



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:25 PM BST

PDB ID : 3J9Q  
EMDB ID: : EMD-6270  
Title : Atomic structures of a bactericidal contractile nanotube in its pre- and post-contraction states  
Authors : Ge, P.; Scholl, D.; Leiman, P.G.; Yu, X.; Miller, J.F.; Zhou, Z.H.  
Deposited on : 2015-02-17  
Resolution : 3.50 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

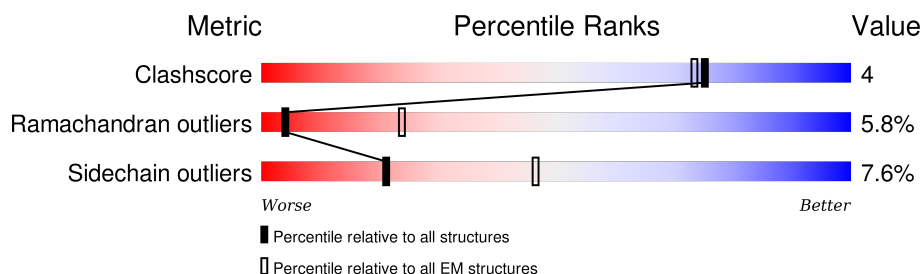
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.50 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	386	81% 15% ..
1	B	386	83% 14% ..
1	C	386	83% 14% ..
1	D	386	82% 15% ..
1	E	386	82% 15% ..
1	F	386	84% 13% ..
1	G	386	82% 15% ..
1	H	386	84% 13% ..
1	I	386	83% 14% ..


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Mol	Chain	Length	Quality of chain
1	J	386	 83% 13% ..
1	K	386	 83% 13% ..
1	L	386	 84% 12% ..
1	M	386	 82% 14% ..
1	N	386	 84% 13% ..
1	O	386	 83% 14% ..
1	P	386	 84% 12% ..
1	Q	386	 83% 14% ..
1	R	386	 84% 13% ..
1	X	386	 84% 13% ..
1	a	386	 92% 7% .
1	d	386	 91% 7% .
1	g	386	 91% 7% .
1	j	386	 91% 7% .
1	m	386	 91% 7% .
2	S	168	 74% 24% ..
2	T	168	 74% 22% ..
2	U	168	 74% 21% ..
2	V	168	 73% 23% ..
2	W	168	 74% 23% ..
2	Y	168	 74% 22% ..
2	Z	168	 74% 22% ..
2	b	168	 83% 16% .
2	c	168	 82% 17% .
2	e	168	 83% 16% .

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Mol	Chain	Length	Quality of chain
2	f	168	 83% 16% .
2	h	168	 83% 16% .
2	i	168	 83% 16% .
2	k	168	 82% 17% .
2	l	168	 83% 16% .
2	n	168	 83% 16% .
2	o	168	 83% 16% .
2	p	168	 83% 16% .
2	q	168	 82% 17% ..
2	r	168	 82% 16% ..
2	s	168	 82% 17% ..
2	t	168	 82% 17% ..
2	u	168	 83% 16% .
2	v	168	 82% 17% .

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 99648 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 sheath.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	385	Total	C	N	O	S	0	0
			2897	1825	506	558	8		
1	B	385	Total	C	N	O	S	0	0
			2897	1825	506	558	8		
1	C	385	Total	C	N	O	S	0	0
			2897	1825	506	558	8		
1	D	385	Total	C	N	O	S	0	0
			2897	1825	506	558	8		
1	E	385	Total	C	N	O	S	0	0
			2897	1825	506	558	8		
1	F	385	Total	C	N	O	S	0	0
			2897	1825	506	558	8		
1	G	385	Total	C	N	O	S	0	0
			2897	1825	506	558	8		
1	K	385	Total	C	N	O	S	0	0
			2897	1825	506	558	8		
1	I	385	Total	C	N	O	S	0	0
			2897	1825	506	558	8		
1	O	385	Total	C	N	O	S	0	0
			2897	1825	506	558	8		
1	M	385	Total	C	N	O	S	0	0
			2897	1825	506	558	8		
1	Q	385	Total	C	N	O	S	0	0
			2897	1825	506	558	8		
1	H	385	Total	C	N	O	S	0	0
			2897	1825	506	558	8		
1	L	385	Total	C	N	O	S	0	0
			2897	1825	506	558	8		
1	J	385	Total	C	N	O	S	0	0
			2897	1825	506	558	8		
1	P	385	Total	C	N	O	S	0	0
			2897	1825	506	558	8		
1	N	385	Total	C	N	O	S	0	0
			2897	1825	506	558	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	385	Total	C	N	O	S	0	0
			2897	1825	506	558	8		
1	X	385	Total	C	N	O	S	0	0
			2897	1825	506	558	8		
1	d	385	Total	C	N	O	S	0	0
			2897	1825	506	558	8		
1	a	385	Total	C	N	O	S	0	0
			2897	1825	506	558	8		
1	j	385	Total	C	N	O	S	0	0
			2897	1825	506	558	8		
1	g	385	Total	C	N	O	S	0	0
			2897	1825	506	558	8		
1	m	385	Total	C	N	O	S	0	0
			2897	1825	506	558	8		

- Molecule 2 is a protein called tube.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S	166	Total	C	N	O	S	0	0
			1255	795	214	242	4		
2	U	166	Total	C	N	O	S	0	0
			1255	795	214	242	4		
2	T	166	Total	C	N	O	S	0	0
			1255	795	214	242	4		
2	W	166	Total	C	N	O	S	0	0
			1255	795	214	242	4		
2	V	166	Total	C	N	O	S	0	0
			1255	795	214	242	4		
2	Z	166	Total	C	N	O	S	0	0
			1255	795	214	242	4		
2	Y	166	Total	C	N	O	S	0	0
			1255	795	214	242	4		
2	e	166	Total	C	N	O	S	0	0
			1255	795	214	242	4		
2	b	166	Total	C	N	O	S	0	0
			1255	795	214	242	4		
2	k	166	Total	C	N	O	S	0	0
			1255	795	214	242	4		
2	h	166	Total	C	N	O	S	0	0
			1255	795	214	242	4		
2	n	166	Total	C	N	O	S	0	0
			1255	795	214	242	4		

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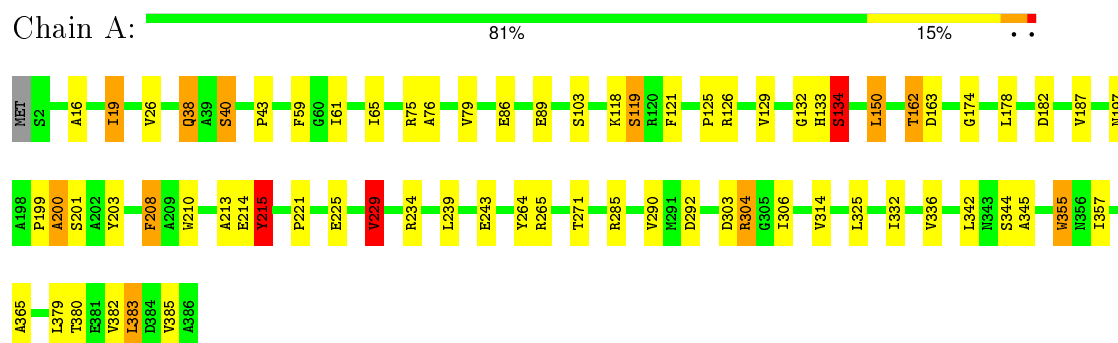
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Mol	Chain	Residues	Atoms					AltConf	Trace
2	c	166	Total	C	N	O	S	0	0
			1255	795	214	242	4		
2	i	166	Total	C	N	O	S	0	0
			1255	795	214	242	4		
2	f	166	Total	C	N	O	S	0	0
			1255	795	214	242	4		
2	o	166	Total	C	N	O	S	0	0
			1255	795	214	242	4		
2	l	166	Total	C	N	O	S	0	0
			1255	795	214	242	4		
2	p	166	Total	C	N	O	S	0	0
			1255	795	214	242	4		
2	q	166	Total	C	N	O	S	0	0
			1255	795	214	242	4		
2	s	166	Total	C	N	O	S	0	0
			1255	795	214	242	4		
2	r	166	Total	C	N	O	S	0	0
			1255	795	214	242	4		
2	u	166	Total	C	N	O	S	0	0
			1255	795	214	242	4		
2	t	166	Total	C	N	O	S	0	0
			1255	795	214	242	4		
2	v	166	Total	C	N	O	S	0	0
			1255	795	214	242	4		

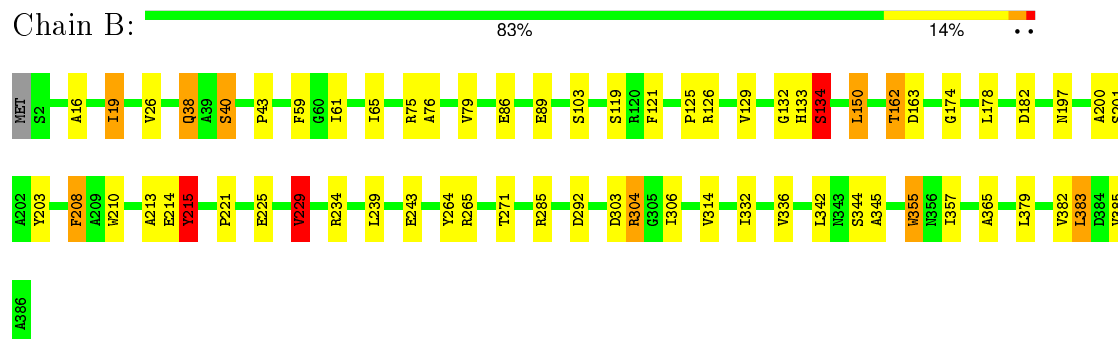
### 3 Residue-property plots

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

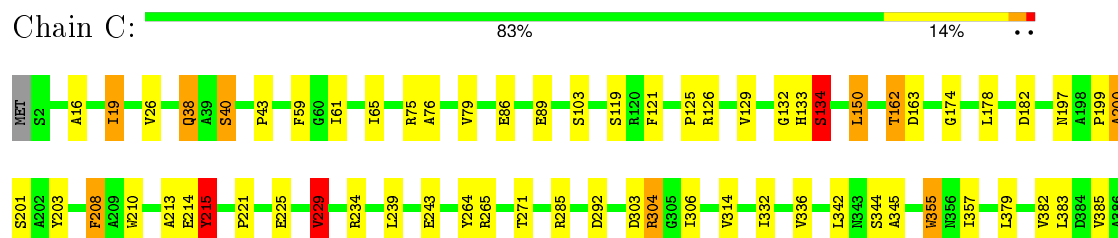
- Molecule 1: sheath



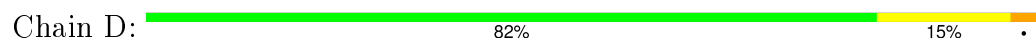
- Molecule 1: sheath



- Molecule 1: sheath



- Molecule 1: sheath

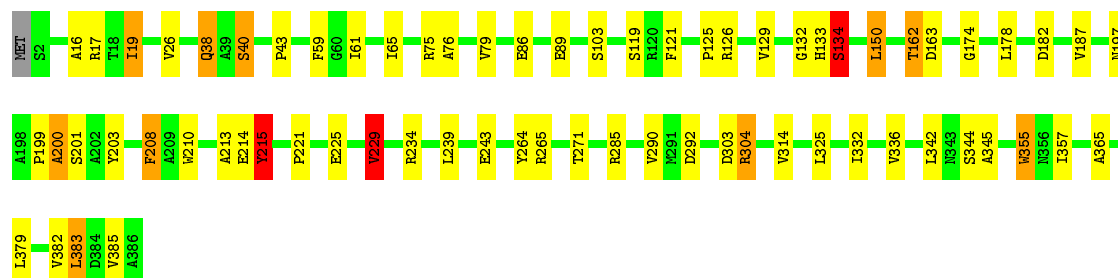






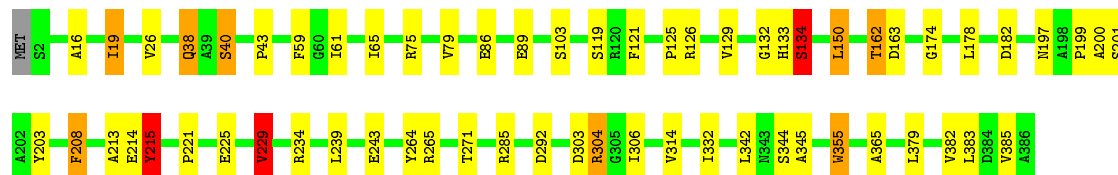
- Molecule 1: sheath

Chain E: 82% 15% ..



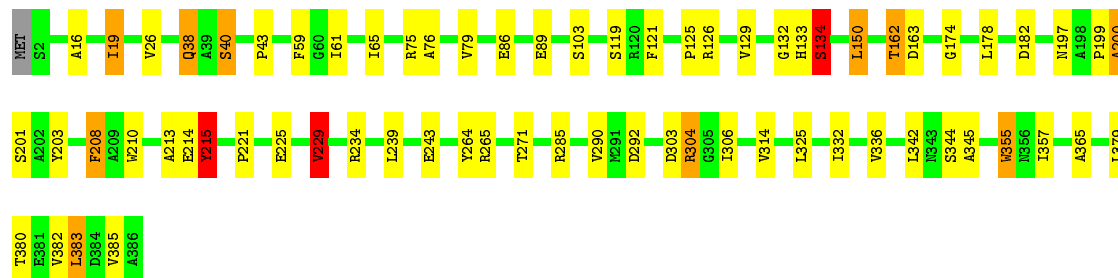
- Molecule 1: sheath

Chain F: 84% 13% ..



- Molecule 1: sheath

Chain G: 82% 15% ..



- Molecule 1: sheath

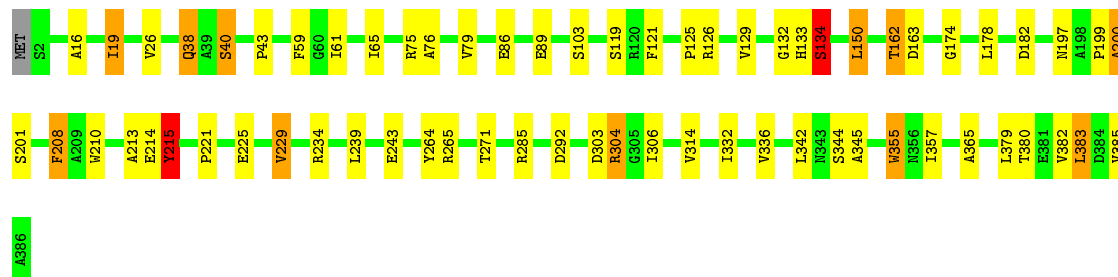
Chain K: 83% 13% ..





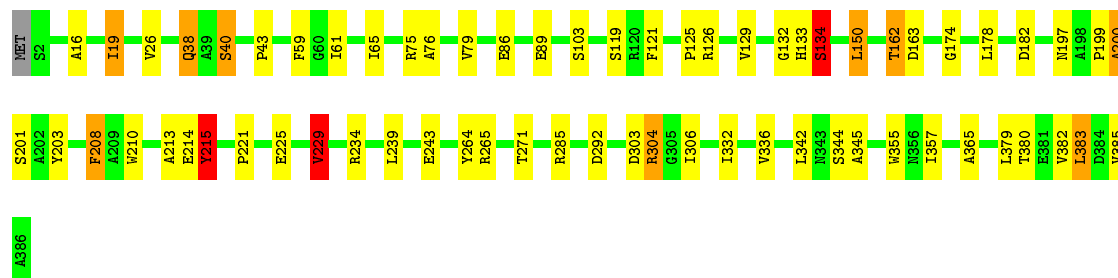
- Molecule 1: sheath

Chain I: 83% 14% ..



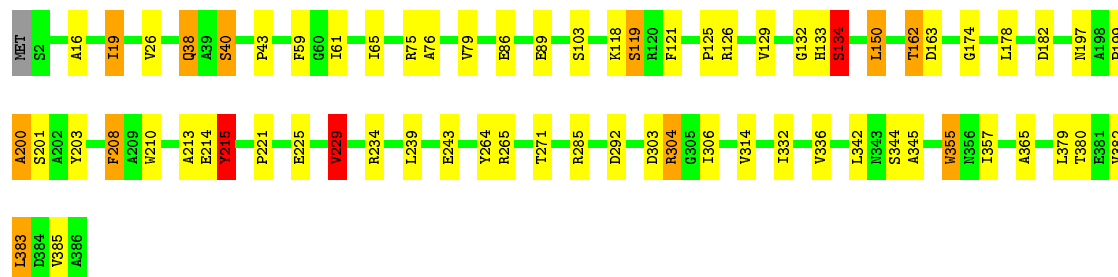
- Molecule 1: sheath

Chain O: 83% 14% ..



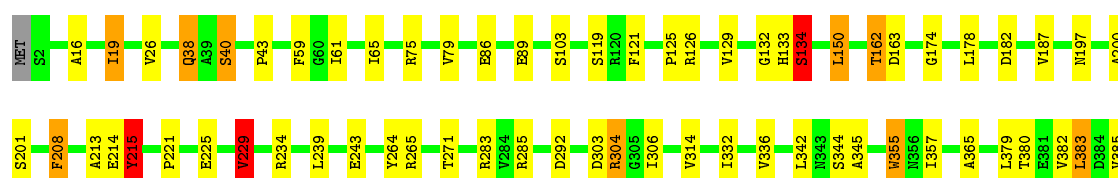
- Molecule 1: sheath

Chain M: 82% 14% ..




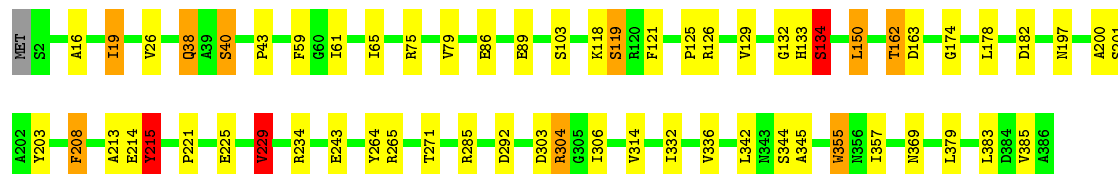
- Molecule 1: sheath

Chain Q: 83% 14% ..


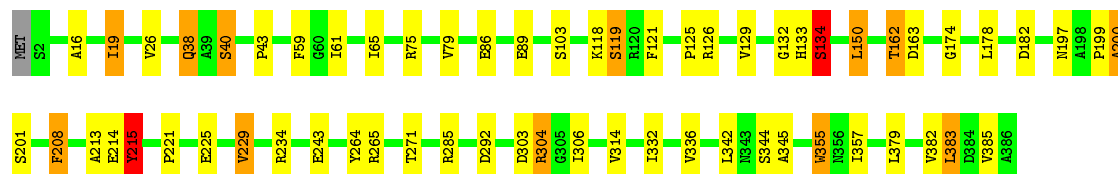


A386


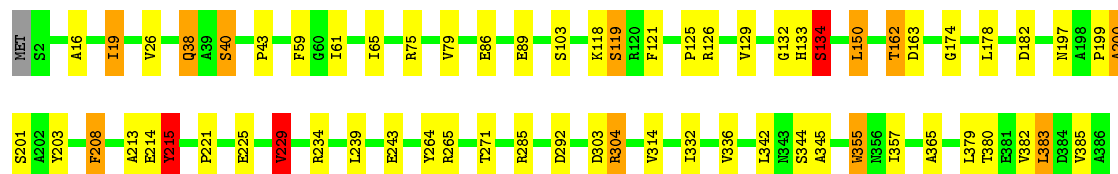
- Molecule 1: sheath

Chain H:  84% 13% ..


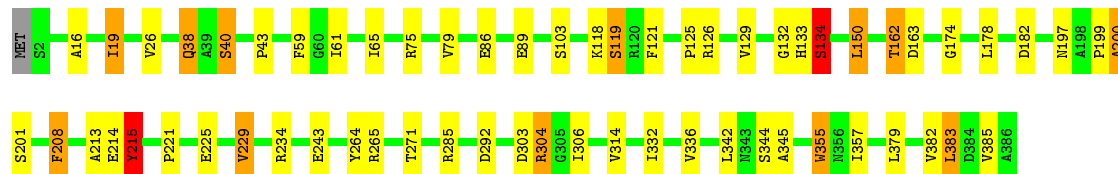
- Molecule 1: sheath

Chain L:  84% 12% ..


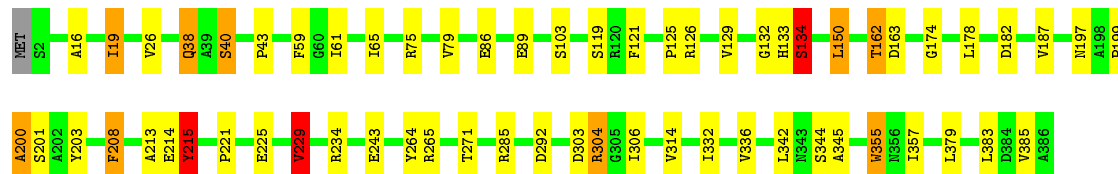
- Molecule 1: sheath

Chain J:  83% 13% ..

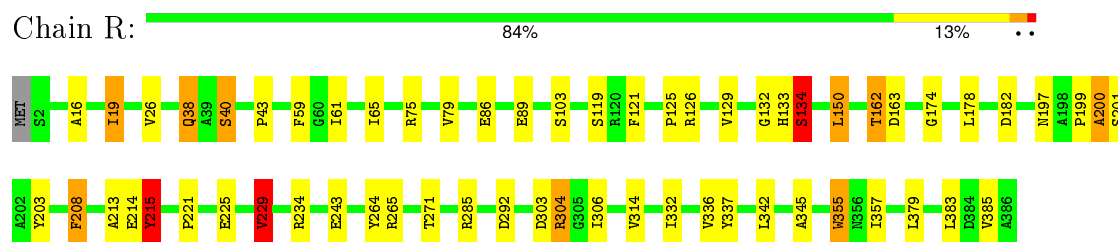
- Molecule 1: sheath

Chain P:  84% 12% ..

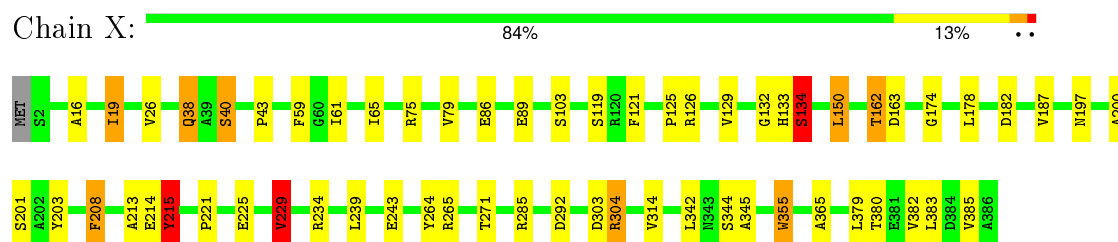
- Molecule 1: sheath

Chain N:  84% 13% ..

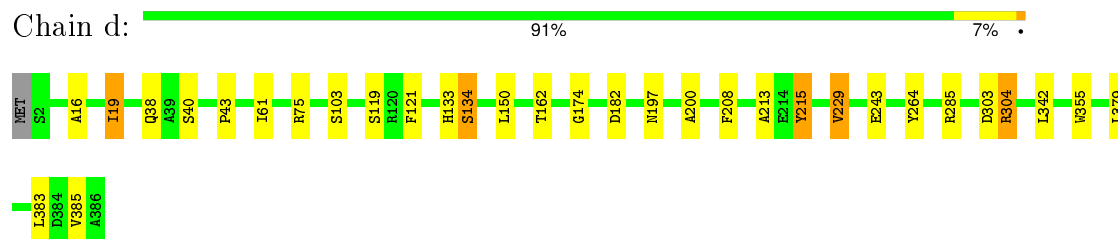
- Molecule 1: sheath



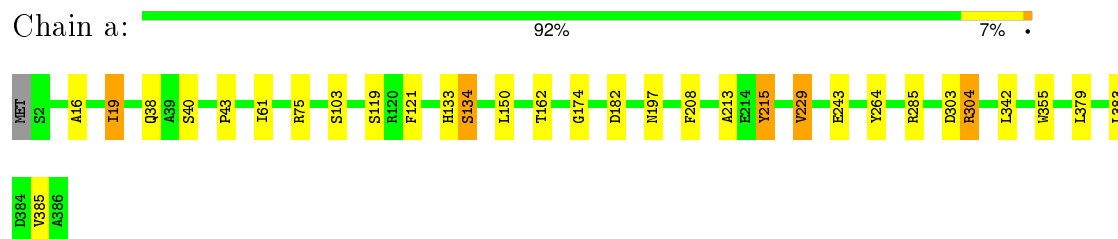
- Molecule 1: sheath



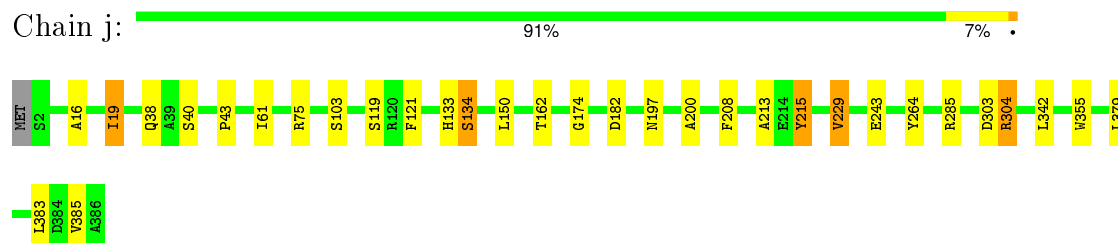
- Molecule 1: sheath



- Molecule 1: sheath

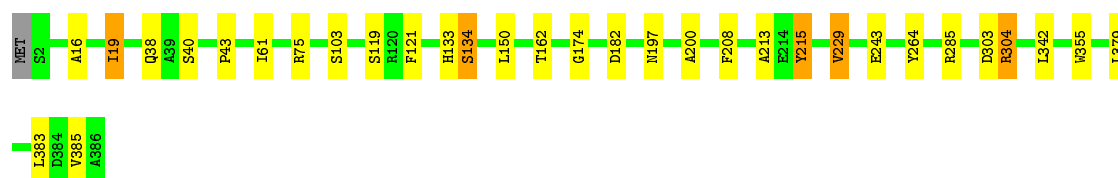


- Molecule 1: sheath



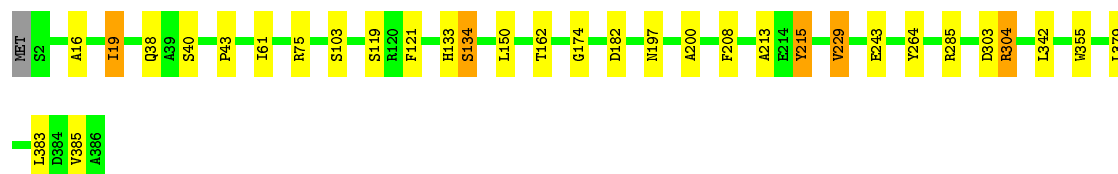
- Molecule 1: sheath

Chain g:  91% 7% .



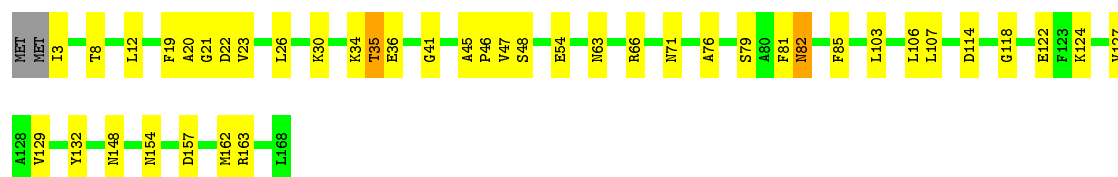
- Molecule 1: sheath

Chain m:  91% 7% .



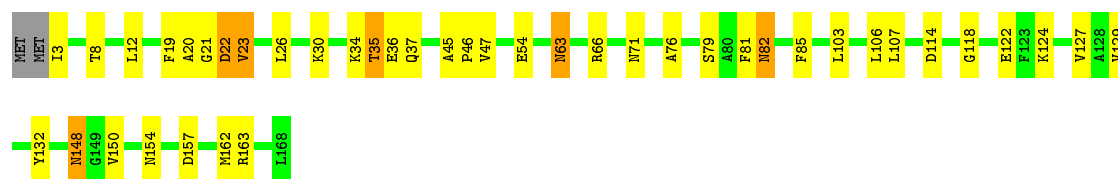
- Molecule 2: tube

Chain S:  74% 24% ..



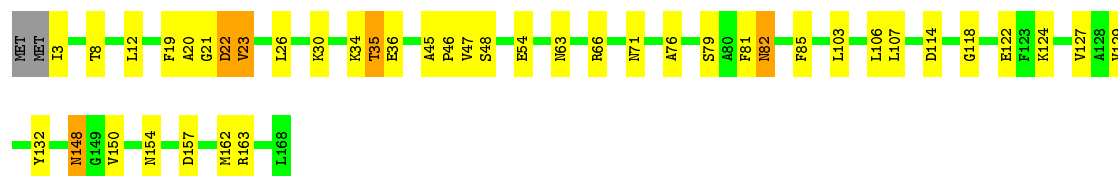
- Molecule 2: tube

Chain U:  74% 21% ..




- Molecule 2: tube

Chain T:  74% 22% ..



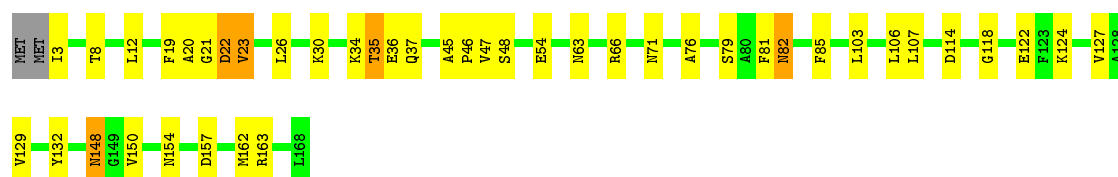
- Molecule 2: tube

Chain W:  74% 23% ..



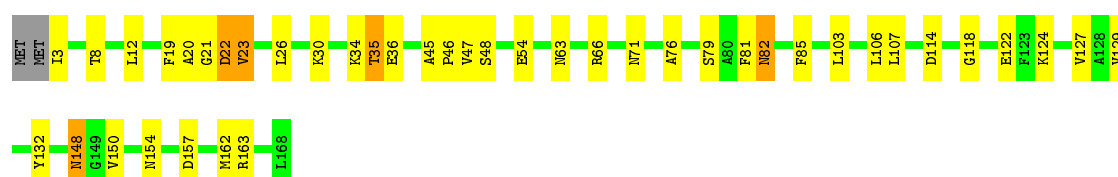
- Molecule 2: tube

Chain V: 73% 23%



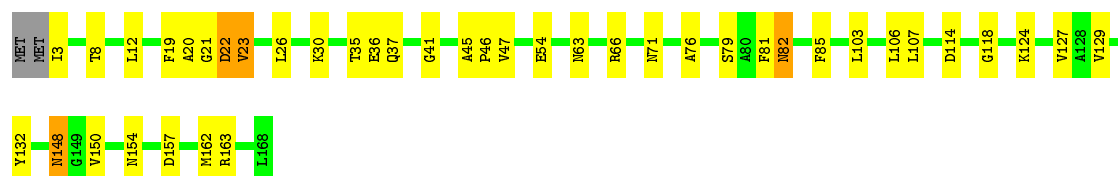
- Molecule 2: tube

Chain Z: 74% 22%



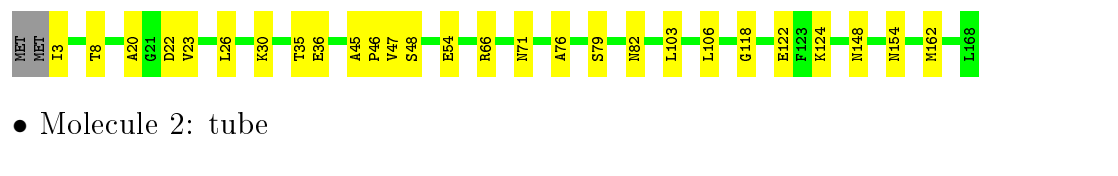
- Molecule 2: tube

Chain Y: 74% 22%



- Molecule 2: tube


Chain e: 83% 16%



- Molecule 2: tube


Chain b: 83% 16%

- Molecule 2: tube

Chain k:  82% 17%




- Molecule 2: tube

Chain h:  83% 16%




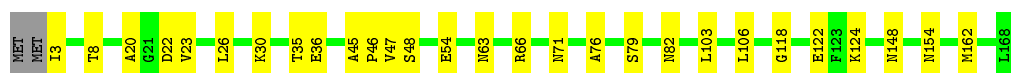
- Molecule 2: tube

Chain n:  83% 16%




- Molecule 2: tube

Chain c:  82% 17%




- Molecule 2: tube

Chain i:  83% 16%




- Molecule 2: tube

Chain f:  83% 16%




- Molecule 2: tube

Chain o:  83% 16%

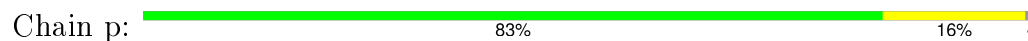


- Molecule 2: tube

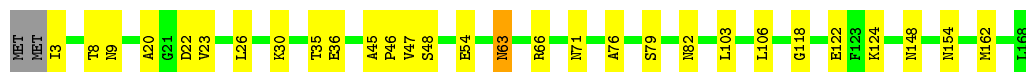
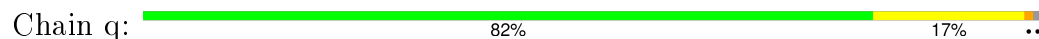
Chain l:  83% 16%



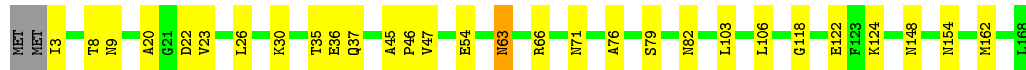
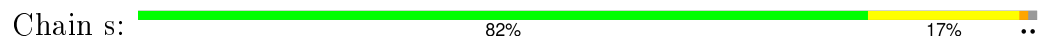
- Molecule 2: tube



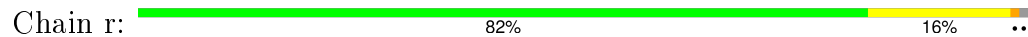
- Molecule 2: tube



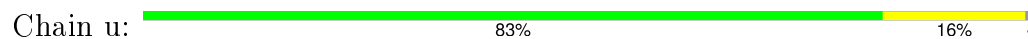
- Molecule 2: tube



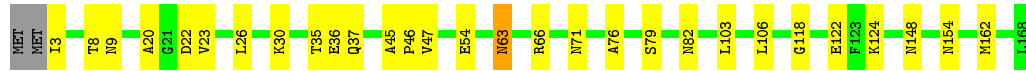
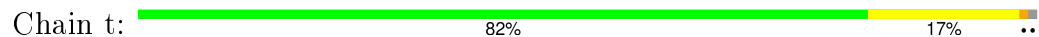
- Molecule 2: tube



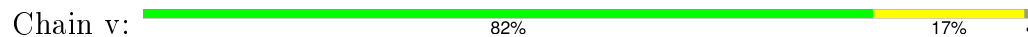
- Molecule 2: tube



- Molecule 2: tube



- Molecule 2: tube





## 4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	25	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	59000	Depositor
Image detector	KODAK SO-163 FILM	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  >2	RMSZ	# Z  >2
1	A	0.30	0/2955	0.53	0/4027
1	B	0.30	0/2955	0.53	0/4027
1	C	0.30	0/2955	0.53	0/4027
1	D	0.31	0/2955	0.54	0/4027
1	E	0.31	0/2955	0.54	0/4027
1	F	0.31	0/2955	0.54	0/4027
1	G	0.30	0/2955	0.53	0/4027
1	H	0.40	2/2955 (0.1%)	0.53	0/4027
1	I	0.31	0/2955	0.54	0/4027
1	J	0.30	0/2955	0.53	0/4027
1	K	0.30	0/2955	0.54	0/4027
1	L	0.30	0/2955	0.53	0/4027
1	M	0.31	0/2955	0.53	0/4027
1	N	0.31	0/2955	0.53	0/4027
1	O	0.31	0/2955	0.53	0/4027
1	P	0.30	0/2955	0.53	0/4027
1	Q	0.31	0/2955	0.54	0/4027
1	R	0.31	0/2955	0.53	0/4027
1	X	0.31	0/2955	0.53	0/4027
1	a	0.31	0/2955	0.53	0/4027
1	d	0.30	0/2955	0.54	0/4027
1	g	0.31	0/2955	0.53	0/4027
1	j	0.31	0/2955	0.54	0/4027
1	m	0.30	0/2955	0.53	0/4027
2	S	0.38	0/1277	0.62	0/1724
2	T	0.39	0/1277	0.62	0/1724
2	U	0.38	0/1277	0.62	0/1724
2	V	0.37	0/1277	0.62	0/1724
2	W	0.38	0/1277	0.62	0/1724
2	Y	0.38	0/1277	0.62	0/1724
2	Z	0.38	0/1277	0.62	0/1724
2	b	0.37	0/1277	0.62	0/1724
2	c	0.37	0/1277	0.62	0/1724
2	e	0.38	0/1277	0.62	0/1724

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
2	f	0.37	0/1277	0.62	0/1724
2	h	0.37	0/1277	0.62	0/1724
2	i	0.37	0/1277	0.62	0/1724
2	k	0.38	0/1277	0.62	0/1724
2	l	0.37	0/1277	0.62	0/1724
2	n	0.38	0/1277	0.62	0/1724
2	o	0.36	0/1277	0.62	0/1724
2	p	0.37	0/1277	0.62	0/1724
2	q	0.58	4/1277 (0.3%)	0.62	0/1724
2	r	0.58	4/1277 (0.3%)	0.62	0/1724
2	s	0.57	4/1277 (0.3%)	0.62	0/1724
2	t	0.57	4/1277 (0.3%)	0.62	0/1724
2	u	0.48	2/1277 (0.2%)	0.62	0/1724
2	v	0.48	2/1277 (0.2%)	0.62	0/1724
All	All	0.35	22/101568 (0.0%)	0.56	0/138024

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	369	ASN	CG-ND2	-11.21	1.04	1.32
2	q	63	ASN	CG-ND2	-9.36	1.09	1.32
2	r	63	ASN	CG-ND2	-9.34	1.09	1.32
2	s	63	ASN	CG-ND2	-9.12	1.10	1.32
2	t	63	ASN	CG-ND2	-9.07	1.10	1.32
1	H	369	ASN	CG-OD1	-8.87	1.04	1.24
2	v	9	ASN	CG-ND2	-8.82	1.10	1.32
2	q	9	ASN	CG-ND2	-8.78	1.10	1.32
2	r	9	ASN	CG-ND2	-8.72	1.11	1.32
2	t	9	ASN	CG-ND2	-8.44	1.11	1.32
2	s	9	ASN	CG-ND2	-8.35	1.11	1.32
2	u	9	ASN	CG-ND2	-8.34	1.11	1.32
2	r	9	ASN	CG-OD1	-7.56	1.07	1.24
2	v	9	ASN	CG-OD1	-7.47	1.07	1.24
2	s	9	ASN	CG-OD1	-7.24	1.08	1.24
2	t	9	ASN	CG-OD1	-7.14	1.08	1.24
2	q	9	ASN	CG-OD1	-7.13	1.08	1.24
2	u	9	ASN	CG-OD1	-6.75	1.09	1.24
2	q	63	ASN	CG-OD1	-6.69	1.09	1.24
2	r	63	ASN	CG-OD1	-6.49	1.09	1.24
2	s	63	ASN	CG-OD1	-6.29	1.10	1.24
2	t	63	ASN	CG-OD1	-6.26	1.10	1.24

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	A	2897	0	2855	38	0
1	B	2897	0	2855	29	0
1	C	2897	0	2855	29	0
1	D	2897	0	2855	37	0
1	E	2897	0	2855	33	0
1	F	2897	0	2855	28	0
1	G	2897	0	2855	36	0
1	H	2897	0	2855	26	0
1	I	2897	0	2855	30	0
1	J	2897	0	2855	31	0
1	K	2897	0	2855	29	0
1	L	2897	0	2855	27	0
1	M	2897	0	2855	34	0
1	N	2897	0	2855	26	0
1	O	2897	0	2855	30	0
1	P	2897	0	2855	27	0
1	Q	2897	0	2855	29	0
1	R	2897	0	2855	26	0
1	X	2897	0	2855	25	0
1	a	2897	0	2855	0	0
1	d	2897	0	2855	0	0
1	g	2897	0	2855	0	0
1	j	2897	0	2855	0	0
1	m	2897	0	2855	0	0
2	S	1255	0	1246	13	0
2	T	1255	0	1246	14	0
2	U	1255	0	1246	13	0
2	V	1255	0	1246	13	0
2	W	1255	0	1246	11	0
2	Y	1255	0	1246	14	0
2	Z	1255	0	1246	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	b	1255	0	1246	0	0
2	c	1255	0	1246	0	0
2	e	1255	0	1246	0	0
2	f	1255	0	1246	0	0
2	h	1255	0	1246	0	0
2	i	1255	0	1246	0	0
2	k	1255	0	1246	0	0
2	l	1255	0	1246	0	0
2	n	1255	0	1246	0	0
2	o	1255	0	1246	0	0
2	p	1255	0	1246	0	0
2	q	1255	0	1246	0	0
2	r	1255	0	1246	0	0
2	s	1255	0	1246	0	0
2	t	1255	0	1246	0	0
2	u	1255	0	1246	0	0
2	v	1255	0	1246	0	0
All	All	99648	0	98424	597	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 4.

All (597) 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)
2:U:81:PHE:CE2	2:U:127:VAL:HG11	2.24	0.73
2:Y:81:PHE:CE2	2:Y:127:VAL:HG11	2.24	0.73
2:S:81:PHE:CE2	2:S:127:VAL:HG11	2.30	0.72
2:T:81:PHE:CE2	2:T:127:VAL:HG11	2.30	0.72
2:V:81:PHE:CE2	2:V:127:VAL:HG11	2.24	0.71
2:W:81:PHE:CE2	2:W:127:VAL:HG11	2.30	0.66
2:Z:81:PHE:CE2	2:Z:127:VAL:HG11	2.30	0.66
1:D:225:GLU:OE2	1:D:265:ARG:NH2	2.30	0.66
1:O:225:GLU:OE2	1:O:265:ARG:NH2	2.29	0.66
1:C:225:GLU:OE2	1:C:265:ARG:NH2	2.29	0.66
1:X:225:GLU:OE2	1:X:265:ARG:NH2	2.29	0.65
1:L:225:GLU:OE2	1:L:265:ARG:NH2	2.29	0.65
1:N:225:GLU:OE2	1:N:265:ARG:NH2	2.29	0.65
1:I:225:GLU:OE2	1:I:265:ARG:NH2	2.29	0.65
1:G:225:GLU:OE2	1:G:265:ARG:NH2	2.29	0.65
1:J:225:GLU:OE2	1:J:265:ARG:NH2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:225:GLU:OE2	1:F:265:ARG:NH2	2.29	0.65
1:B:225:GLU:OE2	1:B:265:ARG:NH2	2.30	0.65
1:M:225:GLU:OE2	1:M:265:ARG:NH2	2.30	0.65
1:A:225:GLU:OE2	1:A:265:ARG:NH2	2.30	0.65
1:H:225:GLU:OE2	1:H:265:ARG:NH2	2.30	0.65
1:R:225:GLU:OE2	1:R:265:ARG:NH2	2.29	0.65
1:P:225:GLU:OE2	1:P:265:ARG:NH2	2.30	0.65
1:Q:225:GLU:OE2	1:Q:265:ARG:NH2	2.29	0.65
1:E:225:GLU:OE2	1:E:265:ARG:NH2	2.30	0.64
1:K:225:GLU:OE2	1:K:265:ARG:NH2	2.30	0.64
1:J:225:GLU:N	1:J:225:GLU:OE1	2.32	0.63
1:K:225:GLU:OE1	1:K:225:GLU:N	2.32	0.63
1:D:225:GLU:N	1:D:225:GLU:OE1	2.32	0.63
1:Q:225:GLU:N	1:Q:225:GLU:OE1	2.32	0.63
1:H:225:GLU:N	1:H:225:GLU:OE1	2.32	0.63
1:P:225:GLU:N	1:P:225:GLU:OE1	2.32	0.63
1:E:225:GLU:N	1:E:225:GLU:OE1	2.32	0.63
1:C:225:GLU:OE1	1:C:225:GLU:N	2.32	0.63
1:I:225:GLU:OE1	1:I:225:GLU:N	2.32	0.63
1:G:225:GLU:N	1:G:225:GLU:OE1	2.32	0.63
1:X:225:GLU:N	1:X:225:GLU:OE1	2.32	0.63
1:L:225:GLU:OE1	1:L:225:GLU:N	2.32	0.63
1:F:225:GLU:OE1	1:F:225:GLU:N	2.32	0.63
1:A:225:GLU:N	1:A:225:GLU:OE1	2.32	0.63
1:M:225:GLU:OE1	1:M:225:GLU:N	2.32	0.62
1:O:225:GLU:N	1:O:225:GLU:OE1	2.32	0.62
1:R:225:GLU:OE1	1:R:225:GLU:N	2.32	0.62
2:U:63:ASN:O	2:U:63:ASN:ND2	2.31	0.62
1:N:225:GLU:OE1	1:N:225:GLU:N	2.32	0.62
1:B:225:GLU:OE1	1:B:225:GLU:N	2.32	0.62
2:T:107:LEU:HA	2:T:127:VAL:HG12	1.92	0.60
2:V:107:LEU:HA	2:V:127:VAL:HG12	1.82	0.60
2:W:63:ASN:O	2:W:63:ASN:ND2	2.35	0.60
2:Y:107:LEU:HA	2:Y:127:VAL:HG12	1.83	0.60
2:S:107:LEU:HA	2:S:127:VAL:HG12	1.93	0.60
2:V:63:ASN:ND2	2:V:63:ASN:O	2.34	0.60
1:B:126:ARG:NH1	1:B:292:ASP:OD1	2.35	0.60
1:K:126:ARG:NH1	1:K:292:ASP:OD1	2.35	0.60
1:J:126:ARG:NH1	1:J:292:ASP:OD1	2.35	0.60
1:C:126:ARG:NH1	1:C:292:ASP:OD1	2.35	0.60
1:L:126:ARG:NH1	1:L:292:ASP:OD1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ARG:NH1	1:A:292:ASP:OD1	2.35	0.59
1:G:126:ARG:NH1	1:G:292:ASP:OD1	2.35	0.59
2:Z:63:ASN:ND2	2:Z:63:ASN:O	2.35	0.59
1:N:126:ARG:NH1	1:N:292:ASP:OD1	2.35	0.59
1:D:126:ARG:NH1	1:D:292:ASP:OD1	2.35	0.59
2:Z:23:VAL:HG23	2:Y:41:GLY:HA3	1.84	0.59
1:X:126:ARG:NH1	1:X:292:ASP:OD1	2.35	0.59
2:Y:63:ASN:ND2	2:Y:63:ASN:O	2.35	0.59
1:I:126:ARG:NH1	1:I:292:ASP:OD1	2.35	0.59
1:Q:126:ARG:NH1	1:Q:292:ASP:OD1	2.35	0.59
1:G:89:GLU:OE1	1:G:89:GLU:N	2.36	0.59
1:A:89:GLU:OE1	1:A:89:GLU:N	2.36	0.59
1:O:126:ARG:NH1	1:O:292:ASP:OD1	2.35	0.59
2:T:63:ASN:ND2	2:T:63:ASN:O	2.35	0.59
1:D:89:GLU:N	1:D:89:GLU:OE1	2.36	0.59
1:Q:89:GLU:N	1:Q:89:GLU:OE1	2.36	0.59
1:F:126:ARG:NH1	1:F:292:ASP:OD1	2.35	0.59
1:M:126:ARG:NH1	1:M:292:ASP:OD1	2.35	0.59
1:H:126:ARG:NH1	1:H:292:ASP:OD1	2.35	0.59
1:H:89:GLU:N	1:H:89:GLU:OE1	2.36	0.59
1:J:89:GLU:N	1:J:89:GLU:OE1	2.36	0.59
1:E:126:ARG:NH1	1:E:292:ASP:OD1	2.35	0.59
1:C:89:GLU:OE1	1:C:89:GLU:N	2.36	0.59
1:K:89:GLU:N	1:K:89:GLU:OE1	2.36	0.59
1:X:89:GLU:OE1	1:X:89:GLU:N	2.36	0.59
2:U:107:LEU:HA	2:U:127:VAL:HG12	1.84	0.59
2:S:19:PHE:O	2:S:21:GLY:N	2.36	0.59
1:R:126:ARG:NH1	1:R:292:ASP:OD1	2.35	0.59
1:M:89:GLU:OE1	1:M:89:GLU:N	2.36	0.59
1:F:89:GLU:N	1:F:89:GLU:OE1	2.36	0.59
1:N:89:GLU:N	1:N:89:GLU:OE1	2.36	0.59
1:R:89:GLU:N	1:R:89:GLU:OE1	2.36	0.59
2:S:41:GLY:HA3	2:Y:23:VAL:HG23	87.17	0.58
1:E:89:GLU:N	1:E:89:GLU:OE1	2.36	0.58
1:P:126:ARG:NH1	1:P:292:ASP:OD1	2.35	0.58
1:I:89:GLU:OE1	1:I:89:GLU:N	2.36	0.58
1:P:89:GLU:OE1	1:P:89:GLU:N	2.36	0.58
2:V:19:PHE:O	2:V:21:GLY:N	2.37	0.58
1:B:89:GLU:N	1:B:89:GLU:OE1	2.36	0.58
1:L:89:GLU:OE1	1:L:89:GLU:N	2.36	0.58
2:W:19:PHE:O	2:W:21:GLY:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:89:GLU:OE1	1:O:89:GLU:N	2.36	0.58
2:T:19:PHE:O	2:T:21:GLY:N	2.37	0.58
2:U:19:PHE:O	2:U:21:GLY:N	2.37	0.58
2:S:63:ASN:O	2:S:63:ASN:ND2	2.35	0.58
2:Y:19:PHE:O	2:Y:21:GLY:N	2.36	0.58
2:Z:19:PHE:O	2:Z:21:GLY:N	2.37	0.56
1:A:26:VAL:HG23	1:A:125:PRO:HA	1.90	0.55
1:D:26:VAL:HG23	1:D:125:PRO:HA	1.89	0.55
1:P:26:VAL:HG23	1:P:125:PRO:HA	1.89	0.55
1:J:26:VAL:HG23	1:J:125:PRO:HA	1.89	0.55
1:F:26:VAL:HG23	1:F:125:PRO:HA	1.89	0.55
1:I:26:VAL:HG23	1:I:125:PRO:HA	1.90	0.54
1:X:26:VAL:HG23	1:X:125:PRO:HA	1.89	0.54
1:G:26:VAL:HG23	1:G:125:PRO:HA	1.90	0.54
1:B:26:VAL:HG23	1:B:125:PRO:HA	1.89	0.54
1:E:26:VAL:HG23	1:E:125:PRO:HA	1.89	0.54
1:M:26:VAL:HG23	1:M:125:PRO:HA	1.89	0.54
1:O:26:VAL:HG23	1:O:125:PRO:HA	1.90	0.54
1:L:26:VAL:HG23	1:L:125:PRO:HA	1.90	0.54
1:N:26:VAL:HG23	1:N:125:PRO:HA	1.89	0.54
1:H:26:VAL:HG23	1:H:125:PRO:HA	1.90	0.54
1:C:26:VAL:HG23	1:C:125:PRO:HA	1.90	0.54
1:K:26:VAL:HG23	1:K:125:PRO:HA	1.90	0.54
1:Q:26:VAL:HG23	1:Q:125:PRO:HA	1.90	0.54
1:R:26:VAL:HG23	1:R:125:PRO:HA	1.90	0.53
1:A:26:VAL:HG12	1:A:79:VAL:HB	1.93	0.52
1:J:382:VAL:HG23	1:J:383:LEU:HG	1.91	0.52
1:H:26:VAL:HG12	1:H:79:VAL:HB	1.92	0.52
1:Q:382:VAL:HG23	1:Q:383:LEU:HG	1.91	0.52
1:I:382:VAL:HG23	1:I:383:LEU:HG	1.91	0.52
1:D:382:VAL:HG23	1:D:383:LEU:HG	2.03	0.52
1:E:382:VAL:HG23	1:E:383:LEU:HG	1.92	0.52
1:L:382:VAL:HG23	1:L:383:LEU:HG	1.91	0.52
2:V:34:LYS:C	2:V:35:THR:HG1	2.17	0.51
1:D:26:VAL:HG12	1:D:79:VAL:HB	2.00	0.51
2:T:81:PHE:CZ	2:T:127:VAL:HG11	2.49	0.51
2:V:81:PHE:CZ	2:V:127:VAL:HG11	2.46	0.51
1:P:382:VAL:HG23	1:P:383:LEU:HG	1.93	0.51
1:G:382:VAL:HG23	1:G:383:LEU:HG	2.03	0.51
2:W:107:LEU:HA	2:W:127:VAL:HG12	1.93	0.50
2:Z:107:LEU:HA	2:Z:127:VAL:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:VAL:HG23	1:A:383:LEU:HG	1.93	0.50
1:O:26:VAL:HG12	1:O:79:VAL:HB	1.93	0.50
1:C:26:VAL:HG12	1:C:79:VAL:HB	1.92	0.50
1:I:26:VAL:HG12	1:I:79:VAL:HB	1.93	0.50
1:K:26:VAL:HG12	1:K:79:VAL:HB	1.92	0.50
2:Y:81:PHE:CZ	2:Y:127:VAL:HG11	2.46	0.49
2:S:81:PHE:CZ	2:S:127:VAL:HG11	2.50	0.49
2:S:157:ASP:OD2	2:S:163:ARG:NH2	2.45	0.49
2:U:157:ASP:OD2	2:U:163:ARG:NH2	2.46	0.49
1:P:129:VAL:HG23	1:P:201:SER:HB3	1.94	0.49
2:T:157:ASP:OD2	2:T:163:ARG:NH2	2.46	0.49
2:V:157:ASP:OD2	2:V:163:ARG:NH2	2.46	0.49
1:B:382:VAL:HG23	1:B:383:LEU:HG	1.94	0.49
1:P:118:LYS:O	1:P:119:SER:OG	2.29	0.49
1:K:382:VAL:HG23	1:K:383:LEU:HG	1.93	0.49
1:X:129:VAL:HG23	1:X:201:SER:HB3	1.95	0.49
1:G:129:VAL:HG23	1:G:201:SER:HB3	2.00	0.49
2:U:81:PHE:CZ	2:U:127:VAL:HG11	2.47	0.49
2:W:157:ASP:OD2	2:W:163:ARG:NH2	2.46	0.48
1:J:129:VAL:HG23	1:J:201:SER:HB3	2.00	0.48
1:D:129:VAL:HG23	1:D:201:SER:HB3	1.95	0.48
2:Z:157:ASP:OD2	2:Z:163:ARG:NH2	2.45	0.48
1:E:129:VAL:HG23	1:E:201:SER:HB3	1.95	0.48
2:Y:157:ASP:OD2	2:Y:163:ARG:NH2	2.46	0.48
1:Q:129:VAL:HG23	1:Q:201:SER:HB3	1.95	0.48
2:T:63:ASN:H	2:T:63:ASN:HD22	4.01	0.47
1:F:129:VAL:HG23	1:F:201:SER:HB3	1.95	0.47
1:A:129:VAL:HG23	1:A:201:SER:HB3	1.96	0.47
1:N:129:VAL:HG23	1:N:201:SER:HB3	1.96	0.47
2:W:82:ASN:OD1	2:W:82:ASN:N	2.48	0.47
2:W:81:PHE:CZ	2:W:127:VAL:HG11	2.49	0.47
2:S:34:LYS:C	2:S:35:THR:HG1	2.22	0.47
2:U:34:LYS:C	2:U:35:THR:HG1	2.24	0.47
2:T:12:LEU:HD23	2:T:85:PHE:CD2	2.50	0.47
2:U:12:LEU:HD23	2:U:85:PHE:CD2	2.49	0.47
2:S:12:LEU:HD23	2:S:85:PHE:CD2	2.50	0.47
2:T:34:LYS:C	2:T:35:THR:HG1	2.18	0.47
2:Z:12:LEU:HD23	2:Z:85:PHE:CD2	2.50	0.47
2:U:82:ASN:N	2:U:82:ASN:OD1	2.47	0.47
2:Z:81:PHE:CZ	2:Z:127:VAL:HG11	2.49	0.47
2:W:12:LEU:HD23	2:W:85:PHE:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:12:LEU:HD23	2:V:85:PHE:CD2	2.50	0.46
2:S:82:ASN:OD1	2:S:82:ASN:N	2.48	0.46
2:V:82:ASN:N	2:V:82:ASN:OD1	2.48	0.46
1:R:178:LEU:O	1:R:271:THR:OG1	2.33	0.46
1:X:178:LEU:O	1:X:271:THR:OG1	2.34	0.46
1:J:178:LEU:O	1:J:271:THR:OG1	2.33	0.46
2:Y:82:ASN:N	2:Y:82:ASN:OD1	2.47	0.46
2:T:82:ASN:OD1	2:T:82:ASN:N	2.48	0.46
2:Z:82:ASN:OD1	2:Z:82:ASN:N	2.48	0.46
2:Y:12:LEU:HD23	2:Y:85:PHE:CD2	2.50	0.46
1:D:118:LYS:O	1:D:119:SER:OG	2.28	0.46
1:C:178:LEU:O	1:C:271:THR:OG1	2.34	0.46
1:K:178:LEU:O	1:K:271:THR:OG1	2.34	0.46
1:L:118:LYS:O	1:L:119:SER:OG	2.29	0.46
2:Z:129:VAL:HG11	2:Z:132:TYR:HB2	1.98	0.46
1:Q:178:LEU:O	1:Q:271:THR:OG1	2.33	0.46
2:S:63:ASN:H	2:S:63:ASN:HD22	4.01	0.45
1:B:178:LEU:O	1:B:271:THR:OG1	2.34	0.45
1:A:178:LEU:O	1:A:271:THR:OG1	2.34	0.45
1:M:118:LYS:O	1:M:119:SER:OG	2.30	0.45
1:M:178:LEU:O	1:M:271:THR:OG1	2.34	0.45
1:D:178:LEU:O	1:D:271:THR:OG1	2.34	0.45
1:H:118:LYS:O	1:H:119:SER:OG	2.29	0.45
1:D:382:VAL:HG21	1:K:332:ILE:HB	99.79	0.45
1:H:208:PHE:CE2	1:H:221:PRO:HG3	2.52	0.45
1:J:118:LYS:O	1:J:119:SER:OG	2.29	0.45
1:H:178:LEU:O	1:H:271:THR:OG1	2.35	0.45
2:Z:34:LYS:C	2:Z:35:THR:HG1	2.18	0.45
1:J:208:PHE:CE2	1:J:221:PRO:HG3	2.52	0.45
1:E:178:LEU:O	1:E:271:THR:OG1	2.34	0.45
1:B:382:VAL:HG21	1:L:332:ILE:HB	1.98	0.45
1:P:208:PHE:CE2	1:P:221:PRO:HG3	2.52	0.45
1:F:178:LEU:O	1:F:271:THR:OG1	2.35	0.45
2:W:129:VAL:HG11	2:W:132:TYR:HB2	1.98	0.45
1:Q:208:PHE:CE2	1:Q:221:PRO:HG3	2.52	0.45
1:B:332:ILE:HB	1:K:382:VAL:HG21	1.99	0.45
2:U:129:VAL:HG11	2:U:132:TYR:HB2	1.99	0.45
1:J:214:GLU:O	1:J:215:TYR:CG	2.70	0.45
1:J:314:VAL:HG11	1:J:355:TRP:CZ2	2.52	0.45
1:O:178:LEU:O	1:O:271:THR:OG1	2.34	0.45
2:Z:114:ASP:N	2:Z:114:ASP:OD1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:114:ASP:OD1	2:T:114:ASP:N	2.50	0.45
1:O:332:ILE:HB	1:J:382:VAL:HG21	141.97	0.45
1:N:314:VAL:HG11	1:N:355:TRP:CZ2	2.52	0.45
1:A:214:GLU:O	1:A:215:TYR:CG	2.71	0.45
2:U:114:ASP:OD1	2:U:114:ASP:N	2.50	0.45
1:C:314:VAL:HG11	1:C:355:TRP:CZ2	2.52	0.44
1:M:208:PHE:CE2	1:M:221:PRO:HG3	2.52	0.44
1:R:208:PHE:CE2	1:R:221:PRO:HG3	2.52	0.44
2:V:114:ASP:OD1	2:V:114:ASP:N	2.51	0.44
1:I:208:PHE:CE2	1:I:221:PRO:HG3	2.53	0.44
1:O:214:GLU:O	1:O:215:TYR:CG	2.70	0.44
1:P:214:GLU:O	1:P:215:TYR:CG	2.70	0.44
1:L:214:GLU:O	1:L:215:TYR:CG	2.70	0.44
1:B:214:GLU:O	1:B:215:TYR:CG	2.70	0.44
1:O:129:VAL:HG23	1:O:201:SER:HB3	2.00	0.44
1:C:129:VAL:HG23	1:C:201:SER:HB3	1.99	0.44
1:G:163:ASP:OD2	1:G:234:ARG:NH1	2.51	0.44
1:F:332:ILE:HB	1:Q:382:VAL:HG21	1.99	0.44
1:N:178:LEU:O	1:N:271:THR:OG1	2.34	0.44
1:R:129:VAL:HG23	1:R:201:SER:HB3	1.99	0.44
1:L:314:VAL:HG11	1:L:355:TRP:CZ2	2.52	0.44
1:P:178:LEU:O	1:P:271:THR:OG1	2.35	0.44
1:A:314:VAL:HG11	1:A:355:TRP:CZ2	2.54	0.44
1:H:314:VAL:HG11	1:H:355:TRP:CZ2	2.53	0.44
1:I:214:GLU:O	1:I:215:TYR:CG	2.70	0.44
1:C:214:GLU:O	1:C:215:TYR:CG	2.70	0.44
1:P:314:VAL:HG11	1:P:355:TRP:CZ2	2.53	0.44
1:K:208:PHE:CE2	1:K:221:PRO:HG3	2.52	0.44
1:X:208:PHE:CE2	1:X:221:PRO:HG3	2.53	0.44
1:R:163:ASP:OD2	1:R:234:ARG:NH1	2.51	0.44
1:D:214:GLU:O	1:D:215:TYR:CG	2.71	0.44
1:X:214:GLU:O	1:X:215:TYR:CG	2.70	0.44
2:S:114:ASP:OD1	2:S:114:ASP:N	2.50	0.44
1:J:38:GLN:O	1:J:40:SER:N	2.51	0.44
1:A:382:VAL:HG21	1:H:332:ILE:HB	2.00	0.44
1:H:163:ASP:OD2	1:H:234:ARG:NH1	2.51	0.44
1:K:163:ASP:OD2	1:K:234:ARG:NH1	2.51	0.44
1:E:163:ASP:OD2	1:E:234:ARG:NH1	2.51	0.44
1:G:214:GLU:O	1:G:215:TYR:CG	2.70	0.44
1:K:214:GLU:O	1:K:215:TYR:CG	2.71	0.44
1:E:214:GLU:O	1:E:215:TYR:CG	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:208:PHE:CE2	1:L:221:PRO:HG3	2.52	0.44
1:I:178:LEU:O	1:I:271:THR:OG1	2.35	0.44
2:Y:129:VAL:HG11	2:Y:132:TYR:HB2	2.00	0.44
1:G:208:PHE:CE2	1:G:221:PRO:HG3	2.53	0.44
1:N:214:GLU:O	1:N:215:TYR:CG	2.70	0.44
1:X:163:ASP:OD2	1:X:234:ARG:NH1	2.51	0.44
1:G:382:VAL:HG21	1:M:332:ILE:HB	83.29	0.44
1:Q:163:ASP:OD2	1:Q:234:ARG:NH1	2.51	0.44
1:M:163:ASP:OD2	1:M:234:ARG:NH1	2.51	0.44
1:N:208:PHE:CE2	1:N:221:PRO:HG3	2.53	0.44
1:C:38:GLN:O	1:C:40:SER:N	2.51	0.44
1:E:208:PHE:CE2	1:E:221:PRO:HG3	2.53	0.44
1:J:163:ASP:OD2	1:J:234:ARG:NH1	2.51	0.44
1:I:38:GLN:O	1:I:40:SER:N	2.51	0.44
1:D:336:VAL:HG22	1:D:357:ILE:HG23	2.00	0.44
1:H:129:VAL:HG23	1:H:201:SER:HB3	2.00	0.44
1:F:163:ASP:OD2	1:F:234:ARG:NH1	2.51	0.43
1:B:314:VAL:HG11	1:B:355:TRP:CZ2	2.53	0.43
1:M:38:GLN:O	1:M:40:SER:N	2.51	0.43
1:F:382:VAL:HG21	1:R:332:ILE:HB	2.00	0.43
1:E:336:VAL:HG22	1:E:357:ILE:HG23	2.00	0.43
1:C:163:ASP:OD2	1:C:234:ARG:NH1	2.51	0.43
1:I:314:VAL:HG11	1:I:355:TRP:CZ2	2.53	0.43
1:D:208:PHE:CE2	1:D:221:PRO:HG3	2.53	0.43
1:G:38:GLN:O	1:G:40:SER:N	2.51	0.43
1:A:38:GLN:O	1:A:40:SER:N	2.51	0.43
1:R:214:GLU:O	1:R:215:TYR:CG	2.70	0.43
1:L:129:VAL:HG23	1:L:201:SER:HB3	2.01	0.43
1:D:38:GLN:O	1:D:40:SER:N	2.51	0.43
1:A:208:PHE:CE2	1:A:221:PRO:HG3	2.54	0.43
1:E:382:VAL:HG21	1:N:332:ILE:HB	1.98	0.43
1:Q:38:GLN:O	1:Q:40:SER:N	2.51	0.43
1:A:163:ASP:OD2	1:A:234:ARG:NH1	2.51	0.43
1:C:208:PHE:CE2	1:C:221:PRO:HG3	2.53	0.43
1:M:214:GLU:O	1:M:215:TYR:CG	2.71	0.43
1:F:208:PHE:CE2	1:F:221:PRO:HG3	2.53	0.43
1:R:314:VAL:HG11	1:R:355:TRP:CZ2	2.53	0.43
1:C:332:ILE:HB	1:I:382:VAL:HG21	1.99	0.43
1:I:163:ASP:OD2	1:I:234:ARG:NH1	2.51	0.43
1:B:208:PHE:CE2	1:B:221:PRO:HG3	2.53	0.43
1:X:38:GLN:O	1:X:40:SER:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:38:GLN:O	1:O:40:SER:N	2.51	0.43
1:O:336:VAL:HG22	1:O:357:ILE:HG23	2.01	0.43
1:N:336:VAL:HG22	1:N:357:ILE:HG23	2.00	0.43
1:I:336:VAL:HG22	1:I:357:ILE:HG23	2.00	0.43
1:X:314:VAL:HG11	1:X:355:TRP:CZ2	2.53	0.43
1:Q:336:VAL:HG22	1:Q:357:ILE:HG23	2.00	0.43
1:M:26:VAL:HG12	1:M:79:VAL:HB	2.01	0.43
1:O:163:ASP:OD2	1:O:234:ARG:NH1	2.51	0.43
1:B:163:ASP:OD2	1:B:234:ARG:NH1	2.51	0.43
1:K:129:VAL:HG23	1:K:201:SER:HB3	2.01	0.43
1:L:38:GLN:O	1:L:40:SER:N	2.51	0.43
1:G:178:LEU:O	1:G:271:THR:OG1	2.34	0.43
1:Q:214:GLU:O	1:Q:215:TYR:CG	2.70	0.43
1:G:59:PHE:CG	1:G:65:ILE:HG21	2.53	0.43
1:D:163:ASP:OD2	1:D:234:ARG:NH1	2.51	0.43
2:W:34:LYS:C	2:W:35:THR:HG1	2.19	0.43
1:E:150:LEU:HA	1:M:239:LEU:CD2	2.48	0.43
1:D:162:THR:OG1	1:D:163:ASP:N	2.53	0.43
1:A:336:VAL:HG22	1:A:357:ILE:HG23	2.00	0.43
1:B:38:GLN:O	1:B:40:SER:N	2.51	0.43
1:G:150:LEU:HA	1:X:239:LEU:CD2	2.49	0.43
1:N:163:ASP:OD2	1:N:234:ARG:NH1	2.51	0.43
1:B:162:THR:OG1	1:B:163:ASP:N	2.52	0.43
1:R:336:VAL:HG22	1:R:357:ILE:HG23	2.00	0.43
1:L:178:LEU:O	1:L:271:THR:OG1	2.36	0.43
1:Q:59:PHE:CG	1:Q:65:ILE:HG21	2.54	0.43
1:A:380:THR:HG22	1:C:345:ALA:HB2	131.56	0.43
1:A:59:PHE:CG	1:A:65:ILE:HG21	2.54	0.43
1:C:382:VAL:HG21	1:J:332:ILE:HB	2.01	0.43
1:A:332:ILE:HB	1:G:382:VAL:HG21	2.01	0.43
1:F:162:THR:OG1	1:F:163:ASP:N	2.52	0.43
1:P:162:THR:OG1	1:P:163:ASP:N	2.52	0.43
1:P:163:ASP:OD2	1:P:234:ARG:NH1	2.51	0.43
1:X:162:THR:OG1	1:X:163:ASP:N	2.52	0.43
1:B:129:VAL:HG23	1:B:201:SER:HB3	2.01	0.43
1:F:59:PHE:CG	1:F:65:ILE:HG21	2.54	0.43
1:O:380:THR:HG22	1:P:345:ALA:HB2	2.01	0.43
1:F:214:GLU:O	1:F:215:TYR:CG	2.70	0.43
1:F:314:VAL:HG11	1:F:355:TRP:CZ2	2.54	0.43
1:A:118:LYS:O	1:A:119:SER:OG	2.28	0.43
1:A:150:LEU:HA	1:G:239:LEU:CD2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:150:LEU:HA	1:Q:239:LEU:CD2	2.49	0.43
1:L:163:ASP:OD2	1:L:234:ARG:NH1	2.52	0.43
1:Q:187:VAL:HG23	1:Q:229:VAL:HA	2.00	0.43
1:H:59:PHE:CG	1:H:65:ILE:HG21	2.54	0.43
1:M:59:PHE:CG	1:M:65:ILE:HG21	2.54	0.43
1:N:38:GLN:O	1:N:40:SER:N	2.51	0.43
1:P:336:VAL:HG22	1:P:357:ILE:HG23	2.01	0.43
1:H:214:GLU:O	1:H:215:TYR:CG	2.71	0.43
1:G:239:LEU:CD2	1:M:150:LEU:HA	107.56	0.43
1:G:26:VAL:HG12	1:G:79:VAL:HB	2.00	0.43
1:L:26:VAL:HG12	1:L:79:VAL:HB	2.00	0.43
1:K:162:THR:OG1	1:K:163:ASP:N	2.52	0.43
1:K:38:GLN:O	1:K:40:SER:N	2.51	0.43
1:G:332:ILE:HB	1:X:382:VAL:HG21	2.01	0.43
1:O:208:PHE:CE2	1:O:221:PRO:HG3	2.54	0.43
1:M:336:VAL:HG22	1:M:357:ILE:HG23	2.06	0.43
1:R:38:GLN:O	1:R:40:SER:N	2.51	0.43
1:M:314:VAL:HG11	1:M:355:TRP:CZ2	2.54	0.43
1:M:129:VAL:HG23	1:M:201:SER:HB3	2.01	0.43
2:W:114:ASP:N	2:W:114:ASP:OD1	2.51	0.43
1:O:59:PHE:CG	1:O:65:ILE:HG21	2.54	0.43
1:M:239:LEU:CD2	1:Q:150:LEU:HA	88.43	0.42
1:R:26:VAL:HG12	1:R:79:VAL:HB	2.01	0.42
1:G:162:THR:OG1	1:G:163:ASP:N	2.52	0.42
1:M:162:THR:OG1	1:M:163:ASP:N	2.52	0.42
1:P:59:PHE:CG	1:P:65:ILE:HG21	2.54	0.42
1:C:203:TYR:CE1	1:C:229:VAL:HG12	2.54	0.42
1:G:336:VAL:HG22	1:G:357:ILE:HG23	2.01	0.42
1:D:239:LEU:CD2	1:K:150:LEU:HA	114.71	0.42
1:Q:26:VAL:HG12	1:Q:79:VAL:HB	2.01	0.42
1:J:162:THR:OG1	1:J:163:ASP:N	2.52	0.42
1:I:129:VAL:HG23	1:I:201:SER:HB3	2.01	0.42
1:J:59:PHE:CG	1:J:65:ILE:HG21	2.54	0.42
1:D:59:PHE:CG	1:D:65:ILE:HG21	2.54	0.42
1:K:344:SER:OG	1:K:345:ALA:N	2.53	0.42
1:K:59:PHE:CG	1:K:65:ILE:HG21	2.54	0.42
1:P:38:GLN:O	1:P:40:SER:N	2.51	0.42
1:H:38:GLN:O	1:H:40:SER:N	2.51	0.42
1:E:203:TYR:CE1	1:E:229:VAL:HG12	2.54	0.42
1:G:314:VAL:HG11	1:G:355:TRP:CZ2	2.56	0.42
1:C:59:PHE:CG	1:C:65:ILE:HG21	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:59:PHE:CG	1:I:65:ILE:HG21	2.54	0.42
1:F:38:GLN:O	1:F:40:SER:N	2.51	0.42
1:X:59:PHE:CG	1:X:65:ILE:HG21	2.54	0.42
1:L:59:PHE:CG	1:L:65:ILE:HG21	2.54	0.42
1:R:203:TYR:CE1	1:R:229:VAL:HG12	2.55	0.42
1:M:382:VAL:HG21	1:Q:332:ILE:HB	73.35	0.42
1:J:344:SER:OG	1:J:345:ALA:N	2.53	0.42
1:G:203:TYR:CE1	1:G:229:VAL:HG12	2.54	0.42
2:Z:22:ASP:O	2:Z:23:VAL:HG13	2.20	0.42
1:A:239:LEU:CD2	1:H:150:LEU:HA	2.50	0.42
1:B:26:VAL:HG12	1:B:79:VAL:HB	2.00	0.42
1:G:344:SER:OG	1:G:345:ALA:N	2.53	0.42
1:A:344:SER:OG	1:A:345:ALA:N	2.53	0.42
1:F:365:ALA:HB2	1:R:306:ILE:CG1	2.49	0.42
1:K:203:TYR:CE1	1:K:229:VAL:HG12	2.54	0.42
1:R:59:PHE:CG	1:R:65:ILE:HG21	2.54	0.42
1:I:344:SER:OG	1:I:345:ALA:N	2.53	0.42
1:N:203:TYR:CE1	1:N:229:VAL:HG12	2.55	0.42
1:J:336:VAL:HG22	1:J:357:ILE:HG23	2.00	0.42
1:L:336:VAL:HG22	1:L:357:ILE:HG23	2.00	0.42
1:J:126:ARG:NH2	1:J:150:LEU:O	2.53	0.42
1:A:239:LEU:CD2	1:I:150:LEU:HA	146.84	0.42
1:R:162:THR:OG1	1:R:163:ASP:N	2.52	0.42
1:Q:344:SER:OG	1:Q:345:ALA:N	2.52	0.42
1:E:59:PHE:CG	1:E:65:ILE:HG21	2.54	0.42
1:F:306:ILE:CG1	1:Q:365:ALA:HB2	2.50	0.42
1:B:150:LEU:HA	1:K:239:LEU:CD2	2.49	0.42
1:M:126:ARG:NH2	1:M:150:LEU:O	2.53	0.42
1:Q:162:THR:OG1	1:Q:163:ASP:N	2.52	0.42
1:E:332:ILE:HB	1:M:382:VAL:HG21	2.01	0.42
1:O:203:TYR:CE1	1:O:229:VAL:HG12	2.55	0.42
1:O:344:SER:OG	1:O:345:ALA:N	2.53	0.42
1:K:314:VAL:HG11	1:K:355:TRP:CZ2	2.54	0.42
2:Y:114:ASP:OD1	2:Y:114:ASP:N	2.50	0.42
1:X:344:SER:OG	1:X:345:ALA:N	2.53	0.42
1:O:150:LEU:HA	1:J:239:LEU:CD2	156.51	0.42
1:N:187:VAL:HG23	1:N:229:VAL:HA	2.01	0.42
1:D:344:SER:OG	1:D:345:ALA:N	2.53	0.42
1:B:59:PHE:CG	1:B:65:ILE:HG21	2.54	0.42
1:M:344:SER:OG	1:M:345:ALA:N	2.53	0.42
1:D:314:VAL:HG11	1:D:355:TRP:CZ2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:86:GLU:N	1:J:86:GLU:OE2	2.53	0.42
1:K:336:VAL:HG22	1:K:357:ILE:HG23	2.00	0.42
1:E:126:ARG:NH2	1:E:150:LEU:O	2.53	0.42
1:R:126:ARG:NH2	1:R:150:LEU:O	2.53	0.42
2:T:22:ASP:O	2:T:23:VAL:HG13	2.20	0.42
1:L:162:THR:OG1	1:L:163:ASP:N	2.52	0.42
1:C:344:SER:OG	1:C:345:ALA:N	2.53	0.42
1:G:306:ILE:CG1	1:X:365:ALA:HB2	2.50	0.42
1:B:344:SER:OG	1:B:345:ALA:N	2.53	0.42
1:B:336:VAL:HG22	1:B:357:ILE:HG23	2.00	0.42
1:F:203:TYR:CE1	1:F:229:VAL:HG12	2.55	0.42
1:O:86:GLU:N	1:O:86:GLU:OE2	2.53	0.42
1:C:150:LEU:HA	1:I:239:LEU:CD2	2.49	0.42
1:G:126:ARG:NH2	1:G:150:LEU:O	2.53	0.42
1:C:162:THR:OG1	1:C:163:ASP:N	2.53	0.42
1:I:380:THR:HG22	1:J:345:ALA:HB2	2.02	0.42
1:Q:380:THR:HG22	1:R:345:ALA:HB2	2.02	0.42
1:D:132:GLY:O	1:D:134:SER:N	2.53	0.42
1:D:332:ILE:HB	1:O:382:VAL:HG21	2.01	0.42
1:G:290:VAL:HG23	1:G:325:LEU:HD13	2.10	0.42
1:N:59:PHE:CG	1:N:65:ILE:HG21	2.54	0.42
1:G:86:GLU:OE2	1:G:86:GLU:N	2.53	0.42
1:I:86:GLU:OE2	1:I:86:GLU:N	2.53	0.42
1:D:150:LEU:HA	1:O:239:LEU:CD2	2.49	0.42
1:I:162:THR:OG1	1:I:163:ASP:N	2.53	0.42
1:J:203:TYR:CE1	1:J:229:VAL:HG12	2.55	0.42
1:H:203:TYR:CE1	1:H:229:VAL:HG12	2.54	0.42
1:A:86:GLU:N	1:A:86:GLU:OE2	2.54	0.42
1:P:86:GLU:OE2	1:P:86:GLU:N	2.53	0.42
1:D:86:GLU:OE2	1:D:86:GLU:N	2.53	0.42
1:A:365:ALA:HB2	1:H:306:ILE:CG1	2.50	0.42
1:L:126:ARG:NH2	1:L:150:LEU:O	2.53	0.41
1:A:126:ARG:NH2	1:A:150:LEU:O	2.53	0.41
1:H:126:ARG:NH2	1:H:150:LEU:O	2.53	0.41
1:O:126:ARG:NH2	1:O:150:LEU:O	2.53	0.41
1:F:239:LEU:CD2	1:R:150:LEU:HA	2.50	0.41
1:P:26:VAL:HG12	1:P:79:VAL:HB	2.01	0.41
1:F:26:VAL:HG12	1:F:79:VAL:HB	2.01	0.41
1:E:26:VAL:HG12	1:E:79:VAL:HB	2.01	0.41
1:O:162:THR:OG1	1:O:163:ASP:N	2.52	0.41
1:H:162:THR:OG1	1:H:163:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:38:GLN:O	1:E:40:SER:N	2.51	0.41
1:A:306:ILE:CG1	1:G:365:ALA:HB2	2.50	0.41
1:G:365:ALA:HB2	1:M:306:ILE:CG1	90.75	0.41
1:J:132:GLY:O	1:J:134:SER:N	2.54	0.41
1:C:336:VAL:HG22	1:C:357:ILE:HG23	2.00	0.41
1:O:306:ILE:CG1	1:J:365:ALA:HB2	145.73	0.41
1:C:86:GLU:OE2	1:C:86:GLU:N	2.53	0.41
1:L:344:SER:OG	1:L:345:ALA:N	2.53	0.41
1:J:26:VAL:HG12	1:J:79:VAL:HB	2.01	0.41
1:N:26:VAL:HG12	1:N:79:VAL:HB	2.01	0.41
1:A:382:VAL:HG21	1:I:332:ILE:HB	122.22	0.41
1:C:132:GLY:O	1:C:134:SER:N	2.53	0.41
1:I:132:GLY:O	1:I:134:SER:N	2.53	0.41
1:N:344:SER:OG	1:N:345:ALA:N	2.53	0.41
1:X:86:GLU:OE2	1:X:86:GLU:N	2.53	0.41
1:B:126:ARG:NH2	1:B:150:LEU:O	2.53	0.41
1:P:126:ARG:NH2	1:P:150:LEU:O	2.53	0.41
1:N:126:ARG:NH2	1:N:150:LEU:O	2.53	0.41
1:D:126:ARG:NH2	1:D:150:LEU:O	2.53	0.41
1:F:132:GLY:O	1:F:134:SER:N	2.53	0.41
1:H:132:GLY:O	1:H:134:SER:N	2.53	0.41
1:P:344:SER:OG	1:P:345:ALA:N	2.53	0.41
1:M:86:GLU:OE2	1:M:86:GLU:N	2.54	0.41
1:N:86:GLU:OE2	1:N:86:GLU:N	2.53	0.41
1:Q:86:GLU:N	1:Q:86:GLU:OE2	2.53	0.41
2:Y:148:ASN:HB3	2:Y:150:VAL:HG23	2.02	0.41
1:D:239:LEU:CD2	1:P:150:LEU:HA	2.49	0.41
1:I:126:ARG:NH2	1:I:150:LEU:O	2.53	0.41
1:A:365:ALA:HB2	1:I:306:ILE:CG1	128.39	0.41
2:U:148:ASN:HB3	2:U:150:VAL:HG23	2.07	0.41
1:H:336:VAL:HG22	1:H:357:ILE:HG23	2.00	0.41
1:F:126:ARG:NH2	1:F:150:LEU:O	2.54	0.41
1:D:382:VAL:HG21	1:P:332:ILE:HB	2.01	0.41
1:N:132:GLY:O	1:N:134:SER:N	2.53	0.41
1:K:132:GLY:O	1:K:134:SER:N	2.54	0.41
1:A:162:THR:OG1	1:A:163:ASP:N	2.53	0.41
1:E:345:ALA:HB2	1:G:380:THR:HG22	92.95	0.41
1:B:365:ALA:HB2	1:L:306:ILE:CG1	2.50	0.41
1:E:132:GLY:O	1:E:134:SER:N	2.53	0.41
1:K:86:GLU:N	1:K:86:GLU:OE2	2.53	0.41
1:E:86:GLU:OE2	1:E:86:GLU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:ARG:NH2	1:C:150:LEU:O	2.53	0.41
2:V:22:ASP:O	2:V:23:VAL:HG13	2.20	0.41
1:E:187:VAL:HG23	1:E:229:VAL:HA	2.01	0.41
1:D:365:ALA:HB2	1:P:306:ILE:CG1	2.50	0.41
1:M:365:ALA:HB2	1:Q:306:ILE:CG1	76.21	0.41
1:N:199:PRO:O	1:N:200:ALA:HB3	2.21	0.41
1:A:290:VAL:HG23	1:A:325:LEU:HD13	2.01	0.41
1:X:203:TYR:CE1	1:X:229:VAL:HG12	2.55	0.41
1:A:132:GLY:O	1:A:134:SER:N	2.53	0.41
1:E:239:LEU:CD2	1:N:150:LEU:HA	2.50	0.41
1:X:126:ARG:NH2	1:X:150:LEU:O	2.53	0.41
1:Q:126:ARG:NH2	1:Q:150:LEU:O	2.53	0.41
1:X:26:VAL:HG12	1:X:79:VAL:HB	2.01	0.41
1:E:162:THR:OG1	1:E:163:ASP:N	2.53	0.41
1:E:344:SER:OG	1:E:345:ALA:N	2.53	0.41
1:H:344:SER:OG	1:H:345:ALA:N	2.53	0.41
1:D:365:ALA:HB2	1:K:306:ILE:CG1	105.37	0.41
1:F:345:ALA:HB2	1:M:380:THR:HG22	78.87	0.41
1:R:199:PRO:O	1:R:200:ALA:HB3	2.21	0.41
1:M:132:GLY:O	1:M:134:SER:N	2.54	0.41
1:D:306:ILE:CG1	1:O:365:ALA:HB2	2.51	0.41
1:R:132:GLY:O	1:R:134:SER:N	2.53	0.41
2:S:129:VAL:HG11	2:S:132:TYR:HB2	2.02	0.41
1:H:86:GLU:OE2	1:H:86:GLU:N	2.53	0.41
1:B:86:GLU:N	1:B:86:GLU:OE2	2.53	0.41
1:F:86:GLU:N	1:F:86:GLU:OE2	2.53	0.41
2:Y:22:ASP:O	2:Y:23:VAL:HG13	2.20	0.41
1:G:380:THR:HG22	1:H:345:ALA:HB2	2.02	0.41
1:X:187:VAL:HG23	1:X:229:VAL:HA	2.03	0.41
2:Z:148:ASN:HB3	2:Z:150:VAL:HG23	2.03	0.41
1:D:187:VAL:HG23	1:D:229:VAL:HA	2.02	0.41
1:C:306:ILE:CG1	1:I:365:ALA:HB2	2.50	0.41
1:O:199:PRO:O	1:O:200:ALA:HB3	2.21	0.41
1:C:239:LEU:CD2	1:J:150:LEU:HA	2.50	0.41
1:B:239:LEU:CD2	1:L:150:LEU:HA	2.50	0.41
2:U:22:ASP:O	2:U:23:VAL:HG13	2.21	0.41
1:O:132:GLY:O	1:O:134:SER:N	2.54	0.41
1:A:345:ALA:HB2	1:X:380:THR:HG22	2.03	0.41
1:D:203:TYR:CE1	1:D:229:VAL:HG12	2.56	0.41
1:C:199:PRO:O	1:C:200:ALA:HB3	2.21	0.41
1:P:199:PRO:O	1:P:200:ALA:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:199:PRO:O	1:L:200:ALA:HB3	2.21	0.41
1:E:314:VAL:HG11	1:E:355:TRP:CZ2	2.56	0.41
1:M:199:PRO:O	1:M:200:ALA:HB3	2.22	0.41
1:L:132:GLY:O	1:L:134:SER:N	2.54	0.41
1:Q:132:GLY:O	1:Q:134:SER:N	2.53	0.41
1:F:199:PRO:O	1:F:200:ALA:HB3	2.21	0.41
1:X:132:GLY:O	1:X:134:SER:N	2.53	0.41
1:L:86:GLU:OE2	1:L:86:GLU:N	2.53	0.41
1:D:199:PRO:O	1:D:200:ALA:HB3	2.22	0.41
1:O:382:VAL:HG23	1:O:383:LEU:HG	2.03	0.41
2:T:129:VAL:HG11	2:T:132:TYR:HB2	2.02	0.41
1:I:199:PRO:O	1:I:200:ALA:HB3	2.21	0.41
2:V:129:VAL:HG11	2:V:132:TYR:HB2	2.03	0.41
1:A:199:PRO:O	1:A:200:ALA:HB3	2.21	0.41
1:R:86:GLU:N	1:R:86:GLU:OE2	2.54	0.41
1:A:203:TYR:CE1	1:A:229:VAL:HG12	2.57	0.41
1:E:365:ALA:HB2	1:N:306:ILE:CG1	2.50	0.41
1:K:126:ARG:NH2	1:K:150:LEU:O	2.53	0.40
1:M:382:VAL:HG23	1:M:383:LEU:HG	2.04	0.40
1:F:344:SER:OG	1:F:345:ALA:N	2.53	0.40
2:V:148:ASN:HB3	2:V:150:VAL:HG23	2.03	0.40
1:D:290:VAL:HG23	1:D:325:LEU:HD13	2.10	0.40
1:M:203:TYR:CE1	1:M:229:VAL:HG12	2.56	0.40
1:P:132:GLY:O	1:P:134:SER:N	2.54	0.40
1:B:203:TYR:CE1	1:B:229:VAL:HG12	2.56	0.40
1:D:76:ALA:HB2	1:D:210:TRP:HB2	2.04	0.40
1:G:199:PRO:O	1:G:200:ALA:HB3	2.21	0.40
1:Q:314:VAL:HG11	1:Q:355:TRP:CZ2	2.56	0.40
1:G:132:GLY:O	1:G:134:SER:N	2.53	0.40
1:D:345:ALA:HB2	1:J:380:THR:HG22	146.80	0.40
1:O:76:ALA:HB2	1:O:210:TRP:HB2	2.04	0.40
1:I:76:ALA:HB2	1:I:210:TRP:HB2	2.04	0.40
1:E:199:PRO:O	1:E:200:ALA:HB3	2.21	0.40
1:E:17:ARG:HG2	1:R:337:TYR:CE2	2.56	0.40
1:J:199:PRO:O	1:J:200:ALA:HB3	2.21	0.40
1:K:380:THR:HG22	1:L:345:ALA:HB2	2.03	0.40
1:C:76:ALA:HB2	1:C:210:TRP:HB2	2.04	0.40
1:B:76:ALA:HB2	1:B:210:TRP:HB2	2.04	0.40
1:A:76:ALA:HB2	1:A:210:TRP:HB2	2.04	0.40
1:N:162:THR:OG1	1:N:163:ASP:N	2.53	0.40
1:B:132:GLY:O	1:B:134:SER:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:VAL:HG23	1:A:229:VAL:HA	2.04	0.40
2:T:148:ASN:HB3	2:T:150:VAL:HG23	2.07	0.40
1:E:290:VAL:HG23	1:E:325:LEU:HD13	2.04	0.40
1:E:76:ALA:HB2	1:E:210:TRP:HB2	2.04	0.40
1:M:76:ALA:HB2	1:M:210:TRP:HB2	2.04	0.40
1:G:76:ALA:HB2	1:G:210:TRP:HB2	2.04	0.40
1:B:306:ILE:CG1	1:K:365:ALA:HB2	2.50	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	A	383/386 (99%)	296 (77%)	68 (18%)	19 (5%)	3	27
1	B	383/386 (99%)	296 (77%)	68 (18%)	19 (5%)	3	27
1	C	383/386 (99%)	297 (78%)	67 (18%)	19 (5%)	3	27
1	D	383/386 (99%)	297 (78%)	67 (18%)	19 (5%)	3	27
1	E	383/386 (99%)	297 (78%)	67 (18%)	19 (5%)	3	27
1	F	383/386 (99%)	298 (78%)	67 (18%)	18 (5%)	3	29
1	G	383/386 (99%)	299 (78%)	65 (17%)	19 (5%)	3	27
1	H	383/386 (99%)	297 (78%)	67 (18%)	19 (5%)	3	27
1	I	383/386 (99%)	295 (77%)	69 (18%)	19 (5%)	3	27
1	J	383/386 (99%)	295 (77%)	69 (18%)	19 (5%)	3	27
1	K	383/386 (99%)	296 (77%)	68 (18%)	19 (5%)	3	27
1	L	383/386 (99%)	298 (78%)	66 (17%)	19 (5%)	3	27
1	M	383/386 (99%)	295 (77%)	69 (18%)	19 (5%)	3	27
1	N	383/386 (99%)	296 (77%)	68 (18%)	19 (5%)	3	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	383/386 (99%)	296 (77%)	68 (18%)	19 (5%)	3	27
1	P	383/386 (99%)	297 (78%)	67 (18%)	19 (5%)	3	27
1	Q	383/386 (99%)	298 (78%)	66 (17%)	19 (5%)	3	27
1	R	383/386 (99%)	298 (78%)	66 (17%)	19 (5%)	3	27
1	X	383/386 (99%)	296 (77%)	68 (18%)	19 (5%)	3	27
1	a	383/386 (99%)	297 (78%)	68 (18%)	18 (5%)	3	29
1	d	383/386 (99%)	295 (77%)	69 (18%)	19 (5%)	3	27
1	g	383/386 (99%)	297 (78%)	67 (18%)	19 (5%)	3	27
1	j	383/386 (99%)	296 (77%)	68 (18%)	19 (5%)	3	27
1	m	383/386 (99%)	298 (78%)	66 (17%)	19 (5%)	3	27
2	S	164/168 (98%)	113 (69%)	38 (23%)	13 (8%)	1	14
2	T	164/168 (98%)	114 (70%)	37 (23%)	13 (8%)	1	14
2	U	164/168 (98%)	114 (70%)	37 (23%)	13 (8%)	1	14
2	V	164/168 (98%)	114 (70%)	36 (22%)	14 (8%)	1	13
2	W	164/168 (98%)	114 (70%)	37 (23%)	13 (8%)	1	14
2	Y	164/168 (98%)	114 (70%)	38 (23%)	12 (7%)	1	16
2	Z	164/168 (98%)	114 (70%)	37 (23%)	13 (8%)	1	14
2	b	164/168 (98%)	114 (70%)	37 (23%)	13 (8%)	1	14
2	c	164/168 (98%)	114 (70%)	37 (23%)	13 (8%)	1	14
2	e	164/168 (98%)	114 (70%)	37 (23%)	13 (8%)	1	14
2	f	164/168 (98%)	114 (70%)	37 (23%)	13 (8%)	1	14
2	h	164/168 (98%)	114 (70%)	37 (23%)	13 (8%)	1	14
2	i	164/168 (98%)	114 (70%)	37 (23%)	13 (8%)	1	14
2	k	164/168 (98%)	114 (70%)	36 (22%)	14 (8%)	1	13
2	l	164/168 (98%)	114 (70%)	37 (23%)	13 (8%)	1	14
2	n	164/168 (98%)	114 (70%)	37 (23%)	13 (8%)	1	14
2	o	164/168 (98%)	114 (70%)	37 (23%)	13 (8%)	1	14
2	p	164/168 (98%)	114 (70%)	37 (23%)	13 (8%)	1	14
2	q	164/168 (98%)	114 (70%)	37 (23%)	13 (8%)	1	14
2	r	164/168 (98%)	114 (70%)	38 (23%)	12 (7%)	1	16
2	s	164/168 (98%)	114 (70%)	37 (23%)	13 (8%)	1	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	t	164/168 (98%)	114 (70%)	37 (23%)	13 (8%)	1	14
2	u	164/168 (98%)	114 (70%)	38 (23%)	12 (7%)	1	16
2	v	164/168 (98%)	114 (70%)	37 (23%)	13 (8%)	1	14
All	All	13128/13296 (99%)	9855 (75%)	2508 (19%)	765 (6%)	4	23

All (765) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	150	LEU
1	A	162	THR
1	A	215	TYR
1	A	229	VAL
1	A	303	ASP
2	S	20	ALA
2	S	148	ASN
1	B	150	LEU
1	B	162	THR
1	B	215	TYR
1	B	229	VAL
1	B	303	ASP
1	C	150	LEU
1	C	162	THR
1	C	215	TYR
1	C	229	VAL
1	C	303	ASP
1	D	150	LEU
1	D	162	THR
1	D	215	TYR
1	D	229	VAL
1	D	303	ASP
1	E	150	LEU
1	E	162	THR
1	E	215	TYR
1	E	229	VAL
1	E	303	ASP
1	F	150	LEU
1	F	162	THR
1	F	215	TYR
1	F	229	VAL
1	F	303	ASP
1	G	150	LEU

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Mol	Chain	Res	Type
1	G	162	THR
1	G	215	TYR
1	G	229	VAL
1	G	303	ASP
1	K	150	LEU
1	K	162	THR
1	K	215	TYR
1	K	229	VAL
1	K	303	ASP
1	I	150	LEU
1	I	162	THR
1	I	215	TYR
1	I	229	VAL
1	I	303	ASP
1	O	150	LEU
1	O	162	THR
1	O	215	TYR
1	O	229	VAL
1	O	303	ASP
1	M	150	LEU
1	M	162	THR
1	M	215	TYR
1	M	229	VAL
1	M	303	ASP
1	Q	150	LEU
1	Q	162	THR
1	Q	215	TYR
1	Q	229	VAL
1	Q	303	ASP
1	H	150	LEU
1	H	162	THR
1	H	215	TYR
1	H	229	VAL
1	H	303	ASP
1	L	150	LEU
1	L	162	THR
1	L	215	TYR
1	L	229	VAL
1	L	303	ASP
1	J	150	LEU
1	J	162	THR
1	J	215	TYR

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Mol	Chain	Res	Type
1	J	229	VAL
1	J	303	ASP
1	P	150	LEU
1	P	162	THR
1	P	215	TYR
1	P	229	VAL
1	P	303	ASP
1	N	150	LEU
1	N	162	THR
1	N	215	TYR
1	N	229	VAL
1	N	303	ASP
1	R	150	LEU
1	R	162	THR
1	R	215	TYR
1	R	229	VAL
1	R	303	ASP
1	X	150	LEU
1	X	162	THR
1	X	215	TYR
1	X	229	VAL
1	X	303	ASP
1	d	150	LEU
1	d	162	THR
1	d	215	TYR
1	d	229	VAL
1	d	303	ASP
1	a	150	LEU
1	a	162	THR
1	a	215	TYR
1	a	229	VAL
1	a	303	ASP
1	j	150	LEU
1	j	162	THR
1	j	215	TYR
1	j	229	VAL
1	j	303	ASP
1	g	150	LEU
1	g	162	THR
1	g	215	TYR
1	g	229	VAL
1	g	303	ASP

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Mol	Chain	Res	Type
1	m	150	LEU
1	m	162	THR
1	m	215	TYR
1	m	229	VAL
1	m	303	ASP
2	U	20	ALA
2	U	76	ALA
2	U	148	ASN
2	T	20	ALA
2	T	148	ASN
2	W	20	ALA
2	W	148	ASN
2	V	20	ALA
2	V	148	ASN
2	Z	20	ALA
2	Z	148	ASN
2	Y	20	ALA
2	Y	148	ASN
2	e	20	ALA
2	e	148	ASN
2	b	20	ALA
2	b	148	ASN
2	k	20	ALA
2	k	148	ASN
2	h	20	ALA
2	h	148	ASN
2	n	20	ALA
2	n	148	ASN
2	c	20	ALA
2	c	76	ALA
2	c	148	ASN
2	i	20	ALA
2	i	148	ASN
2	f	20	ALA
2	f	148	ASN
2	o	20	ALA
2	o	76	ALA
2	o	148	ASN
2	l	20	ALA
2	l	148	ASN
2	p	20	ALA
2	p	148	ASN

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Mol	Chain	Res	Type
2	q	20	ALA
2	q	148	ASN
2	s	20	ALA
2	s	148	ASN
2	r	20	ALA
2	r	148	ASN
2	u	20	ALA
2	u	148	ASN
2	t	20	ALA
2	t	148	ASN
2	v	20	ALA
2	v	148	ASN
1	A	19	ILE
1	A	103	SER
1	A	134	SER
1	A	174	GLY
1	A	342	LEU
1	A	385	VAL
2	S	76	ALA
2	S	118	GLY
1	B	19	ILE
1	B	103	SER
1	B	134	SER
1	B	174	GLY
1	B	342	LEU
1	B	385	VAL
1	C	19	ILE
1	C	103	SER
1	C	134	SER
1	C	174	GLY
1	C	342	LEU
1	C	385	VAL
1	D	19	ILE
1	D	103	SER
1	D	134	SER
1	D	174	GLY
1	D	342	LEU
1	D	385	VAL
1	E	19	ILE
1	E	103	SER
1	E	134	SER
1	E	174	GLY

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Mol	Chain	Res	Type
1	E	342	LEU
1	E	385	VAL
1	F	19	ILE
1	F	103	SER
1	F	134	SER
1	F	174	GLY
1	F	342	LEU
1	F	385	VAL
1	G	19	ILE
1	G	103	SER
1	G	134	SER
1	G	174	GLY
1	G	342	LEU
1	G	385	VAL
1	K	19	ILE
1	K	103	SER
1	K	134	SER
1	K	174	GLY
1	K	342	LEU
1	K	385	VAL
1	I	19	ILE
1	I	103	SER
1	I	134	SER
1	I	174	GLY
1	I	342	LEU
1	I	385	VAL
1	O	19	ILE
1	O	103	SER
1	O	134	SER
1	O	174	GLY
1	O	342	LEU
1	O	385	VAL
1	M	19	ILE
1	M	103	SER
1	M	134	SER
1	M	174	GLY
1	M	342	LEU
1	M	385	VAL
1	Q	19	ILE
1	Q	103	SER
1	Q	134	SER
1	Q	174	GLY

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Mol	Chain	Res	Type
1	Q	342	LEU
1	Q	385	VAL
1	H	19	ILE
1	H	103	SER
1	H	134	SER
1	H	174	GLY
1	H	342	LEU
1	H	385	VAL
1	L	19	ILE
1	L	103	SER
1	L	134	SER
1	L	174	GLY
1	L	342	LEU
1	L	385	VAL
1	J	19	ILE
1	J	103	SER
1	J	134	SER
1	J	174	GLY
1	J	342	LEU
1	J	385	VAL
1	P	19	ILE
1	P	103	SER
1	P	134	SER
1	P	174	GLY
1	P	342	LEU
1	P	385	VAL
1	N	19	ILE
1	N	103	SER
1	N	134	SER
1	N	174	GLY
1	N	342	LEU
1	N	385	VAL
1	R	19	ILE
1	R	103	SER
1	R	134	SER
1	R	174	GLY
1	R	342	LEU
1	R	385	VAL
1	X	19	ILE
1	X	103	SER
1	X	134	SER
1	X	174	GLY

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Mol	Chain	Res	Type
1	X	342	LEU
1	X	385	VAL
1	d	19	ILE
1	d	103	SER
1	d	134	SER
1	d	174	GLY
1	d	342	LEU
1	d	385	VAL
1	a	19	ILE
1	a	103	SER
1	a	134	SER
1	a	174	GLY
1	a	342	LEU
1	a	385	VAL
1	j	19	ILE
1	j	103	SER
1	j	134	SER
1	j	174	GLY
1	j	342	LEU
1	j	385	VAL
1	g	19	ILE
1	g	103	SER
1	g	134	SER
1	g	174	GLY
1	g	342	LEU
1	g	385	VAL
1	m	19	ILE
1	m	103	SER
1	m	134	SER
1	m	174	GLY
1	m	342	LEU
1	m	385	VAL
2	T	76	ALA
2	W	76	ALA
2	V	76	ALA
2	V	118	GLY
2	Z	76	ALA
2	Y	76	ALA
2	e	76	ALA
2	b	76	ALA
2	k	76	ALA
2	h	76	ALA

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Mol	Chain	Res	Type
2	n	76	ALA
2	i	76	ALA
2	f	76	ALA
2	l	76	ALA
2	p	76	ALA
2	q	76	ALA
2	q	118	GLY
2	s	76	ALA
2	s	118	GLY
2	r	76	ALA
2	r	118	GLY
2	u	76	ALA
2	u	118	GLY
2	t	76	ALA
2	t	118	GLY
2	v	76	ALA
2	v	118	GLY
1	A	133	HIS
2	S	30	LYS
2	S	35	THR
1	B	133	HIS
1	D	133	HIS
1	E	133	HIS
1	F	133	HIS
1	G	133	HIS
1	G	383	LEU
1	K	133	HIS
1	I	133	HIS
1	O	133	HIS
1	O	383	LEU
1	M	133	HIS
1	M	383	LEU
1	Q	383	LEU
1	H	133	HIS
1	L	133	HIS
1	J	133	HIS
1	P	133	HIS
1	N	133	HIS
1	R	133	HIS
1	X	133	HIS
1	X	383	LEU
1	a	133	HIS

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Mol	Chain	Res	Type
1	a	383	LEU
1	g	133	HIS
1	m	133	HIS
1	m	383	LEU
2	U	35	THR
2	U	118	GLY
2	T	35	THR
2	T	118	GLY
2	W	35	THR
2	W	118	GLY
2	V	35	THR
2	Z	35	THR
2	Z	118	GLY
2	Y	30	LYS
2	Y	35	THR
2	Y	118	GLY
2	e	35	THR
2	e	118	GLY
2	b	35	THR
2	b	118	GLY
2	k	35	THR
2	k	118	GLY
2	h	35	THR
2	h	118	GLY
2	n	35	THR
2	n	118	GLY
2	c	35	THR
2	c	118	GLY
2	c	154	ASN
2	i	35	THR
2	i	118	GLY
2	f	35	THR
2	f	118	GLY
2	o	35	THR
2	o	118	GLY
2	o	154	ASN
2	l	35	THR
2	l	118	GLY
2	p	35	THR
2	p	118	GLY
2	q	35	THR
2	s	35	THR

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Mol	Chain	Res	Type
2	s	154	ASN
2	r	35	THR
2	u	35	THR
2	t	35	THR
2	v	35	THR
1	A	16	ALA
1	A	213	ALA
1	A	383	LEU
2	S	45	ALA
2	S	154	ASN
1	B	16	ALA
1	B	213	ALA
1	B	383	LEU
1	C	16	ALA
1	C	119	SER
1	C	133	HIS
1	C	213	ALA
1	C	383	LEU
1	D	16	ALA
1	D	213	ALA
1	D	383	LEU
1	E	16	ALA
1	E	119	SER
1	E	213	ALA
1	E	383	LEU
1	F	16	ALA
1	F	213	ALA
1	F	383	LEU
1	G	16	ALA
1	G	213	ALA
1	K	16	ALA
1	K	213	ALA
1	K	383	LEU
1	I	16	ALA
1	I	213	ALA
1	I	383	LEU
1	O	16	ALA
1	O	119	SER
1	O	213	ALA
1	M	16	ALA
1	M	213	ALA
1	Q	16	ALA

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Mol	Chain	Res	Type
1	Q	119	SER
1	Q	133	HIS
1	Q	213	ALA
1	H	16	ALA
1	H	213	ALA
1	H	383	LEU
1	L	16	ALA
1	L	213	ALA
1	L	383	LEU
1	J	16	ALA
1	J	213	ALA
1	J	383	LEU
1	P	16	ALA
1	P	213	ALA
1	P	383	LEU
1	N	16	ALA
1	N	213	ALA
1	N	383	LEU
1	R	16	ALA
1	R	213	ALA
1	R	383	LEU
1	X	16	ALA
1	X	213	ALA
1	d	16	ALA
1	d	133	HIS
1	d	213	ALA
1	d	383	LEU
1	a	16	ALA
1	a	213	ALA
1	j	16	ALA
1	j	133	HIS
1	j	213	ALA
1	j	383	LEU
1	g	16	ALA
1	g	213	ALA
1	g	383	LEU
1	m	16	ALA
1	m	213	ALA
2	U	30	LYS
2	U	45	ALA
2	U	154	ASN
2	T	30	LYS

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Mol	Chain	Res	Type
2	T	45	ALA
2	T	154	ASN
2	W	30	LYS
2	W	45	ALA
2	W	154	ASN
2	V	30	LYS
2	V	45	ALA
2	V	154	ASN
2	Z	30	LYS
2	Z	45	ALA
2	Z	154	ASN
2	Y	45	ALA
2	Y	154	ASN
2	e	30	LYS
2	e	45	ALA
2	e	154	ASN
2	b	30	LYS
2	b	45	ALA
2	b	154	ASN
2	k	30	LYS
2	k	45	ALA
2	k	154	ASN
2	h	30	LYS
2	h	45	ALA
2	h	154	ASN
2	n	30	LYS
2	n	45	ALA
2	n	154	ASN
2	c	30	LYS
2	c	45	ALA
2	i	30	LYS
2	i	45	ALA
2	i	154	ASN
2	f	30	LYS
2	f	45	ALA
2	f	154	ASN
2	o	30	LYS
2	o	45	ALA
2	l	30	LYS
2	l	45	ALA
2	l	154	ASN
2	p	30	LYS

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Mol	Chain	Res	Type
2	p	45	ALA
2	p	154	ASN
2	q	30	LYS
2	q	45	ALA
2	q	154	ASN
2	s	30	LYS
2	s	45	ALA
2	r	30	LYS
2	r	45	ALA
2	r	154	ASN
2	u	30	LYS
2	u	45	ALA
2	u	154	ASN
2	t	30	LYS
2	t	45	ALA
2	t	154	ASN
2	v	30	LYS
2	v	45	ALA
2	v	154	ASN
1	A	119	SER
1	A	304	ARG
2	S	36	GLU
2	S	46	PRO
1	B	119	SER
1	B	304	ARG
1	C	304	ARG
1	D	119	SER
1	D	304	ARG
1	E	304	ARG
1	F	119	SER
1	F	304	ARG
1	G	119	SER
1	G	304	ARG
1	K	119	SER
1	K	304	ARG
1	I	119	SER
1	I	304	ARG
1	O	304	ARG
1	M	119	SER
1	M	304	ARG
1	Q	304	ARG
1	H	119	SER

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Mol	Chain	Res	Type
1	L	119	SER
1	J	119	SER
1	P	119	SER
1	N	119	SER
1	R	119	SER
1	X	119	SER
1	d	119	SER
1	j	119	SER
1	g	119	SER
1	m	119	SER
2	U	36	GLU
2	U	37	GLN
2	U	46	PRO
2	T	46	PRO
2	W	36	GLU
2	W	46	PRO
2	V	46	PRO
2	Z	36	GLU
2	Z	46	PRO
2	Y	36	GLU
2	Y	37	GLN
2	Y	46	PRO
2	e	46	PRO
2	b	36	GLU
2	b	37	GLN
2	b	46	PRO
2	k	36	GLU
2	k	46	PRO
2	h	37	GLN
2	h	46	PRO
2	n	36	GLU
2	n	37	GLN
2	n	46	PRO
2	c	46	PRO
2	i	36	GLU
2	i	46	PRO
2	f	36	GLU
2	f	46	PRO
2	o	36	GLU
2	o	46	PRO
2	l	36	GLU
2	l	37	GLN

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Mol	Chain	Res	Type
2	l	46	PRO
2	p	36	GLU
2	p	37	GLN
2	p	46	PRO
2	q	46	PRO
2	s	36	GLU
2	s	37	GLN
2	s	46	PRO
2	r	46	PRO
2	r	122	GLU
2	u	36	GLU
2	u	46	PRO
2	t	36	GLU
2	t	37	GLN
2	t	46	PRO
2	v	36	GLU
2	v	37	GLN
2	v	46	PRO
1	A	200	ALA
2	S	47	VAL
2	S	48	SER
2	S	122	GLU
1	B	200	ALA
1	C	200	ALA
1	D	200	ALA
1	E	200	ALA
1	G	200	ALA
1	K	200	ALA
1	I	200	ALA
1	O	200	ALA
1	M	200	ALA
1	Q	200	ALA
1	H	200	ALA
1	H	304	ARG
1	L	200	ALA
1	L	304	ARG
1	J	200	ALA
1	J	304	ARG
1	P	200	ALA
1	P	304	ARG
1	N	200	ALA
1	N	304	ARG

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Mol	Chain	Res	Type
1	R	200	ALA
1	R	304	ARG
1	X	200	ALA
1	X	304	ARG
1	d	200	ALA
1	d	304	ARG
1	a	119	SER
1	a	304	ARG
1	j	200	ALA
1	j	304	ARG
1	g	200	ALA
1	g	304	ARG
1	m	200	ALA
1	m	304	ARG
2	U	122	GLU
2	T	36	GLU
2	T	47	VAL
2	T	48	SER
2	T	122	GLU
2	W	47	VAL
2	W	48	SER
2	W	122	GLU
2	V	36	GLU
2	V	37	GLN
2	V	47	VAL
2	V	48	SER
2	V	122	GLU
2	Z	47	VAL
2	Z	48	SER
2	Z	122	GLU
2	Y	47	VAL
2	e	36	GLU
2	e	47	VAL
2	e	48	SER
2	e	122	GLU
2	b	47	VAL
2	b	122	GLU
2	k	37	GLN
2	k	47	VAL
2	k	48	SER
2	k	122	GLU
2	h	36	GLU

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Mol	Chain	Res	Type
2	h	47	VAL
2	h	122	GLU
2	n	47	VAL
2	n	122	GLU
2	c	36	GLU
2	c	47	VAL
2	c	48	SER
2	c	122	GLU
2	i	37	GLN
2	i	47	VAL
2	i	122	GLU
2	f	47	VAL
2	f	48	SER
2	f	122	GLU
2	o	47	VAL
2	o	48	SER
2	o	122	GLU
2	l	47	VAL
2	l	122	GLU
2	p	47	VAL
2	p	122	GLU
2	q	36	GLU
2	q	47	VAL
2	q	48	SER
2	q	122	GLU
2	s	47	VAL
2	s	122	GLU
2	r	36	GLU
2	r	47	VAL
2	u	47	VAL
2	u	122	GLU
2	t	47	VAL
2	t	122	GLU
2	v	47	VAL
2	v	122	GLU
2	U	47	VAL
1	A	43	PRO
1	B	43	PRO
1	C	43	PRO
1	D	43	PRO
1	E	43	PRO
1	F	43	PRO

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Mol	Chain	Res	Type
1	G	43	PRO
1	K	43	PRO
1	I	43	PRO
1	O	43	PRO
1	M	43	PRO
1	Q	43	PRO
1	H	43	PRO
1	L	43	PRO
1	J	43	PRO
1	P	43	PRO
1	N	43	PRO
1	R	43	PRO
1	X	43	PRO
1	d	43	PRO
1	a	43	PRO
1	j	43	PRO
1	g	43	PRO
1	m	43	PRO

### 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	A	297/298 (100%)	279 (94%)	18 (6%)	23	64
1	B	297/298 (100%)	279 (94%)	18 (6%)	23	64
1	C	297/298 (100%)	279 (94%)	18 (6%)	23	64
1	D	297/298 (100%)	279 (94%)	18 (6%)	23	64
1	E	297/298 (100%)	279 (94%)	18 (6%)	23	64
1	F	297/298 (100%)	279 (94%)	18 (6%)	23	64
1	G	297/298 (100%)	279 (94%)	18 (6%)	23	64
1	H	297/298 (100%)	279 (94%)	18 (6%)	23	64
1	I	297/298 (100%)	279 (94%)	18 (6%)	23	64
1	J	297/298 (100%)	279 (94%)	18 (6%)	23	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	297/298 (100%)	279 (94%)	18 (6%)	23	64
1	L	297/298 (100%)	279 (94%)	18 (6%)	23	64
1	M	297/298 (100%)	279 (94%)	18 (6%)	23	64
1	N	297/298 (100%)	279 (94%)	18 (6%)	23	64
1	O	297/298 (100%)	279 (94%)	18 (6%)	23	64
1	P	297/298 (100%)	279 (94%)	18 (6%)	23	64
1	Q	297/298 (100%)	278 (94%)	19 (6%)	22	62
1	R	297/298 (100%)	279 (94%)	18 (6%)	23	64
1	X	297/298 (100%)	279 (94%)	18 (6%)	23	64
1	a	297/298 (100%)	279 (94%)	18 (6%)	23	64
1	d	297/298 (100%)	279 (94%)	18 (6%)	23	64
1	g	297/298 (100%)	279 (94%)	18 (6%)	23	64
1	j	297/298 (100%)	279 (94%)	18 (6%)	23	64
1	m	297/298 (100%)	279 (94%)	18 (6%)	23	64
2	S	129/131 (98%)	115 (89%)	14 (11%)	8	37
2	T	129/131 (98%)	115 (89%)	14 (11%)	8	37
2	U	129/131 (98%)	114 (88%)	15 (12%)	7	33
2	V	129/131 (98%)	115 (89%)	14 (11%)	8	37
2	W	129/131 (98%)	115 (89%)	14 (11%)	8	37
2	Y	129/131 (98%)	115 (89%)	14 (11%)	8	37
2	Z	129/131 (98%)	115 (89%)	14 (11%)	8	37
2	b	129/131 (98%)	115 (89%)	14 (11%)	8	37
2	c	129/131 (98%)	114 (88%)	15 (12%)	7	33
2	e	129/131 (98%)	115 (89%)	14 (11%)	8	37
2	f	129/131 (98%)	115 (89%)	14 (11%)	8	37
2	h	129/131 (98%)	115 (89%)	14 (11%)	8	37
2	i	129/131 (98%)	115 (89%)	14 (11%)	8	37
2	k	129/131 (98%)	115 (89%)	14 (11%)	8	37
2	l	129/131 (98%)	115 (89%)	14 (11%)	8	37
2	n	129/131 (98%)	115 (89%)	14 (11%)	8	37
2	o	129/131 (98%)	115 (89%)	14 (11%)	8	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	p	129/131 (98%)	115 (89%)	14 (11%)	8	37
2	q	129/131 (98%)	114 (88%)	15 (12%)	7	33
2	r	129/131 (98%)	114 (88%)	15 (12%)	7	33
2	s	129/131 (98%)	114 (88%)	15 (12%)	7	33
2	t	129/131 (98%)	114 (88%)	15 (12%)	7	33
2	u	129/131 (98%)	115 (89%)	14 (11%)	8	37
2	v	129/131 (98%)	115 (89%)	14 (11%)	8	37
All	All	10224/10296 (99%)	9449 (92%)	775 (8%)	21	55

All (775) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ILE
1	A	38	GLN
1	A	40	SER
1	A	61	ILE
1	A	75	ARG
1	A	121	PHE
1	A	134	SER
1	A	182	ASP
1	A	197	ASN
1	A	208	PHE
1	A	215	TYR
1	A	229	VAL
1	A	243	GLU
1	A	264	TYR
1	A	285	ARG
1	A	304	ARG
1	A	355	TRP
1	A	379	LEU
2	S	3	ILE
2	S	8	THR
2	S	22	ASP
2	S	23	VAL
2	S	26	LEU
2	S	54	GLU
2	S	66	ARG
2	S	71	ASN
2	S	79	SER
2	S	82	ASN

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Mol	Chain	Res	Type
2	S	103	LEU
2	S	106	LEU
2	S	124	LYS
2	S	162	MET
1	B	19	ILE
1	B	38	GLN
1	B	40	SER
1	B	61	ILE
1	B	75	ARG
1	B	121	PHE
1	B	134	SER
1	B	182	ASP
1	B	197	ASN
1	B	208	PHE
1	B	215	TYR
1	B	229	VAL
1	B	243	GLU
1	B	264	TYR
1	B	285	ARG
1	B	304	ARG
1	B	355	TRP
1	B	379	LEU
1	C	19	ILE
1	C	38	GLN
1	C	40	SER
1	C	61	ILE
1	C	75	ARG
1	C	121	PHE
1	C	134	SER
1	C	182	ASP
1	C	197	ASN
1	C	208	PHE
1	C	215	TYR
1	C	229	VAL
1	C	243	GLU
1	C	264	TYR
1	C	285	ARG
1	C	304	ARG
1	C	355	TRP
1	C	379	LEU
1	D	19	ILE
1	D	38	GLN

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Mol	Chain	Res	Type
1	D	40	SER
1	D	61	ILE
1	D	75	ARG
1	D	121	PHE
1	D	134	SER
1	D	182	ASP
1	D	197	ASN
1	D	208	PHE
1	D	215	TYR
1	D	229	VAL
1	D	243	GLU
1	D	264	TYR
1	D	285	ARG
1	D	304	ARG
1	D	355	TRP
1	D	379	LEU
1	E	19	ILE
1	E	38	GLN
1	E	40	SER
1	E	61	ILE
1	E	75	ARG
1	E	121	PHE
1	E	134	SER
1	E	182	ASP
1	E	197	ASN
1	E	208	PHE
1	E	215	TYR
1	E	229	VAL
1	E	243	GLU
1	E	264	TYR
1	E	285	ARG
1	E	304	ARG
1	E	355	TRP
1	E	379	LEU
1	F	19	ILE
1	F	38	GLN
1	F	40	SER
1	F	61	ILE
1	F	75	ARG
1	F	121	PHE
1	F	134	SER
1	F	182	ASP

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Mol	Chain	Res	Type
1	F	197	ASN
1	F	208	PHE
1	F	215	TYR
1	F	229	VAL
1	F	243	GLU
1	F	264	TYR
1	F	285	ARG
1	F	304	ARG
1	F	355	TRP
1	F	379	LEU
1	G	19	ILE
1	G	38	GLN
1	G	40	SER
1	G	61	ILE
1	G	75	ARG
1	G	121	PHE
1	G	134	SER
1	G	182	ASP
1	G	197	ASN
1	G	208	PHE
1	G	215	TYR
1	G	229	VAL
1	G	243	GLU
1	G	264	TYR
1	G	285	ARG
1	G	304	ARG
1	G	355	TRP
1	G	379	LEU
1	K	19	ILE
1	K	38	GLN
1	K	40	SER
1	K	61	ILE
1	K	75	ARG
1	K	121	PHE
1	K	134	SER
1	K	182	ASP
1	K	197	ASN
1	K	208	PHE
1	K	215	TYR
1	K	229	VAL
1	K	243	GLU
1	K	264	TYR

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Mol	Chain	Res	Type
1	K	285	ARG
1	K	304	ARG
1	K	355	TRP
1	K	379	LEU
1	I	19	ILE
1	I	38	GLN
1	I	40	SER
1	I	61	ILE
1	I	75	ARG
1	I	121	PHE
1	I	134	SER
1	I	182	ASP
1	I	197	ASN
1	I	208	PHE
1	I	215	TYR
1	I	229	VAL
1	I	243	GLU
1	I	264	TYR
1	I	285	ARG
1	I	304	ARG
1	I	355	TRP
1	I	379	LEU
1	O	19	ILE
1	O	38	GLN
1	O	40	SER
1	O	61	ILE
1	O	75	ARG
1	O	121	PHE
1	O	134	SER
1	O	182	ASP
1	O	197	ASN
1	O	208	PHE
1	O	215	TYR
1	O	229	VAL
1	O	243	GLU
1	O	264	TYR
1	O	285	ARG
1	O	304	ARG
1	O	355	TRP
1	O	379	LEU
1	M	19	ILE
1	M	38	GLN

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Mol	Chain	Res	Type
1	M	40	SER
1	M	61	ILE
1	M	75	ARG
1	M	121	PHE
1	M	134	SER
1	M	182	ASP
1	M	197	ASN
1	M	208	PHE
1	M	215	TYR
1	M	229	VAL
1	M	243	GLU
1	M	264	TYR
1	M	285	ARG
1	M	304	ARG
1	M	355	TRP
1	M	379	LEU
1	Q	19	ILE
1	Q	38	GLN
1	Q	40	SER
1	Q	61	ILE
1	Q	75	ARG
1	Q	121	PHE
1	Q	134	SER
1	Q	182	ASP
1	Q	197	ASN
1	Q	208	PHE
1	Q	215	TYR
1	Q	229	VAL
1	Q	243	GLU
1	Q	264	TYR
1	Q	283	ARG
1	Q	285	ARG
1	Q	304	ARG
1	Q	355	TRP
1	Q	379	LEU
1	H	19	ILE
1	H	38	GLN
1	H	40	SER
1	H	61	ILE
1	H	75	ARG
1	H	121	PHE
1	H	134	SER

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Mol	Chain	Res	Type
1	H	182	ASP
1	H	197	ASN
1	H	208	PHE
1	H	215	TYR
1	H	229	VAL
1	H	243	GLU
1	H	264	TYR
1	H	285	ARG
1	H	304	ARG
1	H	355	TRP
1	H	379	LEU
1	L	19	ILE
1	L	38	GLN
1	L	40	SER
1	L	61	ILE
1	L	75	ARG
1	L	121	PHE
1	L	134	SER
1	L	182	ASP
1	L	197	ASN
1	L	208	PHE
1	L	215	TYR
1	L	229	VAL
1	L	243	GLU
1	L	264	TYR
1	L	285	ARG
1	L	304	ARG
1	L	355	TRP
1	L	379	LEU
1	J	19	ILE
1	J	38	GLN
1	J	40	SER
1	J	61	ILE
1	J	75	ARG
1	J	121	PHE
1	J	134	SER
1	J	182	ASP
1	J	197	ASN
1	J	208	PHE
1	J	215	TYR
1	J	229	VAL
1	J	243	GLU

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Mol	Chain	Res	Type
1	J	264	TYR
1	J	285	ARG
1	J	304	ARG
1	J	355	TRP
1	J	379	LEU
1	P	19	ILE
1	P	38	GLN
1	P	40	SER
1	P	61	ILE
1	P	75	ARG
1	P	121	PHE
1	P	134	SER
1	P	182	ASP
1	P	197	ASN
1	P	208	PHE
1	P	215	TYR
1	P	229	VAL
1	P	243	GLU
1	P	264	TYR
1	P	285	ARG
1	P	304	ARG
1	P	355	TRP
1	P	379	LEU
1	N	19	ILE
1	N	38	GLN
1	N	40	SER
1	N	61	ILE
1	N	75	ARG
1	N	121	PHE
1	N	134	SER
1	N	182	ASP
1	N	197	ASN
1	N	208	PHE
1	N	215	TYR
1	N	229	VAL
1	N	243	GLU
1	N	264	TYR
1	N	285	ARG
1	N	304	ARG
1	N	355	TRP
1	N	379	LEU
1	R	19	ILE

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Mol	Chain	Res	Type
1	R	38	GLN
1	R	40	SER
1	R	61	ILE
1	R	75	ARG
1	R	121	PHE
1	R	134	SER
1	R	182	ASP
1	R	197	ASN
1	R	208	PHE
1	R	215	TYR
1	R	229	VAL
1	R	243	GLU
1	R	264	TYR
1	R	285	ARG
1	R	304	ARG
1	R	355	TRP
1	R	379	LEU
1	X	19	ILE
1	X	38	GLN
1	X	40	SER
1	X	61	ILE
1	X	75	ARG
1	X	121	PHE
1	X	134	SER
1	X	182	ASP
1	X	197	ASN
1	X	208	PHE
1	X	215	TYR
1	X	229	VAL
1	X	243	GLU
1	X	264	TYR
1	X	285	ARG
1	X	304	ARG
1	X	355	TRP
1	X	379	LEU
1	d	19	ILE
1	d	38	GLN
1	d	40	SER
1	d	61	ILE
1	d	75	ARG
1	d	121	PHE
1	d	134	SER

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Mol	Chain	Res	Type
1	d	182	ASP
1	d	197	ASN
1	d	208	PHE
1	d	215	TYR
1	d	229	VAL
1	d	243	GLU
1	d	264	TYR
1	d	285	ARG
1	d	304	ARG
1	d	355	TRP
1	d	379	LEU
1	a	19	ILE
1	a	38	GLN
1	a	40	SER
1	a	61	ILE
1	a	75	ARG
1	a	121	PHE
1	a	134	SER
1	a	182	ASP
1	a	197	ASN
1	a	208	PHE
1	a	215	TYR
1	a	229	VAL
1	a	243	GLU
1	a	264	TYR
1	a	285	ARG
1	a	304	ARG
1	a	355	TRP
1	a	379	LEU
1	j	19	ILE
1	j	38	GLN
1	j	40	SER
1	j	61	ILE
1	j	75	ARG
1	j	121	PHE
1	j	134	SER
1	j	182	ASP
1	j	197	ASN
1	j	208	PHE
1	j	215	TYR
1	j	229	VAL
1	j	243	GLU

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Mol	Chain	Res	Type
1	j	264	TYR
1	j	285	ARG
1	j	304	ARG
1	j	355	TRP
1	j	379	LEU
1	g	19	ILE
1	g	38	GLN
1	g	40	SER
1	g	61	ILE
1	g	75	ARG
1	g	121	PHE
1	g	134	SER
1	g	182	ASP
1	g	197	ASN
1	g	208	PHE
1	g	215	TYR
1	g	229	VAL
1	g	243	GLU
1	g	264	TYR
1	g	285	ARG
1	g	304	ARG
1	g	355	TRP
1	g	379	LEU
1	m	19	ILE
1	m	38	GLN
1	m	40	SER
1	m	61	ILE
1	m	75	ARG
1	m	121	PHE
1	m	134	SER
1	m	182	ASP
1	m	197	ASN
1	m	208	PHE
1	m	215	TYR
1	m	229	VAL
1	m	243	GLU
1	m	264	TYR
1	m	285	ARG
1	m	304	ARG
1	m	355	TRP
1	m	379	LEU
2	U	3	ILE

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Mol	Chain	Res	Type
2	U	8	THR
2	U	22	ASP
2	U	23	VAL
2	U	26	LEU
2	U	54	GLU
2	U	63	ASN
2	U	66	ARG
2	U	71	ASN
2	U	79	SER
2	U	82	ASN
2	U	103	LEU
2	U	106	LEU
2	U	124	LYS
2	U	162	MET
2	T	3	ILE
2	T	8	THR
2	T	22	ASP
2	T	23	VAL
2	T	26	LEU
2	T	54	GLU
2	T	66	ARG
2	T	71	ASN
2	T	79	SER
2	T	82	ASN
2	T	103	LEU
2	T	106	LEU
2	T	124	LYS
2	T	162	MET
2	W	3	ILE
2	W	8	THR
2	W	22	ASP
2	W	23	VAL
2	W	26	LEU
2	W	54	GLU
2	W	66	ARG
2	W	71	ASN
2	W	79	SER
2	W	82	ASN
2	W	103	LEU
2	W	106	LEU
2	W	124	LYS
2	W	162	MET

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Mol	Chain	Res	Type
2	V	3	ILE
2	V	8	THR
2	V	22	ASP
2	V	23	VAL
2	V	26	LEU
2	V	54	GLU
2	V	66	ARG
2	V	71	ASN
2	V	79	SER
2	V	82	ASN
2	V	103	LEU
2	V	106	LEU
2	V	124	LYS
2	V	162	MET
2	Z	3	ILE
2	Z	8	THR
2	Z	22	ASP
2	Z	23	VAL
2	Z	26	LEU
2	Z	54	GLU
2	Z	66	ARG
2	Z	71	ASN
2	Z	79	SER
2	Z	82	ASN
2	Z	103	LEU
2	Z	106	LEU
2	Z	124	LYS
2	Z	162	MET
2	Y	3	ILE
2	Y	8	THR
2	Y	22	ASP
2	Y	23	VAL
2	Y	26	LEU
2	Y	54	GLU
2	Y	66	ARG
2	Y	71	ASN
2	Y	79	SER
2	Y	82	ASN
2	Y	103	LEU
2	Y	106	LEU
2	Y	124	LYS
2	Y	162	MET

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Mol	Chain	Res	Type
2	e	3	ILE
2	e	8	THR
2	e	22	ASP
2	e	23	VAL
2	e	26	LEU
2	e	54	GLU
2	e	66	ARG
2	e	71	ASN
2	e	79	SER
2	e	82	ASN
2	e	103	LEU
2	e	106	LEU
2	e	124	LYS
2	e	162	MET
2	b	3	ILE
2	b	8	THR
2	b	22	ASP
2	b	23	VAL
2	b	26	LEU
2	b	54	GLU
2	b	66	ARG
2	b	71	ASN
2	b	79	SER
2	b	82	ASN
2	b	103	LEU
2	b	106	LEU
2	b	124	LYS
2	b	162	MET
2	k	3	ILE
2	k	8	THR
2	k	22	ASP
2	k	23	VAL
2	k	26	LEU
2	k	54	GLU
2	k	66	ARG
2	k	71	ASN
2	k	79	SER
2	k	82	ASN
2	k	103	LEU
2	k	106	LEU
2	k	124	LYS
2	k	162	MET

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Mol	Chain	Res	Type
2	h	3	ILE
2	h	8	THR
2	h	22	ASP
2	h	23	VAL
2	h	26	LEU
2	h	54	GLU
2	h	66	ARG
2	h	71	ASN
2	h	79	SER
2	h	82	ASN
2	h	103	LEU
2	h	106	LEU
2	h	124	LYS
2	h	162	MET
2	n	3	ILE
2	n	8	THR
2	n	22	ASP
2	n	23	VAL
2	n	26	LEU
2	n	54	GLU
2	n	66	ARG
2	n	71	ASN
2	n	79	SER
2	n	82	ASN
2	n	103	LEU
2	n	106	LEU
2	n	124	LYS
2	n	162	MET
2	c	3	ILE
2	c	8	THR
2	c	22	ASP
2	c	23	VAL
2	c	26	LEU
2	c	54	GLU
2	c	63	ASN
2	c	66	ARG
2	c	71	ASN
2	c	79	SER
2	c	82	ASN
2	c	103	LEU
2	c	106	LEU
2	c	124	LYS

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Mol	Chain	Res	Type
2	c	162	MET
2	i	3	ILE
2	i	8	THR
2	i	22	ASP
2	i	23	VAL
2	i	26	LEU
2	i	54	GLU
2	i	66	ARG
2	i	71	ASN
2	i	79	SER
2	i	82	ASN
2	i	103	LEU
2	i	106	LEU
2	i	124	LYS
2	i	162	MET
2	f	3	ILE
2	f	8	THR
2	f	22	ASP
2	f	23	VAL
2	f	26	LEU
2	f	54	GLU
2	f	66	ARG
2	f	71	ASN
2	f	79	SER
2	f	82	ASN
2	f	103	LEU
2	f	106	LEU
2	f	124	LYS
2	f	162	MET
2	o	3	ILE
2	o	8	THR
2	o	22	ASP
2	o	23	VAL
2	o	26	LEU
2	o	54	GLU
2	o	66	ARG
2	o	71	ASN
2	o	79	SER
2	o	82	ASN
2	o	103	LEU
2	o	106	LEU
2	o	124	LYS

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Mol	Chain	Res	Type
2	o	162	MET
2	l	3	ILE
2	l	8	THR
2	l	22	ASP
2	l	23	VAL
2	l	26	LEU
2	l	54	GLU
2	l	66	ARG
2	l	71	ASN
2	l	79	SER
2	l	82	ASN
2	l	103	LEU
2	l	106	LEU
2	l	124	LYS
2	l	162	MET
2	p	3	ILE
2	p	8	THR
2	p	22	ASP
2	p	23	VAL
2	p	26	LEU
2	p	54	GLU
2	p	66	ARG
2	p	71	ASN
2	p	79	SER
2	p	82	ASN
2	p	103	LEU
2	p	106	LEU
2	p	124	LYS
2	p	162	MET
2	q	3	ILE
2	q	8	THR
2	q	22	ASP
2	q	23	VAL
2	q	26	LEU
2	q	54	GLU
2	q	63	ASN
2	q	66	ARG
2	q	71	ASN
2	q	79	SER
2	q	82	ASN
2	q	103	LEU
2	q	106	LEU

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Mol	Chain	Res	Type
2	q	124	LYS
2	q	162	MET
2	s	3	ILE
2	s	8	THR
2	s	22	ASP
2	s	23	VAL
2	s	26	LEU
2	s	54	GLU
2	s	63	ASN
2	s	66	ARG
2	s	71	ASN
2	s	79	SER
2	s	82	ASN
2	s	103	LEU
2	s	106	LEU
2	s	124	LYS
2	s	162	MET
2	r	3	ILE
2	r	8	THR
2	r	22	ASP
2	r	23	VAL
2	r	26	LEU
2	r	54	GLU
2	r	63	ASN
2	r	66	ARG
2	r	71	ASN
2	r	79	SER
2	r	82	ASN
2	r	103	LEU
2	r	106	LEU
2	r	124	LYS
2	r	162	MET
2	u	3	ILE
2	u	8	THR
2	u	22	ASP
2	u	23	VAL
2	u	26	LEU
2	u	54	GLU
2	u	66	ARG
2	u	71	ASN
2	u	79	SER
2	u	82	ASN

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Mol	Chain	Res	Type
2	u	103	LEU
2	u	106	LEU
2	u	124	LYS
2	u	162	MET
2	t	3	ILE
2	t	8	THR
2	t	22	ASP
2	t	23	VAL
2	t	26	LEU
2	t	54	GLU
2	t	63	ASN
2	t	66	ARG
2	t	71	ASN
2	t	79	SER
2	t	82	ASN
2	t	103	LEU
2	t	106	LEU
2	t	124	LYS
2	t	162	MET
2	v	3	ILE
2	v	8	THR
2	v	22	ASP
2	v	23	VAL
2	v	26	LEU
2	v	54	GLU
2	v	66	ARG
2	v	71	ASN
2	v	79	SER
2	v	82	ASN
2	v	103	LEU
2	v	106	LEU
2	v	124	LYS
2	v	162	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	N	369	ASN
2	q	63	ASN
2	s	63	ASN
2	r	63	ASN
2	t	63	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates 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.