



# wwPDB X-ray Structure Validation Summary Report i

Feb 27, 2014 – 11:00 AM GMT

PDB ID : 3MT6  
Title : Structure of ClpP from Escherichia coli in complex with ADEP1  
Authors : Chung, Y.S.  
Deposited on : 2010-04-30  
Resolution : 1.90 Å(reported)

This is a wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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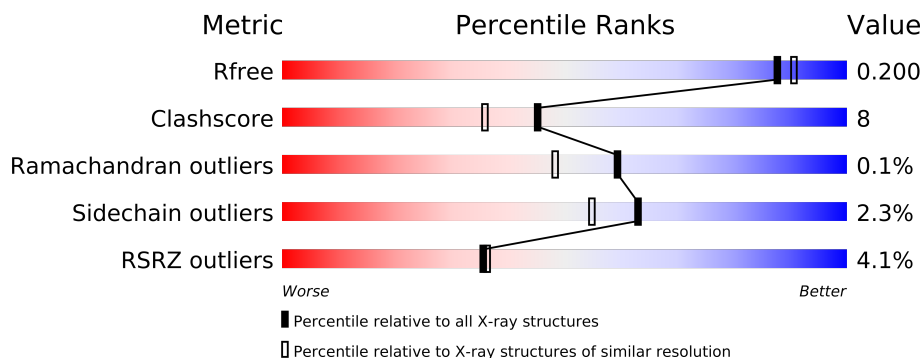
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.90 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))
$R_{free}$	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	207	
1	B	207	
1	C	207	
1	D	207	
1	E	207	
1	F	207	
1	G	207	
1	H	207	
1	I	207	
1	J	207	
1	K	207	
1	L	207	
1	M	207	
1	N	207	

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Mol	Chain	Length	Quality of chain
1	O	207	
1	P	207	
1	Q	207	
1	R	207	
1	S	207	
1	T	207	
1	U	207	
1	V	207	
1	W	207	
1	X	207	
1	Y	207	
1	Z	207	
1	a	207	
1	b	207	
2	1	7	
2	2	7	
2	3	7	
2	4	7	
2	c	7	
2	d	7	
2	e	7	
2	f	7	
2	g	7	
2	h	7	
2	i	7	
2	j	7	
2	k	7	
2	l	7	
2	m	7	
2	n	7	
2	o	7	
2	p	7	
2	q	7	
2	r	7	
2	s	7	
2	t	7	
2	u	7	
2	v	7	
2	w	7	
2	x	7	
2	y	7	
2	z	7	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	MPD	A	801	-	X
3	MPD	B	800	-	X
3	MPD	B	801	-	X
3	MPD	C	800	-	X
3	MPD	C	801	-	X
3	MPD	D	800	-	X
3	MPD	E	801	-	X
3	MPD	H	800	-	X
3	MPD	I	801	-	X
3	MPD	K	800	-	X
3	MPD	K	801	-	X
3	MPD	L	800	-	X
3	MPD	L	801	-	X
3	MPD	M	201	-	X
3	MPD	M	203	-	X
3	MPD	N	800	-	X
3	MPD	N	801	-	X
3	MPD	O	800	-	X
3	MPD	O	801	-	X
3	MPD	P	800	-	X
3	MPD	P	801	-	X
3	MPD	R	202	-	X
3	MPD	R	203	-	X
3	MPD	S	800	-	X
3	MPD	T	800	-	X
3	MPD	T	801	-	X
3	MPD	U	202	-	X
3	MPD	V	201	-	X
3	MPD	V	202	-	X
3	MPD	W	800	-	X
3	MPD	W	801	-	X
3	MPD	X	201	-	X
3	MPD	X	202	-	X
3	MPD	Y	800	-	X
3	MPD	Z	801	-	X
3	MPD	Z	802	-	X
3	MPD	Z	803	-	X
3	MPD	a	800	-	X
3	MPD	b	800	-	X
3	MPD	b	801	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 46463 atoms, of which 0 are hydrogen and 0 are deuterium.

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	R	180	Total	C	N	O	S	0	1	0
			1408	893	238	265	12			
1	S	184	Total	C	N	O	S	0	1	0
			1440	914	245	269	12			
1	T	186	Total	C	N	O	S	0	4	0
			1481	938	253	278	12			
1	U	186	Total	C	N	O	S	0	2	0
			1466	929	251	274	12			
1	O	189	Total	C	N	O	S	0	2	0
			1487	939	256	280	12			
1	P	190	Total	C	N	O	S	0	0	0
			1484	937	255	280	12			
1	Q	187	Total	C	N	O	S	0	1	0
			1459	923	247	277	12			
1	Y	186	Total	C	N	O	S	0	2	0
			1468	930	251	275	12			
1	Z	183	Total	C	N	O	S	0	1	0
			1432	909	242	269	12			
1	a	183	Total	C	N	O	S	0	1	0
			1435	909	245	269	12			
1	b	180	Total	C	N	O	S	0	0	0
			1404	892	238	262	12			
1	V	183	Total	C	N	O	S	0	2	0
			1438	912	244	270	12			
1	W	183	Total	C	N	O	S	0	1	0
			1429	908	241	268	12			
1	X	190	Total	C	N	O	S	0	1	0
			1478	935	250	281	12			
1	M	190	Total	C	N	O	S	0	1	0
			1484	938	253	281	12			
1	L	187	Total	C	N	O	S	0	0	0
			1454	921	246	275	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	K	188	Total	C	N	O	S	0	1	0
			1464	927	248	277	12			
1	J	190	Total	C	N	O	S	0	1	0
			1492	942	258	280	12			
1	I	190	Total	C	N	O	S	0	2	0
			1498	946	258	282	12			
1	H	186	Total	C	N	O	S	0	2	0
			1462	927	250	273	12			
1	N	187	Total	C	N	O	S	0	0	0
			1456	922	249	273	12			
1	F	190	Total	C	N	O	S	0	0	0
			1484	937	255	280	12			
1	E	188	Total	C	N	O	S	0	0	0
			1467	928	250	277	12			
1	D	188	Total	C	N	O	S	0	1	0
			1473	932	251	278	12			
1	C	188	Total	C	N	O	S	0	0	0
			1467	928	250	277	12			
1	B	188	Total	C	N	O	S	0	0	0
			1468	929	250	277	12			
1	A	192	Total	C	N	O	S	0	1	0
			1508	951	261	283	13			
1	G	190	Total	C	N	O	S	0	1	0
			1490	941	255	282	12			

- Molecule 2 is a protein called ACYLDEPSIPEPTIDE 1.

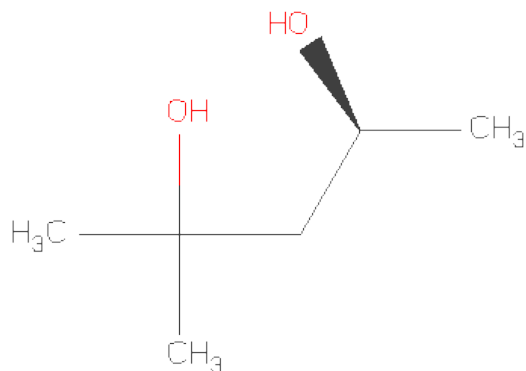
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	1	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	2	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	c	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	d	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	e	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	f	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	g	7	Total	C	N	O	0	0	0
			52	38	6	8			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	h	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	i	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	j	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	k	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	l	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	m	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	n	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	o	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	p	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	q	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	r	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	s	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	t	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	v	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	w	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	x	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	y	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	z	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	3	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	4	7	Total	C	N	O	0	0	0
			52	38	6	8			
2	u	7	Total	C	N	O	0	0	0
			52	38	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	R	1	Total	C	O	0	0
			8	6	2		
3	R	1	Total	C	O	0	0
			8	6	2		
3	R	1	Total	C	O	0	0
			8	6	2		
3	S	1	Total	C	O	0	0
			8	6	2		
3	T	1	Total	C	O	0	0
			8	6	2		
3	T	1	Total	C	O	0	0
			8	6	2		
3	U	1	Total	C	O	0	0
			8	6	2		
3	U	1	Total	C	O	0	0
			8	6	2		
3	O	1	Total	C	O	0	0
			8	6	2		
3	O	1	Total	C	O	0	0
			8	6	2		
3	P	1	Total	C	O	0	0
			8	6	2		
3	P	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	Q	1	Total	C	O	0	0
			8	6	2		
3	Q	1	Total	C	O	0	0
			8	6	2		
3	Y	1	Total	C	O	0	0
			8	6	2		
3	Z	1	Total	C	O	0	0
			8	6	2		
3	Z	1	Total	C	O	0	0
			8	6	2		
3	Z	1	Total	C	O	0	0
			8	6	2		
3	a	1	Total	C	O	0	0
			8	6	2		
3	b	1	Total	C	O	0	0
			8	6	2		
3	b	1	Total	C	O	0	0
			8	6	2		
3	V	1	Total	C	O	0	0
			8	6	2		
3	V	1	Total	C	O	0	0
			8	6	2		
3	W	1	Total	C	O	0	0
			8	6	2		
3	W	1	Total	C	O	0	0
			8	6	2		
3	X	1	Total	C	O	0	0
			8	6	2		
3	X	1	Total	C	O	0	0
			8	6	2		
3	M	1	Total	C	O	0	0
			8	6	2		
3	M	1	Total	C	O	0	0
			8	6	2		
3	M	1	Total	C	O	0	0
			8	6	2		
3	L	1	Total	C	O	0	0
			8	6	2		
3	L	1	Total	C	O	0	0
			8	6	2		
3	K	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	K	1	Total	C	O	0	0
			8	6	2		
3	J	1	Total	C	O	0	0
			8	6	2		
3	J	1	Total	C	O	0	0
			8	6	2		
3	I	1	Total	C	O	0	0
			8	6	2		
3	I	1	Total	C	O	0	0
			8	6	2		
3	H	1	Total	C	O	0	0
			8	6	2		
3	N	1	Total	C	O	0	0
			8	6	2		
3	N	1	Total	C	O	0	0
			8	6	2		
3	F	1	Total	C	O	0	0
			8	6	2		
3	E	1	Total	C	O	0	0
			8	6	2		
3	E	1	Total	C	O	0	0
			8	6	2		
3	E	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	G	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	0	0
			8	6	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	R	130	Total	O		0	0
			130	130			
4	S	105	Total	O		0	0
			105	105			
4	T	141	Total	O		0	0
			141	141			
4	U	136	Total	O		0	0
			136	136			
4	O	123	Total	O		0	0
			123	123			
4	P	120	Total	O		0	0
			120	120			
4	Q	125	Total	O		0	0
			125	125			
4	Y	142	Total	O		0	0
			142	142			
4	Z	124	Total	O		0	0
			124	124			
4	a	129	Total	O		0	0
			129	129			
4	b	114	Total	O		0	0
			114	114			
4	V	108	Total	O		0	0
			108	108			
4	W	102	Total	O		0	0
			102	102			
4	X	118	Total	O		0	0
			118	118			
4	M	133	Total	O		0	0
			133	133			
4	L	132	Total	O		0	0
			132	132			
4	K	130	Total	O		0	0
			130	130			
4	J	137	Total	O		0	0
			137	137			

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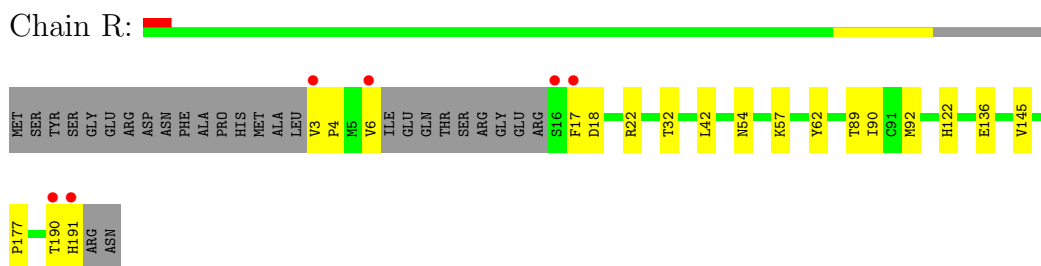
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	147	Total 147	O 147	0	0
4	H	123	Total 123	O 123	0	0
4	N	137	Total 137	O 137	0	0
4	F	123	Total 123	O 123	0	0
4	E	125	Total 125	O 125	0	0
4	D	147	Total 147	O 147	0	0
4	C	137	Total 137	O 137	0	0
4	B	134	Total 134	O 134	0	0
4	A	125	Total 125	O 125	0	0
4	G	143	Total 143	O 143	0	0
4	f	1	Total 1	O 1	0	0

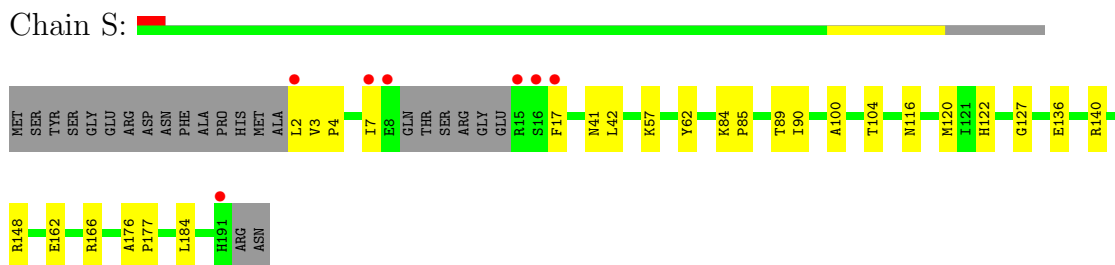
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

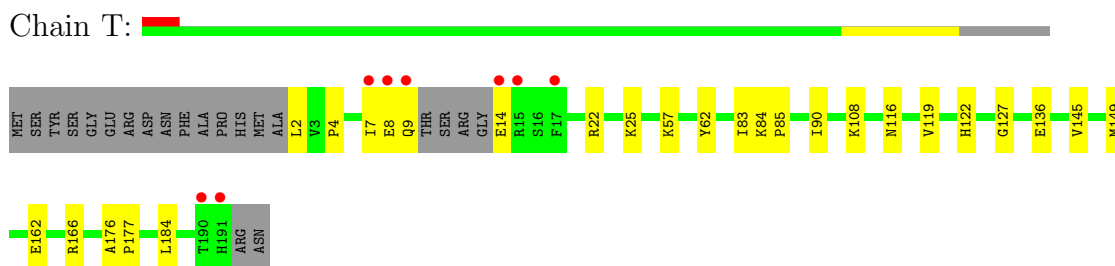
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



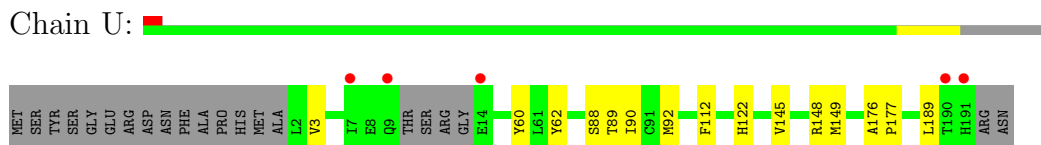
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



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- Molecule 1: ATP-dependent Clp protease proteolytic subunit



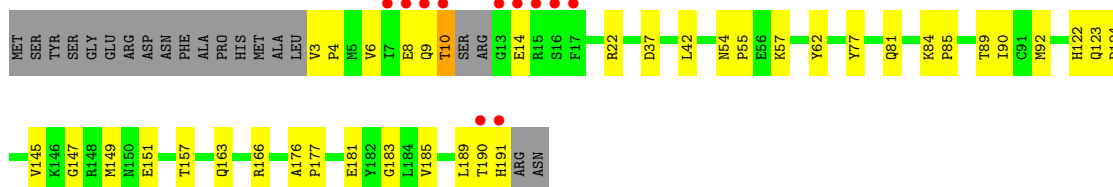
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



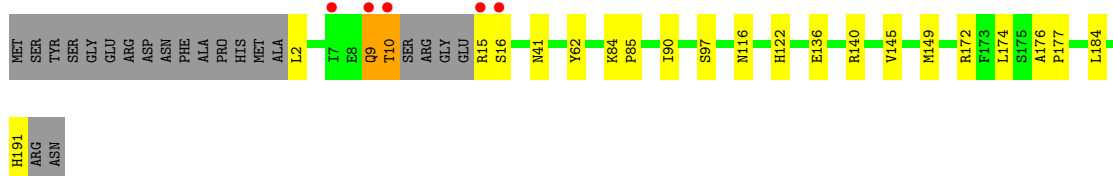
Chain P: 



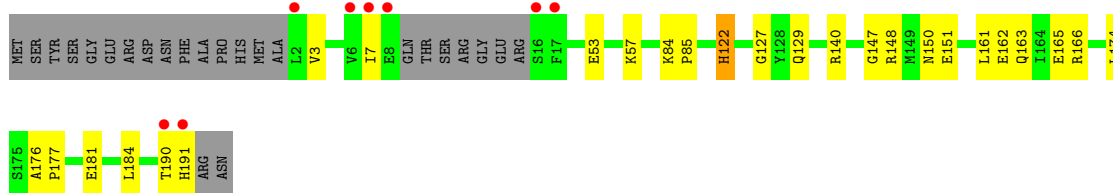
Chain Q: 



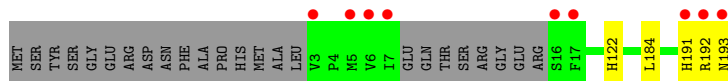
Chain Y:



Chain Z: 



Chain a: 



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain b:

- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain V:

- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain W:

- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain X:

- Molecule 1: ATP-dependent Clp protease proteolytic subunit

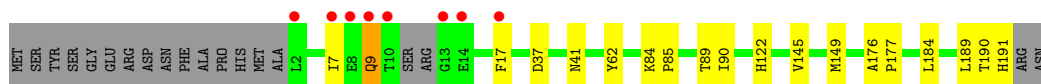
Chain M:

- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain L:

- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain K:



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain J:



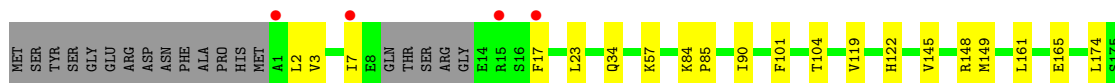
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain I:



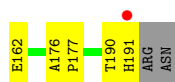
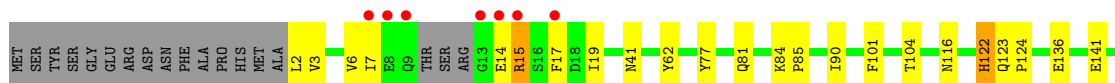
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain H:



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain N:



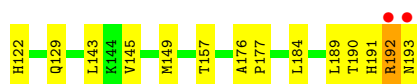
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain F:



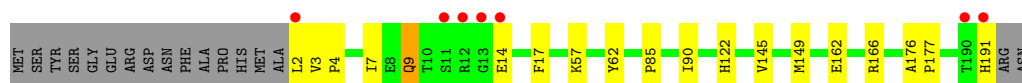






- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain G:



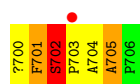
- Molecule 2: ACYLDEPSIPEPTIDE 1

Chain 1:



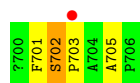
- Molecule 2: ACYLDEPSIPEPTIDE 1

Chain 2:



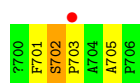
- Molecule 2: ACYLDEPSIPEPTIDE 1

Chain c:



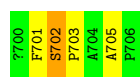
- Molecule 2: ACYLDEPSIPEPTIDE 1

Chain d:



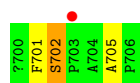
- Molecule 2: ACYLDEPSIPEPTIDE 1

Chain e:



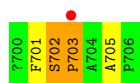
- Molecule 2: ACYLDEPSIPEPTIDE 1

Chain f:



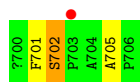
- Molecule 2: ACYLDEPSIPEPTIDE 1

Chain g: 



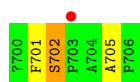
- Molecule 2: ACYLDEPSIPEPTIDE 1

Chain h: 



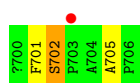
- Molecule 2: ACYLDEPSIPEPTIDE 1

Chain i: 



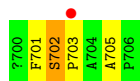
- Molecule 2: ACYLDEPSIPEPTIDE 1

Chain j: 



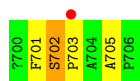
- Molecule 2: ACYLDEPSIPEPTIDE 1

Chain k: 



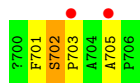
- Molecule 2: ACYLDEPSIPEPTIDE 1

Chain l: 



- Molecule 2: ACYLDEPSIPEPTIDE 1

Chain m: 



- Molecule 2: ACYLDEPSIPEPTIDE 1

Chain n: 



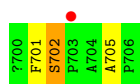
- Molecule 2: ACYLDEPSIPEPTIDE 1

Chain o: 



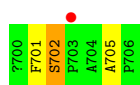
- Molecule 2: ACYLDEPSIPEPTIDE 1

Chain p: 



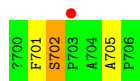
- Molecule 2: ACYLDEPSIPEPTIDE 1

Chain q: 



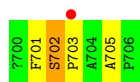
- Molecule 2: ACYLDEPSIPEPTIDE 1

Chain r: 



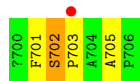
- Molecule 2: ACYLDEPSIPEPTIDE 1

Chain s: 



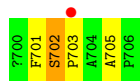
- Molecule 2: ACYLDEPSIPEPTIDE 1

Chain t: 



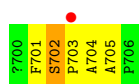
- Molecule 2: ACYLDEPSIPEPTIDE 1

Chain v: 



- Molecule 2: ACYLDEPSIPEPTIDE 1

Chain w: 



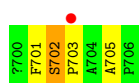
- Molecule 2: ACYLDEPSIPEPTIDE 1

Chain x: 



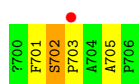
- Molecule 2: ACYLDEPSIPEPTIDE 1

Chain y: 



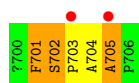
- Molecule 2: ACYLDEPSIPEPTIDE 1

Chain z: 



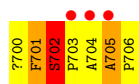
- Molecule 2: ACYLDEPSIPEPTIDE 1

Chain 3: 



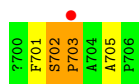
- Molecule 2: ACYLDEPSIPEPTIDE 1

Chain 4: 



- Molecule 2: ACYLDEPSIPEPTIDE 1

Chain u: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.25Å 121.15Å 276.17Å 90.00° 91.38° 90.00°	Depositor
Resolution (Å)	29.90 – 1.90 29.99 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.1 (29.90-1.90) 98.2 (29.99-1.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.26 (at 1.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.4_159)	Depositor
R, $R_{free}$	0.178 , 0.204 0.175 , 0.200	Depositor DCC
$R_{free}$ test set	5191 reflections (1.10%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.9	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 34.9	EDS
Estimated twinning fraction	0.013 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 472016 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	46463	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MAA, MPD, OTT, 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	0.23	0/1535	0.42	0/2068
1	B	0.24	0/1491	0.42	0/2010
1	C	0.24	0/1490	0.42	0/2008
1	D	0.24	0/1499	0.42	0/2020
1	E	0.24	0/1490	0.42	0/2008
1	F	0.23	0/1508	0.41	0/2033
1	G	0.23	0/1517	0.42	0/2045
1	H	0.23	0/1491	0.41	0/2009
1	I	0.25	0/1528	0.43	0/2059
1	J	0.24	0/1519	0.43	0/2047
1	K	0.23	0/1490	0.41	0/2009
1	L	0.24	0/1477	0.41	0/1991
1	M	0.23	0/1511	0.41	0/2038
1	N	0.23	0/1479	0.41	0/1993
1	O	0.23	0/1516	0.42	0/2043
1	P	0.23	0/1508	0.41	0/2033
1	Q	0.23	0/1485	0.42	0/2002
1	R	0.23	0/1434	0.42	0/1933
1	S	0.23	0/1466	0.42	0/1976
1	T	0.23	0/1516	0.42	0/2042
1	U	0.24	0/1495	0.43	0/2014
1	V	0.23	0/1467	0.41	0/1977
1	W	0.23	0/1455	0.41	0/1962
1	X	0.25	0/1505	0.43	0/2031
1	Y	0.23	0/1497	0.42	0/2017
1	Z	0.23	0/1458	0.41	0/1966
1	a	0.23	0/1461	0.41	0/1969
1	b	0.23	0/1427	0.41	0/1924
2	1	2.88	4/29 (13.8%)	3.44	7/37 (18.9%)
2	2	2.89	4/29 (13.8%)	3.43	6/37 (16.2%)
2	3	2.92	4/29 (13.8%)	3.39	6/37 (16.2%)
2	4	2.92	4/29 (13.8%)	3.51	8/37 (21.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
2	c	2.90	4/29 (13.8%)	3.44	7/37 (18.9%)
2	d	2.88	4/29 (13.8%)	3.43	6/37 (16.2%)
2	e	2.90	4/29 (13.8%)	3.46	7/37 (18.9%)
2	f	2.91	4/29 (13.8%)	3.42	6/37 (16.2%)
2	g	2.93	4/29 (13.8%)	3.45	7/37 (18.9%)
2	h	2.93	4/29 (13.8%)	3.45	5/37 (13.5%)
2	i	2.89	4/29 (13.8%)	3.45	5/37 (13.5%)
2	j	2.89	4/29 (13.8%)	3.42	6/37 (16.2%)
2	k	2.91	4/29 (13.8%)	3.45	7/37 (18.9%)
2	l	2.92	4/29 (13.8%)	3.46	7/37 (18.9%)
2	m	2.88	4/29 (13.8%)	3.47	8/37 (21.6%)
2	n	2.92	4/29 (13.8%)	3.44	6/37 (16.2%)
2	o	2.84	4/29 (13.8%)	3.39	6/37 (16.2%)
2	p	2.91	4/29 (13.8%)	3.46	6/37 (16.2%)
2	q	2.91	4/29 (13.8%)	3.47	5/37 (13.5%)
2	r	2.91	4/29 (13.8%)	3.47	6/37 (16.2%)
2	s	2.88	4/29 (13.8%)	3.47	7/37 (18.9%)
2	t	2.91	4/29 (13.8%)	3.45	6/37 (16.2%)
2	u	2.92	4/29 (13.8%)	3.45	6/37 (16.2%)
2	v	2.92	4/29 (13.8%)	3.52	7/37 (18.9%)
2	w	2.89	4/29 (13.8%)	3.43	6/37 (16.2%)
2	x	2.96	4/29 (13.8%)	3.51	8/37 (21.6%)
2	y	2.89	4/29 (13.8%)	3.45	6/37 (16.2%)
2	z	2.91	4/29 (13.8%)	3.45	7/37 (18.9%)
All	All	0.46	112/42527 (0.3%)	0.62	180/57263 (0.3%)

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
2	g	0	1
2	w	0	1
2	x	0	1
All	All	0	3

The worst 5 of 112 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	x	702	SER	CA-CB	7.23	1.63	1.52
2	n	702	SER	CA-CB	7.20	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	l	702	SER	CA-CB	7.18	1.63	1.52
2	p	702	SER	CA-CB	7.17	1.63	1.52
2	z	702	SER	CA-CB	7.15	1.63	1.52

The worst 5 of 180 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	q	701	PHE	O-C-N	10.39	139.32	122.70
2	y	701	PHE	O-C-N	10.32	139.21	122.70
2	g	701	PHE	O-C-N	10.24	139.09	122.70
2	2	701	PHE	O-C-N	10.18	138.99	122.70
2	u	701	PHE	O-C-N	10.18	138.98	122.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	g	703	PRO	Mainchain
2	w	704	MAA	Mainchain
2	x	705	ALA	Mainchain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1508	0	1522	54	0
1	B	1468	0	1480	43	0
1	C	1467	0	1475	23	0
1	D	1473	0	1483	20	0
1	E	1467	0	1475	17	0
1	F	1484	0	1494	26	0
1	G	1490	0	1500	18	0
1	H	1462	0	1480	15	0
1	I	1498	0	1513	18	0
1	J	1492	0	1507	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	1464	0	1465	20	0
1	L	1454	0	1457	20	0
1	M	1484	0	1491	24	0
1	N	1456	0	1464	27	0
1	O	1487	0	1506	22	0
1	P	1484	0	1494	26	0
1	Q	1459	0	1461	31	0
1	R	1408	0	1416	22	0
1	S	1440	0	1453	30	0
1	T	1481	0	1498	26	0
1	U	1466	0	1480	13	0
1	V	1438	0	1448	24	0
1	W	1429	0	1440	22	0
1	X	1478	0	1480	30	0
1	Y	1468	0	1485	23	0
1	Z	1432	0	1444	23	0
1	a	1435	0	1446	0	0
1	b	1404	0	1416	0	0
2	1	52	0	49	12	0
2	2	52	0	48	6	0
2	3	52	0	49	7	0
2	4	52	0	49	10	0
2	c	52	0	49	0	0
2	d	52	0	49	0	0
2	e	52	0	49	0	0
2	f	52	0	49	0	0
2	g	52	0	49	0	0
2	h	52	0	49	0	0
2	i	52	0	49	0	0
2	j	52	0	49	0	0
2	k	52	0	49	0	0
2	l	52	0	49	0	0
2	m	52	0	49	0	0
2	n	52	0	49	0	0
2	o	52	0	49	0	0
2	p	52	0	49	0	0
2	q	52	0	49	0	0
2	r	52	0	49	0	0
2	s	52	0	49	0	0
2	t	52	0	49	0	0
2	u	52	0	49	0	0
2	v	52	0	49	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	w	52	0	49	0	0
2	x	52	0	49	0	0
2	y	52	0	49	0	0
2	z	52	0	48	0	0
3	A	16	0	28	1	0
3	B	16	0	28	0	0
3	C	16	0	28	1	0
3	D	16	0	28	1	0
3	E	24	0	42	1	0
3	F	8	0	14	2	0
3	G	16	0	28	0	0
3	H	8	0	14	0	0
3	I	16	0	28	1	0
3	J	16	0	28	1	0
3	K	16	0	28	1	0
3	L	16	0	28	2	0
3	M	24	0	42	1	0
3	N	16	0	28	0	0
3	O	16	0	28	0	0
3	P	16	0	28	1	0
3	Q	16	0	28	0	0
3	R	24	0	42	1	0
3	S	8	0	14	0	0
3	T	16	0	28	0	0
3	U	16	0	28	1	0
3	V	16	0	28	0	0
3	W	16	0	28	1	0
3	X	16	0	28	2	0
3	Y	8	0	14	1	0
3	Z	24	0	42	0	0
3	a	8	0	14	0	0
3	b	16	0	28	0	0
4	A	125	0	0	1	0
4	B	134	0	0	4	0
4	C	137	0	0	2	0
4	D	147	0	0	0	0
4	E	125	0	0	0	0
4	F	123	0	0	0	0
4	G	143	0	0	0	0
4	H	123	0	0	1	0
4	I	147	0	0	0	0
4	J	137	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	130	0	0	1	0
4	L	132	0	0	0	0
4	M	133	0	0	1	0
4	N	137	0	0	4	0
4	O	123	0	0	0	0
4	P	120	0	0	1	0
4	Q	125	0	0	3	0
4	R	130	0	0	2	0
4	S	105	0	0	1	0
4	T	141	0	0	2	0
4	U	136	0	0	0	0
4	V	108	0	0	0	0
4	W	102	0	0	0	0
4	X	118	0	0	6	0
4	Y	142	0	0	3	0
4	Z	124	0	0	6	0
4	a	129	0	0	0	0
4	b	114	0	0	0	0
4	f	1	0	0	0	0
All	All	46463	0	43413	558	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

The worst 5 of 558 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:192:ARG:HG3	2:1:703:PRO:HD2	1.24	1.15
1:B:7:ILE:HD11	1:A:17:PHE:HZ	1.05	1.13
1:T:9:GLN:HE22	1:T:14:GLU:HG2	1.11	1.08
1:B:7:ILE:HD11	1:A:17:PHE:CZ	1.91	1.05
1:O:15:ARG:HD3	1:O:17:PHE:CZ	1.99	0.96

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	191/207 (92%)	187 (98%)	4 (2%)	0	100	100
1	B	184/207 (89%)	180 (98%)	4 (2%)	0	100	100
1	C	184/207 (89%)	182 (99%)	2 (1%)	0	100	100
1	D	185/207 (89%)	182 (98%)	3 (2%)	0	100	100
1	E	184/207 (89%)	182 (99%)	2 (1%)	0	100	100
1	F	188/207 (91%)	186 (99%)	2 (1%)	0	100	100
1	G	189/207 (91%)	187 (99%)	2 (1%)	0	100	100
1	H	184/207 (89%)	182 (99%)	2 (1%)	0	100	100
1	I	190/207 (92%)	186 (98%)	4 (2%)	0	100	100
1	J	189/207 (91%)	186 (98%)	3 (2%)	0	100	100
1	K	185/207 (89%)	181 (98%)	4 (2%)	0	100	100
1	L	183/207 (88%)	180 (98%)	3 (2%)	0	100	100
1	M	189/207 (91%)	185 (98%)	4 (2%)	0	100	100
1	N	183/207 (88%)	180 (98%)	3 (2%)	0	100	100
1	O	189/207 (91%)	187 (99%)	2 (1%)	0	100	100
1	P	188/207 (91%)	185 (98%)	3 (2%)	0	100	100
1	Q	184/207 (89%)	181 (98%)	3 (2%)	0	100	100
1	R	177/207 (86%)	175 (99%)	2 (1%)	0	100	100
1	S	181/207 (87%)	179 (99%)	2 (1%)	0	100	100
1	T	186/207 (90%)	183 (98%)	3 (2%)	0	100	100
1	U	184/207 (89%)	181 (98%)	3 (2%)	0	100	100
1	V	181/207 (87%)	179 (99%)	2 (1%)	0	100	100
1	W	180/207 (87%)	177 (98%)	3 (2%)	0	100	100
1	X	189/207 (91%)	187 (99%)	2 (1%)	0	100	100
1	Y	184/207 (89%)	181 (98%)	3 (2%)	0	100	100
1	Z	180/207 (87%)	178 (99%)	2 (1%)	0	100	100
1	a	180/207 (87%)	176 (98%)	2 (1%)	2 (1%)	21	7
1	b	176/207 (85%)	173 (98%)	3 (2%)	0	100	100
2	1	3/7 (43%)	1 (33%)	2 (67%)	0	100	100
2	2	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	3	3/7 (43%)	1 (33%)	2 (67%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	4	3/7 (43%)	3 (100%)	0	0	100	100
2	c	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	d	3/7 (43%)	1 (33%)	2 (67%)	0	100	100
2	e	3/7 (43%)	3 (100%)	0	0	100	100
2	f	3/7 (43%)	1 (33%)	2 (67%)	0	100	100
2	g	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	h	3/7 (43%)	1 (33%)	2 (67%)	0	100	100
2	i	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	j	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	k	3/7 (43%)	1 (33%)	2 (67%)	0	100	100
2	l	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	m	3/7 (43%)	1 (33%)	2 (67%)	0	100	100
2	n	3/7 (43%)	1 (33%)	2 (67%)	0	100	100
2	o	3/7 (43%)	1 (33%)	2 (67%)	0	100	100
2	p	3/7 (43%)	1 (33%)	2 (67%)	0	100	100
2	q	3/7 (43%)	1 (33%)	2 (67%)	0	100	100
2	r	3/7 (43%)	1 (33%)	2 (67%)	0	100	100
2	s	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	t	3/7 (43%)	3 (100%)	0	0	100	100
2	u	3/7 (43%)	1 (33%)	1 (33%)	1 (33%)	0	0
2	v	3/7 (43%)	3 (100%)	0	0	100	100
2	w	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	x	3/7 (43%)	1 (33%)	2 (67%)	0	100	100
2	y	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	z	3/7 (43%)	1 (33%)	2 (67%)	0	100	100
All	All	5251/5992 (88%)	5133 (98%)	115 (2%)	3 (0%)	59	48

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	a	191	HIS
1	a	192	ARG
2	u	703	PRO

### 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	164/175 (94%)	161 (98%)	3 (2%)	71	66
1	B	159/175 (91%)	155 (98%)	4 (2%)	60	50
1	C	159/175 (91%)	154 (97%)	5 (3%)	52	41
1	D	160/175 (91%)	158 (99%)	2 (1%)	80	77
1	E	159/175 (91%)	156 (98%)	3 (2%)	69	63
1	F	161/175 (92%)	157 (98%)	4 (2%)	60	50
1	G	162/175 (93%)	160 (99%)	2 (1%)	82	80
1	H	158/175 (90%)	154 (98%)	4 (2%)	60	50
1	I	163/175 (93%)	157 (96%)	6 (4%)	45	32
1	J	162/175 (93%)	158 (98%)	4 (2%)	60	50
1	K	158/175 (90%)	155 (98%)	3 (2%)	69	63
1	L	157/175 (90%)	155 (99%)	2 (1%)	80	77
1	M	161/175 (92%)	159 (99%)	2 (1%)	82	80
1	N	157/175 (90%)	155 (99%)	2 (1%)	80	77
1	O	162/175 (93%)	160 (99%)	2 (1%)	82	80
1	P	161/175 (92%)	158 (98%)	3 (2%)	69	63
1	Q	158/175 (90%)	155 (98%)	3 (2%)	69	63
1	R	153/175 (87%)	153 (100%)	0	100	100
1	S	156/175 (89%)	156 (100%)	0	100	100
1	T	162/175 (93%)	161 (99%)	1 (1%)	92	92
1	U	159/175 (91%)	158 (99%)	1 (1%)	92	92
1	V	156/175 (89%)	153 (98%)	3 (2%)	69	63
1	W	155/175 (89%)	153 (99%)	2 (1%)	80	77
1	X	160/175 (91%)	157 (98%)	3 (2%)	69	63
1	Y	160/175 (91%)	156 (98%)	4 (2%)	60	50
1	Z	156/175 (89%)	155 (99%)	1 (1%)	92	92
1	a	156/175 (89%)	153 (98%)	3 (2%)	69	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	b	152/175 (87%)	150 (99%)	2 (1%)	80	77
2	1	3/3 (100%)	1 (33%)	2 (67%)	0	0
2	2	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	3	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	4	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	c	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	d	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	e	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	f	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	g	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	h	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	i	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	j	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	k	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	l	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	m	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	n	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	o	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	p	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	q	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	r	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	s	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	t	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	u	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	v	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	w	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	x	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	y	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	z	3/3 (100%)	2 (67%)	1 (33%)	0	0
All	All	4530/4984 (91%)	4427 (98%)	103 (2%)	63	55

5 of 103 residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	H	7	ILE
1	E	191	HIS
2	v	702	SER
1	H	23	LEU
1	F	15	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
1	W	41	ASN
1	K	9	GLN
1	B	191	HIS
1	X	64	ASN
1	L	34	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

56 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	MAA	1	704	2	5,5,6	7.89	2 (40%)	3,5,7	8.62	3 (100%)
2	MP8	1	706	2	8,8,9	7.71	2 (25%)	8,10,12	1.30	1 (12%)
2	MAA	2	704	2	5,5,6	7.85	2 (40%)	3,5,7	8.85	3 (100%)
2	MP8	2	706	2	8,8,9	7.63	2 (25%)	8,10,12	1.29	0
2	MAA	3	704	2	5,5,6	7.77	2 (40%)	3,5,7	7.84	3 (100%)
2	MP8	3	706	2	8,8,9	7.85	2 (25%)	8,10,12	1.30	0
2	MAA	4	704	2	5,5,6	7.82	2 (40%)	3,5,7	8.57	3 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MP8	4	706	2	8,8,9	7.71	2 (25%)	8,10,12	1.36	0
2	MAA	c	704	2	5,5,6	7.76	2 (40%)	3,5,7	8.61	3 (100%)
2	MP8	c	706	2	8,8,9	7.61	2 (25%)	8,10,12	1.27	0
2	MAA	d	704	2	5,5,6	7.79	1 (20%)	3,5,7	8.49	3 (100%)
2	MP8	d	706	2	8,8,9	7.66	2 (25%)	8,10,12	1.27	0
2	MAA	e	704	2	5,5,6	7.74	1 (20%)	3,5,7	7.99	3 (100%)
2	MP8	e	706	2	8,8,9	7.70	2 (25%)	8,10,12	1.28	0
2	MAA	f	704	2	5,5,6	7.81	2 (40%)	3,5,7	8.03	3 (100%)
2	MP8	f	706	2	8,8,9	7.73	2 (25%)	8,10,12	1.34	1 (12%)
2	MAA	g	704	2	5,5,6	7.85	1 (20%)	3,5,7	8.07	3 (100%)
2	MP8	g	706	2	8,8,9	7.61	2 (25%)	8,10,12	1.22	0
2	MAA	h	704	2	5,5,6	7.68	2 (40%)	3,5,7	8.18	3 (100%)
2	MP8	h	706	2	8,8,9	7.68	2 (25%)	8,10,12	1.30	0
2	MAA	i	704	2	5,5,6	7.78	2 (40%)	3,5,7	8.34	3 (100%)
2	MP8	i	706	2	8,8,9	7.75	2 (25%)	8,10,12	1.30	1 (12%)
2	MAA	j	704	2	5,5,6	7.74	1 (20%)	3,5,7	8.43	3 (100%)
2	MP8	j	706	2	8,8,9	7.70	2 (25%)	8,10,12	1.26	0
2	MAA	k	704	2	5,5,6	7.83	2 (40%)	3,5,7	8.85	3 (100%)
2	MP8	k	706	2	8,8,9	7.69	2 (25%)	8,10,12	1.31	0
2	MAA	l	704	2	5,5,6	7.79	2 (40%)	3,5,7	8.35	3 (100%)
2	MP8	l	706	2	8,8,9	7.60	2 (25%)	8,10,12	1.28	0
2	MAA	m	704	2	5,5,6	7.76	2 (40%)	3,5,7	8.37	3 (100%)
2	MP8	m	706	2	8,8,9	7.72	2 (25%)	8,10,12	1.31	0
2	MAA	n	704	2	5,5,6	7.72	2 (40%)	3,5,7	7.93	3 (100%)
2	MP8	n	706	2	8,8,9	7.70	2 (25%)	8,10,12	1.26	0
2	MAA	o	704	2	5,5,6	7.73	2 (40%)	3,5,7	8.37	3 (100%)
2	MP8	o	706	2	8,8,9	7.77	2 (25%)	8,10,12	1.26	0
2	MAA	p	704	2	5,5,6	7.84	2 (40%)	3,5,7	7.89	3 (100%)
2	MP8	p	706	2	8,8,9	7.65	2 (25%)	8,10,12	1.23	0
2	MAA	q	704	2	5,5,6	7.86	2 (40%)	3,5,7	8.16	3 (100%)
2	MP8	q	706	2	8,8,9	7.64	2 (25%)	8,10,12	1.33	0
2	MAA	r	704	2	5,5,6	7.75	2 (40%)	3,5,7	8.57	3 (100%)
2	MP8	r	706	2	8,8,9	7.83	2 (25%)	8,10,12	1.34	1 (12%)
2	MAA	s	704	2	5,5,6	7.85	2 (40%)	3,5,7	8.56	3 (100%)
2	MP8	s	706	2	8,8,9	7.59	2 (25%)	8,10,12	1.31	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MAA	t	704	2	5,5,6	7.78	2 (40%)	3,5,7	8.09	3 (100%)
2	MP8	t	706	2	8,8,9	7.76	2 (25%)	8,10,12	1.29	0
2	MAA	u	704	2	5,5,6	7.88	2 (40%)	3,5,7	8.57	3 (100%)
2	MP8	u	706	2	8,8,9	7.74	2 (25%)	8,10,12	1.32	1 (12%)
2	MAA	v	704	2	5,5,6	7.88	2 (40%)	3,5,7	8.13	3 (100%)
2	MP8	v	706	2	8,8,9	7.61	2 (25%)	8,10,12	1.33	0
2	MAA	w	704	2	5,5,6	7.86	2 (40%)	3,5,7	8.76	3 (100%)
2	MP8	w	706	2	8,8,9	7.70	2 (25%)	8,10,12	1.24	0
2	MAA	x	704	2	5,5,6	7.82	1 (20%)	3,5,7	8.27	3 (100%)
2	MP8	x	706	2	8,8,9	7.68	2 (25%)	8,10,12	1.28	0
2	MAA	y	704	2	5,5,6	7.71	2 (40%)	3,5,7	8.23	3 (100%)
2	MP8	y	706	2	8,8,9	7.76	2 (25%)	8,10,12	1.37	1 (12%)
2	MAA	z	704	2	5,5,6	7.80	2 (40%)	3,5,7	8.27	3 (100%)
2	MP8	z	706	2	8,8,9	7.63	2 (25%)	8,10,12	1.36	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAA	1	704	2	-	1/2/4/6	0/0/0/0
2	MP8	1	706	2	-	0/0/11/13	0/1/1/1
2	MAA	2	704	2	-	1/2/4/6	0/0/0/0
2	MP8	2	706	2	-	0/0/11/13	0/1/1/1
2	MAA	3	704	2	-	1/2/4/6	0/0/0/0
2	MP8	3	706	2	-	0/0/11/13	0/1/1/1
2	MAA	4	704	2	-	1/2/4/6	0/0/0/0
2	MP8	4	706	2	-	0/0/11/13	0/1/1/1
2	MAA	c	704	2	-	1/2/4/6	0/0/0/0
2	MP8	c	706	2	-	0/0/11/13	0/1/1/1
2	MAA	d	704	2	-	1/2/4/6	0/0/0/0
2	MP8	d	706	2	-	0/0/11/13	0/1/1/1
2	MAA	e	704	2	-	1/2/4/6	0/0/0/0
2	MP8	e	706	2	-	0/0/11/13	0/1/1/1
2	MAA	f	704	2	-	1/2/4/6	0/0/0/0
2	MP8	f	706	2	-	0/0/11/13	0/1/1/1
2	MAA	g	704	2	-	1/2/4/6	0/0/0/0
2	MP8	g	706	2	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAA	h	704	2	-	1/2/4/6	0/0/0/0
2	MP8	h	706	2	-	0/0/11/13	0/1/1/1
2	MAA	i	704	2	-	1/2/4/6	0/0/0/0
2	MP8	i	706	2	-	0/0/11/13	0/1/1/1
2	MAA	j	704	2	-	1/2/4/6	0/0/0/0
2	MP8	j	706	2	-	0/0/11/13	0/1/1/1
2	MAA	k	704	2	-	1/2/4/6	0/0/0/0
2	MP8	k	706	2	-	0/0/11/13	0/1/1/1
2	MAA	l	704	2	-	1/2/4/6	0/0/0/0
2	MP8	l	706	2	-	0/0/11/13	0/1/1/1
2	MAA	m	704	2	-	1/2/4/6	0/0/0/0
2	MP8	m	706	2	-	0/0/11/13	0/1/1/1
2	MAA	n	704	2	-	1/2/4/6	0/0/0/0
2	MP8	n	706	2	-	0/0/11/13	0/1/1/1
2	MAA	o	704	2	-	1/2/4/6	0/0/0/0
2	MP8	o	706	2	-	0/0/11/13	0/1/1/1
2	MAA	p	704	2	-	1/2/4/6	0/0/0/0
2	MP8	p	706	2	-	0/0/11/13	0/1/1/1
2	MAA	q	704	2	-	1/2/4/6	0/0/0/0
2	MP8	q	706	2	-	0/0/11/13	0/1/1/1
2	MAA	r	704	2	-	1/2/4/6	0/0/0/0
2	MP8	r	706	2	-	0/0/11/13	0/1/1/1
2	MAA	s	704	2	-	1/2/4/6	0/0/0/0
2	MP8	s	706	2	-	0/0/11/13	0/1/1/1
2	MAA	t	704	2	-	1/2/4/6	0/0/0/0
2	MP8	t	706	2	-	0/0/11/13	0/1/1/1
2	MAA	u	704	2	-	1/2/4/6	0/0/0/0
2	MP8	u	706	2	-	0/0/11/13	0/1/1/1
2	MAA	v	704	2	-	1/2/4/6	0/0/0/0
2	MP8	v	706	2	-	0/0/11/13	0/1/1/1
2	MAA	w	704	2	-	1/2/4/6	0/0/0/0
2	MP8	w	706	2	-	0/0/11/13	0/1/1/1
2	MAA	x	704	2	-	1/2/4/6	0/0/0/0
2	MP8	x	706	2	-	0/0/11/13	0/1/1/1
2	MAA	y	704	2	-	1/2/4/6	0/0/0/0
2	MP8	y	706	2	-	0/0/11/13	0/1/1/1
2	MAA	z	704	2	-	1/2/4/6	0/0/0/0
2	MP8	z	706	2	-	0/0/11/13	0/1/1/1

The worst 5 of 107 bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	3	706	MP8	O-C	21.96	1.26	1.11
2	r	706	MP8	O-C	21.91	1.26	1.11
2	o	706	MP8	O-C	21.74	1.26	1.11
2	y	706	MP8	O-C	21.69	1.26	1.11
2	t	706	MP8	O-C	21.69	1.26	1.11

The worst 5 of 91 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	k	704	MAA	CB-CA-C	13.63	114.54	108.46
2	2	704	MAA	CB-CA-C	13.59	114.52	108.46
2	w	704	MAA	CB-CA-C	13.45	114.46	108.46
2	1	704	MAA	CB-CA-C	13.24	114.37	108.46
2	u	704	MAA	CB-CA-C	13.22	114.35	108.46

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	l	704	MAA	C-CA-N-CM
2	n	704	MAA	C-CA-N-CM
2	d	704	MAA	C-CA-N-CM
2	v	704	MAA	C-CA-N-CM
2	3	704	MAA	C-CA-N-CM

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

55 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	A	800	-	7,7,7	0.25	0	10,10,10	0.25	0
3	MPD	A	801	-	7,7,7	0.25	0	10,10,10	0.30	0
3	MPD	B	800	-	7,7,7	0.24	0	10,10,10	0.28	0
3	MPD	B	801	-	7,7,7	0.27	0	10,10,10	0.32	0
3	MPD	C	800	-	7,7,7	0.26	0	10,10,10	0.27	0
3	MPD	C	801	-	7,7,7	0.26	0	10,10,10	0.31	0
3	MPD	D	800	-	7,7,7	0.25	0	10,10,10	0.25	0
3	MPD	D	801	-	7,7,7	0.25	0	10,10,10	0.32	0
3	MPD	E	801	-	7,7,7	0.27	0	10,10,10	0.31	0
3	MPD	E	802	-	7,7,7	0.25	0	10,10,10	0.26	0
3	MPD	E	803	-	7,7,7	0.25	0	10,10,10	0.29	0
3	MPD	F	800	-	7,7,7	0.25	0	10,10,10	0.27	0
3	MPD	G	800	-	7,7,7	0.26	0	10,10,10	0.28	0
3	MPD	G	801	-	7,7,7	0.26	0	10,10,10	0.32	0
3	MPD	H	800	-	7,7,7	0.24	0	10,10,10	0.26	0
3	MPD	I	800	-	7,7,7	0.24	0	10,10,10	0.26	0
3	MPD	I	801	-	7,7,7	0.25	0	10,10,10	0.33	0
3	MPD	J	800	-	7,7,7	0.25	0	10,10,10	0.24	0
3	MPD	J	801	-	7,7,7	0.27	0	10,10,10	0.34	0
3	MPD	K	800	-	7,7,7	0.25	0	10,10,10	0.26	0
3	MPD	K	801	-	7,7,7	0.24	0	10,10,10	0.29	0
3	MPD	L	800	-	7,7,7	0.25	0	10,10,10	0.26	0
3	MPD	L	801	-	7,7,7	0.25	0	10,10,10	0.35	0
3	MPD	M	201	-	7,7,7	0.25	0	10,10,10	0.25	0
3	MPD	M	202	-	7,7,7	0.26	0	10,10,10	0.36	0
3	MPD	M	203	-	7,7,7	0.26	0	10,10,10	0.29	0
3	MPD	N	800	-	7,7,7	0.27	0	10,10,10	0.25	0
3	MPD	N	801	-	7,7,7	0.24	0	10,10,10	0.29	0
3	MPD	O	800	-	7,7,7	0.24	0	10,10,10	0.26	0
3	MPD	O	801	-	7,7,7	0.24	0	10,10,10	0.31	0
3	MPD	P	800	-	7,7,7	0.26	0	10,10,10	0.32	0
3	MPD	P	801	-	7,7,7	0.25	0	10,10,10	0.36	0
3	MPD	Q	800	-	7,7,7	0.26	0	10,10,10	0.28	0
3	MPD	Q	801	-	7,7,7	0.25	0	10,10,10	0.32	0
3	MPD	R	201	-	7,7,7	0.25	0	10,10,10	0.33	0
3	MPD	R	202	-	7,7,7	0.26	0	10,10,10	0.28	0
3	MPD	R	203	-	7,7,7	0.26	0	10,10,10	0.32	0
3	MPD	S	800	-	7,7,7	0.27	0	10,10,10	0.23	0
3	MPD	T	800	-	7,7,7	0.26	0	10,10,10	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	MPD	T	801	-	7,7,7	0.27	0	10,10,10	0.36	0
3	MPD	U	201	-	7,7,7	0.26	0	10,10,10	0.34	0
3	MPD	U	202	-	7,7,7	0.26	0	10,10,10	0.25	0
3	MPD	V	201	-	7,7,7	0.24	0	10,10,10	0.26	0
3	MPD	V	202	-	7,7,7	0.26	0	10,10,10	0.35	0
3	MPD	W	800	-	7,7,7	0.27	0	10,10,10	0.30	0
3	MPD	W	801	-	7,7,7	0.27	0	10,10,10	0.33	0
3	MPD	X	201	-	7,7,7	0.25	0	10,10,10	0.27	0
3	MPD	X	202	-	7,7,7	0.24	0	10,10,10	0.30	0
3	MPD	Y	800	-	7,7,7	0.26	0	10,10,10	0.22	0
3	MPD	Z	801	-	7,7,7	0.24	0	10,10,10	0.30	0
3	MPD	Z	802	-	7,7,7	0.25	0	10,10,10	0.35	0
3	MPD	Z	803	-	7,7,7	0.25	0	10,10,10	0.35	0
3	MPD	a	800	-	7,7,7	0.25	0	10,10,10	0.24	0
3	MPD	b	800	-	7,7,7	0.26	0	10,10,10	0.25	0
3	MPD	b	801	-	7,7,7	0.25	0	10,10,10	0.35	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MPD	A	800	-	-	0/5/5/5	0/0/0/0
3	MPD	A	801	-	-	0/5/5/5	0/0/0/0
3	MPD	B	800	-	-	0/5/5/5	0/0/0/0
3	MPD	B	801	-	-	0/5/5/5	0/0/0/0
3	MPD	C	800	-	-	0/5/5/5	0/0/0/0
3	MPD	C	801	-	-	0/5/5/5	0/0/0/0
3	MPD	D	800	-	-	0/5/5/5	0/0/0/0
3	MPD	D	801	-	-	0/5/5/5	0/0/0/0
3	MPD	E	801	-	-	0/5/5/5	0/0/0/0
3	MPD	E	802	-	-	0/5/5/5	0/0/0/0
3	MPD	E	803	-	-	0/5/5/5	0/0/0/0
3	MPD	F	800	-	-	0/5/5/5	0/0/0/0
3	MPD	G	800	-	-	0/5/5/5	0/0/0/0
3	MPD	G	801	-	-	0/5/5/5	0/0/0/0
3	MPD	H	800	-	-	0/5/5/5	0/0/0/0
3	MPD	I	800	-	-	0/5/5/5	0/0/0/0
3	MPD	I	801	-	-	0/5/5/5	0/0/0/0
3	MPD	J	800	-	-	0/5/5/5	0/0/0/0
3	MPD	J	801	-	-	0/5/5/5	0/0/0/0
3	MPD	K	800	-	-	0/5/5/5	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MPD	K	801	-	-	0/5/5/5	0/0/0/0
3	MPD	L	800	-	-	0/5/5/5	0/0/0/0
3	MPD	L	801	-	-	0/5/5/5	0/0/0/0
3	MPD	M	201	-	-	0/5/5/5	0/0/0/0
3	MPD	M	202	-	-	0/5/5/5	0/0/0/0
3	MPD	M	203	-	-	0/5/5/5	0/0/0/0
3	MPD	N	800	-	-	0/5/5/5	0/0/0/0
3	MPD	N	801	-	-	0/5/5/5	0/0/0/0
3	MPD	O	800	-	-	0/5/5/5	0/0/0/0
3	MPD	O	801	-	-	0/5/5/5	0/0/0/0
3	MPD	P	800	-	-	0/5/5/5	0/0/0/0
3	MPD	P	801	-	-	0/5/5/5	0/0/0/0
3	MPD	Q	800	-	-	0/5/5/5	0/0/0/0
3	MPD	Q	801	-	-	0/5/5/5	0/0/0/0
3	MPD	R	201	-	-	0/5/5/5	0/0/0/0
3	MPD	R	202	-	-	0/5/5/5	0/0/0/0
3	MPD	R	203	-	-	0/5/5/5	0/0/0/0
3	MPD	S	800	-	-	0/5/5/5	0/0/0/0
3	MPD	T	800	-	-	0/5/5/5	0/0/0/0
3	MPD	T	801	-	-	0/5/5/5	0/0/0/0
3	MPD	U	201	-	-	0/5/5/5	0/0/0/0
3	MPD	U	202	-	-	0/5/5/5	0/0/0/0
3	MPD	V	201	-	-	0/5/5/5	0/0/0/0
3	MPD	V	202	-	-	0/5/5/5	0/0/0/0
3	MPD	W	800	-	-	0/5/5/5	0/0/0/0
3	MPD	W	801	-	-	0/5/5/5	0/0/0/0
3	MPD	X	201	-	-	0/5/5/5	0/0/0/0
3	MPD	X	202	-	-	0/5/5/5	0/0/0/0
3	MPD	Y	800	-	-	0/5/5/5	0/0/0/0
3	MPD	Z	801	-	-	0/5/5/5	0/0/0/0
3	MPD	Z	802	-	-	0/5/5/5	0/0/0/0
3	MPD	Z	803	-	-	0/5/5/5	0/0/0/0
3	MPD	a	800	-	-	0/5/5/5	0/0/0/0
3	MPD	b	800	-	-	0/5/5/5	0/0/0/0
3	MPD	b	801	-	-	0/5/5/5	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.



## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	192/207 (92%)	-0.19	3 (1%) 68 70	14, 20, 36, 48	0
1	B	188/207 (90%)	-0.22	6 (3%) 45 46	13, 18, 40, 71	0
1	C	188/207 (90%)	-0.12	7 (3%) 39 41	12, 19, 42, 78	0
1	D	188/207 (90%)	-0.15	7 (3%) 39 41	13, 18, 40, 68	0
1	E	188/207 (90%)	-0.10	5 (2%) 52 53	15, 20, 40, 62	0
1	F	190/207 (91%)	-0.05	8 (4%) 35 35	16, 21, 45, 79	0
1	G	190/207 (91%)	-0.08	7 (3%) 39 41	16, 22, 44, 62	0
1	H	186/207 (89%)	-0.20	6 (3%) 45 46	13, 19, 40, 61	0
1	I	190/207 (91%)	-0.22	3 (1%) 68 70	13, 18, 37, 54	0
1	J	190/207 (91%)	-0.17	6 (3%) 45 46	12, 18, 45, 63	0
1	K	188/207 (90%)	-0.15	8 (4%) 34 34	13, 19, 45, 70	0
1	L	187/207 (90%)	-0.15	2 (1%) 77 79	15, 21, 44, 72	0
1	M	190/207 (91%)	0.01	10 (5%) 25 26	16, 22, 45, 68	0
1	N	187/207 (90%)	-0.11	8 (4%) 34 34	15, 20, 45, 66	0
1	O	189/207 (91%)	-0.15	5 (2%) 53 55	16, 21, 38, 65	0
1	P	190/207 (91%)	-0.03	7 (3%) 39 41	17, 22, 42, 62	0
1	Q	187/207 (90%)	0.06	11 (5%) 22 22	14, 21, 49, 75	0
1	R	180/207 (86%)	-0.04	6 (3%) 44 45	15, 20, 37, 59	0
1	S	184/207 (88%)	-0.05	7 (3%) 38 40	14, 20, 38, 61	0
1	T	186/207 (89%)	-0.10	8 (4%) 34 34	13, 19, 40, 71	0
1	U	186/207 (89%)	-0.16	5 (2%) 52 53	14, 19, 37, 68	0
1	V	183/207 (88%)	0.10	9 (4%) 28 28	17, 25, 47, 71	0
1	W	183/207 (88%)	0.02	7 (3%) 38 40	17, 25, 44, 66	0
1	X	190/207 (91%)	0.07	12 (6%) 19 19	15, 22, 50, 71	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	Y	186/207 (89%)	-0.16	5 (2%)	52	53	13, 19, 35, 66	0
1	Z	183/207 (88%)	-0.12	8 (4%)	33	33	14, 20, 39, 60	0
1	a	183/207 (88%)	0.10	9 (4%)	28	28	15, 21, 41, 73	0
1	b	180/207 (86%)	0.04	7 (3%)	37	38	15, 24, 43, 63	0
2	1	7/7 (100%)	0.47	1 (14%)	3	3	24, 28, 35, 40	0
2	2	7/7 (100%)	0.32	1 (14%)	3	3	22, 25, 34, 43	0
2	3	7/7 (100%)	1.37	2 (28%)	1	1	27, 28, 39, 44	0
2	4	7/7 (100%)	1.82	3 (42%)	1	0	34, 40, 51, 52	0
2	c	7/7 (100%)	0.50	1 (14%)	3	3	22, 27, 38, 43	0
2	d	7/7 (100%)	0.35	1 (14%)	3	3	20, 25, 38, 40	0
2	e	7/7 (100%)	0.31	0	100	100	23, 28, 39, 39	0
2	f	7/7 (100%)	0.44	1 (14%)	3	3	24, 27, 37, 46	0
2	g	7/7 (100%)	0.82	1 (14%)	3	3	26, 29, 37, 48	0
2	h	7/7 (100%)	0.29	1 (14%)	3	3	23, 29, 38, 44	0
2	i	7/7 (100%)	0.37	1 (14%)	3	3	21, 25, 35, 44	0
2	j	7/7 (100%)	0.54	1 (14%)	3	3	22, 25, 35, 44	0
2	k	7/7 (100%)	0.48	1 (14%)	3	3	24, 27, 37, 45	0
2	l	7/7 (100%)	0.55	1 (14%)	3	3	24, 29, 40, 44	0
2	m	7/7 (100%)	0.61	2 (28%)	1	1	27, 29, 36, 41	0
2	n	7/7 (100%)	0.25	0	100	100	24, 31, 42, 46	0
2	o	7/7 (100%)	-0.11	0	100	100	20, 23, 32, 36	0
2	p	7/7 (100%)	0.45	1 (14%)	3	3	25, 30, 40, 43	0
2	q	7/7 (100%)	0.83	1 (14%)	3	3	25, 27, 39, 45	0
2	r	7/7 (100%)	0.49	1 (14%)	3	3	22, 25, 35, 41	0
2	s	7/7 (100%)	0.53	1 (14%)	3	3	24, 27, 39, 44	0
2	t	7/7 (100%)	0.51	1 (14%)	3	3	23, 26, 40, 48	0
2	u	7/7 (100%)	0.19	1 (14%)	3	3	22, 24, 37, 43	0
2	v	7/7 (100%)	1.13	1 (14%)	3	3	33, 39, 52, 54	0
2	w	7/7 (100%)	0.23	1 (14%)	3	3	28, 33, 39, 42	0
2	x	7/7 (100%)	3.19	7 (100%)	0	0	27, 32, 38, 39	7 (100%)
2	y	7/7 (100%)	0.52	1 (14%)	3	3	22, 25, 37, 42	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
2	z	7/7 (100%)	0.90	1 (14%) 3 3	26, 30, 42, 45	0
All	All	5428/5992 (90%)	-0.06	227 (4%) 35 35	12, 21, 44, 79	7 (0%)

The worst 5 of 227 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	V	7	ILE	9.9
1	b	17	PHE	9.0
1	a	7	ILE	8.0
1	a	16	SER	7.2
1	b	2	LEU	7.2

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	MAA	4	704	6/7	0.39	4.86	45,50,54,54	0
2	MAA	v	704	6/7	0.30	3.25	45,52,55,55	0
2	MAA	e	704	6/7	0.21	2.57	30,39,41,44	0
2	MAA	y	704	6/7	0.24	2.33	31,35,41,42	0
2	MAA	n	704	6/7	0.22	2.01	32,42,44,48	0
2	MAA	o	704	6/7	0.18	1.91	25,32,35,35	0
2	MAA	d	704	6/7	0.23	1.84	32,38,40,41	0
2	MAA	l	704	6/7	0.25	1.79	31,37,44,47	0
2	MAA	u	704	6/7	0.23	1.79	31,36,39,41	0
2	MAA	x	704	6/7	0.35	1.69	36,38,39,39	6
2	MAA	q	704	6/7	0.26	1.66	35,39,40,42	0
2	MAA	h	704	6/7	0.22	1.48	33,37,40,41	0
2	MAA	p	704	6/7	0.20	1.42	35,36,42,46	0
2	MAA	j	704	6/7	0.22	1.21	27,33,39,41	0
2	MAA	r	704	6/7	0.22	1.19	30,32,39,41	0
2	MAA	s	704	6/7	0.20	1.16	31,38,40,46	0
2	MAA	i	704	6/7	0.20	1.07	29,33,36,41	0
2	MAA	f	704	6/7	0.19	1.02	32,35,41,42	0
2	MAA	c	704	6/7	0.18	0.79	30,35,42,43	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MAA	t	704	6/7	0.20	0.78	35,40,41,42	0
2	MAA	l	704	6/7	0.17	0.76	30,32,36,38	0
2	MAA	m	704	6/7	0.19	0.75	33,35,38,38	0
2	MAA	k	704	6/7	0.19	0.62	30,35,40,43	0
2	MAA	3	704	6/7	0.27	0.62	32,37,43,43	0
2	MAA	g	704	6/7	0.20	0.61	30,35,41,42	0
2	MAA	z	704	6/7	0.22	0.60	38,39,42,50	0
2	MAA	w	704	6/7	0.15	0.54	34,38,39,41	0
2	MP8	4	706	8/9	0.16	0.14	35,38,44,47	0
2	MAA	2	704	6/7	0.15	0.08	31,33,36,38	0
2	MP8	f	706	8/9	0.13	0.07	23,26,31,32	0
2	MP8	x	706	8/9	0.22	0.06	28,30,34,37	8
2	MP8	s	706	8/9	0.12	-0.16	24,25,30,31	0
2	MP8	3	706	8/9	0.13	-0.30	24,27,30,30	0
2	MP8	l	706	8/9	0.11	-0.30	24,27,30,33	0
2	MP8	j	706	8/9	0.10	-0.35	21,22,27,27	0
2	MP8	g	706	8/9	0.11	-0.38	26,28,32,35	0
2	MP8	q	706	8/9	0.10	-0.43	21,24,30,31	0
2	MP8	z	706	8/9	0.11	-0.47	24,28,34,34	0
2	MP8	n	706	8/9	0.09	-0.51	27,28,31,41	0
2	MP8	d	706	8/9	0.09	-0.52	20,24,30,30	0
2	MP8	2	706	8/9	0.10	-0.53	19,23,27,28	0
2	MP8	c	706	8/9	0.10	-0.59	23,25,31,33	0
2	MP8	r	706	8/9	0.09	-0.60	20,25,28,28	0
2	MP8	m	706	8/9	0.10	-0.61	26,28,32,32	0
2	MP8	o	706	8/9	0.09	-0.63	18,22,25,25	0
2	MP8	k	706	8/9	0.08	-0.73	23,27,29,30	0
2	MP8	u	706	8/9	0.08	-0.73	19,23,28,30	0
2	MP8	y	706	8/9	0.10	-0.75	21,22,28,31	0
2	MP8	p	706	8/9	0.10	-0.79	26,29,32,33	0
2	MP8	l	706	8/9	0.09	-0.79	24,28,31,35	0
2	MP8	v	706	8/9	0.10	-0.84	34,39,41,42	0
2	MP8	e	706	8/9	0.10	-0.89	24,26,33,34	0
2	MP8	w	706	8/9	0.10	-0.93	31,33,34,34	0
2	MP8	t	706	8/9	0.08	-0.93	22,25,28,30	0
2	MP8	h	706	8/9	0.07	-0.95	24,27,30,32	0
2	MP8	i	706	8/9	0.07	-1.06	21,23,26,30	0

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	MPD	P	800	8/8	0.17	7.83	21,27,35,38	0
3	MPD	Z	802	8/8	0.16	7.25	24,31,32,32	0
3	MPD	A	801	8/8	0.24	7.25	33,39,42,43	0
3	MPD	R	203	8/8	0.19	6.56	32,35,38,40	0
3	MPD	O	800	8/8	0.15	6.28	22,24,28,30	0
3	MPD	T	801	8/8	0.18	6.09	26,34,36,38	0
3	MPD	Y	800	8/8	0.17	5.97	19,23,27,27	0
3	MPD	B	800	8/8	0.15	5.40	16,21,23,31	0
3	MPD	C	801	8/8	0.12	5.39	25,30,32,35	0
3	MPD	V	202	8/8	0.20	5.25	30,37,39,41	0
3	MPD	L	801	8/8	0.13	4.90	28,32,34,36	0
3	MPD	Z	801	8/8	0.17	4.87	29,32,36,36	0
3	MPD	W	801	8/8	0.18	4.76	29,34,35,40	0
3	MPD	X	201	8/8	0.18	4.44	23,27,29,31	0
3	MPD	N	801	8/8	0.14	4.44	32,34,36,42	0
3	MPD	I	801	8/8	0.17	4.11	26,32,34,35	0
3	MPD	V	201	8/8	0.12	3.99	23,29,33,33	0
3	MPD	b	801	8/8	0.16	3.90	30,34,40,42	0
3	MPD	W	800	8/8	0.16	3.70	24,31,33,34	0
3	MPD	Z	803	8/8	0.17	3.68	30,36,38,40	0
3	MPD	H	800	8/8	0.12	3.68	16,21,23,26	0
3	MPD	M	203	8/8	0.14	3.33	29,34,36,39	0
3	MPD	K	800	8/8	0.14	3.15	18,22,26,27	0
3	MPD	U	202	8/8	0.13	3.14	19,24,29,30	0
3	MPD	D	800	8/8	0.16	3.12	17,20,23,26	0
3	MPD	K	801	8/8	0.13	2.88	26,30,37,40	0
3	MPD	E	801	8/8	0.14	2.87	28,35,36,36	0
3	MPD	T	800	8/8	0.11	2.79	18,22,24,28	0
3	MPD	S	800	8/8	0.16	2.75	19,22,27,29	0
3	MPD	C	800	8/8	0.13	2.73	16,21,25,26	0
3	MPD	X	202	8/8	0.16	2.63	29,33,35,38	0
3	MPD	B	801	8/8	0.12	2.60	24,29,33,34	0
3	MPD	b	800	8/8	0.13	2.46	22,26,29,32	0
3	MPD	R	202	8/8	0.17	2.36	30,34,39,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MPD	P	801	8/8	0.15	2.30	30,39,43,43	0
3	MPD	O	801	8/8	0.11	2.24	28,30,34,35	0
3	MPD	M	201	8/8	0.14	2.13	18,26,27,28	0
3	MPD	N	800	8/8	0.14	2.05	20,26,27,27	0
3	MPD	a	800	8/8	0.16	2.01	21,24,28,29	0
3	MPD	L	800	8/8	0.14	2.01	21,24,28,29	0
3	MPD	A	800	8/8	0.12	1.94	17,25,28,31	0
3	MPD	E	803	8/8	0.14	1.83	25,30,32,34	0
3	MPD	F	800	8/8	0.11	1.71	22,25,26,31	0
3	MPD	Q	800	8/8	0.13	1.70	22,27,29,30	0
3	MPD	R	201	8/8	0.13	1.59	24,28,31,35	0
3	MPD	D	801	8/8	0.11	1.23	25,29,31,33	0
3	MPD	U	201	8/8	0.11	1.22	27,30,32,35	0
3	MPD	J	800	8/8	0.11	1.16	16,21,24,28	0
3	MPD	J	801	8/8	0.09	1.08	26,30,32,35	0
3	MPD	G	800	8/8	0.12	0.81	22,25,28,30	0
3	MPD	M	202	8/8	0.13	0.77	24,35,39,40	0
3	MPD	E	802	8/8	0.10	0.73	19,24,26,28	0
3	MPD	Q	801	8/8	0.10	0.53	26,36,40,41	0
3	MPD	I	800	8/8	0.10	0.38	16,20,21,25	0
3	MPD	G	801	8/8	0.10	0.17	28,33,35,36	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.