



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 05:14 PM UTC

PDB ID : 3J9Q / pdb_00003j9q
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 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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

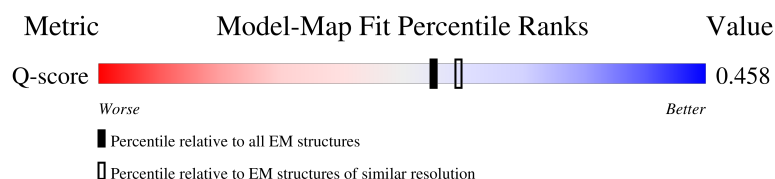
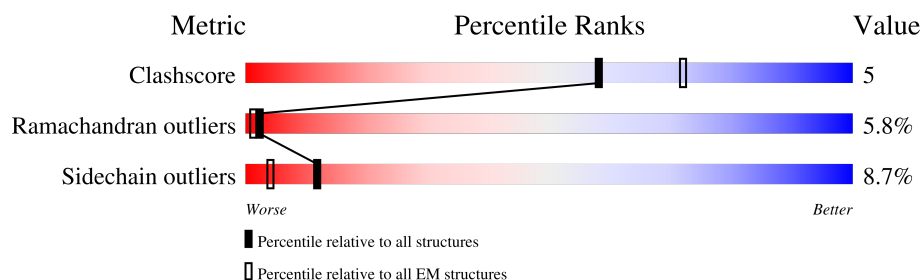
1 Overall quality at a glance

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	A	386	12% 81% 15% ..
1	B	386	12% 81% 15% ..
1	C	386	13% 82% 15% ..
1	D	386	12% 82% 15% ..

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Mol	Chain	Length	Quality of chain
1	E	386	12% 80% 16% ..
1	F	386	13% 82% 15% ..
1	G	386	13% 82% 14% ..
1	H	386	14% 83% 13% ..
1	I	386	13% 81% 15% .
1	J	386	13% 82% 13% ..
1	K	386	13% 82% 14% ..
1	L	386	13% 83% 13% .
1	M	386	13% 83% 13% .
1	N	386	13% 83% 13% ..
1	O	386	13% 81% 15% ..
1	P	386	14% 83% 13% .
1	Q	386	12% 82% 14% ..
1	R	386	13% 82% 14% ..
1	X	386	13% 83% 14% ..
1	a	386	12% 81% 15% ..
1	d	386	13% 81% 15% ..
1	g	386	12% 81% 15% ..
1	j	386	13% 82% 14% .
1	m	386	12% 81% 15% .
2	S	168	5% 74% 23% ..
2	T	168	. 73% 23% ..
2	U	168	5% 73% 23% ..
2	V	168	5% 71% 24% ..
2	W	168	5% 74% 23% ..

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Mol	Chain	Length	Quality of chain
2	Y	168	
2	Z	168	
2	b	168	
2	c	168	
2	e	168	
2	f	168	
2	h	168	
2	i	168	
2	k	168	
2	l	168	
2	n	168	
2	o	168	
2	p	168	
2	q	168	
2	r	168	
2	s	168	
2	t	168	
2	u	168	
2	v	168	

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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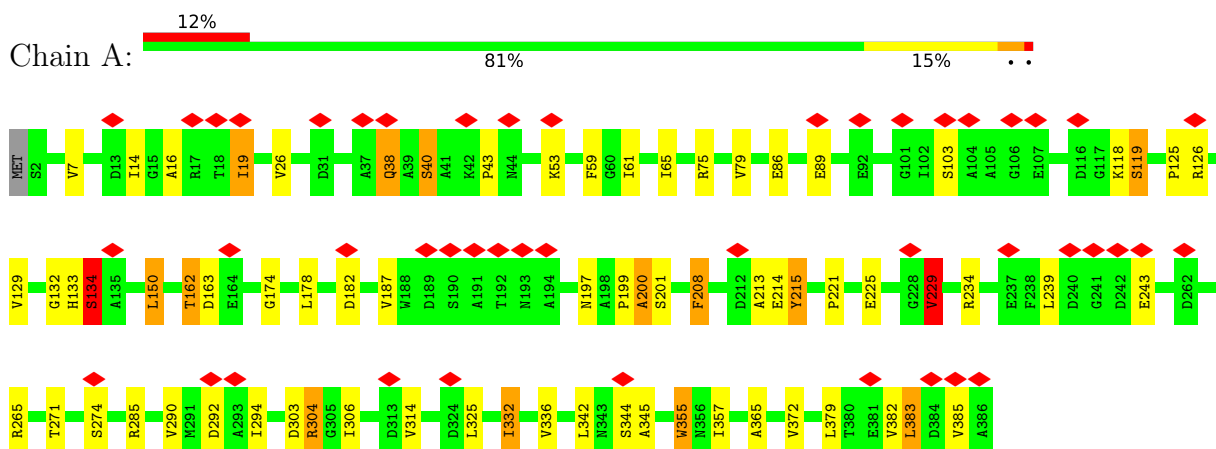
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Mol	Chain	Residues	Atoms					AltConf	Trace
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			1255	795	214	242	4		
2	i	166	Total	C	N	O	S	0	0
			1255	795	214	242	4		
2	f	166	Total	C	N	O	S	0	0
			1255	795	214	242	4		
2	o	166	Total	C	N	O	S	0	0
			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		

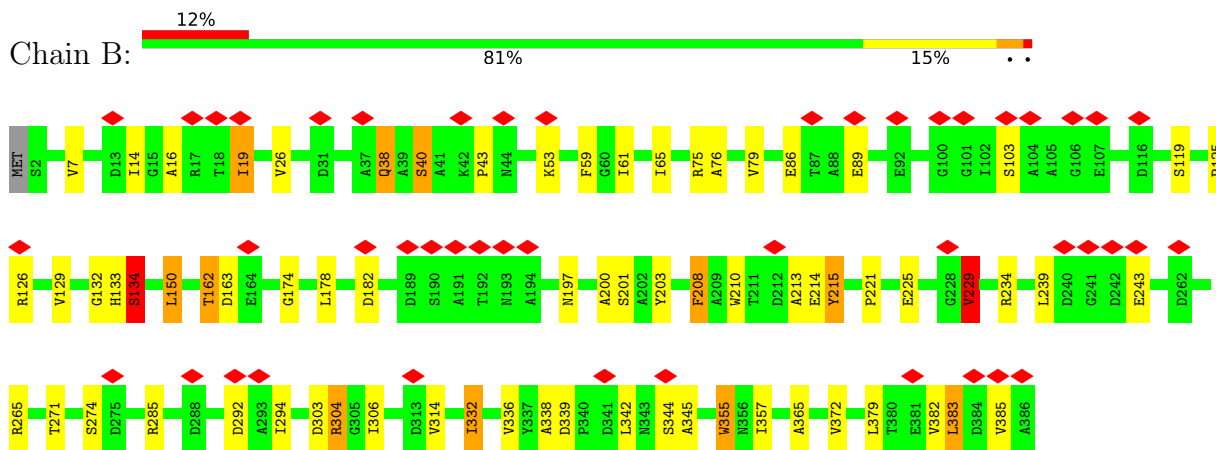
3 Residue-property plots

These plots are drawn for all protein, RNA, 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.

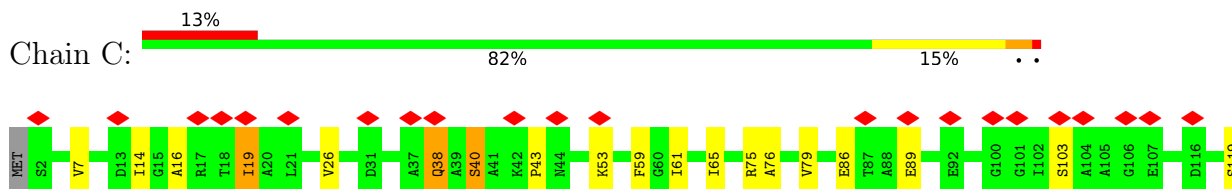
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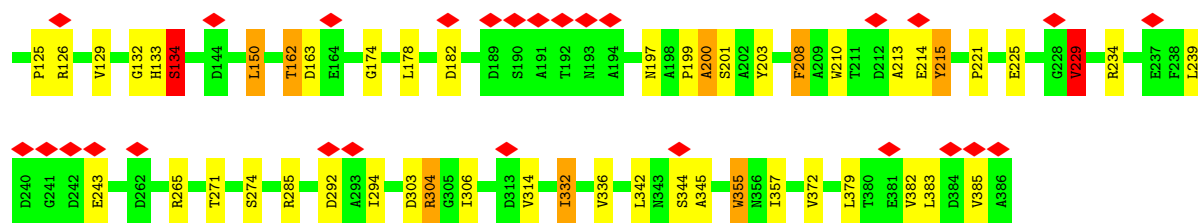


- Molecule 1: sheath

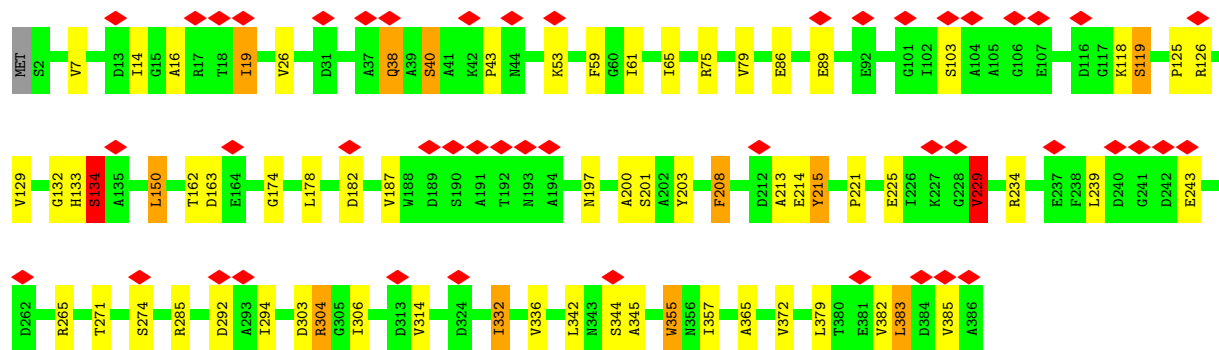
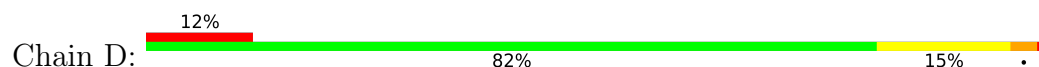


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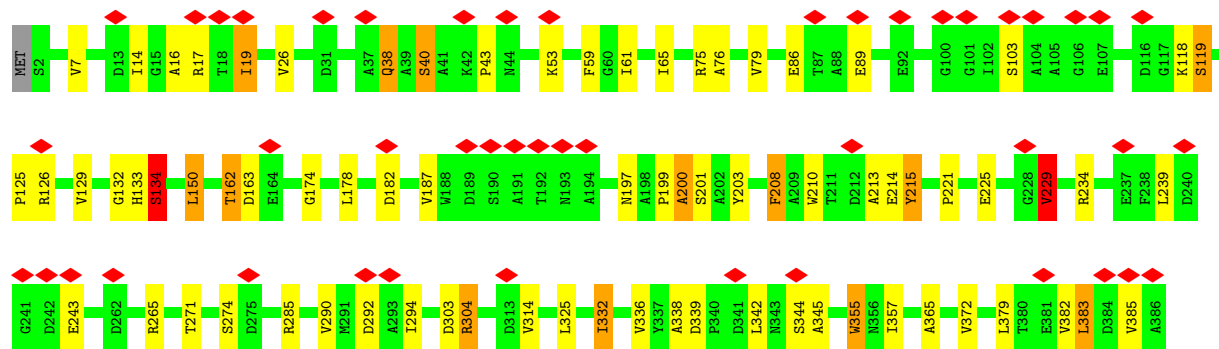
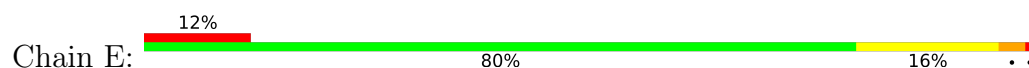




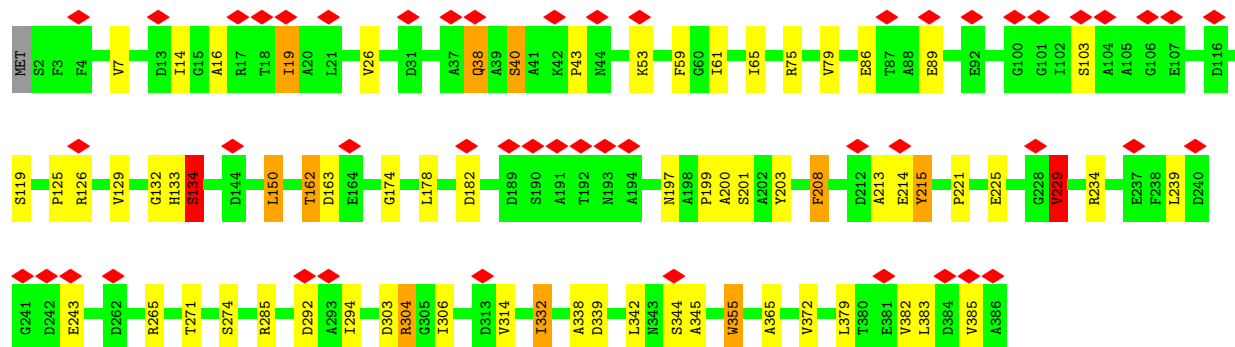
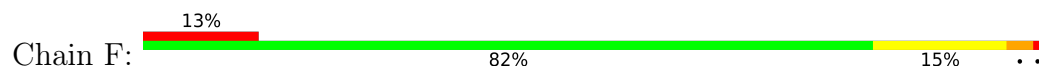
- Molecule 1: sheath



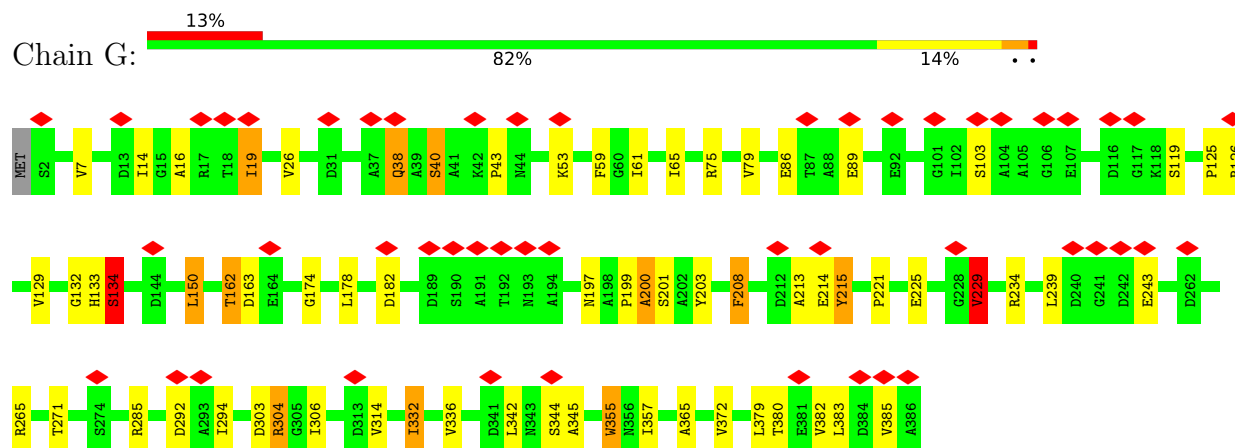
- Molecule 1: sheath



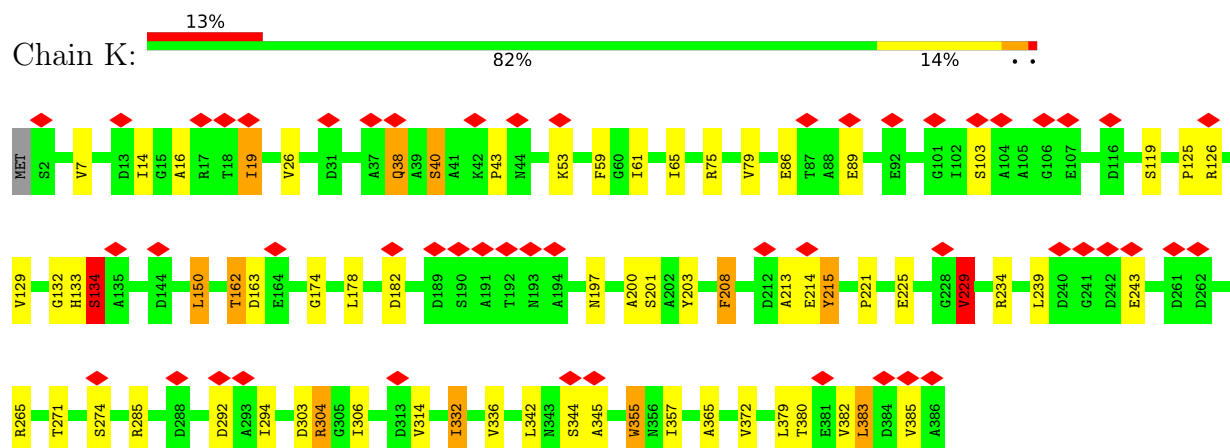
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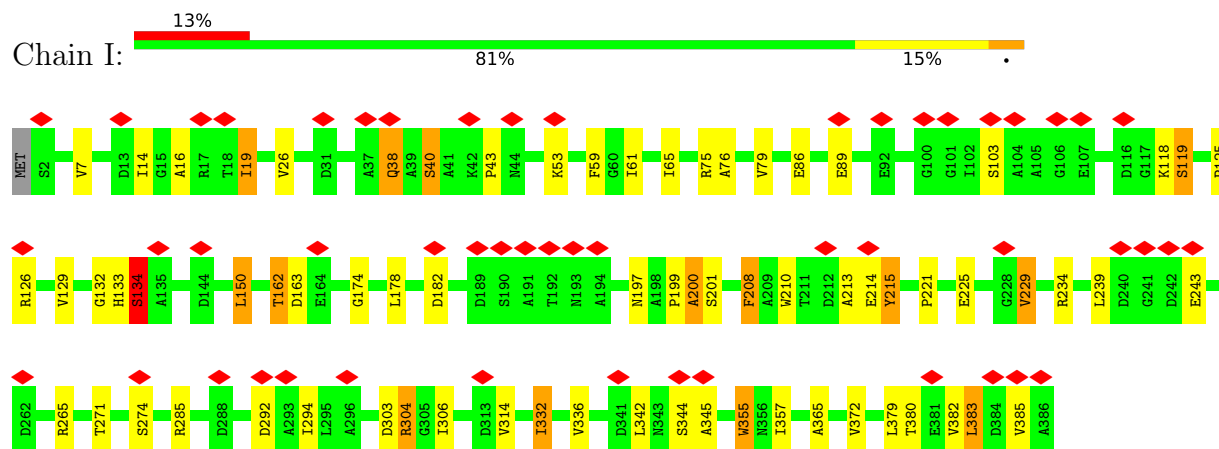
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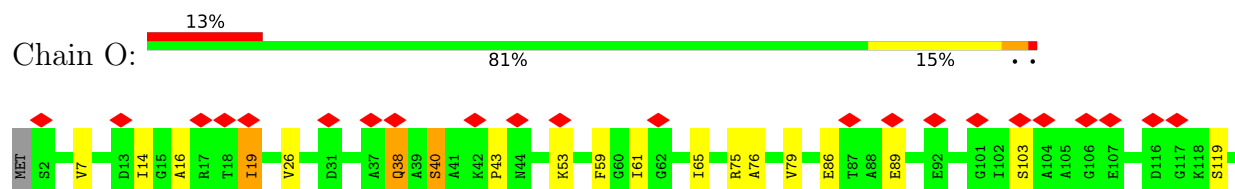
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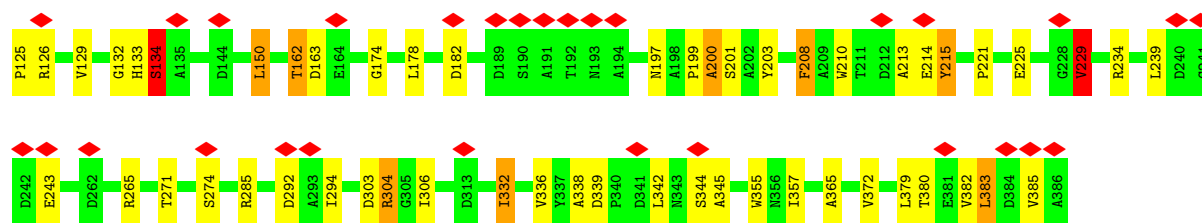


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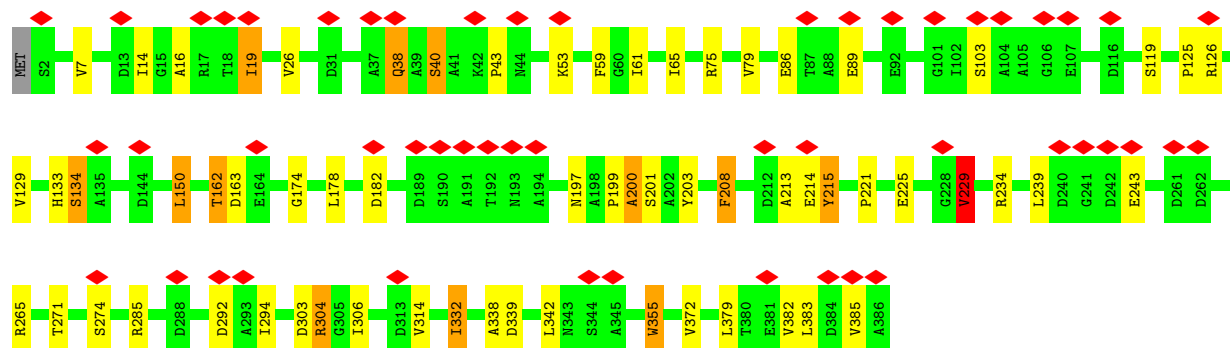
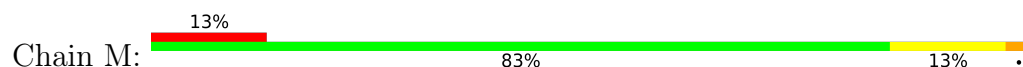


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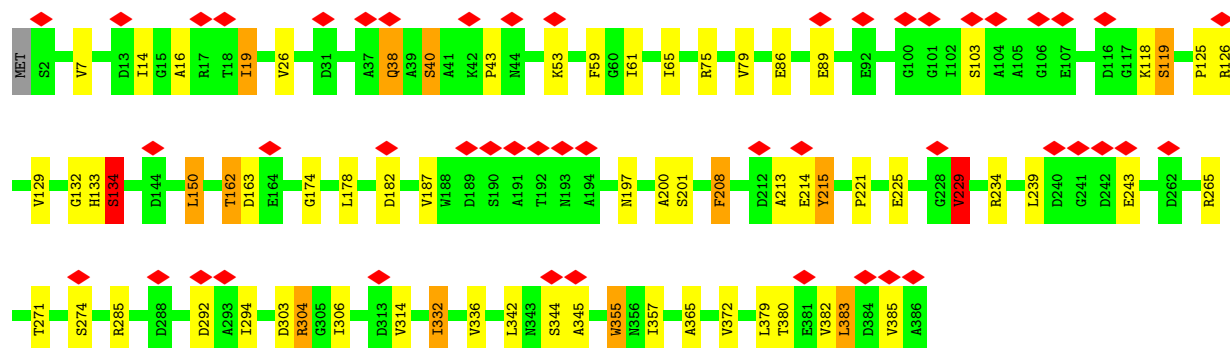
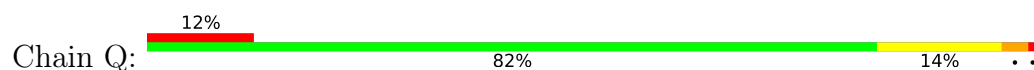




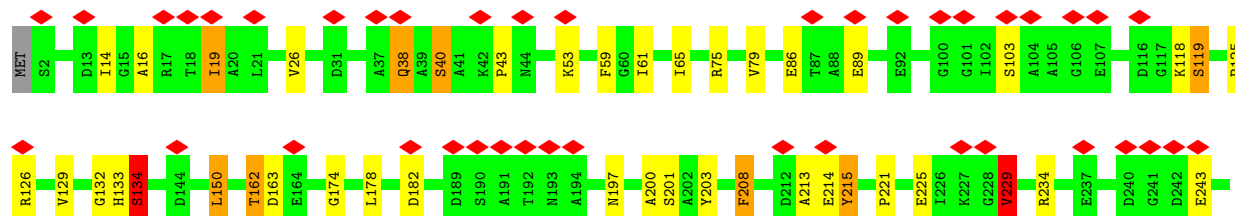
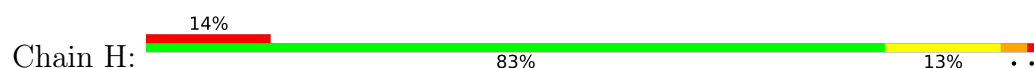
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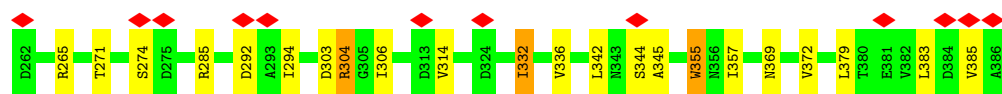


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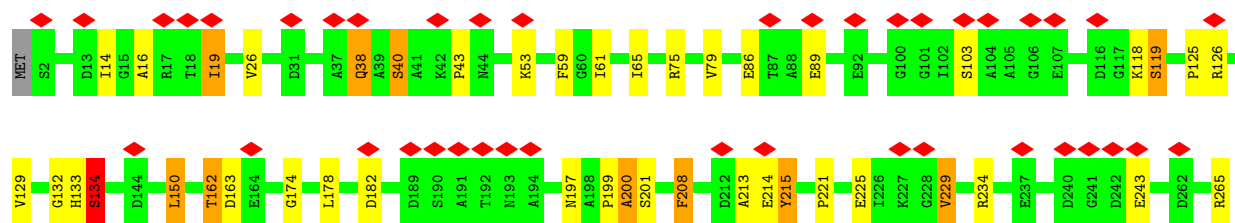
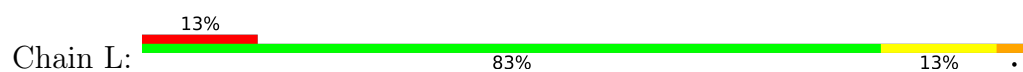


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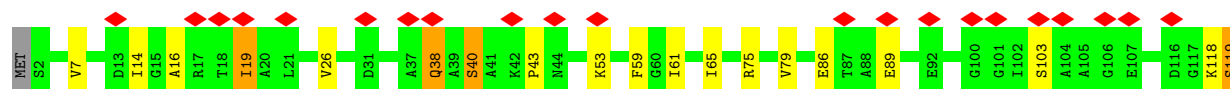
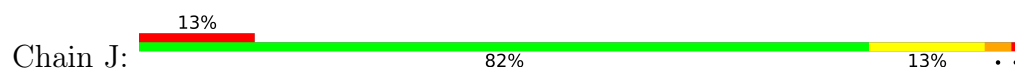




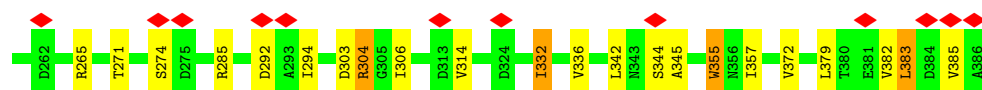
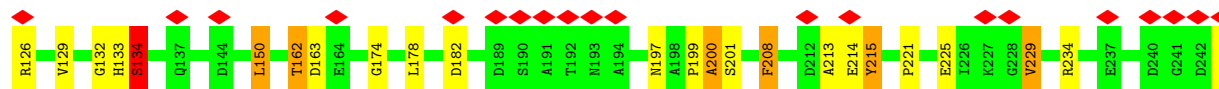
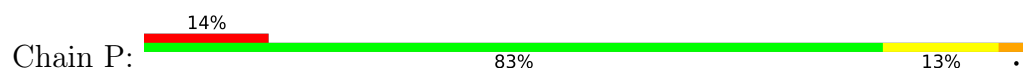
- Molecule 1: sheath



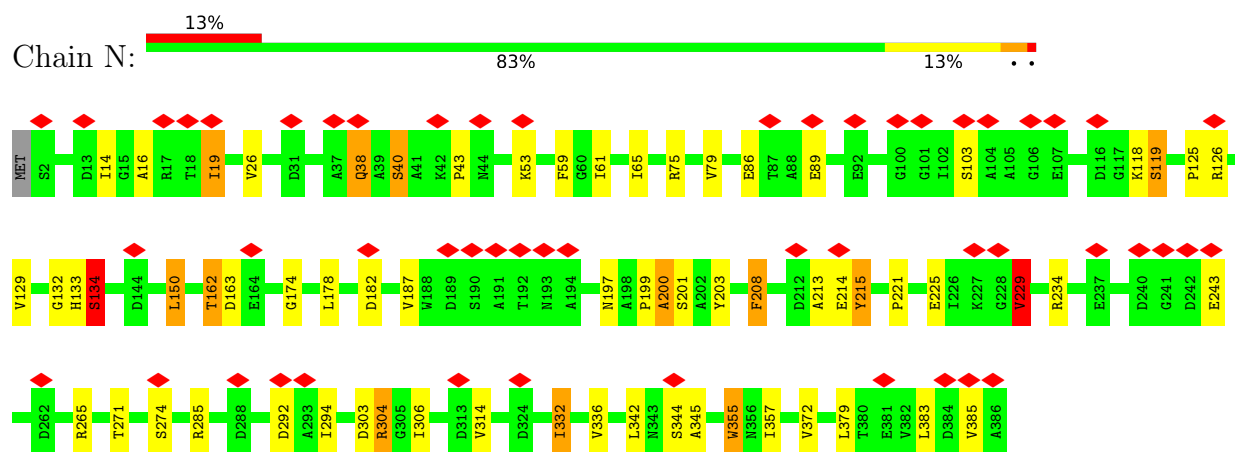
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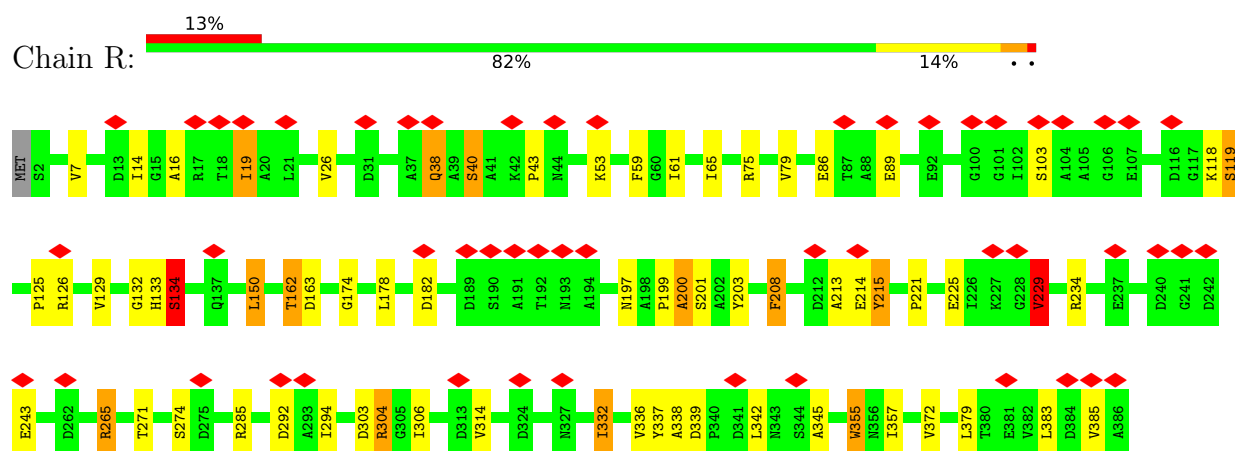
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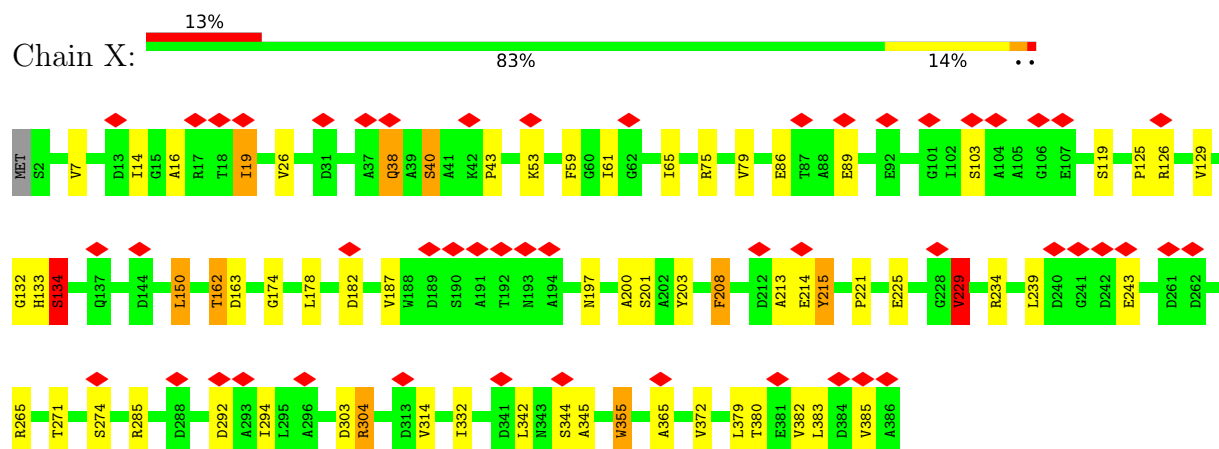
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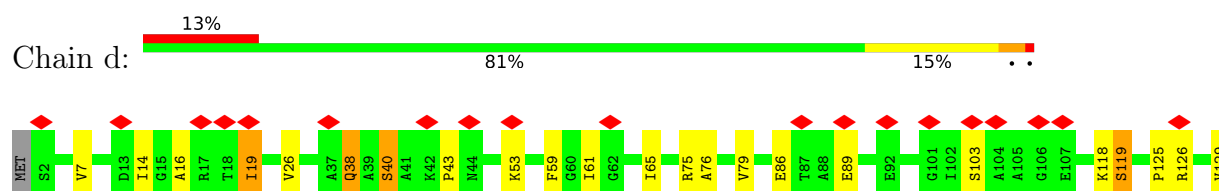
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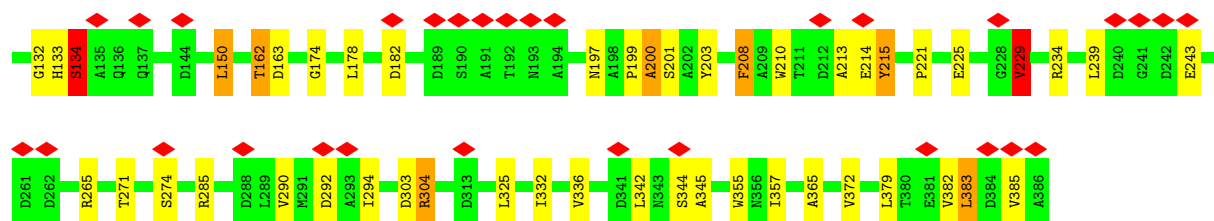


• Molecule 1: sheath

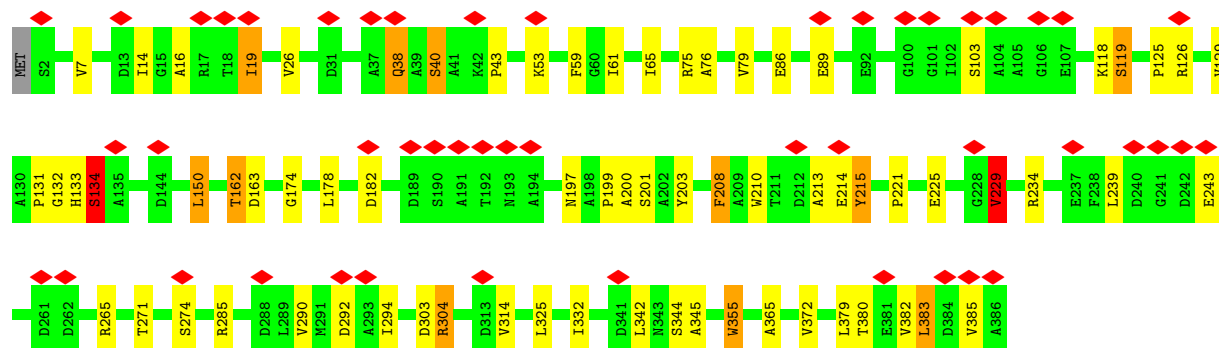
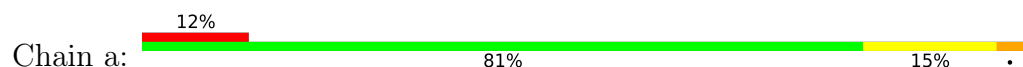


• Molecule 1: sheath

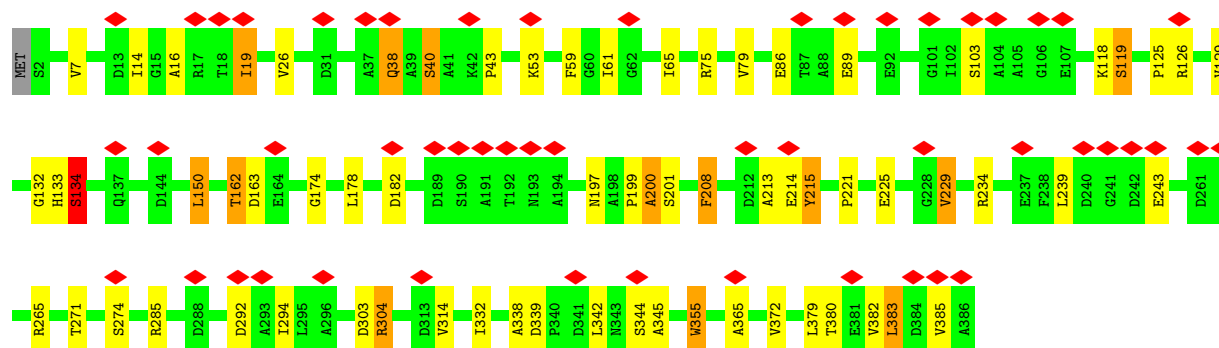
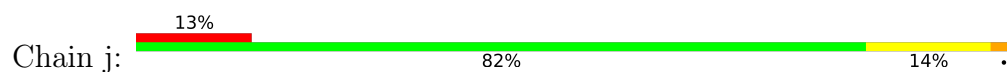




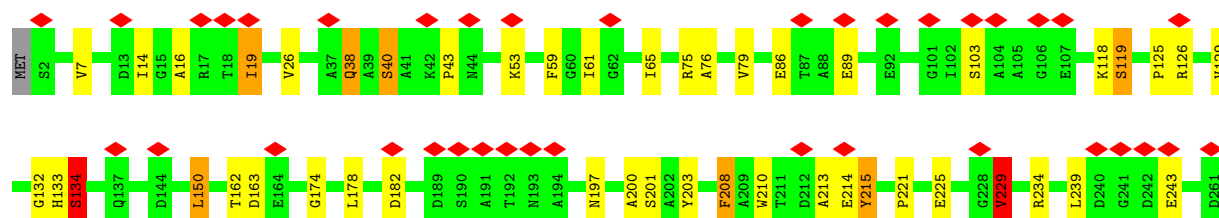
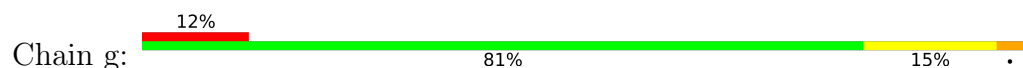
• Molecule 1: sheath



• Molecule 1: sheath

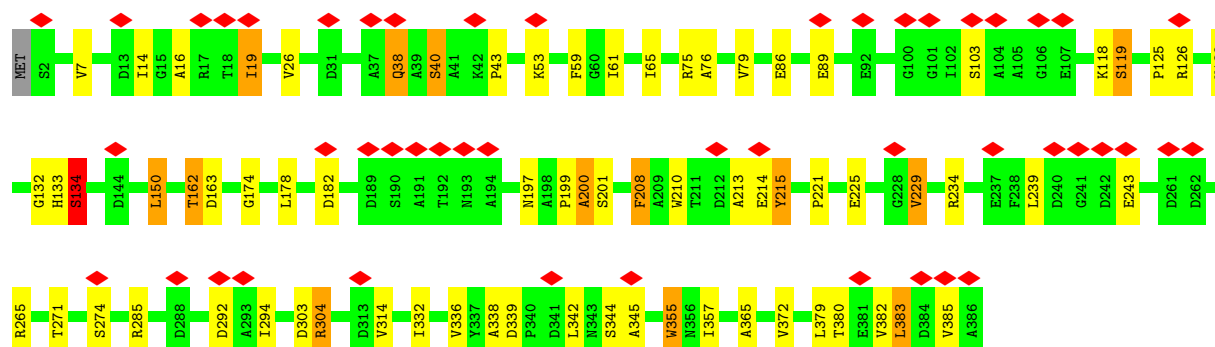
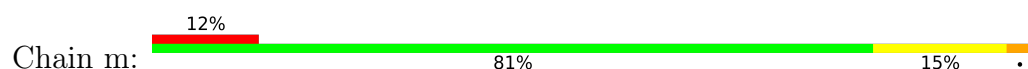


• Molecule 1: sheath

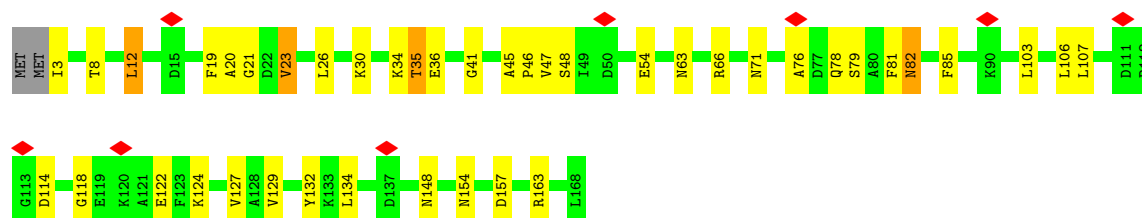
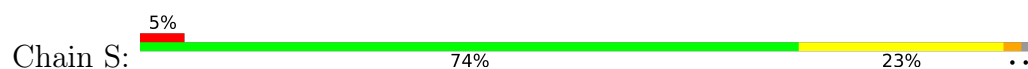




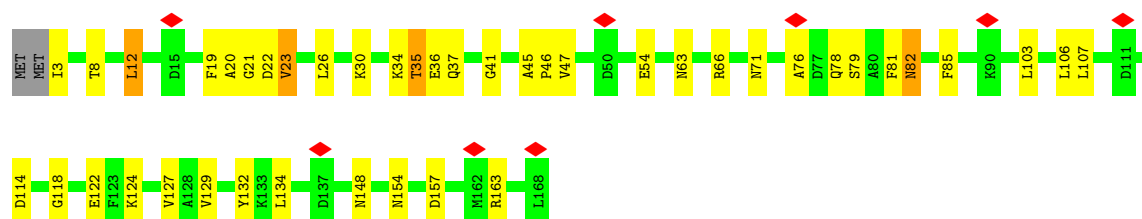
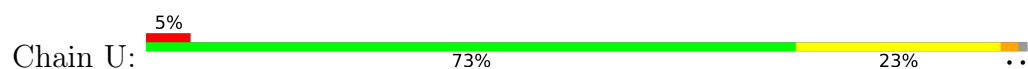
- Molecule 1: sheath



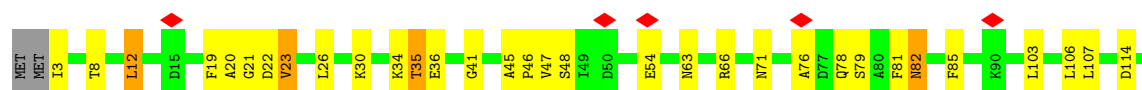
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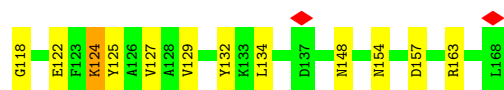


- Molecule 2: tube

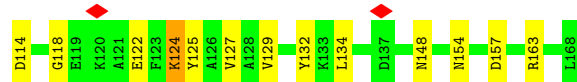
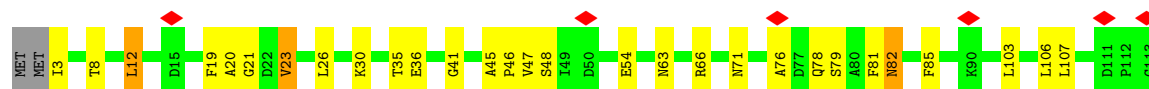
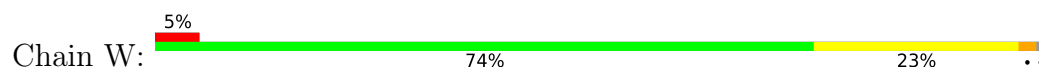


- Molecule 2: tube

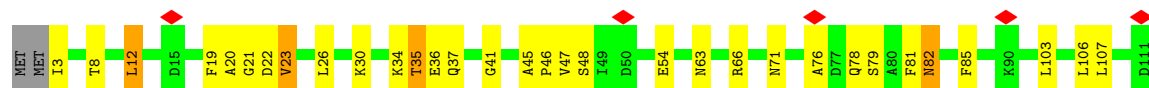




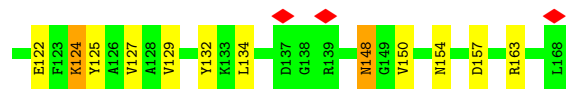
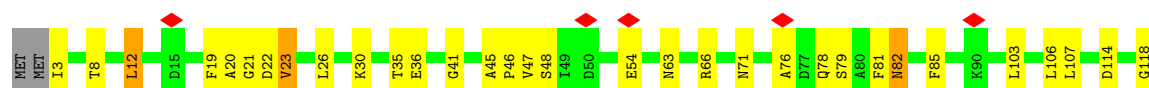
- Molecule 2: tube



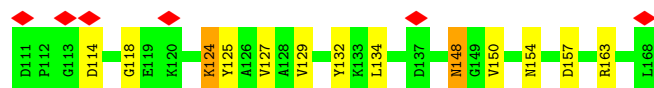
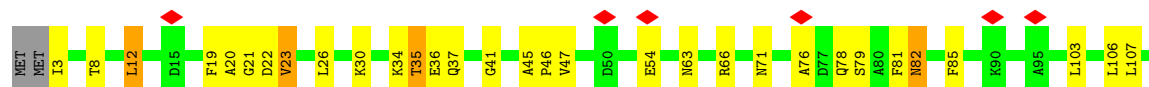
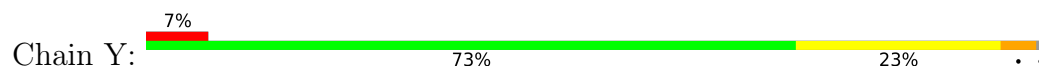
- Molecule 2: tube



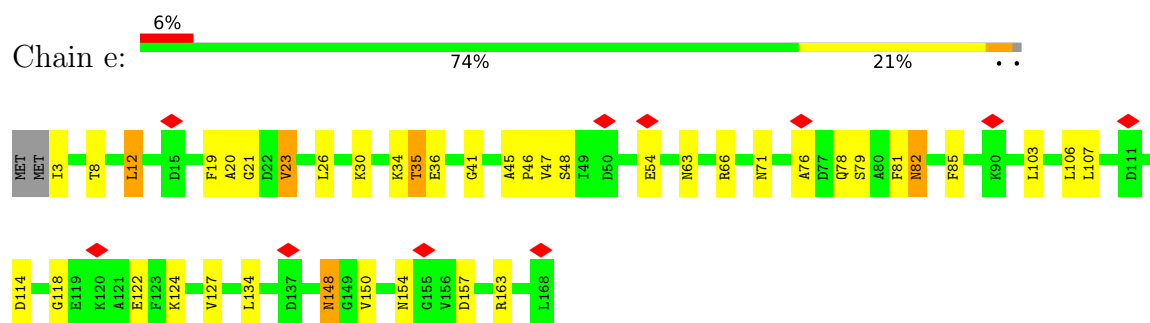
- Molecule 2: tube



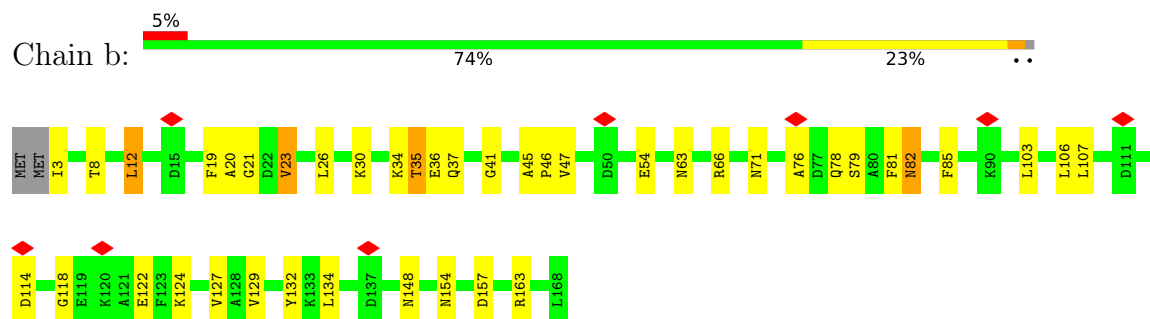
- Molecule 2: tube



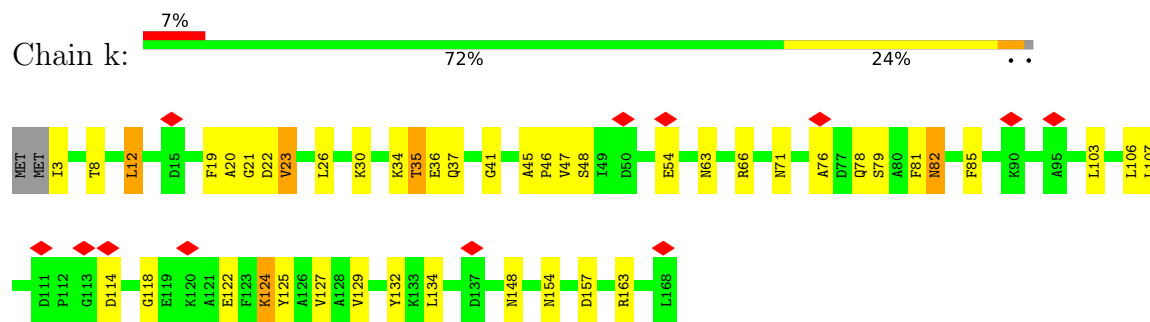
- Molecule 2: tube



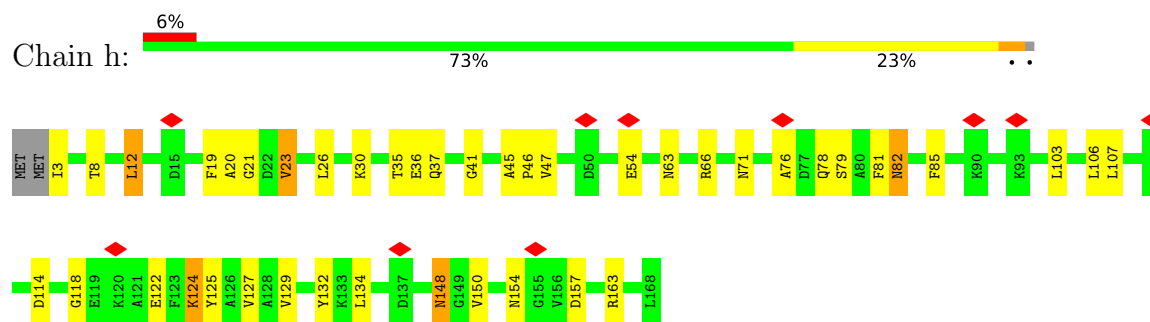
- Molecule 2: tube



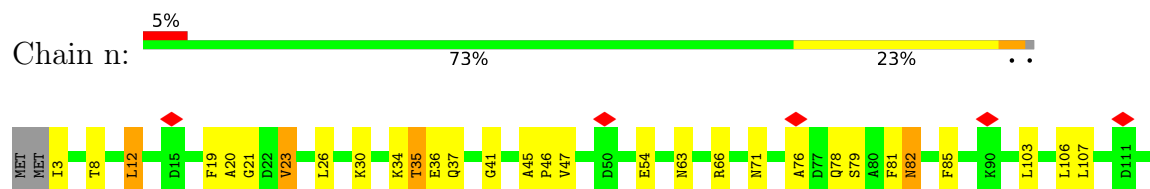
- Molecule 2: tube

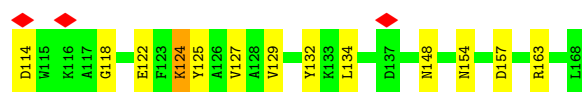


- Molecule 2: tube

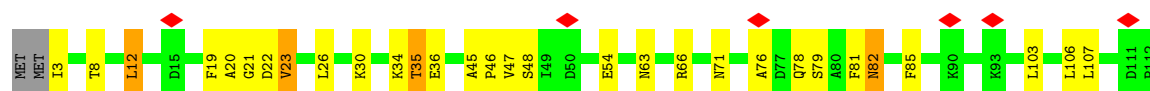


- Molecule 2: tube

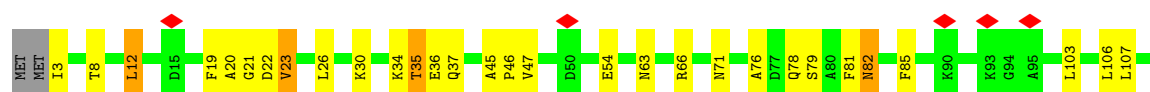




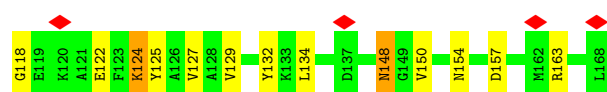
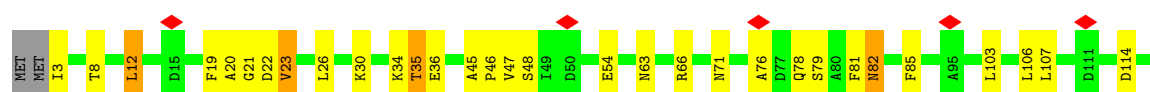
- Molecule 2: tube



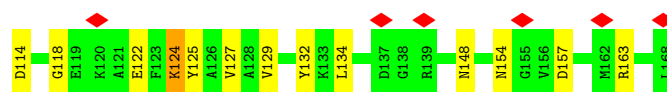
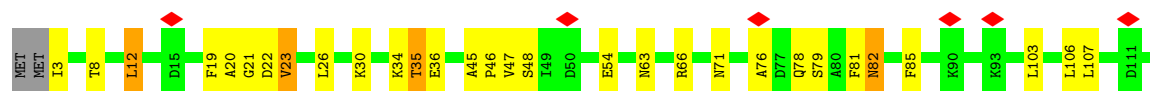
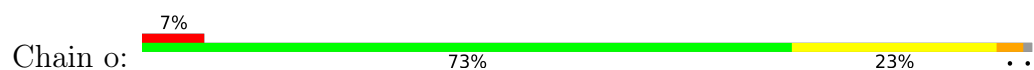
- Molecule 2: tube



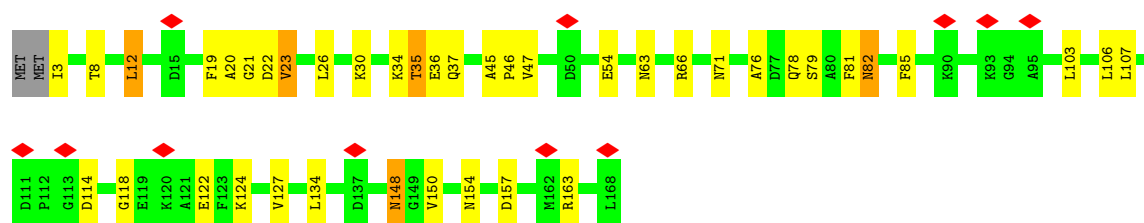
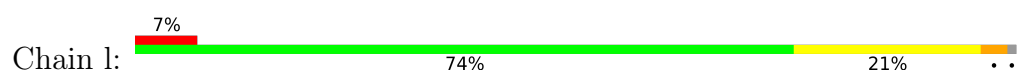
- Molecule 2: tube



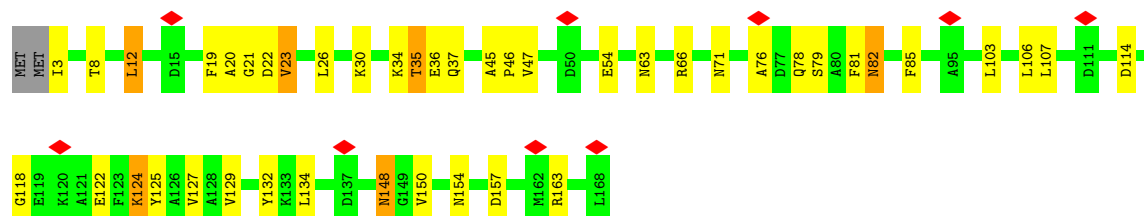
- Molecule 2: tube



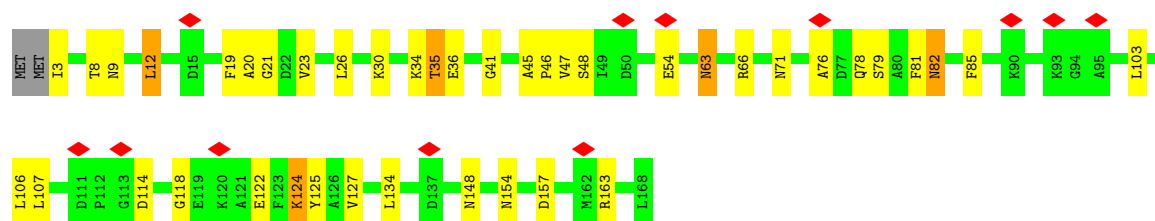
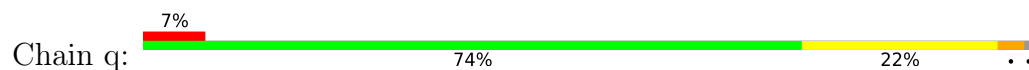
- Molecule 2: tube



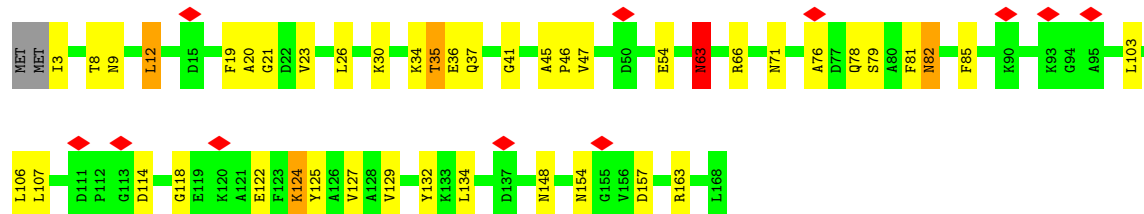
• Molecule 2: tube



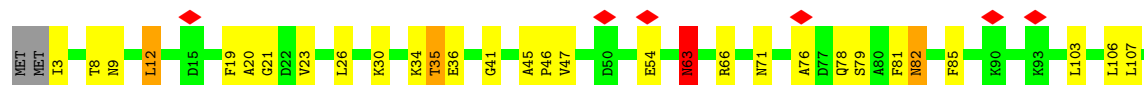
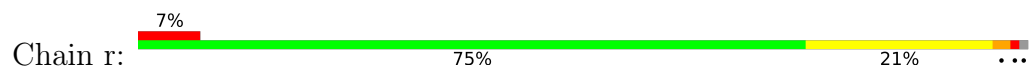
• Molecule 2: tube

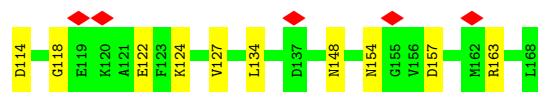


• Molecule 2: tube

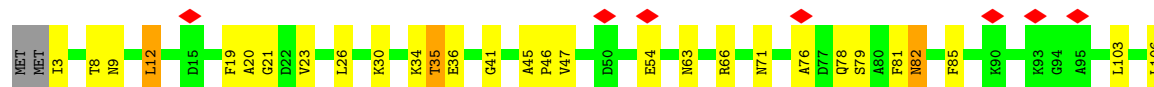
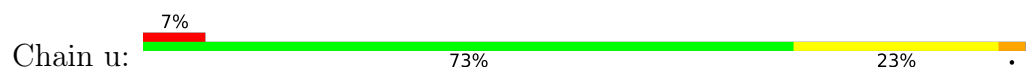


• Molecule 2: tube

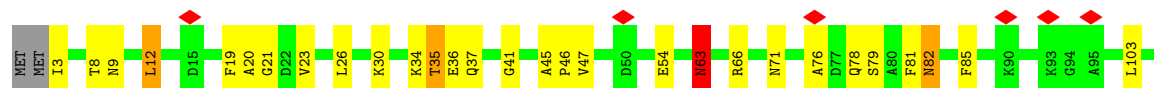




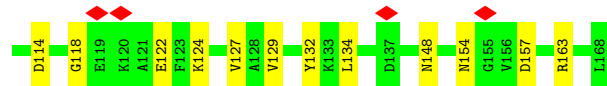
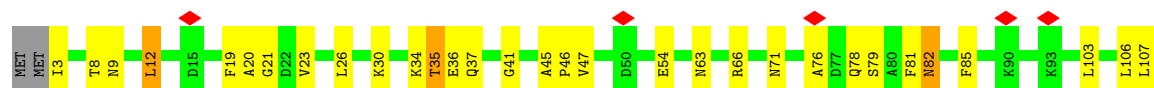
- Molecule 2: tube



- Molecule 2: tube



- Molecule 2: tube



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=18.3°, rise=38.4 Å, axial sym=C6	Depositor
Number of segments used	Not provided	
Resolution determination method	FSC 0.143 CUT-OFF	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
Maximum map value	0.295	Depositor
Minimum map value	-0.183	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	463.68, 463.68, 463.68	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.104, 1.104, 1.104	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	A	0.42	0/2955	0.73	0/4027
1	B	0.42	0/2955	0.73	0/4027
1	C	0.41	0/2955	0.72	0/4027
1	D	0.43	0/2955	0.73	0/4027
1	E	0.42	0/2955	0.73	0/4027
1	F	0.42	0/2955	0.73	0/4027
1	G	0.42	0/2955	0.73	0/4027
1	H	0.52	2/2955 (0.1%)	0.73	1/4027 (0.0%)
1	I	0.42	0/2955	0.73	0/4027
1	J	0.41	0/2955	0.72	1/4027 (0.0%)
1	K	0.42	0/2955	0.73	0/4027
1	L	0.42	0/2955	0.73	0/4027
1	M	0.42	0/2955	0.73	0/4027
1	N	0.42	0/2955	0.73	0/4027
1	O	0.42	0/2955	0.73	0/4027
1	P	0.42	0/2955	0.73	0/4027
1	Q	0.42	0/2955	0.73	0/4027
1	R	0.42	0/2955	0.73	1/4027 (0.0%)
1	X	0.42	0/2955	0.72	0/4027
1	a	0.43	1/2955 (0.0%)	0.72	0/4027
1	d	0.41	0/2955	0.73	0/4027
1	g	0.42	0/2955	0.73	1/4027 (0.0%)
1	j	0.43	0/2955	0.73	0/4027
1	m	0.41	0/2955	0.73	0/4027
2	S	0.47	0/1277	0.78	0/1724
2	T	0.47	0/1277	0.78	0/1724
2	U	0.47	0/1277	0.78	0/1724
2	V	0.47	0/1277	0.77	0/1724
2	W	0.47	0/1277	0.77	0/1724
2	Y	0.47	0/1277	0.78	0/1724
2	Z	0.47	0/1277	0.78	0/1724
2	b	0.47	0/1277	0.78	0/1724
2	c	0.47	0/1277	0.78	0/1724
2	e	0.47	0/1277	0.78	0/1724

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	f	0.47	0/1277	0.78	0/1724
2	h	0.47	0/1277	0.78	0/1724
2	i	0.46	0/1277	0.78	0/1724
2	k	0.47	0/1277	0.77	0/1724
2	l	0.46	0/1277	0.78	0/1724
2	n	0.47	0/1277	0.78	0/1724
2	o	0.46	0/1277	0.78	0/1724
2	p	0.47	0/1277	0.78	0/1724
2	q	0.70	4/1277 (0.3%)	0.79	0/1724
2	r	0.70	4/1277 (0.3%)	0.79	0/1724
2	s	0.68	4/1277 (0.3%)	0.79	0/1724
2	t	0.68	4/1277 (0.3%)	0.79	0/1724
2	u	0.58	2/1277 (0.2%)	0.78	0/1724
2	v	0.59	2/1277 (0.2%)	0.78	0/1724
All	All	0.46	23/101568 (0.0%)	0.74	4/138024 (0.0%)

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	369	ASN	CG-ND2	-13.53	1.04	1.33
2	q	63	ASN	CG-ND2	-11.33	1.09	1.33
2	r	63	ASN	CG-ND2	-11.31	1.09	1.33
2	s	63	ASN	CG-ND2	-11.05	1.10	1.33
2	t	63	ASN	CG-ND2	-10.99	1.10	1.33
2	v	9	ASN	CG-ND2	-10.69	1.10	1.33
2	q	9	ASN	CG-ND2	-10.64	1.10	1.33
2	r	9	ASN	CG-ND2	-10.58	1.11	1.33
2	t	9	ASN	CG-ND2	-10.24	1.11	1.33
2	s	9	ASN	CG-ND2	-10.13	1.11	1.33
2	u	9	ASN	CG-ND2	-10.12	1.11	1.33
1	H	369	ASN	CG-OD1	-10.06	1.04	1.23
2	r	9	ASN	CG-OD1	-8.54	1.07	1.23
2	v	9	ASN	CG-OD1	-8.44	1.07	1.23
2	s	9	ASN	CG-OD1	-8.18	1.08	1.23
2	t	9	ASN	CG-OD1	-8.05	1.08	1.23
2	q	9	ASN	CG-OD1	-8.05	1.08	1.23
2	u	9	ASN	CG-OD1	-7.61	1.09	1.23
2	q	63	ASN	CG-OD1	-7.54	1.09	1.23
2	r	63	ASN	CG-OD1	-7.30	1.09	1.23
2	s	63	ASN	CG-OD1	-7.07	1.10	1.23
2	t	63	ASN	CG-OD1	-7.03	1.10	1.23
1	a	131	PRO	C-O	5.30	1.30	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	369	ASN	OD1-CG-ND2	-5.68	116.92	122.60
1	R	265	ARG	N-CA-C	5.02	116.44	108.96
1	g	265	ARG	N-CA-C	5.01	116.43	108.96
1	J	265	ARG	N-CA-C	5.01	116.42	108.96

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	32	0
1	B	2897	0	2855	30	0
1	C	2897	0	2855	29	0
1	D	2897	0	2855	30	0
1	E	2897	0	2855	35	0
1	F	2897	0	2855	29	0
1	G	2897	0	2855	29	0
1	H	2897	0	2855	26	0
1	I	2897	0	2855	31	0
1	J	2897	0	2855	27	0
1	K	2897	0	2855	29	0
1	L	2897	0	2855	27	0
1	M	2897	0	2855	25	0
1	N	2897	0	2855	27	0
1	O	2897	0	2855	31	0
1	P	2897	0	2855	27	0
1	Q	2897	0	2855	30	0
1	R	2897	0	2855	28	0
1	X	2897	0	2855	25	0
1	a	2897	0	2855	29	0
1	d	2897	0	2855	28	0
1	g	2897	0	2855	28	0
1	j	2897	0	2855	27	0
1	m	2897	0	2855	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	S	1255	0	1246	13	0
2	T	1255	0	1246	15	0
2	U	1255	0	1246	14	0
2	V	1255	0	1246	16	0
2	W	1255	0	1246	13	0
2	Y	1255	0	1246	16	0
2	Z	1255	0	1246	15	0
2	b	1255	0	1246	13	0
2	c	1255	0	1246	15	0
2	e	1255	0	1246	13	0
2	f	1255	0	1246	15	0
2	h	1255	0	1246	14	0
2	i	1255	0	1246	14	0
2	k	1255	0	1246	15	0
2	l	1255	0	1246	13	0
2	n	1255	0	1246	14	0
2	o	1255	0	1246	14	0
2	p	1255	0	1246	15	0
2	q	1255	0	1246	11	0
2	r	1255	0	1246	11	0
2	s	1255	0	1246	13	0
2	t	1255	0	1246	13	0
2	u	1255	0	1246	14	0
2	v	1255	0	1246	12	0
All	All	99648	0	98424	938	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 5.

All (938) 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:p:81:PHE:CE2	2:p:127:VAL:HG11	2.24	0.72
2:s:81:PHE:CE2	2:s:127:VAL:HG11	2.24	0.72
2:b:81:PHE:CE2	2:b:127:VAL:HG11	2.24	0.72
2:n:81:PHE:CE2	2:n:127:VAL:HG11	2.24	0.72
2:o:81:PHE:CE2	2:o:127:VAL:HG11	2.24	0.72
2:c:81:PHE:CE2	2:c:127:VAL:HG11	2.24	0.72
2:t:81:PHE:CE2	2:t:127:VAL:HG11	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:81:PHE:CE2	2:f:127:VAL:HG11	2.24	0.72
2:h:81:PHE:CE2	2:h:127:VAL:HG11	2.24	0.71
2:v:81:PHE:CE2	2:v:127:VAL:HG11	2.24	0.71
2:k:81:PHE:CE2	2:k:127:VAL:HG11	2.25	0.71
2:V:81:PHE:CE2	2:V:127:VAL:HG11	2.24	0.71
2:i:81:PHE:CE2	2:i:127:VAL:HG11	2.29	0.68
2:T:81:PHE:CE2	2:T:127:VAL:HG11	2.30	0.67
2:u:81:PHE:CE2	2:u:127:VAL:HG11	2.30	0.67
2:e:81:PHE:CE2	2:e:127:VAL:HG11	2.30	0.67
2:q:81:PHE:CE2	2:q:127:VAL:HG11	2.30	0.66
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
2:r:81:PHE:CE2	2:r:127:VAL:HG11	2.31	0.66
1:d:225:GLU:OE2	1:d:265:ARG:NH2	2.29	0.66
2:l:81:PHE:CE2	2:l:127:VAL:HG11	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
2:S:81:PHE:CE2	2:S:127:VAL:HG11	2.30	0.65
1:L:225:GLU:OE2	1:L:265:ARG:NH2	2.29	0.65
1:X:225:GLU:OE2	1:X:265:ARG:NH2	2.29	0.65
1:N:225:GLU:OE2	1:N:265:ARG:NH2	2.29	0.65
1:G:225:GLU:OE2	1:G:265:ARG:NH2	2.29	0.65
1:I:225:GLU:OE2	1:I:265:ARG:NH2	2.29	0.65
1:J:225:GLU:OE2	1:J:265:ARG:NH2	2.29	0.65
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:g:225:GLU:OE2	1:g:265:ARG:NH2	2.29	0.65
1:a:225:GLU:OE2	1:a:265:ARG:NH2	2.30	0.65
1:m:225:GLU:OE2	1:m:265:ARG:NH2	2.29	0.65
1:Q:225:GLU:OE2	1:Q:265:ARG:NH2	2.29	0.65
1:H:225:GLU:OE2	1:H:265:ARG:NH2	2.30	0.65
1:P:225:GLU:OE2	1:P:265:ARG:NH2	2.30	0.65
1:R:225:GLU:OE2	1:R:265:ARG:NH2	2.29	0.65
1:D:225:GLU:OE2	1:D:265:ARG:NH2	2.30	0.65
1:j:225:GLU:OE2	1:j:265:ARG:NH2	2.29	0.65
1:A:225:GLU:OE2	1:A:265:ARG:NH2	2.30	0.64
1:M:225:GLU:OE2	1:M:265:ARG:NH2	2.30	0.64
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:K:225:GLU:OE1	1:K:225:GLU:N	2.32	0.63
1:j:225:GLU:N	1:j:225:GLU:OE1	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:225:GLU:N	1:Q:225:GLU:OE1	2.32	0.63
1:d:225:GLU:OE1	1:d:225:GLU:N	2.32	0.63
1:E:225:GLU:N	1:E: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:OE1	1:P:225:GLU:N	2.32	0.63
1:C:225:GLU:N	1:C:225:GLU:OE1	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:A:225:GLU:OE1	1:A:225:GLU:N	2.32	0.63
1:F:225:GLU:OE1	1:F:225:GLU:N	2.32	0.63
1:L:225:GLU:N	1:L:225:GLU:OE1	2.32	0.63
1:J:225:GLU:N	1:J:225:GLU:OE1	2.32	0.63
1:X:225:GLU:N	1:X:225:GLU:OE1	2.32	0.63
1:a:225:GLU:OE1	1:a:225:GLU:N	2.32	0.62
1:D:225:GLU:OE1	1:D:225:GLU:N	2.32	0.62
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:M:225:GLU:N	1:M:225:GLU:OE1	2.32	0.62
1:R:225:GLU:N	1:R:225:GLU:OE1	2.32	0.62
2:U:63:ASN:O	2:U:63:ASN:ND2	2.31	0.62
1:G:225:GLU:N	1:G:225:GLU:OE1	2.32	0.62
1:N:225:GLU:N	1:N:225:GLU:OE1	2.32	0.62
1:B:225:GLU:N	1:B:225:GLU:OE1	2.32	0.62
2:k:107:LEU:HA	2:k:127:VAL:HG12	1.82	0.62
2:o:107:LEU:HA	2:o:127:VAL:HG12	1.82	0.61
2:c:63:ASN:O	2:c:63:ASN:ND2	2.32	0.61
2:e:63:ASN:O	2:e:63:ASN:ND2	2.34	0.61
2:b:63:ASN:ND2	2:b:63:ASN:O	2.34	0.60
2:c:107:LEU:HA	2:c:127:VAL:HG12	1.83	0.60
2:W:63:ASN:O	2:W:63:ASN:ND2	2.35	0.60
2:V:107:LEU:HA	2:V:127:VAL:HG12	1.82	0.60
2:t:107:LEU:HA	2:t:127:VAL:HG12	1.82	0.60
2:Y:107:LEU:HA	2:Y:127:VAL:HG12	1.83	0.60
2:h:63:ASN:O	2:h:63:ASN:ND2	2.34	0.60
1:B:126:ARG:NH1	1:B:292:ASP:OD1	2.35	0.60
2:V:63:ASN:ND2	2:V:63:ASN:O	2.34	0.60
2:i:63:ASN:O	2:i:63:ASN:ND2	2.35	0.60
2:s:107:LEU:HA	2:s:127:VAL:HG12	1.84	0.60
1:K:126:ARG:NH1	1:K:292:ASP:OD1	2.35	0.60
2:f:107:LEU:HA	2:f:127:VAL:HG12	1.84	0.60
2:l:63:ASN:ND2	2:l:63:ASN:O	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:p:107:LEU:HA	2:p:127:VAL:HG12	1.84	0.60
1:C:126:ARG:NH1	1:C:292:ASP:OD1	2.35	0.60
1:J:126:ARG:NH1	1:J:292:ASP:OD1	2.35	0.60
1:L:126:ARG:NH1	1:L:292:ASP:OD1	2.35	0.60
2:o:63:ASN:O	2:o:63:ASN:ND2	2.35	0.60
1:A:126:ARG:NH1	1:A:292:ASP:OD1	2.35	0.59
1:N:126:ARG:NH1	1:N: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:O	2:Z:63:ASN:ND2	2.35	0.59
2:k:63:ASN:O	2:k:63:ASN:ND2	2.35	0.59
1:G:126:ARG:NH1	1:G: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:O	2:Y:63:ASN:ND2	2.35	0.59
2:h:107:LEU:HA	2:h:127:VAL:HG12	1.83	0.59
2:f:63:ASN:O	2:f:63:ASN:ND2	2.35	0.59
1:I:126:ARG:NH1	1:I:292:ASP:OD1	2.35	0.59
2:b:107:LEU:HA	2:b:127:VAL:HG12	1.84	0.59
1:Q:126:ARG:NH1	1:Q:292:ASP:OD1	2.35	0.59
1:a:89:GLU:N	1:a:89:GLU:OE1	2.36	0.59
1:g:89:GLU:N	1:g:89:GLU:OE1	2.36	0.59
1:D:89:GLU:OE1	1:D:89:GLU:N	2.36	0.59
1:F:126:ARG:NH1	1:F:292:ASP:OD1	2.35	0.59
1:O:126:ARG:NH1	1:O:292:ASP:OD1	2.35	0.59
1:Q:89:GLU:N	1:Q:89:GLU:OE1	2.36	0.59
2:T:63:ASN:O	2:T:63:ASN:ND2	2.35	0.59
1:D:126:ARG:NH1	1:D:292:ASP:OD1	2.35	0.59
1:M:126:ARG:NH1	1:M:292:ASP:OD1	2.35	0.59
1:H:89:GLU:N	1:H:89:GLU:OE1	2.36	0.59
1:H:126:ARG:NH1	1:H:292:ASP:OD1	2.35	0.59
1:J:89:GLU:N	1:J:89:GLU:OE1	2.36	0.59
2:e:19:PHE:O	2:e:21:GLY:N	2.36	0.59
2:b:19:PHE:O	2:b:21:GLY:N	2.36	0.59
2:f:19:PHE:O	2:f:21:GLY:N	2.36	0.59
1:C:89:GLU:N	1:C:89:GLU:OE1	2.36	0.59
1:E:126:ARG:NH1	1:E:292:ASP:OD1	2.35	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
1:d:89:GLU:OE1	1:d:89:GLU:N	2.36	0.59
1:j:89:GLU:N	1:j:89:GLU:OE1	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:j:126:ARG:NH1	1:j:292:ASP:OD1	2.35	0.59
2:n:63:ASN:O	2:n:63:ASN:ND2	2.34	0.59
1:F:89:GLU:N	1:F:89:GLU:OE1	2.36	0.59
1:M:89:GLU:N	1:M:89:GLU:OE1	2.36	0.59
1:R:126:ARG:NH1	1:R:292:ASP:OD1	2.35	0.59
1:a:126:ARG:NH1	1:a:292:ASP:OD1	2.35	0.59
2:U:107:LEU:HA	2:U:127:VAL:HG12	1.84	0.59
2:n:107:LEU:HA	2:n:127:VAL:HG12	1.84	0.59
2:s:19:PHE:O	2:s:21:GLY:N	2.36	0.59
1:N:89:GLU:OE1	1:N:89:GLU:N	2.36	0.59
1:R:89:GLU:N	1:R:89:GLU:OE1	2.36	0.59
2:U:23:VAL:HG23	2:b:41:GLY:HA3	1.85	0.59
1:E:89:GLU:N	1:E:89:GLU:OE1	2.36	0.58
2:Y:23:VAL:HG23	2:s:41:GLY:HA3	1.85	0.58
1:A:89:GLU:N	1:A:89:GLU:OE1	2.36	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
1:P:126:ARG:NH1	1:P:292:ASP:OD1	2.35	0.58
2:h:19:PHE:O	2:h:21:GLY:N	2.36	0.58
2:c:19:PHE:O	2:c:21:GLY:N	2.36	0.58
2:i:19:PHE:O	2:i:21:GLY:N	2.36	0.58
2:o:19:PHE:O	2:o:21:GLY:N	2.36	0.58
2:p:63:ASN:O	2:p:63:ASN:ND2	2.34	0.58
2:v:107:LEU:HA	2:v:127:VAL:HG12	1.84	0.58
2:r:19:PHE:O	2:r:21:GLY:N	2.36	0.58
2:v:19:PHE:O	2:v:21:GLY:N	2.36	0.58
1:B:89:GLU:OE1	1:B:89:GLU:N	2.36	0.58
1:L:89:GLU:N	1:L:89:GLU:OE1	2.36	0.58
1:m:126:ARG:NH1	1:m:292:ASP:OD1	2.35	0.58
1:O:89:GLU:N	1:O:89:GLU:OE1	2.36	0.58
1:m:89:GLU:N	1:m:89:GLU:OE1	2.36	0.58
2:W:19:PHE:O	2:W:21:GLY:N	2.36	0.58
1:G:89:GLU:N	1:G:89:GLU:OE1	2.36	0.58
2:U:19:PHE:O	2:U:21:GLY:N	2.37	0.58
2:T:19:PHE:O	2:T:21:GLY:N	2.37	0.58
2:V:23:VAL:HG23	2:n:41:GLY:HA3	1.85	0.58
2:q:19:PHE:O	2:q:21:GLY:N	2.36	0.58
2:S:63:ASN:O	2:S:63:ASN:ND2	2.35	0.58
2:p:19:PHE:O	2:p:21:GLY:N	2.36	0.58
2:Y:19:PHE:O	2:Y:21:GLY:N	2.36	0.58
2:l:19:PHE:O	2:l:21:GLY:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:19:PHE:O	2:V:21:GLY:N	2.37	0.58
2:k:19:PHE:O	2:k:21:GLY:N	2.36	0.58
2:n:19:PHE:O	2:n:21:GLY:N	2.37	0.58
2:t:19:PHE:O	2:t:21:GLY:N	2.36	0.58
2:S:19:PHE:O	2:S:21:GLY:N	2.36	0.57
2:U:34:LYS:C	2:U:35:THR:HG1	2.12	0.57
2:u:19:PHE:O	2:u:21:GLY:N	2.36	0.57
2:k:23:VAL:HG23	2:t:41:GLY:HA3	1.86	0.57
2:Z:19:PHE:O	2:Z:21:GLY:N	2.37	0.56
2:e:34:LYS:C	2:e:35:THR:HG1	2.13	0.56
2:T:23:VAL:HG23	2:k:41:GLY:HA3	1.86	0.56
2:U:41:GLY:HA3	2:c:23:VAL:HG23	1.88	0.56
2:n:23:VAL:HG23	2:q:41:GLY:HA3	1.88	0.56
2:W:23:VAL:HG23	2:h:41:GLY:HA3	1.87	0.55
2:Y:34:LYS:C	2:Y:35:THR:HG1	2.15	0.55
1:a:26:VAL:HG23	1:a:125:PRO:HA	1.89	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
2:s:34:LYS:C	2:s:35:THR:HG1	2.14	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:d:26:VAL:HG23	1:d: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:B:26:VAL:HG23	1:B:125:PRO:HA	1.89	0.54
1:G:26:VAL:HG23	1:G:125:PRO:HA	1.90	0.54
1:j:26:VAL:HG23	1:j: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
2:v:63:ASN:ND2	2:v:63:ASN:O	2.41	0.54
1:A:26:VAL:HG23	1:A:125:PRO:HA	1.90	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:m:26:VAL:HG23	1:m:125:PRO:HA	1.90	0.54
1:H:26:VAL:HG23	1:H:125:PRO:HA	1.90	0.54
1:g:26:VAL:HG23	1:g:125:PRO:HA	1.89	0.54
2:q:34:LYS:C	2:q:35:THR:HG1	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:u:34:LYS:C	2:u:35:THR:HG1	2.15	0.54
1:R:26:VAL:HG23	1:R:125:PRO:HA	1.90	0.53
2:p:34:LYS:C	2:p:35:THR:HG1	2.14	0.53
2:u:63:ASN:O	2:u:63:ASN:ND2	2.41	0.53
2:c:34:LYS:C	2:c:35:THR:HG1	2.15	0.52
1:a:26:VAL:HG12	1:a:79:VAL:HB	1.90	0.52
1:J:382:VAL:HG23	1:J:383:LEU:HG	1.91	0.52
1:j:382:VAL:HG23	1:j:383:LEU:HG	1.92	0.52
1:I:382:VAL:HG23	1:I:383:LEU:HG	1.91	0.52
1:Q:382:VAL:HG23	1:Q:383:LEU:HG	1.91	0.52
1:H:26:VAL:HG12	1:H:79:VAL:HB	1.92	0.52
2:T:107:LEU:HA	2:T:127:VAL:HG12	1.92	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
1:d:382:VAL:HG23	1:d:383:LEU:HG	1.91	0.52
2:h:81:PHE:CZ	2:h:127:VAL:HG11	2.45	0.52
2:l:34:LYS:C	2:l:35:THR:HG1	2.16	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	1.92	0.51
2:q:107:LEU:HA	2:q:127:VAL:HG12	1.92	0.51
1:m:118:LYS:O	1:m:119:SER:OG	2.29	0.51
2:u:107:LEU:HA	2:u:127:VAL:HG12	1.93	0.51
2:t:81:PHE:CZ	2:t:127:VAL:HG11	2.46	0.51
1:P:382:VAL:HG23	1:P:383:LEU:HG	1.93	0.51
2:V:81:PHE:CZ	2:V:127:VAL:HG11	2.46	0.51
2:k:34:LYS:C	2:k:35:THR:HG1	2.18	0.51
1:g:382:VAL:HG23	1:g:383:LEU:HG	1.93	0.51
2:o:81:PHE:CZ	2:o:127:VAL:HG11	2.46	0.51
2:r:34:LYS:C	2:r:35:THR:HG1	2.17	0.51
2:l:107:LEU:HA	2:l:127:VAL:HG12	1.93	0.51
2:k:81:PHE:CZ	2:k:127:VAL:HG11	2.46	0.51
2:W:107:LEU:HA	2:W:127:VAL:HG12	1.93	0.50
2:r:107:LEU:HA	2:r:127:VAL:HG12	1.93	0.50
1:A:382:VAL:HG23	1:A:383:LEU:HG	1.93	0.50
2:Z:107:LEU:HA	2:Z:127:VAL:HG12	1.93	0.50
2:n:81:PHE:CZ	2:n:127:VAL:HG11	2.46	0.50
2:c:81:PHE:CZ	2:c:127:VAL:HG11	2.46	0.50
2:e:107:LEU:HA	2:e:127:VAL:HG12	1.93	0.50
2:i:107:LEU:HA	2:i:127:VAL:HG12	1.92	0.50
1:C:26:VAL:HG12	1:C:79:VAL:HB	1.92	0.50
1:O:26:VAL:HG12	1:O:79:VAL:HB	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:o:157:ASP:OD2	2:o:163:ARG:NH2	2.45	0.50
2:v:81:PHE:CZ	2:v:127:VAL:HG11	2.46	0.50
1:A:26:VAL:HG12	1:A:79:VAL:HB	1.93	0.50
2:S:107:LEU:HA	2:S:127:VAL:HG12	1.93	0.50
1:I:26:VAL:HG12	1:I:79:VAL:HB	1.93	0.50
2:n:34:LYS:C	2:n:35:THR:HG1	2.18	0.50
1:K:26:VAL:HG12	1:K:79:VAL:HB	1.92	0.50
2:l:157:ASP:OD2	2:l:163:ARG:NH2	2.45	0.50
1:D:118:LYS:O	1:D:119:SER:OG	2.28	0.50
1:N:118:LYS:O	1:N:119:SER:OG	2.29	0.50
2:q:157:ASP:OD2	2:q:163:ARG:NH2	2.45	0.50
2:r:157:ASP:OD2	2:r:163:ARG:NH2	2.45	0.50
2:f:157:ASP:OD2	2:f:163:ARG:NH2	2.45	0.50
1:I:118:LYS:O	1:I:119:SER:OG	2.28	0.49
2:Y:81:PHE:CZ	2:Y:127:VAL:HG11	2.46	0.49
2:p:81:PHE:CZ	2:p:127:VAL:HG11	2.46	0.49
2:s:81:PHE:CZ	2:s:127:VAL:HG11	2.46	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	2.45	0.49
2:p:157:ASP:OD2	2:p:163:ARG:NH2	2.45	0.49
1:P:129:VAL:HG23	1:P:201:SER:HB3	1.94	0.49
2:U:157:ASP:OD2	2:U:163:ARG:NH2	2.46	0.49
2:T:157:ASP:OD2	2:T:163:ARG:NH2	2.46	0.49
2:h:157:ASP:OD2	2:h:163:ARG:NH2	2.46	0.49
2:i:157:ASP:OD2	2:i:163:ARG:NH2	2.45	0.49
1:B:382:VAL:HG23	1:B:383:LEU:HG	1.94	0.49
2:v:157:ASP:OD2	2:v:163:ARG:NH2	2.45	0.49
2:b:81:PHE:CZ	2:b:127:VAL:HG11	2.46	0.49
1:K:382:VAL:HG23	1:K:383:LEU:HG	1.93	0.49
1:P:118:LYS:O	1:P:119:SER:OG	2.29	0.49
2:f:81:PHE:CZ	2:f:127:VAL:HG11	2.46	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	1.94	0.49
2:k:157:ASP:OD2	2:k:163:ARG:NH2	2.46	0.49
2:U:81:PHE:CZ	2:U:127:VAL:HG11	2.47	0.49
2:c:157:ASP:OD2	2:c:163:ARG:NH2	2.45	0.49
2:S:157:ASP:OD2	2:S:163:ARG:NH2	2.45	0.49
2:n:157:ASP:OD2	2:n:163:ARG:NH2	2.45	0.49
2:t:157:ASP:OD2	2:t:163:ARG:NH2	2.46	0.49
2:b:157:ASP:OD2	2:b:163:ARG:NH2	2.46	0.48
2:f:34:LYS:C	2:f:35:THR:HG1	2.18	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:t:34:LYS:C	2:t:35:THR:HG1	2.20	0.48
1:j:118:LYS:O	1:j:119:SER:OG	2.29	0.48
2:o:34:LYS:C	2:o:35:THR:HG1	2.19	0.48
2:T:34:LYS:C	2:T:35:THR:HG1	2.18	0.48
2:W:157:ASP:OD2	2:W:163:ARG:NH2	2.46	0.48
2:b:34:LYS:C	2:b:35:THR:HG1	2.19	0.48
2:S:34:LYS:C	2:S:35:THR:HG1	2.19	0.48
1:j:129:VAL:HG23	1:j:201:SER:HB3	1.95	0.48
2:V:157:ASP:OD2	2:V:163:ARG:NH2	2.46	0.48
1:D:129:VAL:HG23	1:D:201:SER:HB3	1.95	0.48
1:E:129:VAL:HG23	1:E:201:SER:HB3	1.95	0.48
1:d:129:VAL:HG23	1:d:201:SER:HB3	1.96	0.48
2:Z:157:ASP:OD2	2:Z:163:ARG:NH2	2.45	0.48
1:J:118:LYS:O	1:J:119:SER:OG	2.29	0.48
2:e:157:ASP:OD2	2:e:163:ARG:NH2	2.46	0.48
1:Q:129:VAL:HG23	1:Q:201:SER:HB3	1.95	0.48
2:Y:157:ASP:OD2	2:Y:163:ARG:NH2	2.46	0.48
1:F:129:VAL:HG23	1:F:201:SER:HB3	1.95	0.47
2:t:63:ASN:H	2:t:63:ASN:HD22	1.62	0.47
1:A:129:VAL:HG23	1:A:201:SER:HB3	1.96	0.47
1:Q:118:LYS:O	1:Q:119:SER:OG	2.32	0.47
2:h:82:ASN:N	2:h:82:ASN:OD1	2.48	0.47
2:r:12:LEU:HD23	2:r:85:PHE:CD2	2.50	0.47
1:N:129:VAL:HG23	1:N:201:SER:HB3	1.96	0.47
2:k:82:ASN:OD1	2:k:82:ASN:N	2.47	0.47
2:l:82:ASN:OD1	2:l:82:ASN:N	2.48	0.47
1:g:118:LYS:O	1:g:119:SER:OG	2.29	0.47
2:W:82:ASN:N	2:W:82:ASN:OD1	2.48	0.47
2:p:82:ASN:OD1	2:p:82:ASN:N	2.47	0.47
1:E:118:LYS:O	1:E:119:SER:OG	2.31	0.47
2:W:81:PHE:CZ	2:W:127:VAL:HG11	2.49	0.47
2:e:81:PHE:CZ	2:e:127:VAL:HG11	2.49	0.47
2:l:81:PHE:CZ	2:l:127:VAL:HG11	2.50	0.47
2:p:12:LEU:HD23	2:p:85:PHE:CD2	2.49	0.47
2:r:82:ASN:OD1	2:r:82:ASN:N	2.48	0.47
2:t:12:LEU:HD23	2:t:85:PHE:CD2	2.50	0.47
2:k:12:LEU:HD23	2:k:85:PHE:CD2	2.50	0.47
2:h:12:LEU:HD23	2:h:85:PHE:CD2	2.50	0.47
2:s:12:LEU:HD23	2:s:85:PHE:CD2	2.50	0.47
2:u:12:LEU:HD23	2:u:85:PHE:CD2	2.50	0.47
2:S:12:LEU:HD23	2:S:85:PHE:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:12:LEU:HD23	2:Z:85:PHE:CD2	2.50	0.47
2:n:12:LEU:HD23	2:n:85:PHE:CD2	2.50	0.47
2:i:12:LEU:HD23	2:i:85:PHE:CD2	2.50	0.47
2:u:82:ASN:OD1	2:u:82:ASN:N	2.48	0.47
2:Z:81:PHE:CZ	2:Z:127:VAL:HG11	2.49	0.47
2:b:12:LEU:HD23	2:b:85:PHE:CD2	2.50	0.47
2:c:12:LEU:HD23	2:c:85:PHE:CD2	2.50	0.47
2:i:82:ASN:OD1	2:i:82:ASN:N	2.48	0.47
2:q:81:PHE:CZ	2:q:127:VAL:HG11	2.50	0.47
2:S:82:ASN:OD1	2:S:82:ASN:N	2.48	0.46
2:W:12:LEU:HD23	2:W:85:PHE:CD2	2.50	0.46
2:V:12:LEU:HD23	2:V:85:PHE:CD2	2.50	0.46
2:V:82:ASN:OD1	2:V:82:ASN:N	2.48	0.46
2:q:82:ASN:N	2:q:82:ASN:OD1	2.47	0.46
1:R:178:LEU:O	1:R:271:THR:OG1	2.33	0.46
2:U:12:LEU:HD23	2:U:85:PHE:CD2	2.49	0.46
2:T:81:PHE:CZ	2:T:127:VAL:HG11	2.49	0.46
2:e:82:ASN:N	2:e:82:ASN:OD1	2.48	0.46
2:f:12:LEU:HD23	2:f:85:PHE:CD2	2.50	0.46
2:q:12:LEU:HD23	2:q:85:PHE:CD2	2.50	0.46
1:J:178:LEU:O	1:J:271:THR:OG1	2.33	0.46
1:X:178:LEU:O	1:X:271:THR:OG1	2.34	0.46
2:T:82:ASN:N	2:T:82:ASN:OD1	2.48	0.46
2:Y:82:ASN:N	2:Y:82:ASN:OD1	2.47	0.46
2:n:82:ASN:OD1	2:n:82:ASN:N	2.47	0.46
2:o:12:LEU:HD23	2:o:85:PHE:CD2	2.50	0.46
2:t:82:ASN:N	2:t:82:ASN:OD1	2.47	0.46
2:f:82:ASN:OD1	2:f:82:ASN:N	2.47	0.46
2:o:82:ASN:OD1	2:o:82:ASN:N	2.47	0.46
2:u:81:PHE:CZ	2:u:127:VAL:HG11	2.49	0.46
2:v:82:ASN:N	2:v:82:ASN:OD1	2.48	0.46
2:S:81:PHE:CZ	2:S:127:VAL:HG11	2.50	0.46
2:T:12:LEU:HD23	2:T:85:PHE:CD2	2.50	0.46
2:Z:82:ASN:OD1	2:Z:82:ASN:N	2.48	0.46
1:C:178:LEU:O	1:C:271:THR:OG1	2.34	0.46
1:d:118:LYS:O	1:d:119:SER:OG	2.32	0.46
2:Y:12:LEU:HD23	2:Y:85:PHE:CD2	2.50	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:U:82:ASN:OD1	2:U:82:ASN:N	2.47	0.46
2:i:81:PHE:CZ	2:i:127:VAL:HG11	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:s:82:ASN:OD1	2:s:82:ASN:N	2.48	0.46
2:r:81:PHE:CZ	2:r:127:VAL:HG11	2.50	0.46
2:v:12:LEU:HD23	2:v:85:PHE:CD2	2.50	0.46
1:Q:178:LEU:O	1:Q:271:THR:OG1	2.33	0.46
2:Z:129:VAL:HG11	2:Z:132:TYR:HB2	1.98	0.46
2:e:12:LEU:HD23	2:e:85:PHE:CD2	2.50	0.46
2:l:12:LEU:HD23	2:l:85:PHE:CD2	2.50	0.46
2:b:23:VAL:HG23	2:u:41:GLY:HA3	1.97	0.46
2:b:82:ASN:OD1	2:b:82:ASN:N	2.47	0.46
2:c:82:ASN:OD1	2:c:82:ASN:N	2.48	0.46
1:B:178:LEU:O	1:B:271:THR:OG1	2.34	0.45
2:s:63:ASN:HD22	2:s:63:ASN:H	1.63	0.45
1:A:178:LEU:O	1:A:271:THR:OG1	2.34	0.45
2:S:41:GLY:HA3	2:p:23:VAL:HG23	1.98	0.45
2:v:34:LYS:C	2:v:35:THR:HG1	2.22	0.45
1:G:178:LEU:O	1:G:271:THR:OG1	2.34	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:m:178:LEU:O	1:m:271:THR:OG1	2.34	0.45
2:e:23:VAL:HG23	2:r:41:GLY:HA3	1.98	0.45
1:K:332:ILE:HB	1:d:382:VAL:HG21	1.98	0.45
1:H:178:LEU:O	1:H:271:THR:OG1	2.35	0.45
1:H:208:PHE:CE2	1:H:221:PRO:HG3	2.52	0.45
1:E:178:LEU:O	1:E:271:THR:OG1	2.34	0.45
1:J:208:PHE:CE2	1:J:221:PRO:HG3	2.52	0.45
2:h:23:VAL:HG23	2:v:41:GLY:HA3	1.97	0.45
2:S:23:VAL:HG23	2:e:41:GLY:HA3	1.98	0.45
1:B:382:VAL:HG21	1:L:332:ILE:HB	1.98	0.45
1:F:178:LEU:O	1:F:271:THR:OG1	2.35	0.45
1:Q:208:PHE:CE2	1:Q:221:PRO:HG3	2.52	0.45
1:P:208:PHE:CE2	1:P:221:PRO:HG3	2.52	0.45
2:W:129:VAL:HG11	2:W:132:TYR:HB2	1.98	0.45
2:b:114:ASP:N	2:b:114:ASP:OD1	2.50	0.45
1:A:118:LYS:O	1:A:119:SER:OG	2.28	0.45
1:B:332:ILE:HB	1:K:382:VAL:HG21	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:R:118:LYS:O	1:R:119:SER:OG	2.29	0.45
2:u:129:VAL:HG11	2:u:132:TYR:HB2	1.99	0.45
1:O:178:LEU:O	1:O:271:THR:OG1	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:178:LEU:O	1:a:271:THR:OG1	2.34	0.45
1:j:208:PHE:CE2	1:j:221:PRO:HG3	2.52	0.45
2:Z:114:ASP:N	2:Z:114:ASP:OD1	2.50	0.45
2:o:114:ASP:OD1	2:o:114:ASP:N	2.50	0.45
2:t:114:ASP:OD1	2:t:114:ASP:N	2.50	0.45
1:O:332:ILE:HB	1:j:382:VAL:HG21	1.98	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	2.70	0.45
2:i:34:LYS:C	2:i:35:THR:HG1	2.23	0.45
2:o:129:VAL:HG11	2:o:132:TYR:HB2	1.98	0.45
2:u:114:ASP:N	2:u:114:ASP:OD1	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:f:129:VAL:HG11	2:f:132:TYR:HB2	1.98	0.44
2:v:114:ASP:OD1	2:v:114:ASP:N	2.50	0.44
1:B:214:GLU:O	1:B:215:TYR:CG	2.70	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:L:214:GLU:O	1:L:215:TYR:CG	2.70	0.44
1:P:214:GLU:O	1:P:215:TYR:CG	2.70	0.44
2:l:114:ASP:OD1	2:l:114:ASP:N	2.50	0.44
1:C:129:VAL:HG23	1:C:201:SER:HB3	1.99	0.44
1:O:129:VAL:HG23	1:O:201:SER:HB3	2.00	0.44
1:g:163:ASP:OD2	1:g:234:ARG:NH1	2.50	0.44
1:F:332:ILE:HB	1:Q:382:VAL:HG21	1.99	0.44
1:L:314:VAL:HG11	1:L:355:TRP:CZ2	2.52	0.44
1:J:129:VAL:HG23	1:J:201:SER:HB3	2.00	0.44
1:P:178:LEU:O	1:P:271:THR:OG1	2.35	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:a:129:VAL:HG23	1:a:201:SER:HB3	2.00	0.44
1:a:314:VAL:HG11	1:a:355:TRP:CZ2	2.52	0.44
2:k:114:ASP:N	2:k:114:ASP:OD1	2.50	0.44
1:C:214:GLU:O	1:C:215:TYR:CG	2.70	0.44
1:K:208:PHE:CE2	1:K:221:PRO:HG3	2.52	0.44
1:I:214:GLU:O	1:I:215:TYR:CG	2.70	0.44
1:H:314:VAL:HG11	1:H:355:TRP:CZ2	2.53	0.44
1:P:314:VAL:HG11	1:P:355:TRP:CZ2	2.53	0.44
1:X:208:PHE:CE2	1:X:221:PRO:HG3	2.53	0.44
2:T:41:GLY:HA3	2:i:23:VAL:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:114:ASP:OD1	2:V:114:ASP:N	2.51	0.44
2:S:114:ASP:N	2:S:114:ASP:OD1	2.50	0.44
1:J:38:GLN:O	1:J:40:SER:N	2.51	0.44
1:R:163:ASP:OD2	1:R:234:ARG:NH1	2.51	0.44
1:X:214:GLU:O	1:X:215:TYR:CG	2.70	0.44
1:d:214:GLU:O	1:d:215:TYR:CG	2.70	0.44
1:j:214:GLU:O	1:j:215:TYR:CG	2.70	0.44
2:W:41:GLY:HA3	2:f:23:VAL:HG23	1.99	0.44
1:A:382:VAL:HG21	1:H:332:ILE:HB	2.00	0.44
1:E:163:ASP:OD2	1:E:234:ARG:NH1	2.51	0.44
1:E:214:GLU:O	1:E:215:TYR:CG	2.70	0.44
1:G:208:PHE:CE2	1:G:221:PRO:HG3	2.53	0.44
1:G:214:GLU:O	1:G:215:TYR:CG	2.70	0.44
1:K:163:ASP:OD2	1:K:234:ARG:NH1	2.51	0.44
1:K:214:GLU:O	1:K:215:TYR:CG	2.71	0.44
1:I:178:LEU:O	1:I:271:THR:OG1	2.35	0.44
1:H:163:ASP:OD2	1:H:234:ARG:NH1	2.51	0.44
1:L:208:PHE:CE2	1:L:221:PRO:HG3	2.52	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
2:U:129:VAL:HG11	2:U:132:TYR:HB2	1.99	0.44
2:Y:129:VAL:HG11	2:Y:132:TYR:HB2	2.00	0.44
2:k:129:VAL:HG11	2:k:132:TYR:HB2	1.99	0.44
1:D:178:LEU:O	1:D:271:THR:OG1	2.34	0.44
1:D:214:GLU:O	1:D:215:TYR:CG	2.71	0.44
1:M:163:ASP:OD2	1:M:234:ARG:NH1	2.51	0.44
1:M:332:ILE:HB	1:g:382:VAL:HG21	1.99	0.44
1:Q:163:ASP:OD2	1:Q:234:ARG:NH1	2.51	0.44
1:g:208:PHE:CE2	1:g:221:PRO:HG3	2.53	0.44
2:V:41:GLY:HA3	2:o:23:VAL:HG23	1.99	0.44
2:Z:41:GLY:HA3	2:l:23:VAL:HG23	1.99	0.44
2:i:114:ASP:N	2:i:114:ASP:OD1	2.50	0.44
1:C:38:GLN:O	1:C:40:SER:N	2.51	0.44
1:D:336:VAL:HG22	1:D:357:ILE:HG23	2.00	0.44
1:E:208:PHE:CE2	1:E:221:PRO:HG3	2.53	0.44
1:I:38:GLN:O	1:I:40:SER:N	2.51	0.44
1:H:129:VAL:HG23	1:H:201:SER:HB3	2.00	0.44
1:N:208:PHE:CE2	1:N:221:PRO:HG3	2.53	0.44
1:j:163:ASP:OD2	1:j:234:ARG:NH1	2.51	0.44
2:q:114:ASP:OD1	2:q:114:ASP:N	2.50	0.44
1:B:314:VAL:HG11	1:B:355:TRP:CZ2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:336:VAL:HG22	1:E:357:ILE:HG23	2.00	0.43
1:F:163:ASP:OD2	1:F:234:ARG:NH1	2.51	0.43
1:F:382:VAL:HG21	1:R:332:ILE:HB	2.00	0.43
1:G:129:VAL:HG23	1:G:201:SER:HB3	2.00	0.43
1:M:38:GLN:O	1:M:40:SER:N	2.51	0.43
1:j:178:LEU:O	1:j:271:THR:OG1	2.36	0.43
2:U:114:ASP:OD1	2:U:114:ASP:N	2.50	0.43
1:C:163:ASP:OD2	1:C:234:ARG:NH1	2.51	0.43
1:D:38:GLN:O	1:D:40:SER:N	2.51	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:G:163:ASP:OD2	1:G:234:ARG:NH1	2.51	0.43
1:I:314:VAL:HG11	1:I:355:TRP:CZ2	2.53	0.43
1:L:129:VAL:HG23	1:L:201:SER:HB3	2.01	0.43
1:R:214:GLU:O	1:R:215:TYR:CG	2.70	0.43
1:a:38:GLN:O	1:a:40:SER:N	2.51	0.43
1:a:208:PHE:CE2	1:a:221:PRO:HG3	2.52	0.43
2:h:114:ASP:OD1	2:h:114:ASP:N	2.50	0.43
2:c:129:VAL:HG11	2:c:132:TYR:HB2	2.00	0.43
2:s:114:ASP:N	2:s:114:ASP:OD1	2.50	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:E:382:VAL:HG21	1:N:332:ILE:HB	1.98	0.43
1:F:208:PHE:CE2	1:F:221:PRO:HG3	2.53	0.43
1:Q:38:GLN:O	1:Q:40:SER:N	2.51	0.43
1:R:314:VAL:HG11	1:R:355:TRP:CZ2	2.53	0.43
1:m:214:GLU:O	1:m:215:TYR:CG	2.71	0.43
2:T:114:ASP:OD1	2:T:114:ASP:N	2.50	0.43
1:B:208:PHE:CE2	1:B:221:PRO:HG3	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:I:336:VAL:HG22	1:I:357:ILE:HG23	2.00	0.43
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:Q:336:VAL:HG22	1:Q:357:ILE:HG23	2.00	0.43
1:N:336:VAL:HG22	1:N:357:ILE:HG23	2.00	0.43
1:X:38:GLN:O	1:X:40:SER:N	2.51	0.43
1:X:314:VAL:HG11	1:X:355:TRP:CZ2	2.53	0.43
1:a:163:ASP:OD2	1:a:234:ARG:NH1	2.51	0.43
2:p:114:ASP:N	2:p:114:ASP:OD1	2.50	0.43
1:B:163:ASP:OD2	1:B:234:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:59:PHE:CG	1:G:65:ILE:HG21	2.53	0.43
1:K:129:VAL:HG23	1:K:201:SER:HB3	2.01	0.43
1:O:163:ASP:OD2	1:O:234:ARG:NH1	2.51	0.43
1:Q:214:GLU:O	1:Q:215:TYR:CG	2.70	0.43
1:L:38:GLN:O	1:L:40:SER:N	2.51	0.43
1:J:163:ASP:OD2	1:J:234:ARG:NH1	2.51	0.43
1:d:163:ASP:OD2	1:d:234:ARG:NH1	2.51	0.43
1:d:208:PHE:CE2	1:d:221:PRO:HG3	2.53	0.43
1:g:178:LEU:O	1:g:271:THR:OG1	2.36	0.43
1:m:26:VAL:HG12	1:m:79:VAL:HB	2.00	0.43
2:r:114:ASP:OD1	2:r:114:ASP:N	2.50	0.43
1:A:214:GLU:O	1:A:215:TYR:CG	2.71	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:E:150:LEU:HA	1:M:239:LEU:CD2	2.48	0.43
1:d:162:THR:OG1	1:d:163:ASP:N	2.52	0.43
1:j:38:GLN:O	1:j:40:SER:N	2.51	0.43
1:m:163:ASP:OD2	1:m:234:ARG:NH1	2.51	0.43
1:A:59:PHE:CG	1:A:65:ILE:HG21	2.54	0.43
1:A:208:PHE:CE2	1:A:221:PRO:HG3	2.54	0.43
1:B:162:THR:OG1	1:B:163:ASP:N	2.52	0.43
1:C:345:ALA:HB2	1:a:380:THR:HG22	2.01	0.43
1:C:382:VAL:HG21	1:J:332:ILE:HB	2.01	0.43
1:G:150:LEU:HA	1:X:239:LEU:CD2	2.49	0.43
1:Q:59:PHE:CG	1:Q:65:ILE:HG21	2.54	0.43
1:L:178:LEU:O	1:L:271:THR:OG1	2.36	0.43
1:N:163:ASP:OD2	1:N:234:ARG:NH1	2.51	0.43
1:R:336:VAL:HG22	1:R:357:ILE:HG23	2.00	0.43
1:d:38:GLN:O	1:d:40:SER:N	2.51	0.43
1:j:314:VAL:HG11	1:j:355:TRP:CZ2	2.53	0.43
1:m:208:PHE:CE2	1:m:221:PRO:HG3	2.53	0.43
1:A:332:ILE:HB	1:G:382:VAL:HG21	2.01	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:F:162:THR:OG1	1:F:163:ASP:N	2.52	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:O:380:THR:HG22	1:P:345:ALA:HB2	2.01	0.43
1:M:214:GLU:O	1:M:215:TYR:CG	2.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:162:THR:OG1	1:X:163:ASP:N	2.52	0.43
1:A:150:LEU:HA	1:G:239:LEU:CD2	2.49	0.43
1:F:150:LEU:HA	1:Q:239:LEU:CD2	2.49	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:H:214:GLU:O	1:H:215:TYR:CG	2.71	0.43
1:L:163:ASP:OD2	1:L:234:ARG:NH1	2.52	0.43
1:P:336:VAL:HG22	1:P:357:ILE:HG23	2.01	0.43
1:N:38:GLN:O	1:N:40:SER:N	2.51	0.43
1:g:59:PHE:CG	1:g:65:ILE:HG21	2.54	0.43
1:g:214:GLU:O	1:g:215:TYR:CG	2.70	0.43
1:m:59:PHE:CG	1:m:65:ILE:HG21	2.54	0.43
2:i:129:VAL:HG11	2:i:132:TYR:HB2	2.00	0.43
1:D:163:ASP:OD2	1:D:234:ARG:NH1	2.51	0.43
1:G:332:ILE:HB	1:X:382:VAL:HG21	2.01	0.43
1:K:38:GLN:O	1:K:40:SER:N	2.51	0.43
1:K:162:THR:OG1	1:K:163:ASP:N	2.52	0.43
1:O:59:PHE:CG	1:O:65:ILE:HG21	2.54	0.43
1:O:208:PHE:CE2	1:O:221:PRO:HG3	2.54	0.43
1:M:129:VAL:HG23	1:M:201:SER:HB3	2.01	0.43
1:M:150:LEU:HA	1:g:239:LEU:CD2	2.49	0.43
1:M:314:VAL:HG11	1:M:355:TRP:CZ2	2.54	0.43
1:L:26:VAL:HG12	1:L:79:VAL:HB	2.00	0.43
1:R:38:GLN:O	1:R:40:SER:N	2.51	0.43
1:g:26:VAL:HG12	1:g:79:VAL:HB	2.01	0.43
1:m:129:VAL:HG23	1:m:201:SER:HB3	2.01	0.43
1:m:336:VAL:HG22	1:m:357:ILE:HG23	2.00	0.43
2:W:114:ASP:OD1	2:W:114:ASP:N	2.51	0.43
1:C:203:TYR:CE1	1:C:229:VAL:HG12	2.54	0.42
1:G:162:THR:OG1	1:G:163:ASP:N	2.52	0.42
1:G:336:VAL:HG22	1:G:357:ILE:HG23	2.01	0.42
1:Q:150:LEU:HA	1:m:239:LEU:CD2	2.49	0.42
1:P:59:PHE:CG	1:P:65:ILE:HG21	2.54	0.42
1:R:26:VAL:HG12	1:R:79:VAL:HB	2.01	0.42
1:d:336:VAL:HG22	1:d:357:ILE:HG23	2.00	0.42
1:a:118:LYS:O	1:a:119:SER:OG	2.32	0.42
1:g:336:VAL:HG22	1:g:357:ILE:HG23	2.00	0.42
1:m:162:THR:OG1	1:m:163:ASP:N	2.52	0.42
1:C:59:PHE:CG	1:C:65:ILE:HG21	2.54	0.42
1:D:59:PHE:CG	1:D:65:ILE:HG21	2.54	0.42
1:E:203:TYR:CE1	1:E:229:VAL:HG12	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:59:PHE:CG	1:K:65:ILE:HG21	2.54	0.42
1:K:150:LEU:HA	1:d:239:LEU:CD2	2.49	0.42
1:I:59:PHE:CG	1:I:65:ILE:HG21	2.54	0.42
1:I:129:VAL:HG23	1:I:201:SER:HB3	2.01	0.42
1:M:26:VAL:HG12	1:M:79:VAL:HB	2.01	0.42
1:Q:26:VAL:HG12	1:Q:79:VAL:HB	2.01	0.42
1:H:38:GLN:O	1:H:40:SER:N	2.51	0.42
1:J:162:THR:OG1	1:J:163:ASP:N	2.52	0.42
1:P:38:GLN:O	1:P:40:SER:N	2.51	0.42
1:a:59:PHE:CG	1:a:65:ILE:HG21	2.54	0.42
1:j:59:PHE:CG	1:j:65:ILE:HG21	2.54	0.42
1:j:162:THR:OG1	1:j:163:ASP:N	2.52	0.42
1:g:38:GLN:O	1:g:40:SER:N	2.51	0.42
1:g:314:VAL:HG11	1:g:355:TRP:CZ2	2.54	0.42
1:A:314:VAL:HG11	1:A:355:TRP:CZ2	2.54	0.42
1:F:38:GLN:O	1:F:40:SER:N	2.51	0.42
1:K:344:SER:OG	1:K:345:ALA:N	2.53	0.42
1:M:59:PHE:CG	1:M:65:ILE:HG21	2.54	0.42
1:Q:332:ILE:HB	1:m:382:VAL:HG21	2.01	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:X:59:PHE:CG	1:X:65:ILE:HG21	2.54	0.42
1:j:344:SER:OG	1:j:345:ALA:N	2.52	0.42
1:g:203:TYR:CE1	1:g:229:VAL:HG12	2.54	0.42
1:m:38:GLN:O	1:m:40:SER:N	2.51	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:D:26:VAL:HG12	1:D:79:VAL:HB	2.00	0.42
1:F:365:ALA:HB2	1:R:306:ILE:CG1	2.49	0.42
1:G:344:SER:OG	1:G:345:ALA:N	2.53	0.42
1:K:203:TYR:CE1	1:K:229:VAL:HG12	2.54	0.42
1:I:344:SER:OG	1:I:345:ALA:N	2.53	0.42
1:M:162:THR:OG1	1:M:163:ASP:N	2.52	0.42
1:L:336:VAL:HG22	1:L:357:ILE:HG23	2.00	0.42
1:J:59:PHE:CG	1:J:65:ILE:HG21	2.54	0.42
1:J:336:VAL:HG22	1:J:357:ILE:HG23	2.00	0.42
1:N:203:TYR:CE1	1:N:229:VAL:HG12	2.55	0.42
1:R:59:PHE:CG	1:R:65:ILE:HG21	2.54	0.42
1:d:59:PHE:CG	1:d:65:ILE:HG21	2.54	0.42
1:a:344:SER:OG	1:a:345:ALA:N	2.53	0.42
2:Z:22:ASP:O	2:Z:23:VAL:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:150:LEU:HA	1:a:239:LEU:CD2	2.49	0.42
1:Q:344:SER:OG	1:Q:345:ALA:N	2.52	0.42
1:R:162:THR:OG1	1:R:163:ASP:N	2.52	0.42
1:j:126:ARG:NH2	1:j:150:LEU:O	2.53	0.42
1:B:150:LEU:HA	1:K:239:LEU:CD2	2.49	0.42
1:E:332:ILE:HB	1:M:382:VAL:HG21	2.01	0.42
1:G:26:VAL:HG12	1:G:79:VAL:HB	2.00	0.42
1:K:314:VAL:HG11	1:K:355:TRP:CZ2	2.54	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: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:X:344:SER:OG	1:X:345:ALA:N	2.53	0.42
2:Y:114:ASP:OD1	2:Y:114:ASP:N	2.50	0.42
2:b:129:VAL:HG11	2:b:132:TYR:HB2	2.00	0.42
2:n:114:ASP:N	2:n:114:ASP:OD1	2.50	0.42
1:A:38:GLN:O	1:A:40:SER:N	2.51	0.42
1:B:59:PHE:CG	1:B:65:ILE:HG21	2.54	0.42
1:D:314:VAL:HG11	1:D:355:TRP:CZ2	2.54	0.42
1:K:336:VAL:HG22	1:K:357:ILE:HG23	2.00	0.42
1:O:150:LEU:HA	1:j:239:LEU:CD2	2.49	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:j:86:GLU:OE2	1:j:86:GLU:N	2.53	0.42
1:m:126:ARG:NH2	1:m:150:LEU:O	2.53	0.42
1:m:344:SER:OG	1:m:345:ALA:N	2.53	0.42
1:B:336:VAL:HG22	1:B:357:ILE:HG23	2.00	0.42
1:B:344:SER:OG	1:B:345:ALA:N	2.53	0.42
1:E:126:ARG:NH2	1:E:150:LEU:O	2.53	0.42
1:F:203:TYR:CE1	1:F:229:VAL:HG12	2.55	0.42
1:G:306:ILE:CG1	1:X:365:ALA:HB2	2.50	0.42
1:O:86:GLU:OE2	1:O:86:GLU:N	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:C:150:LEU:HA	1:I:239:LEU:CD2	2.49	0.42
1:C:162:THR:OG1	1:C:163:ASP:N	2.53	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:126:ARG:NH2	1:G:150:LEU:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:86:GLU:OE2	1:I:86:GLU: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: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:g:290:VAL:HG23	1:g:325:LEU:HD13	2.02	0.42
2:f:148:ASN:HB3	2:f:150:VAL:HG23	2.02	0.42
1:A:344:SER:OG	1:A:345:ALA:N	2.53	0.42
1:A:365:ALA:HB2	1:H:306:ILE:CG1	2.50	0.42
1:D:86:GLU:OE2	1:D: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:H:203:TYR:CE1	1:H:229:VAL:HG12	2.54	0.42
1:L:162:THR:OG1	1:L:163:ASP:N	2.52	0.42
1:J:203:TYR:CE1	1:J:229:VAL:HG12	2.55	0.42
1:P:86:GLU:OE2	1:P:86:GLU:N	2.53	0.42
1:d:132:GLY:O	1:d:134:SER:N	2.53	0.42
1:a:86:GLU:OE2	1:a:86:GLU:N	2.53	0.42
2:p:22:ASP:O	2:p:23:VAL:HG13	2.20	0.42
1:A:126:ARG:NH2	1:A:150:LEU:O	2.53	0.41
1:A:306:ILE:CG1	1:G:365:ALA:HB2	2.50	0.41
1:C:86:GLU:N	1:C:86:GLU:OE2	2.53	0.41
1:C:336:VAL:HG22	1:C:357:ILE:HG23	2.00	0.41
1:C:344:SER:OG	1:C:345:ALA:N	2.53	0.41
1:E:26:VAL:HG12	1:E:79:VAL:HB	2.01	0.41
1:E:38:GLN:O	1:E:40:SER:N	2.51	0.41
1:F:26:VAL:HG12	1:F:79:VAL:HB	2.01	0.41
1:F:239:LEU:CD2	1:R:150:LEU:HA	2.50	0.41
1:G:86:GLU:OE2	1:G:86:GLU:N	2.53	0.41
1:O:126:ARG:NH2	1:O:150:LEU:O	2.53	0.41
1:O:162:THR:OG1	1:O:163:ASP:N	2.52	0.41
1:O:306:ILE:CG1	1:j:365:ALA:HB2	2.50	0.41
1:M:306:ILE:CG1	1:g:365:ALA:HB2	2.49	0.41
1:H:126:ARG:NH2	1:H:150:LEU:O	2.53	0.41
1:H:162:THR:OG1	1:H:163:ASP:N	2.53	0.41
1:L:126:ARG:NH2	1:L:150:LEU:O	2.53	0.41
1:L:344:SER:OG	1:L:345:ALA:N	2.53	0.41
1:P:26:VAL:HG12	1:P:79:VAL:HB	2.01	0.41
1:j:132:GLY:O	1:j:134:SER:N	2.53	0.41
2:f:22:ASP:O	2:f:23:VAL:HG13	2.20	0.41
1:C:132:GLY:O	1:C:134:SER:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:132:GLY:O	1:I:134:SER:N	2.53	0.41
1:I:332:ILE:HB	1:a:382:VAL:HG21	2.02	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: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:j:26:VAL:HG12	1:j:79:VAL:HB	2.01	0.41
2:i:22:ASP:O	2:i:23:VAL:HG13	2.20	0.41
1:B:126:ARG:NH2	1:B: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:M:86:GLU:OE2	1:M:86:GLU:N	2.54	0.41
1:Q:86:GLU:OE2	1:Q:86:GLU:N	2.53	0.41
1:H:132:GLY:O	1:H:134:SER:N	2.53	0.41
1:J:86:GLU:N	1:J:86:GLU:OE2	2.53	0.41
1:P:126:ARG:NH2	1:P:150:LEU:O	2.53	0.41
1:N:86:GLU:OE2	1:N:86:GLU:N	2.53	0.41
1:N:126:ARG:NH2	1:N:150:LEU:O	2.53	0.41
1:m:86:GLU:OE2	1:m:86:GLU:N	2.53	0.41
2:Y:148:ASN:HB3	2:Y:150:VAL:HG23	2.02	0.41
2:c:114:ASP:OD1	2:c:114:ASP:N	2.51	0.41
1:D:239:LEU:CD2	1:P:150:LEU:HA	2.49	0.41
1:D:344:SER:OG	1:D:345:ALA:N	2.53	0.41
1:I:126:ARG:NH2	1:I:150:LEU:O	2.53	0.41
1:I:306:ILE:CG1	1:a:365:ALA:HB2	2.50	0.41
1:H:336:VAL:HG22	1:H:357:ILE:HG23	2.00	0.41
1:J:132:GLY:O	1:J:134:SER:N	2.54	0.41
2:k:22:ASP:O	2:k:23:VAL:HG13	2.20	0.41
2:p:148:ASN:HB3	2:p:150:VAL:HG23	2.02	0.41
2:r:63:ASN:HD22	2:r:63:ASN:H	1.68	0.41
2:u:148:ASN:HB3	2:u:150:VAL:HG23	2.02	0.41
1:A:162:THR:OG1	1:A:163:ASP:N	2.53	0.41
1:B:365:ALA:HB2	1:L:306:ILE:CG1	2.50	0.41
1:D:382:VAL:HG21	1:P:332:ILE:HB	2.01	0.41
1:E:86:GLU:OE2	1:E:86:GLU:N	2.54	0.41
1:E:132:GLY:O	1:E:134:SER:N	2.53	0.41
1:E:345:ALA:HB2	1:g:380:THR:HG22	2.01	0.41
1:F:126:ARG:NH2	1:F:150:LEU:O	2.54	0.41
1:G:314:VAL:HG11	1:G:355:TRP:CZ2	2.56	0.41
1:K:86:GLU:OE2	1:K:86:GLU:N	2.53	0.41
1:K:132:GLY:O	1:K:134:SER:N	2.54	0.41

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:199:PRO:O	1:O:200:ALA:HB3	2.21	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
2:Y:22:ASP:O	2:Y:23:VAL:HG13	2.20	0.41
2:Y:124:LYS:C	2:Y:125:TYR:CD1	2.99	0.41
1:A:132:GLY:O	1:A:134:SER:N	2.53	0.41
1:A:345:ALA:HB2	1:X:380:THR:HG22	2.03	0.41
1:B:239:LEU:CD2	1:L:150:LEU:HA	2.50	0.41
1:C:199:PRO:O	1:C:200:ALA:HB3	2.21	0.41
1:C:239:LEU:CD2	1:J:150:LEU:HA	2.50	0.41
1:D:203:TYR:CE1	1:D:229:VAL:HG12	2.56	0.41
1:E:314:VAL:HG11	1:E:355:TRP:CZ2	2.56	0.41
1:E:338:ALA:O	1:E:339:ASP:C	2.64	0.41
1:F:199:PRO:O	1:F:200:ALA:HB3	2.21	0.41
1:O:132:GLY:O	1:O:134:SER:N	2.54	0.41
1:Q:132:GLY:O	1:Q:134:SER:N	2.53	0.41
1:L:86:GLU:OE2	1:L:86:GLU:N	2.53	0.41
1:L:132:GLY:O	1:L:134:SER:N	2.54	0.41
1:L:199:PRO:O	1:L:200:ALA:HB3	2.21	0.41
1:P:199:PRO:O	1:P:200:ALA:HB3	2.21	0.41
1:P:344:SER:OG	1:P:345:ALA:N	2.53	0.41
1:R:338:ALA:O	1:R:339:ASP:C	2.64	0.41
1:X:132:GLY:O	1:X:134:SER:N	2.53	0.41
1:d:199:PRO:O	1:d:200:ALA:HB3	2.21	0.41
1:g:126:ARG:NH2	1:g:150:LEU:O	2.53	0.41
1:m:199:PRO:O	1:m:200:ALA:HB3	2.21	0.41
2:U:22:ASP:O	2:U:23:VAL:HG13	2.21	0.41
2:Z:124:LYS:C	2:Z:125:TYR:CD1	2.99	0.41
2:c:124:LYS:C	2:c:125:TYR:CD1	2.99	0.41
2:i:148:ASN:HB3	2:i:150:VAL:HG23	2.03	0.41
2:o:22:ASP:O	2:o:23:VAL:HG13	2.21	0.41
2:o:124:LYS:C	2:o:125:TYR:CD1	2.99	0.41
1:E:365:ALA:HB2	1:N:306:ILE:CG1	2.50	0.41
1:I:199:PRO:O	1:I:200:ALA:HB3	2.21	0.41
1:O:382:VAL:HG23	1:O:383:LEU:HG	2.03	0.41
1:R:86:GLU:OE2	1:R:86:GLU:N	2.54	0.41
1:a:199:PRO:O	1:a:200:ALA:HB3	2.21	0.41
1:a:203:TYR:CE1	1:a:229:VAL:HG12	2.56	0.41
2:T:129:VAL:HG11	2:T:132:TYR:HB2	2.02	0.41
2:W:124:LYS:C	2:W:125:TYR:CD1	2.99	0.41
2:V:124:LYS:C	2:V:125:TYR:CD1	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:129:VAL:HG11	2:V:132:TYR:HB2	2.03	0.41
2:f:114:ASP:OD1	2:f:114:ASP:N	2.50	0.41
2:p:124:LYS:C	2:p:125:TYR:CD1	2.99	0.41
1:A:199:PRO:O	1:A:200:ALA:HB3	2.21	0.40
1:F:344:SER:OG	1:F:345:ALA:N	2.53	0.40
1:K:126:ARG:NH2	1:K:150:LEU:O	2.53	0.40
1:M:203:TYR:CE1	1:M:229:VAL:HG12	2.56	0.40
1:M:338:ALA:O	1:M:339:ASP:C	2.64	0.40
1:d:290:VAL:HG23	1:d:325:LEU:HD13	2.01	0.40
1:m:382:VAL:HG23	1:m:383:LEU:HG	2.03	0.40
2:V:148:ASN:HB3	2:V:150:VAL:HG23	2.03	0.40
2:e:114:ASP:OD1	2:e:114:ASP:N	2.51	0.40
2:n:124:LYS:C	2:n:125:TYR:CD1	2.99	0.40
2:l:22:ASP:O	2:l:23:VAL:HG13	2.21	0.40
2:v:129:VAL:HG11	2:v:132:TYR:HB2	2.03	0.40
1:B:203:TYR:CE1	1:B:229:VAL:HG12	2.56	0.40
1:F:338:ALA:O	1:F:339:ASP:C	2.64	0.40
1:G:132:GLY:O	1:G:134:SER:N	2.53	0.40
1:G:199:PRO:O	1:G:200:ALA:HB3	2.21	0.40
1:O:338:ALA:O	1:O:339:ASP:C	2.64	0.40
1:M:199:PRO:O	1:M:200:ALA:HB3	2.22	0.40
1:Q:314:VAL:HG11	1:Q:355:TRP:CZ2	2.56	0.40
1:P:132:GLY:O	1:P:134:SER:N	2.54	0.40
1:d:76:ALA:HB2	1:d:210:TRP:HB2	2.04	0.40
1:j:338:ALA:O	1:j:339:ASP:C	2.64	0.40
1:g:132:GLY:O	1:g:134:SER:N	2.53	0.40
2:T:124:LYS:C	2:T:125:TYR:CD1	2.99	0.40
2:e:148:ASN:HB3	2:e:150:VAL:HG23	2.02	0.40
2:h:124:LYS:C	2:h:125:TYR:CD1	3.00	0.40
2:c:22:ASP:O	2:c:23:VAL:HG13	2.20	0.40
2:l:148:ASN:HB3	2:l:150:VAL:HG23	2.03	0.40
1:D:345:ALA:HB2	1:j:380:THR:HG22	2.03	0.40
1:E:17:ARG:HG2	1:R:337:TYR:CE2	2.56	0.40
1:E:199:PRO:O	1:E:200:ALA:HB3	2.21	0.40
1:I:76:ALA:HB2	1:I:210:TRP:HB2	2.04	0.40
1:O:76:ALA:HB2	1:O:210:TRP:HB2	2.04	0.40
1:J:338:ALA:O	1:J:339:ASP:C	2.64	0.40
1:j:199:PRO:O	1:j:200:ALA:HB3	2.21	0.40
1:m:314:VAL:HG11	1:m:355:TRP:CZ2	2.56	0.40
2:k:124:LYS:C	2:k:125:TYR:CD1	3.00	0.40
2:f:124:LYS:C	2:f:125:TYR:CD1	2.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:q:124:LYS:C	2:q:125:TYR:CD1	2.99	0.40
1:B:76:ALA:HB2	1:B:210:TRP:HB2	2.04	0.40
1:C:76:ALA:HB2	1:C:210:TRP:HB2	2.04	0.40
1:D:382:VAL:HG23	1:D:383:LEU:HG	2.03	0.40
1:K:380:THR:HG22	1:L:345:ALA:HB2	2.03	0.40
1:a:76:ALA:HB2	1:a:210:TRP:HB2	2.04	0.40
1:a:162:THR:OG1	1:a:163:ASP:N	2.53	0.40
1:a:382:VAL:HG23	1:a:383:LEU:HG	2.03	0.40
2:h:148:ASN:HB3	2:h:150:VAL:HG23	2.03	0.40
2:s:124:LYS:C	2:s:125:TYR:CD1	2.99	0.40
2:u:124:LYS:C	2:u:125:TYR:CD1	3.00	0.40
2:t:124:LYS:C	2:t:125:TYR:CD1	3.00	0.40
1:A:187:VAL:HG23	1:A:229:VAL:HA	2.04	0.40
1:B:132:GLY:O	1:B:134:SER:N	2.54	0.40
1:B:306:ILE:CG1	1:K:365:ALA:HB2	2.50	0.40
1:B:338:ALA:O	1:B:339:ASP:C	2.64	0.40
1:E:76:ALA:HB2	1:E:210:TRP:HB2	2.04	0.40
1:E:290:VAL:HG23	1:E:325:LEU:HD13	2.04	0.40
1:N:162:THR:OG1	1:N:163:ASP:N	2.53	0.40
1:d:203:TYR:CE1	1:d:229:VAL:HG12	2.57	0.40
1:g:76:ALA:HB2	1:g:210:TRP:HB2	2.04	0.40
1:m:76:ALA:HB2	1:m:210:TRP:HB2	2.04	0.40
1:m:338:ALA:O	1:m:339:ASP:C	2.64	0.40
2:h:129:VAL:HG11	2:h:132:TYR:HB2	2.03	0.40
2:n:129:VAL:HG11	2:n:132:TYR:HB2	2.04	0.40
2:s:129:VAL:HG11	2:s:132:TYR:HB2	2.03	0.40
2:t:148:ASN:HB3	2:t:150:VAL:HG23	2.03	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%)	1	15
1	B	383/386 (99%)	296 (77%)	68 (18%)	19 (5%)	1	15
1	C	383/386 (99%)	297 (78%)	67 (18%)	19 (5%)	1	15
1	D	383/386 (99%)	297 (78%)	67 (18%)	19 (5%)	1	15
1	E	383/386 (99%)	297 (78%)	67 (18%)	19 (5%)	1	15
1	F	383/386 (99%)	298 (78%)	67 (18%)	18 (5%)	2	17
1	G	383/386 (99%)	299 (78%)	65 (17%)	19 (5%)	1	15
1	H	383/386 (99%)	297 (78%)	67 (18%)	19 (5%)	1	15
1	I	383/386 (99%)	295 (77%)	69 (18%)	19 (5%)	1	15
1	J	383/386 (99%)	295 (77%)	69 (18%)	19 (5%)	1	15
1	K	383/386 (99%)	296 (77%)	68 (18%)	19 (5%)	1	15
1	L	383/386 (99%)	298 (78%)	66 (17%)	19 (5%)	1	15
1	M	383/386 (99%)	295 (77%)	69 (18%)	19 (5%)	1	15
1	N	383/386 (99%)	296 (77%)	68 (18%)	19 (5%)	1	15
1	O	383/386 (99%)	296 (77%)	68 (18%)	19 (5%)	1	15
1	P	383/386 (99%)	297 (78%)	67 (18%)	19 (5%)	1	15
1	Q	383/386 (99%)	298 (78%)	66 (17%)	19 (5%)	1	15
1	R	383/386 (99%)	298 (78%)	66 (17%)	19 (5%)	1	15
1	X	383/386 (99%)	296 (77%)	68 (18%)	19 (5%)	1	15
1	a	383/386 (99%)	297 (78%)	68 (18%)	18 (5%)	2	17
1	d	383/386 (99%)	295 (77%)	69 (18%)	19 (5%)	1	15
1	g	383/386 (99%)	297 (78%)	67 (18%)	19 (5%)	1	15
1	j	383/386 (99%)	296 (77%)	68 (18%)	19 (5%)	1	15
1	m	383/386 (99%)	298 (78%)	66 (17%)	19 (5%)	1	15
2	S	164/168 (98%)	113 (69%)	38 (23%)	13 (8%)	1	8
2	T	164/168 (98%)	114 (70%)	37 (23%)	13 (8%)	1	8
2	U	164/168 (98%)	114 (70%)	37 (23%)	13 (8%)	1	8
2	V	164/168 (98%)	114 (70%)	36 (22%)	14 (8%)	0	7
2	W	164/168 (98%)	114 (70%)	37 (23%)	13 (8%)	1	8
2	Y	164/168 (98%)	114 (70%)	38 (23%)	12 (7%)	1	9
2	Z	164/168 (98%)	114 (70%)	37 (23%)	13 (8%)	1	8
2	b	164/168 (98%)	114 (70%)	37 (23%)	13 (8%)	1	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	c	164/168 (98%)	114 (70%)	37 (23%)	13 (8%)	1	8
2	e	164/168 (98%)	114 (70%)	37 (23%)	13 (8%)	1	8
2	f	164/168 (98%)	114 (70%)	37 (23%)	13 (8%)	1	8
2	h	164/168 (98%)	114 (70%)	37 (23%)	13 (8%)	1	8
2	i	164/168 (98%)	114 (70%)	37 (23%)	13 (8%)	1	8
2	k	164/168 (98%)	114 (70%)	36 (22%)	14 (8%)	0	7
2	l	164/168 (98%)	114 (70%)	37 (23%)	13 (8%)	1	8
2	n	164/168 (98%)	114 (70%)	37 (23%)	13 (8%)	1	8
2	o	164/168 (98%)	114 (70%)	37 (23%)	13 (8%)	1	8
2	p	164/168 (98%)	114 (70%)	37 (23%)	13 (8%)	1	8
2	q	164/168 (98%)	114 (70%)	37 (23%)	13 (8%)	1	8
2	r	164/168 (98%)	114 (70%)	38 (23%)	12 (7%)	1	9
2	s	164/168 (98%)	114 (70%)	37 (23%)	13 (8%)	1	8
2	t	164/168 (98%)	114 (70%)	37 (23%)	13 (8%)	1	8
2	u	164/168 (98%)	114 (70%)	38 (23%)	12 (7%)	1	9
2	v	164/168 (98%)	114 (70%)	37 (23%)	13 (8%)	1	8
All	All	13128/13296 (99%)	9855 (75%)	2508 (19%)	765 (6%)	2	13

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 [i](#)

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%)	275 (93%)	22 (7%)	13	37
1	B	297/298 (100%)	275 (93%)	22 (7%)	13	37
1	C	297/298 (100%)	275 (93%)	22 (7%)	13	37
1	D	297/298 (100%)	275 (93%)	22 (7%)	13	37
1	E	297/298 (100%)	275 (93%)	22 (7%)	13	37
1	F	297/298 (100%)	275 (93%)	22 (7%)	13	37
1	G	297/298 (100%)	276 (93%)	21 (7%)	13	38
1	H	297/298 (100%)	276 (93%)	21 (7%)	13	38
1	I	297/298 (100%)	275 (93%)	22 (7%)	13	37
1	J	297/298 (100%)	275 (93%)	22 (7%)	13	37
1	K	297/298 (100%)	275 (93%)	22 (7%)	13	37
1	L	297/298 (100%)	276 (93%)	21 (7%)	13	38
1	M	297/298 (100%)	275 (93%)	22 (7%)	13	37
1	N	297/298 (100%)	276 (93%)	21 (7%)	13	38
1	O	297/298 (100%)	275 (93%)	22 (7%)	13	37
1	P	297/298 (100%)	276 (93%)	21 (7%)	13	38
1	Q	297/298 (100%)	275 (93%)	22 (7%)	13	37
1	R	297/298 (100%)	275 (93%)	22 (7%)	13	37
1	X	297/298 (100%)	275 (93%)	22 (7%)	13	37
1	a	297/298 (100%)	275 (93%)	22 (7%)	13	37
1	d	297/298 (100%)	275 (93%)	22 (7%)	13	37
1	g	297/298 (100%)	275 (93%)	22 (7%)	13	37
1	j	297/298 (100%)	275 (93%)	22 (7%)	13	37
1	m	297/298 (100%)	275 (93%)	22 (7%)	13	37
2	S	129/131 (98%)	114 (88%)	15 (12%)	5	24
2	T	129/131 (98%)	114 (88%)	15 (12%)	5	24
2	U	129/131 (98%)	114 (88%)	15 (12%)	5	24
2	V	129/131 (98%)	114 (88%)	15 (12%)	5	24
2	W	129/131 (98%)	114 (88%)	15 (12%)	5	24
2	Y	129/131 (98%)	114 (88%)	15 (12%)	5	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Z	129/131 (98%)	114 (88%)	15 (12%)	5	24
2	b	129/131 (98%)	114 (88%)	15 (12%)	5	24
2	c	129/131 (98%)	114 (88%)	15 (12%)	5	24
2	e	129/131 (98%)	114 (88%)	15 (12%)	5	24
2	f	129/131 (98%)	114 (88%)	15 (12%)	5	24
2	h	129/131 (98%)	114 (88%)	15 (12%)	5	24
2	i	129/131 (98%)	114 (88%)	15 (12%)	5	24
2	k	129/131 (98%)	114 (88%)	15 (12%)	5	24
2	l	129/131 (98%)	114 (88%)	15 (12%)	5	24
2	n	129/131 (98%)	114 (88%)	15 (12%)	5	24
2	o	129/131 (98%)	114 (88%)	15 (12%)	5	24
2	p	129/131 (98%)	114 (88%)	15 (12%)	5	24
2	q	129/131 (98%)	113 (88%)	16 (12%)	4	22
2	r	129/131 (98%)	113 (88%)	16 (12%)	4	22
2	s	129/131 (98%)	113 (88%)	16 (12%)	4	22
2	t	129/131 (98%)	113 (88%)	16 (12%)	4	22
2	u	129/131 (98%)	114 (88%)	15 (12%)	5	24
2	v	129/131 (98%)	114 (88%)	15 (12%)	5	24
All	All	10224/10296 (99%)	9337 (91%)	887 (9%)	12	33

All (887) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	14	ILE
1	A	19	ILE
1	A	38	GLN
1	A	40	SER
1	A	53	LYS
1	A	61	ILE
1	A	75	ARG
1	A	134	SER
1	A	182	ASP
1	A	197	ASN
1	A	208	PHE
1	A	229	VAL

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Mol	Chain	Res	Type
1	A	243	GLU
1	A	274	SER
1	A	285	ARG
1	A	294	ILE
1	A	304	ARG
1	A	332	ILE
1	A	355	TRP
1	A	372	VAL
1	A	379	LEU
2	S	3	ILE
2	S	8	THR
2	S	12	LEU
2	S	23	VAL
2	S	26	LEU
2	S	54	GLU
2	S	66	ARG
2	S	71	ASN
2	S	78	GLN
2	S	79	SER
2	S	82	ASN
2	S	103	LEU
2	S	106	LEU
2	S	124	LYS
2	S	134	LEU
1	B	7	VAL
1	B	14	ILE
1	B	19	ILE
1	B	38	GLN
1	B	40	SER
1	B	53	LYS
1	B	61	ILE
1	B	75	ARG
1	B	134	SER
1	B	182	ASP
1	B	197	ASN
1	B	208	PHE
1	B	229	VAL
1	B	243	GLU
1	B	274	SER
1	B	285	ARG
1	B	294	ILE
1	B	304	ARG

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Mol	Chain	Res	Type
1	B	332	ILE
1	B	355	TRP
1	B	372	VAL
1	B	379	LEU
1	C	7	VAL
1	C	14	ILE
1	C	19	ILE
1	C	38	GLN
1	C	40	SER
1	C	53	LYS
1	C	61	ILE
1	C	75	ARG
1	C	134	SER
1	C	182	ASP
1	C	197	ASN
1	C	208	PHE
1	C	229	VAL
1	C	243	GLU
1	C	274	SER
1	C	285	ARG
1	C	294	ILE
1	C	304	ARG
1	C	332	ILE
1	C	355	TRP
1	C	372	VAL
1	C	379	LEU
1	D	7	VAL
1	D	14	ILE
1	D	19	ILE
1	D	38	GLN
1	D	40	SER
1	D	53	LYS
1	D	61	ILE
1	D	75	ARG
1	D	134	SER
1	D	182	ASP
1	D	197	ASN
1	D	208	PHE
1	D	229	VAL
1	D	243	GLU
1	D	274	SER
1	D	285	ARG

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Mol	Chain	Res	Type
1	D	294	ILE
1	D	304	ARG
1	D	332	ILE
1	D	355	TRP
1	D	372	VAL
1	D	379	LEU
1	E	7	VAL
1	E	14	ILE
1	E	19	ILE
1	E	38	GLN
1	E	40	SER
1	E	53	LYS
1	E	61	ILE
1	E	75	ARG
1	E	134	SER
1	E	182	ASP
1	E	197	ASN
1	E	208	PHE
1	E	229	VAL
1	E	243	GLU
1	E	274	SER
1	E	285	ARG
1	E	294	ILE
1	E	304	ARG
1	E	332	ILE
1	E	355	TRP
1	E	372	VAL
1	E	379	LEU
1	F	7	VAL
1	F	14	ILE
1	F	19	ILE
1	F	38	GLN
1	F	40	SER
1	F	53	LYS
1	F	61	ILE
1	F	75	ARG
1	F	134	SER
1	F	182	ASP
1	F	197	ASN
1	F	208	PHE
1	F	229	VAL
1	F	243	GLU

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Mol	Chain	Res	Type
1	F	274	SER
1	F	285	ARG
1	F	294	ILE
1	F	304	ARG
1	F	332	ILE
1	F	355	TRP
1	F	372	VAL
1	F	379	LEU
1	G	7	VAL
1	G	14	ILE
1	G	19	ILE
1	G	38	GLN
1	G	40	SER
1	G	53	LYS
1	G	61	ILE
1	G	75	ARG
1	G	134	SER
1	G	182	ASP
1	G	197	ASN
1	G	208	PHE
1	G	229	VAL
1	G	243	GLU
1	G	285	ARG
1	G	294	ILE
1	G	304	ARG
1	G	332	ILE
1	G	355	TRP
1	G	372	VAL
1	G	379	LEU
1	K	7	VAL
1	K	14	ILE
1	K	19	ILE
1	K	38	GLN
1	K	40	SER
1	K	53	LYS
1	K	61	ILE
1	K	75	ARG
1	K	134	SER
1	K	182	ASP
1	K	197	ASN
1	K	208	PHE
1	K	229	VAL

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Mol	Chain	Res	Type
1	K	243	GLU
1	K	274	SER
1	K	285	ARG
1	K	294	ILE
1	K	304	ARG
1	K	332	ILE
1	K	355	TRP
1	K	372	VAL
1	K	379	LEU
1	I	7	VAL
1	I	14	ILE
1	I	19	ILE
1	I	38	GLN
1	I	40	SER
1	I	53	LYS
1	I	61	ILE
1	I	75	ARG
1	I	134	SER
1	I	182	ASP
1	I	197	ASN
1	I	208	PHE
1	I	229	VAL
1	I	243	GLU
1	I	274	SER
1	I	285	ARG
1	I	294	ILE
1	I	304	ARG
1	I	332	ILE
1	I	355	TRP
1	I	372	VAL
1	I	379	LEU
1	O	7	VAL
1	O	14	ILE
1	O	19	ILE
1	O	38	GLN
1	O	40	SER
1	O	53	LYS
1	O	61	ILE
1	O	75	ARG
1	O	134	SER
1	O	182	ASP
1	O	197	ASN

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Mol	Chain	Res	Type
1	O	208	PHE
1	O	229	VAL
1	O	243	GLU
1	O	274	SER
1	O	285	ARG
1	O	294	ILE
1	O	304	ARG
1	O	332	ILE
1	O	355	TRP
1	O	372	VAL
1	O	379	LEU
1	M	7	VAL
1	M	14	ILE
1	M	19	ILE
1	M	38	GLN
1	M	40	SER
1	M	53	LYS
1	M	61	ILE
1	M	75	ARG
1	M	134	SER
1	M	182	ASP
1	M	197	ASN
1	M	208	PHE
1	M	229	VAL
1	M	243	GLU
1	M	274	SER
1	M	285	ARG
1	M	294	ILE
1	M	304	ARG
1	M	332	ILE
1	M	355	TRP
1	M	372	VAL
1	M	379	LEU
1	Q	7	VAL
1	Q	14	ILE
1	Q	19	ILE
1	Q	38	GLN
1	Q	40	SER
1	Q	53	LYS
1	Q	61	ILE
1	Q	75	ARG
1	Q	134	SER

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Mol	Chain	Res	Type
1	Q	182	ASP
1	Q	197	ASN
1	Q	208	PHE
1	Q	229	VAL
1	Q	243	GLU
1	Q	274	SER
1	Q	285	ARG
1	Q	294	ILE
1	Q	304	ARG
1	Q	332	ILE
1	Q	355	TRP
1	Q	372	VAL
1	Q	379	LEU
1	H	14	ILE
1	H	19	ILE
1	H	38	GLN
1	H	40	SER
1	H	53	LYS
1	H	61	ILE
1	H	75	ARG
1	H	134	SER
1	H	182	ASP
1	H	197	ASN
1	H	208	PHE
1	H	229	VAL
1	H	243	GLU
1	H	274	SER
1	H	285	ARG
1	H	294	ILE
1	H	304	ARG
1	H	332	ILE
1	H	355	TRP
1	H	372	VAL
1	H	379	LEU
1	L	14	ILE
1	L	19	ILE
1	L	38	GLN
1	L	40	SER
1	L	53	LYS
1	L	61	ILE
1	L	75	ARG
1	L	134	SER

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Mol	Chain	Res	Type
1	L	182	ASP
1	L	197	ASN
1	L	208	PHE
1	L	229	VAL
1	L	243	GLU
1	L	274	SER
1	L	285	ARG
1	L	294	ILE
1	L	304	ARG
1	L	332	ILE
1	L	355	TRP
1	L	372	VAL
1	L	379	LEU
1	J	7	VAL
1	J	14	ILE
1	J	19	ILE
1	J	38	GLN
1	J	40	SER
1	J	53	LYS
1	J	61	ILE
1	J	75	ARG
1	J	134	SER
1	J	182	ASP
1	J	197	ASN
1	J	208	PHE
1	J	229	VAL
1	J	243	GLU
1	J	274	SER
1	J	285	ARG
1	J	294	ILE
1	J	304	ARG
1	J	332	ILE
1	J	355	TRP
1	J	372	VAL
1	J	379	LEU
1	P	14	ILE
1	P	19	ILE
1	P	38	GLN
1	P	40	SER
1	P	53	LYS
1	P	61	ILE
1	P	75	ARG

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Mol	Chain	Res	Type
1	P	134	SER
1	P	182	ASP
1	P	197	ASN
1	P	208	PHE
1	P	229	VAL
1	P	243	GLU
1	P	274	SER
1	P	285	ARG
1	P	294	ILE
1	P	304	ARG
1	P	332	ILE
1	P	355	TRP
1	P	372	VAL
1	P	379	LEU
1	N	14	ILE
1	N	19	ILE
1	N	38	GLN
1	N	40	SER
1	N	53	LYS
1	N	61	ILE
1	N	75	ARG
1	N	134	SER
1	N	182	ASP
1	N	197	ASN
1	N	208	PHE
1	N	229	VAL
1	N	243	GLU
1	N	274	SER
1	N	285	ARG
1	N	294	ILE
1	N	304	ARG
1	N	332	ILE
1	N	355	TRP
1	N	372	VAL
1	N	379	LEU
1	R	7	VAL
1	R	14	ILE
1	R	19	ILE
1	R	38	GLN
1	R	40	SER
1	R	53	LYS
1	R	61	ILE

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Mol	Chain	Res	Type
1	R	75	ARG
1	R	134	SER
1	R	182	ASP
1	R	197	ASN
1	R	208	PHE
1	R	229	VAL
1	R	243	GLU
1	R	274	SER
1	R	285	ARG
1	R	294	ILE
1	R	304	ARG
1	R	332	ILE
1	R	355	TRP
1	R	372	VAL
1	R	379	LEU
1	X	7	VAL
1	X	14	ILE
1	X	19	ILE
1	X	38	GLN
1	X	40	SER
1	X	53	LYS
1	X	61	ILE
1	X	75	ARG
1	X	134	SER
1	X	182	ASP
1	X	197	ASN
1	X	208	PHE
1	X	229	VAL
1	X	243	GLU
1	X	274	SER
1	X	285	ARG
1	X	294	ILE
1	X	304	ARG
1	X	332	ILE
1	X	355	TRP
1	X	372	VAL
1	X	379	LEU
1	d	7	VAL
1	d	14	ILE
1	d	19	ILE
1	d	38	GLN
1	d	40	SER

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Mol	Chain	Res	Type
1	d	53	LYS
1	d	61	ILE
1	d	75	ARG
1	d	134	SER
1	d	182	ASP
1	d	197	ASN
1	d	208	PHE
1	d	229	VAL
1	d	243	GLU
1	d	274	SER
1	d	285	ARG
1	d	294	ILE
1	d	304	ARG
1	d	332	ILE
1	d	355	TRP
1	d	372	VAL
1	d	379	LEU
1	a	7	VAL
1	a	14	ILE
1	a	19	ILE
1	a	38	GLN
1	a	40	SER
1	a	53	LYS
1	a	61	ILE
1	a	75	ARG
1	a	134	SER
1	a	182	ASP
1	a	197	ASN
1	a	208	PHE
1	a	229	VAL
1	a	243	GLU
1	a	274	SER
1	a	285	ARG
1	a	294	ILE
1	a	304	ARG
1	a	332	ILE
1	a	355	TRP
1	a	372	VAL
1	a	379	LEU
1	j	7	VAL
1	j	14	ILE
1	j	19	ILE

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Mol	Chain	Res	Type
1	j	38	GLN
1	j	40	SER
1	j	53	LYS
1	j	61	ILE
1	j	75	ARG
1	j	134	SER
1	j	182	ASP
1	j	197	ASN
1	j	208	PHE
1	j	229	VAL
1	j	243	GLU
1	j	274	SER
1	j	285	ARG
1	j	294	ILE
1	j	304	ARG
1	j	332	ILE
1	j	355	TRP
1	j	372	VAL
1	j	379	LEU
1	g	7	VAL
1	g	14	ILE
1	g	19	ILE
1	g	38	GLN
1	g	40	SER
1	g	53	LYS
1	g	61	ILE
1	g	75	ARG
1	g	134	SER
1	g	182	ASP
1	g	197	ASN
1	g	208	PHE
1	g	229	VAL
1	g	243	GLU
1	g	274	SER
1	g	285	ARG
1	g	294	ILE
1	g	304	ARG
1	g	332	ILE
1	g	355	TRP
1	g	372	VAL
1	g	379	LEU
1	m	7	VAL

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Mol	Chain	Res	Type
1	m	14	ILE
1	m	19	ILE
1	m	38	GLN
1	m	40	SER
1	m	53	LYS
1	m	61	ILE
1	m	75	ARG
1	m	134	SER
1	m	182	ASP
1	m	197	ASN
1	m	208	PHE
1	m	229	VAL
1	m	243	GLU
1	m	274	SER
1	m	285	ARG
1	m	294	ILE
1	m	304	ARG
1	m	332	ILE
1	m	355	TRP
1	m	372	VAL
1	m	379	LEU
2	U	3	ILE
2	U	8	THR
2	U	12	LEU
2	U	23	VAL
2	U	26	LEU
2	U	54	GLU
2	U	66	ARG
2	U	71	ASN
2	U	78	GLN
2	U	79	SER
2	U	82	ASN
2	U	103	LEU
2	U	106	LEU
2	U	124	LYS
2	U	134	LEU
2	T	3	ILE
2	T	8	THR
2	T	12	LEU
2	T	23	VAL
2	T	26	LEU
2	T	54	GLU

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Mol	Chain	Res	Type
2	T	66	ARG
2	T	71	ASN
2	T	78	GLN
2	T	79	SER
2	T	82	ASN
2	T	103	LEU
2	T	106	LEU
2	T	124	LYS
2	T	134	LEU
2	W	3	ILE
2	W	8	THR
2	W	12	LEU
2	W	23	VAL
2	W	26	LEU
2	W	54	GLU
2	W	66	ARG
2	W	71	ASN
2	W	78	GLN
2	W	79	SER
2	W	82	ASN
2	W	103	LEU
2	W	106	LEU
2	W	124	LYS
2	W	134	LEU
2	V	3	ILE
2	V	8	THR
2	V	12	LEU
2	V	23	VAL
2	V	26	LEU
2	V	54	GLU
2	V	66	ARG
2	V	71	ASN
2	V	78	GLN
2	V	79	SER
2	V	82	ASN
2	V	103	LEU
2	V	106	LEU
2	V	124	LYS
2	V	134	LEU
2	Z	3	ILE
2	Z	8	THR
2	Z	12	LEU

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Mol	Chain	Res	Type
2	Z	23	VAL
2	Z	26	LEU
2	Z	54	GLU
2	Z	66	ARG
2	Z	71	ASN
2	Z	78	GLN
2	Z	79	SER
2	Z	82	ASN
2	Z	103	LEU
2	Z	106	LEU
2	Z	124	LYS
2	Z	134	LEU
2	Y	3	ILE
2	Y	8	THR
2	Y	12	LEU
2	Y	23	VAL
2	Y	26	LEU
2	Y	54	GLU
2	Y	66	ARG
2	Y	71	ASN
2	Y	78	GLN
2	Y	79	SER
2	Y	82	ASN
2	Y	103	LEU
2	Y	106	LEU
2	Y	124	LYS
2	Y	134	LEU
2	e	3	ILE
2	e	8	THR
2	e	12	LEU
2	e	23	VAL
2	e	26	LEU
2	e	54	GLU
2	e	66	ARG
2	e	71	ASN
2	e	78	GLN
2	e	79	SER
2	e	82	ASN
2	e	103	LEU
2	e	106	LEU
2	e	124	LYS
2	e	134	LEU

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Mol	Chain	Res	Type
2	b	3	ILE
2	b	8	THR
2	b	12	LEU
2	b	23	VAL
2	b	26	LEU
2	b	54	GLU
2	b	66	ARG
2	b	71	ASN
2	b	78	GLN
2	b	79	SER
2	b	82	ASN
2	b	103	LEU
2	b	106	LEU
2	b	124	LYS
2	b	134	LEU
2	k	3	ILE
2	k	8	THR
2	k	12	LEU
2	k	23	VAL
2	k	26	LEU
2	k	54	GLU
2	k	66	ARG
2	k	71	ASN
2	k	78	GLN
2	k	79	SER
2	k	82	ASN
2	k	103	LEU
2	k	106	LEU
2	k	124	LYS
2	k	134	LEU
2	h	3	ILE
2	h	8	THR
2	h	12	LEU
2	h	23	VAL
2	h	26	LEU
2	h	54	GLU
2	h	66	ARG
2	h	71	ASN
2	h	78	GLN
2	h	79	SER
2	h	82	ASN
2	h	103	LEU

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Mol	Chain	Res	Type
2	h	106	LEU
2	h	124	LYS
2	h	134	LEU
2	n	3	ILE
2	n	8	THR
2	n	12	LEU
2	n	23	VAL
2	n	26	LEU
2	n	54	GLU
2	n	66	ARG
2	n	71	ASN
2	n	78	GLN
2	n	79	SER
2	n	82	ASN
2	n	103	LEU
2	n	106	LEU
2	n	124	LYS
2	n	134	LEU
2	c	3	ILE
2	c	8	THR
2	c	12	LEU
2	c	23	VAL
2	c	26	LEU
2	c	54	GLU
2	c	66	ARG
2	c	71	ASN
2	c	78	GLN
2	c	79	SER
2	c	82	ASN
2	c	103	LEU
2	c	106	LEU
2	c	124	LYS
2	c	134	LEU
2	i	3	ILE
2	i	8	THR
2	i	12	LEU
2	i	23	VAL
2	i	26	LEU
2	i	54	GLU
2	i	66	ARG
2	i	71	ASN
2	i	78	GLN

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Mol	Chain	Res	Type
2	i	79	SER
2	i	82	ASN
2	i	103	LEU
2	i	106	LEU
2	i	124	LYS
2	i	134	LEU
2	f	3	ILE
2	f	8	THR
2	f	12	LEU
2	f	23	VAL
2	f	26	LEU
2	f	54	GLU
2	f	66	ARG
2	f	71	ASN
2	f	78	GLN
2	f	79	SER
2	f	82	ASN
2	f	103	LEU
2	f	106	LEU
2	f	124	LYS
2	f	134	LEU
2	o	3	ILE
2	o	8	THR
2	o	12	LEU
2	o	23	VAL
2	o	26	LEU
2	o	54	GLU
2	o	66	ARG
2	o	71	ASN
2	o	78	GLN
2	o	79	SER
2	o	82	ASN
2	o	103	LEU
2	o	106	LEU
2	o	124	LYS
2	o	134	LEU
2	l	3	ILE
2	l	8	THR
2	l	12	LEU
2	l	23	VAL
2	l	26	LEU
2	l	54	GLU

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Mol	Chain	Res	Type
2	l	66	ARG
2	l	71	ASN
2	l	78	GLN
2	l	79	SER
2	l	82	ASN
2	l	103	LEU
2	l	106	LEU
2	l	124	LYS
2	l	134	LEU
2	p	3	ILE
2	p	8	THR
2	p	12	LEU
2	p	23	VAL
2	p	26	LEU
2	p	54	GLU
2	p	66	ARG
2	p	71	ASN
2	p	78	GLN
2	p	79	SER
2	p	82	ASN
2	p	103	LEU
2	p	106	LEU
2	p	124	LYS
2	p	134	LEU
2	q	3	ILE
2	q	8	THR
2	q	12	LEU
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	78	GLN
2	q	79	SER
2	q	82	ASN
2	q	103	LEU
2	q	106	LEU
2	q	124	LYS
2	q	134	LEU
2	s	3	ILE
2	s	8	THR

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Mol	Chain	Res	Type
2	s	12	LEU
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	78	GLN
2	s	79	SER
2	s	82	ASN
2	s	103	LEU
2	s	106	LEU
2	s	124	LYS
2	s	134	LEU
2	r	3	ILE
2	r	8	THR
2	r	12	LEU
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	78	GLN
2	r	79	SER
2	r	82	ASN
2	r	103	LEU
2	r	106	LEU
2	r	124	LYS
2	r	134	LEU
2	u	3	ILE
2	u	8	THR
2	u	12	LEU
2	u	23	VAL
2	u	26	LEU
2	u	54	GLU
2	u	66	ARG
2	u	71	ASN
2	u	78	GLN
2	u	79	SER
2	u	82	ASN
2	u	103	LEU

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Mol	Chain	Res	Type
2	u	106	LEU
2	u	124	LYS
2	u	134	LEU
2	t	3	ILE
2	t	8	THR
2	t	12	LEU
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	78	GLN
2	t	79	SER
2	t	82	ASN
2	t	103	LEU
2	t	106	LEU
2	t	124	LYS
2	t	134	LEU
2	v	3	ILE
2	v	8	THR
2	v	12	LEU
2	v	23	VAL
2	v	26	LEU
2	v	54	GLU
2	v	66	ARG
2	v	71	ASN
2	v	78	GLN
2	v	79	SER
2	v	82	ASN
2	v	103	LEU
2	v	106	LEU
2	v	124	LYS
2	v	134	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (117) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	193	ASN
1	A	298	HIS
1	A	327	ASN
2	S	11	ASN

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Mol	Chain	Res	Type
1	B	193	ASN
1	B	298	HIS
1	B	327	ASN
1	C	193	ASN
1	C	298	HIS
1	C	327	ASN
1	D	193	ASN
1	D	327	ASN
1	E	193	ASN
1	E	298	HIS
1	E	327	ASN
1	F	193	ASN
1	F	298	HIS
1	F	327	ASN
1	G	193	ASN
1	G	298	HIS
1	G	327	ASN
1	K	193	ASN
1	K	298	HIS
1	K	327	ASN
1	I	193	ASN
1	I	298	HIS
1	I	327	ASN
1	O	193	ASN
1	O	298	HIS
1	O	327	ASN
1	M	193	ASN
1	M	298	HIS
1	M	327	ASN
1	Q	193	ASN
1	Q	298	HIS
1	Q	327	ASN
1	H	193	ASN
1	H	298	HIS
1	H	327	ASN
1	L	193	ASN
1	L	298	HIS
1	L	327	ASN
1	J	193	ASN
1	J	298	HIS
1	J	327	ASN
1	P	193	ASN

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Mol	Chain	Res	Type
1	P	298	HIS
1	P	327	ASN
1	N	193	ASN
1	N	298	HIS
1	N	327	ASN
1	R	193	ASN
1	R	298	HIS
1	R	327	ASN
1	X	193	ASN
1	X	298	HIS
1	X	327	ASN
1	d	193	ASN
1	d	298	HIS
1	d	327	ASN
1	a	193	ASN
1	a	327	ASN
1	j	193	ASN
1	j	298	HIS
1	j	327	ASN
1	g	193	ASN
1	g	298	HIS
1	g	327	ASN
1	m	193	ASN
1	m	298	HIS
1	m	327	ASN
2	U	11	ASN
2	T	11	ASN
2	W	11	ASN
2	W	148	ASN
2	V	11	ASN
2	V	148	ASN
2	Z	11	ASN
2	Z	148	ASN
2	Y	11	ASN
2	e	11	ASN
2	e	148	ASN
2	b	11	ASN
2	b	148	ASN
2	k	11	ASN
2	k	148	ASN
2	h	11	ASN
2	h	148	ASN

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Mol	Chain	Res	Type
2	n	11	ASN
2	c	11	ASN
2	c	148	ASN
2	i	11	ASN
2	f	11	ASN
2	o	11	ASN
2	o	148	ASN
2	l	11	ASN
2	l	148	ASN
2	p	11	ASN
2	q	11	ASN
2	q	63	ASN
2	q	148	ASN
2	s	11	ASN
2	s	63	ASN
2	s	148	ASN
2	r	9	ASN
2	r	11	ASN
2	r	63	ASN
2	u	11	ASN
2	u	63	ASN
2	u	148	ASN
2	t	11	ASN
2	t	63	ASN
2	t	148	ASN
2	v	9	ASN
2	v	11	ASN
2	v	63	ASN
2	v	148	ASN

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 ⓘ

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.

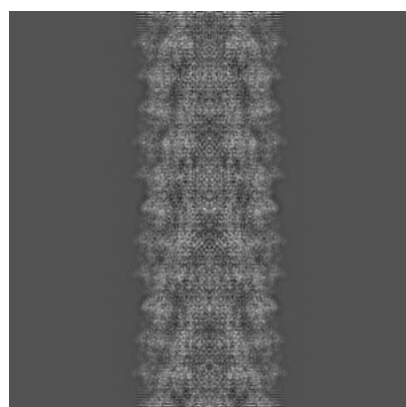
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6270. These allow visual inspection of the internal detail of the map and identification of artifacts.

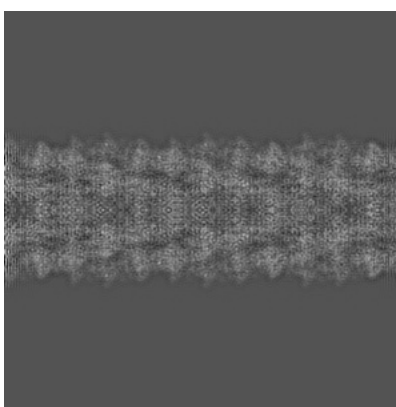
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

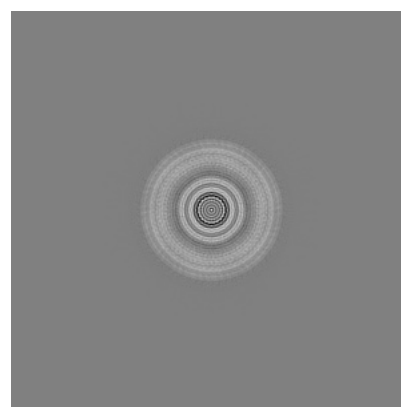
6.1.1 Primary map



X



Y

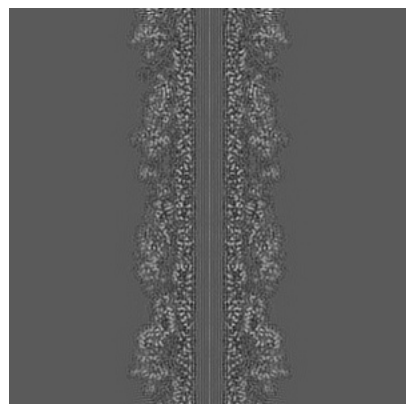


Z

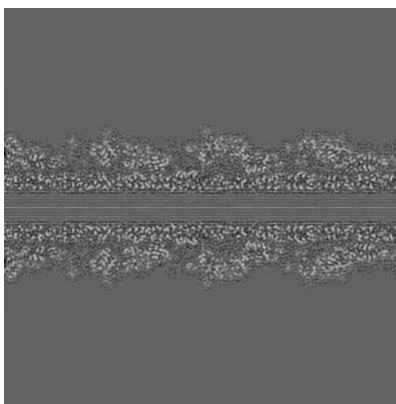
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

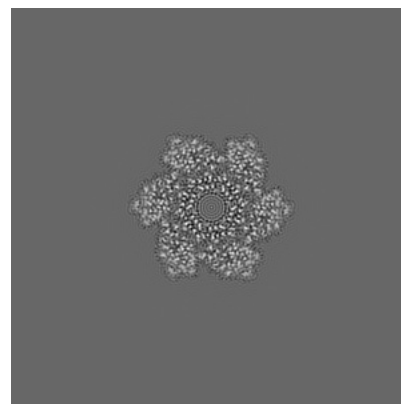
6.2.1 Primary map



X Index: 210



Y Index: 210

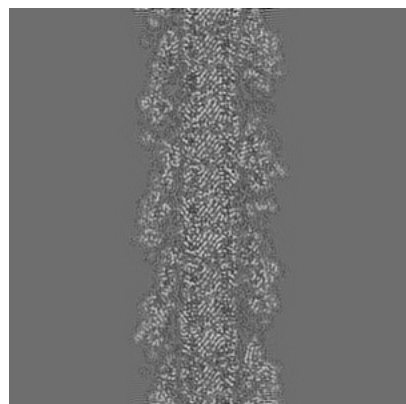


Z Index: 210

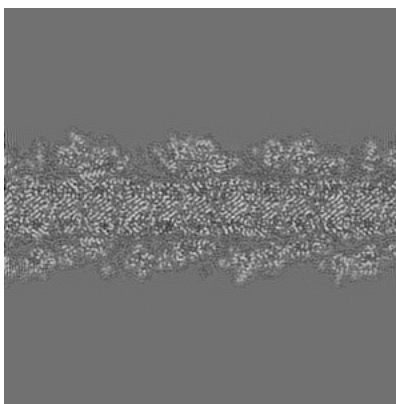
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

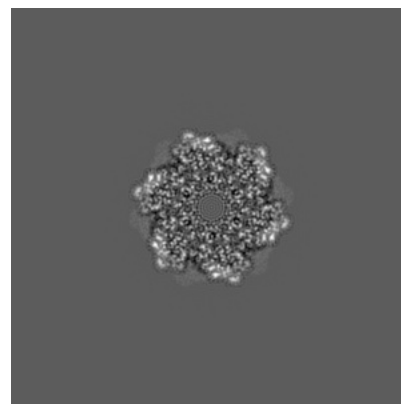
6.3.1 Primary map



X Index: 230



Y Index: 190

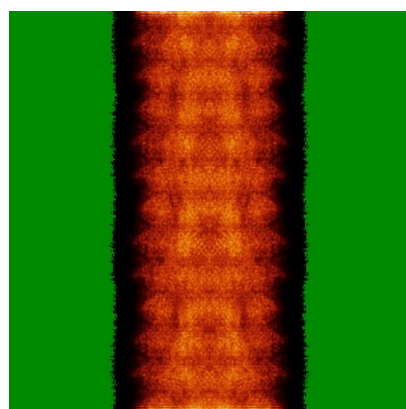


Z Index: 418

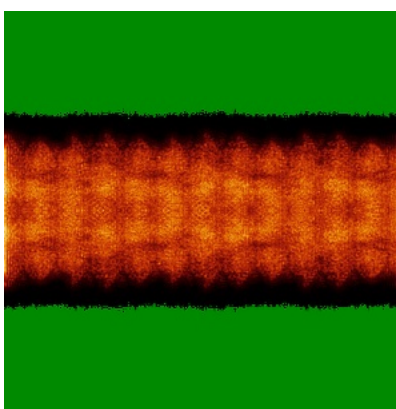
The images above show the largest variance slices of the map in three orthogonal directions.

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

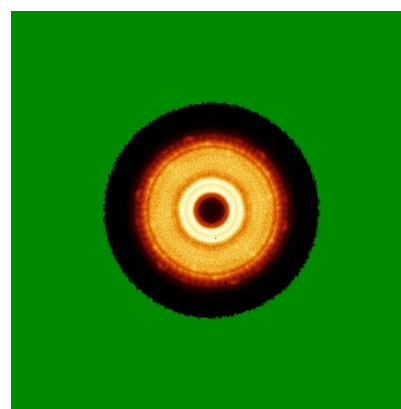
6.4.1 Primary map



X



Y

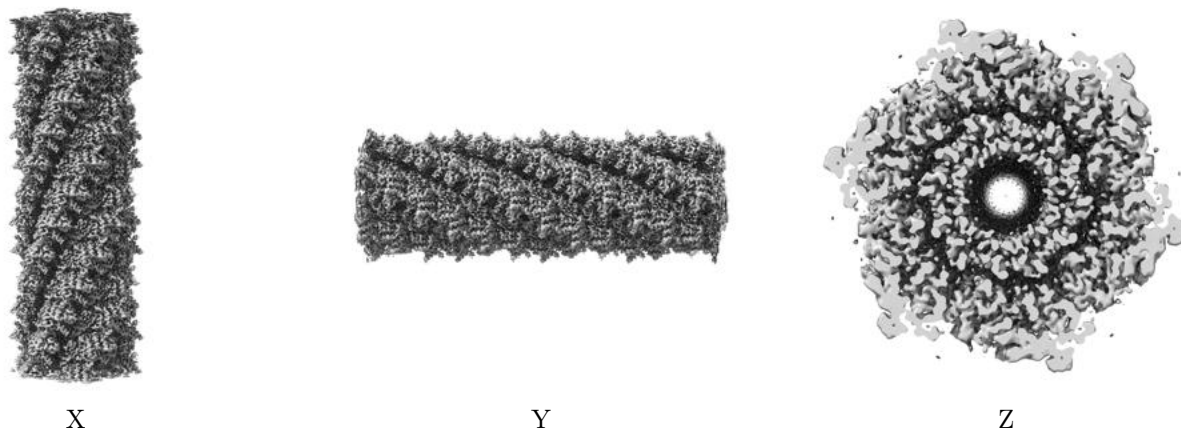


Z

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 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

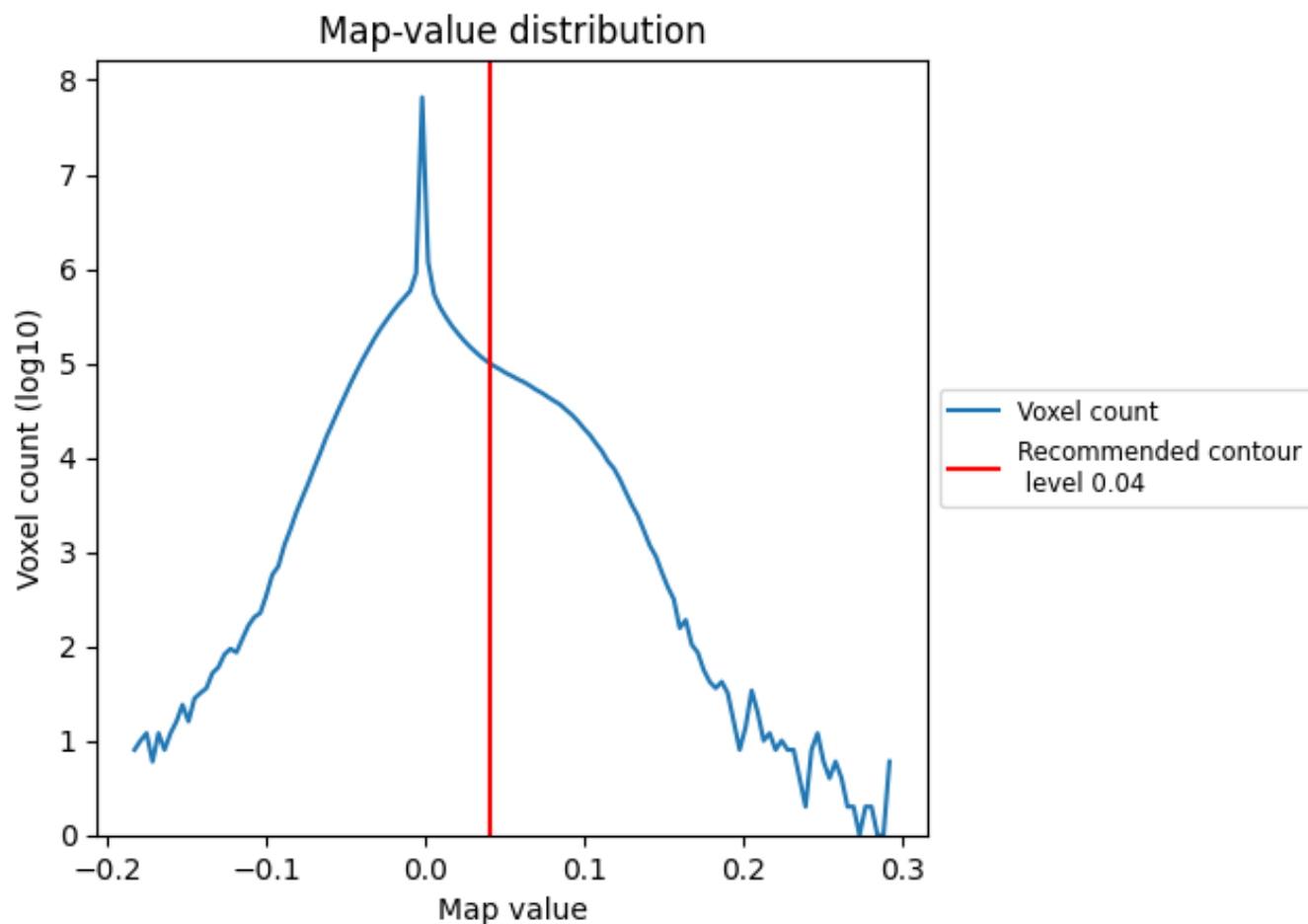
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

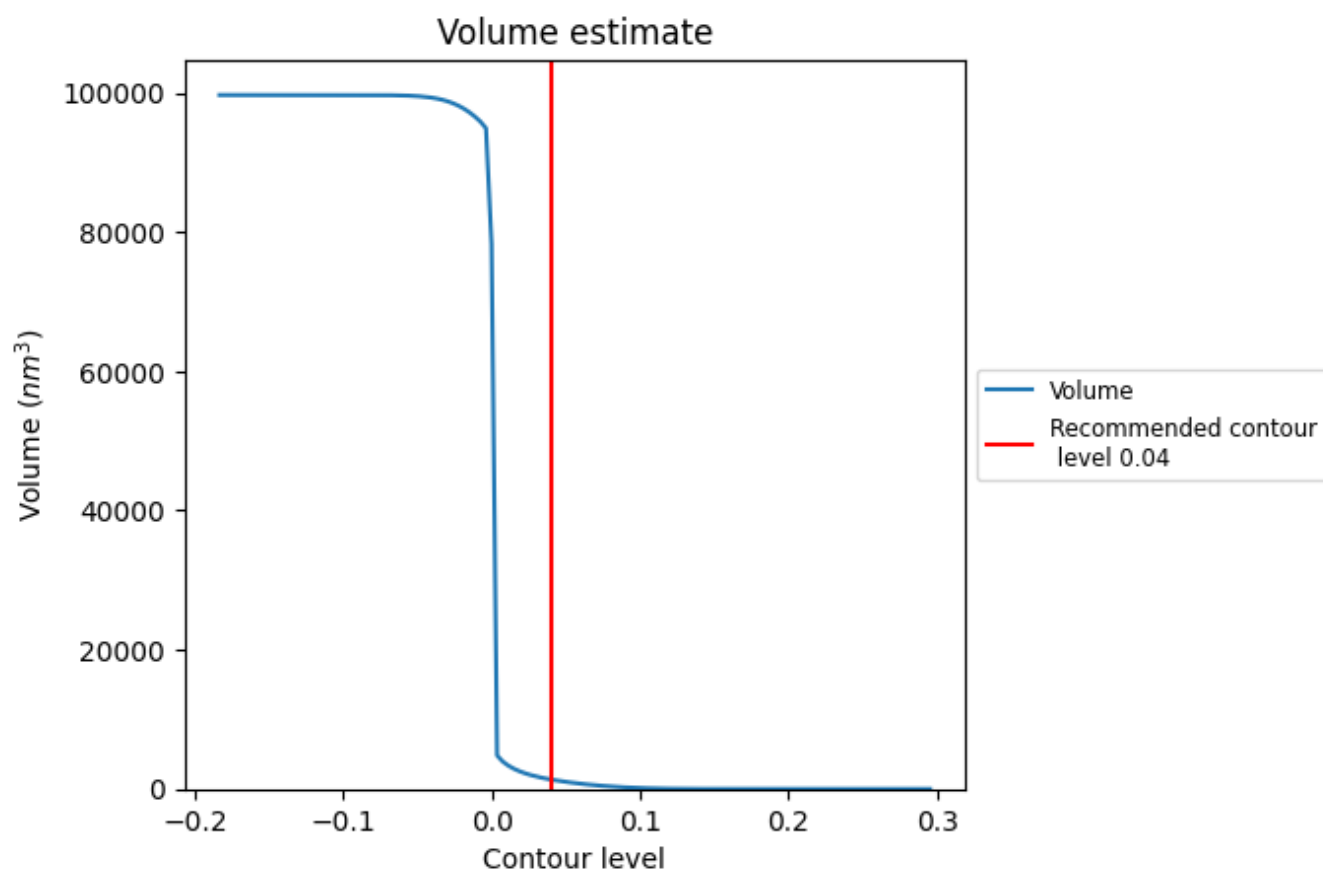
This section contains the results of statistical analysis of the map.

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.

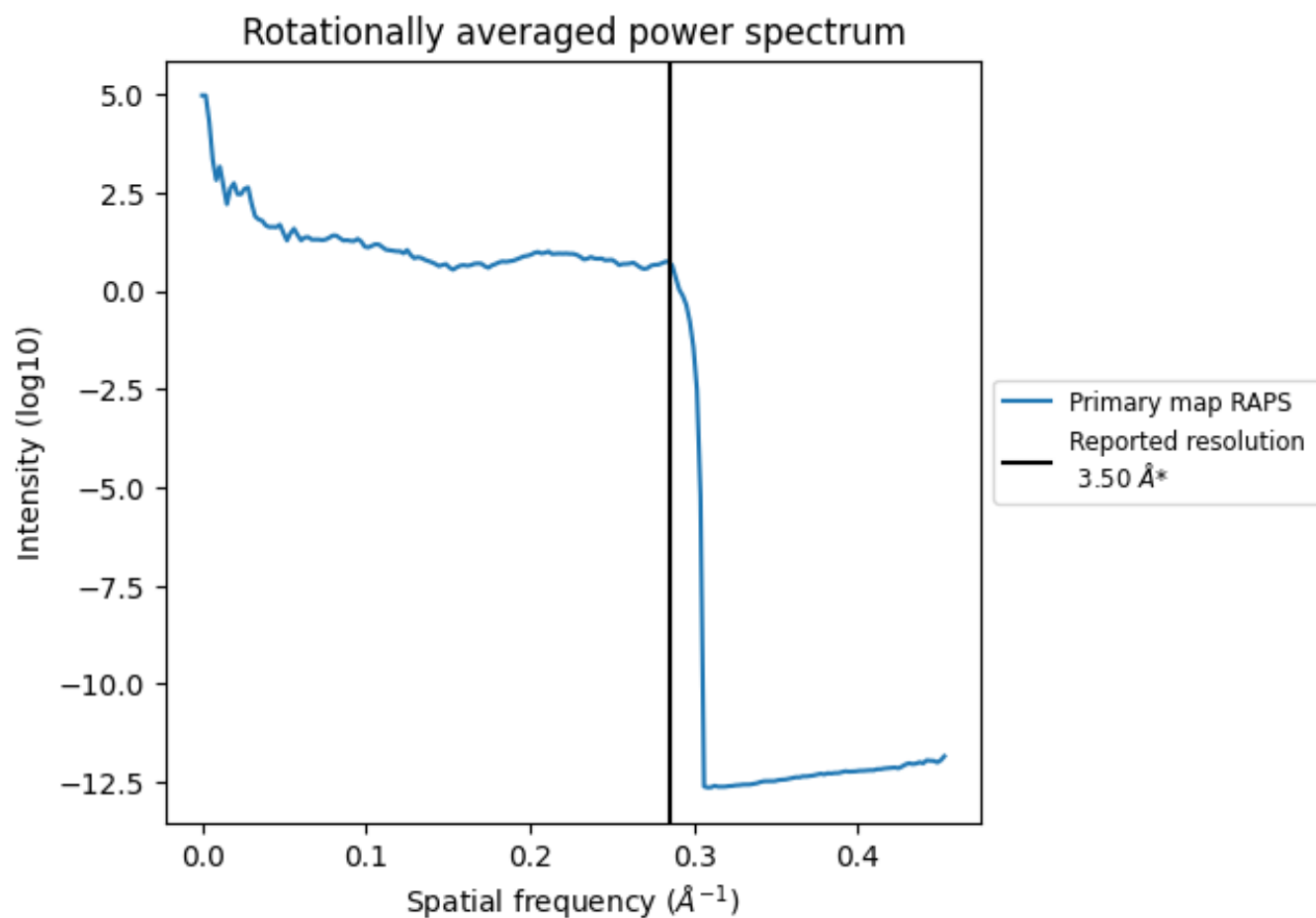
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1353 nm^3 ; this corresponds to an approximate mass of 1222 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 0.286 Å⁻¹

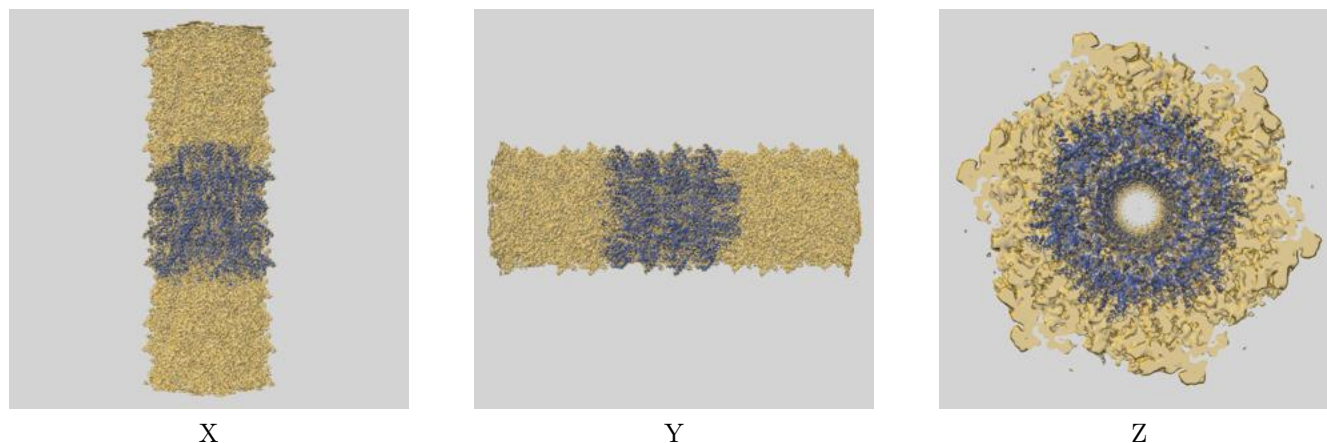
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

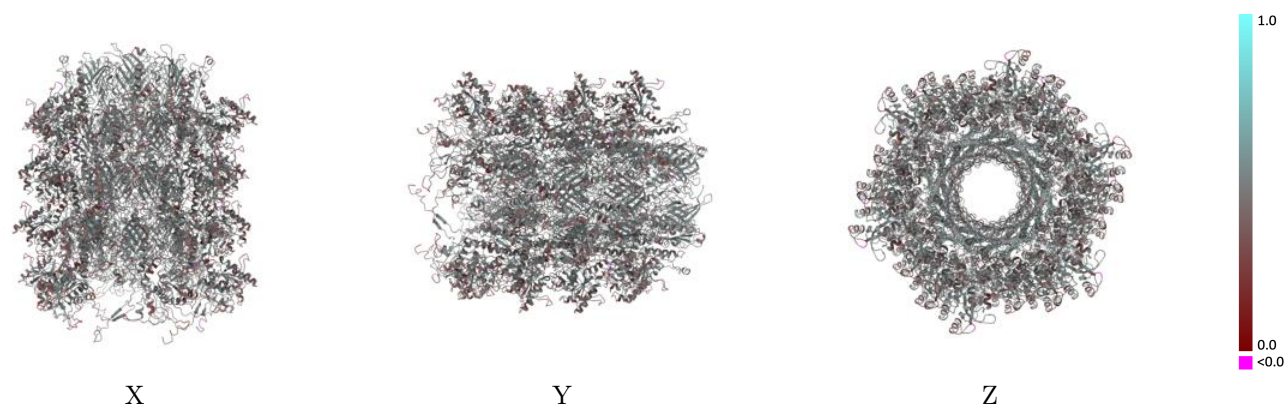
This section contains information regarding the fit between EMDB map EMD-6270 and PDB model 3J9Q. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

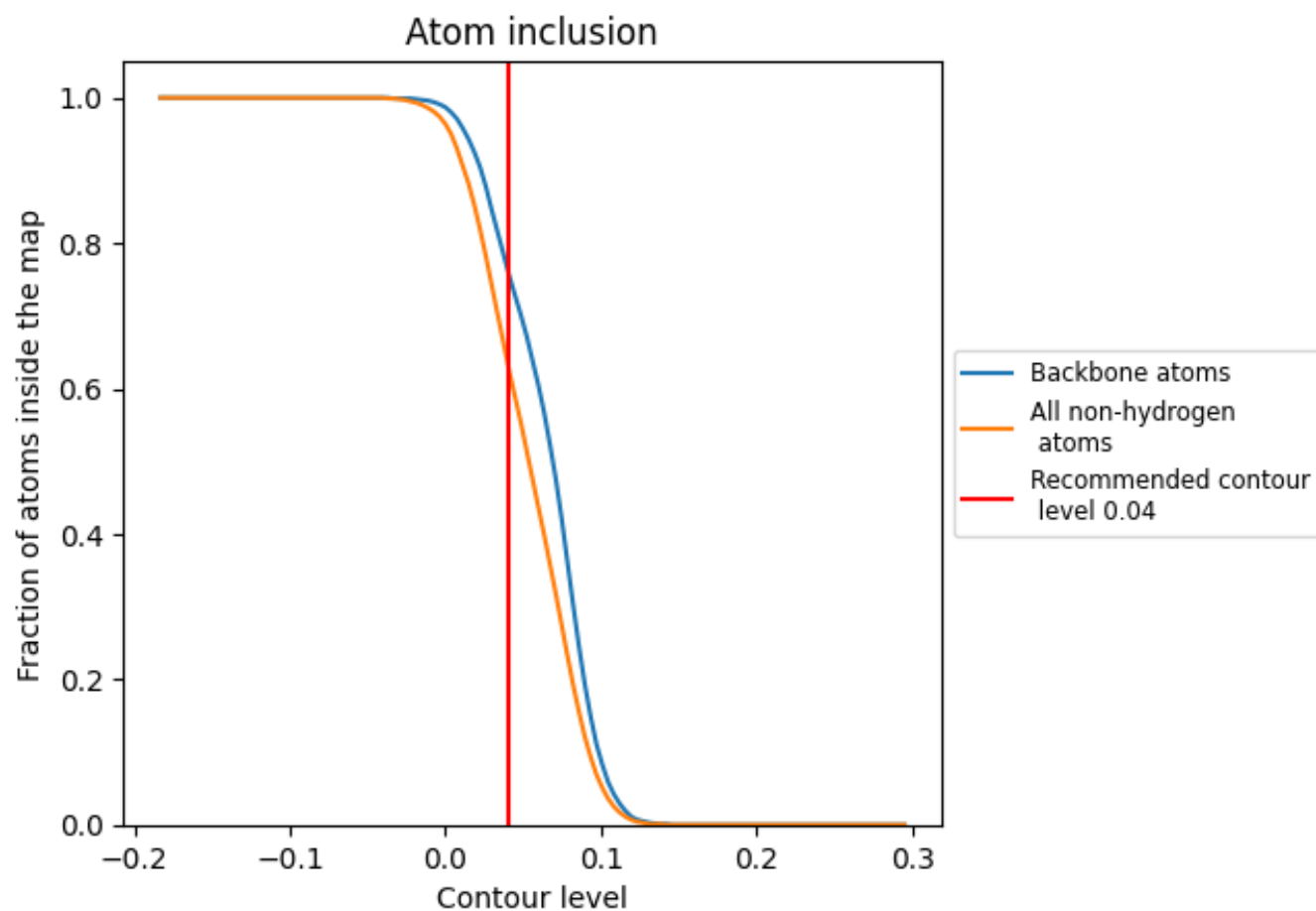


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 64% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6350	 0.4580
A	 0.6280	 0.4430
B	 0.6260	 0.4450
C	 0.6300	 0.4430
D	 0.6270	 0.4450
E	 0.6270	 0.4450
F	 0.6310	 0.4430
G	 0.6330	 0.4450
H	 0.6150	 0.4430
I	 0.6320	 0.4470
J	 0.6200	 0.4440
K	 0.6310	 0.4450
L	 0.6160	 0.4420
M	 0.6300	 0.4450
N	 0.6190	 0.4430
O	 0.6290	 0.4460
P	 0.6170	 0.4440
Q	 0.6330	 0.4450
R	 0.6190	 0.4440
S	 0.6670	 0.4940
T	 0.6680	 0.4910
U	 0.6670	 0.4910
V	 0.6690	 0.4920
W	 0.6650	 0.4930
X	 0.6250	 0.4440
Y	 0.6540	 0.4910
Z	 0.6700	 0.4920
a	 0.6230	 0.4450
b	 0.6540	 0.4890
c	 0.6540	 0.4890
d	 0.6270	 0.4440
e	 0.6560	 0.4900
f	 0.6560	 0.4880
g	 0.6260	 0.4430
h	 0.6500	 0.4890



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Chain	Atom inclusion	Q-score
i	 0.6630	 0.4900
j	 0.6250	 0.4450
k	 0.6580	 0.4890
l	 0.6620	 0.4890
m	 0.6250	 0.4440
n	 0.6520	 0.4900
o	 0.6560	 0.4890
p	 0.6560	 0.4880
q	 0.6410	 0.4880
r	 0.6440	 0.4840
s	 0.6470	 0.4860
t	 0.6470	 0.4860
u	 0.6460	 0.4870
v	 0.6470	 0.4840