wwPDB X-ray Structure Validation Summary Report (i)

Nov 5, 2023 – 01:33 AM EST

PDB ID	:	6NAH
Title	:	Crystal structure of Neisseria meningitidis ClpP protease in complex with Acyldepsipeptide-14 (ADEP-14)
Authors	:	Mabanglo, M.F.; Houry, W.A.
Deposited on	:	2018-12-05
Resolution	:	2.70 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

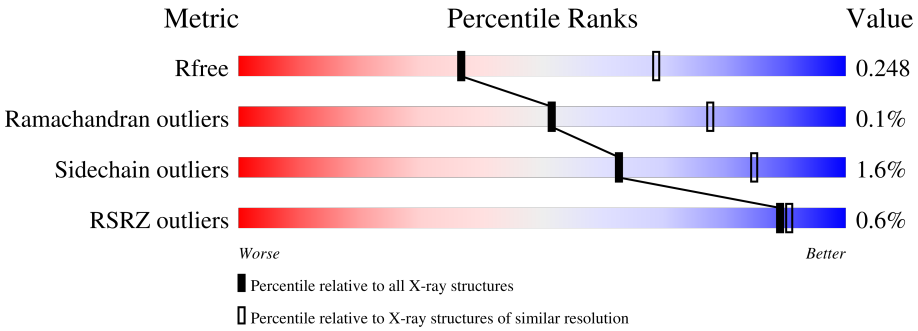
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	217	79% · 19%
1	B	217	% 77% · 20%
1	C	217	76% · 20%
1	D	217	% 77% · 20%
1	E	217	78% · 20%
1	F	217	78% · 21%

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Mol	Chain	Length	Quality of chain
1	G	217	78% 20%
1	H	217	76% 20%
1	I	217	76% 21%
1	J	217	78% 21%
1	K	217	78% 20%
1	L	217	78% 20%
1	M	217	76% 21%
1	N	217	77% 20%
1	O	217	76% 21%
1	P	217	78% 20%
1	Q	217	77% 20%
1	R	217	78% 19%
1	S	217	77% 20%
1	T	217	77% 21%
1	U	217	76% 20%
1	V	217	78% 21%
1	W	217	78% 20%
1	X	217	77% 20%
1	Y	217	77% 21%
1	Z	217	77% 21%
1	a	217	78% 20%
1	b	217	76% 21%
2	0	6	33% 67%
2	1	6	33% 67%
2	2	6	33% 67%

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Mol	Chain	Length	Quality of chain
2	3	6	33% 67%
2	4	6	33% 50% 17%
2	c	6	33% 67%
2	e	6	33% 67%
2	f	6	33% 67%
2	g	6	33% 67%
2	h	6	33% 67%
2	i	6	33% 67%
2	j	6	33% 67%
2	k	6	33% 67%
2	l	6	33% 67%
2	m	6	33% 67%
2	n	6	33% 67%
2	o	6	33% 67%
2	p	6	33% 67%
2	q	6	33% 67%
2	r	6	33% 67%
2	s	6	17% 83%
2	t	6	33% 67%
2	u	6	33% 67%
2	v	6	17% 83%
2	w	6	17% 83%
2	x	6	33% 67%
2	y	6	17% 83%
2	z	6	33% 67%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 40076 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	175	Total	C	N	O	S	0	0	0
			1359	858	230	263	8			
1	B	173	Total	C	N	O	S	0	0	0
			1347	850	228	261	8			
1	C	173	Total	C	N	O	S	0	0	0
			1346	851	228	259	8			
1	D	173	Total	C	N	O	S	0	0	0
			1351	852	229	262	8			
1	E	174	Total	C	N	O	S	0	0	0
			1359	858	230	263	8			
1	F	171	Total	C	N	O	S	0	0	0
			1339	846	226	259	8			
1	G	173	Total	C	N	O	S	0	0	0
			1351	854	228	261	8			
1	H	174	Total	C	N	O	S	0	0	0
			1359	858	230	263	8			
1	I	171	Total	C	N	O	S	0	0	0
			1339	846	226	259	8			
1	J	172	Total	C	N	O	S	0	0	0
			1347	850	228	261	8			
1	K	174	Total	C	N	O	S	0	0	0
			1359	858	230	263	8			
1	L	174	Total	C	N	O	S	0	0	0
			1355	856	229	262	8			
1	M	171	Total	C	N	O	S	0	0	0
			1339	846	226	259	8			
1	N	173	Total	C	N	O	S	0	0	0
			1347	850	228	261	8			
1	O	172	Total	C	N	O	S	0	0	0
			1347	850	228	261	8			
1	P	173	Total	C	N	O	S	0	0	0
			1347	850	228	261	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	173	Total	C	N	O	S	0	0	0
			1351	854	228	261	8			
1	R	175	Total	C	N	O	S	0	0	0
			1363	860	231	264	8			
1	S	173	Total	C	N	O	S	0	0	0
			1351	852	229	262	8			
1	T	171	Total	C	N	O	S	0	0	0
			1339	846	227	258	8			
1	U	174	Total	C	N	O	S	0	0	0
			1350	853	229	260	8			
1	V	171	Total	C	N	O	S	0	0	0
			1341	847	227	259	8			
1	W	173	Total	C	N	O	S	0	0	0
			1347	850	228	261	8			
1	X	174	Total	C	N	O	S	0	0	0
			1355	856	229	262	8			
1	Y	172	Total	C	N	O	S	0	0	0
			1347	850	228	261	8			
1	Z	172	Total	C	N	O	S	0	0	0
			1343	848	227	260	8			
1	a	173	Total	C	N	O	S	0	0	0
			1351	852	229	262	8			
1	b	172	Total	C	N	O	S	0	0	0
			1345	851	227	259	8			

There are 364 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	HIS	-	expression tag	UNP I4E574
A	-11	HIS	-	expression tag	UNP I4E574
A	-10	HIS	-	expression tag	UNP I4E574
A	-9	HIS	-	expression tag	UNP I4E574
A	-8	HIS	-	expression tag	UNP I4E574
A	-7	HIS	-	expression tag	UNP I4E574
A	-6	GLU	-	expression tag	UNP I4E574
A	-5	ASN	-	expression tag	UNP I4E574
A	-4	LEU	-	expression tag	UNP I4E574
A	-3	TYR	-	expression tag	UNP I4E574
A	-2	PHE	-	expression tag	UNP I4E574
A	-1	GLN	-	expression tag	UNP I4E574
A	0	GLY	-	expression tag	UNP I4E574
B	-12	HIS	-	expression tag	UNP I4E574
B	-11	HIS	-	expression tag	UNP I4E574

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	HIS	-	expression tag	UNP I4E574
B	-9	HIS	-	expression tag	UNP I4E574
B	-8	HIS	-	expression tag	UNP I4E574
B	-7	HIS	-	expression tag	UNP I4E574
B	-6	GLU	-	expression tag	UNP I4E574
B	-5	ASN	-	expression tag	UNP I4E574
B	-4	LEU	-	expression tag	UNP I4E574
B	-3	TYR	-	expression tag	UNP I4E574
B	-2	PHE	-	expression tag	UNP I4E574
B	-1	GLN	-	expression tag	UNP I4E574
B	0	GLY	-	expression tag	UNP I4E574
C	-12	HIS	-	expression tag	UNP I4E574
C	-11	HIS	-	expression tag	UNP I4E574
C	-10	HIS	-	expression tag	UNP I4E574
C	-9	HIS	-	expression tag	UNP I4E574
C	-8	HIS	-	expression tag	UNP I4E574
C	-7	HIS	-	expression tag	UNP I4E574
C	-6	GLU	-	expression tag	UNP I4E574
C	-5	ASN	-	expression tag	UNP I4E574
C	-4	LEU	-	expression tag	UNP I4E574
C	-3	TYR	-	expression tag	UNP I4E574
C	-2	PHE	-	expression tag	UNP I4E574
C	-1	GLN	-	expression tag	UNP I4E574
C	0	GLY	-	expression tag	UNP I4E574
D	-12	HIS	-	expression tag	UNP I4E574
D	-11	HIS	-	expression tag	UNP I4E574
D	-10	HIS	-	expression tag	UNP I4E574
D	-9	HIS	-	expression tag	UNP I4E574
D	-8	HIS	-	expression tag	UNP I4E574
D	-7	HIS	-	expression tag	UNP I4E574
D	-6	GLU	-	expression tag	UNP I4E574
D	-5	ASN	-	expression tag	UNP I4E574
D	-4	LEU	-	expression tag	UNP I4E574
D	-3	TYR	-	expression tag	UNP I4E574
D	-2	PHE	-	expression tag	UNP I4E574
D	-1	GLN	-	expression tag	UNP I4E574
D	0	GLY	-	expression tag	UNP I4E574
E	-12	HIS	-	expression tag	UNP I4E574
E	-11	HIS	-	expression tag	UNP I4E574
E	-10	HIS	-	expression tag	UNP I4E574
E	-9	HIS	-	expression tag	UNP I4E574
E	-8	HIS	-	expression tag	UNP I4E574

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-7	HIS	-	expression tag	UNP I4E574
E	-6	GLU	-	expression tag	UNP I4E574
E	-5	ASN	-	expression tag	UNP I4E574
E	-4	LEU	-	expression tag	UNP I4E574
E	-3	TYR	-	expression tag	UNP I4E574
E	-2	PHE	-	expression tag	UNP I4E574
E	-1	GLN	-	expression tag	UNP I4E574
E	0	GLY	-	expression tag	UNP I4E574
F	-12	HIS	-	expression tag	UNP I4E574
F	-11	HIS	-	expression tag	UNP I4E574
F	-10	HIS	-	expression tag	UNP I4E574
F	-9	HIS	-	expression tag	UNP I4E574
F	-8	HIS	-	expression tag	UNP I4E574
F	-7	HIS	-	expression tag	UNP I4E574
F	-6	GLU	-	expression tag	UNP I4E574
F	-5	ASN	-	expression tag	UNP I4E574
F	-4	LEU	-	expression tag	UNP I4E574
F	-3	TYR	-	expression tag	UNP I4E574
F	-2	PHE	-	expression tag	UNP I4E574
F	-1	GLN	-	expression tag	UNP I4E574
F	0	GLY	-	expression tag	UNP I4E574
G	-12	HIS	-	expression tag	UNP I4E574
G	-11	HIS	-	expression tag	UNP I4E574
G	-10	HIS	-	expression tag	UNP I4E574
G	-9	HIS	-	expression tag	UNP I4E574
G	-8	HIS	-	expression tag	UNP I4E574
G	-7	HIS	-	expression tag	UNP I4E574
G	-6	GLU	-	expression tag	UNP I4E574
G	-5	ASN	-	expression tag	UNP I4E574
G	-4	LEU	-	expression tag	UNP I4E574
G	-3	TYR	-	expression tag	UNP I4E574
G	-2	PHE	-	expression tag	UNP I4E574
G	-1	GLN	-	expression tag	UNP I4E574
G	0	GLY	-	expression tag	UNP I4E574
H	-12	HIS	-	expression tag	UNP I4E574
H	-11	HIS	-	expression tag	UNP I4E574
H	-10	HIS	-	expression tag	UNP I4E574
H	-9	HIS	-	expression tag	UNP I4E574
H	-8	HIS	-	expression tag	UNP I4E574
H	-7	HIS	-	expression tag	UNP I4E574
H	-6	GLU	-	expression tag	UNP I4E574
H	-5	ASN	-	expression tag	UNP I4E574

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-4	LEU	-	expression tag	UNP I4E574
H	-3	TYR	-	expression tag	UNP I4E574
H	-2	PHE	-	expression tag	UNP I4E574
H	-1	GLN	-	expression tag	UNP I4E574
H	0	GLY	-	expression tag	UNP I4E574
I	-12	HIS	-	expression tag	UNP I4E574
I	-11	HIS	-	expression tag	UNP I4E574
I	-10	HIS	-	expression tag	UNP I4E574
I	-9	HIS	-	expression tag	UNP I4E574
I	-8	HIS	-	expression tag	UNP I4E574
I	-7	HIS	-	expression tag	UNP I4E574
I	-6	GLU	-	expression tag	UNP I4E574
I	-5	ASN	-	expression tag	UNP I4E574
I	-4	LEU	-	expression tag	UNP I4E574
I	-3	TYR	-	expression tag	UNP I4E574
I	-2	PHE	-	expression tag	UNP I4E574
I	-1	GLN	-	expression tag	UNP I4E574
I	0	GLY	-	expression tag	UNP I4E574
J	-12	HIS	-	expression tag	UNP I4E574
J	-11	HIS	-	expression tag	UNP I4E574
J	-10	HIS	-	expression tag	UNP I4E574
J	-9	HIS	-	expression tag	UNP I4E574
J	-8	HIS	-	expression tag	UNP I4E574
J	-7	HIS	-	expression tag	UNP I4E574
J	-6	GLU	-	expression tag	UNP I4E574
J	-5	ASN	-	expression tag	UNP I4E574
J	-4	LEU	-	expression tag	UNP I4E574
J	-3	TYR	-	expression tag	UNP I4E574
J	-2	PHE	-	expression tag	UNP I4E574
J	-1	GLN	-	expression tag	UNP I4E574
J	0	GLY	-	expression tag	UNP I4E574
K	-12	HIS	-	expression tag	UNP I4E574
K	-11	HIS	-	expression tag	UNP I4E574
K	-10	HIS	-	expression tag	UNP I4E574
K	-9	HIS	-	expression tag	UNP I4E574
K	-8	HIS	-	expression tag	UNP I4E574
K	-7	HIS	-	expression tag	UNP I4E574
K	-6	GLU	-	expression tag	UNP I4E574
K	-5	ASN	-	expression tag	UNP I4E574
K	-4	LEU	-	expression tag	UNP I4E574
K	-3	TYR	-	expression tag	UNP I4E574
K	-2	PHE	-	expression tag	UNP I4E574

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-1	GLN	-	expression tag	UNP I4E574
K	0	GLY	-	expression tag	UNP I4E574
L	-12	HIS	-	expression tag	UNP I4E574
L	-11	HIS	-	expression tag	UNP I4E574
L	-10	HIS	-	expression tag	UNP I4E574
L	-9	HIS	-	expression tag	UNP I4E574
L	-8	HIS	-	expression tag	UNP I4E574
L	-7	HIS	-	expression tag	UNP I4E574
L	-6	GLU	-	expression tag	UNP I4E574
L	-5	ASN	-	expression tag	UNP I4E574
L	-4	LEU	-	expression tag	UNP I4E574
L	-3	TYR	-	expression tag	UNP I4E574
L	-2	PHE	-	expression tag	UNP I4E574
L	-1	GLN	-	expression tag	UNP I4E574
L	0	GLY	-	expression tag	UNP I4E574
M	-12	HIS	-	expression tag	UNP I4E574
M	-11	HIS	-	expression tag	UNP I4E574
M	-10	HIS	-	expression tag	UNP I4E574
M	-9	HIS	-	expression tag	UNP I4E574
M	-8	HIS	-	expression tag	UNP I4E574
M	-7	HIS	-	expression tag	UNP I4E574
M	-6	GLU	-	expression tag	UNP I4E574
M	-5	ASN	-	expression tag	UNP I4E574
M	-4	LEU	-	expression tag	UNP I4E574
M	-3	TYR	-	expression tag	UNP I4E574
M	-2	PHE	-	expression tag	UNP I4E574
M	-1	GLN	-	expression tag	UNP I4E574
M	0	GLY	-	expression tag	UNP I4E574
N	-12	HIS	-	expression tag	UNP I4E574
N	-11	HIS	-	expression tag	UNP I4E574
N	-10	HIS	-	expression tag	UNP I4E574
N	-9	HIS	-	expression tag	UNP I4E574
N	-8	HIS	-	expression tag	UNP I4E574
N	-7	HIS	-	expression tag	UNP I4E574
N	-6	GLU	-	expression tag	UNP I4E574
N	-5	ASN	-	expression tag	UNP I4E574
N	-4	LEU	-	expression tag	UNP I4E574
N	-3	TYR	-	expression tag	UNP I4E574
N	-2	PHE	-	expression tag	UNP I4E574
N	-1	GLN	-	expression tag	UNP I4E574
N	0	GLY	-	expression tag	UNP I4E574
O	-12	HIS	-	expression tag	UNP I4E574

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-11	HIS	-	expression tag	UNP I4E574
O	-10	HIS	-	expression tag	UNP I4E574
O	-9	HIS	-	expression tag	UNP I4E574
O	-8	HIS	-	expression tag	UNP I4E574
O	-7	HIS	-	expression tag	UNP I4E574
O	-6	GLU	-	expression tag	UNP I4E574
O	-5	ASN	-	expression tag	UNP I4E574
O	-4	LEU	-	expression tag	UNP I4E574
O	-3	TYR	-	expression tag	UNP I4E574
O	-2	PHE	-	expression tag	UNP I4E574
O	-1	GLN	-	expression tag	UNP I4E574
O	0	GLY	-	expression tag	UNP I4E574
P	-12	HIS	-	expression tag	UNP I4E574
P	-11	HIS	-	expression tag	UNP I4E574
P	-10	HIS	-	expression tag	UNP I4E574
P	-9	HIS	-	expression tag	UNP I4E574
P	-8	HIS	-	expression tag	UNP I4E574
P	-7	HIS	-	expression tag	UNP I4E574
P	-6	GLU	-	expression tag	UNP I4E574
P	-5	ASN	-	expression tag	UNP I4E574
P	-4	LEU	-	expression tag	UNP I4E574
P	-3	TYR	-	expression tag	UNP I4E574
P	-2	PHE	-	expression tag	UNP I4E574
P	-1	GLN	-	expression tag	UNP I4E574
P	0	GLY	-	expression tag	UNP I4E574
Q	-12	HIS	-	expression tag	UNP I4E574
Q	-11	HIS	-	expression tag	UNP I4E574
Q	-10	HIS	-	expression tag	UNP I4E574
Q	-9	HIS	-	expression tag	UNP I4E574
Q	-8	HIS	-	expression tag	UNP I4E574
Q	-7	HIS	-	expression tag	UNP I4E574
Q	-6	GLU	-	expression tag	UNP I4E574
Q	-5	ASN	-	expression tag	UNP I4E574
Q	-4	LEU	-	expression tag	UNP I4E574
Q	-3	TYR	-	expression tag	UNP I4E574
Q	-2	PHE	-	expression tag	UNP I4E574
Q	-1	GLN	-	expression tag	UNP I4E574
Q	0	GLY	-	expression tag	UNP I4E574
R	-12	HIS	-	expression tag	UNP I4E574
R	-11	HIS	-	expression tag	UNP I4E574
R	-10	HIS	-	expression tag	UNP I4E574
R	-9	HIS	-	expression tag	UNP I4E574

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-8	HIS	-	expression tag	UNP I4E574
R	-7	HIS	-	expression tag	UNP I4E574
R	-6	GLU	-	expression tag	UNP I4E574
R	-5	ASN	-	expression tag	UNP I4E574
R	-4	LEU	-	expression tag	UNP I4E574
R	-3	TYR	-	expression tag	UNP I4E574
R	-2	PHE	-	expression tag	UNP I4E574
R	-1	GLN	-	expression tag	UNP I4E574
R	0	GLY	-	expression tag	UNP I4E574
S	-12	HIS	-	expression tag	UNP I4E574
S	-11	HIS	-	expression tag	UNP I4E574
S	-10	HIS	-	expression tag	UNP I4E574
S	-9	HIS	-	expression tag	UNP I4E574
S	-8	HIS	-	expression tag	UNP I4E574
S	-7	HIS	-	expression tag	UNP I4E574
S	-6	GLU	-	expression tag	UNP I4E574
S	-5	ASN	-	expression tag	UNP I4E574
S	-4	LEU	-	expression tag	UNP I4E574
S	-3	TYR	-	expression tag	UNP I4E574
S	-2	PHE	-	expression tag	UNP I4E574
S	-1	GLN	-	expression tag	UNP I4E574
S	0	GLY	-	expression tag	UNP I4E574
T	-12	HIS	-	expression tag	UNP I4E574
T	-11	HIS	-	expression tag	UNP I4E574
T	-10	HIS	-	expression tag	UNP I4E574
T	-9	HIS	-	expression tag	UNP I4E574
T	-8	HIS	-	expression tag	UNP I4E574
T	-7	HIS	-	expression tag	UNP I4E574
T	-6	GLU	-	expression tag	UNP I4E574
T	-5	ASN	-	expression tag	UNP I4E574
T	-4	LEU	-	expression tag	UNP I4E574
T	-3	TYR	-	expression tag	UNP I4E574
T	-2	PHE	-	expression tag	UNP I4E574
T	-1	GLN	-	expression tag	UNP I4E574
T	0	GLY	-	expression tag	UNP I4E574
U	-12	HIS	-	expression tag	UNP I4E574
U	-11	HIS	-	expression tag	UNP I4E574
U	-10	HIS	-	expression tag	UNP I4E574
U	-9	HIS	-	expression tag	UNP I4E574
U	-8	HIS	-	expression tag	UNP I4E574
U	-7	HIS	-	expression tag	UNP I4E574
U	-6	GLU	-	expression tag	UNP I4E574

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Chain	Residue	Modelled	Actual	Comment	Reference
U	-5	ASN	-	expression tag	UNP I4E574
U	-4	LEU	-	expression tag	UNP I4E574
U	-3	TYR	-	expression tag	UNP I4E574
U	-2	PHE	-	expression tag	UNP I4E574
U	-1	GLN	-	expression tag	UNP I4E574
U	0	GLY	-	expression tag	UNP I4E574
V	-12	HIS	-	expression tag	UNP I4E574
V	-11	HIS	-	expression tag	UNP I4E574
V	-10	HIS	-	expression tag	UNP I4E574
V	-9	HIS	-	expression tag	UNP I4E574
V	-8	HIS	-	expression tag	UNP I4E574
V	-7	HIS	-	expression tag	UNP I4E574
V	-6	GLU	-	expression tag	UNP I4E574
V	-5	ASN	-	expression tag	UNP I4E574
V	-4	LEU	-	expression tag	UNP I4E574
V	-3	TYR	-	expression tag	UNP I4E574
V	-2	PHE	-	expression tag	UNP I4E574
V	-1	GLN	-	expression tag	UNP I4E574
V	0	GLY	-	expression tag	UNP I4E574
W	-12	HIS	-	expression tag	UNP I4E574
W	-11	HIS	-	expression tag	UNP I4E574
W	-10	HIS	-	expression tag	UNP I4E574
W	-9	HIS	-	expression tag	UNP I4E574
W	-8	HIS	-	expression tag	UNP I4E574
W	-7	HIS	-	expression tag	UNP I4E574
W	-6	GLU	-	expression tag	UNP I4E574
W	-5	ASN	-	expression tag	UNP I4E574
W	-4	LEU	-	expression tag	UNP I4E574
W	-3	TYR	-	expression tag	UNP I4E574
W	-2	PHE	-	expression tag	UNP I4E574
W	-1	GLN	-	expression tag	UNP I4E574
W	0	GLY	-	expression tag	UNP I4E574
X	-12	HIS	-	expression tag	UNP I4E574
X	-11	HIS	-	expression tag	UNP I4E574
X	-10	HIS	-	expression tag	UNP I4E574
X	-9	HIS	-	expression tag	UNP I4E574
X	-8	HIS	-	expression tag	UNP I4E574
X	-7	HIS	-	expression tag	UNP I4E574
X	-6	GLU	-	expression tag	UNP I4E574
X	-5	ASN	-	expression tag	UNP I4E574
X	-4	LEU	-	expression tag	UNP I4E574
X	-3	TYR	-	expression tag	UNP I4E574

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Chain	Residue	Modelled	Actual	Comment	Reference
X	-2	PHE	-	expression tag	UNP I4E574
X	-1	GLN	-	expression tag	UNP I4E574
X	0	GLY	-	expression tag	UNP I4E574
Y	-12	HIS	-	expression tag	UNP I4E574
Y	-11	HIS	-	expression tag	UNP I4E574
Y	-10	HIS	-	expression tag	UNP I4E574
Y	-9	HIS	-	expression tag	UNP I4E574
Y	-8	HIS	-	expression tag	UNP I4E574
Y	-7	HIS	-	expression tag	UNP I4E574
Y	-6	GLU	-	expression tag	UNP I4E574
Y	-5	ASN	-	expression tag	UNP I4E574
Y	-4	LEU	-	expression tag	UNP I4E574
Y	-3	TYR	-	expression tag	UNP I4E574
Y	-2	PHE	-	expression tag	UNP I4E574
Y	-1	GLN	-	expression tag	UNP I4E574
Y	0	GLY	-	expression tag	UNP I4E574
Z	-12	HIS	-	expression tag	UNP I4E574
Z	-11	HIS	-	expression tag	UNP I4E574
Z	-10	HIS	-	expression tag	UNP I4E574
Z	-9	HIS	-	expression tag	UNP I4E574
Z	-8	HIS	-	expression tag	UNP I4E574
Z	-7	HIS	-	expression tag	UNP I4E574
Z	-6	GLU	-	expression tag	UNP I4E574
Z	-5	ASN	-	expression tag	UNP I4E574
Z	-4	LEU	-	expression tag	UNP I4E574
Z	-3	TYR	-	expression tag	UNP I4E574
Z	-2	PHE	-	expression tag	UNP I4E574
Z	-1	GLN	-	expression tag	UNP I4E574
Z	0	GLY	-	expression tag	UNP I4E574
a	-12	HIS	-	expression tag	UNP I4E574
a	-11	HIS	-	expression tag	UNP I4E574
a	-10	HIS	-	expression tag	UNP I4E574
a	-9	HIS	-	expression tag	UNP I4E574
a	-8	HIS	-	expression tag	UNP I4E574
a	-7	HIS	-	expression tag	UNP I4E574
a	-6	GLU	-	expression tag	UNP I4E574
a	-5	ASN	-	expression tag	UNP I4E574
a	-4	LEU	-	expression tag	UNP I4E574
a	-3	TYR	-	expression tag	UNP I4E574
a	-2	PHE	-	expression tag	UNP I4E574
a	-1	GLN	-	expression tag	UNP I4E574
a	0	GLY	-	expression tag	UNP I4E574

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Chain	Residue	Modelled	Actual	Comment	Reference
b	-12	HIS	-	expression tag	UNP I4E574
b	-11	HIS	-	expression tag	UNP I4E574
b	-10	HIS	-	expression tag	UNP I4E574
b	-9	HIS	-	expression tag	UNP I4E574
b	-8	HIS	-	expression tag	UNP I4E574
b	-7	HIS	-	expression tag	UNP I4E574
b	-6	GLU	-	expression tag	UNP I4E574
b	-5	ASN	-	expression tag	UNP I4E574
b	-4	LEU	-	expression tag	UNP I4E574
b	-3	TYR	-	expression tag	UNP I4E574
b	-2	PHE	-	expression tag	UNP I4E574
b	-1	GLN	-	expression tag	UNP I4E574
b	0	GLY	-	expression tag	UNP I4E574

- Molecule 2 is a protein called Acyldepsipeptide-14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	c	6	Total	C	F	N	O	0	0	0
			48	33	2	6	7			
2	e	6	Total	C	F	N	O	0	0	0
			48	33	2	6	7			
2	f	6	Total	C	F	N	O	0	0	0
			48	33	2	6	7			
2	g	6	Total	C	F	N	O	0	0	0
			48	33	2	6	7			
2	h	6	Total	C	F	N	O	0	0	0
			48	33	2	6	7			
2	i	6	Total	C	F	N	O	0	0	0
			48	33	2	6	7			
2	j	6	Total	C	F	N	O	0	0	0
			48	33	2	6	7			
2	k	6	Total	C	F	N	O	0	0	0
			48	33	2	6	7			
2	l	6	Total	C	F	N	O	0	0	0
			48	33	2	6	7			
2	m	6	Total	C	F	N	O	0	0	0
			48	33	2	6	7			
2	n	6	Total	C	F	N	O	0	0	0
			48	33	2	6	7			
2	o	6	Total	C	F	N	O	0	0	0
			48	33	2	6	7			
2	p	6	Total	C	F	N	O	0	0	0
			48	33	2	6	7			

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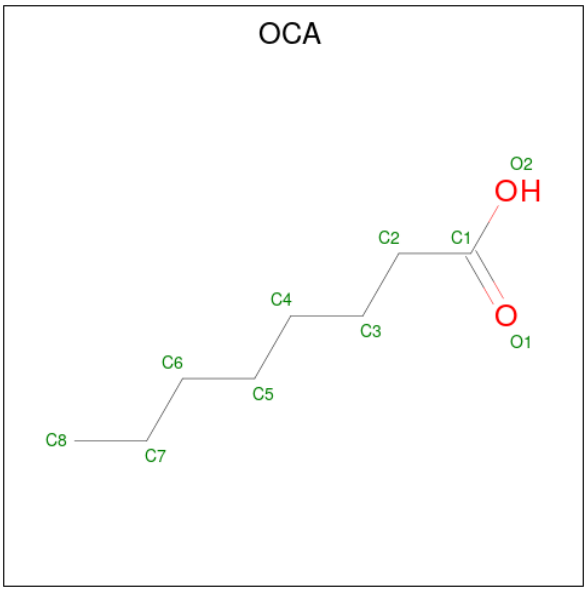
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	q	6	Total	C	F	N	O	0	0	0
			48	33	2	6	7			
2	r	6	Total	C	F	N	O	0	0	0
			48	33	2	6	7			
2	s	6	Total	C	F	N	O	0	0	0
			48	33	2	6	7			
2	t	6	Total	C	F	N	O	0	0	0
			48	33	2	6	7			
2	u	6	Total	C	F	N	O	0	0	0
			48	33	2	6	7			
2	v	6	Total	C	F	N	O	0	0	0
			48	33	2	6	7			
2	w	6	Total	C	F	N	O	0	0	0
			48	33	2	6	7			
2	x	6	Total	C	F	N	O	0	0	0
			48	33	2	6	7			
2	y	6	Total	C	F	N	O	0	0	0
			48	33	2	6	7			
2	z	6	Total	C	F	N	O	0	0	0
			48	33	2	6	7			
2	0	6	Total	C	F	N	O	0	0	0
			48	33	2	6	7			
2	1	6	Total	C	F	N	O	0	0	0
			48	33	2	6	7			
2	2	6	Total	C	F	N	O	0	0	0
			48	33	2	6	7			
2	3	6	Total	C	F	N	O	0	0	0
			48	33	2	6	7			
2	4	6	Total	C	F	N	O	0	0	0
			48	33	2	6	7			

- Molecule 3 is OCTANOIC ACID (CAPRYLIC ACID) (three-letter code: OCA) (formula: $C_8H_{16}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	c	1	Total C O 9 8 1	0	0
3	e	1	Total C O 9 8 1	0	0
3	f	1	Total C O 9 8 1	0	0
3	g	1	Total C O 9 8 1	0	0
3	h	1	Total C O 9 8 1	0	0
3	i	1	Total C O 9 8 1	0	0
3	j	1	Total C O 9 8 1	0	0
3	k	1	Total C O 9 8 1	0	0
3	l	1	Total C O 9 8 1	0	0
3	m	1	Total C O 9 8 1	0	0
3	n	1	Total C O 9 8 1	0	0
3	o	1	Total C O 9 8 1	0	0
3	p	1	Total C O 9 8 1	0	0
3	q	1	Total C O 9 8 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	r	1	Total C O 9 8 1	0	0
3	s	1	Total C O 9 8 1	0	0
3	t	1	Total C O 9 8 1	0	0
3	u	1	Total C O 9 8 1	0	0
3	v	1	Total C O 9 8 1	0	0
3	w	1	Total C O 9 8 1	0	0
3	x	1	Total C O 9 8 1	0	0
3	y	1	Total C O 9 8 1	0	0
3	z	1	Total C O 9 8 1	0	0
3	0	1	Total C O 9 8 1	0	0
3	1	1	Total C O 9 8 1	0	0
3	2	1	Total C O 9 8 1	0	0
3	3	1	Total C O 9 8 1	0	0
3	4	1	Total C O 9 8 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	25	Total O 25 25	0	0
4	B	27	Total O 27 27	0	0
4	C	21	Total O 21 21	0	0
4	D	17	Total O 17 17	0	0
4	E	24	Total O 24 24	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	22	Total O 22 22	0	0
4	G	26	Total O 26 26	0	0
4	H	19	Total O 19 19	0	0
4	I	20	Total O 20 20	0	0
4	J	21	Total O 21 21	0	0
4	K	32	Total O 32 32	0	0
4	L	26	Total O 26 26	0	0
4	M	31	Total O 31 31	0	0
4	N	35	Total O 35 35	0	0
4	O	22	Total O 22 22	0	0
4	P	30	Total O 30 30	0	0
4	Q	22	Total O 22 22	0	0
4	R	27	Total O 27 27	0	0
4	S	17	Total O 17 17	0	0
4	T	24	Total O 24 24	0	0
4	U	25	Total O 25 25	0	0
4	V	29	Total O 29 29	0	0
4	W	24	Total O 24 24	0	0
4	X	24	Total O 24 24	0	0
4	Y	17	Total O 17 17	0	0
4	Z	32	Total O 32 32	0	0

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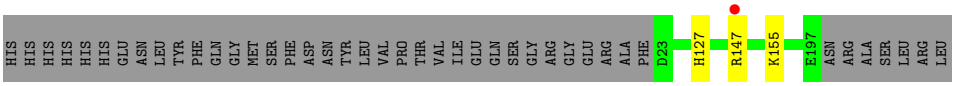
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	a	29	Total O 29 29	0	0
4	b	37	Total O 37 37	0	0
4	0	1	Total O 1 1	0	0

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.

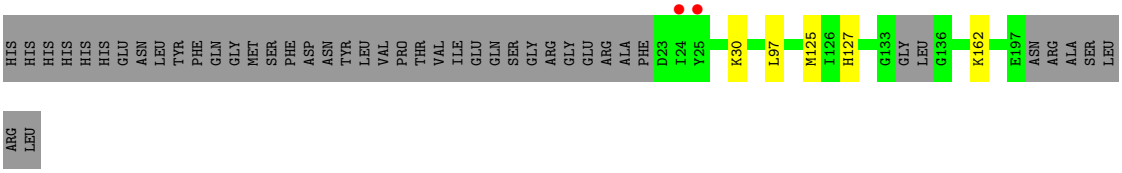
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain A:



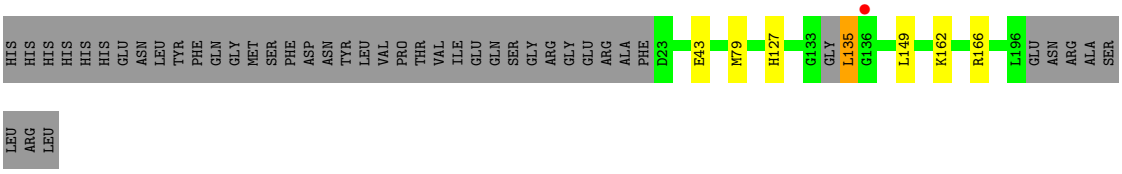
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain B:



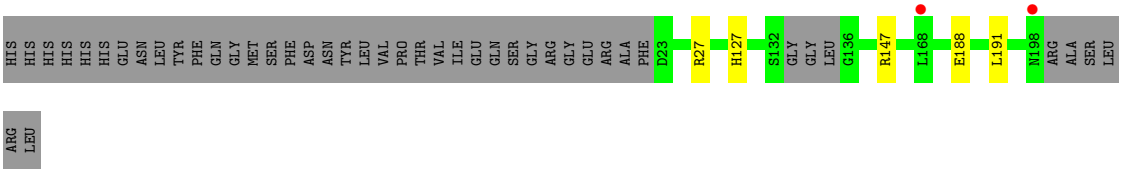
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain C:



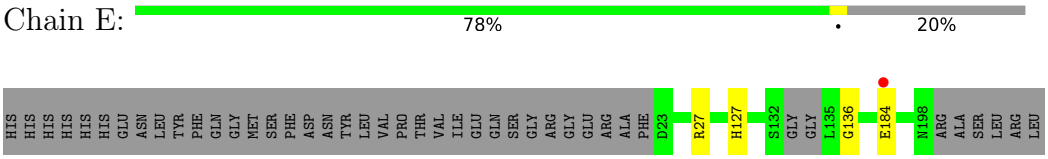
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain D:



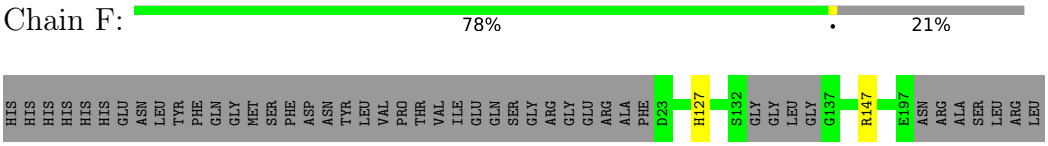
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain E:



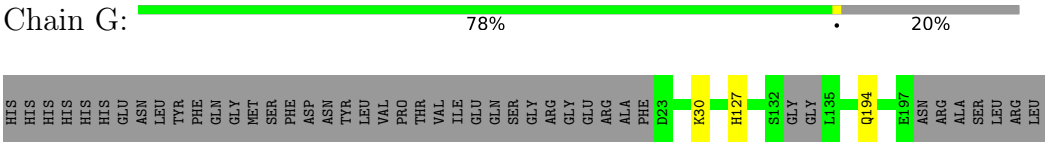
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain F:



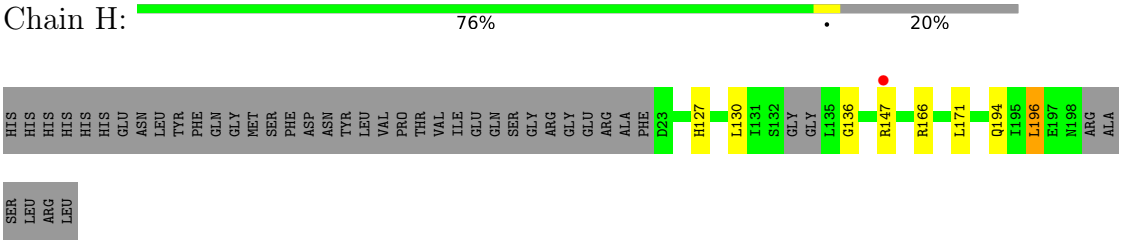
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain G:



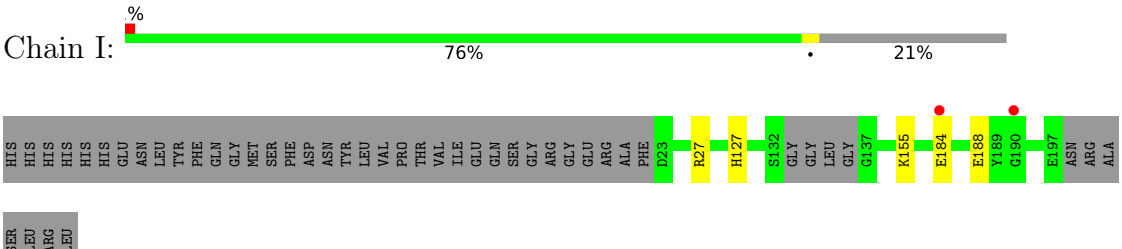
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain H:



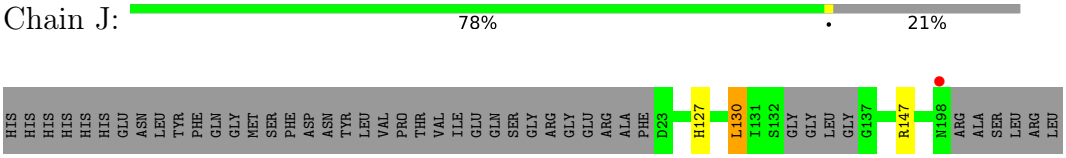
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain I:



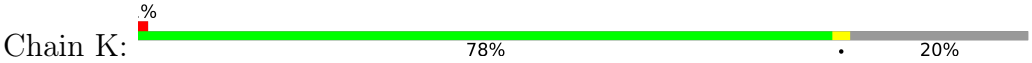
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

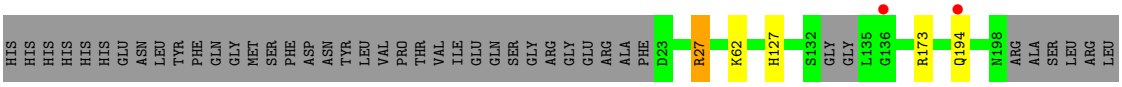
Chain J:



• Molecule 1: ATP-dependent Clp protease proteolytic subunit

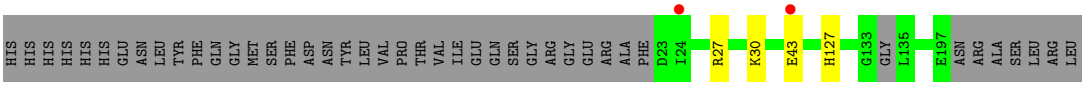
Chain K:





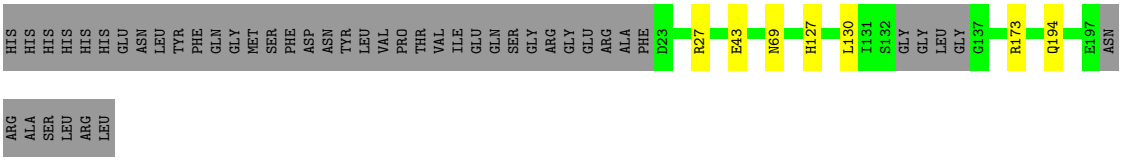
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain L:



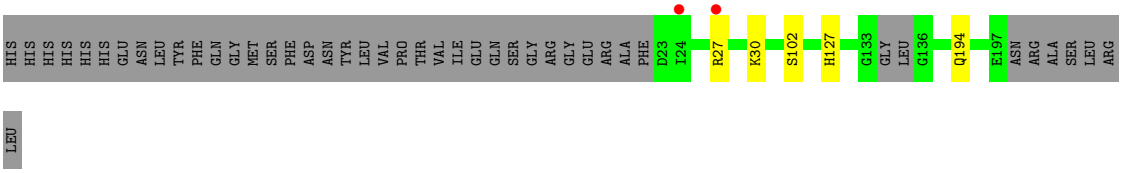
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain M:



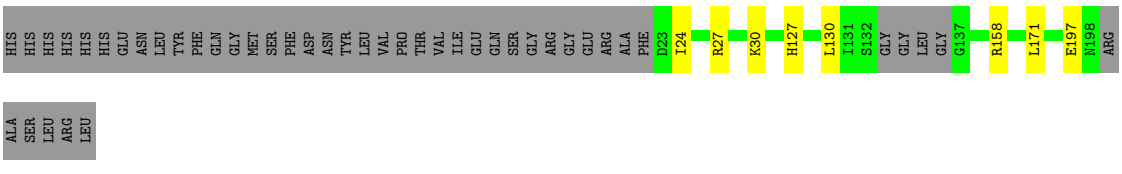
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain N:



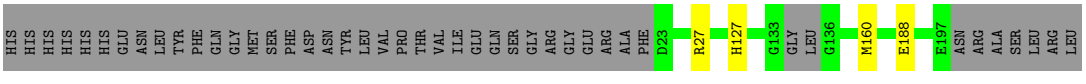
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain O:



• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain P:

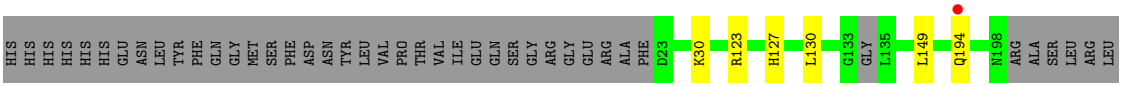


• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Q:

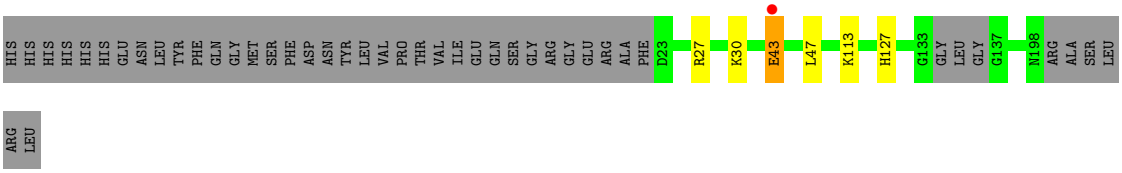
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain R:



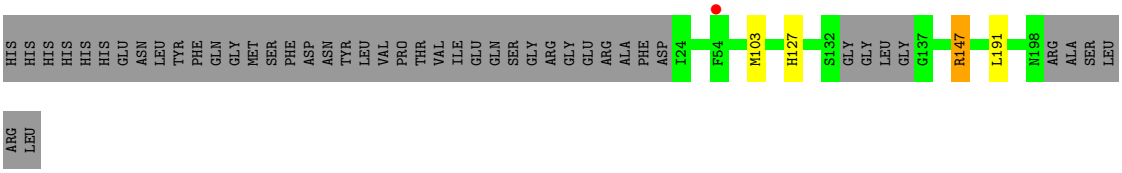
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain S:



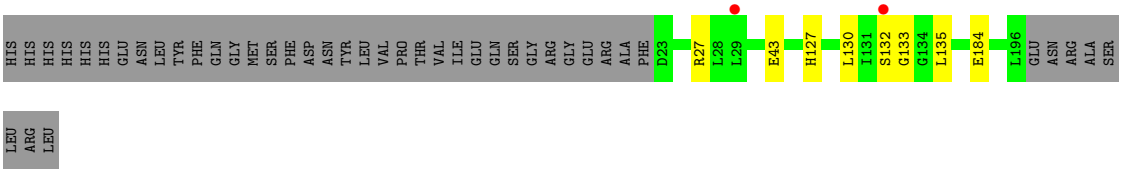
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain T:



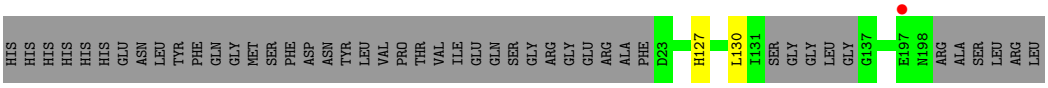
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain U:



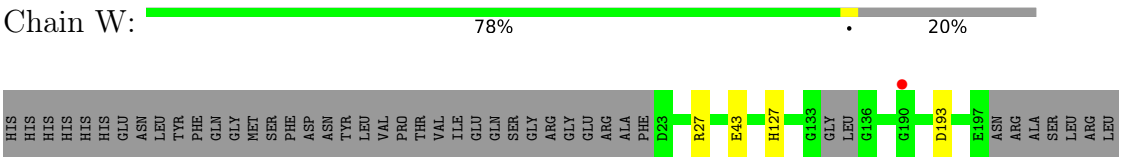
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain V:



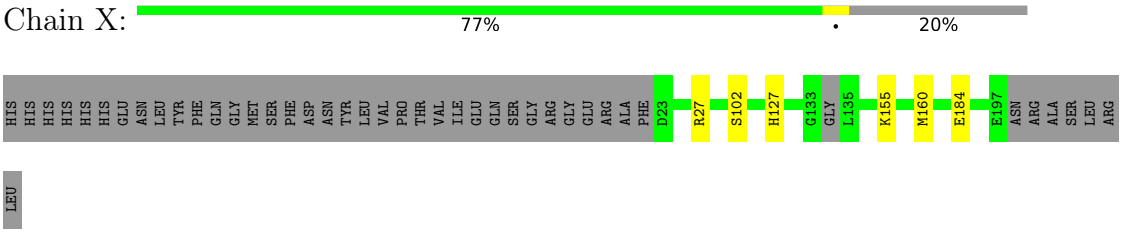
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain W:



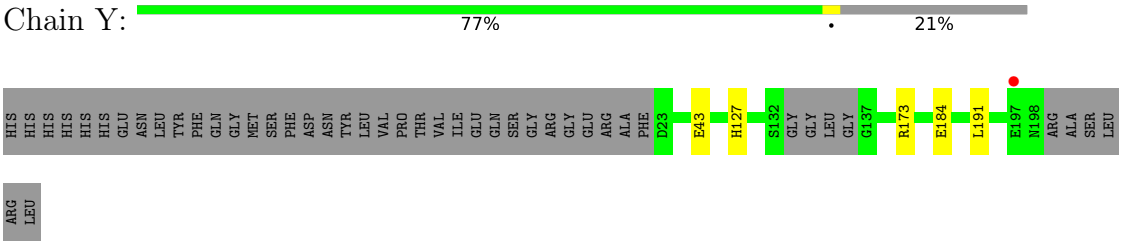
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain X:



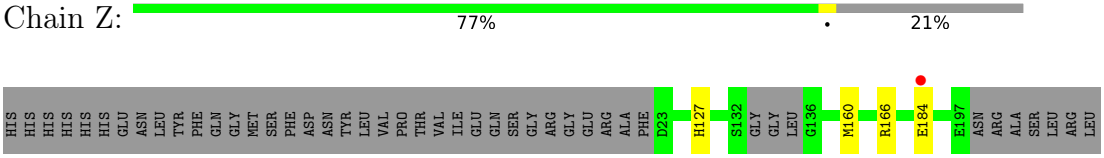
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Y:



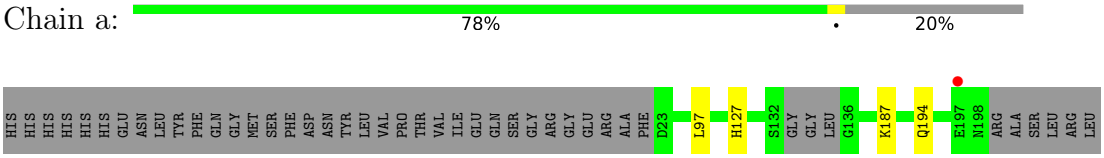
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Z:



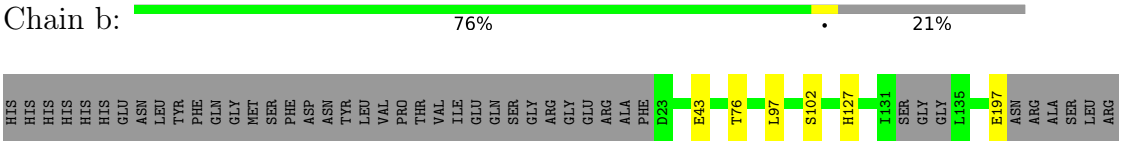
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain a:



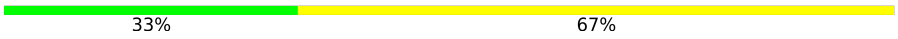
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

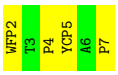
Chain b:



• Molecule 2: Acyldepsipeptide-14

Chain c:





• Molecule 2: Acyldepsipeptide-14

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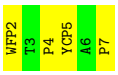
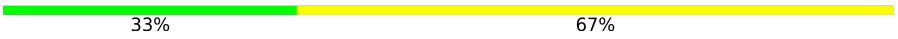
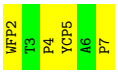


• Molecule 2: Acyldepsipeptide-14

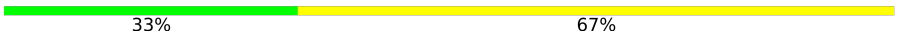
Chain f:

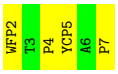




• Molecule 2: Acyldepsipeptide-14

Chain g:





• Molecule 2: Acyldepsipeptide-14

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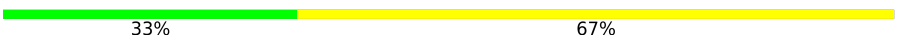
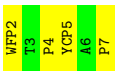
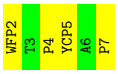




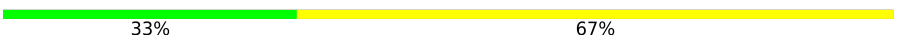
• Molecule 2: Acyldepsipeptide-14

Chain i:



• Molecule 2: Acyldepsipeptide-14

Chain j:



• Molecule 2: Acyldepsipeptide-14

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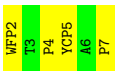

• Molecule 2: Acyldepsipeptide-14

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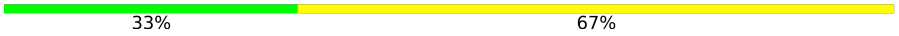

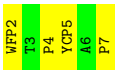

• Molecule 2: Acyldepsipeptide-14

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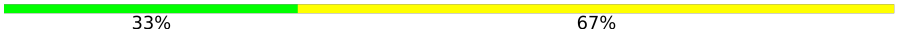

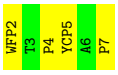

• Molecule 2: Acyldepsipeptide-14

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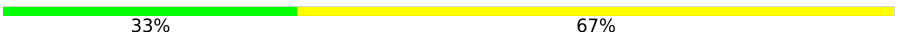

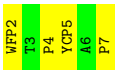

• Molecule 2: Acyldepsipeptide-14

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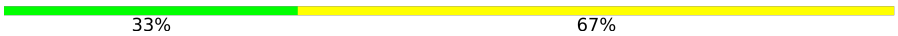
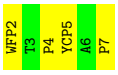
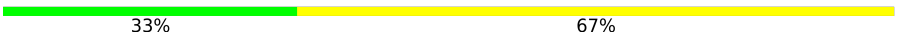
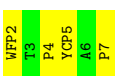




• Molecule 2: Acyldepsipeptide-14

Chain p:





• Molecule 2: Acyldepsipeptide-14

Chain q:

• Molecule 2: Acyldepsipeptide-14

Chain r:

• Molecule 2: Acyldepsipeptide-14

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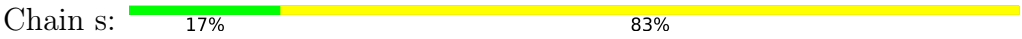

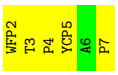

• Molecule 2: Acyldepsipeptide-14

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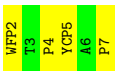

• Molecule 2: Acyldepsipeptide-14

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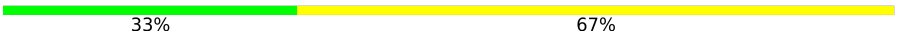
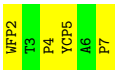
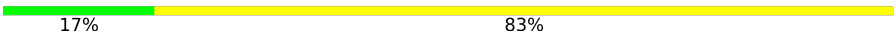
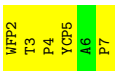




• Molecule 2: Acyldepsipeptide-14

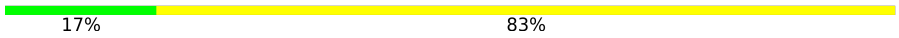
Chain v:

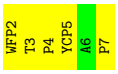




• Molecule 2: Acyldepsipeptide-14

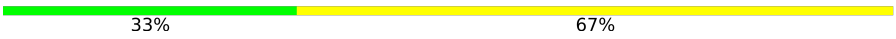
Chain w:

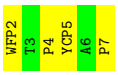




• Molecule 2: Acyldepsipeptide-14

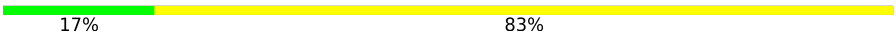
Chain x:

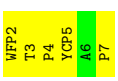




• Molecule 2: Acyldepsipeptide-14

Chain y:



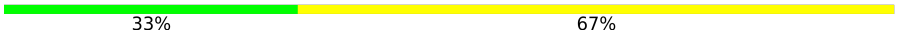


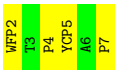
• Molecule 2: Acyldepsipeptide-14

Chain z:

• Molecule 2: Acyldepsipeptide-14

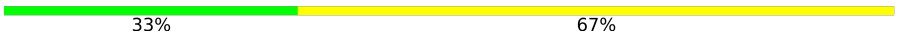
Chain 0:

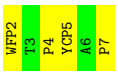




• Molecule 2: Acyldepsipeptide-14

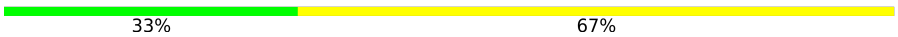
Chain 1:

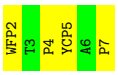




• Molecule 2: Acyldepsipeptide-14

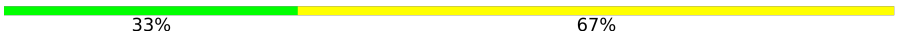
Chain 2:

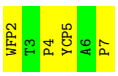




• Molecule 2: Acyldepsipeptide-14

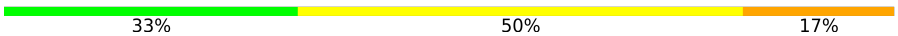
Chain 3:

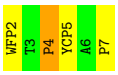




• Molecule 2: Acyldepsipeptide-14

Chain 4:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	117.24Å 195.98Å 139.89Å 90.00° 97.42° 90.00°	Depositor
Resolution (Å)	49.63 – 2.70 49.63 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.63-2.70) 98.6 (49.63-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, R_{free}	0.192 , 0.248 0.192 , 0.248	Depositor DCC
R_{free} test set	1999 reflections (1.19%)	wwPDB-VP
Wilson B-factor (Å^2)	43.2	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 55.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	40076	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.46	0/1379	0.77	2/1856 (0.1%)
1	B	0.54	1/1366 (0.1%)	0.80	5/1837 (0.3%)
1	C	0.45	0/1365	0.76	2/1836 (0.1%)
1	D	0.51	0/1370	0.82	7/1843 (0.4%)
1	E	0.53	1/1378 (0.1%)	0.83	5/1854 (0.3%)
1	F	0.52	1/1358 (0.1%)	0.72	2/1827 (0.1%)
1	G	0.49	0/1370	0.72	2/1843 (0.1%)
1	H	0.49	0/1378	0.80	4/1854 (0.2%)
1	I	0.51	2/1358 (0.1%)	0.76	3/1827 (0.2%)
1	J	0.48	0/1366	0.79	5/1838 (0.3%)
1	K	0.56	0/1378	0.92	6/1854 (0.3%)
1	L	0.51	1/1374 (0.1%)	0.76	4/1848 (0.2%)
1	M	0.52	1/1358 (0.1%)	0.82	5/1827 (0.3%)
1	N	0.45	0/1366	0.80	7/1837 (0.4%)
1	O	0.49	0/1366	0.87	7/1838 (0.4%)
1	P	0.54	1/1366 (0.1%)	0.93	4/1837 (0.2%)
1	Q	0.46	0/1370	0.79	3/1843 (0.2%)
1	R	0.46	0/1382	0.75	3/1859 (0.2%)
1	S	0.53	0/1370	0.82	6/1843 (0.3%)
1	T	0.43	0/1358	0.70	1/1827 (0.1%)
1	U	0.54	2/1370 (0.1%)	0.86	7/1844 (0.4%)
1	V	0.46	0/1360	0.68	0/1830
1	W	0.46	0/1366	0.72	1/1837 (0.1%)
1	X	0.46	0/1374	0.74	4/1848 (0.2%)
1	Y	0.46	1/1366 (0.1%)	0.74	3/1838 (0.2%)
1	Z	0.46	0/1362	0.68	1/1832 (0.1%)
1	a	0.47	0/1370	0.71	4/1843 (0.2%)
1	b	0.53	0/1364	0.76	3/1835 (0.2%)
2	0	4.18	2/11 (18.2%)	1.21	0/12
2	1	4.14	1/11 (9.1%)	1.35	0/12
2	2	4.25	2/11 (18.2%)	1.90	0/12
2	3	4.18	2/11 (18.2%)	1.42	0/12

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	4	4.21	2/11 (18.2%)	1.20	0/12
2	c	4.13	2/11 (18.2%)	1.33	0/12
2	e	4.30	2/11 (18.2%)	1.17	0/12
2	f	4.11	2/11 (18.2%)	1.52	0/12
2	g	4.29	2/11 (18.2%)	1.43	0/12
2	h	4.34	2/11 (18.2%)	1.42	0/12
2	i	4.26	2/11 (18.2%)	1.44	0/12
2	j	4.20	2/11 (18.2%)	1.61	0/12
2	k	4.17	2/11 (18.2%)	1.38	0/12
2	l	4.20	2/11 (18.2%)	1.34	0/12
2	m	4.20	2/11 (18.2%)	2.16	0/12
2	n	4.17	2/11 (18.2%)	1.57	0/12
2	o	4.14	2/11 (18.2%)	1.45	0/12
2	p	4.08	2/11 (18.2%)	1.44	0/12
2	q	4.17	2/11 (18.2%)	1.24	0/12
2	r	4.31	2/11 (18.2%)	1.32	0/12
2	s	4.25	2/11 (18.2%)	1.53	0/12
2	t	4.30	2/11 (18.2%)	1.57	0/12
2	u	4.11	1/11 (9.1%)	2.06	0/12
2	v	4.11	2/11 (18.2%)	1.79	0/12
2	w	4.22	2/11 (18.2%)	1.27	0/12
2	x	4.15	2/11 (18.2%)	1.70	0/12
2	y	4.08	1/11 (9.1%)	1.50	0/12
2	z	4.22	2/11 (18.2%)	1.59	0/12
All	All	0.62	64/38616 (0.2%)	0.79	106/51871 (0.2%)

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	S	0	1
1	W	0	1
All	All	0	2

The worst 5 of 64 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	i	4	PRO	N-CD	-11.16	1.32	1.47
2	h	4	PRO	N-CD	-11.16	1.32	1.47
2	e	4	PRO	N-CD	-11.15	1.32	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	r	4	PRO	N-CD	-11.09	1.32	1.47
2	s	4	PRO	N-CD	-11.02	1.32	1.47

The worst 5 of 106 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	27	ARG	NE-CZ-NH2	16.30	128.45	120.30
1	P	27	ARG	NE-CZ-NH1	-14.57	113.02	120.30
1	K	27	ARG	NE-CZ-NH2	-11.86	114.37	120.30
1	E	27	ARG	CA-CB-CG	11.69	139.13	113.40
1	K	27	ARG	CG-CD-NE	-11.65	87.34	111.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	S	43	GLU	Sidechain
1	W	193	ASP	Peptide

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	173/217 (80%)	168 (97%)	5 (3%)	0	100	100
1	B	169/217 (78%)	166 (98%)	3 (2%)	0	100	100
1	C	169/217 (78%)	166 (98%)	3 (2%)	0	100	100
1	D	169/217 (78%)	165 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	170/217 (78%)	165 (97%)	4 (2%)	1 (1%)	25 50
1	F	167/217 (77%)	165 (99%)	2 (1%)	0	100 100
1	G	169/217 (78%)	165 (98%)	4 (2%)	0	100 100
1	H	170/217 (78%)	165 (97%)	3 (2%)	2 (1%)	13 32
1	I	167/217 (77%)	165 (99%)	2 (1%)	0	100 100
1	J	168/217 (77%)	166 (99%)	2 (1%)	0	100 100
1	K	170/217 (78%)	165 (97%)	5 (3%)	0	100 100
1	L	170/217 (78%)	166 (98%)	4 (2%)	0	100 100
1	M	167/217 (77%)	165 (99%)	2 (1%)	0	100 100
1	N	169/217 (78%)	167 (99%)	2 (1%)	0	100 100
1	O	168/217 (77%)	164 (98%)	3 (2%)	1 (1%)	25 50
1	P	169/217 (78%)	167 (99%)	2 (1%)	0	100 100
1	Q	169/217 (78%)	166 (98%)	3 (2%)	0	100 100
1	R	171/217 (79%)	168 (98%)	3 (2%)	0	100 100
1	S	169/217 (78%)	165 (98%)	4 (2%)	0	100 100
1	T	167/217 (77%)	165 (99%)	2 (1%)	0	100 100
1	U	172/217 (79%)	165 (96%)	5 (3%)	2 (1%)	13 32
1	V	167/217 (77%)	164 (98%)	2 (1%)	1 (1%)	25 50
1	W	169/217 (78%)	167 (99%)	2 (1%)	0	100 100
1	X	170/217 (78%)	165 (97%)	5 (3%)	0	100 100
1	Y	168/217 (77%)	165 (98%)	3 (2%)	0	100 100
1	Z	168/217 (77%)	165 (98%)	3 (2%)	0	100 100
1	a	169/217 (78%)	167 (99%)	2 (1%)	0	100 100
1	b	168/217 (77%)	166 (99%)	2 (1%)	0	100 100
2	0	2/6 (33%)	1 (50%)	1 (50%)	0	100 100
2	1	2/6 (33%)	1 (50%)	1 (50%)	0	100 100
2	2	2/6 (33%)	1 (50%)	1 (50%)	0	100 100
2	3	2/6 (33%)	1 (50%)	1 (50%)	0	100 100
2	4	2/6 (33%)	1 (50%)	1 (50%)	0	100 100
2	c	2/6 (33%)	1 (50%)	1 (50%)	0	100 100
2	e	2/6 (33%)	1 (50%)	1 (50%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	f	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
2	g	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
2	h	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
2	i	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
2	j	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
2	k	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
2	l	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
2	m	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
2	n	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
2	o	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
2	p	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
2	q	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
2	r	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
2	s	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
2	t	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
2	u	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
2	v	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
2	w	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
2	x	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
2	y	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
2	z	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
All	All	4787/6244 (77%)	4666 (98%)	114 (2%)	7 (0%)	51	78

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	136	GLY
1	H	136	GLY
1	H	196	LEU
1	U	132	SER
1	U	133	GLY

5.3.2 Protein sidechains (i)

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	148/185 (80%)	146 (99%)	2 (1%)	67	86
1	B	147/185 (80%)	145 (99%)	2 (1%)	67	86
1	C	147/185 (80%)	141 (96%)	6 (4%)	30	59
1	D	148/185 (80%)	147 (99%)	1 (1%)	84	94
1	E	149/185 (80%)	148 (99%)	1 (1%)	84	94
1	F	147/185 (80%)	146 (99%)	1 (1%)	84	94
1	G	148/185 (80%)	147 (99%)	1 (1%)	84	94
1	H	149/185 (80%)	146 (98%)	3 (2%)	55	81
1	I	147/185 (80%)	145 (99%)	2 (1%)	67	86
1	J	148/185 (80%)	146 (99%)	2 (1%)	67	86
1	K	149/185 (80%)	146 (98%)	3 (2%)	55	81
1	L	148/185 (80%)	146 (99%)	2 (1%)	67	86
1	M	147/185 (80%)	145 (99%)	2 (1%)	67	86
1	N	147/185 (80%)	144 (98%)	3 (2%)	55	81
1	O	148/185 (80%)	146 (99%)	2 (1%)	67	86
1	P	147/185 (80%)	145 (99%)	2 (1%)	67	86
1	Q	148/185 (80%)	145 (98%)	3 (2%)	55	81
1	R	149/185 (80%)	146 (98%)	3 (2%)	55	81
1	S	148/185 (80%)	146 (99%)	2 (1%)	67	86
1	T	147/185 (80%)	143 (97%)	4 (3%)	44	74
1	U	147/185 (80%)	145 (99%)	2 (1%)	67	86
1	V	147/185 (80%)	146 (99%)	1 (1%)	84	94
1	W	147/185 (80%)	145 (99%)	2 (1%)	67	86
1	X	148/185 (80%)	144 (97%)	4 (3%)	44	74
1	Y	148/185 (80%)	146 (99%)	2 (1%)	67	86
1	Z	147/185 (80%)	144 (98%)	3 (2%)	55	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	a	148/185 (80%)	147 (99%)	1 (1%)	84 94
1	b	147/185 (80%)	143 (97%)	4 (3%)	44 74
2	0	1/1 (100%)	1 (100%)	0	100 100
2	1	1/1 (100%)	1 (100%)	0	100 100
2	2	1/1 (100%)	1 (100%)	0	100 100
2	3	1/1 (100%)	1 (100%)	0	100 100
2	4	1/1 (100%)	0	1 (100%)	0 0
2	c	1/1 (100%)	1 (100%)	0	100 100
2	e	1/1 (100%)	1 (100%)	0	100 100
2	f	1/1 (100%)	1 (100%)	0	100 100
2	g	1/1 (100%)	1 (100%)	0	100 100
2	h	1/1 (100%)	1 (100%)	0	100 100
2	i	1/1 (100%)	1 (100%)	0	100 100
2	j	1/1 (100%)	1 (100%)	0	100 100
2	k	1/1 (100%)	1 (100%)	0	100 100
2	l	1/1 (100%)	1 (100%)	0	100 100
2	m	1/1 (100%)	1 (100%)	0	100 100
2	n	1/1 (100%)	1 (100%)	0	100 100
2	o	1/1 (100%)	1 (100%)	0	100 100
2	p	1/1 (100%)	1 (100%)	0	100 100
2	q	1/1 (100%)	1 (100%)	0	100 100
2	r	1/1 (100%)	1 (100%)	0	100 100
2	s	1/1 (100%)	1 (100%)	0	100 100
2	t	1/1 (100%)	1 (100%)	0	100 100
2	u	1/1 (100%)	1 (100%)	0	100 100
2	v	1/1 (100%)	1 (100%)	0	100 100
2	w	1/1 (100%)	1 (100%)	0	100 100
2	x	1/1 (100%)	1 (100%)	0	100 100
2	y	1/1 (100%)	1 (100%)	0	100 100
2	z	1/1 (100%)	1 (100%)	0	100 100
All	All	4163/5208 (80%)	4096 (98%)	67 (2%)	62 85

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Y	191	LEU
1	Z	160	MET
1	b	197	GLU
1	L	30	LYS
1	K	173	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	69	ASN
1	P	59	ASN
1	b	46	ASN
1	Z	127	HIS
1	J	59	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

112 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	ALO	y	3	2	5,6,7	0.78	0	6,7,9	1.35	1 (16%)
2	YCP	w	5	2	6,8,9	1.35	2 (33%)	5,9,11	1.83	3 (60%)
2	WFP	s	2	2,3	12,13,14	1.29	0	14,17,19	1.88	6 (42%)
2	YCP	4	5	2	6,8,9	1.45	2 (33%)	5,9,11	1.33	0
2	WFP	v	2	2,3	12,13,14	1.24	0	14,17,19	1.64	4 (28%)
2	ALO	f	3	2	5,6,7	0.64	0	6,7,9	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	WFP	0	2	2,3	12,13,14	1.06	0	14,17,19	1.74	4 (28%)
2	YCP	e	5	2	6,8,9	1.33	2 (33%)	5,9,11	1.07	0
2	MP8	1	7	2	5,8,9	2.94	2 (40%)	3,10,12	1.13	0
2	WFP	g	2	2,3	12,13,14	1.02	0	14,17,19	1.90	4 (28%)
2	WFP	q	2	2,3	12,13,14	0.94	0	14,17,19	1.79	4 (28%)
2	ALO	e	3	2	5,6,7	0.78	0	6,7,9	0.90	0
2	ALO	m	3	2	5,6,7	0.65	0	6,7,9	0.53	0
2	YCP	2	5	2	6,8,9	1.36	1 (16%)	5,9,11	1.32	0
2	MP8	o	7	2	5,8,9	2.92	2 (40%)	3,10,12	1.40	0
2	ALO	v	3	2	5,6,7	0.56	0	6,7,9	1.15	1 (16%)
2	MP8	w	7	2	5,8,9	2.99	2 (40%)	3,10,12	1.29	0
2	YCP	l	5	2	6,8,9	1.36	2 (33%)	5,9,11	1.36	1 (20%)
2	YCP	3	5	2	6,8,9	1.25	1 (16%)	5,9,11	2.46	3 (60%)
2	YCP	1	5	2	6,8,9	1.25	0	5,9,11	2.68	2 (40%)
2	WFP	w	2	2,3	12,13,14	1.15	1 (8%)	14,17,19	1.60	4 (28%)
2	ALO	t	3	2	5,6,7	0.55	0	6,7,9	0.63	0
2	MP8	h	7	2	5,8,9	2.94	3 (60%)	3,10,12	1.42	1 (33%)
2	ALO	j	3	2	5,6,7	0.59	0	6,7,9	0.85	0
2	ALO	h	3	2	5,6,7	0.80	0	6,7,9	0.74	0
2	ALO	c	3	2	5,6,7	0.83	0	6,7,9	0.93	0
2	WFP	p	2	2,3	12,13,14	1.08	0	14,17,19	1.87	6 (42%)
2	WFP	k	2	2,3	12,13,14	1.03	0	14,17,19	1.94	4 (28%)
2	ALO	p	3	2	5,6,7	0.74	0	6,7,9	0.74	0
2	MP8	i	7	2	5,8,9	3.02	3 (60%)	3,10,12	0.77	0
2	MP8	t	7	2	5,8,9	2.95	3 (60%)	3,10,12	1.49	0
2	ALO	u	3	2	5,6,7	0.64	0	6,7,9	0.87	0
2	MP8	l	7	2	5,8,9	2.91	2 (40%)	3,10,12	1.19	0
2	WFP	x	2	2,3	12,13,14	1.03	0	14,17,19	1.55	3 (21%)
2	WFP	y	2	2,3	12,13,14	0.97	0	14,17,19	1.79	5 (35%)
2	WFP	r	2	2,3	12,13,14	1.21	0	14,17,19	1.72	3 (21%)
2	MP8	n	7	2	5,8,9	2.88	2 (40%)	3,10,12	1.43	0
2	MP8	x	7	2	5,8,9	2.88	2 (40%)	3,10,12	1.30	0
2	MP8	2	7	2	5,8,9	2.91	2 (40%)	3,10,12	1.42	1 (33%)
2	YCP	o	5	2	6,8,9	1.31	1 (16%)	5,9,11	2.03	3 (60%)
2	ALO	o	3	2	5,6,7	0.56	0	6,7,9	0.67	0
2	YCP	f	5	2	6,8,9	1.30	1 (16%)	5,9,11	1.30	1 (20%)
2	ALO	0	3	2	5,6,7	0.67	0	6,7,9	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	WFP	4	2	2,3	12,13,14	1.01	0	14,17,19	1.82	5 (35%)
2	MP8	f	7	2	5,8,9	2.97	3 (60%)	3,10,12	1.38	0
2	WFP	e	2	2,3	12,13,14	1.07	0	14,17,19	1.95	5 (35%)
2	ALO	g	3	2	5,6,7	0.67	0	6,7,9	1.21	0
2	MP8	y	7	2	5,8,9	2.92	3 (60%)	3,10,12	1.16	0
2	YCP	j	5	2	6,8,9	1.41	2 (33%)	5,9,11	1.55	1 (20%)
2	YCP	y	5	2	6,8,9	1.41	1 (16%)	5,9,11	1.12	0
2	MP8	z	7	2	5,8,9	2.91	2 (40%)	3,10,12	1.43	1 (33%)
2	MP8	m	7	2	5,8,9	2.91	2 (40%)	3,10,12	1.44	0
2	ALO	k	3	2	5,6,7	0.64	0	6,7,9	0.95	0
2	YCP	s	5	2	6,8,9	1.47	2 (33%)	5,9,11	1.44	1 (20%)
2	YCP	h	5	2	6,8,9	1.47	2 (33%)	5,9,11	1.48	1 (20%)
2	MP8	e	7	2	5,8,9	3.01	3 (60%)	3,10,12	1.52	0
2	WFP	2	2	2,3	12,13,14	1.12	0	14,17,19	1.77	4 (28%)
2	MP8	c	7	2	5,8,9	2.84	3 (60%)	3,10,12	1.25	0
2	ALO	i	3	2	5,6,7	0.68	0	6,7,9	0.58	0
2	ALO	w	3	2	5,6,7	0.69	0	6,7,9	1.09	1 (16%)
2	WFP	3	2	2,3	12,13,14	1.01	0	14,17,19	1.62	4 (28%)
2	YCP	p	5	2	6,8,9	1.46	2 (33%)	5,9,11	1.76	2 (40%)
2	MP8	0	7	2	5,8,9	2.91	3 (60%)	3,10,12	1.33	0
2	YCP	c	5	2	6,8,9	1.35	1 (16%)	5,9,11	1.61	2 (40%)
2	YCP	g	5	2	6,8,9	1.42	2 (33%)	5,9,11	1.34	0
2	WFP	n	2	2,3	12,13,14	1.08	0	14,17,19	1.75	5 (35%)
2	YCP	v	5	2	6,8,9	1.52	2 (33%)	5,9,11	1.29	1 (20%)
2	YCP	0	5	2	6,8,9	1.54	2 (33%)	5,9,11	1.30	1 (20%)
2	ALO	2	3	2	5,6,7	0.62	0	6,7,9	0.67	0
2	MP8	3	7	2	5,8,9	2.84	3 (60%)	3,10,12	1.49	0
2	MP8	s	7	2	5,8,9	2.89	3 (60%)	3,10,12	1.20	0
2	ALO	s	3	2	5,6,7	0.66	0	6,7,9	0.94	1 (16%)
2	WFP	1	2	2,3	12,13,14	1.02	0	14,17,19	1.84	4 (28%)
2	MP8	q	7	2	5,8,9	2.89	2 (40%)	3,10,12	1.63	1 (33%)
2	MP8	p	7	2	5,8,9	2.87	3 (60%)	3,10,12	0.91	0
2	ALO	n	3	2	5,6,7	0.59	0	6,7,9	0.60	0
2	ALO	x	3	2	5,6,7	0.53	0	6,7,9	0.86	0
2	YCP	m	5	2	6,8,9	1.42	2 (33%)	5,9,11	1.53	1 (20%)
2	ALO	r	3	2	5,6,7	0.71	0	6,7,9	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	YCP	k	5	2	6,8,9	1.42	2 (33%)	5,9,11	1.49	1 (20%)
2	ALO	z	3	2	5,6,7	0.79	0	6,7,9	0.73	0
2	MP8	4	7	2	5,8,9	2.90	2 (40%)	3,10,12	1.09	0
2	YCP	i	5	2	6,8,9	1.28	1 (16%)	5,9,11	1.41	1 (20%)
2	MP8	g	7	2	5,8,9	3.03	3 (60%)	3,10,12	1.05	0
2	YCP	u	5	2	6,8,9	1.48	2 (33%)	5,9,11	0.87	0
2	WFP	o	2	2,3	12,13,14	1.07	0	14,17,19	1.79	4 (28%)
2	WFP	f	2	2,3	12,13,14	0.99	0	14,17,19	1.85	4 (28%)
2	WFP	u	2	2,3	12,13,14	1.07	1 (8%)	14,17,19	1.87	5 (35%)
2	ALO	3	3	2	5,6,7	0.68	0	6,7,9	0.42	0
2	YCP	t	5	2	6,8,9	1.44	2 (33%)	5,9,11	1.38	1 (20%)
2	ALO	4	3	2	5,6,7	0.68	0	6,7,9	0.91	0
2	ALO	q	3	2	5,6,7	0.67	0	6,7,9	0.58	0
2	WFP	m	2	2,3	12,13,14	1.15	0	14,17,19	2.06	4 (28%)
2	MP8	k	7	2	5,8,9	2.90	2 (40%)	3,10,12	1.37	0
2	WFP	i	2	2,3	12,13,14	1.06	0	14,17,19	2.19	4 (28%)
2	MP8	u	7	2	5,8,9	2.96	3 (60%)	3,10,12	1.24	0
2	YCP	r	5	2	6,8,9	1.34	1 (16%)	5,9,11	1.48	1 (20%)
2	WFP	z	2	2,3	12,13,14	1.20	1 (8%)	14,17,19	2.12	5 (35%)
2	ALO	l	3	2	5,6,7	0.66	0	6,7,9	0.75	0
2	MP8	r	7	2	5,8,9	3.07	3 (60%)	3,10,12	1.33	0
2	WFP	l	2	2,3	12,13,14	1.09	1 (8%)	14,17,19	1.73	4 (28%)
2	MP8	v	7	2	5,8,9	3.12	3 (60%)	3,10,12	1.18	0
2	ALO	1	3	2	5,6,7	0.72	0	6,7,9	1.03	0
2	WFP	t	2	2,3	12,13,14	1.09	0	14,17,19	1.70	2 (14%)
2	YCP	q	5	2	6,8,9	1.33	1 (16%)	5,9,11	1.41	1 (20%)
2	WFP	j	2	2,3	12,13,14	1.13	1 (8%)	14,17,19	1.51	4 (28%)
2	YCP	n	5	2	6,8,9	1.37	2 (33%)	5,9,11	1.73	1 (20%)
2	YCP	x	5	2	6,8,9	1.42	1 (16%)	5,9,11	2.32	3 (60%)
2	WFP	h	2	2,3	12,13,14	1.08	0	14,17,19	1.58	3 (21%)
2	MP8	j	7	2	5,8,9	2.91	2 (40%)	3,10,12	1.69	1 (33%)
2	WFP	c	2	2,3	12,13,14	1.19	0	14,17,19	1.76	2 (14%)
2	YCP	z	5	2	6,8,9	1.39	1 (16%)	5,9,11	1.21	1 (20%)

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	ALO	y	3	2	-	1/5/6/8	-
2	YCP	w	5	2	-	0/1/10/12	0/1/1/1
2	WFP	s	2	2,3	-	0/5/6/8	0/1/1/1
2	YCP	4	5	2	-	0/1/10/12	1/1/1/1
2	WFP	v	2	2,3	-	0/5/6/8	0/1/1/1
2	ALO	f	3	2	-	1/5/6/8	-
2	WFP	0	2	2,3	-	0/5/6/8	0/1/1/1
2	YCP	e	5	2	-	0/1/10/12	1/1/1/1
2	MP8	1	7	2	-	0/0/11/13	0/1/1/1
2	WFP	g	2	2,3	-	0/5/6/8	0/1/1/1
2	WFP	q	2	2,3	-	0/5/6/8	0/1/1/1
2	ALO	e	3	2	-	1/5/6/8	-
2	ALO	m	3	2	-	1/5/6/8	-
2	YCP	2	5	2	-	1/1/10/12	0/1/1/1
2	MP8	o	7	2	-	0/0/11/13	0/1/1/1
2	ALO	v	3	2	-	1/5/6/8	-
2	MP8	w	7	2	-	0/0/11/13	0/1/1/1
2	YCP	l	5	2	-	0/1/10/12	1/1/1/1
2	YCP	3	5	2	-	0/1/10/12	0/1/1/1
2	YCP	1	5	2	-	0/1/10/12	0/1/1/1
2	WFP	w	2	2,3	-	0/5/6/8	0/1/1/1
2	ALO	t	3	2	-	1/5/6/8	-
2	MP8	h	7	2	-	0/0/11/13	0/1/1/1
2	ALO	j	3	2	-	1/5/6/8	-
2	ALO	h	3	2	-	1/5/6/8	-
2	ALO	c	3	2	-	1/5/6/8	-
2	WFP	p	2	2,3	-	0/5/6/8	0/1/1/1
2	WFP	k	2	2,3	-	0/5/6/8	0/1/1/1
2	ALO	p	3	2	-	1/5/6/8	-
2	MP8	i	7	2	-	0/0/11/13	0/1/1/1
2	MP8	t	7	2	-	0/0/11/13	0/1/1/1
2	ALO	u	3	2	-	1/5/6/8	-
2	MP8	l	7	2	-	0/0/11/13	0/1/1/1
2	WFP	x	2	2,3	-	0/5/6/8	0/1/1/1
2	WFP	y	2	2,3	-	0/5/6/8	0/1/1/1
2	WFP	r	2	2,3	-	0/5/6/8	0/1/1/1
2	MP8	n	7	2	-	0/0/11/13	0/1/1/1
2	MP8	x	7	2	-	0/0/11/13	0/1/1/1
2	MP8	2	7	2	-	0/0/11/13	0/1/1/1
2	YCP	o	5	2	-	0/1/10/12	1/1/1/1
2	ALO	o	3	2	-	1/5/6/8	-
2	YCP	f	5	2	-	0/1/10/12	1/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ALO	0	3	2	-	1/5/6/8	-
2	WFP	4	2	2,3	-	0/5/6/8	0/1/1/1
2	MP8	f	7	2	-	0/0/11/13	0/1/1/1
2	WFP	e	2	2,3	-	0/5/6/8	0/1/1/1
2	ALO	g	3	2	-	1/5/6/8	-
2	MP8	y	7	2	-	0/0/11/13	0/1/1/1
2	YCP	j	5	2	-	1/1/10/12	1/1/1/1
2	YCP	y	5	2	-	1/1/10/12	1/1/1/1
2	MP8	z	7	2	-	0/0/11/13	0/1/1/1
2	MP8	m	7	2	-	0/0/11/13	0/1/1/1
2	ALO	k	3	2	-	1/5/6/8	-
2	YCP	s	5	2	-	0/1/10/12	1/1/1/1
2	YCP	h	5	2	-	1/1/10/12	1/1/1/1
2	MP8	e	7	2	-	0/0/11/13	0/1/1/1
2	WFP	2	2	2,3	-	0/5/6/8	0/1/1/1
2	MP8	c	7	2	-	0/0/11/13	0/1/1/1
2	ALO	i	3	2	-	1/5/6/8	-
2	ALO	w	3	2	-	1/5/6/8	-
2	WFP	3	2	2,3	-	0/5/6/8	0/1/1/1
2	YCP	p	5	2	-	1/1/10/12	1/1/1/1
2	MP8	0	7	2	-	0/0/11/13	0/1/1/1
2	YCP	c	5	2	-	1/1/10/12	1/1/1/1
2	YCP	g	5	2	-	0/1/10/12	1/1/1/1
2	WFP	n	2	2,3	-	0/5/6/8	0/1/1/1
2	YCP	v	5	2	-	1/1/10/12	1/1/1/1
2	YCP	0	5	2	-	0/1/10/12	1/1/1/1
2	ALO	2	3	2	-	1/5/6/8	-
2	MP8	3	7	2	-	0/0/11/13	0/1/1/1
2	MP8	s	7	2	-	0/0/11/13	0/1/1/1
2	ALO	s	3	2	-	1/5/6/8	-
2	WFP	1	2	2,3	-	0/5/6/8	0/1/1/1
2	MP8	q	7	2	-	0/0/11/13	0/1/1/1
2	MP8	p	7	2	-	0/0/11/13	0/1/1/1
2	ALO	n	3	2	-	1/5/6/8	-
2	ALO	x	3	2	-	1/5/6/8	-
2	YCP	m	5	2	-	1/1/10/12	1/1/1/1
2	ALO	r	3	2	-	1/5/6/8	-
2	YCP	k	5	2	-	0/1/10/12	1/1/1/1
2	ALO	z	3	2	-	1/5/6/8	-
2	MP8	4	7	2	-	0/0/11/13	0/1/1/1
2	YCP	i	5	2	-	0/1/10/12	1/1/1/1
2	MP8	g	7	2	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	YCP	u	5	2	-	1/1/10/12	1/1/1/1
2	WFP	o	2	2,3	-	0/5/6/8	0/1/1/1
2	WFP	f	2	2,3	-	0/5/6/8	0/1/1/1
2	WFP	u	2	2,3	-	0/5/6/8	0/1/1/1
2	ALO	3	3	2	-	1/5/6/8	-
2	YCP	t	5	2	-	1/1/10/12	1/1/1/1
2	ALO	4	3	2	-	1/5/6/8	-
2	ALO	q	3	2	-	1/5/6/8	-
2	WFP	m	2	2,3	-	0/5/6/8	0/1/1/1
2	MP8	k	7	2	-	0/0/11/13	0/1/1/1
2	WFP	i	2	2,3	-	0/5/6/8	0/1/1/1
2	MP8	u	7	2	-	0/0/11/13	0/1/1/1
2	YCP	r	5	2	-	0/1/10/12	1/1/1/1
2	WFP	z	2	2,3	-	0/5/6/8	0/1/1/1
2	ALO	l	3	2	-	1/5/6/8	-
2	MP8	r	7	2	-	0/0/11/13	0/1/1/1
2	WFP	l	2	2,3	-	0/5/6/8	0/1/1/1
2	MP8	v	7	2	-	0/0/11/13	0/1/1/1
2	ALO	1	3	2	-	1/5/6/8	-
2	WFP	t	2	2,3	-	0/5/6/8	0/1/1/1
2	YCP	q	5	2	-	0/1/10/12	1/1/1/1
2	WFP	j	2	2,3	-	0/5/6/8	0/1/1/1
2	YCP	n	5	2	-	1/1/10/12	1/1/1/1
2	YCP	x	5	2	-	0/1/10/12	0/1/1/1
2	WFP	h	2	2,3	-	0/5/6/8	0/1/1/1
2	MP8	j	7	2	-	0/0/11/13	0/1/1/1
2	WFP	c	2	2,3	-	0/5/6/8	0/1/1/1
2	YCP	z	5	2	-	1/1/10/12	1/1/1/1

The worst 5 of 119 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	u	7	MP8	CD-N	5.68	1.67	1.47
2	e	7	MP8	CD-N	5.66	1.67	1.47
2	r	7	MP8	CD-N	5.66	1.67	1.47
2	1	7	MP8	CD-N	5.65	1.67	1.47
2	g	7	MP8	CD-N	5.65	1.67	1.47

The worst 5 of 157 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	m	2	WFP	CG-CB-CA	-4.93	104.12	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	e	2	WFP	CG-CB-CA	-4.78	104.42	114.10
2	i	2	WFP	CG-CB-CA	-4.74	104.51	114.10
2	g	2	WFP	CG-CB-CA	-4.73	104.53	114.10
2	z	2	WFP	CG-CB-CA	-4.72	104.53	114.10

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	e	3	ALO	O-C-CA-CB
2	f	3	ALO	O-C-CA-CB
2	g	3	ALO	O-C-CA-CB
2	h	3	ALO	O-C-CA-CB
2	i	3	ALO	O-C-CA-CB

5 of 23 ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	t	5	YCP	CA-CB-CD-CE-CG-N
2	o	5	YCP	CA-CB-CD-CE-CG-N
2	z	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

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

28 ligands 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	$\#\|Z\|>2$
3	OCA	k	101	2	8,8,9	1.79	2 (25%)	7,7,9	0.89	0
3	OCA	l	101	2	8,8,9	1.83	2 (25%)	7,7,9	0.84	0
3	OCA	v	101	2	8,8,9	1.70	2 (25%)	7,7,9	1.01	0
3	OCA	s	101	2	8,8,9	1.89	2 (25%)	7,7,9	0.74	0
3	OCA	n	101	2	8,8,9	1.70	2 (25%)	7,7,9	0.99	0
3	OCA	2	101	2	8,8,9	1.74	2 (25%)	7,7,9	0.91	0
3	OCA	r	101	2	8,8,9	1.73	2 (25%)	7,7,9	1.02	0
3	OCA	y	101	2	8,8,9	1.75	2 (25%)	7,7,9	1.00	0
3	OCA	u	101	2	8,8,9	1.81	2 (25%)	7,7,9	0.88	0
3	OCA	w	101	2	8,8,9	1.72	2 (25%)	7,7,9	1.05	0
3	OCA	t	101	2	8,8,9	1.76	2 (25%)	7,7,9	1.06	0
3	OCA	j	101	2	8,8,9	1.67	2 (25%)	7,7,9	1.11	0
3	OCA	h	101	2	8,8,9	1.76	2 (25%)	7,7,9	0.90	0
3	OCA	m	101	2	8,8,9	1.76	2 (25%)	7,7,9	1.01	0
3	OCA	p	101	2	8,8,9	1.74	2 (25%)	7,7,9	0.90	0
3	OCA	4	101	2	8,8,9	1.69	2 (25%)	7,7,9	1.08	0
3	OCA	i	101	2	8,8,9	1.71	2 (25%)	7,7,9	0.93	0
3	OCA	e	101	2	8,8,9	1.72	2 (25%)	7,7,9	0.95	0
3	OCA	z	101	2	8,8,9	1.72	2 (25%)	7,7,9	1.02	0
3	OCA	f	101	2	8,8,9	1.68	2 (25%)	7,7,9	0.92	0
3	OCA	o	101	2	8,8,9	1.73	2 (25%)	7,7,9	1.11	0
3	OCA	3	101	2	8,8,9	1.77	2 (25%)	7,7,9	0.92	0
3	OCA	1	101	2	8,8,9	1.71	2 (25%)	7,7,9	1.05	0
3	OCA	g	101	2	8,8,9	1.75	2 (25%)	7,7,9	0.94	0
3	OCA	c	101	2	8,8,9	1.75	2 (25%)	7,7,9	0.83	0
3	OCA	q	101	2	8,8,9	1.75	2 (25%)	7,7,9	0.91	0
3	OCA	x	101	2	8,8,9	1.66	2 (25%)	7,7,9	1.08	0
3	OCA	0	101	2	8,8,9	1.72	2 (25%)	7,7,9	1.10	0

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
3	OCA	k	101	2	-	1/5/6/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OCA	l	101	2	-	2/5/6/7	-
3	OCA	v	101	2	-	1/5/6/7	-
3	OCA	s	101	2	-	2/5/6/7	-
3	OCA	n	101	2	-	2/5/6/7	-
3	OCA	2	101	2	-	2/5/6/7	-
3	OCA	r	101	2	-	2/5/6/7	-
3	OCA	y	101	2	-	1/5/6/7	-
3	OCA	u	101	2	-	1/5/6/7	-
3	OCA	w	101	2	-	3/5/6/7	-
3	OCA	t	101	2	-	2/5/6/7	-
3	OCA	j	101	2	-	2/5/6/7	-
3	OCA	h	101	2	-	2/5/6/7	-
3	OCA	m	101	2	-	1/5/6/7	-
3	OCA	p	101	2	-	1/5/6/7	-
3	OCA	4	101	2	-	2/5/6/7	-
3	OCA	i	101	2	-	1/5/6/7	-
3	OCA	e	101	2	-	2/5/6/7	-
3	OCA	z	101	2	-	1/5/6/7	-
3	OCA	f	101	2	-	2/5/6/7	-
3	OCA	o	101	2	-	2/5/6/7	-
3	OCA	3	101	2	-	2/5/6/7	-
3	OCA	1	101	2	-	0/5/6/7	-
3	OCA	g	101	2	-	2/5/6/7	-
3	OCA	c	101	2	-	1/5/6/7	-
3	OCA	q	101	2	-	2/5/6/7	-
3	OCA	x	101	2	-	1/5/6/7	-
3	OCA	0	101	2	-	1/5/6/7	-

The worst 5 of 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	s	101	OCA	C3-C2	-4.17	1.35	1.52
3	u	101	OCA	C3-C2	-3.96	1.36	1.52
3	l	101	OCA	C3-C2	-3.96	1.36	1.52
3	k	101	OCA	C3-C2	-3.83	1.37	1.52
3	3	101	OCA	C3-C2	-3.81	1.37	1.52

There are no bond angle outliers.

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	u	101	OCA	C4-C5-C6-C7
3	x	101	OCA	C4-C5-C6-C7
3	i	101	OCA	C4-C5-C6-C7
3	s	101	OCA	C4-C5-C6-C7
3	t	101	OCA	C4-C5-C6-C7

There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} 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	175/217 (80%)	0.17	1 (0%) 89 91	29, 39, 60, 74	0
1	B	173/217 (79%)	0.16	2 (1%) 79 80	30, 38, 60, 72	0
1	C	173/217 (79%)	0.19	1 (0%) 89 91	32, 42, 60, 80	0
1	D	173/217 (79%)	0.21	2 (1%) 79 80	32, 43, 63, 76	0
1	E	174/217 (80%)	0.15	1 (0%) 89 91	32, 41, 59, 79	0
1	F	171/217 (78%)	0.15	0 100 100	31, 37, 53, 76	0
1	G	173/217 (79%)	0.05	0 100 100	30, 39, 57, 69	0
1	H	174/217 (80%)	0.17	1 (0%) 89 91	32, 42, 59, 70	0
1	I	171/217 (78%)	0.20	2 (1%) 79 80	34, 43, 62, 76	0
1	J	172/217 (79%)	0.19	1 (0%) 89 91	33, 42, 60, 76	0
1	K	174/217 (80%)	0.16	2 (1%) 80 82	32, 39, 61, 72	0
1	L	174/217 (80%)	0.09	2 (1%) 80 82	29, 37, 57, 79	0
1	M	171/217 (78%)	0.12	0 100 100	27, 37, 56, 76	0
1	N	173/217 (79%)	0.10	2 (1%) 79 80	31, 38, 55, 68	0
1	O	172/217 (79%)	0.13	0 100 100	30, 41, 64, 90	0
1	P	173/217 (79%)	0.04	0 100 100	27, 37, 59, 75	0
1	Q	173/217 (79%)	0.14	0 100 100	30, 39, 58, 70	0
1	R	175/217 (80%)	0.14	1 (0%) 89 91	32, 40, 59, 69	0
1	S	173/217 (79%)	0.23	1 (0%) 89 91	32, 42, 65, 77	0
1	T	171/217 (78%)	0.20	1 (0%) 89 91	35, 46, 61, 72	0
1	U	174/217 (80%)	0.20	2 (1%) 80 82	30, 42, 63, 79	0
1	V	171/217 (78%)	0.17	1 (0%) 89 91	28, 36, 53, 69	0
1	W	173/217 (79%)	0.16	1 (0%) 89 91	30, 38, 56, 69	0
1	X	174/217 (80%)	0.13	0 100 100	31, 40, 59, 76	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	Y	172/217 (79%)	0.09	1 (0%)	89	91	28, 39, 56, 80	0
1	Z	172/217 (79%)	0.10	1 (0%)	89	91	28, 37, 56, 66	0
1	a	173/217 (79%)	0.15	1 (0%)	89	91	28, 38, 55, 72	0
1	b	172/217 (79%)	0.05	0	100	100	30, 36, 49, 70	0
2	0	2/6 (33%)	0.25	0	100	100	41, 41, 41, 45	0
2	1	2/6 (33%)	0.01	0	100	100	40, 40, 40, 42	0
2	2	2/6 (33%)	0.57	0	100	100	41, 41, 41, 45	0
2	3	2/6 (33%)	0.43	0	100	100	37, 37, 37, 41	0
2	4	2/6 (33%)	0.08	0	100	100	39, 39, 39, 41	0
2	c	2/6 (33%)	0.22	0	100	100	45, 45, 45, 50	0
2	e	2/6 (33%)	-0.16	0	100	100	45, 45, 45, 48	0
2	f	2/6 (33%)	0.14	0	100	100	51, 51, 51, 52	0
2	g	2/6 (33%)	0.03	0	100	100	47, 47, 47, 47	0
2	h	2/6 (33%)	0.52	0	100	100	44, 44, 44, 47	0
2	i	2/6 (33%)	0.18	0	100	100	42, 42, 42, 42	0
2	j	2/6 (33%)	-0.23	0	100	100	46, 46, 46, 49	0
2	k	2/6 (33%)	0.05	0	100	100	42, 42, 42, 43	0
2	l	2/6 (33%)	0.70	0	100	100	44, 44, 44, 49	0
2	m	2/6 (33%)	0.48	0	100	100	44, 44, 44, 44	0
2	n	2/6 (33%)	0.27	0	100	100	46, 46, 46, 56	0
2	o	2/6 (33%)	-0.14	0	100	100	39, 39, 39, 44	0
2	p	2/6 (33%)	0.09	0	100	100	46, 46, 46, 48	0
2	q	2/6 (33%)	0.10	0	100	100	43, 43, 43, 44	0
2	r	2/6 (33%)	0.12	0	100	100	44, 44, 44, 49	0
2	s	2/6 (33%)	-0.17	0	100	100	46, 46, 46, 51	0
2	t	2/6 (33%)	0.00	0	100	100	40, 40, 40, 42	0
2	u	2/6 (33%)	-0.04	0	100	100	43, 43, 43, 48	0
2	v	2/6 (33%)	1.53	0	100	100	45, 45, 45, 48	0
2	w	2/6 (33%)	0.54	0	100	100	51, 51, 51, 56	0
2	x	2/6 (33%)	0.21	0	100	100	47, 47, 47, 51	0
2	y	2/6 (33%)	-0.07	0	100	100	43, 43, 43, 43	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
2	z	2/6 (33%)	0.44	0 100 100	45, 45, 45, 46	0
All	All	4895/6244 (78%)	0.14	27 (0%) 89 91	27, 40, 59, 90	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	136	GLY	3.6
1	B	25	TYR	3.3
1	N	24	ILE	3.2
1	S	43	GLU	3.1
1	B	24	ILE	3.1

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	ALO	3	3	7/8	0.91	0.19	36,42,44,48	0
2	ALO	1	3	7/8	0.93	0.17	39,41,44,46	0
2	YCP	3	5	8/9	0.93	0.24	24,35,39,42	0
2	ALO	p	3	7/8	0.94	0.18	43,45,50,53	0
2	ALO	w	3	7/8	0.94	0.16	46,53,56,56	0
2	WFP	e	2	13/14	0.94	0.19	41,43,47,49	0
2	ALO	c	3	7/8	0.94	0.16	39,45,47,51	0
2	ALO	4	3	7/8	0.94	0.24	35,37,42,43	0
2	YCP	c	5	8/9	0.94	0.18	39,46,49,52	0
2	YCP	e	5	8/9	0.94	0.22	45,49,51,53	0
2	YCP	u	5	8/9	0.94	0.16	42,46,48,50	0
2	ALO	m	3	7/8	0.94	0.19	39,48,50,55	0
2	MP8	w	7	8/9	0.94	0.22	46,50,53,56	0
2	ALO	x	3	7/8	0.95	0.18	42,51,54,56	0
2	ALO	z	3	7/8	0.95	0.18	37,43,46,52	0
2	WFP	c	2	13/14	0.95	0.21	38,46,50,50	0
2	ALO	f	3	7/8	0.95	0.19	46,46,50,53	0
2	ALO	k	3	7/8	0.95	0.18	38,42,44,47	0
2	WFP	n	2	13/14	0.95	0.21	43,46,51,55	0
2	WFP	s	2	13/14	0.95	0.21	39,47,52,55	0
2	YCP	f	5	8/9	0.95	0.19	43,50,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	YCP	j	5	8/9	0.95	0.19	47,48,53,53	0
2	ALO	q	3	7/8	0.95	0.16	31,42,44,44	0
2	YCP	x	5	8/9	0.95	0.20	47,50,51,52	0
2	YCP	y	5	8/9	0.95	0.15	41,45,46,48	0
2	YCP	z	5	8/9	0.95	0.19	39,44,47,50	0
2	ALO	r	3	7/8	0.95	0.20	39,45,51,51	0
2	YCP	4	5	8/9	0.95	0.14	37,42,43,44	0
2	MP8	n	7	8/9	0.95	0.21	37,46,47,47	0
2	WFP	1	2	13/14	0.95	0.19	36,40,43,43	0
2	WFP	x	2	13/14	0.96	0.20	45,48,53,55	0
2	ALO	s	3	7/8	0.96	0.17	45,50,53,57	0
2	ALO	t	3	7/8	0.96	0.14	34,38,40,42	0
2	ALO	u	3	7/8	0.96	0.22	44,46,50,56	0
2	YCP	k	5	8/9	0.96	0.19	38,43,45,45	0
2	YCP	l	5	8/9	0.96	0.17	34,44,48,49	0
2	YCP	p	5	8/9	0.96	0.20	41,44,47,47	0
2	YCP	r	5	8/9	0.96	0.14	46,49,54,54	0
2	YCP	t	5	8/9	0.96	0.19	36,40,41,42	0
2	ALO	g	3	7/8	0.96	0.16	37,44,49,52	0
2	YCP	v	5	8/9	0.96	0.20	40,43,44,47	0
2	ALO	i	3	7/8	0.96	0.24	41,44,46,46	0
2	ALO	y	3	7/8	0.96	0.18	37,43,46,46	0
2	WFP	z	2	13/14	0.96	0.19	39,42,45,46	0
2	YCP	0	5	8/9	0.96	0.17	37,43,45,47	0
2	ALO	0	3	7/8	0.96	0.15	38,41,44,45	0
2	WFP	t	2	13/14	0.96	0.22	37,41,47,49	0
2	MP8	e	7	8/9	0.96	0.20	46,47,48,48	0
2	MP8	f	7	8/9	0.96	0.17	43,46,48,49	0
2	MP8	g	7	8/9	0.96	0.18	35,41,45,45	0
2	MP8	h	7	8/9	0.96	0.21	37,39,42,43	0
2	MP8	k	7	8/9	0.96	0.26	39,43,48,51	0
2	WFP	u	2	13/14	0.96	0.25	38,43,47,48	0
2	MP8	p	7	8/9	0.96	0.23	39,44,47,50	0
2	ALO	e	3	7/8	0.96	0.16	46,47,48,51	0
2	MP8	x	7	8/9	0.96	0.20	46,49,52,54	0
2	MP8	1	7	8/9	0.96	0.15	39,41,43,44	0
2	MP8	3	7	8/9	0.96	0.21	31,37,40,41	0
2	WFP	g	2	13/14	0.97	0.21	36,41,44,45	0
2	ALO	n	3	7/8	0.97	0.18	41,52,53,53	0
2	YCP	m	5	8/9	0.97	0.20	38,44,46,47	0
2	YCP	n	5	8/9	0.97	0.15	46,51,55,57	0
2	YCP	o	5	8/9	0.97	0.23	39,40,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	WFP	h	2	13/14	0.97	0.23	41,45,47,48	0
2	WFP	i	2	13/14	0.97	0.25	42,43,46,49	0
2	YCP	s	5	8/9	0.97	0.20	44,48,53,53	0
2	WFP	v	2	13/14	0.97	0.26	35,40,44,48	0
2	WFP	w	2	13/14	0.97	0.22	45,50,53,53	0
2	WFP	j	2	13/14	0.97	0.18	41,44,47,48	0
2	WFP	k	2	13/14	0.97	0.22	36,41,45,48	0
2	WFP	0	2	13/14	0.97	0.18	35,43,49,49	0
2	WFP	l	2	13/14	0.97	0.19	39,44,48,51	0
2	WFP	2	2	13/14	0.97	0.21	34,39,45,46	0
2	YCP	1	5	8/9	0.97	0.14	39,43,47,48	0
2	YCP	2	5	8/9	0.97	0.18	36,38,42,42	0
2	WFP	m	2	13/14	0.97	0.19	45,47,50,50	0
2	WFP	f	2	13/14	0.97	0.20	44,48,50,52	0
2	MP8	c	7	8/9	0.97	0.16	39,43,47,48	0
2	WFP	o	2	13/14	0.97	0.17	34,40,44,45	0
2	ALO	2	3	7/8	0.97	0.16	39,41,44,55	0
2	WFP	p	2	13/14	0.97	0.21	35,39,47,47	0
2	ALO	h	3	7/8	0.97	0.16	41,44,48,52	0
2	MP8	j	7	8/9	0.97	0.18	38,43,47,47	0
2	WFP	q	2	13/14	0.97	0.22	39,43,47,51	0
2	MP8	l	7	8/9	0.97	0.24	34,42,43,49	0
2	MP8	m	7	8/9	0.97	0.19	38,42,45,46	0
2	ALO	j	3	7/8	0.97	0.21	40,44,49,54	0
2	MP8	o	7	8/9	0.97	0.18	38,43,45,47	0
2	WFP	r	2	13/14	0.97	0.22	35,40,47,49	0
2	MP8	q	7	8/9	0.97	0.19	36,39,42,42	0
2	MP8	r	7	8/9	0.97	0.19	41,44,49,49	0
2	MP8	s	7	8/9	0.97	0.18	45,50,51,51	0
2	MP8	v	7	8/9	0.97	0.14	37,40,42,44	0
2	YCP	g	5	8/9	0.97	0.20	41,45,50,51	0
2	YCP	h	5	8/9	0.97	0.18	37,45,48,50	0
2	YCP	i	5	8/9	0.97	0.27	40,41,47,48	0
2	MP8	2	7	8/9	0.97	0.21	36,39,43,43	0
2	ALO	l	3	7/8	0.97	0.14	41,43,47,53	0
2	WFP	3	2	13/14	0.98	0.21	34,37,41,43	0
2	MP8	t	7	8/9	0.98	0.15	35,37,43,45	0
2	MP8	u	7	8/9	0.98	0.22	41,43,44,44	0
2	ALO	o	3	7/8	0.98	0.14	41,42,45,52	0
2	YCP	w	5	8/9	0.98	0.23	46,52,54,55	0
2	WFP	4	2	13/14	0.98	0.22	33,38,43,47	0
2	MP8	y	7	8/9	0.98	0.15	37,39,42,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MP8	z	7	8/9	0.98	0.23	39,40,44,44	0
2	MP8	0	7	8/9	0.98	0.17	36,40,41,44	0
2	MP8	i	7	8/9	0.98	0.21	36,42,44,44	0
2	WFP	y	2	13/14	0.98	0.18	33,37,43,43	0
2	ALO	v	3	7/8	0.98	0.16	37,44,47,48	0
2	MP8	4	7	8/9	0.98	0.19	28,36,38,41	0
2	YCP	q	5	8/9	0.99	0.17	39,43,44,46	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (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
3	OCA	w	101	9/10	0.90	0.32	41,48,52,56	0
3	OCA	t	101	9/10	0.92	0.27	38,41,49,54	0
3	OCA	j	101	9/10	0.93	0.34	43,45,50,52	0
3	OCA	i	101	9/10	0.94	0.35	43,44,58,61	0
3	OCA	e	101	9/10	0.95	0.28	40,49,55,58	0
3	OCA	m	101	9/10	0.95	0.33	42,46,56,59	0
3	OCA	r	101	9/10	0.95	0.41	39,45,53,69	0
3	OCA	g	101	9/10	0.95	0.24	38,44,53,58	0
3	OCA	u	101	9/10	0.95	0.28	40,43,51,57	0
3	OCA	c	101	9/10	0.95	0.27	35,40,46,47	0
3	OCA	1	101	9/10	0.95	0.26	37,41,44,48	0
3	OCA	h	101	9/10	0.96	0.23	39,48,53,56	0
3	OCA	s	101	9/10	0.96	0.26	38,46,53,56	0
3	OCA	l	101	9/10	0.96	0.25	31,40,50,50	0
3	OCA	f	101	9/10	0.96	0.45	43,49,63,66	0
3	OCA	v	101	9/10	0.96	0.19	38,43,48,49	0
3	OCA	o	101	9/10	0.96	0.25	38,40,49,52	0
3	OCA	x	101	9/10	0.96	0.24	45,46,53,53	0
3	OCA	z	101	9/10	0.96	0.29	37,43,54,56	0
3	OCA	p	101	9/10	0.96	0.23	38,45,51,51	0
3	OCA	2	101	9/10	0.96	0.28	38,43,54,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	OCA	y	101	9/10	0.97	0.26	40,42,45,49	0
3	OCA	n	101	9/10	0.97	0.25	44,48,55,57	0
3	OCA	0	101	9/10	0.97	0.21	30,34,44,46	0
3	OCA	q	101	9/10	0.97	0.29	37,41,50,59	0
3	OCA	k	101	9/10	0.97	0.28	31,37,52,53	0
3	OCA	3	101	9/10	0.97	0.25	40,41,43,49	0
3	OCA	4	101	9/10	0.97	0.24	31,35,41,44	0

6.5 Other polymers (i)

There are no such residues in this entry.