



Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 05:48 PM EST

PDB ID : 6WL7
EMDB ID : EMD-21816
Title : Cryo-EM of Form 2 like peptide filament, 29-20-2
Authors : Wang, F.; Gnewou, O.M.; Modlin, C.; Egelman, E.H.; Conticello, V.P.
Deposited on : 2020-04-18
Resolution : 3.80 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

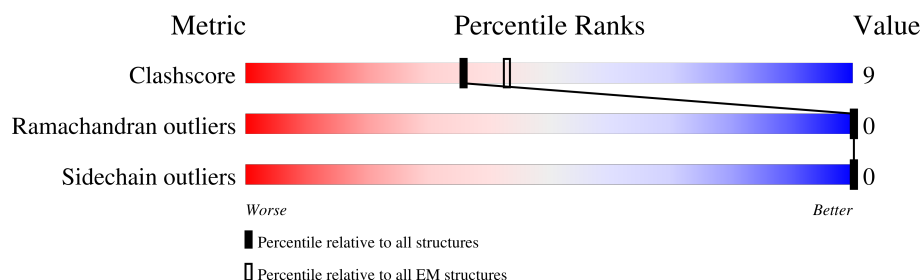
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	29	<div> <div>28%</div> <div>90%</div> <div>10%</div> </div>
1	0A	29	<div> <div>24%</div> <div>90%</div> <div>10%</div> </div>
1	1	29	<div> <div>7%</div> <div>83%</div> <div>17%</div> </div>
1	1A	29	<div> <div>28%</div> <div>93%</div> <div>7%</div> </div>
1	2	29	<div> <div>24%</div> <div>93%</div> <div>7%</div> </div>
1	2A	29	<div> <div>83%</div> <div>17%</div> </div>
1	3	29	<div> <div>28%</div> <div>90%</div> <div>10%</div> </div>
1	3A	29	<div> <div>28%</div> <div>97%</div> </div>

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Mol	Chain	Length	Quality of chain
1	4	29	
1	4A	29	
1	5	29	
1	5A	29	
1	6	29	
1	6A	29	
1	7	29	
1	7A	29	
1	8	29	
1	8A	29	
1	9	29	
1	9A	29	
1	A	29	
1	AA	29	
1	AB	29	
1	B	29	
1	BA	29	
1	BB	29	
1	C	29	
1	CA	29	
1	CB	29	
1	D	29	
1	DA	29	
1	DB	29	
1	E	29	

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Mol	Chain	Length	Quality of chain
1	EA	29	
1	EB	29	
1	F	29	
1	FA	29	
1	FB	29	
1	G	29	
1	GA	29	
1	GB	29	
1	H	29	
1	HA	29	
1	HB	29	
1	I	29	
1	IA	29	
1	IB	29	
1	J	29	
1	JA	29	
1	JB	29	
1	K	29	
1	KA	29	
1	KB	29	
1	L	29	
1	LA	29	
1	LB	29	
1	M	29	
1	MA	29	




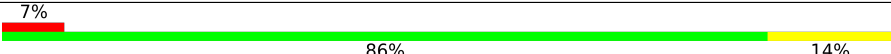
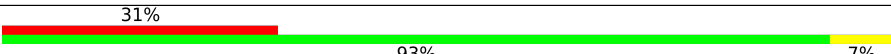
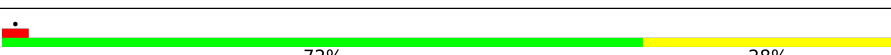
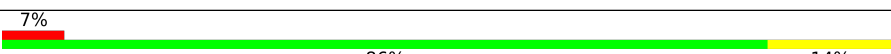
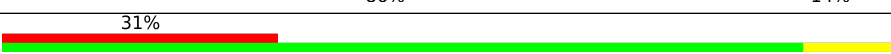
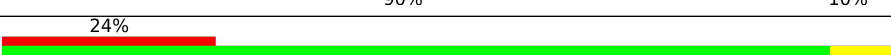
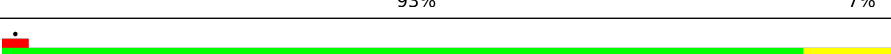
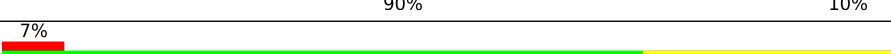
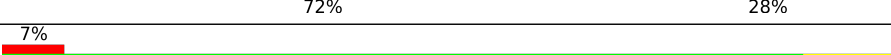
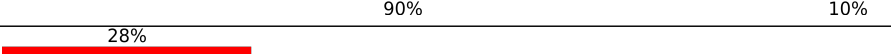
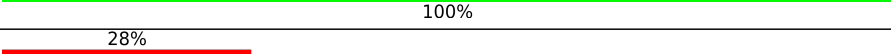
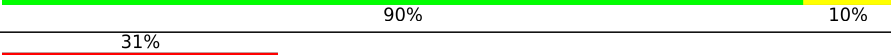
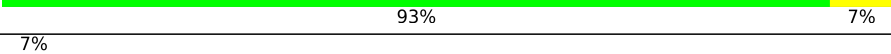
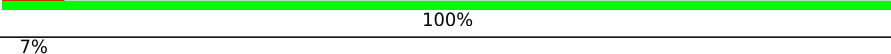
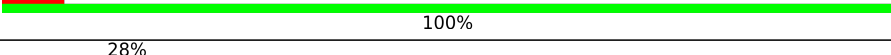
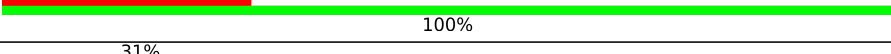
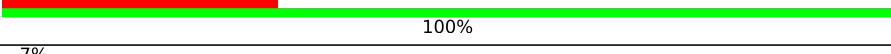
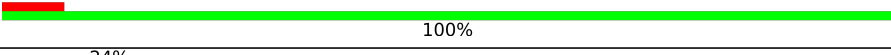
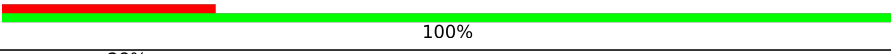
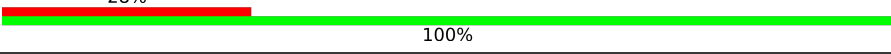
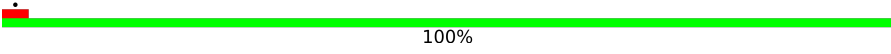
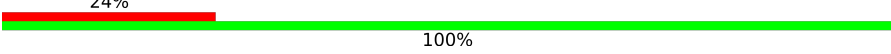
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Mol	Chain	Length	Quality of chain
1	MB	29	
1	N	29	
1	NA	29	
1	NB	29	
1	O	29	
1	OA	29	
1	OB	29	
1	P	29	
1	PA	29	
1	PB	29	
1	Q	29	
1	QA	29	
1	QB	29	
1	R	29	
1	RA	29	
1	RB	29	
1	S	29	
1	SA	29	
1	SB	29	
1	T	29	
1	TA	29	
1	TB	29	
1	U	29	
1	UA	29	
1	UB	29	

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Mol	Chain	Length	Quality of chain
1	V	29	
1	VA	29	
1	VB	29	
1	W	29	
1	WA	29	
1	WB	29	
1	X	29	
1	XA	29	
1	XB	29	
1	Y	29	
1	YA	29	
1	YB	29	
1	Z	29	
1	ZA	29	
1	ZB	29	
1	a	29	
1	aA	29	
1	b	29	
1	bA	29	
1	c	29	
1	cA	29	
1	d	29	
1	dA	29	
1	e	29	
1	eA	29	

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Mol	Chain	Length	Quality of chain
1	f	29	7% 100%
1	fA	29	7% 100%
1	g	29	28% 100%
1	gA	29	31% 100%
1	h	29	7% 100%
1	hA	29	28% 100%
1	i	29	31% 100%
1	iA	29	7% 100%
1	j	29	28% 100%
1	jA	29	24% 100%
1	k	29	7% 100%
1	kA	29	7% 100%
1	l	29	28% 100%
1	lA	29	28% 100%
1	m	29	7% 100%
1	mA	29	28% 100%
1	n	29	28% 100%
1	nA	29	• 100%
1	o	29	21% 100%
1	oA	29	28% 100%
1	p	29	7% 100%
1	pA	29	7% 100%
1	q	29	28% 100%
1	qA	29	28% 100%
1	r	29	• 100%

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Mol	Chain	Length	Quality of chain
1	rA	29	<div> <div>31%</div> <div>100%</div> </div>
1	s	29	<div> <div>28%</div> <div>100%</div> </div>
1	sA	29	<div> <div>7%</div> <div>100%</div> </div>
1	t	29	<div> <div>28%</div> <div>100%</div> </div>
1	tA	29	<div> <div>31%</div> <div>100%</div> </div>
1	u	29	<div> <div>7%</div> <div>100%</div> </div>
1	uA	29	<div> <div>7%</div> <div>100%</div> </div>
1	v	29	<div> <div>28%</div> <div>100%</div> </div>
1	vA	29	<div> <div>31%</div> <div>100%</div> </div>
1	w	29	<div> <div>7%</div> <div>100%</div> </div>
1	wA	29	<div> <div>31%</div> <div>100%</div> </div>
1	x	29	<div> <div>28%</div> <div>100%</div> </div>
1	xA	29	<div> <div>7%</div> <div>100%</div> </div>
1	y	29	<div> <div>28%</div> <div>100%</div> </div>
1	yA	29	<div> <div>28%</div> <div>100%</div> </div>
1	z	29	<div> <div>7%</div> <div>100%</div> </div>
1	zA	29	<div> <div>7%</div> <div>100%</div> </div>

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 34350 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 peptide 29-20-2.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	29	Total	C	N	O	0	0
			229	145	41	43		
1	Z	29	Total	C	N	O	0	0
			229	145	41	43		
1	a	29	Total	C	N	O	0	0
			229	145	41	43		
1	b	29	Total	C	N	O	0	0
			229	145	41	43		
1	c	29	Total	C	N	O	0	0
			229	145	41	43		
1	d	29	Total	C	N	O	0	0
			229	145	41	43		
1	B	29	Total	C	N	O	0	0
			229	145	41	43		
1	e	29	Total	C	N	O	0	0
			229	145	41	43		
1	f	29	Total	C	N	O	0	0
			229	145	41	43		
1	g	29	Total	C	N	O	0	0
			229	145	41	43		
1	h	29	Total	C	N	O	0	0
			229	145	41	43		
1	i	29	Total	C	N	O	0	0
			229	145	41	43		
1	C	29	Total	C	N	O	0	0
			229	145	41	43		
1	j	29	Total	C	N	O	0	0
			229	145	41	43		
1	k	29	Total	C	N	O	0	0
			229	145	41	43		
1	l	29	Total	C	N	O	0	0
			229	145	41	43		
1	m	29	Total	C	N	O	0	0
			229	145	41	43		

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	n	29	Total	C	N	O	0	0
			229	145	41	43		
1	D	29	Total	C	N	O	0	0
			229	145	41	43		
1	o	29	Total	C	N	O	0	0
			229	145	41	43		
1	p	29	Total	C	N	O	0	0
			229	145	41	43		
1	q	29	Total	C	N	O	0	0
			229	145	41	43		
1	r	29	Total	C	N	O	0	0
			229	145	41	43		
1	s	29	Total	C	N	O	0	0
			229	145	41	43		
1	E	29	Total	C	N	O	0	0
			229	145	41	43		
1	t	29	Total	C	N	O	0	0
			229	145	41	43		
1	u	29	Total	C	N	O	0	0
			229	145	41	43		
1	v	29	Total	C	N	O	0	0
			229	145	41	43		
1	w	29	Total	C	N	O	0	0
			229	145	41	43		
1	x	29	Total	C	N	O	0	0
			229	145	41	43		
1	F	29	Total	C	N	O	0	0
			229	145	41	43		
1	y	29	Total	C	N	O	0	0
			229	145	41	43		
1	z	29	Total	C	N	O	0	0
			229	145	41	43		
1	0	29	Total	C	N	O	0	0
			229	145	41	43		
1	1	29	Total	C	N	O	0	0
			229	145	41	43		
1	2	29	Total	C	N	O	0	0
			229	145	41	43		
1	G	29	Total	C	N	O	0	0
			229	145	41	43		
1	3	29	Total	C	N	O	0	0
			229	145	41	43		

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	4	29	Total	C	N	O	0	0
			229	145	41	43		
1	5	29	Total	C	N	O	0	0
			229	145	41	43		
1	6	29	Total	C	N	O	0	0
			229	145	41	43		
1	7	29	Total	C	N	O	0	0
			229	145	41	43		
1	H	29	Total	C	N	O	0	0
			229	145	41	43		
1	8	29	Total	C	N	O	0	0
			229	145	41	43		
1	9	29	Total	C	N	O	0	0
			229	145	41	43		
1	AA	29	Total	C	N	O	0	0
			229	145	41	43		
1	BA	29	Total	C	N	O	0	0
			229	145	41	43		
1	CA	29	Total	C	N	O	0	0
			229	145	41	43		
1	I	29	Total	C	N	O	0	0
			229	145	41	43		
1	DA	29	Total	C	N	O	0	0
			229	145	41	43		
1	EA	29	Total	C	N	O	0	0
			229	145	41	43		
1	FA	29	Total	C	N	O	0	0
			229	145	41	43		
1	GA	29	Total	C	N	O	0	0
			229	145	41	43		
1	HA	29	Total	C	N	O	0	0
			229	145	41	43		
1	J	29	Total	C	N	O	0	0
			229	145	41	43		
1	IA	29	Total	C	N	O	0	0
			229	145	41	43		
1	JA	29	Total	C	N	O	0	0
			229	145	41	43		
1	KA	29	Total	C	N	O	0	0
			229	145	41	43		
1	LA	29	Total	C	N	O	0	0
			229	145	41	43		

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	MA	29	Total	C	N	O	0	0
			229	145	41	43		
1	K	29	Total	C	N	O	0	0
			229	145	41	43		
1	NA	29	Total	C	N	O	0	0
			229	145	41	43		
1	OA	29	Total	C	N	O	0	0
			229	145	41	43		
1	PA	29	Total	C	N	O	0	0
			229	145	41	43		
1	QA	29	Total	C	N	O	0	0
			229	145	41	43		
1	RA	29	Total	C	N	O	0	0
			229	145	41	43		
1	L	29	Total	C	N	O	0	0
			229	145	41	43		
1	SA	29	Total	C	N	O	0	0
			229	145	41	43		
1	TA	29	Total	C	N	O	0	0
			229	145	41	43		
1	UA	29	Total	C	N	O	0	0
			229	145	41	43		
1	VA	29	Total	C	N	O	0	0
			229	145	41	43		
1	WA	29	Total	C	N	O	0	0
			229	145	41	43		
1	M	29	Total	C	N	O	0	0
			229	145	41	43		
1	XA	29	Total	C	N	O	0	0
			229	145	41	43		
1	YA	29	Total	C	N	O	0	0
			229	145	41	43		
1	ZA	29	Total	C	N	O	0	0
			229	145	41	43		
1	aA	29	Total	C	N	O	0	0
			229	145	41	43		
1	bA	29	Total	C	N	O	0	0
			229	145	41	43		
1	N	29	Total	C	N	O	0	0
			229	145	41	43		
1	cA	29	Total	C	N	O	0	0
			229	145	41	43		

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	dA	29	Total	C	N	O	0	0
			229	145	41	43		
1	eA	29	Total	C	N	O	0	0
			229	145	41	43		
1	fA	29	Total	C	N	O	0	0
			229	145	41	43		
1	gA	29	Total	C	N	O	0	0
			229	145	41	43		
1	O	29	Total	C	N	O	0	0
			229	145	41	43		
1	hA	29	Total	C	N	O	0	0
			229	145	41	43		
1	iA	29	Total	C	N	O	0	0
			229	145	41	43		
1	jA	29	Total	C	N	O	0	0
			229	145	41	43		
1	kA	29	Total	C	N	O	0	0
			229	145	41	43		
1	lA	29	Total	C	N	O	0	0
			229	145	41	43		
1	P	29	Total	C	N	O	0	0
			229	145	41	43		
1	mA	29	Total	C	N	O	0	0
			229	145	41	43		
1	nA	29	Total	C	N	O	0	0
			229	145	41	43		
1	oA	29	Total	C	N	O	0	0
			229	145	41	43		
1	pA	29	Total	C	N	O	0	0
			229	145	41	43		
1	qA	29	Total	C	N	O	0	0
			229	145	41	43		
1	Q	29	Total	C	N	O	0	0
			229	145	41	43		
1	rA	29	Total	C	N	O	0	0
			229	145	41	43		
1	sA	29	Total	C	N	O	0	0
			229	145	41	43		
1	tA	29	Total	C	N	O	0	0
			229	145	41	43		
1	uA	29	Total	C	N	O	0	0
			229	145	41	43		

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	vA	29	Total	C	N	O	0	0
			229	145	41	43		
1	R	29	Total	C	N	O	0	0
			229	145	41	43		
1	wA	29	Total	C	N	O	0	0
			229	145	41	43		
1	xA	29	Total	C	N	O	0	0
			229	145	41	43		
1	yA	29	Total	C	N	O	0	0
			229	145	41	43		
1	zA	29	Total	C	N	O	0	0
			229	145	41	43		
1	0A	29	Total	C	N	O	0	0
			229	145	41	43		
1	S	29	Total	C	N	O	0	0
			229	145	41	43		
1	1A	29	Total	C	N	O	0	0
			229	145	41	43		
1	2A	29	Total	C	N	O	0	0
			229	145	41	43		
1	3A	29	Total	C	N	O	0	0
			229	145	41	43		
1	4A	29	Total	C	N	O	0	0
			229	145	41	43		
1	5A	29	Total	C	N	O	0	0
			229	145	41	43		
1	T	29	Total	C	N	O	0	0
			229	145	41	43		
1	6A	29	Total	C	N	O	0	0
			229	145	41	43		
1	7A	29	Total	C	N	O	0	0
			229	145	41	43		
1	8A	29	Total	C	N	O	0	0
			229	145	41	43		
1	9A	29	Total	C	N	O	0	0
			229	145	41	43		
1	AB	29	Total	C	N	O	0	0
			229	145	41	43		
1	U	29	Total	C	N	O	0	0
			229	145	41	43		
1	BB	29	Total	C	N	O	0	0
			229	145	41	43		

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	CB	29	Total	C	N	O	0	0
			229	145	41	43		
1	DB	29	Total	C	N	O	0	0
			229	145	41	43		
1	EB	29	Total	C	N	O	0	0
			229	145	41	43		
1	FB	29	Total	C	N	O	0	0
			229	145	41	43		
1	V	29	Total	C	N	O	0	0
			229	145	41	43		
1	GB	29	Total	C	N	O	0	0
			229	145	41	43		
1	HB	29	Total	C	N	O	0	0
			229	145	41	43		
1	IB	29	Total	C	N	O	0	0
			229	145	41	43		
1	JB	29	Total	C	N	O	0	0
			229	145	41	43		
1	KB	29	Total	C	N	O	0	0
			229	145	41	43		
1	W	29	Total	C	N	O	0	0
			229	145	41	43		
1	LB	29	Total	C	N	O	0	0
			229	145	41	43		
1	MB	29	Total	C	N	O	0	0
			229	145	41	43		
1	NB	29	Total	C	N	O	0	0
			229	145	41	43		
1	OB	29	Total	C	N	O	0	0
			229	145	41	43		
1	PB	29	Total	C	N	O	0	0
			229	145	41	43		
1	X	29	Total	C	N	O	0	0
			229	145	41	43		
1	QB	29	Total	C	N	O	0	0
			229	145	41	43		
1	RB	29	Total	C	N	O	0	0
			229	145	41	43		
1	SB	29	Total	C	N	O	0	0
			229	145	41	43		
1	TB	29	Total	C	N	O	0	0
			229	145	41	43		

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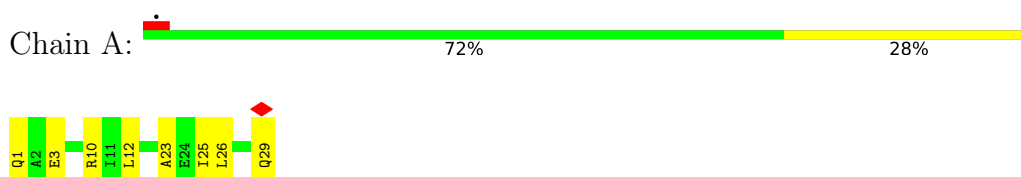
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Mol	Chain	Residues	Atoms				AltConf	Trace
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1	Y	29	Total 229	C 145	N 41	O 43	0	0
1	VB	29	Total 229	C 145	N 41	O 43	0	0
1	WB	29	Total 229	C 145	N 41	O 43	0	0
1	XB	29	Total 229	C 145	N 41	O 43	0	0
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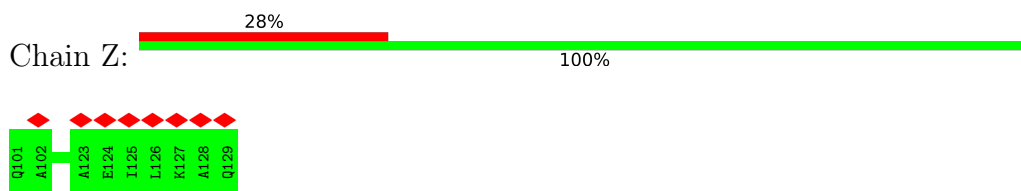
3 Residue-property plots [i](#)

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

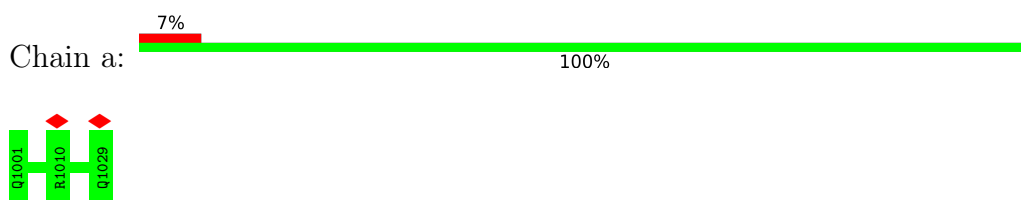
- Molecule 1: peptide 29-20-2



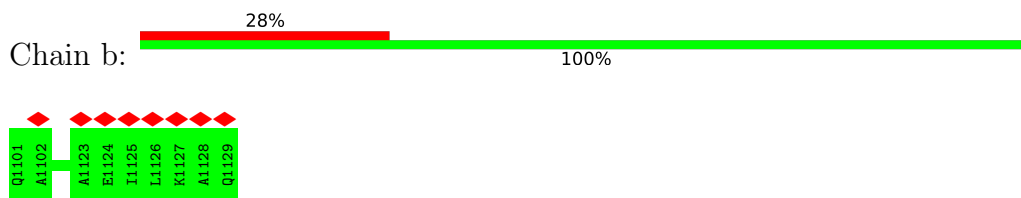
- Molecule 1: peptide 29-20-2



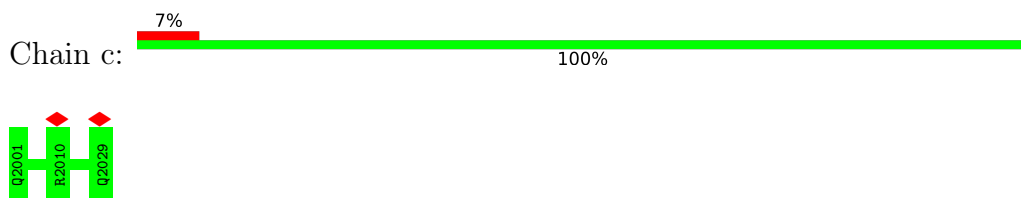
- Molecule 1: peptide 29-20-2



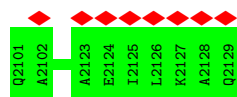
- Molecule 1: peptide 29-20-2



- Molecule 1: peptide 29-20-2



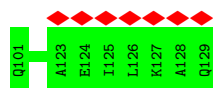
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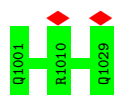
- Molecule 1: peptide 29-20-2



- Molecule 1: peptide 29-20-2



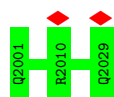
- Molecule 1: peptide 29-20-2



- Molecule 1: peptide 29-20-2

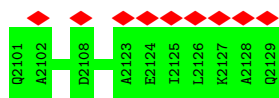


- Molecule 1: peptide 29-20-2

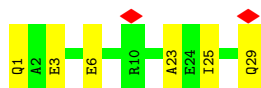
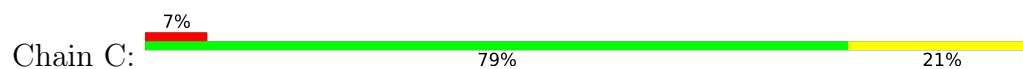


- Molecule 1: peptide 29-20-2

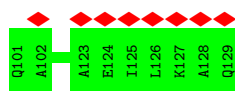




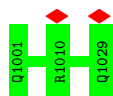
- Molecule 1: peptide 29-20-2



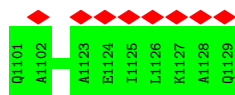
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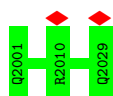
- Molecule 1: peptide 29-20-2



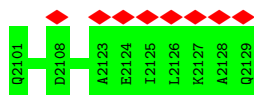
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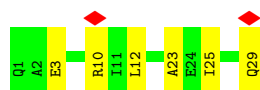
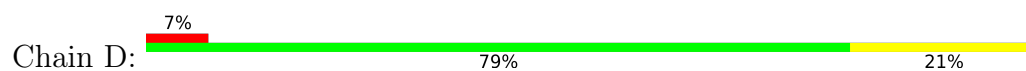
- Molecule 1: peptide 29-20-2



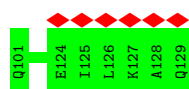
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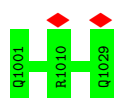
- Molecule 1: peptide 29-20-2



- Molecule 1: peptide 29-20-2



- Molecule 1: peptide 29-20-2



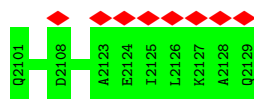
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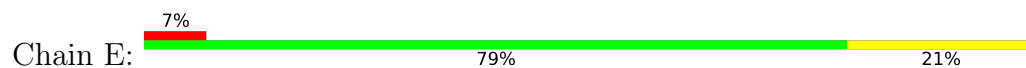
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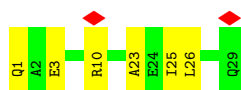


- Molecule 1: peptide 29-20-2

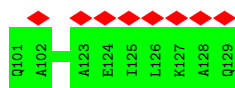


- Molecule 1: peptide 29-20-2

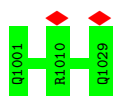




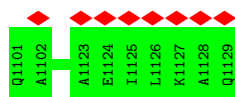
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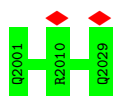
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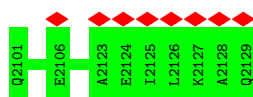
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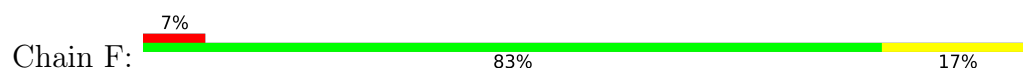
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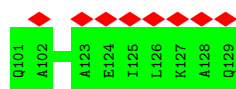
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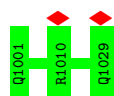
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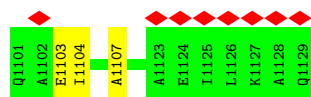
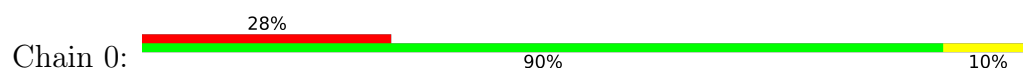
- Molecule 1: peptide 29-20-2



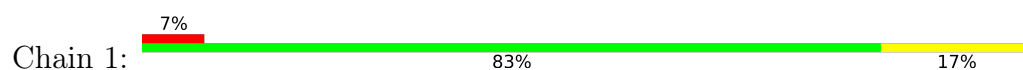
- Molecule 1: peptide 29-20-2



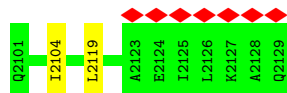
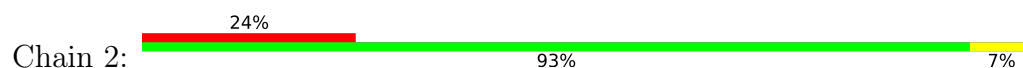
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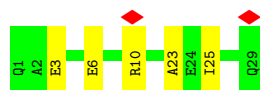
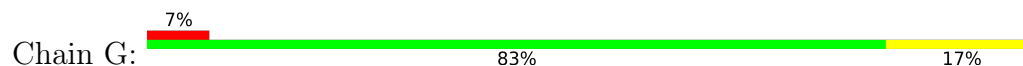
- Molecule 1: peptide 29-20-2



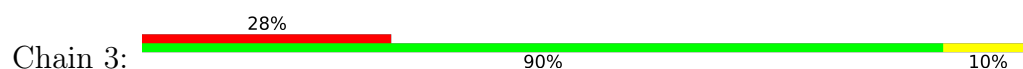
- Molecule 1: peptide 29-20-2



- Molecule 1: peptide 29-20-2

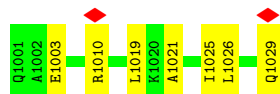
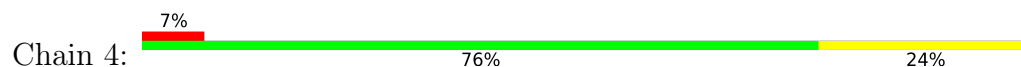


- Molecule 1: peptide 29-20-2

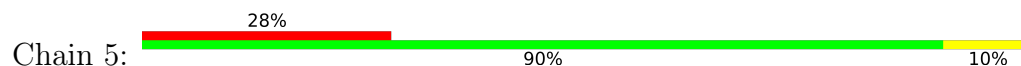




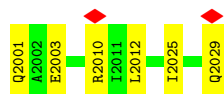
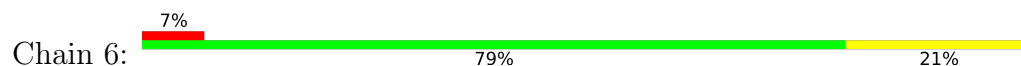
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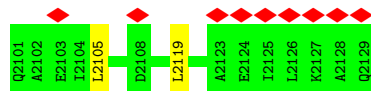
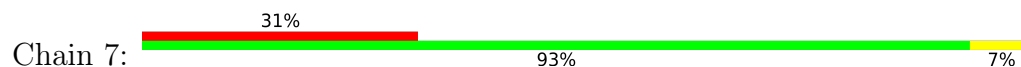
- Molecule 1: peptide 29-20-2



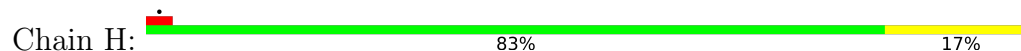
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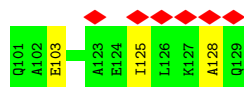
- Molecule 1: peptide 29-20-2



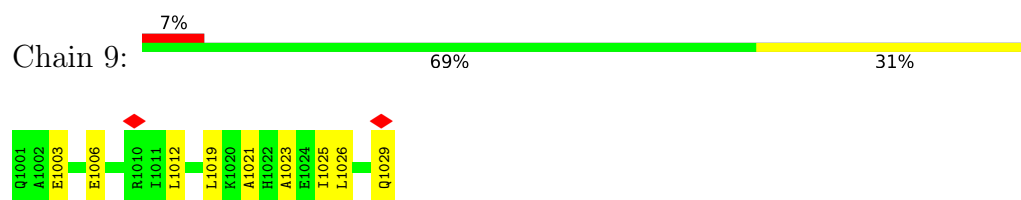
- Molecule 1: peptide 29-20-2



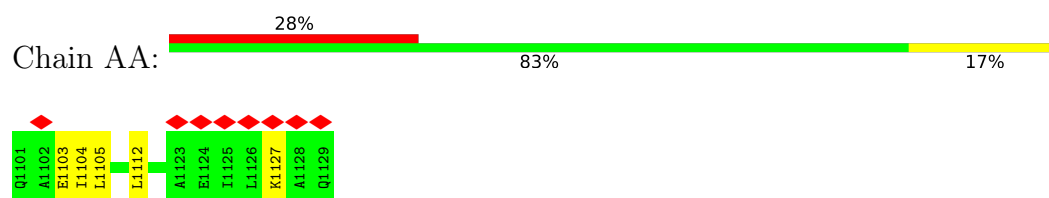
- Molecule 1: peptide 29-20-2



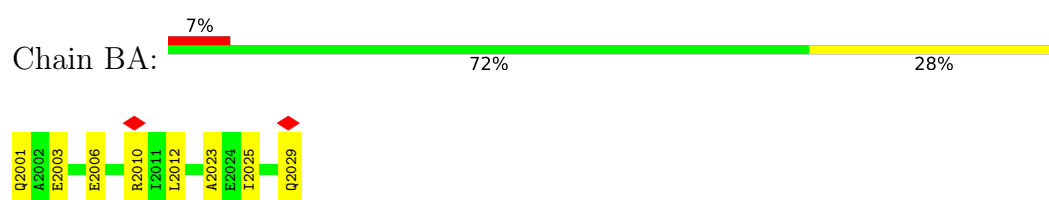
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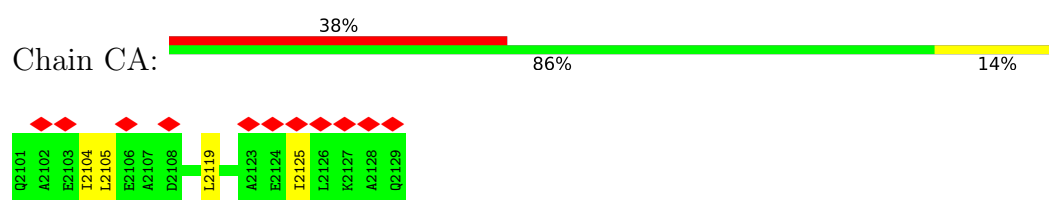
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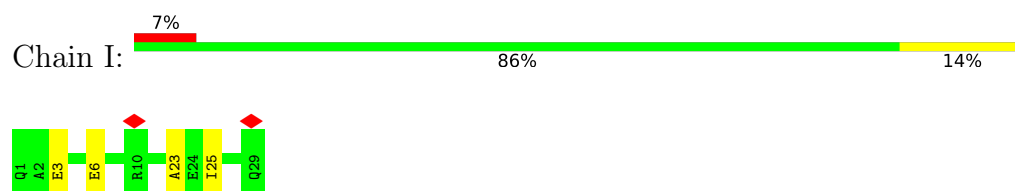
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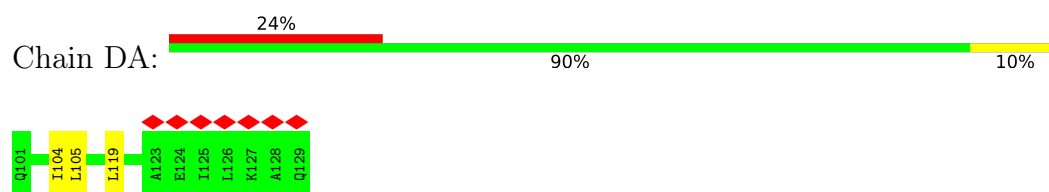
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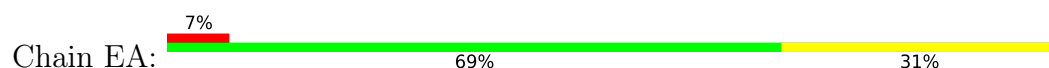
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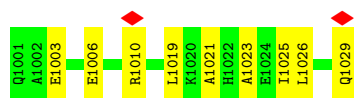


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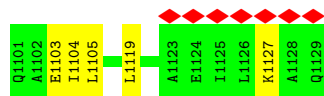
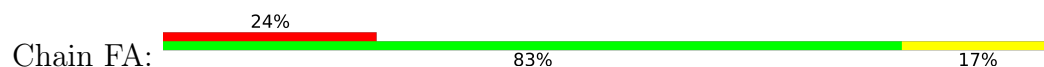


- Molecule 1: peptide 29-20-2

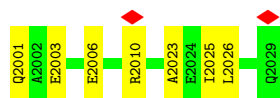
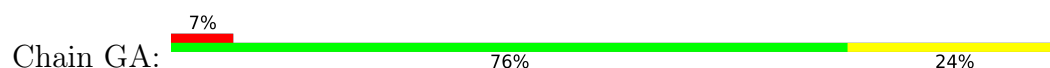




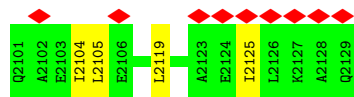
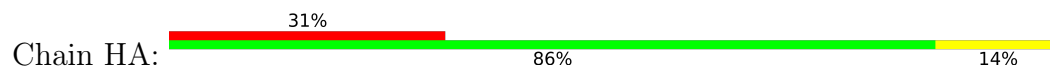
- Molecule 1: peptide 29-20-2



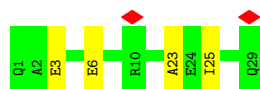
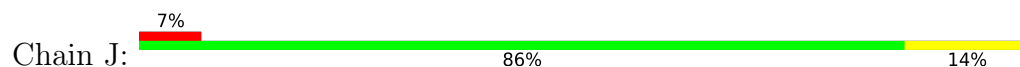
- Molecule 1: peptide 29-20-2



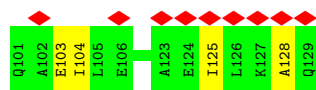
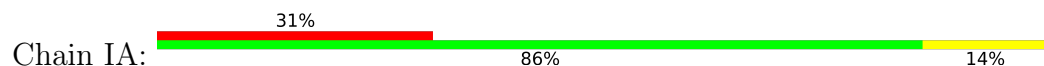
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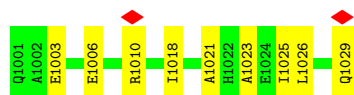
- Molecule 1: peptide 29-20-2



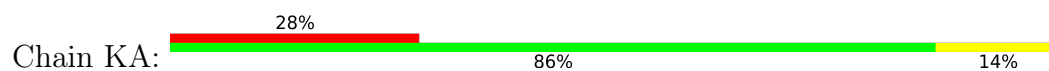
- Molecule 1: peptide 29-20-2



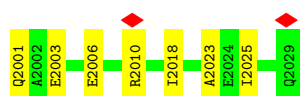
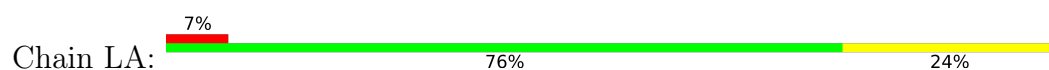
- Molecule 1: peptide 29-20-2



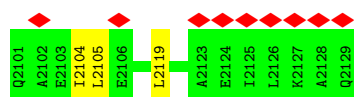
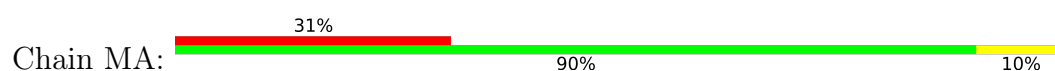
- Molecule 1: peptide 29-20-2



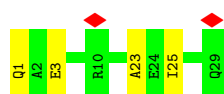
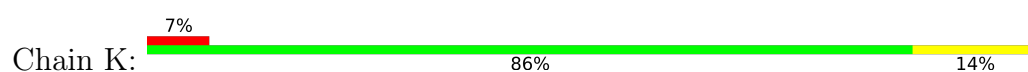
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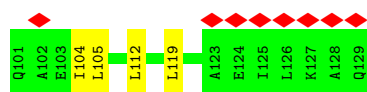
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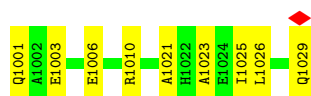
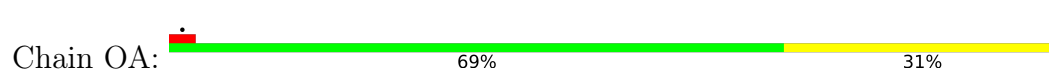
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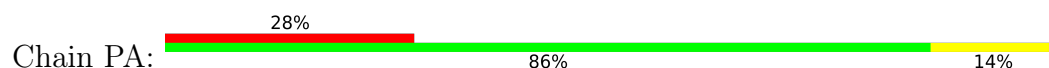
- Molecule 1: peptide 29-20-2



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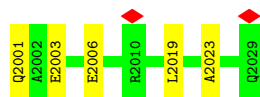
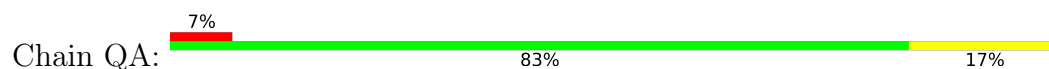


- Molecule 1: peptide 29-20-2

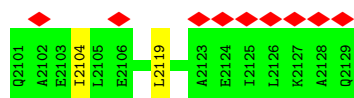




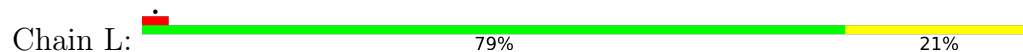
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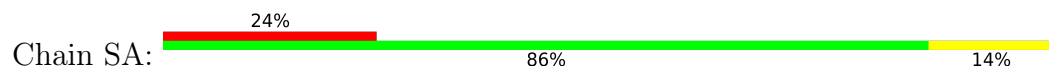
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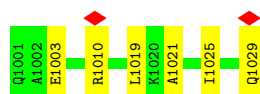
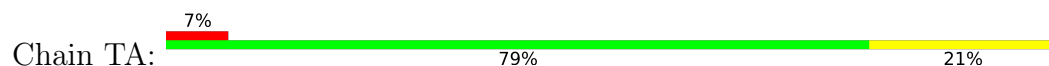
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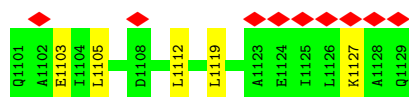
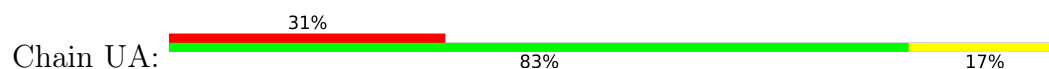
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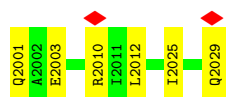
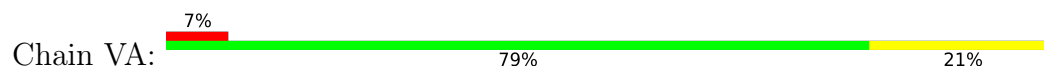
- Molecule 1: peptide 29-20-2



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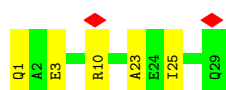
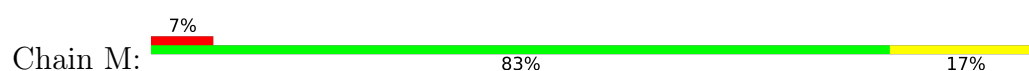
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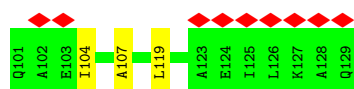
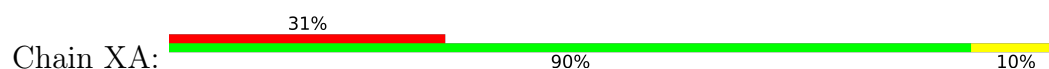
- Molecule 1: peptide 29-20-2



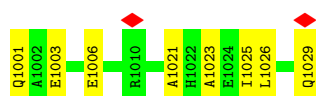
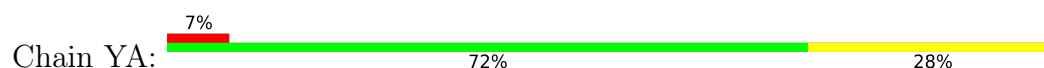
- Molecule 1: peptide 29-20-2



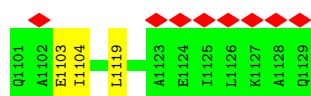
- Molecule 1: peptide 29-20-2



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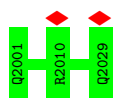


- Molecule 1: peptide 29-20-2

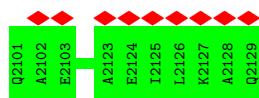


- Molecule 1: peptide 29-20-2

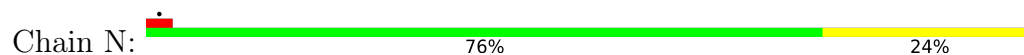




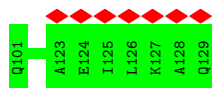
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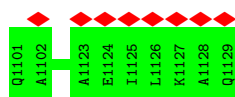
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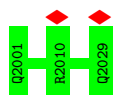
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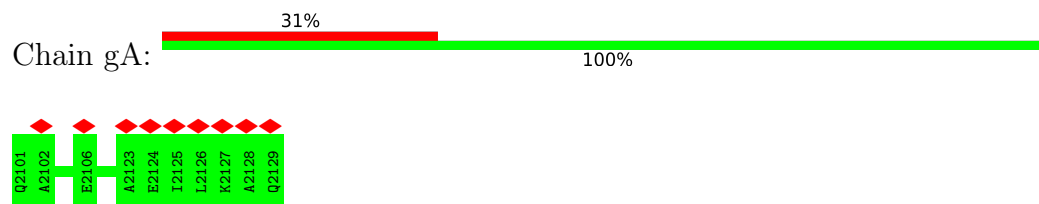
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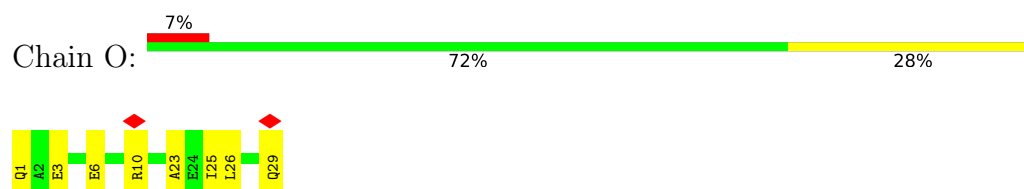
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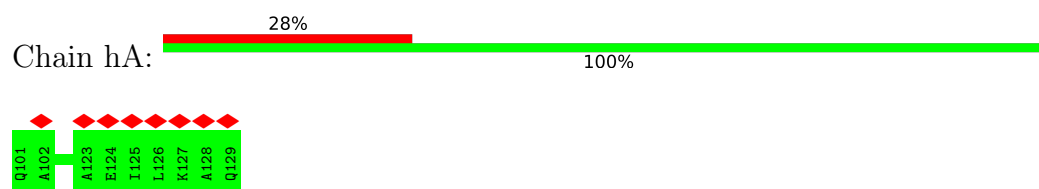
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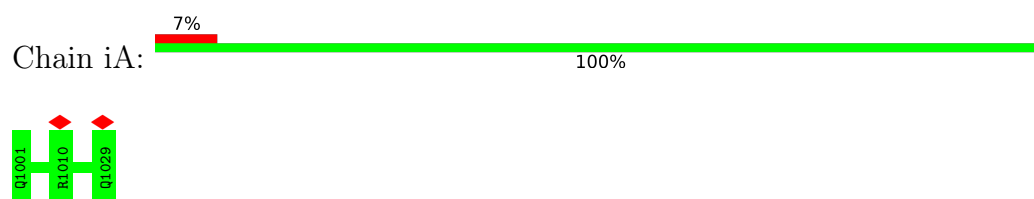
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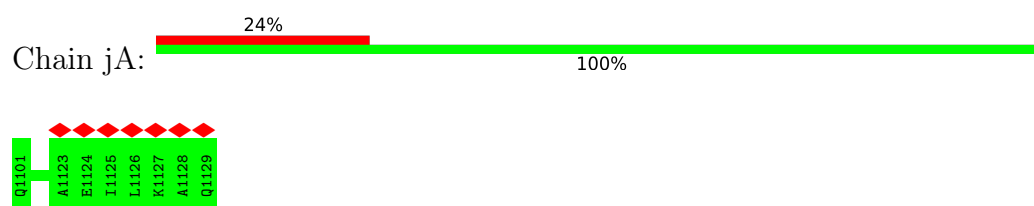
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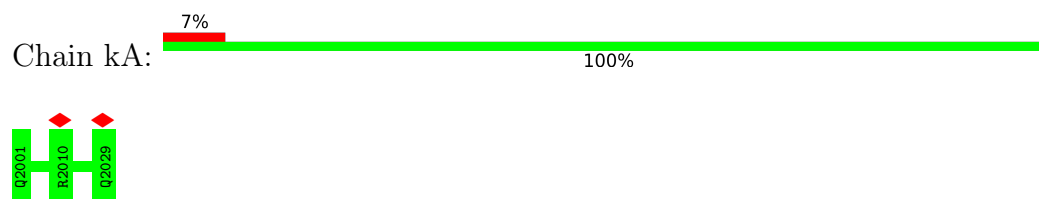
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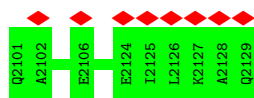


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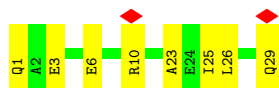
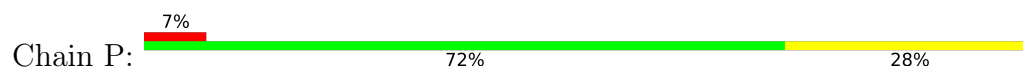


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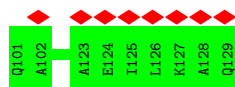




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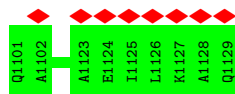
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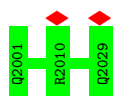
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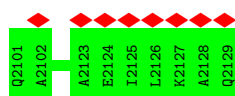
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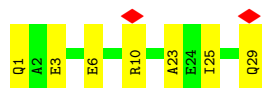
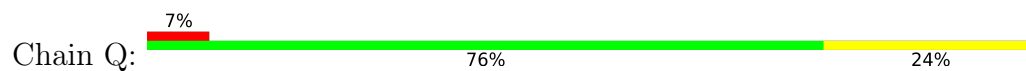
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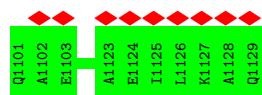
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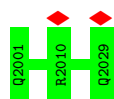
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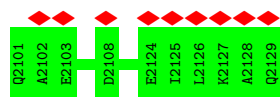
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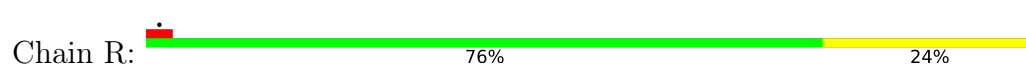
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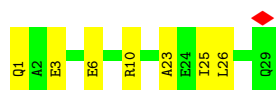


- Molecule 1: peptide 29-20-2



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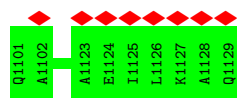
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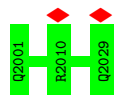
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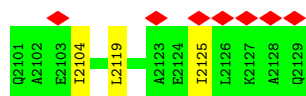
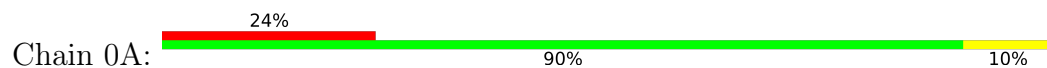
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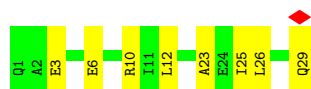
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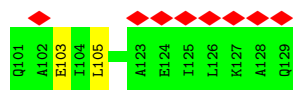
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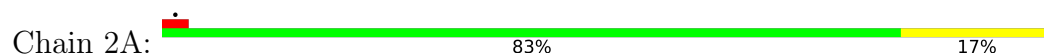
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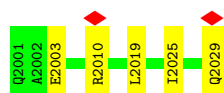
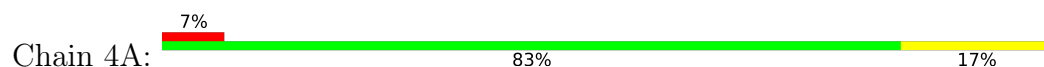
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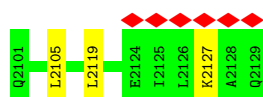
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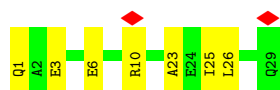
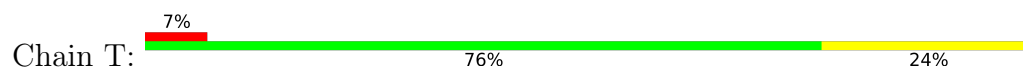
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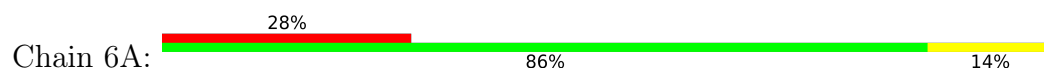
- Molecule 1: peptide 29-20-2



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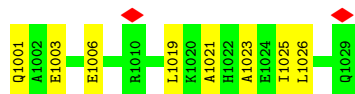
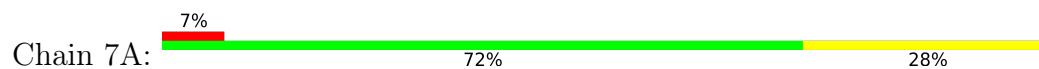


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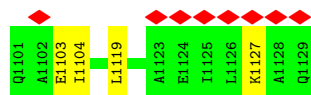
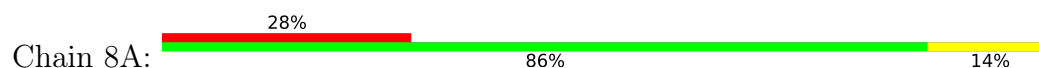




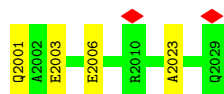
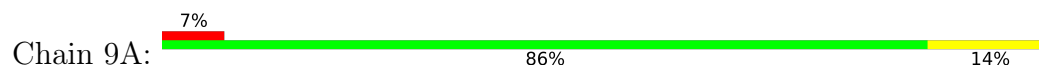
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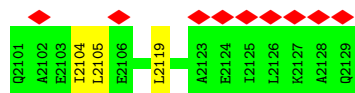
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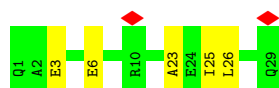
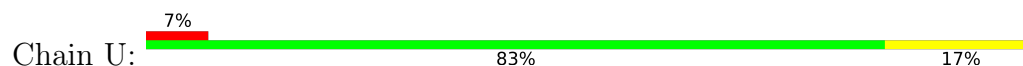
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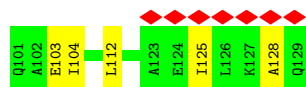
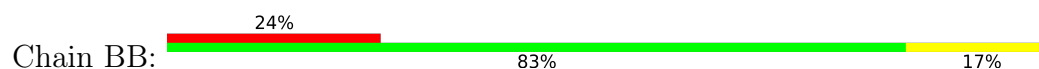
- Molecule 1: peptide 29-20-2




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Chain CB:  76% 24%



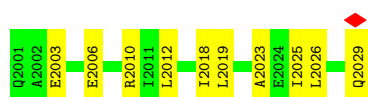
- Molecule 1: peptide 29-20-2

Chain DB:  28% 93% 7%




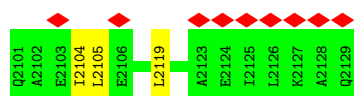
- Molecule 1: peptide 29-20-2

Chain EB:  66% 34%




- Molecule 1: peptide 29-20-2

Chain FB:  31% 90% 10%




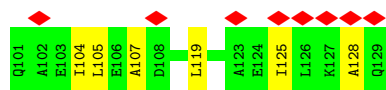
- Molecule 1: peptide 29-20-2

Chain V:  76% 24%




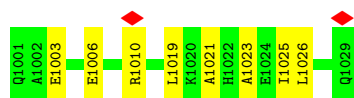
- Molecule 1: peptide 29-20-2

Chain GB:  28% 79% 21%

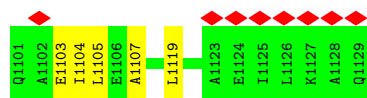
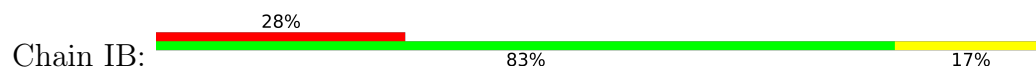


- Molecule 1: peptide 29-20-2

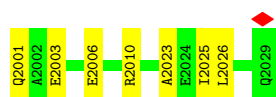
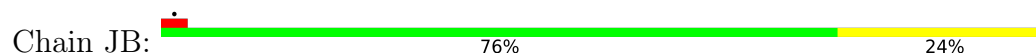
Chain HB:  7% 72% 28%



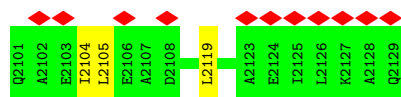
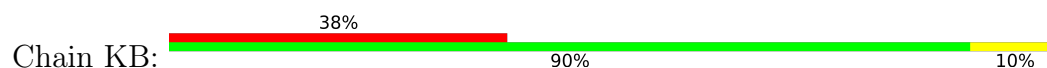
- Molecule 1: peptide 29-20-2



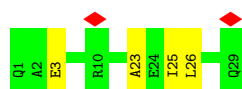
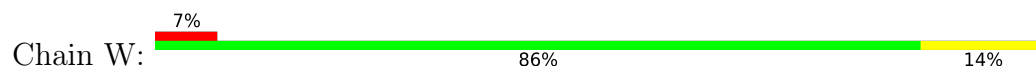
- Molecule 1: peptide 29-20-2



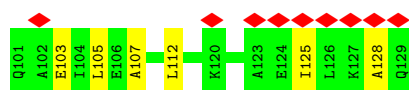
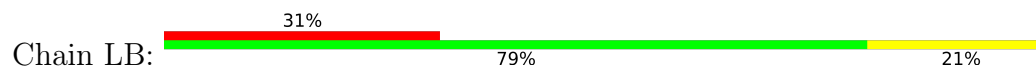
- Molecule 1: peptide 29-20-2



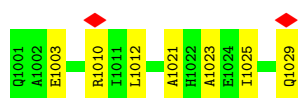
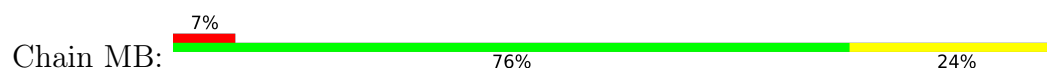
- Molecule 1: peptide 29-20-2



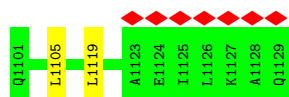
- Molecule 1: peptide 29-20-2



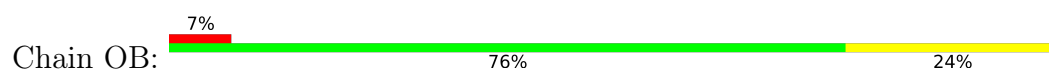
- Molecule 1: peptide 29-20-2



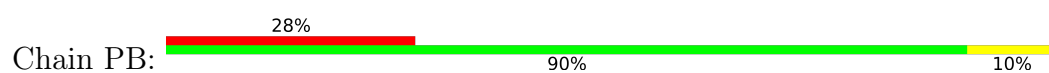
- Molecule 1: peptide 29-20-2



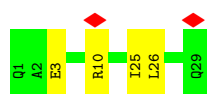
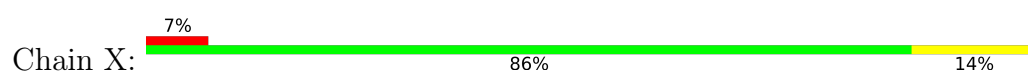
- Molecule 1: peptide 29-20-2



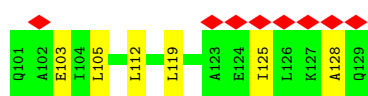
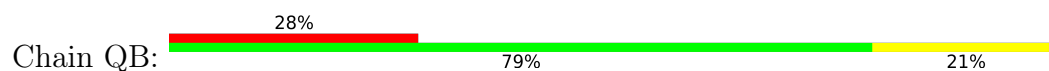
- Molecule 1: peptide 29-20-2



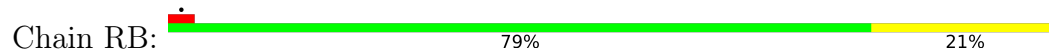
- Molecule 1: peptide 29-20-2



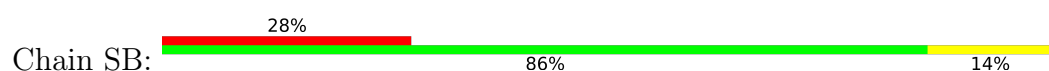
- Molecule 1: peptide 29-20-2

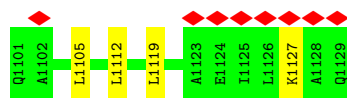


- Molecule 1: peptide 29-20-2

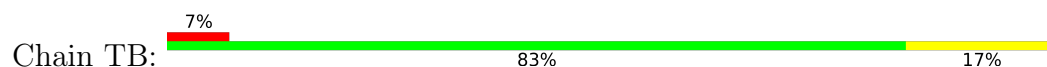


- Molecule 1: peptide 29-20-2

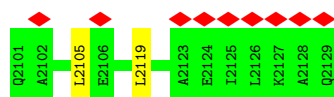




- Molecule 1: peptide 29-20-2



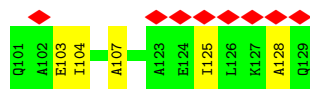
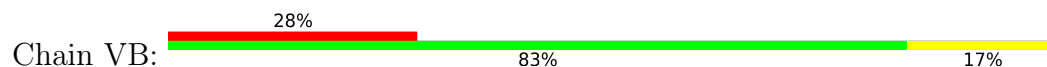
- Molecule 1: peptide 29-20-2



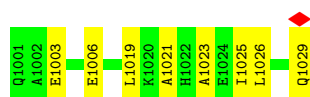
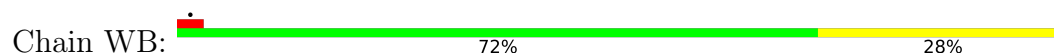
- Molecule 1: peptide 29-20-2



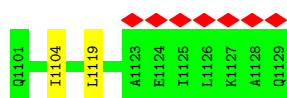
- Molecule 1: peptide 29-20-2



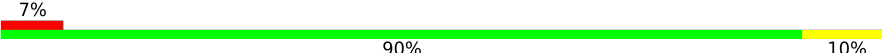
- Molecule 1: peptide 29-20-2



- Molecule 1: peptide 29-20-2

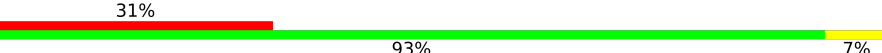


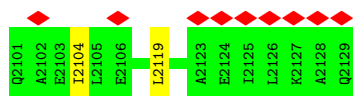
- Molecule 1: peptide 29-20-2

Chain YB:  7% 90% 10%



- Molecule 1: peptide 29-20-2

Chain ZB:  31% 93% 7%



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=12.90°, rise=5.63 Å, axial sym=C3	Depositor
Number of segments used	67941	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{Å}^2$)	55	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.027	Depositor
Minimum map value	-0.010	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0111	Depositor
Map size (Å)	332.8, 332.8, 332.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

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	0	0.34	0/230	0.36	0/307
1	0A	0.34	0/230	0.36	0/307
1	1	0.39	0/230	0.40	0/307
1	1A	0.34	0/230	0.36	0/307
1	2	0.34	0/230	0.36	0/307
1	2A	0.40	0/230	0.39	0/307
1	3	0.34	0/230	0.36	0/307
1	3A	0.33	0/230	0.36	0/307
1	4	0.40	0/230	0.39	0/307
1	4A	0.39	0/230	0.40	0/307
1	5	0.33	0/230	0.36	0/307
1	5A	0.34	0/230	0.36	0/307
1	6	0.39	0/230	0.40	0/307
1	6A	0.34	0/230	0.37	0/307
1	7	0.34	0/230	0.36	0/307
1	7A	0.40	0/230	0.39	0/307
1	8	0.34	0/230	0.37	0/307
1	8A	0.34	0/230	0.36	0/307
1	9	0.40	0/230	0.39	0/307
1	9A	0.39	0/230	0.40	0/307
1	A	0.40	0/230	0.41	0/307
1	AA	0.33	0/230	0.36	0/307
1	AB	0.34	0/230	0.36	0/307
1	B	0.40	0/230	0.41	0/307
1	BA	0.39	0/230	0.40	0/307
1	BB	0.34	0/230	0.37	0/307
1	C	0.40	0/230	0.41	0/307
1	CA	0.33	0/230	0.36	0/307
1	CB	0.40	0/230	0.39	0/307
1	D	0.40	0/230	0.41	0/307
1	DA	0.34	0/230	0.37	0/307
1	DB	0.34	0/230	0.36	0/307
1	E	0.40	0/230	0.41	0/307
1	EA	0.40	0/230	0.39	0/307

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	EB	0.39	0/230	0.40	0/307
1	F	0.39	0/230	0.41	0/307
1	FA	0.33	0/230	0.36	0/307
1	FB	0.34	0/230	0.36	0/307
1	G	0.40	0/230	0.41	0/307
1	GA	0.39	0/230	0.40	0/307
1	GB	0.34	0/230	0.37	0/307
1	H	0.40	0/230	0.41	0/307
1	HA	0.34	0/230	0.36	0/307
1	HB	0.40	0/230	0.39	0/307
1	I	0.40	0/230	0.41	0/307
1	IA	0.34	0/230	0.36	0/307
1	IB	0.33	0/230	0.36	0/307
1	J	0.39	0/230	0.41	0/307
1	JA	0.40	0/230	0.39	0/307
1	JB	0.39	0/230	0.40	0/307
1	K	0.40	0/230	0.41	0/307
1	KA	0.34	0/230	0.36	0/307
1	KB	0.34	0/230	0.36	0/307
1	L	0.40	0/230	0.41	0/307
1	LA	0.39	0/230	0.40	0/307
1	LB	0.34	0/230	0.37	0/307
1	M	0.40	0/230	0.41	0/307
1	MA	0.34	0/230	0.36	0/307
1	MB	0.40	0/230	0.39	0/307
1	N	0.39	0/230	0.41	0/307
1	NA	0.34	0/230	0.37	0/307
1	NB	0.34	0/230	0.36	0/307
1	O	0.40	0/230	0.41	0/307
1	OA	0.40	0/230	0.39	0/307
1	OB	0.39	0/230	0.40	0/307
1	P	0.40	0/230	0.41	0/307
1	PA	0.34	0/230	0.36	0/307
1	PB	0.34	0/230	0.36	0/307
1	Q	0.40	0/230	0.41	0/307
1	QA	0.39	0/230	0.40	0/307
1	QB	0.33	0/230	0.37	0/307
1	R	0.39	0/230	0.41	0/307
1	RA	0.34	0/230	0.36	0/307
1	RB	0.40	0/230	0.39	0/307
1	S	0.40	0/230	0.41	0/307
1	SA	0.34	0/230	0.36	0/307
1	SB	0.33	0/230	0.36	0/307

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	T	0.40	0/230	0.41	0/307
1	TA	0.40	0/230	0.39	0/307
1	TB	0.39	0/230	0.40	0/307
1	U	0.40	0/230	0.41	0/307
1	UA	0.33	0/230	0.36	0/307
1	UB	0.34	0/230	0.36	0/307
1	V	0.40	0/230	0.41	0/307
1	VA	0.39	0/230	0.40	0/307
1	VB	0.34	0/230	0.37	0/307
1	W	0.40	0/230	0.41	0/307
1	WA	0.34	0/230	0.36	0/307
1	WB	0.40	0/230	0.39	0/307
1	X	0.40	0/230	0.41	0/307
1	XA	0.34	0/230	0.36	0/307
1	XB	0.34	0/230	0.36	0/307
1	Y	0.39	0/230	0.41	0/307
1	YA	0.40	0/230	0.39	0/307
1	YB	0.39	0/230	0.40	0/307
1	Z	0.34	0/230	0.37	0/307
1	ZA	0.34	0/230	0.36	0/307
1	ZB	0.33	0/230	0.36	0/307
1	a	0.40	0/230	0.39	0/307
1	aA	0.39	0/230	0.40	0/307
1	b	0.34	0/230	0.36	0/307
1	bA	0.34	0/230	0.36	0/307
1	c	0.39	0/230	0.40	0/307
1	cA	0.34	0/230	0.37	0/307
1	d	0.33	0/230	0.36	0/307
1	dA	0.40	0/230	0.39	0/307
1	e	0.33	0/230	0.36	0/307
1	eA	0.34	0/230	0.36	0/307
1	f	0.40	0/230	0.39	0/307
1	fA	0.39	0/230	0.40	0/307
1	g	0.33	0/230	0.36	0/307
1	gA	0.34	0/230	0.36	0/307
1	h	0.39	0/230	0.39	0/307
1	hA	0.33	0/230	0.37	0/307
1	i	0.33	0/230	0.36	0/307
1	iA	0.40	0/230	0.39	0/307
1	j	0.34	0/230	0.37	0/307
1	jA	0.33	0/230	0.36	0/307
1	k	0.40	0/230	0.39	0/307
1	kA	0.39	0/230	0.40	0/307

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	l	0.34	0/230	0.36	0/307
1	lA	0.34	0/230	0.36	0/307
1	m	0.39	0/230	0.40	0/307
1	mA	0.33	0/230	0.37	0/307
1	n	0.34	0/230	0.36	0/307
1	nA	0.40	0/230	0.39	0/307
1	o	0.34	0/230	0.37	0/307
1	oA	0.33	0/230	0.36	0/307
1	p	0.40	0/230	0.39	0/307
1	pA	0.39	0/230	0.40	0/307
1	q	0.33	0/230	0.36	0/307
1	qA	0.33	0/230	0.36	0/307
1	r	0.39	0/230	0.40	0/307
1	rA	0.34	0/230	0.37	0/307
1	s	0.34	0/230	0.36	0/307
1	sA	0.40	0/230	0.39	0/307
1	t	0.34	0/230	0.37	0/307
1	tA	0.33	0/230	0.36	0/307
1	u	0.40	0/230	0.39	0/307
1	uA	0.39	0/230	0.40	0/307
1	v	0.34	0/230	0.36	0/307
1	vA	0.34	0/230	0.36	0/307
1	w	0.39	0/230	0.40	0/307
1	wA	0.34	0/230	0.37	0/307
1	x	0.33	0/230	0.36	0/307
1	xA	0.40	0/230	0.39	0/307
1	y	0.33	0/230	0.37	0/307
1	yA	0.34	0/230	0.36	0/307
1	z	0.40	0/230	0.39	0/307
1	zA	0.39	0/230	0.40	0/307
All	All	0.37	0/34500	0.38	0/46050

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	229	0	239	3	0
1	0A	229	0	239	3	0
1	1	229	0	239	5	0
1	1A	229	0	239	2	0
1	2	229	0	239	2	0
1	2A	229	0	239	5	0
1	3	229	0	239	3	0
1	3A	229	0	239	1	0
1	4	229	0	239	7	0
1	4A	229	0	239	6	0
1	5	229	0	239	3	0
1	5A	229	0	239	3	0
1	6	229	0	239	6	0
1	6A	229	0	239	4	0
1	7	229	0	239	2	0
1	7A	229	0	239	7	0
1	8	229	0	239	2	0
1	8A	229	0	239	5	0
1	9	229	0	239	8	0
1	9A	229	0	239	4	0
1	A	229	0	242	9	0
1	AA	229	0	239	5	0
1	AB	229	0	239	4	0
1	B	229	0	242	9	0
1	BA	229	0	239	8	0
1	BB	229	0	239	4	0
1	C	229	0	242	7	0
1	CA	229	0	239	4	0
1	CB	229	0	239	7	0
1	D	229	0	242	7	0
1	DA	229	0	239	3	0
1	DB	229	0	239	2	0
1	E	229	0	242	7	0
1	EA	229	0	239	9	0
1	EB	229	0	239	10	0
1	F	229	0	242	6	0
1	FA	229	0	239	6	0
1	FB	229	0	239	4	0
1	G	229	0	242	7	0
1	GA	229	0	239	7	0
1	GB	229	0	239	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	229	0	242	6	0
1	HA	229	0	239	4	0
1	HB	229	0	239	8	0
1	I	229	0	242	5	0
1	IA	229	0	239	3	0
1	IB	229	0	239	5	0
1	J	229	0	242	5	0
1	JA	229	0	239	9	0
1	JB	229	0	239	7	0
1	K	229	0	242	4	0
1	KA	229	0	239	4	0
1	KB	229	0	239	3	0
1	L	229	0	242	8	0
1	LA	229	0	239	7	0
1	LB	229	0	239	5	0
1	M	229	0	242	6	0
1	MA	229	0	239	4	0
1	MB	229	0	239	7	0
1	N	229	0	242	8	0
1	NA	229	0	239	4	0
1	NB	229	0	239	2	0
1	O	229	0	242	10	0
1	OA	229	0	239	9	0
1	OB	229	0	239	8	0
1	P	229	0	242	9	0
1	PA	229	0	239	4	0
1	PB	229	0	239	4	0
1	Q	229	0	242	9	0
1	QA	229	0	239	5	0
1	QB	229	0	239	5	0
1	R	229	0	242	9	0
1	RA	229	0	239	2	0
1	RB	229	0	239	6	0
1	S	229	0	242	10	0
1	SA	229	0	239	3	0
1	SB	229	0	239	4	0
1	T	229	0	242	9	0
1	TA	229	0	239	6	0
1	TB	229	0	239	5	0
1	U	229	0	242	6	0
1	UA	229	0	239	5	0
1	UB	229	0	239	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	V	229	0	242	8	0
1	VA	229	0	239	6	0
1	VB	229	0	239	4	0
1	W	229	0	242	4	0
1	WA	229	0	239	2	0
1	WB	229	0	239	7	0
1	X	229	0	242	4	0
1	XA	229	0	239	4	0
1	XB	229	0	239	2	0
1	Y	229	0	242	3	0
1	YA	229	0	239	7	0
1	YB	229	0	239	3	0
1	Z	229	0	239	0	0
1	ZA	229	0	239	3	0
1	ZB	229	0	239	2	0
1	a	229	0	239	0	0
1	aA	229	0	239	0	0
1	b	229	0	239	0	0
1	bA	229	0	239	0	0
1	c	229	0	239	0	0
1	cA	229	0	239	0	0
1	d	229	0	239	0	0
1	dA	229	0	239	0	0
1	e	229	0	239	0	0
1	eA	229	0	239	0	0
1	f	229	0	239	0	0
1	fA	229	0	239	0	0
1	g	229	0	239	0	0
1	gA	229	0	239	0	0
1	h	229	0	239	0	0
1	hA	229	0	239	0	0
1	i	229	0	239	0	0
1	iA	229	0	239	0	0
1	j	229	0	239	0	0
1	jA	229	0	239	0	0
1	k	229	0	239	0	0
1	kA	229	0	239	0	0
1	l	229	0	239	0	0
1	lA	229	0	239	0	0
1	m	229	0	239	0	0
1	mA	229	0	239	0	0
1	n	229	0	239	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	nA	229	0	239	0	0
1	o	229	0	239	0	0
1	oA	229	0	239	0	0
1	p	229	0	239	0	0
1	pA	229	0	239	0	0
1	q	229	0	239	0	0
1	qA	229	0	239	0	0
1	r	229	0	239	0	0
1	rA	229	0	239	0	0
1	s	229	0	239	0	0
1	sA	229	0	239	0	0
1	t	229	0	239	0	0
1	tA	229	0	239	0	0
1	u	229	0	239	0	0
1	uA	229	0	239	0	0
1	v	229	0	239	0	0
1	vA	229	0	239	0	0
1	w	229	0	239	0	0
1	wA	229	0	239	0	0
1	x	229	0	239	0	0
1	xA	229	0	239	0	0
1	y	229	0	239	0	0
1	yA	229	0	239	0	0
1	z	229	0	239	0	0
1	zA	229	0	239	0	0
All	All	34350	0	35925	353	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (353) 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)
1:4:1025:ILE:HG12	1:EA:1023:ALA:HB2	1.58	0.84
1:2A:1025:ILE:HG12	1:CB:1023:ALA:HB2	1.57	0.84
1:JA:1023:ALA:HB2	1:TA:1025:ILE:HG12	1.59	0.83
1:HB:1023:ALA:HB2	1:RB:1025:ILE:HG12	1.61	0.82
1:7A:1023:ALA:HB2	1:HB:1025:ILE:HG12	1.59	0.82
1:OA:1025:ILE:HG12	1:YA:1023:ALA:HB2	1.61	0.81
1:EA:1025:ILE:HG12	1:OA:1023:ALA:HB2	1.63	0.80
1:MB:1025:ILE:HG12	1:WB:1023:ALA:HB2	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:9:1023:ALA:HB2	1:JA:1025:ILE:HG12	1.64	0.78
1:CB:1025:ILE:HG12	1:MB:1023:ALA:HB2	1.66	0.76
1:JB:2023:ALA:HB2	1:TB:2025:ILE:HG12	1.71	0.72
1:1:2023:ALA:HB2	1:BA:2025:ILE:HG12	1.72	0.72
1:6:2025:ILE:HG12	1:GA:2023:ALA:HB2	1.72	0.71
1:4A:2025:ILE:HG12	1:EB:2023:ALA:HB2	1.72	0.71
1:GA:2001:GLN:N	1:Q:29:GLN:O	2.24	0.70
1:LA:2023:ALA:HB2	1:VA:2025:ILE:HG12	1.74	0.69
1:B:1:GLN:N	1:4:1029:GLN:O	2.22	0.69
1:9:1029:GLN:O	1:P:1:GLN:N	2.26	0.69
1:C:29:GLN:O	1:1:2001:GLN:N	2.27	0.68
1:GA:2025:ILE:HG12	1:QA:2023:ALA:HB2	1.76	0.68
1:5A:2105:LEU:HD12	1:FB:2104:ILE:HD11	1.76	0.67
1:2:2104:ILE:HD11	1:CA:2105:LEU:HD12	1.77	0.67
1:BA:2023:ALA:HB2	1:LA:2025:ILE:HG12	1.77	0.66
1:9A:2023:ALA:HB2	1:JB:2025:ILE:HG12	1.76	0.66
1:D:29:GLN:O	1:VA:2001:GLN:N	2.28	0.66
1:OB:2025:ILE:HG12	1:YB:2023:ALA:HB2	1.76	0.66
1:6:2001:GLN:N	1:O:29:GLN:O	2.29	0.65
1:1:2006:GLU:OE1	1:BA:2010:ARG:NH1	2.26	0.65
1:B:29:GLN:O	1:LA:2001:GLN:N	2.29	0.65
1:2A:1010:ARG:NH1	1:CB:1006:GLU:OE1	2.28	0.64
1:EB:2025:ILE:HG12	1:OB:2023:ALA:HB2	1.78	0.64
1:7:2105:LEU:HD12	1:HA:2104:ILE:HD11	1.80	0.63
1:A:29:GLN:O	1:BA:2001:GLN:N	2.32	0.63
1:O:3:GLU:OE1	1:O:3:GLU:N	2.26	0.62
1:P:3:GLU:OE1	1:P:3:GLU:N	2.25	0.62
1:C:1:GLN:N	1:OA:1029:GLN:O	2.28	0.62
1:E:1:GLN:N	1:YA:1029:GLN:O	2.28	0.62
1:E:3:GLU:OE1	1:E:3:GLU:N	2.26	0.62
1:6:2010:ARG:NH1	1:GA:2006:GLU:OE1	2.29	0.62
1:9A:2006:GLU:OE1	1:JB:2010:ARG:NH1	2.31	0.61
1:F:3:GLU:OE1	1:F:3:GLU:N	2.25	0.61
1:D:3:GLU:OE1	1:D:3:GLU:N	2.26	0.61
1:JB:2003:GLU:OE1	1:JB:2003:GLU:N	2.25	0.61
1:9A:2003:GLU:OE1	1:9A:2003:GLU:N	2.25	0.60
1:YB:2003:GLU:OE1	1:YB:2003:GLU:N	2.25	0.60
1:LA:2006:GLU:OE1	1:VA:2010:ARG:NH1	2.31	0.60
1:R:3:GLU:OE1	1:R:3:GLU:N	2.26	0.60
1:M:3:GLU:OE1	1:M:3:GLU:N	2.25	0.60
1:Y:3:GLU:OE1	1:Y:3:GLU:N	2.25	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:2003:GLU:OE1	1:QA:2003:GLU:N	2.25	0.59
1:H:3:GLU:OE1	1:H:3:GLU:N	2.26	0.59
1:Q:1:GLN:N	1:WB:1029:GLN:O	2.31	0.59
1:C:3:GLU:OE1	1:C:3:GLU:N	2.25	0.59
1:0A:2104:ILE:HD11	1:AB:2105:LEU:HD12	1.85	0.59
1:J:3:GLU:OE1	1:J:3:GLU:N	2.25	0.59
1:4A:2010:ARG:NH1	1:EB:2006:GLU:OE1	2.26	0.58
1:TB:2003:GLU:OE1	1:TB:2003:GLU:N	2.25	0.58
1:MA:2104:ILE:HD11	1:WA:2105:LEU:HD12	1.85	0.58
1:AB:2104:ILE:HD11	1:KB:2105:LEU:HD12	1.85	0.58
1:X:3:GLU:OE1	1:X:3:GLU:N	2.25	0.58
1:GA:2003:GLU:OE1	1:GA:2003:GLU:N	2.25	0.58
1:VA:2029:GLN:O	1:7A:1001:GLN:N	2.36	0.58
1:T:3:GLU:OE1	1:T:3:GLU:N	2.25	0.58
1:W:3:GLU:OE1	1:W:3:GLU:N	2.25	0.58
1:OB:2003:GLU:OE1	1:OB:2003:GLU:N	2.25	0.58
1:L:3:GLU:OE1	1:L:3:GLU:N	2.25	0.58
1:K:3:GLU:OE1	1:K:3:GLU:N	2.25	0.57
1:I:3:GLU:OE1	1:I:3:GLU:N	2.25	0.57
1:7A:1003:GLU:OE1	1:7A:1003:GLU:N	2.32	0.57
1:0:1104:ILE:HD11	1:AA:1105:LEU:HD12	1.87	0.57
1:WB:1003:GLU:OE1	1:WB:1003:GLU:N	2.32	0.57
1:Q:3:GLU:OE1	1:Q:3:GLU:N	2.25	0.57
1:OA:1001:GLN:N	1:4A:2029:GLN:O	2.37	0.57
1:N:3:GLU:OE1	1:N:3:GLU:N	2.25	0.57
1:P:29:GLN:O	1:TB:2001:GLN:N	2.38	0.57
1:G:3:GLU:OE1	1:G:3:GLU:N	2.26	0.56
1:S:3:GLU:OE1	1:S:3:GLU:N	2.25	0.56
1:1:2003:GLU:OE1	1:1:2003:GLU:N	2.25	0.56
1:4:1003:GLU:OE1	1:4:1003:GLU:N	2.32	0.56
1:7A:1006:GLU:OE1	1:HB:1010:ARG:NH1	2.35	0.56
1:HB:1003:GLU:OE1	1:HB:1003:GLU:N	2.32	0.56
1:3A:1105:LEU:HD12	1:DB:1104:ILE:HD11	1.87	0.56
1:6:2003:GLU:OE1	1:6:2003:GLU:N	2.25	0.56
1:KB:2104:ILE:HD11	1:UB:2105:LEU:HD12	1.86	0.56
1:U:3:GLU:OE1	1:U:3:GLU:N	2.26	0.56
1:HB:1006:GLU:OE1	1:RB:1010:ARG:NH1	2.32	0.56
1:S:10:ARG:NH1	1:U:6:GLU:OE2	2.36	0.56
1:V:3:GLU:OE1	1:V:3:GLU:N	2.25	0.56
1:A:3:GLU:OE1	1:A:3:GLU:N	2.25	0.56
1:QA:2001:GLN:N	1:S:29:GLN:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EB:2003:GLU:OE1	1:EB:2003:GLU:N	2.25	0.56
1:1A:105:LEU:HD12	1:BB:104:ILE:HD11	1.89	0.55
1:RB:1003:GLU:OE1	1:RB:1003:GLU:N	2.32	0.55
1:TA:1003:GLU:OE1	1:TA:1003:GLU:N	2.32	0.55
1:MB:1003:GLU:OE1	1:MB:1003:GLU:N	2.32	0.55
1:9:1003:GLU:OE1	1:9:1003:GLU:N	2.32	0.54
1:BA:2003:GLU:OE1	1:BA:2003:GLU:N	2.25	0.54
1:4:1010:ARG:NH1	1:EA:1006:GLU:OE1	2.31	0.54
1:N:29:GLN:O	1:JB:2001:GLN:N	2.41	0.54
1:LA:2003:GLU:OE1	1:LA:2003:GLU:N	2.25	0.54
1:TA:1029:GLN:O	1:T:1:GLN:N	2.40	0.54
1:A:1:GLN:N	1:EA:1029:GLN:O	2.36	0.54
1:YA:1003:GLU:OE1	1:YA:1003:GLU:N	2.32	0.54
1:JA:1003:GLU:OE1	1:JA:1003:GLU:N	2.32	0.54
1:5:1105:LEU:HD12	1:FA:1104:ILE:HD11	1.91	0.53
1:VA:2003:GLU:OE1	1:VA:2003:GLU:N	2.25	0.53
1:4A:2003:GLU:OE1	1:4A:2003:GLU:N	2.25	0.53
1:B:3:GLU:OE1	1:B:3:GLU:N	2.25	0.53
1:3:105:LEU:HD12	1:DA:104:ILE:HD11	1.91	0.53
1:F:23:ALA:HB2	1:H:25:ILE:HG12	1.90	0.53
1:O:1:GLN:N	1:MB:1029:GLN:O	2.39	0.52
1:R:23:ALA:HB2	1:T:25:ILE:HG12	1.91	0.52
1:L:23:ALA:HB2	1:N:25:ILE:HG12	1.91	0.52
1:Q:25:ILE:HG12	1:S:23:ALA:HB2	1.90	0.52
1:CB:1003:GLU:OE1	1:CB:1003:GLU:N	2.32	0.52
1:J:23:ALA:HB2	1:L:25:ILE:HG12	1.91	0.52
1:S:25:ILE:HG12	1:U:23:ALA:HB2	1.90	0.52
1:IB:1104:ILE:HD11	1:SB:1105:LEU:HD12	1.92	0.52
1:B:23:ALA:HB2	1:D:25:ILE:HG12	1.91	0.52
1:A:25:ILE:HG12	1:C:23:ALA:HB2	1.90	0.52
1:V:23:ALA:HB2	1:X:25:ILE:HG12	1.92	0.52
1:L:29:GLN:O	1:9A:2001:GLN:N	2.43	0.52
1:K:1:GLN:N	1:2A:1029:GLN:O	2.40	0.52
1:N:23:ALA:HB2	1:P:25:ILE:HG12	1.92	0.52
1:E:25:ILE:HG12	1:G:23:ALA:HB2	1.91	0.52
1:G:25:ILE:HG12	1:I:23:ALA:HB2	1.91	0.51
1:T:23:ALA:HB2	1:V:25:ILE:HG12	1.92	0.51
1:PB:2105:LEU:HD12	1:ZB:2104:ILE:HD11	1.91	0.51
1:O:25:ILE:HG12	1:Q:23:ALA:HB2	1.92	0.51
1:W:25:ILE:HG12	1:Y:23:ALA:HB2	1.92	0.51
1:A:23:ALA:HB2	1:B:25:ILE:HG12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:25:ILE:HG12	1:O:23:ALA:HB2	1.92	0.51
1:D:23:ALA:HB2	1:F:25:ILE:HG12	1.93	0.51
1:K:25:ILE:HG12	1:M:23:ALA:HB2	1.92	0.51
1:C:25:ILE:HG12	1:E:23:ALA:HB2	1.93	0.51
1:HA:2105:LEU:HD12	1:RA:2104:ILE:HD11	1.92	0.51
1:I:25:ILE:HG12	1:K:23:ALA:HB2	1.93	0.51
1:P:23:ALA:HB2	1:R:25:ILE:HG12	1.92	0.51
1:H:23:ALA:HB2	1:J:25:ILE:HG12	1.93	0.50
1:OA:1003:GLU:OE1	1:OA:1003:GLU:N	2.32	0.50
1:JA:1006:GLU:OE1	1:TA:1010:ARG:NH1	2.34	0.50
1:U:25:ILE:HG12	1:W:23:ALA:HB2	1.94	0.50
1:Q:10:ARG:NH1	1:S:6:GLU:OE2	2.35	0.50
1:2A:1003:GLU:OE1	1:2A:1003:GLU:N	2.32	0.50
1:CA:2104:ILE:HD11	1:MA:2105:LEU:HD12	1.94	0.49
1:JB:2006:GLU:OE1	1:TB:2010:ARG:NH1	2.36	0.49
1:B:6:GLU:OE2	1:D:10:ARG:NH1	2.40	0.49
1:P:6:GLU:OE2	1:R:10:ARG:NH1	2.36	0.49
1:F:6:GLU:OE2	1:H:10:ARG:NH1	2.36	0.49
1:IA:104:ILE:HD11	1:SA:105:LEU:HD12	1.94	0.49
1:7A:1021:ALA:O	1:7A:1025:ILE:HG13	2.13	0.49
1:OB:2010:ARG:NH1	1:YB:2006:GLU:OE1	2.36	0.49
1:WB:1021:ALA:O	1:WB:1025:ILE:HG13	2.13	0.49
1:KA:1104:ILE:HD11	1:UA:1105:LEU:HD12	1.95	0.49
1:CB:1021:ALA:O	1:CB:1025:ILE:HG13	2.13	0.48
1:HB:1021:ALA:O	1:HB:1025:ILE:HG13	2.13	0.48
1:MB:1021:ALA:O	1:MB:1025:ILE:HG13	2.13	0.48
1:2A:1021:ALA:O	1:2A:1025:ILE:HG13	2.13	0.48
1:MB:1010:ARG:NH1	1:WB:1006:GLU:OE1	2.39	0.48
1:RB:1021:ALA:O	1:RB:1025:ILE:HG13	2.13	0.48
1:G:10:ARG:NH1	1:I:6:GLU:OE2	2.38	0.48
1:YA:1021:ALA:O	1:YA:1025:ILE:HG13	2.13	0.48
1:4:1021:ALA:O	1:4:1025:ILE:HG13	2.13	0.48
1:9:1021:ALA:O	1:9:1025:ILE:HG13	2.13	0.48
1:6A:104:ILE:HD11	1:GB:105:LEU:HD12	1.96	0.48
1:JA:1021:ALA:O	1:JA:1025:ILE:HG13	2.13	0.48
1:T:6:GLU:OE2	1:V:10:ARG:NH1	2.40	0.48
1:8A:1104:ILE:HD11	1:IB:1105:LEU:HD12	1.96	0.48
1:EA:1021:ALA:O	1:EA:1025:ILE:HG13	2.13	0.48
1:M:10:ARG:NH1	1:O:6:GLU:OE2	2.41	0.48
1:EA:1003:GLU:OE1	1:EA:1003:GLU:N	2.32	0.48
1:TA:1021:ALA:O	1:TA:1025:ILE:HG13	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:OA:1010:ARG:NH1	1:YA:1006:GLU:OE1	2.37	0.47
1:OA:1021:ALA:O	1:OA:1025:ILE:HG13	2.13	0.47
1:GA:2010:ARG:NH1	1:QA:2006:GLU:OE1	2.36	0.47
1:KA:1119:LEU:HD23	1:KA:1119:LEU:HA	1.73	0.47
1:L:6:GLU:OE2	1:N:10:ARG:NH1	2.40	0.47
1:J:6:GLU:OE2	1:L:10:ARG:NH1	2.41	0.47
1:E:10:ARG:NH1	1:G:6:GLU:OE2	2.43	0.46
1:UA:1119:LEU:HD23	1:UA:1119:LEU:HA	1.73	0.46
1:SB:1119:LEU:HD23	1:SB:1119:LEU:HA	1.74	0.46
1:WB:1019:LEU:HD23	1:WB:1019:LEU:HA	1.82	0.46
1:EA:1010:ARG:NH1	1:OA:1006:GLU:OE1	2.38	0.46
1:IB:1119:LEU:HD23	1:IB:1119:LEU:HA	1.73	0.46
1:O:10:ARG:NH1	1:Q:6:GLU:OE2	2.41	0.46
1:P:26:LEU:HD12	1:P:26:LEU:HA	1.77	0.46
1:R:6:GLU:OE2	1:T:10:ARG:NH1	2.42	0.46
1:8A:1119:LEU:HD23	1:8A:1119:LEU:HA	1.73	0.46
1:JB:2026:LEU:HD21	1:TB:2029:GLN:HG2	1.97	0.46
1:QB:103:GLU:OE1	1:QB:103:GLU:N	2.34	0.46
1:EB:2010:ARG:NH1	1:OB:2006:GLU:OE1	2.40	0.46
1:NA:105:LEU:HD12	1:XA:104:ILE:HD11	1.98	0.46
1:HB:1026:LEU:HD12	1:HB:1026:LEU:HA	1.79	0.46
1:IB:1107:ALA:HB1	1:SB:1112:LEU:HB3	1.98	0.46
1:PA:1105:LEU:HD12	1:ZA:1104:ILE:HD11	1.99	0.45
1:UA:1103:GLU:OE1	1:UA:1103:GLU:N	2.34	0.45
1:S:25:ILE:CG1	1:U:23:ALA:HB2	2.47	0.45
1:CB:1018:ILE:HD11	1:MB:1012:LEU:HD12	1.99	0.45
1:YA:1001:GLN:N	1:EB:2029:GLN:O	2.50	0.45
1:Q:25:ILE:CG1	1:S:23:ALA:HB2	2.47	0.45
1:VB:103:GLU:OE1	1:VB:103:GLU:N	2.34	0.45
1:F:23:ALA:HB2	1:H:25:ILE:CG1	2.47	0.45
1:F:26:LEU:HD12	1:F:26:LEU:HA	1.77	0.45
1:GB:104:ILE:HD11	1:QB:105:LEU:HD12	1.97	0.45
1:QA:2019:LEU:HD23	1:QA:2019:LEU:HA	1.84	0.45
1:5:1119:LEU:HA	1:5:1119:LEU:HD23	1.74	0.44
1:4A:2029:GLN:HG2	1:EB:2026:LEU:HD21	1.99	0.44
1:GB:107:ALA:HB1	1:QB:112:LEU:HB3	1.99	0.44
1:M:1:GLN:N	1:CB:1029:GLN:O	2.50	0.44
1:PA:1119:LEU:HD23	1:PA:1119:LEU:HA	1.73	0.44
1:WA:2119:LEU:HA	1:WA:2119:LEU:HD23	1.74	0.44
1:ZA:1119:LEU:HA	1:ZA:1119:LEU:HD23	1.73	0.44
1:9:1026:LEU:HD12	1:9:1026:LEU:HA	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FA:1119:LEU:HD23	1:FA:1119:LEU:HA	1.74	0.44
1:O:26:LEU:HD12	1:O:26:LEU:HA	1.77	0.44
1:H:26:LEU:HD12	1:H:26:LEU:HA	1.77	0.44
1:FB:2105:LEU:HD12	1:PB:2104:ILE:HD11	1.99	0.44
1:LB:103:GLU:OE1	1:LB:103:GLU:N	2.34	0.44
1:O:1103:GLU:OE1	1:O:1103:GLU:N	2.34	0.44
1:SA:103:GLU:OE1	1:SA:103:GLU:N	2.34	0.43
1:VA:2012:LEU:HD13	1:VA:2012:LEU:HA	1.90	0.43
1:N:26:LEU:HD12	1:N:26:LEU:HA	1.77	0.43
1:MA:2119:LEU:HD23	1:MA:2119:LEU:HA	1.74	0.43
1:5A:2119:LEU:HA	1:5A:2119:LEU:HD23	1.74	0.43
1:W:26:LEU:HD12	1:W:26:LEU:HA	1.77	0.43
1:XA:119:LEU:HA	1:XA:119:LEU:HD23	1.79	0.43
1:YA:1026:LEU:HD12	1:YA:1026:LEU:HA	1.79	0.43
1:RB:1019:LEU:HD23	1:RB:1019:LEU:HA	1.82	0.43
1:G:25:ILE:CG1	1:I:23:ALA:HB2	2.49	0.43
1:RB:1026:LEU:HD12	1:RB:1026:LEU:HA	1.79	0.43
1:9:1006:GLU:OE1	1:JA:1010:ARG:NH1	2.40	0.43
1:IA:103:GLU:OE1	1:IA:103:GLU:N	2.34	0.43
1:RA:2119:LEU:HD23	1:RA:2119:LEU:HA	1.74	0.43
1:A:12:LEU:HD13	1:A:12:LEU:HA	1.92	0.43
1:6:2012:LEU:HD13	1:6:2012:LEU:HA	1.90	0.43
1:CA:2119:LEU:HD23	1:CA:2119:LEU:HA	1.74	0.43
1:E:26:LEU:HD12	1:E:26:LEU:HA	1.77	0.43
1:P:23:ALA:HB2	1:R:25:ILE:CG1	2.49	0.43
1:HB:1019:LEU:HA	1:HB:1019:LEU:HD23	1.82	0.43
1:OB:2012:LEU:HD13	1:OB:2012:LEU:HA	1.91	0.43
1:A:25:ILE:CG1	1:C:23:ALA:HB2	2.49	0.43
1:1:2026:LEU:HD21	1:BA:2029:GLN:HG2	2.00	0.43
1:NA:119:LEU:HA	1:NA:119:LEU:HD23	1.79	0.43
1:B:26:LEU:HD12	1:B:26:LEU:HA	1.77	0.43
1:FA:1105:LEU:HD12	1:PA:1104:ILE:HD11	2.01	0.43
1:FB:2119:LEU:HA	1:FB:2119:LEU:HD23	1.74	0.43
1:EA:1019:LEU:HD23	1:EA:1019:LEU:HA	1.82	0.42
1:OA:2119:LEU:HA	1:OA:2119:LEU:HD23	1.74	0.42
1:7A:1019:LEU:HD23	1:7A:1019:LEU:HA	1.82	0.42
1:FA:1103:GLU:OE1	1:FA:1103:GLU:N	2.34	0.42
1:HA:2119:LEU:HD23	1:HA:2119:LEU:HA	1.74	0.42
1:N:6:GLU:OE2	1:P:10:ARG:NH1	2.43	0.42
1:B:23:ALA:HB2	1:D:25:ILE:CG1	2.49	0.42
1:8:103:GLU:OE1	1:8:103:GLU:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:PA:1103:GLU:OE1	1:PA:1103:GLU:N	2.34	0.42
1:2:2119:LEU:HD23	1:2:2119:LEU:HA	1.74	0.42
1:5:1103:GLU:OE1	1:5:1103:GLU:N	2.34	0.42
1:7:2119:LEU:HD23	1:7:2119:LEU:HA	1.74	0.42
1:L:23:ALA:HB2	1:N:25:ILE:CG1	2.49	0.42
1:BB:103:GLU:OE1	1:BB:103:GLU:N	2.34	0.42
1:FB:2104:ILE:H	1:FB:2104:ILE:HG13	1.67	0.42
1:B:12:LEU:HD13	1:B:12:LEU:HA	1.91	0.42
1:S:26:LEU:HD12	1:S:26:LEU:HA	1.77	0.42
1:8A:1103:GLU:OE1	1:8A:1103:GLU:N	2.34	0.42
1:LB:105:LEU:HD12	1:VB:104:ILE:HD11	2.02	0.42
1:XB:1119:LEU:HA	1:XB:1119:LEU:HD23	1.74	0.42
1:A:10:ARG:NH1	1:C:6:GLU:OE2	2.41	0.42
1:AA:1103:GLU:OE1	1:AA:1103:GLU:N	2.34	0.42
1:DA:119:LEU:HA	1:DA:119:LEU:HD23	1.79	0.42
1:ZA:1103:GLU:OE1	1:ZA:1103:GLU:N	2.34	0.42
1:R:26:LEU:HD12	1:R:26:LEU:HA	1.77	0.42
1:AB:2119:LEU:HA	1:AB:2119:LEU:HD23	1.74	0.42
1:PB:2119:LEU:HD23	1:PB:2119:LEU:HA	1.75	0.42
1:X:26:LEU:HD12	1:X:26:LEU:HA	1.77	0.42
1:MA:2104:ILE:H	1:MA:2104:ILE:HG13	1.67	0.42
1:V:12:LEU:HD13	1:V:12:LEU:HA	1.91	0.42
1:FA:1127:LYS:HE2	1:FA:1127:LYS:HB2	1.92	0.42
1:JA:1029:GLN:O	1:R:1:GLN:N	2.42	0.42
1:EB:2018:ILE:HD11	1:OB:2012:LEU:HD12	2.02	0.42
1:NB:1105:LEU:HD12	1:XB:1104:ILE:HD11	2.02	0.42
1:ZB:2119:LEU:HD23	1:ZB:2119:LEU:HA	1.74	0.42
1:DA:105:LEU:HD12	1:NA:104:ILE:HD11	2.02	0.41
1:OA:1026:LEU:HD12	1:OA:1026:LEU:HA	1.79	0.41
1:QB:119:LEU:HA	1:QB:119:LEU:HD23	1.79	0.41
1:1A:103:GLU:OE1	1:1A:103:GLU:N	2.34	0.41
1:EB:2012:LEU:HD13	1:EB:2012:LEU:HA	1.90	0.41
1:4:1019:LEU:HD23	1:4:1019:LEU:HA	1.82	0.41
1:V:26:LEU:HD12	1:V:26:LEU:HA	1.77	0.41
1:O:1107:ALA:HB1	1:AA:1112:LEU:HB3	2.03	0.41
1:9:1019:LEU:HD23	1:9:1019:LEU:HA	1.82	0.41
1:BA:2006:GLU:OE1	1:LA:2010:ARG:NH1	2.38	0.41
1:FA:1104:ILE:H	1:FA:1104:ILE:HG13	1.69	0.41
1:HA:2125:ILE:HD13	1:HA:2125:ILE:HA	1.91	0.41
1:JA:1026:LEU:HD12	1:JA:1026:LEU:HA	1.79	0.41
1:KA:1107:ALA:HB1	1:UA:1112:LEU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:26:LEU:HA	1:U:26:LEU:HD12	1.77	0.41
1:NB:1119:LEU:HA	1:NB:1119:LEU:HD23	1.73	0.41
1:EA:1026:LEU:HA	1:EA:1026:LEU:HD12	1.79	0.41
1:4A:2019:LEU:HD23	1:4A:2019:LEU:HA	1.83	0.41
1:KB:2119:LEU:HD23	1:KB:2119:LEU:HA	1.74	0.41
1:UB:2119:LEU:HD23	1:UB:2119:LEU:HA	1.74	0.41
1:WB:1026:LEU:HD12	1:WB:1026:LEU:HA	1.78	0.41
1:9:1012:LEU:HD12	1:JA:1018:ILE:HD11	2.03	0.41
1:6A:104:ILE:H	1:6A:104:ILE:HG13	1.68	0.41
1:E:25:ILE:CG1	1:G:23:ALA:HB2	2.51	0.41
1:CA:2125:ILE:HD13	1:CA:2125:ILE:HA	1.91	0.41
1:J:23:ALA:HB2	1:L:25:ILE:CG1	2.50	0.41
1:UA:1127:LYS:HE2	1:UA:1127:LYS:HB2	1.92	0.41
1:T:23:ALA:HB2	1:V:25:ILE:CG1	2.50	0.41
1:IB:1103:GLU:OE1	1:IB:1103:GLU:N	2.34	0.41
1:LB:112:LEU:HB3	1:VB:107:ALA:HB1	2.03	0.41
1:3:119:LEU:HA	1:3:119:LEU:HD23	1.79	0.41
1:AA:1127:LYS:HE2	1:AA:1127:LYS:HB2	1.92	0.41
1:BA:2012:LEU:HD12	1:LA:2018:ILE:HD11	2.03	0.41
1:NA:112:LEU:HB3	1:XA:107:ALA:HB1	2.03	0.41
1:M:25:ILE:CG1	1:O:23:ALA:HB2	2.51	0.41
1:XA:104:ILE:H	1:XA:104:ILE:HG13	1.68	0.41
1:O:25:ILE:CG1	1:Q:23:ALA:HB2	2.51	0.41
1:0A:2125:ILE:HD13	1:0A:2125:ILE:HA	1.91	0.41
1:T:26:LEU:HD12	1:T:26:LEU:HA	1.77	0.41
1:6A:103:GLU:OE1	1:6A:103:GLU:N	2.34	0.41
1:8A:1127:LYS:HE2	1:8A:1127:LYS:HB2	1.92	0.41
1:GB:119:LEU:HA	1:GB:119:LEU:HD23	1.79	0.41
1:D:12:LEU:HD13	1:D:12:LEU:HA	1.91	0.41
1:AB:2104:ILE:H	1:AB:2104:ILE:HG13	1.67	0.41
1:LB:125:ILE:HD12	1:LB:128:ALA:HB3	2.03	0.41
1:PB:2104:ILE:H	1:PB:2104:ILE:HG13	1.67	0.41
1:A:26:LEU:HD12	1:A:26:LEU:HA	1.77	0.40
1:IA:125:ILE:HD12	1:IA:128:ALA:HB3	2.03	0.40
1:DB:1119:LEU:HA	1:DB:1119:LEU:HD23	1.74	0.40
1:VB:125:ILE:HD12	1:VB:128:ALA:HB3	2.04	0.40
1:4:1026:LEU:HA	1:4:1026:LEU:HD12	1.78	0.40
1:6:2029:GLN:HG2	1:GA:2026:LEU:HD21	2.02	0.40
1:8:125:ILE:HD12	1:8:128:ALA:HB3	2.03	0.40
1:S:12:LEU:HD13	1:S:12:LEU:HA	1.91	0.40
1:QB:125:ILE:HD12	1:QB:128:ALA:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:104:ILE:H	1:3:104:ILE:HG13	1.68	0.40
1:SA:125:ILE:HD12	1:SA:128:ALA:HB3	2.04	0.40
1:R:23:ALA:HB2	1:T:25:ILE:CG1	2.51	0.40
1:5A:2127:LYS:HE2	1:5A:2127:LYS:HB2	1.94	0.40
1:7A:1026:LEU:HA	1:7A:1026:LEU:HD12	1.78	0.40
1:V:6:GLU:OE2	1:X:10:ARG:NH1	2.44	0.40
1:6A:125:ILE:HD12	1:6A:128:ALA:HB3	2.04	0.40
1:BB:125:ILE:HD12	1:BB:128:ALA:HB3	2.03	0.40
1:EB:2019:LEU:HD23	1:EB:2019:LEU:HA	1.84	0.40
1:GB:125:ILE:HD12	1:GB:128:ALA:HB3	2.04	0.40
1:SB:1127:LYS:HE2	1:SB:1127:LYS:HB2	1.92	0.40
1:Y:26:LEU:HD12	1:Y:26:LEU:HA	1.77	0.40
1:AA:1104:ILE:HD11	1:KA:1105:LEU:HD12	2.03	0.40
1:TA:1019:LEU:HD23	1:TA:1019:LEU:HA	1.82	0.40
1:8A:1104:ILE:H	1:8A:1104:ILE:HG13	1.69	0.40
1:BB:112:LEU:HB3	1:LB:107:ALA:HB1	2.04	0.40
1:OB:2019:LEU:HD23	1:OB:2019:LEU:HA	1.83	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	0	27/29 (93%)	27 (100%)	0	0	100	100
1	0A	27/29 (93%)	27 (100%)	0	0	100	100
1	1	27/29 (93%)	27 (100%)	0	0	100	100
1	1A	27/29 (93%)	27 (100%)	0	0	100	100
1	2	27/29 (93%)	27 (100%)	0	0	100	100
1	2A	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	3	27/29 (93%)	27 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3A	27/29 (93%)	27 (100%)	0	0	100	100
1	4	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	4A	27/29 (93%)	27 (100%)	0	0	100	100
1	5	27/29 (93%)	27 (100%)	0	0	100	100
1	5A	27/29 (93%)	27 (100%)	0	0	100	100
1	6	27/29 (93%)	27 (100%)	0	0	100	100
1	6A	27/29 (93%)	27 (100%)	0	0	100	100
1	7	27/29 (93%)	27 (100%)	0	0	100	100
1	7A	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	8	27/29 (93%)	27 (100%)	0	0	100	100
1	8A	27/29 (93%)	27 (100%)	0	0	100	100
1	9	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	9A	27/29 (93%)	27 (100%)	0	0	100	100
1	A	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	AA	27/29 (93%)	27 (100%)	0	0	100	100
1	AB	27/29 (93%)	27 (100%)	0	0	100	100
1	B	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	BA	27/29 (93%)	27 (100%)	0	0	100	100
1	BB	27/29 (93%)	27 (100%)	0	0	100	100
1	C	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	CA	27/29 (93%)	27 (100%)	0	0	100	100
1	CB	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	D	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	DA	27/29 (93%)	27 (100%)	0	0	100	100
1	DB	27/29 (93%)	27 (100%)	0	0	100	100
1	E	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	EA	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	EB	27/29 (93%)	27 (100%)	0	0	100	100
1	F	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	FA	27/29 (93%)	27 (100%)	0	0	100	100
1	FB	27/29 (93%)	27 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	GA	27/29 (93%)	27 (100%)	0	0	100	100
1	GB	27/29 (93%)	27 (100%)	0	0	100	100
1	H	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	HA	27/29 (93%)	27 (100%)	0	0	100	100
1	HB	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	I	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	IA	27/29 (93%)	27 (100%)	0	0	100	100
1	IB	27/29 (93%)	27 (100%)	0	0	100	100
1	J	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	JA	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	JB	27/29 (93%)	27 (100%)	0	0	100	100
1	K	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	KA	27/29 (93%)	27 (100%)	0	0	100	100
1	KB	27/29 (93%)	27 (100%)	0	0	100	100
1	L	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	LA	27/29 (93%)	27 (100%)	0	0	100	100
1	LB	27/29 (93%)	27 (100%)	0	0	100	100
1	M	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	MA	27/29 (93%)	27 (100%)	0	0	100	100
1	MB	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	N	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	NA	27/29 (93%)	27 (100%)	0	0	100	100
1	NB	27/29 (93%)	27 (100%)	0	0	100	100
1	O	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	OA	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	OB	27/29 (93%)	27 (100%)	0	0	100	100
1	P	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	PA	27/29 (93%)	27 (100%)	0	0	100	100
1	PB	27/29 (93%)	27 (100%)	0	0	100	100
1	Q	27/29 (93%)	26 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	QA	27/29 (93%)	27 (100%)	0	0	100	100
1	QB	27/29 (93%)	27 (100%)	0	0	100	100
1	R	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	RA	27/29 (93%)	27 (100%)	0	0	100	100
1	RB	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	S	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	SA	27/29 (93%)	27 (100%)	0	0	100	100
1	SB	27/29 (93%)	27 (100%)	0	0	100	100
1	T	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	TA	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	TB	27/29 (93%)	27 (100%)	0	0	100	100
1	U	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	UA	27/29 (93%)	27 (100%)	0	0	100	100
1	UB	27/29 (93%)	27 (100%)	0	0	100	100
1	V	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	VA	27/29 (93%)	27 (100%)	0	0	100	100
1	VB	27/29 (93%)	27 (100%)	0	0	100	100
1	W	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	WA	27/29 (93%)	27 (100%)	0	0	100	100
1	WB	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	X	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	XA	27/29 (93%)	27 (100%)	0	0	100	100
1	XB	27/29 (93%)	27 (100%)	0	0	100	100
1	Y	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	YA	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	YB	27/29 (93%)	27 (100%)	0	0	100	100
1	Z	27/29 (93%)	27 (100%)	0	0	100	100
1	ZA	27/29 (93%)	27 (100%)	0	0	100	100
1	ZB	27/29 (93%)	27 (100%)	0	0	100	100
1	a	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	aA	27/29 (93%)	27 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	b	27/29 (93%)	27 (100%)	0	0	100	100
1	bA	27/29 (93%)	27 (100%)	0	0	100	100
1	c	27/29 (93%)	27 (100%)	0	0	100	100
1	cA	27/29 (93%)	27 (100%)	0	0	100	100
1	d	27/29 (93%)	27 (100%)	0	0	100	100
1	dA	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	e	27/29 (93%)	27 (100%)	0	0	100	100
1	eA	27/29 (93%)	27 (100%)	0	0	100	100
1	f	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	fA	27/29 (93%)	27 (100%)	0	0	100	100
1	g	27/29 (93%)	27 (100%)	0	0	100	100
1	gA	27/29 (93%)	27 (100%)	0	0	100	100
1	h	27/29 (93%)	27 (100%)	0	0	100	100
1	hA	27/29 (93%)	27 (100%)	0	0	100	100
1	i	27/29 (93%)	27 (100%)	0	0	100	100
1	iA	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	j	27/29 (93%)	27 (100%)	0	0	100	100
1	jA	27/29 (93%)	27 (100%)	0	0	100	100
1	k	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	kA	27/29 (93%)	27 (100%)	0	0	100	100
1	l	27/29 (93%)	27 (100%)	0	0	100	100
1	lA	27/29 (93%)	27 (100%)	0	0	100	100
1	m	27/29 (93%)	27 (100%)	0	0	100	100
1	mA	27/29 (93%)	27 (100%)	0	0	100	100
1	n	27/29 (93%)	27 (100%)	0	0	100	100
1	nA	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	o	27/29 (93%)	27 (100%)	0	0	100	100
1	oA	27/29 (93%)	27 (100%)	0	0	100	100
1	p	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	pA	27/29 (93%)	27 (100%)	0	0	100	100
1	q	27/29 (93%)	27 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	qA	27/29 (93%)	27 (100%)	0	0	100	100
1	r	27/29 (93%)	27 (100%)	0	0	100	100
1	rA	27/29 (93%)	27 (100%)	0	0	100	100
1	s	27/29 (93%)	27 (100%)	0	0	100	100
1	sA	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	t	27/29 (93%)	27 (100%)	0	0	100	100
1	tA	27/29 (93%)	27 (100%)	0	0	100	100
1	u	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	uA	27/29 (93%)	27 (100%)	0	0	100	100
1	v	27/29 (93%)	27 (100%)	0	0	100	100
1	vA	27/29 (93%)	27 (100%)	0	0	100	100
1	w	27/29 (93%)	27 (100%)	0	0	100	100
1	wA	27/29 (93%)	27 (100%)	0	0	100	100
1	x	27/29 (93%)	27 (100%)	0	0	100	100
1	xA	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	y	27/29 (93%)	27 (100%)	0	0	100	100
1	yA	27/29 (93%)	27 (100%)	0	0	100	100
1	z	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	zA	27/29 (93%)	27 (100%)	0	0	100	100
All	All	4050/4350 (93%)	4000 (99%)	50 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	0	21/21 (100%)	21 (100%)	0	100	100
1	0A	21/21 (100%)	21 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	21/21 (100%)	21 (100%)	0	100	100
1	1A	21/21 (100%)	21 (100%)	0	100	100
1	2	21/21 (100%)	21 (100%)	0	100	100
1	2A	21/21 (100%)	21 (100%)	0	100	100
1	3	21/21 (100%)	21 (100%)	0	100	100
1	3A	21/21 (100%)	21 (100%)	0	100	100
1	4	21/21 (100%)	21 (100%)	0	100	100
1	4A	21/21 (100%)	21 (100%)	0	100	100
1	5	21/21 (100%)	21 (100%)	0	100	100
1	5A	21/21 (100%)	21 (100%)	0	100	100
1	6	21/21 (100%)	21 (100%)	0	100	100
1	6A	21/21 (100%)	21 (100%)	0	100	100
1	7	21/21 (100%)	21 (100%)	0	100	100
1	7A	21/21 (100%)	21 (100%)	0	100	100
1	8	21/21 (100%)	21 (100%)	0	100	100
1	8A	21/21 (100%)	21 (100%)	0	100	100
1	9	21/21 (100%)	21 (100%)	0	100	100
1	9A	21/21 (100%)	21 (100%)	0	100	100
1	A	21/21 (100%)	21 (100%)	0	100	100
1	AA	21/21 (100%)	21 (100%)	0	100	100
1	AB	21/21 (100%)	21 (100%)	0	100	100
1	B	21/21 (100%)	21 (100%)	0	100	100
1	BA	21/21 (100%)	21 (100%)	0	100	100
1	BB	21/21 (100%)	21 (100%)	0	100	100
1	C	21/21 (100%)	21 (100%)	0	100	100
1	CA	21/21 (100%)	21 (100%)	0	100	100
1	CB	21/21 (100%)	21 (100%)	0	100	100
1	D	21/21 (100%)	21 (100%)	0	100	100
1	DA	21/21 (100%)	21 (100%)	0	100	100
1	DB	21/21 (100%)	21 (100%)	0	100	100
1	E	21/21 (100%)	21 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	EA	21/21 (100%)	21 (100%)	0	100	100
1	EB	21/21 (100%)	21 (100%)	0	100	100
1	F	21/21 (100%)	21 (100%)	0	100	100
1	FA	21/21 (100%)	21 (100%)	0	100	100
1	FB	21/21 (100%)	21 (100%)	0	100	100
1	G	21/21 (100%)	21 (100%)	0	100	100
1	GA	21/21 (100%)	21 (100%)	0	100	100
1	GB	21/21 (100%)	21 (100%)	0	100	100
1	H	21/21 (100%)	21 (100%)	0	100	100
1	HA	21/21 (100%)	21 (100%)	0	100	100
1	HB	21/21 (100%)	21 (100%)	0	100	100
1	I	21/21 (100%)	21 (100%)	0	100	100
1	IA	21/21 (100%)	21 (100%)	0	100	100
1	IB	21/21 (100%)	21 (100%)	0	100	100
1	J	21/21 (100%)	21 (100%)	0	100	100
1	JA	21/21 (100%)	21 (100%)	0	100	100
1	JB	21/21 (100%)	21 (100%)	0	100	100
1	K	21/21 (100%)	21 (100%)	0	100	100
1	KA	21/21 (100%)	21 (100%)	0	100	100
1	KB	21/21 (100%)	21 (100%)	0	100	100
1	L	21/21 (100%)	21 (100%)	0	100	100
1	LA	21/21 (100%)	21 (100%)	0	100	100
1	LB	21/21 (100%)	21 (100%)	0	100	100
1	M	21/21 (100%)	21 (100%)	0	100	100
1	MA	21/21 (100%)	21 (100%)	0	100	100
1	MB	21/21 (100%)	21 (100%)	0	100	100
1	N	21/21 (100%)	21 (100%)	0	100	100
1	NA	21/21 (100%)	21 (100%)	0	100	100
1	NB	21/21 (100%)	21 (100%)	0	100	100
1	O	21/21 (100%)	21 (100%)	0	100	100
1	OA	21/21 (100%)	21 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	OB	21/21 (100%)	21 (100%)	0	100	100
1	P	21/21 (100%)	21 (100%)	0	100	100
1	PA	21/21 (100%)	21 (100%)	0	100	100
1	PB	21/21 (100%)	21 (100%)	0	100	100
1	Q	21/21 (100%)	21 (100%)	0	100	100
1	QA	21/21 (100%)	21 (100%)	0	100	100
1	QB	21/21 (100%)	21 (100%)	0	100	100
1	R	21/21 (100%)	21 (100%)	0	100	100
1	RA	21/21 (100%)	21 (100%)	0	100	100
1	RB	21/21 (100%)	21 (100%)	0	100	100
1	S	21/21 (100%)	21 (100%)	0	100	100
1	SA	21/21 (100%)	21 (100%)	0	100	100
1	SB	21/21 (100%)	21 (100%)	0	100	100
1	T	21/21 (100%)	21 (100%)	0	100	100
1	TA	21/21 (100%)	21 (100%)	0	100	100
1	TB	21/21 (100%)	21 (100%)	0	100	100
1	U	21/21 (100%)	21 (100%)	0	100	100
1	UA	21/21 (100%)	21 (100%)	0	100	100
1	UB	21/21 (100%)	21 (100%)	0	100	100
1	V	21/21 (100%)	21 (100%)	0	100	100
1	VA	21/21 (100%)	21 (100%)	0	100	100
1	VB	21/21 (100%)	21 (100%)	0	100	100
1	W	21/21 (100%)	21 (100%)	0	100	100
1	WA	21/21 (100%)	21 (100%)	0	100	100
1	WB	21/21 (100%)	21 (100%)	0	100	100
1	X	21/21 (100%)	21 (100%)	0	100	100
1	XA	21/21 (100%)	21 (100%)	0	100	100
1	XB	21/21 (100%)	21 (100%)	0	100	100
1	Y	21/21 (100%)	21 (100%)	0	100	100
1	YA	21/21 (100%)	21 (100%)	0	100	100
1	YB	21/21 (100%)	21 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Z	21/21 (100%)	21 (100%)	0	100	100
1	ZA	21/21 (100%)	21 (100%)	0	100	100
1	ZB	21/21 (100%)	21 (100%)	0	100	100
1	a	21/21 (100%)	21 (100%)	0	100	100
1	aA	21/21 (100%)	21 (100%)	0	100	100
1	b	21/21 (100%)	21 (100%)	0	100	100
1	bA	21/21 (100%)	21 (100%)	0	100	100
1	c	21/21 (100%)	21 (100%)	0	100	100
1	cA	21/21 (100%)	21 (100%)	0	100	100
1	d	21/21 (100%)	21 (100%)	0	100	100
1	dA	21/21 (100%)	21 (100%)	0	100	100
1	e	21/21 (100%)	21 (100%)	0	100	100
1	eA	21/21 (100%)	21 (100%)	0	100	100
1	f	21/21 (100%)	21 (100%)	0	100	100
1	fA	21/21 (100%)	21 (100%)	0	100	100
1	g	21/21 (100%)	21 (100%)	0	100	100
1	gA	21/21 (100%)	21 (100%)	0	100	100
1	h	21/21 (100%)	21 (100%)	0	100	100
1	hA	21/21 (100%)	21 (100%)	0	100	100
1	i	21/21 (100%)	21 (100%)	0	100	100
1	iA	21/21 (100%)	21 (100%)	0	100	100
1	j	21/21 (100%)	21 (100%)	0	100	100
1	jA	21/21 (100%)	21 (100%)	0	100	100
1	k	21/21 (100%)	21 (100%)	0	100	100
1	kA	21/21 (100%)	21 (100%)	0	100	100
1	l	21/21 (100%)	21 (100%)	0	100	100
1	lA	21/21 (100%)	21 (100%)	0	100	100
1	m	21/21 (100%)	21 (100%)	0	100	100
1	mA	21/21 (100%)	21 (100%)	0	100	100
1	n	21/21 (100%)	21 (100%)	0	100	100
1	nA	21/21 (100%)	21 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	o	21/21 (100%)	21 (100%)	0	100	100
1	oA	21/21 (100%)	21 (100%)	0	100	100
1	p	21/21 (100%)	21 (100%)	0	100	100
1	pA	21/21 (100%)	21 (100%)	0	100	100
1	q	21/21 (100%)	21 (100%)	0	100	100
1	qA	21/21 (100%)	21 (100%)	0	100	100
1	r	21/21 (100%)	21 (100%)	0	100	100
1	rA	21/21 (100%)	21 (100%)	0	100	100
1	s	21/21 (100%)	21 (100%)	0	100	100
1	sA	21/21 (100%)	21 (100%)	0	100	100
1	t	21/21 (100%)	21 (100%)	0	100	100
1	tA	21/21 (100%)	21 (100%)	0	100	100
1	u	21/21 (100%)	21 (100%)	0	100	100
1	uA	21/21 (100%)	21 (100%)	0	100	100
1	v	21/21 (100%)	21 (100%)	0	100	100
1	vA	21/21 (100%)	21 (100%)	0	100	100
1	w	21/21 (100%)	21 (100%)	0	100	100
1	wA	21/21 (100%)	21 (100%)	0	100	100
1	x	21/21 (100%)	21 (100%)	0	100	100
1	xA	21/21 (100%)	21 (100%)	0	100	100
1	y	21/21 (100%)	21 (100%)	0	100	100
1	yA	21/21 (100%)	21 (100%)	0	100	100
1	z	21/21 (100%)	21 (100%)	0	100	100
1	zA	21/21 (100%)	21 (100%)	0	100	100
All	All	3150/3150 (100%)	3150 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

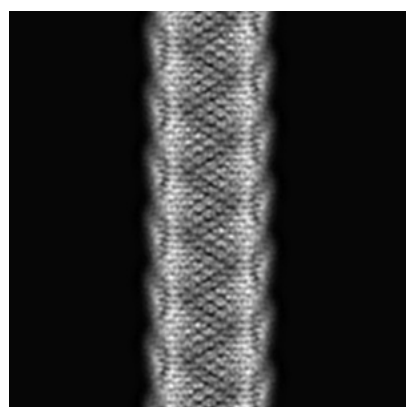
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21816. These allow visual inspection of the internal detail of the map and identification of artifacts.

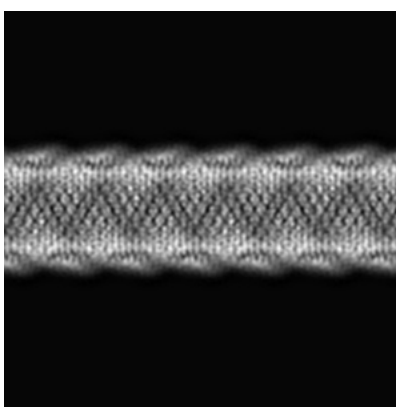
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y



Z

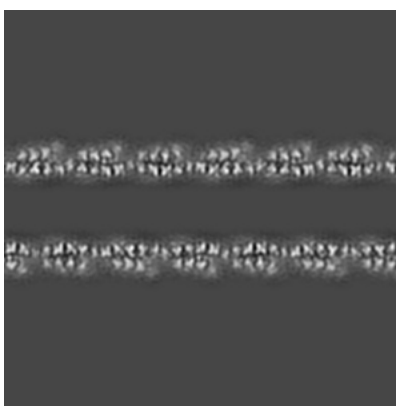
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

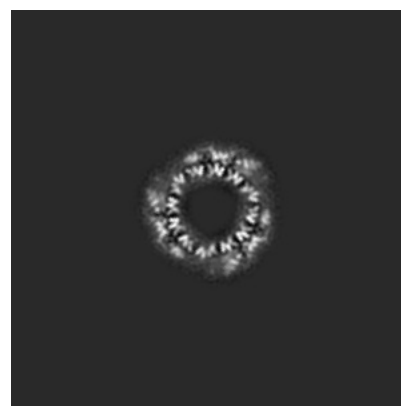
6.2.1 Primary map



X Index: 160



Y Index: 160

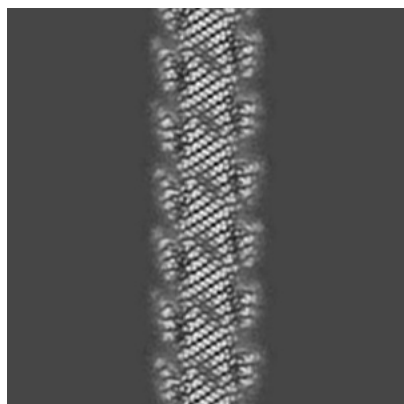


Z Index: 160

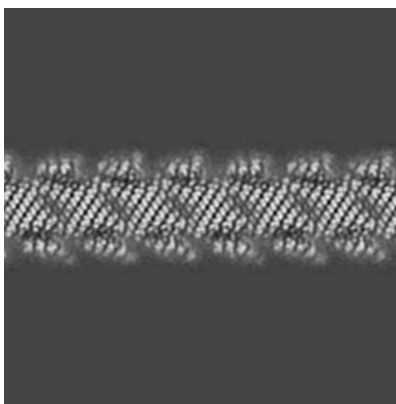
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

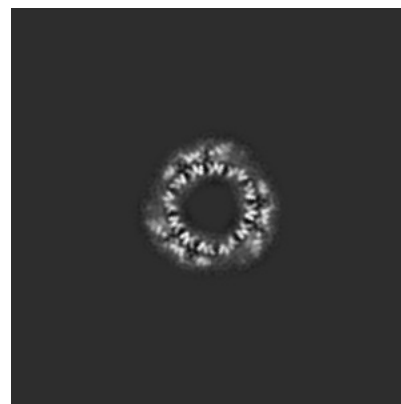
6.3.1 Primary map



X Index: 130



Y Index: 190



Z Index: 122

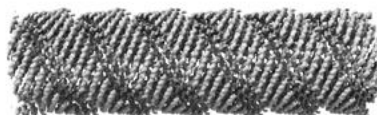
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

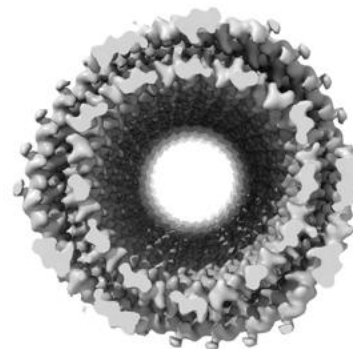
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0111. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

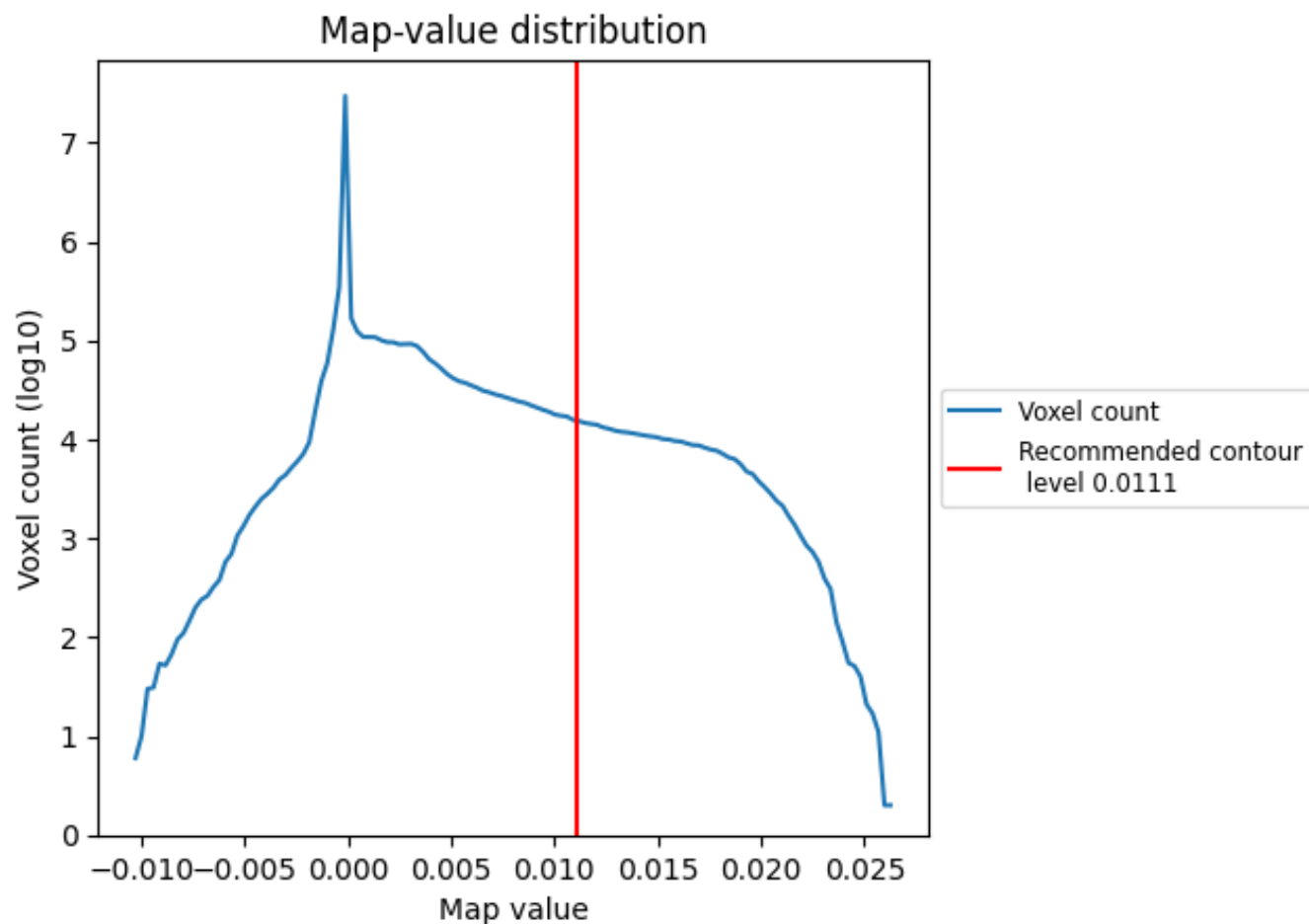
6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

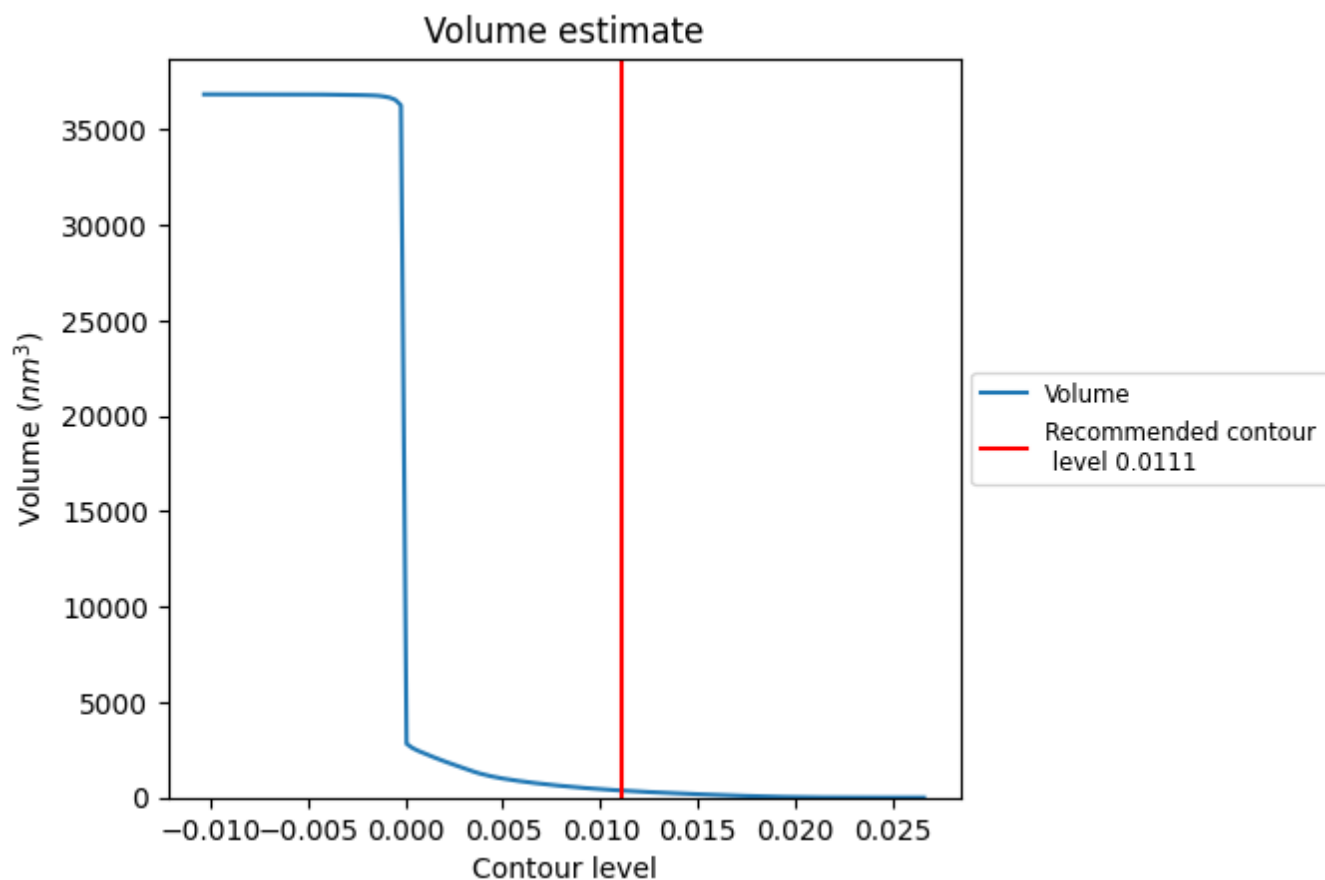
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

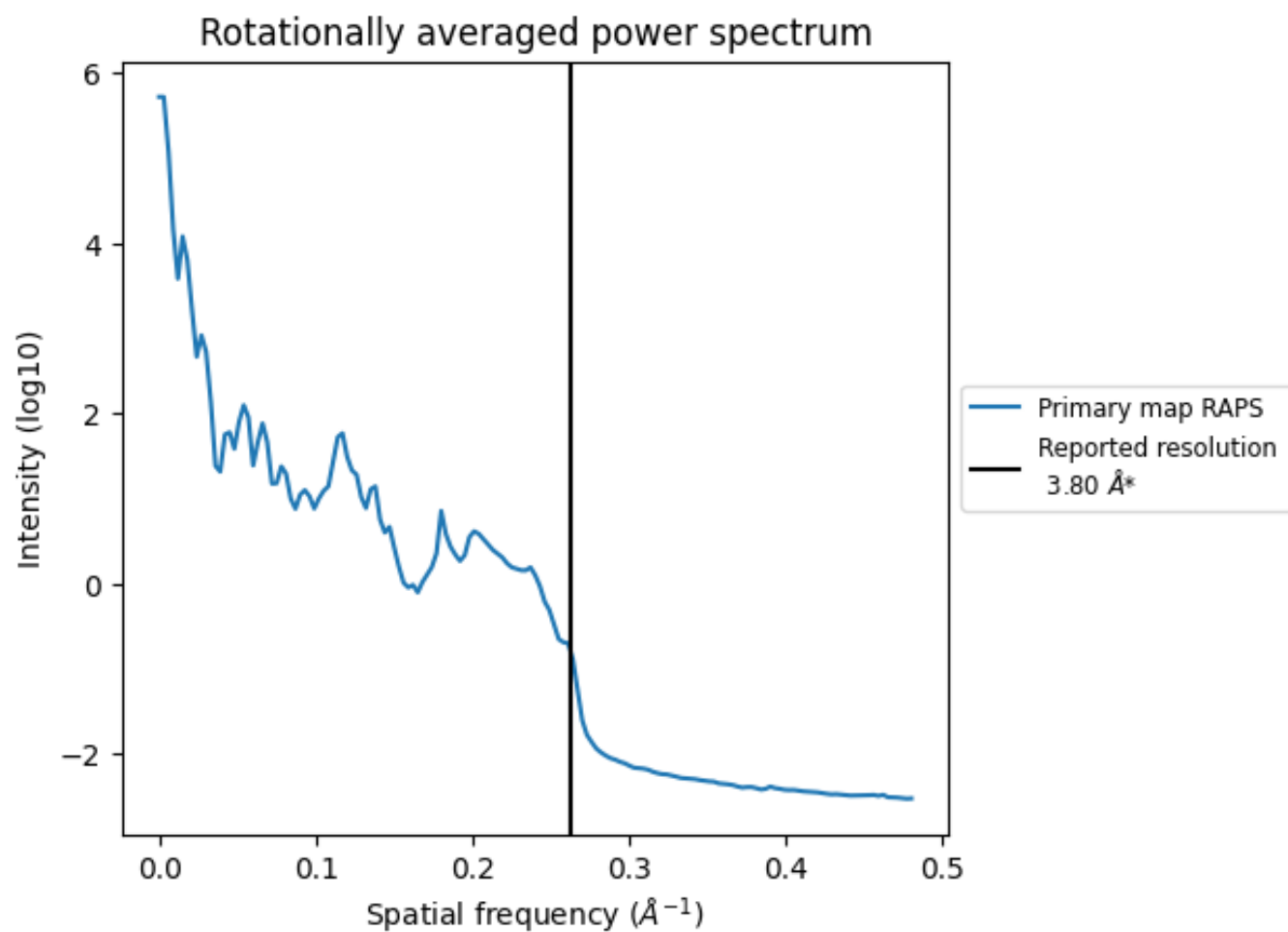
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 367 nm³; this corresponds to an approximate mass of 331 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

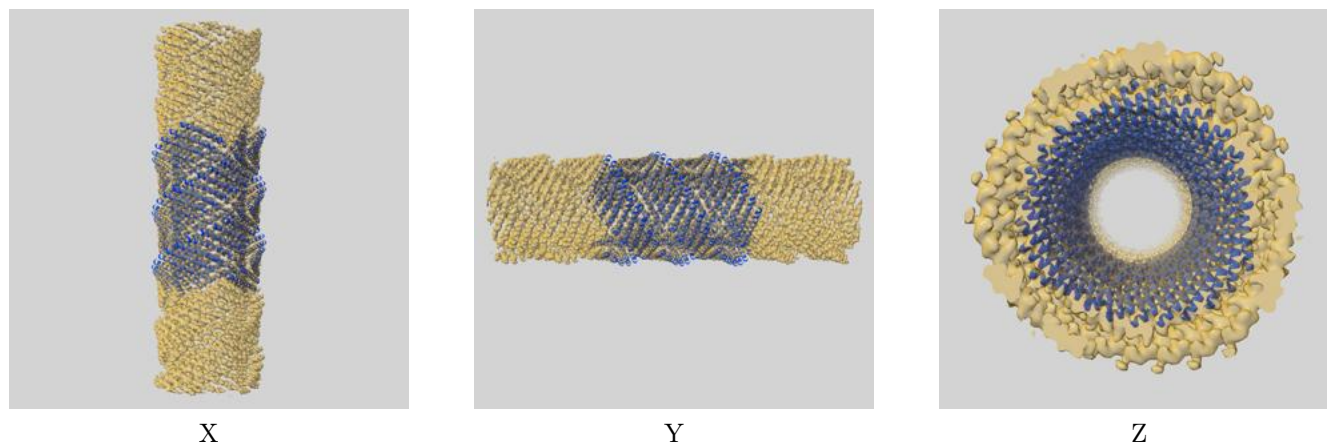
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

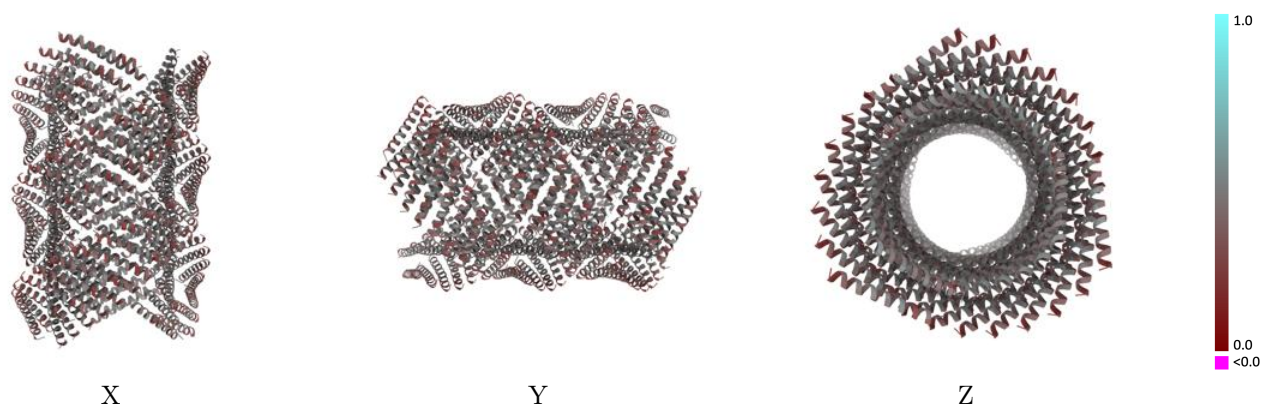
This section contains information regarding the fit between EMDB map EMD-21816 and PDB model 6WL7. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay [i](#)



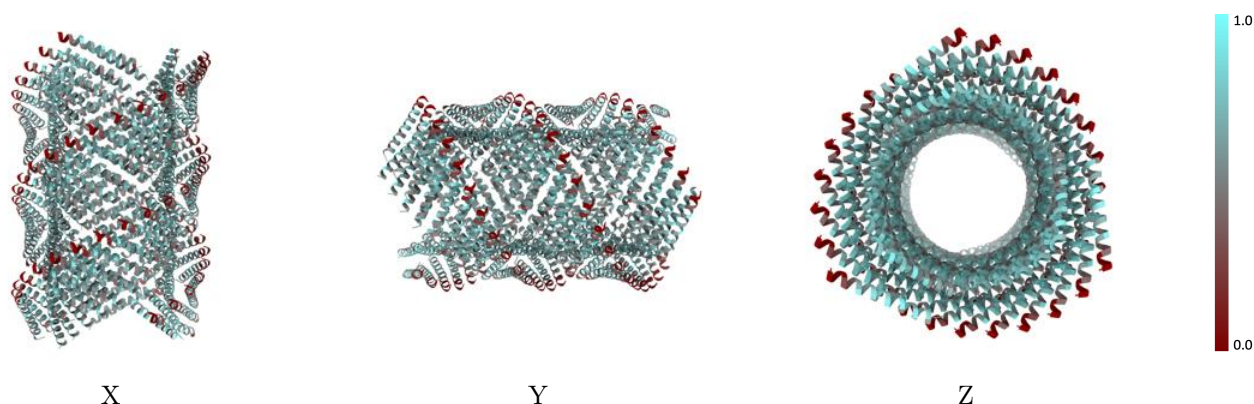
The images above show the 3D surface view of the map at the recommended contour level 0.0111 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



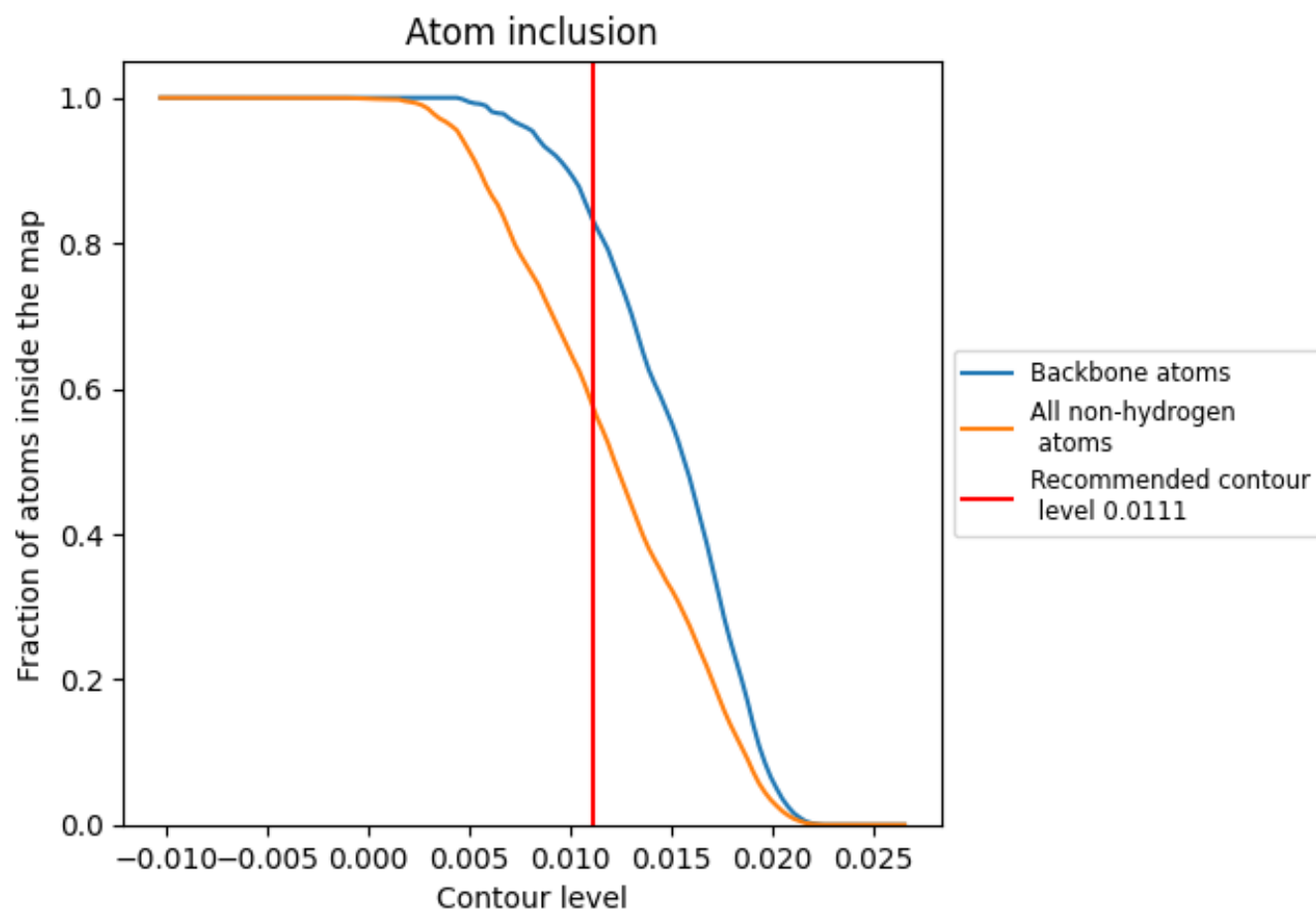
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0111).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 58% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ





















































































The table lists the average atom inclusion at the recommended contour level (0.0111) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5778	 0.4070
0	 0.5268	 0.3790
0A	 0.5268	 0.3770
1	 0.6429	 0.4330
1A	 0.5223	 0.3810
2	 0.5134	 0.3720
2A	 0.6607	 0.4370
3	 0.5179	 0.3800
3A	 0.5134	 0.3770
4	 0.6250	 0.4380
4A	 0.6562	 0.4350
5	 0.5179	 0.3850
5A	 0.5179	 0.3750
6	 0.6429	 0.4330
6A	 0.5268	 0.3820
7	 0.5045	 0.3720
7A	 0.6429	 0.4300
8	 0.5268	 0.3840
8A	 0.5223	 0.3780
9	 0.6384	 0.4340
9A	 0.6339	 0.4320
A	 0.6562	 0.4310
AA	 0.5089	 0.3830
AB	 0.5179	 0.3840
B	 0.6429	 0.4340
BA	 0.6429	 0.4330
BB	 0.5000	 0.3790
C	 0.6384	 0.4360
CA	 0.5089	 0.3750
CB	 0.6473	 0.4300
D	 0.6518	 0.4330
DA	 0.5312	 0.3820
DB	 0.5000	 0.3770
E	 0.6473	 0.4340
EA	 0.6473	 0.4350























































































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Chain	Atom inclusion	Q-score
EB	 0.6384	 0.4320
F	 0.6429	 0.4330
FA	 0.5179	 0.3800
FB	 0.4911	 0.3690
G	 0.6384	 0.4330
GA	 0.6384	 0.4410
GB	 0.5134	 0.3800
H	 0.6384	 0.4340
HA	 0.5000	 0.3770
HB	 0.6429	 0.4350
I	 0.6473	 0.4270
IA	 0.5045	 0.3810
IB	 0.5089	 0.3770
J	 0.6429	 0.4310
JA	 0.6429	 0.4370
JB	 0.6295	 0.4310
K	 0.6473	 0.4290
KA	 0.5179	 0.3840
KB	 0.5045	 0.3720
L	 0.6473	 0.4360
LA	 0.6295	 0.4350
LB	 0.5000	 0.3740
M	 0.6339	 0.4300
MA	 0.5134	 0.3800
MB	 0.6473	 0.4340
N	 0.6429	 0.4280
NA	 0.5000	 0.3830
NB	 0.5134	 0.3750
O	 0.6384	 0.4330
OA	 0.6384	 0.4300
OB	 0.6429	 0.4420
P	 0.6339	 0.4340
PA	 0.5134	 0.3840
PB	 0.5179	 0.3800
Q	 0.6384	 0.4340
QA	 0.6339	 0.4370
QB	 0.5134	 0.3810
R	 0.6473	 0.4340
RA	 0.5045	 0.3780
RB	 0.6429	 0.4330
S	 0.6607	 0.4350
SA	 0.5134	 0.3830

































































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Chain	Atom inclusion	Q-score
SB	 0.5089	 0.3790
T	 0.6384	 0.4300
TA	 0.6518	 0.4360
TB	 0.6339	 0.4340
U	 0.6384	 0.4340
UA	 0.5000	 0.3790
UB	 0.5268	 0.3770
V	 0.6339	 0.4290
VA	 0.6518	 0.4380
VB	 0.5134	 0.3830
W	 0.6429	 0.4340
WA	 0.5223	 0.3760
WB	 0.6518	 0.4360
X	 0.6384	 0.4310
XA	 0.5089	 0.3810
XB	 0.5134	 0.3790
Y	 0.6518	 0.4300
YA	 0.6429	 0.4370
YB	 0.6339	 0.4360
Z	 0.5402	 0.3840
ZA	 0.5000	 0.3770
ZB	 0.5045	 0.3810
a	 0.6473	 0.4350
aA	 0.6429	 0.4370
b	 0.4955	 0.3800
bA	 0.5134	 0.3730
c	 0.6473	 0.4380
cA	 0.5223	 0.3830
d	 0.5179	 0.3720
dA	 0.6384	 0.4310
e	 0.5089	 0.3800
eA	 0.5134	 0.3830
f	 0.6473	 0.4310
fA	 0.6339	 0.4360
g	 0.5045	 0.3780
gA	 0.5000	 0.3750
h	 0.6384	 0.4380
hA	 0.5000	 0.3810
i	 0.5179	 0.3780
iA	 0.6339	 0.4320
j	 0.5134	 0.3840
jA	 0.5312	 0.3830

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Chain	Atom inclusion	Q-score
k	 0.6429	 0.4340
kA	 0.6473	 0.4330
l	 0.5089	 0.3820
lA	 0.5268	 0.3830
m	 0.6429	 0.4360
mA	 0.5089	 0.3810
n	 0.5089	 0.3770
nA	 0.6473	 0.4330
o	 0.5357	 0.3880
oA	 0.5134	 0.3860
p	 0.6339	 0.4300
pA	 0.6473	 0.4350
q	 0.5089	 0.3790
qA	 0.5179	 0.3760
r	 0.6518	 0.4400
rA	 0.5134	 0.3800
s	 0.4955	 0.3780
sA	 0.6429	 0.4320
t	 0.5223	 0.3800
tA	 0.5179	 0.3870
u	 0.6429	 0.4340
uA	 0.6429	 0.4360
v	 0.5089	 0.3800
vA	 0.5089	 0.3770
w	 0.6518	 0.4340
wA	 0.5045	 0.3810
x	 0.5134	 0.3760
xA	 0.6429	 0.4380
y	 0.5268	 0.3840
yA	 0.5089	 0.3740
z	 0.6384	 0.4340
zA	 0.6384	 0.4330