



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 30, 2018 – 10:38 AM EDT

PDB ID : 6CFD  
Title : ADEP4 bound to E. faecium ClpP  
Authors : Lee, R.E.; Griffith, E.C.  
Deposited on : 2018-02-14  
Resolution : 2.57 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](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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : rb-20031172  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031172

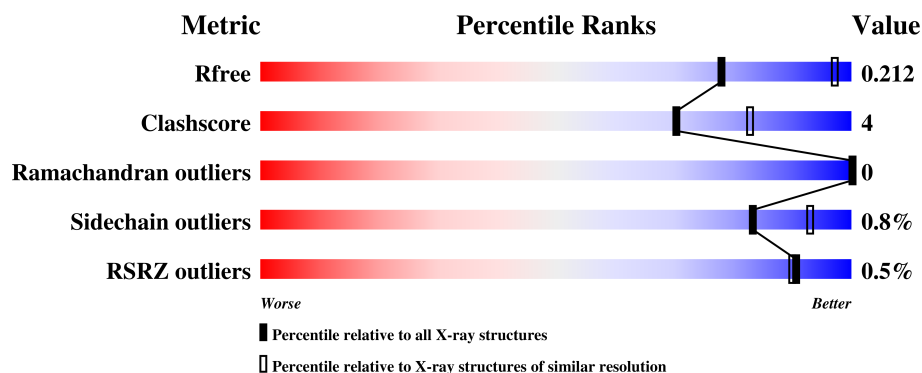
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.57 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))
$R_{free}$	111664	3182 (2.60-2.56)
Clashscore	122126	3541 (2.60-2.56)
Ramachandran outliers	120053	3489 (2.60-2.56)
Sidechain outliers	120020	3489 (2.60-2.56)
RSRZ outliers	108989	3120 (2.60-2.56)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	210	<div> <div>80%</div> <div>6%</div> <div>14%</div> </div>
1	B	210	<div> <div>83%</div> <div>•</div> <div>13%</div> </div>
1	C	210	<div> <div>%</div> <div>80%</div> <div>5%</div> <div>14%</div> </div>
1	D	210	<div> <div>81%</div> <div>•</div> <div>14%</div> </div>
1	E	210	<div> <div>81%</div> <div>6%</div> <div>12%</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	210	 83% 13%
1	G	210	 82% 5% 13%
1	I	210	 2% 82% 7% 10%
1	K	210	 82% 5% 13%
1	L	210	 79% 7% 14%
1	M	210	 81% 5% 14%
1	N	210	 82% 5% 13%
1	S	210	 81% 5% 14%
1	T	210	 80% 7% 14%

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	MPD	A	401	-	-	X	-
2	MPD	C	401	-	-	X	-
2	MPD	E	401	-	-	X	-
2	MPD	I	401	-	-	X	-
2	MPD	K	401	-	-	X	-
3	EZA	A	402	X	-	-	-
3	EZA	C	402	X	-	-	-
3	EZA	D	402	X	-	-	-
3	EZA	E	402	X	-	-	-
3	EZA	F	402	X	-	-	-
3	EZA	I	402	X	-	-	X
3	EZA	L	402	X	-	-	-
3	EZA	M	402	X	-	-	-
3	EZA	N	402	X	-	-	-
3	EZA	S	402	X	-	-	X
3	EZA	T	402	X	-	-	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20070 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	181	Total	C	N	O	S	0	0	0
			1370	862	231	268	9			
1	B	182	Total	C	N	O	S	0	0	0
			1375	864	231	271	9			
1	C	180	Total	C	N	O	S	0	0	0
			1361	856	229	267	9			
1	D	181	Total	C	N	O	S	0	0	0
			1362	856	229	268	9			
1	E	184	Total	C	N	O	S	0	0	0
			1385	871	234	271	9			
1	F	183	Total	C	N	O	S	0	0	0
			1380	868	233	270	9			
1	G	182	Total	C	N	O	S	0	0	0
			1367	859	230	269	9			
1	I	188	Total	C	N	O	S	0	0	0
			1405	881	237	278	9			
1	K	183	Total	C	N	O	S	0	0	0
			1380	868	233	270	9			
1	L	180	Total	C	N	O	S	0	0	0
			1361	855	228	269	9			
1	M	181	Total	C	N	O	S	0	0	0
			1370	862	231	268	9			
1	N	182	Total	C	N	O	S	0	0	0
			1371	862	231	269	9			
1	S	180	Total	C	N	O	S	0	0	0
			1357	853	228	267	9			
1	T	181	Total	C	N	O	S	0	0	0
			1370	862	231	268	9			

There are 196 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	197	LYS	-	expression tag	UNP A0A133CH35

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	198	ILE	-	expression tag	UNP A0A133CH35
A	199	GLU	-	expression tag	UNP A0A133CH35
A	200	GLY	-	expression tag	UNP A0A133CH35
A	201	ARG	-	expression tag	UNP A0A133CH35
A	202	GLY	-	expression tag	UNP A0A133CH35
A	203	LEU	-	expression tag	UNP A0A133CH35
A	204	GLU	-	expression tag	UNP A0A133CH35
A	205	HIS	-	expression tag	UNP A0A133CH35
A	206	HIS	-	expression tag	UNP A0A133CH35
A	207	HIS	-	expression tag	UNP A0A133CH35
A	208	HIS	-	expression tag	UNP A0A133CH35
A	209	HIS	-	expression tag	UNP A0A133CH35
A	210	HIS	-	expression tag	UNP A0A133CH35
B	197	LYS	-	expression tag	UNP A0A133CH35
B	198	ILE	-	expression tag	UNP A0A133CH35
B	199	GLU	-	expression tag	UNP A0A133CH35
B	200	GLY	-	expression tag	UNP A0A133CH35
B	201	ARG	-	expression tag	UNP A0A133CH35
B	202	GLY	-	expression tag	UNP A0A133CH35
B	203	LEU	-	expression tag	UNP A0A133CH35
B	204	GLU	-	expression tag	UNP A0A133CH35
B	205	HIS	-	expression tag	UNP A0A133CH35
B	206	HIS	-	expression tag	UNP A0A133CH35
B	207	HIS	-	expression tag	UNP A0A133CH35
B	208	HIS	-	expression tag	UNP A0A133CH35
B	209	HIS	-	expression tag	UNP A0A133CH35
B	210	HIS	-	expression tag	UNP A0A133CH35
C	197	LYS	-	expression tag	UNP A0A133CH35
C	198	ILE	-	expression tag	UNP A0A133CH35
C	199	GLU	-	expression tag	UNP A0A133CH35
C	200	GLY	-	expression tag	UNP A0A133CH35
C	201	ARG	-	expression tag	UNP A0A133CH35
C	202	GLY	-	expression tag	UNP A0A133CH35
C	203	LEU	-	expression tag	UNP A0A133CH35
C	204	GLU	-	expression tag	UNP A0A133CH35
C	205	HIS	-	expression tag	UNP A0A133CH35
C	206	HIS	-	expression tag	UNP A0A133CH35
C	207	HIS	-	expression tag	UNP A0A133CH35
C	208	HIS	-	expression tag	UNP A0A133CH35
C	209	HIS	-	expression tag	UNP A0A133CH35
C	210	HIS	-	expression tag	UNP A0A133CH35
D	197	LYS	-	expression tag	UNP A0A133CH35

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	198	ILE	-	expression tag	UNP A0A133CH35
D	199	GLU	-	expression tag	UNP A0A133CH35
D	200	GLY	-	expression tag	UNP A0A133CH35
D	201	ARG	-	expression tag	UNP A0A133CH35
D	202	GLY	-	expression tag	UNP A0A133CH35
D	203	LEU	-	expression tag	UNP A0A133CH35
D	204	GLU	-	expression tag	UNP A0A133CH35
D	205	HIS	-	expression tag	UNP A0A133CH35
D	206	HIS	-	expression tag	UNP A0A133CH35
D	207	HIS	-	expression tag	UNP A0A133CH35
D	208	HIS	-	expression tag	UNP A0A133CH35
D	209	HIS	-	expression tag	UNP A0A133CH35
D	210	HIS	-	expression tag	UNP A0A133CH35
E	197	LYS	-	expression tag	UNP A0A133CH35
E	198	ILE	-	expression tag	UNP A0A133CH35
E	199	GLU	-	expression tag	UNP A0A133CH35
E	200	GLY	-	expression tag	UNP A0A133CH35
E	201	ARG	-	expression tag	UNP A0A133CH35
E	202	GLY	-	expression tag	UNP A0A133CH35
E	203	LEU	-	expression tag	UNP A0A133CH35
E	204	GLU	-	expression tag	UNP A0A133CH35
E	205	HIS	-	expression tag	UNP A0A133CH35
E	206	HIS	-	expression tag	UNP A0A133CH35
E	207	HIS	-	expression tag	UNP A0A133CH35
E	208	HIS	-	expression tag	UNP A0A133CH35
E	209	HIS	-	expression tag	UNP A0A133CH35
E	210	HIS	-	expression tag	UNP A0A133CH35
F	197	LYS	-	expression tag	UNP A0A133CH35
F	198	ILE	-	expression tag	UNP A0A133CH35
F	199	GLU	-	expression tag	UNP A0A133CH35
F	200	GLY	-	expression tag	UNP A0A133CH35
F	201	ARG	-	expression tag	UNP A0A133CH35
F	202	GLY	-	expression tag	UNP A0A133CH35
F	203	LEU	-	expression tag	UNP A0A133CH35
F	204	GLU	-	expression tag	UNP A0A133CH35
F	205	HIS	-	expression tag	UNP A0A133CH35
F	206	HIS	-	expression tag	UNP A0A133CH35
F	207	HIS	-	expression tag	UNP A0A133CH35
F	208	HIS	-	expression tag	UNP A0A133CH35
F	209	HIS	-	expression tag	UNP A0A133CH35
F	210	HIS	-	expression tag	UNP A0A133CH35
G	197	LYS	-	expression tag	UNP A0A133CH35

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
G	198	ILE	-	expression tag	UNP A0A133CH35
G	199	GLU	-	expression tag	UNP A0A133CH35
G	200	GLY	-	expression tag	UNP A0A133CH35
G	201	ARG	-	expression tag	UNP A0A133CH35
G	202	GLY	-	expression tag	UNP A0A133CH35
G	203	LEU	-	expression tag	UNP A0A133CH35
G	204	GLU	-	expression tag	UNP A0A133CH35
G	205	HIS	-	expression tag	UNP A0A133CH35
G	206	HIS	-	expression tag	UNP A0A133CH35
G	207	HIS	-	expression tag	UNP A0A133CH35
G	208	HIS	-	expression tag	UNP A0A133CH35
G	209	HIS	-	expression tag	UNP A0A133CH35
G	210	HIS	-	expression tag	UNP A0A133CH35
I	197	LYS	-	expression tag	UNP A0A133CH35
I	198	ILE	-	expression tag	UNP A0A133CH35
I	199	GLU	-	expression tag	UNP A0A133CH35
I	200	GLY	-	expression tag	UNP A0A133CH35
I	201	ARG	-	expression tag	UNP A0A133CH35
I	202	GLY	-	expression tag	UNP A0A133CH35
I	203	LEU	-	expression tag	UNP A0A133CH35
I	204	GLU	-	expression tag	UNP A0A133CH35
I	205	HIS	-	expression tag	UNP A0A133CH35
I	206	HIS	-	expression tag	UNP A0A133CH35
I	207	HIS	-	expression tag	UNP A0A133CH35
I	208	HIS	-	expression tag	UNP A0A133CH35
I	209	HIS	-	expression tag	UNP A0A133CH35
I	210	HIS	-	expression tag	UNP A0A133CH35
K	197	LYS	-	expression tag	UNP A0A133CH35
K	198	ILE	-	expression tag	UNP A0A133CH35
K	199	GLU	-	expression tag	UNP A0A133CH35
K	200	GLY	-	expression tag	UNP A0A133CH35
K	201	ARG	-	expression tag	UNP A0A133CH35
K	202	GLY	-	expression tag	UNP A0A133CH35
K	203	LEU	-	expression tag	UNP A0A133CH35
K	204	GLU	-	expression tag	UNP A0A133CH35
K	205	HIS	-	expression tag	UNP A0A133CH35
K	206	HIS	-	expression tag	UNP A0A133CH35
K	207	HIS	-	expression tag	UNP A0A133CH35
K	208	HIS	-	expression tag	UNP A0A133CH35
K	209	HIS	-	expression tag	UNP A0A133CH35
K	210	HIS	-	expression tag	UNP A0A133CH35
L	197	LYS	-	expression tag	UNP A0A133CH35

*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
L	198	ILE	-	expression tag	UNP A0A133CH35
L	199	GLU	-	expression tag	UNP A0A133CH35
L	200	GLY	-	expression tag	UNP A0A133CH35
L	201	ARG	-	expression tag	UNP A0A133CH35
L	202	GLY	-	expression tag	UNP A0A133CH35
L	203	LEU	-	expression tag	UNP A0A133CH35
L	204	GLU	-	expression tag	UNP A0A133CH35
L	205	HIS	-	expression tag	UNP A0A133CH35
L	206	HIS	-	expression tag	UNP A0A133CH35
L	207	HIS	-	expression tag	UNP A0A133CH35
L	208	HIS	-	expression tag	UNP A0A133CH35
L	209	HIS	-	expression tag	UNP A0A133CH35
L	210	HIS	-	expression tag	UNP A0A133CH35
M	197	LYS	-	expression tag	UNP A0A133CH35
M	198	ILE	-	expression tag	UNP A0A133CH35
M	199	GLU	-	expression tag	UNP A0A133CH35
M	200	GLY	-	expression tag	UNP A0A133CH35
M	201	ARG	-	expression tag	UNP A0A133CH35
M	202	GLY	-	expression tag	UNP A0A133CH35
M	203	LEU	-	expression tag	UNP A0A133CH35
M	204	GLU	-	expression tag	UNP A0A133CH35
M	205	HIS	-	expression tag	UNP A0A133CH35
M	206	HIS	-	expression tag	UNP A0A133CH35
M	207	HIS	-	expression tag	UNP A0A133CH35
M	208	HIS	-	expression tag	UNP A0A133CH35
M	209	HIS	-	expression tag	UNP A0A133CH35
M	210	HIS	-	expression tag	UNP A0A133CH35
N	197	LYS	-	expression tag	UNP A0A133CH35
N	198	ILE	-	expression tag	UNP A0A133CH35
N	199	GLU	-	expression tag	UNP A0A133CH35
N	200	GLY	-	expression tag	UNP A0A133CH35
N	201	ARG	-	expression tag	UNP A0A133CH35
N	202	GLY	-	expression tag	UNP A0A133CH35
N	203	LEU	-	expression tag	UNP A0A133CH35
N	204	GLU	-	expression tag	UNP A0A133CH35
N	205	HIS	-	expression tag	UNP A0A133CH35
N	206	HIS	-	expression tag	UNP A0A133CH35
N	207	HIS	-	expression tag	UNP A0A133CH35
N	208	HIS	-	expression tag	UNP A0A133CH35
N	209	HIS	-	expression tag	UNP A0A133CH35
N	210	HIS	-	expression tag	UNP A0A133CH35
S	197	LYS	-	expression tag	UNP A0A133CH35

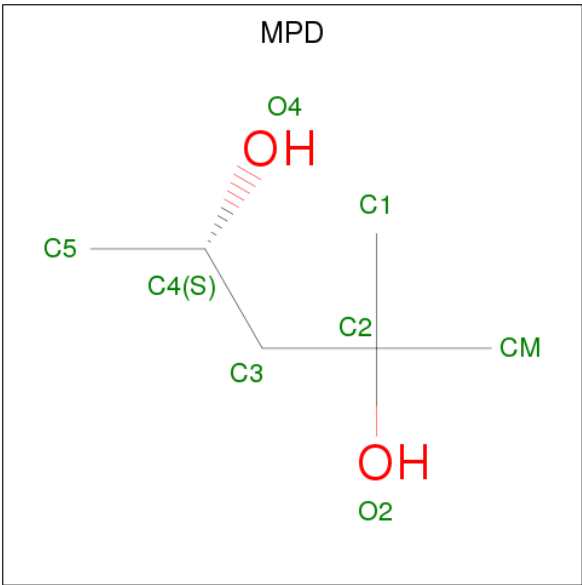
*Continued on next page...*



*Continued from previous page...*

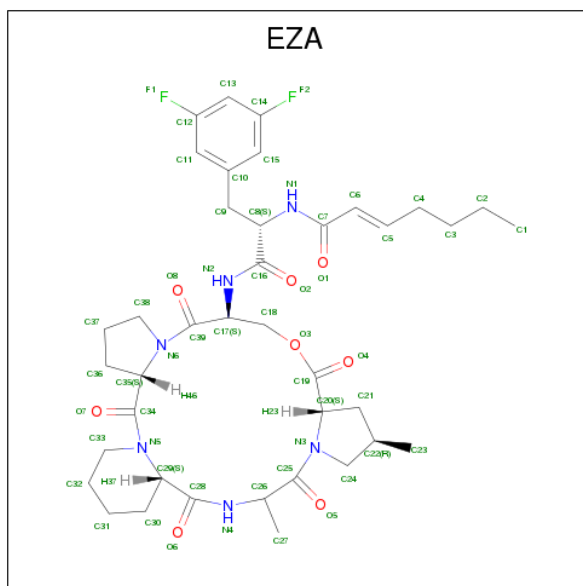
Chain	Residue	Modelled	Actual	Comment	Reference
S	198	ILE	-	expression tag	UNP A0A133CH35
S	199	GLU	-	expression tag	UNP A0A133CH35
S	200	GLY	-	expression tag	UNP A0A133CH35
S	201	ARG	-	expression tag	UNP A0A133CH35
S	202	GLY	-	expression tag	UNP A0A133CH35
S	203	LEU	-	expression tag	UNP A0A133CH35
S	204	GLU	-	expression tag	UNP A0A133CH35
S	205	HIS	-	expression tag	UNP A0A133CH35
S	206	HIS	-	expression tag	UNP A0A133CH35
S	207	HIS	-	expression tag	UNP A0A133CH35
S	208	HIS	-	expression tag	UNP A0A133CH35
S	209	HIS	-	expression tag	UNP A0A133CH35
S	210	HIS	-	expression tag	UNP A0A133CH35
T	197	LYS	-	expression tag	UNP A0A133CH35
T	198	ILE	-	expression tag	UNP A0A133CH35
T	199	GLU	-	expression tag	UNP A0A133CH35
T	200	GLY	-	expression tag	UNP A0A133CH35
T	201	ARG	-	expression tag	UNP A0A133CH35
T	202	GLY	-	expression tag	UNP A0A133CH35
T	203	LEU	-	expression tag	UNP A0A133CH35
T	204	GLU	-	expression tag	UNP A0A133CH35
T	205	HIS	-	expression tag	UNP A0A133CH35
T	206	HIS	-	expression tag	UNP A0A133CH35
T	207	HIS	-	expression tag	UNP A0A133CH35
T	208	HIS	-	expression tag	UNP A0A133CH35
T	209	HIS	-	expression tag	UNP A0A133CH35
T	210	HIS	-	expression tag	UNP A0A133CH35

- Molecule 2 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
2	A	1	Total	C	O	0	0
			8	6	2		
2	B	1	Total	C	O	0	0
			8	6	2		
2	C	1	Total	C	O	0	0
			8	6	2		
2	D	1	Total	C	O	0	0
			8	6	2		
2	E	1	Total	C	O	0	0
			8	6	2		
2	F	1	Total	C	O	0	0
			8	6	2		
2	G	1	Total	C	O	0	0
			8	6	2		
2	I	1	Total	C	O	0	0
			8	6	2		
2	K	1	Total	C	O	0	0
			8	6	2		
2	L	1	Total	C	O	0	0
			8	6	2		
2	M	1	Total	C	O	0	0
			8	6	2		
2	N	1	Total	C	O	0	0
			8	6	2		
2	S	1	Total	C	O	0	0
			8	6	2		
2	T	1	Total	C	O	0	0
			8	6	2		

- Molecule 3 is N-[(6aS,12S,15aS,17R,21R,23aS)-17,21-dimethyl-6,11,15,20,23-pentaoxooctadecahydro-2H,6H,11H,15H-pyrido[2,1-i]dipyrrolo[2,1-c:2',1'-l][1,4,7,10,13]oxatetraazacyclohexadecin-12-yl]-3,5-difluoro-Nalpha-[(2E)-hept-2-enoyl]-L-phenylalaninamide (three-letter code: EZA) (formula: C<sub>39</sub>H<sub>52</sub>F<sub>2</sub>N<sub>6</sub>O<sub>8</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 55	C 39	F 2	N 6	O 8	0	0
3	C	1	Total 55	C 39	F 2	N 6	O 8	0	0
3	D	1	Total 55	C 39	F 2	N 6	O 8	0	0
3	E	1	Total 55	C 39	F 2	N 6	O 8	0	0
3	F	1	Total 55	C 39	F 2	N 6	O 8	0	0
3	I	1	Total 55	C 39	F 2	N 6	O 8	0	0
3	L	1	Total 55	C 39	F 2	N 6	O 8	0	0
3	M	1	Total 55	C 39	F 2	N 6	O 8	0	0
3	N	1	Total 55	C 39	F 2	N 6	O 8	0	0
3	S	1	Total 55	C 39	F 2	N 6	O 8	0	0
3	T	1	Total 55	C 39	F 2	N 6	O 8	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	9	Total O 9 9	0	0
4	B	11	Total O 11 11	0	0
4	C	8	Total O 8 8	0	0
4	D	8	Total O 8 8	0	0
4	E	6	Total O 6 6	0	0
4	F	11	Total O 11 11	0	0
4	G	15	Total O 15 15	0	0
4	I	9	Total O 9 9	0	0
4	K	14	Total O 14 14	0	0
4	L	10	Total O 10 10	0	0
4	M	7	Total O 7 7	0	0
4	N	12	Total O 12 12	0	0
4	S	13	Total O 13 13	0	0
4	T	6	Total O 6 6	0	0





- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain G: 82% 5% 13%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain I: 82% 7% 10%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain K: 82% 5% 13%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain L: 79% 7% 14%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain M: 81% 5% 14%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain N: 82% 5% 13%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain S: 

81%

5%

14%



● Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain T: 

80%

7%

14%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.39Å 202.17Å 97.39Å 90.00° 102.69° 90.00°	Depositor
Resolution (Å)	101.08 – 2.57 47.50 – 2.57	Depositor EDS
% Data completeness (in resolution range)	98.9 (101.08-2.57) 99.0 (47.50-2.57)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 2.58Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.175 , 0.209 0.179 , 0.212	Depositor DCC
$R_{free}$ test set	5708 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.9	Xtriage
Anisotropy	0.569	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 29.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.176 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	20070	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, EZA

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	0.67	0/1386	0.80	1/1875 (0.1%)
1	B	0.75	0/1391	0.79	0/1883
1	C	0.74	0/1377	0.82	0/1864
1	D	0.73	0/1378	0.80	0/1867
1	E	0.71	0/1401	0.77	1/1896 (0.1%)
1	F	0.71	0/1396	0.81	0/1889
1	G	0.73	0/1383	0.78	0/1874
1	I	0.74	0/1421	0.81	0/1924
1	K	0.74	0/1396	0.80	0/1889
1	L	0.72	0/1377	0.80	0/1865
1	M	0.71	0/1386	0.80	0/1875
1	N	0.68	0/1387	0.78	0/1878
1	S	0.74	0/1373	0.80	0/1860
1	T	0.74	0/1386	0.81	0/1875
All	All	0.72	0/19438	0.80	2/26314 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	93	MET	CG-SD-CE	-7.94	87.50	100.20
1	E	79	ASP	CB-CG-OD1	5.03	122.82	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1370	0	1363	15	0
1	B	1375	0	1358	8	0
1	C	1361	0	1347	12	0
1	D	1362	0	1341	10	0
1	E	1385	0	1369	13	0
1	F	1380	0	1367	7	0
1	G	1367	0	1343	8	0
1	I	1405	0	1374	13	0
1	K	1380	0	1367	10	0
1	L	1361	0	1343	10	0
1	M	1370	0	1363	8	0
1	N	1371	0	1354	5	0
1	S	1357	0	1339	10	0
1	T	1370	0	1363	11	0
2	A	8	0	14	6	0
2	B	8	0	14	5	0
2	C	8	0	14	7	0
2	D	8	0	14	4	0
2	E	8	0	14	7	0
2	F	8	0	14	4	0
2	G	8	0	14	5	0
2	I	8	0	14	6	0
2	K	8	0	14	6	0
2	L	8	0	14	4	0
2	M	8	0	14	4	0
2	N	8	0	14	2	0
2	S	8	0	14	5	0
2	T	8	0	14	4	0
3	A	55	0	0	3	0
3	C	55	0	0	0	0
3	D	55	0	0	1	0
3	E	55	0	0	0	0
3	F	55	0	0	0	0
3	I	55	0	0	0	0
3	L	55	0	0	0	0
3	M	55	0	0	1	0
3	N	55	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	S	55	0	0	2	0
3	T	55	0	0	0	0
4	A	9	0	0	1	0
4	B	11	0	0	0	0
4	C	8	0	0	0	0
4	D	8	0	0	0	0
4	E	6	0	0	0	0
4	F	11	0	0	0	0
4	G	15	0	0	0	0
4	I	9	0	0	0	0
4	K	14	0	0	1	0
4	L	10	0	0	0	0
4	M	7	0	0	0	0
4	N	12	0	0	0	0
4	S	13	0	0	0	0
4	T	6	0	0	0	0
All	All	20070	0	19187	154	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 4.

The worst 5 of 154 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:147:ARG:HD2	4:K:513:HOH:O	1.80	0.80
1:B:99:MET:HE2	2:B:401:MPD:C1	2.19	0.73
1:S:99:MET:HE2	2:S:401:MPD:H12	1.72	0.71
2:B:401:MPD:HM2	2:B:401:MPD:H52	1.73	0.69
1:S:98:SER:HA	2:S:401:MPD:H32	1.75	0.68

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	177/210 (84%)	174 (98%)	3 (2%)	0	100	100
1	B	178/210 (85%)	175 (98%)	3 (2%)	0	100	100
1	C	176/210 (84%)	173 (98%)	3 (2%)	0	100	100
1	D	177/210 (84%)	173 (98%)	4 (2%)	0	100	100
1	E	180/210 (86%)	177 (98%)	3 (2%)	0	100	100
1	F	179/210 (85%)	177 (99%)	2 (1%)	0	100	100
1	G	178/210 (85%)	175 (98%)	3 (2%)	0	100	100
1	I	184/210 (88%)	181 (98%)	3 (2%)	0	100	100
1	K	179/210 (85%)	175 (98%)	4 (2%)	0	100	100
1	L	176/210 (84%)	173 (98%)	3 (2%)	0	100	100
1	M	177/210 (84%)	174 (98%)	3 (2%)	0	100	100
1	N	178/210 (85%)	175 (98%)	3 (2%)	0	100	100
1	S	176/210 (84%)	174 (99%)	2 (1%)	0	100	100
1	T	177/210 (84%)	175 (99%)	2 (1%)	0	100	100
All	All	2492/2940 (85%)	2451 (98%)	41 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	142/174 (82%)	141 (99%)	1 (1%)	85	94
1	B	142/174 (82%)	141 (99%)	1 (1%)	85	94
1	C	141/174 (81%)	140 (99%)	1 (1%)	85	94
1	D	140/174 (80%)	139 (99%)	1 (1%)	85	94
1	E	142/174 (82%)	141 (99%)	1 (1%)	85	94

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	142/174 (82%)	141 (99%)	1 (1%)	85	94
1	G	140/174 (80%)	139 (99%)	1 (1%)	85	94
1	I	143/174 (82%)	141 (99%)	2 (1%)	69	86
1	K	142/174 (82%)	141 (99%)	1 (1%)	85	94
1	L	141/174 (81%)	140 (99%)	1 (1%)	85	94
1	M	142/174 (82%)	141 (99%)	1 (1%)	85	94
1	N	141/174 (81%)	140 (99%)	1 (1%)	85	94
1	S	140/174 (80%)	139 (99%)	1 (1%)	85	94
1	T	142/174 (82%)	141 (99%)	1 (1%)	85	94
All	All	1980/2436 (81%)	1965 (99%)	15 (1%)	83	93

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	123	HIS
1	I	11	SER
1	N	123	HIS
1	F	123	HIS
1	M	123	HIS

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

25 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
2	MPD	A	401	-	7,7,7	0.46	0	9,10,10	0.26	0
3	EZA	A	402	-	59,59,59	2.76	16 (27%)	81,83,83	1.90	14 (17%)
2	MPD	B	401	-	7,7,7	0.46	0	9,10,10	0.77	0
2	MPD	C	401	-	7,7,7	0.77	0	9,10,10	1.03	1 (11%)
3	EZA	C	402	-	59,59,59	2.78	17 (28%)	81,83,83	2.37	26 (32%)
2	MPD	D	401	-	7,7,7	0.42	0	9,10,10	0.45	0
3	EZA	D	402	-	59,59,59	2.77	16 (27%)	81,83,83	2.22	17 (20%)
2	MPD	E	401	-	7,7,7	0.59	0	9,10,10	0.67	0
3	EZA	E	402	-	59,59,59	2.72	14 (23%)	81,83,83	2.41	21 (25%)
2	MPD	F	401	-	7,7,7	0.50	0	9,10,10	0.76	0
3	EZA	F	402	-	59,59,59	2.85	16 (27%)	81,83,83	2.15	19 (23%)
2	MPD	G	401	-	7,7,7	0.63	0	9,10,10	1.30	1 (11%)
2	MPD	I	401	-	7,7,7	0.44	0	9,10,10	0.54	0
3	EZA	I	402	-	59,59,59	2.65	17 (28%)	81,83,83	2.46	24 (29%)
2	MPD	K	401	-	7,7,7	0.63	0	9,10,10	0.85	1 (11%)
2	MPD	L	401	-	7,7,7	0.53	0	9,10,10	0.75	0
3	EZA	L	402	-	59,59,59	2.77	14 (23%)	81,83,83	2.16	20 (24%)
2	MPD	M	401	-	7,7,7	0.38	0	9,10,10	0.96	1 (11%)
3	EZA	M	402	-	59,59,59	2.82	17 (28%)	81,83,83	2.41	22 (27%)
2	MPD	N	401	-	7,7,7	0.72	0	9,10,10	0.95	1 (11%)
3	EZA	N	402	-	59,59,59	2.83	17 (28%)	81,83,83	2.25	23 (28%)
2	MPD	S	401	-	7,7,7	0.69	0	9,10,10	0.76	0
3	EZA	S	402	-	59,59,59	2.74	18 (30%)	81,83,83	2.31	31 (38%)
2	MPD	T	401	-	7,7,7	0.78	0	9,10,10	0.90	0
3	EZA	T	402	-	59,59,59	2.79	17 (28%)	81,83,83	2.31	19 (23%)

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	MPD	A	401	-	-	0/5/5/5	0/0/0/0
3	EZA	A	402	-	1/1/17/22	0/63/96/96	0/4/5/5
2	MPD	B	401	-	-	0/5/5/5	0/0/0/0
2	MPD	C	401	-	-	0/5/5/5	0/0/0/0
3	EZA	C	402	-	2/2/17/22	0/63/96/96	0/4/5/5
2	MPD	D	401	-	-	0/5/5/5	0/0/0/0
3	EZA	D	402	-	1/1/17/22	0/63/96/96	0/4/5/5
2	MPD	E	401	-	-	0/5/5/5	0/0/0/0
3	EZA	E	402	-	2/2/17/22	0/63/96/96	0/4/5/5
2	MPD	F	401	-	-	0/5/5/5	0/0/0/0
3	EZA	F	402	-	1/1/17/22	0/63/96/96	0/4/5/5
2	MPD	G	401	-	-	0/5/5/5	0/0/0/0
2	MPD	I	401	-	-	0/5/5/5	0/0/0/0
3	EZA	I	402	-	2/2/17/22	0/63/96/96	0/4/5/5
2	MPD	K	401	-	-	0/5/5/5	0/0/0/0
2	MPD	L	401	-	-	0/5/5/5	0/0/0/0
3	EZA	L	402	-	1/1/17/22	0/63/96/96	0/4/5/5
2	MPD	M	401	-	-	0/5/5/5	0/0/0/0
3	EZA	M	402	-	2/2/17/22	0/63/96/96	0/4/5/5
2	MPD	N	401	-	-	0/5/5/5	0/0/0/0
3	EZA	N	402	-	1/1/17/22	0/63/96/96	0/4/5/5
2	MPD	S	401	-	-	0/5/5/5	0/0/0/0
3	EZA	S	402	-	2/2/17/22	1/63/96/96	0/4/5/5
2	MPD	T	401	-	-	0/5/5/5	0/0/0/0
3	EZA	T	402	-	1/1/17/22	0/63/96/96	0/4/5/5

The worst 5 of 179 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	EZA	C20-C19	-7.83	1.37	1.52
3	F	402	EZA	C20-C19	-7.49	1.37	1.52
3	L	402	EZA	C20-C19	-7.45	1.37	1.52
3	N	402	EZA	C20-C19	-6.85	1.39	1.52
3	T	402	EZA	C20-C19	-6.63	1.39	1.52

The worst 5 of 241 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	402	EZA	C24-N3-C20	-6.55	101.87	111.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	402	EZA	C24-N3-C20	-6.52	101.91	111.70
3	I	402	EZA	C24-N3-C20	-6.49	101.96	111.70
3	T	402	EZA	C24-N3-C20	-6.37	102.14	111.70
3	N	402	EZA	C24-N3-C20	-6.33	102.19	111.70

5 of 16 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	N	402	EZA	C26
3	C	402	EZA	C26
3	C	402	EZA	C20
3	F	402	EZA	C26
3	D	402	EZA	C26

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	S	402	EZA	C18-O3-C19-C20

There are no ring outliers.

18 monomers are involved in 76 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	MPD	6	0
3	A	402	EZA	3	0
2	B	401	MPD	5	0
2	C	401	MPD	7	0
2	D	401	MPD	4	0
3	D	402	EZA	1	0
2	E	401	MPD	7	0
2	F	401	MPD	4	0
2	G	401	MPD	5	0
2	I	401	MPD	6	0
2	K	401	MPD	6	0
2	L	401	MPD	4	0
2	M	401	MPD	4	0
3	M	402	EZA	1	0
2	N	401	MPD	2	0
2	S	401	MPD	5	0
3	S	402	EZA	2	0
2	T	401	MPD	4	0

## 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<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	181/210 (86%)	-0.18	0 100 100	40, 53, 83, 104	0
1	B	182/210 (86%)	-0.17	1 (0%) 90 90	37, 50, 84, 106	0
1	C	180/210 (85%)	-0.08	2 (1%) 80 78	36, 49, 83, 108	0
1	D	181/210 (86%)	-0.19	0 100 100	38, 53, 84, 101	0
1	E	184/210 (87%)	-0.16	1 (0%) 90 90	37, 50, 87, 114	0
1	F	183/210 (87%)	-0.19	0 100 100	35, 49, 82, 110	0
1	G	182/210 (86%)	-0.18	0 100 100	36, 49, 81, 106	0
1	I	188/210 (89%)	-0.17	4 (2%) 63 60	36, 53, 90, 121	0
1	K	183/210 (87%)	-0.17	1 (0%) 90 90	36, 48, 87, 115	0
1	L	180/210 (85%)	-0.16	1 (0%) 89 88	36, 50, 82, 108	0
1	M	181/210 (86%)	-0.15	1 (0%) 89 88	36, 50, 83, 105	0
1	N	182/210 (86%)	-0.15	0 100 100	41, 53, 87, 109	0
1	S	180/210 (85%)	-0.15	0 100 100	37, 51, 80, 96	0
1	T	181/210 (86%)	-0.14	1 (0%) 89 88	35, 50, 81, 101	0
All	All	2548/2940 (86%)	-0.16	12 (0%) 90 90	35, 51, 85, 121	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	18	TYR	2.6
1	I	63	TYR	2.6
1	E	18	TYR	2.5
1	L	18	TYR	2.3
1	M	4	ILE	2.3

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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
3	EZA	I	402	55/55	0.75	0.49	93,132,159,187	0
3	EZA	S	402	55/55	0.79	0.55	96,135,177,184	0
3	EZA	N	402	55/55	0.80	0.39	98,127,147,158	0
3	EZA	M	402	55/55	0.82	0.42	96,129,159,162	0
3	EZA	D	402	55/55	0.83	0.43	85,118,141,147	0
3	EZA	C	402	55/55	0.83	0.33	84,111,147,153	0
3	EZA	T	402	55/55	0.85	0.36	84,111,135,138	0
3	EZA	E	402	55/55	0.86	0.36	92,116,138,177	0
2	MPD	B	401	8/8	0.90	0.22	65,68,73,79	0
3	EZA	F	402	55/55	0.91	0.43	77,102,123,130	0
3	EZA	L	402	55/55	0.91	0.49	80,101,122,130	0
2	MPD	D	401	8/8	0.92	0.30	72,77,80,82	0
2	MPD	C	401	8/8	0.92	0.27	51,68,74,80	0
2	MPD	I	401	8/8	0.93	0.31	65,71,76,78	0
3	EZA	A	402	55/55	0.94	0.28	64,78,93,98	0
2	MPD	F	401	8/8	0.94	0.38	58,68,74,76	0
2	MPD	M	401	8/8	0.94	0.28	55,68,69,73	0
2	MPD	L	401	8/8	0.94	0.26	57,64,66,73	0
2	MPD	T	401	8/8	0.94	0.30	66,76,83,85	0
2	MPD	E	401	8/8	0.95	0.24	68,74,82,84	0
2	MPD	S	401	8/8	0.95	0.30	63,65,78,79	0
2	MPD	K	401	8/8	0.95	0.23	67,69,72,74	0
2	MPD	N	401	8/8	0.95	0.26	62,67,70,75	0
2	MPD	G	401	8/8	0.95	0.24	58,60,66,67	0
2	MPD	A	401	8/8	0.96	0.37	65,68,71,71	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.