



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2023 – 07:13 AM EST

PDB ID : 6PMD  
Title : Structure of ClpP from Staphylococcus aureus in complex with Acyldepsipeptide  
Authors : Griffith, E.C.; Lee, R.E.  
Deposited on : 2019-07-01  
Resolution : 2.21 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) 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

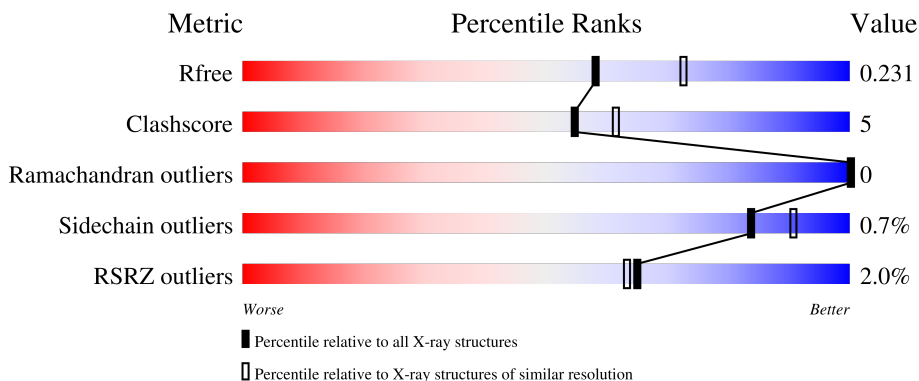
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.21 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.





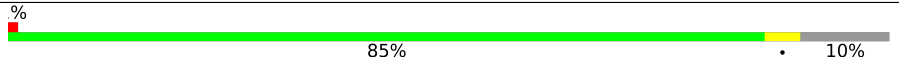
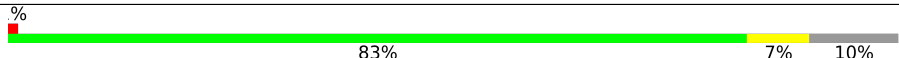
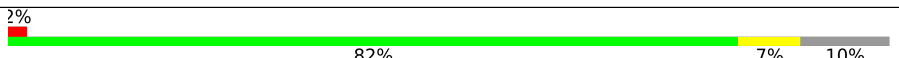
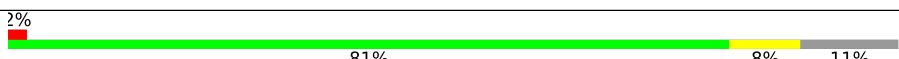
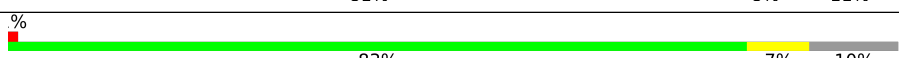
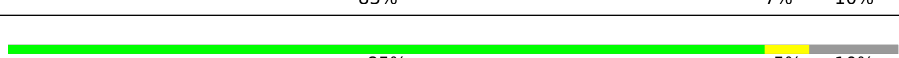
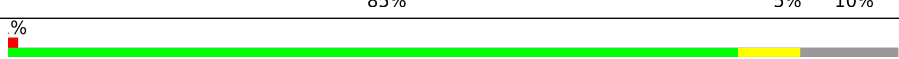

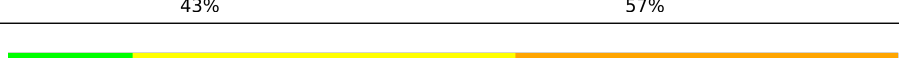

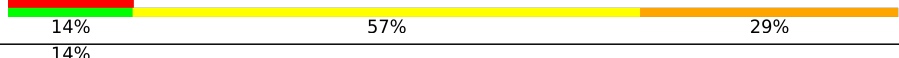




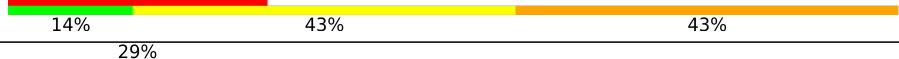

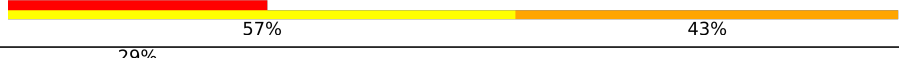
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	203	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 86%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 5%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 9%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">2% 86% 5% 9%</p>
1	B	203	<div style="display: flex; align-items: center;"> <div style="width: 1%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 82%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 7%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">% 82% 7% 10%</p>
1	C	203	<div style="display: flex; align-items: center;"> <div style="width: 82%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 7%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">82% 7% 10%</p>
1	D	203	<div style="display: flex; align-items: center;"> <div style="width: 1%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 82%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 7%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">% 82% 7% 10%</p>
1	E	203	<div style="display: flex; align-items: center;"> <div style="width: 1%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 82%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 7%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">% 82% 7% 10%</p>

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Mol	Chain	Length	Quality of chain
1	F	203	
1	G	203	
1	I	203	
1	K	203	
1	L	203	
1	M	203	
1	N	203	
1	S	203	
1	T	203	
2	H	7	
2	J	7	
2	O	7	
2	P	7	
2	Q	7	
2	R	7	
2	U	7	
2	V	7	
2	X	7	
2	Y	7	
2	Z	7	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	WFP	O	2	-	-	-	X
2	WFP	V	2	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 21307 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
			Total	C	N	O	S			
1	A	184	1388	873	238	271	6	0	0	0
1	B	182	1392	878	240	268	6	0	1	0
1	C	182	1386	876	236	268	6	0	0	0
1	D	182	1394	881	237	270	6	0	0	0
1	E	182	1385	873	236	270	6	0	0	0
1	F	181	1373	863	234	270	6	0	0	0
1	G	181	1386	875	235	270	6	0	0	0
1	I	183	1396	880	237	273	6	0	0	0
1	K	183	1399	884	238	271	6	0	0	0
1	L	182	1390	875	237	272	6	0	0	0
1	M	181	1371	864	235	266	6	0	0	0
1	N	182	1393	878	237	272	6	0	0	0
1	S	182	1390	878	235	271	6	0	0	0
1	T	181	1380	871	236	267	6	0	0	0

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	196	LEU	-	expression tag	UNP Q2G036

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Chain	Residue	Modelled	Actual	Comment	Reference
A	197	GLU	-	expression tag	UNP Q2G036
A	198	HIS	-	expression tag	UNP Q2G036
A	199	HIS	-	expression tag	UNP Q2G036
A	200	HIS	-	expression tag	UNP Q2G036
A	201	HIS	-	expression tag	UNP Q2G036
A	202	HIS	-	expression tag	UNP Q2G036
A	203	HIS	-	expression tag	UNP Q2G036
B	196	LEU	-	expression tag	UNP Q2G036
B	197	GLU	-	expression tag	UNP Q2G036
B	198	HIS	-	expression tag	UNP Q2G036
B	199	HIS	-	expression tag	UNP Q2G036
B	200	HIS	-	expression tag	UNP Q2G036
B	201	HIS	-	expression tag	UNP Q2G036
B	202	HIS	-	expression tag	UNP Q2G036
B	203	HIS	-	expression tag	UNP Q2G036
C	196	LEU	-	expression tag	UNP Q2G036
C	197	GLU	-	expression tag	UNP Q2G036
C	198	HIS	-	expression tag	UNP Q2G036
C	199	HIS	-	expression tag	UNP Q2G036
C	200	HIS	-	expression tag	UNP Q2G036
C	201	HIS	-	expression tag	UNP Q2G036
C	202	HIS	-	expression tag	UNP Q2G036
C	203	HIS	-	expression tag	UNP Q2G036
D	196	LEU	-	expression tag	UNP Q2G036
D	197	GLU	-	expression tag	UNP Q2G036
D	198	HIS	-	expression tag	UNP Q2G036
D	199	HIS	-	expression tag	UNP Q2G036
D	200	HIS	-	expression tag	UNP Q2G036
D	201	HIS	-	expression tag	UNP Q2G036
D	202	HIS	-	expression tag	UNP Q2G036
D	203	HIS	-	expression tag	UNP Q2G036
E	196	LEU	-	expression tag	UNP Q2G036
E	197	GLU	-	expression tag	UNP Q2G036
E	198	HIS	-	expression tag	UNP Q2G036
E	199	HIS	-	expression tag	UNP Q2G036
E	200	HIS	-	expression tag	UNP Q2G036
E	201	HIS	-	expression tag	UNP Q2G036
E	202	HIS	-	expression tag	UNP Q2G036
E	203	HIS	-	expression tag	UNP Q2G036
F	196	LEU	-	expression tag	UNP Q2G036
F	197	GLU	-	expression tag	UNP Q2G036
F	198	HIS	-	expression tag	UNP Q2G036

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Chain	Residue	Modelled	Actual	Comment	Reference
F	199	HIS	-	expression tag	UNP Q2G036
F	200	HIS	-	expression tag	UNP Q2G036
F	201	HIS	-	expression tag	UNP Q2G036
F	202	HIS	-	expression tag	UNP Q2G036
F	203	HIS	-	expression tag	UNP Q2G036
G	196	LEU	-	expression tag	UNP Q2G036
G	197	GLU	-	expression tag	UNP Q2G036
G	198	HIS	-	expression tag	UNP Q2G036
G	199	HIS	-	expression tag	UNP Q2G036
G	200	HIS	-	expression tag	UNP Q2G036
G	201	HIS	-	expression tag	UNP Q2G036
G	202	HIS	-	expression tag	UNP Q2G036
G	203	HIS	-	expression tag	UNP Q2G036
I	196	LEU	-	expression tag	UNP Q2G036
I	197	GLU	-	expression tag	UNP Q2G036
I	198	HIS	-	expression tag	UNP Q2G036
I	199	HIS	-	expression tag	UNP Q2G036
I	200	HIS	-	expression tag	UNP Q2G036
I	201	HIS	-	expression tag	UNP Q2G036
I	202	HIS	-	expression tag	UNP Q2G036
I	203	HIS	-	expression tag	UNP Q2G036
K	196	LEU	-	expression tag	UNP Q2G036
K	197	GLU	-	expression tag	UNP Q2G036
K	198	HIS	-	expression tag	UNP Q2G036
K	199	HIS	-	expression tag	UNP Q2G036
K	200	HIS	-	expression tag	UNP Q2G036
K	201	HIS	-	expression tag	UNP Q2G036
K	202	HIS	-	expression tag	UNP Q2G036
K	203	HIS	-	expression tag	UNP Q2G036
L	196	LEU	-	expression tag	UNP Q2G036
L	197	GLU	-	expression tag	UNP Q2G036
L	198	HIS	-	expression tag	UNP Q2G036
L	199	HIS	-	expression tag	UNP Q2G036
L	200	HIS	-	expression tag	UNP Q2G036
L	201	HIS	-	expression tag	UNP Q2G036
L	202	HIS	-	expression tag	UNP Q2G036
L	203	HIS	-	expression tag	UNP Q2G036
M	196	LEU	-	expression tag	UNP Q2G036
M	197	GLU	-	expression tag	UNP Q2G036
M	198	HIS	-	expression tag	UNP Q2G036
M	199	HIS	-	expression tag	UNP Q2G036
M	200	HIS	-	expression tag	UNP Q2G036

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Chain	Residue	Modelled	Actual	Comment	Reference
M	201	HIS	-	expression tag	UNP Q2G036
M	202	HIS	-	expression tag	UNP Q2G036
M	203	HIS	-	expression tag	UNP Q2G036
N	196	LEU	-	expression tag	UNP Q2G036
N	197	GLU	-	expression tag	UNP Q2G036
N	198	HIS	-	expression tag	UNP Q2G036
N	199	HIS	-	expression tag	UNP Q2G036
N	200	HIS	-	expression tag	UNP Q2G036
N	201	HIS	-	expression tag	UNP Q2G036
N	202	HIS	-	expression tag	UNP Q2G036
N	203	HIS	-	expression tag	UNP Q2G036
S	196	LEU	-	expression tag	UNP Q2G036
S	197	GLU	-	expression tag	UNP Q2G036
S	198	HIS	-	expression tag	UNP Q2G036
S	199	HIS	-	expression tag	UNP Q2G036
S	200	HIS	-	expression tag	UNP Q2G036
S	201	HIS	-	expression tag	UNP Q2G036
S	202	HIS	-	expression tag	UNP Q2G036
S	203	HIS	-	expression tag	UNP Q2G036
T	196	LEU	-	expression tag	UNP Q2G036
T	197	GLU	-	expression tag	UNP Q2G036
T	198	HIS	-	expression tag	UNP Q2G036
T	199	HIS	-	expression tag	UNP Q2G036
T	200	HIS	-	expression tag	UNP Q2G036
T	201	HIS	-	expression tag	UNP Q2G036
T	202	HIS	-	expression tag	UNP Q2G036
T	203	HIS	-	expression tag	UNP Q2G036

- Molecule 2 is a protein called SHV-WFP-SER-PRO-YCP-ALA-MP8 Acyldepsipeptide.

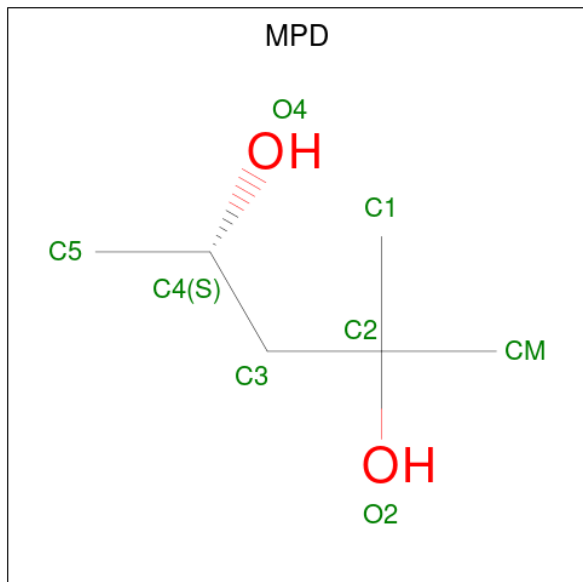
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	7	Total	C	F	N	O	0	0	0
			55	39	2	6	8			
2	J	7	Total	C	F	N	O	0	0	0
			55	39	2	6	8			
2	O	7	Total	C	F	N	O	0	0	0
			55	39	2	6	8			
2	P	7	Total	C	F	N	O	0	0	0
			55	39	2	6	8			
2	Q	7	Total	C	F	N	O	0	0	0
			55	39	2	6	8			
2	R	7	Total	C	F	N	O	0	0	0
			55	39	2	6	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	U	7	Total	C	F	N	O	0	0	0
			55	39	2	6	8			
2	V	7	Total	C	F	N	O	0	0	0
			55	39	2	6	8			
2	X	7	Total	C	F	N	O	0	0	0
			55	39	2	6	8			
2	Y	7	Total	C	F	N	O	0	0	0
			55	39	2	6	8			
2	Z	7	Total	C	F	N	O	0	0	0
			55	39	2	6	8			

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C O	0	0
			8	6 2		
3	B	1	Total	C O	0	0
			8	6 2		
3	C	1	Total	C O	0	0
			8	6 2		
3	D	1	Total	C O	0	0
			8	6 2		
3	E	1	Total	C O	0	0
			8	6 2		
3	F	1	Total	C O	0	0
			8	6 2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total C O 8 6 2	0	0
3	I	1	Total C O 8 6 2	0	0
3	K	1	Total C O 8 6 2	0	0
3	L	1	Total C O 8 6 2	0	0
3	M	1	Total C O 8 6 2	0	0
3	N	1	Total C O 8 6 2	0	0
3	S	1	Total C O 8 6 2	0	0
3	T	1	Total C O 8 6 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	54	Total O 54 54	0	0
4	B	81	Total O 81 81	0	0
4	C	99	Total O 99 99	0	0
4	D	102	Total O 102 102	0	0
4	E	81	Total O 81 81	0	0
4	F	65	Total O 65 65	0	0
4	G	58	Total O 58 58	0	0
4	I	91	Total O 91 91	0	0
4	K	113	Total O 113 113	0	0
4	L	120	Total O 120 120	0	0
4	M	95	Total O 95 95	0	0

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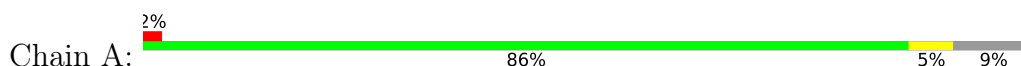
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	N	69	Total O 69 69	0	0
4	S	67	Total O 67 67	0	0
4	T	67	Total O 67 67	0	0
4	J	1	Total O 1 1	0	0
4	Q	1	Total O 1 1	0	0
4	R	1	Total O 1 1	0	0
4	X	1	Total O 1 1	0	0
4	Z	1	Total O 1 1	0	0

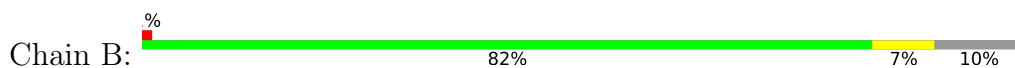
### 3 Residue-property plots [i](#)

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.

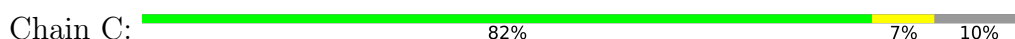
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



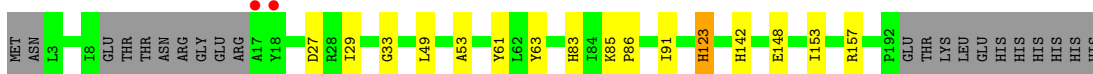
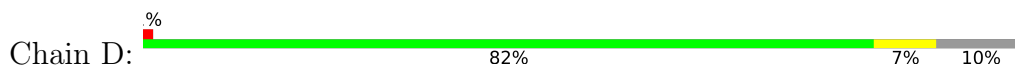
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



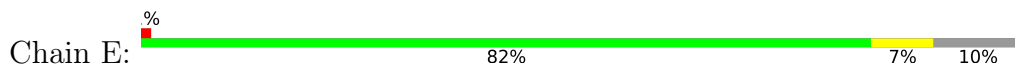
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



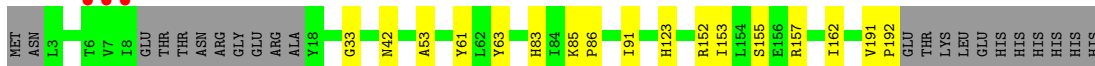
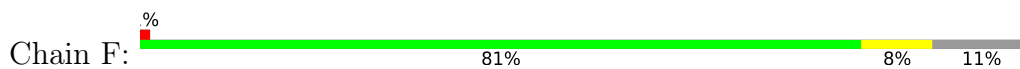
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



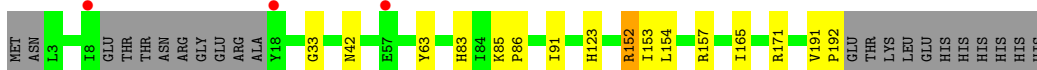
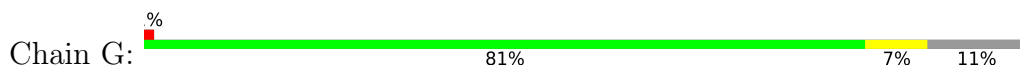
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



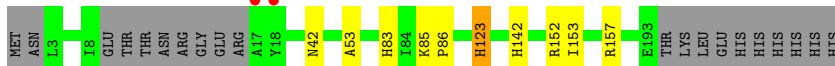
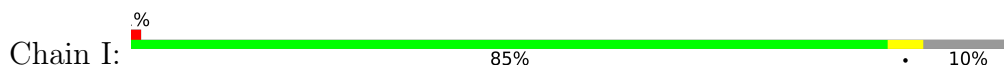
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



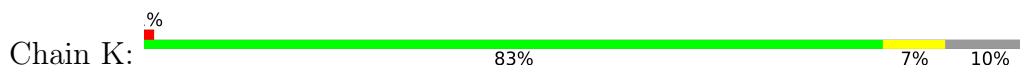
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



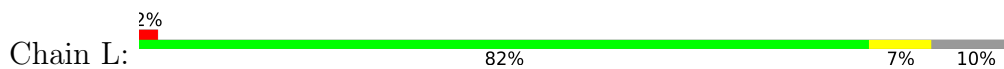
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



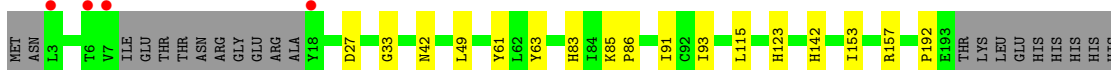
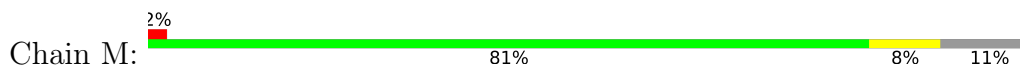
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

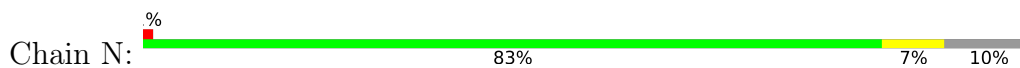


- Molecule 1: ATP-dependent Clp protease proteolytic subunit



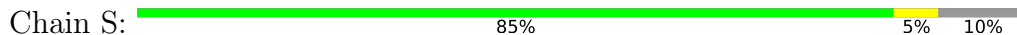
HIS

- Molecule 1: ATP-dependent Clp protease proteolytic subunit

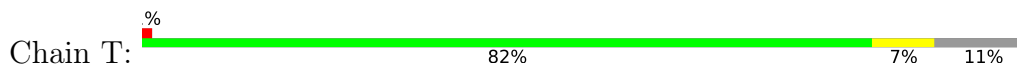




● Molecule 1: ATP-dependent Clp protease proteolytic subunit



● Molecule 1: ATP-dependent Clp protease proteolytic subunit



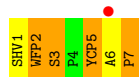
● Molecule 2: SHV-WFP-SER-PRO-YCP-ALA-MP8 Acyldepsipeptide



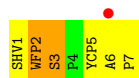
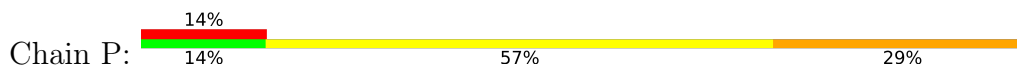
● Molecule 2: SHV-WFP-SER-PRO-YCP-ALA-MP8 Acyldepsipeptide



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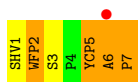


● Molecule 2: SHV-WFP-SER-PRO-YCP-ALA-MP8 Acyldepsipeptide

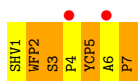


● Molecule 2: SHV-WFP-SER-PRO-YCP-ALA-MP8 Acyldepsipeptide

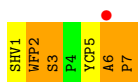




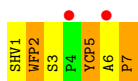
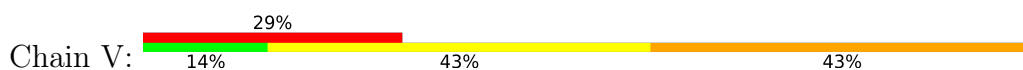
- Molecule 2: SHV-WFP-SER-PRO-YCP-ALA-MP8 Acyldepsipeptide



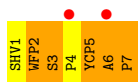
- Molecule 2: SHV-WFP-SER-PRO-YCP-ALA-MP8 Acyldepsipeptide



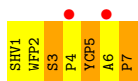
- Molecule 2: SHV-WFP-SER-PRO-YCP-ALA-MP8 Acyldepsipeptide



- Molecule 2: SHV-WFP-SER-PRO-YCP-ALA-MP8 Acyldepsipeptide



- Molecule 2: SHV-WFP-SER-PRO-YCP-ALA-MP8 Acyldepsipeptide



- Molecule 2: SHV-WFP-SER-PRO-YCP-ALA-MP8 Acyldepsipeptide



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.38Å 125.97Å 145.60Å 90.00° 93.77° 90.00°	Depositor
Resolution (Å)	38.80 – 2.21 38.78 – 2.21	Depositor EDS
% Data completeness (in resolution range)	98.1 (38.80-2.21) 98.1 (38.78-2.21)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.71 (at 2.22Å)	Xtrriage
Refinement program	REFMAC 5.8.0222	Depositor
R, $R_{free}$	0.200 , 0.227 0.204 , 0.231	Depositor DCC
$R_{free}$ test set	8358 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.1	Xtrriage
Anisotropy	0.066	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 42.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	21307	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: YCP, SHV, WFP, MPD, 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	0.45	0/1405	0.63	1/1899 (0.1%)
1	B	0.50	0/1413	0.64	0/1908
1	C	0.53	0/1404	0.67	0/1898
1	D	0.56	1/1412 (0.1%)	0.67	0/1907
1	E	0.49	0/1403	0.64	0/1896
1	F	0.44	0/1390	0.62	0/1879
1	G	0.47	0/1404	0.65	2/1896 (0.1%)
1	I	0.49	0/1414	0.63	0/1911
1	K	0.56	0/1417	0.69	0/1914
1	L	0.54	0/1408	0.71	1/1901 (0.1%)
1	M	0.50	0/1388	0.64	0/1876
1	N	0.49	0/1411	0.64	0/1905
1	S	0.45	0/1408	0.64	0/1903
1	T	0.44	0/1398	0.63	0/1888
2	H	2.28	1/17 (5.9%)	1.74	0/21
2	J	2.40	1/17 (5.9%)	2.17	1/21 (4.8%)
2	O	2.35	1/17 (5.9%)	1.62	0/21
2	P	2.00	1/17 (5.9%)	1.78	0/21
2	Q	2.28	1/17 (5.9%)	2.32	2/21 (9.5%)
2	R	1.98	1/17 (5.9%)	1.46	0/21
2	U	2.24	1/17 (5.9%)	2.03	1/21 (4.8%)
2	V	2.07	1/17 (5.9%)	1.87	0/21
2	X	2.22	1/17 (5.9%)	2.23	1/21 (4.8%)
2	Y	2.28	1/17 (5.9%)	1.85	0/21
2	Z	2.32	1/17 (5.9%)	1.95	0/21
All	All	0.54	12/19862 (0.1%)	0.67	9/26812 (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	G	0	1
1	I	0	1
All	All	0	2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	3	SER	C-N	7.49	1.48	1.34
2	J	3	SER	C-N	7.43	1.48	1.34
2	H	3	SER	C-N	7.20	1.48	1.34
2	V	3	SER	C-N	7.08	1.47	1.34
2	Z	3	SER	C-N	7.06	1.47	1.34
2	X	3	SER	C-N	6.97	1.47	1.34
2	Q	3	SER	C-N	6.96	1.47	1.34
2	Y	3	SER	C-N	6.90	1.47	1.34
2	R	3	SER	C-N	6.54	1.46	1.34
2	U	3	SER	C-N	6.54	1.46	1.34
2	P	3	SER	C-N	6.20	1.46	1.34
1	D	148	GLU	CD-OE2	5.16	1.31	1.25

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	6	ALA	N-CA-CB	-7.87	99.09	110.10
1	L	55	ASP	CB-CG-OD2	-6.67	112.29	118.30
2	X	6	ALA	N-CA-CB	-6.59	100.88	110.10
2	Q	6	ALA	N-CA-C	5.59	126.08	111.00
2	U	6	ALA	N-CA-CB	-5.55	102.32	110.10
2	Q	6	ALA	N-CA-CB	-5.41	102.52	110.10
1	G	152	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	G	171	ARG	NE-CZ-NH1	-5.13	117.74	120.30
1	A	171	ARG	NE-CZ-NH1	-5.05	117.78	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	152	ARG	Sidechain
1	I	152	ARG	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1388	0	1380	10	0
1	B	1392	0	1401	15	0
1	C	1386	0	1393	21	0
1	D	1394	0	1410	17	0
1	E	1385	0	1380	13	0
1	F	1373	0	1364	18	0
1	G	1386	0	1394	12	0
1	I	1396	0	1396	8	0
1	K	1399	0	1412	15	0
1	L	1390	0	1389	18	0
1	M	1371	0	1374	18	0
1	N	1393	0	1395	12	0
1	S	1390	0	1397	7	0
1	T	1380	0	1385	14	0
2	H	55	0	53	10	0
2	J	55	0	53	6	0
2	O	55	0	53	18	0
2	P	55	0	53	10	0
2	Q	55	0	52	9	0
2	R	55	0	52	9	0
2	U	55	0	52	12	0
2	V	55	0	52	10	0
2	X	55	0	52	8	0
2	Y	55	0	52	8	0
2	Z	55	0	52	6	0
3	A	8	0	14	0	0
3	B	8	0	14	0	0
3	C	8	0	14	0	0
3	D	8	0	14	1	0
3	E	8	0	14	0	0
3	F	8	0	14	0	0
3	G	8	0	14	0	0
3	I	8	0	14	1	0
3	K	8	0	14	0	0
3	L	8	0	14	0	0
3	M	8	0	14	0	0
3	N	8	0	14	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	S	8	0	14	0	0
3	T	8	0	14	0	0
4	A	54	0	0	0	0
4	B	81	0	0	0	0
4	C	99	0	0	0	0
4	D	102	0	0	1	0
4	E	81	0	0	1	0
4	F	65	0	0	0	0
4	G	58	0	0	0	0
4	I	91	0	0	0	0
4	J	1	0	0	0	0
4	K	113	0	0	0	0
4	L	120	0	0	0	0
4	M	95	0	0	0	0
4	N	69	0	0	0	0
4	Q	1	0	0	1	0
4	R	1	0	0	0	0
4	S	67	0	0	0	0
4	T	67	0	0	0	0
4	X	1	0	0	0	0
4	Z	1	0	0	1	0
All	All	21307	0	20242	210	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 5.

All (210) 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)
2:O:5:YCP:HD	2:O:5:YCP:C	1.88	1.01
1:F:152:ARG:HA	1:F:162:ILE:HD11	1.50	0.92
4:D:514:HOH:O	2:O:1:SHV:H32	1.72	0.89
2:V:1:SHV:H22	2:V:7:MP8:HD	1.52	0.89
2:X:1:SHV:H22	2:X:7:MP8:HD	1.56	0.87
2:O:5:YCP:C	2:O:5:YCP:CD	2.49	0.87
1:L:33:GLY:HA3	1:M:42:ASN:OD1	1.75	0.87
2:H:1:SHV:O2	2:H:3:SER:N	2.10	0.85
1:N:33:GLY:HA3	1:S:42:ASN:OD1	1.76	0.84
2:R:5:YCP:HD	2:R:5:YCP:C	2.12	0.80
1:N:93:ILE:HG22	1:N:115:LEU:HD12	1.63	0.80
1:C:63:TYR:CD2	2:O:2:WFP:F2	2.24	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:42:ASN:OD1	1:T:33:GLY:HA3	1.83	0.79
2:O:1:SHV:H22	2:O:7:MP8:HD	1.65	0.78
1:K:27:ASP:OD2	2:U:1:SHV:H62	1.83	0.78
1:M:33:GLY:HA3	1:N:42:ASN:OD1	1.85	0.77
1:A:42:ASN:OD1	1:G:33:GLY:HA3	1.85	0.75
1:L:63:TYR:CZ	2:V:2:WFP:HD2	2.21	0.75
2:R:5:YCP:C	2:R:5:YCP:CD	2.64	0.74
1:F:33:GLY:HA3	1:G:42:ASN:OD1	1.89	0.72
1:E:93:ILE:HG22	1:E:115:LEU:HD12	1.72	0.71
2:P:1:SHV:O2	2:P:3:SER:N	2.24	0.71
1:C:63:TYR:CZ	2:O:2:WFP:HD2	2.26	0.71
2:O:1:SHV:O2	2:O:3:SER:N	2.24	0.70
1:M:93:ILE:HG22	1:M:115:LEU:HD12	1.73	0.70
1:L:63:TYR:CE1	1:L:91:ILE:HD12	2.28	0.69
1:K:63:TYR:CZ	2:U:2:WFP:HD2	2.27	0.69
1:D:63:TYR:CE1	1:D:91:ILE:HD12	2.28	0.69
1:C:63:TYR:CE1	1:C:91:ILE:HD12	2.28	0.68
1:T:63:TYR:CE1	1:T:91:ILE:HD12	2.29	0.68
1:A:61:TYR:CE2	2:H:6:ALA:HA	2.29	0.68
1:F:152:ARG:HA	1:F:162:ILE:CD1	2.23	0.68
1:G:63:TYR:CE1	1:G:91:ILE:HD12	2.28	0.68
1:S:63:TYR:CE1	1:S:91:ILE:HD12	2.29	0.68
2:U:1:SHV:H22	2:U:7:MP8:HD	1.76	0.67
1:B:63:TYR:CE1	1:B:91:ILE:HD12	2.30	0.67
2:Q:1:SHV:H32	4:Q:101:HOH:O	1.95	0.67
1:M:63:TYR:CE1	1:M:91:ILE:HD12	2.29	0.67
2:H:5:YCP:HE	2:H:6:ALA:N	2.08	0.67
1:B:61:TYR:CE2	2:J:6:ALA:HA	2.29	0.67
1:E:63:TYR:CE1	1:E:91:ILE:HD12	2.29	0.66
1:F:63:TYR:CE1	1:F:91:ILE:HD12	2.30	0.66
1:T:63:TYR:CZ	2:Z:2:WFP:HD2	2.30	0.66
1:C:29:ILE:CD1	2:O:1:SHV:H41	2.26	0.66
1:E:33:GLY:HA3	1:F:42:ASN:OD1	1.95	0.66
1:D:27:ASP:OD2	2:P:1:SHV:H71	1.95	0.66
1:M:63:TYR:CZ	2:X:2:WFP:HD2	2.33	0.63
2:Y:5:YCP:HE	2:Y:6:ALA:N	2.13	0.63
1:M:63:TYR:CE2	2:X:2:WFP:HD2	2.34	0.62
2:H:1:SHV:H22	2:H:7:MP8:HD	1.80	0.62
1:F:155:SER:HB2	1:F:162:ILE:HD13	1.81	0.62
1:K:27:ASP:OD2	2:U:1:SHV:C6	2.48	0.61
1:C:61:TYR:CE2	2:O:6:ALA:HA	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:TYR:CE2	2:P:2:WFP:HD2	2.36	0.61
1:L:63:TYR:CE2	2:V:2:WFP:HD2	2.35	0.61
1:D:33:GLY:HA3	1:E:42:ASN:OD1	2.01	0.61
1:T:63:TYR:CE2	2:Z:2:WFP:HD2	2.36	0.60
1:B:63:TYR:CE2	2:J:2:WFP:HD2	2.36	0.60
1:K:63:TYR:CD2	2:U:2:WFP:F2	2.45	0.60
2:Y:5:YCP:CE	2:Y:6:ALA:N	2.65	0.60
2:Y:5:YCP:HE	2:Y:6:ALA:H	1.66	0.60
1:F:191:VAL:HG22	1:F:192:PRO:HD2	1.84	0.59
2:Y:3:SER:HA	2:Y:4:PRO:C	2.22	0.58
1:D:61:TYR:CE2	2:P:6:ALA:HA	2.40	0.57
2:Z:1:SHV:H32	4:Z:101:HOH:O	2.05	0.57
2:X:5:YCP:HE	2:X:6:ALA:N	2.18	0.57
1:B:33:GLY:HA3	1:C:42:ASN:OD1	2.04	0.56
1:I:53:ALA:HB2	2:Z:1:SHV:H51	1.87	0.56
1:C:63:TYR:HE2	1:D:49:LEU:HD13	1.71	0.56
1:C:119:GLU:CD	1:D:142:HIS:HE2	2.08	0.56
1:L:61:TYR:CE2	2:V:6:ALA:HA	2.40	0.56
1:A:63:TYR:CE2	2:H:2:WFP:HD2	2.41	0.56
1:A:33:GLY:HA3	1:B:42:ASN:OD1	2.06	0.55
2:Y:1:SHV:H22	2:Y:7:MP8:HD	1.86	0.55
1:A:115:LEU:HD21	1:A:190:MET:HE3	1.88	0.55
1:L:24:LEU:HD12	2:V:1:SHV:H73	1.88	0.55
1:K:29:ILE:CD1	2:U:1:SHV:H42	2.37	0.54
1:B:63:TYR:CZ	2:J:2:WFP:HD2	2.42	0.54
2:Q:1:SHV:H22	2:Q:7:MP8:HD	1.88	0.54
1:L:63:TYR:CD2	2:V:2:WFP:F2	2.51	0.53
1:C:191:VAL:HG13	1:C:192:PRO:HD2	1.89	0.53
1:C:63:TYR:HE2	1:D:49:LEU:CD1	2.21	0.53
1:T:24:LEU:HD12	2:Z:1:SHV:H73	1.91	0.53
1:B:191:VAL:HG22	1:B:192:PRO:HD2	1.91	0.53
1:S:192:PRO:HB3	1:T:83:HIS:HA	1.91	0.53
1:L:27:ASP:OD2	2:V:1:SHV:H71	2.09	0.52
1:C:63:TYR:CE2	2:O:2:WFP:F2	2.52	0.52
1:G:191:VAL:HG13	1:G:192:PRO:HD2	1.91	0.52
2:R:3:SER:HA	2:R:4:PRO:C	2.28	0.52
1:K:29:ILE:HD11	2:U:1:SHV:H42	1.92	0.52
1:B:119:GLU:CD	1:C:142:HIS:HE2	2.13	0.52
1:T:61:TYR:CE2	2:Z:6:ALA:HA	2.46	0.51
2:H:3:SER:HA	2:H:4:PRO:C	2.30	0.51
1:N:191:VAL:HG13	1:N:192:PRO:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:ASP:OD2	2:O:1:SHV:H71	2.10	0.51
1:S:24:LEU:HD12	2:Y:1:SHV:H73	1.93	0.51
4:E:511:HOH:O	2:P:1:SHV:H31	2.08	0.51
1:C:153:ILE:O	1:C:157:ARG:HG2	2.11	0.50
1:D:63:TYR:CZ	2:P:2:WFP:HD2	2.46	0.50
1:I:153:ILE:O	1:I:157:ARG:HG2	2.11	0.50
2:R:3:SER:HB3	2:R:4:PRO:HA	1.93	0.50
1:K:153:ILE:O	1:K:157:ARG:HG2	2.11	0.50
2:U:1:SHV:O2	2:U:3:SER:N	2.45	0.50
1:B:153:ILE:O	1:B:157:ARG:HG2	2.11	0.50
1:E:153:ILE:O	1:E:157:ARG:HG2	2.12	0.50
1:L:153:ILE:O	1:L:157:ARG:HG2	2.11	0.50
2:H:5:YCP:CE	2:H:6:ALA:N	2.71	0.50
1:G:153:ILE:O	1:G:157:ARG:HG2	2.12	0.50
1:S:153:ILE:O	1:S:157:ARG:HG2	2.12	0.50
1:F:61:TYR:CE2	2:R:6:ALA:HA	2.47	0.50
1:K:63:TYR:CE2	2:U:2:WFP:HD2	2.46	0.50
1:M:153:ILE:O	1:M:157:ARG:HG2	2.11	0.50
1:A:153:ILE:O	1:A:157:ARG:HG2	2.12	0.50
1:B:61:TYR:CD2	2:J:6:ALA:C	2.85	0.50
1:F:153:ILE:O	1:F:157:ARG:HG2	2.12	0.50
1:D:153:ILE:O	1:D:157:ARG:HG2	2.12	0.49
1:K:33:GLY:HA3	1:L:42:ASN:OD1	2.12	0.49
1:T:153:ILE:O	1:T:157:ARG:HG2	2.11	0.49
1:K:191:VAL:HG13	1:K:192:PRO:HD2	1.93	0.49
1:N:191:VAL:CG1	1:N:192:PRO:HD2	2.42	0.49
1:D:29:ILE:CD1	2:P:1:SHV:H41	2.42	0.49
1:F:191:VAL:CG2	1:F:192:PRO:HD2	2.42	0.49
1:K:61:TYR:CE2	2:U:6:ALA:HA	2.48	0.49
1:E:49:LEU:HB3	2:P:1:SHV:H32	1.95	0.49
2:H:1:SHV:O2	2:H:2:WFP:C	2.59	0.48
1:B:191:VAL:CG2	1:B:192:PRO:HD2	2.44	0.48
1:E:93:ILE:HG22	1:E:115:LEU:CD1	2.43	0.48
1:N:153:ILE:O	1:N:157:ARG:HG2	2.12	0.48
1:S:33:GLY:HA3	1:T:42:ASN:OD1	2.14	0.48
1:D:53:ALA:HB2	2:O:1:SHV:H51	1.96	0.47
2:X:5:YCP:CE	2:X:6:ALA:N	2.77	0.47
1:I:123:HIS:O	3:I:400:MPD:H12	2.15	0.47
1:I:42:ASN:OD1	1:T:33:GLY:CA	2.60	0.46
1:M:61:TYR:CE2	2:X:6:ALA:HA	2.50	0.46
1:F:53:ALA:HB2	2:Q:1:SHV:H51	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:ILE:HD13	2:O:1:SHV:H41	1.97	0.46
1:G:191:VAL:CG1	1:G:192:PRO:HD2	2.46	0.46
1:M:115:LEU:HD13	1:N:79:ASP:HB3	1.97	0.46
1:C:191:VAL:CG1	1:C:192:PRO:HD2	2.46	0.46
1:C:29:ILE:CD1	2:O:1:SHV:C4	2.94	0.45
1:A:63:TYR:CZ	2:H:2:WFP:HD2	2.51	0.45
1:K:191:VAL:CG1	1:K:192:PRO:HD2	2.47	0.45
2:V:5:YCP:HE	2:V:6:ALA:N	2.31	0.45
1:B:29:ILE:CD1	2:J:1:SHV:H41	2.47	0.45
1:B:53:ALA:HB2	2:H:1:SHV:H51	1.99	0.45
1:D:91:ILE:HD11	2:P:6:ALA:CB	2.46	0.45
1:F:192:PRO:HB3	1:G:83:HIS:HA	1.99	0.45
2:X:3:SER:HA	2:X:4:PRO:C	2.37	0.45
2:Q:5:YCP:HE	2:Q:6:ALA:N	2.31	0.45
1:M:192:PRO:HB3	1:N:83:HIS:HA	1.99	0.45
1:N:93:ILE:HG22	1:N:115:LEU:CD1	2.41	0.45
2:Y:4:PRO:HA	2:Y:5:YCP:HA	1.83	0.45
1:E:61:TYR:CE2	2:Q:6:ALA:HA	2.52	0.44
1:F:63:TYR:CE2	2:R:2:WFP:HD2	2.52	0.44
2:U:5:YCP:HE	2:U:6:ALA:N	2.33	0.44
1:M:93:ILE:HG22	1:M:115:LEU:CD1	2.44	0.44
2:O:5:YCP:HD	2:O:6:ALA:HB2	1.99	0.44
1:N:115:LEU:HD13	1:S:79:ASP:HB3	2.00	0.44
1:F:63:TYR:CZ	2:R:2:WFP:HD2	2.52	0.44
1:I:83:HIS:HA	1:T:192:PRO:HB3	2.00	0.44
1:L:33:GLY:CA	1:M:42:ASN:OD1	2.58	0.44
1:G:83:HIS:CD2	2:R:2:WFP:HD1	2.53	0.44
2:O:1:SHV:C1	2:O:3:SER:N	2.81	0.44
1:E:91:ILE:HD11	2:Q:6:ALA:CB	2.48	0.43
1:F:83:HIS:CD2	2:Q:2:WFP:HD1	2.52	0.43
1:L:63:TYR:HE2	1:M:49:LEU:CD1	2.31	0.43
2:Y:5:YCP:C	2:Y:5:YCP:CD	2.93	0.43
1:E:192:PRO:HB3	1:F:83:HIS:HA	2.01	0.43
2:P:1:SHV:C1	2:P:3:SER:N	2.80	0.43
1:L:63:TYR:CE2	2:V:2:WFP:CD2	3.01	0.43
1:L:119:GLU:OE2	1:M:142:HIS:CE1	2.72	0.42
1:C:61:TYR:CZ	2:O:7:MP8:HA	2.54	0.42
1:L:192:PRO:HB3	1:M:83:HIS:HA	2.01	0.42
2:R:1:SHV:H22	2:R:7:MP8:HD	2.02	0.42
1:L:61:TYR:CZ	2:V:7:MP8:HB	2.53	0.42
1:E:27:ASP:OD2	2:Q:1:SHV:C6	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:91:ILE:HD11	2:Q:6:ALA:HB1	2.02	0.42
1:M:85:LYS:N	1:M:86:PRO:CD	2.83	0.42
1:N:150:LEU:HD13	3:N:400:MPD:H52	2.02	0.42
1:A:42:ASN:OD1	1:G:33:GLY:CA	2.62	0.42
1:E:85:LYS:N	1:E:86:PRO:CD	2.83	0.41
1:L:63:TYR:N	1:L:63:TYR:CD1	2.88	0.41
1:M:27:ASP:OD2	2:X:1:SHV:H62	2.20	0.41
1:T:85:LYS:N	1:T:86:PRO:CD	2.83	0.41
1:B:119:GLU:OE2	1:C:142:HIS:NE2	2.48	0.41
1:C:85:LYS:N	1:C:86:PRO:CD	2.83	0.41
1:B:85:LYS:N	1:B:86:PRO:CD	2.84	0.41
1:D:83:HIS:CD2	2:O:2:WFP:HD1	2.55	0.41
1:L:85:LYS:N	1:L:86:PRO:CD	2.84	0.41
1:N:85:LYS:N	1:N:86:PRO:CD	2.84	0.41
1:C:63:TYR:N	1:C:63:TYR:CD1	2.88	0.41
1:D:85:LYS:N	1:D:86:PRO:CD	2.83	0.41
1:G:154:LEU:HB3	1:G:165:ILE:HD13	2.03	0.41
1:K:63:TYR:N	1:K:63:TYR:CD1	2.88	0.41
1:G:63:TYR:CD1	1:G:63:TYR:N	2.88	0.41
1:G:85:LYS:N	1:G:86:PRO:CD	2.84	0.41
1:A:63:TYR:CD1	1:A:63:TYR:N	2.89	0.41
1:D:63:TYR:N	1:D:63:TYR:CD1	2.89	0.41
1:F:85:LYS:N	1:F:86:PRO:CD	2.84	0.41
1:K:85:LYS:N	1:K:86:PRO:CD	2.84	0.41
1:K:154:LEU:HB3	1:K:165:ILE:HD13	2.03	0.41
1:D:123:HIS:O	3:D:400:MPD:H12	2.22	0.40
1:I:85:LYS:N	1:I:86:PRO:CD	2.83	0.40
1:M:63:TYR:N	1:M:63:TYR:CD1	2.89	0.40
2:U:5:YCP:CE	2:U:6:ALA:N	2.84	0.40
1:F:63:TYR:CD1	1:F:63:TYR:N	2.89	0.40
2:J:5:YCP:C	2:J:5:YCP:CD	2.97	0.40
1:A:115:LEU:HD21	1:A:190:MET:CE	2.51	0.40
1:I:142:HIS:HE2	1:T:119:GLU:CD	2.25	0.40
1:T:63:TYR:N	1:T:63:TYR:CD1	2.89	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	180/203 (89%)	176 (98%)	4 (2%)	0	100	100
1	B	179/203 (88%)	176 (98%)	3 (2%)	0	100	100
1	C	178/203 (88%)	175 (98%)	3 (2%)	0	100	100
1	D	178/203 (88%)	175 (98%)	3 (2%)	0	100	100
1	E	178/203 (88%)	175 (98%)	3 (2%)	0	100	100
1	F	177/203 (87%)	174 (98%)	3 (2%)	0	100	100
1	G	177/203 (87%)	174 (98%)	3 (2%)	0	100	100
1	I	179/203 (88%)	176 (98%)	3 (2%)	0	100	100
1	K	179/203 (88%)	176 (98%)	3 (2%)	0	100	100
1	L	178/203 (88%)	175 (98%)	3 (2%)	0	100	100
1	M	177/203 (87%)	174 (98%)	3 (2%)	0	100	100
1	N	178/203 (88%)	175 (98%)	3 (2%)	0	100	100
1	S	178/203 (88%)	175 (98%)	3 (2%)	0	100	100
1	T	177/203 (87%)	174 (98%)	3 (2%)	0	100	100
2	H	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	J	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	U	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	V	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	X	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	Y	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	Z	3/7 (43%)	2 (67%)	1 (33%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2526/2919 (86%)	2472 (98%)	54 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	145/171 (85%)	144 (99%)	1 (1%)	84	91
1	B	147/171 (86%)	146 (99%)	1 (1%)	84	91
1	C	147/171 (86%)	146 (99%)	1 (1%)	84	91
1	D	149/171 (87%)	148 (99%)	1 (1%)	84	91
1	E	146/171 (85%)	145 (99%)	1 (1%)	84	91
1	F	145/171 (85%)	144 (99%)	1 (1%)	84	91
1	G	148/171 (86%)	147 (99%)	1 (1%)	84	91
1	I	148/171 (86%)	147 (99%)	1 (1%)	84	91
1	K	149/171 (87%)	148 (99%)	1 (1%)	84	91
1	L	147/171 (86%)	146 (99%)	1 (1%)	84	91
1	M	145/171 (85%)	144 (99%)	1 (1%)	84	91
1	N	148/171 (86%)	147 (99%)	1 (1%)	84	91
1	S	148/171 (86%)	147 (99%)	1 (1%)	84	91
1	T	146/171 (85%)	145 (99%)	1 (1%)	84	91
2	H	2/2 (100%)	2 (100%)	0	100	100
2	J	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	U	2/2 (100%)	2 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	V	2/2 (100%)	2 (100%)	0	100	100
2	X	2/2 (100%)	2 (100%)	0	100	100
2	Y	2/2 (100%)	2 (100%)	0	100	100
2	Z	2/2 (100%)	2 (100%)	0	100	100
All	All	2080/2416 (86%)	2066 (99%)	14 (1%)	84	91

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	HIS
1	B	123	HIS
1	C	123	HIS
1	D	123	HIS
1	E	123	HIS
1	F	123	HIS
1	G	123	HIS
1	I	123	HIS
1	K	123	HIS
1	L	123	HIS
1	M	123	HIS
1	N	123	HIS
1	S	123	HIS
1	T	123	HIS

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

Mol	Chain	Res	Type
1	G	83	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

33 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	YCP	X	5	2	6,8,9	0.68	0	5,9,11	1.55	1 (20%)
2	WFP	R	2	2	12,13,14	1.32	1 (8%)	14,17,19	1.50	2 (14%)
2	WFP	Z	2	2	12,13,14	1.41	2 (16%)	14,17,19	1.53	2 (14%)
2	MP8	Q	7	2	5,8,9	2.54	1 (20%)	3,10,12	1.20	0
2	MP8	V	7	2	5,8,9	2.47	1 (20%)	3,10,12	1.10	0
2	YCP	Q	5	2	6,8,9	0.73	0	5,9,11	1.54	1 (20%)
2	WFP	P	2	2	12,13,14	1.63	4 (33%)	14,17,19	1.71	5 (35%)
2	MP8	P	7	2	5,8,9	2.41	1 (20%)	3,10,12	1.15	0
2	WFP	O	2	2	12,13,14	2.16	5 (41%)	14,17,19	2.20	6 (42%)
2	YCP	U	5	2	6,8,9	0.86	0	5,9,11	1.15	0
2	YCP	Z	5	2	6,8,9	0.66	0	5,9,11	1.40	1 (20%)
2	MP8	X	7	2	5,8,9	2.38	1 (20%)	3,10,12	1.33	1 (33%)
2	WFP	U	2	2	12,13,14	1.95	3 (25%)	14,17,19	1.70	4 (28%)
2	YCP	Y	5	2	6,8,9	0.87	0	5,9,11	1.54	2 (40%)
2	YCP	P	5	2	6,8,9	0.70	0	5,9,11	2.34	2 (40%)
2	MP8	O	7	2	5,8,9	2.14	1 (20%)	3,10,12	1.43	1 (33%)
2	YCP	H	5	2	6,8,9	0.85	0	5,9,11	1.14	1 (20%)
2	WFP	H	2	2	12,13,14	1.52	2 (16%)	14,17,19	1.67	3 (21%)
2	MP8	H	7	2	5,8,9	2.97	1 (20%)	3,10,12	0.98	0
2	YCP	R	5	2	6,8,9	0.68	0	5,9,11	1.43	1 (20%)
2	MP8	Z	7	2	5,8,9	1.62	1 (20%)	3,10,12	0.93	0
2	WFP	V	2	2	12,13,14	1.85	5 (41%)	14,17,19	1.85	4 (28%)
2	MP8	Y	7	2	5,8,9	3.06	1 (20%)	3,10,12	1.05	0
2	WFP	Y	2	2	12,13,14	1.31	1 (8%)	14,17,19	1.62	3 (21%)
2	MP8	R	7	2	5,8,9	3.15	2 (40%)	3,10,12	2.11	1 (33%)
2	WFP	X	2	2	12,13,14	1.65	3 (25%)	14,17,19	1.54	4 (28%)
2	YCP	J	5	2	6,8,9	0.73	0	5,9,11	2.00	2 (40%)
2	WFP	Q	2	2	12,13,14	1.29	1 (8%)	14,17,19	1.14	0
2	YCP	O	5	2	6,8,9	0.74	0	5,9,11	1.50	1 (20%)
2	WFP	J	2	2	12,13,14	1.88	4 (33%)	14,17,19	1.66	4 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MP8	J	7	2	5,8,9	1.60	1 (20%)	3,10,12	1.39	1 (33%)
2	MP8	U	7	2	5,8,9	2.98	1 (20%)	3,10,12	1.89	1 (33%)
2	YCP	V	5	2	6,8,9	0.81	0	5,9,11	1.47	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	YCP	X	5	2	-	1/1/10/12	1/1/1/1
2	WFP	R	2	2	-	1/5/6/8	0/1/1/1
2	WFP	Z	2	2	-	0/5/6/8	0/1/1/1
2	MP8	Q	7	2	-	0/0/11/13	0/1/1/1
2	MP8	V	7	2	-	0/0/11/13	0/1/1/1
2	YCP	Q	5	2	-	1/1/10/12	1/1/1/1
2	WFP	P	2	2	-	1/5/6/8	0/1/1/1
2	MP8	P	7	2	-	0/0/11/13	0/1/1/1
2	WFP	O	2	2	-	0/5/6/8	0/1/1/1
2	YCP	U	5	2	-	0/1/10/12	1/1/1/1
2	YCP	Z	5	2	-	1/1/10/12	1/1/1/1
2	MP8	X	7	2	-	0/0/11/13	0/1/1/1
2	WFP	U	2	2	-	0/5/6/8	0/1/1/1
2	YCP	Y	5	2	-	1/1/10/12	1/1/1/1
2	YCP	P	5	2	-	0/1/10/12	1/1/1/1
2	MP8	O	7	2	-	0/0/11/13	0/1/1/1
2	YCP	H	5	2	-	1/1/10/12	1/1/1/1
2	WFP	H	2	2	-	0/5/6/8	0/1/1/1
2	MP8	H	7	2	-	0/0/11/13	0/1/1/1
2	YCP	R	5	2	-	0/1/10/12	1/1/1/1
2	MP8	Z	7	2	-	0/0/11/13	0/1/1/1
2	WFP	V	2	2	-	0/5/6/8	0/1/1/1
2	MP8	Y	7	2	-	0/0/11/13	0/1/1/1
2	WFP	Y	2	2	-	0/5/6/8	0/1/1/1
2	MP8	R	7	2	-	0/0/11/13	0/1/1/1
2	WFP	X	2	2	-	0/5/6/8	0/1/1/1
2	YCP	J	5	2	-	0/1/10/12	0/1/1/1
2	WFP	Q	2	2	-	0/5/6/8	0/1/1/1
2	YCP	O	5	2	-	0/1/10/12	1/1/1/1
2	WFP	J	2	2	-	0/5/6/8	0/1/1/1
2	MP8	J	7	2	-	0/0/11/13	0/1/1/1
2	MP8	U	7	2	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	YCP	V	5	2	-	1/1/10/12	1/1/1/1

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	7	MP8	CB-CA	-6.60	1.39	1.54
2	Y	7	MP8	CB-CA	-6.54	1.40	1.54
2	H	7	MP8	CB-CA	-6.36	1.40	1.54
2	U	7	MP8	CB-CA	-6.24	1.40	1.54
2	Q	7	MP8	CB-CA	-5.26	1.42	1.54
2	V	7	MP8	CB-CA	-5.18	1.43	1.54
2	P	7	MP8	CB-CA	-5.10	1.43	1.54
2	X	7	MP8	CB-CA	-4.83	1.43	1.54
2	O	2	WFP	CZ-CE2	4.66	1.45	1.37
2	O	7	MP8	CB-CA	-4.31	1.45	1.54
2	U	2	WFP	CZ-CE2	4.01	1.44	1.37
2	J	2	WFP	CD2-CG	3.47	1.45	1.39
2	Z	7	MP8	CB-CA	-3.24	1.47	1.54
2	Y	2	WFP	CA-N	-3.18	1.38	1.48
2	V	2	WFP	CA-N	-3.16	1.38	1.48
2	H	2	WFP	CA-N	-3.15	1.38	1.48
2	J	2	WFP	CD2-CE2	3.11	1.42	1.37
2	O	2	WFP	CA-N	-2.99	1.39	1.48
2	J	7	MP8	CB-CA	-2.99	1.47	1.54
2	V	2	WFP	CZ-CE2	2.97	1.42	1.37
2	P	2	WFP	CA-N	-2.97	1.39	1.48
2	U	2	WFP	CA-N	-2.71	1.40	1.48
2	V	2	WFP	CD2-CG	2.70	1.43	1.39
2	X	2	WFP	CD2-CG	2.68	1.43	1.39
2	O	2	WFP	CD2-CE2	2.66	1.42	1.37
2	Z	2	WFP	CA-N	-2.64	1.40	1.48
2	Q	2	WFP	CA-N	-2.63	1.40	1.48
2	O	2	WFP	CD2-CG	2.61	1.43	1.39
2	J	2	WFP	CA-N	-2.58	1.40	1.48
2	X	2	WFP	CA-N	-2.54	1.40	1.48
2	H	2	WFP	CD2-CE2	2.49	1.41	1.37
2	P	2	WFP	CD2-CE2	2.46	1.41	1.37
2	X	2	WFP	CD2-CE2	2.37	1.41	1.37
2	Z	2	WFP	CD2-CE2	2.37	1.41	1.37
2	R	2	WFP	CA-N	-2.36	1.41	1.48
2	U	2	WFP	F1-CE1	-2.28	1.30	1.36
2	V	2	WFP	CD2-CE2	2.27	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	2	WFP	F1-CE1	-2.20	1.31	1.36
2	O	2	WFP	F1-CE1	-2.18	1.31	1.36
2	R	7	MP8	CB-CG	-2.15	1.45	1.52
2	P	2	WFP	F1-CE1	-2.10	1.31	1.36
2	J	2	WFP	CZ-CE2	2.08	1.41	1.37
2	P	2	WFP	CD1-CG	-2.04	1.35	1.39

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	2	WFP	CB-CA-C	-4.77	102.52	111.47
2	P	5	YCP	CG-CB-CA	4.55	117.73	110.98
2	Z	2	WFP	CG-CB-CA	-3.87	106.27	114.10
2	R	7	MP8	CE-CG-CB	-3.60	104.94	114.05
2	Y	2	WFP	CG-CD1-CE1	3.56	122.05	118.81
2	U	2	WFP	F2-CE2-CZ	3.48	123.23	118.25
2	J	5	YCP	CG-CB-CA	3.30	115.87	110.98
2	H	2	WFP	CG-CB-CA	-3.28	107.46	114.10
2	O	2	WFP	CG-CB-CA	-3.23	107.56	114.10
2	U	7	MP8	CE-CG-CB	-3.12	106.14	114.05
2	H	2	WFP	CG-CD1-CE1	2.92	121.46	118.81
2	J	5	YCP	O-C-CA	-2.91	117.15	124.78
2	V	2	WFP	CB-CG-CD1	-2.88	115.49	120.44
2	V	2	WFP	CB-CA-C	-2.86	106.11	111.47
2	U	2	WFP	F1-CE1-CD1	-2.85	114.18	118.25
2	P	2	WFP	CG-CD1-CE1	2.81	121.36	118.81
2	O	2	WFP	F2-CE2-CZ	2.73	122.15	118.25
2	J	2	WFP	CE2-CZ-CE1	2.68	120.30	116.13
2	R	2	WFP	CG-CD1-CE1	2.67	121.24	118.81
2	O	2	WFP	CD2-CE2-CZ	-2.64	120.18	123.52
2	X	2	WFP	CG-CD1-CE1	2.63	121.20	118.81
2	O	2	WFP	F1-CE1-CZ	2.63	122.00	118.25
2	J	2	WFP	F2-CE2-CD2	2.57	121.92	118.25
2	R	5	YCP	CG-CB-CA	2.56	114.79	110.98
2	Q	5	YCP	O-C-CA	-2.46	118.32	124.78
2	Y	5	YCP	O-C-CA	-2.44	118.37	124.78
2	P	2	WFP	CG-CB-CA	-2.43	109.18	114.10
2	Y	2	WFP	CD1-CE1-CZ	-2.42	120.47	123.52
2	H	2	WFP	CD1-CE1-CZ	-2.40	120.49	123.52
2	Y	2	WFP	F1-CE1-CZ	2.39	121.67	118.25
2	J	7	MP8	CE-CG-CB	-2.37	108.05	114.05
2	P	2	WFP	CB-CA-C	-2.34	107.08	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	2	WFP	CD2-CE2-CZ	-2.33	120.57	123.52
2	X	2	WFP	CB-CA-C	-2.33	107.10	111.47
2	X	5	YCP	O-C-CA	-2.32	118.69	124.78
2	O	7	MP8	CE-CG-CB	-2.30	108.23	114.05
2	R	2	WFP	F1-CE1-CZ	2.27	121.50	118.25
2	V	2	WFP	CG-CD2-CE2	-2.26	116.76	118.81
2	V	5	YCP	O-C-CA	-2.25	118.89	124.78
2	V	2	WFP	F1-CE1-CZ	2.22	121.43	118.25
2	O	2	WFP	F1-CE1-CD1	-2.22	115.08	118.25
2	J	2	WFP	CD1-CE1-CZ	-2.22	120.72	123.52
2	Z	5	YCP	O-C-CA	-2.21	118.99	124.78
2	U	2	WFP	F2-CE2-CD2	-2.17	115.15	118.25
2	X	7	MP8	CE-CG-CB	-2.15	108.61	114.05
2	P	2	WFP	F1-CE1-CD1	-2.14	115.20	118.25
2	P	2	WFP	CB-CG-CD2	2.13	124.09	120.44
2	U	2	WFP	F1-CE1-CZ	2.11	121.27	118.25
2	P	5	YCP	O-C-CA	-2.11	119.24	124.78
2	Y	5	YCP	CG-CB-CA	2.11	114.11	110.98
2	Z	2	WFP	F2-CE2-CD2	2.09	121.24	118.25
2	H	5	YCP	O-C-CA	-2.04	119.43	124.78
2	O	5	YCP	O-C-CA	-2.03	119.45	124.78
2	X	2	WFP	CD2-CE2-CZ	-2.02	120.97	123.52
2	X	2	WFP	F1-CE1-CZ	2.01	121.12	118.25

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Q	5	YCP	O-C-CA-CB
2	X	5	YCP	O-C-CA-CB
2	Y	5	YCP	O-C-CA-CB
2	Z	5	YCP	O-C-CA-CB
2	H	5	YCP	O-C-CA-CB
2	V	5	YCP	O-C-CA-CB
2	P	2	WFP	N-CA-CB-CG
2	R	2	WFP	N-CA-CB-CG

All (10) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	P	5	YCP	CA-CB-CD-CE-CG-N
2	U	5	YCP	CA-CB-CD-CE-CG-N

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Mol	Chain	Res	Type	Atoms
2	Y	5	YCP	CA-CB-CD-CE-CG-N
2	V	5	YCP	CA-CB-CD-CE-CG-N
2	O	5	YCP	CA-CB-CD-CE-CG-N
2	R	5	YCP	CA-CB-CD-CE-CG-N
2	X	5	YCP	CA-CB-CD-CE-CG-N
2	H	5	YCP	CA-CB-CD-CE-CG-N
2	Q	5	YCP	CA-CB-CD-CE-CG-N
2	Z	5	YCP	CA-CB-CD-CE-CG-N

27 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	X	5	YCP	2	0
2	R	2	WFP	3	0
2	Z	2	WFP	2	0
2	Q	7	MP8	1	0
2	V	7	MP8	2	0
2	Q	5	YCP	1	0
2	P	2	WFP	2	0
2	O	2	WFP	4	0
2	U	5	YCP	2	0
2	X	7	MP8	1	0
2	U	2	WFP	3	0
2	Y	5	YCP	5	0
2	O	7	MP8	2	0
2	H	5	YCP	2	0
2	H	2	WFP	3	0
2	H	7	MP8	1	0
2	R	5	YCP	2	0
2	V	2	WFP	4	0
2	Y	7	MP8	1	0
2	R	7	MP8	1	0
2	X	2	WFP	2	0
2	J	5	YCP	1	0
2	Q	2	WFP	1	0
2	O	5	YCP	3	0
2	J	2	WFP	2	0
2	U	7	MP8	1	0
2	V	5	YCP	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

14 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	MPD	K	400	-	7,7,7	0.55	0	9,10,10	0.93	0
3	MPD	D	400	-	7,7,7	0.40	0	9,10,10	1.26	1 (11%)
3	MPD	S	400	-	7,7,7	0.42	0	9,10,10	1.37	1 (11%)
3	MPD	E	400	-	7,7,7	0.77	0	9,10,10	1.08	0
3	MPD	M	400	-	7,7,7	0.66	0	9,10,10	1.21	1 (11%)
3	MPD	L	400	-	7,7,7	0.46	0	9,10,10	0.63	0
3	MPD	C	400	-	7,7,7	0.71	0	9,10,10	1.13	0
3	MPD	N	400	-	7,7,7	0.81	0	9,10,10	1.01	0
3	MPD	I	400	-	7,7,7	0.40	0	9,10,10	1.07	0
3	MPD	G	400	-	7,7,7	0.36	0	9,10,10	1.03	1 (11%)
3	MPD	F	400	-	7,7,7	0.40	0	9,10,10	0.64	0
3	MPD	T	400	-	7,7,7	0.65	0	9,10,10	0.80	0
3	MPD	A	400	-	7,7,7	0.40	0	9,10,10	1.22	1 (11%)
3	MPD	B	400	-	7,7,7	0.52	0	9,10,10	1.24	1 (11%)

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	MPD	K	400	-	-	0/5/5/5	-
3	MPD	D	400	-	-	0/5/5/5	-
3	MPD	S	400	-	-	0/5/5/5	-
3	MPD	E	400	-	-	0/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MPD	M	400	-	-	0/5/5/5	-
3	MPD	L	400	-	-	0/5/5/5	-
3	MPD	C	400	-	-	0/5/5/5	-
3	MPD	N	400	-	-	0/5/5/5	-
3	MPD	I	400	-	-	0/5/5/5	-
3	MPD	G	400	-	-	0/5/5/5	-
3	MPD	F	400	-	-	1/5/5/5	-
3	MPD	T	400	-	-	0/5/5/5	-
3	MPD	A	400	-	-	0/5/5/5	-
3	MPD	B	400	-	-	0/5/5/5	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	400	MPD	O2-C2-CM	-3.01	98.43	108.08
3	A	400	MPD	O2-C2-CM	-2.75	99.24	108.08
3	S	400	MPD	O4-C4-C5	-2.30	99.40	109.38
3	M	400	MPD	CM-C2-C1	-2.06	106.28	110.57
3	G	400	MPD	O2-C2-CM	-2.02	101.59	108.08
3	B	400	MPD	O2-C2-CM	-2.02	101.60	108.08

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	400	MPD	O2-C2-C3-C4

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	400	MPD	1	0
3	N	400	MPD	1	0
3	I	400	MPD	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	184/203 (90%)	0.05	4 (2%) 62 60	29, 39, 60, 84	0
1	B	182/203 (89%)	-0.20	3 (1%) 72 70	17, 28, 49, 62	0
1	C	182/203 (89%)	-0.30	0 100 100	13, 21, 41, 63	0
1	D	182/203 (89%)	-0.34	2 (1%) 80 79	14, 22, 43, 58	0
1	E	182/203 (89%)	-0.18	2 (1%) 80 79	17, 29, 50, 73	0
1	F	181/203 (89%)	0.09	3 (1%) 70 68	21, 40, 60, 86	0
1	G	181/203 (89%)	0.17	3 (1%) 70 68	30, 41, 61, 74	0
1	I	183/203 (90%)	-0.18	2 (1%) 80 79	18, 29, 52, 67	0
1	K	183/203 (90%)	-0.20	2 (1%) 80 79	14, 23, 40, 56	0
1	L	182/203 (89%)	-0.27	4 (2%) 62 60	14, 22, 42, 65	0
1	M	181/203 (89%)	-0.24	4 (2%) 62 60	17, 25, 49, 74	0
1	N	182/203 (89%)	-0.11	3 (1%) 72 70	22, 33, 54, 79	0
1	S	182/203 (89%)	-0.13	1 (0%) 91 90	26, 35, 61, 97	0
1	T	181/203 (89%)	-0.03	3 (1%) 70 68	27, 37, 58, 73	0
2	H	3/7 (42%)	3.04	2 (66%) 0 0	39, 39, 43, 45	3 (100%)
2	J	3/7 (42%)	1.12	0 100 100	24, 24, 26, 26	3 (100%)
2	O	3/7 (42%)	2.14	1 (33%) 0 0	35, 35, 38, 45	3 (100%)
2	P	3/7 (42%)	1.93	1 (33%) 0 0	27, 27, 30, 31	3 (100%)
2	Q	3/7 (42%)	1.20	1 (33%) 0 0	34, 34, 34, 38	3 (100%)
2	R	3/7 (42%)	3.08	2 (66%) 0 0	40, 40, 42, 47	3 (100%)
2	U	3/7 (42%)	1.90	1 (33%) 0 0	29, 29, 30, 34	3 (100%)
2	V	3/7 (42%)	3.19	2 (66%) 0 0	37, 37, 39, 42	3 (100%)
2	X	3/7 (42%)	2.14	2 (66%) 0 0	44, 44, 45, 46	3 (100%)
2	Y	3/7 (42%)	2.84	2 (66%) 0 0	46, 46, 48, 50	3 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
2	Z	3/7 (42%)	2.44	2 (66%) 0 0	41, 41, 47, 50	3 (100%)
All	All	2581/2919 (88%)	-0.10	52 (2%) 65 63	13, 32, 55, 97	33 (1%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	17	ALA	7.7
2	R	6	ALA	5.6
2	Y	6	ALA	4.9
1	B	17	ALA	4.8
2	V	4	PRO	4.1
2	H	4	PRO	4.1
2	Z	6	ALA	3.9
2	U	6	ALA	3.9
2	P	6	ALA	3.9
1	T	18	TYR	3.9
1	F	8	ILE	3.8
2	V	6	ALA	3.8
2	O	6	ALA	3.7
2	H	6	ALA	3.7
1	F	7	VAL	3.7
1	I	18	TYR	3.7
1	E	18	TYR	3.6
1	F	6	THR	3.4
1	M	18	TYR	3.4
1	D	17	ALA	3.4
1	T	3	LEU	3.4
1	S	8	ILE	3.3
1	A	194	THR	3.0
2	Z	4	PRO	3.0
1	I	17	ALA	3.0
1	M	3	LEU	2.7
1	A	17	ALA	2.7
1	B	18	TYR	2.7
1	G	18	TYR	2.7
1	L	16	ARG	2.6
1	L	8	ILE	2.6
2	Y	4	PRO	2.5
1	N	18	TYR	2.5
1	M	7	VAL	2.5
1	E	192	PRO	2.5
2	X	6	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	18	TYR	2.4
1	G	8	ILE	2.3
2	X	4	PRO	2.3
2	Q	6	ALA	2.2
1	B	16	ARG	2.2
1	N	7	VAL	2.2
1	T	162	ILE	2.2
1	K	17	ALA	2.2
2	R	4	PRO	2.1
1	M	6	THR	2.1
1	G	57	GLU	2.1
1	A	56	SER	2.1
1	N	8	ILE	2.0
1	L	63	TYR	2.0
1	A	4	ILE	2.0
1	K	8	ILE	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	MP8	O	7	8/9	0.56	0.33	30,34,37,37	8
2	MP8	P	7	8/9	0.58	0.33	25,27,29,29	8
2	MP8	U	7	8/9	0.62	0.37	22,25,28,30	8
2	YCP	O	5	8/9	0.63	0.24	43,44,45,45	8
2	WFP	O	2	13/14	0.63	0.43	22,26,32,35	13
2	MP8	X	7	8/9	0.64	0.33	39,43,46,47	8
2	YCP	V	5	8/9	0.65	0.27	37,40,40,42	8
2	YCP	Y	5	8/9	0.65	0.22	43,45,46,48	8
2	WFP	X	2	13/14	0.65	0.39	25,29,35,36	13
2	MP8	V	7	8/9	0.69	0.36	34,37,39,39	8
2	YCP	Z	5	8/9	0.69	0.23	47,49,50,50	8
2	YCP	Q	5	8/9	0.70	0.23	31,37,38,38	8
2	WFP	V	2	13/14	0.74	0.41	20,23,31,35	13
2	YCP	J	5	8/9	0.74	0.27	24,27,28,28	8
2	MP8	R	7	8/9	0.75	0.25	37,39,40,40	8
2	MP8	Q	7	8/9	0.76	0.22	27,30,32,32	8
2	MP8	Z	7	8/9	0.76	0.27	42,44,46,46	8

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	YCP	R	5	8/9	0.77	0.25	37,46,49,50	8
2	WFP	U	2	13/14	0.77	0.40	16,19,26,27	13
2	WFP	P	2	13/14	0.77	0.38	20,22,26,27	13
2	WFP	R	2	13/14	0.78	0.36	30,32,36,36	13
2	WFP	Z	2	13/14	0.78	0.39	27,30,34,35	13
2	YCP	H	5	8/9	0.78	0.33	42,44,44,44	8
2	MP8	J	7	8/9	0.79	0.25	25,25,27,27	8
2	WFP	Q	2	13/14	0.82	0.29	25,26,30,31	13
2	WFP	Y	2	13/14	0.82	0.39	26,29,36,38	13
2	YCP	U	5	8/9	0.84	0.23	31,35,37,37	8
2	WFP	J	2	13/14	0.84	0.33	13,16,18,20	13
2	MP8	H	7	8/9	0.84	0.30	40,42,42,43	8
2	YCP	P	5	8/9	0.85	0.21	26,28,29,30	8
2	WFP	H	2	13/14	0.86	0.33	24,26,34,36	13
2	MP8	Y	7	8/9	0.88	0.25	43,44,45,46	8
2	YCP	X	5	8/9	0.88	0.15	33,42,45,45	8

### 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	MPD	E	400	8/8	0.73	0.25	36,41,46,50	0
3	MPD	M	400	8/8	0.74	0.25	38,44,46,50	0
3	MPD	N	400	8/8	0.79	0.21	41,44,49,60	0
3	MPD	T	400	8/8	0.83	0.22	41,48,50,57	0
3	MPD	K	400	8/8	0.84	0.21	33,38,40,49	0
3	MPD	A	400	8/8	0.84	0.26	43,49,54,64	0
3	MPD	L	400	8/8	0.85	0.17	31,36,42,54	0
3	MPD	G	400	8/8	0.85	0.24	52,59,63,67	0
3	MPD	S	400	8/8	0.88	0.21	38,47,51,59	0
3	MPD	F	400	8/8	0.89	0.16	40,50,56,61	0
3	MPD	C	400	8/8	0.89	0.19	27,36,38,46	0
3	MPD	D	400	8/8	0.90	0.21	31,39,46,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MPD	I	400	8/8	0.90	0.20	38,44,47,56	0
3	MPD	B	400	8/8	0.91	0.19	32,39,45,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.