



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 05:53 PM BST

PDB ID : 5DKP  
Title : Crystal Structure of *N. meningitidis* ClpP in complex with agonist ADEP A54556.  
Authors : Goodreid, J.D.; Janetzko, J.; Santa Maria Jr., J.P.; Wong, K.; Leung, E.; Eger, B.T.; Bryson, S.; Pai, E.F.; Gray-Owen, S.D.; Walker, S.; Houry, W.A.; Batey, R.A.  
Deposited on : 2015-09-03  
Resolution : 2.38 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13

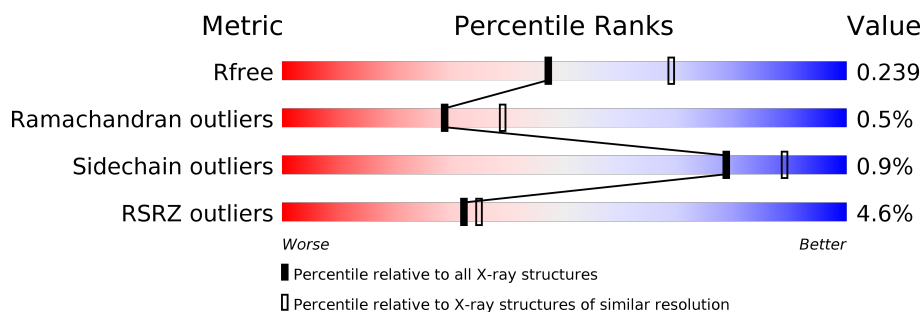
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.38 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5509 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	206	<div> <div>4%</div> <div>90%</div> <div>8%</div> </div>
1	B	206	<div> <div>%</div> <div>90%</div> <div>9%</div> </div>
1	C	206	<div> <div>5%</div> <div>92%</div> <div>7%</div> </div>
1	D	206	<div> <div>4%</div> <div>91%</div> <div>7%</div> </div>
1	E	206	<div> <div>2%</div> <div>92%</div> <div>7%</div> </div>
1	F	206	<div> <div>5%</div> <div>91%</div> <div>7%</div> </div>
1	G	206	<div> <div>5%</div> <div>91%</div> <div>6%</div> </div>













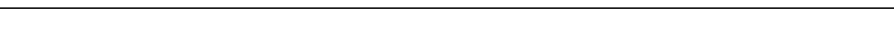











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Mol	Chain	Length	Quality of chain
1	H	206	
1	I	206	
1	J	206	
1	K	206	
1	L	206	
1	M	206	
1	N	206	
1	a	206	
1	b	206	
1	c	206	
1	d	206	
1	e	206	
1	f	206	
1	g	206	
1	h	206	
1	i	206	
1	j	206	
1	k	206	
1	l	206	
1	m	206	
1	n	206	
2	0	7	
2	1	7	
2	2	7	
2	3	7	

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Mol	Chain	Length	Quality of chain
2	O	7	 71%29%
2	P	7	 57%29%14%
2	Q	7	 57%43%
2	R	7	 57%43%
2	S	7	 71%29%
2	T	7	 71%29%
2	U	7	 71%29%
2	V	7	 71%29%
2	W	7	 71%29%
2	X	7	 71%29%
2	Y	7	 57%43%
2	Z	7	 43%57%
2	o	7	 57%43%
2	p	7	 71%29%
2	q	7	 57%43%
2	r	7	 57%29%14%
2	s	7	 57%43%
2	t	7	 57%29%14%
2	u	7	 71%29%
2	v	7	 57%43%
2	w	7	 57%43%
2	x	7	 57%43%
2	y	7	 57%43%
2	z	7	 71%29%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 43749 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	190	Total	C	N	O	S	0	0	0
			1473	930	252	283	8			
1	B	187	Total	C	N	O	S	0	0	0
			1456	921	246	281	8			
1	C	191	Total	C	N	O	S	0	0	0
			1482	933	254	287	8			
1	D	191	Total	C	N	O	S	0	0	0
			1482	935	253	286	8			
1	E	192	Total	C	N	O	S	0	0	0
			1494	944	254	288	8			
1	F	191	Total	C	N	O	S	0	0	0
			1485	939	253	285	8			
1	G	193	Total	C	N	O	S	0	0	0
			1502	948	256	290	8			
1	H	191	Total	C	N	O	S	0	0	0
			1485	939	253	285	8			
1	I	191	Total	C	N	O	S	0	0	0
			1482	935	253	286	8			
1	J	193	Total	C	N	O	S	0	0	0
			1502	948	256	290	8			
1	K	193	Total	C	N	O	S	0	0	0
			1501	945	259	289	8			
1	L	193	Total	C	N	O	S	0	0	0
			1502	948	256	290	8			
1	M	191	Total	C	N	O	S	0	0	0
			1485	939	253	285	8			
1	N	193	Total	C	N	O	S	0	0	0
			1502	948	256	290	8			
1	a	191	Total	C	N	O	S	0	0	0
			1485	939	253	285	8			
1	b	188	Total	C	N	O	S	0	0	0
			1462	924	248	282	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	c	177	Total	C	N	O	S	0	0	0
			1378	871	233	266	8			
1	d	184	Total	C	N	O	S	0	0	0
			1430	907	242	273	8			
1	e	191	Total	C	N	O	S	0	0	0
			1482	935	253	286	8			
1	f	183	Total	C	N	O	S	0	0	0
			1421	902	241	270	8			
1	g	192	Total	C	N	O	S	0	0	0
			1490	939	255	288	8			
1	h	191	Total	C	N	O	S	0	0	0
			1485	939	253	285	8			
1	i	191	Total	C	N	O	S	0	0	0
			1482	935	253	286	8			
1	j	191	Total	C	N	O	S	0	0	0
			1482	933	254	287	8			
1	k	194	Total	C	N	O	S	0	0	0
			1513	954	260	291	8			
1	l	193	Total	C	N	O	S	0	0	0
			1502	948	256	290	8			
1	m	190	Total	C	N	O	S	0	0	0
			1473	930	252	283	8			
1	n	192	Total	C	N	O	S	0	0	0
			1490	939	255	288	8			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q9JZ38
A	0	HIS	-	expression tag	UNP Q9JZ38
B	-1	GLY	-	expression tag	UNP Q9JZ38
B	0	HIS	-	expression tag	UNP Q9JZ38
C	-1	GLY	-	expression tag	UNP Q9JZ38
C	0	HIS	-	expression tag	UNP Q9JZ38
D	-1	GLY	-	expression tag	UNP Q9JZ38
D	0	HIS	-	expression tag	UNP Q9JZ38
E	-1	GLY	-	expression tag	UNP Q9JZ38
E	0	HIS	-	expression tag	UNP Q9JZ38
F	-1	GLY	-	expression tag	UNP Q9JZ38
F	0	HIS	-	expression tag	UNP Q9JZ38
G	-1	GLY	-	expression tag	UNP Q9JZ38
G	0	HIS	-	expression tag	UNP Q9JZ38
H	-1	GLY	-	expression tag	UNP Q9JZ38

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Chain	Residue	Modelled	Actual	Comment	Reference
H	0	HIS	-	expression tag	UNP Q9JZ38
I	-1	GLY	-	expression tag	UNP Q9JZ38
I	0	HIS	-	expression tag	UNP Q9JZ38
J	-1	GLY	-	expression tag	UNP Q9JZ38
J	0	HIS	-	expression tag	UNP Q9JZ38
K	-1	GLY	-	expression tag	UNP Q9JZ38
K	0	HIS	-	expression tag	UNP Q9JZ38
L	-1	GLY	-	expression tag	UNP Q9JZ38
L	0	HIS	-	expression tag	UNP Q9JZ38
M	-1	GLY	-	expression tag	UNP Q9JZ38
M	0	HIS	-	expression tag	UNP Q9JZ38
N	-1	GLY	-	expression tag	UNP Q9JZ38
N	0	HIS	-	expression tag	UNP Q9JZ38
a	-1	GLY	-	expression tag	UNP Q9JZ38
a	0	HIS	-	expression tag	UNP Q9JZ38
b	-1	GLY	-	expression tag	UNP Q9JZ38
b	0	HIS	-	expression tag	UNP Q9JZ38
c	-1	GLY	-	expression tag	UNP Q9JZ38
c	0	HIS	-	expression tag	UNP Q9JZ38
d	-1	GLY	-	expression tag	UNP Q9JZ38
d	0	HIS	-	expression tag	UNP Q9JZ38
e	-1	GLY	-	expression tag	UNP Q9JZ38
e	0	HIS	-	expression tag	UNP Q9JZ38
f	-1	GLY	-	expression tag	UNP Q9JZ38
f	0	HIS	-	expression tag	UNP Q9JZ38
g	-1	GLY	-	expression tag	UNP Q9JZ38
g	0	HIS	-	expression tag	UNP Q9JZ38
h	-1	GLY	-	expression tag	UNP Q9JZ38
h	0	HIS	-	expression tag	UNP Q9JZ38
i	-1	GLY	-	expression tag	UNP Q9JZ38
i	0	HIS	-	expression tag	UNP Q9JZ38
j	-1	GLY	-	expression tag	UNP Q9JZ38
j	0	HIS	-	expression tag	UNP Q9JZ38
k	-1	GLY	-	expression tag	UNP Q9JZ38
k	0	HIS	-	expression tag	UNP Q9JZ38
l	-1	GLY	-	expression tag	UNP Q9JZ38
l	0	HIS	-	expression tag	UNP Q9JZ38
m	-1	GLY	-	expression tag	UNP Q9JZ38
m	0	HIS	-	expression tag	UNP Q9JZ38
n	-1	GLY	-	expression tag	UNP Q9JZ38
n	0	HIS	-	expression tag	UNP Q9JZ38

- Molecule 2 is a protein called agonist ADEP A54556.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
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	U	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	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	u	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			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
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	0	7	Total	C	N	O	0	0	0
			52	38	6	8			
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	3	7	Total	C	N	O	0	0	0
			52	38	6	8			

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	g	1	Total	K	0	0
			1	1		
3	K	1	Total	K	0	0
			1	1		
3	h	1	Total	K	0	0
			1	1		
3	B	1	Total	K	0	0
			1	1		
3	c	1	Total	K	0	0
			1	1		
3	N	1	Total	K	0	0
			1	1		
3	f	1	Total	K	0	0
			1	1		
3	J	1	Total	K	0	0
			1	1		
3	k	1	Total	K	0	0
			1	1		
3	E	1	Total	K	0	0
			1	1		
3	b	1	Total	K	0	0
			1	1		
3	A	1	Total	K	0	0
			1	1		
3	n	1	Total	K	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	M	1	Total K 1 1	0	0
3	j	1	Total K 1 1	0	0
3	D	1	Total K 1 1	0	0
3	e	1	Total K 1 1	0	0
3	I	1	Total K 1 1	0	0
3	a	1	Total K 1 1	0	0
3	L	1	Total K 1 1	0	0
3	m	1	Total K 1 1	0	0
3	G	1	Total K 1 1	0	0
3	d	1	Total K 1 1	0	0
3	H	1	Total K 1 1	0	0
3	i	1	Total K 1 1	0	0
3	C	1	Total K 1 1	0	0
3	l	1	Total K 1 1	0	0
3	F	1	Total K 1 1	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	h	1	Total Na 1 1	0	0
4	c	1	Total Na 1 1	0	0
4	k	1	Total Na 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	35	Total 35	O 35	0	0
5	B	42	Total 42	O 42	0	0
5	C	35	Total 35	O 35	0	0
5	D	29	Total 29	O 29	0	0
5	E	34	Total 34	O 34	0	0
5	F	27	Total 27	O 27	0	0
5	G	31	Total 31	O 31	0	0
5	H	27	Total 27	O 27	0	0
5	I	34	Total 34	O 34	0	0
5	J	31	Total 31	O 31	0	0
5	K	41	Total 41	O 41	0	0
5	L	32	Total 32	O 32	0	0
5	M	37	Total 37	O 37	0	0
5	N	32	Total 32	O 32	0	0
5	a	27	Total 27	O 27	0	0
5	b	26	Total 26	O 26	0	0
5	c	34	Total 34	O 34	0	0
5	d	33	Total 33	O 33	0	0
5	e	26	Total 26	O 26	0	0
5	f	28	Total 28	O 28	0	0
5	g	16	Total 16	O 16	0	0
5	h	24	Total 24	O 24	0	0

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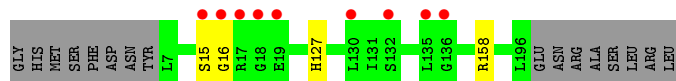
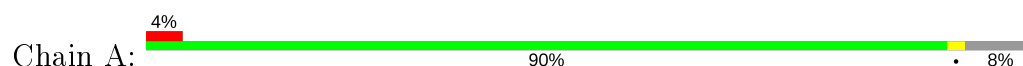
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	i	24	Total 24	O 24	0	0
5	j	35	Total 35	O 35	0	0
5	k	30	Total 30	O 30	0	0
5	l	29	Total 29	O 29	0	0
5	m	28	Total 28	O 28	0	0
5	n	24	Total 24	O 24	0	0
5	O	2	Total 2	O 2	0	0
5	t	1	Total 1	O 1	0	0

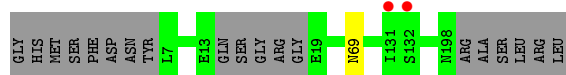
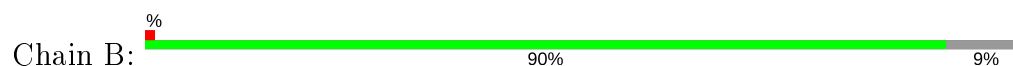
### 3 Residue-property plots [i](#)

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

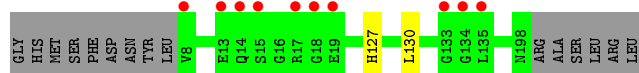
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



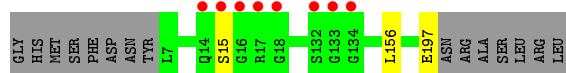
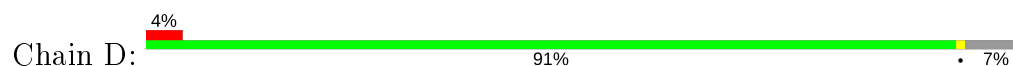
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



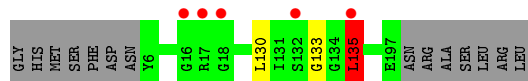
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



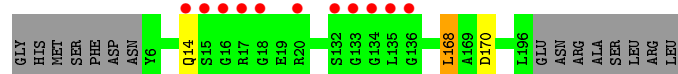
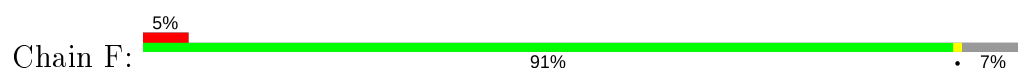
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



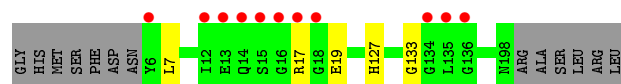
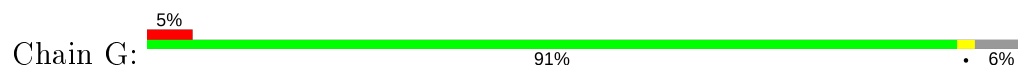
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



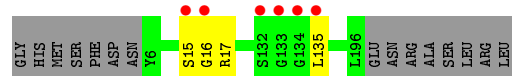
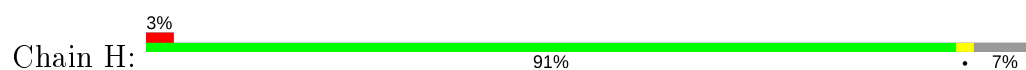
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



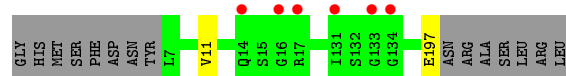
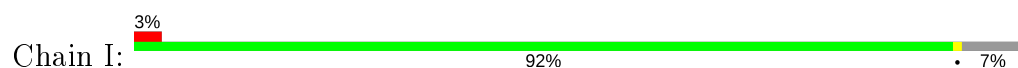
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



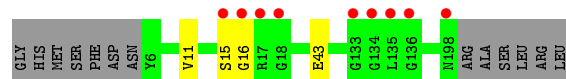
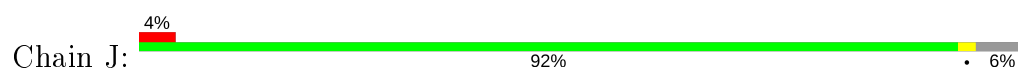
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



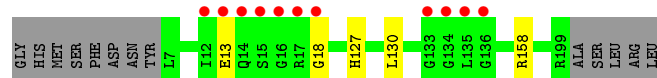
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



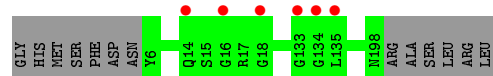
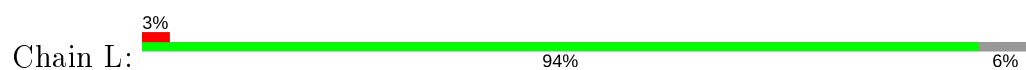
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



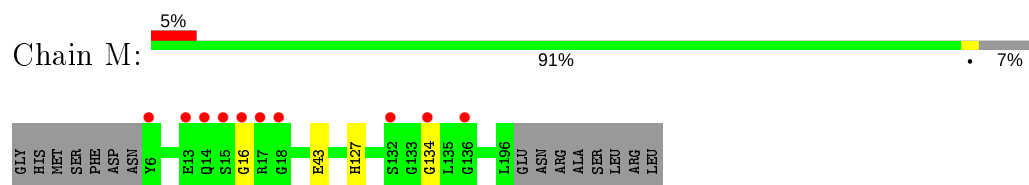
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



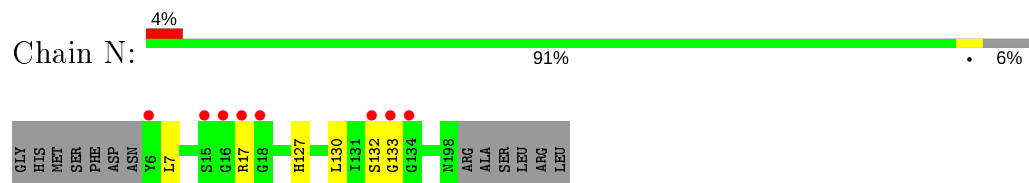
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



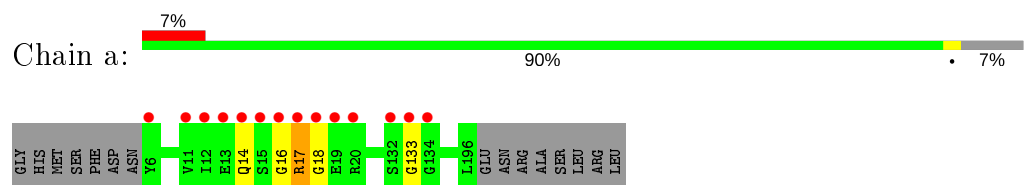
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



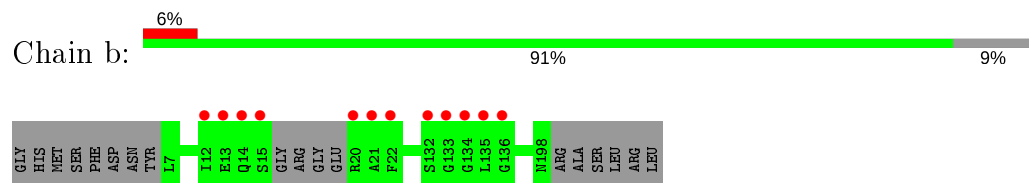
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



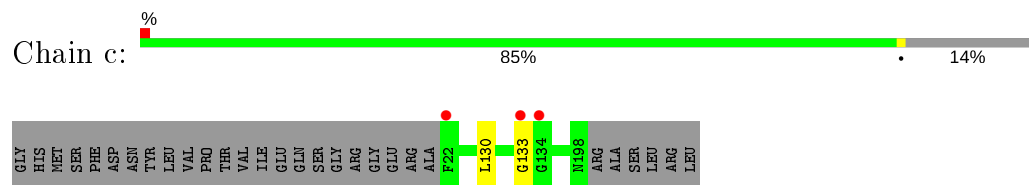
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



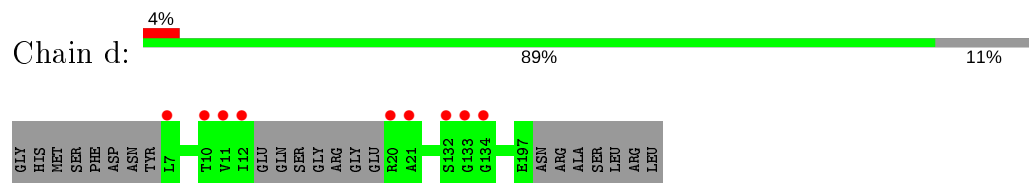
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



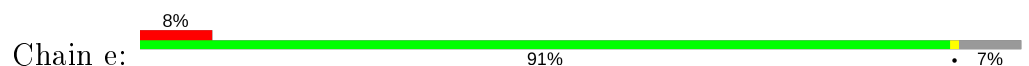
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

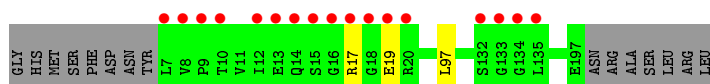


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

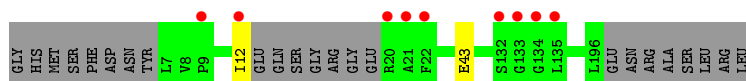
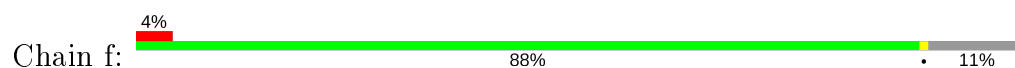


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

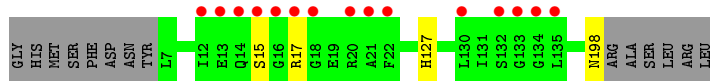
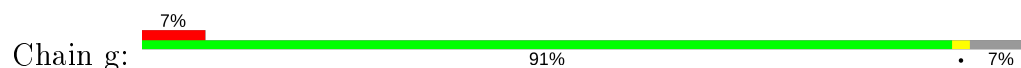




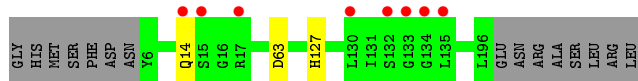
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



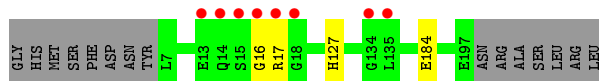
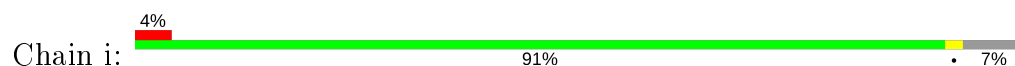
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



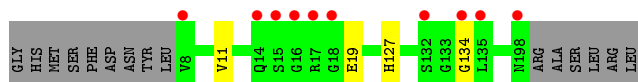
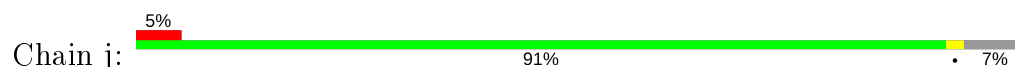
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



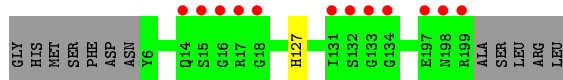
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

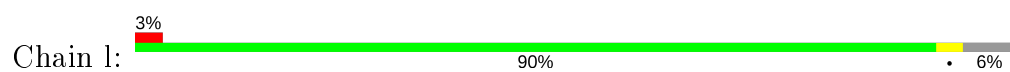


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

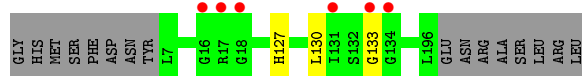
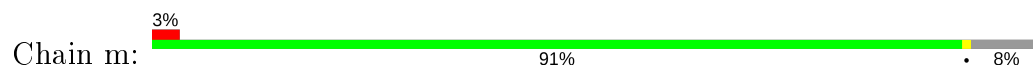


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

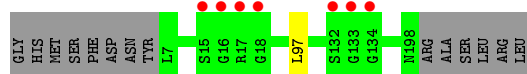




- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 2: agonist ADEP A54556



- Molecule 2: agonist ADEP A54556



- Molecule 2: agonist ADEP A54556



- Molecule 2: agonist ADEP A54556



- Molecule 2: agonist ADEP A54556



- Molecule 2: agonist ADEP A54556



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- Molecule 2: agonist ADEP A54556



- Molecule 2: agonist ADEP A54556



- Molecule 2: agonist ADEP A54556



- Molecule 2: agonist ADEP A54556

Chain Z:  43% 57%



- Molecule 2: agonist ADEP A54556

Chain o:  57% 43%



- Molecule 2: agonist ADEP A54556

Chain p:  71% 29%



- Molecule 2: agonist ADEP A54556

Chain q:  57% 43%



- Molecule 2: agonist ADEP A54556

Chain r:  57% 29% 14%



- Molecule 2: agonist ADEP A54556

Chain s:  57% 43%



- Molecule 2: agonist ADEP A54556

Chain t:  57% 29% 14%

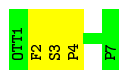


- Molecule 2: agonist ADEP A54556

Chain u:  71% 29%



- Molecule 2: agonist ADEP A54556



- Molecule 2: agonist ADEP A54556



- Molecule 2: agonist ADEP A54556



- Molecule 2: agonist ADEP A54556



- Molecule 2: agonist ADEP A54556



- Molecule 2: agonist ADEP A54556



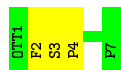
- Molecule 2: agonist ADEP A54556





- Molecule 2: agonist ADEP A54556

Chain 2:  57% 43%



- Molecule 2: agonist ADEP A54556

Chain 3:  71% 29%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.64Å 198.85Å 144.04Å 90.00° 97.81° 90.00°	Depositor
Resolution (Å)	42.40 – 2.38 142.70 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.4 (42.40-2.38) 99.4 (142.70-2.38)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.01 (at 2.37Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.196 , 0.239 0.197 , 0.239	Depositor DCC
$R_{free}$ test set	10329 reflections (3.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.2	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	43749	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.18% 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: MAA, NA, K, 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	0.44	0/1495	0.61	0/2013
1	B	0.45	0/1477	0.64	0/1989
1	C	0.45	0/1504	0.64	1/2025 (0.0%)
1	D	0.44	0/1504	0.60	0/2025
1	E	0.46	0/1517	0.67	2/2043 (0.1%)
1	F	0.45	0/1508	0.64	1/2031 (0.0%)
1	G	0.45	0/1525	0.64	1/2054 (0.0%)
1	H	0.48	0/1508	0.65	2/2031 (0.1%)
1	I	0.46	0/1504	0.63	0/2025
1	J	0.42	0/1525	0.63	0/2054
1	K	0.42	0/1523	0.59	1/2050 (0.0%)
1	L	0.44	0/1525	0.60	0/2054
1	M	0.44	0/1508	0.61	1/2031 (0.0%)
1	N	0.45	0/1525	0.65	2/2054 (0.1%)
1	a	0.44	0/1508	0.67	2/2031 (0.1%)
1	b	0.45	0/1483	0.60	0/1997
1	c	0.43	0/1399	0.62	2/1883 (0.1%)
1	d	0.43	0/1451	0.59	0/1954
1	e	0.44	0/1504	0.63	1/2025 (0.0%)
1	f	0.42	0/1442	0.60	0/1942
1	g	0.43	0/1512	0.61	0/2036
1	h	0.44	0/1508	0.62	0/2031
1	i	0.44	0/1504	0.63	0/2025
1	j	0.42	0/1504	0.64	0/2025
1	k	0.44	0/1536	0.62	0/2068
1	l	0.44	0/1525	0.64	1/2054 (0.0%)
1	m	0.43	0/1495	0.64	2/2013 (0.1%)
1	n	0.44	0/1512	0.63	1/2036 (0.0%)
2	0	2.18	3/29 (10.3%)	1.01	0/37
2	1	2.15	2/29 (6.9%)	1.04	0/37
2	2	2.33	3/29 (10.3%)	1.15	0/37
2	3	2.06	2/29 (6.9%)	1.10	0/37

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
2	O	2.16	2/29 (6.9%)	0.96	0/37
2	P	2.13	3/29 (10.3%)	0.94	0/37
2	Q	2.18	2/29 (6.9%)	1.07	0/37
2	R	2.27	3/29 (10.3%)	1.09	0/37
2	S	1.98	2/29 (6.9%)	0.95	0/37
2	T	2.08	2/29 (6.9%)	1.09	0/37
2	U	2.16	2/29 (6.9%)	1.07	0/37
2	V	2.10	2/29 (6.9%)	1.08	0/37
2	W	2.32	2/29 (6.9%)	0.86	0/37
2	X	2.14	2/29 (6.9%)	1.08	0/37
2	Y	2.21	3/29 (10.3%)	1.02	0/37
2	Z	2.11	3/29 (10.3%)	0.85	0/37
2	o	2.07	3/29 (10.3%)	1.15	0/37
2	p	2.12	2/29 (6.9%)	1.11	0/37
2	q	2.26	2/29 (6.9%)	0.99	0/37
2	r	2.20	3/29 (10.3%)	0.99	0/37
2	s	2.20	3/29 (10.3%)	0.88	0/37
2	t	2.21	3/29 (10.3%)	1.03	0/37
2	u	2.27	2/29 (6.9%)	1.06	0/37
2	v	2.18	3/29 (10.3%)	0.95	0/37
2	w	2.15	2/29 (6.9%)	1.02	0/37
2	x	2.06	2/29 (6.9%)	0.87	0/37
2	y	2.11	2/29 (6.9%)	1.06	0/37
2	z	2.18	2/29 (6.9%)	1.10	0/37
All	All	0.53	67/42843 (0.2%)	0.64	20/57635 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	N	0	1
1	a	0	2
1	l	0	1
All	All	0	4

The worst 5 of 67 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	W	2	PHE	CB-CG	-7.21	1.39	1.51
2	u	2	PHE	CB-CG	-7.09	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	2	PHE	CB-CG	-6.97	1.39	1.51
2	t	2	PHE	CB-CG	-6.94	1.39	1.51
2	R	2	PHE	CB-CG	-6.94	1.39	1.51

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	135	LEU	CA-CB-CG	9.63	137.46	115.30
1	N	133	GLY	N-CA-C	-6.88	95.91	113.10
1	G	133	GLY	N-CA-C	-6.41	97.07	113.10
1	M	134	GLY	N-CA-C	6.11	128.36	113.10
1	a	18	GLY	N-CA-C	-6.06	97.95	113.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	N	132	SER	Peptide
1	a	16	GLY	Peptide
1	a	17	ARG	Peptide
1	l	14	GLN	Peptide

## 5.2 Too-close contacts [i](#)

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

## 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	188/206 (91%)	180 (96%)	6 (3%)	2 (1%)	14	18
1	B	183/206 (89%)	180 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	189/206 (92%)	184 (97%)	5 (3%)	0	100	100
1	D	189/206 (92%)	184 (97%)	4 (2%)	1 (0%)	29	39
1	E	190/206 (92%)	184 (97%)	4 (2%)	2 (1%)	14	18
1	F	189/206 (92%)	181 (96%)	7 (4%)	1 (0%)	29	39
1	G	191/206 (93%)	184 (96%)	7 (4%)	0	100	100
1	H	189/206 (92%)	182 (96%)	4 (2%)	3 (2%)	9	11
1	I	189/206 (92%)	184 (97%)	5 (3%)	0	100	100
1	J	191/206 (93%)	184 (96%)	5 (3%)	2 (1%)	15	21
1	K	191/206 (93%)	182 (95%)	8 (4%)	1 (0%)	29	39
1	L	191/206 (93%)	184 (96%)	7 (4%)	0	100	100
1	M	189/206 (92%)	183 (97%)	5 (3%)	1 (0%)	29	39
1	N	191/206 (93%)	184 (96%)	5 (3%)	2 (1%)	15	21
1	a	189/206 (92%)	183 (97%)	5 (3%)	1 (0%)	29	39
1	b	184/206 (89%)	180 (98%)	4 (2%)	0	100	100
1	c	175/206 (85%)	171 (98%)	4 (2%)	0	100	100
1	d	180/206 (87%)	176 (98%)	4 (2%)	0	100	100
1	e	189/206 (92%)	180 (95%)	7 (4%)	2 (1%)	14	18
1	f	179/206 (87%)	176 (98%)	3 (2%)	0	100	100
1	g	190/206 (92%)	180 (95%)	9 (5%)	1 (0%)	29	39
1	h	189/206 (92%)	185 (98%)	4 (2%)	0	100	100
1	i	189/206 (92%)	183 (97%)	4 (2%)	2 (1%)	14	18
1	j	189/206 (92%)	181 (96%)	7 (4%)	1 (0%)	29	39
1	k	192/206 (93%)	188 (98%)	4 (2%)	0	100	100
1	l	191/206 (93%)	185 (97%)	4 (2%)	2 (1%)	15	21
1	m	188/206 (91%)	184 (98%)	4 (2%)	0	100	100
1	n	190/206 (92%)	185 (97%)	5 (3%)	0	100	100
2	0	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	1	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	2	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	3	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	O	3/7 (43%)	2 (67%)	1 (33%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	P	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	Q	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	R	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	S	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	T	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	U	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	V	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	W	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	X	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	Y	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	Z	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	o	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	p	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	q	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	r	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	s	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	t	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	u	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	v	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	w	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	x	3/7 (43%)	2 (67%)	0	1 (33%)	0	0
2	y	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	z	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
All	All	5348/5964 (90%)	5153 (96%)	170 (3%)	25 (0%)	29	39

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	133	GLY
1	J	15	SER
1	N	17	ARG
1	g	15	SER
1	j	134	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	160/174 (92%)	158 (99%)	2 (1%)	69	82
1	B	159/174 (91%)	158 (99%)	1 (1%)	86	93
1	C	161/174 (92%)	160 (99%)	1 (1%)	86	93
1	D	161/174 (92%)	159 (99%)	2 (1%)	71	84
1	E	162/174 (93%)	161 (99%)	1 (1%)	86	93
1	F	161/174 (92%)	160 (99%)	1 (1%)	86	93
1	G	163/174 (94%)	160 (98%)	3 (2%)	59	75
1	H	161/174 (92%)	161 (100%)	0	100	100
1	I	161/174 (92%)	159 (99%)	2 (1%)	71	84
1	J	163/174 (94%)	161 (99%)	2 (1%)	71	84
1	K	163/174 (94%)	161 (99%)	2 (1%)	71	84
1	L	163/174 (94%)	163 (100%)	0	100	100
1	M	161/174 (92%)	159 (99%)	2 (1%)	71	84
1	N	163/174 (94%)	162 (99%)	1 (1%)	86	93
1	a	161/174 (92%)	160 (99%)	1 (1%)	86	93
1	b	160/174 (92%)	160 (100%)	0	100	100
1	c	150/174 (86%)	150 (100%)	0	100	100
1	d	156/174 (90%)	156 (100%)	0	100	100
1	e	161/174 (92%)	161 (100%)	0	100	100
1	f	155/174 (89%)	153 (99%)	2 (1%)	69	82
1	g	162/174 (93%)	159 (98%)	3 (2%)	57	73
1	h	161/174 (92%)	159 (99%)	2 (1%)	71	84
1	i	161/174 (92%)	159 (99%)	2 (1%)	71	84
1	j	161/174 (92%)	158 (98%)	3 (2%)	57	73
1	k	164/174 (94%)	163 (99%)	1 (1%)	86	93
1	l	163/174 (94%)	160 (98%)	3 (2%)	59	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	m	160/174 (92%)	159 (99%)	1 (1%)	86	93
1	n	162/174 (93%)	162 (100%)	0	100	100
2	0	3/3 (100%)	3 (100%)	0	100	100
2	1	3/3 (100%)	3 (100%)	0	100	100
2	2	3/3 (100%)	3 (100%)	0	100	100
2	3	3/3 (100%)	3 (100%)	0	100	100
2	O	3/3 (100%)	3 (100%)	0	100	100
2	P	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	Q	3/3 (100%)	3 (100%)	0	100	100
2	R	3/3 (100%)	3 (100%)	0	100	100
2	S	3/3 (100%)	3 (100%)	0	100	100
2	T	3/3 (100%)	3 (100%)	0	100	100
2	U	3/3 (100%)	3 (100%)	0	100	100
2	V	3/3 (100%)	3 (100%)	0	100	100
2	W	3/3 (100%)	3 (100%)	0	100	100
2	X	3/3 (100%)	3 (100%)	0	100	100
2	Y	3/3 (100%)	3 (100%)	0	100	100
2	Z	3/3 (100%)	3 (100%)	0	100	100
2	o	3/3 (100%)	3 (100%)	0	100	100
2	p	3/3 (100%)	3 (100%)	0	100	100
2	q	3/3 (100%)	3 (100%)	0	100	100
2	r	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	s	3/3 (100%)	3 (100%)	0	100	100
2	t	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	u	3/3 (100%)	3 (100%)	0	100	100
2	v	3/3 (100%)	3 (100%)	0	100	100
2	w	3/3 (100%)	3 (100%)	0	100	100
2	x	3/3 (100%)	3 (100%)	0	100	100
2	y	3/3 (100%)	3 (100%)	0	100	100
2	z	3/3 (100%)	3 (100%)	0	100	100
All	All	4583/4956 (92%)	4542 (99%)	41 (1%)	78	89

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	127	HIS
1	f	43	GLU
1	m	127	HIS
1	N	127	HIS
1	a	14	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	127	HIS
1	k	127	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	x	5	2	4,5,6	0.82	0	1,5,7	1.40	0
2	MAA	p	5	2	4,5,6	0.76	0	1,5,7	1.39	0
2	MP8	q	7	2	5,8,9	0.54	0	3,10,12	1.35	1 (33%)
2	MP8	r	7	2	5,8,9	0.74	0	3,10,12	1.16	0
2	MP8	P	7	2	5,8,9	0.69	0	3,10,12	1.27	0
2	MP8	u	7	2	5,8,9	0.76	0	3,10,12	1.03	0
2	MP8	T	7	2	5,8,9	0.62	0	3,10,12	1.18	0
2	MAA	y	5	2	4,5,6	0.67	0	1,5,7	0.38	0
2	MP8	Z	7	2	5,8,9	0.84	0	3,10,12	1.69	1 (33%)
2	MAA	Z	5	2	4,5,6	0.63	0	1,5,7	1.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MP8	o	7	2	5,8,9	0.83	0	3,10,12	1.16	0
2	MAA	2	5	2	4,5,6	0.57	0	1,5,7	0.86	0
2	MP8	s	7	2	5,8,9	0.68	0	3,10,12	1.24	0
2	MP8	Q	7	2	5,8,9	0.74	0	3,10,12	1.31	1 (33%)
2	MP8	R	7	2	5,8,9	0.67	0	3,10,12	1.41	0
2	MP8	0	7	2	5,8,9	0.87	0	3,10,12	0.94	0
2	MP8	U	7	2	5,8,9	0.93	0	3,10,12	1.33	0
2	MP8	v	7	2	5,8,9	0.64	0	3,10,12	1.15	0
2	MP8	y	7	2	5,8,9	0.85	0	3,10,12	1.39	1 (33%)
2	MAA	W	5	2	4,5,6	1.06	0	1,5,7	0.14	0
2	MP8	x	7	2	5,8,9	0.61	0	3,10,12	1.36	0
2	MAA	3	5	2	4,5,6	0.84	0	1,5,7	0.33	0
2	MAA	1	5	2	4,5,6	0.92	0	1,5,7	0.73	0
2	MAA	O	5	2	4,5,6	0.84	0	1,5,7	0.12	0
2	MAA	z	5	2	4,5,6	0.80	0	1,5,7	0.45	0
2	MAA	V	5	2	4,5,6	0.76	0	1,5,7	0.04	0
2	MP8	O	7	2	5,8,9	0.73	0	3,10,12	1.12	0
2	MAA	T	5	2	4,5,6	0.63	0	1,5,7	0.96	0
2	MAA	R	5	2	4,5,6	0.83	0	1,5,7	0.05	0
2	MP8	S	7	2	5,8,9	0.74	0	3,10,12	1.30	0
2	MAA	0	5	2	4,5,6	0.68	0	1,5,7	0.22	0
2	MP8	1	7	2	5,8,9	0.66	0	3,10,12	1.22	0
2	MP8	2	7	2	5,8,9	0.78	0	3,10,12	1.16	0
2	MP8	w	7	2	5,8,9	0.82	0	3,10,12	1.31	1 (33%)
2	MP8	V	7	2	5,8,9	0.74	0	3,10,12	1.13	0
2	MP8	Y	7	2	5,8,9	0.65	0	3,10,12	1.36	0
2	MAA	w	5	2	4,5,6	0.77	0	1,5,7	0.89	0
2	MP8	X	7	2	5,8,9	0.58	0	3,10,12	1.30	0
2	MAA	U	5	2	4,5,6	0.71	0	1,5,7	0.70	0
2	MAA	S	5	2	4,5,6	0.63	0	1,5,7	0.76	0
2	MAA	Q	5	2	4,5,6	0.94	0	1,5,7	0.05	0
2	MAA	o	5	2	4,5,6	0.52	0	1,5,7	0.40	0
2	MAA	X	5	2	4,5,6	0.86	0	1,5,7	0.12	0
2	MAA	v	5	2	4,5,6	0.69	0	1,5,7	1.36	0
2	MAA	t	5	2	4,5,6	0.49	0	1,5,7	0.53	0
2	MAA	r	5	2	4,5,6	0.67	0	1,5,7	0.18	0
2	MP8	3	7	2	5,8,9	0.64	0	3,10,12	1.43	0
2	MAA	P	5	2	4,5,6	0.86	0	1,5,7	0.39	0
2	MP8	W	7	2	5,8,9	0.83	0	3,10,12	1.14	0
2	MP8	p	7	2	5,8,9	0.65	0	3,10,12	1.36	0
2	MP8	t	7	2	5,8,9	0.83	0	3,10,12	0.95	0
2	MAA	Y	5	2	4,5,6	0.94	0	1,5,7	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MP8	z	7	2	5,8,9	0.69	0	3,10,12	1.21	0
2	MAA	u	5	2	4,5,6	0.71	0	1,5,7	0.57	0
2	MAA	s	5	2	4,5,6	0.74	0	1,5,7	0.41	0
2	MAA	q	5	2	4,5,6	0.74	0	1,5,7	0.61	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	x	5	2	-	0/1/4/6	-
2	MAA	p	5	2	-	0/1/4/6	-
2	MP8	q	7	2	-	0/0/11/13	0/1/1/1
2	MP8	r	7	2	-	0/0/11/13	0/1/1/1
2	MP8	P	7	2	-	0/0/11/13	0/1/1/1
2	MP8	u	7	2	-	0/0/11/13	0/1/1/1
2	MP8	T	7	2	-	0/0/11/13	0/1/1/1
2	MAA	y	5	2	-	0/1/4/6	-
2	MP8	Z	7	2	-	0/0/11/13	0/1/1/1
2	MAA	Z	5	2	-	0/1/4/6	-
2	MP8	o	7	2	-	0/0/11/13	0/1/1/1
2	MAA	2	5	2	-	0/1/4/6	-
2	MP8	s	7	2	-	0/0/11/13	0/1/1/1
2	MP8	Q	7	2	-	0/0/11/13	0/1/1/1
2	MP8	R	7	2	-	0/0/11/13	0/1/1/1
2	MP8	0	7	2	-	0/0/11/13	0/1/1/1
2	MP8	U	7	2	-	0/0/11/13	0/1/1/1
2	MP8	v	7	2	-	0/0/11/13	0/1/1/1
2	MP8	y	7	2	-	0/0/11/13	0/1/1/1
2	MAA	W	5	2	-	0/1/4/6	-
2	MP8	x	7	2	-	0/0/11/13	0/1/1/1
2	MAA	3	5	2	-	0/1/4/6	-
2	MAA	1	5	2	-	0/1/4/6	-
2	MAA	O	5	2	-	0/1/4/6	-
2	MAA	z	5	2	-	0/1/4/6	-
2	MAA	V	5	2	-	0/1/4/6	-
2	MP8	O	7	2	-	0/0/11/13	0/1/1/1
2	MAA	T	5	2	-	0/1/4/6	-
2	MAA	R	5	2	-	0/1/4/6	-
2	MP8	S	7	2	-	0/0/11/13	0/1/1/1
2	MAA	0	5	2	-	0/1/4/6	-
2	MP8	1	7	2	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MP8	2	7	2	-	0/0/11/13	0/1/1/1
2	MP8	w	7	2	-	0/0/11/13	0/1/1/1
2	MP8	V	7	2	-	0/0/11/13	0/1/1/1
2	MP8	Y	7	2	-	0/0/11/13	0/1/1/1
2	MAA	w	5	2	-	0/1/4/6	-
2	MP8	X	7	2	-	0/0/11/13	0/1/1/1
2	MAA	U	5	2	-	0/1/4/6	-
2	MAA	S	5	2	-	0/1/4/6	-
2	MAA	Q	5	2	-	0/1/4/6	-
2	MAA	o	5	2	-	0/1/4/6	-
2	MAA	X	5	2	-	0/1/4/6	-
2	MAA	v	5	2	-	0/1/4/6	-
2	MAA	t	5	2	-	1/1/4/6	-
2	MAA	r	5	2	-	0/1/4/6	-
2	MP8	3	7	2	-	0/0/11/13	0/1/1/1
2	MAA	P	5	2	-	0/1/4/6	-
2	MP8	W	7	2	-	0/0/11/13	0/1/1/1
2	MP8	p	7	2	-	0/0/11/13	0/1/1/1
2	MP8	t	7	2	-	0/0/11/13	0/1/1/1
2	MAA	Y	5	2	-	0/1/4/6	-
2	MP8	z	7	2	-	0/0/11/13	0/1/1/1
2	MAA	u	5	2	-	0/1/4/6	-
2	MAA	s	5	2	-	0/1/4/6	-
2	MAA	q	5	2	-	0/1/4/6	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	y	7	MP8	O-C-CA	-2.25	118.89	124.78
2	q	7	MP8	O-C-CA	-2.11	119.26	124.78
2	Q	7	MP8	O-C-CA	-2.06	119.37	124.78
2	w	7	MP8	O-C-CA	-2.05	119.42	124.78
2	Z	7	MP8	O-C-CA	-2.04	119.44	124.78

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	t	5	MAA	CB-CA-N-CM

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 31 ligands modelled in this entry, 31 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

## 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	190/206 (92%)	0.15	9 (4%) 31 34	14, 20, 58, 87	0
1	B	187/206 (90%)	0.15	2 (1%) 80 81	13, 20, 46, 85	0
1	C	191/206 (92%)	0.18	10 (5%) 27 30	14, 20, 66, 96	0
1	D	191/206 (92%)	0.17	8 (4%) 36 39	13, 20, 63, 93	0
1	E	192/206 (93%)	0.10	5 (2%) 56 57	13, 21, 60, 91	0
1	F	191/206 (92%)	0.22	11 (5%) 23 25	14, 21, 73, 105	0
1	G	193/206 (93%)	0.25	11 (5%) 23 26	14, 21, 68, 98	0
1	H	191/206 (92%)	0.11	6 (3%) 49 51	14, 22, 61, 90	0
1	I	191/206 (92%)	0.18	6 (3%) 49 51	14, 21, 59, 90	0
1	J	193/206 (93%)	0.21	9 (4%) 31 34	15, 22, 66, 103	0
1	K	193/206 (93%)	0.27	11 (5%) 23 26	12, 21, 69, 102	0
1	L	193/206 (93%)	0.23	6 (3%) 49 51	14, 21, 65, 111	0
1	M	191/206 (92%)	0.21	10 (5%) 27 30	14, 20, 62, 103	0
1	N	193/206 (93%)	0.24	8 (4%) 37 40	14, 21, 61, 99	0
1	a	191/206 (92%)	0.30	14 (7%) 15 16	15, 22, 75, 117	0
1	b	188/206 (91%)	0.25	12 (6%) 19 21	14, 22, 64, 107	0
1	c	177/206 (85%)	0.02	3 (1%) 70 71	14, 20, 41, 86	0
1	d	184/206 (89%)	0.19	9 (4%) 29 32	14, 20, 52, 90	0
1	e	191/206 (92%)	0.39	17 (8%) 9 10	13, 22, 72, 108	0
1	f	183/206 (88%)	0.16	9 (4%) 29 32	16, 22, 64, 88	0
1	g	192/206 (93%)	0.29	15 (7%) 13 14	15, 22, 75, 120	0
1	h	191/206 (92%)	0.14	8 (4%) 36 39	15, 21, 57, 88	0
1	i	191/206 (92%)	0.13	8 (4%) 36 39	14, 21, 57, 103	0
1	j	191/206 (92%)	0.21	10 (5%) 27 30	14, 21, 68, 97	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	k	194/206 (94%)	0.29	12 (6%)	20	22	14, 21, 69, 105	0
1	l	193/206 (93%)	0.08	6 (3%)	49	51	14, 22, 64, 91	0
1	m	190/206 (92%)	0.07	6 (3%)	47	50	13, 21, 52, 90	0
1	n	192/206 (93%)	0.14	7 (3%)	42	46	15, 22, 63, 102	0
2	0	4/7 (57%)	-0.27	0	100	100	21, 26, 27, 34	0
2	1	4/7 (57%)	-0.05	0	100	100	22, 26, 27, 30	0
2	2	4/7 (57%)	-0.04	0	100	100	27, 28, 28, 30	0
2	3	4/7 (57%)	-0.09	0	100	100	25, 27, 29, 32	0
2	O	4/7 (57%)	-0.00	0	100	100	21, 23, 27, 28	0
2	P	4/7 (57%)	-0.03	0	100	100	19, 21, 27, 28	0
2	Q	4/7 (57%)	-0.26	0	100	100	19, 23, 23, 23	0
2	R	4/7 (57%)	-0.27	0	100	100	18, 22, 26, 28	0
2	S	4/7 (57%)	0.01	0	100	100	21, 22, 25, 27	0
2	T	4/7 (57%)	-0.02	0	100	100	24, 26, 27, 31	0
2	U	4/7 (57%)	-0.18	0	100	100	26, 27, 27, 33	0
2	V	4/7 (57%)	0.14	0	100	100	24, 24, 34, 34	0
2	W	4/7 (57%)	-0.04	0	100	100	24, 29, 30, 33	0
2	X	4/7 (57%)	0.23	0	100	100	23, 26, 26, 30	0
2	Y	4/7 (57%)	0.07	0	100	100	23, 29, 31, 41	0
2	Z	4/7 (57%)	-0.20	0	100	100	17, 20, 23, 24	0
2	o	4/7 (57%)	0.02	0	100	100	22, 24, 24, 30	0
2	p	4/7 (57%)	-0.29	0	100	100	21, 23, 28, 30	0
2	q	4/7 (57%)	0.25	0	100	100	24, 33, 35, 36	0
2	r	4/7 (57%)	-0.23	0	100	100	27, 28, 30, 36	0
2	s	4/7 (57%)	-0.51	0	100	100	24, 26, 26, 28	0
2	t	4/7 (57%)	0.10	0	100	100	23, 24, 25, 30	0
2	u	4/7 (57%)	0.36	0	100	100	19, 31, 32, 34	0
2	v	4/7 (57%)	0.09	0	100	100	24, 30, 33, 44	0
2	w	4/7 (57%)	-0.03	0	100	100	23, 32, 35, 37	0
2	x	4/7 (57%)	0.20	0	100	100	28, 28, 31, 32	0
2	y	4/7 (57%)	-0.01	0	100	100	24, 25, 26, 27	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
2	z	4/7 (57%)	0.46	0	100	100	24, 27, 27, 28	0
All	All	5440/5964 (91%)	0.19	248 (4%)	32	35	12, 21, 64, 120	0

The worst 5 of 248 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	n	16	GLY	10.8
1	G	15	SER	10.4
1	g	16	GLY	9.4
1	e	16	GLY	9.2
1	J	18	GLY	9.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MAA	p	5	6/7	0.92	0.12	22,32,34,36	0
2	MP8	r	7	8/9	0.93	0.10	17,21,32,37	0
2	MP8	u	7	8/9	0.93	0.13	13,23,28,32	0
2	MP8	o	7	8/9	0.93	0.11	14,19,30,31	0
2	MP8	U	7	8/9	0.93	0.13	18,23,30,38	0
2	MP8	p	7	8/9	0.93	0.11	17,21,24,32	0
2	MP8	t	7	8/9	0.93	0.13	22,24,33,41	0
2	MAA	W	5	6/7	0.94	0.16	25,31,34,35	0
2	MAA	z	5	6/7	0.94	0.13	21,28,30,34	0
2	MP8	S	7	8/9	0.94	0.14	14,21,28,35	0
2	MP8	2	7	8/9	0.94	0.14	13,17,25,25	0
2	MP8	0	7	8/9	0.94	0.12	16,23,27,28	0
2	MP8	v	7	8/9	0.94	0.12	18,24,28,38	0
2	MAA	S	5	6/7	0.95	0.11	18,25,31,32	0
2	MAA	r	5	6/7	0.95	0.14	24,32,39,41	0
2	MP8	3	7	8/9	0.95	0.12	15,20,23,27	0
2	MP8	W	7	8/9	0.95	0.12	18,27,33,36	0
2	MAA	x	5	6/7	0.95	0.17	32,44,53,65	0
2	MP8	w	7	8/9	0.95	0.10	26,32,38,39	0
2	MAA	q	5	6/7	0.95	0.15	32,34,39,43	0
2	MAA	y	5	6/7	0.96	0.13	17,22,27,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MP8	P	7	8/9	0.96	0.11	19,24,25,26	0
2	MP8	Y	7	8/9	0.96	0.10	14,19,23,31	0
2	MAA	w	5	6/7	0.96	0.14	27,32,36,45	0
2	MP8	X	7	8/9	0.96	0.10	19,24,29,29	0
2	MP8	Q	7	8/9	0.96	0.12	10,18,27,27	0
2	MAA	X	5	6/7	0.96	0.15	21,30,34,45	0
2	MAA	v	5	6/7	0.96	0.14	29,35,39,40	0
2	MAA	t	5	6/7	0.96	0.14	29,34,35,39	0
2	MP8	x	7	8/9	0.96	0.11	19,23,32,32	0
2	MP8	R	7	8/9	0.96	0.12	10,20,25,32	0
2	MAA	V	5	6/7	0.96	0.12	26,28,32,36	0
2	MAA	T	5	6/7	0.96	0.17	25,31,34,36	0
2	MP8	q	7	8/9	0.96	0.15	19,29,33,38	0
2	MAA	Y	5	6/7	0.96	0.11	22,28,38,44	0
2	MP8	z	7	8/9	0.96	0.13	15,20,27,33	0
2	MAA	u	5	6/7	0.96	0.17	20,36,44,46	0
2	MP8	1	7	8/9	0.96	0.11	20,23,28,30	0
2	MP8	O	7	8/9	0.97	0.12	22,26,31,34	0
2	MAA	Q	5	6/7	0.97	0.13	24,25,29,30	0
2	MP8	s	7	8/9	0.97	0.12	17,25,27,27	0
2	MAA	R	5	6/7	0.97	0.10	23,28,30,33	0
2	MP8	y	7	8/9	0.97	0.12	16,19,24,24	0
2	MAA	0	5	6/7	0.97	0.11	24,30,33,36	0
2	MP8	Z	7	8/9	0.97	0.11	16,22,28,30	0
2	MAA	P	5	6/7	0.97	0.13	24,27,30,35	0
2	MAA	Z	5	6/7	0.97	0.14	14,18,26,31	0
2	MAA	3	5	6/7	0.97	0.13	27,35,38,40	0
2	MP8	V	7	8/9	0.97	0.12	11,25,29,30	0
2	MAA	1	5	6/7	0.97	0.12	21,33,35,37	0
2	MP8	T	7	8/9	0.97	0.11	12,16,21,28	0
2	MAA	2	5	6/7	0.97	0.10	21,25,27,32	0
2	MAA	s	5	6/7	0.97	0.09	20,25,34,39	0
2	MAA	U	5	6/7	0.97	0.13	18,26,31,32	0
2	MAA	O	5	6/7	0.98	0.13	18,21,35,36	0
2	MAA	o	5	6/7	0.99	0.14	20,26,27,27	0

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	NA	h	302	1/1	0.97	0.13	37,37,37,37	0
3	K	J	301	1/1	0.97	0.07	31,31,31,31	0
3	K	k	301	1/1	0.97	0.07	26,26,26,26	0
3	K	M	301	1/1	0.97	0.10	26,26,26,26	0
3	K	d	301	1/1	0.97	0.07	27,27,27,27	0
4	NA	k	302	1/1	0.98	0.10	40,40,40,40	0
3	K	i	301	1/1	0.98	0.11	28,28,28,28	0
3	K	h	301	1/1	0.98	0.11	30,30,30,30	0
3	K	f	301	1/1	0.98	0.07	32,32,32,32	0
4	NA	c	302	1/1	0.98	0.08	25,25,25,25	0
3	K	e	301	1/1	0.98	0.07	32,32,32,32	0
3	K	n	301	1/1	0.98	0.05	26,26,26,26	0
3	K	a	301	1/1	0.98	0.07	31,31,31,31	0
3	K	E	301	1/1	0.98	0.07	30,30,30,30	0
3	K	H	301	1/1	0.98	0.08	35,35,35,35	0
3	K	m	301	1/1	0.98	0.07	29,29,29,29	0
3	K	L	301	1/1	0.99	0.12	25,25,25,25	0
3	K	g	301	1/1	0.99	0.07	31,31,31,31	0
3	K	D	301	1/1	0.99	0.09	26,26,26,26	0
3	K	I	301	1/1	0.99	0.08	30,30,30,30	0
3	K	K	301	1/1	0.99	0.07	29,29,29,29	0
3	K	B	301	1/1	0.99	0.07	22,22,22,22	0
3	K	G	301	1/1	0.99	0.10	25,25,25,25	0
3	K	c	301	1/1	0.99	0.08	25,25,25,25	0
3	K	A	301	1/1	0.99	0.09	24,24,24,24	0
3	K	l	301	1/1	0.99	0.08	27,27,27,27	0
3	K	C	301	1/1	0.99	0.09	24,24,24,24	0
3	K	N	301	1/1	0.99	0.09	25,25,25,25	0
3	K	F	301	1/1	0.99	0.07	26,26,26,26	0
3	K	b	301	1/1	0.99	0.09	40,40,40,40	0
3	K	j	301	1/1	1.00	0.09	22,22,22,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.