



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 28, 2016 – 12:44 PM EDT

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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027107  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027107

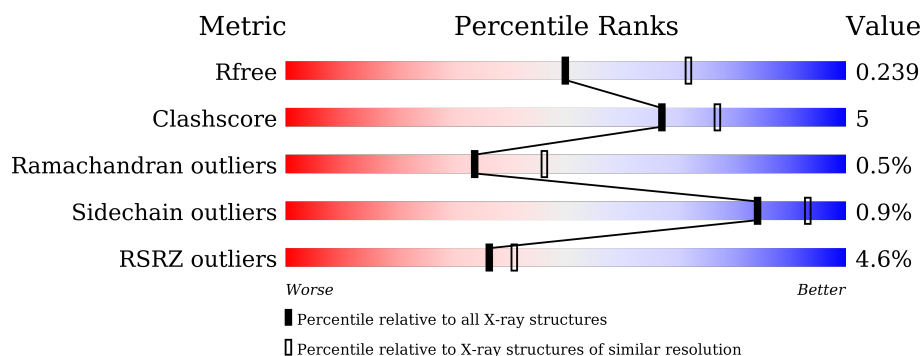
# 1 Overall quality at a glance

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))
$R_{free}$	91344	4019 (2.40-2.36)
Clashscore	102246	4595 (2.40-2.36)
Ramachandran outliers	100387	4520 (2.40-2.36)
Sidechain outliers	100360	4522 (2.40-2.36)
RSRZ outliers	91569	4034 (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. 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> <div></div> <div>74%</div> <div>17%</div> <div>8%</div> </div> </div>
1	B	206	<div> <div>0%</div> <div> <div></div> <div>74%</div> <div>17%</div> <div>9%</div> </div> </div>
1	C	206	<div> <div>5%</div> <div> <div></div> <div>75%</div> <div>17%</div> <div>7%</div> </div> </div>
1	D	206	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>16%</div> <div>7%</div> </div> </div>
1	E	206	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>17%</div> <div>7%</div> </div> </div>
1	F	206	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>18%</div> <div>7%</div> </div> </div>

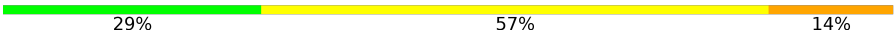
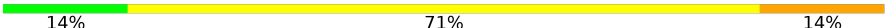

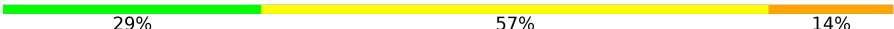
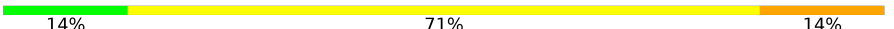
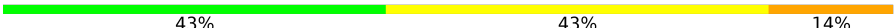
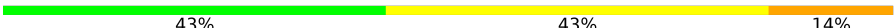


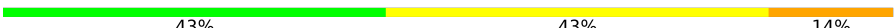
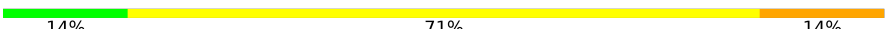
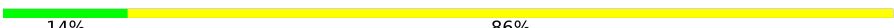
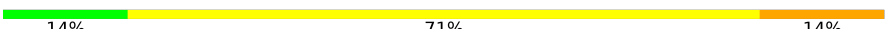












*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	206	
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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	3	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	
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	

## 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			

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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			

Continued on next page...



*Continued from previous page...*

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		

*Continued on next page...*

*Continued from previous page...*

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

Continued on next page...

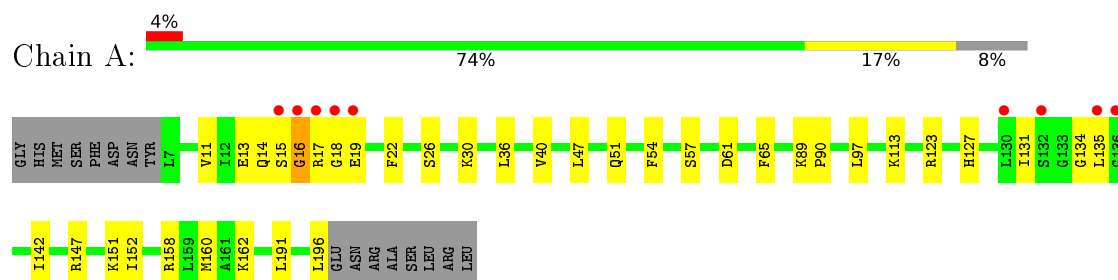
*Continued from previous page...*

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

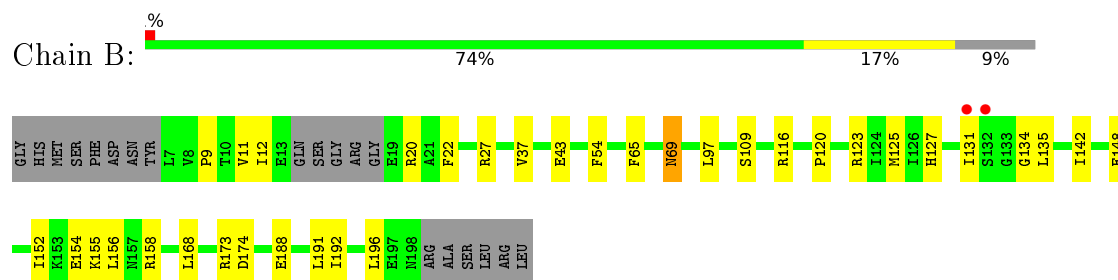
### 3 Residue-property plots

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.

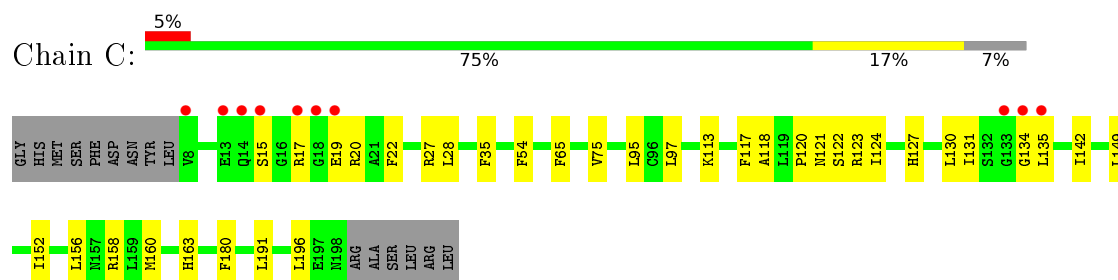
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



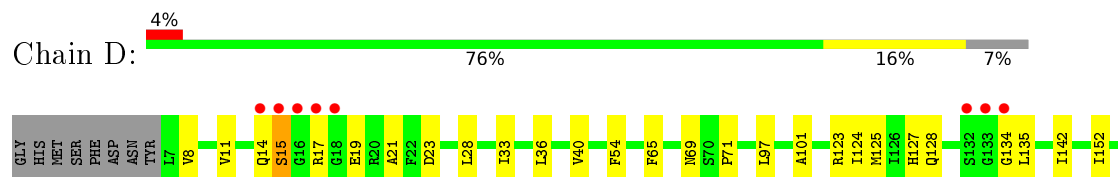
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

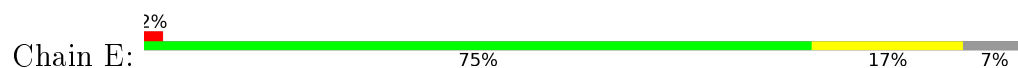


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

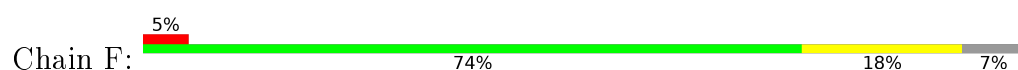




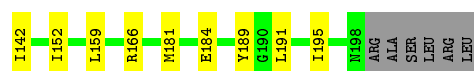
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



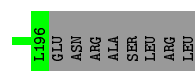
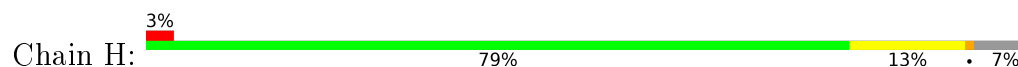
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

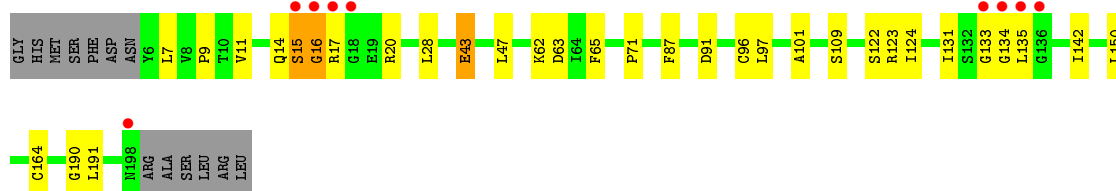
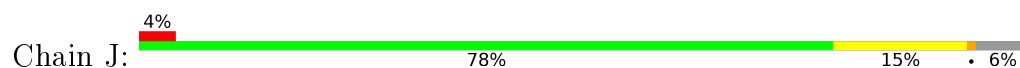


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

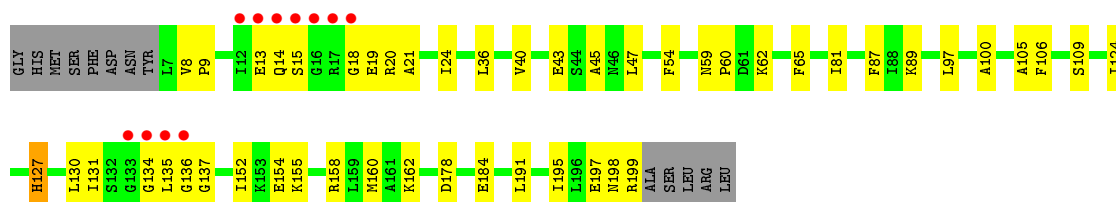




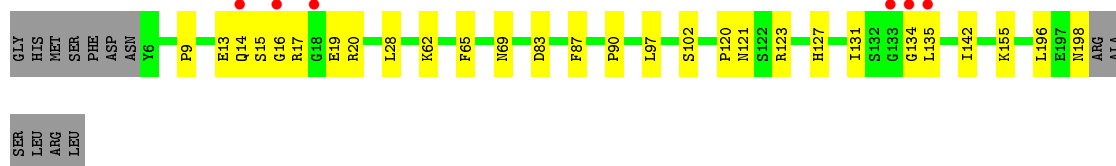
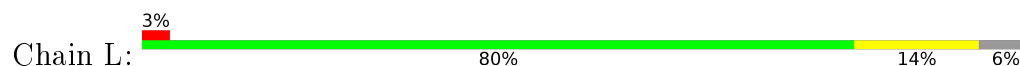
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



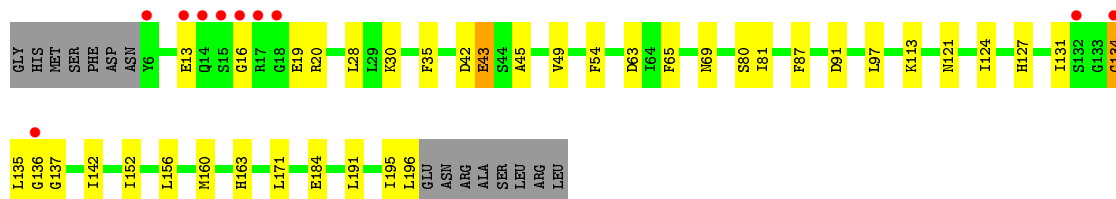
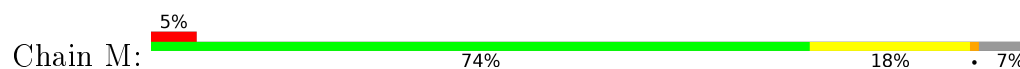
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



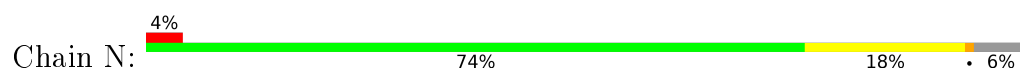
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

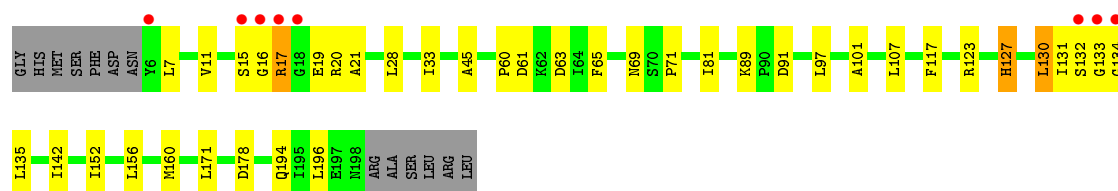


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

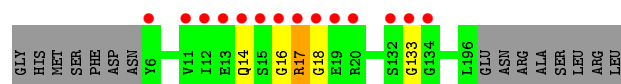


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

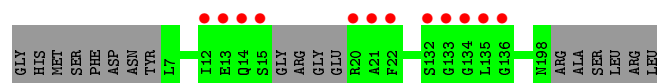




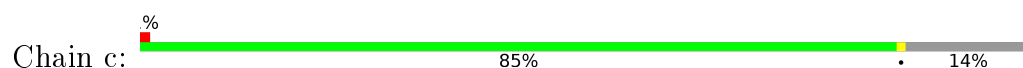
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



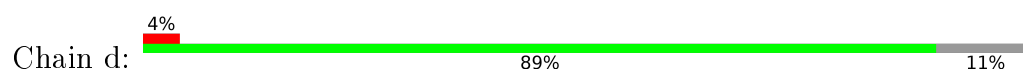
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



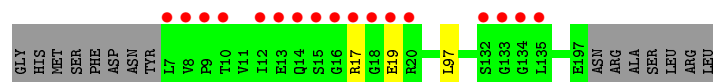
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



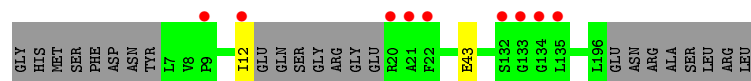
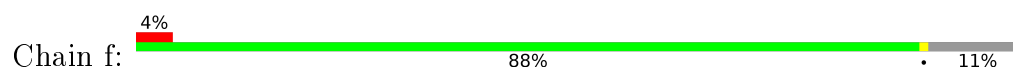
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

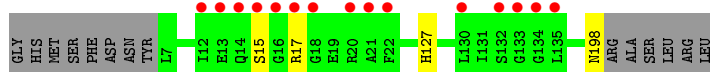
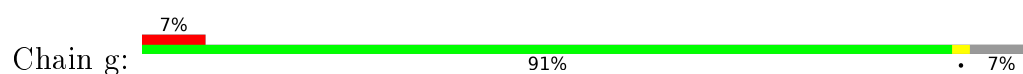


- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit





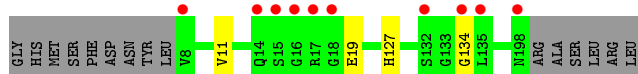
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit



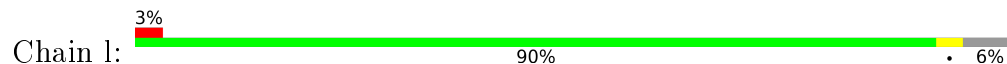
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit



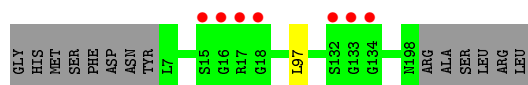
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- 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



- Molecule 2: agonist ADEP A54556



- Molecule 2: agonist ADEP A54556

Chain V:  29% 57% 14%



- Molecule 2: agonist ADEP A54556

Chain W:  43% 43% 14%



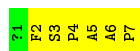
- Molecule 2: agonist ADEP A54556

Chain X:  14% 71% 14%



- Molecule 2: agonist ADEP A54556

Chain Y:  14% 86%



- Molecule 2: agonist ADEP A54556

Chain Z:  14% 71% 14%



- Molecule 2: agonist ADEP A54556

Chain o:  57% 43%



- Molecule 2: agonist ADEP A54556

Chain p:  71% 29%



- Molecule 2: agonist ADEP A54556

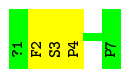
Chain q:  71% 29%



- 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 y:  71% 29%




- Molecule 2: agonist ADEP A54556

Chain z:  71% 29%




- Molecule 2: agonist ADEP A54556

Chain 0:  29% 57% 14%



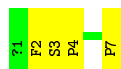
- Molecule 2: agonist ADEP A54556

Chain 1:  57% 43%




- Molecule 2: agonist ADEP A54556

Chain 2:  43% 57%



- Molecule 2: agonist ADEP A54556

Chain 3:  29% 57% 14%



## 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 0.196 , 0.239	Depositor DCC
$R_{free}$ test set	10332 reflections (3.98%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	3 of 259707 reflections (0.001%)	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, 0.375 respectively for untwinned datasets, and 0.333, 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

All (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

*Continued on next page...*



*Continued from previous page...*

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
2	p	4	PRO	CA-C	-6.74	1.39	1.52
2	U	2	PHE	CB-CG	-6.62	1.40	1.51
2	O	2	PHE	CB-CG	-6.51	1.40	1.51
2	q	2	PHE	CB-CG	-6.51	1.40	1.51
2	X	2	PHE	CB-CG	-6.49	1.40	1.51
2	r	2	PHE	CB-CG	-6.47	1.40	1.51
2	z	2	PHE	CB-CG	-6.39	1.40	1.51
2	s	2	PHE	CB-CG	-6.35	1.40	1.51
2	Q	4	PRO	CA-C	-6.35	1.40	1.52
2	z	4	PRO	CA-C	-6.33	1.40	1.52
2	v	2	PHE	CB-CG	-6.30	1.40	1.51
2	Y	2	PHE	CB-CG	-6.22	1.40	1.51
2	w	2	PHE	CB-CG	-6.20	1.40	1.51
2	3	2	PHE	CB-CG	-6.14	1.41	1.51
2	V	2	PHE	CB-CG	-6.13	1.41	1.51
2	1	2	PHE	CB-CG	-6.13	1.41	1.51
2	0	2	PHE	CB-CG	-6.08	1.41	1.51
2	U	4	PRO	CA-C	-6.07	1.40	1.52
2	3	4	PRO	CA-C	-6.04	1.40	1.52
2	q	4	PRO	CA-C	-6.00	1.40	1.52
2	2	4	PRO	CA-C	-5.98	1.40	1.52
2	y	4	PRO	CA-C	-5.95	1.41	1.52
2	x	2	PHE	CB-CG	-5.93	1.41	1.51
2	s	4	PRO	CA-C	-5.89	1.41	1.52
2	u	4	PRO	CA-C	-5.89	1.41	1.52
2	R	4	PRO	CA-C	-5.87	1.41	1.52
2	x	4	PRO	CA-C	-5.87	1.41	1.52
2	O	4	PRO	CA-C	-5.84	1.41	1.52
2	v	4	PRO	CA-C	-5.82	1.41	1.52
2	1	4	PRO	CA-C	-5.82	1.41	1.52
2	V	4	PRO	CA-C	-5.80	1.41	1.52
2	Q	2	PHE	CB-CG	-5.79	1.41	1.51
2	P	2	PHE	CB-CG	-5.79	1.41	1.51
2	o	4	PRO	CA-C	-5.76	1.41	1.52
2	T	4	PRO	CA-C	-5.75	1.41	1.52
2	w	4	PRO	CA-C	-5.74	1.41	1.52
2	0	4	PRO	CA-C	-5.74	1.41	1.52
2	Y	6	ALA	CA-C	-5.72	1.38	1.52
2	S	4	PRO	CA-C	-5.70	1.41	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	2	PHE	CB-CG	-5.70	1.41	1.51
2	Z	4	PRO	CA-C	-5.65	1.41	1.52
2	X	4	PRO	CA-C	-5.52	1.41	1.52
2	r	3	SER	CA-C	-5.51	1.38	1.52
2	s	3	SER	CA-C	-5.48	1.38	1.52
2	r	4	PRO	CA-C	-5.47	1.42	1.52
2	W	4	PRO	CA-C	-5.46	1.42	1.52
2	P	4	PRO	CA-C	-5.32	1.42	1.52
2	v	3	SER	CA-C	-5.31	1.39	1.52
2	Z	2	PHE	CB-CG	-5.26	1.42	1.51
2	2	3	SER	CA-C	-5.20	1.39	1.52
2	t	4	PRO	CA-C	-5.19	1.42	1.52
2	y	2	PHE	CB-CG	-5.17	1.42	1.51
2	Y	3	SER	CA-C	-5.11	1.39	1.52
2	o	6	ALA	CA-C	-5.09	1.39	1.52
2	S	2	PHE	CB-CG	-5.06	1.42	1.51
2	o	2	PHE	CB-CG	-5.06	1.42	1.51
2	p	2	PHE	CB-CG	-5.05	1.42	1.51
2	0	3	SER	CA-C	-5.05	1.39	1.52
2	t	6	ALA	CA-C	-5.04	1.39	1.52
2	P	3	SER	CA-C	-5.04	1.39	1.52
2	R	3	SER	CA-C	-5.03	1.39	1.52
2	Z	3	SER	CA-C	-5.01	1.40	1.52

All (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
1	K	130	LEU	CA-CB-CG	6.02	129.14	115.30
1	E	130	LEU	CA-CB-CG	5.94	128.96	115.30
1	H	135	LEU	CB-CG-CD1	-5.86	101.04	111.00
1	c	133	GLY	N-CA-C	-5.81	98.57	113.10
1	l	133	GLY	N-CA-C	-5.81	98.58	113.10
1	N	130	LEU	CA-CB-CG	5.62	128.22	115.30
1	m	130	LEU	CA-CB-CG	5.51	127.97	115.30
1	F	168	LEU	CA-CB-CG	5.50	127.96	115.30
1	m	133	GLY	N-CA-C	-5.44	99.51	113.10
1	c	130	LEU	CA-CB-CG	5.26	127.40	115.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	n	97	LEU	CA-CB-CG	5.25	127.38	115.30
1	a	133	GLY	N-CA-C	-5.23	100.03	113.10
1	e	97	LEU	CA-CB-CG	5.21	127.28	115.30
1	H	135	LEU	CA-CB-CG	5.15	127.14	115.30
1	C	130	LEU	CA-CB-CG	5.12	127.08	115.30

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1473	0	1484	36	0
1	B	1456	0	1463	37	0
1	C	1482	0	1485	32	0
1	D	1482	0	1490	29	0
1	E	1494	0	1499	36	0
1	F	1485	0	1493	34	1
1	G	1502	0	1505	39	1
1	H	1485	0	1493	27	0
1	I	1482	0	1490	43	0
1	J	1502	0	1505	36	0
1	K	1501	0	1509	42	1
1	L	1502	0	1505	33	0
1	M	1485	0	1493	34	0
1	N	1502	0	1505	42	0
1	a	1485	0	1493	0	0
1	b	1462	0	1470	0	0
1	c	1378	0	1380	0	0
1	d	1430	0	1445	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	e	1482	0	1490	0	0
1	f	1421	0	1439	0	0
1	g	1490	0	1496	0	0
1	h	1485	0	1493	0	1
1	i	1482	0	1490	0	0
1	j	1482	0	1485	0	0
1	k	1513	0	1518	0	0
1	l	1502	0	1505	0	0
1	m	1473	0	1484	0	0
1	n	1490	0	1496	0	0
2	0	52	0	49	2	0
2	1	52	0	49	2	0
2	2	52	0	49	1	0
2	3	52	0	49	3	0
2	O	52	0	49	4	0
2	P	52	0	49	2	0
2	Q	52	0	49	3	0
2	R	52	0	49	6	0
2	S	52	0	49	4	0
2	T	52	0	49	3	0
2	U	52	0	49	4	0
2	V	52	0	49	3	0
2	W	52	0	49	3	0
2	X	52	0	49	6	0
2	Y	52	0	49	4	0
2	Z	52	0	49	4	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
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	49	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	a	1	0	0	0	0
3	b	1	0	0	0	0
3	c	1	0	0	0	0
3	d	1	0	0	0	0
3	e	1	0	0	0	0
3	f	1	0	0	0	0
3	g	1	0	0	0	0
3	h	1	0	0	0	0
3	i	1	0	0	0	0
3	j	1	0	0	0	0
3	k	1	0	0	0	0
3	l	1	0	0	0	0
3	m	1	0	0	0	0
3	n	1	0	0	0	0
4	c	1	0	0	0	0
4	h	1	0	0	0	0
4	k	1	0	0	0	0
5	A	35	0	0	2	0
5	B	42	0	0	1	0
5	C	35	0	0	1	0
5	D	29	0	0	0	0
5	E	34	0	0	1	0
5	F	27	0	0	1	0
5	G	31	0	0	1	0
5	H	27	0	0	1	0
5	I	34	0	0	1	0
5	J	31	0	0	1	0
5	K	41	0	0	1	0
5	L	32	0	0	0	0
5	M	37	0	0	2	0
5	N	32	0	0	3	0
5	O	2	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	a	27	0	0	0	0
5	b	26	0	0	0	0
5	c	34	0	0	0	0
5	d	33	0	0	0	0
5	e	26	0	0	0	0
5	f	28	0	0	0	0
5	g	16	0	0	0	0
5	h	24	0	0	0	0
5	i	24	0	0	0	0
5	j	35	0	0	0	0
5	k	30	0	0	0	0
5	l	29	0	0	0	0
5	m	28	0	0	0	0
5	n	24	0	0	0	0
5	t	1	0	0	0	0
All	All	43749	0	42975	408	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (408) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:LEU:H	1:I:135:LEU:H	1.08	0.94
1:N:117:PHE:HB3	1:N:196:LEU:HD11	1.52	0.91
1:B:135:LEU:H	1:K:135:LEU:H	1.18	0.91
1:G:181:MET:HE1	1:G:191:LEU:HD12	3.47	0.89
1:G:135:LEU:H	1:M:135:LEU:H	1.20	0.87
1:F:135:LEU:H	1:N:135:LEU:H	1.26	0.85
1:I:158:ARG:O	1:I:162:LYS:HD3	1.80	0.82
1:E:135:LEU:HB2	1:H:135:LEU:HB2	4.61	0.80
1:L:155:LYS:NZ	1:M:121:ASN:OD1	3.18	0.78
1:A:135:LEU:H	1:L:135:LEU:H	1.29	0.78
1:E:135:LEU:H	1:H:135:LEU:H	4.20	0.78
1:A:61:ASP:OD1	1:A:89:LYS:NZ	3.35	0.77
1:L:69:ASN:HB2	1:L:97:LEU:HD12	1.67	0.77
1:L:15:SER:OG	1:L:16:GLY:N	2.17	0.77
1:G:69:ASN:HB2	1:G:97:LEU:HD12	1.67	0.77
1:I:69:ASN:HB2	1:I:97:LEU:HD12	1.67	0.77
1:A:19:GLU:OE1	1:G:20:ARG:NH2	4.88	0.76
1:A:135:LEU:HB2	1:L:135:LEU:HB2	1.87	0.75

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:LEU:HB2	1:I:135:LEU:HB2	1.68	0.75
1:I:14:GLN:OE1	1:I:27:ARG:NH2	2.20	0.75
1:I:152:ILE:HD11	1:J:123:ARG:HH21	3.82	0.73
1:J:20:ARG:NH1	1:K:19:GLU:OE2	2.21	0.73
1:C:135:LEU:H	1:J:135:LEU:H	1.36	0.73
1:H:123:ARG:HH21	1:N:152:ILE:HD11	1.62	0.73
1:B:69:ASN:HB2	1:B:97:LEU:HD12	1.95	0.73
1:F:135:LEU:HB2	1:N:135:LEU:HB2	1.72	0.72
1:C:135:LEU:HB2	1:J:135:LEU:HB2	1.69	0.72
1:N:69:ASN:HB2	1:N:97:LEU:HD12	1.71	0.72
1:F:17:ARG:NH1	5:F:401:HOH:O	2.22	0.71
1:G:59:ASN:ND2	1:G:62:LYS:HE2	2.06	0.71
1:B:135:LEU:HB2	1:K:135:LEU:HB2	1.75	0.70
1:G:135:LEU:N	1:M:135:LEU:H	1.89	0.70
1:F:134:GLY:HA3	1:N:134:GLY:HA3	1.74	0.70
1:B:158:ARG:HE	1:B:168:LEU:HD22	1.57	0.69
1:F:22:PHE:HZ	1:G:12:ILE:HD11	3.61	0.69
1:E:132:SER:O	1:E:134:GLY:N	2.27	0.68
1:E:69:ASN:HB2	1:E:97:LEU:HD12	1.75	0.68
1:M:80:SER:HB2	1:N:97:LEU:HG	4.54	0.68
1:C:135:LEU:HB2	1:J:135:LEU:HD22	4.77	0.68
1:B:135:LEU:O	1:K:134:GLY:HA2	2.26	0.68
1:D:135:LEU:N	1:I:135:LEU:H	1.86	0.68
1:L:28:LEU:HD23	2:1:1:OTT:H6	133.27	0.68
1:D:69:ASN:HB2	1:D:97:LEU:HD12	1.80	0.67
1:B:20:ARG:NH2	1:C:19:GLU:OE1	2.27	0.66
1:E:142:ILE:HG12	1:H:131:ILE:HD11	1.76	0.66
1:C:152:ILE:HD11	1:D:123:ARG:HH21	1.60	0.66
1:K:106:PHE:HA	1:K:160:MET:HE1	1.78	0.66
1:L:17:ARG:HH11	1:L:17:ARG:HG2	1.59	0.65
1:N:17:ARG:NH2	5:N:401:HOH:O	35.65	0.65
1:G:181:MET:SD	5:G:404:HOH:O	31.44	0.65
1:B:142:ILE:HD11	1:K:131:ILE:HG12	1.86	0.64
1:L:20:ARG:NH2	1:M:19:GLU:OE1	3.08	0.64
1:F:117:PHE:HB3	1:F:196:LEU:HD11	3.24	0.64
1:K:59:ASN:ND2	1:K:62:LYS:HE2	4.80	0.64
1:M:152:ILE:HD11	1:N:123:ARG:HH21	1.63	0.64
1:I:143:GLU:HG2	1:I:147:ARG:HH12	1.63	0.63
1:E:16:GLY:O	1:E:17:ARG:HB3	3.49	0.63
1:J:133:GLY:O	1:J:135:LEU:N	4.60	0.63
1:L:83:ASP:OD1	1:M:121:ASN:ND2	2.41	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:69:ASN:HB2	1:M:97:LEU:HD12	4.68	0.62
1:F:69:ASN:HB2	1:F:97:LEU:HD12	4.65	0.62
1:B:173:ARG:NH1	1:B:174:ASP:OD1	2.91	0.62
1:N:28:LEU:HD22	1:N:33:ILE:HD12	1.82	0.61
1:F:20:ARG:HD2	1:F:21:ALA:H	1.64	0.61
1:D:152:ILE:HD11	1:E:123:ARG:HH21	6.25	0.61
1:I:158:ARG:NH2	1:I:170:ASP:OD2	12.24	0.61
1:A:131:ILE:HG12	1:L:142:ILE:HD11	2.01	0.61
1:K:154:GLU:O	1:K:158:ARG:HG3	2.00	0.61
1:C:142:ILE:HD11	1:J:131:ILE:HG12	1.83	0.61
1:F:142:ILE:HD11	1:N:131:ILE:HG12	2.28	0.60
1:H:152:ILE:HD11	1:I:123:ARG:HH21	1.67	0.60
1:I:124:ILE:HG21	1:I:191:LEU:HD13	1.84	0.60
1:E:20:ARG:NH1	1:F:19:GLU:OE2	2.34	0.59
1:F:20:ARG:HD2	1:F:21:ALA:N	2.18	0.59
1:F:135:LEU:N	1:N:135:LEU:H	2.01	0.59
1:D:135:LEU:H	1:I:135:LEU:N	1.91	0.59
1:D:142:ILE:HD11	1:I:131:ILE:HG12	1.92	0.59
1:A:134:GLY:HA3	1:L:134:GLY:HA3	1.85	0.59
1:I:27:ARG:NH1	1:I:27:ARG:O	2.35	0.58
1:K:152:ILE:HD11	1:L:123:ARG:HH21	1.93	0.58
1:F:131:ILE:HG12	1:N:142:ILE:HD11	1.86	0.58
1:I:47:LEU:HD11	1:J:9:PRO:HD3	3.07	0.58
1:E:131:ILE:HG12	1:H:142:ILE:HD11	1.87	0.58
1:F:135:LEU:H	1:N:135:LEU:N	1.98	0.58
1:G:14:GLN:HA	1:G:19:GLU:HA	1.85	0.58
1:I:15:SER:O	1:I:17:ARG:N	3.46	0.58
1:K:47:LEU:HD11	1:L:9:PRO:HD2	1.85	0.58
1:C:131:ILE:HG12	1:J:142:ILE:HD11	1.86	0.58
1:F:160:MET:HB3	1:F:171:LEU:HG	1.86	0.57
1:A:142:ILE:HD11	1:L:131:ILE:HG12	2.05	0.57
1:F:113:LYS:HE2	1:F:163:HIS:O	2.05	0.57
1:C:124:ILE:HG21	1:C:191:LEU:HD23	1.87	0.57
1:I:28:LEU:HD22	1:I:33:ILE:HD12	4.84	0.57
1:E:166:ARG:NH1	1:E:170:ASP:OD2	3.56	0.56
1:E:32:ARG:NH1	1:E:62:LYS:O	4.68	0.56
1:H:47:LEU:HD11	1:I:9:PRO:HD2	1.87	0.56
1:C:20:ARG:NH1	1:D:19:GLU:OE2	2.38	0.56
1:I:154:GLU:O	1:I:158:ARG:HG3	2.27	0.56
1:B:22:PHE:HE1	1:B:27:ARG:N	6.57	0.56
1:B:188:GLU:HG3	5:B:425:HOH:O	31.92	0.56

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:LYS:NZ	1:C:163:HIS:O	2.39	0.56
1:D:127:HIS:HD2	1:D:128:GLN:O	5.30	0.56
1:I:65:PHE:CE2	2:Y:7:MP8:HB	47.71	0.56
1:N:97:LEU:HD21	5:N:420:HOH:O	23.64	0.56
1:N:65:PHE:CE2	2:3:7:MP8:HB	140.26	0.56
1:B:173:ARG:HD2	1:B:174:ASP:OD1	2.05	0.55
1:F:22:PHE:CZ	1:G:12:ILE:HD11	3.87	0.55
1:G:15:SER:OG	1:G:16:GLY:N	4.05	0.55
1:B:154:GLU:OE2	1:B:158:ARG:HD2	2.05	0.55
1:D:135:LEU:O	1:I:131:ILE:HD11	2.31	0.55
1:A:22:PHE:CZ	1:A:30:LYS:HE2	6.10	0.55
1:N:60:PRO:O	1:N:89:LYS:HG3	3.98	0.55
1:L:65:PHE:CE2	2:Z:7:MP8:HB	2.42	0.55
1:I:27:ARG:NH1	1:I:30:LYS:HB2	2.22	0.54
1:I:59:ASN:ND2	1:I:62:LYS:HE2	5.08	0.54
1:L:13:GLU:HG2	1:L:14:GLN:N	2.44	0.54
1:M:28:LEU:HD22	2:O:1:OTT:H6	79.19	0.54
1:F:155:LYS:NZ	1:G:121:ASN:OD1	3.72	0.54
1:A:65:PHE:CE2	2:Q:7:MP8:HB	47.80	0.54
1:M:160:MET:HB3	1:M:171:LEU:CD2	4.28	0.54
1:N:60:PRO:HB2	1:N:89:LYS:HD3	1.90	0.54
1:C:28:LEU:HD13	1:C:35:PHE:HE2	4.59	0.54
1:I:113:LYS:HE2	1:I:163:HIS:O	2.08	0.54
1:M:54:PHE:HA	2:3:1:OTT:H7	139.96	0.54
1:B:120:PRO:HD3	1:B:196:LEU:O	2.39	0.54
1:I:65:PHE:CE2	2:W:7:MP8:HB	2.43	0.54
1:A:14:GLN:HG3	1:A:17:ARG:HD2	12.59	0.53
1:F:154:GLU:OE2	1:F:158:ARG:NH1	5.31	0.53
1:E:45:ALA:HA	1:E:81:ILE:HD11	1.90	0.53
1:K:87:PHE:HE2	1:L:196:LEU:HB3	1.94	0.53
1:E:133:GLY:HA2	1:H:136:GLY:HA3	1.90	0.53
1:E:32:ARG:NH2	1:E:55:LEU:O	3.37	0.53
1:K:197:GLU:HG2	1:K:198:ASN:N	2.24	0.53
1:J:71:PRO:HA	1:J:101:ALA:HB3	1.91	0.53
1:N:45:ALA:HA	1:N:81:ILE:HD11	1.91	0.52
1:G:131:ILE:HG12	1:M:142:ILE:HD11	1.91	0.52
1:A:123:ARG:HH21	1:G:152:ILE:HD11	1.75	0.52
1:A:47:LEU:HD11	1:B:9:PRO:HD2	1.93	0.52
1:D:54:PHE:CZ	1:E:11:VAL:HB	2.69	0.52
1:L:87:PHE:HE2	1:M:196:LEU:HB3	1.74	0.52
1:C:54:PHE:HA	2:R:1:OTT:H7	1.92	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:ARG:HG2	1:B:168:LEU:HD13	1.91	0.52
1:D:125:MET:SD	1:D:127:HIS:ND1	4.93	0.52
1:J:28:LEU:HD23	2:X:1:OTT:H6	1.91	0.52
1:N:20:ARG:NH1	1:N:21:ALA:O	2.42	0.52
1:F:152:ILE:HD11	1:G:123:ARG:HH21	1.89	0.52
1:E:134:GLY:HA3	1:H:134:GLY:HA3	5.38	0.52
1:D:134:GLY:HA3	1:I:134:GLY:HA3	1.93	0.52
1:I:158:ARG:HH22	1:I:170:ASP:CG	11.90	0.51
1:E:135:LEU:HD21	1:H:135:LEU:HB2	1.93	0.51
1:E:135:LEU:N	1:H:135:LEU:H	4.14	0.51
1:H:123:ARG:NH2	1:N:152:ILE:HD11	2.44	0.51
1:D:71:PRO:HA	1:D:101:ALA:HB3	1.99	0.51
1:J:124:ILE:HG21	1:J:191:LEU:HD13	1.98	0.51
1:H:109:SER:HB3	1:H:191:LEU:HD23	2.67	0.51
1:K:65:PHE:CE2	2:O:7:MP8:HB	112.51	0.51
1:J:109:SER:HB3	1:J:191:LEU:HD23	1.92	0.51
1:L:14:GLN:NE2	1:L:15:SER:HB2	5.85	0.51
1:G:14:GLN:HG2	1:G:19:GLU:HG2	7.71	0.51
1:K:59:ASN:HD22	1:K:62:LYS:HE2	4.80	0.50
1:N:71:PRO:HA	1:N:101:ALA:HB3	1.92	0.50
1:N:117:PHE:HB3	1:N:196:LEU:CD1	2.33	0.50
1:M:49:VAL:HG11	1:N:97:LEU:HD11	4.59	0.50
1:F:65:PHE:CE2	2:T:7:MP8:HB	2.46	0.50
1:L:28:LEU:CD2	2:1:1:OTT:H6	133.21	0.50
1:I:97:LEU:H	1:I:97:LEU:HD23	4.38	0.50
1:K:8:VAL:HG13	1:K:24:ILE:HG22	1.92	0.50
1:M:124:ILE:HG21	1:M:191:LEU:HD13	2.33	0.50
1:B:148:GLU:O	1:B:152:ILE:HG12	2.31	0.50
1:C:28:LEU:HD13	1:C:35:PHE:CE2	5.39	0.50
1:J:62:LYS:HB3	5:J:420:HOH:O	11.93	0.50
1:A:196:LEU:HB3	1:G:87:PHE:HE2	1.81	0.50
1:G:131:ILE:HD11	1:M:135:LEU:O	2.21	0.50
1:J:65:PHE:CE2	2:Z:7:MP8:HB	48.09	0.50
1:J:43:GLU:H	1:J:43:GLU:CD	2.15	0.50
1:C:65:PHE:CE2	2:S:7:MP8:HB	47.49	0.49
1:H:157:ASN:ND2	1:H:172:GLU:HG2	3.02	0.49
1:H:154:GLU:OE2	1:H:158:ARG:NH1	6.43	0.49
1:M:184:GLU:HA	1:M:195:ILE:HD11	2.17	0.49
1:K:14:GLN:NE2	1:K:15:SER:O	2.74	0.49
1:A:152:ILE:HD11	1:B:123:ARG:HH21	1.98	0.49
1:D:65:PHE:CE2	2:R:7:MP8:HB	2.48	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:65:PHE:CE2	2:O:7:MP8:HB	79.98	0.49
1:A:135:LEU:H	1:L:135:LEU:N	2.02	0.49
1:D:17:ARG:NH2	1:E:12:ILE:HG21	2.28	0.49
1:D:65:PHE:CE2	2:T:7:MP8:HB	47.67	0.49
1:B:65:PHE:CE2	2:R:7:MP8:HB	47.84	0.48
1:J:65:PHE:CE2	2:X:7:MP8:HB	2.48	0.48
1:K:199:ARG:C	2:Y:4:PRO:HD2	2.33	0.48
1:B:134:GLY:HA3	1:K:134:GLY:HA3	1.94	0.48
1:K:155:LYS:HE2	1:L:121:ASN:OD1	2.14	0.48
1:A:89:LYS:N	1:A:90:PRO:HD2	2.66	0.48
1:F:97:LEU:HD12	1:F:97:LEU:O	4.68	0.48
1:M:113:LYS:HE2	1:M:163:HIS:O	2.65	0.48
1:E:61:ASP:OD1	1:E:89:LYS:NZ	2.34	0.48
1:F:85:MET:HG2	1:F:92:VAL:HG11	2.19	0.48
1:E:65:PHE:CE2	2:U:7:MP8:HB	48.11	0.48
1:B:116:ARG:O	1:B:192:ILE:HG13	4.76	0.47
1:G:15:SER:N	1:G:18:GLY:O	2.36	0.47
1:L:17:ARG:NH1	1:L:17:ARG:HG2	2.26	0.47
1:A:47:LEU:HG	1:A:51:GLN:HE21	2.36	0.47
1:I:184:GLU:HA	1:I:195:ILE:HD11	2.22	0.47
1:D:124:ILE:HG21	1:D:191:LEU:HD13	2.67	0.47
1:C:158:ARG:HB3	1:C:158:ARG:HE	2.63	0.47
1:I:127:HIS:HD2	1:I:128:GLN:O	1.97	0.47
1:G:142:ILE:HD11	1:M:131:ILE:HG12	1.96	0.47
1:B:97:LEU:HD12	1:B:97:LEU:O	2.22	0.47
1:N:15:SER:OG	1:N:16:GLY:N	2.48	0.47
1:C:120:PRO:HD3	1:C:196:LEU:O	2.15	0.47
1:D:184:GLU:HA	1:D:195:ILE:HD11	1.97	0.47
1:J:16:GLY:O	1:J:17:ARG:HB3	4.48	0.47
1:J:20:ARG:HH21	1:K:21:ALA:HB2	9.52	0.47
1:N:156:LEU:HA	1:N:156:LEU:HD23	1.97	0.47
1:A:147:ARG:O	1:A:151:LYS:HG3	2.49	0.47
1:A:36:LEU:HD21	1:A:40:VAL:HG22	2.13	0.47
1:F:142:ILE:CD1	1:N:131:ILE:HG12	2.72	0.47
1:I:47:LEU:HD11	1:J:9:PRO:HD2	1.97	0.47
1:G:135:LEU:HD23	1:G:142:ILE:HA	5.28	0.47
1:A:196:LEU:HB3	1:G:87:PHE:CE2	2.50	0.47
1:C:135:LEU:N	1:J:135:LEU:H	2.10	0.47
1:J:97:LEU:HD23	1:J:97:LEU:H	1.80	0.46
1:M:42:ASP:OD2	5:M:401:HOH:O	2.21	0.46
2:V:4:PRO:HA	2:V:5:MAA:HA	1.61	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:GLU:OE1	1:A:30:LYS:HD3	2.15	0.46
1:C:134:GLY:HA3	1:J:134:GLY:HA3	1.96	0.46
1:D:11:VAL:O	1:D:21:ALA:HB1	3.89	0.46
1:G:62:LYS:O	1:G:90:PRO:HB3	2.27	0.46
1:E:97:LEU:HD12	1:E:97:LEU:O	2.15	0.46
1:G:166:ARG:HD2	1:G:189:TYR:O	2.52	0.46
1:H:170:ASP:HA	1:H:173:ARG:NH1	2.31	0.46
1:H:65:PHE:CE2	2:X:7:MP8:HB	47.78	0.46
1:J:28:LEU:CD2	2:X:1:OTT:H6	2.45	0.46
1:G:134:GLY:HA3	1:M:134:GLY:HA3	1.96	0.46
1:N:61:ASP:OD1	1:N:89:LYS:HE3	3.80	0.46
1:A:113:LYS:HG3	5:A:423:HOH:O	29.17	0.46
1:F:97:LEU:HD23	1:F:97:LEU:H	1.80	0.46
1:B:125:MET:SD	1:B:127:HIS:HD2	2.38	0.46
1:E:166:ARG:HG3	5:E:406:HOH:O	2.14	0.46
1:H:65:PHE:CE2	2:V:7:MP8:HB	2.51	0.46
5:N:405:HOH:O	2:V:1:OTT:H3	2.16	0.46
1:G:27:ARG:O	1:G:30:LYS:HB3	2.16	0.46
1:A:54:PHE:CZ	1:B:11:VAL:HB	2.52	0.46
2:P:4:PRO:HA	2:P:5:MAA:HA	1.67	0.46
1:K:36:LEU:HD21	1:K:40:VAL:HG22	2.22	0.45
1:M:43:GLU:HG3	5:M:425:HOH:O	7.80	0.45
1:B:65:PHE:CE2	2:P:7:MP8:HB	2.51	0.45
1:I:138:GLN:O	1:I:142:ILE:HD12	2.16	0.45
1:J:14:GLN:H	1:J:14:GLN:CD	2.19	0.45
1:A:142:ILE:CD1	1:L:131:ILE:HG12	2.48	0.45
1:E:87:PHE:CE1	1:F:196:LEU:HB3	2.98	0.45
1:I:184:GLU:HB2	5:I:423:HOH:O	27.55	0.45
1:K:65:PHE:CE2	2:Y:7:MP8:HB	2.51	0.45
1:N:63:ASP:OD1	1:N:91:ASP:HB2	2.17	0.45
1:C:191:LEU:HD12	1:C:191:LEU:HA	1.70	0.45
1:C:75:VAL:HG23	5:C:424:HOH:O	15.94	0.45
1:K:97:LEU:H	1:K:97:LEU:HD23	1.85	0.45
2:T:4:PRO:HA	2:T:5:MAA:HA	1.70	0.45
1:G:136:GLY:HA2	1:G:137:GLY:HA2	1.78	0.45
1:G:135:LEU:HB2	1:M:135:LEU:HB2	1.97	0.45
1:M:20:ARG:NH1	1:N:19:GLU:OE1	7.64	0.45
1:A:57:SER:CB	2:R:1:OTT:H7	41.42	0.45
1:C:15:SER:HB2	1:C:17:ARG:H	1.81	0.45
1:K:109:SER:HB3	1:K:191:LEU:HD23	1.99	0.45
1:K:124:ILE:HG21	1:K:191:LEU:HD13	1.99	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:43:GLU:HB2	5:K:413:HOH:O	2.16	0.45
1:A:97:LEU:H	1:A:97:LEU:HD23	1.85	0.45
1:G:69:ASN:HB2	1:G:97:LEU:CD1	2.43	0.45
1:M:87:PHE:HE2	1:N:196:LEU:HB3	1.82	0.45
1:N:20:ARG:HD2	1:N:20:ARG:HA	1.71	0.45
1:C:97:LEU:HD23	1:C:97:LEU:H	1.82	0.45
1:G:28:LEU:HD22	1:G:33:ILE:HD12	1.99	0.45
1:M:63:ASP:OD1	1:M:91:ASP:HB2	2.22	0.45
1:C:118:ALA:HB1	1:C:122:SER:OG	2.17	0.45
1:G:184:GLU:HA	1:G:195:ILE:HD11	2.10	0.45
1:J:87:PHE:CZ	1:K:199:ARG:HA	6.30	0.45
1:D:170:ASP:HA	1:D:173:ARG:HH11	1.82	0.44
1:H:146:ALA:O	1:H:150:LEU:HD13	2.17	0.44
1:N:69:ASN:HB2	1:N:97:LEU:CD1	2.45	0.44
1:C:95:LEU:HD23	1:C:117:PHE:HB2	1.99	0.44
1:E:184:GLU:HA	1:E:195:ILE:HD11	1.98	0.44
1:A:11:VAL:N	1:A:22:PHE:O	2.82	0.44
1:F:47:LEU:O	1:F:51:GLN:HG3	2.38	0.44
2:W:4:PRO:HA	2:W:5:MAA:HA	1.59	0.44
1:L:62:LYS:O	1:L:90:PRO:HB3	2.16	0.44
1:C:22:PHE:CE1	1:C:27:ARG:HB2	6.40	0.44
1:E:65:PHE:CE2	2:S:7:MP8:HB	2.53	0.44
1:B:142:ILE:CD1	1:K:131:ILE:HG12	2.57	0.44
1:K:184:GLU:HA	1:K:195:ILE:HD11	1.99	0.44
1:M:54:PHE:CZ	1:N:11:VAL:HB	2.54	0.44
1:A:113:LYS:NZ	1:A:162:LYS:O	2.79	0.44
1:C:156:LEU:O	1:C:160:MET:HB2	2.76	0.44
1:F:56:GLU:HG3	1:F:90:PRO:HD3	2.12	0.44
1:I:69:ASN:HB2	1:I:97:LEU:CD1	2.43	0.44
1:B:131:ILE:N	1:K:137:GLY:O	2.42	0.44
1:G:109:SER:HB3	1:G:191:LEU:HD22	4.08	0.44
1:A:26:SER:O	1:A:30:LYS:HG2	4.34	0.44
1:H:71:PRO:HA	1:H:101:ALA:HB3	2.22	0.43
1:I:131:ILE:CD1	1:I:135:LEU:HD13	2.59	0.43
2:R:4:PRO:HA	2:R:5:MAA:HA	1.71	0.43
2:3:4:PRO:HA	2:3:5:MAA:HA	1.69	0.43
1:A:131:ILE:HG12	1:L:142:ILE:CD1	2.63	0.43
1:E:12:ILE:O	1:E:12:ILE:HG13	5.13	0.43
1:B:135:LEU:N	1:K:135:LEU:H	2.00	0.43
2:Q:4:PRO:HA	2:Q:5:MAA:HA	1.81	0.43
1:C:149:LEU:HA	1:C:149:LEU:HD12	1.79	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:95:LEU:HD12	1:I:96:CYS:N	5.36	0.43
1:L:14:GLN:O	1:L:15:SER:HB3	4.19	0.43
1:H:97:LEU:H	1:H:97:LEU:HD23	1.83	0.43
1:A:57:SER:HB3	2:R:1:OTT:H7	41.35	0.43
1:B:156:LEU:HD23	1:B:156:LEU:HA	1.87	0.43
1:D:17:ARG:HH22	1:E:12:ILE:HG21	1.82	0.43
1:G:135:LEU:HB3	1:G:142:ILE:HG12	2.01	0.43
1:J:96:CYS:SG	1:J:122:SER:HB2	2.57	0.43
1:K:127:HIS:HD2	1:K:178:ASP:OD1	2.23	0.43
1:N:117:PHE:CD1	1:N:194:GLN:HB2	2.62	0.43
1:E:135:LEU:HD21	1:H:135:LEU:HD12	2.01	0.43
2:Z:4:PRO:HA	2:Z:5:MAA:HA	1.77	0.43
1:A:160:MET:HE2	1:A:191:LEU:HD21	4.32	0.43
1:A:18:GLY:O	1:A:19:GLU:HB2	2.19	0.43
1:L:120:PRO:HD3	1:L:196:LEU:O	2.55	0.43
1:M:28:LEU:HD12	1:M:35:PHE:HE2	1.84	0.43
2:X:6:ALA:H	2:X:7:MP8:C	3.15	0.43
1:B:22:PHE:HE1	1:B:27:ARG:CA	7.05	0.43
1:C:123:ARG:HD3	1:C:180:PHE:HD1	3.70	0.43
1:D:36:LEU:HD21	1:D:40:VAL:HG22	2.01	0.43
1:E:129:PRO:HG3	1:E:156:LEU:HD12	2.00	0.43
1:K:136:GLY:HA2	1:K:137:GLY:HA2	1.72	0.43
1:C:142:ILE:CD1	1:J:131:ILE:HG12	2.58	0.43
1:A:16:GLY:O	1:A:17:ARG:HB2	4.64	0.42
1:H:17:ARG:HD3	1:I:19:GLU:OE2	11.73	0.42
1:B:54:PHE:HA	2:Q:1:OTT:H7	2.00	0.42
1:F:168:LEU:HG	1:F:172:GLU:OE2	7.24	0.42
1:M:45:ALA:HA	1:M:81:ILE:HD11	2.01	0.42
1:B:109:SER:HB3	1:B:191:LEU:HD12	4.41	0.42
1:E:120:PRO:HD3	1:E:196:LEU:O	2.36	0.42
1:I:136:GLY:HA2	1:I:137:GLY:HA2	1.64	0.42
1:K:162:LYS:HA	1:K:162:LYS:HD3	1.84	0.42
2:U:4:PRO:HA	2:U:5:MAA:HA	1.75	0.42
1:N:130:LEU:HD12	1:N:130:LEU:O	5.33	0.42
1:K:100:ALA:O	1:K:105:ALA:HB2	2.19	0.42
1:L:198:ASN:OD1	1:L:198:ASN:N	3.14	0.42
2:O:3:SER:HA	2:O:4:PRO:C	2.39	0.42
2:S:4:PRO:HA	2:S:5:MAA:HA	1.74	0.42
1:A:30:LYS:HE3	1:B:12:ILE:HG12	5.63	0.42
1:D:152:ILE:HD11	1:E:123:ARG:NH2	5.47	0.42
1:I:8:VAL:HG21	1:J:7:LEU:HD12	2.02	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:LEU:HD22	1:D:33:ILE:HD12	2.02	0.42
1:E:62:LYS:O	1:E:90:PRO:HB3	2.25	0.42
1:E:8:VAL:HG12	1:E:24:ILE:HG22	3.07	0.42
1:L:97:LEU:O	1:L:97:LEU:HD12	2.25	0.42
1:N:160:MET:HB3	1:N:171:LEU:HD23	5.02	0.42
1:B:155:LYS:HE2	1:C:121:ASN:OD1	4.18	0.41
1:C:22:PHE:CD1	1:C:27:ARG:HB2	5.37	0.41
1:F:156:LEU:HD23	1:F:156:LEU:HA	1.87	0.41
1:K:54:PHE:HA	2:Z:1:OTT:H7	2.02	0.41
2:O:4:PRO:HA	2:O:5:MAA:HA	1.72	0.41
2:Y:4:PRO:HA	2:Y:5:MAA:HA	1.65	0.41
1:B:12:ILE:HA	1:B:20:ARG:O	2.71	0.41
1:I:102:SER:OG	1:I:127:HIS:CE1	2.73	0.41
1:K:45:ALA:HA	1:K:81:ILE:HD11	2.03	0.41
1:N:127:HIS:ND1	1:N:178:ASP:OD1	2.33	0.41
2:X:4:PRO:HA	2:X:5:MAA:HA	1.77	0.41
1:B:69:ASN:HB2	1:B:97:LEU:CD1	2.58	0.41
1:E:135:LEU:O	1:E:135:LEU:HD12	2.20	0.41
1:J:63:ASP:OD1	1:J:91:ASP:HB2	2.21	0.41
5:A:432:HOH:O	1:B:37:VAL:HG13	2.20	0.41
1:D:8:VAL:HG11	1:D:23:ASP:HB2	2.48	0.41
1:G:65:PHE:CE2	2:U:7:MP8:HB	2.56	0.41
1:K:20:ARG:HH12	1:L:19:GLU:HG3	1.85	0.41
1:L:102:SER:OG	1:L:127:HIS:NE2	2.39	0.41
1:L:135:LEU:HA	1:L:135:LEU:HD23	1.86	0.41
1:M:156:LEU:HD23	1:M:156:LEU:HA	1.98	0.41
1:N:107:LEU:HA	1:N:107:LEU:HD23	1.97	0.41
1:D:54:PHE:HA	2:U:1:OTT:H7	40.43	0.41
1:H:154:GLU:CD	1:H:158:ARG:HH12	7.80	0.41
1:H:19:GLU:OE1	1:N:20:ARG:NH1	8.11	0.41
1:N:160:MET:HB3	1:N:171:LEU:CD2	4.52	0.41
1:G:65:PHE:CE2	2:W:7:MP8:HB	89.68	0.41
1:J:47:LEU:HD11	1:K:9:PRO:HD2	2.11	0.41
1:A:14:GLN:HG3	1:A:17:ARG:CD	12.12	0.41
1:J:150:LEU:HD23	1:J:150:LEU:HA	1.90	0.41
1:K:197:GLU:HG2	1:K:198:ASN:H	1.83	0.41
1:N:97:LEU:O	1:N:97:LEU:HD12	2.20	0.41
1:M:65:PHE:CE2	2:2:7:MP8:HB	160.14	0.41
1:B:43:GLU:CD	1:B:43:GLU:H	2.24	0.41
1:K:60:PRO:HB2	1:K:89:LYS:HD3	2.03	0.41
1:H:155:LYS:NZ	5:H:401:HOH:O	23.63	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:56:GLU:HG3	1:H:90:PRO:HD3	2.02	0.40
1:J:164:CYS:HA	1:J:190:GLY:O	2.21	0.40
1:J:15:SER:OG	1:J:16:GLY:N	3.30	0.40
1:J:17:ARG:HG2	1:J:17:ARG:O	2.21	0.40
1:M:136:GLY:HA2	1:M:137:GLY:HA2	1.69	0.40
1:M:13:GLU:OE2	1:M:30:LYS:NZ	2.30	0.40
1:F:69:ASN:HB2	1:F:97:LEU:CD1	4.38	0.40
1:C:196:LEU:HD22	2:S:5:MAA:HM1	61.27	0.40
1:F:118:ALA:HB1	1:F:122:SER:OG	3.45	0.40
1:F:83:ASP:OD1	1:G:121:ASN:ND2	2.57	0.40
1:G:63:ASP:OD2	1:G:115:LYS:NZ	2.50	0.40
1:I:125:MET:SD	1:I:127:HIS:ND1	2.79	0.40
1:I:27:ARG:HH12	1:I:30:LYS:HB2	1.86	0.40
1:F:60:PRO:HB2	1:F:89:LYS:HD3	2.04	0.40
1:G:159:LEU:HD23	1:G:159:LEU:HA	2.24	0.40
1:G:17:ARG:HH11	1:G:17:ARG:HD3	1.77	0.40
2:0:4:PRO:HA	2:0:5:MAA:HA	1.60	0.40
1:D:14:GLN:HG2	1:D:15:SER:N	2.35	0.40
1:E:13:GLU:O	1:E:19:GLU:HA	2.76	0.40
1:I:114:GLY:N	1:I:193:ASP:OD2	2.53	0.40
1:J:20:ARG:NH2	1:K:21:ALA:HB2	9.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:17:ARG:NH1	1:h:63:ASP:OD2[1_556]	2.09	0.11
1:F:170:ASP:OD2	1:K:158:ARG:NH2[2_646]	2.19	0.01

## 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%)	17	23
1	B	183/206 (89%)	180 (98%)	3 (2%)	0	100	100
1	C	189/206 (92%)	184 (97%)	5 (3%)	0	100	100
1	D	189/206 (92%)	184 (97%)	4 (2%)	1 (0%)	34	46
1	E	190/206 (92%)	184 (97%)	4 (2%)	2 (1%)	17	23
1	F	189/206 (92%)	181 (96%)	7 (4%)	1 (0%)	34	46
1	G	191/206 (93%)	184 (96%)	7 (4%)	0	100	100
1	H	189/206 (92%)	182 (96%)	4 (2%)	3 (2%)	12	14
1	I	189/206 (92%)	184 (97%)	5 (3%)	0	100	100
1	J	191/206 (93%)	184 (96%)	5 (3%)	2 (1%)	19	26
1	K	191/206 (93%)	182 (95%)	8 (4%)	1 (0%)	34	46
1	L	191/206 (93%)	184 (96%)	7 (4%)	0	100	100
1	M	189/206 (92%)	183 (97%)	5 (3%)	1 (0%)	34	46
1	N	191/206 (93%)	184 (96%)	5 (3%)	2 (1%)	19	26
1	a	189/206 (92%)	183 (97%)	5 (3%)	1 (0%)	34	46
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%)	17	23
1	f	179/206 (87%)	176 (98%)	3 (2%)	0	100	100
1	g	190/206 (92%)	180 (95%)	9 (5%)	1 (0%)	34	46
1	h	189/206 (92%)	185 (98%)	4 (2%)	0	100	100
1	i	189/206 (92%)	183 (97%)	4 (2%)	2 (1%)	17	23
1	j	189/206 (92%)	181 (96%)	7 (4%)	1 (0%)	34	46
1	k	192/206 (93%)	188 (98%)	4 (2%)	0	100	100
1	l	191/206 (93%)	185 (97%)	4 (2%)	2 (1%)	19	26
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

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	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%)	34	46

All (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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	l	15	SER
1	H	15	SER
1	H	16	GLY
1	M	16	GLY
1	i	16	GLY
1	i	17	ARG
1	l	16	GLY
1	D	15	SER
1	E	135	LEU
1	F	14	GLN
1	N	7	LEU
1	a	17	ARG
1	A	16	GLY
1	e	19	GLU
1	A	15	SER
1	H	17	ARG
1	e	17	ARG
1	K	18	GLY
2	x	6	ALA
1	J	16	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%)	76	89
1	B	159/174 (91%)	158 (99%)	1 (1%)	90	96
1	C	161/174 (92%)	160 (99%)	1 (1%)	90	96
1	D	161/174 (92%)	159 (99%)	2 (1%)	78	90
1	E	162/174 (93%)	161 (99%)	1 (1%)	90	96
1	F	161/174 (92%)	160 (99%)	1 (1%)	90	96
1	G	163/174 (94%)	160 (98%)	3 (2%)	66	83
1	H	161/174 (92%)	161 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	161/174 (92%)	159 (99%)	2 (1%)	78	90
1	J	163/174 (94%)	161 (99%)	2 (1%)	78	90
1	K	163/174 (94%)	161 (99%)	2 (1%)	78	90
1	L	163/174 (94%)	163 (100%)	0	100	100
1	M	161/174 (92%)	159 (99%)	2 (1%)	78	90
1	N	163/174 (94%)	162 (99%)	1 (1%)	90	96
1	a	161/174 (92%)	160 (99%)	1 (1%)	90	96
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%)	76	89
1	g	162/174 (93%)	159 (98%)	3 (2%)	65	82
1	h	161/174 (92%)	159 (99%)	2 (1%)	78	90
1	i	161/174 (92%)	159 (99%)	2 (1%)	78	90
1	j	161/174 (92%)	158 (98%)	3 (2%)	65	82
1	k	164/174 (94%)	163 (99%)	1 (1%)	90	96
1	l	163/174 (94%)	160 (98%)	3 (2%)	66	83
1	m	160/174 (92%)	159 (99%)	1 (1%)	90	96
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	84	93

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	HIS
1	A	158	ARG
1	B	69	ASN
1	C	127	HIS
1	D	156	LEU
1	D	197	GLU
1	E	135	LEU
1	F	168	LEU
1	G	7	LEU
1	G	19	GLU
1	G	127	HIS
1	I	11	VAL
1	I	197	GLU
1	J	11	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	J	43	GLU
1	K	13	GLU
1	K	127	HIS
1	M	43	GLU
1	M	127	HIS
1	N	127	HIS
1	a	14	GLN
1	f	12	ILE
1	f	43	GLU
1	g	17	ARG
1	g	127	HIS
1	g	198	ASN
1	h	14	GLN
1	h	127	HIS
1	i	127	HIS
1	i	184	GLU
1	j	11	VAL
1	j	19	GLU
1	j	127	HIS
1	k	127	HIS
1	l	20	ARG
1	l	127	HIS
1	l	191	LEU
1	m	127	HIS
2	P	4	PRO
2	r	4	PRO
2	t	4	PRO

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 ⓘ

There are no RNA molecules 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	0	5	2	4,5,6	0.59	0	2,5,7	2.31	1 (50%)
2	MP8	0	7	2	6,8,9	0.79	0	4,10,12	1.24	0
2	MAA	1	5	2	4,5,6	0.84	0	2,5,7	1.83	1 (50%)
2	MP8	1	7	2	6,8,9	0.63	0	4,10,12	1.28	1 (25%)
2	MAA	2	5	2	4,5,6	0.51	0	2,5,7	2.11	1 (50%)
2	MP8	2	7	2	6,8,9	0.71	0	4,10,12	1.03	0
2	MAA	3	5	2	4,5,6	0.81	0	2,5,7	1.62	1 (50%)
2	MP8	3	7	2	6,8,9	0.54	0	4,10,12	1.23	1 (25%)
2	MAA	O	5	2	4,5,6	0.75	0	2,5,7	1.62	1 (50%)
2	MP8	O	7	2	6,8,9	0.67	0	4,10,12	1.17	0
2	MAA	P	5	2	4,5,6	0.85	0	2,5,7	1.77	1 (50%)
2	MP8	P	7	2	6,8,9	0.59	0	4,10,12	1.18	0
2	MAA	Q	5	2	4,5,6	0.97	0	2,5,7	1.24	0
2	MP8	Q	7	2	6,8,9	0.66	0	4,10,12	1.35	1 (25%)
2	MAA	R	5	2	4,5,6	0.81	0	2,5,7	2.14	1 (50%)
2	MP8	R	7	2	6,8,9	0.61	0	4,10,12	1.35	1 (25%)
2	MAA	S	5	2	4,5,6	0.58	0	2,5,7	1.68	1 (50%)
2	MP8	S	7	2	6,8,9	0.67	0	4,10,12	1.16	1 (25%)
2	MAA	T	5	2	4,5,6	0.56	0	2,5,7	2.17	1 (50%)
2	MP8	T	7	2	6,8,9	0.64	0	4,10,12	1.13	0
2	MAA	U	5	2	4,5,6	0.62	0	2,5,7	1.83	1 (50%)
2	MP8	U	7	2	6,8,9	0.78	0	4,10,12	1.24	0
2	MAA	V	5	2	4,5,6	0.66	0	2,5,7	1.87	1 (50%)
2	MP8	V	7	2	6,8,9	0.64	0	4,10,12	1.18	0
2	MAA	W	5	2	4,5,6	1.12	0	2,5,7	1.61	1 (50%)
2	MP8	W	7	2	6,8,9	0.78	0	4,10,12	1.31	0
2	MAA	X	5	2	4,5,6	0.72	0	2,5,7	1.72	1 (50%)
2	MP8	X	7	2	6,8,9	0.52	0	4,10,12	1.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MAA	Y	5	2	4,5,6	0.87	0	2,5,7	1.65	1 (50%)
2	MP8	Y	7	2	6,8,9	0.56	0	4,10,12	1.26	1 (25%)
2	MAA	Z	5	2	4,5,6	0.58	0	2,5,7	1.19	0
2	MP8	Z	7	2	6,8,9	0.77	0	4,10,12	1.43	1 (25%)
2	MAA	o	5	2	4,5,6	0.47	0	2,5,7	1.85	1 (50%)
2	MP8	o	7	2	6,8,9	0.75	0	4,10,12	1.25	1 (25%)
2	MAA	p	5	2	4,5,6	0.65	0	2,5,7	2.04	1 (50%)
2	MP8	p	7	2	6,8,9	0.58	0	4,10,12	1.32	1 (25%)
2	MAA	q	5	2	4,5,6	0.64	0	2,5,7	2.07	1 (50%)
2	MP8	q	7	2	6,8,9	0.50	0	4,10,12	1.45	1 (25%)
2	MAA	r	5	2	4,5,6	0.60	0	2,5,7	1.85	1 (50%)
2	MP8	r	7	2	6,8,9	0.79	0	4,10,12	1.18	0
2	MAA	s	5	2	4,5,6	0.65	0	2,5,7	1.42	0
2	MP8	s	7	2	6,8,9	0.72	0	4,10,12	1.12	1 (25%)
2	MAA	t	5	2	4,5,6	0.44	0	2,5,7	2.58	1 (50%)
2	MP8	t	7	2	6,8,9	0.73	0	4,10,12	1.16	0
2	MAA	u	5	2	4,5,6	0.62	0	2,5,7	1.93	1 (50%)
2	MP8	u	7	2	6,8,9	0.67	0	4,10,12	1.12	0
2	MAA	v	5	2	4,5,6	0.62	0	2,5,7	1.98	1 (50%)
2	MP8	v	7	2	6,8,9	0.57	0	4,10,12	1.30	0
2	MAA	w	5	2	4,5,6	0.71	0	2,5,7	1.90	1 (50%)
2	MP8	w	7	2	6,8,9	0.75	0	4,10,12	1.47	1 (25%)
2	MAA	x	5	2	4,5,6	0.81	0	2,5,7	1.79	1 (50%)
2	MP8	x	7	2	6,8,9	0.54	0	4,10,12	1.49	1 (25%)
2	MAA	y	5	2	4,5,6	0.61	0	2,5,7	1.85	1 (50%)
2	MP8	y	7	2	6,8,9	0.72	0	4,10,12	1.63	1 (25%)
2	MAA	z	5	2	4,5,6	0.70	0	2,5,7	1.60	1 (50%)
2	MP8	z	7	2	6,8,9	0.68	0	4,10,12	1.22	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	0	5	2	-	0/1/4/6	0/0/0/0
2	MP8	0	7	2	-	0/0/11/13	0/1/1/1
2	MAA	1	5	2	-	0/1/4/6	0/0/0/0

*Continued on next page...*



*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MP8	u	7	2	-	0/0/11/13	0/1/1/1
2	MAA	v	5	2	-	0/1/4/6	0/0/0/0
2	MP8	v	7	2	-	0/0/11/13	0/1/1/1
2	MAA	w	5	2	-	0/1/4/6	0/0/0/0
2	MP8	w	7	2	-	0/0/11/13	0/1/1/1
2	MAA	x	5	2	-	0/1/4/6	0/0/0/0
2	MP8	x	7	2	-	0/0/11/13	0/1/1/1
2	MAA	y	5	2	-	0/1/4/6	0/0/0/0
2	MP8	y	7	2	-	0/0/11/13	0/1/1/1
2	MAA	z	5	2	-	0/1/4/6	0/0/0/0
2	MP8	z	7	2	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	t	5	MAA	O-C-CA	-3.61	118.39	124.97
2	0	5	MAA	O-C-CA	-3.26	119.03	124.97
2	R	5	MAA	O-C-CA	-3.02	119.47	124.97
2	T	5	MAA	O-C-CA	-2.93	119.62	124.97
2	2	5	MAA	O-C-CA	-2.87	119.73	124.97
2	q	5	MAA	O-C-CA	-2.87	119.75	124.97
2	u	5	MAA	O-C-CA	-2.67	120.10	124.97
2	V	5	MAA	O-C-CA	-2.64	120.15	124.97
2	r	5	MAA	O-C-CA	-2.61	120.22	124.97
2	y	5	MAA	O-C-CA	-2.59	120.25	124.97
2	o	5	MAA	O-C-CA	-2.59	120.26	124.97
2	p	5	MAA	O-C-CA	-2.58	120.27	124.97
2	w	5	MAA	O-C-CA	-2.55	120.32	124.97
2	U	5	MAA	O-C-CA	-2.50	120.41	124.97
2	1	5	MAA	O-C-CA	-2.50	120.42	124.97
2	v	5	MAA	O-C-CA	-2.49	120.43	124.97
2	y	7	MP8	O-C-CA	-2.49	118.89	125.69
2	P	5	MAA	O-C-CA	-2.48	120.45	124.97
2	X	5	MAA	O-C-CA	-2.44	120.53	124.97
2	q	7	MP8	O-C-CA	-2.35	119.26	125.69
2	Y	5	MAA	O-C-CA	-2.32	120.74	124.97
2	Q	7	MP8	O-C-CA	-2.31	119.37	125.69
2	w	7	MP8	O-C-CA	-2.30	119.42	125.69
2	Z	7	MP8	O-C-CA	-2.29	119.44	125.69
2	O	5	MAA	O-C-CA	-2.29	120.81	124.97
2	W	5	MAA	O-C-CA	-2.27	120.83	124.97

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	5	MAA	O-C-CA	-2.27	120.83	124.97
2	S	5	MAA	O-C-CA	-2.27	120.84	124.97
2	z	5	MAA	O-C-CA	-2.23	120.92	124.97
2	x	7	MP8	O-C-CA	-2.22	119.63	125.69
2	x	5	MAA	O-C-CA	-2.20	120.97	124.97
2	p	7	MP8	O-C-CA	-2.13	119.86	125.69
2	S	7	MP8	O-C-CA	-2.06	120.05	125.69
2	Y	7	MP8	O-C-CA	-2.05	120.09	125.69
2	3	7	MP8	O-C-CA	-2.04	120.11	125.69
2	1	7	MP8	O-C-CA	-2.04	120.11	125.69
2	s	7	MP8	O-C-CA	-2.04	120.12	125.69
2	R	7	MP8	O-C-CA	-2.04	120.12	125.69
2	o	7	MP8	O-C-CA	-2.02	120.17	125.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

29 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	0	5	MAA	1	0
2	0	7	MP8	1	0
2	2	7	MP8	1	0
2	3	5	MAA	1	0
2	3	7	MP8	1	0
2	O	5	MAA	1	0
2	O	7	MP8	1	0
2	P	5	MAA	1	0
2	P	7	MP8	1	0
2	Q	5	MAA	1	0
2	Q	7	MP8	1	0
2	R	5	MAA	1	0
2	R	7	MP8	2	0
2	S	5	MAA	2	0
2	S	7	MP8	2	0
2	T	5	MAA	1	0
2	T	7	MP8	2	0
2	U	5	MAA	1	0
2	U	7	MP8	2	0
2	V	5	MAA	1	0
2	V	7	MP8	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	W	5	MAA	1	0
2	W	7	MP8	2	0
2	X	5	MAA	1	0
2	X	7	MP8	3	0
2	Y	5	MAA	1	0
2	Y	7	MP8	2	0
2	Z	5	MAA	1	0
2	Z	7	MP8	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	190/206 (92%)	0.15	9 (4%) 35 40	14, 20, 58, 87	0
1	B	187/206 (90%)	0.15	2 (1%) 82 84	13, 20, 46, 85	0
1	C	191/206 (92%)	0.18	10 (5%) 31 35	14, 20, 66, 96	0
1	D	191/206 (92%)	0.17	8 (4%) 40 45	13, 20, 63, 93	0
1	E	192/206 (93%)	0.10	5 (2%) 59 62	13, 21, 60, 91	0
1	F	191/206 (92%)	0.22	11 (5%) 26 31	14, 21, 73, 105	0
1	G	193/206 (93%)	0.25	11 (5%) 27 31	14, 21, 68, 98	0
1	H	191/206 (92%)	0.11	6 (3%) 52 56	14, 22, 61, 90	0
1	I	191/206 (92%)	0.18	6 (3%) 52 56	14, 21, 59, 90	0
1	J	193/206 (93%)	0.21	9 (4%) 35 40	15, 22, 66, 103	0
1	K	193/206 (93%)	0.27	11 (5%) 27 31	12, 21, 69, 102	0
1	L	193/206 (93%)	0.23	6 (3%) 52 56	14, 21, 65, 111	0
1	M	191/206 (92%)	0.21	10 (5%) 31 35	14, 20, 62, 103	0
1	N	193/206 (93%)	0.24	8 (4%) 41 46	14, 21, 61, 99	0
1	a	191/206 (92%)	0.30	14 (7%) 18 20	15, 22, 75, 117	0
1	b	188/206 (91%)	0.25	12 (6%) 23 26	14, 22, 64, 107	0
1	c	177/206 (85%)	0.02	3 (1%) 73 75	14, 20, 41, 86	0
1	d	184/206 (89%)	0.19	9 (4%) 33 38	14, 20, 52, 90	0
1	e	191/206 (92%)	0.39	17 (8%) 12 14	13, 22, 72, 108	0
1	f	183/206 (88%)	0.16	9 (4%) 33 38	16, 22, 64, 88	0
1	g	192/206 (93%)	0.29	15 (7%) 16 18	15, 22, 75, 120	0
1	h	191/206 (92%)	0.14	8 (4%) 40 45	15, 21, 57, 88	0
1	i	191/206 (92%)	0.13	8 (4%) 40 45	14, 21, 57, 103	0
1	j	191/206 (92%)	0.21	10 (5%) 31 35	14, 21, 68, 97	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	k	194/206 (94%)	0.29	12 (6%)	24	28	14, 21, 69, 105	0
1	l	193/206 (93%)	0.08	6 (3%)	52	56	14, 22, 64, 91	0
1	m	190/206 (92%)	0.07	6 (3%)	51	55	13, 21, 52, 90	0
1	n	192/206 (93%)	0.14	7 (3%)	46	51	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%)	-0.26	0	100	100	18, 22, 26, 28	0
2	S	4/7 (57%)	0.00	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%)	-0.03	0	100	100	24, 29, 30, 33	0
2	X	4/7 (57%)	0.22	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%)	-0.28	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%)	0.11	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%)	0.08	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%)	-0.02	0	100	100	24, 25, 26, 27	0

*Continued on next page...*

*Continued from previous page...*

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%)	36	41	12, 21, 64, 120	0

All (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
1	k	133	GLY	8.8
1	d	21	ALA	8.7
1	a	16	GLY	8.5
1	b	133	GLY	8.1
1	D	134	GLY	7.9
1	i	16	GLY	7.7
1	b	20	ARG	7.7
1	I	133	GLY	7.7
1	a	18	GLY	7.6
1	I	14	GLN	7.6
1	K	133	GLY	7.4
1	j	16	GLY	7.3
1	F	135	LEU	7.3
1	e	17	ARG	7.0
1	C	134	GLY	7.0
1	M	17	ARG	7.0
1	d	20	ARG	7.0
1	m	134	GLY	6.8
1	e	13	GLU	6.6
1	K	18	GLY	6.4
1	D	133	GLY	6.4
1	J	134	GLY	6.4
1	a	17	ARG	6.4
1	C	133	GLY	6.4
1	I	134	GLY	6.4
1	N	18	GLY	6.4
1	k	198	ASN	6.3
1	k	15	SER	6.3
1	F	15	SER	6.2
1	H	133	GLY	6.2
1	i	15	SER	6.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	j	17	ARG	6.2
1	f	20	ARG	6.0
1	F	134	GLY	6.0
1	k	134	GLY	5.9
1	a	15	SER	5.9
1	L	16	GLY	5.8
1	c	22	PHE	5.8
1	G	16	GLY	5.8
1	H	15	SER	5.7
1	e	15	SER	5.7
1	f	133	GLY	5.7
1	h	134	GLY	5.6
1	A	17	ARG	5.6
1	M	18	GLY	5.6
1	g	134	GLY	5.5
1	H	134	GLY	5.5
1	N	17	ARG	5.5
1	N	16	GLY	5.5
1	C	15	SER	5.4
1	f	132	SER	5.4
1	J	17	ARG	5.4
1	n	133	GLY	5.3
1	a	14	GLN	5.2
1	E	17	ARG	5.1
1	H	16	GLY	5.1
1	b	12	ILE	5.1
1	F	16	GLY	5.1
1	L	134	GLY	5.0
1	e	134	GLY	5.0
1	F	132	SER	5.0
1	C	18	GLY	5.0
1	B	132	SER	4.9
1	b	14	GLN	4.9
1	E	18	GLY	4.9
1	f	12	ILE	4.8
1	e	18	GLY	4.8
1	K	15	SER	4.8
1	f	134	GLY	4.8
1	J	135	LEU	4.7
1	F	18	GLY	4.7
1	e	133	GLY	4.7
1	b	22	PHE	4.7

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	l	15	SER	4.6
1	D	15	SER	4.6
1	H	135	LEU	4.6
1	K	16	GLY	4.5
1	G	134	GLY	4.5
1	K	134	GLY	4.5
1	h	15	SER	4.5
1	G	17	ARG	4.5
1	k	14	GLN	4.4
1	g	17	ARG	4.3
1	l	17	ARG	4.3
1	J	16	GLY	4.3
1	b	13	GLU	4.2
1	J	198	ASN	4.2
1	L	133	GLY	4.2
1	K	14	GLN	4.2
1	h	14	GLN	4.2
1	N	134	GLY	4.2
1	g	15	SER	4.1
1	g	18	GLY	4.1
1	J	15	SER	4.1
1	C	17	ARG	4.1
1	n	17	ARG	4.1
1	e	14	GLN	4.0
1	g	133	GLY	4.0
1	b	21	ALA	4.0
1	n	134	GLY	3.9
1	i	135	LEU	3.9
1	j	18	GLY	3.9
1	k	16	GLY	3.9
1	n	15	SER	3.9
1	a	6	TYR	3.8
1	j	15	SER	3.8
1	F	14	GLN	3.8
1	k	199	ARG	3.8
1	G	14	GLN	3.8
1	a	132	SER	3.8
1	C	14	GLN	3.8
1	e	8	VAL	3.7
1	F	133	GLY	3.7
1	D	16	GLY	3.7
1	D	18	GLY	3.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	l	134	GLY	3.7
1	n	132	SER	3.7
1	a	133	GLY	3.7
1	A	18	GLY	3.6
1	G	18	GLY	3.6
1	j	8	VAL	3.6
1	g	14	GLN	3.6
1	c	134	GLY	3.6
1	a	134	GLY	3.6
1	D	17	ARG	3.5
1	G	135	LEU	3.5
1	K	17	ARG	3.5
1	b	134	GLY	3.5
1	b	135	LEU	3.4
1	C	13	GLU	3.4
1	l	133	GLY	3.3
1	h	135	LEU	3.3
1	G	13	GLU	3.3
1	k	18	GLY	3.3
1	e	12	ILE	3.2
1	g	22	PHE	3.2
1	a	12	ILE	3.2
1	f	22	PHE	3.2
1	h	133	GLY	3.2
1	g	135	LEU	3.2
1	g	20	ARG	3.1
1	M	134	GLY	3.1
1	c	133	GLY	3.1
1	M	15	SER	3.1
1	i	134	GLY	3.1
1	D	132	SER	3.1
1	j	135	LEU	3.0
1	l	14	GLN	3.0
1	d	12	ILE	3.0
1	g	130	LEU	3.0
1	k	17	ARG	3.0
1	m	133	GLY	3.0
1	b	15	SER	2.9
1	d	11	VAL	2.9
1	g	12	ILE	2.9
1	i	18	GLY	2.9
1	e	9	PRO	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	J	136	GLY	2.8
1	A	15	SER	2.8
1	d	132	SER	2.8
1	M	16	GLY	2.8
1	N	6	TYR	2.8
1	C	135	LEU	2.8
1	m	131	ILE	2.8
1	h	132	SER	2.8
1	L	18	GLY	2.7
1	m	18	GLY	2.7
1	g	21	ALA	2.7
1	h	130	LEU	2.7
1	M	14	GLN	2.7
1	n	18	GLY	2.7
1	b	132	SER	2.7
1	e	10	THR	2.7
1	M	132	SER	2.7
1	N	133	GLY	2.7
1	e	19	GLU	2.7
1	e	135	LEU	2.7
1	N	132	SER	2.6
1	l	16	GLY	2.6
1	h	17	ARG	2.6
1	g	13	GLU	2.6
1	d	7	LEU	2.6
1	f	9	PRO	2.6
1	f	21	ALA	2.6
1	G	12	ILE	2.6
1	F	136	GLY	2.6
1	j	134	GLY	2.6
1	L	14	GLN	2.5
1	A	19	GLU	2.5
1	A	135	LEU	2.5
1	e	7	LEU	2.5
1	F	17	ARG	2.5
1	K	136	GLY	2.5
1	j	132	SER	2.5
1	m	17	ARG	2.5
1	K	12	ILE	2.5
1	I	17	ARG	2.4
1	m	16	GLY	2.4
1	k	131	ILE	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	i	17	ARG	2.4
1	a	11	VAL	2.4
1	G	6	TYR	2.4
1	G	136	GLY	2.4
1	i	13	GLU	2.4
1	e	132	SER	2.4
1	E	135	LEU	2.4
1	A	136	GLY	2.4
1	K	13	GLU	2.4
1	E	16	GLY	2.4
1	d	133	GLY	2.4
1	A	130	LEU	2.3
1	g	132	SER	2.3
1	B	131	ILE	2.3
1	a	13	GLU	2.3
1	F	20	ARG	2.3
1	e	20	ARG	2.3
1	b	136	GLY	2.3
1	j	14	GLN	2.3
1	M	13	GLU	2.3
1	E	132	SER	2.3
1	H	132	SER	2.3
1	K	135	LEU	2.3
1	I	131	ILE	2.2
1	a	20	ARG	2.2
1	D	14	GLN	2.2
1	J	133	GLY	2.2
1	M	136	GLY	2.2
1	N	15	SER	2.2
1	k	132	SER	2.2
1	a	19	GLU	2.2
1	A	132	SER	2.2
1	i	14	GLN	2.2
1	j	198	ASN	2.2
1	d	134	GLY	2.2
1	M	6	TYR	2.1
1	k	197	GLU	2.1
1	C	19	GLU	2.1
1	A	16	GLY	2.1
1	C	8	VAL	2.1
1	I	16	GLY	2.1
1	d	10	THR	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	L	135	LEU	2.0
1	f	135	LEU	2.0

## 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	MAA	x	5	6/7	0.95	0.17	-	32,44,53,65	0
2	MAA	p	5	6/7	0.92	0.12	-	22,32,34,36	0
2	MP8	q	7	8/9	0.96	0.15	-	19,29,33,38	0
2	MP8	r	7	8/9	0.93	0.10	-	17,21,32,37	0
2	MP8	P	7	8/9	0.96	0.11	-	19,24,25,26	0
2	MP8	u	7	8/9	0.93	0.13	-	13,23,28,32	0
2	MP8	T	7	8/9	0.97	0.11	-	12,16,21,28	0
2	MAA	y	5	6/7	0.96	0.13	-	17,22,27,32	0
2	MP8	Z	7	8/9	0.97	0.11	-	16,22,28,30	0
2	MAA	Z	5	6/7	0.97	0.14	-	14,18,26,31	0
2	MP8	o	7	8/9	0.93	0.11	-	14,19,30,31	0
2	MAA	2	5	6/7	0.97	0.10	-	21,25,27,32	0
2	MP8	s	7	8/9	0.97	0.12	-	17,25,27,27	0
2	MP8	Q	7	8/9	0.96	0.12	-	10,18,27,27	0
2	MP8	R	7	8/9	0.96	0.12	-	10,20,25,32	0
2	MP8	0	7	8/9	0.94	0.12	-	16,23,27,28	0
2	MP8	U	7	8/9	0.93	0.13	-	18,23,30,38	0
2	MP8	v	7	8/9	0.94	0.12	-	18,24,28,38	0
2	MP8	y	7	8/9	0.97	0.12	-	16,19,24,24	0
2	MAA	W	5	6/7	0.94	0.16	-	25,31,34,35	0
2	MP8	x	7	8/9	0.96	0.11	-	19,23,32,32	0
2	MAA	3	5	6/7	0.97	0.13	-	27,35,38,40	0
2	MAA	1	5	6/7	0.97	0.12	-	21,33,35,37	0
2	MAA	O	5	6/7	0.98	0.13	-	18,21,35,36	0
2	MAA	z	5	6/7	0.94	0.13	-	21,28,30,34	0
2	MAA	V	5	6/7	0.96	0.12	-	26,28,32,36	0
2	MP8	O	7	8/9	0.97	0.12	-	22,26,31,34	0
2	MAA	T	5	6/7	0.96	0.17	-	25,31,34,36	0
2	MAA	R	5	6/7	0.97	0.10	-	23,28,30,33	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	MP8	S	7	8/9	0.94	0.14	-	14,21,28,35	0
2	MAA	0	5	6/7	0.97	0.11	-	24,30,33,36	0
2	MP8	1	7	8/9	0.96	0.11	-	20,23,28,30	0
2	MP8	2	7	8/9	0.94	0.14	-	13,17,25,25	0
2	MP8	w	7	8/9	0.95	0.10	-	26,32,38,39	0
2	MP8	V	7	8/9	0.97	0.12	-	11,25,29,30	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	MAA	U	5	6/7	0.97	0.13	-	18,26,31,32	0
2	MAA	S	5	6/7	0.95	0.11	-	18,25,31,32	0
2	MAA	Q	5	6/7	0.97	0.13	-	24,25,29,30	0
2	MAA	o	5	6/7	0.99	0.14	-	20,26,27,27	0
2	MAA	X	5	6/7	0.96	0.15	-	21,30,34,45	0
2	MAA	v	5	6/7	0.96	0.15	-	29,35,39,40	0
2	MAA	t	5	6/7	0.96	0.14	-	29,34,35,39	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	MAA	P	5	6/7	0.97	0.13	-	24,27,30,35	0
2	MP8	W	7	8/9	0.95	0.12	-	18,27,33,36	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	Y	5	6/7	0.96	0.10	-	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	MAA	s	5	6/7	0.97	0.09	-	20,25,34,39	0
2	MAA	q	5	6/7	0.95	0.15	-	32,34,39,43	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	K	F	301	1/1	0.99	0.07	-1.06	26,26,26,26	0
3	K	h	301	1/1	0.98	0.11	-1.18	30,30,30,30	0
3	K	l	301	1/1	0.99	0.08	-1.19	27,27,27,27	0
3	K	e	301	1/1	0.98	0.07	-1.37	32,32,32,32	0
4	NA	h	302	1/1	0.97	0.13	-1.38	37,37,37,37	0
3	K	b	301	1/1	0.99	0.09	-1.38	40,40,40,40	0
3	K	L	301	1/1	0.99	0.12	-1.63	25,25,25,25	0
3	K	M	301	1/1	0.97	0.10	-1.71	26,26,26,26	0
3	K	i	301	1/1	0.98	0.11	-1.88	28,28,28,28	0
3	K	H	301	1/1	0.98	0.08	-2.35	35,35,35,35	0
3	K	c	301	1/1	0.99	0.08	-2.35	25,25,25,25	0
4	NA	k	302	1/1	0.98	0.10	-2.48	40,40,40,40	0
3	K	N	301	1/1	0.99	0.09	-2.90	25,25,25,25	0
3	K	C	301	1/1	0.99	0.08	-3.12	24,24,24,24	0
3	K	m	301	1/1	0.98	0.07	-3.32	29,29,29,29	0
3	K	d	301	1/1	0.97	0.07	-3.36	27,27,27,27	0
3	K	a	301	1/1	0.98	0.07	-3.42	31,31,31,31	0
3	K	D	301	1/1	0.99	0.09	-3.56	26,26,26,26	0
3	K	K	301	1/1	0.99	0.07	-3.57	29,29,29,29	0
4	NA	c	302	1/1	0.98	0.08	-3.61	25,25,25,25	0
3	K	I	301	1/1	0.99	0.08	-3.94	30,30,30,30	0
3	K	E	301	1/1	0.98	0.07	-4.06	30,30,30,30	0
3	K	J	301	1/1	0.97	0.07	-4.14	31,31,31,31	0
3	K	j	301	1/1	1.00	0.09	-4.14	22,22,22,22	0
3	K	g	301	1/1	0.99	0.07	-4.38	31,31,31,31	0
3	K	G	301	1/1	0.99	0.10	-4.52	25,25,25,25	0
3	K	A	301	1/1	0.99	0.09	-4.77	24,24,24,24	0
3	K	B	301	1/1	0.99	0.07	-4.95	22,22,22,22	0
3	K	f	301	1/1	0.98	0.07	-4.96	32,32,32,32	0
3	K	k	301	1/1	0.97	0.07	-6.65	26,26,26,26	0
3	K	n	301	1/1	0.98	0.05	-7.90	26,26,26,26	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.