



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 30, 2026 – 10:19 AM UTC

PDB ID : 7P81 / pdb_00007p81
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)

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
Mogul	:	2022.3.0, CSD as543be (2022)
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

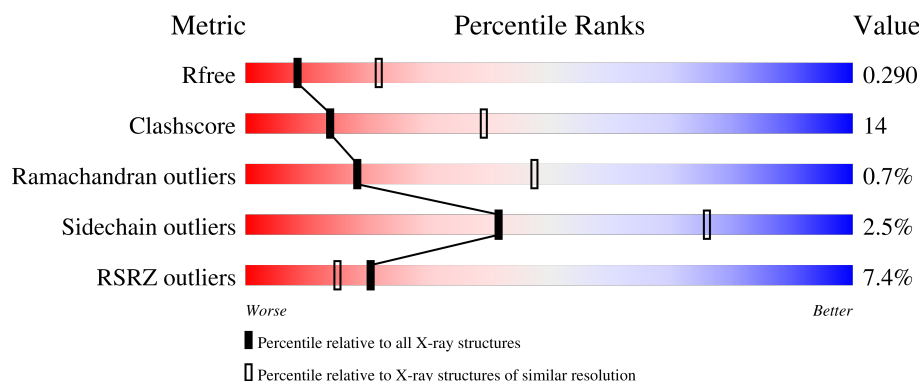
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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}	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	199	
1	B	199	
1	C	199	
1	D	199	
1	E	199	

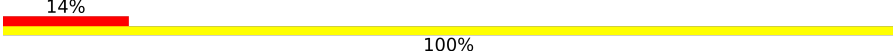
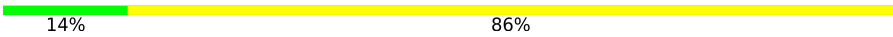
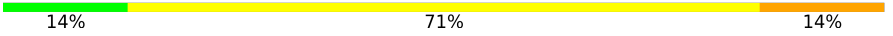
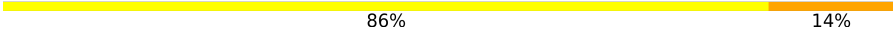
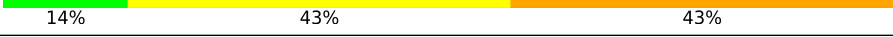
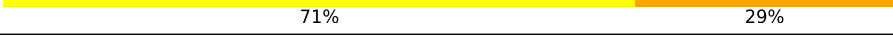
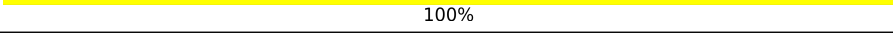
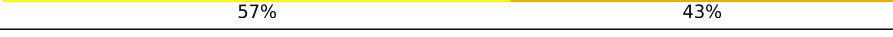
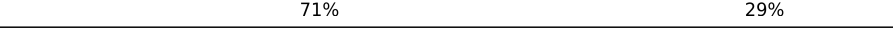
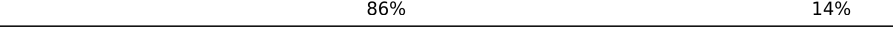
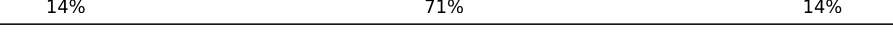
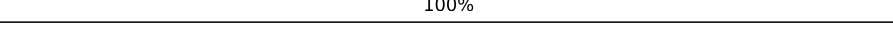
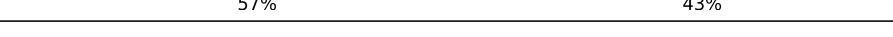
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Mol	Chain	Length	Quality of chain
1	F	199	
1	G	199	
1	H	199	
1	I	199	
1	J	199	
1	K	199	
1	L	199	
1	M	199	
1	N	199	
1	O	199	
1	P	199	
1	Q	199	
1	R	199	
1	S	199	
1	T	199	
1	U	199	
1	V	199	
1	W	199	
1	X	199	
1	Y	199	
1	Z	199	
1	a	199	
1	b	199	
2	c	7	
2	d	7	

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Mol	Chain	Length	Quality of chain
2	e	7	
2	f	7	
2	g	7	
2	h	7	
2	i	7	
2	j	7	
2	k	7	
2	l	7	
2	m	7	
2	n	7	
2	o	7	
2	p	7	
2	q	7	
2	r	7	
2	t	7	
2	u	7	
2	v	7	
2	w	7	

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

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

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

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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

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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

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Chain	Residue	Modelled	Actual	Comment	Reference
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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

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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

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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...

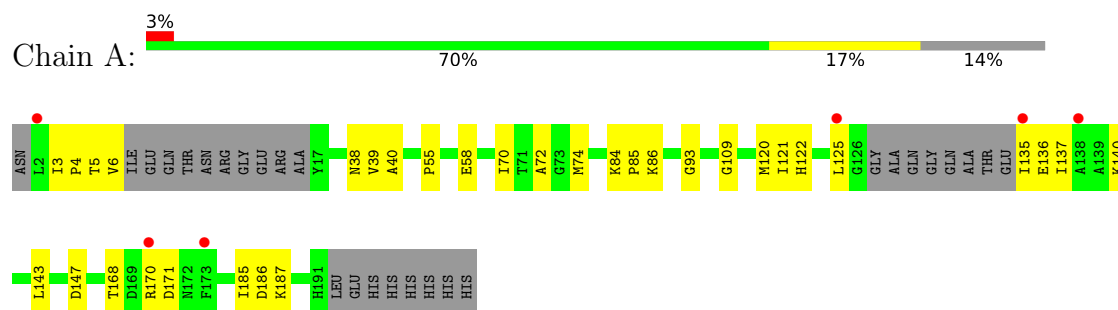
Continued from previous page...

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

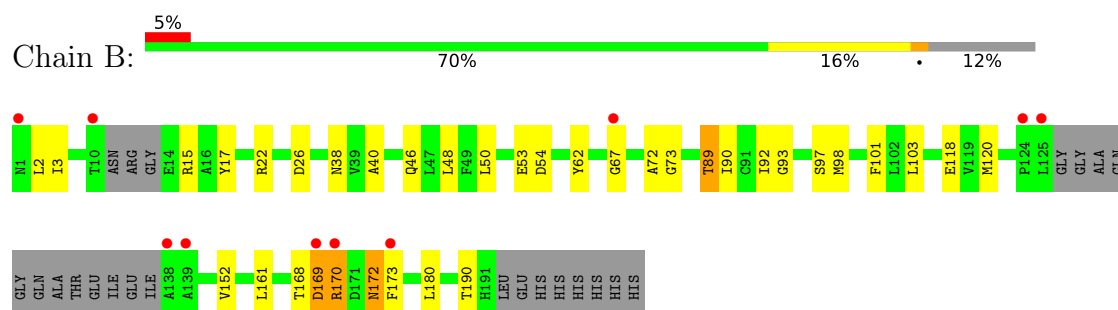
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

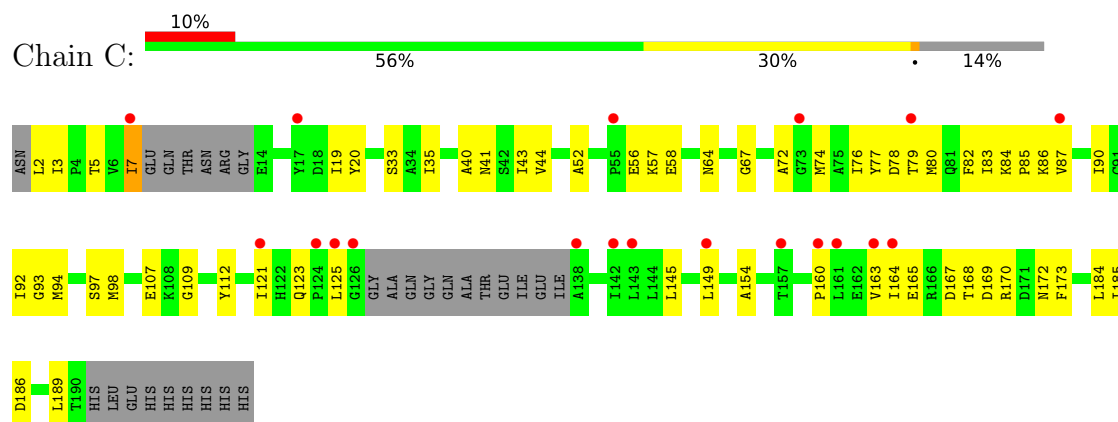
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



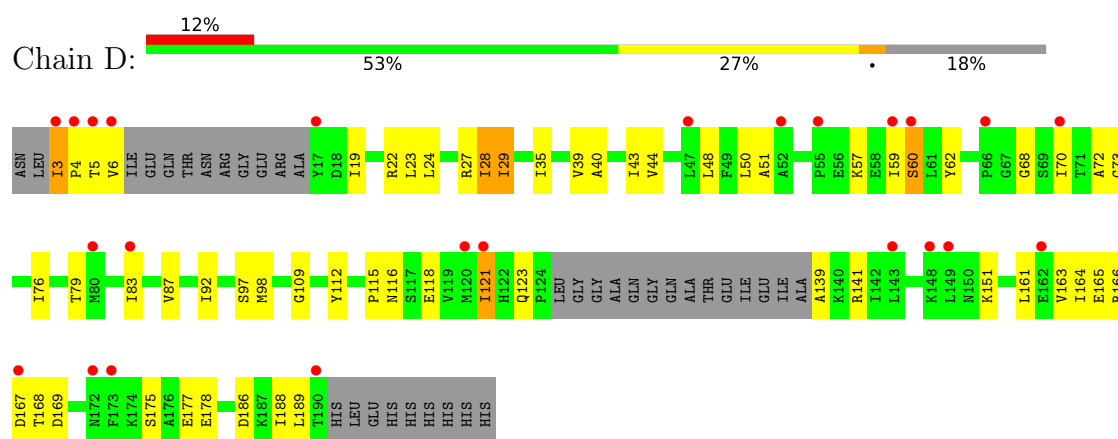
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



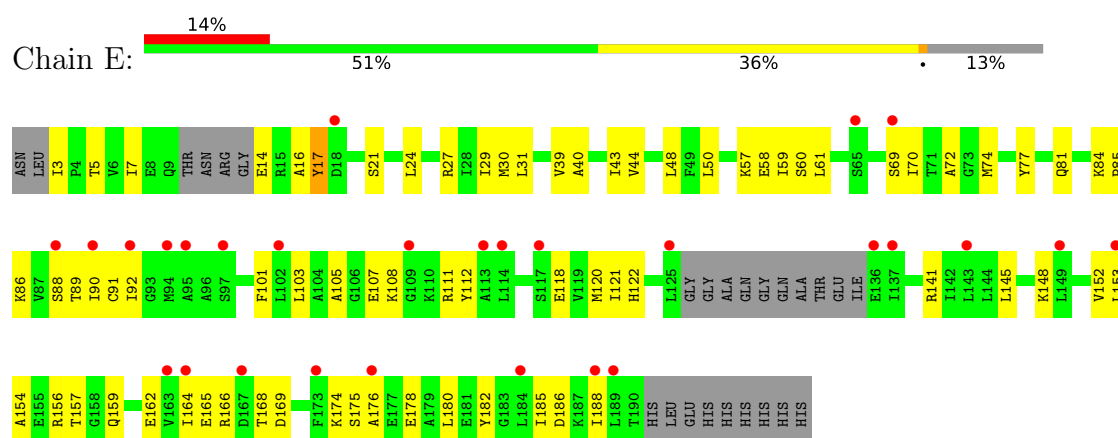
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



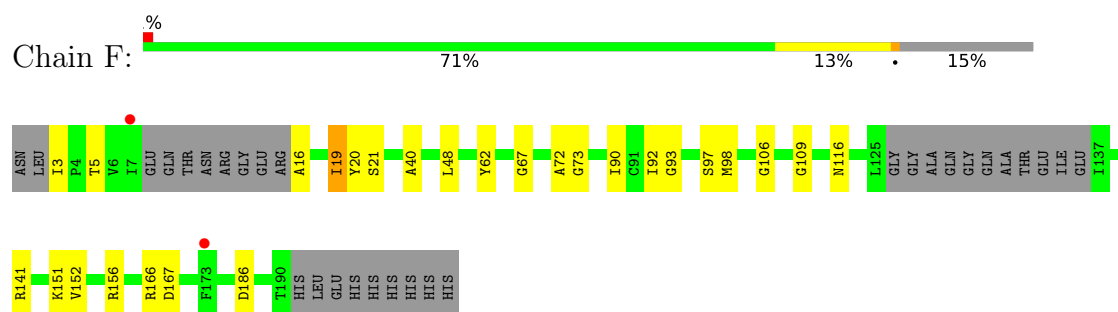
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



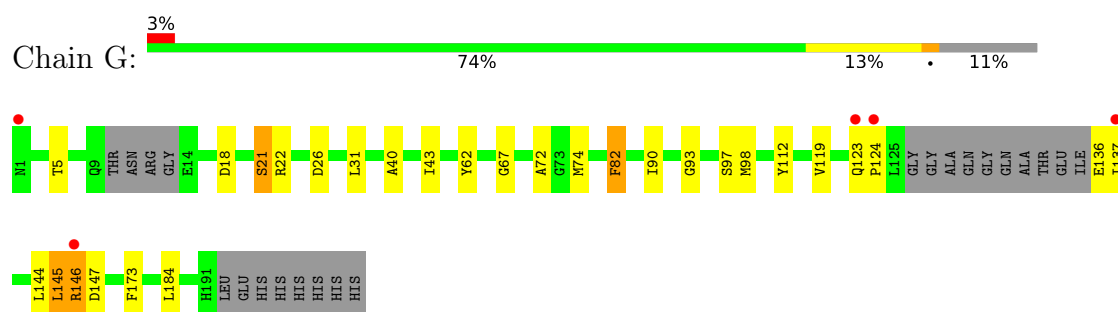
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



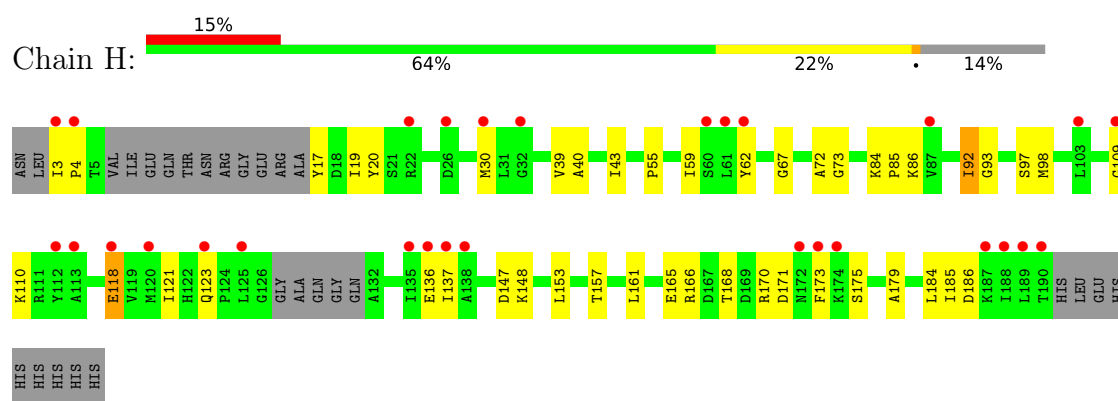
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



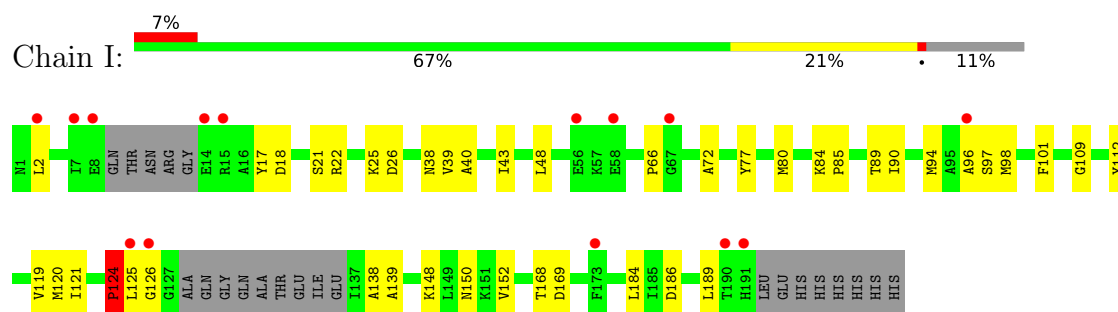
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



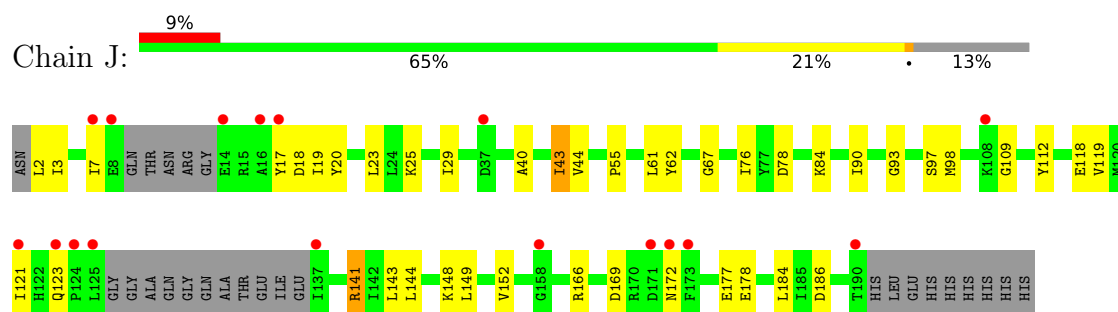
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



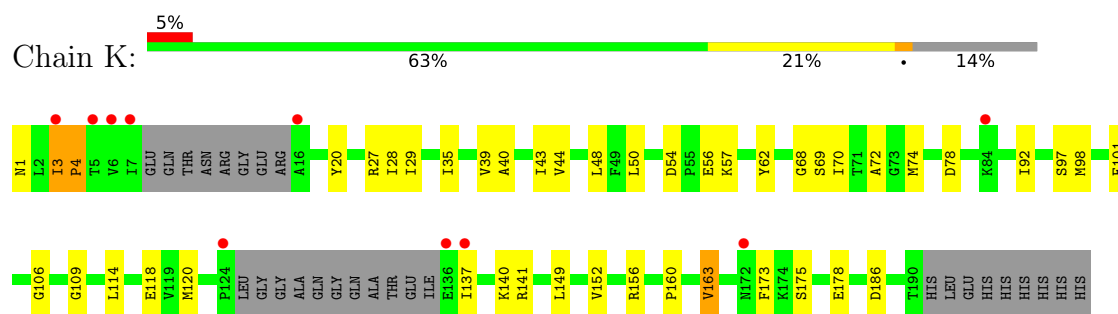
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

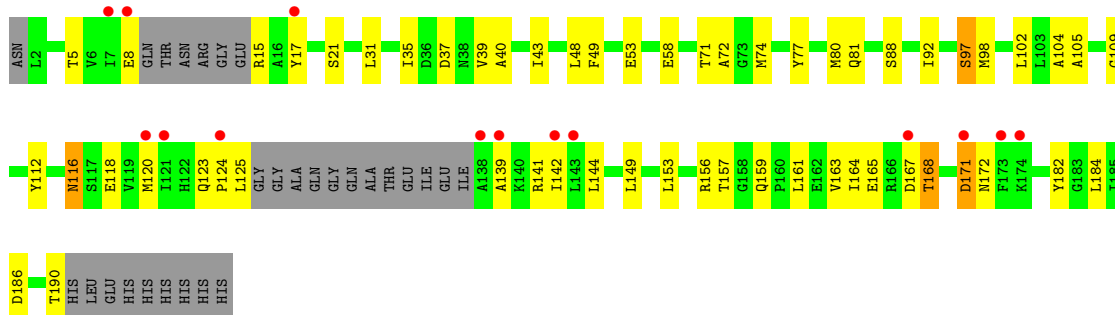


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

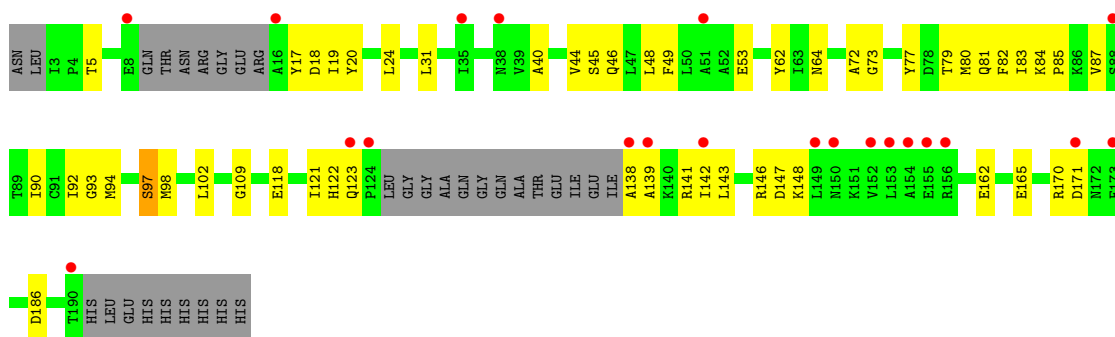


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

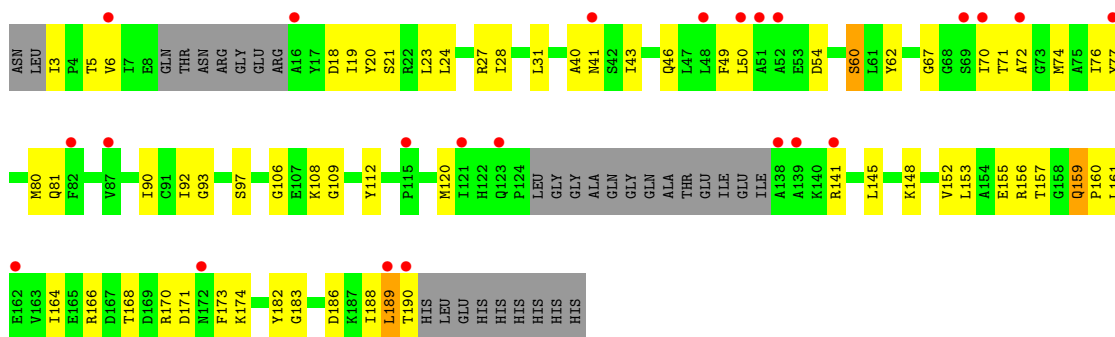




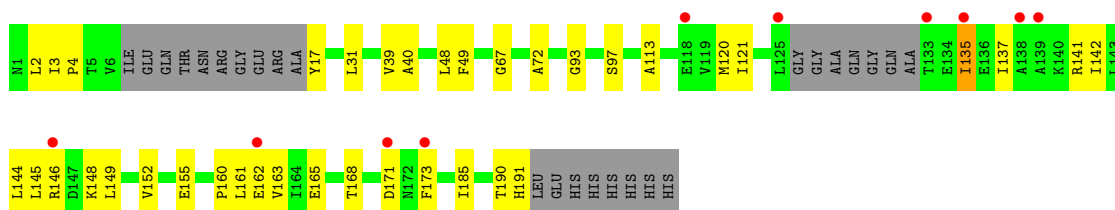
• Molecule 1: ATP-dependent Clp protease proteolytic subunit



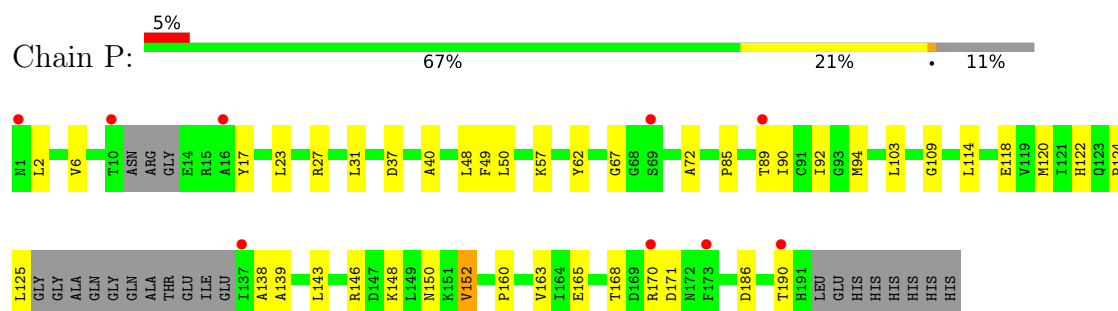
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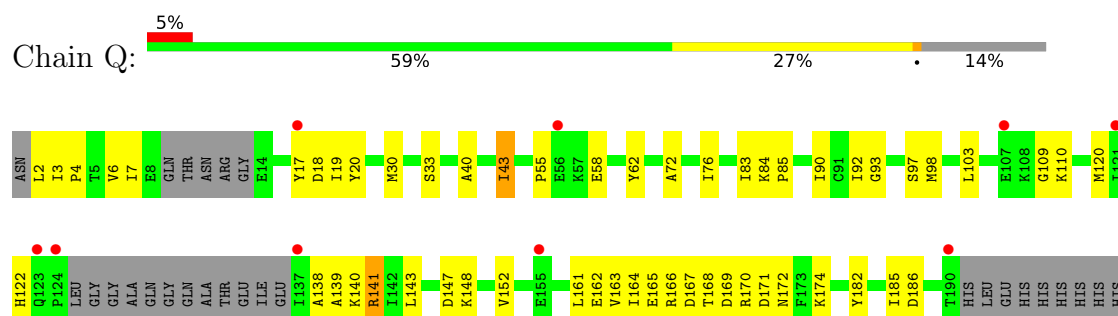
• Molecule 1: ATP-dependent Clp protease proteolytic subunit



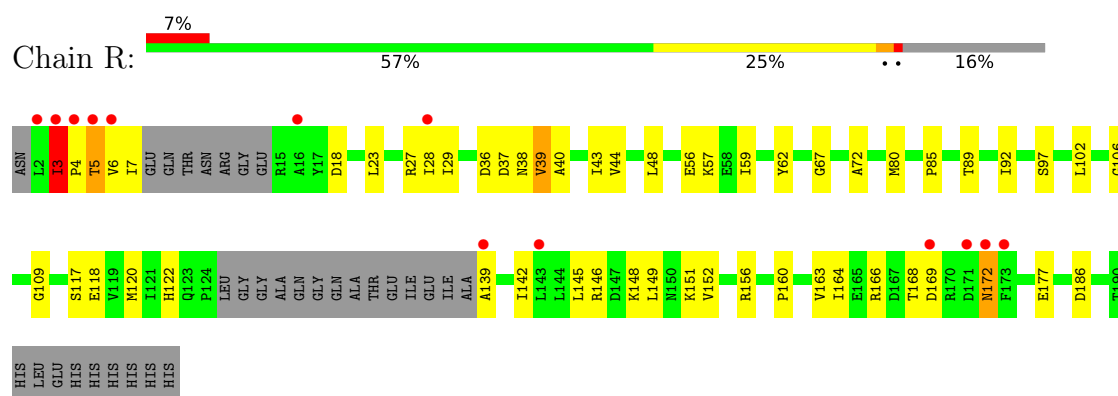
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



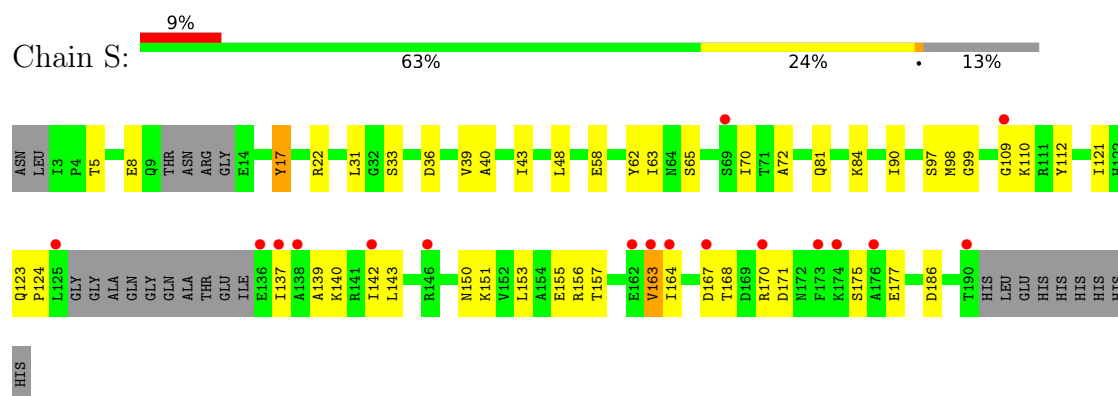
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



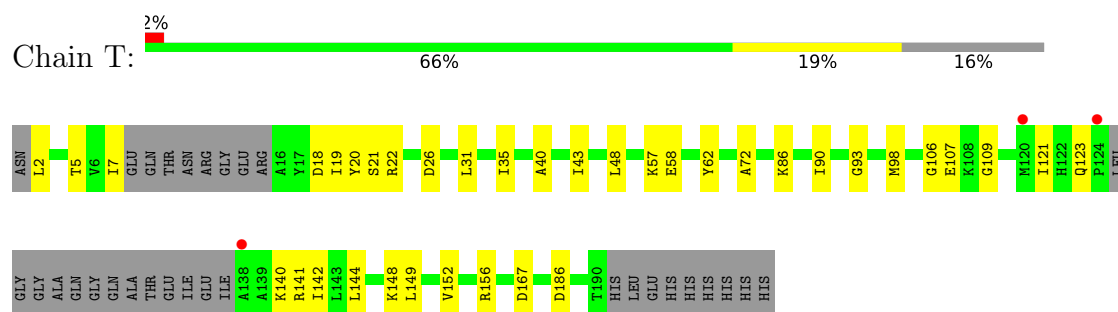
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



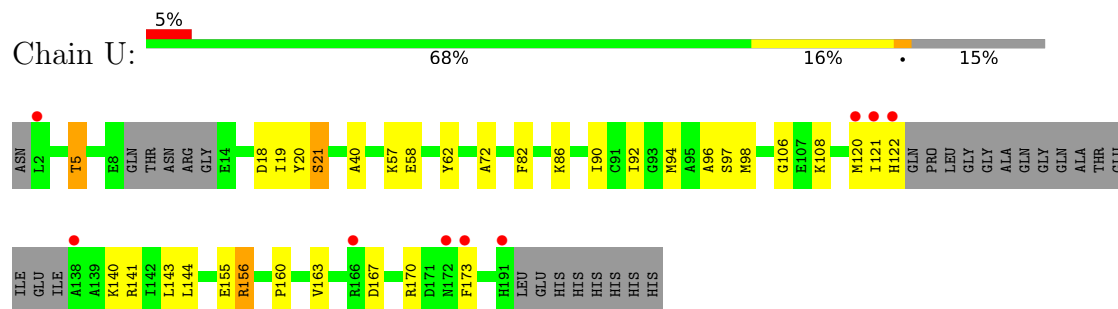
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



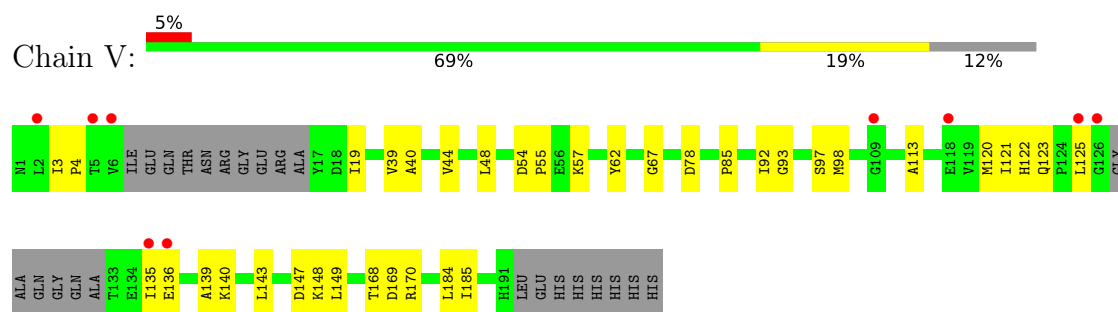
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



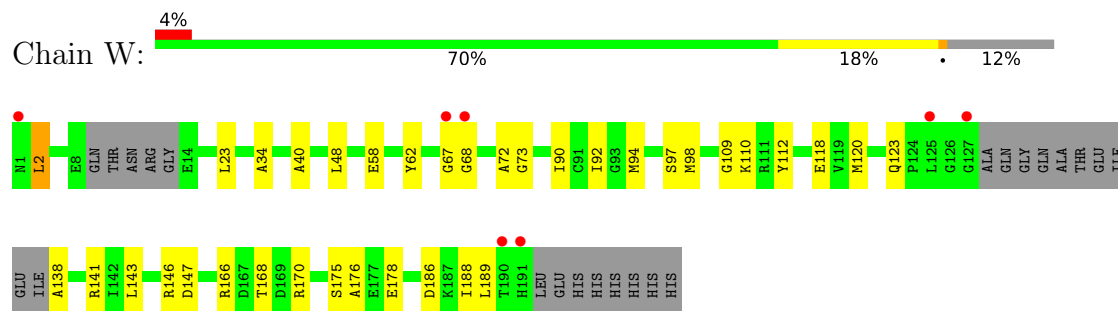
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



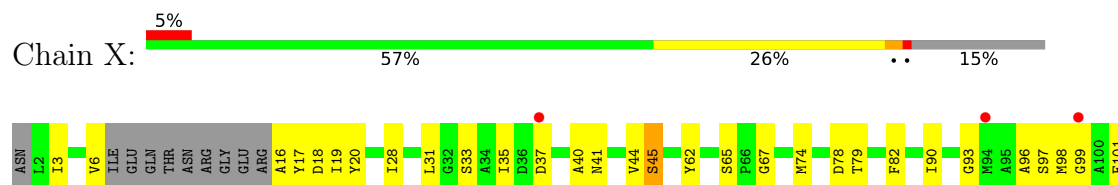
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

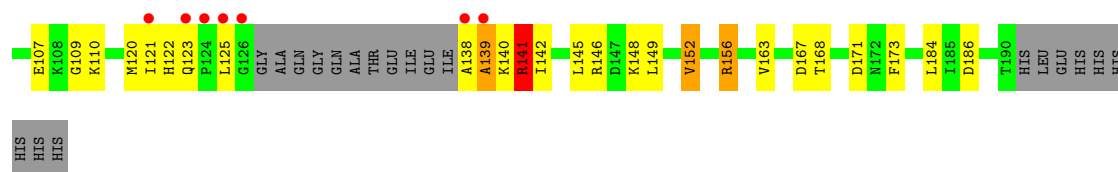


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

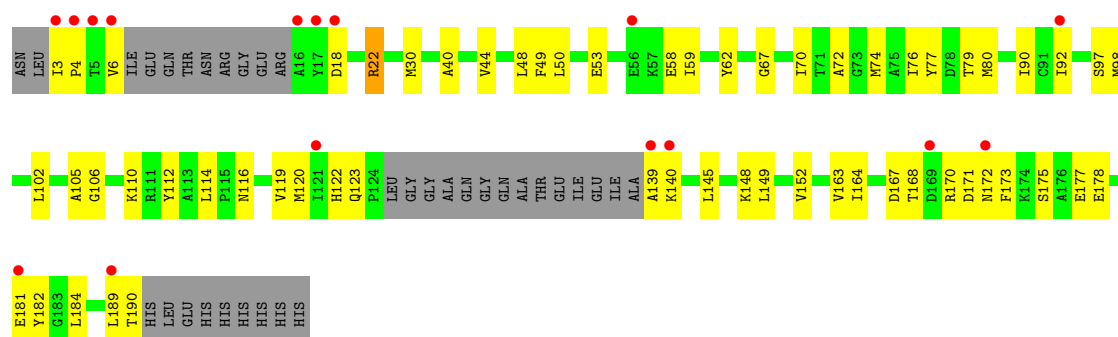


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

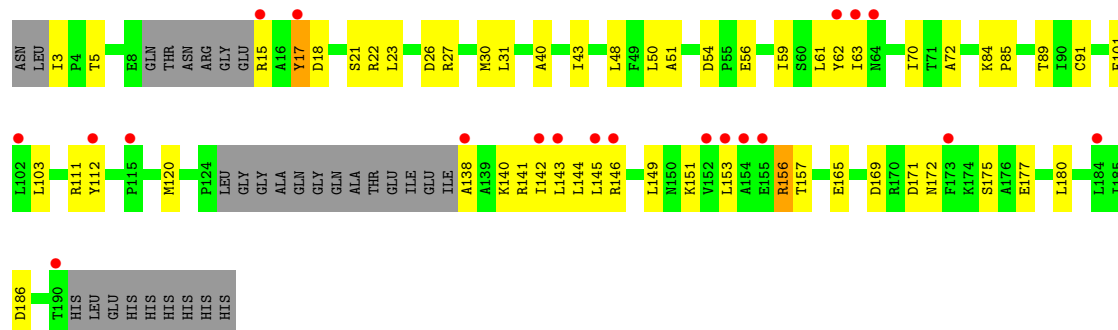




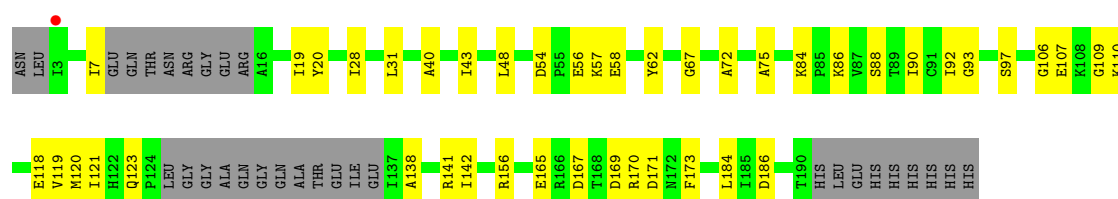
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



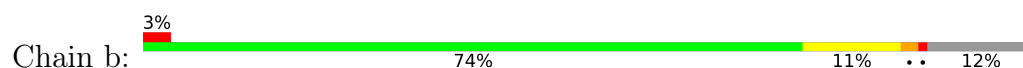
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

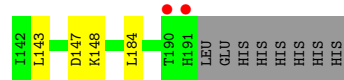


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

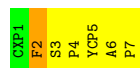


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

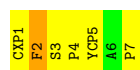




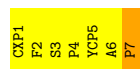
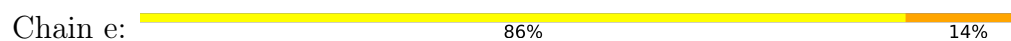
● Molecule 2: ADEP2



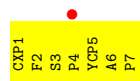
● Molecule 2: ADEP2



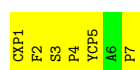
● Molecule 2: ADEP2



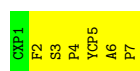
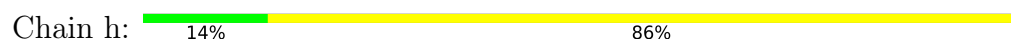
● Molecule 2: ADEP2



● Molecule 2: ADEP2

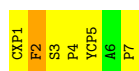


● Molecule 2: ADEP2

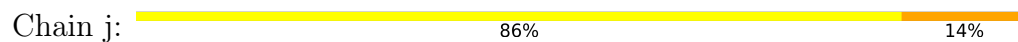


● Molecule 2: ADEP2





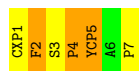
- Molecule 2: ADEP2



- Molecule 2: ADEP2



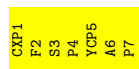
- Molecule 2: ADEP2



- Molecule 2: ADEP2



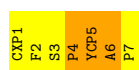
- Molecule 2: ADEP2



- Molecule 2: ADEP2

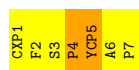


- Molecule 2: ADEP2



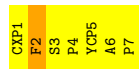
- Molecule 2: ADEP2

Chain q:  71% 29%



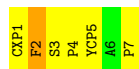
- Molecule 2: ADEP2

Chain r:  86% 14%



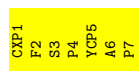
- Molecule 2: ADEP2

Chain t:  14% 71% 14%



- Molecule 2: ADEP2

Chain u:  100%



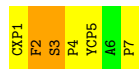
- Molecule 2: ADEP2

Chain v:  57% 43%



- Molecule 2: ADEP2

Chain w:  14% 57% 29%



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) 91.4 (45.51-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.65 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.235 , 0.290 0.235 , 0.290	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)	0.34 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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.*

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 ⓘ

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

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	0.18	0/1334	0.37	0/1798
1	B	0.30	0/1370	0.49	1/1847 (0.1%)
1	C	0.21	0/1330	0.39	0/1793
1	D	0.21	0/1274	0.44	0/1716
1	E	0.22	0/1338	0.46	0/1805
1	F	0.16	0/1307	0.33	0/1762
1	G	0.32	0/1373	0.55	0/1851
1	H	0.23	0/1332	0.46	0/1795
1	I	0.32	1/1367 (0.1%)	0.58	6/1843 (0.3%)
1	J	0.28	1/1333 (0.1%)	0.48	0/1798
1	K	0.22	0/1326	0.40	0/1788
1	L	0.18	0/1326	0.41	0/1788
1	M	0.33	0/1299	0.60	1/1751 (0.1%)
1	N	0.17	0/1309	0.36	0/1764
1	O	0.18	0/1348	0.34	0/1818
1	P	0.25	0/1378	0.44	0/1858
1	Q	0.30	1/1332 (0.1%)	0.49	3/1796 (0.2%)
1	R	0.30	0/1308	0.56	2/1763 (0.1%)
1	S	0.24	0/1342	0.46	0/1810
1	T	0.16	0/1305	0.33	0/1759
1	U	0.27	0/1321	0.46	1/1779 (0.1%)
1	V	0.22	0/1358	0.40	0/1831
1	W	0.16	0/1364	0.34	0/1838
1	X	0.30	1/1309 (0.1%)	0.48	1/1764 (0.1%)
1	Y	0.26	0/1276	0.54	0/1719
1	Z	0.34	0/1307	0.54	0/1762
1	a	0.16	0/1305	0.33	0/1759
1	b	0.34	1/1359 (0.1%)	0.53	2/1831 (0.1%)
2	c	4.33	3/17 (17.6%)	1.47	0/21
2	d	4.35	3/17 (17.6%)	1.37	0/21
2	e	4.49	4/17 (23.5%)	1.55	0/21
2	f	4.42	4/17 (23.5%)	1.36	0/21

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	g	4.31	3/17 (17.6%)	1.64	0/21
2	h	4.54	4/17 (23.5%)	1.66	0/21
2	i	4.42	3/17 (17.6%)	1.29	0/21
2	j	4.44	3/17 (17.6%)	1.33	0/21
2	k	4.48	4/17 (23.5%)	1.24	0/21
2	l	4.58	4/17 (23.5%)	1.48	0/21
2	m	4.42	3/17 (17.6%)	1.48	0/21
2	n	4.48	3/17 (17.6%)	1.44	0/21
2	o	4.50	4/17 (23.5%)	1.37	0/21
2	p	4.39	4/17 (23.5%)	1.82	1/21 (4.8%)
2	q	4.46	3/17 (17.6%)	1.41	0/21
2	r	4.49	3/17 (17.6%)	1.49	0/21
2	t	4.34	3/17 (17.6%)	1.50	0/21
2	u	4.35	4/17 (23.5%)	1.34	0/21
2	v	4.28	3/17 (17.6%)	1.61	0/21
2	w	4.50	4/17 (23.5%)	1.40	0/21
All	All	0.49	74/37570 (0.2%)	0.47	18/50606 (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 (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	f	4	PRO	N-CD	12.36	1.65	1.47
2	h	4	PRO	N-CD	12.18	1.64	1.47
2	l	4	PRO	N-CD	12.07	1.64	1.47
2	r	4	PRO	N-CD	11.89	1.64	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	k	4	PRO	N-CD	11.79	1.64	1.47
2	w	4	PRO	N-CD	11.76	1.64	1.47
2	j	4	PRO	N-CD	11.72	1.64	1.47
2	e	4	PRO	N-CD	11.61	1.64	1.47
2	i	4	PRO	N-CD	11.61	1.64	1.47
2	p	4	PRO	N-CD	11.59	1.64	1.47
2	q	4	PRO	N-CD	11.53	1.63	1.47
2	c	4	PRO	N-CD	11.48	1.63	1.47
2	u	4	PRO	N-CD	11.47	1.63	1.47
2	d	4	PRO	N-CD	11.42	1.63	1.47
2	t	4	PRO	N-CD	11.38	1.63	1.47
2	v	4	PRO	N-CD	11.29	1.63	1.47
2	o	4	PRO	N-CD	11.27	1.63	1.47
2	m	4	PRO	N-CD	11.24	1.63	1.47
2	n	4	PRO	N-CD	11.19	1.63	1.47
2	g	4	PRO	N-CD	10.99	1.63	1.47
2	n	4	PRO	N-CA	-9.80	1.32	1.47
2	o	4	PRO	N-CA	-9.73	1.32	1.47
2	w	4	PRO	N-CA	-9.24	1.33	1.47
2	r	4	PRO	N-CA	-9.20	1.33	1.47
2	g	4	PRO	N-CA	-9.17	1.33	1.47
2	l	4	PRO	N-CA	-9.16	1.33	1.47
2	k	4	PRO	N-CA	-9.12	1.33	1.47
2	q	4	PRO	N-CA	-9.09	1.33	1.47
2	t	4	PRO	N-CA	-8.89	1.33	1.47
2	j	4	PRO	N-CA	-8.83	1.33	1.47
2	i	4	PRO	N-CA	-8.76	1.33	1.47
2	h	4	PRO	N-CA	-8.75	1.33	1.47
2	p	4	PRO	N-CA	-8.67	1.34	1.47
2	u	4	PRO	N-CA	-8.64	1.34	1.47
2	c	4	PRO	N-CA	-8.63	1.34	1.47
2	m	4	PRO	N-CA	-8.55	1.34	1.47
2	d	4	PRO	N-CA	-8.35	1.34	1.47
2	v	4	PRO	N-CA	-8.21	1.34	1.47
2	f	4	PRO	N-CA	-8.00	1.35	1.47
2	e	4	PRO	N-CA	-7.90	1.35	1.47
1	b	124	PRO	N-CD	7.79	1.58	1.47
1	Q	141	ARG	C-O	-7.50	1.15	1.24
2	e	3	SER	C-N	7.48	1.46	1.34
2	d	3	SER	C-N	6.83	1.45	1.34
2	h	3	SER	C-N	6.69	1.45	1.34
2	c	3	SER	C-N	6.59	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	l	3	SER	C-N	6.48	1.45	1.34
1	X	141	ARG	C-O	-6.40	1.16	1.24
2	t	3	SER	C-N	6.21	1.44	1.34
2	q	3	SER	C-N	6.18	1.44	1.34
2	i	3	SER	C-N	6.16	1.44	1.34
2	f	3	SER	C-N	6.14	1.44	1.34
2	p	3	SER	C-N	6.12	1.44	1.34
2	j	3	SER	C-N	6.01	1.44	1.34
2	r	3	SER	C-N	5.91	1.44	1.34
2	g	3	SER	C-N	5.76	1.43	1.34
2	w	3	SER	C-N	5.68	1.43	1.34
2	m	3	SER	C-N	5.64	1.43	1.34
2	u	3	SER	C-N	5.53	1.43	1.34
2	k	3	SER	C-N	5.52	1.43	1.34
1	I	139	ALA	C-O	-5.48	1.17	1.24
2	o	3	SER	C-N	5.48	1.43	1.34
1	J	141	ARG	C-O	-5.40	1.17	1.24
2	v	3	SER	C-N	5.33	1.43	1.34
2	p	4	PRO	CA-CB	5.33	1.64	1.53
2	k	4	PRO	CA-CB	5.25	1.64	1.53
2	e	4	PRO	CA-CB	5.20	1.63	1.53
2	l	4	PRO	CA-CB	5.19	1.63	1.53
2	h	4	PRO	CA-CB	5.19	1.63	1.53
2	u	4	PRO	CA-CB	5.19	1.63	1.53
2	f	4	PRO	CA-CB	5.18	1.63	1.53
2	w	4	PRO	CA-CB	5.17	1.63	1.53
2	n	3	SER	C-N	5.16	1.42	1.34
2	o	4	PRO	CA-CB	5.04	1.63	1.53

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	b	125	LEU	N-CA-CB	-11.01	93.12	110.19
1	I	124	PRO	CB-CA-C	-8.43	97.65	111.56
1	I	124	PRO	N-CA-CB	-8.41	94.42	103.25
1	b	124	PRO	N-CA-C	-7.17	97.69	112.47
1	I	124	PRO	N-CA-C	6.89	126.66	112.47
1	B	169	ASP	CA-C-O	-6.51	112.75	120.10
1	I	139	ALA	CA-C-O	-6.06	114.13	120.55
1	X	141	ARG	CA-C-O	-5.98	114.54	120.82
1	Q	138	ALA	N-CA-C	-5.97	103.74	111.02
1	M	147	ASP	N-CA-C	-5.86	104.89	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	141	ARG	CA-C-O	-5.81	114.69	120.90
1	Q	138	ALA	CA-C-O	-5.72	114.77	121.07
2	p	6	ALA	N-CA-CB	-5.55	102.08	110.40
1	U	120	MET	CA-C-O	-5.47	115.17	121.19
1	R	5	THR	CB-CA-C	-5.40	103.28	110.79
1	R	151	LYS	CA-C-O	-5.24	115.00	120.55
1	I	139	ALA	CA-C-N	5.17	127.16	120.44
1	I	139	ALA	C-N-CA	5.17	127.16	120.44

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1319	0	1362	44	0
1	B	1354	0	1395	36	0
1	C	1315	0	1361	52	0
1	D	1260	0	1304	56	0
1	E	1323	0	1355	83	0
1	F	1292	0	1327	21	0
1	G	1358	0	1396	17	0
1	H	1317	0	1358	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	1351	0	1388	28	0
1	J	1318	0	1353	48	0
1	K	1311	0	1361	42	0
1	L	1311	0	1358	46	0
1	M	1284	0	1316	59	0
1	N	1294	0	1338	61	0
1	O	1333	0	1377	48	0
1	P	1362	0	1406	42	0
1	Q	1317	0	1355	52	0
1	R	1293	0	1340	49	0
1	S	1327	0	1359	42	0
1	T	1290	0	1334	28	0
1	U	1307	0	1351	26	0
1	V	1343	0	1384	38	0
1	W	1348	0	1393	29	0
1	X	1294	0	1337	54	0
1	Y	1262	0	1300	50	0
1	Z	1292	0	1327	50	0
1	a	1290	0	1334	37	0
1	b	1344	0	1388	20	0
2	c	57	0	55	3	0
2	d	57	0	55	2	0
2	e	57	0	55	3	0
2	f	57	0	55	3	0
2	g	57	0	55	2	0
2	h	57	0	55	1	0
2	i	57	0	55	2	0
2	j	57	0	55	6	0
2	k	57	0	55	5	0
2	l	57	0	55	6	0
2	m	57	0	55	9	0
2	n	57	0	55	5	0
2	o	57	0	55	5	0
2	p	57	0	55	5	0
2	q	57	0	55	4	0
2	r	57	0	55	6	0
2	t	57	0	55	3	0
2	u	57	0	55	4	0
2	v	57	0	55	9	0
2	w	57	0	55	4	0
3	A	6	0	0	0	0
3	B	17	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	11	0	0	4	0
3	D	13	0	0	4	0
3	E	16	0	0	12	0
3	F	10	0	0	3	0
3	G	17	0	0	1	0
3	H	6	0	0	2	0
3	I	3	0	0	1	0
3	J	9	0	0	3	0
3	K	19	0	0	2	0
3	L	13	0	0	5	0
3	M	11	0	0	15	0
3	N	5	0	0	11	0
3	O	7	0	0	2	0
3	P	6	0	0	2	0
3	Q	15	0	0	3	0
3	R	10	0	0	6	0
3	S	12	0	0	4	0
3	T	14	0	0	2	0
3	U	12	0	0	0	0
3	V	5	0	0	1	0
3	W	9	0	0	4	0
3	X	8	0	0	6	0
3	Y	5	0	0	1	0
3	Z	9	0	0	2	0
3	a	10	0	0	2	0
3	b	12	0	0	3	0
3	f	1	0	0	0	0
3	g	2	0	0	0	0
3	h	1	0	0	0	0
3	j	1	0	0	0	0
3	m	2	0	0	5	0
3	o	1	0	0	0	0
3	v	1	0	0	5	0
All	All	38248	0	39057	1106	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 14.

All (1106) 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:Z:145:LEU:HD12	1:Z:146:ARG:N	1.43	1.31
1:A:170:ARG:NE	1:J:169:ASP:CB	2.09	1.15
1:N:70:ILE:O	3:N:201:HOH:O	1.66	1.13
1:A:170:ARG:HG3	1:J:169:ASP:HB3	1.25	1.13
1:O:137:ILE:HD11	1:P:170:ARG:NH2	1.62	1.12
1:A:170:ARG:CG	1:J:169:ASP:HB3	1.77	1.12
1:A:170:ARG:HE	1:J:169:ASP:CB	1.61	1.12
1:J:123:GLN:HE22	1:J:149:LEU:CD1	1.62	1.12
1:a:56:GLU:OE2	1:a:84:LYS:NZ	1.81	1.12
1:J:123:GLN:NE2	1:J:149:LEU:HD13	1.62	1.11
1:A:170:ARG:NE	1:J:169:ASP:HB2	1.63	1.09
1:Z:142:ILE:O	1:Z:145:LEU:HG	1.53	1.07
1:S:156:ARG:NH1	3:S:201:HOH:O	1.75	1.04
1:A:170:ARG:HE	1:J:169:ASP:CG	1.62	1.04
1:M:139:ALA:O	3:M:201:HOH:O	1.74	1.04
1:M:44:VAL:O	3:M:202:HOH:O	1.77	1.03
1:E:166:ARG:HH12	1:M:170:ARG:NH1	1.56	1.01
1:R:6:VAL:O	1:R:7:ILE:HG22	1.59	1.00
1:M:142:ILE:N	3:M:201:HOH:O	1.93	0.99
1:E:166:ARG:NH1	1:M:170:ARG:HH12	1.59	0.98
1:V:136:GLU:OE2	1:V:140:LYS:HE3	1.64	0.96
1:B:50:LEU:O	3:B:201:HOH:O	1.83	0.96
1:E:120:MET:HE1	1:E:122:HIS:HB3	1.47	0.95
1:R:139:ALA:CA	1:R:142:ILE:HD12	1.97	0.94
1:J:123:GLN:NE2	1:J:149:LEU:CD1	2.26	0.94
1:N:166:ARG:O	3:N:202:HOH:O	1.85	0.93
1:S:8:GLU:OE2	1:S:17:TYR:OH	1.86	0.93
1:N:54:ASP:OD2	3:N:203:HOH:O	1.86	0.93
1:E:166:ARG:HH12	1:M:170:ARG:HH12	0.98	0.93
1:O:113:ALA:HB3	1:O:185:ILE:HD13	1.52	0.92
1:O:113:ALA:CB	1:O:185:ILE:HD13	1.98	0.92
1:Z:145:LEU:HD12	1:Z:146:ARG:H	1.27	0.92
1:S:153:LEU:O	1:S:157:THR:HG23	1.70	0.91
1:Y:80:MET:HE1	1:Y:102:LEU:HD22	1.52	0.91
1:O:137:ILE:CD1	1:P:170:ARG:NH2	2.33	0.91
1:D:168:THR:OG1	3:D:201:HOH:O	1.73	0.91
1:Z:145:LEU:CD1	1:Z:146:ARG:N	2.32	0.91
1:a:106:GLY:O	1:a:156:ARG:NH2	2.05	0.90
1:P:94:MET:HE1	1:P:120:MET:SD	2.14	0.88
1:Z:31:LEU:HD13	1:Z:43:ILE:HD11	1.56	0.88
1:W:143:LEU:O	1:W:147:ASP:OD1	1.91	0.87
1:A:170:ARG:HG3	1:J:169:ASP:CB	2.05	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:122:HIS:ND1	1:Y:171:ASP:OD1	2.07	0.87
1:J:123:GLN:HE22	1:J:149:LEU:HD11	1.38	0.86
1:R:6:VAL:O	1:R:7:ILE:CG2	2.25	0.85
1:O:137:ILE:HD11	1:P:170:ARG:HH22	1.42	0.85
1:R:168:THR:O	3:R:201:HOH:O	1.95	0.85
1:O:113:ALA:HB3	1:O:185:ILE:CD1	2.05	0.85
1:D:48:LEU:HB3	2:e:1:CXP:H71	1.58	0.84
1:E:166:ARG:NH1	1:M:170:ARG:NH1	2.19	0.84
1:D:98:MET:SD	1:D:123:GLN:NE2	2.50	0.84
1:J:98:MET:CE	1:J:123:GLN:OE1	2.26	0.84
1:N:3:ILE:N	3:N:204:HOH:O	2.09	0.84
1:E:58:GLU:OE2	1:E:88:SER:OG	1.96	0.83
1:N:18:ASP:OD1	1:N:21:SER:OG	1.96	0.83
1:R:139:ALA:N	1:R:142:ILE:HD12	1.94	0.82
1:O:160:PRO:HB2	1:O:162:GLU:OE1	1.79	0.82
1:D:164:ILE:O	1:D:168:THR:HG23	1.79	0.82
1:Z:145:LEU:CD1	1:Z:146:ARG:H	1.93	0.81
1:V:113:ALA:CB	1:V:185:ILE:HD13	2.11	0.81
1:C:44:VAL:HG23	1:C:79:THR:HG21	1.62	0.80
1:S:153:LEU:N	3:S:203:HOH:O	2.14	0.80
1:E:3:ILE:N	3:E:203:HOH:O	2.12	0.80
1:O:137:ILE:HD11	1:P:170:ARG:HH21	1.43	0.80
1:B:46:GLN:OE1	3:B:202:HOH:O	2.00	0.79
1:b:9:GLN:O	3:b:201:HOH:O	2.00	0.79
1:Y:48:LEU:HB3	2:u:1:CXP:H71	1.63	0.79
1:Q:139:ALA:HB1	1:b:143:LEU:HD11	1.65	0.79
1:R:139:ALA:CA	1:R:142:ILE:CD1	2.60	0.79
1:W:48:LEU:HB3	2:t:1:CXP:H72	1.65	0.79
2:v:6:ALA:N	3:v:101:HOH:O	2.14	0.79
1:E:27:ARG:O	3:E:201:HOH:O	2.01	0.78
1:L:164:ILE:O	1:L:168:THR:OG1	2.02	0.78
1:L:8:GLU:O	3:L:201:HOH:O	2.01	0.78
1:P:89:THR:HG21	1:P:103:LEU:HA	1.65	0.78
1:Y:58:GLU:OE1	1:Y:110:LYS:NZ	2.16	0.78
1:B:54:ASP:N	3:B:201:HOH:O	2.06	0.78
1:L:74:MET:HA	1:L:74:MET:HE3	1.66	0.78
1:V:113:ALA:HB3	1:V:185:ILE:HD13	1.65	0.77
2:m:2:WFP:C	3:m:101:HOH:O	2.32	0.77
1:A:170:ARG:CG	1:J:169:ASP:CB	2.62	0.77
1:B:38:ASN:OD1	3:B:203:HOH:O	2.02	0.77
1:M:97:SER:OG	1:M:98:MET:N	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:106:GLY:O	1:N:156:ARG:NH2	2.17	0.77
1:A:143:LEU:O	1:A:147:ASP:OD1	2.00	0.77
1:J:20:TYR:N	3:J:201:HOH:O	2.17	0.76
1:M:138:ALA:HB3	1:M:141:ARG:HB3	1.68	0.76
1:Q:3:ILE:HD12	1:Q:4:PRO:HD2	1.67	0.76
1:R:139:ALA:N	1:R:142:ILE:CD1	2.47	0.76
1:R:139:ALA:HA	1:R:142:ILE:CD1	2.14	0.76
1:X:78:ASP:OD2	1:Y:116:ASN:ND2	2.18	0.76
1:K:1:ASN:N	3:K:202:HOH:O	2.19	0.76
1:B:118:GLU:OE1	1:B:173:PHE:HE1	1.69	0.76
1:L:141:ARG:HA	1:L:144:LEU:HD13	1.66	0.76
1:N:170:ARG:HG2	3:N:202:HOH:O	1.86	0.76
1:N:90:ILE:HG23	1:N:112:TYR:HB2	1.69	0.75
1:N:148:LYS:O	1:N:152:VAL:HG23	1.86	0.75
1:Q:122:HIS:ND1	1:Q:171:ASP:OD1	2.19	0.75
1:K:48:LEU:HB3	2:j:1:CXP:H72	1.67	0.75
1:S:139:ALA:O	3:S:202:HOH:O	2.04	0.74
1:L:153:LEU:O	1:L:157:THR:HG23	1.87	0.74
1:S:170:ARG:NH2	1:a:170:ARG:HG3	2.01	0.74
1:D:115:PRO:O	3:D:202:HOH:O	2.06	0.74
1:E:60:SER:O	3:E:201:HOH:O	2.06	0.74
1:J:62:TYR:CE1	1:J:90:ILE:HD13	2.22	0.74
1:K:156:ARG:NH1	3:K:203:HOH:O	2.21	0.74
1:Q:169:ASP:OD2	1:V:170:ARG:NH2	2.20	0.73
1:G:18:ASP:OD2	3:G:201:HOH:O	2.06	0.73
1:Y:70:ILE:HG21	1:Y:145:LEU:HD13	1.70	0.73
1:O:121:ILE:HG22	1:O:168:THR:HG22	1.70	0.73
1:S:137:ILE:HG23	1:S:140:LYS:HD3	1.69	0.73
1:a:7:ILE:O	3:a:201:HOH:O	2.07	0.73
1:Q:2:LEU:N	3:Q:202:HOH:O	2.21	0.73
1:C:52:ALA:O	3:C:201:HOH:O	2.06	0.72
1:L:190:THR:O	3:L:202:HOH:O	2.06	0.72
1:R:48:LEU:HB3	2:o:1:CXP:H72	1.70	0.72
1:Z:48:LEU:HB3	2:v:1:CXP:H72	1.70	0.72
1:b:53:GLU:OE2	3:b:202:HOH:O	2.08	0.72
1:Z:145:LEU:HD12	1:Z:146:ARG:CA	2.18	0.72
1:K:118:GLU:OE1	1:K:173:PHE:HB3	1.90	0.72
1:L:15:ARG:N	3:L:201:HOH:O	2.23	0.72
1:V:121:ILE:HD11	1:V:184:LEU:HD21	1.71	0.72
1:E:77:TYR:OH	1:E:152:VAL:HG21	1.90	0.72
1:O:137:ILE:CD1	1:P:170:ARG:HH22	2.00	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:92:ILE:O	3:E:202:HOH:O	2.07	0.71
1:E:30:MET:HE3	1:E:31:LEU:H	1.56	0.71
1:Q:3:ILE:HD11	1:Q:19:ILE:HG22	1.70	0.71
1:M:143:LEU:N	3:M:201:HOH:O	2.02	0.71
1:X:146:ARG:NH2	3:X:202:HOH:O	2.23	0.71
1:X:121:ILE:HD11	1:X:184:LEU:HD11	1.71	0.71
1:X:122:HIS:ND1	1:X:171:ASP:OD1	2.23	0.71
1:Q:3:ILE:HD11	1:Q:19:ILE:CG2	2.19	0.71
1:W:138:ALA:N	3:W:201:HOH:O	2.23	0.71
1:C:58:GLU:OE1	1:C:58:GLU:N	2.19	0.70
1:M:49:PHE:HE2	1:N:6:VAL:HG11	1.56	0.70
1:S:48:LEU:HB3	2:p:1:CXP:H72	1.72	0.70
1:E:60:SER:N	3:E:201:HOH:O	2.25	0.70
1:M:45:SER:HB3	1:N:23:LEU:HD11	1.71	0.70
1:H:39:VAL:HG22	1:I:2:LEU:HD11	1.71	0.70
1:L:74:MET:HE3	1:L:77:TYR:HB3	1.71	0.70
1:U:90:ILE:HD11	2:q:6:ALA:HB3	1.74	0.70
1:A:170:ARG:CD	1:J:169:ASP:CB	2.70	0.70
1:V:113:ALA:HB3	1:V:185:ILE:CD1	2.21	0.70
1:T:109:GLY:N	1:T:186:ASP:OD2	2.25	0.70
1:K:97:SER:OG	1:K:98:MET:N	2.20	0.70
1:K:118:GLU:OE1	1:K:173:PHE:HD2	1.75	0.70
1:T:106:GLY:O	1:T:156:ARG:NH2	2.24	0.70
1:Z:89:THR:HG21	1:Z:103:LEU:HA	1.73	0.70
1:B:53:GLU:N	3:B:201:HOH:O	2.23	0.69
1:B:89:THR:CG2	1:B:103:LEU:HD12	2.22	0.69
1:M:64:ASN:O	3:M:203:HOH:O	2.10	0.69
1:R:37:ASP:OD2	3:R:202:HOH:O	2.09	0.69
1:Q:17:TYR:HA	1:R:6:VAL:HG23	1.74	0.69
1:J:62:TYR:HE1	1:J:90:ILE:HD13	1.57	0.69
1:O:113:ALA:HB2	1:O:185:ILE:HD13	1.73	0.69
1:E:91:CYS:HB2	1:E:103:LEU:HD22	1.73	0.69
1:J:90:ILE:HG23	1:J:112:TYR:HB2	1.75	0.69
1:Q:97:SER:OG	1:Q:98:MET:N	2.23	0.69
1:Z:70:ILE:HD13	1:Z:145:LEU:HD13	1.73	0.69
1:F:48:LEU:HB3	2:g:1:CXP:H72	1.75	0.69
1:Q:103:LEU:HD21	1:Q:185:ILE:HD11	1.73	0.69
1:Y:76:ILE:HG22	1:Y:80:MET:HE2	1.74	0.69
1:E:30:MET:HE3	1:E:31:LEU:N	2.08	0.68
1:F:106:GLY:O	1:F:156:ARG:NH2	2.27	0.68
1:A:135:ILE:N	1:I:126:GLY:HA2	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:136:GLU:OE2	3:H:201:HOH:O	2.11	0.68
1:L:125:LEU:O	3:L:203:HOH:O	2.11	0.68
1:N:153:LEU:O	1:N:157:THR:OG1	2.12	0.68
1:B:48:LEU:HB3	2:d:1:CXP:H72	1.74	0.68
1:P:62:TYR:CE1	1:P:90:ILE:HD13	2.28	0.68
1:D:178:GLU:N	1:D:178:GLU:OE1	2.27	0.68
1:S:137:ILE:HG23	1:S:140:LYS:CD	2.22	0.68
1:D:62:TYR:CD2	1:D:92:ILE:HD11	2.30	0.67
1:A:170:ARG:NE	1:J:169:ASP:CG	2.39	0.67
1:N:170:ARG:N	3:N:202:HOH:O	2.27	0.67
1:D:97:SER:OG	1:D:98:MET:N	2.21	0.67
1:b:148:LYS:NZ	3:b:204:HOH:O	2.27	0.67
2:v:2:WFP:O	3:v:101:HOH:O	2.11	0.67
1:Y:178:GLU:HA	1:Y:181:GLU:OE1	1.94	0.67
1:U:62:TYR:HB3	1:U:92:ILE:HD11	1.76	0.67
1:A:74:MET:HE3	1:A:74:MET:HA	1.76	0.67
1:R:6:VAL:C	1:R:7:ILE:HG22	2.19	0.67
1:H:121:ILE:CG2	1:H:168:THR:HG22	2.25	0.67
1:I:48:LEU:HB3	2:i:1:CXP:H72	1.77	0.67
1:M:80:MET:CE	1:M:102:LEU:HD12	2.25	0.67
1:O:17:TYR:N	3:O:201:HOH:O	2.27	0.67
1:D:59:ILE:HD11	1:D:87:VAL:HG23	1.77	0.66
1:a:90:ILE:HD11	2:v:6:ALA:HB3	1.76	0.66
1:F:3:ILE:N	3:F:201:HOH:O	2.28	0.66
1:I:94:MET:HE1	1:I:120:MET:SD	2.35	0.66
1:J:17:TYR:OH	1:J:25:LYS:NZ	2.28	0.66
1:M:48:LEU:N	3:M:202:HOH:O	2.09	0.66
1:E:162:GLU:O	3:E:204:HOH:O	2.13	0.66
1:V:98:MET:HE1	1:V:149:LEU:HD21	1.78	0.66
1:X:40:ALA:O	1:X:44:VAL:HG12	1.96	0.66
1:A:147:ASP:OD1	1:A:147:ASP:N	2.28	0.66
1:B:15:ARG:HG3	1:B:15:ARG:HH11	1.59	0.66
1:B:40:ALA:HB2	1:B:72:ALA:HB1	1.78	0.65
1:J:98:MET:HE1	1:J:123:GLN:OE1	1.96	0.65
1:M:48:LEU:HB3	2:l:1:CXP:H72	1.79	0.65
1:Q:147:ASP:OD2	3:Q:201:HOH:O	2.14	0.65
1:X:62:TYR:HE1	1:X:90:ILE:HD13	1.61	0.65
1:A:170:ARG:NH1	1:J:166:ARG:HA	2.12	0.65
1:N:71:THR:O	3:N:201:HOH:O	2.15	0.65
1:T:148:LYS:O	1:T:152:VAL:HG23	1.97	0.65
1:a:170:ARG:HG2	1:a:171:ASP:N	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:ILE:HG23	1:A:3:ILE:O	1.96	0.64
1:B:89:THR:HG21	1:B:103:LEU:HA	1.78	0.64
1:E:61:LEU:HD22	1:E:89:THR:HG23	1.79	0.64
1:O:148:LYS:O	1:O:152:VAL:HG23	1.97	0.64
1:H:17:TYR:N	3:H:202:HOH:O	2.28	0.64
1:Y:148:LYS:O	1:Y:152:VAL:HG23	1.98	0.64
1:I:109:GLY:N	1:I:186:ASP:OD2	2.30	0.64
1:S:170:ARG:HH22	1:a:170:ARG:HG3	1.62	0.64
1:V:136:GLU:OE2	1:V:140:LYS:CE	2.41	0.64
1:W:68:GLY:N	3:W:204:HOH:O	2.30	0.64
1:P:37:ASP:OD2	3:P:201:HOH:O	2.15	0.64
1:X:62:TYR:CE1	1:X:90:ILE:HD13	2.32	0.64
1:H:118:GLU:HG3	1:H:173:PHE:CD2	2.32	0.64
1:A:170:ARG:CD	1:J:169:ASP:HB3	2.28	0.64
1:B:89:THR:HG22	1:B:103:LEU:HD12	1.80	0.64
1:A:170:ARG:CD	1:J:169:ASP:HB2	2.28	0.63
1:F:62:TYR:CE1	1:F:90:ILE:HD12	2.33	0.63
1:K:48:LEU:HD11	2:j:2:WFP:CE1	2.28	0.63
1:J:40:ALA:O	1:J:44:VAL:HG13	1.97	0.63
1:N:24:LEU:HD11	1:N:50:LEU:HD21	1.80	0.63
1:N:74:MET:N	3:N:201:HOH:O	2.04	0.63
1:S:31:LEU:HD13	1:S:43:ILE:HD11	1.79	0.63
1:X:139:ALA:N	3:X:203:HOH:O	2.30	0.63
1:Y:98:MET:SD	1:Y:123:GLN:NE2	2.71	0.63
1:a:62:TYR:HB3	1:a:92:ILE:HD11	1.79	0.63
1:R:172:ASN:HD22	1:R:172:ASN:C	2.05	0.63
1:L:37:ASP:OD2	3:M:203:HOH:O	2.15	0.63
1:a:31:LEU:HD13	1:a:43:ILE:CD1	2.29	0.63
1:X:98:MET:HE1	1:X:149:LEU:HD11	1.81	0.63
1:W:62:TYR:CE1	1:W:90:ILE:HD13	2.33	0.63
1:E:178:GLU:OE1	3:E:205:HOH:O	2.15	0.63
1:M:62:TYR:CE1	1:M:90:ILE:HD12	2.33	0.63
1:Y:44:VAL:HG23	1:Y:79:THR:OG1	1.98	0.63
1:Z:40:ALA:HB2	1:Z:72:ALA:HB1	1.81	0.63
1:O:171:ASP:OD1	1:X:125:LEU:HD21	1.97	0.62
1:R:56:GLU:OE1	3:R:203:HOH:O	2.16	0.62
1:Y:80:MET:CE	1:Y:102:LEU:HD22	2.26	0.62
1:K:118:GLU:OE1	1:K:173:PHE:CD2	2.52	0.62
1:T:48:LEU:HB3	2:q:1:CXP:H71	1.82	0.62
1:U:62:TYR:CE1	1:U:90:ILE:HD12	2.34	0.62
1:D:62:TYR:CE2	1:D:92:ILE:HD11	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:LEU:O	1:D:165:GLU:HG3	2.00	0.62
1:H:62:TYR:HD2	1:H:92:ILE:HD13	1.64	0.62
1:I:38:ASN:ND2	3:I:201:HOH:O	2.32	0.62
1:N:109:GLY:N	1:N:186:ASP:OD2	2.33	0.62
1:U:106:GLY:O	1:U:156:ARG:NH2	2.31	0.62
1:K:3:ILE:HB	1:K:4:PRO:HD2	1.82	0.62
1:O:40:ALA:HB2	1:O:72:ALA:HB1	1.80	0.62
1:O:135:ILE:HD12	1:P:171:ASP:CB	2.29	0.62
1:X:31:LEU:HD23	1:X:31:LEU:O	2.00	0.62
1:Q:90:ILE:HD11	2:n:6:ALA:HB3	1.81	0.62
1:C:167:ASP:OD1	1:C:170:ARG:NH2	2.33	0.62
1:T:140:LYS:O	1:T:144:LEU:HD13	1.99	0.62
1:a:40:ALA:HB2	1:a:72:ALA:HB1	1.82	0.62
1:E:108:LYS:NZ	1:E:156:ARG:O	2.28	0.61
1:W:40:ALA:HB2	1:W:72:ALA:HB1	1.81	0.61
1:X:120:MET:HE1	1:X:173:PHE:CZ	2.34	0.61
1:H:109:GLY:N	1:H:186:ASP:OD2	2.31	0.61
1:V:120:MET:HE3	1:V:122:HIS:HB3	1.83	0.61
1:P:40:ALA:HB2	1:P:72:ALA:HB1	1.82	0.61
1:Q:143:LEU:HD21	1:b:143:LEU:HD22	1.81	0.61
1:W:141:ARG:HD3	1:X:173:PHE:CD2	2.36	0.61
1:R:109:GLY:N	1:R:186:ASP:OD2	2.33	0.61
1:W:90:ILE:HD11	2:r:6:ALA:HB1	1.83	0.61
1:X:18:ASP:OD1	1:X:19:ILE:N	2.34	0.61
1:L:40:ALA:HB2	1:L:72:ALA:HB1	1.82	0.61
1:Z:3:ILE:N	3:Z:202:HOH:O	2.33	0.61
1:R:139:ALA:C	1:R:142:ILE:HD12	2.25	0.61
1:X:78:ASP:HB3	1:Y:114:LEU:HD13	1.82	0.61
1:a:170:ARG:NH1	1:a:171:ASP:O	2.34	0.61
1:T:2:LEU:N	3:T:203:HOH:O	2.34	0.60
1:G:62:TYR:CE1	1:G:90:ILE:HD12	2.36	0.60
1:Q:163:VAL:HG22	1:Q:166:ARG:NH2	2.16	0.60
1:W:62:TYR:HE1	1:W:90:ILE:HD13	1.64	0.60
1:Y:163:VAL:HG22	1:Y:167:ASP:OD2	2.01	0.60
1:M:80:MET:SD	1:M:87:VAL:HG11	2.40	0.60
1:M:82:PHE:HE2	1:N:189:LEU:HD22	1.66	0.60
1:E:86:LYS:HD3	1:E:107:GLU:OE2	2.00	0.60
1:M:170:ARG:HG2	1:M:171:ASP:N	2.16	0.60
1:Y:77:TYR:HE1	1:Y:105:ALA:HB1	1.65	0.60
1:M:49:PHE:CE2	1:N:6:VAL:HG11	2.35	0.60
1:a:48:LEU:HB3	2:w:1:CXP:H72	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:TYR:CA	1:C:185:ILE:HD11	2.31	0.60
1:M:48:LEU:HB2	3:M:202:HOH:O	2.01	0.60
1:M:122:HIS:N	3:M:205:HOH:O	2.26	0.60
1:V:113:ALA:HB2	1:V:185:ILE:HD13	1.83	0.60
1:E:27:ARG:HD3	1:E:57:LYS:HD2	1.84	0.60
1:B:118:GLU:OE1	1:B:173:PHE:CE1	2.54	0.59
1:U:170:ARG:HB3	1:Y:170:ARG:HB3	1.83	0.59
1:N:108:LYS:HD3	1:N:156:ARG:NH2	2.17	0.59
1:R:29:ILE:CD1	1:R:43:ILE:HG23	2.32	0.59
1:A:40:ALA:HB2	1:A:72:ALA:HB1	1.85	0.59
1:A:121:ILE:HD12	1:A:121:ILE:H	1.67	0.59
1:M:121:ILE:N	3:M:205:HOH:O	2.33	0.59
1:O:49:PHE:CZ	1:P:6:VAL:HG11	2.37	0.59
1:X:120:MET:HE1	1:X:173:PHE:CE1	2.37	0.59
1:P:85:PRO:O	3:P:202:HOH:O	2.17	0.59
1:U:122:HIS:CG	1:U:122:HIS:O	2.54	0.59
1:Y:77:TYR:CE1	1:Y:105:ALA:HB1	2.38	0.59
1:E:7:ILE:HG12	1:E:16:ALA:HB2	1.84	0.59
1:E:120:MET:CE	1:E:122:HIS:HB3	2.27	0.59
1:X:16:ALA:O	1:Y:6:VAL:HG21	2.02	0.59
1:C:3:ILE:HD11	1:C:20:TYR:CE2	2.37	0.59
1:E:89:THR:HG22	1:E:103:LEU:HD12	1.85	0.59
1:N:71:THR:C	3:N:201:HOH:O	2.45	0.59
1:Q:161:LEU:O	1:Q:161:LEU:HD23	2.03	0.59
1:T:7:ILE:O	3:T:201:HOH:O	2.17	0.59
1:X:148:LYS:O	1:X:152:VAL:HG12	2.01	0.59
1:C:2:LEU:HD22	1:C:3:ILE:H	1.67	0.59
1:C:78:ASP:OD2	1:D:116:ASN:HB2	2.03	0.59
1:F:62:TYR:HB3	1:F:92:ILE:HD11	1.83	0.59
1:Q:148:LYS:NZ	3:Q:206:HOH:O	2.34	0.58
2:v:3:SER:HA	3:v:101:HOH:O	2.03	0.58
1:E:145:LEU:HD12	1:E:145:LEU:H	1.68	0.58
2:m:6:ALA:C	3:m:101:HOH:O	2.46	0.58
1:D:29:ILE:HD11	1:D:43:ILE:HG12	1.84	0.58
1:K:109:GLY:N	1:K:186:ASP:OD2	2.36	0.58
1:S:175:SER:OG	1:S:177:GLU:OE1	2.16	0.58
1:T:18:ASP:OD1	1:T:19:ILE:O	2.21	0.58
1:C:2:LEU:HD13	1:C:3:ILE:N	2.19	0.58
1:E:101:PHE:CZ	1:E:152:VAL:HG11	2.39	0.58
1:Q:7:ILE:HD12	1:Q:7:ILE:O	2.03	0.58
1:L:144:LEU:HD12	1:L:144:LEU:H	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:90:ILE:HD11	2:m:6:ALA:CB	2.33	0.58
1:Y:74:MET:HE2	1:Y:149:LEU:HD21	1.85	0.58
1:V:3:ILE:HG22	1:V:19:ILE:HB	1.84	0.58
1:Y:74:MET:HE2	1:Y:149:LEU:CD2	2.34	0.58
1:E:101:PHE:CE1	1:E:152:VAL:CG1	2.87	0.58
1:Y:164:ILE:O	1:Y:168:THR:HG23	2.02	0.58
1:J:109:GLY:N	1:J:186:ASP:OD2	2.33	0.58
1:P:124:PRO:O	1:P:125:LEU:HB2	2.03	0.58
2:m:2:WFP:O	3:m:101:HOH:O	2.17	0.58
1:Q:163:VAL:HG22	1:Q:166:ARG:HH22	1.69	0.58
1:E:39:VAL:HG22	1:E:43:ILE:HD12	1.86	0.57
1:L:97:SER:OG	1:L:98:MET:N	2.37	0.57
1:S:33:SER:O	1:S:65:SER:OG	2.16	0.57
1:b:31:LEU:HD13	1:b:43:ILE:HG13	1.86	0.57
1:L:139:ALA:O	1:L:142:ILE:HD12	2.04	0.57
1:M:123:GLN:O	1:M:146:ARG:NH2	2.37	0.57
1:R:18:ASP:OD2	3:R:204:HOH:O	2.16	0.57
1:T:18:ASP:OD1	1:T:18:ASP:C	2.47	0.57
1:V:3:ILE:O	1:V:3:ILE:HG23	2.04	0.57
1:a:109:GLY:N	1:a:186:ASP:OD2	2.34	0.57
1:J:2:LEU:HD23	1:J:3:ILE:N	2.20	0.57
1:O:113:ALA:CB	1:O:185:ILE:CD1	2.74	0.57
1:W:94:MET:HE1	1:W:120:MET:HE1	1.85	0.57
1:E:40:ALA:HB2	1:E:72:ALA:HB1	1.85	0.56
1:S:170:ARG:CZ	1:a:170:ARG:HG3	2.35	0.56
1:F:73:GLY:HA3	1:F:98:MET:HE2	1.88	0.56
1:B:169:ASP:OD1	1:B:170:ARG:NH1	2.39	0.56
1:E:166:ARG:N	3:E:204:HOH:O	2.37	0.56
1:L:77:TYR:CE2	1:L:81:GLN:NE2	2.71	0.56
1:Q:143:LEU:HD21	1:b:143:LEU:CD2	2.35	0.56
1:R:38:ASN:OD1	3:R:205:HOH:O	2.17	0.56
1:S:58:GLU:OE2	1:S:110:LYS:NZ	2.36	0.56
1:Z:15:ARG:N	3:Z:204:HOH:O	2.37	0.56
1:L:141:ARG:NH1	1:M:118:GLU:OE1	2.38	0.56
1:O:49:PHE:HA	2:m:1:CXP:H52	1.86	0.56
1:A:109:GLY:N	1:A:186:ASP:OD2	2.35	0.56
1:O:135:ILE:HD12	1:P:171:ASP:HB3	1.87	0.56
1:Q:139:ALA:HB1	1:b:143:LEU:CD1	2.35	0.56
1:B:92:ILE:HD12	2:c:2:WFP:F1	1.96	0.56
1:E:153:LEU:O	1:E:157:THR:HG23	2.06	0.56
1:A:170:ARG:CZ	1:J:169:ASP:HB2	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:40:ALA:HB2	1:I:72:ALA:HB1	1.88	0.55
1:J:119:VAL:HG11	1:J:184:LEU:HD13	1.88	0.55
1:Q:18:ASP:OD1	1:Q:19:ILE:N	2.39	0.55
1:V:40:ALA:O	1:V:44:VAL:HG23	2.06	0.55
1:C:40:ALA:O	1:C:44:VAL:HG12	2.07	0.55
1:H:118:GLU:HG2	1:N:141:ARG:HD3	1.88	0.55
1:O:141:ARG:NH1	1:P:118:GLU:OE1	2.40	0.55
1:V:147:ASP:OD1	1:V:148:LYS:N	2.40	0.55
1:Y:177:GLU:O	1:Y:181:GLU:HG3	2.06	0.55
1:S:70:ILE:HD12	1:S:70:ILE:H	1.72	0.55
1:V:121:ILE:HD11	1:V:184:LEU:CD2	2.35	0.55
1:F:16:ALA:N	3:F:202:HOH:O	2.38	0.55
1:H:3:ILE:HG23	1:H:3:ILE:O	2.06	0.55
1:X:163:VAL:HG12	1:X:167:ASP:OD2	2.07	0.55
1:I:150:ASN:OD1	1:I:168:THR:HG21	2.07	0.55
1:N:46:GLN:O	1:N:50:LEU:HD23	2.07	0.55
1:U:140:LYS:O	1:U:144:LEU:HD13	2.07	0.55
1:C:74:MET:HE3	1:C:74:MET:HA	1.89	0.55
1:D:87:VAL:HG13	1:D:87:VAL:O	2.07	0.55
1:B:90:ILE:HD11	2:c:6:ALA:HB1	1.88	0.54
1:X:3:ILE:HD11	1:X:20:TYR:HE2	1.72	0.54
1:E:101:PHE:HE1	1:E:152:VAL:CG1	2.20	0.54
1:I:89:THR:C	1:I:90:ILE:HD12	2.32	0.54
1:Y:62:TYR:HD2	1:Y:92:ILE:HD11	1.70	0.54
1:H:73:GLY:HA3	1:H:98:MET:HE2	1.89	0.54
1:I:17:TYR:OH	1:J:7:ILE:HG12	2.06	0.54
1:S:40:ALA:HB2	1:S:72:ALA:HB1	1.89	0.54
1:R:120:MET:HE3	1:R:122:HIS:HB3	1.90	0.54
1:Z:140:LYS:H	1:Z:140:LYS:HD2	1.73	0.54
1:D:112:TYR:HB3	1:D:189:LEU:HD21	1.90	0.54
1:P:17:TYR:OH	1:Q:7:ILE:HG12	2.08	0.54
1:Z:31:LEU:HD13	1:Z:43:ILE:CD1	2.33	0.54
1:H:3:ILE:HG22	1:H:19:ILE:HB	1.90	0.54
1:E:101:PHE:HE1	1:E:152:VAL:HG13	1.73	0.54
1:K:27:ARG:HD3	1:K:57:LYS:HE3	1.90	0.54
1:X:74:MET:HG3	1:X:145:LEU:HD23	1.89	0.54
1:L:120:MET:HE1	1:L:171:ASP:CB	2.38	0.54
1:Z:141:ARG:HA	1:Z:144:LEU:HD13	1.89	0.54
1:Z:153:LEU:O	1:Z:157:THR:HG23	2.08	0.54
1:R:62:TYR:HD2	1:R:92:ILE:HD11	1.73	0.53
1:T:40:ALA:HB2	1:T:72:ALA:HB1	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:62:TYR:CD2	1:Y:92:ILE:HD11	2.43	0.53
1:Z:61:LEU:CD2	1:Z:63:ILE:HD11	2.38	0.53
1:S:109:GLY:N	1:S:186:ASP:OD2	2.39	0.53
1:Z:50:LEU:HD13	1:Z:59:ILE:HD12	1.90	0.53
1:Q:120:MET:HE1	1:Q:171:ASP:CG	2.33	0.53
1:S:151:LYS:O	1:S:155:GLU:HG3	2.08	0.53
1:C:78:ASP:OD2	1:D:116:ASN:ND2	2.36	0.53
1:N:31:LEU:HD13	1:N:43:ILE:HG13	1.91	0.53
1:K:3:ILE:HD11	1:K:20:TYR:CE2	2.44	0.53
1:K:160:PRO:HG2	1:K:163:VAL:HG13	1.90	0.53
1:O:120:MET:HE3	1:O:171:ASP:O	2.08	0.53
1:O:137:ILE:CD1	1:P:170:ARG:HH21	2.08	0.53
1:O:173:PHE:HZ	1:U:144:LEU:CD2	2.21	0.53
1:X:6:VAL:HG23	1:X:17:TYR:HB2	1.91	0.53
1:Y:40:ALA:HB2	1:Y:72:ALA:HB1	1.89	0.53
1:K:35:ILE:HA	1:K:39:VAL:HG21	1.89	0.53
1:L:92:ILE:HD13	2:j:2:WFP:F1	1.98	0.53
1:L:112:TYR:CE2	2:j:6:ALA:HB2	2.44	0.53
1:R:139:ALA:N	1:R:142:ILE:HD11	2.22	0.53
1:T:142:ILE:HD11	1:Y:139:ALA:HB1	1.90	0.53
1:Y:50:LEU:HD13	1:Y:59:ILE:HG12	1.89	0.53
1:C:98:MET:HE3	1:C:98:MET:HA	1.90	0.53
1:E:101:PHE:HZ	1:E:152:VAL:HG11	1.72	0.53
1:S:31:LEU:HD13	1:S:43:ILE:CD1	2.39	0.53
1:C:121:ILE:HD11	1:C:184:LEU:HD21	1.89	0.53
1:O:171:ASP:CG	1:X:125:LEU:HD21	2.33	0.53
1:Q:40:ALA:HB2	1:Q:72:ALA:HB1	1.91	0.53
1:R:27:ARG:NH2	1:R:57:LYS:O	2.41	0.53
1:W:109:GLY:N	1:W:186:ASP:OD2	2.41	0.53
2:v:2:WFP:C	3:v:101:HOH:O	2.57	0.53
1:C:40:ALA:HB2	1:C:72:ALA:HB1	1.90	0.53
1:Q:174:LYS:HE3	1:Q:182:TYR:CD1	2.43	0.53
1:K:137:ILE:HD13	1:L:172:ASN:HA	1.91	0.53
1:L:80:MET:HE2	1:L:102:LEU:HD22	1.89	0.53
1:S:97:SER:OG	1:S:98:MET:N	2.42	0.53
1:C:86:LYS:HD3	1:C:107:GLU:HG3	1.91	0.52
1:R:3:ILE:O	1:R:4:PRO:C	2.53	0.52
1:H:121:ILE:HD11	1:H:184:LEU:HD21	1.92	0.52
1:I:48:LEU:HD11	2:i:2:WFP:CE1	2.39	0.52
1:O:191:HIS:N	3:O:204:HOH:O	2.40	0.52
1:P:148:LYS:O	1:P:152:VAL:HG12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:3:ILE:O	1:V:3:ILE:CG2	2.57	0.52
1:a:67:GLY:HA3	1:a:97:SER:HB3	1.91	0.52
1:a:123:GLN:OE1	3:a:202:HOH:O	2.18	0.52
1:b:125:LEU:O	1:b:126:GLY:C	2.53	0.52
1:C:43:ILE:HD11	1:C:76:ILE:HG21	1.91	0.52
1:E:101:PHE:CE1	1:E:152:VAL:HG13	2.45	0.52
1:R:40:ALA:O	1:R:44:VAL:HG13	2.09	0.52
1:R:62:TYR:CD2	1:R:92:ILE:HD11	2.45	0.52
1:U:40:ALA:HB2	1:U:72:ALA:HB1	1.90	0.52
1:A:58:GLU:HB3	1:A:86:LYS:HE2	1.92	0.52
1:A:136:GLU:HA	1:A:136:GLU:OE1	2.08	0.52
1:P:146:ARG:HD2	1:V:135:ILE:HD12	1.90	0.52
1:W:92:ILE:HD11	2:r:2:WFP:F1	2.00	0.52
1:Z:70:ILE:CD1	1:Z:145:LEU:HD13	2.39	0.52
1:A:5:THR:OG1	1:A:6:VAL:N	2.42	0.52
1:P:146:ARG:HB2	1:V:135:ILE:HD12	1.91	0.52
1:D:59:ILE:C	1:D:59:ILE:HD12	2.34	0.52
1:G:22:ARG:NH1	1:G:26:ASP:OD1	2.34	0.52
1:K:54:ASP:OD1	1:K:56:GLU:N	2.42	0.52
1:R:36:ASP:OD1	1:R:39:VAL:HG13	2.10	0.52
1:D:59:ILE:HD11	1:D:87:VAL:CG2	2.40	0.52
1:F:62:TYR:HB3	1:F:92:ILE:CD1	2.39	0.52
1:O:39:VAL:HG22	1:P:2:LEU:HD11	1.91	0.52
1:O:135:ILE:HD12	1:P:171:ASP:HB2	1.92	0.52
1:N:159:GLN:HG3	1:N:160:PRO:HD2	1.91	0.52
1:R:172:ASN:O	1:R:172:ASN:ND2	2.38	0.52
1:V:39:VAL:HG22	1:W:2:LEU:HD11	1.91	0.52
1:D:40:ALA:O	1:D:44:VAL:HG12	2.09	0.51
1:E:77:TYR:OH	1:E:152:VAL:CG2	2.59	0.51
1:S:168:THR:O	1:S:168:THR:HG22	2.11	0.51
1:U:143:LEU:HD21	1:X:140:LYS:HE3	1.92	0.51
1:W:92:ILE:CD1	2:r:2:WFP:F1	2.49	0.51
1:D:27:ARG:HA	1:D:50:LEU:HD11	1.92	0.51
1:R:40:ALA:HB2	1:R:72:ALA:HB1	1.92	0.51
1:T:90:ILE:HD11	2:p:6:ALA:HB3	1.92	0.51
1:H:4:PRO:O	1:N:21:SER:OG	2.29	0.51
1:M:109:GLY:N	1:M:186:ASP:OD2	2.44	0.51
1:P:138:ALA:HA	1:V:125:LEU:HD22	1.93	0.51
1:W:141:ARG:HD3	1:X:173:PHE:CE2	2.45	0.51
1:X:120:MET:CE	1:X:173:PHE:CE1	2.93	0.51
1:A:137:ILE:O	1:A:140:LYS:HD3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:ARG:NE	1:E:118:GLU:OE2	2.38	0.51
1:N:108:LYS:HD3	1:N:156:ARG:HH21	1.74	0.51
1:N:120:MET:HE2	1:N:173:PHE:CZ	2.46	0.51
1:S:137:ILE:HG12	1:S:140:LYS:HD2	1.91	0.51
1:D:39:VAL:O	1:D:43:ILE:HD12	2.10	0.51
1:D:40:ALA:HB2	1:D:72:ALA:HB1	1.93	0.51
1:V:48:LEU:HB3	2:r:1:CXP:H82	1.93	0.51
1:F:40:ALA:HB2	1:F:72:ALA:HB1	1.92	0.51
1:D:87:VAL:O	1:D:87:VAL:CG1	2.59	0.51
1:E:48:LEU:HD12	2:f:1:CXP:O2	2.11	0.51
1:E:69:SER:OG	3:E:206:HOH:O	2.16	0.51
1:E:169:ASP:OD2	1:M:170:ARG:NH2	2.44	0.51
1:N:19:ILE:HG23	1:N:20:TYR:N	2.25	0.51
1:T:22:ARG:NH1	1:T:26:ASP:OD1	2.38	0.51
1:H:30:MET:HE1	1:N:41:ASN:OD1	2.10	0.51
1:S:112:TYR:CE2	2:o:6:ALA:HB2	2.46	0.51
1:V:78:ASP:O	3:V:201:HOH:O	2.17	0.51
1:G:90:ILE:HG23	1:G:112:TYR:HB2	1.92	0.50
1:H:59:ILE:HD12	1:H:85:PRO:HB2	1.92	0.50
1:N:74:MET:HB2	3:N:201:HOH:O	2.11	0.50
1:Z:146:ARG:NH2	1:Z:165:GLU:O	2.44	0.50
1:C:123:GLN:HE21	1:C:149:LEU:HD21	1.74	0.50
1:Q:161:LEU:HD23	1:Q:165:GLU:HG3	1.93	0.50
1:R:80:MET:CE	1:R:102:LEU:HD22	2.41	0.50
1:V:98:MET:HE1	1:V:149:LEU:CD2	2.40	0.50
1:V:147:ASP:OD1	1:V:147:ASP:C	2.54	0.50
1:Y:120:MET:HG3	1:Y:173:PHE:CD1	2.45	0.50
1:H:40:ALA:HB2	1:H:72:ALA:HB1	1.93	0.50
1:O:160:PRO:HG2	1:O:163:VAL:HG13	1.92	0.50
1:V:121:ILE:CG2	1:V:168:THR:HG22	2.42	0.50
1:Y:6:VAL:HG12	1:Y:6:VAL:O	2.11	0.50
1:a:58:GLU:OE1	1:a:110:LYS:HE3	2.12	0.50
1:D:35:ILE:HA	1:D:39:VAL:HG21	1.92	0.50
1:H:39:VAL:O	1:H:43:ILE:HG12	2.11	0.50
1:P:62:TYR:CE1	1:P:90:ILE:CD1	2.93	0.50
1:S:121:ILE:O	1:S:168:THR:HG23	2.11	0.50
1:A:38:ASN:HB3	1:B:2:LEU:HD21	1.93	0.50
1:G:97:SER:OG	1:G:98:MET:N	2.44	0.50
1:H:121:ILE:HG22	1:H:168:THR:HG22	1.93	0.50
1:O:171:ASP:OD1	1:O:171:ASP:O	2.29	0.50
1:M:77:TYR:CD1	1:M:77:TYR:C	2.89	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:76:ILE:O	1:N:80:MET:HG3	2.12	0.50
1:O:48:LEU:HD11	2:m:2:WFP:CE1	2.41	0.50
1:P:23:LEU:CD2	2:m:1:CXP:H51	2.40	0.50
1:J:148:LYS:O	1:J:152:VAL:HG12	2.11	0.50
1:E:27:ARG:NH2	1:E:59:ILE:HD11	2.27	0.50
1:U:18:ASP:OD1	1:U:21:SER:HB2	2.12	0.50
1:Y:112:TYR:HB3	1:Y:189:LEU:HD21	1.92	0.50
1:b:123:GLN:C	1:b:123:GLN:CD	2.79	0.50
1:C:3:ILE:HD11	1:C:20:TYR:HE2	1.77	0.50
1:C:154:ALA:HB2	1:C:164:ILE:HD12	1.94	0.50
1:D:6:VAL:HG12	1:D:6:VAL:O	2.12	0.50
1:E:77:TYR:CZ	1:E:152:VAL:HG21	2.47	0.50
1:U:160:PRO:HG2	1:U:163:VAL:HG23	1.93	0.50
1:W:23:LEU:CD2	2:r:1:CXP:H51	2.41	0.50
1:Z:145:LEU:HD12	1:Z:145:LEU:C	2.27	0.50
1:a:31:LEU:HD13	1:a:43:ILE:HD11	1.94	0.50
1:a:170:ARG:CG	1:a:171:ASP:N	2.75	0.50
1:Q:2:LEU:HD22	1:Q:3:ILE:H	1.77	0.49
1:E:17:TYR:HB2	1:E:21:SER:HB2	1.93	0.49
1:N:159:GLN:HG3	1:N:160:PRO:CD	2.42	0.49
1:Z:27:ARG:NH2	1:Z:59:ILE:HD11	2.26	0.49
1:J:172:ASN:OD1	1:J:172:ASN:O	2.30	0.49
1:L:77:TYR:CZ	1:L:81:GLN:NE2	2.72	0.49
1:M:80:MET:HE2	1:M:102:LEU:HD12	1.94	0.49
1:U:97:SER:OG	1:U:98:MET:N	2.44	0.49
1:B:17:TYR:OH	1:C:7:ILE:HG12	2.12	0.49
1:E:121:ILE:HD12	1:E:168:THR:HA	1.95	0.49
1:Q:170:ARG:NH1	1:Q:172:ASN:HB3	2.28	0.49
1:H:19:ILE:HG23	1:H:20:TYR:N	2.28	0.49
1:b:40:ALA:HB2	1:b:72:ALA:HB1	1.93	0.49
1:D:62:TYR:HD2	1:D:92:ILE:HD11	1.76	0.49
1:H:118:GLU:HG2	1:N:141:ARG:CD	2.43	0.49
1:K:40:ALA:HB2	1:K:72:ALA:HB1	1.95	0.49
1:N:62:TYR:HD2	1:N:92:ILE:HD11	1.78	0.49
1:O:171:ASP:OD1	1:O:171:ASP:C	2.55	0.49
1:O:190:THR:OG1	1:O:191:HIS:N	2.45	0.49
1:V:121:ILE:HG22	1:V:168:THR:HG22	1.94	0.49
1:Z:18:ASP:OD1	1:Z:21:SER:OG	2.27	0.49
1:L:81:GLN:HE22	1:L:156:ARG:HH22	1.60	0.49
1:V:62:TYR:CD2	1:V:92:ILE:HD11	2.48	0.49
1:B:97:SER:OG	1:B:98:MET:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:ILE:HD11	1:C:76:ILE:CG2	2.42	0.49
1:H:121:ILE:HD11	1:H:184:LEU:CD2	2.42	0.49
1:X:122:HIS:CE1	1:X:171:ASP:OD1	2.66	0.49
1:a:62:TYR:CE1	1:a:90:ILE:HD12	2.48	0.49
1:A:170:ARG:HG3	1:J:169:ASP:O	2.13	0.49
1:C:165:GLU:O	1:C:169:ASP:OD1	2.30	0.49
1:K:74:MET:HE2	1:K:149:LEU:HD21	1.95	0.49
1:Q:58:GLU:OE2	1:Q:110:LYS:NZ	2.45	0.49
1:Q:109:GLY:N	1:Q:186:ASP:OD2	2.45	0.49
1:Q:170:ARG:HD2	1:V:169:ASP:OD2	2.12	0.49
1:X:107:GLU:OE2	1:X:110:LYS:HG3	2.12	0.49
1:Y:44:VAL:O	1:Y:48:LEU:HG	2.13	0.49
1:Y:67:GLY:HA2	1:Y:97:SER:HB2	1.93	0.49
1:L:53:GLU:OE1	3:L:204:HOH:O	2.20	0.49
1:Q:166:ARG:HH11	1:Q:166:ARG:CB	2.26	0.49
1:W:67:GLY:N	3:W:204:HOH:O	2.46	0.49
1:A:170:ARG:HG3	1:J:169:ASP:C	2.38	0.48
1:M:24:LEU:HD13	1:M:46:GLN:OE1	2.12	0.48
1:M:49:PHE:CE1	1:M:53:GLU:OE2	2.65	0.48
1:Z:141:ARG:NH1	1:a:118:GLU:OE2	2.46	0.48
1:B:172:ASN:C	1:B:172:ASN:ND2	2.71	0.48
1:T:31:LEU:HD13	1:T:43:ILE:CD1	2.44	0.48
1:E:89:THR:HG21	1:E:103:LEU:HA	1.95	0.48
1:H:147:ASP:OD1	1:H:148:LYS:N	2.46	0.48
1:L:149:LEU:O	1:L:153:LEU:HD23	2.12	0.48
1:Q:7:ILE:O	1:Q:7:ILE:CD1	2.61	0.48
1:Q:30:MET:HE1	1:Q:92:ILE:HD11	1.94	0.48
1:D:70:ILE:HD12	1:D:70:ILE:N	2.29	0.48
1:K:29:ILE:HD12	1:K:43:ILE:HG23	1.94	0.48
1:K:74:MET:CE	1:K:149:LEU:HD21	2.43	0.48
1:X:37:ASP:O	1:X:41:ASN:OD1	2.30	0.48
1:D:27:ARG:HA	1:D:50:LEU:HD21	1.95	0.48
1:I:90:ILE:HD11	2:h:6:ALA:HB1	1.96	0.48
1:N:70:ILE:HD11	1:N:145:LEU:HB3	1.96	0.48
1:R:152:VAL:O	1:R:156:ARG:HG2	2.12	0.48
1:T:19:ILE:O	1:T:20:TYR:HB2	2.14	0.48
1:E:120:MET:HE1	1:E:122:HIS:CB	2.33	0.48
1:E:141:ARG:HD2	1:E:141:ARG:O	2.13	0.48
1:M:45:SER:C	3:M:202:HOH:O	2.55	0.48
1:W:112:TYR:CD1	1:W:189:LEU:HD21	2.48	0.48
1:Z:172:ASN:CG	1:Z:172:ASN:O	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:PRO:HG2	1:D:19:ILE:HB	1.94	0.48
1:G:40:ALA:HB2	1:G:72:ALA:HB1	1.95	0.48
1:C:80:MET:HG3	1:C:87:VAL:HG21	1.94	0.48
1:F:151:LYS:NZ	3:F:203:HOH:O	2.46	0.48
1:I:77:TYR:HA	1:I:80:MET:HE2	1.96	0.48
1:K:27:ARG:HG2	1:K:50:LEU:HD22	1.96	0.48
1:K:39:VAL:O	1:K:43:ILE:HG13	2.14	0.48
1:M:165:GLU:OE1	3:M:204:HOH:O	2.20	0.48
1:V:62:TYR:HD2	1:V:92:ILE:HD11	1.78	0.48
1:V:98:MET:HG2	1:V:123:GLN:HE21	1.79	0.48
1:D:27:ARG:HD3	1:D:57:LYS:HE3	1.95	0.48
1:U:108:LYS:H	1:U:108:LYS:HD2	1.78	0.48
1:Z:138:ALA:N	1:Z:140:LYS:HZ3	2.12	0.48
1:H:86:LYS:HD2	1:H:110:LYS:NZ	2.28	0.47
1:L:35:ILE:HA	1:L:39:VAL:HG11	1.96	0.47
1:H:118:GLU:HG2	1:N:141:ARG:NH1	2.29	0.47
1:R:139:ALA:HA	1:R:142:ILE:HD13	1.96	0.47
1:X:35:ILE:HD12	1:X:98:MET:HB2	1.94	0.47
1:A:170:ARG:HH21	1:J:169:ASP:CG	2.21	0.47
1:B:22:ARG:NH1	1:B:26:ASP:OD1	2.45	0.47
1:D:109:GLY:N	1:D:186:ASP:OD2	2.37	0.47
1:E:77:TYR:CE1	1:E:81:GLN:HG3	2.49	0.47
1:H:84:LYS:HD2	1:H:84:LYS:C	2.39	0.47
1:M:170:ARG:CG	1:M:171:ASP:N	2.76	0.47
1:E:159:GLN:OE1	1:E:182:TYR:HA	2.14	0.47
1:S:171:ASP:OD1	1:S:171:ASP:O	2.32	0.47
1:Z:145:LEU:CG	1:Z:146:ARG:H	2.27	0.47
1:N:60:SER:OG	1:N:62:TYR:HE1	1.98	0.47
1:R:139:ALA:O	1:R:142:ILE:HD12	2.14	0.47
1:S:177:GLU:CD	1:S:177:GLU:H	2.22	0.47
2:p:1:CXP:H22	2:p:1:CXP:H81	1.61	0.47
1:A:120:MET:HE1	1:A:171:ASP:HB2	1.96	0.47
1:E:159:GLN:OE1	1:E:182:TYR:CG	2.67	0.47
1:K:137:ILE:HA	1:K:140:LYS:HD2	1.96	0.47
1:M:48:LEU:CB	3:M:202:HOH:O	2.58	0.47
1:P:150:ASN:OD1	1:P:168:THR:HG21	2.14	0.47
1:T:62:TYR:CE1	1:T:90:ILE:HD12	2.49	0.47
2:g:1:CXP:H22	2:g:1:CXP:H81	1.74	0.47
1:B:90:ILE:HD11	2:c:6:ALA:CB	2.45	0.47
1:C:82:PHE:CD1	1:C:82:PHE:C	2.92	0.47
1:C:109:GLY:N	1:C:186:ASP:OD2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:LEU:O	1:C:149:LEU:N	2.44	0.47
1:E:165:GLU:O	1:E:168:THR:HG22	2.15	0.47
1:K:40:ALA:O	1:K:44:VAL:HG13	2.15	0.47
1:M:90:ILE:HD11	2:k:6:ALA:HB3	1.97	0.47
1:U:57:LYS:HG3	1:U:58:GLU:H	1.80	0.47
1:B:180:LEU:HD12	3:B:204:HOH:O	2.14	0.47
1:C:19:ILE:O	1:C:20:TYR:HB2	2.15	0.47
1:H:161:LEU:O	1:H:165:GLU:HG3	2.15	0.47
1:I:97:SER:OG	1:I:98:MET:N	2.48	0.47
1:W:98:MET:HE2	1:W:98:MET:HA	1.97	0.47
1:X:44:VAL:CG2	1:X:79:THR:HG21	2.44	0.47
1:a:86:LYS:HD2	1:a:107:GLU:HG2	1.96	0.47
1:E:17:TYR:CD1	1:E:17:TYR:N	2.83	0.47
1:G:18:ASP:OD1	1:G:21:SER:HB2	2.15	0.47
1:O:142:ILE:HG22	1:O:146:ARG:HD2	1.96	0.47
1:T:123:GLN:OE1	1:T:149:LEU:HD13	2.15	0.47
1:a:58:GLU:OE2	1:a:88:SER:HB2	2.15	0.47
2:j:1:CXP:H22	2:j:1:CXP:H81	1.67	0.47
2:m:7:MP8:C	3:m:101:HOH:O	2.63	0.47
1:N:161:LEU:O	1:N:164:ILE:HB	2.14	0.47
1:P:139:ALA:HB3	1:V:143:LEU:CD1	2.45	0.47
1:Q:140:LYS:O	1:Q:143:LEU:HG	2.15	0.47
1:a:138:ALA:HB3	1:a:141:ARG:HB3	1.97	0.47
1:J:19:ILE:O	1:J:20:TYR:HB2	2.15	0.46
1:L:81:GLN:HE22	1:L:156:ARG:NH2	2.12	0.46
1:M:92:ILE:HD12	2:k:2:WFP:F1	2.05	0.46
1:Q:43:ILE:HD11	1:Q:76:ILE:CG2	2.45	0.46
1:a:48:LEU:HD11	2:w:2:WFP:CE1	2.45	0.46
1:O:171:ASP:OD1	1:X:125:LEU:CD2	2.63	0.46
1:U:121:ILE:HG23	1:U:167:ASP:O	2.15	0.46
1:F:166:ARG:NH2	1:F:167:ASP:OD1	2.48	0.46
1:O:120:MET:CE	1:O:171:ASP:HB2	2.45	0.46
1:P:146:ARG:HD2	1:V:135:ILE:CD1	2.45	0.46
1:R:29:ILE:HD11	1:R:43:ILE:HG23	1.97	0.46
1:C:168:THR:HG23	3:C:208:HOH:O	2.15	0.46
1:F:152:VAL:O	1:F:156:ARG:HG2	2.15	0.46
1:H:30:MET:CE	1:N:41:ASN:OD1	2.64	0.46
1:I:119:VAL:HG11	1:I:184:LEU:HD13	1.97	0.46
1:Q:19:ILE:O	1:Q:20:TYR:HB2	2.16	0.46
1:Y:70:ILE:CG2	1:Y:145:LEU:HD13	2.44	0.46
1:Z:143:LEU:O	1:Z:144:LEU:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:LYS:HD2	1:A:84:LYS:O	2.16	0.46
1:M:49:PHE:HA	2:l:1:CXP:H61	1.98	0.46
1:R:6:VAL:O	1:R:6:VAL:HG13	2.16	0.46
1:R:164:ILE:O	1:R:168:THR:HG23	2.16	0.46
1:U:94:MET:HE2	1:U:96:ALA:HB2	1.98	0.46
1:C:79:THR:O	1:C:83:ILE:HG12	2.16	0.46
1:D:60:SER:O	1:D:60:SER:OG	2.34	0.46
1:G:137:ILE:HG12	1:G:137:ILE:O	2.15	0.46
1:K:35:ILE:HB	1:K:68:GLY:HA3	1.98	0.46
1:K:70:ILE:O	1:K:74:MET:HG2	2.16	0.46
1:X:96:ALA:O	1:X:99:GLY:N	2.49	0.46
1:A:125:LEU:HD22	1:I:138:ALA:HA	1.97	0.46
1:C:41:ASN:HA	1:C:44:VAL:CG1	2.46	0.46
1:P:143:LEU:HD22	1:V:136:GLU:OE1	2.16	0.46
1:P:143:LEU:HD21	1:V:139:ALA:HB3	1.96	0.46
1:Q:161:LEU:CD2	1:Q:165:GLU:HG3	2.46	0.46
1:H:118:GLU:CG	1:N:141:ARG:HD3	2.46	0.46
1:H:118:GLU:HA	1:H:118:GLU:OE1	2.16	0.46
1:T:86:LYS:HD3	1:T:107:GLU:HG2	1.97	0.46
1:X:3:ILE:HD11	1:X:20:TYR:CE2	2.50	0.46
1:Y:167:ASP:OD2	1:Y:182:TYR:OH	2.31	0.46
1:E:58:GLU:O	1:E:59:ILE:HD13	2.16	0.46
1:E:84:LYS:HB3	1:E:85:PRO:HD3	1.98	0.46
1:P:122:HIS:C	1:P:124:PRO:HD3	2.41	0.46
1:Z:142:ILE:HG23	1:Z:145:LEU:HD21	1.97	0.46
1:A:70:ILE:O	1:A:74:MET:HG2	2.16	0.46
1:C:160:PRO:C	3:C:202:HOH:O	2.59	0.46
1:E:153:LEU:CD1	1:E:164:ILE:HG21	2.46	0.46
1:Z:22:ARG:NH2	1:Z:26:ASP:OD1	2.49	0.46
1:Z:120:MET:HE1	1:Z:171:ASP:HB2	1.97	0.46
1:C:121:ILE:HG22	1:C:168:THR:HG22	1.98	0.45
1:C:170:ARG:HD3	1:H:166:ARG:HH12	1.81	0.45
1:D:35:ILE:HB	1:D:68:GLY:HA3	1.99	0.45
1:E:48:LEU:HD12	2:f:1:CXP:C9	2.46	0.45
1:N:67:GLY:HA3	1:N:97:SER:HB3	1.97	0.45
1:O:161:LEU:O	1:O:165:GLU:HG3	2.15	0.45
1:E:148:LYS:HG2	1:F:116:ASN:OD1	2.16	0.45
1:F:21:SER:OG	1:G:5:THR:O	2.34	0.45
1:J:29:ILE:HG22	1:J:61:LEU:HD12	1.98	0.45
1:C:170:ARG:HG3	1:H:170:ARG:HG2	1.98	0.45
1:J:118:GLU:OE1	3:J:202:HOH:O	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:152:VAL:O	1:T:156:ARG:HG2	2.15	0.45
1:E:77:TYR:CD1	1:E:77:TYR:C	2.93	0.45
1:L:48:LEU:HB3	2:k:1:CXP:H82	1.97	0.45
1:S:137:ILE:HG23	1:S:140:LYS:HD2	1.98	0.45
1:E:112:TYR:CE2	2:e:6:ALA:HB2	2.51	0.45
1:J:177:GLU:HG3	1:J:178:GLU:N	2.32	0.45
1:K:3:ILE:HD11	1:K:20:TYR:HE2	1.81	0.45
1:N:27:ARG:HG2	1:N:50:LEU:HD12	1.99	0.45
1:O:162:GLU:H	1:O:162:GLU:CD	2.24	0.45
1:R:145:LEU:O	1:R:149:LEU:HG	2.16	0.45
1:Y:3:ILE:CB	1:Y:4:PRO:CD	2.94	0.45
1:Y:80:MET:HE1	1:Y:102:LEU:CD2	2.36	0.45
1:Z:111:ARG:O	1:Z:186:ASP:N	2.38	0.45
2:v:1:CXP:H22	2:v:1:CXP:H81	1.67	0.45
1:B:120:MET:HE3	1:B:173:PHE:HD1	1.81	0.45
1:D:51:ALA:HB2	1:D:83:ILE:HD12	1.99	0.45
1:E:153:LEU:HD12	1:E:154:ALA:N	2.31	0.45
1:E:180:LEU:HG	1:E:185:ILE:HG13	1.99	0.45
1:H:121:ILE:O	1:H:123:GLN:OE1	2.35	0.45
1:N:188:ILE:O	1:N:190:THR:N	2.50	0.45
1:U:57:LYS:HG3	1:U:58:GLU:N	2.32	0.45
1:a:120:MET:SD	1:a:173:PHE:CE2	3.10	0.45
1:a:165:GLU:O	1:a:169:ASP:HB2	2.16	0.45
1:J:143:LEU:HD12	1:J:144:LEU:N	2.32	0.45
1:K:141:ARG:NH1	1:L:118:GLU:OE2	2.49	0.45
1:M:19:ILE:O	1:M:20:TYR:HB2	2.15	0.45
1:Z:145:LEU:CG	1:Z:146:ARG:N	2.79	0.45
1:C:112:TYR:C	1:C:185:ILE:HD11	2.41	0.45
1:D:24:LEU:O	3:D:203:HOH:O	2.21	0.45
1:M:73:GLY:HA3	1:M:98:MET:HE2	1.99	0.45
1:N:24:LEU:HD22	1:N:46:GLN:OE1	2.16	0.45
1:Q:185:ILE:HG22	1:Q:186:ASP:N	2.31	0.45
2:n:1:CXP:H82	2:n:1:CXP:H61	1.78	0.45
1:E:89:THR:CG2	1:E:103:LEU:HD12	2.47	0.45
1:L:109:GLY:N	1:L:186:ASP:OD2	2.50	0.45
1:N:174:LYS:HE3	1:N:182:TYR:CD1	2.52	0.45
1:Q:166:ARG:HH11	1:Q:166:ARG:HB2	1.82	0.45
1:Z:91:CYS:HB2	1:Z:103:LEU:HD22	1.98	0.45
1:M:45:SER:HB3	1:N:23:LEU:CD1	2.42	0.45
1:O:142:ILE:HG22	1:O:146:ARG:CD	2.47	0.45
1:P:27:ARG:HG2	1:P:50:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:p:4:PRO:HA	2:p:5:YCP:HA	1.74	0.45
1:A:121:ILE:HG22	1:A:168:THR:HG22	1.98	0.44
1:B:89:THR:HG21	1:B:103:LEU:HD12	1.96	0.44
1:E:27:ARG:HG2	1:E:50:LEU:HD22	1.98	0.44
1:I:148:LYS:O	1:I:152:VAL:HG12	2.17	0.44
1:M:146:ARG:NE	3:M:207:HOH:O	2.29	0.44
1:P:27:ARG:HD3	1:P:57:LYS:HG2	2.00	0.44
1:U:90:ILE:HD11	2:q:6:ALA:CB	2.44	0.44
1:D:70:ILE:HD12	1:D:70:ILE:H	1.83	0.44
1:H:86:LYS:HD2	1:H:110:LYS:HZ2	1.83	0.44
1:J:23:LEU:N	3:J:201:HOH:O	2.31	0.44
1:N:164:ILE:O	1:N:168:THR:HG23	2.18	0.44
1:Z:141:ARG:O	1:Z:144:LEU:HB2	2.17	0.44
1:b:123:GLN:HB3	1:b:124:PRO:HD3	1.98	0.44
1:B:101:PHE:CZ	1:B:152:VAL:HG11	2.51	0.44
1:D:151:LYS:HA	1:D:161:LEU:HD11	2.00	0.44
1:P:160:PRO:HD2	1:P:163:VAL:HG11	1.99	0.44
1:S:17:TYR:N	1:S:17:TYR:CD1	2.86	0.44
1:S:62:TYR:CD1	1:S:90:ILE:CG2	3.00	0.44
1:S:170:ARG:NH1	1:a:170:ARG:HG3	2.32	0.44
1:U:108:LYS:H	1:U:108:LYS:CD	2.30	0.44
1:V:54:ASP:OD2	1:V:57:LYS:HE2	2.17	0.44
1:X:139:ALA:C	3:X:203:HOH:O	2.61	0.44
1:a:170:ARG:HG2	1:a:171:ASP:H	1.79	0.44
1:E:105:ALA:HA	1:E:156:ARG:CD	2.48	0.44
1:H:179:ALA:HB1	1:H:184:LEU:HD12	2.00	0.44
1:K:78:ASP:OD2	1:L:116:ASN:OD1	2.35	0.44
1:K:101:PHE:CZ	1:K:149:LEU:HD23	2.53	0.44
1:M:82:PHE:CE2	1:N:189:LEU:HD22	2.50	0.44
1:S:8:GLU:OE1	1:S:22:ARG:NH1	2.51	0.44
1:T:21:SER:OG	1:U:5:THR:O	2.35	0.44
1:T:31:LEU:HD11	1:T:35:ILE:HG12	2.00	0.44
1:Y:3:ILE:N	3:Y:202:HOH:O	2.49	0.44
1:E:29:ILE:HD11	1:E:50:LEU:HD12	1.98	0.44
1:K:152:VAL:O	1:K:156:ARG:HG2	2.17	0.44
1:a:28:ILE:HD11	2:v:7:MP8:HE	1.99	0.44
1:B:15:ARG:HG3	1:B:15:ARG:NH1	2.29	0.44
1:C:112:TYR:CD1	1:C:189:LEU:HD21	2.53	0.44
1:D:73:GLY:HA2	1:D:76:ILE:HD12	2.00	0.44
1:E:111:ARG:O	1:E:186:ASP:N	2.47	0.44
1:E:176:ALA:HB1	1:E:188:ILE:CD1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:123:GLN:OE1	1:L:124:PRO:HD3	2.17	0.44
1:N:28:ILE:HD11	2:l:1:CXP:H82	2.00	0.44
1:V:55:PRO:HA	1:V:85:PRO:HG3	2.00	0.44
1:X:19:ILE:O	1:X:20:TYR:HB2	2.17	0.44
1:C:64:ASN:HB2	1:C:92:ILE:HD11	1.99	0.44
1:E:152:VAL:HG13	1:E:153:LEU:N	2.32	0.44
1:G:67:GLY:HA3	1:G:97:SER:HB3	1.99	0.44
1:H:118:GLU:OE1	1:H:175:SER:HA	2.18	0.44
1:T:121:ILE:HD11	1:T:167:ASP:HB3	1.99	0.44
1:X:31:LEU:HD21	1:X:65:SER:HB3	2.00	0.44
1:D:112:TYR:HB3	1:D:189:LEU:CD2	2.48	0.44
1:D:163:VAL:HG22	1:D:167:ASP:OD1	2.18	0.44
1:G:123:GLN:CB	1:G:146:ARG:HH22	2.31	0.44
1:K:74:MET:CE	1:K:149:LEU:CD2	2.96	0.44
1:M:49:PHE:CE1	1:M:53:GLU:CD	2.96	0.44
1:M:77:TYR:CE1	1:M:81:GLN:HG3	2.52	0.44
1:Q:43:ILE:HD11	1:Q:76:ILE:HG21	2.00	0.44
1:Q:161:LEU:HD23	1:Q:161:LEU:C	2.43	0.44
1:R:146:ARG:HG3	1:R:146:ARG:HH11	1.82	0.44
1:K:3:ILE:O	1:K:4:PRO:C	2.60	0.43
1:K:62:TYR:CD2	1:K:92:ILE:HD11	2.53	0.43
1:L:31:LEU:HD13	1:L:43:ILE:HD11	2.00	0.43
1:L:105:ALA:HA	1:L:156:ARG:HD2	1.99	0.43
1:N:72:ALA:O	1:N:76:ILE:HG13	2.18	0.43
1:Q:6:VAL:O	1:Q:17:TYR:N	2.51	0.43
1:U:122:HIS:O	1:U:122:HIS:ND1	2.51	0.43
1:U:160:PRO:HG2	1:U:163:VAL:CG2	2.47	0.43
1:A:171:ASP:C	1:A:171:ASP:OD1	2.62	0.43
1:C:163:VAL:HB	3:C:202:HOH:O	2.17	0.43
1:E:24:LEU:N	3:E:210:HOH:O	2.51	0.43
1:E:61:LEU:HD22	1:E:89:THR:CG2	2.46	0.43
1:F:109:GLY:N	1:F:186:ASP:OD2	2.46	0.43
1:G:74:MET:HE2	1:G:98:MET:HE1	2.00	0.43
1:I:17:TYR:OH	1:I:25:LYS:HD2	2.17	0.43
1:P:48:LEU:HB3	2:n:1:CXP:H82	2.00	0.43
1:Q:148:LYS:O	1:Q:152:VAL:HG12	2.18	0.43
1:X:98:MET:HE2	1:X:123:GLN:OE1	2.18	0.43
1:I:101:PHE:HE1	1:I:152:VAL:HG13	1.83	0.43
1:a:119:VAL:HG11	1:a:184:LEU:HD13	2.01	0.43
2:o:4:PRO:HA	2:o:5:YCP:HA	1.81	0.43
2:w:1:CXP:H81	2:w:1:CXP:H22	1.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:ALA:O	1:D:76:ILE:HG13	2.17	0.43
1:E:70:ILE:O	1:E:74:MET:HG2	2.18	0.43
1:F:19:ILE:HD12	1:F:19:ILE:HA	1.92	0.43
1:H:84:LYS:HD2	1:H:84:LYS:O	2.18	0.43
1:L:74:MET:HE1	1:L:77:TYR:CG	2.52	0.43
1:M:19:ILE:HD12	1:M:19:ILE:HA	1.94	0.43
1:X:82:PHE:HB2	1:Y:189:LEU:HB3	2.00	0.43
1:Y:3:ILE:CB	1:Y:4:PRO:HD2	2.49	0.43
1:b:114:LEU:N	1:b:117:SER:HG	2.15	0.43
1:B:62:TYR:CE1	1:B:90:ILE:HD13	2.54	0.43
1:C:125:LEU:HD11	1:H:171:ASP:OD2	2.18	0.43
1:D:177:GLU:OE1	1:D:188:ILE:HD12	2.18	0.43
1:K:175:SER:OG	1:K:178:GLU:HG3	2.17	0.43
1:L:80:MET:CE	1:L:102:LEU:HD22	2.48	0.43
1:X:17:TYR:HA	1:Y:6:VAL:HG21	2.01	0.43
2:o:1:CXP:H81	2:o:1:CXP:H22	1.61	0.43
1:E:174:LYS:HG3	1:E:175:SER:H	1.84	0.43
1:G:119:VAL:HG11	1:G:184:LEU:HD13	1.99	0.43
1:L:120:MET:HE1	1:L:171:ASP:CA	2.49	0.43
1:O:3:ILE:HD12	1:O:3:ILE:N	2.34	0.43
1:Y:48:LEU:HD13	2:u:1:CXP:H82	2.00	0.43
2:l:1:CXP:H22	2:l:1:CXP:H81	1.81	0.43
2:v:6:ALA:C	3:v:101:HOH:O	2.62	0.43
1:D:175:SER:OG	1:D:178:GLU:OE1	2.36	0.43
1:E:174:LYS:HD2	1:E:178:GLU:CB	2.49	0.43
1:E:174:LYS:HD2	1:E:178:GLU:HB3	2.01	0.43
1:S:137:ILE:HD12	1:Z:169:ASP:OD2	2.18	0.43
1:T:142:ILE:HD11	1:Y:139:ALA:CB	2.48	0.43
1:W:34:ALA:HA	3:W:204:HOH:O	2.17	0.43
1:Z:62:TYR:OH	2:u:6:ALA:O	2.30	0.43
1:a:75:ALA:HB1	1:b:92:ILE:HG22	2.01	0.43
1:M:83:ILE:HD12	1:M:85:PRO:HD2	2.01	0.43
1:Q:162:GLU:O	1:Q:166:ARG:HG3	2.19	0.43
1:S:150:ASN:C	3:S:203:HOH:O	2.61	0.43
1:W:23:LEU:HD22	2:r:1:CXP:H51	2.00	0.43
1:X:45:SER:OG	1:Y:30:MET:HE2	2.19	0.43
1:Z:89:THR:HG22	1:Z:103:LEU:HD12	2.00	0.43
1:A:39:VAL:HG22	1:B:2:LEU:HD11	2.01	0.43
1:C:92:ILE:HG21	2:d:2:WFP:F1	2.08	0.43
1:D:169:ASP:O	1:N:170:ARG:HB2	2.18	0.43
1:E:86:LYS:HD3	1:E:107:GLU:CD	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:84:LYS:HB3	1:M:85:PRO:HD3	2.01	0.43
1:N:77:TYR:CE1	1:N:81:GLN:CG	3.02	0.43
1:Q:83:ILE:HD12	1:Q:85:PRO:HG2	2.00	0.43
1:U:19:ILE:HG23	1:U:20:TYR:N	2.33	0.43
1:W:166:ARG:HE	1:W:170:ARG:HH22	1.65	0.43
1:X:142:ILE:HG12	3:X:203:HOH:O	2.18	0.43
1:Z:112:TYR:CE2	2:u:6:ALA:HB2	2.54	0.43
2:t:1:CXP:H22	2:t:1:CXP:H81	1.61	0.43
1:C:74:MET:CE	1:C:77:TYR:HD2	2.32	0.43
1:D:44:VAL:O	1:D:48:LEU:HG	2.19	0.43
1:J:67:GLY:HA3	1:J:97:SER:HB2	2.01	0.43
1:M:17:TYR:CD1	1:M:17:TYR:N	2.87	0.43
1:O:67:GLY:HA3	1:O:97:SER:HB3	2.01	0.43
1:X:67:GLY:HA3	1:X:97:SER:HB2	2.01	0.43
1:A:3:ILE:O	1:A:3:ILE:CG2	2.66	0.42
1:B:118:GLU:CD	1:B:173:PHE:HE1	2.26	0.42
1:C:35:ILE:HD12	1:C:67:GLY:HA2	1.99	0.42
1:K:120:MET:HG3	1:K:173:PHE:CD1	2.53	0.42
1:X:28:ILE:HD13	1:X:62:TYR:CZ	2.54	0.42
1:D:28:ILE:HD11	1:D:62:TYR:CE1	2.54	0.42
1:H:84:LYS:O	1:H:85:PRO:C	2.63	0.42
1:M:49:PHE:HE1	1:M:53:GLU:OE2	2.02	0.42
1:M:82:PHE:CD1	2:l:2:WFP:HD2	2.54	0.42
1:O:2:LEU:C	1:O:3:ILE:HD12	2.44	0.42
1:R:160:PRO:HG2	1:R:163:VAL:HG13	2.01	0.42
1:X:109:GLY:N	1:X:186:ASP:OD2	2.49	0.42
1:Z:17:TYR:HB2	1:Z:21:SER:HB2	2.01	0.42
1:Z:70:ILE:CD1	1:Z:145:LEU:HD22	2.48	0.42
1:Z:101:PHE:CD2	1:Z:149:LEU:HD22	2.54	0.42
1:J:62:TYR:CD1	1:J:90:ILE:HD13	2.53	0.42
1:L:182:TYR:HB3	1:L:184:LEU:HG	2.01	0.42
1:O:141:ARG:HG2	1:O:145:LEU:CD1	2.50	0.42
1:X:138:ALA:C	3:X:203:HOH:O	2.60	0.42
1:C:67:GLY:HA3	1:C:97:SER:HB2	2.01	0.42
1:D:23:LEU:HG	1:D:28:ILE:HG23	2.01	0.42
1:D:116:ASN:O	1:D:118:GLU:OE1	2.37	0.42
1:K:27:ARG:CD	1:K:57:LYS:HE3	2.49	0.42
1:L:161:LEU:O	1:L:165:GLU:HG3	2.19	0.42
1:N:155:GLU:C	1:N:155:GLU:OE1	2.62	0.42
1:N:157:THR:HG22	1:N:183:GLY:C	2.45	0.42
1:W:97:SER:OG	1:W:98:MET:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:138:ALA:O	1:X:139:ALA:HB3	2.19	0.42
1:Y:76:ILE:HG22	1:Y:80:MET:CE	2.47	0.42
1:Y:119:VAL:HG11	1:Y:184:LEU:HD13	2.02	0.42
1:Z:54:ASP:OD1	1:Z:56:GLU:HG3	2.19	0.42
2:w:1:CXP:C9	2:w:3:SER:N	2.83	0.42
1:J:55:PRO:HB2	1:J:84:LYS:HD3	2.01	0.42
2:q:4:PRO:HA	2:q:5:YCP:HA	1.83	0.42
1:A:55:PRO:HA	1:A:85:PRO:HG3	2.01	0.42
1:E:44:VAL:O	1:E:48:LEU:HD23	2.19	0.42
1:G:82:PHE:CD1	1:G:82:PHE:C	2.98	0.42
1:X:98:MET:HE1	1:X:149:LEU:CD1	2.48	0.42
1:X:121:ILE:HG22	1:X:168:THR:HG22	2.00	0.42
1:Z:31:LEU:HD23	1:Z:63:ILE:HG12	2.01	0.42
1:b:119:VAL:HG11	1:b:184:LEU:HD13	2.01	0.42
1:B:161:LEU:HD23	1:B:161:LEU:O	2.20	0.42
1:D:163:VAL:HG23	1:D:166:ARG:NH1	2.34	0.42
1:E:90:ILE:HA	1:E:112:TYR:O	2.19	0.42
1:K:48:LEU:HD22	2:j:1:CXP:O2	2.19	0.42
1:M:40:ALA:HB2	1:M:72:ALA:HB1	2.02	0.42
1:T:2:LEU:N	1:T:2:LEU:HD23	2.34	0.42
1:U:155:GLU:C	1:U:155:GLU:OE1	2.62	0.42
1:W:123:GLN:CG	1:W:168:THR:HG23	2.49	0.42
1:Y:49:PHE:CZ	1:Y:53:GLU:OE2	2.73	0.42
1:Z:142:ILE:O	1:Z:143:LEU:C	2.61	0.42
1:B:73:GLY:HA3	1:B:98:MET:HG2	2.01	0.42
1:C:90:ILE:HG13	1:C:112:TYR:HB2	2.00	0.42
1:D:3:ILE:HG22	3:D:209:HOH:O	2.20	0.42
1:N:148:LYS:HE2	1:N:148:LYS:HA	2.01	0.42
1:R:67:GLY:HA2	1:R:97:SER:HB3	2.01	0.42
1:S:123:GLN:OE1	1:S:124:PRO:HD3	2.19	0.42
1:W:58:GLU:OE1	1:W:110:LYS:NZ	2.48	0.42
1:Y:112:TYR:HB3	1:Y:189:LEU:CD2	2.49	0.42
1:a:54:ASP:OD2	1:a:57:LYS:HB2	2.19	0.42
1:A:170:ARG:HE	1:J:169:ASP:HB3	1.68	0.42
1:N:74:MET:CB	3:N:201:HOH:O	2.67	0.42
1:b:7:ILE:HD13	1:b:16:ALA:HB2	2.02	0.42
1:C:112:TYR:N	1:C:185:ILE:HD11	2.35	0.42
1:E:14:GLU:N	3:E:211:HOH:O	2.53	0.42
1:F:90:ILE:HD11	2:f:6:ALA:CB	2.50	0.42
1:J:3:ILE:HG22	1:J:18:ASP:OD1	2.20	0.42
1:L:58:GLU:OE2	1:L:88:SER:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:161:LEU:O	1:N:161:LEU:HD23	2.20	0.42
1:O:137:ILE:HD12	1:P:170:ARG:NH2	2.30	0.42
1:S:81:GLN:NE2	1:S:156:ARG:HH12	2.17	0.42
1:S:163:VAL:O	1:S:167:ASP:HB2	2.20	0.42
1:X:44:VAL:HG23	1:X:79:THR:HG21	2.02	0.42
1:a:121:ILE:HD11	1:a:167:ASP:HB3	2.02	0.42
1:I:66:PRO:HA	1:I:96:ALA:HB3	2.02	0.41
1:K:27:ARG:NH1	1:K:50:LEU:O	2.38	0.41
1:P:92:ILE:O	1:P:114:LEU:HD12	2.20	0.41
1:Q:55:PRO:O	1:Q:84:LYS:HG2	2.20	0.41
1:Q:167:ASP:HB3	1:Q:172:ASN:HD21	1.85	0.41
1:R:23:LEU:HG	1:R:28:ILE:HG23	2.02	0.41
1:S:70:ILE:HD12	1:S:70:ILE:N	2.32	0.41
1:T:90:ILE:HD11	2:p:6:ALA:CB	2.48	0.41
1:I:22:ARG:NH1	1:I:26:ASP:OD2	2.52	0.41
1:I:84:LYS:HB3	1:I:85:PRO:HD3	2.02	0.41
1:L:163:VAL:O	1:L:167:ASP:HB2	2.20	0.41
1:M:170:ARG:HG2	1:M:171:ASP:H	1.85	0.41
1:O:145:LEU:HD21	1:P:118:GLU:OE2	2.20	0.41
1:W:175:SER:OG	1:W:178:GLU:HG3	2.20	0.41
1:X:3:ILE:O	1:X:3:ILE:CG2	2.68	0.41
1:Y:90:ILE:HG23	1:Y:112:TYR:HB2	2.02	0.41
1:K:62:TYR:HD2	1:K:92:ILE:HD11	1.85	0.41
1:A:120:MET:CE	1:A:171:ASP:HB2	2.51	0.41
1:B:89:THR:C	1:B:90:ILE:HD12	2.45	0.41
1:B:101:PHE:HZ	1:B:152:VAL:HG11	1.85	0.41
1:D:139:ALA:CB	1:M:142:ILE:HD11	2.51	0.41
1:E:57:LYS:NZ	2:e:7:MP8:HEB	2.35	0.41
1:E:61:LEU:C	1:E:61:LEU:HD23	2.45	0.41
1:R:139:ALA:CB	1:a:142:ILE:HD11	2.51	0.41
1:R:172:ASN:C	1:R:172:ASN:ND2	2.74	0.41
1:T:57:LYS:HG3	1:T:58:GLU:N	2.35	0.41
1:W:176:ALA:HB1	1:W:188:ILE:HD13	2.02	0.41
2:l:4:PRO:HA	2:l:5:YCP:HA	1.90	0.41
1:B:62:TYR:HE1	1:B:90:ILE:HD13	1.85	0.41
1:D:121:ILE:HD12	1:D:168:THR:HG22	2.02	0.41
1:L:49:PHE:HA	2:k:1:CXP:H52	2.02	0.41
1:O:155:GLU:OE1	1:O:155:GLU:C	2.64	0.41
1:S:142:ILE:O	1:S:143:LEU:C	2.64	0.41
1:Z:23:LEU:HD12	1:Z:30:MET:HE3	2.02	0.41
1:a:19:ILE:O	1:a:20:TYR:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:49:PHE:HD2	1:N:50:LEU:HD22	1.85	0.41
1:b:19:ILE:HG23	1:b:20:TYR:N	2.35	0.41
1:b:141:ARG:HG2	1:b:141:ARG:HH11	1.85	0.41
2:k:1:CXP:O2	2:k:3:SER:N	2.50	0.41
1:J:43:ILE:HD11	1:J:76:ILE:HG21	2.01	0.41
1:N:40:ALA:HB2	1:N:72:ALA:HB1	2.02	0.41
1:V:122:HIS:HB2	1:V:170:ARG:O	2.21	0.41
1:X:101:PHE:HE1	1:X:152:VAL:HG13	1.85	0.41
1:B:172:ASN:C	1:B:172:ASN:HD22	2.27	0.41
1:F:141:ARG:HD3	1:G:173:PHE:CD1	2.56	0.41
1:G:31:LEU:HD13	1:G:43:ILE:HG13	2.01	0.41
1:I:112:TYR:CD1	1:I:189:LEU:HD21	2.55	0.41
1:M:162:GLU:OE1	1:M:162:GLU:N	2.52	0.41
1:X:62:TYR:CZ	2:t:2:WFP:HD1	2.55	0.41
1:Z:51:ALA:HA	1:Z:85:PRO:HG2	2.02	0.41
2:m:1:CXP:H61	2:m:1:CXP:H82	1.76	0.41
1:A:120:MET:HE3	1:A:122:HIS:HB3	2.03	0.41
1:A:185:ILE:HD12	1:A:187:LYS:N	2.36	0.41
1:C:94:MET:HE1	1:C:173:PHE:HE1	1.86	0.41
1:I:18:ASP:OD1	1:I:21:SER:OG	2.24	0.41
1:I:90:ILE:HD12	1:I:90:ILE:N	2.36	0.41
1:K:118:GLU:OE1	1:K:173:PHE:CB	2.66	0.41
1:O:137:ILE:HG23	1:W:146:ARG:CZ	2.50	0.41
1:O:144:LEU:HD12	1:O:144:LEU:O	2.20	0.41
1:P:49:PHE:HA	2:n:1:CXP:H52	2.03	0.41
1:R:48:LEU:HD11	2:o:2:WFP:CE1	2.50	0.41
1:R:59:ILE:HD12	1:R:85:PRO:HB2	2.03	0.41
1:S:36:ASP:OD1	1:S:39:VAL:HG12	2.20	0.41
1:S:63:ILE:HD11	1:S:99:GLY:CA	2.51	0.41
1:T:98:MET:HE1	1:T:149:LEU:HD22	2.01	0.41
1:V:67:GLY:HA3	1:V:97:SER:HB3	2.02	0.41
1:Y:172:ASN:O	1:Y:172:ASN:OD1	2.39	0.41
1:C:57:LYS:HG3	1:C:58:GLU:OE1	2.21	0.41
1:C:84:LYS:N	1:C:85:PRO:HD2	2.35	0.41
1:I:94:MET:HE3	1:I:94:MET:HA	2.03	0.41
1:J:78:ASP:HB3	1:K:114:LEU:HD13	2.03	0.41
1:L:17:TYR:HB2	1:L:21:SER:HB2	2.03	0.41
1:L:104:ALA:O	1:L:156:ARG:HD2	2.20	0.41
1:R:166:ARG:CB	1:R:166:ARG:HH11	2.34	0.41
1:D:22:ARG:HH11	1:D:22:ARG:HG3	1.85	0.40
1:L:71:THR:HG21	1:M:94:MET:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:103:LEU:CD2	1:Q:185:ILE:HD11	2.44	0.40
1:R:89:THR:HG21	1:R:102:LEU:O	2.21	0.40
1:W:73:GLY:HA3	1:W:98:MET:HG2	2.02	0.40
1:C:74:MET:HE1	1:C:77:TYR:HD2	1.86	0.40
1:D:44:VAL:HG23	1:D:79:THR:HG21	2.03	0.40
1:F:19:ILE:O	1:F:20:TYR:HB2	2.21	0.40
1:H:55:PRO:O	1:H:84:LYS:HG3	2.21	0.40
1:H:153:LEU:O	1:H:157:THR:HG23	2.21	0.40
1:I:39:VAL:O	1:I:43:ILE:HG12	2.21	0.40
1:Q:164:ILE:O	1:Q:168:THR:HG23	2.21	0.40
1:R:37:ASP:N	3:R:202:HOH:O	2.39	0.40
1:T:141:ARG:HD3	1:U:173:PHE:CG	2.56	0.40
1:Y:140:LYS:H	1:Y:140:LYS:CD	2.34	0.40
1:A:137:ILE:HD11	1:I:169:ASP:OD2	2.21	0.40
1:C:41:ASN:HA	1:C:44:VAL:HG12	2.03	0.40
1:E:148:LYS:HE3	1:F:116:ASN:OD1	2.21	0.40
1:F:67:GLY:HA3	1:F:97:SER:HB3	2.04	0.40
1:G:74:MET:HG3	1:G:145:LEU:HD13	2.03	0.40
1:M:5:THR:HA	1:M:18:ASP:HA	2.02	0.40
1:N:24:LEU:CD1	1:N:50:LEU:HD21	2.49	0.40
1:Q:62:TYR:CE1	1:Q:90:ILE:HD12	2.56	0.40
1:Z:180:LEU:HD11	1:Z:186:ASP:C	2.46	0.40
1:a:170:ARG:CG	1:a:171:ASP:H	2.33	0.40
1:E:165:GLU:N	3:E:204:HOH:O	2.54	0.40
1:L:77:TYR:O	1:L:81:GLN:HG2	2.22	0.40
1:P:109:GLY:N	1:P:186:ASP:OD2	2.53	0.40
1:R:117:SER:C	1:R:118:GLU:OE1	2.63	0.40
1:X:156:ARG:NH1	3:X:201:HOH:O	2.53	0.40
1:Z:84:LYS:HB3	1:Z:85:PRO:HD3	2.03	0.40
1:b:114:LEU:N	1:b:117:SER:OG	2.54	0.40
2:m:6:ALA:N	3:m:101:HOH:O	2.55	0.40
1:C:2:LEU:HD13	1:C:2:LEU:C	2.47	0.40
1:D:22:ARG:HH11	1:D:22:ARG:CG	2.34	0.40
1:E:153:LEU:CD1	1:E:164:ILE:CG2	3.00	0.40
1:H:67:GLY:HA3	1:H:97:SER:HB3	2.04	0.40
1:M:146:ARG:CD	3:M:207:HOH:O	2.68	0.40
1:P:62:TYR:CD1	1:P:90:ILE:HD13	2.56	0.40
1:S:153:LEU:HD11	1:S:164:ILE:CG2	2.51	0.40
1:b:108:LYS:HD3	1:b:108:LYS:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	166/199 (83%)	157 (95%)	7 (4%)	2 (1%)	10	34
1	B	170/199 (85%)	162 (95%)	6 (4%)	2 (1%)	10	34
1	C	166/199 (83%)	155 (93%)	10 (6%)	1 (1%)	21	51
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%)	21	51
1	G	171/199 (86%)	162 (95%)	7 (4%)	2 (1%)	10	34
1	H	166/199 (83%)	157 (95%)	8 (5%)	1 (1%)	21	51
1	I	171/199 (86%)	159 (93%)	11 (6%)	1 (1%)	21	51
1	J	167/199 (84%)	156 (93%)	10 (6%)	1 (1%)	21	51
1	K	165/199 (83%)	155 (94%)	8 (5%)	2 (1%)	10	34
1	L	165/199 (83%)	153 (93%)	12 (7%)	0	100	100
1	M	162/199 (81%)	152 (94%)	9 (6%)	1 (1%)	21	51
1	N	162/199 (81%)	155 (96%)	5 (3%)	2 (1%)	10	34
1	O	168/199 (84%)	159 (95%)	6 (4%)	3 (2%)	6	23
1	P	171/199 (86%)	160 (94%)	10 (6%)	1 (1%)	21	51
1	Q	166/199 (83%)	152 (92%)	13 (8%)	1 (1%)	21	51
1	R	162/199 (81%)	153 (94%)	7 (4%)	2 (1%)	10	34
1	S	168/199 (84%)	157 (94%)	11 (6%)	0	100	100
1	T	162/199 (81%)	153 (94%)	8 (5%)	1 (1%)	21	51
1	U	164/199 (82%)	156 (95%)	8 (5%)	0	100	100
1	V	169/199 (85%)	163 (96%)	4 (2%)	2 (1%)	10	34
1	W	170/199 (85%)	158 (93%)	12 (7%)	0	100	100
1	X	163/199 (82%)	155 (95%)	6 (4%)	2 (1%)	10	34
1	Y	159/199 (80%)	150 (94%)	8 (5%)	1 (1%)	21	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Z	163/199 (82%)	150 (92%)	13 (8%)	0	100	100
1	a	162/199 (81%)	153 (94%)	8 (5%)	1 (1%)	21	51
1	b	169/199 (85%)	162 (96%)	5 (3%)	2 (1%)	10	34
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
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%)	18	47

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

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Mol	Chain	Res	Type
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
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%)	142 (100%)	0	100	100
1	B	145/165 (88%)	140 (97%)	5 (3%)	32	68
1	C	141/165 (86%)	136 (96%)	5 (4%)	32	67
1	D	137/165 (83%)	131 (96%)	6 (4%)	25	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	140/165 (85%)	138 (99%)	2 (1%)	59	85
1	F	138/165 (84%)	136 (99%)	2 (1%)	59	85
1	G	145/165 (88%)	139 (96%)	6 (4%)	27	62
1	H	141/165 (86%)	137 (97%)	4 (3%)	38	73
1	I	144/165 (87%)	141 (98%)	3 (2%)	47	79
1	J	140/165 (85%)	138 (99%)	2 (1%)	59	85
1	K	141/165 (86%)	137 (97%)	4 (3%)	38	73
1	L	141/165 (86%)	135 (96%)	6 (4%)	26	60
1	M	137/165 (83%)	133 (97%)	4 (3%)	37	73
1	N	140/165 (85%)	136 (97%)	4 (3%)	37	73
1	O	143/165 (87%)	141 (99%)	2 (1%)	59	85
1	P	146/165 (88%)	142 (97%)	4 (3%)	39	74
1	Q	141/165 (86%)	139 (99%)	2 (1%)	59	85
1	R	140/165 (85%)	133 (95%)	7 (5%)	22	54
1	S	141/165 (86%)	137 (97%)	4 (3%)	38	73
1	T	139/165 (84%)	138 (99%)	1 (1%)	76	91
1	U	140/165 (85%)	136 (97%)	4 (3%)	37	73
1	V	145/165 (88%)	145 (100%)	0	100	100
1	W	144/165 (87%)	142 (99%)	2 (1%)	59	85
1	X	139/165 (84%)	135 (97%)	4 (3%)	37	73
1	Y	136/165 (82%)	132 (97%)	4 (3%)	37	73
1	Z	138/165 (84%)	132 (96%)	6 (4%)	26	60
1	a	139/165 (84%)	139 (100%)	0	100	100
1	b	144/165 (87%)	139 (96%)	5 (4%)	32	67
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	3889 (98%)	98 (2%)	42	76

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	3	ILE
1	B	89	THR
1	B	168	THR
1	B	172	ASN
1	B	190	THR
1	C	5	THR
1	C	7	ILE
1	C	33	SER
1	C	56	GLU
1	C	172	ASN
1	D	3	ILE
1	D	5	THR
1	D	28	ILE
1	D	29	ILE
1	D	60	SER
1	D	121	ILE
1	E	5	THR
1	E	17	TYR
1	F	5	THR

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Mol	Chain	Res	Type
1	F	19	ILE
1	G	21	SER
1	G	82	PHE
1	G	136	GLU
1	G	144	LEU
1	G	145	LEU
1	G	147	ASP
1	H	92	ILE
1	H	118	GLU
1	H	137	ILE
1	H	185	ILE
1	I	121	ILE
1	I	124	PRO
1	I	125	LEU
1	J	43	ILE
1	J	121	ILE
1	K	3	ILE
1	K	28	ILE
1	K	69	SER
1	K	163	VAL
1	L	5	THR
1	L	97	SER
1	L	116	ASN
1	L	159	GLN
1	L	168	THR
1	L	171	ASP
1	M	31	LEU
1	M	79	THR
1	M	97	SER
1	M	148	LYS
1	N	5	THR
1	N	60	SER
1	N	159	GLN
1	N	171	ASP
1	O	31	LEU
1	O	149	LEU
1	P	31	LEU
1	P	152	VAL
1	P	165	GLU
1	P	190	THR
1	Q	33	SER
1	Q	43	ILE

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Mol	Chain	Res	Type
1	R	3	ILE
1	R	5	THR
1	R	39	VAL
1	R	148	LYS
1	R	169	ASP
1	R	172	ASN
1	R	177	GLU
1	S	5	THR
1	S	17	TYR
1	S	84	LYS
1	S	163	VAL
1	T	5	THR
1	U	5	THR
1	U	21	SER
1	U	82	PHE
1	U	86	LYS
1	W	2	LEU
1	W	118	GLU
1	X	33	SER
1	X	45	SER
1	X	141	ARG
1	X	152	VAL
1	Y	18	ASP
1	Y	22	ARG
1	Y	175	SER
1	Y	190	THR
1	Z	5	THR
1	Z	17	TYR
1	Z	151	LYS
1	Z	156	ARG
1	Z	175	SER
1	Z	177	GLU
1	b	5	THR
1	b	82	PHE
1	b	117	SER
1	b	123	GLN
1	b	147	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN

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Mol	Chain	Res	Type
1	B	41	ASN
1	C	64	ASN
1	F	159	GLN
1	G	38	ASN
1	G	172	ASN
1	I	41	ASN
1	I	64	ASN
1	I	81	GLN
1	J	64	ASN
1	J	123	GLN
1	J	150	ASN
1	K	64	ASN
1	L	159	GLN
1	M	159	GLN
1	N	38	ASN
1	O	41	ASN
1	O	81	GLN
1	P	1	ASN
1	P	64	ASN
1	Q	38	ASN
1	R	122	HIS
1	R	172	ASN
1	U	150	ASN
1	W	41	ASN
1	W	116	ASN
1	W	122	HIS
1	W	172	ASN
1	X	46	GLN
1	X	64	ASN
1	Y	41	ASN
1	Y	46	GLN
1	Y	172	ASN

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	MP8	q	7	2	6,8,9	6.14	4 (66%)	3,10,12	1.64	1 (33%)
2	MP8	w	7	2	6,8,9	6.08	4 (66%)	3,10,12	2.27	3 (100%)
2	WFP	i	2	2	12,13,14	1.00	0	12,17,19	1.60	3 (25%)
2	WFP	d	2	2	12,13,14	1.12	0	12,17,19	1.54	3 (25%)
2	MP8	k	7	2	6,8,9	6.04	4 (66%)	3,10,12	1.54	1 (33%)
2	MP8	i	7	2	6,8,9	6.08	4 (66%)	3,10,12	1.53	1 (33%)
2	YCP	v	5	2	6,8,9	1.88	2 (33%)	7,9,11	0.84	0
2	MP8	g	7	2	6,8,9	5.96	4 (66%)	3,10,12	2.11	1 (33%)
2	WFP	u	2	2	12,13,14	1.00	0	12,17,19	2.01	5 (41%)
2	WFP	h	2	2	12,13,14	1.11	0	12,17,19	1.70	5 (41%)
2	WFP	q	2	2	12,13,14	0.82	0	12,17,19	1.78	4 (33%)
2	WFP	w	2	2	12,13,14	1.02	0	12,17,19	1.55	3 (25%)
2	YCP	e	5	2	6,8,9	1.74	2 (33%)	7,9,11	1.35	1 (14%)
2	YCP	r	5	2	6,8,9	1.56	1 (16%)	7,9,11	2.66	3 (42%)
2	WFP	t	2	2	12,13,14	0.96	0	12,17,19	1.57	3 (25%)
2	MP8	n	7	2	6,8,9	5.98	4 (66%)	3,10,12	1.56	1 (33%)
2	MP8	u	7	2	6,8,9	6.25	4 (66%)	3,10,12	2.31	2 (66%)
2	WFP	g	2	2	12,13,14	0.82	0	12,17,19	1.39	1 (8%)
2	WFP	k	2	2	12,13,14	0.88	0	12,17,19	1.62	2 (16%)
2	YCP	q	5	2	6,8,9	1.59	1 (16%)	7,9,11	2.67	3 (42%)
2	YCP	w	5	2	6,8,9	1.64	1 (16%)	7,9,11	1.82	2 (28%)
2	YCP	i	5	2	6,8,9	1.60	1 (16%)	7,9,11	2.63	3 (42%)
2	YCP	d	5	2	6,8,9	1.66	1 (16%)	7,9,11	2.63	4 (57%)
2	YCP	g	5	2	6,8,9	1.63	1 (16%)	7,9,11	2.45	2 (28%)
2	MP8	p	7	2	6,8,9	5.86	4 (66%)	3,10,12	0.61	0
2	YCP	t	5	2	6,8,9	1.64	1 (16%)	7,9,11	2.30	2 (28%)
2	MP8	m	7	2	6,8,9	5.96	4 (66%)	3,10,12	0.77	0
2	MP8	j	7	2	6,8,9	6.14	4 (66%)	3,10,12	2.00	2 (66%)
2	MP8	l	7	2	6,8,9	6.16	4 (66%)	3,10,12	1.88	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	WFP	r	2	2	12,13,14	0.89	0	12,17,19	1.78	4 (33%)
2	MP8	o	7	2	6,8,9	6.00	4 (66%)	3,10,12	2.35	3 (100%)
2	YCP	f	5	2	6,8,9	1.76	1 (16%)	7,9,11	1.30	1 (14%)
2	MP8	h	7	2	6,8,9	6.23	4 (66%)	3,10,12	1.38	0
2	YCP	n	5	2	6,8,9	1.72	1 (16%)	7,9,11	1.50	2 (28%)
2	WFP	o	2	2	12,13,14	0.83	0	12,17,19	1.62	4 (33%)
2	WFP	v	2	2	12,13,14	1.03	0	12,17,19	1.50	3 (25%)
2	YCP	m	5	2	6,8,9	1.69	1 (16%)	7,9,11	1.96	2 (28%)
2	YCP	o	5	2	6,8,9	1.81	1 (16%)	7,9,11	1.68	2 (28%)
2	YCP	j	5	2	6,8,9	1.86	1 (16%)	7,9,11	1.32	2 (28%)
2	MP8	f	7	2	6,8,9	6.26	4 (66%)	3,10,12	1.69	1 (33%)
2	MP8	t	7	2	6,8,9	6.15	4 (66%)	3,10,12	1.61	1 (33%)
2	YCP	l	5	2	6,8,9	1.65	1 (16%)	7,9,11	2.11	3 (42%)
2	WFP	p	2	2	12,13,14	1.06	0	12,17,19	1.35	1 (8%)
2	WFP	n	2	2	12,13,14	0.91	0	12,17,19	1.70	5 (41%)
2	MP8	e	7	2	6,8,9	6.24	4 (66%)	3,10,12	1.87	1 (33%)
2	WFP	l	2	2	12,13,14	1.17	1 (8%)	12,17,19	2.91	8 (66%)
2	WFP	f	2	2	12,13,14	0.95	1 (8%)	12,17,19	1.66	5 (41%)
2	MP8	c	7	2	6,8,9	6.01	4 (66%)	3,10,12	1.38	0
2	YCP	p	5	2	6,8,9	1.85	2 (33%)	7,9,11	1.61	1 (14%)
2	YCP	k	5	2	6,8,9	1.74	1 (16%)	7,9,11	1.58	2 (28%)
2	WFP	m	2	2	12,13,14	0.84	1 (8%)	12,17,19	1.59	3 (25%)
2	WFP	e	2	2	12,13,14	1.20	1 (8%)	12,17,19	2.16	4 (33%)
2	YCP	u	5	2	6,8,9	1.85	2 (33%)	7,9,11	1.38	1 (14%)
2	MP8	d	7	2	6,8,9	6.16	4 (66%)	3,10,12	1.40	1 (33%)
2	WFP	j	2	2	12,13,14	1.07	1 (8%)	12,17,19	1.63	4 (33%)
2	MP8	v	7	2	6,8,9	6.14	4 (66%)	3,10,12	0.65	0
2	WFP	c	2	2	12,13,14	0.93	1 (8%)	12,17,19	2.26	6 (50%)
2	MP8	r	7	2	6,8,9	5.96	4 (66%)	3,10,12	1.45	1 (33%)
2	YCP	h	5	2	6,8,9	1.64	1 (16%)	7,9,11	2.20	3 (42%)
2	YCP	c	5	2	6,8,9	1.77	1 (16%)	7,9,11	2.04	4 (57%)

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	MP8	q	7	2	-	0/0/11/13	0/1/1/1
2	MP8	w	7	2	-	0/0/11/13	0/1/1/1
2	WFP	i	2	2	-	2/5/6/8	0/1/1/1
2	WFP	d	2	2	-	2/5/6/8	0/1/1/1
2	MP8	k	7	2	-	0/0/11/13	0/1/1/1
2	MP8	i	7	2	-	0/0/11/13	0/1/1/1
2	YCP	v	5	2	-	1/1/10/12	1/1/1/1
2	MP8	g	7	2	-	0/0/11/13	0/1/1/1
2	WFP	u	2	2	-	0/5/6/8	0/1/1/1
2	WFP	h	2	2	-	2/5/6/8	0/1/1/1
2	WFP	q	2	2	-	1/5/6/8	0/1/1/1
2	WFP	w	2	2	-	1/5/6/8	0/1/1/1
2	YCP	e	5	2	-	0/1/10/12	1/1/1/1
2	YCP	r	5	2	-	0/1/10/12	0/1/1/1
2	WFP	t	2	2	-	1/5/6/8	0/1/1/1
2	MP8	n	7	2	-	0/0/11/13	0/1/1/1
2	MP8	u	7	2	-	0/0/11/13	0/1/1/1
2	WFP	g	2	2	-	1/5/6/8	0/1/1/1
2	WFP	k	2	2	-	0/5/6/8	0/1/1/1
2	YCP	q	5	2	-	0/1/10/12	0/1/1/1
2	YCP	w	5	2	-	0/1/10/12	0/1/1/1
2	YCP	i	5	2	-	0/1/10/12	0/1/1/1
2	YCP	d	5	2	-	0/1/10/12	0/1/1/1
2	YCP	g	5	2	-	0/1/10/12	0/1/1/1
2	MP8	p	7	2	-	0/0/11/13	0/1/1/1
2	YCP	t	5	2	-	0/1/10/12	0/1/1/1
2	MP8	m	7	2	-	0/0/11/13	0/1/1/1
2	MP8	j	7	2	-	0/0/11/13	0/1/1/1
2	MP8	l	7	2	-	0/0/11/13	0/1/1/1
2	WFP	r	2	2	-	2/5/6/8	0/1/1/1
2	MP8	o	7	2	-	0/0/11/13	0/1/1/1
2	YCP	f	5	2	-	0/1/10/12	1/1/1/1
2	MP8	h	7	2	-	0/0/11/13	0/1/1/1
2	YCP	n	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	v	2	2	-	2/5/6/8	0/1/1/1
2	YCP	m	5	2	-	0/1/10/12	0/1/1/1
2	YCP	o	5	2	-	0/1/10/12	1/1/1/1
2	YCP	j	5	2	-	0/1/10/12	1/1/1/1
2	MP8	f	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	l	5	2	-	0/1/10/12	0/1/1/1

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

All (110) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	h	7	MP8	CB-CA	-10.85	1.30	1.54
2	o	7	MP8	CB-CA	-10.84	1.30	1.54
2	j	7	MP8	CB-CA	-10.82	1.30	1.54
2	f	7	MP8	CB-CA	-10.81	1.30	1.54
2	w	7	MP8	CB-CA	-10.80	1.30	1.54
2	u	7	MP8	CB-CA	-10.79	1.30	1.54
2	t	7	MP8	CB-CA	-10.66	1.31	1.54
2	q	7	MP8	CB-CA	-10.61	1.31	1.54
2	c	7	MP8	CB-CA	-10.56	1.31	1.54
2	i	7	MP8	CB-CA	-10.56	1.31	1.54
2	e	7	MP8	CB-CA	-10.54	1.31	1.54
2	l	7	MP8	CB-CA	-10.52	1.31	1.54
2	d	7	MP8	CB-CA	-10.48	1.31	1.54
2	v	7	MP8	CB-CA	-10.38	1.31	1.54
2	n	7	MP8	CB-CA	-10.30	1.31	1.54
2	g	7	MP8	CB-CA	-10.28	1.31	1.54
2	m	7	MP8	CB-CA	-10.24	1.32	1.54
2	k	7	MP8	CB-CA	-10.18	1.32	1.54
2	p	7	MP8	CB-CA	-10.10	1.32	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	r	7	MP8	CB-CA	-10.09	1.32	1.54
2	e	7	MP8	CA-N	7.71	1.62	1.48
2	v	7	MP8	CA-N	7.37	1.61	1.48
2	u	7	MP8	CA-N	7.31	1.61	1.48
2	f	7	MP8	CA-N	7.27	1.61	1.48
2	d	7	MP8	CA-N	7.19	1.61	1.48
2	h	7	MP8	CA-N	7.14	1.61	1.48
2	l	7	MP8	CA-N	7.13	1.61	1.48
2	t	7	MP8	CA-N	7.11	1.61	1.48
2	q	7	MP8	CA-N	7.10	1.61	1.48
2	j	7	MP8	CA-N	7.04	1.61	1.48
2	i	7	MP8	CA-N	7.01	1.61	1.48
2	k	7	MP8	CA-N	6.93	1.60	1.48
2	p	7	MP8	CA-N	6.89	1.60	1.48
2	n	7	MP8	CA-N	6.80	1.60	1.48
2	r	7	MP8	CA-N	6.70	1.60	1.48
2	w	7	MP8	CA-N	6.67	1.60	1.48
2	g	7	MP8	CA-N	6.65	1.60	1.48
2	m	7	MP8	CA-N	6.63	1.60	1.48
2	c	7	MP8	CA-N	6.62	1.60	1.48
2	f	7	MP8	O-C	6.41	1.44	1.20
2	l	7	MP8	O-C	6.41	1.44	1.20
2	d	7	MP8	O-C	6.38	1.44	1.20
2	t	7	MP8	O-C	6.33	1.44	1.20
2	k	7	MP8	O-C	6.33	1.44	1.20
2	h	7	MP8	O-C	6.29	1.43	1.20
2	e	7	MP8	O-C	6.29	1.43	1.20
2	r	7	MP8	O-C	6.29	1.43	1.20
2	m	7	MP8	O-C	6.27	1.43	1.20
2	u	7	MP8	O-C	6.16	1.43	1.20
2	v	7	MP8	O-C	6.15	1.43	1.20
2	q	7	MP8	O-C	6.15	1.43	1.20
2	i	7	MP8	O-C	6.13	1.43	1.20
2	o	7	MP8	O-C	6.11	1.43	1.20
2	c	7	MP8	O-C	6.06	1.43	1.20
2	o	7	MP8	CA-N	5.97	1.59	1.48
2	g	7	MP8	O-C	5.96	1.42	1.20
2	j	7	MP8	O-C	5.96	1.42	1.20
2	n	7	MP8	O-C	5.91	1.42	1.20
2	w	7	MP8	O-C	5.85	1.42	1.20
2	p	7	MP8	O-C	5.77	1.41	1.20
2	r	7	MP8	CD-N	-5.00	1.30	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	n	7	MP8	CD-N	-4.99	1.30	1.47
2	g	7	MP8	CD-N	-4.97	1.30	1.47
2	k	7	MP8	CD-N	-4.94	1.30	1.47
2	u	7	MP8	CD-N	-4.93	1.30	1.47
2	w	7	MP8	CD-N	-4.91	1.30	1.47
2	v	7	MP8	CD-N	-4.85	1.31	1.47
2	o	7	MP8	CD-N	-4.83	1.31	1.47
2	q	7	MP8	CD-N	-4.81	1.31	1.47
2	d	7	MP8	CD-N	-4.79	1.31	1.47
2	l	7	MP8	CD-N	-4.70	1.31	1.47
2	j	7	MP8	CD-N	-4.69	1.31	1.47
2	m	7	MP8	CD-N	-4.65	1.31	1.47
2	h	7	MP8	CD-N	-4.64	1.31	1.47
2	c	7	MP8	CD-N	-4.64	1.31	1.47
2	f	7	MP8	CD-N	-4.63	1.31	1.47
2	e	7	MP8	CD-N	-4.61	1.31	1.47
2	i	7	MP8	CD-N	-4.58	1.32	1.47
2	t	7	MP8	CD-N	-4.49	1.32	1.47
2	p	7	MP8	CD-N	-4.45	1.32	1.47
2	j	5	YCP	CG-CB	-3.66	1.44	1.53
2	o	5	YCP	CG-CB	-3.53	1.44	1.53
2	p	5	YCP	CG-CB	-3.50	1.44	1.53
2	v	5	YCP	CG-CB	-3.49	1.44	1.53
2	u	5	YCP	CG-CB	-3.48	1.44	1.53
2	m	5	YCP	CG-CB	-3.44	1.44	1.53
2	f	5	YCP	CG-CB	-3.42	1.44	1.53
2	c	5	YCP	CG-CB	-3.41	1.44	1.53
2	n	5	YCP	CG-CB	-3.40	1.44	1.53
2	k	5	YCP	CG-CB	-3.34	1.44	1.53
2	e	5	YCP	CG-CB	-3.33	1.44	1.53
2	i	5	YCP	CG-CB	-3.28	1.45	1.53
2	w	5	YCP	CG-CB	-3.23	1.45	1.53
2	g	5	YCP	CG-CB	-3.22	1.45	1.53
2	t	5	YCP	CG-CB	-3.20	1.45	1.53
2	l	5	YCP	CG-CB	-3.20	1.45	1.53
2	r	5	YCP	CG-CB	-3.17	1.45	1.53
2	d	5	YCP	CG-CB	-3.14	1.45	1.53
2	h	5	YCP	CG-CB	-3.11	1.45	1.53
2	q	5	YCP	CG-CB	-3.02	1.45	1.53
2	c	2	WFP	CZ-CE1	2.30	1.41	1.37
2	v	5	YCP	CE-N	2.23	1.53	1.47
2	u	5	YCP	CE-N	2.21	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	e	2	WFP	CZ-CE1	2.21	1.41	1.37
2	p	5	YCP	CE-N	2.07	1.52	1.47
2	j	2	WFP	CZ-CE1	2.07	1.41	1.37
2	m	2	WFP	CD2-CE2	2.06	1.41	1.37
2	e	5	YCP	CE-N	2.05	1.52	1.47
2	f	2	WFP	CB-CA	-2.03	1.49	1.53
2	l	2	WFP	CZ-CE1	2.02	1.41	1.37

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	q	5	YCP	CG-CB-CA	5.31	118.47	110.93
2	r	5	YCP	CD-CG-CB	4.85	121.39	111.42
2	i	5	YCP	CD-CG-CB	4.66	121.01	111.42
2	d	5	YCP	CD-CG-CB	4.51	120.68	111.42
2	l	2	WFP	CD1-CE1-CZ	-4.50	118.03	123.50
2	r	5	YCP	CG-CB-CA	4.39	117.16	110.93
2	g	5	YCP	CG-CB-CA	4.34	117.09	110.93
2	i	5	YCP	CG-CB-CA	4.18	116.86	110.93
2	m	5	YCP	CD-CG-CB	4.09	119.83	111.42
2	l	2	WFP	F2-CE2-CD2	4.09	124.10	118.28
2	l	2	WFP	CE2-CZ-CE1	4.06	121.99	116.08
2	g	5	YCP	CD-CG-CB	4.04	119.72	111.42
2	d	5	YCP	CG-CB-CA	4.04	116.66	110.93
2	t	5	YCP	CD-CG-CB	3.97	119.57	111.42
2	l	2	WFP	CB-CG-CD1	-3.96	113.63	120.43
2	q	5	YCP	CD-CG-CB	3.85	119.34	111.42
2	e	2	WFP	CE2-CZ-CE1	3.75	121.55	116.08
2	t	5	YCP	CG-CB-CA	3.70	116.19	110.93
2	l	5	YCP	CD-CG-CB	3.63	118.88	111.42
2	h	5	YCP	CG-CB-CA	3.61	116.06	110.93
2	e	2	WFP	CD2-CE2-CZ	-3.59	119.14	123.50
2	e	2	WFP	CD1-CE1-CZ	-3.56	119.17	123.50
2	c	2	WFP	CD2-CE2-CZ	-3.50	119.25	123.50
2	w	5	YCP	CG-CB-CA	3.49	115.89	110.93
2	c	2	WFP	CB-CG-CD2	-3.43	114.55	120.43
2	u	2	WFP	CD2-CE2-CZ	-3.34	119.44	123.50
2	k	2	WFP	CD2-CE2-CZ	-3.32	119.47	123.50
2	g	7	MP8	O-C-CA	-3.32	116.23	124.77
2	c	2	WFP	CD2-CG-CD1	3.30	123.49	119.01
2	u	2	WFP	CE2-CZ-CE1	3.23	120.79	116.08
2	q	2	WFP	CD2-CE2-CZ	-3.20	119.61	123.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	h	5	YCP	CD-CG-CB	3.18	117.95	111.42
2	p	5	YCP	O-C-CA	-3.05	116.93	124.77
2	m	2	WFP	F2-CE2-CD2	3.01	122.56	118.28
2	c	5	YCP	CD-CG-CB	3.01	117.60	111.42
2	l	5	YCP	CG-CB-CA	2.95	115.12	110.93
2	w	5	YCP	CD-CG-CB	2.94	117.46	111.42
2	r	2	WFP	CD2-CE2-CZ	-2.93	119.94	123.50
2	w	2	WFP	CD2-CE2-CZ	-2.92	119.95	123.50
2	t	2	WFP	CD1-CE1-CZ	-2.92	119.96	123.50
2	c	2	WFP	CG-CD1-CE1	-2.90	116.23	118.75
2	u	2	WFP	CD1-CE1-CZ	-2.87	120.01	123.50
2	h	5	YCP	O-C-CA	-2.84	117.47	124.77
2	q	2	WFP	CE2-CZ-CE1	2.82	120.19	116.08
2	l	2	WFP	CD2-CE2-CZ	-2.79	120.12	123.50
2	c	2	WFP	F2-CE2-CZ	2.77	122.22	118.28
2	c	5	YCP	CB-CA-N	-2.77	104.27	109.23
2	o	5	YCP	O-C-CA	-2.76	117.66	124.77
2	r	2	WFP	CE2-CZ-CE1	2.73	120.05	116.08
2	h	2	WFP	F1-CE1-CD1	2.72	122.14	118.28
2	j	2	WFP	CD2-CE2-CZ	-2.71	120.21	123.50
2	u	7	MP8	O-C-CA	-2.70	117.82	124.77
2	k	5	YCP	O-C-CA	-2.69	117.84	124.77
2	r	2	WFP	CD2-CG-CD1	2.69	122.67	119.01
2	t	7	MP8	O-C-CA	-2.68	117.88	124.77
2	o	5	YCP	CG-CB-CA	2.67	114.72	110.93
2	f	2	WFP	CD2-CE2-CZ	-2.64	120.29	123.50
2	i	2	WFP	CD2-CE2-CZ	-2.64	120.29	123.50
2	n	2	WFP	CD1-CE1-CZ	-2.64	120.30	123.50
2	t	2	WFP	CE2-CZ-CE1	2.60	119.87	116.08
2	n	5	YCP	CD-CG-CB	2.60	116.76	111.42
2	d	2	WFP	CD1-CE1-CZ	-2.60	120.35	123.50
2	m	5	YCP	CG-CB-CA	2.59	114.60	110.93
2	u	7	MP8	CE-CG-CB	-2.59	107.61	114.00
2	k	7	MP8	O-C-CA	-2.57	118.16	124.77
2	q	2	WFP	CD2-CG-CD1	2.55	122.48	119.01
2	u	5	YCP	CG-CB-CA	2.53	114.53	110.93
2	j	7	MP8	CE-CG-CB	-2.53	107.75	114.00
2	c	2	WFP	CE2-CZ-CE1	2.53	119.77	116.08
2	v	2	WFP	CD1-CE1-CZ	-2.53	120.43	123.50
2	f	2	WFP	CD2-CG-CD1	2.52	122.44	119.01
2	o	2	WFP	CD2-CE2-CZ	-2.51	120.45	123.50
2	k	2	WFP	CE2-CZ-CE1	2.51	119.73	116.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	n	2	WFP	CE2-CZ-CE1	2.50	119.73	116.08
2	o	2	WFP	CD2-CG-CD1	2.50	122.41	119.01
2	o	7	MP8	O-C-CA	-2.50	118.34	124.77
2	o	2	WFP	CE2-CZ-CE1	2.50	119.72	116.08
2	n	5	YCP	O-C-CA	-2.50	118.35	124.77
2	r	7	MP8	O-C-CA	-2.50	118.35	124.77
2	l	5	YCP	O-C-CA	-2.48	118.39	124.77
2	j	2	WFP	CD2-CG-CD1	2.46	122.36	119.01
2	i	7	MP8	O-C-CA	-2.46	118.45	124.77
2	h	2	WFP	CE2-CZ-CE1	2.45	119.65	116.08
2	g	2	WFP	CD2-CE2-CZ	-2.45	120.53	123.50
2	f	2	WFP	CE2-CZ-CE1	2.44	119.64	116.08
2	d	2	WFP	CD2-CE2-CZ	-2.44	120.54	123.50
2	h	2	WFP	CD2-CE2-CZ	-2.44	120.54	123.50
2	h	2	WFP	F2-CE2-CD2	2.44	121.74	118.28
2	k	5	YCP	CG-CB-CA	2.43	114.38	110.93
2	m	2	WFP	CB-CG-CD1	-2.43	116.26	120.43
2	e	5	YCP	O-C-CA	-2.42	118.54	124.77
2	d	2	WFP	CE2-CZ-CE1	2.42	119.61	116.08
2	w	7	MP8	CE-CG-CB	-2.42	108.03	114.00
2	l	7	MP8	O-C-CA	-2.40	118.59	124.77
2	d	5	YCP	O-C-CA	-2.40	118.59	124.77
2	o	7	MP8	CE-CG-CB	-2.39	108.08	114.00
2	j	2	WFP	CE2-CZ-CE1	2.39	119.56	116.08
2	n	2	WFP	F1-CE1-CD1	2.38	121.66	118.28
2	j	5	YCP	O-C-CA	-2.38	118.65	124.77
2	r	5	YCP	O-C-CA	-2.38	118.65	124.77
2	v	2	WFP	CD2-CE2-CZ	-2.37	120.62	123.50
2	i	5	YCP	O-C-CA	-2.36	118.71	124.77
2	n	7	MP8	O-C-CA	-2.36	118.71	124.77
2	p	2	WFP	CD2-CE2-CZ	-2.35	120.64	123.50
2	l	2	WFP	F1-CE1-CD1	2.34	121.61	118.28
2	j	7	MP8	O-C-CA	-2.32	118.79	124.77
2	i	2	WFP	F1-CE1-CD1	2.30	121.55	118.28
2	o	2	WFP	CD1-CE1-CZ	-2.30	120.71	123.50
2	d	7	MP8	O-C-CA	-2.30	118.86	124.77
2	v	2	WFP	CE2-CZ-CE1	2.29	119.42	116.08
2	f	7	MP8	O-C-CA	-2.28	118.90	124.77
2	n	2	WFP	CD2-CG-CD1	2.28	122.10	119.01
2	l	2	WFP	CB-CG-CD2	2.28	124.33	120.43
2	t	2	WFP	CD2-CE2-CZ	-2.26	120.75	123.50
2	m	2	WFP	CD2-CE2-CZ	-2.26	120.75	123.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	w	2	WFP	CE2-CZ-CE1	2.26	119.37	116.08
2	f	5	YCP	O-C-CA	-2.25	118.99	124.77
2	q	5	YCP	O-C-CA	-2.23	119.04	124.77
2	l	2	WFP	CD2-CG-CD1	2.22	122.03	119.01
2	r	2	WFP	CD1-CE1-CZ	-2.20	120.82	123.50
2	e	7	MP8	O-C-CA	-2.20	119.10	124.77
2	i	2	WFP	CE2-CZ-CE1	2.20	119.29	116.08
2	u	2	WFP	F1-CE1-CD1	2.20	121.41	118.28
2	f	2	WFP	CD1-CE1-CZ	-2.20	120.83	123.50
2	w	7	MP8	O-C-CA	-2.20	119.12	124.77
2	w	7	MP8	CG-CD-N	-2.19	104.01	106.65
2	e	2	WFP	CD2-CG-CD1	2.18	121.98	119.01
2	j	5	YCP	CG-CB-CA	2.18	114.03	110.93
2	n	2	WFP	CD2-CE2-CZ	-2.17	120.87	123.50
2	c	5	YCP	CG-CB-CA	2.15	113.97	110.93
2	o	7	MP8	CG-CD-N	-2.13	104.08	106.65
2	j	2	WFP	CD1-CE1-CZ	-2.12	120.92	123.50
2	f	2	WFP	F2-CE2-CZ	2.11	121.27	118.28
2	h	2	WFP	CD1-CE1-CZ	-2.10	120.94	123.50
2	q	2	WFP	CD1-CE1-CZ	-2.08	120.98	123.50
2	c	5	YCP	O-C-CA	-2.04	119.52	124.77
2	d	5	YCP	CD-CE-N	2.04	116.04	110.84
2	q	7	MP8	CE-CG-CB	-2.02	109.01	114.00
2	u	2	WFP	CB-CG-CD2	-2.01	116.97	120.43
2	w	2	WFP	CD1-CE1-CZ	-2.01	121.06	123.50

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	c	2	WFP	C-CA-CB-CG
2	d	2	WFP	C-CA-CB-CG
2	d	2	WFP	N-CA-CB-CG
2	f	2	WFP	N-CA-CB-CG
2	i	2	WFP	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	i	2	WFP	N-CA-CB-CG
2	j	2	WFP	C-CA-CB-CG
2	j	2	WFP	N-CA-CB-CG
2	l	2	WFP	C-CA-CB-CG
2	l	2	WFP	N-CA-CB-CG
2	m	2	WFP	C-CA-CB-CG
2	o	2	WFP	C-CA-CB-CG
2	o	2	WFP	N-CA-CB-CG
2	p	2	WFP	N-CA-CB-CG
2	r	2	WFP	C-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	5	YCP	O-C-CA-CB
2	h	2	WFP	C-CA-CB-CG
2	p	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

19 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	i	2	WFP	1	0
2	d	2	WFP	1	0
2	w	2	WFP	1	0
2	t	2	WFP	1	0
2	k	2	WFP	1	0
2	q	5	YCP	1	0
2	m	7	MP8	1	0
2	r	2	WFP	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	o	2	WFP	1	0
2	v	2	WFP	2	0
2	o	5	YCP	1	0
2	l	5	YCP	1	0
2	e	7	MP8	1	0
2	l	2	WFP	1	0
2	p	5	YCP	1	0
2	m	2	WFP	3	0
2	j	2	WFP	2	0
2	v	7	MP8	1	0
2	c	2	WFP	1	0

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	172/199 (86%)	0.19	6 (3%) 47 38	30, 45, 71, 78	0
1	B	176/199 (88%)	0.27	10 (5%) 29 22	30, 44, 70, 87	0
1	C	172/199 (86%)	0.93	19 (11%) 10 8	42, 61, 85, 92	0
1	D	164/199 (82%)	1.03	24 (14%) 6 4	36, 62, 82, 91	0
1	E	174/199 (87%)	1.14	28 (16%) 4 4	42, 67, 84, 88	0
1	F	169/199 (84%)	0.11	2 (1%) 76 68	30, 42, 61, 73	0
1	G	177/199 (88%)	0.01	5 (2%) 55 45	28, 38, 59, 77	0
1	H	172/199 (86%)	1.10	29 (16%) 4 3	45, 68, 84, 91	0
1	I	177/199 (88%)	0.71	14 (7%) 18 13	30, 59, 79, 95	0
1	J	173/199 (86%)	0.63	17 (9%) 13 9	36, 54, 74, 84	0
1	K	171/199 (85%)	0.46	10 (5%) 29 22	32, 46, 67, 78	0
1	L	171/199 (85%)	0.71	14 (8%) 17 13	42, 57, 84, 98	0
1	M	168/199 (84%)	0.95	21 (12%) 8 6	43, 67, 84, 102	0
1	N	168/199 (84%)	1.20	23 (13%) 6 5	49, 72, 87, 96	0
1	O	174/199 (87%)	0.28	10 (5%) 29 22	28, 50, 74, 85	0
1	P	177/199 (88%)	0.32	9 (5%) 33 25	26, 43, 71, 79	0
1	Q	172/199 (86%)	0.37	9 (5%) 33 25	29, 44, 68, 81	0
1	R	168/199 (84%)	0.30	13 (7%) 19 14	29, 41, 63, 72	0
1	S	174/199 (87%)	0.65	17 (9%) 13 9	31, 49, 85, 98	0
1	T	168/199 (84%)	0.16	3 (1%) 67 58	33, 45, 69, 83	0
1	U	170/199 (85%)	0.29	9 (5%) 32 24	31, 46, 68, 80	0
1	V	175/199 (87%)	0.30	9 (5%) 33 25	35, 47, 69, 84	0
1	W	176/199 (88%)	0.52	7 (3%) 42 33	41, 55, 75, 91	0
1	X	169/199 (84%)	0.67	10 (5%) 28 21	46, 63, 80, 90	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	Y	165/199 (82%)	0.89	16 (9%) 13 10	30, 66, 80, 93	0
1	Z	169/199 (84%)	1.02	20 (11%) 9 7	43, 67, 86, 99	0
1	a	168/199 (84%)	0.17	1 (0%) 85 80	33, 45, 63, 77	0
1	b	175/199 (87%)	0.01	5 (2%) 53 43	27, 41, 64, 78	0
2	c	3/7 (42%)	-0.58	0 100 100	40, 40, 46, 50	0
2	d	3/7 (42%)	0.11	0 100 100	53, 53, 60, 62	0
2	e	3/7 (42%)	0.43	0 100 100	68, 68, 70, 73	0
2	f	3/7 (42%)	1.02	1 (33%) 1 1	55, 55, 56, 71	0
2	g	3/7 (42%)	-0.02	0 100 100	47, 47, 49, 53	0
2	h	3/7 (42%)	0.28	0 100 100	71, 71, 72, 73	0
2	i	3/7 (42%)	0.12	0 100 100	64, 64, 73, 74	0
2	j	3/7 (42%)	0.17	0 100 100	53, 53, 56, 66	0
2	k	3/7 (42%)	0.92	0 100 100	64, 64, 68, 77	0
2	l	3/7 (42%)	0.47	0 100 100	82, 82, 83, 84	0
2	m	3/7 (42%)	-0.00	0 100 100	45, 45, 45, 53	0
2	n	3/7 (42%)	0.08	0 100 100	49, 49, 50, 58	0
2	o	3/7 (42%)	-0.22	0 100 100	47, 47, 51, 52	0
2	p	3/7 (42%)	-0.03	0 100 100	45, 45, 51, 56	0
2	q	3/7 (42%)	0.02	0 100 100	52, 52, 52, 56	0
2	r	3/7 (42%)	-0.01	0 100 100	50, 50, 51, 55	0
2	t	3/7 (42%)	0.71	0 100 100	68, 68, 68, 72	0
2	u	3/7 (42%)	0.37	0 100 100	65, 65, 68, 71	0
2	v	3/7 (42%)	0.59	0 100 100	51, 51, 58, 61	0
2	w	3/7 (42%)	0.01	0 100 100	47, 47, 51, 55	0
All	All	4864/5712 (85%)	0.54	361 (7%) 20 15	26, 54, 80, 102	0

All (361) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Y	5	THR	7.0
1	Q	124	PRO	5.7
1	J	123	GLN	5.1
1	V	125	LEU	4.9
1	U	121	ILE	4.9

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Mol	Chain	Res	Type	RSRZ
1	H	118	GLU	4.9
1	S	125	LEU	4.8
1	V	2	LEU	4.8
1	M	138	ALA	4.5
1	J	124	PRO	4.5
1	M	155	GLU	4.4
1	Q	123	GLN	4.4
1	R	139	ALA	4.3
1	I	126	GLY	4.3
1	b	124	PRO	4.3
1	J	37	ASP	4.2
1	S	136	GLU	4.2
1	E	92	ILE	4.1
1	J	137	ILE	4.1
1	L	138	ALA	4.0
1	S	137	ILE	4.0
1	N	52	ALA	4.0
1	Y	6	VAL	4.0
1	H	135	ILE	3.9
1	E	125	LEU	3.9
1	U	122	HIS	3.9
1	A	170	ARG	3.9
1	A	2	LEU	3.9
1	D	3	ILE	3.9
1	Y	18	ASP	3.9
1	R	3	ILE	3.8
1	H	189	LEU	3.8
1	P	173	PHE	3.7
1	D	4	PRO	3.7
1	Q	56	GLU	3.7
1	D	173	PHE	3.7
1	J	121	ILE	3.6
1	S	163	VAL	3.6
1	b	125	LEU	3.6
1	I	125	LEU	3.6
1	L	173	PHE	3.5
1	N	72	ALA	3.5
1	J	17	TYR	3.5
1	A	135	ILE	3.5
1	P	10	THR	3.5
1	B	138	ALA	3.5
1	N	51	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	V	5	THR	3.4
1	W	127	GLY	3.4
1	V	118	GLU	3.4
1	N	189	LEU	3.4
1	N	50	LEU	3.4
1	Z	145	LEU	3.4
1	S	173	PHE	3.4
1	M	123	GLN	3.4
1	M	171	ASP	3.4
1	N	16	ALA	3.3
1	S	146	ARG	3.3
1	N	138	ALA	3.3
1	S	138	ALA	3.3
1	M	150	ASN	3.3
1	D	80	MET	3.2
1	H	60	SER	3.2
1	S	69	SER	3.2
1	N	87	VAL	3.2
1	D	172	ASN	3.2
1	N	172	ASN	3.2
1	L	8	GLU	3.2
1	Z	102	LEU	3.2
1	H	138	ALA	3.2
1	C	125	LEU	3.1
1	H	125	LEU	3.1
1	E	136	GLU	3.1
1	Z	17	TYR	3.1
1	I	67	GLY	3.1
1	L	17	TYR	3.1
1	M	139	ALA	3.1
1	U	172	ASN	3.1
1	Y	56	GLU	3.0
1	P	16	ALA	3.0
1	C	163	VAL	3.0
1	U	191	HIS	3.0
1	Z	115	PRO	3.0
1	N	190	THR	3.0
1	G	124	PRO	3.0
1	H	62	TYR	3.0
1	X	124	PRO	3.0
1	Y	17	TYR	3.0
1	E	94	MET	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	73	GLY	3.0
1	V	135	ILE	3.0
1	R	143	LEU	3.0
1	U	120	MET	3.0
1	L	142	ILE	3.0
1	H	137	ILE	2.9
1	W	190	THR	2.9
1	X	138	ALA	2.9
1	Y	139	ALA	2.9
1	E	102	LEU	2.9
1	H	136	GLU	2.9
1	D	5	THR	2.9
1	B	67	GLY	2.9
1	S	162	GLU	2.9
1	C	138	ALA	2.9
1	J	125	LEU	2.9
1	O	125	LEU	2.9
1	Y	189	LEU	2.9
1	G	146	ARG	2.8
1	N	141	ARG	2.8
1	G	137	ILE	2.8
1	C	17	TYR	2.8
1	Y	140	LYS	2.8
1	L	139	ALA	2.8
1	Q	155	GLU	2.8
1	Z	173	PHE	2.8
1	O	135	ILE	2.8
1	Y	3	ILE	2.8
1	E	184	LEU	2.8
1	H	112	TYR	2.8
1	I	14	GLU	2.8
1	Z	155	GLU	2.8
1	M	153	LEU	2.7
1	X	139	ALA	2.7
1	Y	16	ALA	2.7
1	Z	190	THR	2.7
1	D	47	LEU	2.7
1	I	15	ARG	2.7
1	R	6	VAL	2.7
1	D	17	TYR	2.7
1	C	7	ILE	2.7
1	O	146	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	W	1	ASN	2.7
1	N	139	ALA	2.7
2	f	4	PRO	2.7
1	S	142	ILE	2.7
1	a	3	ILE	2.7
1	Y	181	GLU	2.7
1	D	6	VAL	2.7
1	D	52	ALA	2.7
1	K	6	VAL	2.7
1	N	82	PHE	2.7
1	O	133	THR	2.7
1	R	173	PHE	2.7
1	B	169	ASP	2.7
1	D	167	ASP	2.7
1	K	3	ILE	2.6
1	K	7	ILE	2.6
1	Z	63	ILE	2.6
1	C	126	GLY	2.6
1	N	115	PRO	2.6
1	R	5	THR	2.6
1	E	117	SER	2.6
1	V	6	VAL	2.6
1	D	70	ILE	2.6
1	D	121	ILE	2.6
1	K	137	ILE	2.6
1	S	170	ARG	2.6
1	O	138	ALA	2.6
1	X	37	ASP	2.6
1	H	120	MET	2.6
1	E	137	ILE	2.6
1	H	188	ILE	2.6
1	D	148	LYS	2.6
1	M	154	ALA	2.6
1	O	139	ALA	2.6
1	Z	152	VAL	2.6
1	E	69	SER	2.5
1	S	190	THR	2.5
1	H	30	MET	2.5
1	X	121	ILE	2.5
1	W	191	HIS	2.5
1	C	55	PRO	2.5
1	I	173	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	K	16	ALA	2.5
1	J	172	ASN	2.5
1	S	167	ASP	2.5
1	Q	137	ILE	2.5
1	H	22	ARG	2.5
1	R	2	LEU	2.5
1	I	56	GLU	2.5
1	C	87	VAL	2.5
1	E	173	PHE	2.5
1	T	138	ALA	2.5
1	P	69	SER	2.5
1	B	125	LEU	2.5
1	D	149	LEU	2.5
1	Y	169	ASP	2.5
1	Z	15	ARG	2.5
1	E	109	GLY	2.5
1	I	190	THR	2.5
1	B	170	ARG	2.5
1	D	143	LEU	2.5
1	E	164	ILE	2.5
1	Z	64	ASN	2.4
1	E	188	ILE	2.4
1	V	136	GLU	2.4
1	E	163	VAL	2.4
1	H	174	LYS	2.4
1	M	152	VAL	2.4
1	N	6	VAL	2.4
1	E	95	ALA	2.4
1	E	113	ALA	2.4
1	K	5	THR	2.4
1	C	142	ILE	2.4
1	E	189	LEU	2.4
1	H	87	VAL	2.4
1	H	113	ALA	2.4
1	R	171	ASP	2.4
1	D	66	PRO	2.4
1	Y	4	PRO	2.4
1	A	138	ALA	2.4
1	F	173	PHE	2.4
1	R	16	ALA	2.4
1	E	143	LEU	2.4
1	Z	143	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	Y	172	ASN	2.4
1	K	136	GLU	2.4
1	M	8	GLU	2.4
1	H	187	LYS	2.4
1	U	138	ALA	2.4
1	I	7	ILE	2.3
1	Q	121	ILE	2.3
1	E	97	SER	2.3
1	B	173	PHE	2.3
1	M	173	PHE	2.3
1	U	2	LEU	2.3
1	R	172	ASN	2.3
1	I	8	GLU	2.3
1	J	173	PHE	2.3
1	E	176	ALA	2.3
1	M	51	ALA	2.3
1	H	190	THR	2.3
1	J	14	GLU	2.3
1	K	84	LYS	2.3
1	O	118	GLU	2.3
1	B	124	PRO	2.3
1	K	124	PRO	2.3
1	R	4	PRO	2.3
1	V	109	GLY	2.3
1	E	153	LEU	2.3
1	H	61	LEU	2.3
1	J	16	ALA	2.3
1	D	120	MET	2.3
1	P	190	THR	2.3
1	N	77	TYR	2.3
1	Q	107	GLU	2.3
1	M	38	ASN	2.3
1	N	69	SER	2.3
1	W	67	GLY	2.3
1	N	48	LEU	2.3
1	A	173	PHE	2.3
1	C	164	ILE	2.2
1	N	70	ILE	2.2
1	B	10	THR	2.2
1	U	166	ARG	2.2
1	C	160	PRO	2.2
1	E	65	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	R	169	ASP	2.2
1	A	125	LEU	2.2
1	X	94	MET	2.2
1	Z	62	TYR	2.2
1	M	124	PRO	2.2
1	T	124	PRO	2.2
1	J	158	GLY	2.2
1	L	167	ASP	2.2
1	L	171	ASP	2.2
1	X	126	GLY	2.2
1	C	143	LEU	2.2
1	W	125	LEU	2.2
1	Z	184	LEU	2.2
1	D	59	ILE	2.2
1	F	7	ILE	2.2
1	L	7	ILE	2.2
1	L	121	ILE	2.2
1	N	162	GLU	2.2
1	P	89	THR	2.2
1	N	41	ASN	2.2
1	Q	17	TYR	2.2
1	X	123	GLN	2.2
1	C	161	LEU	2.2
1	J	108	LYS	2.2
1	W	68	GLY	2.2
1	X	99	GLY	2.2
1	L	120	MET	2.2
1	H	173	PHE	2.2
1	N	121	ILE	2.2
1	P	137	ILE	2.2
1	B	139	ALA	2.2
1	Z	138	ALA	2.2
1	C	157	THR	2.2
1	M	156	ARG	2.2
1	K	172	ASN	2.2
1	G	123	GLN	2.2
1	C	149	LEU	2.2
1	V	126	GLY	2.2
1	D	60	SER	2.2
1	Z	142	ILE	2.2
1	b	191	HIS	2.2
1	Z	154	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	M	190	THR	2.1
1	C	124	PRO	2.1
1	X	125	LEU	2.1
1	H	32	GLY	2.1
1	S	109	GLY	2.1
1	E	18	ASP	2.1
1	H	3	ILE	2.1
1	J	7	ILE	2.1
1	M	88	SER	2.1
1	O	173	PHE	2.1
1	M	16	ALA	2.1
1	I	58	GLU	2.1
1	B	1	ASN	2.1
1	N	123	GLN	2.1
1	H	109	GLY	2.1
1	D	83	ILE	2.1
1	I	191	HIS	2.1
1	Y	121	ILE	2.1
1	I	96	ALA	2.1
1	Z	146	ARG	2.1
1	b	190	THR	2.1
1	L	124	PRO	2.1
1	T	120	MET	2.1
1	b	123	GLN	2.1
1	H	103	LEU	2.1
1	Z	112	TYR	2.1
1	M	142	ILE	2.1
1	H	26	ASP	2.1
1	J	171	ASP	2.1
1	E	88	SER	2.1
1	J	8	GLU	2.1
1	S	176	ALA	2.1
1	J	190	THR	2.1
1	H	4	PRO	2.1
1	E	114	LEU	2.1
1	E	149	LEU	2.1
1	G	1	ASN	2.1
1	E	90	ILE	2.1
1	R	28	ILE	2.1
1	E	167	ASP	2.0
1	O	171	ASP	2.0
1	D	162	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	O	162	GLU	2.0
1	L	174	LYS	2.0
1	S	174	LYS	2.0
1	C	79	THR	2.0
1	D	190	THR	2.0
1	H	123	GLN	2.0
1	L	143	LEU	2.0
1	Z	153	LEU	2.0
1	M	35	ILE	2.0
1	Y	92	ILE	2.0
1	U	173	PHE	2.0
1	D	55	PRO	2.0
1	Q	190	THR	2.0
1	I	2	LEU	2.0
1	M	149	LEU	2.0
1	C	121	ILE	2.0
1	H	172	ASN	2.0
1	P	1	ASN	2.0
1	S	164	ILE	2.0
1	P	170	ARG	2.0

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

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, 95th 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	YCP	e	5	8/9	0.76	0.14	62,65,69,70	0
2	MP8	e	7	8/9	0.78	0.14	64,68,69,70	0
2	YCP	l	5	8/9	0.79	0.15	79,84,86,89	0
2	MP8	l	7	8/9	0.80	0.15	82,84,89,90	0
2	WFP	l	2	13/14	0.84	0.16	62,76,83,84	0
2	YCP	k	5	8/9	0.85	0.15	59,68,70,72	0
2	MP8	k	7	8/9	0.86	0.15	59,64,70,74	0
2	WFP	e	2	13/14	0.87	0.16	58,64,70,70	0
2	MP8	h	7	8/9	0.87	0.13	69,71,75,75	0
2	YCP	t	5	8/9	0.88	0.12	69,70,71,73	0
2	MP8	q	7	8/9	0.88	0.12	39,46,53,54	0
2	MP8	t	7	8/9	0.88	0.13	67,69,71,74	0
2	YCP	o	5	8/9	0.89	0.12	45,49,53,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MP8	v	7	8/9	0.89	0.12	43,48,51,53	0
2	YCP	h	5	8/9	0.90	0.12	58,67,73,74	0
2	YCP	p	5	8/9	0.90	0.11	39,48,49,49	0
2	YCP	q	5	8/9	0.90	0.10	51,56,58,60	0
2	YCP	d	5	8/9	0.90	0.10	59,65,71,71	0
2	YCP	v	5	8/9	0.90	0.10	45,50,52,54	0
2	WFP	h	2	13/14	0.90	0.11	57,60,66,73	0
2	MP8	o	7	8/9	0.91	0.11	44,45,57,60	0
2	MP8	i	7	8/9	0.91	0.12	56,61,63,65	0
2	MP8	f	7	8/9	0.91	0.10	47,49,52,55	0
2	MP8	u	7	8/9	0.91	0.14	63,67,71,73	0
2	WFP	v	2	13/14	0.91	0.11	51,54,60,61	0
2	WFP	i	2	13/14	0.92	0.10	54,61,66,67	0
2	YCP	u	5	8/9	0.92	0.09	63,68,69,72	0
2	WFP	d	2	13/14	0.92	0.11	37,50,53,59	0
2	YCP	w	5	8/9	0.92	0.10	50,52,55,57	0
2	WFP	u	2	13/14	0.92	0.11	58,62,69,70	0
2	YCP	f	5	8/9	0.93	0.09	49,56,58,60	0
2	WFP	k	2	13/14	0.93	0.11	52,55,62,68	0
2	MP8	p	7	8/9	0.93	0.08	37,41,44,44	0
2	YCP	r	5	8/9	0.93	0.10	53,56,57,66	0
2	MP8	r	7	8/9	0.93	0.10	40,51,54,57	0
2	WFP	f	2	13/14	0.93	0.09	43,47,59,61	0
2	WFP	r	2	13/14	0.93	0.09	43,45,60,63	0
2	WFP	t	2	13/14	0.93	0.12	49,57,65,66	0
2	MP8	j	7	8/9	0.94	0.10	44,51,61,61	0
2	YCP	g	5	8/9	0.94	0.09	43,45,47,52	0
2	WFP	n	2	13/14	0.94	0.09	36,43,49,61	0
2	MP8	c	7	8/9	0.94	0.09	39,42,44,50	0
2	MP8	d	7	8/9	0.94	0.10	49,57,59,61	0
2	YCP	j	5	8/9	0.94	0.10	57,59,61,62	0
2	WFP	w	2	13/14	0.94	0.10	38,42,44,52	0
2	MP8	g	7	8/9	0.94	0.09	35,45,49,51	0
2	YCP	c	5	8/9	0.94	0.09	35,39,44,45	0
2	YCP	n	5	8/9	0.94	0.09	53,58,58,61	0
2	YCP	i	5	8/9	0.95	0.08	58,66,68,70	0
2	WFP	q	2	13/14	0.95	0.08	36,43,47,49	0
2	WFP	j	2	13/14	0.95	0.09	39,44,48,59	0
2	MP8	m	7	8/9	0.95	0.08	36,39,43,48	0
2	MP8	n	7	8/9	0.95	0.09	34,45,46,50	0
2	WFP	g	2	13/14	0.95	0.08	31,37,48,48	0
2	MP8	w	7	8/9	0.95	0.10	39,44,49,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	WFP	p	2	13/14	0.96	0.08	39,42,46,47	0
2	WFP	m	2	13/14	0.96	0.07	31,39,47,51	0
2	YCP	m	5	8/9	0.96	0.07	37,47,50,50	0
2	WFP	c	2	13/14	0.96	0.07	26,39,42,43	0
2	WFP	o	2	13/14	0.97	0.07	36,41,46,47	0

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.