



Full wwPDB EM Validation Report ⓘ

May 4, 2025 – 04:02 PM EDT

PDB ID : 6WL9 / pdb_00006wl9
EMDB ID : EMD-21818
Title : Cryo-EM of Form 2 like peptide filament, Form2a
Authors : Wang, F.; Beltran, L.C.; Gnewou, O.M.; Egelman, E.H.; Conticello, V.P.
Deposited on : 2020-04-18
Resolution : 4.20 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.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

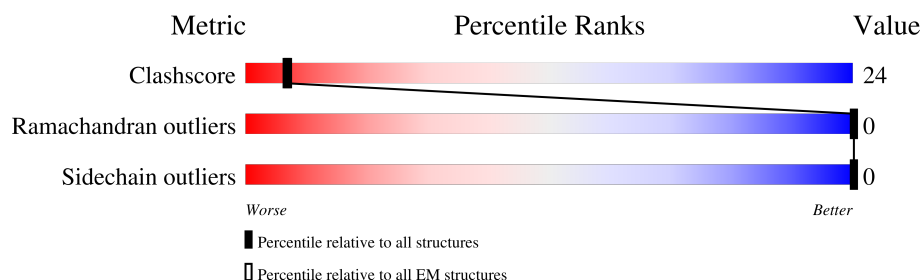
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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>7%</div> <div>52%</div> <div>48%</div> </div>
1	1	29	<div> <div>7%</div> <div>55%</div> <div>45%</div> </div>
1	2	29	<div> <div>14%</div> <div>55%</div> <div>45%</div> </div>
1	3	29	<div> <div>10%</div> <div>52%</div> <div>48%</div> </div>
1	4	29	<div> <div>7%</div> <div>55%</div> <div>45%</div> </div>
1	5	29	<div> <div>10%</div> <div>52%</div> <div>48%</div> </div>
1	6	29	<div> <div>7%</div> <div>52%</div> <div>48%</div> </div>
1	7	29	<div> <div>7%</div> <div>52%</div> <div>48%</div> </div>

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Mol	Chain	Length	Quality of chain
1	8	29	<div> <div>10%</div> <div>52%</div> <div>48%</div> </div>
1	9	29	<div> <div>7%</div> <div>48%</div> <div>52%</div> </div>
1	A	29	<div> <div>55%</div> <div>45%</div> </div>
1	AA	29	<div> <div>7%</div> <div>55%</div> <div>45%</div> </div>
1	B	29	<div> <div>52%</div> <div>48%</div> </div>
1	BA	29	<div> <div>7%</div> <div>52%</div> <div>48%</div> </div>
1	C	29	<div> <div>52%</div> <div>48%</div> </div>
1	CA	29	<div> <div>7%</div> <div>48%</div> <div>52%</div> </div>
1	D	29	<div> <div>55%</div> <div>45%</div> </div>
1	DA	29	<div> <div>7%</div> <div>52%</div> <div>48%</div> </div>
1	E	29	<div> <div>48%</div> <div>52%</div> </div>
1	EA	29	<div> <div>7%</div> <div>59%</div> <div>41%</div> </div>
1	F	29	<div> <div>55%</div> <div>45%</div> </div>
1	FA	29	<div> <div>7%</div> <div>48%</div> <div>52%</div> </div>
1	G	29	<div> <div>45%</div> <div>55%</div> </div>
1	GA	29	<div> <div>7%</div> <div>55%</div> <div>45%</div> </div>
1	H	29	<div> <div>48%</div> <div>52%</div> </div>
1	HA	29	<div> <div>7%</div> <div>59%</div> <div>41%</div> </div>
1	I	29	<div> <div>45%</div> <div>55%</div> </div>
1	IA	29	<div> <div>7%</div> <div>52%</div> <div>48%</div> </div>
1	J	29	<div> <div>45%</div> <div>55%</div> </div>
1	JA	29	<div> <div>7%</div> <div>62%</div> <div>38%</div> </div>
1	K	29	<div> <div>55%</div> <div>45%</div> </div>
1	KA	29	<div> <div>7%</div> <div>55%</div> <div>45%</div> </div>
1	L	29	<div> <div>52%</div> <div>48%</div> </div>









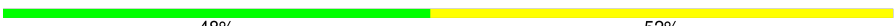






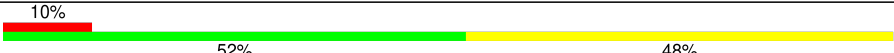
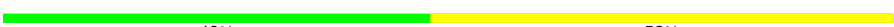
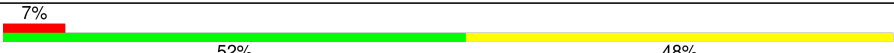


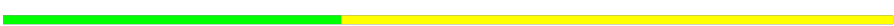


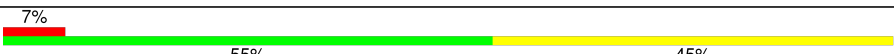

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Mol	Chain	Length	Quality of chain
1	LA	29	
1	M	29	
1	MA	29	
1	N	29	
1	NA	29	
1	O	29	
1	OA	29	
1	P	29	
1	PA	29	
1	Q	29	
1	QA	29	
1	R	29	
1	RA	29	
1	S	29	
1	SA	29	
1	T	29	
1	TA	29	
1	U	29	
1	UA	29	
1	V	29	
1	VA	29	
1	W	29	
1	WA	29	
1	X	29	
1	XA	29	

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Mol	Chain	Length	Quality of chain
1	Y	29	
1	YA	29	
1	Z	29	
1	ZA	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	
1	f	29	
1	fA	29	
1	g	29	
1	gA	29	
1	h	29	
1	hA	29	
1	i	29	
1	iA	29	
1	j	29	
1	jA	29	
1	k	29	

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Mol	Chain	Length	Quality of chain
1	kA	29	
1	l	29	
1	lA	29	
1	m	29	
1	mA	29	
1	n	29	
1	nA	29	
1	o	29	
1	oA	29	
1	p	29	
1	pA	29	
1	q	29	
1	r	29	
1	s	29	
1	t	29	
1	u	29	
1	v	29	
1	w	29	
1	x	29	
1	y	29	
1	z	29	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 23400 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 Form2a.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	29	Total	C	N	O	0	0
			225	145	37	43		
1	0	29	Total	C	N	O	0	0
			225	145	37	43		
1	B	29	Total	C	N	O	0	0
			225	145	37	43		
1	1	29	Total	C	N	O	0	0
			225	145	37	43		
1	C	29	Total	C	N	O	0	0
			225	145	37	43		
1	2	29	Total	C	N	O	0	0
			225	145	37	43		
1	D	29	Total	C	N	O	0	0
			225	145	37	43		
1	3	29	Total	C	N	O	0	0
			225	145	37	43		
1	E	29	Total	C	N	O	0	0
			225	145	37	43		
1	4	29	Total	C	N	O	0	0
			225	145	37	43		
1	F	29	Total	C	N	O	0	0
			225	145	37	43		
1	5	29	Total	C	N	O	0	0
			225	145	37	43		
1	G	29	Total	C	N	O	0	0
			225	145	37	43		
1	6	29	Total	C	N	O	0	0
			225	145	37	43		
1	H	29	Total	C	N	O	0	0
			225	145	37	43		
1	7	29	Total	C	N	O	0	0
			225	145	37	43		
1	I	29	Total	C	N	O	0	0
			225	145	37	43		

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	8	29	Total	C	N	O	0	0
			225	145	37	43		
1	J	29	Total	C	N	O	0	0
			225	145	37	43		
1	9	29	Total	C	N	O	0	0
			225	145	37	43		
1	K	29	Total	C	N	O	0	0
			225	145	37	43		
1	AA	29	Total	C	N	O	0	0
			225	145	37	43		
1	L	29	Total	C	N	O	0	0
			225	145	37	43		
1	BA	29	Total	C	N	O	0	0
			225	145	37	43		
1	M	29	Total	C	N	O	0	0
			225	145	37	43		
1	CA	29	Total	C	N	O	0	0
			225	145	37	43		
1	N	29	Total	C	N	O	0	0
			225	145	37	43		
1	DA	29	Total	C	N	O	0	0
			225	145	37	43		
1	O	29	Total	C	N	O	0	0
			225	145	37	43		
1	EA	29	Total	C	N	O	0	0
			225	145	37	43		
1	P	29	Total	C	N	O	0	0
			225	145	37	43		
1	FA	29	Total	C	N	O	0	0
			225	145	37	43		
1	Q	29	Total	C	N	O	0	0
			225	145	37	43		
1	GA	29	Total	C	N	O	0	0
			225	145	37	43		
1	R	29	Total	C	N	O	0	0
			225	145	37	43		
1	HA	29	Total	C	N	O	0	0
			225	145	37	43		
1	S	29	Total	C	N	O	0	0
			225	145	37	43		
1	IA	29	Total	C	N	O	0	0
			225	145	37	43		

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	T	29	Total 225	C 145	N 37	O 43	0	0
1	JA	29	Total 225	C 145	N 37	O 43	0	0
1	U	29	Total 225	C 145	N 37	O 43	0	0
1	KA	29	Total 225	C 145	N 37	O 43	0	0
1	V	29	Total 225	C 145	N 37	O 43	0	0
1	LA	29	Total 225	C 145	N 37	O 43	0	0
1	W	29	Total 225	C 145	N 37	O 43	0	0
1	MA	29	Total 225	C 145	N 37	O 43	0	0
1	X	29	Total 225	C 145	N 37	O 43	0	0
1	NA	29	Total 225	C 145	N 37	O 43	0	0
1	Y	29	Total 225	C 145	N 37	O 43	0	0
1	OA	29	Total 225	C 145	N 37	O 43	0	0
1	Z	29	Total 225	C 145	N 37	O 43	0	0
1	PA	29	Total 225	C 145	N 37	O 43	0	0
1	a	29	Total 225	C 145	N 37	O 43	0	0
1	QA	29	Total 225	C 145	N 37	O 43	0	0
1	b	29	Total 225	C 145	N 37	O 43	0	0
1	RA	29	Total 225	C 145	N 37	O 43	0	0
1	c	29	Total 225	C 145	N 37	O 43	0	0
1	SA	29	Total 225	C 145	N 37	O 43	0	0
1	d	29	Total 225	C 145	N 37	O 43	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	TA	29	Total 225	C 145	N 37	O 43	0	0
1	e	29	Total 225	C 145	N 37	O 43	0	0
1	UA	29	Total 225	C 145	N 37	O 43	0	0
1	f	29	Total 225	C 145	N 37	O 43	0	0
1	VA	29	Total 225	C 145	N 37	O 43	0	0
1	g	29	Total 225	C 145	N 37	O 43	0	0
1	WA	29	Total 225	C 145	N 37	O 43	0	0
1	h	29	Total 225	C 145	N 37	O 43	0	0
1	XA	29	Total 225	C 145	N 37	O 43	0	0
1	i	29	Total 225	C 145	N 37	O 43	0	0
1	YA	29	Total 225	C 145	N 37	O 43	0	0
1	j	29	Total 225	C 145	N 37	O 43	0	0
1	ZA	29	Total 225	C 145	N 37	O 43	0	0
1	k	29	Total 225	C 145	N 37	O 43	0	0
1	aA	29	Total 225	C 145	N 37	O 43	0	0
1	l	29	Total 225	C 145	N 37	O 43	0	0
1	bA	29	Total 225	C 145	N 37	O 43	0	0
1	m	29	Total 225	C 145	N 37	O 43	0	0
1	cA	29	Total 225	C 145	N 37	O 43	0	0
1	n	29	Total 225	C 145	N 37	O 43	0	0
1	dA	29	Total 225	C 145	N 37	O 43	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	o	29	Total 225	C 145	N 37	O 43	0	0
1	eA	29	Total 225	C 145	N 37	O 43	0	0
1	p	29	Total 225	C 145	N 37	O 43	0	0
1	fA	29	Total 225	C 145	N 37	O 43	0	0
1	q	29	Total 225	C 145	N 37	O 43	0	0
1	gA	29	Total 225	C 145	N 37	O 43	0	0
1	r	29	Total 225	C 145	N 37	O 43	0	0
1	hA	29	Total 225	C 145	N 37	O 43	0	0
1	s	29	Total 225	C 145	N 37	O 43	0	0
1	iA	29	Total 225	C 145	N 37	O 43	0	0
1	t	29	Total 225	C 145	N 37	O 43	0	0
1	jA	29	Total 225	C 145	N 37	O 43	0	0
1	u	29	Total 225	C 145	N 37	O 43	0	0
1	kA	29	Total 225	C 145	N 37	O 43	0	0
1	v	29	Total 225	C 145	N 37	O 43	0	0
1	lA	29	Total 225	C 145	N 37	O 43	0	0
1	w	29	Total 225	C 145	N 37	O 43	0	0
1	mA	29	Total 225	C 145	N 37	O 43	0	0
1	x	29	Total 225	C 145	N 37	O 43	0	0
1	nA	29	Total 225	C 145	N 37	O 43	0	0
1	y	29	Total 225	C 145	N 37	O 43	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	oA	29	Total 225	C 145	N 37	O 43	0	0
1	z	29	Total 225	C 145	N 37	O 43	0	0
1	pA	29	Total 225	C 145	N 37	O 43	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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 Form2a

Chain A:  55% 45%



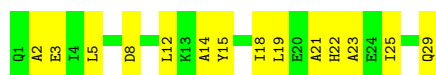
- Molecule 1: peptide Form2a

Chain 0:  7% 52% 48%



- Molecule 1: peptide Form2a

Chain B:  52% 48%



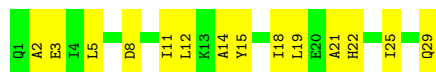
- Molecule 1: peptide Form2a

Chain 1:  7% 55% 45%



- Molecule 1: peptide Form2a

Chain C:  52% 48%



- Molecule 1: peptide Form2a



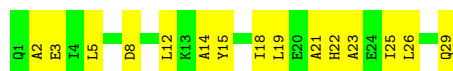
- Molecule 1: peptide Form2a



- Molecule 1: peptide Form2a



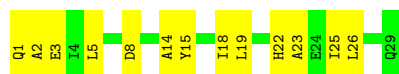
- Molecule 1: peptide Form2a



- Molecule 1: peptide Form2a



- Molecule 1: peptide Form2a



- Molecule 1: peptide Form2a



- Molecule 1: peptide Form2a

Chain G:  45% 55%



- Molecule 1: peptide Form2a

Chain 6:  7% 52% 48%



- Molecule 1: peptide Form2a

Chain H:  48% 52%



- Molecule 1: peptide Form2a

Chain 7:  7% 52% 48%



- Molecule 1: peptide Form2a

Chain I:  45% 55%



- Molecule 1: peptide Form2a

Chain 8:  10% 52% 48%



- Molecule 1: peptide Form2a

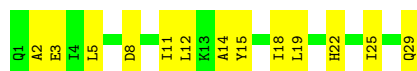
Chain J:  45% 55%



- Molecule 1: peptide Form2a



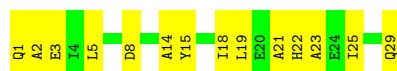
- Molecule 1: peptide Form2a



- Molecule 1: peptide Form2a



- Molecule 1: peptide Form2a



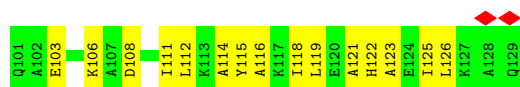
- Molecule 1: peptide Form2a



- Molecule 1: peptide Form2a

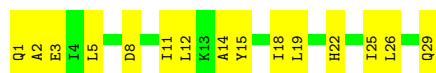


- Molecule 1: peptide Form2a



- Molecule 1: peptide Form2a

Chain N:  48% 52%



- Molecule 1: peptide Form2a

Chain DA:  7% 52% 48%



- Molecule 1: peptide Form2a

Chain O:  52% 48%



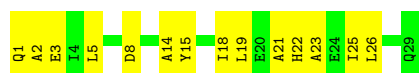
- Molecule 1: peptide Form2a

Chain EA:  7% 59% 41%



- Molecule 1: peptide Form2a

Chain P:  52% 48%



- Molecule 1: peptide Form2a

Chain FA:  7% 48% 52%



- Molecule 1: peptide Form2a

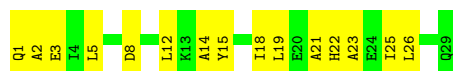
Chain Q:  52% 48%



- Molecule 1: peptide Form2a



- Molecule 1: peptide Form2a



- Molecule 1: peptide Form2a



- Molecule 1: peptide Form2a



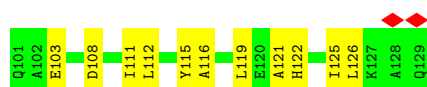
- Molecule 1: peptide Form2a



- Molecule 1: peptide Form2a

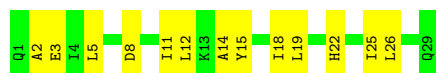


- Molecule 1: peptide Form2a



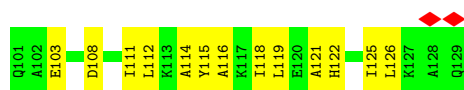
- Molecule 1: peptide Form2a

Chain U:  55% 45%



- Molecule 1: peptide Form2a

Chain KA:  7% 55% 45%



- Molecule 1: peptide Form2a

Chain V:  45% 55%



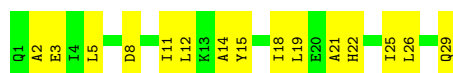
- Molecule 1: peptide Form2a

Chain LA:  10% 48% 52%



- Molecule 1: peptide Form2a

Chain W:  48% 52%



- Molecule 1: peptide Form2a

Chain MA:  7% 52% 48%



- Molecule 1: peptide Form2a

Chain X:  45% 55%



- Molecule 1: peptide Form2a



- Molecule 1: peptide Form2a



- Molecule 1: peptide Form2a



- Molecule 1: peptide Form2a



- Molecule 1: peptide Form2a



- Molecule 1: peptide Form2a

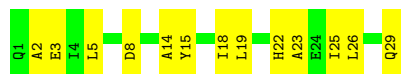


- Molecule 1: peptide Form2a



- Molecule 1: peptide Form2a

Chain b:  55% 45%



- Molecule 1: peptide Form2a

Chain RA:  7% 52% 48%



- Molecule 1: peptide Form2a

Chain c:  48% 52%



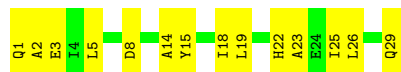
- Molecule 1: peptide Form2a

Chain SA:  7% 62% 38%



- Molecule 1: peptide Form2a

Chain d:  52% 48%



- Molecule 1: peptide Form2a

Chain TA:  7% 48% 52%



- Molecule 1: peptide Form2a

Chain e:  52% 48%



● Molecule 1: peptide Form2a



● Molecule 1: peptide Form2a



● Molecule 1: peptide Form2a



● Molecule 1: peptide Form2a



● Molecule 1: peptide Form2a



● Molecule 1: peptide Form2a



● Molecule 1: peptide Form2a





- Molecule 1: peptide Form2a



- Molecule 1: peptide Form2a



- Molecule 1: peptide Form2a



- Molecule 1: peptide Form2a



- Molecule 1: peptide Form2a



- Molecule 1: peptide Form2a



- Molecule 1: peptide Form2a

Chain l:  55% 45%



• Molecule 1: peptide Form2a

Chain bA:  14% 62% 38%



• Molecule 1: peptide Form2a

Chain m:  55% 45%



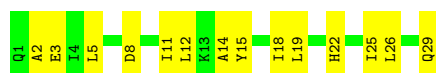
• Molecule 1: peptide Form2a

Chain cA:  7% 55% 45%



• Molecule 1: peptide Form2a

Chain n:  52% 48%



• Molecule 1: peptide Form2a

Chain dA:  10% 59% 41%

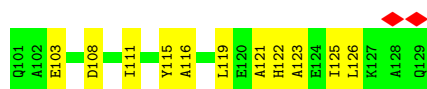


• Molecule 1: peptide Form2a

Chain o:  59% 41%



• Molecule 1: peptide Form2a



- Molecule 1: peptide Form2a



- Molecule 1: peptide Form2a



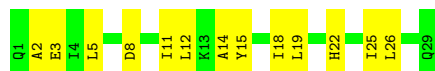
- Molecule 1: peptide Form2a



- Molecule 1: peptide Form2a



- Molecule 1: peptide Form2a



- Molecule 1: peptide Form2a



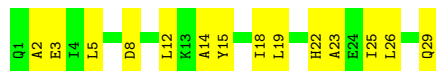
● Molecule 1: peptide Form2a

Chain s:  55% 45%

● Molecule 1: peptide Form2a

Chain iA:  7% 55% 45%

● Molecule 1: peptide Form2a

Chain t:  52% 48%

● Molecule 1: peptide Form2a

Chain jA:  7% 55% 45%

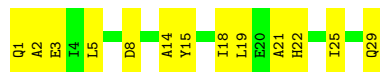
● Molecule 1: peptide Form2a

Chain u:  59% 41%

● Molecule 1: peptide Form2a

Chain kA:  10% 59% 41%

● Molecule 1: peptide Form2a

Chain v:  55% 45%

- Molecule 1: peptide Form2a



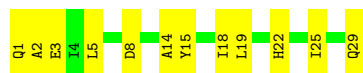
- Molecule 1: peptide Form2a



- Molecule 1: peptide Form2a



- Molecule 1: peptide Form2a



- Molecule 1: peptide Form2a



- Molecule 1: peptide Form2a



- Molecule 1: peptide Form2a





• Molecule 1: peptide Form2a



• Molecule 1: peptide Form2a



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=124.37°, rise=1.92 Å, axial sym=C1	Depositor
Number of segments used	288990	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	51	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.042	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0118	Depositor
Map size (Å)	345.6, 345.6, 345.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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	0.28	0/226	0.33	0/301
1	1	0.28	0/226	0.33	0/301
1	2	0.28	0/226	0.32	0/301
1	3	0.28	0/226	0.33	0/301
1	4	0.28	0/226	0.33	0/301
1	5	0.28	0/226	0.33	0/301
1	6	0.28	0/226	0.33	0/301
1	7	0.28	0/226	0.33	0/301
1	8	0.28	0/226	0.33	0/301
1	9	0.28	0/226	0.33	0/301
1	A	0.35	0/226	0.35	0/301
1	AA	0.28	0/226	0.33	0/301
1	B	0.35	0/226	0.35	0/301
1	BA	0.28	0/226	0.33	0/301
1	C	0.35	0/226	0.35	0/301
1	CA	0.28	0/226	0.33	0/301
1	D	0.35	0/226	0.35	0/301
1	DA	0.28	0/226	0.33	0/301
1	E	0.35	0/226	0.35	0/301
1	EA	0.28	0/226	0.33	0/301
1	F	0.35	0/226	0.35	0/301
1	FA	0.28	0/226	0.33	0/301
1	G	0.35	0/226	0.35	0/301
1	GA	0.28	0/226	0.33	0/301
1	H	0.35	0/226	0.35	0/301
1	HA	0.28	0/226	0.33	0/301
1	I	0.35	0/226	0.35	0/301
1	IA	0.28	0/226	0.33	0/301
1	J	0.35	0/226	0.35	0/301
1	JA	0.28	0/226	0.33	0/301
1	K	0.35	0/226	0.35	0/301
1	KA	0.28	0/226	0.33	0/301
1	L	0.35	0/226	0.35	0/301
1	LA	0.28	0/226	0.33	0/301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	M	0.35	0/226	0.35	0/301
1	MA	0.28	0/226	0.33	0/301
1	N	0.35	0/226	0.35	0/301
1	NA	0.28	0/226	0.32	0/301
1	O	0.35	0/226	0.35	0/301
1	OA	0.28	0/226	0.33	0/301
1	P	0.35	0/226	0.35	0/301
1	PA	0.28	0/226	0.33	0/301
1	Q	0.35	0/226	0.35	0/301
1	QA	0.28	0/226	0.33	0/301
1	R	0.35	0/226	0.35	0/301
1	RA	0.28	0/226	0.33	0/301
1	S	0.35	0/226	0.35	0/301
1	SA	0.28	0/226	0.32	0/301
1	T	0.35	0/226	0.35	0/301
1	TA	0.28	0/226	0.32	0/301
1	U	0.35	0/226	0.35	0/301
1	UA	0.28	0/226	0.33	0/301
1	V	0.35	0/226	0.35	0/301
1	VA	0.28	0/226	0.33	0/301
1	W	0.35	0/226	0.35	0/301
1	WA	0.28	0/226	0.33	0/301
1	X	0.35	0/226	0.35	0/301
1	XA	0.28	0/226	0.33	0/301
1	Y	0.35	0/226	0.35	0/301
1	YA	0.28	0/226	0.33	0/301
1	Z	0.35	0/226	0.35	0/301
1	ZA	0.28	0/226	0.33	0/301
1	a	0.35	0/226	0.35	0/301
1	aA	0.28	0/226	0.33	0/301
1	b	0.35	0/226	0.35	0/301
1	bA	0.28	0/226	0.33	0/301
1	c	0.35	0/226	0.35	0/301
1	cA	0.28	0/226	0.33	0/301
1	d	0.35	0/226	0.35	0/301
1	dA	0.28	0/226	0.33	0/301
1	e	0.35	0/226	0.35	0/301
1	eA	0.28	0/226	0.32	0/301
1	f	0.35	0/226	0.35	0/301
1	fA	0.28	0/226	0.33	0/301
1	g	0.35	0/226	0.35	0/301
1	gA	0.28	0/226	0.33	0/301
1	h	0.35	0/226	0.35	0/301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	hA	0.28	0/226	0.33	0/301
1	i	0.35	0/226	0.35	0/301
1	iA	0.28	0/226	0.33	0/301
1	j	0.35	0/226	0.35	0/301
1	jA	0.28	0/226	0.32	0/301
1	k	0.35	0/226	0.35	0/301
1	kA	0.28	0/226	0.33	0/301
1	l	0.35	0/226	0.35	0/301
1	lA	0.28	0/226	0.32	0/301
1	m	0.35	0/226	0.35	0/301
1	mA	0.28	0/226	0.33	0/301
1	n	0.35	0/226	0.35	0/301
1	nA	0.28	0/226	0.32	0/301
1	o	0.35	0/226	0.35	0/301
1	oA	0.28	0/226	0.33	0/301
1	p	0.35	0/226	0.35	0/301
1	pA	0.28	0/226	0.33	0/301
1	q	0.35	0/226	0.35	0/301
1	r	0.35	0/226	0.35	0/301
1	s	0.35	0/226	0.35	0/301
1	t	0.35	0/226	0.35	0/301
1	u	0.35	0/226	0.35	0/301
1	v	0.35	0/226	0.35	0/301
1	w	0.35	0/226	0.35	0/301
1	x	0.35	0/226	0.35	0/301
1	y	0.35	0/226	0.35	0/301
1	z	0.35	0/226	0.35	0/301
All	All	0.31	0/23504	0.34	0/31304

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	225	0	239	12	0
1	1	225	0	239	11	0
1	2	225	0	239	12	0
1	3	225	0	239	15	0
1	4	225	0	239	12	0
1	5	225	0	239	12	0
1	6	225	0	239	12	0
1	7	225	0	239	12	0
1	8	225	0	239	13	0
1	9	225	0	239	15	0
1	A	225	0	242	16	0
1	AA	225	0	239	11	0
1	B	225	0	242	19	0
1	BA	225	0	239	12	0
1	C	225	0	242	16	0
1	CA	225	0	239	13	0
1	D	225	0	242	13	0
1	DA	225	0	239	11	0
1	E	225	0	242	17	0
1	EA	225	0	239	11	0
1	F	225	0	242	14	0
1	FA	225	0	239	15	0
1	G	225	0	242	17	0
1	GA	225	0	239	11	0
1	H	225	0	242	20	0
1	HA	225	0	239	10	0
1	I	225	0	242	20	0
1	IA	225	0	239	12	0
1	J	225	0	242	16	0
1	JA	225	0	239	9	0
1	K	225	0	242	17	0
1	KA	225	0	239	11	0
1	L	225	0	242	17	0
1	LA	225	0	239	13	0
1	M	225	0	242	17	0
1	MA	225	0	239	11	0
1	N	225	0	242	17	0
1	NA	225	0	239	12	0
1	O	225	0	242	18	0
1	OA	225	0	239	14	0
1	P	225	0	242	16	0
1	PA	225	0	239	10	0
1	Q	225	0	242	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	225	0	239	13	0
1	R	225	0	242	20	0
1	RA	225	0	239	13	0
1	S	225	0	242	17	0
1	SA	225	0	239	11	0
1	T	225	0	242	14	0
1	TA	225	0	239	15	0
1	U	225	0	242	15	0
1	UA	225	0	239	13	0
1	V	225	0	242	16	0
1	VA	225	0	239	11	0
1	W	225	0	242	18	0
1	WA	225	0	239	15	0
1	X	225	0	242	21	0
1	XA	225	0	239	13	0
1	Y	225	0	242	19	0
1	YA	225	0	239	12	0
1	Z	225	0	242	14	0
1	ZA	225	0	239	13	0
1	a	225	0	242	17	0
1	aA	225	0	239	13	0
1	b	225	0	242	16	0
1	bA	225	0	239	10	0
1	c	225	0	242	24	0
1	cA	225	0	239	11	0
1	d	225	0	242	19	0
1	dA	225	0	239	10	0
1	e	225	0	242	17	0
1	eA	225	0	239	10	0
1	f	225	0	242	15	0
1	fA	225	0	239	12	0
1	g	225	0	242	19	0
1	gA	225	0	239	12	0
1	h	225	0	242	19	0
1	hA	225	0	239	12	0
1	i	225	0	242	24	0
1	iA	225	0	239	12	0
1	j	225	0	242	18	0
1	jA	225	0	239	12	0
1	k	225	0	242	18	0
1	kA	225	0	239	9	0
1	l	225	0	242	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	lA	225	0	239	9	0
1	m	225	0	242	16	0
1	mA	225	0	239	11	0
1	n	225	0	242	17	0
1	nA	225	0	239	11	0
1	o	225	0	242	14	0
1	oA	225	0	239	11	0
1	p	225	0	242	19	0
1	pA	225	0	239	12	0
1	q	225	0	242	14	0
1	r	225	0	242	18	0
1	s	225	0	242	13	0
1	t	225	0	242	16	0
1	u	225	0	242	12	0
1	v	225	0	242	15	0
1	w	225	0	242	11	0
1	x	225	0	242	14	0
1	y	225	0	242	11	0
1	z	225	0	242	14	0
All	All	23400	0	25012	1173	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 24.

All (1173) 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:H:29:GLN:O	1:d:2:ALA:N	2.05	0.89
1:c:25:ILE:HG12	1:i:23:ALA:HB2	1.54	0.89
1:l:12:LEU:HD12	1:r:18:ILE:HD11	1.54	0.89
1:SA:123:ALA:HB2	1:YA:118:ILE:HG12	1.55	0.88
1:K:29:GLN:O	1:L:1:GLN:N	2.10	0.85
1:B:29:GLN:O	1:X:2:ALA:N	2.11	0.83
1:Y:1:GLN:N	1:u:29:GLN:O	2.13	0.79
1:c:25:ILE:CG1	1:i:23:ALA:HB2	2.17	0.73
1:O:1:GLN:N	1:k:29:GLN:O	2.19	0.71
1:YA:112:LEU:HD12	1:eA:111:ILE:HD11	1.72	0.71
1:b:26:LEU:HD21	1:h:29:GLN:HG2	1.72	0.71
1:LA:108:ASP:HA	1:LA:111:ILE:HD12	1.73	0.71
1:BA:108:ASP:HA	1:BA:111:ILE:HD12	1.73	0.70
1:CA:108:ASP:HA	1:CA:111:ILE:HD12	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:aA:108:ASP:HA	1:aA:111:ILE:HD12	1.74	0.70
1:ZA:108:ASP:HA	1:ZA:111:ILE:HD12	1.73	0.70
1:l:19:LEU:HD12	1:r:25:ILE:HD11	1.71	0.70
1:jA:108:ASP:HA	1:jA:111:ILE:HD12	1.74	0.70
1:A:1:GLN:N	1:W:29:GLN:O	2.18	0.70
1:GA:108:ASP:HA	1:GA:111:ILE:HD12	1.74	0.70
1:6:108:ASP:HA	1:6:111:ILE:HD12	1.74	0.70
1:FA:108:ASP:HA	1:FA:111:ILE:HD12	1.73	0.70
1:HA:108:ASP:HA	1:HA:111:ILE:HD12	1.73	0.70
1:MA:108:ASP:HA	1:MA:111:ILE:HD12	1.73	0.70
1:dA:108:ASP:HA	1:dA:111:ILE:HD12	1.74	0.70
1:UA:108:ASP:HA	1:UA:111:ILE:HD12	1.74	0.70
1:eA:108:ASP:HA	1:eA:111:ILE:HD12	1.74	0.70
1:b:29:GLN:O	1:x:1:GLN:N	2.16	0.70
1:iA:108:ASP:HA	1:iA:111:ILE:HD12	1.73	0.70
1:kA:108:ASP:HA	1:kA:111:ILE:HD12	1.74	0.70
1:fA:108:ASP:HA	1:fA:111:ILE:HD12	1.74	0.70
1:gA:108:ASP:HA	1:gA:111:ILE:HD12	1.73	0.70
1:5:108:ASP:HA	1:5:111:ILE:HD12	1.73	0.70
1:TA:108:ASP:HA	1:TA:111:ILE:HD12	1.73	0.70
1:RA:108:ASP:HA	1:RA:111:ILE:HD12	1.73	0.70
1:IA:108:ASP:HA	1:IA:111:ILE:HD12	1.73	0.70
1:RA:118:ILE:HG12	1:XA:123:ALA:HB2	1.73	0.70
1:cA:108:ASP:HA	1:cA:111:ILE:HD12	1.73	0.70
1:pA:108:ASP:HA	1:pA:111:ILE:HD12	1.73	0.70
1:AA:108:ASP:HA	1:AA:111:ILE:HD12	1.73	0.69
1:DA:108:ASP:HA	1:DA:111:ILE:HD12	1.73	0.69
1:bA:111:ILE:HD11	1:hA:112:LEU:HD12	1.74	0.69
1:7:108:ASP:HA	1:7:111:ILE:HD12	1.74	0.69
1:8:108:ASP:HA	1:8:111:ILE:HD12	1.73	0.69
1:EA:108:ASP:HA	1:EA:111:ILE:HD12	1.74	0.69
1:YA:108:ASP:HA	1:YA:111:ILE:HD12	1.73	0.69
1:oA:108:ASP:HA	1:oA:111:ILE:HD12	1.73	0.69
1:OA:108:ASP:HA	1:OA:111:ILE:HD12	1.73	0.69
1:SA:108:ASP:HA	1:SA:111:ILE:HD12	1.73	0.69
1:hA:108:ASP:HA	1:hA:111:ILE:HD12	1.73	0.69
1:K:29:GLN:O	1:L:2:ALA:N	2.22	0.69
1:nA:108:ASP:HA	1:nA:111:ILE:HD12	1.73	0.69
1:9:108:ASP:HA	1:9:111:ILE:HD12	1.74	0.69
1:XA:108:ASP:HA	1:XA:111:ILE:HD12	1.73	0.69
1:A:29:GLN:O	1:V:1:GLN:N	2.17	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JA:108:ASP:HA	1:JA:111:ILE:HD12	1.73	0.69
1:NA:108:ASP:HA	1:NA:111:ILE:HD12	1.73	0.69
1:bA:108:ASP:HA	1:bA:111:ILE:HD12	1.73	0.69
1:0:108:ASP:HA	1:0:111:ILE:HD12	1.74	0.69
1:2:108:ASP:HA	1:2:111:ILE:HD12	1.73	0.69
1:1:108:ASP:HA	1:1:111:ILE:HD12	1.73	0.69
1:a:1:GLN:N	1:w:29:GLN:O	2.19	0.68
1:WA:108:ASP:HA	1:WA:111:ILE:HD12	1.73	0.68
1:KA:108:ASP:HA	1:KA:111:ILE:HD12	1.73	0.68
1:IA:108:ASP:HA	1:IA:111:ILE:HD12	1.73	0.68
1:mA:108:ASP:HA	1:mA:111:ILE:HD12	1.74	0.68
1:3:108:ASP:HA	1:3:111:ILE:HD12	1.73	0.68
1:4:108:ASP:HA	1:4:111:ILE:HD12	1.73	0.68
1:ZA:111:ILE:HD11	1:fA:112:LEU:HD12	1.75	0.68
1:VA:108:ASP:HA	1:VA:111:ILE:HD12	1.74	0.68
1:jA:111:ILE:HD11	1:pA:112:LEU:HD12	1.75	0.68
1:E:29:GLN:O	1:R:2:ALA:N	2.18	0.68
1:F:1:GLN:N	1:Q:29:GLN:O	2.20	0.67
1:PA:108:ASP:HA	1:PA:111:ILE:HD12	1.73	0.67
1:QA:108:ASP:HA	1:QA:111:ILE:HD12	1.73	0.67
1:b:23:ALA:HB2	1:h:25:ILE:HG12	1.77	0.67
1:r:12:LEU:HD12	1:x:18:ILE:HD11	1.76	0.66
1:l:12:LEU:HD12	1:r:18:ILE:CD1	2.24	0.66
1:l:19:LEU:HD12	1:r:25:ILE:CD1	2.25	0.66
1:2:111:ILE:HD11	1:3:112:LEU:HD12	1.78	0.65
1:b:23:ALA:HB2	1:h:25:ILE:CG1	2.27	0.65
1:hA:111:ILE:HD11	1:nA:112:LEU:HD12	1.78	0.65
1:J:1:GLN:N	1:M:29:GLN:O	2.24	0.65
1:iA:112:LEU:HD12	1:oA:111:ILE:HD11	1.79	0.65
1:SA:123:ALA:HB2	1:YA:118:ILE:CG1	2.26	0.65
1:WA:112:LEU:HD12	1:cA:111:ILE:HD11	1.80	0.65
1:A:29:GLN:HG2	1:G:26:LEU:HD21	1.80	0.64
1:2:116:ALA:HA	1:2:119:LEU:HD12	1.81	0.63
1:8:116:ALA:HA	1:8:119:LEU:HD12	1.81	0.63
1:QA:112:LEU:HD12	1:WA:111:ILE:HD11	1.78	0.63
1:3:111:ILE:HD11	1:9:112:LEU:HD12	1.81	0.63
1:3:116:ALA:HA	1:3:119:LEU:HD12	1.81	0.63
1:8:112:LEU:HD12	1:EA:111:ILE:HD11	1.81	0.63
1:AA:116:ALA:HA	1:AA:119:LEU:HD12	1.81	0.63
1:DA:116:ALA:HA	1:DA:119:LEU:HD12	1.81	0.63
1:p:12:LEU:HD12	1:v:18:ILE:HD11	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:nA:116:ALA:HA	1:nA:119:LEU:HD12	1.81	0.63
1:1:116:ALA:HA	1:1:119:LEU:HD12	1.81	0.63
1:4:116:ALA:HA	1:4:119:LEU:HD12	1.81	0.63
1:7:116:ALA:HA	1:7:119:LEU:HD12	1.81	0.63
1:EA:116:ALA:HA	1:EA:119:LEU:HD12	1.81	0.63
1:GA:116:ALA:HA	1:GA:119:LEU:HD12	1.81	0.63
1:JA:116:ALA:HA	1:JA:119:LEU:HD12	1.81	0.63
1:ZA:116:ALA:HA	1:ZA:119:LEU:HD12	1.81	0.63
1:hA:116:ALA:HA	1:hA:119:LEU:HD12	1.81	0.63
1:lA:116:ALA:HA	1:lA:119:LEU:HD12	1.81	0.63
1:oA:116:ALA:HA	1:oA:119:LEU:HD12	1.81	0.63
1:TA:116:ALA:HA	1:TA:119:LEU:HD12	1.81	0.63
1:bA:116:ALA:HA	1:bA:119:LEU:HD12	1.81	0.63
1:cA:116:ALA:HA	1:cA:119:LEU:HD12	1.81	0.63
1:fA:116:ALA:HA	1:fA:119:LEU:HD12	1.81	0.63
1:iA:116:ALA:HA	1:iA:119:LEU:HD12	1.81	0.63
1:mA:116:ALA:HA	1:mA:119:LEU:HD12	1.81	0.63
1:5:116:ALA:HA	1:5:119:LEU:HD12	1.81	0.63
1:9:116:ALA:HA	1:9:119:LEU:HD12	1.81	0.63
1:NA:116:ALA:HA	1:NA:119:LEU:HD12	1.81	0.63
1:PA:116:ALA:HA	1:PA:119:LEU:HD12	1.81	0.63
1:VA:111:ILE:HD11	1:bA:112:LEU:HD12	1.81	0.63
1:WA:116:ALA:HA	1:WA:119:LEU:HD12	1.81	0.63
1:0:116:ALA:HA	1:0:119:LEU:HD12	1.81	0.63
1:BA:116:ALA:HA	1:BA:119:LEU:HD12	1.81	0.63
1:KA:116:ALA:HA	1:KA:119:LEU:HD12	1.81	0.63
1:SA:116:ALA:HA	1:SA:119:LEU:HD12	1.81	0.63
1:FA:116:ALA:HA	1:FA:119:LEU:HD12	1.81	0.62
1:HA:116:ALA:HA	1:HA:119:LEU:HD12	1.81	0.62
1:MA:116:ALA:HA	1:MA:119:LEU:HD12	1.81	0.62
1:jA:116:ALA:HA	1:jA:119:LEU:HD12	1.81	0.62
1:pA:116:ALA:HA	1:pA:119:LEU:HD12	1.81	0.62
1:QA:116:ALA:HA	1:QA:119:LEU:HD12	1.81	0.62
1:VA:116:ALA:HA	1:VA:119:LEU:HD12	1.81	0.62
1:YA:116:ALA:HA	1:YA:119:LEU:HD12	1.81	0.62
1:eA:116:ALA:HA	1:eA:119:LEU:HD12	1.81	0.62
1:gA:116:ALA:HA	1:gA:119:LEU:HD12	1.81	0.62
1:6:116:ALA:HA	1:6:119:LEU:HD12	1.81	0.62
1:CA:116:ALA:HA	1:CA:119:LEU:HD12	1.81	0.62
1:dA:116:ALA:HA	1:dA:119:LEU:HD12	1.81	0.62
1:LA:116:ALA:HA	1:LA:119:LEU:HD12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:TA:111:ILE:HD11	1:ZA:112:LEU:HD12	1.80	0.62
1:i:22:HIS:HA	1:i:25:ILE:HD12	1.82	0.62
1:o:22:HIS:HA	1:o:25:ILE:HD12	1.82	0.62
1:kA:116:ALA:HA	1:kA:119:LEU:HD12	1.81	0.62
1:E:22:HIS:HA	1:E:25:ILE:HD12	1.82	0.62
1:K:22:HIS:HA	1:K:25:ILE:HD12	1.82	0.62
1:L:22:HIS:HA	1:L:25:ILE:HD12	1.82	0.62
1:M:1:GLN:N	1:i:29:GLN:O	2.32	0.62
1:aA:116:ALA:HA	1:aA:119:LEU:HD12	1.81	0.62
1:u:22:HIS:HA	1:u:25:ILE:HD12	1.82	0.62
1:v:22:HIS:HA	1:v:25:ILE:HD12	1.82	0.62
1:B:22:HIS:HA	1:B:25:ILE:HD12	1.82	0.62
1:Q:22:HIS:HA	1:Q:25:ILE:HD12	1.82	0.62
1:p:22:HIS:HA	1:p:25:ILE:HD12	1.82	0.62
1:y:22:HIS:HA	1:y:25:ILE:HD12	1.82	0.62
1:F:22:HIS:HA	1:F:25:ILE:HD12	1.82	0.62
1:FA:118:ILE:HG12	1:LA:123:ALA:HB2	1.81	0.62
1:R:22:HIS:HA	1:R:25:ILE:HD12	1.82	0.62
1:IA:116:ALA:HA	1:IA:119:LEU:HD12	1.81	0.62
1:W:22:HIS:HA	1:W:25:ILE:HD12	1.82	0.62
1:OA:116:ALA:HA	1:OA:119:LEU:HD12	1.81	0.62
1:RA:116:ALA:HA	1:RA:119:LEU:HD12	1.81	0.62
1:s:22:HIS:HA	1:s:25:ILE:HD12	1.82	0.62
1:A:22:HIS:HA	1:A:25:ILE:HD12	1.82	0.62
1:c:22:HIS:HA	1:c:25:ILE:HD12	1.82	0.62
1:XA:116:ALA:HA	1:XA:119:LEU:HD12	1.81	0.62
1:H:22:HIS:HA	1:H:25:ILE:HD12	1.82	0.62
1:X:22:HIS:HA	1:X:25:ILE:HD12	1.82	0.62
1:d:22:HIS:HA	1:d:25:ILE:HD12	1.82	0.62
1:UA:116:ALA:HA	1:UA:119:LEU:HD12	1.81	0.62
1:j:22:HIS:HA	1:j:25:ILE:HD12	1.82	0.62
1:z:22:HIS:HA	1:z:25:ILE:HD12	1.82	0.62
1:U:18:ILE:HD11	1:a:12:LEU:HD12	1.81	0.61
1:a:22:HIS:HA	1:a:25:ILE:HD12	1.82	0.61
1:d:26:LEU:HD21	1:j:29:GLN:HG2	1.83	0.61
1:f:22:HIS:HA	1:f:25:ILE:HD12	1.82	0.61
1:g:22:HIS:HA	1:g:25:ILE:HD12	1.82	0.61
1:h:22:HIS:HA	1:h:25:ILE:HD12	1.82	0.61
1:M:22:HIS:HA	1:M:25:ILE:HD12	1.82	0.61
1:EA:112:LEU:HD12	1:KA:111:ILE:HD11	1.82	0.61
1:n:22:HIS:HA	1:n:25:ILE:HD12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:18:ILE:HD11	1:O:12:LEU:HD12	1.82	0.61
1:N:22:HIS:HA	1:N:25:ILE:HD12	1.82	0.61
1:S:22:HIS:HA	1:S:25:ILE:HD12	1.82	0.61
1:T:22:HIS:HA	1:T:25:ILE:HD12	1.82	0.61
1:Z:22:HIS:HA	1:Z:25:ILE:HD12	1.82	0.61
1:l:22:HIS:HA	1:l:25:ILE:HD12	1.82	0.61
1:m:22:HIS:HA	1:m:25:ILE:HD12	1.82	0.61
1:t:22:HIS:HA	1:t:25:ILE:HD12	1.82	0.61
1:G:22:HIS:HA	1:G:25:ILE:HD12	1.82	0.61
1:U:22:HIS:HA	1:U:25:ILE:HD12	1.82	0.61
1:Y:22:HIS:HA	1:Y:25:ILE:HD12	1.82	0.61
1:b:22:HIS:HA	1:b:25:ILE:HD12	1.82	0.61
1:O:22:HIS:HA	1:O:25:ILE:HD12	1.82	0.61
1:Y:1:GLN:H3	1:u:29:GLN:C	2.04	0.61
1:e:22:HIS:HA	1:e:25:ILE:HD12	1.82	0.61
1:h:12:LEU:HD12	1:n:18:ILE:HD11	1.82	0.61
1:r:22:HIS:HA	1:r:25:ILE:HD12	1.82	0.61
1:V:22:HIS:HA	1:V:25:ILE:HD12	1.82	0.61
1:OA:112:LEU:HD12	1:UA:111:ILE:HD11	1.82	0.61
1:w:22:HIS:HA	1:w:25:ILE:HD12	1.82	0.60
1:x:22:HIS:HA	1:x:25:ILE:HD12	1.82	0.60
1:k:22:HIS:HA	1:k:25:ILE:HD12	1.82	0.60
1:q:22:HIS:HA	1:q:25:ILE:HD12	1.82	0.60
1:J:22:HIS:HA	1:J:25:ILE:HD12	1.82	0.60
1:A:2:ALA:N	1:W:29:GLN:O	2.29	0.60
1:C:22:HIS:HA	1:C:25:ILE:HD12	1.82	0.60
1:D:22:HIS:HA	1:D:25:ILE:HD12	1.82	0.60
1:P:22:HIS:HA	1:P:25:ILE:HD12	1.82	0.60
1:I:22:HIS:HA	1:I:25:ILE:HD12	1.82	0.60
1:H:29:GLN:OXT	1:d:2:ALA:HB3	2.03	0.59
1:R:26:LEU:HD21	1:X:29:GLN:HG2	1.84	0.59
1:E:29:GLN:O	1:R:1:GLN:N	2.21	0.59
1:SA:123:ALA:CB	1:YA:118:ILE:HG12	2.30	0.59
1:B:29:GLN:O	1:X:1:GLN:N	2.23	0.59
1:g:29:GLN:HG2	1:m:26:LEU:HD21	1.86	0.58
1:o:25:ILE:HG12	1:u:23:ALA:HB2	1.85	0.57
1:Z:12:LEU:HD12	1:f:18:ILE:HD11	1.85	0.57
1:b:3:GLU:OE1	1:b:3:GLU:N	2.37	0.57
1:cA:112:LEU:HD12	1:iA:111:ILE:HD11	1.86	0.57
1:P:23:ALA:HB2	1:V:25:ILE:HG12	1.85	0.57
1:Z:26:LEU:HD21	1:f:29:GLN:HG2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:t:12:LEU:HD12	1:z:18:ILE:HD11	1.85	0.57
1:B:3:GLU:N	1:B:3:GLU:OE1	2.37	0.57
1:J:3:GLU:OE1	1:J:3:GLU:N	2.37	0.57
1:f:26:LEU:HD21	1:l:29:GLN:HG2	1.85	0.57
1:M:25:ILE:HG12	1:S:23:ALA:HB2	1.87	0.57
1:T:3:GLU:OE1	1:T:3:GLU:N	2.37	0.56
1:a:3:GLU:OE1	1:a:3:GLU:N	2.37	0.56
1:C:12:LEU:HD12	1:D:18:ILE:HD11	1.88	0.56
1:O:18:ILE:HD11	1:U:12:LEU:HD12	1.86	0.56
1:e:3:GLU:OE1	1:e:3:GLU:N	2.37	0.56
1:h:3:GLU:OE1	1:h:3:GLU:N	2.37	0.56
1:I:29:GLN:O	1:N:2:ALA:N	2.28	0.56
1:M:3:GLU:OE1	1:M:3:GLU:N	2.37	0.56
1:g:18:ILE:HD11	1:m:12:LEU:HD12	1.87	0.56
1:I:3:GLU:OE1	1:I:3:GLU:N	2.37	0.56
1:j:3:GLU:OE1	1:j:3:GLU:N	2.37	0.56
1:l:3:GLU:N	1:l:3:GLU:OE1	2.37	0.56
1:z:3:GLU:OE1	1:z:3:GLU:N	2.37	0.56
1:GA:112:LEU:HD12	1:MA:111:ILE:HD11	1.86	0.56
1:XA:111:ILE:HD11	1:dA:112:LEU:HD12	1.87	0.56
1:F:3:GLU:OE1	1:F:3:GLU:N	2.37	0.56
1:R:15:TYR:HA	1:R:18:ILE:HD12	1.88	0.56
1:o:3:GLU:OE1	1:o:3:GLU:N	2.37	0.56
1:o:15:TYR:HA	1:o:18:ILE:HD12	1.88	0.56
1:X:15:TYR:HA	1:X:18:ILE:HD12	1.88	0.56
1:PA:111:ILE:HD11	1:VA:112:LEU:HD12	1.86	0.56
1:d:15:TYR:HA	1:d:18:ILE:HD12	1.88	0.56
1:L:15:TYR:HA	1:L:18:ILE:HD12	1.88	0.56
1:i:15:TYR:HA	1:i:18:ILE:HD12	1.88	0.56
1:t:15:TYR:HA	1:t:18:ILE:HD12	1.88	0.56
1:u:15:TYR:HA	1:u:18:ILE:HD12	1.88	0.56
1:P:3:GLU:OE1	1:P:3:GLU:N	2.37	0.56
1:j:15:TYR:HA	1:j:18:ILE:HD12	1.88	0.56
1:w:3:GLU:OE1	1:w:3:GLU:N	2.37	0.56
1:K:3:GLU:OE1	1:K:3:GLU:N	2.37	0.55
1:FA:111:ILE:HD11	1:LA:112:LEU:HD12	1.88	0.55
1:W:15:TYR:HA	1:W:18:ILE:HD12	1.88	0.55
1:Y:11:ILE:HD11	1:e:8:ASP:HB2	1.88	0.55
1:c:15:TYR:HA	1:c:18:ILE:HD12	1.88	0.55
1:F:15:TYR:HA	1:F:18:ILE:HD12	1.88	0.55
1:M:15:TYR:HA	1:M:18:ILE:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:UA:112:LEU:HD12	1:aA:111:ILE:HD11	1.89	0.55
1:h:15:TYR:HA	1:h:18:ILE:HD12	1.88	0.55
1:n:15:TYR:HA	1:n:18:ILE:HD12	1.88	0.55
1:v:15:TYR:HA	1:v:18:ILE:HD12	1.88	0.55
1:E:15:TYR:HA	1:E:18:ILE:HD12	1.88	0.55
1:L:23:ALA:HB2	1:R:25:ILE:HG12	1.87	0.55
1:S:15:TYR:HA	1:S:18:ILE:HD12	1.88	0.55
1:p:15:TYR:HA	1:p:18:ILE:HD12	1.88	0.55
1:s:15:TYR:HA	1:s:18:ILE:HD12	1.88	0.55
1:z:15:TYR:HA	1:z:18:ILE:HD12	1.88	0.55
1:G:15:TYR:HA	1:G:18:ILE:HD12	1.88	0.55
1:K:15:TYR:HA	1:K:18:ILE:HD12	1.88	0.55
1:y:15:TYR:HA	1:y:18:ILE:HD12	1.88	0.55
1:A:15:TYR:HA	1:A:18:ILE:HD12	1.88	0.55
1:B:15:TYR:HA	1:B:18:ILE:HD12	1.88	0.55
1:H:15:TYR:HA	1:H:18:ILE:HD12	1.88	0.55
1:Q:15:TYR:HA	1:Q:18:ILE:HD12	1.88	0.55
1:Y:15:TYR:HA	1:Y:18:ILE:HD12	1.88	0.55
1:Y:25:ILE:HG12	1:e:23:ALA:HB2	1.87	0.55
1:m:3:GLU:OE1	1:m:3:GLU:N	2.37	0.55
1:X:3:GLU:OE1	1:X:3:GLU:N	2.37	0.55
1:b:15:TYR:HA	1:b:18:ILE:HD12	1.88	0.55
1:2:112:LEU:HD12	1:8:111:ILE:HD11	1.89	0.55
1:m:15:TYR:HA	1:m:18:ILE:HD12	1.88	0.55
1:N:15:TYR:HA	1:N:18:ILE:HD12	1.88	0.55
1:k:15:TYR:HA	1:k:18:ILE:HD12	1.88	0.55
1:e:15:TYR:HA	1:e:18:ILE:HD12	1.88	0.55
1:H:3:GLU:OE1	1:H:3:GLU:N	2.37	0.55
1:q:15:TYR:HA	1:q:18:ILE:HD12	1.88	0.55
1:KA:112:LEU:HD12	1:QA:111:ILE:HD11	1.90	0.54
1:a:15:TYR:HA	1:a:18:ILE:HD12	1.88	0.54
1:f:15:TYR:HA	1:f:18:ILE:HD12	1.88	0.54
1:T:15:TYR:HA	1:T:18:ILE:HD12	1.88	0.54
1:V:15:TYR:HA	1:V:18:ILE:HD12	1.88	0.54
1:g:15:TYR:HA	1:g:18:ILE:HD12	1.88	0.54
1:w:15:TYR:HA	1:w:18:ILE:HD12	1.88	0.54
1:J:15:TYR:HA	1:J:18:ILE:HD12	1.88	0.54
1:Z:15:TYR:HA	1:Z:18:ILE:HD12	1.88	0.54
1:C:3:GLU:OE1	1:C:3:GLU:N	2.37	0.54
1:P:15:TYR:HA	1:P:18:ILE:HD12	1.88	0.54
1:l:15:TYR:HA	1:l:18:ILE:HD12	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:15:TYR:HA	1:O:18:ILE:HD12	1.88	0.54
1:r:15:TYR:HA	1:r:18:ILE:HD12	1.88	0.54
1:D:15:TYR:HA	1:D:18:ILE:HD12	1.88	0.54
1:BA:118:ILE:HG12	1:HA:123:ALA:HB2	1.90	0.54
1:Y:3:GLU:OE1	1:Y:3:GLU:N	2.37	0.54
1:Z:3:GLU:OE1	1:Z:3:GLU:N	2.37	0.54
1:U:15:TYR:HA	1:U:18:ILE:HD12	1.88	0.54
1:W:3:GLU:OE1	1:W:3:GLU:N	2.37	0.54
1:i:3:GLU:OE1	1:i:3:GLU:N	2.37	0.54
1:U:3:GLU:OE1	1:U:3:GLU:N	2.37	0.54
1:x:15:TYR:HA	1:x:18:ILE:HD12	1.88	0.54
1:I:15:TYR:HA	1:I:18:ILE:HD12	1.88	0.54
1:CA:123:ALA:HB2	1:IA:118:ILE:HG12	1.89	0.54
1:V:12:LEU:HD12	1:b:18:ILE:HD11	1.90	0.54
1:d:3:GLU:OE1	1:d:3:GLU:N	2.37	0.54
1:r:3:GLU:OE1	1:r:3:GLU:N	2.37	0.54
1:v:3:GLU:OE1	1:v:3:GLU:N	2.37	0.54
1:Q:3:GLU:OE1	1:Q:3:GLU:N	2.37	0.54
1:OA:123:ALA:HB2	1:UA:118:ILE:HG12	1.89	0.54
1:n:3:GLU:OE1	1:n:3:GLU:N	2.37	0.54
1:q:3:GLU:OE1	1:q:3:GLU:N	2.37	0.54
1:G:3:GLU:OE1	1:G:3:GLU:N	2.37	0.53
1:C:15:TYR:HA	1:C:18:ILE:HD12	1.88	0.53
1:V:3:GLU:N	1:V:3:GLU:OE1	2.37	0.53
1:MA:112:LEU:HD12	1:SA:111:ILE:HD11	1.90	0.53
1:r:26:LEU:HD21	1:x:29:GLN:HG2	1.90	0.53
1:H:26:LEU:HD21	1:N:29:GLN:HG2	1.90	0.53
1:5:118:ILE:HG12	1:BA:123:ALA:HB2	1.90	0.53
1:DA:111:ILE:HD11	1:JA:112:LEU:HD12	1.90	0.53
1:F:23:ALA:HB2	1:L:25:ILE:HG12	1.90	0.53
1:c:3:GLU:OE1	1:c:3:GLU:N	2.37	0.53
1:k:29:GLN:HG2	1:q:26:LEU:HD21	1.91	0.53
1:y:3:GLU:OE1	1:y:3:GLU:N	2.37	0.53
1:L:3:GLU:OE1	1:L:3:GLU:N	2.37	0.53
1:j:26:LEU:HD21	1:p:29:GLN:HG2	1.91	0.53
1:E:3:GLU:OE1	1:E:3:GLU:N	2.37	0.53
1:J:29:GLN:O	1:f:1:GLN:N	2.30	0.53
1:Q:18:ILE:HD11	1:W:12:LEU:HD12	1.90	0.53
1:p:3:GLU:OE1	1:p:3:GLU:N	2.37	0.53
1:t:8:ASP:HB2	1:z:11:ILE:HD11	1.91	0.53
1:s:3:GLU:N	1:s:3:GLU:OE1	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:j:8:ASP:HB2	1:p:11:ILE:HD11	1.91	0.52
1:j:12:LEU:HD12	1:p:18:ILE:HD11	1.90	0.52
1:s:29:GLN:HG2	1:y:26:LEU:HD21	1.89	0.52
1:u:3:GLU:OE1	1:u:3:GLU:N	2.37	0.52
1:A:3:GLU:OE1	1:A:3:GLU:N	2.37	0.52
1:I:11:ILE:HD11	1:O:8:ASP:HB2	1.90	0.52
1:a:11:ILE:HD11	1:g:8:ASP:HB2	1.91	0.52
1:r:12:LEU:HD12	1:x:18:ILE:CD1	2.39	0.52
1:R:3:GLU:OE1	1:R:3:GLU:N	2.37	0.52
1:IA:112:LEU:HD12	1:OA:111:ILE:HD11	1.90	0.52
1:N:3:GLU:OE1	1:N:3:GLU:N	2.37	0.52
1:g:3:GLU:OE1	1:g:3:GLU:N	2.37	0.52
1:n:12:LEU:HD12	1:t:18:ILE:HD11	1.90	0.52
1:r:19:LEU:HD12	1:x:25:ILE:HD11	1.92	0.52
1:C:29:GLN:O	1:T:2:ALA:N	2.27	0.52
1:G:29:GLN:O	1:P:1:GLN:N	2.34	0.52
1:D:3:GLU:OE1	1:D:3:GLU:N	2.37	0.52
1:7:111:ILE:HD11	1:DA:112:LEU:HD12	1.92	0.52
1:a:18:ILE:HD11	1:g:12:LEU:HD12	1.91	0.52
1:c:11:ILE:HD11	1:i:8:ASP:HB2	1.92	0.52
1:t:26:LEU:HD21	1:z:29:GLN:HG2	1.92	0.52
1:TA:111:ILE:CD1	1:ZA:112:LEU:HD12	2.40	0.51
1:AA:112:LEU:HD12	1:GA:111:ILE:HD11	1.91	0.51
1:W:25:ILE:HG12	1:c:23:ALA:HB2	1.92	0.51
1:c:25:ILE:HD11	1:i:19:LEU:HB3	1.91	0.51
1:C:29:GLN:O	1:T:1:GLN:N	2.30	0.51
1:M:29:GLN:HG2	1:S:26:LEU:HD21	1.92	0.51
1:R:23:ALA:HB2	1:X:25:ILE:HG12	1.93	0.51
1:r:19:LEU:HD12	1:x:25:ILE:CD1	2.41	0.51
1:t:3:GLU:OE1	1:t:3:GLU:N	2.37	0.51
1:D:12:LEU:HD12	1:J:18:ILE:HD11	1.92	0.51
1:G:25:ILE:HG12	1:M:23:ALA:HB2	1.91	0.51
1:iA:112:LEU:HD12	1:oA:111:ILE:CD1	2.40	0.51
1:N:12:LEU:HD12	1:T:18:ILE:HD11	1.91	0.51
1:ZA:111:ILE:CD1	1:fA:112:LEU:HD12	2.40	0.51
1:k:3:GLU:OE1	1:k:3:GLU:N	2.37	0.51
1:O:123:ALA:HB2	1:6:118:ILE:HG12	1.93	0.51
1:p:12:LEU:HD12	1:v:18:ILE:CD1	2.41	0.51
1:HA:111:ILE:HD11	1:NA:112:LEU:HD12	1.93	0.51
1:i:18:ILE:HD11	1:o:12:LEU:HD12	1.92	0.51
1:x:3:GLU:OE1	1:x:3:GLU:N	2.37	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ALA:HB2	1:F:25:ILE:HG12	1.93	0.51
1:B:29:GLN:C	1:X:2:ALA:H	2.14	0.51
1:O:3:GLU:OE1	1:O:3:GLU:N	2.37	0.51
1:e:18:ILE:HD11	1:k:12:LEU:HD12	1.92	0.51
1:JA:111:ILE:HD11	1:PA:112:LEU:HD12	1.92	0.50
1:jA:118:ILE:HG12	1:pA:123:ALA:HB2	1.93	0.50
1:0:112:LEU:HD12	1:6:111:ILE:HD11	1.93	0.50
1:S:3:GLU:OE1	1:S:3:GLU:N	2.37	0.50
1:S:25:ILE:HG12	1:Y:23:ALA:HB2	1.93	0.50
1:H:1:GLN:N	1:O:29:GLN:O	2.26	0.50
1:H:12:LEU:HD12	1:N:18:ILE:HD11	1.94	0.50
1:P:23:ALA:HB2	1:V:25:ILE:CG1	2.41	0.50
1:B:29:GLN:C	1:X:1:GLN:H3	2.11	0.50
1:f:3:GLU:OE1	1:f:3:GLU:N	2.37	0.50
1:aA:112:LEU:HD12	1:gA:111:ILE:HD11	1.94	0.50
1:dA:111:ILE:HD11	1:jA:112:LEU:HD12	1.94	0.50
1:jA:111:ILE:CD1	1:pA:112:LEU:HD12	2.41	0.50
1:a:25:ILE:HG12	1:g:23:ALA:HB2	1.94	0.50
1:6:123:ALA:HB2	1:CA:118:ILE:HG12	1.94	0.50
1:CA:115:TYR:CE2	1:CA:119:LEU:HD11	2.47	0.50
1:GA:115:TYR:CE2	1:GA:119:LEU:HD11	2.47	0.50
1:HA:118:ILE:HG12	1:NA:123:ALA:HB2	1.93	0.50
1:OA:115:TYR:CE2	1:OA:119:LEU:HD11	2.47	0.50
1:eA:115:TYR:CE2	1:eA:119:LEU:HD11	2.47	0.50
1:kA:115:TYR:CE2	1:kA:119:LEU:HD11	2.47	0.50
1:aA:115:TYR:CE2	1:aA:119:LEU:HD11	2.48	0.49
1:m:18:ILE:HD11	1:s:12:LEU:HD12	1.93	0.49
1:iA:115:TYR:CE2	1:iA:119:LEU:HD11	2.47	0.49
1:jA:115:TYR:CE2	1:jA:119:LEU:HD11	2.47	0.49
1:pA:115:TYR:CE2	1:pA:119:LEU:HD11	2.47	0.49
1:1:103:GLU:OE1	1:1:103:GLU:N	2.33	0.49
1:C:18:ILE:HD11	1:I:12:LEU:HD12	1.93	0.49
1:4:115:TYR:CE2	1:4:119:LEU:HD11	2.48	0.49
1:RA:115:TYR:CE2	1:RA:119:LEU:HD11	2.47	0.49
1:SA:115:TYR:CE2	1:SA:119:LEU:HD11	2.47	0.49
1:YA:115:TYR:CE2	1:YA:119:LEU:HD11	2.47	0.49
1:fA:103:GLU:OE1	1:fA:103:GLU:N	2.33	0.49
1:0:115:TYR:CE2	1:0:119:LEU:HD11	2.47	0.49
1:7:115:TYR:CE2	1:7:119:LEU:HD11	2.47	0.49
1:MA:115:TYR:CE2	1:MA:119:LEU:HD11	2.47	0.49
1:UA:115:TYR:CE2	1:UA:119:LEU:HD11	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:ZA:115:TYR:CE2	1:ZA:119:LEU:HD11	2.47	0.49
1:fA:115:TYR:CE2	1:fA:119:LEU:HD11	2.47	0.49
1:gA:115:TYR:CE2	1:gA:119:LEU:HD11	2.47	0.49
1:lA:115:TYR:CE2	1:lA:119:LEU:HD11	2.47	0.49
1:mA:115:TYR:CE2	1:mA:119:LEU:HD11	2.47	0.49
1:oA:115:TYR:CE2	1:oA:119:LEU:HD11	2.47	0.49
1:BA:115:TYR:CE2	1:BA:119:LEU:HD11	2.47	0.49
1:M:25:ILE:CG1	1:S:23:ALA:HB2	2.42	0.49
1:FA:115:TYR:CE2	1:FA:119:LEU:HD11	2.47	0.49
1:IA:115:TYR:CE2	1:IA:119:LEU:HD11	2.47	0.49
1:WA:115:TYR:CE2	1:WA:119:LEU:HD11	2.47	0.49
1:dA:115:TYR:CE2	1:dA:119:LEU:HD11	2.47	0.49
1:TA:115:TYR:CE2	1:TA:119:LEU:HD11	2.47	0.49
1:l:2:ALA:HA	1:l:5:LEU:HD13	1.95	0.49
1:cA:115:TYR:CE2	1:cA:119:LEU:HD11	2.47	0.49
1:r:2:ALA:HA	1:r:5:LEU:HD13	1.95	0.49
1:4:112:LEU:HD12	1:AA:111:ILE:HD11	1.94	0.49
1:R:23:ALA:HB2	1:X:25:ILE:CG1	2.43	0.49
1:z:2:ALA:HA	1:z:5:LEU:HD13	1.94	0.49
1:A:2:ALA:HA	1:A:5:LEU:HD13	1.94	0.49
1:6:115:TYR:CE2	1:6:119:LEU:HD11	2.47	0.49
1:NA:115:TYR:CE2	1:NA:119:LEU:HD11	2.47	0.49
1:a:2:ALA:HA	1:a:5:LEU:HD13	1.95	0.49
1:RA:111:ILE:HD11	1:XA:112:LEU:HD12	1.95	0.49
1:XA:115:TYR:CE2	1:XA:119:LEU:HD11	2.47	0.49
1:i:2:ALA:HA	1:i:5:LEU:HD13	1.94	0.49
1:u:2:ALA:HA	1:u:5:LEU:HD13	1.95	0.49
1:E:29:GLN:C	1:R:1:GLN:H3	2.15	0.49
1:G:2:ALA:HA	1:G:5:LEU:HD13	1.94	0.49
1:H:2:ALA:HA	1:H:5:LEU:HD13	1.94	0.49
1:AA:115:TYR:CE2	1:AA:119:LEU:HD11	2.47	0.49
1:N:2:ALA:HA	1:N:5:LEU:HD13	1.95	0.49
1:3:115:TYR:CE2	1:3:119:LEU:HD11	2.47	0.49
1:F:2:ALA:HA	1:F:5:LEU:HD13	1.94	0.49
1:R:2:ALA:HA	1:R:5:LEU:HD13	1.94	0.49
1:U:2:ALA:HA	1:U:5:LEU:HD13	1.94	0.49
1:LA:111:ILE:HD11	1:RA:112:LEU:HD12	1.94	0.49
1:Y:2:ALA:HA	1:Y:5:LEU:HD13	1.95	0.49
1:b:2:ALA:HA	1:b:5:LEU:HD13	1.94	0.49
1:e:2:ALA:HA	1:e:5:LEU:HD13	1.94	0.49
1:g:2:ALA:HA	1:g:5:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YA:112:LEU:HD12	1:eA:111:ILE:CD1	2.42	0.49
1:k:18:ILE:HD11	1:q:12:LEU:HD12	1.94	0.49
1:o:2:ALA:HA	1:o:5:LEU:HD13	1.95	0.49
1:B:2:ALA:HA	1:B:5:LEU:HD13	1.94	0.49
1:5:115:TYR:CE2	1:5:119:LEU:HD11	2.47	0.49
1:M:2:ALA:HA	1:M:5:LEU:HD13	1.94	0.49
1:S:2:ALA:HA	1:S:5:LEU:HD13	1.94	0.49
1:JA:115:TYR:CE2	1:JA:119:LEU:HD11	2.47	0.49
1:LA:115:TYR:CE2	1:LA:119:LEU:HD11	2.47	0.49
1:X:2:ALA:HA	1:X:5:LEU:HD13	1.94	0.49
1:Y:18:ILE:HD11	1:e:12:LEU:HD12	1.95	0.49
1:QA:115:TYR:CE2	1:QA:119:LEU:HD11	2.47	0.49
1:h:2:ALA:HA	1:h:5:LEU:HD13	1.94	0.49
1:t:2:ALA:HA	1:t:5:LEU:HD13	1.95	0.49
1:x:2:ALA:HA	1:x:5:LEU:HD13	1.94	0.49
1:1:115:TYR:CE2	1:1:119:LEU:HD11	2.47	0.48
1:C:2:ALA:HA	1:C:5:LEU:HD13	1.95	0.48
1:9:115:TYR:CE2	1:9:119:LEU:HD11	2.47	0.48
1:L:2:ALA:HA	1:L:5:LEU:HD13	1.94	0.48
1:DA:115:TYR:CE2	1:DA:119:LEU:HD11	2.47	0.48
1:HA:115:TYR:CE2	1:HA:119:LEU:HD11	2.47	0.48
1:f:2:ALA:HA	1:f:5:LEU:HD13	1.95	0.48
1:v:2:ALA:HA	1:v:5:LEU:HD13	1.95	0.48
1:nA:115:TYR:CE2	1:nA:119:LEU:HD11	2.47	0.48
1:9:111:ILE:HD11	1:FA:112:LEU:HD12	1.94	0.48
1:K:25:ILE:HG12	1:Q:23:ALA:HB2	1.95	0.48
1:V:2:ALA:HA	1:V:5:LEU:HD13	1.95	0.48
1:c:2:ALA:HA	1:c:5:LEU:HD13	1.95	0.48
1:n:2:ALA:HA	1:n:5:LEU:HD13	1.94	0.48
1:hA:115:TYR:CE2	1:hA:119:LEU:HD11	2.47	0.48
1:B:29:GLN:OXT	1:X:2:ALA:HB3	2.12	0.48
1:D:2:ALA:HA	1:D:5:LEU:HD13	1.95	0.48
1:D:26:LEU:HD21	1:J:29:GLN:HG2	1.95	0.48
1:8:115:TYR:CE2	1:8:119:LEU:HD11	2.47	0.48
1:KA:115:TYR:CE2	1:KA:119:LEU:HD11	2.47	0.48
1:PA:115:TYR:CE2	1:PA:119:LEU:HD11	2.47	0.48
1:e:11:ILE:HD11	1:k:8:ASP:HB2	1.95	0.48
1:k:2:ALA:HA	1:k:5:LEU:HD13	1.94	0.48
1:bA:115:TYR:CE2	1:bA:119:LEU:HD11	2.47	0.48
1:C:29:GLN:HG2	1:I:26:LEU:HD21	1.96	0.48
1:T:2:ALA:HA	1:T:5:LEU:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:2:ALA:HA	1:d:5:LEU:HD13	1.94	0.48
1:f:8:ASP:HB2	1:l:11:ILE:HD11	1.95	0.48
1:VA:115:TYR:CE2	1:VA:119:LEU:HD11	2.47	0.48
1:g:11:ILE:HD11	1:m:8:ASP:HB2	1.95	0.48
1:m:2:ALA:HA	1:m:5:LEU:HD13	1.95	0.48
1:cA:103:GLU:OE1	1:cA:103:GLU:N	2.33	0.48
1:p:2:ALA:HA	1:p:5:LEU:HD13	1.94	0.48
1:y:2:ALA:HA	1:y:5:LEU:HD13	1.94	0.48
1:I:2:ALA:HA	1:I:5:LEU:HD13	1.94	0.48
1:EA:115:TYR:CE2	1:EA:119:LEU:HD11	2.47	0.48
1:h:8:ASP:HB2	1:n:11:ILE:HD11	1.96	0.48
1:2:103:GLU:OE1	1:2:103:GLU:N	2.33	0.48
1:P:2:ALA:HA	1:P:5:LEU:HD13	1.94	0.48
1:W:2:ALA:HA	1:W:5:LEU:HD13	1.94	0.48
1:e:25:ILE:HG12	1:k:23:ALA:HB2	1.95	0.48
1:q:2:ALA:HA	1:q:5:LEU:HD13	1.94	0.48
1:E:18:ILE:HD11	1:K:12:LEU:HD12	1.95	0.48
1:6:112:LEU:HD12	1:CA:111:ILE:HD11	1.94	0.48
1:IA:123:ALA:HB2	1:OA:118:ILE:HG12	1.95	0.48
1:J:2:ALA:HA	1:J:5:LEU:HD13	1.94	0.48
1:O:2:ALA:HA	1:O:5:LEU:HD13	1.94	0.48
1:U:18:ILE:CD1	1:a:12:LEU:HD12	2.44	0.48
1:MA:103:GLU:OE1	1:MA:103:GLU:N	2.33	0.48
1:3:103:GLU:OE1	1:3:103:GLU:N	2.33	0.48
1:E:2:ALA:HA	1:E:5:LEU:HD13	1.94	0.48
1:Q:2:ALA:HA	1:Q:5:LEU:HD13	1.94	0.48
1:w:2:ALA:HA	1:w:5:LEU:HD13	1.95	0.48
1:2:115:TYR:CE2	1:2:119:LEU:HD11	2.47	0.47
1:eA:123:ALA:HB2	1:kA:118:ILE:HG12	1.96	0.47
1:p:19:LEU:HD12	1:v:25:ILE:CD1	2.44	0.47
1:D:8:ASP:HB2	1:J:11:ILE:HD11	1.95	0.47
1:R:8:ASP:HB2	1:X:11:ILE:HD11	1.96	0.47
1:U:11:ILE:HD11	1:a:8:ASP:HB2	1.95	0.47
1:Z:2:ALA:HA	1:Z:5:LEU:HD13	1.95	0.47
1:UA:123:ALA:HB2	1:aA:118:ILE:HG12	1.95	0.47
1:j:2:ALA:HA	1:j:5:LEU:HD13	1.95	0.47
1:8:103:GLU:OE1	1:8:103:GLU:N	2.33	0.47
1:N:26:LEU:HD21	1:T:29:GLN:HG2	1.96	0.47
1:R:12:LEU:HD12	1:X:18:ILE:HD11	1.96	0.47
1:3:111:ILE:CD1	1:9:112:LEU:HD12	2.44	0.47
1:I:18:ILE:CD1	1:O:12:LEU:HD12	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:s:2:ALA:HA	1:s:5:LEU:HD13	1.95	0.47
1:K:2:ALA:HA	1:K:5:LEU:HD13	1.95	0.47
1:ZA:118:ILE:HG12	1:fA:123:ALA:HB2	1.96	0.47
1:kA:103:GLU:OE1	1:kA:103:GLU:N	2.33	0.47
1:7:103:GLU:OE1	1:7:103:GLU:N	2.33	0.47
1:MA:123:ALA:HB2	1:SA:118:ILE:HG12	1.97	0.47
1:9:103:GLU:OE1	1:9:103:GLU:N	2.33	0.47
1:mA:103:GLU:OE1	1:mA:103:GLU:N	2.33	0.47
1:c:29:GLN:HG2	1:i:26:LEU:HD21	1.97	0.47
1:A:25:ILE:HG12	1:G:23:ALA:HB2	1.97	0.47
1:B:29:GLN:HG2	1:E:26:LEU:HD21	1.96	0.47
1:gA:103:GLU:OE1	1:gA:103:GLU:N	2.33	0.47
1:O:29:GLN:HG2	1:U:26:LEU:HD21	1.97	0.46
1:Q:29:GLN:HG2	1:W:26:LEU:HD21	1.96	0.46
1:h:12:LEU:HD12	1:n:18:ILE:CD1	2.44	0.46
1:i:11:ILE:HD11	1:o:8:ASP:HB2	1.97	0.46
1:lA:103:GLU:OE1	1:lA:103:GLU:N	2.33	0.46
1:VA:111:ILE:CD1	1:bA:112:LEU:HD12	2.44	0.46
1:p:26:LEU:HD21	1:v:29:GLN:HG2	1.97	0.46
1:hA:103:GLU:OE1	1:hA:103:GLU:N	2.33	0.46
1:0:103:GLU:OE1	1:0:103:GLU:N	2.33	0.46
1:c:11:ILE:HD11	1:i:5:LEU:O	2.16	0.46
1:FA:103:GLU:OE1	1:FA:103:GLU:N	2.33	0.46
1:X:23:ALA:HB2	1:d:25:ILE:HG12	1.96	0.46
1:d:8:ASP:HB2	1:j:11:ILE:HD11	1.96	0.46
1:bA:103:GLU:OE1	1:bA:103:GLU:N	2.33	0.46
1:1:111:ILE:HD11	1:7:112:LEU:HD12	1.97	0.46
1:AA:123:ALA:HB2	1:GA:118:ILE:HG12	1.97	0.46
1:Q:11:ILE:HD11	1:W:8:ASP:HB2	1.98	0.46
1:LA:103:GLU:OE1	1:LA:103:GLU:N	2.33	0.46
1:q:25:ILE:HG12	1:w:23:ALA:HB2	1.96	0.46
1:P:26:LEU:HD21	1:V:29:GLN:HG2	1.97	0.46
1:NA:103:GLU:OE1	1:NA:103:GLU:N	2.33	0.46
1:t:12:LEU:HD12	1:z:18:ILE:CD1	2.46	0.46
1:F:23:ALA:HB2	1:L:25:ILE:CG1	2.46	0.46
1:h:26:LEU:HD21	1:n:29:GLN:HG2	1.98	0.46
1:gA:123:ALA:HB2	1:mA:118:ILE:HG12	1.97	0.46
1:nA:103:GLU:OE1	1:nA:103:GLU:N	2.33	0.46
1:0:118:ILE:HG12	1:5:123:ALA:HB2	1.98	0.46
1:EA:103:GLU:OE1	1:EA:103:GLU:N	2.33	0.46
1:c:18:ILE:CD1	1:i:12:LEU:HD12	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:23:ALA:HB2	1:j:25:ILE:CG1	2.46	0.46
1:F:2:ALA:N	1:Q:29:GLN:O	2.35	0.46
1:S:11:ILE:HD11	1:Y:8:ASP:HB2	1.98	0.46
1:m:14:ALA:O	1:m:18:ILE:HG13	2.17	0.46
1:S:14:ALA:O	1:S:18:ILE:HG13	2.16	0.45
1:T:14:ALA:O	1:T:18:ILE:HG13	2.16	0.45
1:KA:103:GLU:OE1	1:KA:103:GLU:N	2.33	0.45
1:Y:14:ALA:O	1:Y:18:ILE:HG13	2.17	0.45
1:Z:14:ALA:O	1:Z:18:ILE:HG13	2.17	0.45
1:a:14:ALA:O	1:a:18:ILE:HG13	2.17	0.45
1:e:14:ALA:O	1:e:18:ILE:HG13	2.17	0.45
1:g:14:ALA:O	1:g:18:ILE:HG13	2.17	0.45
1:fA:111:ILE:HD11	1:lA:112:LEU:HD12	1.99	0.45
1:q:14:ALA:O	1:q:18:ILE:HG13	2.17	0.45
1:s:14:ALA:O	1:s:18:ILE:HG13	2.17	0.45
1:y:14:ALA:O	1:y:18:ILE:HG13	2.16	0.45
1:J:14:ALA:O	1:J:18:ILE:HG13	2.17	0.45
1:U:14:ALA:O	1:U:18:ILE:HG13	2.17	0.45
1:LA:106:LYS:HB3	1:LA:106:LYS:HE2	1.83	0.45
1:k:14:ALA:O	1:k:18:ILE:HG13	2.17	0.45
1:gA:112:LEU:HD12	1:mA:111:ILE:HD11	1.99	0.45
1:x:14:ALA:O	1:x:18:ILE:HG13	2.17	0.45
1:B:14:ALA:O	1:B:18:ILE:HG13	2.17	0.45
1:D:14:ALA:O	1:D:18:ILE:HG13	2.17	0.45
1:E:14:ALA:O	1:E:18:ILE:HG13	2.17	0.45
1:G:14:ALA:O	1:G:18:ILE:HG13	2.17	0.45
1:M:14:ALA:O	1:M:18:ILE:HG13	2.17	0.45
1:O:14:ALA:O	1:O:18:ILE:HG13	2.17	0.45
1:Q:14:ALA:O	1:Q:18:ILE:HG13	2.16	0.45
1:RA:103:GLU:OE1	1:RA:103:GLU:N	2.33	0.45
1:c:18:ILE:HG12	1:i:16:ALA:HB2	1.99	0.45
1:aA:103:GLU:OE1	1:aA:103:GLU:N	2.33	0.45
1:r:14:ALA:O	1:r:18:ILE:HG13	2.17	0.45
1:w:14:ALA:O	1:w:18:ILE:HG13	2.17	0.45
1:A:25:ILE:CG1	1:G:23:ALA:HB2	2.46	0.45
1:H:29:GLN:O	1:d:1:GLN:N	2.34	0.45
1:J:23:ALA:HB2	1:P:25:ILE:HG12	1.98	0.45
1:K:14:ALA:O	1:K:18:ILE:HG13	2.17	0.45
1:W:14:ALA:O	1:W:18:ILE:HG13	2.17	0.45
1:b:14:ALA:O	1:b:18:ILE:HG13	2.17	0.45
1:RA:118:ILE:CG1	1:XA:123:ALA:HB2	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:14:ALA:O	1:c:18:ILE:HG13	2.16	0.45
1:h:14:ALA:O	1:h:18:ILE:HG13	2.17	0.45
1:p:19:LEU:HD12	1:v:25:ILE:HD11	1.98	0.45
1:QA:123:ALA:HB2	1:WA:118:ILE:HG12	1.97	0.45
1:1:112:LEU:HD12	1:4:111:ILE:HD11	1.99	0.45
1:7:118:ILE:HG12	1:DA:123:ALA:HB2	1.98	0.45
1:VA:103:GLU:OE1	1:VA:103:GLU:N	2.33	0.45
1:WA:112:LEU:HD12	1:cA:111:ILE:CD1	2.45	0.45
1:p:14:ALA:O	1:p:18:ILE:HG13	2.16	0.45
1:A:14:ALA:O	1:A:18:ILE:HG13	2.17	0.45
1:F:26:LEU:HD21	1:L:29:GLN:HG2	1.98	0.45
1:H:14:ALA:O	1:H:18:ILE:HG13	2.17	0.45
1:I:14:ALA:O	1:I:18:ILE:HG13	2.17	0.45
1:f:12:LEU:HD12	1:l:18:ILE:HD11	1.99	0.45
1:g:25:ILE:HD11	1:m:19:LEU:HD12	1.99	0.45
1:C:14:ALA:O	1:C:18:ILE:HG13	2.17	0.45
1:F:14:ALA:O	1:F:18:ILE:HG13	2.17	0.45
1:i:14:ALA:O	1:i:18:ILE:HG13	2.17	0.45
1:n:14:ALA:O	1:n:18:ILE:HG13	2.17	0.45
1:o:14:ALA:O	1:o:18:ILE:HG13	2.17	0.45
1:v:14:ALA:O	1:v:18:ILE:HG13	2.17	0.45
1:N:14:ALA:O	1:N:18:ILE:HG13	2.16	0.45
1:P:14:ALA:O	1:P:18:ILE:HG13	2.17	0.45
1:GA:103:GLU:OE1	1:GA:103:GLU:N	2.33	0.45
1:QA:103:GLU:OE1	1:QA:103:GLU:N	2.33	0.45
1:f:14:ALA:O	1:f:18:ILE:HG13	2.17	0.45
1:j:14:ALA:O	1:j:18:ILE:HG13	2.17	0.45
1:S:18:ILE:HD11	1:Y:12:LEU:HD12	1.98	0.45
1:V:14:ALA:O	1:V:18:ILE:HG13	2.17	0.45
1:WA:103:GLU:OE1	1:WA:103:GLU:N	2.33	0.45
1:l:14:ALA:O	1:l:18:ILE:HG13	2.16	0.45
1:m:11:ILE:HD11	1:s:8:ASP:HB2	1.99	0.45
1:u:14:ALA:O	1:u:18:ILE:HG13	2.17	0.45
1:mA:106:LYS:HE2	1:mA:106:LYS:HB3	1.83	0.45
1:R:14:ALA:O	1:R:18:ILE:HG13	2.17	0.44
1:t:14:ALA:O	1:t:18:ILE:HG13	2.17	0.44
1:z:14:ALA:O	1:z:18:ILE:HG13	2.17	0.44
1:L:14:ALA:O	1:L:18:ILE:HG13	2.17	0.44
1:P:8:ASP:HB2	1:V:11:ILE:HD11	2.00	0.44
1:S:15:TYR:CZ	1:S:19:LEU:HD21	2.53	0.44
1:Y:25:ILE:CG1	1:e:23:ALA:HB2	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:15:TYR:CZ	1:b:19:LEU:HD21	2.53	0.44
1:u:15:TYR:CZ	1:u:19:LEU:HD21	2.53	0.44
1:H:23:ALA:HB2	1:N:25:ILE:HG12	1.98	0.44
1:J:5:LEU:H	1:J:5:LEU:HD12	1.83	0.44
1:P:5:LEU:HD12	1:P:5:LEU:H	1.83	0.44
1:k:15:TYR:CZ	1:k:19:LEU:HD21	2.53	0.44
1:jA:103:GLU:OE1	1:jA:103:GLU:N	2.33	0.44
1:w:15:TYR:CZ	1:w:19:LEU:HD21	2.53	0.44
1:z:15:TYR:CZ	1:z:19:LEU:HD21	2.53	0.44
1:A:15:TYR:CZ	1:A:19:LEU:HD21	2.53	0.44
1:J:15:TYR:CZ	1:J:19:LEU:HD21	2.53	0.44
1:S:5:LEU:HD12	1:S:5:LEU:H	1.83	0.44
1:Y:15:TYR:CZ	1:Y:19:LEU:HD21	2.53	0.44
1:OA:112:LEU:HD12	1:UA:111:ILE:CD1	2.47	0.44
1:PA:103:GLU:OE1	1:PA:103:GLU:N	2.33	0.44
1:e:15:TYR:CZ	1:e:19:LEU:HD21	2.53	0.44
1:UA:103:GLU:OE1	1:UA:103:GLU:N	2.33	0.44
1:q:15:TYR:CZ	1:q:19:LEU:HD21	2.53	0.44
1:q:18:ILE:HD11	1:w:12:LEU:HD12	1.99	0.44
1:t:15:TYR:CZ	1:t:19:LEU:HD21	2.53	0.44
1:C:15:TYR:CZ	1:C:19:LEU:HD21	2.53	0.44
1:9:118:ILE:HG12	1:FA:123:ALA:HB2	2.00	0.44
1:M:5:LEU:HD12	1:M:5:LEU:H	1.83	0.44
1:P:15:TYR:CZ	1:P:19:LEU:HD21	2.53	0.44
1:V:5:LEU:HD12	1:V:5:LEU:H	1.83	0.44
1:X:12:LEU:HD12	1:d:18:ILE:HD11	1.98	0.44
1:o:15:TYR:CZ	1:o:19:LEU:HD21	2.53	0.44
1:t:23:ALA:HB2	1:z:25:ILE:HG12	2.00	0.44
1:G:5:LEU:HD12	1:G:5:LEU:H	1.83	0.44
1:I:15:TYR:CZ	1:I:19:LEU:HD21	2.53	0.44
1:O:15:TYR:CZ	1:O:19:LEU:HD21	2.53	0.44
1:R:15:TYR:CZ	1:R:19:LEU:HD21	2.53	0.44
1:IA:103:GLU:OE1	1:IA:103:GLU:N	2.33	0.44
1:X:15:TYR:CZ	1:X:19:LEU:HD21	2.53	0.44
1:OA:103:GLU:OE1	1:OA:103:GLU:N	2.33	0.44
1:b:5:LEU:HD12	1:b:5:LEU:H	1.83	0.44
1:e:5:LEU:H	1:e:5:LEU:HD12	1.83	0.44
1:h:15:TYR:CZ	1:h:19:LEU:HD21	2.53	0.44
1:k:5:LEU:HD12	1:k:5:LEU:H	1.83	0.44
1:n:15:TYR:CZ	1:n:19:LEU:HD21	2.53	0.44
1:q:5:LEU:H	1:q:5:LEU:HD12	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:r:5:LEU:HD12	1:r:5:LEU:H	1.83	0.44
1:w:5:LEU:HD12	1:w:5:LEU:H	1.83	0.44
1:B:25:ILE:HG12	1:E:23:ALA:HB2	1.99	0.44
1:D:5:LEU:HD12	1:D:5:LEU:H	1.83	0.44
1:G:15:TYR:CZ	1:G:19:LEU:HD21	2.53	0.44
1:L:15:TYR:CZ	1:L:19:LEU:HD21	2.53	0.44
1:U:15:TYR:CZ	1:U:19:LEU:HD21	2.53	0.44
1:X:14:ALA:O	1:X:18:ILE:HG13	2.17	0.44
1:Y:5:LEU:H	1:Y:5:LEU:HD12	1.83	0.44
1:d:14:ALA:O	1:d:18:ILE:HG13	2.17	0.44
1:d:15:TYR:CZ	1:d:19:LEU:HD21	2.53	0.44
1:i:15:TYR:CZ	1:i:19:LEU:HD21	2.53	0.44
1:i:25:ILE:HD11	1:o:19:LEU:HD12	1.99	0.44
1:iA:123:ALA:HB2	1:oA:118:ILE:HG12	1.98	0.44
1:x:5:LEU:HD12	1:x:5:LEU:H	1.83	0.44
1:O:25:ILE:HD11	1:U:19:LEU:HD12	1.99	0.44
1:a:15:TYR:CZ	1:a:19:LEU:HD21	2.53	0.44
1:XA:103:GLU:OE1	1:XA:103:GLU:N	2.33	0.44
1:aA:123:ALA:HB2	1:gA:118:ILE:HG12	2.00	0.44
1:H:15:TYR:CZ	1:H:19:LEU:HD21	2.53	0.44
1:M:15:TYR:CZ	1:M:19:LEU:HD21	2.53	0.44
1:b:8:ASP:HB2	1:h:11:ILE:HD11	2.00	0.44
1:TA:118:ILE:HG12	1:ZA:123:ALA:HB2	2.00	0.44
1:A:5:LEU:HD12	1:A:5:LEU:H	1.83	0.43
1:D:15:TYR:CZ	1:D:19:LEU:HD21	2.53	0.43
1:G:1:GLN:N	1:c:29:GLN:O	2.29	0.43
1:I:29:GLN:HG2	1:O:26:LEU:HD21	2.00	0.43
1:L:23:ALA:HB2	1:R:25:ILE:CG1	2.46	0.43
1:DA:103:GLU:OE1	1:DA:103:GLU:N	2.33	0.43
1:j:15:TYR:CZ	1:j:19:LEU:HD21	2.53	0.43
1:l:5:LEU:HD12	1:l:5:LEU:H	1.83	0.43
1:gA:106:LYS:HB3	1:gA:106:LYS:HE2	1.83	0.43
1:x:15:TYR:CZ	1:x:19:LEU:HD21	2.53	0.43
1:N:15:TYR:CZ	1:N:19:LEU:HD21	2.53	0.43
1:c:18:ILE:HD11	1:i:12:LEU:HD12	2.00	0.43
1:g:15:TYR:CZ	1:g:19:LEU:HD21	2.53	0.43
1:j:23:ALA:HB2	1:p:25:ILE:HG12	1.99	0.43
1:B:15:TYR:CZ	1:B:19:LEU:HD21	2.53	0.43
1:E:15:TYR:CZ	1:E:19:LEU:HD21	2.53	0.43
1:F:15:TYR:CZ	1:F:19:LEU:HD21	2.53	0.43
1:JA:103:GLU:OE1	1:JA:103:GLU:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:15:TYR:CZ	1:V:19:LEU:HD21	2.53	0.43
1:f:5:LEU:HD12	1:f:5:LEU:H	1.83	0.43
1:h:5:LEU:HD12	1:h:5:LEU:H	1.83	0.43
1:m:5:LEU:HD12	1:m:5:LEU:H	1.83	0.43
1:o:25:ILE:CG1	1:u:23:ALA:HB2	2.47	0.43
1:jA:122:HIS:NE2	1:jA:126:LEU:HD11	2.34	0.43
1:2:122:HIS:NE2	1:2:126:LEU:HD11	2.34	0.43
1:8:122:HIS:NE2	1:8:126:LEU:HD11	2.34	0.43
1:BA:111:ILE:HD11	1:HA:112:LEU:HD12	2.00	0.43
1:CA:103:GLU:OE1	1:CA:103:GLU:N	2.33	0.43
1:JA:122:HIS:NE2	1:JA:126:LEU:HD11	2.34	0.43
1:OA:122:HIS:NE2	1:OA:126:LEU:HD11	2.34	0.43
1:d:23:ALA:HB1	1:j:24:GLU:HG3	2.01	0.43
1:TA:104:ILE:HD11	1:ZA:105:LEU:HD23	1.99	0.43
1:UA:122:HIS:NE2	1:UA:126:LEU:HD11	2.34	0.43
1:VA:122:HIS:NE2	1:VA:126:LEU:HD11	2.34	0.43
1:g:5:LEU:HD12	1:g:5:LEU:H	1.83	0.43
1:eA:103:GLU:OE1	1:eA:103:GLU:N	2.33	0.43
1:p:15:TYR:CZ	1:p:19:LEU:HD21	2.53	0.43
1:r:15:TYR:CZ	1:r:19:LEU:HD21	2.53	0.43
1:u:5:LEU:HD12	1:u:5:LEU:H	1.83	0.43
1:lA:122:HIS:NE2	1:lA:126:LEU:HD11	2.34	0.43
1:B:18:ILE:HD11	1:E:12:LEU:HD12	2.00	0.43
1:C:5:LEU:H	1:C:5:LEU:HD12	1.83	0.43
1:3:106:LYS:HB3	1:3:106:LYS:HE2	1.83	0.43
1:E:5:LEU:HD12	1:E:5:LEU:H	1.83	0.43
1:F:5:LEU:HD12	1:F:5:LEU:H	1.83	0.43
1:K:5:LEU:HD12	1:K:5:LEU:H	1.83	0.43
1:K:15:TYR:CZ	1:K:19:LEU:HD21	2.53	0.43
1:K:29:GLN:C	1:L:1:GLN:H3	2.10	0.43
1:T:15:TYR:CZ	1:T:19:LEU:HD21	2.53	0.43
1:PA:122:HIS:NE2	1:PA:126:LEU:HD11	2.34	0.43
1:c:15:TYR:CZ	1:c:19:LEU:HD21	2.53	0.43
1:aA:122:HIS:NE2	1:aA:126:LEU:HD11	2.34	0.43
1:o:5:LEU:HD12	1:o:5:LEU:H	1.83	0.43
1:gA:122:HIS:NE2	1:gA:126:LEU:HD11	2.34	0.43
1:pA:122:HIS:NE2	1:pA:126:LEU:HD11	2.34	0.43
1:0:121:ALA:O	1:0:125:ILE:HG12	2.19	0.43
1:B:5:LEU:HD12	1:B:5:LEU:H	1.83	0.43
1:5:103:GLU:OE1	1:5:103:GLU:N	2.33	0.43
1:K:18:ILE:HD11	1:Q:12:LEU:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:121:ALA:O	1:AA:125:ILE:HG12	2.19	0.43
1:EA:122:HIS:NE2	1:EA:126:LEU:HD11	2.34	0.43
1:Q:5:LEU:HD12	1:Q:5:LEU:H	1.83	0.43
1:JA:121:ALA:O	1:JA:125:ILE:HG12	2.19	0.43
1:MA:122:HIS:NE2	1:MA:126:LEU:HD11	2.34	0.43
1:Z:5:LEU:HD12	1:Z:5:LEU:H	1.83	0.43
1:RA:121:ALA:O	1:RA:125:ILE:HG12	2.19	0.43
1:c:5:LEU:HD12	1:c:5:LEU:H	1.83	0.43
1:g:18:ILE:CD1	1:m:12:LEU:HD12	2.48	0.43
1:i:5:LEU:HD12	1:i:5:LEU:H	1.83	0.43
1:aA:106:LYS:HE2	1:aA:106:LYS:HB3	1.83	0.43
1:s:5:LEU:HD12	1:s:5:LEU:H	1.83	0.43
1:3:122:HIS:NE2	1:3:126:LEU:HD11	2.34	0.43
1:CA:106:LYS:HE2	1:CA:106:LYS:HB3	1.83	0.43
1:CA:121:ALA:O	1:CA:125:ILE:HG12	2.19	0.43
1:DA:122:HIS:NE2	1:DA:126:LEU:HD11	2.34	0.43
1:GA:122:HIS:NE2	1:GA:126:LEU:HD11	2.34	0.43
1:HA:122:HIS:NE2	1:HA:126:LEU:HD11	2.34	0.43
1:W:5:LEU:HD12	1:W:5:LEU:H	1.83	0.43
1:W:25:ILE:CG1	1:c:23:ALA:HB2	2.49	0.43
1:Z:15:TYR:CZ	1:Z:19:LEU:HD21	2.53	0.43
1:SA:122:HIS:NE2	1:SA:126:LEU:HD11	2.34	0.43
1:TA:121:ALA:O	1:TA:125:ILE:HG12	2.19	0.43
1:UA:121:ALA:O	1:UA:125:ILE:HG12	2.19	0.43
1:bA:122:HIS:NE2	1:bA:126:LEU:HD11	2.34	0.43
1:m:15:TYR:CZ	1:m:19:LEU:HD21	2.53	0.43
1:cA:121:ALA:O	1:cA:125:ILE:HG12	2.19	0.43
1:dA:122:HIS:NE2	1:dA:126:LEU:HD11	2.34	0.43
1:eA:121:ALA:O	1:eA:125:ILE:HG12	2.19	0.43
1:mA:122:HIS:NE2	1:mA:126:LEU:HD11	2.34	0.43
1:oA:121:ALA:O	1:oA:125:ILE:HG12	2.19	0.43
1:A:18:ILE:HD11	1:G:12:LEU:HD12	1.99	0.43
1:2:123:ALA:HB2	1:8:118:ILE:HG12	2.00	0.43
1:5:122:HIS:NE2	1:5:126:LEU:HD11	2.34	0.43
1:7:122:HIS:NE2	1:7:126:LEU:HD11	2.34	0.43
1:L:5:LEU:HD12	1:L:5:LEU:H	1.83	0.43
1:BA:121:ALA:O	1:BA:125:ILE:HG12	2.19	0.43
1:BA:122:HIS:NE2	1:BA:126:LEU:HD11	2.34	0.43
1:FA:121:ALA:O	1:FA:125:ILE:HG12	2.19	0.43
1:IA:106:LYS:HE2	1:IA:106:LYS:HB3	1.82	0.43
1:IA:122:HIS:NE2	1:IA:126:LEU:HD11	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:KA:121:ALA:O	1:KA:125:ILE:HG12	2.19	0.43
1:W:11:ILE:HD11	1:c:8:ASP:HB2	2.00	0.43
1:a:5:LEU:HD12	1:a:5:LEU:H	1.83	0.43
1:b:26:LEU:CD2	1:h:29:GLN:HG2	2.46	0.43
1:SA:121:ALA:O	1:SA:125:ILE:HG12	2.19	0.43
1:VA:121:ALA:O	1:VA:125:ILE:HG12	2.19	0.43
1:dA:121:ALA:O	1:dA:125:ILE:HG12	2.19	0.43
1:gA:121:ALA:O	1:gA:125:ILE:HG12	2.19	0.43
1:v:15:TYR:CZ	1:v:19:LEU:HD21	2.53	0.43
1:lA:121:ALA:O	1:lA:125:ILE:HG12	2.19	0.43
1:B:23:ALA:HB2	1:H:25:ILE:HG12	2.01	0.43
1:3:121:ALA:O	1:3:125:ILE:HG12	2.19	0.43
1:6:103:GLU:OE1	1:6:103:GLU:N	2.33	0.43
1:H:5:LEU:HD12	1:H:5:LEU:H	1.83	0.43
1:7:121:ALA:O	1:7:125:ILE:HG12	2.19	0.43
1:8:121:ALA:O	1:8:125:ILE:HG12	2.19	0.43
1:9:122:HIS:NE2	1:9:126:LEU:HD11	2.34	0.43
1:S:29:GLN:HG2	1:Y:26:LEU:HD21	2.01	0.43
1:MA:121:ALA:O	1:MA:125:ILE:HG12	2.19	0.43
1:RA:106:LYS:HB3	1:RA:106:LYS:HE2	1.82	0.43
1:n:5:LEU:HD12	1:n:5:LEU:H	1.83	0.43
1:fA:122:HIS:NE2	1:fA:126:LEU:HD11	2.34	0.43
1:y:5:LEU:HD12	1:y:5:LEU:H	1.83	0.43
1:oA:122:HIS:NE2	1:oA:126:LEU:HD11	2.34	0.43
1:pA:121:ALA:O	1:pA:125:ILE:HG12	2.19	0.43
1:1:121:ALA:O	1:1:125:ILE:HG12	2.19	0.43
1:1:123:ALA:HB2	1:4:118:ILE:HG12	2.00	0.43
1:G:18:ILE:HD11	1:M:12:LEU:HD12	2.01	0.43
1:O:5:LEU:H	1:O:5:LEU:HD12	1.83	0.43
1:Q:15:TYR:CZ	1:Q:19:LEU:HD21	2.53	0.43
1:HA:121:ALA:O	1:HA:125:ILE:HG12	2.19	0.43
1:KA:122:HIS:NE2	1:KA:126:LEU:HD11	2.34	0.43
1:OA:106:LYS:HE2	1:OA:106:LYS:HB3	1.82	0.43
1:k:25:ILE:HG12	1:q:23:ALA:HB2	2.01	0.43
1:l:15:TYR:CZ	1:l:19:LEU:HD21	2.53	0.43
1:fA:121:ALA:O	1:fA:125:ILE:HG12	2.19	0.43
1:hA:121:ALA:O	1:hA:125:ILE:HG12	2.19	0.43
1:t:5:LEU:HD12	1:t:5:LEU:H	1.83	0.43
1:kA:121:ALA:O	1:kA:125:ILE:HG12	2.19	0.43
1:y:15:TYR:CZ	1:y:19:LEU:HD21	2.53	0.43
1:z:5:LEU:HD12	1:z:5:LEU:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5:LEU:HA	1:F:8:ASP:OD2	2.19	0.42
1:6:106:LYS:HB3	1:6:106:LYS:HE2	1.83	0.42
1:I:5:LEU:HD12	1:I:5:LEU:H	1.83	0.42
1:N:5:LEU:HD12	1:N:5:LEU:H	1.83	0.42
1:IA:121:ALA:O	1:IA:125:ILE:HG12	2.19	0.42
1:U:5:LEU:HD12	1:U:5:LEU:H	1.83	0.42
1:V:5:LEU:HA	1:V:8:ASP:OD2	2.19	0.42
1:QA:121:ALA:O	1:QA:125:ILE:HG12	2.19	0.42
1:g:25:ILE:CD1	1:m:19:LEU:HD12	2.49	0.42
1:XA:122:HIS:NE2	1:XA:126:LEU:HD11	2.34	0.42
1:l:8:ASP:HB2	1:r:11:ILE:HD11	2.00	0.42
1:hA:122:HIS:NE2	1:hA:126:LEU:HD11	2.34	0.42
1:s:15:TYR:CZ	1:s:19:LEU:HD21	2.53	0.42
1:iA:122:HIS:NE2	1:iA:126:LEU:HD11	2.34	0.42
1:0:111:ILE:HD11	1:5:112:LEU:HD12	2.01	0.42
1:1:122:HIS:NE2	1:1:126:LEU:HD11	2.34	0.42
1:AA:122:HIS:NE2	1:AA:126:LEU:HD11	2.34	0.42
1:S:5:LEU:HA	1:S:8:ASP:OD2	2.20	0.42
1:T:5:LEU:H	1:T:5:LEU:HD12	1.83	0.42
1:X:26:LEU:HD21	1:d:29:GLN:HG2	2.00	0.42
1:NA:122:HIS:NE2	1:NA:126:LEU:HD11	2.34	0.42
1:Y:5:LEU:HA	1:Y:8:ASP:OD2	2.19	0.42
1:RA:122:HIS:NE2	1:RA:126:LEU:HD11	2.34	0.42
1:d:5:LEU:HA	1:d:8:ASP:OD2	2.20	0.42
1:UA:106:LYS:HE2	1:UA:106:LYS:HB3	1.83	0.42
1:f:15:TYR:CZ	1:f:19:LEU:HD21	2.53	0.42
1:h:5:LEU:HA	1:h:8:ASP:OD2	2.20	0.42
1:XA:106:LYS:HB3	1:XA:106:LYS:HE2	1.83	0.42
1:bA:121:ALA:O	1:bA:125:ILE:HG12	2.19	0.42
1:n:5:LEU:HA	1:n:8:ASP:OD2	2.20	0.42
1:dA:103:GLU:OE1	1:dA:103:GLU:N	2.33	0.42
1:dA:106:LYS:HB3	1:dA:106:LYS:HE2	1.83	0.42
1:t:5:LEU:HA	1:t:8:ASP:OD2	2.20	0.42
1:z:5:LEU:HA	1:z:8:ASP:OD2	2.20	0.42
1:A:5:LEU:HA	1:A:8:ASP:OD2	2.19	0.42
1:0:122:HIS:NE2	1:0:126:LEU:HD11	2.34	0.42
1:I:29:GLN:O	1:N:1:GLN:N	2.33	0.42
1:S:25:ILE:CG1	1:Y:23:ALA:HB2	2.48	0.42
1:W:15:TYR:CZ	1:W:19:LEU:HD21	2.53	0.42
1:X:5:LEU:HA	1:X:8:ASP:OD2	2.20	0.42
1:OA:121:ALA:O	1:OA:125:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:122:HIS:NE2	1:QA:126:LEU:HD11	2.34	0.42
1:b:5:LEU:HA	1:b:8:ASP:OD2	2.20	0.42
1:WA:121:ALA:O	1:WA:125:ILE:HG12	2.19	0.42
1:WA:122:HIS:NE2	1:WA:126:LEU:HD11	2.34	0.42
1:j:5:LEU:HA	1:j:8:ASP:OD2	2.19	0.42
1:o:5:LEU:HA	1:o:8:ASP:OD2	2.20	0.42
1:nA:121:ALA:O	1:nA:125:ILE:HG12	2.19	0.42
1:4:121:ALA:O	1:4:125:ILE:HG12	2.19	0.42
1:8:112:LEU:HD12	1:EA:111:ILE:CD1	2.49	0.42
1:CA:122:HIS:NE2	1:CA:126:LEU:HD11	2.34	0.42
1:FA:122:HIS:NE2	1:FA:126:LEU:HD11	2.34	0.42
1:R:5:LEU:HA	1:R:8:ASP:OD2	2.19	0.42
1:LA:122:HIS:NE2	1:LA:126:LEU:HD11	2.34	0.42
1:NA:121:ALA:O	1:NA:125:ILE:HG12	2.19	0.42
1:YA:122:HIS:NE2	1:YA:126:LEU:HD11	2.34	0.42
1:ZA:122:HIS:NE2	1:ZA:126:LEU:HD11	2.34	0.42
1:w:5:LEU:HA	1:w:8:ASP:OD2	2.20	0.42
1:K:5:LEU:HA	1:K:8:ASP:OD2	2.19	0.42
1:L:5:LEU:HA	1:L:8:ASP:OD2	2.20	0.42
1:Q:5:LEU:HA	1:Q:8:ASP:OD2	2.20	0.42
1:GA:121:ALA:O	1:GA:125:ILE:HG12	2.19	0.42
1:R:5:LEU:HD12	1:R:5:LEU:H	1.83	0.42
1:Z:19:LEU:HD12	1:f:25:ILE:HD11	2.01	0.42
1:c:18:ILE:HD11	1:i:12:LEU:HB3	2.01	0.42
1:TA:122:HIS:NE2	1:TA:126:LEU:HD11	2.34	0.42
1:cA:122:HIS:NE2	1:cA:126:LEU:HD11	2.34	0.42
1:p:5:LEU:HA	1:p:8:ASP:OD2	2.20	0.42
1:p:5:LEU:HD12	1:p:5:LEU:H	1.83	0.42
1:q:5:LEU:HA	1:q:8:ASP:OD2	2.20	0.42
1:jA:106:LYS:HB3	1:jA:106:LYS:HE2	1.83	0.42
1:jA:121:ALA:O	1:jA:125:ILE:HG12	2.19	0.42
1:v:5:LEU:H	1:v:5:LEU:HD12	1.83	0.42
1:4:122:HIS:NE2	1:4:126:LEU:HD11	2.34	0.42
1:G:11:ILE:HD11	1:M:8:ASP:HB2	2.02	0.42
1:DA:121:ALA:O	1:DA:125:ILE:HG12	2.19	0.42
1:P:5:LEU:HA	1:P:8:ASP:OD2	2.19	0.42
1:NA:118:ILE:HG12	1:TA:123:ALA:HB2	2.02	0.42
1:i:5:LEU:HA	1:i:8:ASP:OD2	2.20	0.42
1:u:5:LEU:HA	1:u:8:ASP:OD2	2.19	0.42
1:kA:122:HIS:NE2	1:kA:126:LEU:HD11	2.34	0.42
1:nA:122:HIS:NE2	1:nA:126:LEU:HD11	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:121:ALA:O	1:6:125:ILE:HG12	2.19	0.42
1:9:121:ALA:O	1:9:125:ILE:HG12	2.19	0.42
1:M:5:LEU:HA	1:M:8:ASP:OD2	2.19	0.42
1:d:5:LEU:HD12	1:d:5:LEU:H	1.83	0.42
1:e:5:LEU:HA	1:e:8:ASP:OD2	2.19	0.42
1:ZA:121:ALA:O	1:ZA:125:ILE:HG12	2.19	0.42
1:v:5:LEU:HA	1:v:8:ASP:OD2	2.20	0.42
1:5:121:ALA:O	1:5:125:ILE:HG12	2.19	0.42
1:H:23:ALA:HB2	1:N:25:ILE:CG1	2.50	0.42
1:K:11:ILE:HD11	1:Q:8:ASP:HB2	2.02	0.42
1:T:12:LEU:HD12	1:Z:18:ILE:HD11	2.00	0.42
1:QA:105:LEU:HD23	1:WA:104:ILE:HD11	2.02	0.42
1:TA:103:GLU:OE1	1:TA:103:GLU:N	2.33	0.42
1:i:24:GLU:HG3	1:o:23:ALA:HB1	2.01	0.42
1:j:5:LEU:H	1:j:5:LEU:HD12	1.83	0.42
1:CA:112:LEU:HD12	1:IA:111:ILE:HD11	2.01	0.42
1:LA:121:ALA:O	1:LA:125:ILE:HG12	2.19	0.42
1:X:5:LEU:HD12	1:X:5:LEU:H	1.83	0.42
1:QA:112:LEU:HD12	1:WA:111:ILE:CD1	2.45	0.42
1:aA:121:ALA:O	1:aA:125:ILE:HG12	2.19	0.42
1:B:12:LEU:HD12	1:H:18:ILE:HD11	2.02	0.42
1:6:122:HIS:NE2	1:6:126:LEU:HD11	2.34	0.42
1:H:8:ASP:HB2	1:N:11:ILE:HD11	2.01	0.42
1:J:5:LEU:HA	1:J:8:ASP:OD2	2.20	0.42
1:AA:103:GLU:OE1	1:AA:103:GLU:N	2.33	0.42
1:EA:121:ALA:O	1:EA:125:ILE:HG12	2.19	0.42
1:FA:111:ILE:CD1	1:LA:112:LEU:HD12	2.49	0.42
1:PA:121:ALA:O	1:PA:125:ILE:HG12	2.19	0.42
1:a:25:ILE:CG1	1:g:23:ALA:HB2	2.50	0.42
1:g:5:LEU:HA	1:g:8:ASP:OD2	2.20	0.42
1:eA:122:HIS:NE2	1:eA:126:LEU:HD11	2.34	0.42
1:mA:121:ALA:O	1:mA:125:ILE:HG12	2.19	0.42
1:3:112:LEU:HD13	1:3:112:LEU:HA	1.94	0.41
1:YA:121:ALA:O	1:YA:125:ILE:HG12	2.19	0.41
1:n:12:LEU:HD12	1:t:18:ILE:CD1	2.50	0.41
1:iA:121:ALA:O	1:iA:125:ILE:HG12	2.19	0.41
1:5:106:LYS:HB3	1:5:106:LYS:HE2	1.83	0.41
1:AA:115:TYR:CZ	1:AA:119:LEU:HD11	2.56	0.41
1:N:5:LEU:HA	1:N:8:ASP:OD2	2.19	0.41
1:FA:115:TYR:CZ	1:FA:119:LEU:HD11	2.56	0.41
1:LA:115:TYR:CZ	1:LA:119:LEU:HD11	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:5:LEU:HA	1:W:8:ASP:OD2	2.20	0.41
1:a:29:GLN:HG2	1:g:26:LEU:HD21	2.01	0.41
1:RA:115:TYR:CZ	1:RA:119:LEU:HD11	2.56	0.41
1:TA:115:TYR:CZ	1:TA:119:LEU:HD11	2.56	0.41
1:h:19:LEU:HD12	1:n:25:ILE:CD1	2.51	0.41
1:h:19:LEU:HD12	1:n:25:ILE:HD11	2.01	0.41
1:XA:121:ALA:O	1:XA:125:ILE:HG12	2.19	0.41
1:k:5:LEU:HA	1:k:8:ASP:OD2	2.20	0.41
1:iA:103:GLU:OE1	1:iA:103:GLU:N	2.33	0.41
1:pA:106:LYS:HB3	1:pA:106:LYS:HE2	1.82	0.41
1:0:115:TYR:CZ	1:0:119:LEU:HD11	2.56	0.41
1:2:111:ILE:CD1	1:3:112:LEU:HD12	2.47	0.41
1:2:121:ALA:O	1:2:125:ILE:HG12	2.19	0.41
1:E:5:LEU:HA	1:E:8:ASP:OD2	2.20	0.41
1:H:5:LEU:HA	1:H:8:ASP:OD2	2.20	0.41
1:9:115:TYR:CZ	1:9:119:LEU:HD11	2.56	0.41
1:GA:115:TYR:CZ	1:GA:119:LEU:HD11	2.56	0.41
1:T:23:ALA:HB2	1:Z:25:ILE:HG12	2.03	0.41
1:KA:112:LEU:HD13	1:KA:112:LEU:HA	1.95	0.41
1:MA:115:TYR:CZ	1:MA:119:LEU:HD11	2.56	0.41
1:c:5:LEU:HA	1:c:8:ASP:OD2	2.20	0.41
1:WA:115:TYR:CZ	1:WA:119:LEU:HD11	2.56	0.41
1:aA:115:TYR:CZ	1:aA:119:LEU:HD11	2.56	0.41
1:C:5:LEU:HA	1:C:8:ASP:OD2	2.20	0.41
1:D:5:LEU:HA	1:D:8:ASP:OD2	2.20	0.41
1:4:115:TYR:CZ	1:4:119:LEU:HD11	2.56	0.41
1:5:115:TYR:CZ	1:5:119:LEU:HD11	2.56	0.41
1:G:5:LEU:HA	1:G:8:ASP:OD2	2.20	0.41
1:6:115:TYR:CZ	1:6:119:LEU:HD11	2.56	0.41
1:BA:115:TYR:CZ	1:BA:119:LEU:HD11	2.55	0.41
1:CA:115:TYR:CZ	1:CA:119:LEU:HD11	2.56	0.41
1:cA:115:TYR:CZ	1:cA:119:LEU:HD11	2.56	0.41
1:s:5:LEU:HA	1:s:8:ASP:OD2	2.20	0.41
1:lA:115:TYR:CZ	1:lA:119:LEU:HD11	2.56	0.41
1:x:5:LEU:HA	1:x:8:ASP:OD2	2.20	0.41
1:nA:106:LYS:HB3	1:nA:106:LYS:HE2	1.82	0.41
1:y:5:LEU:HA	1:y:8:ASP:OD2	2.20	0.41
1:4:112:LEU:HD13	1:4:112:LEU:HA	1.95	0.41
1:J:12:LEU:HD12	1:P:18:ILE:HD11	2.01	0.41
1:K:25:ILE:CG1	1:Q:23:ALA:HB2	2.51	0.41
1:M:18:ILE:HD11	1:S:12:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HA:115:TYR:CZ	1:HA:119:LEU:HD11	2.55	0.41
1:IA:115:TYR:CZ	1:IA:119:LEU:HD11	2.56	0.41
1:T:5:LEU:HA	1:T:8:ASP:OD2	2.20	0.41
1:a:5:LEU:HA	1:a:8:ASP:OD2	2.20	0.41
1:SA:115:TYR:CZ	1:SA:119:LEU:HD11	2.56	0.41
1:l:5:LEU:HA	1:l:8:ASP:OD2	2.19	0.41
1:m:5:LEU:HA	1:m:8:ASP:OD2	2.20	0.41
1:fA:115:TYR:CZ	1:fA:119:LEU:HD11	2.55	0.41
1:s:18:ILE:HD11	1:y:12:LEU:HD12	2.02	0.41
1:iA:115:TYR:CZ	1:iA:119:LEU:HD11	2.56	0.41
1:jA:115:TYR:CZ	1:jA:119:LEU:HD11	2.55	0.41
1:nA:115:TYR:CZ	1:nA:119:LEU:HD11	2.56	0.41
1:B:5:LEU:HA	1:B:8:ASP:OD2	2.20	0.41
1:l:115:TYR:CZ	1:l:119:LEU:HD11	2.56	0.41
1:9:104:ILE:H	1:9:104:ILE:HG13	1.74	0.41
1:NA:115:TYR:CZ	1:NA:119:LEU:HD11	2.56	0.41
1:Z:5:LEU:HA	1:Z:8:ASP:OD2	2.20	0.41
1:f:5:LEU:HA	1:f:8:ASP:OD2	2.20	0.41
1:XA:115:TYR:CZ	1:XA:119:LEU:HD11	2.56	0.41
1:hA:104:ILE:H	1:hA:104:ILE:HG13	1.73	0.41
1:hA:115:TYR:CZ	1:hA:119:LEU:HD11	2.56	0.41
1:mA:115:TYR:CZ	1:mA:119:LEU:HD11	2.56	0.41
1:oA:115:TYR:CZ	1:oA:119:LEU:HD11	2.56	0.41
1:0:106:LYS:HB3	1:0:106:LYS:HE2	1.82	0.41
1:C:25:ILE:HG12	1:I:23:ALA:HB2	2.02	0.41
1:3:115:TYR:CZ	1:3:119:LEU:HD11	2.56	0.41
1:3:118:ILE:HG12	1:9:123:ALA:HB2	2.02	0.41
1:5:111:ILE:HD11	1:BA:112:LEU:HD12	2.02	0.41
1:I:5:LEU:HA	1:I:8:ASP:OD2	2.20	0.41
1:Z:29:GLN:O	1:v:1:GLN:N	2.32	0.41
1:QA:115:TYR:CZ	1:QA:119:LEU:HD11	2.56	0.41
1:dA:115:TYR:CZ	1:dA:119:LEU:HD11	2.56	0.41
1:r:5:LEU:HA	1:r:8:ASP:OD2	2.20	0.41
1:hA:111:ILE:CD1	1:nA:112:LEU:HD12	2.48	0.41
1:FA:106:LYS:HE2	1:FA:106:LYS:HB3	1.83	0.41
1:gA:115:TYR:CZ	1:gA:119:LEU:HD11	2.56	0.41
1:oA:103:GLU:OE1	1:oA:103:GLU:N	2.33	0.41
1:oA:114:ALA:O	1:oA:118:ILE:HG13	2.21	0.41
1:pA:103:GLU:OE1	1:pA:103:GLU:N	2.33	0.41
1:pA:104:ILE:H	1:pA:104:ILE:HG13	1.74	0.41
1:4:114:ALA:O	1:4:118:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:115:TYR:CZ	1:7:119:LEU:HD11	2.56	0.41
1:K:12:LEU:HD13	1:K:12:LEU:HA	1.96	0.41
1:AA:106:LYS:HB3	1:AA:106:LYS:HE2	1.82	0.41
1:DA:114:ALA:O	1:DA:118:ILE:HG13	2.21	0.41
1:EA:106:LYS:HB3	1:EA:106:LYS:HE2	1.83	0.41
1:JA:115:TYR:CZ	1:JA:119:LEU:HD11	2.56	0.41
1:MA:114:ALA:O	1:MA:118:ILE:HG13	2.21	0.41
1:NA:111:ILE:HD11	1:TA:112:LEU:HD12	2.02	0.41
1:OA:114:ALA:O	1:OA:118:ILE:HG13	2.21	0.41
1:OA:115:TYR:CZ	1:OA:119:LEU:HD11	2.56	0.41
1:c:21:ALA:O	1:c:25:ILE:HG13	2.21	0.41
1:TA:114:ALA:O	1:TA:118:ILE:HG13	2.21	0.41
1:VA:115:TYR:CZ	1:VA:119:LEU:HD11	2.56	0.41
1:YA:114:ALA:O	1:YA:118:ILE:HG13	2.21	0.41
1:YA:115:TYR:CZ	1:YA:119:LEU:HD11	2.56	0.41
1:ZA:115:TYR:CZ	1:ZA:119:LEU:HD11	2.56	0.41
1:bA:115:TYR:CZ	1:bA:119:LEU:HD11	2.56	0.41
1:fA:114:ALA:O	1:fA:118:ILE:HG13	2.21	0.41
1:s:11:ILE:HD11	1:y:8:ASP:HB2	2.03	0.41
1:2:106:LYS:HB3	1:2:106:LYS:HE2	1.83	0.41
1:3:114:ALA:O	1:3:118:ILE:HG13	2.21	0.41
1:DA:115:TYR:CZ	1:DA:119:LEU:HD11	2.56	0.41
1:FA:114:ALA:O	1:FA:118:ILE:HG13	2.21	0.41
1:U:12:LEU:HD13	1:U:12:LEU:HA	1.96	0.41
1:KA:115:TYR:CZ	1:KA:119:LEU:HD11	2.56	0.41
1:PA:114:ALA:O	1:PA:118:ILE:HG13	2.21	0.41
1:QA:112:LEU:HD13	1:QA:112:LEU:HA	1.95	0.41
1:WA:114:ALA:O	1:WA:118:ILE:HG13	2.21	0.41
1:aA:114:ALA:O	1:aA:118:ILE:HG13	2.21	0.41
1:n:26:LEU:HD21	1:t:29:GLN:HG2	2.03	0.41
1:p:21:ALA:O	1:p:25:ILE:HG13	2.21	0.41
1:7:114:ALA:O	1:7:118:ILE:HG13	2.21	0.40
1:8:115:TYR:CZ	1:8:119:LEU:HD11	2.56	0.40
1:CA:114:ALA:O	1:CA:118:ILE:HG13	2.21	0.40
1:GA:114:ALA:O	1:GA:118:ILE:HG13	2.21	0.40
1:KA:114:ALA:O	1:KA:118:ILE:HG13	2.21	0.40
1:W:21:ALA:O	1:W:25:ILE:HG13	2.21	0.40
1:PA:115:TYR:CZ	1:PA:119:LEU:HD11	2.56	0.40
1:RA:114:ALA:O	1:RA:118:ILE:HG13	2.21	0.40
1:e:18:ILE:CD1	1:k:12:LEU:HD12	2.51	0.40
1:UA:115:TYR:CZ	1:UA:119:LEU:HD11	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:i:21:ALA:O	1:i:25:ILE:HG13	2.21	0.40
1:j:21:ALA:O	1:j:25:ILE:HG13	2.21	0.40
1:j:23:ALA:HB2	1:p:25:ILE:CG1	2.51	0.40
1:cA:114:ALA:O	1:cA:118:ILE:HG13	2.21	0.40
1:eA:115:TYR:CZ	1:eA:119:LEU:HD11	2.55	0.40
1:iA:104:ILE:H	1:iA:104:ILE:HG13	1.74	0.40
1:mA:114:ALA:O	1:mA:118:ILE:HG13	2.21	0.40
1:l:118:ILE:HG12	1:7:123:ALA:HB2	2.02	0.40
1:H:29:GLN:C	1:d:1:GLN:H3	2.21	0.40
1:9:106:LYS:HE2	1:9:106:LYS:HB3	1.83	0.40
1:9:112:LEU:HD13	1:9:112:LEU:HA	1.95	0.40
1:L:21:ALA:O	1:L:25:ILE:HG13	2.21	0.40
1:R:21:ALA:O	1:R:25:ILE:HG13	2.21	0.40
1:k:18:ILE:CD1	1:q:12:LEU:HD12	2.51	0.40
1:hA:114:ALA:O	1:hA:118:ILE:HG13	2.21	0.40
1:v:21:ALA:O	1:v:25:ILE:HG13	2.21	0.40
1:B:21:ALA:O	1:B:25:ILE:HG13	2.21	0.40
1:8:114:ALA:O	1:8:118:ILE:HG13	2.21	0.40
1:J:21:ALA:O	1:J:25:ILE:HG13	2.21	0.40
1:BA:106:LYS:HB3	1:BA:106:LYS:HE2	1.83	0.40
1:BA:114:ALA:O	1:BA:118:ILE:HG13	2.21	0.40
1:EA:115:TYR:CZ	1:EA:119:LEU:HD11	2.56	0.40
1:V:26:LEU:HD21	1:b:29:GLN:HG2	2.03	0.40
1:W:18:ILE:HD11	1:c:12:LEU:HD12	2.02	0.40
1:TA:112:LEU:HD13	1:TA:112:LEU:HA	1.95	0.40
1:kA:114:ALA:O	1:kA:118:ILE:HG13	2.21	0.40
1:lA:114:ALA:O	1:lA:118:ILE:HG13	2.21	0.40
1:z:21:ALA:O	1:z:25:ILE:HG13	2.21	0.40
1:pA:115:TYR:CZ	1:pA:119:LEU:HD11	2.56	0.40
1:C:11:ILE:HD11	1:I:8:ASP:HB2	2.03	0.40
1:C:21:ALA:O	1:C:25:ILE:HG13	2.21	0.40
1:2:115:TYR:CZ	1:2:119:LEU:HD11	2.56	0.40
1:D:21:ALA:O	1:D:25:ILE:HG13	2.21	0.40
1:I:25:ILE:HD11	1:O:19:LEU:HD12	2.03	0.40
1:O:5:LEU:HA	1:O:8:ASP:OD2	2.20	0.40
1:P:21:ALA:O	1:P:25:ILE:HG13	2.21	0.40
1:e:29:GLN:HG2	1:k:26:LEU:HD21	2.04	0.40
1:kA:115:TYR:CZ	1:kA:119:LEU:HD11	2.56	0.40
1:E:21:ALA:O	1:E:25:ILE:HG13	2.21	0.40
1:E:29:GLN:OXT	1:R:2:ALA:HB3	2.22	0.40
1:4:103:GLU:OE1	1:4:103:GLU:N	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:21:ALA:O	1:I:25:ILE:HG13	2.21	0.40
1:8:106:LYS:HE2	1:8:106:LYS:HB3	1.83	0.40
1:FA:112:LEU:HD13	1:FA:112:LEU:HA	1.95	0.40
1:U:5:LEU:HA	1:U:8:ASP:OD2	2.19	0.40
1:V:21:ALA:O	1:V:25:ILE:HG13	2.21	0.40
1:LA:114:ALA:O	1:LA:118:ILE:HG13	2.21	0.40
1:NA:114:ALA:O	1:NA:118:ILE:HG13	2.21	0.40
1:VA:114:ALA:O	1:VA:118:ILE:HG13	2.21	0.40
1:WA:104:ILE:H	1:WA:104:ILE:HG13	1.74	0.40
1:XA:114:ALA:O	1:XA:118:ILE:HG13	2.21	0.40
1:nA:114:ALA:O	1:nA:118:ILE:HG13	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	1	27/29 (93%)	27 (100%)	0	0	100	100
1	2	27/29 (93%)	27 (100%)	0	0	100	100
1	3	27/29 (93%)	27 (100%)	0	0	100	100
1	4	27/29 (93%)	27 (100%)	0	0	100	100
1	5	27/29 (93%)	27 (100%)	0	0	100	100
1	6	27/29 (93%)	27 (100%)	0	0	100	100
1	7	27/29 (93%)	27 (100%)	0	0	100	100
1	8	27/29 (93%)	27 (100%)	0	0	100	100
1	9	27/29 (93%)	27 (100%)	0	0	100	100
1	A	27/29 (93%)	26 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	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	C	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	CA	27/29 (93%)	27 (100%)	0	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	E	27/29 (93%)	26 (96%)	1 (4%)	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%)	26 (96%)	1 (4%)	0	100	100
1	GA	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	I	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	IA	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%)	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%)	26 (96%)	1 (4%)	0	100	100
1	LA	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	N	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	NA	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%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	QA	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	S	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	SA	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%)	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%)	26 (96%)	1 (4%)	0	100	100
1	VA	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	X	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	XA	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%)	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
1	a	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	aA	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	c	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	cA	27/29 (93%)	27 (100%)	0	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	e	27/29 (93%)	26 (96%)	1 (4%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	fA	27/29 (93%)	27 (100%)	0	0	100	100
1	g	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	gA	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	i	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	iA	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%)	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%)	26 (96%)	1 (4%)	0	100	100
1	lA	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	n	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	nA	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%)	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%)	26 (96%)	1 (4%)	0	100	100
1	r	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	s	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	t	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	u	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	v	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	w	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	x	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	y	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
1	z	27/29 (93%)	26 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2808/3016 (93%)	2756 (98%)	52 (2%)	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	1	21/21 (100%)	21 (100%)	0	100	100
1	2	21/21 (100%)	21 (100%)	0	100	100
1	3	21/21 (100%)	21 (100%)	0	100	100
1	4	21/21 (100%)	21 (100%)	0	100	100
1	5	21/21 (100%)	21 (100%)	0	100	100
1	6	21/21 (100%)	21 (100%)	0	100	100
1	7	21/21 (100%)	21 (100%)	0	100	100
1	8	21/21 (100%)	21 (100%)	0	100	100
1	9	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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	r	21/21 (100%)	21 (100%)	0	100	100
1	s	21/21 (100%)	21 (100%)	0	100	100
1	t	21/21 (100%)	21 (100%)	0	100	100
1	u	21/21 (100%)	21 (100%)	0	100	100
1	v	21/21 (100%)	21 (100%)	0	100	100
1	w	21/21 (100%)	21 (100%)	0	100	100
1	x	21/21 (100%)	21 (100%)	0	100	100
1	y	21/21 (100%)	21 (100%)	0	100	100
1	z	21/21 (100%)	21 (100%)	0	100	100
All	All	2184/2184 (100%)	2184 (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 ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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.

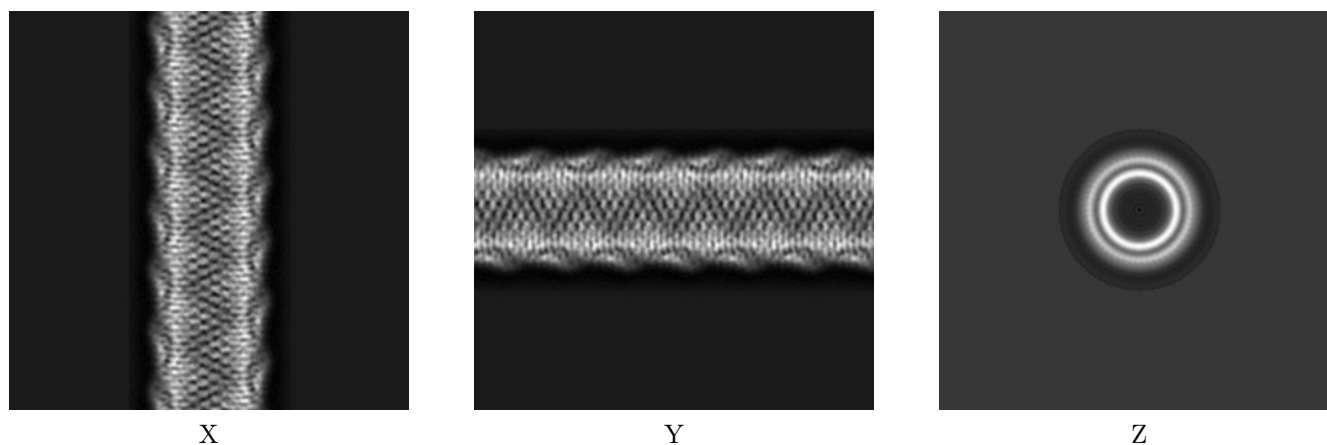
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21818. 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](#)

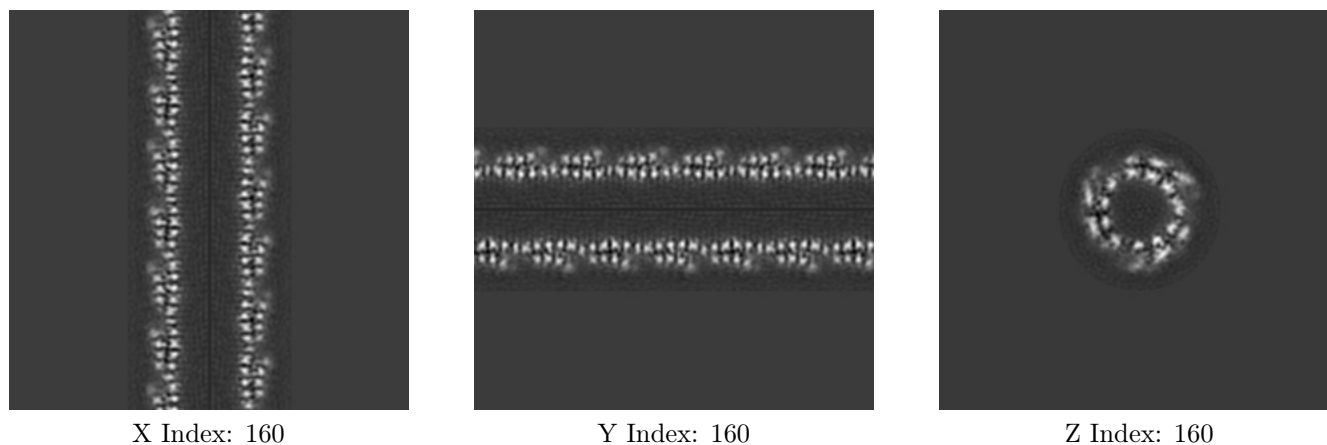
6.1.1 Primary map



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

6.2 Central slices [i](#)

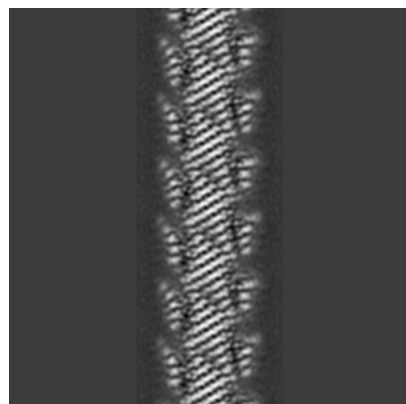
6.2.1 Primary map



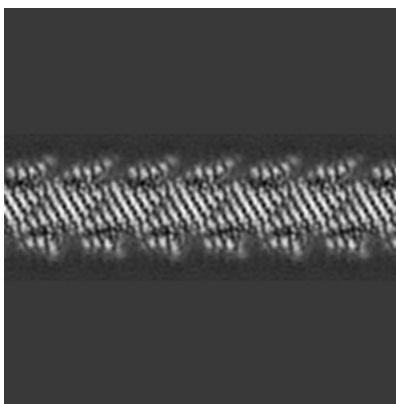
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

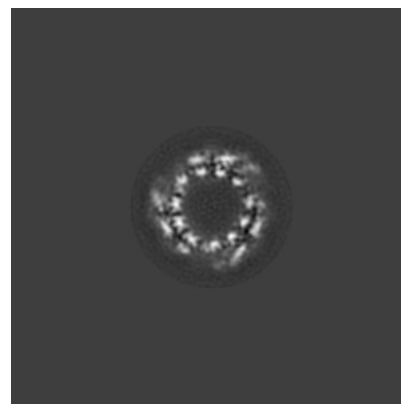
6.3.1 Primary map



X Index: 132



Y Index: 132

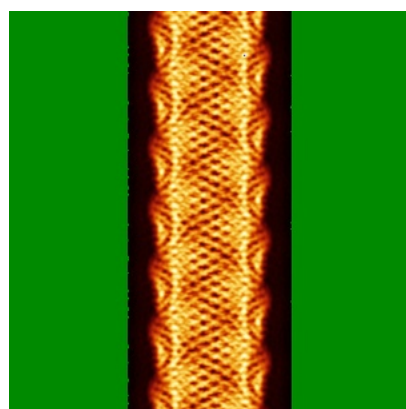


Z Index: 70

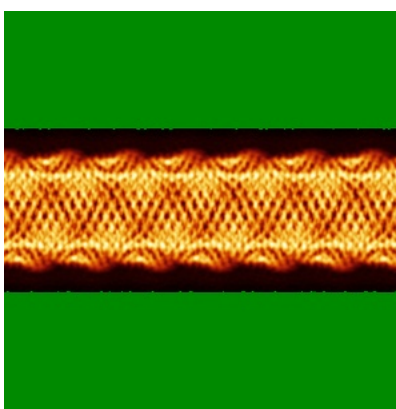
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

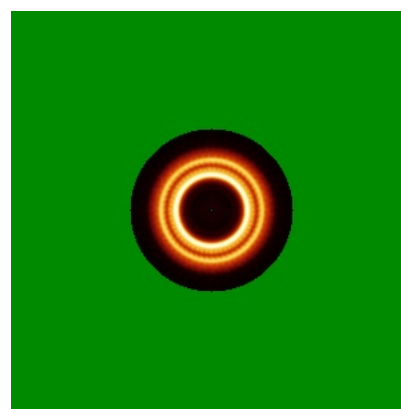
6.4.1 Primary map



X



Y

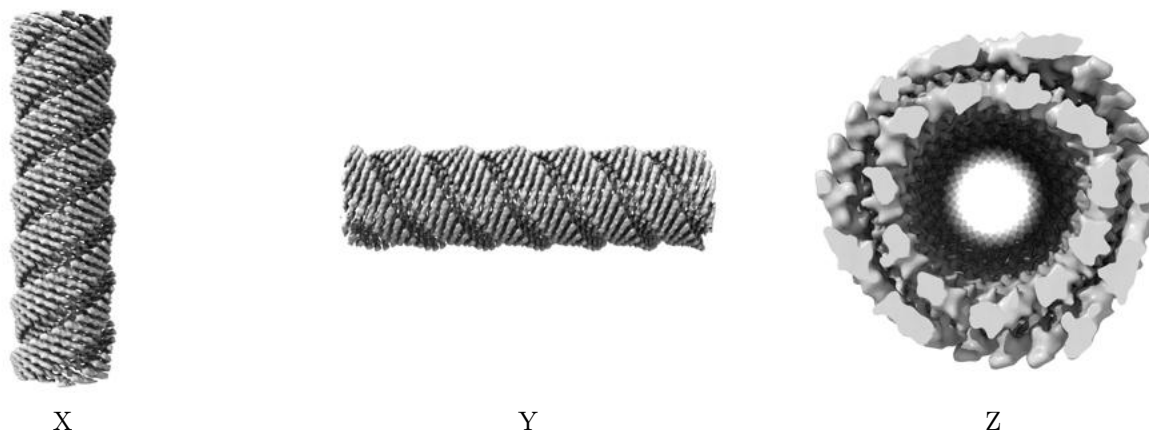


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0118. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

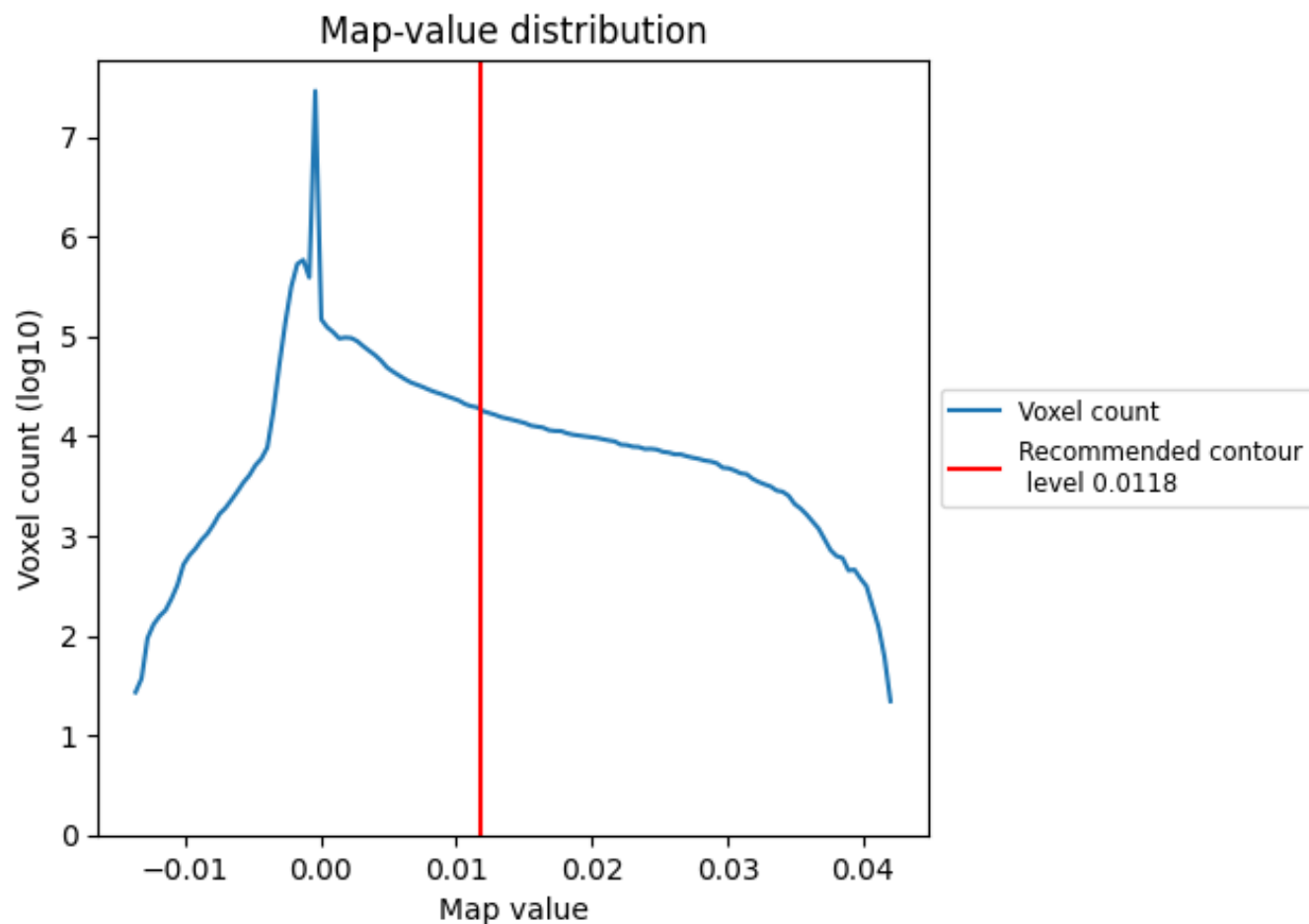
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

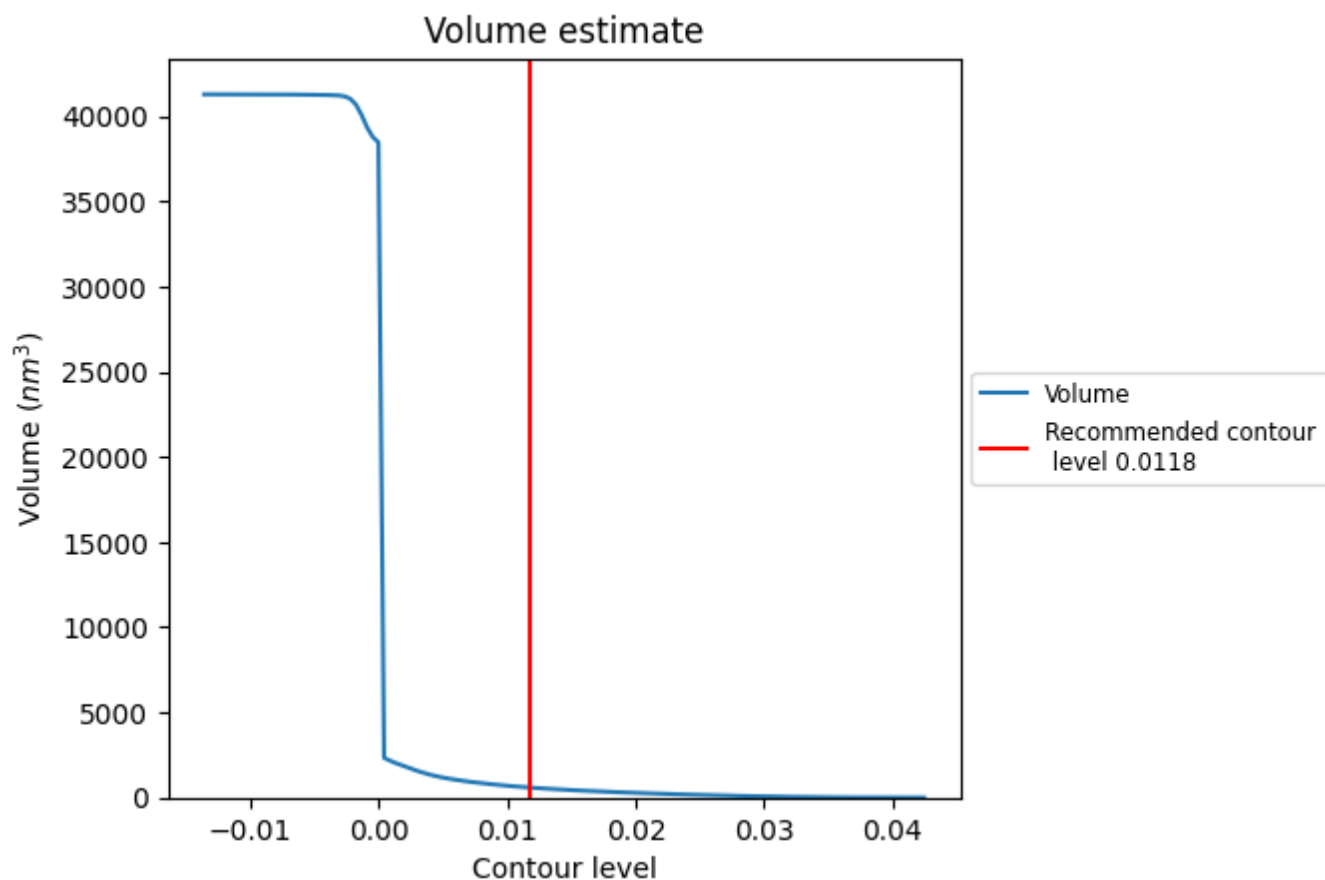
This section contains the results of statistical analysis of the map.

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.

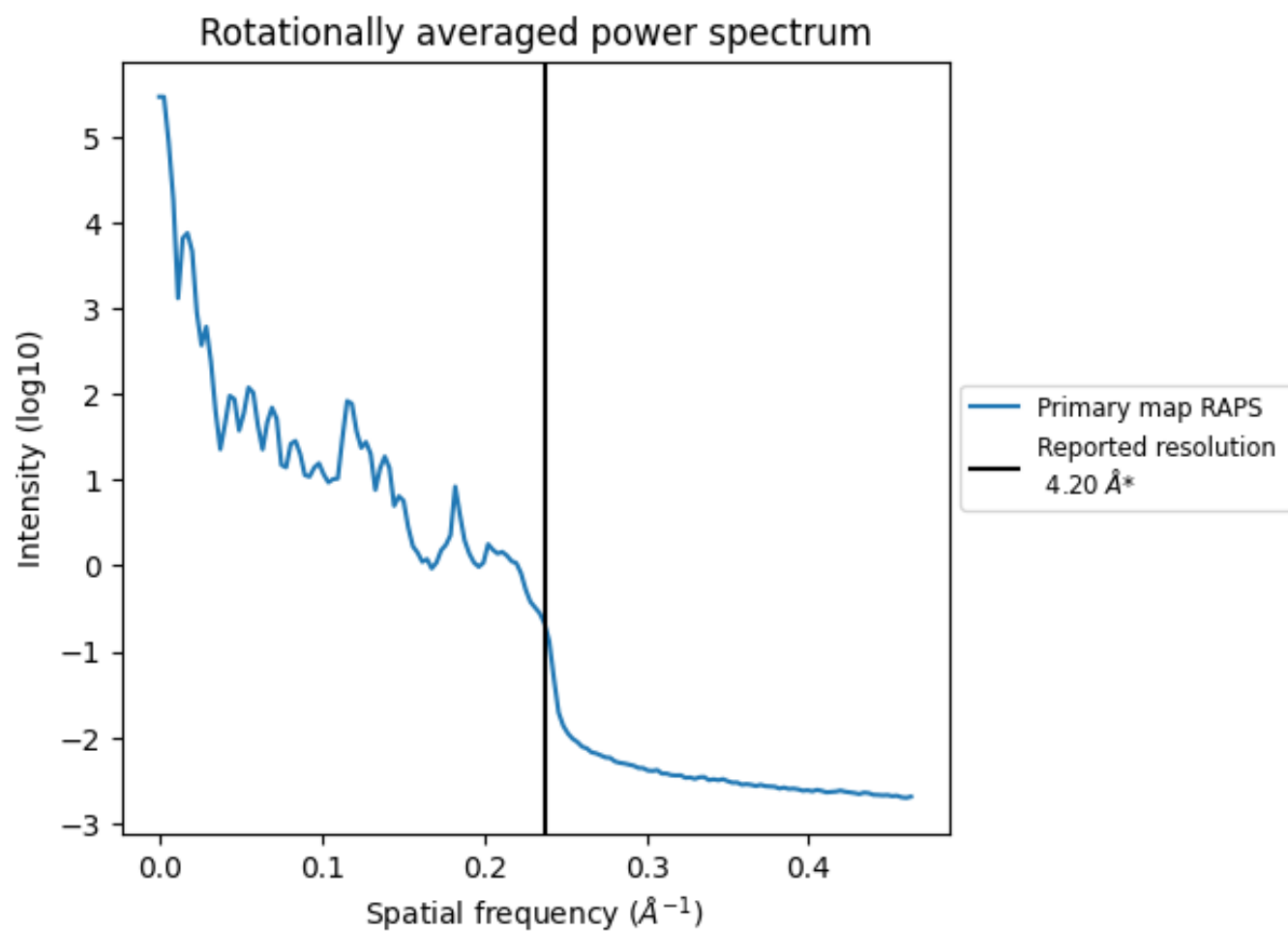
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 583 nm^3 ; this corresponds to an approximate mass of 527 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 0.238 Å⁻¹

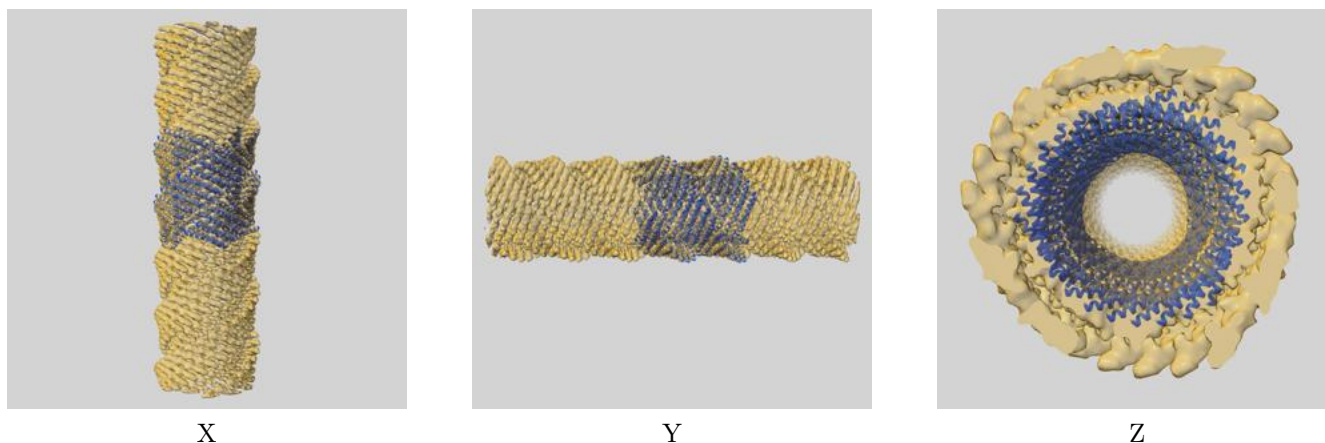
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

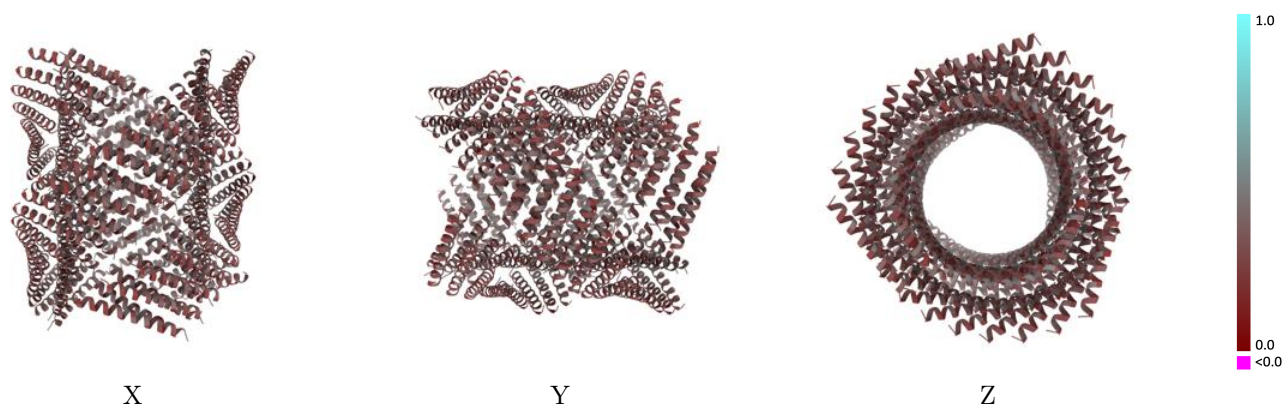
This section contains information regarding the fit between EMDB map EMD-21818 and PDB model 6WL9. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



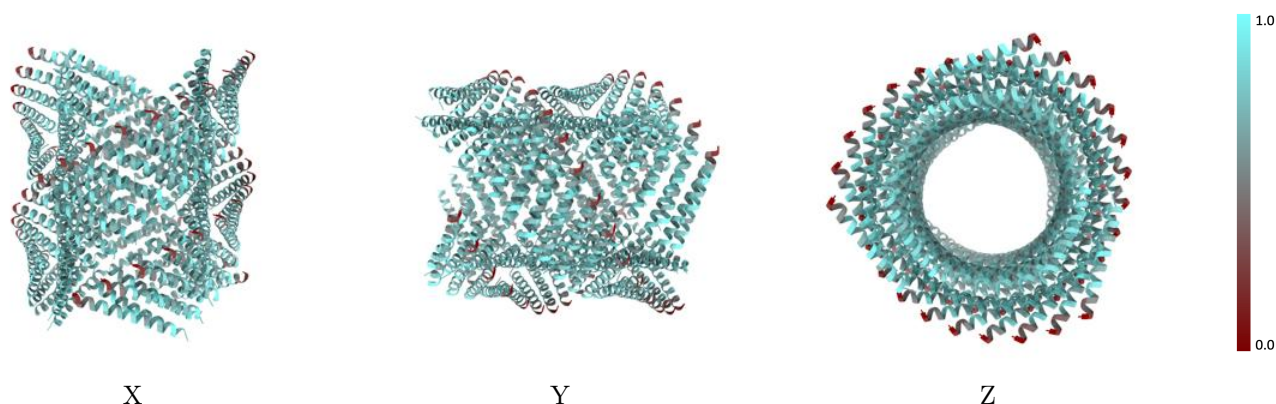
The images above show the 3D surface view of the map at the recommended contour level 0.0118 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



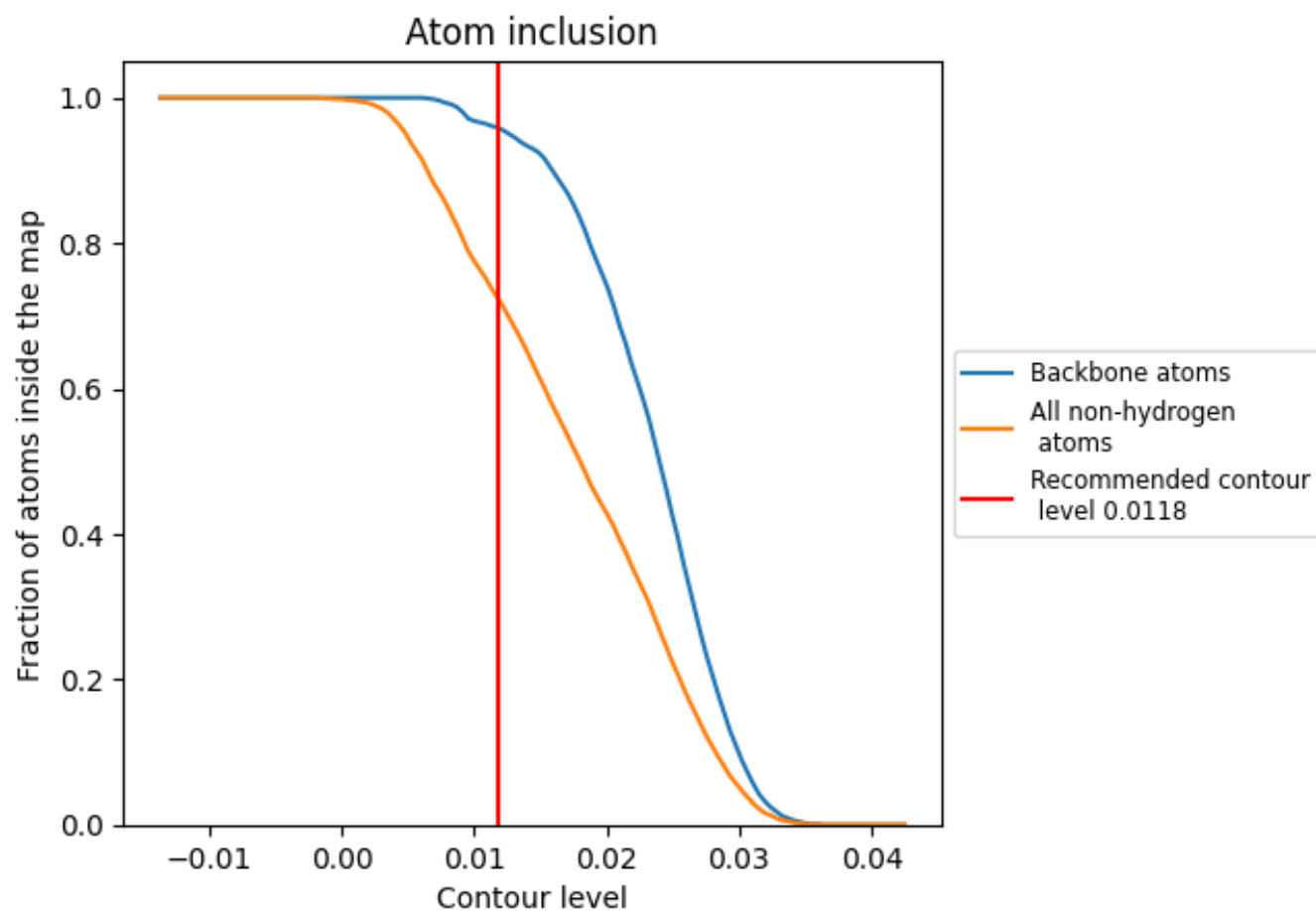
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0118).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 72% 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 (0.0118) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7240	 0.3330
0	 0.6790	 0.3180
1	 0.6880	 0.3170
2	 0.6610	 0.3210
3	 0.6700	 0.3170
4	 0.6830	 0.3180
5	 0.6740	 0.3140
6	 0.6740	 0.3190
7	 0.6880	 0.3190
8	 0.6740	 0.3190
9	 0.6790	 0.3170
A	 0.7630	 0.3540
AA	 0.6960	 0.3170
B	 0.7630	 0.3480
BA	 0.6700	 0.3100
C	 0.7770	 0.3530
CA	 0.6740	 0.3200
D	 0.7680	 0.3530
DA	 0.6830	 0.3200
E	 0.7630	 0.3460
EA	 0.6740	 0.3180
F	 0.7590	 0.3530
FA	 0.6790	 0.3240
G	 0.7540	 0.3510
GA	 0.6880	 0.3130
H	 0.7680	 0.3480
HA	 0.6740	 0.3070
I	 0.7720	 0.3570
IA	 0.6700	 0.3140
J	 0.7720	 0.3530
JA	 0.6880	 0.3220
K	 0.7590	 0.3470
KA	 0.6740	 0.3220
L	 0.7540	 0.3500
LA	 0.6740	 0.3200



























































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Chain	Atom inclusion	Q-score
M	 0.7770	 0.3560
MA	 0.6880	 0.3160
N	 0.7720	 0.3510
NA	 0.6830	 0.3100
O	 0.7860	 0.3560
OA	 0.6920	 0.3170
P	 0.7770	 0.3590
PA	 0.6790	 0.3150
Q	 0.7720	 0.3430
QA	 0.6740	 0.3190
R	 0.7540	 0.3430
RA	 0.6880	 0.3190
S	 0.7540	 0.3520
SA	 0.6880	 0.3130
T	 0.7810	 0.3510
TA	 0.6740	 0.3090
U	 0.7680	 0.3570
UA	 0.6650	 0.3100
V	 0.7770	 0.3550
VA	 0.6830	 0.3140
W	 0.7720	 0.3500
WA	 0.6830	 0.3190
X	 0.7540	 0.3450
XA	 0.6880	 0.3130
Y	 0.7630	 0.3500
YA	 0.6740	 0.3160
Z	 0.7770	 0.3530
ZA	 0.6740	 0.3120
a	 0.7810	 0.3520
aA	 0.6520	 0.3060
b	 0.7860	 0.3520
bA	 0.6740	 0.3140
c	 0.7720	 0.3450
cA	 0.6650	 0.3160
d	 0.7590	 0.3510
dA	 0.6880	 0.3180
e	 0.7680	 0.3520
eA	 0.6700	 0.3100
f	 0.7810	 0.3540
fA	 0.6790	 0.3170
g	 0.7860	 0.3560
gA	 0.6740	 0.3100

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Chain	Atom inclusion	Q-score
h	 0.7950	 0.3520
hA	 0.6650	 0.3200
i	 0.7770	 0.3470
iA	 0.6740	 0.3070
j	 0.7770	 0.3560
jA	 0.6740	 0.3190
k	 0.7720	 0.3490
kA	 0.6880	 0.2970
l	 0.7810	 0.3460
lA	 0.6790	 0.3180
m	 0.7860	 0.3530
mA	 0.6790	 0.3130
n	 0.7720	 0.3490
nA	 0.6610	 0.3180
o	 0.7680	 0.3490
oA	 0.6610	 0.3020
p	 0.7720	 0.3510
pA	 0.6880	 0.3160
q	 0.7590	 0.3530
r	 0.7770	 0.3540
s	 0.7720	 0.3510
t	 0.7810	 0.3490
u	 0.7630	 0.3500
v	 0.7720	 0.3520
w	 0.7810	 0.3500
x	 0.7860	 0.3510
y	 0.7590	 0.3430
z	 0.7680	 0.3490