



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:08 AM UTC

PDB ID : 5DKP / pdb_00005dkp
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

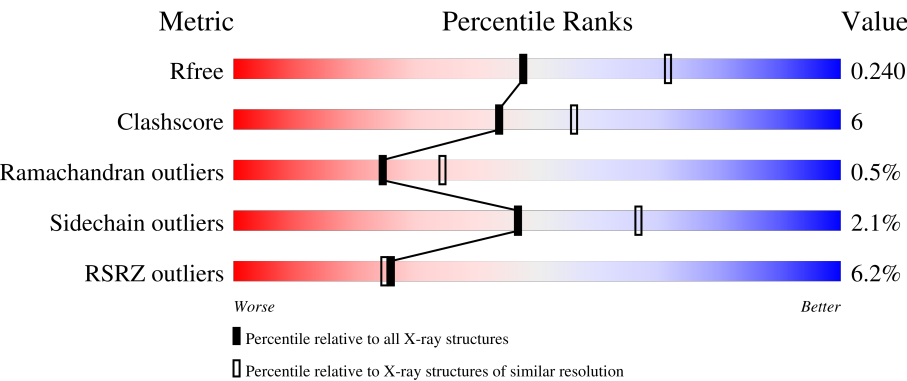
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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}	180053	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	5% 81% 10% • 8%
1	B	206	4% 78% 13% 9%
1	C	206	6% 79% 13% • 7%
1	D	206	5% 81% 11% • 7%

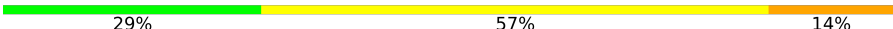
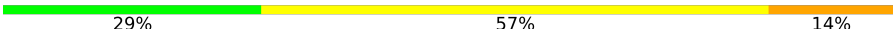
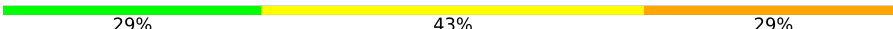
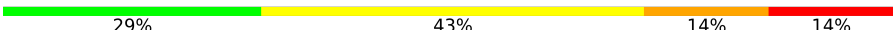
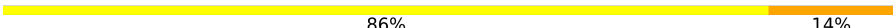
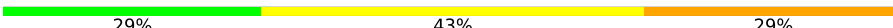
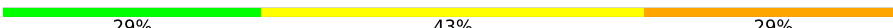
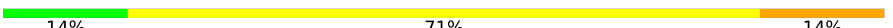
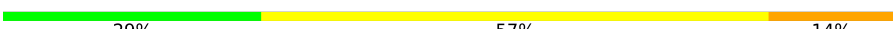
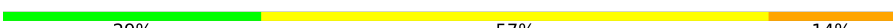
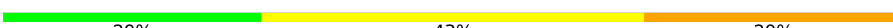
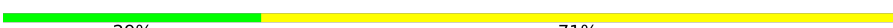
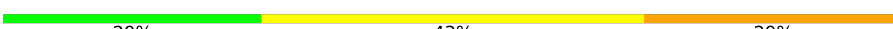
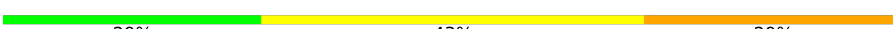
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Mol	Chain	Length	Quality of chain
1	E	206	
1	F	206	
1	G	206	
1	H	206	
1	I	206	
1	J	206	
1	K	206	
1	L	206	
1	M	206	
1	N	206	
1	a	206	
1	b	206	
1	c	206	
1	d	206	
1	e	206	
1	f	206	
1	g	206	
1	h	206	
1	i	206	
1	j	206	
1	k	206	
1	l	206	
1	m	206	
1	n	206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

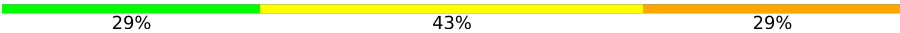
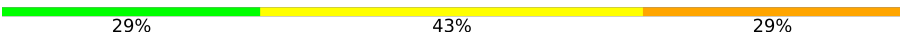
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Mol	Chain	Length	Quality of chain
2	1	7	
2	2	7	
2	3	7	
2	O	7	
2	P	7	
2	Q	7	
2	R	7	
2	S	7	
2	T	7	
2	U	7	
2	V	7	
2	W	7	
2	X	7	
2	Y	7	
2	Z	7	
2	o	7	
2	p	7	
2	q	7	
2	r	7	
2	s	7	
2	t	7	
2	u	7	
2	v	7	
2	w	7	
2	x	7	

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Mol	Chain	Length	Quality of chain
2	y	7	 29% 43% 29%
2	z	7	 29% 43% 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 (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	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	D	1	Total	K	0	0
			1	1		
3	E	1	Total	K	0	0
			1	1		
3	F	1	Total	K	0	0
			1	1		
3	G	1	Total	K	0	0
			1	1		
3	H	1	Total	K	0	0
			1	1		
3	I	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	L	1	Total	K	0	0
			1	1		
3	M	1	Total	K	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	N	1	Total K 1 1	0	0
3	a	1	Total K 1 1	0	0
3	b	1	Total K 1 1	0	0
3	c	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	f	1	Total K 1 1	0	0
3	g	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	j	1	Total K 1 1	0	0
3	k	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	n	1	Total K 1 1	0	0

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

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

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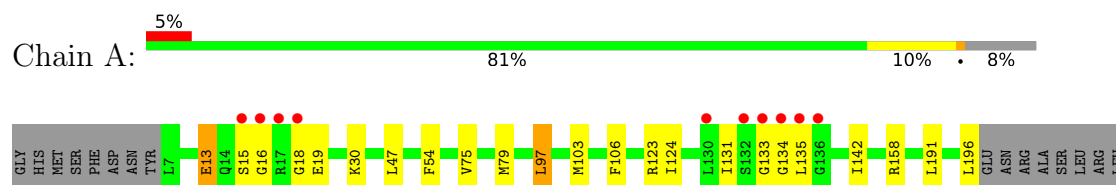
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	i	24	Total 24	O 24	0	0
5	j	35	Total 35	O 35	0	0
5	k	30	Total 30	O 30	0	0
5	l	29	Total 29	O 29	0	0
5	m	28	Total 28	O 28	0	0
5	n	24	Total 24	O 24	0	0
5	O	2	Total 2	O 2	0	0
5	t	1	Total 1	O 1	0	0

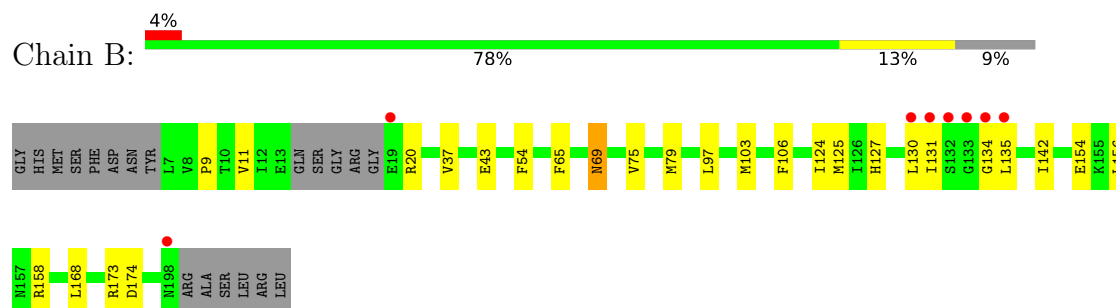
3 Residue-property plots [i](#)

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.

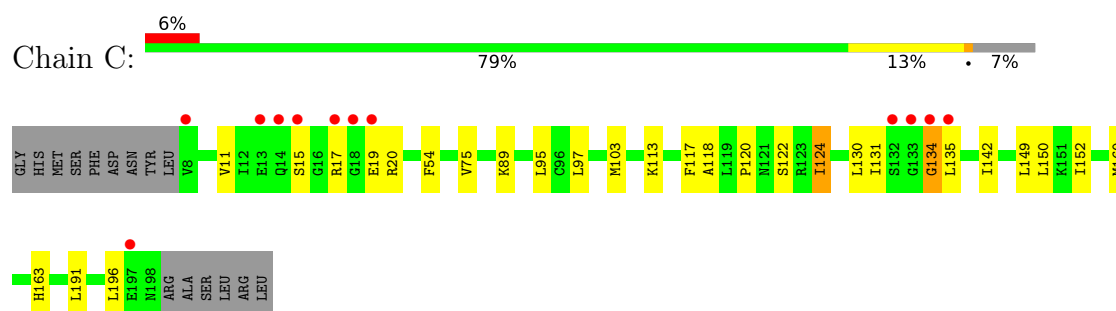
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



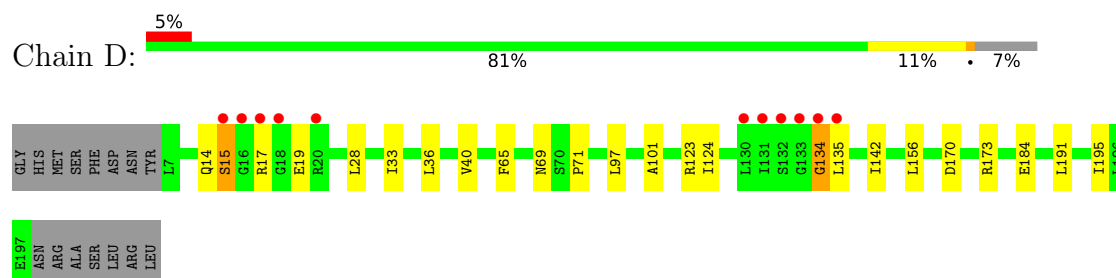
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



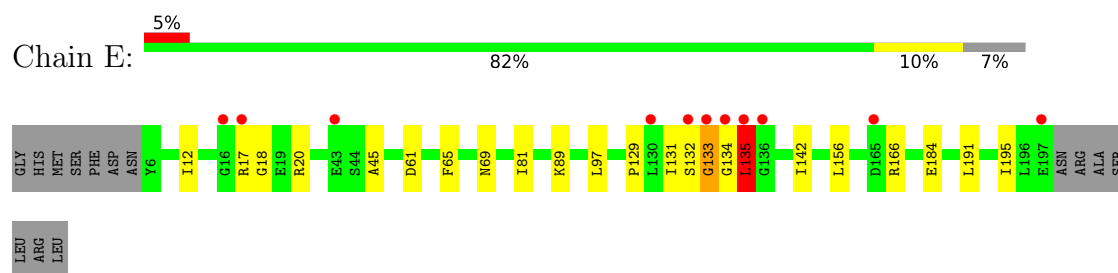
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



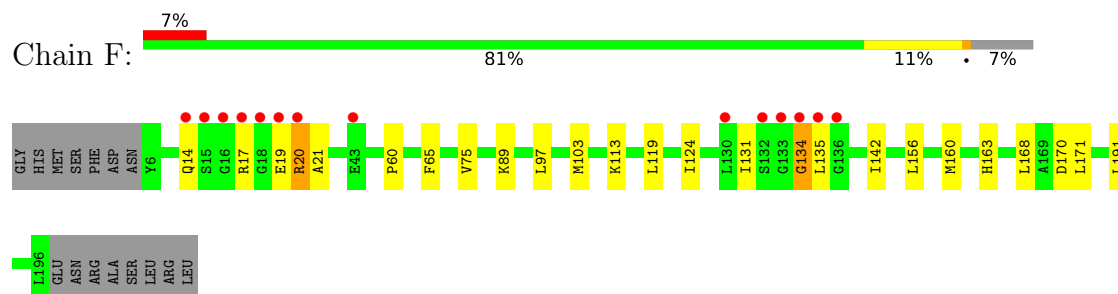
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



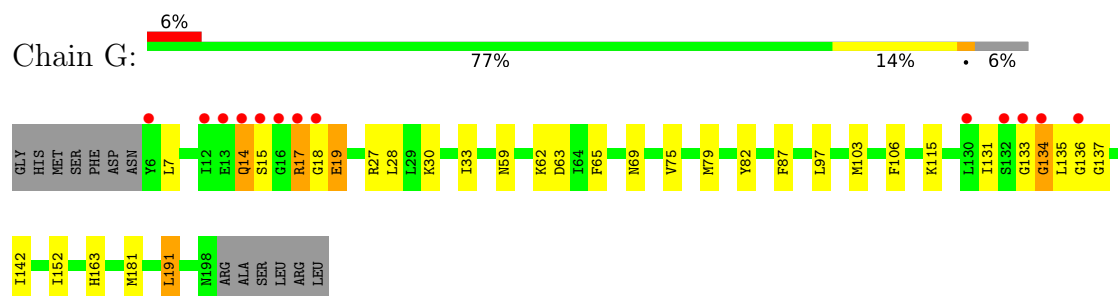
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



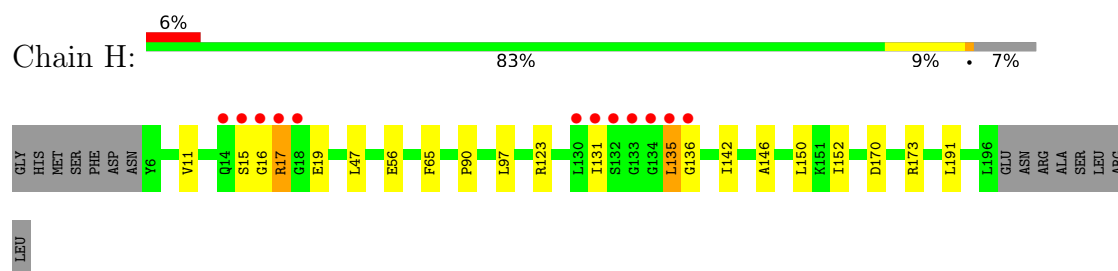
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



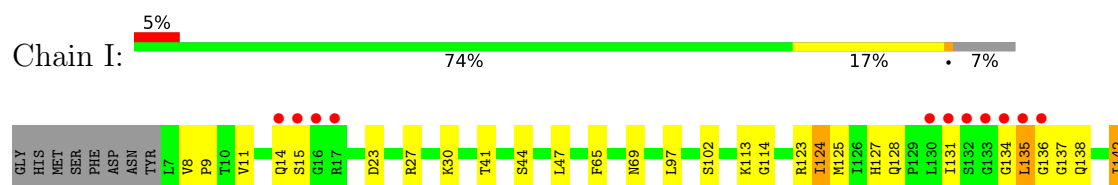
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



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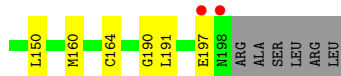
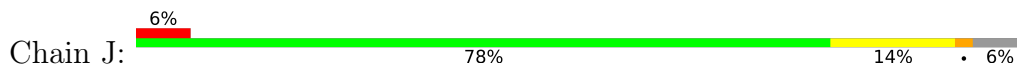


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

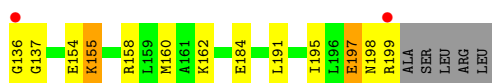
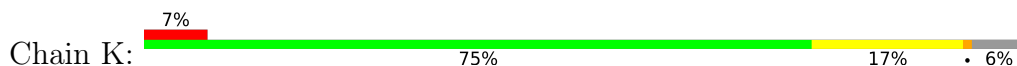




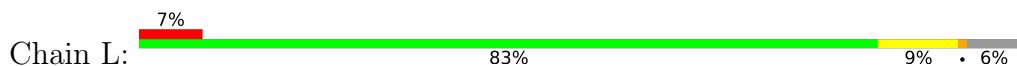
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



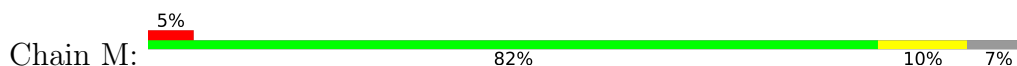
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



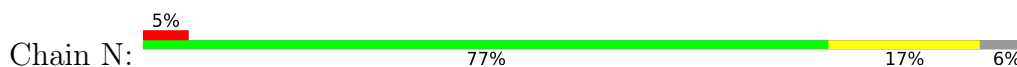
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



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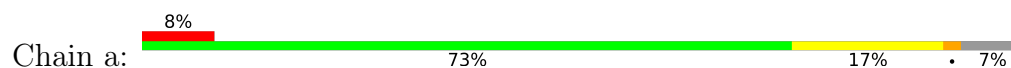


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

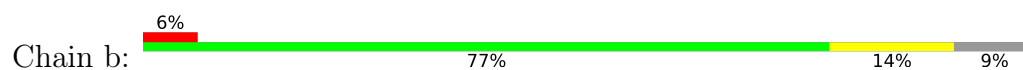




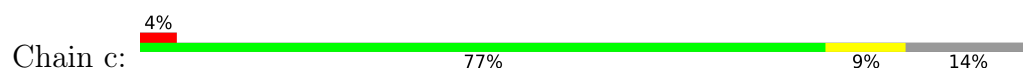
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



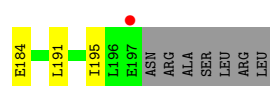
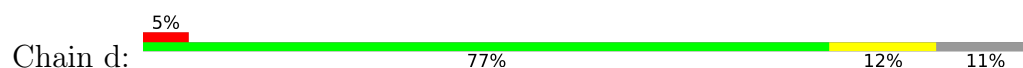
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



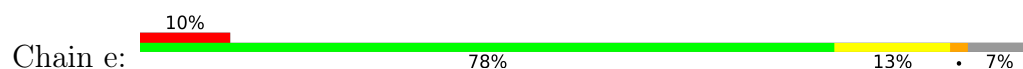
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

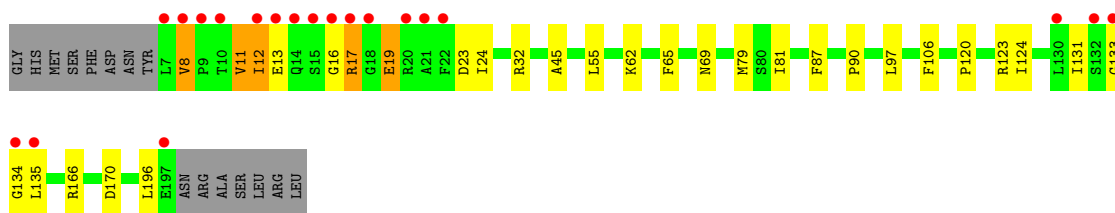


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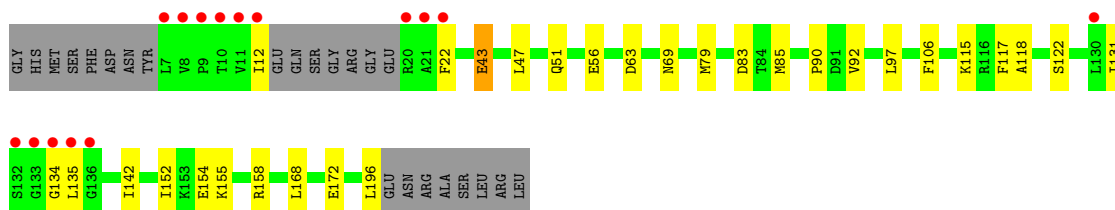
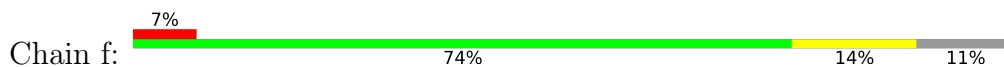


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

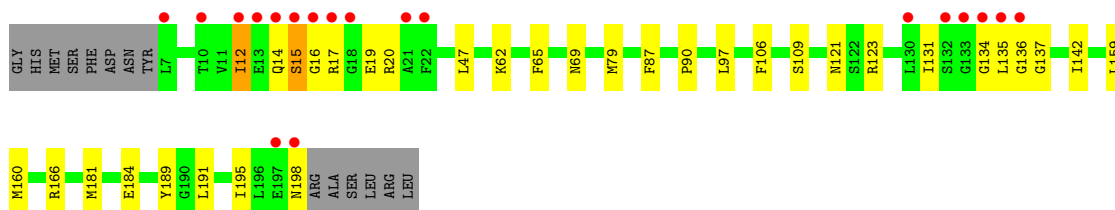
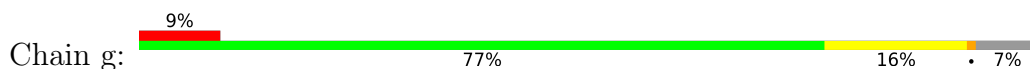




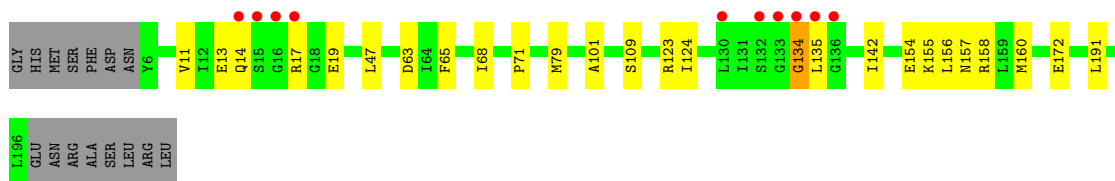
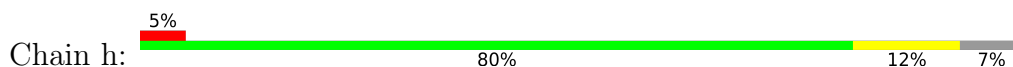
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



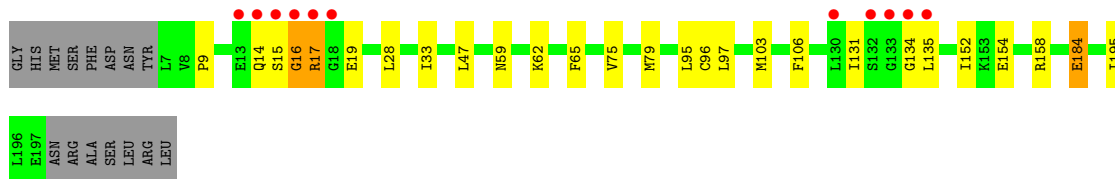
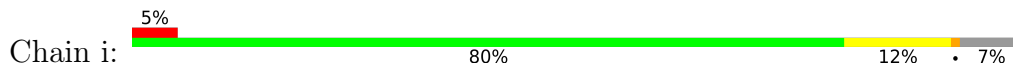
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



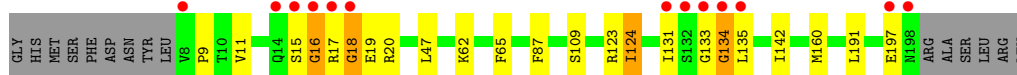
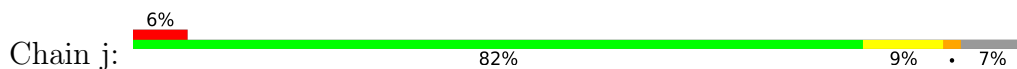
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



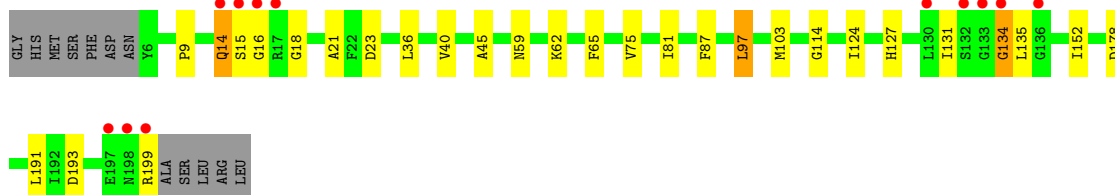
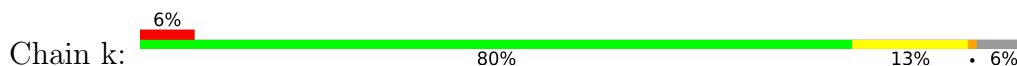
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



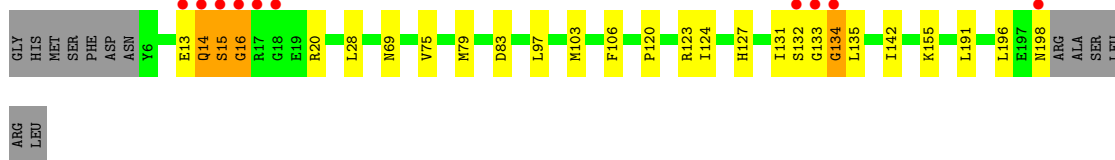
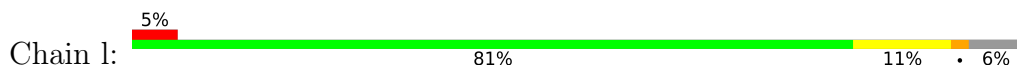
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



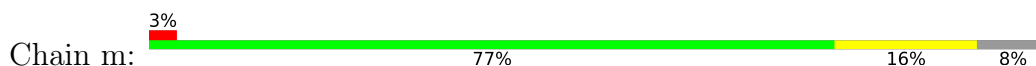
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



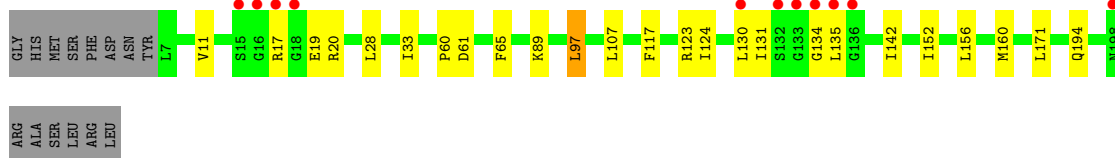
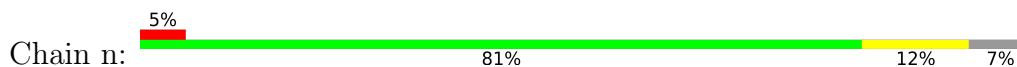
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



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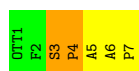


- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 2: agonist ADEP A54556

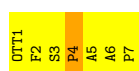
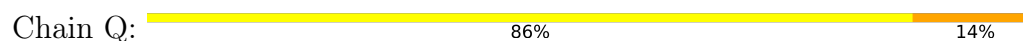




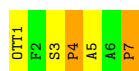
- Molecule 2: agonist ADEP A54556



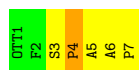
- Molecule 2: agonist ADEP A54556



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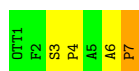
- Molecule 2: agonist ADEP A54556



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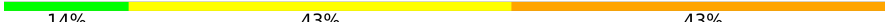
- Molecule 2: agonist ADEP A54556

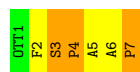


- Molecule 2: agonist ADEP A54556

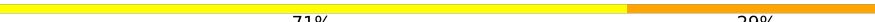


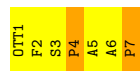
- Molecule 2: agonist ADEP A54556

Chain W:  14% 43% 43%

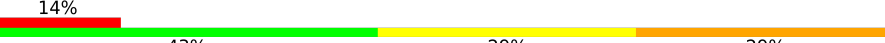


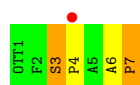
- Molecule 2: agonist ADEP A54556

Chain X:  71% 29%

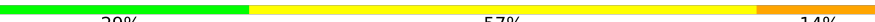


- Molecule 2: agonist ADEP A54556

Chain Y:  14% 43% 29% 29%

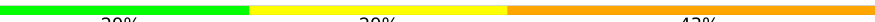


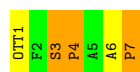
- Molecule 2: agonist ADEP A54556

Chain Z:  29% 57% 14%



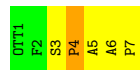
- Molecule 2: agonist ADEP A54556

Chain o:  29% 29% 43%

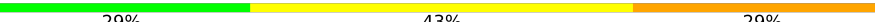


- Molecule 2: agonist ADEP A54556

Chain p:  29% 57% 14%

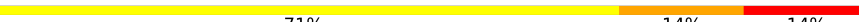


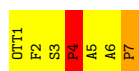
- Molecule 2: agonist ADEP A54556

Chain q:  29% 43% 29%



- Molecule 2: agonist ADEP A54556

Chain r:  71% 14% 14%



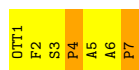
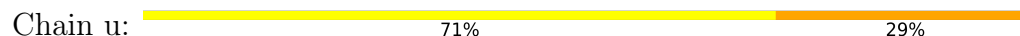
- Molecule 2: agonist ADEP A54556



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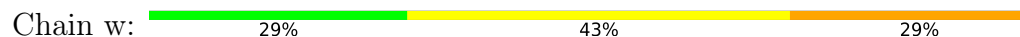
- Molecule 2: agonist ADEP A54556



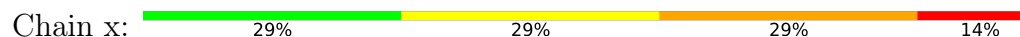
- Molecule 2: agonist ADEP A54556



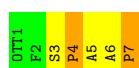
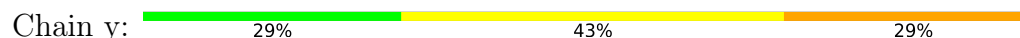
- Molecule 2: agonist ADEP A54556



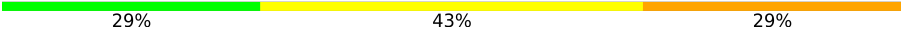
- Molecule 2: agonist ADEP A54556

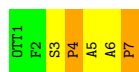


- Molecule 2: agonist ADEP A54556

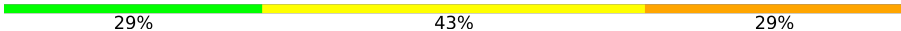


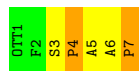
- Molecule 2: agonist ADEP A54556

Chain z:  29% 43% 29%

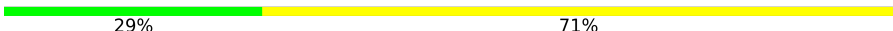


- Molecule 2: agonist ADEP A54556

Chain 0:  29% 43% 29%

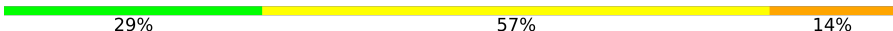


- Molecule 2: agonist ADEP A54556

Chain 1:  29% 71%

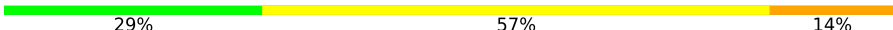


- Molecule 2: agonist ADEP A54556

Chain 2:  29% 57% 14%



- 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, α , β , γ	117.64Å 198.85Å 144.04Å 90.00° 97.81° 90.00°	Depositor
Resolution (Å)	42.40 – 2.38 42.40 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.4 (42.40-2.38) 99.4 (42.40-2.38)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 2.37Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.196 , 0.239 0.199 , 0.240	Depositor DCC
R_{free} test set	10329 reflections (3.98%)	wwPDB-VP
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: OTT, MAA, K, MP8, NA

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	0.57	0/1495	0.87	1/2013 (0.0%)
1	B	0.59	0/1477	0.88	2/1989 (0.1%)
1	C	0.56	0/1504	0.89	1/2025 (0.0%)
1	D	0.55	0/1504	0.83	1/2025 (0.0%)
1	E	0.58	0/1517	0.88	2/2043 (0.1%)
1	F	0.56	0/1508	0.88	1/2031 (0.0%)
1	G	0.55	0/1525	0.87	2/2054 (0.1%)
1	H	0.61	0/1508	0.91	2/2031 (0.1%)
1	I	0.56	0/1504	0.86	1/2025 (0.0%)
1	J	0.53	0/1525	0.87	2/2054 (0.1%)
1	K	0.52	0/1523	0.82	0/2050
1	L	0.55	0/1525	0.85	1/2054 (0.0%)
1	M	0.56	0/1508	0.88	1/2031 (0.0%)
1	N	0.56	0/1525	0.90	2/2054 (0.1%)
1	a	0.56	0/1508	0.96	8/2031 (0.4%)
1	b	0.57	0/1483	0.86	0/1997
1	c	0.56	0/1399	0.88	1/1883 (0.1%)
1	d	0.53	0/1451	0.86	0/1954
1	e	0.58	0/1504	0.86	2/2025 (0.1%)
1	f	0.54	0/1442	0.83	0/1942
1	g	0.53	0/1512	0.87	1/2036 (0.0%)
1	h	0.54	0/1508	0.88	4/2031 (0.2%)
1	i	0.55	0/1504	0.86	0/2025
1	j	0.53	0/1504	0.89	3/2025 (0.1%)
1	k	0.57	0/1536	0.88	4/2068 (0.2%)
1	l	0.54	0/1525	0.94	3/2054 (0.1%)
1	m	0.55	0/1495	0.88	1/2013 (0.0%)
1	n	0.56	0/1512	0.85	0/2036
2	0	3.19	3/29 (10.3%)	1.17	0/37
2	1	3.10	3/29 (10.3%)	1.26	0/37
2	2	2.86	3/29 (10.3%)	1.47	1/37 (2.7%)
2	3	2.54	2/29 (6.9%)	1.32	0/37

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	O	2.63	3/29 (10.3%)	1.11	0/37
2	P	2.70	3/29 (10.3%)	1.04	0/37
2	Q	2.60	3/29 (10.3%)	1.44	1/37 (2.7%)
2	R	3.18	2/29 (6.9%)	1.19	0/37
2	S	2.50	3/29 (10.3%)	1.20	0/37
2	T	2.43	3/29 (10.3%)	1.31	0/37
2	U	2.60	3/29 (10.3%)	1.33	0/37
2	V	2.64	3/29 (10.3%)	1.34	0/37
2	W	3.26	4/29 (13.8%)	1.10	0/37
2	X	2.69	3/29 (10.3%)	1.34	1/37 (2.7%)
2	Y	3.30	2/29 (6.9%)	1.37	0/37
2	Z	2.66	3/29 (10.3%)	1.00	0/37
2	o	2.86	3/29 (10.3%)	1.40	0/37
2	p	2.57	3/29 (10.3%)	1.34	0/37
2	q	3.05	3/29 (10.3%)	1.21	0/37
2	r	2.89	3/29 (10.3%)	1.36	1/37 (2.7%)
2	s	3.39	3/29 (10.3%)	1.02	0/37
2	t	2.96	2/29 (6.9%)	1.29	0/37
2	u	2.75	3/29 (10.3%)	1.41	1/37 (2.7%)
2	v	2.82	3/29 (10.3%)	1.07	0/37
2	w	2.72	3/29 (10.3%)	1.32	0/37
2	x	2.47	3/29 (10.3%)	1.35	0/37
2	y	2.73	3/29 (10.3%)	1.20	0/37
2	z	2.73	3/29 (10.3%)	1.10	0/37
All	All	0.67	81/42843 (0.2%)	0.88	51/57635 (0.1%)

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 (81) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	s	3	SER	CA-C	-15.37	1.38	1.52
2	Y	3	SER	CA-C	-14.30	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	0	3	SER	CA-C	-14.13	1.39	1.52
2	R	3	SER	CA-C	-14.08	1.39	1.52
2	W	3	SER	CA-C	-13.92	1.40	1.52
2	1	3	SER	CA-C	-13.55	1.40	1.52
2	q	3	SER	CA-C	-12.90	1.41	1.52
2	t	3	SER	CA-C	-12.11	1.40	1.52
2	r	3	SER	CA-C	-12.04	1.38	1.52
2	v	3	SER	CA-C	-11.60	1.39	1.52
2	o	3	SER	CA-C	-11.54	1.41	1.52
2	2	3	SER	CA-C	-11.36	1.39	1.52
2	P	3	SER	CA-C	-11.00	1.39	1.52
2	z	3	SER	CA-C	-10.85	1.40	1.52
2	w	3	SER	CA-C	-10.78	1.40	1.52
2	y	3	SER	CA-C	-10.74	1.40	1.52
2	X	3	SER	CA-C	-10.53	1.40	1.52
2	u	3	SER	CA-C	-10.49	1.40	1.52
2	V	3	SER	CA-C	-10.30	1.40	1.52
2	Z	3	SER	CA-C	-10.19	1.40	1.52
2	U	3	SER	CA-C	-10.00	1.41	1.52
2	3	3	SER	CA-C	-9.98	1.41	1.52
2	O	3	SER	CA-C	-9.95	1.41	1.52
2	S	3	SER	CA-C	-9.82	1.41	1.52
2	x	3	SER	CA-C	-9.36	1.41	1.52
2	Q	3	SER	CA-C	-9.32	1.41	1.52
2	p	3	SER	CA-C	-9.22	1.42	1.52
2	T	3	SER	CA-C	-8.99	1.40	1.52
2	Y	6	ALA	CA-C	-7.08	1.38	1.52
2	p	4	PRO	CA-C	-6.46	1.39	1.52
2	o	6	ALA	CA-C	-6.30	1.39	1.52
2	t	6	ALA	CA-C	-6.24	1.39	1.52
2	y	6	ALA	CA-C	-6.18	1.40	1.52
2	Q	4	PRO	CA-C	-6.09	1.40	1.52
2	z	4	PRO	CA-C	-6.08	1.40	1.52
2	u	6	ALA	CA-C	-6.07	1.40	1.52
2	X	6	ALA	CA-C	-6.04	1.40	1.52
2	r	6	ALA	CA-C	-5.91	1.40	1.52
2	V	6	ALA	CA-C	-5.86	1.40	1.52
2	U	4	PRO	CA-C	-5.83	1.40	1.52
2	O	6	ALA	CA-C	-5.82	1.40	1.52
2	3	4	PRO	CA-C	-5.79	1.40	1.52
2	T	6	ALA	CA-C	-5.78	1.40	1.52
2	q	4	PRO	CA-C	-5.76	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	w	6	ALA	CA-C	-5.75	1.40	1.52
2	Z	6	ALA	CA-C	-5.75	1.40	1.52
2	2	4	PRO	CA-C	-5.75	1.40	1.52
2	y	4	PRO	CA-C	-5.71	1.41	1.52
2	W	6	ALA	CA-C	-5.70	1.41	1.52
2	s	4	PRO	CA-C	-5.66	1.41	1.52
2	u	4	PRO	CA-C	-5.66	1.41	1.52
2	R	4	PRO	CA-C	-5.63	1.41	1.52
2	x	4	PRO	CA-C	-5.63	1.41	1.52
2	O	4	PRO	CA-C	-5.61	1.41	1.52
2	P	6	ALA	CA-C	-5.60	1.41	1.52
2	v	4	PRO	CA-C	-5.59	1.41	1.52
2	l	4	PRO	CA-C	-5.59	1.41	1.52
2	S	6	ALA	CA-C	-5.58	1.41	1.52
2	V	4	PRO	CA-C	-5.57	1.41	1.52
2	q	6	ALA	CA-C	-5.57	1.41	1.52
2	l	6	ALA	CA-C	-5.57	1.41	1.52
2	o	4	PRO	CA-C	-5.54	1.41	1.52
2	T	4	PRO	CA-C	-5.52	1.41	1.52
2	p	6	ALA	CA-C	-5.52	1.41	1.52
2	w	4	PRO	CA-C	-5.51	1.41	1.52
2	0	4	PRO	CA-C	-5.51	1.41	1.52
2	U	6	ALA	CA-C	-5.49	1.41	1.52
2	S	4	PRO	CA-C	-5.47	1.41	1.52
2	Z	4	PRO	CA-C	-5.43	1.41	1.52
2	Q	6	ALA	CA-C	-5.33	1.41	1.52
2	X	4	PRO	CA-C	-5.31	1.41	1.52
2	2	6	ALA	CA-C	-5.27	1.41	1.52
2	r	4	PRO	CA-C	-5.26	1.42	1.52
2	W	4	PRO	CA-C	-5.25	1.42	1.52
2	v	6	ALA	CA-C	-5.24	1.42	1.52
2	z	6	ALA	CA-C	-5.21	1.42	1.52
2	s	6	ALA	CA-C	-5.17	1.42	1.52
2	P	4	PRO	CA-C	-5.12	1.42	1.52
2	0	6	ALA	CA-C	-5.06	1.42	1.52
2	x	6	ALA	CA-C	-5.04	1.42	1.52
2	W	2	PHE	CB-CG	-5.03	1.39	1.50

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	134	GLY	N-CA-C	12.36	128.36	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	133	GLY	N-CA-C	-10.67	95.91	112.45
1	m	133	GLY	N-CA-C	-9.71	99.51	111.45
1	k	134	GLY	N-CA-C	9.48	120.95	111.95
1	l	133	GLY	N-CA-C	-9.02	98.58	112.84
1	H	135	LEU	CA-C-N	-8.46	115.90	121.65
1	H	135	LEU	C-N-CA	-8.46	115.90	121.65
1	G	134	GLY	N-CA-C	8.28	122.08	110.74
1	G	133	GLY	N-CA-C	-8.16	97.07	110.95
1	a	13	GLU	CA-C-N	-8.06	111.42	122.30
1	a	13	GLU	C-N-CA	-8.06	111.42	122.30
1	h	134	GLY	N-CA-C	7.78	119.34	111.95
1	N	134	GLY	N-CA-C	7.05	121.47	110.96
1	A	133	GLY	N-CA-C	-7.05	101.70	112.84
1	D	134	GLY	N-CA-C	6.89	118.49	111.95
1	L	134	GLY	N-CA-C	6.67	119.76	112.29
1	a	130	LEU	CA-C-N	-6.65	113.70	122.94
1	a	130	LEU	C-N-CA	-6.65	113.70	122.94
1	h	13	GLU	CA-C-N	-6.54	113.76	122.85
1	h	13	GLU	C-N-CA	-6.54	113.76	122.85
1	a	18	GLY	N-CA-C	-6.42	97.95	113.18
1	E	18	GLY	N-CA-C	6.21	119.00	110.56
1	c	133	GLY	N-CA-C	-6.17	98.57	113.18
1	E	135	LEU	CA-CB-CG	6.04	137.46	116.30
2	2	2	PHE	CA-CB-CG	-5.96	107.84	113.80
1	a	23	ASP	N-CA-C	-5.93	102.13	110.50
1	B	130	LEU	CA-C-N	-5.93	115.83	123.19
1	B	130	LEU	C-N-CA	-5.93	115.83	123.19
1	C	134	GLY	N-CA-C	5.92	117.57	111.95
1	j	16	GLY	N-CA-C	-5.84	104.61	112.14
2	r	2	PHE	CA-CB-CG	-5.80	108.00	113.80
1	a	135	LEU	N-CA-C	-5.79	98.31	108.20
1	k	18	GLY	N-CA-C	5.76	119.07	111.70
2	u	2	PHE	CA-CB-CG	-5.69	108.11	113.80
1	j	18	GLY	N-CA-C	5.65	121.08	111.19
1	l	134	GLY	N-CA-C	5.64	119.37	110.96
2	Q	2	PHE	CA-CB-CG	-5.60	108.20	113.80
1	F	134	GLY	N-CA-C	5.58	117.73	112.04
1	a	133	GLY	N-CA-C	-5.55	100.03	113.18
1	g	12	ILE	N-CA-C	5.48	114.63	106.85
1	I	23	ASP	N-CA-C	-5.34	102.97	110.50
1	J	134	GLY	N-CA-C	5.29	119.33	111.18
1	J	23	ASP	N-CA-C	-5.29	103.04	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	k	16	GLY	N-CA-C	-5.28	104.43	112.51
1	h	68	ILE	N-CA-C	5.17	115.30	107.75
1	e	23	ASP	N-CA-C	-5.14	103.25	110.50
1	k	23	ASP	N-CA-C	-5.12	103.28	110.50
1	l	132	SER	N-CA-C	-5.11	101.83	109.95
1	j	134	GLY	N-CA-C	5.09	125.25	113.18
1	e	133	GLY	N-CA-C	-5.02	101.29	113.18
2	X	2	PHE	CA-CB-CG	-5.01	108.79	113.80

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	16	0
1	B	1456	0	1463	23	0
1	C	1482	0	1485	21	0
1	D	1482	0	1490	18	0
1	E	1494	0	1499	18	0
1	F	1485	0	1493	18	1
1	G	1502	0	1505	27	1
1	H	1485	0	1493	13	0
1	I	1482	0	1490	31	0
1	J	1502	0	1505	25	0
1	K	1501	0	1509	30	1
1	L	1502	0	1505	19	0
1	M	1485	0	1493	19	0
1	N	1502	0	1505	25	0
1	a	1485	0	1493	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	b	1462	0	1470	27	0
1	c	1378	0	1380	17	0
1	d	1430	0	1445	20	0
1	e	1482	0	1490	22	0
1	f	1421	0	1439	27	0
1	g	1490	0	1496	28	0
1	h	1485	0	1493	20	1
1	i	1482	0	1490	23	0
1	j	1482	0	1485	19	0
1	k	1513	0	1518	20	0
1	l	1502	0	1505	24	0
1	m	1473	0	1484	26	0
1	n	1490	0	1496	28	0
2	O	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	2	0
2	P	52	0	49	2	0
2	Q	52	0	49	2	0
2	R	52	0	49	3	0
2	S	52	0	49	2	0
2	T	52	0	49	2	0
2	U	52	0	49	1	0
2	V	52	0	49	3	0
2	W	52	0	49	3	0
2	X	52	0	49	4	0
2	Y	52	0	49	3	0
2	Z	52	0	49	2	0
2	o	52	0	49	3	0
2	p	52	0	49	1	0
2	q	52	0	49	2	0
2	r	52	0	49	4	0
2	s	52	0	49	2	0
2	t	52	0	49	2	0
2	u	52	0	49	3	0
2	v	52	0	49	1	0
2	w	52	0	49	2	0
2	x	52	0	49	3	0
2	y	52	0	49	2	0
2	z	52	0	49	2	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	1	0
5	B	42	0	0	0	0
5	C	35	0	0	0	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	0	0
5	H	27	0	0	0	0
5	I	34	0	0	0	0
5	J	31	0	0	0	0
5	K	41	0	0	1	0
5	L	32	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	M	37	0	0	1	0
5	N	32	0	0	1	0
5	O	2	0	0	0	0
5	a	27	0	0	1	0
5	b	26	0	0	1	0
5	c	34	0	0	1	0
5	d	33	0	0	1	0
5	e	26	0	0	0	0
5	f	28	0	0	0	0
5	g	16	0	0	1	0
5	h	24	0	0	1	0
5	i	24	0	0	1	0
5	j	35	0	0	1	0
5	k	30	0	0	0	0
5	l	29	0	0	0	0
5	m	28	0	0	1	0
5	n	24	0	0	2	0
5	t	1	0	0	0	0
All	All	43749	0	42975	522	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 6.

All (522) 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:g:181:MET:HE1	1:g:191:LEU:HD12	1.48	0.95
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:135:LEU:H	1:M:135:LEU:H	1.20	0.87
1:f:135:LEU:H	1:n:135:LEU:H	1.19	0.85
1:F:135:LEU:H	1:N:135:LEU:H	1.26	0.84
1:h:160:MET:HE1	1:h:191:LEU:HD21	1.61	0.83
1:I:158:ARG:O	1:I:162:LYS:HD3	1.80	0.82
1:e:135:LEU:HB2	1:h:135:LEU:HB2	1.64	0.80
1:l:155:LYS:NZ	1:m:121:ASN:OD1	2.15	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	1.32	0.78
1:a:61:ASP:OD1	1:a:89:LYS:NZ	2.16	0.77
1:L:69:ASN:HB2	1:L:97:LEU:HD12	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	2.18	0.76
1:I:160:MET:HE1	1:I:191:LEU:HD21	1.67	0.76
1:D:135:LEU:HB2	1:I:135:LEU:HB2	1.68	0.75
1:a:135:LEU:HB2	1:l:135:LEU:HB2	1.66	0.75
1:I:14:GLN:OE1	1:I:27:ARG:NH2	2.20	0.75
1:m:160:MET:HE1	1:m:191:LEU:HD21	1.69	0.74
1:i:152:ILE:HD11	1:j:123:ARG:HH21	1.53	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	1.54	0.73
1:G:181:MET:HE1	1:G:191:LEU:HD13	1.71	0.73
1:b:69:ASN:HB2	1:b:97:LEU:HD12	1.71	0.73
1:f:135:LEU:HB2	1:n:135:LEU:HB2	1.70	0.72
1:C:135:LEU:HB2	1:J:135:LEU:HB2	1.69	0.72
1:C:160:MET:HE1	1:C:191:LEU:HD11	1.70	0.72
1:N:69:ASN:HB2	1:N:97:LEU:HD12	1.71	0.72
1:g:160:MET:HE3	1:g:191:LEU:HD21	1.71	0.72
1:F:17:ARG:NH1	5:F:401:HOH:O	2.22	0.71
1:F:160:MET:HE3	1:F:191:LEU:HD21	1.71	0.71
1:F:135:LEU:HB2	1:N:135:LEU:HB2	1.72	0.71
1:G:59:ASN:ND2	1:G:62:LYS:HE2	2.06	0.71
1:a:135:LEU:H	1:l:135:LEU:H	1.39	0.70
1:b:160:MET:HE3	1:b:191:LEU:HD11	1.72	0.70
1:b:135:LEU:HB2	1:k:135:LEU:HB2	1.74	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	1.56	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:B:135:LEU:HB2	1:K:135:LEU:HB2	1.75	0.68
1:m:80:SER:HB2	1:n:97:LEU:HG	1.76	0.68
1:b:135:LEU:O	1:k:134:GLY:HA2	1.94	0.68
1:c:135:LEU:HB2	1:j:135:LEU:HD22	1.73	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	1.75	0.68
1:j:160:MET:HE1	1:j:191:LEU:HD21	1.75	0.67
1:d:69:ASN:HB2	1:d:97:LEU:HD12	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:69:ASN:HB2	1:g:97:LEU:HD12	1.77	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:e:69:ASN:HB2	1:e:97:LEU:HD12	1.79	0.65
1:n:17:ARG:NH2	5:n:401:HOH:O	2.26	0.65
1:H:123:ARG:HH21	1:N:152:ILE:HD11	1.62	0.65
1:g:181:MET:SD	5:g:404:HOH:O	2.55	0.65
1:b:142:ILE:HD11	1:k:131:ILE:HG12	1.79	0.64
1:l:20:ARG:NH2	1:m:19:GLU:OE1	2.31	0.64
1:f:117:PHE:HB3	1:f:196:LEU:HD11	1.80	0.64
1:M:152:ILE:HD11	1:N:123:ARG:HH21	1.63	0.64
1:g:135:LEU:H	1:m:135:LEU:H	1.44	0.64
1:k:59:ASN:ND2	1:k:62:LYS:HE2	2.13	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	1.96	0.63
1:j:133:GLY:O	1:j:135:LEU:N	2.27	0.63
1:l:83:ASP:OD1	1:m:121:ASN:ND2	2.26	0.63
1:D:69:ASN:HB2	1:D:97:LEU:HD12	1.80	0.62
1:m:69:ASN:HB2	1:m:97:LEU:HD12	1.80	0.62
1:f:69:ASN:HB2	1:f:97:LEU:HD12	1.82	0.62
1:b:173:ARG:NH1	1:b:174:ASP:OD1	2.32	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:I:170:ASP:OD2	1:i:158:ARG:NH2	2.34	0.61
1:a:131:ILE:HG12	1:l:142:ILE:HD11	1.82	0.61
1:d:152:ILE:HD11	1:e:123:ARG:HH21	1.65	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:a:160:MET:HE3	1:a:191:LEU:HD21	1.83	0.60
1:f:142:ILE:HD11	1:n:131:ILE:HG12	1.81	0.60
1:J:160:MET:HE1	1:J:191:LEU:HD21	1.81	0.60
1:k:75:VAL:HA	1:k:103:MET:HE3	1.82	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:155:LYS:NZ	1:g:121:ASN:OD1	2.32	0.59
1:f:135:LEU:N	1:n:135:LEU:H	1.96	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:LEU:H	1:I:135:LEU:N	1.91	0.59
1:d:142:ILE:HD11	1:i:131:ILE:HG12	1.85	0.59
1:A:134:GLY:HA3	1:L:134:GLY:HA3	1.85	0.59
1:I:27:ARG:O	1:I:27:ARG:NH1	2.35	0.58
1:k:152:ILE:HD11	1:l:123:ARG:HH21	1.68	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	1.84	0.58
1:c:142:ILE:HD11	1:j:131:ILE:HG12	1.85	0.58
1:e:131:ILE:HG12	1:h:142:ILE:HD11	1.84	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:K:47:LEU:HD11	1:L:9:PRO:HD2	1.85	0.58
1:K:79:MET:HE1	1:K:106:PHE:CE2	2.38	0.58
1:i:15:SER:O	1:i:17:ARG:N	2.37	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:c:131:ILE:HG12	1:j:142:ILE:HD11	1.86	0.57
1:a:142:ILE:HD11	1:l:131:ILE:HG12	1.86	0.57
1:F:113:LYS:HE2	1:F:163:HIS:O	2.05	0.57
1:n:28:LEU:HD22	1:n:33:ILE:HD12	1.85	0.57
1:C:124:ILE:HG21	1:C:191:LEU:HD23	1.87	0.57
1:E:131:ILE:HG12	1:H:142:ILE:HD11	1.87	0.57
1:i:28:LEU:HD22	1:i:33:ILE:HD12	1.85	0.57
1:e:32:ARG:NH1	1:e:62:LYS:O	2.38	0.56
1:e:166:ARG:NH1	1:e:170:ASP:OD2	2.38	0.56
1:A:75:VAL:HA	1:A:103:MET:HE3	1.87	0.56
1:H:47:LEU:HD11	1:I:9:PRO:HD2	1.87	0.56
1:l:69:ASN:HB2	1:l:97:LEU:HD12	1.86	0.56
1:A:135:LEU:HB2	1:L:135:LEU:HB2	1.87	0.56
1:B:142:ILE:HD11	1:K:131:ILE:HG12	1.86	0.56
1:C:20:ARG:NH1	1:D:19:GLU:OE2	2.38	0.56
1:I:170:ASP:CG	1:i:158:ARG:HH22	2.14	0.56
1:i:154:GLU:O	1:i:158:ARG:HG3	2.05	0.56
1:C:75:VAL:HA	1:C:103:MET:HE3	1.87	0.56
1:b:22:PHE:HE1	1:b:27:ARG:N	2.03	0.56
1:C:113:LYS:NZ	1:C:163:HIS:O	2.39	0.56
1:b:188:GLU:HG3	5:b:425:HOH:O	2.06	0.56
1:d:127:HIS:HD2	1:d:128:GLN:O	1.89	0.56
1:i:65:PHE:CE2	2:y:7:MP8:HB	2.40	0.56
1:n:97:LEU:HD21	5:n:420:HOH:O	2.05	0.56
1:n:65:PHE:CE2	2:3:7:MP8:HB	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:ARG:HD2	1:B:174:ASP:OD1	2.05	0.55
1:f:22:PHE:CZ	1:g:12:ILE:HD11	2.40	0.55
1:g:15:SER:OG	1:g:16:GLY:N	2.39	0.55
1:B:154:GLU:OE2	1:B:158:ARG:HD2	2.05	0.55
1:f:134:GLY:HA3	1:n:134:GLY:HA3	1.89	0.55
1:d:135:LEU:O	1:i:131:ILE:HD11	2.06	0.55
1:a:22:PHE:CZ	1:a:30:LYS:HE2	2.42	0.55
1:n:60:PRO:O	1:n:89:LYS:HG3	2.07	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:J:43:GLU:H	1:J:43:GLU:CD	2.15	0.54
1:M:28:LEU:HD22	2:o:1:OTT:H6	1.89	0.54
1:i:59:ASN:ND2	1:i:62:LYS:HE2	2.22	0.54
1:l:13:GLU:HG2	1:l:14:GLN:N	2.22	0.54
1:d:135:LEU:H	1:i:135:LEU:H	1.53	0.54
1:i:75:VAL:HA	1:i:103:MET:HE3	1.88	0.54
1:N:60:PRO:HB2	1:N:89:LYS:HD3	1.90	0.54
1:a:65:PHE:CE2	2:q:7:MP8:HB	2.42	0.54
1:m:160:MET:HB3	1:m:171:LEU:CD2	2.38	0.54
1:I:113:LYS:HE2	1:I:163:HIS:O	2.08	0.54
1:c:28:LEU:HD13	1:c:35:PHE:HE2	1.73	0.54
1:m:54:PHE:HA	2:3:1:OTT:H7	1.88	0.54
1:b:120:PRO:HD3	1:b:196:LEU:O	2.07	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	1.89	0.53
1:f:154:GLU:OE2	1:f:158:ARG:NH1	2.42	0.53
1:E:45:ALA:HA	1:E:81:ILE:HD11	1.90	0.53
1:K:199:ARG:C	2:Y:4:PRO:HD2	2.33	0.53
1:k:87:PHE:HE2	1:l:196:LEU:HB3	1.73	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	2.42	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:A:123:ARG:HH21	1:G:152:ILE:HD11	1.75	0.52
1:G:131:ILE:HG12	1:M:142:ILE:HD11	1.91	0.52
1:C:54:PHE:HA	2:R:1:OTT:H7	1.92	0.52
1:L:87:PHE:HE2	1:M:196:LEU:HB3	1.74	0.52
1:a:47:LEU:HD11	1:b:9:PRO:HD2	1.91	0.52
1:d:54:PHE:CZ	1:e:11:VAL:HB	2.45	0.52
1:g:131:ILE:HG12	1:m:142:ILE:HD11	1.91	0.52

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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: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:d:125:MET:SD	1:d:127:HIS:ND1	2.76	0.52
1:F:135:LEU:N	1:N:135:LEU:H	2.01	0.52
1:d:134:GLY:HA3	1:i:134:GLY:HA3	1.92	0.52
1:e:134:GLY:HA3	1:h:134:GLY:HA3	1.92	0.52
1:f:152:ILE:HD11	1:g:123:ARG:HH21	1.75	0.52
1:h:79:MET:HE3	1:h:155:LYS:HE3	1.91	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	2.04	0.51
1:h:123:ARG:NH2	1:n:152:ILE:HD11	2.25	0.51
1:B:79:MET:HE1	1:B:106:PHE:CE2	2.45	0.51
1:d:71:PRO:HA	1:d:101:ALA:HB3	1.90	0.51
1:j:124:ILE:HG21	1:j:191:LEU:HD13	1.92	0.51
1:h:109:SER:HB3	1:h:191:LEU:HD23	1.93	0.51
1:k:65:PHE:CE2	2:O:7:MP8:HB	2.46	0.51
1:J:109:SER:HB3	1:J:191:LEU:HD23	1.92	0.51
1:j:109:SER:HB3	1:j:191:LEU:HD23	1.91	0.51
1:l:14:GLN:NE2	1:l:15:SER:HB2	2.26	0.51
1:D:134:GLY:HA3	1:I:134:GLY:HA3	1.93	0.51
1:g:14:GLN:HG2	1:g:19:GLU:HG2	1.93	0.51
1:J:75:VAL:HA	1:J:103:MET:HE3	1.93	0.50
1:N:71:PRO:HA	1:N:101:ALA:HB3	1.92	0.50
1:k:59:ASN:HD22	1:k:62:LYS:HE2	1.76	0.50
1:A:47:LEU:HD11	1:B:9:PRO:HD2	1.93	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	1.91	0.50
1:F:65:PHE:CE2	2:T:7:MP8:HB	2.46	0.50
1:K:8:VAL:HG13	1:K:24:ILE:HG22	1.92	0.50
1:i:97:LEU:H	1:i:97:LEU:HD23	1.77	0.50
1:l:15:SER:OG	1:l:16:GLY:N	2.33	0.50
1:l:28:LEU:CD2	2:1:1:OTT:H6	2.41	0.50
1:m:124:ILE:HG21	1:m:191:LEU:HD13	1.91	0.50
1:m:152:ILE:HD11	1:n:123:ARG:HH21	1.77	0.50
1:b:148:GLU:O	1:b:152:ILE:HG12	2.12	0.50
1:c:28:LEU:HD13	1:c:35:PHE:CE2	2.46	0.50
1:j:62:LYS:HB3	5:j:420:HOH:O	2.11	0.50
1:D:142:ILE:HD11	1:I:131:ILE:HG12	1.92	0.50
1:J:14:GLN:H	1:J:14:GLN:CD	2.19	0.50
1:a:196:LEU:HB3	1:g:87:PHE:HE2	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:131:ILE:HD11	1:m:135:LEU:O	2.11	0.50
1:j:65:PHE:CE2	2:z:7:MP8:HB	2.46	0.50
1:c:65:PHE:CE2	2:s:7:MP8:HB	2.47	0.49
1:h:157:ASN:ND2	1:h:172:GLU:HG2	2.27	0.49
1:h:154:GLU:OE2	1:h:158:ARG:NH1	2.35	0.49
1:m:184:GLU:HA	1:m:195:ILE:HD11	1.94	0.49
1:e:45:ALA:HA	1:e:81:ILE:HD11	1.94	0.49
1:k:14:GLN:NE2	1:k:15:SER:O	2.45	0.49
1:a:152:ILE:HD11	1:b:123:ARG:HH21	1.77	0.49
1:D:65:PHE:CE2	2:R:7:MP8:HB	2.48	0.49
1:M:65:PHE:CE2	2:o:7:MP8:HB	2.46	0.49
1:B:69:ASN:HB2	1:B:97:LEU:HD12	1.95	0.49
1:f:135:LEU:H	1:n:135:LEU:N	1.98	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:L:79:MET:HE1	1:L:106:PHE:CE2	2.47	0.49
1:d:65:PHE:CE2	2:t:7:MP8:HB	2.47	0.49
1:J:65:PHE:CE2	2:X:7:MP8:HB	2.48	0.48
1:b:65:PHE:CE2	2:r:7:MP8:HB	2.48	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	2.29	0.48
1:f:97:LEU:HD12	1:f:97:LEU:O	2.13	0.48
1:m:113:LYS:HE2	1:m:163:HIS:O	2.13	0.48
1:f:131:ILE:HG12	1:n:142:ILE:HD11	1.96	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	1.96	0.48
1:e:65:PHE:CE2	2:u:7:MP8:HB	2.49	0.48
1:G:15:SER:N	1:G:18:GLY:O	2.36	0.47
1:L:17:ARG:HG2	1:L:17:ARG:NH1	2.26	0.47
1:b:116:ARG:O	1:b:192:ILE:HG13	2.14	0.47
1:a:47:LEU:HG	1:a:51:GLN:HE21	1.78	0.47
1:i:184:GLU:HA	1:i:195:ILE:HD11	1.95	0.47
1:G:79:MET:HE1	1:G:106:PHE:CE1	2.49	0.47
1:d:124:ILE:HG21	1:d:191:LEU:HD13	1.97	0.47
1:G:142:ILE:HD11	1:M:131:ILE:HG12	1.96	0.47
1:I:127:HIS:HD2	1:I:128:GLN:O	1.97	0.47
1:c:158:ARG:HE	1:c:158:ARG:HB3	1.45	0.47
1:m:160:MET:HE1	1:m:191:LEU:CD2	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:15:SER:OG	1:N:16:GLY:N	2.48	0.47
1:b:97:LEU:HD12	1:b:97:LEU:O	2.15	0.47
1:j:16:GLY:O	1:j:17:ARG:HB3	2.15	0.47
1:j:20:ARG:HH21	1:k:21:ALA:HB2	1.78	0.47
1:n:156:LEU:HD23	1:n:156:LEU:HA	1.79	0.47
2:O:3:SER:HA	2:O:4:PRO:C	2.39	0.47
1:a:147:ARG:O	1:a:151:LYS:HG3	2.14	0.47
1:I:47:LEU:HD11	1:J:9:PRO:HD2	1.97	0.47
1:a:36:LEU:HD21	1:a:40:VAL:HG22	1.97	0.47
1:f:142:ILE:CD1	1:n:131:ILE:HG12	2.45	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:g:135:LEU:HD23	1:g:142:ILE:HA	1.97	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
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	2.15	0.46
1:g:62:LYS:O	1:g:90:PRO:HB3	2.16	0.46
1:E:97:LEU:HD12	1:E:97:LEU:O	2.15	0.46
1:G:134:GLY:HA3	1:M:134:GLY:HA3	1.96	0.46
1:H:170:ASP:HA	1:H:173:ARG:NH1	2.31	0.46
1:J:28:LEU:CD2	2:X:1:OTT:H6	2.45	0.46
1:g:166:ARG:HD2	1:g:189:TYR:O	2.16	0.46
1:h:65:PHE:CE2	2:x:7:MP8:HB	2.50	0.46
1:h:154:GLU:CD	1:h:158:ARG:HH12	2.21	0.46
1:l:79:MET:HE1	1:l:106:PHE:CE2	2.51	0.46
1:n:61:ASP:OD1	1:n:89:LYS:HE3	2.15	0.46
1:F:97:LEU:HD23	1:F:97:LEU:H	1.80	0.46
1:a:113:LYS:HG3	5:a:423:HOH:O	2.15	0.46
1:d:79:MET:HE1	1:d:106:PHE:CE2	2.51	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
2:o:3:SER:HA	2:o:4:PRO:C	2.41	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	2.51	0.46
2:p:4:PRO:HA	2:p:5:MAA:HA	1.70	0.46
1:A:196:LEU:HB3	1:G:87:PHE:HE2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:PHE:CE2	2:P:7:MP8:HB	2.51	0.45
1:N:75:VAL:HA	1:N:103:MET:HE3	1.97	0.45
1:d:113:LYS:HG3	5:d:432:HOH:O	2.17	0.45
1:k:36:LEU:HD21	1:k:40:VAL:HG22	1.98	0.45
1:m:43:GLU:HG3	5:m:425:HOH:O	2.15	0.45
1:D:71:PRO:HA	1:D:101:ALA:HB3	1.99	0.45
1:I:138:GLN:O	1:I:142:ILE:HD12	2.16	0.45
1:d:125:MET:HE1	1:d:127:HIS:CE1	2.51	0.45
1:B:43:GLU:CD	1:B:43:GLU:H	2.24	0.45
1:a:142:ILE:CD1	1:l:131:ILE:HG12	2.45	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:e:87:PHE:CE1	1:f:196:LEU:HB3	2.51	0.45
1:i:184:GLU:HB2	5:i:423:HOH:O	2.17	0.45
1:B:75:VAL:HA	1:B:103:MET:HE3	1.99	0.45
1:C:191:LEU:HA	1:C:191:LEU:HD12	1.70	0.45
1:c:75:VAL:HG23	5:c:424:HOH:O	2.17	0.45
1:k:97:LEU:HD23	1:k:97:LEU:H	1.82	0.45
2:t:4:PRO:HA	2:t:5:MAA:HA	1.66	0.45
1:G:135:LEU:HB2	1:M:135:LEU:HB2	1.97	0.45
1:J:124:ILE:HG21	1:J:191:LEU:HD13	1.98	0.45
1:g:136:GLY:HA2	1:g:137:GLY:HA2	1.56	0.45
1:m:20:ARG:NH1	1:n:19:GLU:OE1	2.49	0.45
1:C:15:SER:HB2	1:C:17:ARG:H	1.81	0.45
1:K:43:GLU:HB2	5:K:413:HOH:O	2.16	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
1:a:57:SER:CB	2:r:1:OTT:H7	2.47	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:a:97:LEU:HD23	1:a:97:LEU:H	1.81	0.45
1:G:28:LEU:HD22	1:G:33:ILE:HD12	1.99	0.45
1:b:75:VAL:HA	1:b:103:MET:HE3	1.99	0.45
1:c:97:LEU:HD23	1:c:97:LEU:H	1.81	0.45
1:m:63:ASP:OD1	1:m:91:ASP:HB2	2.17	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	1.99	0.45
1:j:87:PHE:CZ	1:k:199:ARG:HA	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:69:ASN:HB2	1:N:97:LEU:CD1	2.45	0.44
1:A:54:PHE:CZ	1:B:11:VAL:HB	2.52	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	2.48	0.44
1:f:47:LEU:O	1:f:51:GLN:HG3	2.16	0.44
2:w:4:PRO:HA	2:w:5:MAA:HA	1.62	0.44
1:L:62:LYS:O	1:L:90:PRO:HB3	2.16	0.44
1:a:6:TYR:CE1	1:g:47:LEU:HD22	2.53	0.44
1:E:65:PHE:CE2	2:S:7:MP8:HB	2.53	0.44
1:K:184:GLU:HA	1:K:195:ILE:HD11	1.99	0.44
1:b:142:ILE:CD1	1:k:131:ILE:HG12	2.47	0.44
1:c:22:PHE:CE1	1:c:27:ARG:HB2	2.53	0.44
1:f:63:ASP:CG	1:f:115:LYS:HZ3	2.23	0.44
1:m:54:PHE:CZ	1:n:11:VAL:HB	2.52	0.44
1:B:131:ILE:N	1:K:137:GLY:O	2.42	0.44
1:I:69:ASN:HB2	1:I:97:LEU:CD1	2.43	0.44
1:a:113:LYS:NZ	1:a:162:LYS:O	2.46	0.44
1:c:156:LEU:O	1:c:160:MET:HB2	2.16	0.44
1:f:56:GLU:HG3	1:f:90:PRO:HD3	2.00	0.44
1:G:75:VAL:HA	1:G:103:MET:HE3	1.99	0.44
1:g:109:SER:HB3	1:g:191:LEU:HD22	2.00	0.44
1:l:75:VAL:HA	1:l:103:MET:HE3	2.00	0.44
2:v:4:PRO:HA	2:v:5:MAA:HA	1.75	0.44
1:a:26:SER:O	1:a:30:LYS:HG2	2.16	0.44
1:a:75:VAL:HA	1:a:103:MET:HE3	2.00	0.44
1:a:196:LEU:HB3	1:g:87:PHE:CE2	2.52	0.44
1:C:97:LEU:HD23	1:C:97:LEU:H	1.82	0.44
2:W:4:PRO:HA	2:W:5:MAA:HA	1.59	0.44
1:A:142:ILE:CD1	1:L:131:ILE:HG12	2.48	0.43
1:G:82:TYR:OH	1:G:163:HIS:NE2	2.42	0.43
1:h:71:PRO:HA	1:h:101:ALA:HB3	2.01	0.43
1:i:131:ILE:CD1	1:i:135:LEU:HD13	2.48	0.43
2:R:4:PRO:HA	2:R:5:MAA:HA	1.71	0.43
1:B:135:LEU:N	1:K:135:LEU:H	2.00	0.43
1:a:131:ILE:HG12	1:l:142:ILE:CD1	2.47	0.43
2:q:4:PRO:HA	2:q:5:MAA:HA	1.63	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:HD11	2.01	0.43
1:e:12:ILE:O	1:e:12:ILE:HG13	2.16	0.43
1:C:149:LEU:HD12	1:C:149:LEU:HA	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:54:PHE:CZ	1:N:11:VAL:HB	2.54	0.43
1:i:95:LEU:HD12	1:i:96:CYS:N	2.34	0.43
1:l:14:GLN:O	1:l:15:SER:HB3	2.18	0.43
1:H:97:LEU:HD23	1:H:97:LEU:H	1.83	0.43
1:a:134:GLY:HA3	1:l:134:GLY:HA3	1.99	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:a:57:SER:HB3	2:r:1:OTT:H7	2.00	0.43
1:k:127:HIS:HD2	1:k:178:ASP:OD1	2.02	0.43
1:n:117:PHE:CD1	1:n:194:GLN:HB2	2.53	0.43
1:E:135:LEU:HD21	1:H:135:LEU:HD12	2.01	0.43
1:K:75:VAL:HA	1:K:103:MET:HE3	2.01	0.43
2:z:4:PRO:HA	2:z:5:MAA:HA	1.72	0.43
1:B:69:ASN:HD22	1:B:69:ASN:C	2.27	0.43
1:M:28:LEU:HD12	1:M:35:PHE:HE2	1.84	0.43
1:e:79:MET:HE1	1:e:106:PHE:CE2	2.53	0.43
1:l:120:PRO:HD3	1:l:196:LEU:O	2.19	0.43
2:x:6:ALA:H	2:x:7:MP8:C	2.32	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:F:75:VAL:HA	1:F:103:MET:HE3	2.00	0.43
1:K:136:GLY:HA2	1:K:137:GLY:HA2	1.72	0.43
1:b:22:PHE:HE1	1:b:27:ARG:CA	2.31	0.43
1:c:123:ARG:HD3	1:c:180:PHE:HD1	1.84	0.43
1:c:142:ILE:CD1	1:j:131:ILE:HG12	2.47	0.43
2:T:4:PRO:HA	2:T:5:MAA:HA	1.70	0.43
1:a:16:GLY:O	1:a:17:ARG:HB2	2.18	0.42
1:h:17:ARG:HD3	1:i:19:GLU:OE2	2.19	0.42
1:h:47:LEU:HD11	1:i:9:PRO:HD2	2.00	0.42
2:W:3:SER:HA	2:W:4:PRO:C	2.42	0.42
1:B:54:PHE:HA	2:Q:1:OTT:H7	2.00	0.42
1:I:41:THR:H	1:I:44:SER:HG	1.65	0.42
1:f:168:LEU:HG	1:f:172:GLU:OE2	2.19	0.42
1:j:16:GLY:C	1:j:18:GLY:H	2.27	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	2.02	0.42
1:G:136:GLY:HA2	1:G:137:GLY:HA2	1.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:120:PRO:HD3	1:e:196:LEU:O	2.18	0.42
2:P:4:PRO:HA	2:P:5:MAA:HA	1.67	0.42
2:u:4:PRO:HA	2:u:5:MAA:HA	1.68	0.42
1:n:130:LEU:HD12	1:n:130:LEU:O	2.20	0.42
1:K:100:ALA:O	1:K:105:ALA:HB2	2.19	0.42
1:f:79:MET:HE1	1:f:106:PHE:CE2	2.54	0.42
1:l:198:ASN:OD1	1:l:198:ASN:N	2.52	0.42
2:S:4:PRO:HA	2:S:5:MAA:HA	1.74	0.42
1:A:18:GLY:O	1:A:19:GLU:HB2	2.19	0.42
1:I:8:VAL:HG21	1:J:7:LEU:HD12	2.02	0.42
1:a:30:LYS:HE3	1:b:12:ILE:HG12	2.02	0.42
1:d:152:ILE:HD11	1:e:123:ARG:NH2	2.32	0.42
1:D:28:LEU:HD22	1:D:33:ILE:HD12	2.02	0.42
1:e:62:LYS:O	1:e:90:PRO:HB3	2.20	0.42
1:M:45:ALA:HA	1:M:81:ILE:HD11	2.01	0.42
1:e:8:VAL:HG12	1:e:24:ILE:HG22	2.00	0.42
1:l:97:LEU:HD12	1:l:97:LEU:O	2.20	0.42
1:n:160:MET:HB3	1:n:171:LEU:HD23	2.01	0.42
2:Y:3:SER:HA	2:Y:4:PRO:C	2.45	0.42
1:b:155:LYS:HE2	1:c:121:ASN:OD1	2.19	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
1:M:75:VAL:HA	1:M:103:MET:HE3	2.01	0.41
1:c:22:PHE:CD1	1:c:27:ARG:HB2	2.56	0.41
1:i:79:MET:HE1	1:i:106:PHE:CE2	2.55	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	1.56	0.41
1:I:102:SER:OG	1:I:127:HIS:CE1	2.73	0.41
1:N:127:HIS:ND1	1:N:178:ASP:OD1	2.33	0.41
1:b:12:ILE:HA	1:b:20:ARG:O	2.20	0.41
1:g:134:GLY:HA3	1:m:134:GLY:HA3	2.01	0.41
1:i:16:GLY:C	1:i:17:ARG:HG3	2.45	0.41
1:k:45:ALA:HA	1:k:81:ILE:HD11	2.02	0.41
2:x:4:PRO:HA	2:x:5:MAA:HA	1.64	0.41
1:E:135:LEU:HD12	1:E:135:LEU:O	2.20	0.41
1:J:63:ASP:OD1	1:J:91:ASP:HB2	2.21	0.41
1:b:69:ASN:HB2	1:b:97:LEU:CD1	2.45	0.41
5:A:432:HOH:O	1:B:37:VAL:HG13	2.20	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:b:79:MET:HE1	1:b:106:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:173:ARG:HD2	1:b:174:ASP:OD1	2.20	0.41
1:d:8:VAL:HG11	1:d:23:ASP:HB2	2.02	0.41
1:K:16:GLY:C	1:K:17:ARG:HG3	2.46	0.41
1:L:102:SER:OG	1:L:127:HIS:NE2	2.39	0.41
1:L:135:LEU:HD23	1:L:135:LEU:HA	1.86	0.41
1:c:95:LEU:C	1:c:95:LEU:HD13	2.45	0.41
1:d:54:PHE:HA	2:u:1:OTT:H7	2.02	0.41
1:m:156:LEU:HD23	1:m:156:LEU:HA	1.89	0.41
1:n:107:LEU:HD23	1:n:107:LEU:HA	1.89	0.41
1:A:79:MET:HE1	1:A:106:PHE:CE2	2.56	0.41
1:G:131:ILE:HD11	1:M:135:LEU:O	2.21	0.41
1:h:19:GLU:OE1	1:n:20:ARG:NH1	2.53	0.41
1:g:65:PHE:CE2	2:w:7:MP8:HB	2.55	0.41
1:n:160:MET:HB3	1:n:171:LEU:CD2	2.51	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:HD12	1:N:97:LEU:O	2.20	0.41
1:a:14:GLN:HG3	1:a:17:ARG:CD	2.50	0.41
1:b:160:MET:HE3	1:b:191:LEU:CD1	2.47	0.41
1:d:184:GLU:HA	1:d:195:ILE:HD11	2.02	0.41
1:f:43:GLU:H	1:f:43:GLU:CD	2.29	0.41
1:j:47:LEU:HD11	1:k:9:PRO:HD2	2.02	0.41
1:k:114:GLY:H	1:k:193:ASP:CG	2.28	0.41
2:X:4:PRO:HA	2:X:5:MAA:HA	1.77	0.41
1:K:60:PRO:HB2	1:K:89:LYS:HD3	2.03	0.41
1:m:65:PHE:CE2	2:2:7:MP8:HB	2.55	0.41
1:A:97:LEU:H	1:A:97:LEU:HD23	1.85	0.40
1:G:59:ASN:CG	1:G:62:LYS:HE2	2.47	0.40
1:H:56:GLU:HG3	1:H:90:PRO:HD3	2.02	0.40
1:J:17:ARG:O	1:J:17:ARG:HG2	2.21	0.40
1:J:164:CYS:HA	1:J:190:GLY:O	2.21	0.40
1:M:13:GLU:OE2	1:M:30:LYS:NZ	2.30	0.40
1:M:136:GLY:HA2	1:M:137:GLY:HA2	1.69	0.40
1:h:155:LYS:NZ	5:h:401:HOH:O	2.26	0.40
1:j:15:SER:OG	1:j:16:GLY:N	2.54	0.40
1:c:196:LEU:HD22	2:s:5:MAA:HM1	2.03	0.40
1:f:69:ASN:HB2	1:f:97:LEU:CD1	2.49	0.40
1:g:79:MET:HE1	1:g:106:PHE:CE1	2.56	0.40
1:m:13:GLU:OE2	1:m:30:LYS:NZ	2.47	0.40
1:G:63:ASP:OD2	1:G:115:LYS:NZ	2.50	0.40
1:I:27:ARG:HH12	1:I:30:LYS:HB2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:125:MET:SD	1:I:127:HIS:ND1	2.79	0.40
1:f:83:ASP:OD1	1:g:121:ASN:ND2	2.38	0.40
1:f:118:ALA:HB1	1:f:122:SER:OG	2.22	0.40
1:h:79:MET:HE2	1:h:156:LEU:HD21	2.04	0.40
1:F:60:PRO:HB2	1:F:89:LYS:HD3	2.04	0.40
1:G:17:ARG:HH11	1:G:17:ARG:HD3	1.77	0.40
1:K:97:LEU:HD23	1:K:97:LEU:H	1.85	0.40
1:g:159:LEU:HD23	1:g:159:LEU:HA	1.93	0.40
2:Q:4:PRO:HA	2:Q:5:MAA:HA	1.81	0.40
1:D:14:GLN:HG2	1:D:15:SER:N	2.35	0.40
1:I:114:GLY:N	1:I:193:ASP:OD2	2.53	0.40
1:e:13:GLU:O	1:e:19:GLU:HA	2.21	0.40
1:j:20:ARG:NH2	1:k:21:ALA:HB2	2.36	0.40
2:r:4:PRO:HA	2:r:5:MAA:HA	1.69	0.40
2:0:4:PRO:HA	2:0:5:MAA:HA	1.60	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%)	11	16
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%)	24	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	190/206 (92%)	184 (97%)	4 (2%)	2 (1%)	11	16
1	F	189/206 (92%)	181 (96%)	7 (4%)	1 (0%)	24	34
1	G	191/206 (93%)	184 (96%)	7 (4%)	0	100	100
1	H	189/206 (92%)	182 (96%)	4 (2%)	3 (2%)	7	9
1	I	189/206 (92%)	184 (97%)	5 (3%)	0	100	100
1	J	191/206 (93%)	184 (96%)	5 (3%)	2 (1%)	12	17
1	K	191/206 (93%)	182 (95%)	8 (4%)	1 (0%)	24	34
1	L	191/206 (93%)	184 (96%)	7 (4%)	0	100	100
1	M	189/206 (92%)	183 (97%)	5 (3%)	1 (0%)	24	34
1	N	191/206 (93%)	184 (96%)	5 (3%)	2 (1%)	12	17
1	a	189/206 (92%)	183 (97%)	5 (3%)	1 (0%)	24	34
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%)	11	16
1	f	179/206 (87%)	176 (98%)	3 (2%)	0	100	100
1	g	190/206 (92%)	180 (95%)	9 (5%)	1 (0%)	24	34
1	h	189/206 (92%)	185 (98%)	4 (2%)	0	100	100
1	i	189/206 (92%)	183 (97%)	4 (2%)	2 (1%)	11	16
1	j	189/206 (92%)	181 (96%)	7 (4%)	1 (0%)	24	34
1	k	192/206 (93%)	188 (98%)	4 (2%)	0	100	100
1	l	191/206 (93%)	185 (97%)	4 (2%)	2 (1%)	12	17
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
2	P	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	Q	3/7 (43%)	2 (67%)	1 (33%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	24	34

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
1	l	15	SER
1	H	15	SER
1	H	16	GLY
1	M	16	GLY

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Mol	Chain	Res	Type
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%)	155 (97%)	5 (3%)	35	54
1	B	159/174 (91%)	157 (99%)	2 (1%)	61	78
1	C	161/174 (92%)	156 (97%)	5 (3%)	35	54
1	D	161/174 (92%)	158 (98%)	3 (2%)	50	69
1	E	162/174 (93%)	159 (98%)	3 (2%)	50	69
1	F	161/174 (92%)	156 (97%)	5 (3%)	35	54
1	G	163/174 (94%)	158 (97%)	5 (3%)	35	54
1	H	161/174 (92%)	157 (98%)	4 (2%)	42	61
1	I	161/174 (92%)	155 (96%)	6 (4%)	30	47
1	J	163/174 (94%)	158 (97%)	5 (3%)	35	54
1	K	163/174 (94%)	159 (98%)	4 (2%)	42	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	163/174 (94%)	161 (99%)	2 (1%)	63	79
1	M	161/174 (92%)	160 (99%)	1 (1%)	78	88
1	N	163/174 (94%)	160 (98%)	3 (2%)	51	71
1	a	161/174 (92%)	157 (98%)	4 (2%)	42	61
1	b	160/174 (92%)	158 (99%)	2 (1%)	61	78
1	c	150/174 (86%)	149 (99%)	1 (1%)	76	87
1	d	156/174 (90%)	153 (98%)	3 (2%)	50	69
1	e	161/174 (92%)	157 (98%)	4 (2%)	42	61
1	f	155/174 (89%)	153 (99%)	2 (1%)	61	78
1	g	162/174 (93%)	160 (99%)	2 (1%)	63	79
1	h	161/174 (92%)	158 (98%)	3 (2%)	50	69
1	i	161/174 (92%)	159 (99%)	2 (1%)	63	79
1	j	161/174 (92%)	157 (98%)	4 (2%)	42	61
1	k	164/174 (94%)	160 (98%)	4 (2%)	43	63
1	l	163/174 (94%)	160 (98%)	3 (2%)	51	71
1	m	160/174 (92%)	158 (99%)	2 (1%)	61	78
1	n	162/174 (93%)	160 (99%)	2 (1%)	63	79
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	4489 (98%)	94 (2%)	47	67

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	97	LEU
1	A	124	ILE
1	A	158	ARG
1	A	191	LEU
1	B	69	ASN
1	B	124	ILE
1	C	11	VAL
1	C	89	LYS
1	C	124	ILE
1	C	130	LEU
1	C	150	LEU
1	D	124	ILE
1	D	156	LEU
1	D	191	LEU
1	E	17	ARG
1	E	135	LEU
1	E	191	LEU

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Mol	Chain	Res	Type
1	F	20	ARG
1	F	119	LEU
1	F	124	ILE
1	F	142	ILE
1	F	168	LEU
1	G	7	LEU
1	G	14	GLN
1	G	17	ARG
1	G	19	GLU
1	G	191	LEU
1	H	11	VAL
1	H	17	ARG
1	H	19	GLU
1	H	191	LEU
1	I	11	VAL
1	I	15	SER
1	I	124	ILE
1	I	135	LEU
1	I	142	ILE
1	I	197	GLU
1	J	7	LEU
1	J	11	VAL
1	J	43	GLU
1	J	97	LEU
1	J	197	GLU
1	K	13	GLU
1	K	97	LEU
1	K	155	LYS
1	K	197	GLU
1	L	142	ILE
1	L	191	LEU
1	M	43	GLU
1	N	124	ILE
1	N	191	LEU
1	N	197	GLU
1	a	11	VAL
1	a	12	ILE
1	a	14	GLN
1	a	162	LYS
1	b	155	LYS
1	b	197	GLU
1	c	158	ARG

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Mol	Chain	Res	Type
1	d	11	VAL
1	d	12	ILE
1	d	162	LYS
1	e	8	VAL
1	e	11	VAL
1	e	12	ILE
1	e	124	ILE
1	f	12	ILE
1	f	43	GLU
1	g	17	ARG
1	g	198	ASN
1	h	11	VAL
1	h	14	GLN
1	h	124	ILE
1	i	14	GLN
1	i	184	GLU
1	j	11	VAL
1	j	19	GLU
1	j	124	ILE
1	j	197	GLU
1	k	14	GLN
1	k	97	LEU
1	k	124	ILE
1	k	191	LEU
1	l	124	ILE
1	l	127	HIS
1	l	191	LEU
1	m	11	VAL
1	m	17	ARG
1	n	97	LEU
1	n	124	ILE
2	P	4	PRO
2	r	4	PRO
2	t	4	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	ASN
1	B	51	GLN
1	G	194	GLN
1	J	14	GLN

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Mol	Chain	Res	Type
1	M	127	HIS
1	M	145	HIS
1	N	157	ASN
1	a	46	ASN
1	c	46	ASN
1	c	194	GLN
1	e	99	GLN
1	f	51	GLN
1	g	51	GLN
1	j	121	ASN

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	MP8	U	7	2	6,8,9	1.18	0	3,10,12	2.09	1 (33%)
2	MP8	z	7	2	6,8,9	0.86	0	3,10,12	1.67	1 (33%)
2	MP8	Q	7	2	6,8,9	1.09	1 (16%)	3,10,12	1.63	1 (33%)
2	MAA	Z	5	2	4,5,6	0.66	0	2,5,7	0.84	0
2	MAA	V	5	2	4,5,6	0.79	0	2,5,7	0.86	0
2	MP8	y	7	2	6,8,9	0.89	0	3,10,12	2.06	2 (66%)
2	MAA	2	5	2	4,5,6	0.60	0	2,5,7	1.14	0
2	MAA	3	5	2	4,5,6	0.88	0	2,5,7	0.75	0
2	MAA	o	5	2	4,5,6	0.55	0	2,5,7	0.89	0
2	MP8	3	7	2	6,8,9	0.61	0	3,10,12	1.56	0
2	MAA	r	5	2	4,5,6	0.70	0	2,5,7	0.86	0
2	MP8	1	7	2	6,8,9	1.12	1 (16%)	3,10,12	1.95	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAA	R	5	2	4,5,6	0.87	0	2,5,7	1.02	0
2	MP8	Z	7	2	6,8,9	0.91	0	3,10,12	1.85	1 (33%)
2	MP8	v	7	2	6,8,9	0.85	0	3,10,12	1.88	1 (33%)
2	MP8	V	7	2	6,8,9	0.93	0	3,10,12	1.43	0
2	MP8	2	7	2	6,8,9	0.74	0	3,10,12	1.99	1 (33%)
2	MP8	X	7	2	6,8,9	0.68	0	3,10,12	1.70	1 (33%)
2	MAA	W	5	2	4,5,6	1.11	0	2,5,7	0.71	0
2	MP8	S	7	2	6,8,9	0.83	0	3,10,12	1.55	0
2	MP8	w	7	2	6,8,9	0.94	0	3,10,12	2.18	2 (66%)
2	MP8	x	7	2	6,8,9	0.56	0	3,10,12	1.91	1 (33%)
2	MP8	R	7	2	6,8,9	0.69	0	3,10,12	1.77	1 (33%)
2	MAA	Q	5	2	4,5,6	0.98	0	2,5,7	0.49	0
2	MP8	Y	7	2	6,8,9	0.68	0	3,10,12	2.21	1 (33%)
2	MP8	r	7	2	6,8,9	0.69	0	3,10,12	1.77	1 (33%)
2	MP8	T	7	2	6,8,9	0.66	0	3,10,12	1.89	1 (33%)
2	MAA	z	5	2	4,5,6	0.84	0	2,5,7	0.76	0
2	MP8	s	7	2	6,8,9	0.67	0	3,10,12	1.55	0
2	MP8	t	7	2	6,8,9	0.80	0	3,10,12	1.60	1 (33%)
2	MP8	O	7	2	6,8,9	0.83	0	3,10,12	1.88	1 (33%)
2	MAA	u	5	2	4,5,6	0.75	0	2,5,7	0.97	0
2	MP8	W	7	2	6,8,9	1.05	0	3,10,12	2.01	1 (33%)
2	MAA	p	5	2	4,5,6	0.79	0	2,5,7	1.31	0
2	MAA	q	5	2	4,5,6	0.78	0	2,5,7	1.05	0
2	MAA	y	5	2	4,5,6	0.71	0	2,5,7	0.88	0
2	MAA	X	5	2	4,5,6	0.89	0	2,5,7	0.78	0
2	MAA	S	5	2	4,5,6	0.67	0	2,5,7	0.89	0
2	MAA	v	5	2	4,5,6	0.72	0	2,5,7	1.26	0
2	MAA	w	5	2	4,5,6	0.81	0	2,5,7	1.04	0
2	MAA	0	5	2	4,5,6	0.71	0	2,5,7	1.13	0
2	MAA	P	5	2	4,5,6	0.90	0	2,5,7	0.84	0
2	MP8	0	7	2	6,8,9	1.32	1 (16%)	3,10,12	2.21	1 (33%)
2	MAA	T	5	2	4,5,6	0.66	0	2,5,7	1.20	0
2	MAA	Y	5	2	4,5,6	0.98	0	2,5,7	0.74	0
2	MAA	x	5	2	4,5,6	0.86	0	2,5,7	1.20	0
2	MAA	s	5	2	4,5,6	0.77	0	2,5,7	0.66	0
2	MP8	u	7	2	6,8,9	0.86	0	3,10,12	1.83	1 (33%)
2	MP8	p	7	2	6,8,9	0.83	0	3,10,12	2.38	1 (33%)
2	MAA	1	5	2	4,5,6	0.96	0	2,5,7	0.96	0
2	MP8	o	7	2	6,8,9	0.94	0	3,10,12	2.18	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MP8	q	7	2	6,8,9	0.68	0	3,10,12	2.36	2 (66%)
2	MAA	t	5	2	4,5,6	0.50	0	2,5,7	1.32	0
2	MAA	U	5	2	4,5,6	0.75	0	2,5,7	0.95	0
2	MP8	P	7	2	6,8,9	0.74	0	3,10,12	1.78	1 (33%)
2	MAA	O	5	2	4,5,6	0.89	0	2,5,7	0.72	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	MP8	U	7	2	-	0/0/11/13	0/1/1/1
2	MP8	z	7	2	-	0/0/11/13	0/1/1/1
2	MP8	Q	7	2	-	0/0/11/13	0/1/1/1
2	MAA	Z	5	2	-	0/2/4/6	-
2	MAA	V	5	2	-	0/2/4/6	-
2	MP8	y	7	2	-	0/0/11/13	0/1/1/1
2	MAA	2	5	2	-	0/2/4/6	-
2	MAA	3	5	2	-	0/2/4/6	-
2	MAA	o	5	2	-	0/2/4/6	-
2	MP8	3	7	2	-	0/0/11/13	0/1/1/1
2	MAA	r	5	2	-	0/2/4/6	-
2	MP8	1	7	2	-	0/0/11/13	0/1/1/1
2	MAA	R	5	2	-	0/2/4/6	-
2	MP8	Z	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	V	7	2	-	0/0/11/13	0/1/1/1
2	MP8	2	7	2	-	0/0/11/13	0/1/1/1
2	MP8	X	7	2	-	0/0/11/13	0/1/1/1
2	MAA	W	5	2	-	0/2/4/6	-
2	MP8	S	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	x	7	2	-	0/0/11/13	0/1/1/1
2	MP8	R	7	2	-	0/0/11/13	0/1/1/1
2	MAA	Q	5	2	-	0/2/4/6	-
2	MP8	Y	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	T	7	2	-	0/0/11/13	0/1/1/1
2	MAA	z	5	2	-	0/2/4/6	-
2	MP8	s	7	2	-	0/0/11/13	0/1/1/1
2	MP8	t	7	2	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MP8	O	7	2	-	0/0/11/13	0/1/1/1
2	MAA	u	5	2	-	0/2/4/6	-
2	MP8	W	7	2	-	0/0/11/13	0/1/1/1
2	MAA	p	5	2	-	0/2/4/6	-
2	MAA	q	5	2	-	0/2/4/6	-
2	MAA	y	5	2	-	0/2/4/6	-
2	MAA	X	5	2	-	0/2/4/6	-
2	MAA	S	5	2	-	0/2/4/6	-
2	MAA	v	5	2	-	0/2/4/6	-
2	MAA	w	5	2	-	0/2/4/6	-
2	MAA	0	5	2	-	0/2/4/6	-
2	MAA	P	5	2	-	0/2/4/6	-
2	MP8	0	7	2	-	0/0/11/13	0/1/1/1
2	MAA	T	5	2	-	0/2/4/6	-
2	MAA	Y	5	2	-	0/2/4/6	-
2	MAA	x	5	2	-	0/2/4/6	-
2	MAA	s	5	2	-	0/2/4/6	-
2	MP8	u	7	2	-	0/0/11/13	0/1/1/1
2	MP8	p	7	2	-	0/0/11/13	0/1/1/1
2	MAA	1	5	2	-	0/2/4/6	-
2	MP8	o	7	2	-	0/0/11/13	0/1/1/1
2	MP8	q	7	2	-	0/0/11/13	0/1/1/1
2	MAA	t	5	2	-	1/2/4/6	-
2	MAA	U	5	2	-	0/2/4/6	-
2	MP8	P	7	2	-	0/0/11/13	0/1/1/1
2	MAA	O	5	2	-	0/2/4/6	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	0	7	MP8	CA-N	2.56	1.53	1.48
2	1	7	MP8	CA-N	2.33	1.52	1.48
2	Q	7	MP8	CA-N	2.06	1.52	1.48

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	0	7	MP8	CG-CD-N	-3.46	102.48	106.65
2	p	7	MP8	CG-CD-N	-3.46	102.49	106.65
2	q	7	MP8	CG-CD-N	-3.43	102.53	106.65
2	o	7	MP8	CG-CD-N	-3.24	102.75	106.65
2	Y	7	MP8	CG-CD-N	-3.06	102.97	106.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	w	7	MP8	CG-CD-N	-2.98	103.06	106.65
2	2	7	MP8	CG-CD-N	-2.94	103.11	106.65
2	W	7	MP8	CG-CD-N	-2.89	103.17	106.65
2	U	7	MP8	CG-CD-N	-2.79	103.29	106.65
2	T	7	MP8	CG-CD-N	-2.76	103.33	106.65
2	1	7	MP8	CG-CD-N	-2.76	103.33	106.65
2	O	7	MP8	CG-CD-N	-2.73	103.37	106.65
2	u	7	MP8	CG-CD-N	-2.65	103.46	106.65
2	v	7	MP8	CG-CD-N	-2.62	103.49	106.65
2	y	7	MP8	CG-CD-N	-2.61	103.51	106.65
2	r	7	MP8	CG-CD-N	-2.49	103.65	106.65
2	x	7	MP8	CG-CD-N	-2.35	103.82	106.65
2	y	7	MP8	O-C-CA	-2.29	118.89	124.77
2	t	7	MP8	CG-CD-N	-2.25	103.94	106.65
2	P	7	MP8	CG-CD-N	-2.20	104.00	106.65
2	q	7	MP8	O-C-CA	-2.14	119.26	124.77
2	X	7	MP8	CG-CD-N	-2.14	104.08	106.65
2	Q	7	MP8	O-C-CA	-2.10	119.37	124.77
2	w	7	MP8	O-C-CA	-2.08	119.42	124.77
2	Z	7	MP8	O-C-CA	-2.07	119.44	124.77
2	R	7	MP8	CG-CD-N	-2.03	104.21	106.65
2	z	7	MP8	CG-CD-N	-2.01	104.23	106.65

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.

45 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	U	7	MP8	1	0
2	z	7	MP8	1	0
2	V	5	MAA	1	0
2	y	7	MP8	1	0
2	3	5	MAA	1	0
2	3	7	MP8	1	0
2	r	5	MAA	1	0
2	R	5	MAA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Z	7	MP8	1	0
2	V	7	MP8	1	0
2	2	7	MP8	1	0
2	X	7	MP8	1	0
2	W	5	MAA	1	0
2	S	7	MP8	1	0
2	w	7	MP8	1	0
2	x	7	MP8	2	0
2	R	7	MP8	1	0
2	Q	5	MAA	1	0
2	Y	7	MP8	1	0
2	r	7	MP8	1	0
2	T	7	MP8	1	0
2	z	5	MAA	1	0
2	s	7	MP8	1	0
2	t	7	MP8	1	0
2	u	5	MAA	1	0
2	W	7	MP8	1	0
2	p	5	MAA	1	0
2	q	5	MAA	1	0
2	y	5	MAA	1	0
2	X	5	MAA	1	0
2	S	5	MAA	1	0
2	v	5	MAA	1	0
2	w	5	MAA	1	0
2	0	5	MAA	1	0
2	P	5	MAA	1	0
2	0	7	MP8	1	0
2	T	5	MAA	1	0
2	x	5	MAA	1	0
2	s	5	MAA	1	0
2	u	7	MP8	1	0
2	o	7	MP8	1	0
2	q	7	MP8	1	0
2	t	5	MAA	1	0
2	P	7	MP8	1	0
2	O	5	MAA	1	0

5.5 Carbohydrates

There are no oligosaccharides 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, 95th 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 ²)	Q<0.9
1	A	190/206 (92%)	-0.12	10 (5%)	32 31	14, 20, 58, 87	0
1	B	187/206 (90%)	-0.04	8 (4%)	40 39	13, 20, 46, 85	0
1	C	191/206 (92%)	-0.01	12 (6%)	26 25	14, 20, 66, 96	0
1	D	191/206 (92%)	-0.14	11 (5%)	29 28	13, 20, 63, 93	0
1	E	192/206 (93%)	0.02	11 (5%)	29 28	13, 21, 60, 91	0
1	F	191/206 (92%)	0.02	14 (7%)	21 20	14, 21, 73, 105	0
1	G	193/206 (93%)	0.11	13 (6%)	24 22	14, 21, 68, 98	0
1	H	191/206 (92%)	0.03	12 (6%)	26 25	14, 22, 61, 90	0
1	I	191/206 (92%)	0.02	11 (5%)	29 28	14, 21, 59, 90	0
1	J	193/206 (93%)	0.06	12 (6%)	26 25	15, 22, 66, 103	0
1	K	193/206 (93%)	0.01	15 (7%)	19 17	12, 21, 69, 102	0
1	L	193/206 (93%)	0.06	14 (7%)	21 20	14, 21, 65, 111	0
1	M	191/206 (92%)	-0.12	10 (5%)	33 32	14, 20, 62, 103	0
1	N	193/206 (93%)	0.11	11 (5%)	29 28	14, 21, 61, 99	0
1	a	191/206 (92%)	0.16	16 (8%)	17 15	15, 22, 75, 117	0
1	b	188/206 (91%)	0.06	13 (6%)	23 21	14, 22, 64, 107	0
1	c	177/206 (85%)	-0.10	9 (5%)	33 33	14, 20, 41, 86	0
1	d	184/206 (89%)	-0.06	10 (5%)	31 31	14, 20, 52, 90	0
1	e	191/206 (92%)	0.19	20 (10%)	11 10	13, 22, 72, 108	0
1	f	183/206 (88%)	0.08	15 (8%)	17 16	16, 22, 64, 88	0
1	g	192/206 (93%)	0.13	19 (9%)	13 11	15, 22, 75, 120	0
1	h	191/206 (92%)	-0.02	10 (5%)	33 32	15, 21, 57, 88	0
1	i	191/206 (92%)	0.02	11 (5%)	29 28	14, 21, 57, 103	0
1	j	191/206 (92%)	-0.07	13 (6%)	23 22	14, 21, 68, 97	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	k	194/206 (94%)	0.06	12 (6%)	26	25	14, 21, 68, 105	0
1	l	193/206 (93%)	0.02	10 (5%)	33	32	14, 22, 64, 91	0
1	m	190/206 (92%)	-0.10	6 (3%)	50	50	13, 21, 52, 90	0
1	n	192/206 (93%)	0.08	11 (5%)	29	28	15, 22, 63, 102	0
2	0	4/7 (57%)	0.13	0	100	100	21, 26, 27, 34	0
2	1	4/7 (57%)	-0.30	0	100	100	22, 26, 27, 30	0
2	2	4/7 (57%)	0.29	0	100	100	27, 28, 28, 30	0
2	3	4/7 (57%)	-0.41	0	100	100	25, 27, 29, 32	0
2	O	4/7 (57%)	-0.26	0	100	100	21, 23, 27, 28	0
2	P	4/7 (57%)	-0.14	0	100	100	19, 21, 27, 28	0
2	Q	4/7 (57%)	-0.56	0	100	100	19, 23, 23, 23	0
2	R	4/7 (57%)	-0.38	0	100	100	18, 22, 26, 28	0
2	S	4/7 (57%)	-0.58	0	100	100	21, 22, 25, 27	0
2	T	4/7 (57%)	0.13	0	100	100	24, 26, 27, 31	0
2	U	4/7 (57%)	-0.35	0	100	100	26, 27, 27, 33	0
2	V	4/7 (57%)	-0.39	0	100	100	24, 24, 34, 34	0
2	W	4/7 (57%)	0.50	0	100	100	24, 29, 30, 33	0
2	X	4/7 (57%)	-0.25	0	100	100	23, 26, 26, 30	0
2	Y	4/7 (57%)	0.77	1 (25%)	2	1	23, 29, 31, 41	0
2	Z	4/7 (57%)	-0.70	0	100	100	17, 20, 23, 24	0
2	o	4/7 (57%)	-0.15	0	100	100	22, 24, 24, 30	0
2	p	4/7 (57%)	-0.24	0	100	100	21, 23, 28, 30	0
2	q	4/7 (57%)	0.20	0	100	100	24, 33, 35, 36	0
2	r	4/7 (57%)	0.29	0	100	100	27, 28, 30, 36	0
2	s	4/7 (57%)	-0.44	0	100	100	24, 26, 26, 28	0
2	t	4/7 (57%)	0.09	0	100	100	23, 24, 25, 30	0
2	u	4/7 (57%)	0.05	0	100	100	19, 31, 32, 34	0
2	v	4/7 (57%)	-0.12	0	100	100	24, 30, 33, 44	0
2	w	4/7 (57%)	0.56	0	100	100	23, 32, 35, 37	0
2	x	4/7 (57%)	0.33	0	100	100	28, 28, 31, 32	0
2	y	4/7 (57%)	-0.10	0	100	100	24, 25, 26, 27	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
2	z	4/7 (57%)	0.05	0	100	100	24, 27, 27, 28	0
All	All	5440/5964 (91%)	0.01	340 (6%)	26	25	12, 21, 64, 120	0

All (340) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	i	16	GLY	8.2
1	C	133	GLY	7.4
1	n	16	GLY	7.3
1	C	134	GLY	6.3
1	J	134	GLY	6.1
1	i	15	SER	6.0
1	I	14	GLN	6.0
1	j	8	VAL	5.9
1	K	133	GLY	5.8
1	d	21	ALA	5.7
1	c	22	PHE	5.7
1	N	18	GLY	5.6
1	k	198	ASN	5.6
1	D	134	GLY	5.6
1	I	133	GLY	5.4
1	f	133	GLY	5.4
1	H	133	GLY	5.4
1	d	7	LEU	5.2
1	n	133	GLY	5.2
1	H	16	GLY	5.1
1	N	6	TYR	5.0
1	L	17	ARG	5.0
1	a	16	GLY	5.0
1	l	17	ARG	5.0
1	n	132	SER	5.0
1	j	198	ASN	5.0
1	H	15	SER	4.9
1	J	136	GLY	4.9
1	e	133	GLY	4.9
1	f	134	GLY	4.9
1	l	133	GLY	4.9
1	J	135	LEU	4.9
1	F	133	GLY	4.9
1	B	132	SER	4.8
1	C	18	GLY	4.8
1	F	134	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
1	a	12	ILE	4.8
1	H	134	GLY	4.8
1	k	133	GLY	4.7
1	J	16	GLY	4.7
1	G	15	SER	4.7
1	i	18	GLY	4.6
1	C	8	VAL	4.6
1	K	18	GLY	4.6
1	M	133	GLY	4.6
1	b	13	GLU	4.6
1	E	135	LEU	4.6
1	G	16	GLY	4.5
1	J	18	GLY	4.5
1	F	135	LEU	4.5
1	H	135	LEU	4.5
1	a	6	TYR	4.4
1	M	18	GLY	4.4
1	c	133	GLY	4.4
1	m	134	GLY	4.4
1	J	133	GLY	4.4
1	L	16	GLY	4.4
1	d	133	GLY	4.4
1	c	198	ASN	4.4
1	b	133	GLY	4.3
1	f	12	ILE	4.3
1	h	134	GLY	4.3
1	n	134	GLY	4.3
1	a	18	GLY	4.3
1	k	134	GLY	4.2
1	F	17	ARG	4.2
1	E	134	GLY	4.2
1	G	14	GLN	4.2
1	a	133	GLY	4.1
1	L	18	GLY	4.1
1	C	17	ARG	4.1
1	A	18	GLY	4.0
1	N	16	GLY	4.0
1	F	132	SER	4.0
1	K	15	SER	4.0
1	e	16	GLY	4.0
1	I	134	GLY	4.0
1	b	22	PHE	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	15	SER	4.0
1	G	12	ILE	3.9
1	H	17	ARG	3.9
1	i	17	ARG	3.9
1	h	14	GLN	3.9
1	E	130	LEU	3.9
1	G	17	ARG	3.9
1	a	15	SER	3.9
1	F	14	GLN	3.9
1	K	17	ARG	3.9
1	e	197	GLU	3.8
1	K	16	GLY	3.8
1	g	16	GLY	3.8
1	b	20	ARG	3.8
1	d	20	ARG	3.8
1	g	198	ASN	3.8
1	E	16	GLY	3.8
1	b	134	GLY	3.8
1	A	136	GLY	3.8
1	L	133	GLY	3.8
1	J	198	ASN	3.7
1	a	132	SER	3.7
1	b	15	SER	3.7
1	F	18	GLY	3.7
1	j	197	GLU	3.7
1	l	14	GLN	3.7
1	D	133	GLY	3.7
1	F	136	GLY	3.7
1	K	14	GLN	3.7
1	e	7	LEU	3.7
1	L	14	GLN	3.6
1	I	135	LEU	3.6
1	M	17	ARG	3.6
1	f	9	PRO	3.6
1	D	18	GLY	3.6
1	j	134	GLY	3.6
1	l	18	GLY	3.6
1	M	16	GLY	3.6
1	g	133	GLY	3.6
1	h	15	SER	3.5
1	G	134	GLY	3.5
1	c	134	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	g	134	GLY	3.5
1	f	7	LEU	3.5
1	L	198	ASN	3.5
1	h	133	GLY	3.5
1	N	17	ARG	3.5
1	k	199	ARG	3.5
1	f	22	PHE	3.5
1	g	135	LEU	3.5
1	e	8	VAL	3.4
1	D	15	SER	3.4
1	n	15	SER	3.4
1	F	15	SER	3.4
1	E	197	GLU	3.4
1	L	19	GLU	3.4
1	M	134	GLY	3.4
1	k	16	GLY	3.4
1	d	12	ILE	3.4
1	f	132	SER	3.4
1	E	17	ARG	3.4
1	B	133	GLY	3.4
1	N	133	GLY	3.4
1	l	132	SER	3.4
1	D	16	GLY	3.4
1	N	132	SER	3.3
1	l	15	SER	3.3
1	c	130	LEU	3.3
1	A	17	ARG	3.3
1	C	13	GLU	3.3
1	b	14	GLN	3.3
1	i	14	GLN	3.3
1	n	17	ARG	3.3
1	G	136	GLY	3.3
1	a	134	GLY	3.2
1	a	130	LEU	3.2
1	N	130	LEU	3.2
1	M	6	TYR	3.2
1	g	21	ALA	3.2
1	e	18	GLY	3.2
1	e	17	ARG	3.2
1	L	130	LEU	3.2
1	D	132	SER	3.1
1	E	132	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	K	13	GLU	3.1
1	j	18	GLY	3.1
1	l	134	GLY	3.1
1	e	12	ILE	3.1
1	D	17	ARG	3.1
1	a	17	ARG	3.1
1	e	13	GLU	3.1
1	G	130	LEU	3.1
1	g	130	LEU	3.1
1	j	135	LEU	3.1
1	i	134	GLY	3.1
1	C	14	GLN	3.1
1	G	13	GLU	3.1
1	i	133	GLY	3.1
1	i	135	LEU	3.1
1	a	14	GLN	3.0
1	G	18	GLY	3.0
1	K	136	GLY	3.0
1	j	133	GLY	3.0
1	J	130	LEU	3.0
1	n	130	LEU	3.0
1	d	132	SER	3.0
1	h	132	SER	3.0
1	i	132	SER	3.0
1	k	197	GLU	3.0
1	j	17	ARG	3.0
1	f	8	VAL	3.0
1	G	6	TYR	3.0
1	J	17	ARG	3.0
1	g	17	ARG	3.0
1	c	197	GLU	3.0
1	C	135	LEU	2.9
1	e	14	GLN	2.9
1	I	136	GLY	2.9
1	m	133	GLY	2.9
1	A	130	LEU	2.9
1	e	15	SER	2.9
1	I	16	GLY	2.9
1	M	136	GLY	2.9
1	b	21	ALA	2.9
1	A	132	SER	2.9
1	L	134	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	e	134	GLY	2.9
1	h	16	GLY	2.9
1	L	197	GLU	2.9
1	n	198	ASN	2.9
1	f	135	LEU	2.8
1	N	198	ASN	2.8
1	d	134	GLY	2.8
1	k	14	GLN	2.8
1	g	7	LEU	2.8
1	m	131	ILE	2.8
1	g	14	GLN	2.8
1	i	13	GLU	2.8
1	e	132	SER	2.8
1	F	130	LEU	2.8
1	k	130	LEU	2.8
1	m	130	LEU	2.8
1	g	22	PHE	2.8
1	M	14	GLN	2.7
1	j	16	GLY	2.7
1	d	197	GLU	2.7
1	c	135	LEU	2.7
1	f	21	ALA	2.7
1	C	132	SER	2.7
1	j	15	SER	2.7
1	l	13	GLU	2.7
1	F	16	GLY	2.7
1	K	134	GLY	2.7
1	h	136	GLY	2.7
1	f	130	LEU	2.7
1	h	130	LEU	2.7
1	n	135	LEU	2.7
1	g	13	GLU	2.6
1	g	12	ILE	2.6
1	K	135	LEU	2.6
1	h	135	LEU	2.6
1	D	20	ARG	2.6
1	l	16	GLY	2.6
1	j	132	SER	2.6
1	L	135	LEU	2.6
1	b	7	LEU	2.6
1	j	14	GLN	2.6
1	A	134	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	133	GLY	2.6
1	n	18	GLY	2.6
1	J	132	SER	2.6
1	G	133	GLY	2.6
1	H	136	GLY	2.6
1	N	134	GLY	2.6
1	k	15	SER	2.6
1	b	135	LEU	2.5
1	f	10	THR	2.5
1	H	131	ILE	2.5
1	M	132	SER	2.5
1	a	131	ILE	2.5
1	k	132	SER	2.5
1	N	135	LEU	2.5
1	n	136	GLY	2.5
1	f	136	GLY	2.5
1	C	197	GLU	2.5
1	K	22	PHE	2.5
1	e	20	ARG	2.5
1	f	20	ARG	2.5
1	h	17	ARG	2.5
1	b	136	GLY	2.5
1	I	132	SER	2.4
1	L	15	SER	2.4
1	f	11	VAL	2.4
1	A	135	LEU	2.4
1	I	130	LEU	2.4
1	A	133	GLY	2.4
1	K	199	ARG	2.4
1	e	22	PHE	2.4
1	b	198	ASN	2.4
1	G	132	SER	2.4
1	d	11	VAL	2.4
1	M	13	GLU	2.4
2	Y	4	PRO	2.4
1	b	12	ILE	2.4
1	d	22	PHE	2.4
1	K	130	LEU	2.4
1	e	130	LEU	2.4
1	g	197	GLU	2.4
1	E	165	ASP	2.3
1	L	20	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	130	LEU	2.3
1	a	135	LEU	2.3
1	C	19	GLU	2.3
1	J	197	GLU	2.3
1	l	198	ASN	2.3
1	e	9	PRO	2.3
1	A	16	GLY	2.3
1	F	20	ARG	2.3
1	k	17	ARG	2.3
1	K	12	ILE	2.3
1	F	43	GLU	2.3
1	A	15	SER	2.3
1	m	132	SER	2.3
1	e	135	LEU	2.3
1	a	136	GLY	2.3
1	j	131	ILE	2.3
1	a	20	ARG	2.2
1	I	15	SER	2.2
1	g	132	SER	2.2
1	i	130	LEU	2.2
1	N	20	ARG	2.2
1	E	136	GLY	2.2
1	k	136	GLY	2.2
1	D	131	ILE	2.2
1	H	18	GLY	2.2
1	B	135	LEU	2.2
1	D	130	LEU	2.2
1	g	18	GLY	2.2
1	g	136	GLY	2.2
1	e	21	ALA	2.2
1	g	10	THR	2.2
1	D	135	LEU	2.1
1	I	131	ILE	2.1
1	B	198	ASN	2.1
1	H	132	SER	2.1
1	g	15	SER	2.1
1	E	43	GLU	2.1
1	F	19	GLU	2.1
1	B	131	ILE	2.1
1	J	14	GLN	2.1
1	I	17	ARG	2.1
1	e	10	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	14	GLN	2.1
1	c	131	ILE	2.1
1	B	134	GLY	2.1
1	K	20	ARG	2.1
1	c	132	SER	2.0
1	B	19	GLU	2.0
1	L	154	GLU	2.0
1	m	17	ARG	2.0
1	a	19	GLU	2.0
1	B	130	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. The B-factors column lists the minimum, median, 95th 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 ²)	Q<0.9
2	MAA	x	5	6/7	0.88	0.14	32,44,53,65	0
2	MAA	p	5	6/7	0.89	0.10	22,32,34,36	0
2	MP8	w	7	8/9	0.90	0.10	26,32,38,39	0
2	MP8	q	7	8/9	0.91	0.09	19,29,33,38	0
2	MAA	q	5	6/7	0.91	0.10	32,34,39,43	0
2	MP8	0	7	8/9	0.91	0.10	16,23,27,28	0
2	MP8	p	7	8/9	0.92	0.08	17,21,24,32	0
2	MAA	v	5	6/7	0.92	0.10	29,35,39,40	0
2	MP8	u	7	8/9	0.92	0.09	13,23,28,32	0
2	MP8	S	7	8/9	0.92	0.08	14,21,28,35	0
2	MP8	Y	7	8/9	0.92	0.08	14,19,23,31	0
2	MP8	2	7	8/9	0.92	0.11	13,17,25,25	0
2	MAA	V	5	6/7	0.93	0.09	26,28,32,36	0
2	MAA	r	5	6/7	0.93	0.11	24,32,39,41	0
2	MAA	X	5	6/7	0.93	0.10	21,30,34,45	0
2	MP8	t	7	8/9	0.93	0.09	22,24,33,41	0
2	MAA	Y	5	6/7	0.93	0.09	22,28,38,44	0
2	MAA	U	5	6/7	0.93	0.08	18,26,31,32	0
2	MP8	U	7	8/9	0.93	0.09	18,23,30,38	0
2	MP8	W	7	8/9	0.93	0.09	18,27,33,36	0
2	MP8	P	7	8/9	0.94	0.08	19,24,25,26	0
2	MAA	R	5	6/7	0.94	0.08	23,28,30,33	0
2	MAA	S	5	6/7	0.94	0.08	18,25,31,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MAA	t	5	6/7	0.94	0.09	29,34,35,39	0
2	MAA	u	5	6/7	0.94	0.10	20,36,44,46	0
2	MP8	o	7	8/9	0.94	0.08	14,19,30,31	0
2	MAA	T	5	6/7	0.94	0.09	25,31,34,36	0
2	MAA	w	5	6/7	0.94	0.09	27,32,36,45	0
2	MP8	r	7	8/9	0.94	0.07	17,21,32,37	0
2	MAA	P	5	6/7	0.94	0.09	24,27,30,35	0
2	MAA	y	5	6/7	0.94	0.08	17,22,27,32	0
2	MP8	v	7	8/9	0.94	0.08	18,24,28,38	0
2	MAA	z	5	6/7	0.94	0.08	21,28,30,34	0
2	MAA	0	5	6/7	0.94	0.08	24,30,33,36	0
2	MAA	3	5	6/7	0.94	0.08	27,35,38,40	0
2	MP8	X	7	8/9	0.95	0.07	19,24,29,29	0
2	MAA	W	5	6/7	0.95	0.08	25,31,34,35	0
2	MP8	R	7	8/9	0.95	0.08	10,20,25,32	0
2	MAA	1	5	6/7	0.95	0.08	21,33,35,37	0
2	MP8	z	7	8/9	0.95	0.07	15,20,27,33	0
2	MAA	2	5	6/7	0.95	0.07	21,25,27,32	0
2	MAA	Z	5	6/7	0.95	0.08	14,18,26,31	0
2	MP8	3	7	8/9	0.95	0.06	15,20,23,27	0
2	MAA	Q	5	6/7	0.96	0.07	24,25,29,30	0
2	MAA	O	5	6/7	0.96	0.07	18,21,35,36	0
2	MP8	x	7	8/9	0.96	0.06	19,23,32,32	0
2	MP8	y	7	8/9	0.96	0.07	16,19,24,24	0
2	MAA	o	5	6/7	0.96	0.07	20,26,27,27	0
2	MP8	O	7	8/9	0.96	0.06	22,26,31,34	0
2	MP8	1	7	8/9	0.96	0.07	20,23,28,30	0
2	MAA	s	5	6/7	0.96	0.06	20,25,34,39	0
2	MP8	Q	7	8/9	0.96	0.06	10,18,27,27	0
2	MP8	s	7	8/9	0.97	0.06	17,25,27,27	0
2	MP8	T	7	8/9	0.97	0.05	12,16,21,28	0
2	MP8	Z	7	8/9	0.97	0.05	16,22,28,30	0
2	MP8	V	7	8/9	0.97	0.06	11,25,29,30	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides 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, 95th 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 ²)	Q<0.9
4	NA	k	302	1/1	0.94	0.08	40,40,40,40	0
3	K	f	301	1/1	0.95	0.07	32,32,32,32	0
3	K	N	301	1/1	0.96	0.06	25,25,25,25	0
3	K	n	301	1/1	0.96	0.07	26,26,26,26	0
4	NA	h	302	1/1	0.96	0.09	37,37,37,37	0
3	K	e	301	1/1	0.96	0.05	32,32,32,32	0
3	K	G	301	1/1	0.97	0.08	25,25,25,25	0
3	K	i	301	1/1	0.97	0.13	28,28,28,28	0
3	K	k	301	1/1	0.97	0.07	26,26,26,26	0
3	K	a	301	1/1	0.97	0.07	31,31,31,31	0
3	K	d	301	1/1	0.97	0.06	27,27,27,27	0
3	K	M	301	1/1	0.97	0.05	26,26,26,26	0
3	K	g	301	1/1	0.98	0.05	31,31,31,31	0
3	K	h	301	1/1	0.98	0.07	30,30,30,30	0
3	K	J	301	1/1	0.98	0.10	31,31,31,31	0
3	K	c	301	1/1	0.98	0.08	25,25,25,25	0
3	K	K	301	1/1	0.98	0.08	29,29,29,29	0
3	K	E	301	1/1	0.98	0.05	30,30,30,30	0
3	K	H	301	1/1	0.98	0.08	35,35,35,35	0
3	K	L	301	1/1	0.99	0.11	25,25,25,25	0
3	K	F	301	1/1	0.99	0.10	26,26,26,26	0
3	K	B	301	1/1	0.99	0.05	22,22,22,22	0
3	K	C	301	1/1	0.99	0.09	24,24,24,24	0
3	K	j	301	1/1	0.99	0.04	22,22,22,22	0
3	K	b	301	1/1	0.99	0.08	40,40,40,40	0
3	K	l	301	1/1	0.99	0.10	27,27,27,27	0
3	K	m	301	1/1	0.99	0.06	29,29,29,29	0
3	K	I	301	1/1	0.99	0.04	30,30,30,30	0
4	NA	c	302	1/1	0.99	0.05	25,25,25,25	0
3	K	D	301	1/1	0.99	0.04	26,26,26,26	0
3	K	A	301	1/1	0.99	0.04	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.