



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 03:06 AM UTC

PDB ID : 8BL4 / pdb_00008bl4
EMDB ID : EMD-16101
Title : Cryo-EM structure of a contractile injection system in *Streptomyces coelicolor*, the sheath-tube module in extended state.
Authors : Casu, B.; Sallmen, J.W.; Schlimpert, S.; Pilhofer, M.
Deposited on : 2022-11-09
Resolution : 3.90 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:

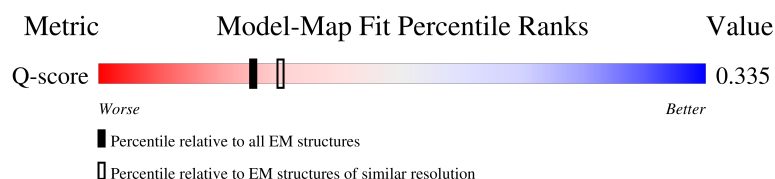
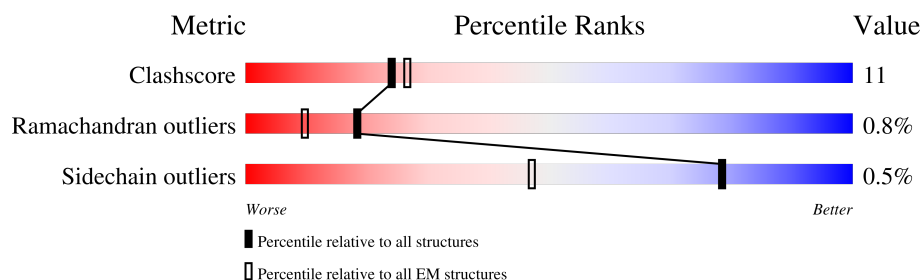
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.90 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	8855 (3.40 - 4.40)

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	539	 5% 57% 11% • 31%
1	B	539	 5% 54% 14% • 31%
1	C	539	 5% 56% 12% • 31%
1	D	539	 5% 56% 12% • 31%

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Mol	Chain	Length	Quality of chain
1	E	539	
1	F	539	
1	G	539	
1	H	539	
1	I	539	
1	J	539	
1	K	539	
1	L	539	
1	M	539	
1	N	539	
1	O	539	
1	P	539	
1	Q	539	
1	R	539	
1	S	539	
1	T	539	
1	U	539	
1	V	539	
1	W	539	
1	X	539	
2	a	149	
2	b	149	
2	c	149	
2	d	149	
2	e	149	

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Mol	Chain	Length	Quality of chain
2	f	149	
2	g	149	
2	h	149	
2	i	149	
2	j	149	
2	k	149	
2	l	149	
2	m	149	
2	n	149	
2	o	149	
2	p	149	
2	q	149	
2	r	149	
2	s	149	
2	t	149	
2	u	149	
2	v	149	
2	w	149	
2	x	149	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 96456 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 Phage tail sheath family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	V	371	Total	C	N	O	S	0	0
			2867	1819	502	538	8		
1	P	371	Total	C	N	O	S	0	0
			2867	1819	502	538	8		
1	J	371	Total	C	N	O	S	0	0
			2867	1819	502	538	8		
1	D	371	Total	C	N	O	S	0	0
			2867	1819	502	538	8		
1	W	371	Total	C	N	O	S	0	0
			2867	1819	502	538	8		
1	Q	371	Total	C	N	O	S	0	0
			2867	1819	502	538	8		
1	K	371	Total	C	N	O	S	0	0
			2867	1819	502	538	8		
1	E	371	Total	C	N	O	S	0	0
			2867	1819	502	538	8		
1	X	371	Total	C	N	O	S	0	0
			2867	1819	502	538	8		
1	R	371	Total	C	N	O	S	0	0
			2867	1819	502	538	8		
1	L	371	Total	C	N	O	S	0	0
			2867	1819	502	538	8		
1	F	371	Total	C	N	O	S	0	0
			2867	1819	502	538	8		
1	S	371	Total	C	N	O	S	0	0
			2867	1819	502	538	8		
1	M	371	Total	C	N	O	S	0	0
			2867	1819	502	538	8		
1	G	371	Total	C	N	O	S	0	0
			2867	1819	502	538	8		
1	A	371	Total	C	N	O	S	0	0
			2867	1819	502	538	8		
1	T	371	Total	C	N	O	S	0	0
			2867	1819	502	538	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	N	371	Total	C	N	O	S	0	0
			2867	1819	502	538	8		
1	H	371	Total	C	N	O	S	0	0
			2867	1819	502	538	8		
1	B	371	Total	C	N	O	S	0	0
			2867	1819	502	538	8		
1	U	371	Total	C	N	O	S	0	0
			2867	1819	502	538	8		
1	O	371	Total	C	N	O	S	0	0
			2867	1819	502	538	8		
1	I	371	Total	C	N	O	S	0	0
			2867	1819	502	538	8		
1	C	371	Total	C	N	O	S	0	0
			2867	1819	502	538	8		

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	26	ILE	-	insertion	UNP Q9L0N8
V	27	GLU	-	insertion	UNP Q9L0N8
V	28	GLY	-	insertion	UNP Q9L0N8
V	29	VAL	-	insertion	UNP Q9L0N8
V	30	GLY	-	insertion	UNP Q9L0N8
P	26	ILE	-	insertion	UNP Q9L0N8
P	27	GLU	-	insertion	UNP Q9L0N8
P	28	GLY	-	insertion	UNP Q9L0N8
P	29	VAL	-	insertion	UNP Q9L0N8
P	30	GLY	-	insertion	UNP Q9L0N8
J	26	ILE	-	insertion	UNP Q9L0N8
J	27	GLU	-	insertion	UNP Q9L0N8
J	28	GLY	-	insertion	UNP Q9L0N8
J	29	VAL	-	insertion	UNP Q9L0N8
J	30	GLY	-	insertion	UNP Q9L0N8
D	26	ILE	-	insertion	UNP Q9L0N8
D	27	GLU	-	insertion	UNP Q9L0N8
D	28	GLY	-	insertion	UNP Q9L0N8
D	29	VAL	-	insertion	UNP Q9L0N8
D	30	GLY	-	insertion	UNP Q9L0N8
W	26	ILE	-	insertion	UNP Q9L0N8
W	27	GLU	-	insertion	UNP Q9L0N8
W	28	GLY	-	insertion	UNP Q9L0N8
W	29	VAL	-	insertion	UNP Q9L0N8
W	30	GLY	-	insertion	UNP Q9L0N8

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	26	ILE	-	insertion	UNP Q9L0N8
Q	27	GLU	-	insertion	UNP Q9L0N8
Q	28	GLY	-	insertion	UNP Q9L0N8
Q	29	VAL	-	insertion	UNP Q9L0N8
Q	30	GLY	-	insertion	UNP Q9L0N8
K	26	ILE	-	insertion	UNP Q9L0N8
K	27	GLU	-	insertion	UNP Q9L0N8
K	28	GLY	-	insertion	UNP Q9L0N8
K	29	VAL	-	insertion	UNP Q9L0N8
K	30	GLY	-	insertion	UNP Q9L0N8
E	26	ILE	-	insertion	UNP Q9L0N8
E	27	GLU	-	insertion	UNP Q9L0N8
E	28	GLY	-	insertion	UNP Q9L0N8
E	29	VAL	-	insertion	UNP Q9L0N8
E	30	GLY	-	insertion	UNP Q9L0N8
X	26	ILE	-	insertion	UNP Q9L0N8
X	27	GLU	-	insertion	UNP Q9L0N8
X	28	GLY	-	insertion	UNP Q9L0N8
X	29	VAL	-	insertion	UNP Q9L0N8
X	30	GLY	-	insertion	UNP Q9L0N8
R	26	ILE	-	insertion	UNP Q9L0N8
R	27	GLU	-	insertion	UNP Q9L0N8
R	28	GLY	-	insertion	UNP Q9L0N8
R	29	VAL	-	insertion	UNP Q9L0N8
R	30	GLY	-	insertion	UNP Q9L0N8
L	26	ILE	-	insertion	UNP Q9L0N8
L	27	GLU	-	insertion	UNP Q9L0N8
L	28	GLY	-	insertion	UNP Q9L0N8
L	29	VAL	-	insertion	UNP Q9L0N8
L	30	GLY	-	insertion	UNP Q9L0N8
F	26	ILE	-	insertion	UNP Q9L0N8
F	27	GLU	-	insertion	UNP Q9L0N8
F	28	GLY	-	insertion	UNP Q9L0N8
F	29	VAL	-	insertion	UNP Q9L0N8
F	30	GLY	-	insertion	UNP Q9L0N8
S	26	ILE	-	insertion	UNP Q9L0N8
S	27	GLU	-	insertion	UNP Q9L0N8
S	28	GLY	-	insertion	UNP Q9L0N8
S	29	VAL	-	insertion	UNP Q9L0N8
S	30	GLY	-	insertion	UNP Q9L0N8
M	26	ILE	-	insertion	UNP Q9L0N8
M	27	GLU	-	insertion	UNP Q9L0N8

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Chain	Residue	Modelled	Actual	Comment	Reference
M	28	GLY	-	insertion	UNP Q9L0N8
M	29	VAL	-	insertion	UNP Q9L0N8
M	30	GLY	-	insertion	UNP Q9L0N8
G	26	ILE	-	insertion	UNP Q9L0N8
G	27	GLU	-	insertion	UNP Q9L0N8
G	28	GLY	-	insertion	UNP Q9L0N8
G	29	VAL	-	insertion	UNP Q9L0N8
G	30	GLY	-	insertion	UNP Q9L0N8
A	26	ILE	-	insertion	UNP Q9L0N8
A	27	GLU	-	insertion	UNP Q9L0N8
A	28	GLY	-	insertion	UNP Q9L0N8
A	29	VAL	-	insertion	UNP Q9L0N8
A	30	GLY	-	insertion	UNP Q9L0N8
T	26	ILE	-	insertion	UNP Q9L0N8
T	27	GLU	-	insertion	UNP Q9L0N8
T	28	GLY	-	insertion	UNP Q9L0N8
T	29	VAL	-	insertion	UNP Q9L0N8
T	30	GLY	-	insertion	UNP Q9L0N8
N	26	ILE	-	insertion	UNP Q9L0N8
N	27	GLU	-	insertion	UNP Q9L0N8
N	28	GLY	-	insertion	UNP Q9L0N8
N	29	VAL	-	insertion	UNP Q9L0N8
N	30	GLY	-	insertion	UNP Q9L0N8
H	26	ILE	-	insertion	UNP Q9L0N8
H	27	GLU	-	insertion	UNP Q9L0N8
H	28	GLY	-	insertion	UNP Q9L0N8
H	29	VAL	-	insertion	UNP Q9L0N8
H	30	GLY	-	insertion	UNP Q9L0N8
B	26	ILE	-	insertion	UNP Q9L0N8
B	27	GLU	-	insertion	UNP Q9L0N8
B	28	GLY	-	insertion	UNP Q9L0N8
B	29	VAL	-	insertion	UNP Q9L0N8
B	30	GLY	-	insertion	UNP Q9L0N8
U	26	ILE	-	insertion	UNP Q9L0N8
U	27	GLU	-	insertion	UNP Q9L0N8
U	28	GLY	-	insertion	UNP Q9L0N8
U	29	VAL	-	insertion	UNP Q9L0N8
U	30	GLY	-	insertion	UNP Q9L0N8
O	26	ILE	-	insertion	UNP Q9L0N8
O	27	GLU	-	insertion	UNP Q9L0N8
O	28	GLY	-	insertion	UNP Q9L0N8
O	29	VAL	-	insertion	UNP Q9L0N8

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Chain	Residue	Modelled	Actual	Comment	Reference
O	30	GLY	-	insertion	UNP Q9L0N8
I	26	ILE	-	insertion	UNP Q9L0N8
I	27	GLU	-	insertion	UNP Q9L0N8
I	28	GLY	-	insertion	UNP Q9L0N8
I	29	VAL	-	insertion	UNP Q9L0N8
I	30	GLY	-	insertion	UNP Q9L0N8
C	26	ILE	-	insertion	UNP Q9L0N8
C	27	GLU	-	insertion	UNP Q9L0N8
C	28	GLY	-	insertion	UNP Q9L0N8
C	29	VAL	-	insertion	UNP Q9L0N8
C	30	GLY	-	insertion	UNP Q9L0N8

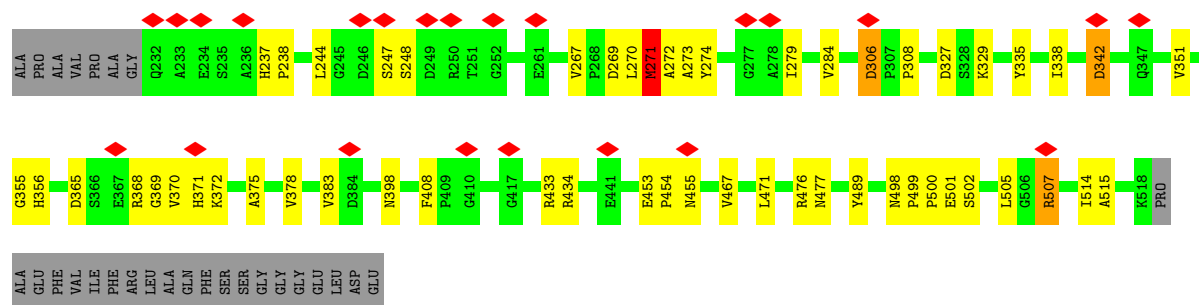
- Molecule 2 is a protein called Phage tail protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	v	149	Total	C	N	O	S	0	0
			1152	717	200	227	8		
2	p	149	Total	C	N	O	S	0	0
			1152	717	200	227	8		
2	j	149	Total	C	N	O	S	0	0
			1152	717	200	227	8		
2	d	149	Total	C	N	O	S	0	0
			1152	717	200	227	8		
2	w	149	Total	C	N	O	S	0	0
			1152	717	200	227	8		
2	q	149	Total	C	N	O	S	0	0
			1152	717	200	227	8		
2	k	149	Total	C	N	O	S	0	0
			1152	717	200	227	8		
2	e	149	Total	C	N	O	S	0	0
			1152	717	200	227	8		
2	x	149	Total	C	N	O	S	0	0
			1152	717	200	227	8		
2	r	149	Total	C	N	O	S	0	0
			1152	717	200	227	8		
2	l	149	Total	C	N	O	S	0	0
			1152	717	200	227	8		
2	f	149	Total	C	N	O	S	0	0
			1152	717	200	227	8		
2	s	149	Total	C	N	O	S	0	0
			1152	717	200	227	8		
2	m	149	Total	C	N	O	S	0	0
			1152	717	200	227	8		

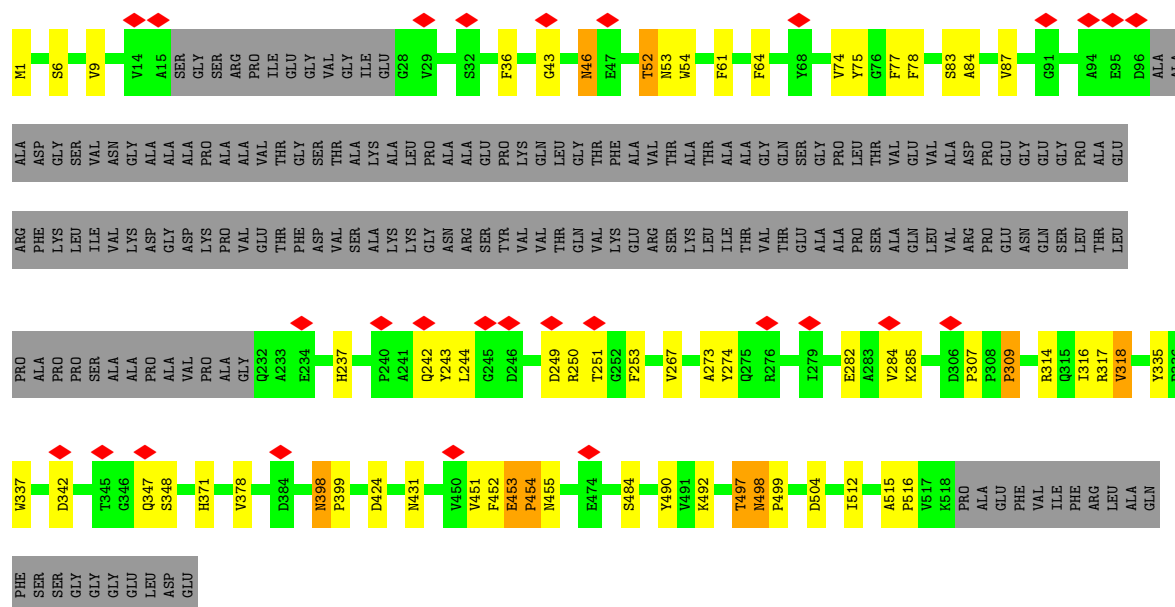
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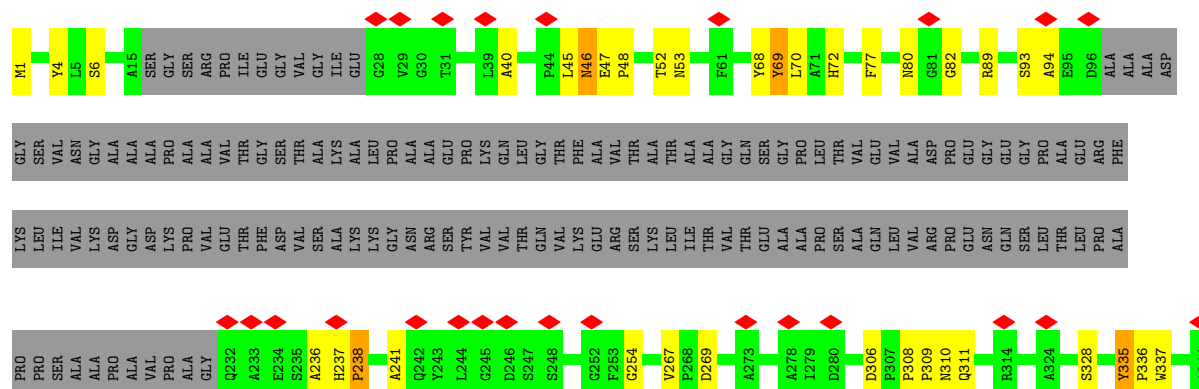
Mol	Chain	Residues	Atoms					AltConf	Trace
2	g	149	Total	C	N	O	S	0	0
			1152	717	200	227	8		
2	a	149	Total	C	N	O	S	0	0
			1152	717	200	227	8		
2	t	149	Total	C	N	O	S	0	0
			1152	717	200	227	8		
2	n	149	Total	C	N	O	S	0	0
			1152	717	200	227	8		
2	h	149	Total	C	N	O	S	0	0
			1152	717	200	227	8		
2	b	149	Total	C	N	O	S	0	0
			1152	717	200	227	8		
2	u	149	Total	C	N	O	S	0	0
			1152	717	200	227	8		
2	o	149	Total	C	N	O	S	0	0
			1152	717	200	227	8		
2	i	149	Total	C	N	O	S	0	0
			1152	717	200	227	8		
2	c	149	Total	C	N	O	S	0	0
			1152	717	200	227	8		

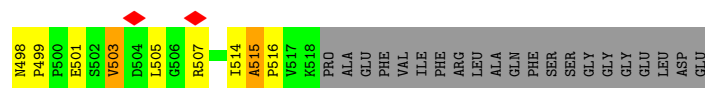


- Molecule 1: Phage tail sheath family protein

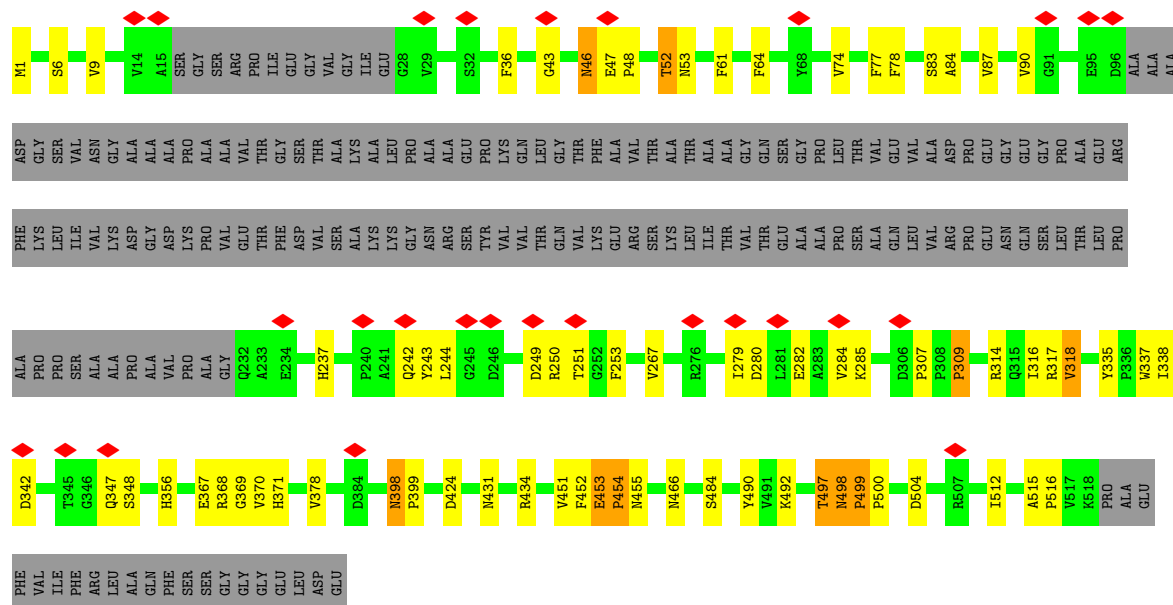


- Molecule 1: Phage tail sheath family protein

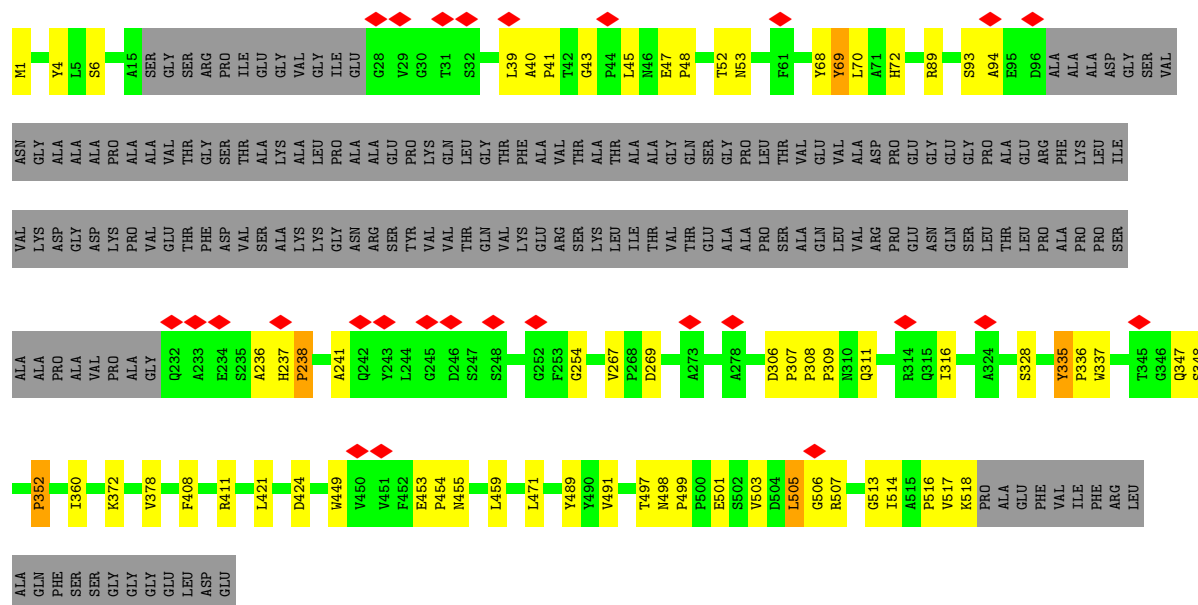




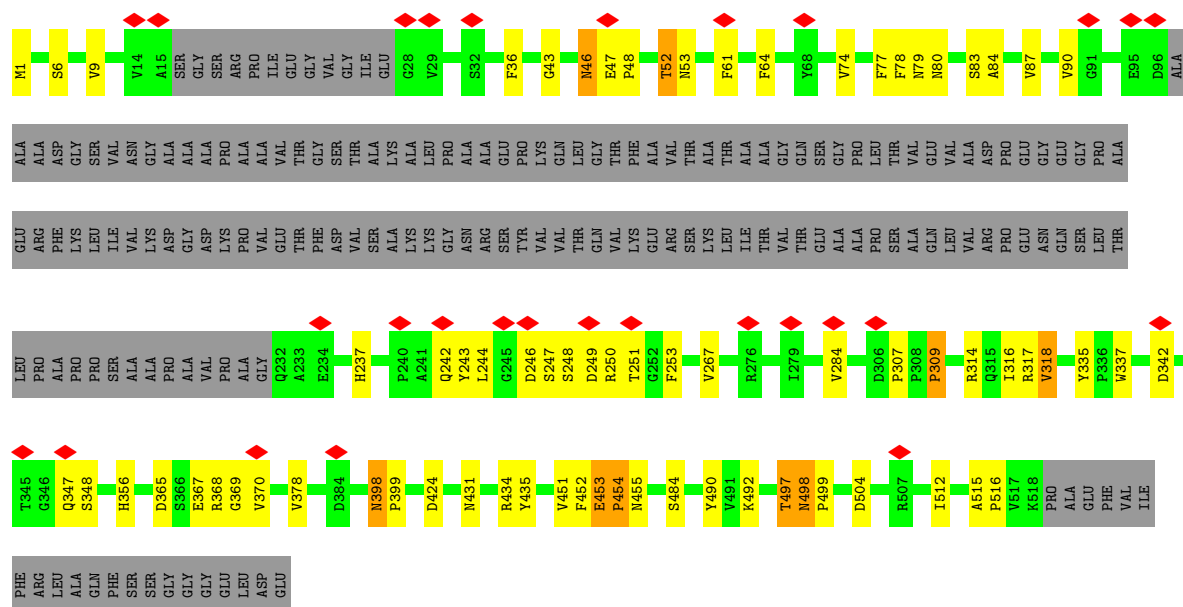
• Molecule 1: Phage tail sheath family protein



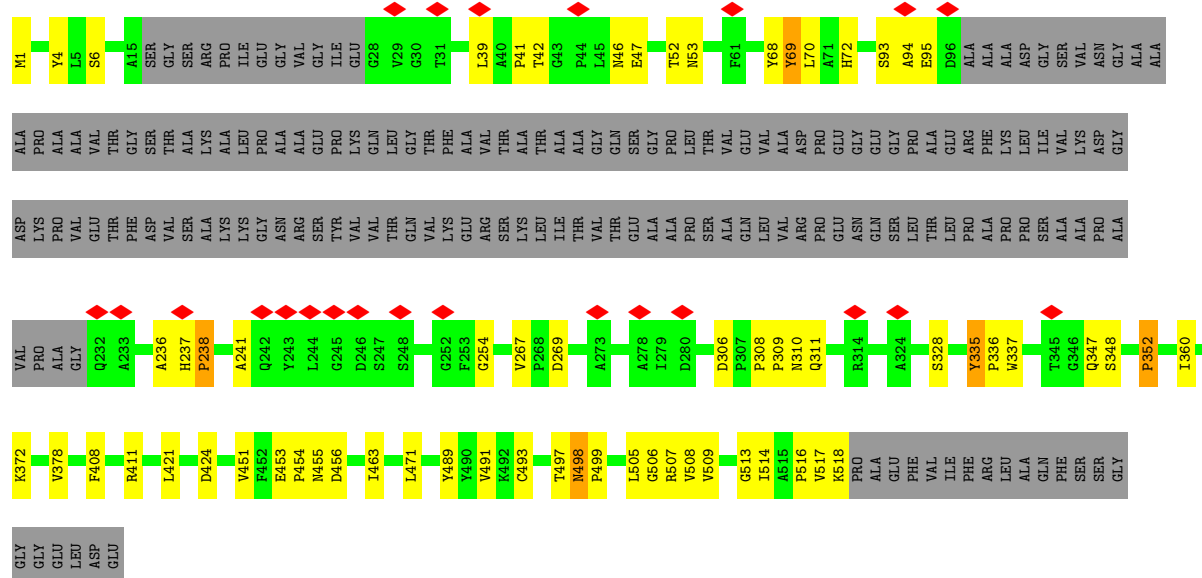
• Molecule 1: Phage tail sheath family protein



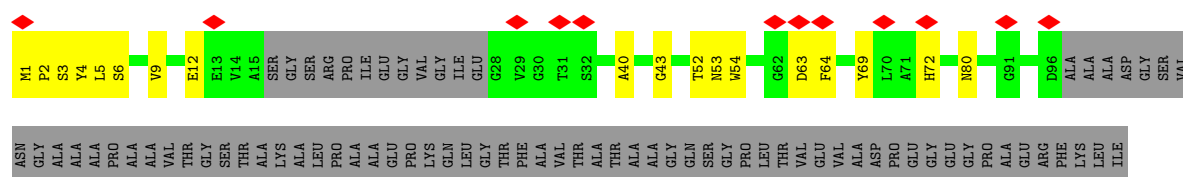
• Molecule 1: Phage tail sheath family protein



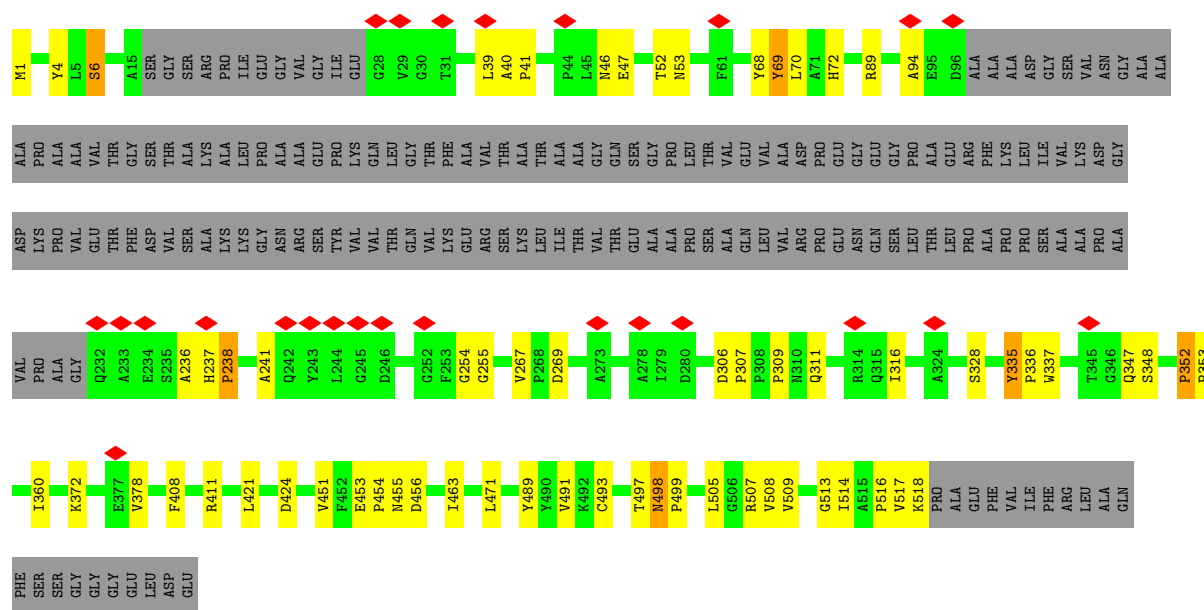
• Molecule 1: Phage tail sheath family protein



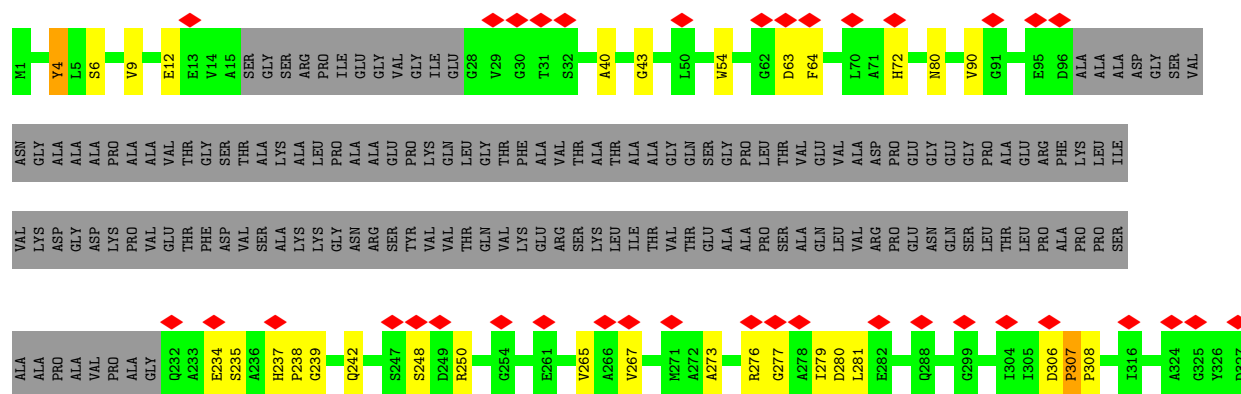
• Molecule 1: Phage tail sheath family protein

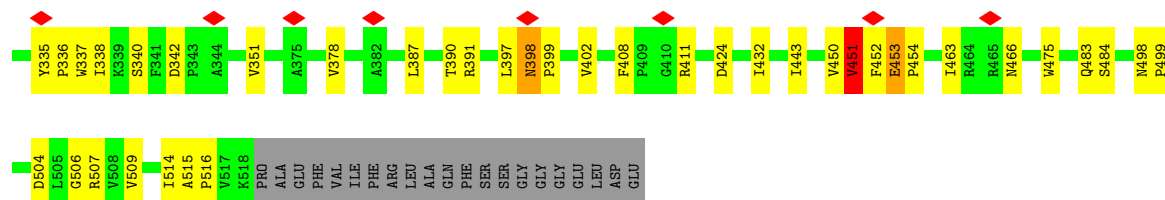


- Molecule 1: Phage tail sheath family protein

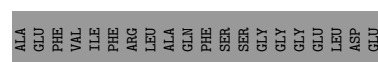
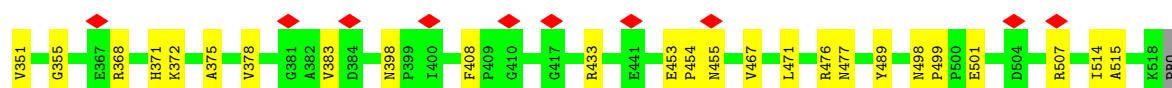
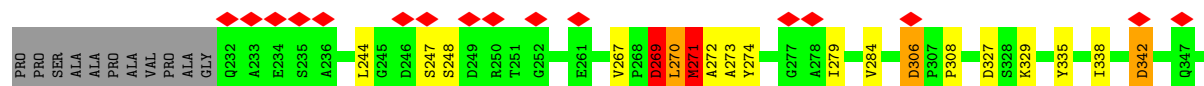
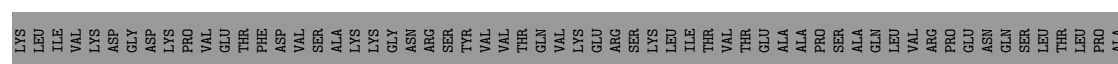
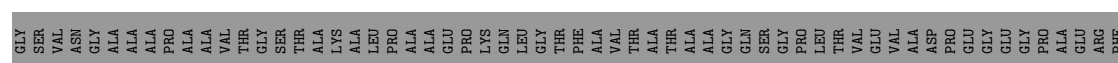
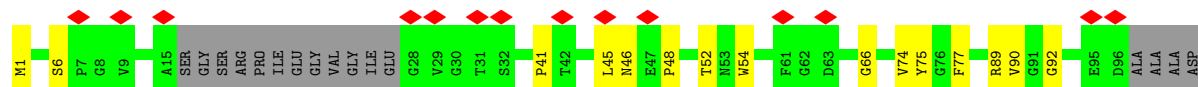


- Molecule 1: Phage tail sheath family protein

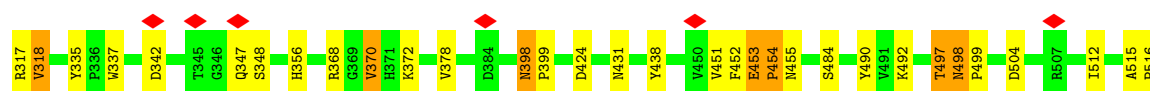
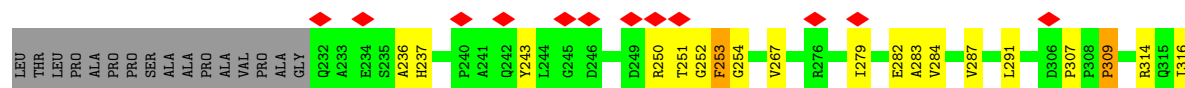
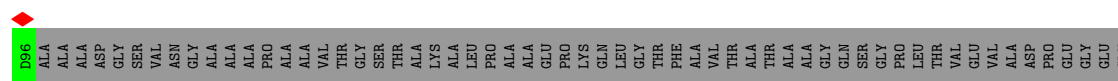
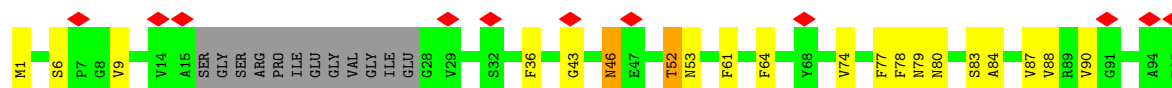


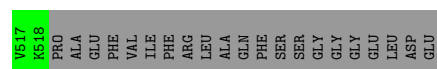


• Molecule 1: Phage tail sheath family protein

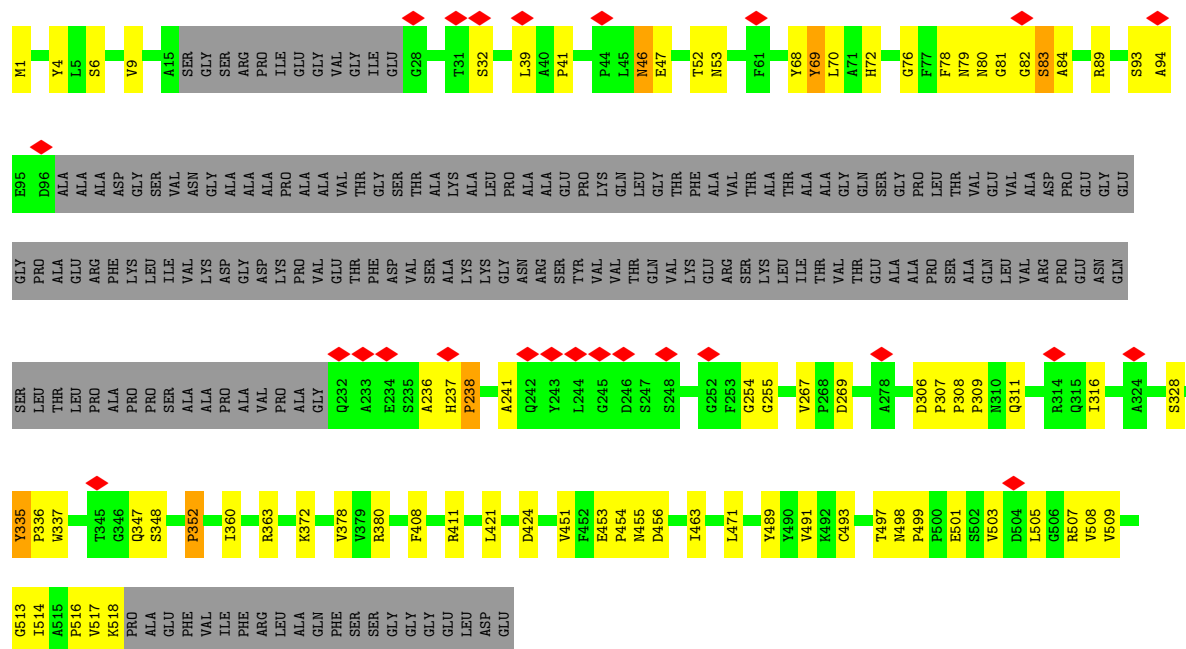


• Molecule 1: Phage tail sheath family protein

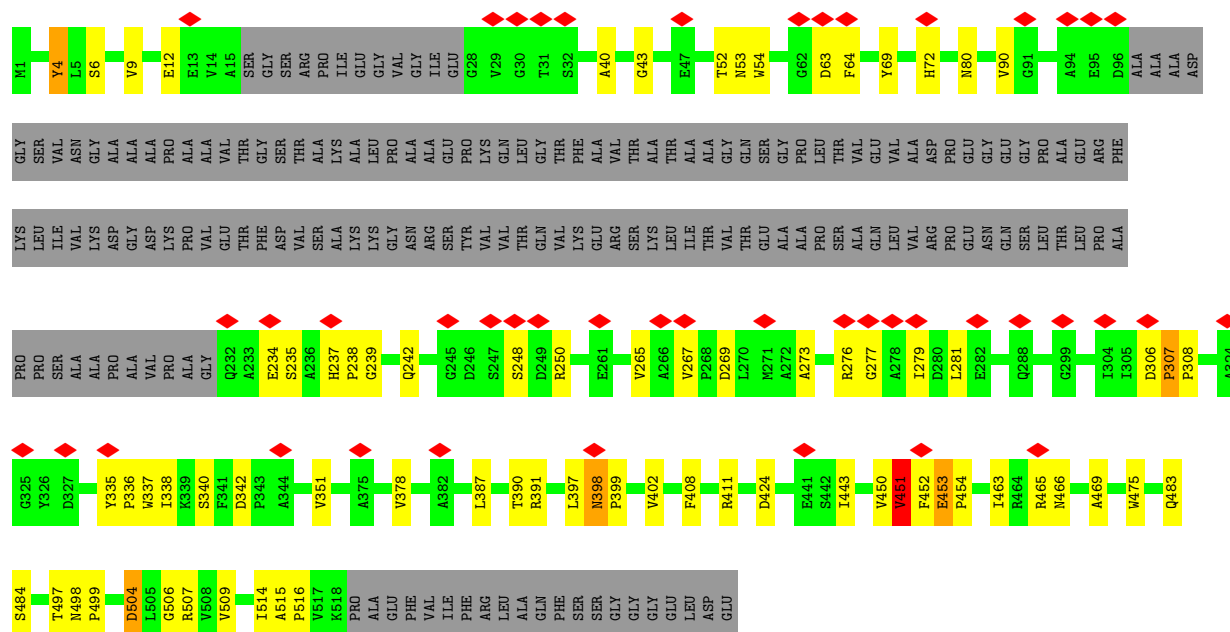




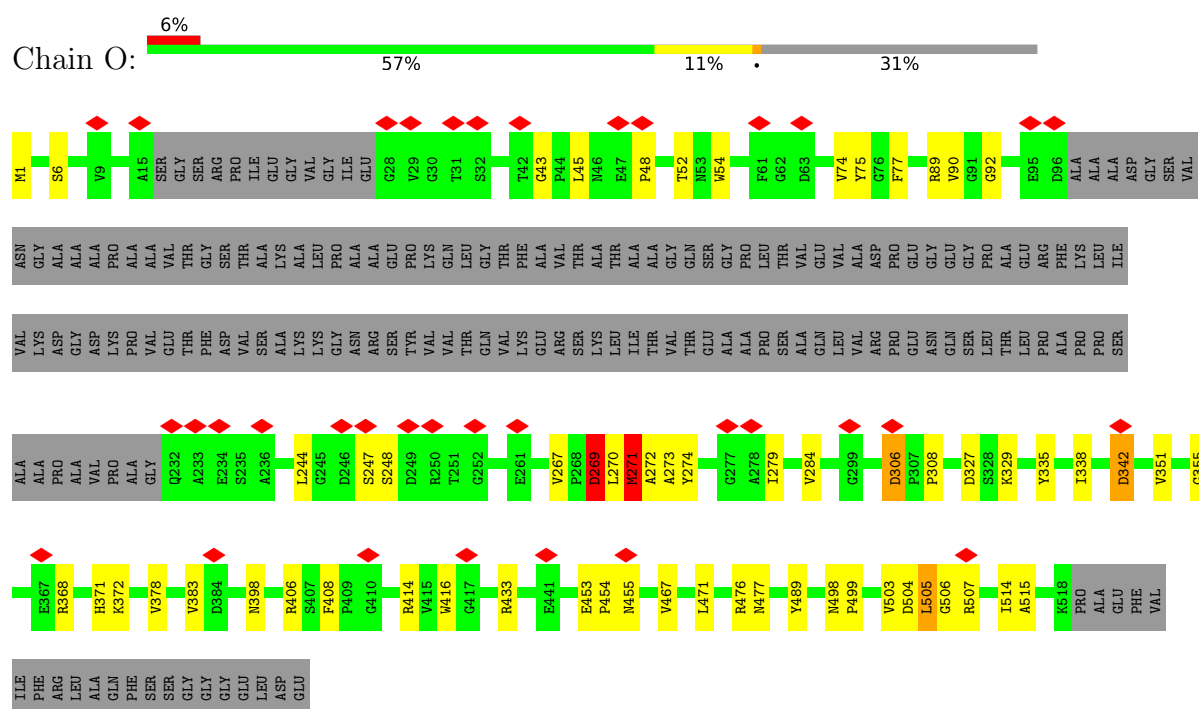
• Molecule 1: Phage tail sheath family protein



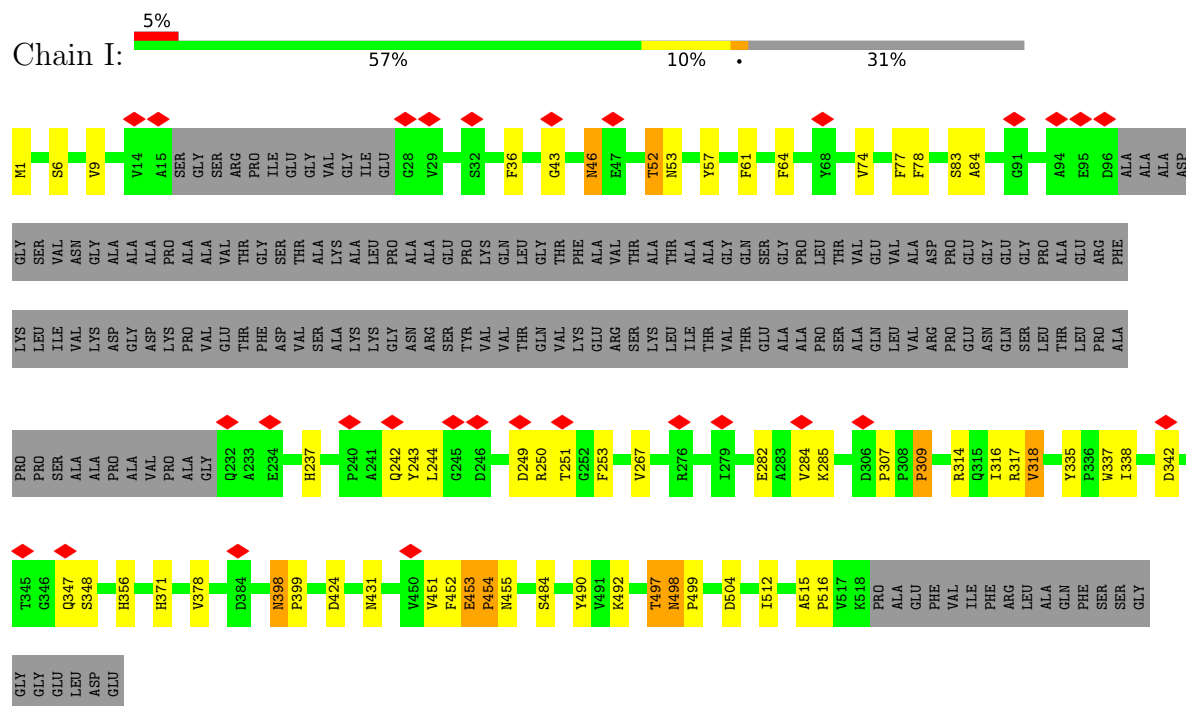
• Molecule 1: Phage tail sheath family protein



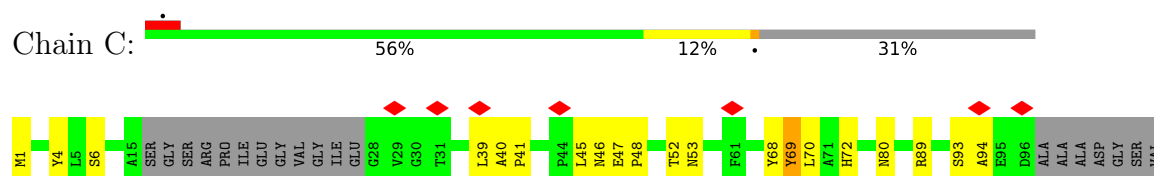
• Molecule 1: Phage tail sheath family protein

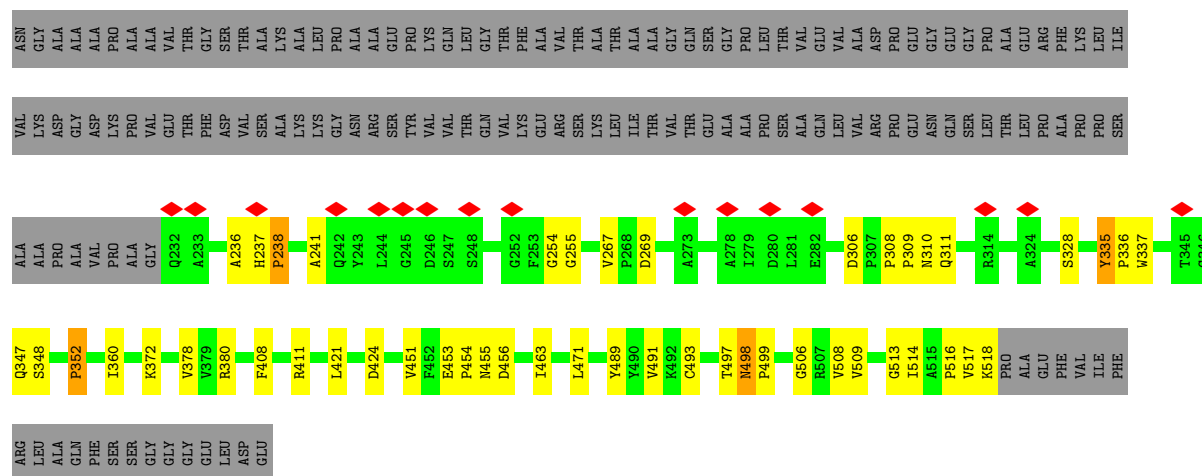


- Molecule 1: Phage tail sheath family protein

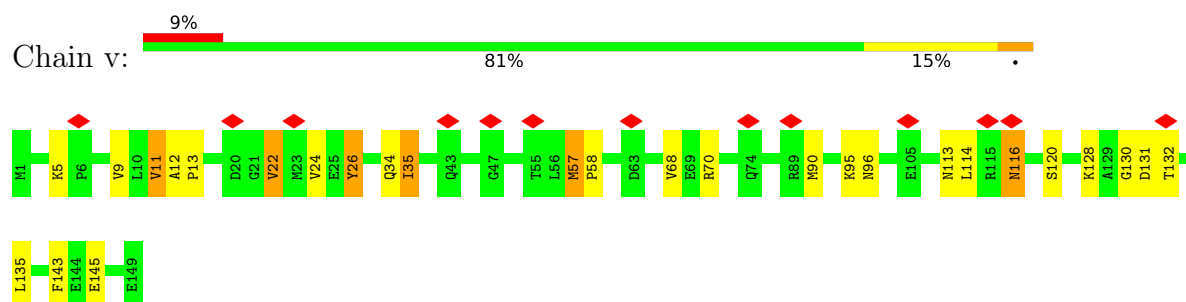


- Molecule 1: Phage tail sheath family protein

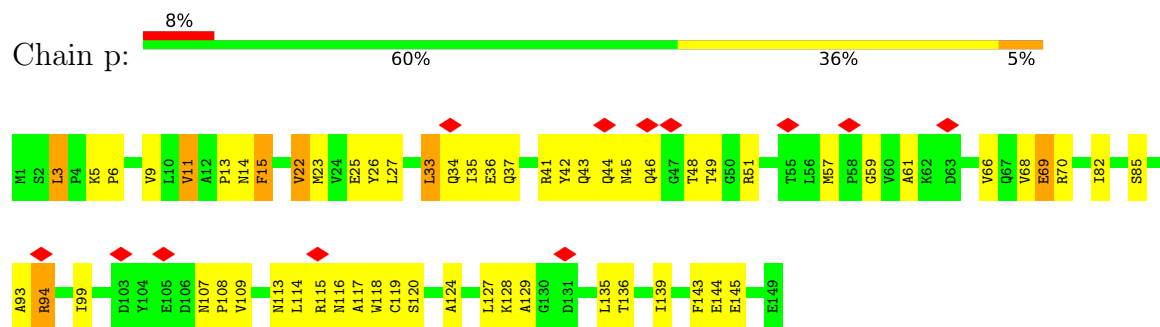




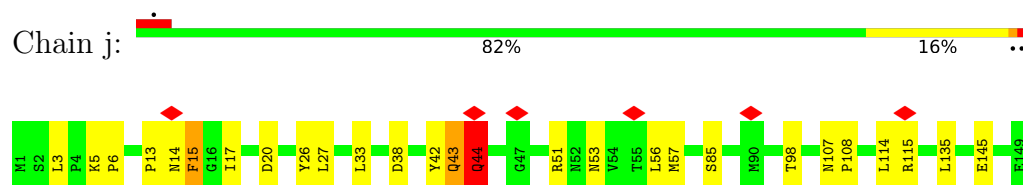
• Molecule 2: Phage tail protein



• Molecule 2: Phage tail protein

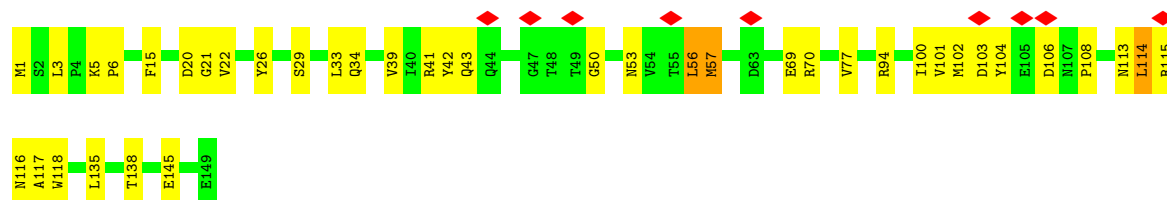


• Molecule 2: Phage tail protein

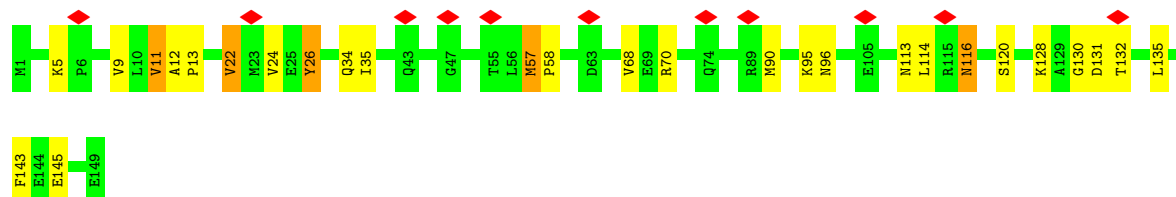
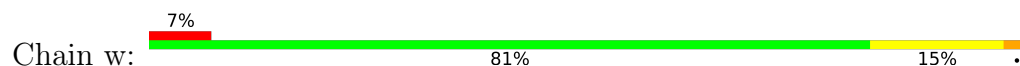


• Molecule 2: Phage tail protein

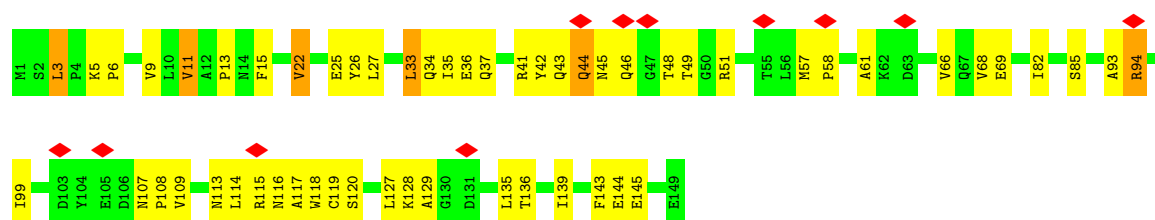




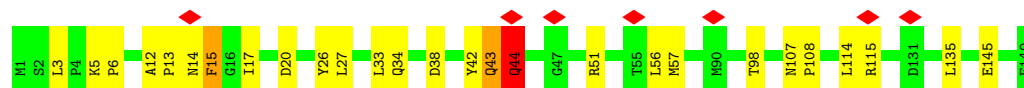
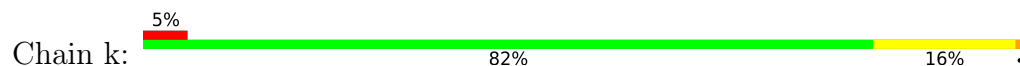
• Molecule 2: Phage tail protein



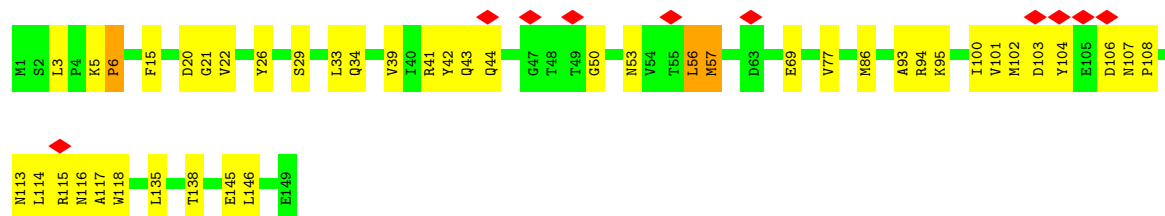
• Molecule 2: Phage tail protein



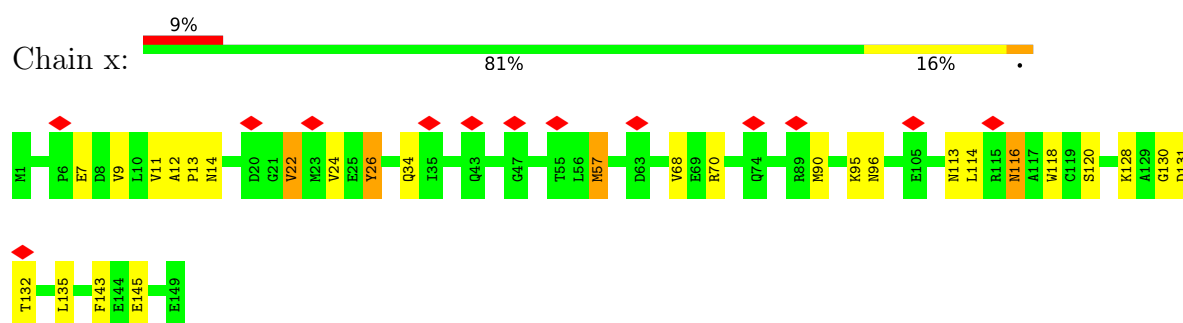
• Molecule 2: Phage tail protein



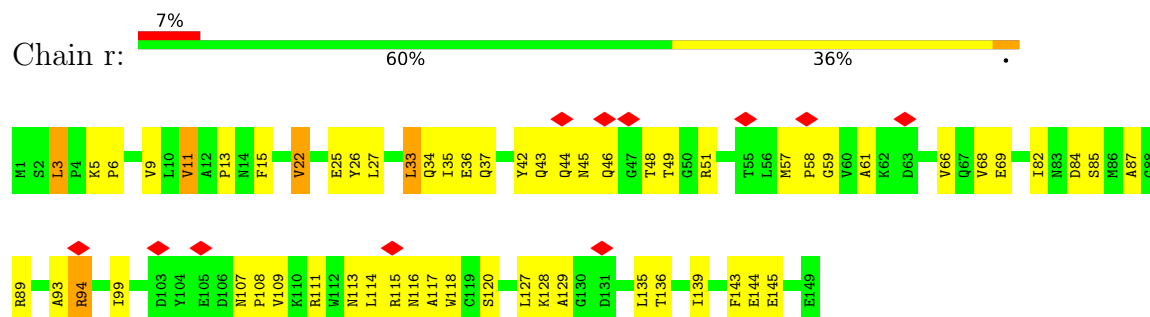
• Molecule 2: Phage tail protein



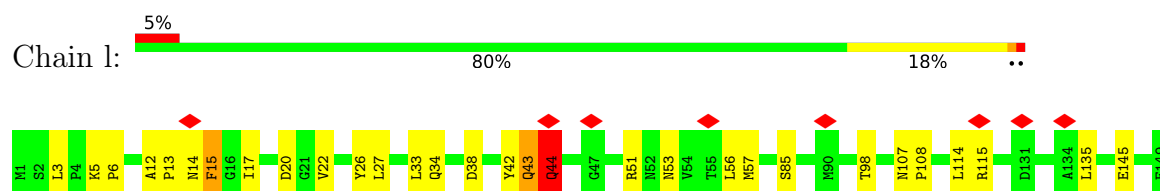
• Molecule 2: Phage tail protein



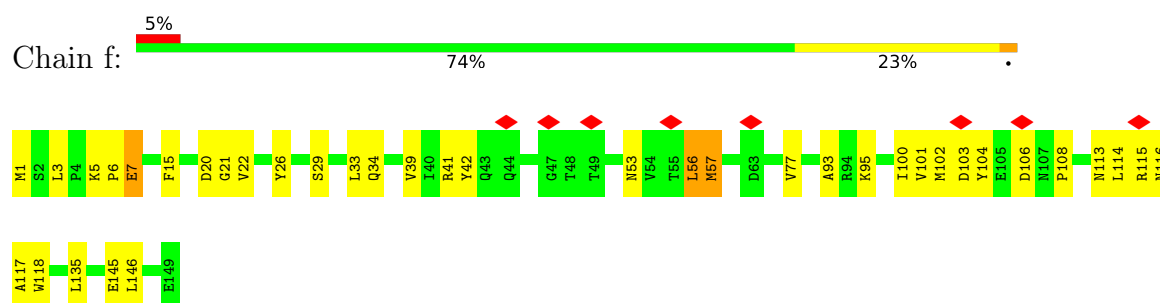
- Molecule 2: Phage tail protein



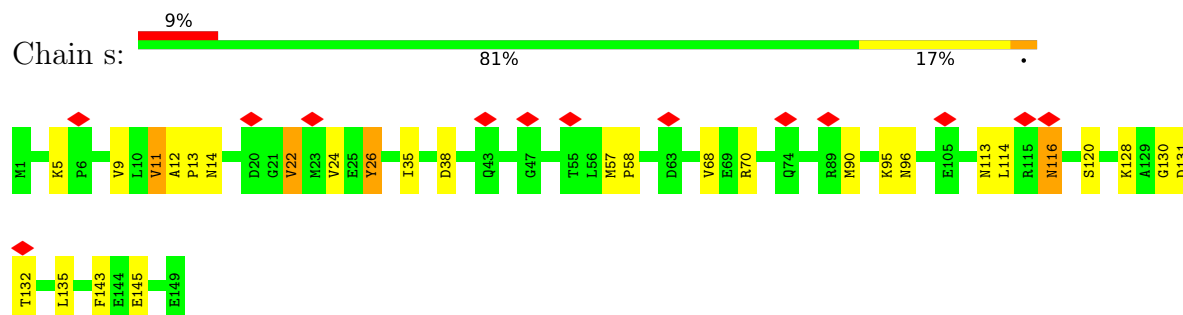
- Molecule 2: Phage tail protein



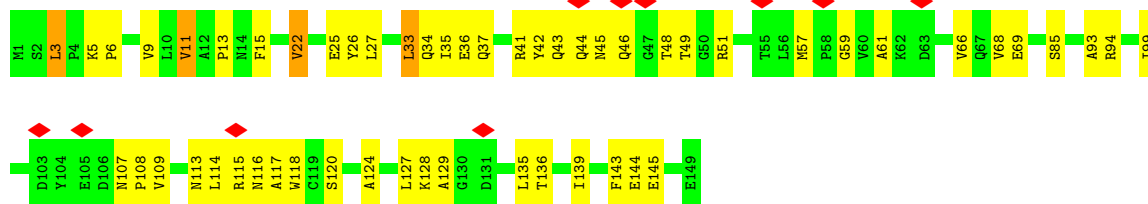
- Molecule 2: Phage tail protein



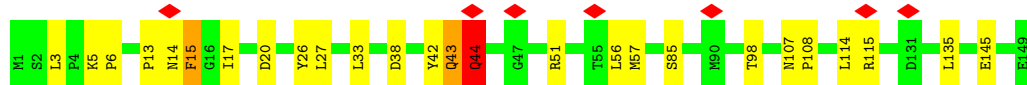
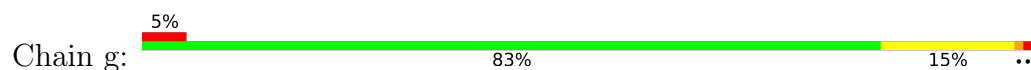
- Molecule 2: Phage tail protein



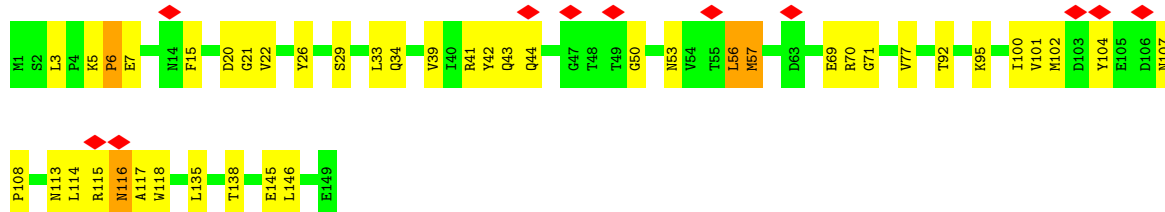
- Molecule 2: Phage tail protein



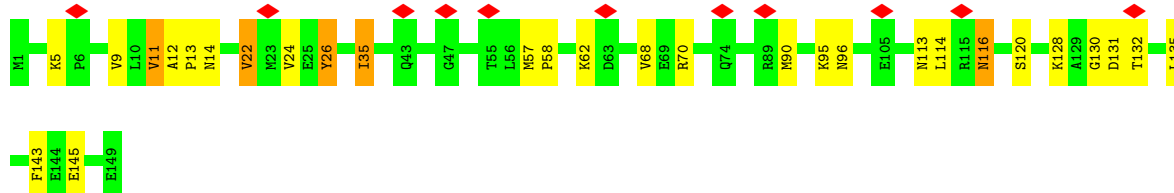
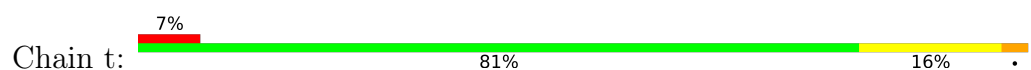
- Molecule 2: Phage tail protein



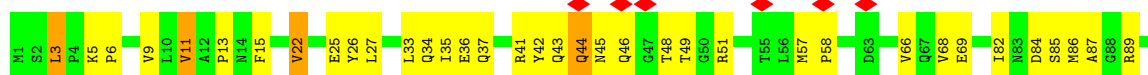
- Molecule 2: Phage tail protein

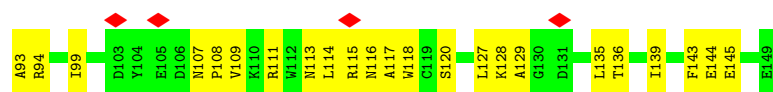


- Molecule 2: Phage tail protein

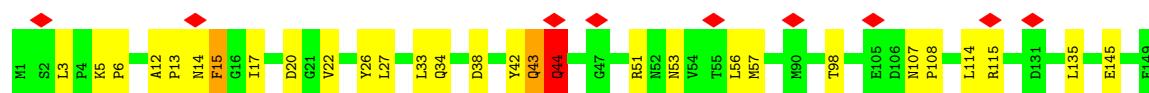
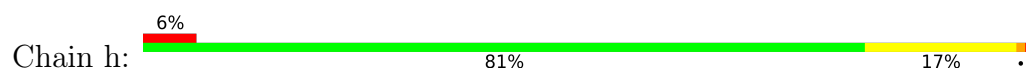


- Molecule 2: Phage tail protein

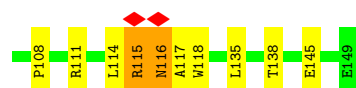
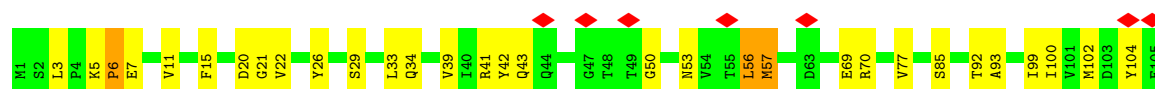




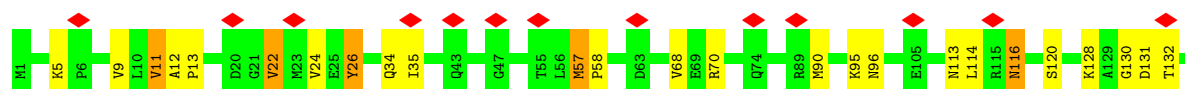
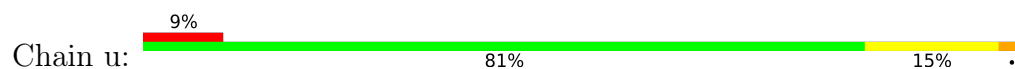
- Molecule 2: Phage tail protein



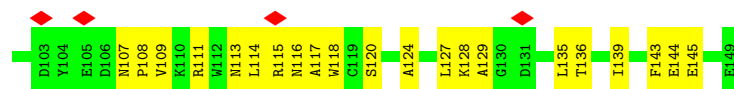
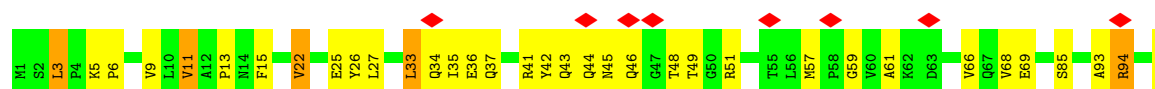
- Molecule 2: Phage tail protein



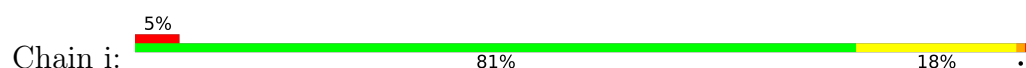
- Molecule 2: Phage tail protein

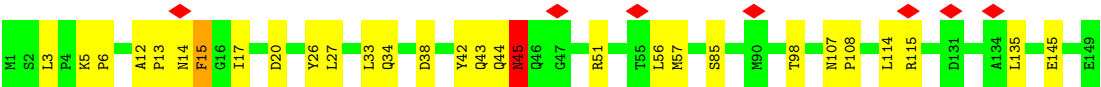


- Molecule 2: Phage tail protein

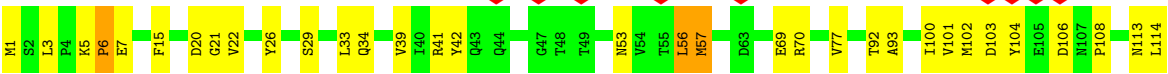


- Molecule 2: Phage tail protein





• Molecule 2: Phage tail protein



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=23.10°, rise=38.50 Å, axial sym=C6	Depositor
Number of segments used	18822	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.183	Depositor
Minimum map value	-0.093	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	448.0, 448.0, 448.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	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	1.01	1/2942 (0.0%)	1.34	32/4014 (0.8%)
1	B	1.01	1/2942 (0.0%)	1.34	32/4014 (0.8%)
1	C	1.01	1/2942 (0.0%)	1.34	31/4014 (0.8%)
1	D	1.02	1/2942 (0.0%)	1.34	33/4014 (0.8%)
1	E	1.02	1/2942 (0.0%)	1.34	30/4014 (0.7%)
1	F	1.02	1/2942 (0.0%)	1.34	31/4014 (0.8%)
1	G	0.99	0/2942	1.36	39/4014 (1.0%)
1	H	0.99	0/2942	1.36	37/4014 (0.9%)
1	I	0.99	0/2942	1.37	38/4014 (0.9%)
1	J	0.99	0/2942	1.37	38/4014 (0.9%)
1	K	0.99	0/2942	1.37	37/4014 (0.9%)
1	L	0.99	0/2942	1.37	38/4014 (0.9%)
1	M	1.01	2/2942 (0.1%)	1.30	31/4014 (0.8%)
1	N	1.02	2/2942 (0.1%)	1.29	30/4014 (0.7%)
1	O	1.02	2/2942 (0.1%)	1.30	30/4014 (0.7%)
1	P	1.01	1/2942 (0.0%)	1.30	30/4014 (0.7%)
1	Q	1.02	2/2942 (0.1%)	1.30	30/4014 (0.7%)
1	R	1.01	2/2942 (0.1%)	1.29	30/4014 (0.7%)
1	S	0.98	0/2942	1.36	39/4014 (1.0%)
1	T	0.99	1/2942 (0.0%)	1.39	43/4014 (1.1%)
1	U	0.99	0/2942	1.39	42/4014 (1.0%)
1	V	0.99	0/2942	1.39	43/4014 (1.1%)
1	W	0.98	0/2942	1.39	43/4014 (1.1%)
1	X	0.98	0/2942	1.39	42/4014 (1.0%)
2	a	1.04	0/1168	1.48	22/1586 (1.4%)
2	b	1.05	0/1168	1.46	20/1586 (1.3%)
2	c	1.04	0/1168	1.45	20/1586 (1.3%)
2	d	1.08	0/1168	1.45	19/1586 (1.2%)
2	e	1.04	0/1168	1.48	22/1586 (1.4%)
2	f	1.05	0/1168	1.44	19/1586 (1.2%)
2	g	1.03	0/1168	1.45	17/1586 (1.1%)
2	h	1.03	0/1168	1.45	17/1586 (1.1%)
2	i	1.03	0/1168	1.44	16/1586 (1.0%)
2	j	1.03	0/1168	1.45	17/1586 (1.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	k	1.03	0/1168	1.45	17/1586 (1.1%)
2	l	1.03	0/1168	1.45	16/1586 (1.0%)
2	m	0.98	0/1168	1.43	14/1586 (0.9%)
2	n	0.98	0/1168	1.43	14/1586 (0.9%)
2	o	0.99	0/1168	1.43	14/1586 (0.9%)
2	p	0.99	0/1168	1.43	14/1586 (0.9%)
2	q	0.99	0/1168	1.43	14/1586 (0.9%)
2	r	0.98	0/1168	1.43	14/1586 (0.9%)
2	s	0.98	0/1168	1.45	11/1586 (0.7%)
2	t	0.98	0/1168	1.45	12/1586 (0.8%)
2	u	0.98	0/1168	1.44	11/1586 (0.7%)
2	v	0.98	0/1168	1.44	12/1586 (0.8%)
2	w	0.98	0/1168	1.44	11/1586 (0.7%)
2	x	0.98	0/1168	1.45	11/1586 (0.7%)
All	All	1.00	18/98640 (0.0%)	1.38	1223/134400 (0.9%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	80	ASN	N-CA	5.96	1.50	1.46
1	Q	269	ASP	C-O	5.86	1.31	1.24
1	M	269	ASP	C-O	5.64	1.31	1.24
1	N	269	ASP	C-O	5.60	1.31	1.24
1	R	269	ASP	C-O	5.26	1.30	1.24
1	O	269	ASP	C-O	5.24	1.30	1.24
1	F	1	MET	C-N	5.20	1.39	1.33
1	C	1	MET	C-N	5.18	1.39	1.33
1	D	1	MET	C-N	5.14	1.39	1.33
1	E	1	MET	C-N	5.13	1.39	1.33
1	B	1	MET	C-N	5.13	1.39	1.33
1	N	1	MET	C-N	5.13	1.39	1.33
1	A	1	MET	C-N	5.12	1.39	1.33
1	O	1	MET	C-N	5.09	1.39	1.33
1	P	1	MET	C-N	5.08	1.39	1.33
1	Q	1	MET	C-N	5.06	1.39	1.33
1	R	1	MET	C-N	5.04	1.39	1.33
1	M	1	MET	C-N	5.03	1.39	1.33

All (1223) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	498	ASN	CA-C-N	9.73	126.76	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	498	ASN	C-N-CA	9.73	126.76	119.66
1	F	498	ASN	CA-C-N	9.70	126.74	119.66
1	F	498	ASN	C-N-CA	9.70	126.74	119.66
1	E	498	ASN	CA-C-N	9.70	126.74	119.66
1	E	498	ASN	C-N-CA	9.70	126.74	119.66
1	X	498	ASN	CA-C-N	9.68	126.73	119.66
1	X	498	ASN	C-N-CA	9.68	126.73	119.66
1	U	498	ASN	CA-C-N	9.68	126.73	119.66
1	U	498	ASN	C-N-CA	9.68	126.73	119.66
1	A	498	ASN	CA-C-N	9.67	126.72	119.66
1	A	498	ASN	C-N-CA	9.67	126.72	119.66
1	B	498	ASN	CA-C-N	9.67	126.72	119.66
1	B	498	ASN	C-N-CA	9.67	126.72	119.66
1	D	498	ASN	CA-C-N	9.65	126.70	119.66
1	D	498	ASN	C-N-CA	9.65	126.70	119.66
1	W	498	ASN	CA-C-N	9.64	126.70	119.66
1	W	498	ASN	C-N-CA	9.64	126.70	119.66
1	T	498	ASN	CA-C-N	9.63	126.69	119.66
1	T	498	ASN	C-N-CA	9.63	126.69	119.66
1	S	498	ASN	CA-C-N	9.59	126.66	119.66
1	S	498	ASN	C-N-CA	9.59	126.66	119.66
1	V	498	ASN	CA-C-N	9.58	126.65	119.66
1	V	498	ASN	C-N-CA	9.58	126.65	119.66
1	G	497	THR	N-CA-C	-9.40	101.94	113.97
1	L	497	THR	N-CA-C	-9.39	101.95	113.97
1	H	497	THR	N-CA-C	-9.38	101.96	113.97
1	K	497	THR	N-CA-C	-9.37	101.98	113.97
1	I	497	THR	N-CA-C	-9.36	101.98	113.97
1	J	497	THR	N-CA-C	-9.35	102.00	113.97
1	E	352	PRO	CA-C-N	8.88	128.62	119.56
1	E	352	PRO	C-N-CA	8.88	128.62	119.56
1	D	352	PRO	CA-C-N	8.85	128.59	119.56
1	D	352	PRO	C-N-CA	8.85	128.59	119.56
1	C	352	PRO	CA-C-N	8.84	128.58	119.56
1	C	352	PRO	C-N-CA	8.84	128.58	119.56
1	J	46	ASN	N-CA-C	8.84	122.08	111.82
1	L	46	ASN	N-CA-C	8.84	122.07	111.82
1	F	352	PRO	CA-C-N	8.84	128.57	119.56
1	F	352	PRO	C-N-CA	8.84	128.57	119.56
1	G	46	ASN	N-CA-C	8.84	122.07	111.82
1	I	46	ASN	N-CA-C	8.83	122.07	111.82
1	K	46	ASN	N-CA-C	8.81	122.05	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	499	PRO	CA-C-N	8.81	128.46	119.82
1	B	499	PRO	C-N-CA	8.81	128.46	119.82
1	H	46	ASN	N-CA-C	8.81	122.04	111.82
1	A	352	PRO	CA-C-N	8.81	128.54	119.56
1	A	352	PRO	C-N-CA	8.81	128.54	119.56
1	B	352	PRO	CA-C-N	8.80	128.54	119.56
1	B	352	PRO	C-N-CA	8.80	128.54	119.56
1	C	499	PRO	CA-C-N	8.79	128.44	119.82
1	C	499	PRO	C-N-CA	8.79	128.44	119.82
1	E	499	PRO	CA-C-N	8.79	128.43	119.82
1	E	499	PRO	C-N-CA	8.79	128.43	119.82
1	D	499	PRO	CA-C-N	8.78	128.42	119.82
1	D	499	PRO	C-N-CA	8.78	128.42	119.82
1	A	499	PRO	CA-C-N	8.74	128.39	119.82
1	A	499	PRO	C-N-CA	8.74	128.39	119.82
1	F	499	PRO	CA-C-N	8.70	128.34	119.82
1	F	499	PRO	C-N-CA	8.70	128.34	119.82
1	J	43	GLY	CA-C-N	8.57	130.56	119.84
1	J	43	GLY	C-N-CA	8.57	130.56	119.84
1	G	43	GLY	CA-C-N	8.56	130.55	119.84
1	G	43	GLY	C-N-CA	8.56	130.55	119.84
1	H	43	GLY	CA-C-N	8.56	130.54	119.84
1	H	43	GLY	C-N-CA	8.56	130.54	119.84
1	L	43	GLY	CA-C-N	8.53	130.50	119.84
1	L	43	GLY	C-N-CA	8.53	130.50	119.84
1	I	43	GLY	CA-C-N	8.53	130.50	119.84
1	I	43	GLY	C-N-CA	8.53	130.50	119.84
1	K	43	GLY	CA-C-N	8.52	130.48	119.84
1	K	43	GLY	C-N-CA	8.52	130.48	119.84
1	P	308	PRO	CA-C-N	8.47	128.20	119.56
1	P	308	PRO	C-N-CA	8.47	128.20	119.56
1	R	308	PRO	CA-C-N	8.46	128.19	119.56
1	R	308	PRO	C-N-CA	8.46	128.19	119.56
2	f	57	MET	CA-C-N	8.46	130.42	119.84
2	f	57	MET	C-N-CA	8.46	130.42	119.84
2	e	57	MET	CA-C-N	8.46	130.41	119.84
2	e	57	MET	C-N-CA	8.46	130.41	119.84
2	d	57	MET	CA-C-N	8.46	130.41	119.84
2	d	57	MET	C-N-CA	8.46	130.41	119.84
1	Q	308	PRO	CA-C-N	8.46	128.19	119.56
1	Q	308	PRO	C-N-CA	8.46	128.19	119.56
2	b	57	MET	CA-C-N	8.46	130.41	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	57	MET	C-N-CA	8.46	130.41	119.84
1	N	308	PRO	CA-C-N	8.45	128.18	119.56
1	N	308	PRO	C-N-CA	8.45	128.18	119.56
2	c	57	MET	CA-C-N	8.44	130.39	119.84
2	c	57	MET	C-N-CA	8.44	130.39	119.84
1	M	308	PRO	CA-C-N	8.44	128.16	119.56
1	M	308	PRO	C-N-CA	8.44	128.16	119.56
1	O	308	PRO	CA-C-N	8.43	128.16	119.56
1	O	308	PRO	C-N-CA	8.43	128.16	119.56
2	a	57	MET	CA-C-N	8.43	130.37	119.84
2	a	57	MET	C-N-CA	8.43	130.37	119.84
2	a	22	VAL	N-CA-C	8.39	118.25	111.62
1	V	499	PRO	CA-C-N	8.36	128.09	119.56
1	V	499	PRO	C-N-CA	8.36	128.09	119.56
2	b	22	VAL	N-CA-C	8.36	118.22	111.62
2	e	22	VAL	N-CA-C	8.35	118.22	111.62
1	S	499	PRO	CA-C-N	8.32	128.04	119.56
1	S	499	PRO	C-N-CA	8.32	128.04	119.56
1	T	499	PRO	CA-C-N	8.32	128.04	119.56
1	T	499	PRO	C-N-CA	8.32	128.04	119.56
2	d	22	VAL	N-CA-C	8.31	118.18	111.62
1	W	499	PRO	CA-C-N	8.30	128.03	119.56
1	W	499	PRO	C-N-CA	8.30	128.03	119.56
2	c	22	VAL	N-CA-C	8.30	118.17	111.62
1	U	499	PRO	CA-C-N	8.29	128.02	119.56
1	U	499	PRO	C-N-CA	8.29	128.02	119.56
2	f	22	VAL	N-CA-C	8.29	118.17	111.62
1	X	499	PRO	CA-C-N	8.27	127.99	119.56
1	X	499	PRO	C-N-CA	8.27	127.99	119.56
1	J	6	SER	N-CA-C	8.26	115.56	108.13
1	K	6	SER	N-CA-C	8.26	115.56	108.13
1	G	6	SER	N-CA-C	8.21	115.52	108.13
1	L	6	SER	N-CA-C	8.21	115.52	108.13
1	H	6	SER	N-CA-C	8.20	115.51	108.13
1	I	6	SER	N-CA-C	8.20	115.51	108.13
1	V	483	GLN	N-CA-C	-8.17	102.22	114.64
1	U	483	GLN	N-CA-C	-8.15	102.25	114.64
1	X	483	GLN	N-CA-C	-8.14	102.27	114.64
1	W	483	GLN	N-CA-C	-8.13	102.28	114.64
1	T	483	GLN	N-CA-C	-8.13	102.28	114.64
1	M	499	PRO	CA-C-N	8.12	127.84	119.56
1	M	499	PRO	C-N-CA	8.12	127.84	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	499	PRO	CA-C-N	8.12	127.84	119.56
1	Q	499	PRO	C-N-CA	8.12	127.84	119.56
1	O	499	PRO	CA-C-N	8.10	127.82	119.56
1	O	499	PRO	C-N-CA	8.10	127.82	119.56
1	L	499	PRO	CA-C-N	8.10	128.86	119.47
1	L	499	PRO	C-N-CA	8.10	128.86	119.47
1	G	499	PRO	CA-C-N	8.10	128.86	119.47
1	G	499	PRO	C-N-CA	8.10	128.86	119.47
1	J	499	PRO	CA-C-N	8.09	128.86	119.47
1	J	499	PRO	C-N-CA	8.09	128.86	119.47
1	S	483	GLN	N-CA-C	-8.07	102.37	114.64
1	H	499	PRO	CA-C-N	8.07	128.84	119.47
1	H	499	PRO	C-N-CA	8.07	128.84	119.47
1	I	499	PRO	CA-C-N	8.07	128.83	119.47
1	I	499	PRO	C-N-CA	8.07	128.83	119.47
1	K	499	PRO	CA-C-N	8.05	128.81	119.47
1	K	499	PRO	C-N-CA	8.05	128.81	119.47
1	W	307	PRO	CA-C-N	8.03	125.52	119.66
1	W	307	PRO	C-N-CA	8.03	125.52	119.66
1	X	307	PRO	CA-C-N	7.99	125.50	119.66
1	X	307	PRO	C-N-CA	7.99	125.50	119.66
1	S	307	PRO	CA-C-N	7.98	125.48	119.66
1	S	307	PRO	C-N-CA	7.98	125.48	119.66
1	U	307	PRO	CA-C-N	7.96	125.47	119.66
1	U	307	PRO	C-N-CA	7.96	125.47	119.66
1	V	307	PRO	CA-C-N	7.93	125.45	119.66
1	V	307	PRO	C-N-CA	7.93	125.45	119.66
1	T	307	PRO	CA-C-N	7.93	125.45	119.66
1	T	307	PRO	C-N-CA	7.93	125.45	119.66
1	N	499	PRO	CA-C-N	7.80	127.86	119.28
1	N	499	PRO	C-N-CA	7.80	127.86	119.28
1	R	499	PRO	CA-C-N	7.78	127.84	119.28
1	R	499	PRO	C-N-CA	7.78	127.84	119.28
1	P	499	PRO	CA-C-N	7.78	127.83	119.28
1	P	499	PRO	C-N-CA	7.78	127.83	119.28
2	t	57	MET	CA-C-N	7.59	127.50	120.21
2	t	57	MET	C-N-CA	7.59	127.50	120.21
2	j	43	GLN	N-CA-C	7.57	120.52	110.53
2	v	57	MET	CA-C-N	7.57	127.47	120.21
2	v	57	MET	C-N-CA	7.57	127.47	120.21
2	s	57	MET	CA-C-N	7.56	127.47	120.21
2	s	57	MET	C-N-CA	7.56	127.47	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	u	57	MET	CA-C-N	7.55	127.45	120.21
2	u	57	MET	C-N-CA	7.55	127.45	120.21
2	x	57	MET	CA-C-N	7.54	127.45	120.21
2	x	57	MET	C-N-CA	7.54	127.45	120.21
2	w	57	MET	CA-C-N	7.53	127.44	120.21
2	w	57	MET	C-N-CA	7.53	127.44	120.21
2	l	43	GLN	N-CA-C	7.51	120.44	110.53
2	h	43	GLN	N-CA-C	7.51	120.44	110.53
2	x	116	ASN	N-CA-C	-7.48	101.37	113.19
2	c	26	TYR	N-CA-C	7.48	120.23	108.79
2	a	26	TYR	N-CA-C	7.47	120.23	108.79
2	w	116	ASN	N-CA-C	-7.47	101.38	113.19
2	g	43	GLN	N-CA-C	7.46	120.38	110.53
2	t	116	ASN	N-CA-C	-7.46	101.39	113.19
2	u	116	ASN	N-CA-C	-7.46	101.41	113.19
2	e	26	TYR	N-CA-C	7.46	120.20	108.79
2	s	116	ASN	N-CA-C	-7.45	101.42	113.19
2	f	26	TYR	N-CA-C	7.45	120.18	108.79
2	b	26	TYR	N-CA-C	7.44	120.18	108.79
2	v	116	ASN	N-CA-C	-7.44	101.43	113.19
2	d	26	TYR	N-CA-C	7.44	120.17	108.79
2	k	43	GLN	N-CA-C	7.43	120.33	110.53
1	B	497	THR	N-CA-C	-7.36	104.82	113.88
1	E	497	THR	N-CA-C	-7.36	104.83	113.88
1	A	497	THR	N-CA-C	-7.34	104.85	113.88
1	D	497	THR	N-CA-C	-7.34	104.85	113.88
1	F	497	THR	N-CA-C	-7.33	104.87	113.88
1	C	497	THR	N-CA-C	-7.33	104.86	113.88
2	q	15	PHE	N-CA-C	7.33	120.36	108.34
2	r	15	PHE	N-CA-C	7.32	120.35	108.34
2	m	15	PHE	N-CA-C	7.32	120.34	108.34
2	o	15	PHE	N-CA-C	7.31	120.33	108.34
2	n	15	PHE	N-CA-C	7.30	120.32	108.34
1	X	424	ASP	CA-C-N	7.30	127.01	119.56
1	X	424	ASP	C-N-CA	7.30	127.01	119.56
1	G	342	ASP	CA-C-N	7.30	127.00	119.56
1	G	342	ASP	C-N-CA	7.30	127.00	119.56
2	p	15	PHE	N-CA-C	7.29	120.30	108.34
1	W	424	ASP	CA-C-N	7.28	126.99	119.56
1	W	424	ASP	C-N-CA	7.28	126.99	119.56
1	V	424	ASP	CA-C-N	7.26	126.97	119.56
1	V	424	ASP	C-N-CA	7.26	126.97	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	43	GLY	CA-C-N	7.26	127.22	120.03
1	W	43	GLY	C-N-CA	7.26	127.22	120.03
1	S	424	ASP	CA-C-N	7.26	126.96	119.56
1	S	424	ASP	C-N-CA	7.26	126.96	119.56
1	J	342	ASP	CA-C-N	7.26	126.96	119.56
1	J	342	ASP	C-N-CA	7.26	126.96	119.56
1	U	43	GLY	CA-C-N	7.25	127.20	120.03
1	U	43	GLY	C-N-CA	7.25	127.20	120.03
1	O	342	ASP	CA-C-N	7.25	126.95	119.56
1	O	342	ASP	C-N-CA	7.25	126.95	119.56
1	U	424	ASP	CA-C-N	7.25	126.95	119.56
1	U	424	ASP	C-N-CA	7.25	126.95	119.56
1	T	424	ASP	CA-C-N	7.24	126.95	119.56
1	T	424	ASP	C-N-CA	7.24	126.95	119.56
1	H	1	MET	CA-C-N	7.24	127.24	119.78
1	H	1	MET	C-N-CA	7.24	127.24	119.78
1	S	43	GLY	CA-C-N	7.24	127.20	120.03
1	S	43	GLY	C-N-CA	7.24	127.20	120.03
1	R	342	ASP	CA-C-N	7.23	126.94	119.56
1	R	342	ASP	C-N-CA	7.23	126.94	119.56
1	L	342	ASP	CA-C-N	7.23	126.94	119.56
1	L	342	ASP	C-N-CA	7.23	126.94	119.56
1	I	1	MET	CA-C-N	7.23	127.23	119.78
1	I	1	MET	C-N-CA	7.23	127.23	119.78
1	K	1	MET	CA-C-N	7.23	127.22	119.78
1	K	1	MET	C-N-CA	7.23	127.22	119.78
1	L	1	MET	CA-C-N	7.23	127.22	119.78
1	L	1	MET	C-N-CA	7.23	127.22	119.78
1	M	342	ASP	CA-C-N	7.23	126.93	119.56
1	M	342	ASP	C-N-CA	7.23	126.93	119.56
1	K	342	ASP	CA-C-N	7.22	126.93	119.56
1	K	342	ASP	C-N-CA	7.22	126.93	119.56
1	Q	342	ASP	CA-C-N	7.22	126.92	119.56
1	Q	342	ASP	C-N-CA	7.22	126.92	119.56
1	X	43	GLY	CA-C-N	7.22	127.18	120.03
1	X	43	GLY	C-N-CA	7.22	127.18	120.03
1	H	342	ASP	CA-C-N	7.22	126.92	119.56
1	H	342	ASP	C-N-CA	7.22	126.92	119.56
1	G	1	MET	CA-C-N	7.21	127.21	119.78
1	G	1	MET	C-N-CA	7.21	127.21	119.78
1	N	342	ASP	CA-C-N	7.21	126.91	119.56
1	N	342	ASP	C-N-CA	7.21	126.91	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	342	ASP	CA-C-N	7.21	126.91	119.56
1	P	342	ASP	C-N-CA	7.21	126.91	119.56
1	I	342	ASP	CA-C-N	7.21	126.91	119.56
1	I	342	ASP	C-N-CA	7.21	126.91	119.56
1	V	43	GLY	CA-C-N	7.18	127.14	120.03
1	V	43	GLY	C-N-CA	7.18	127.14	120.03
1	J	1	MET	CA-C-N	7.18	127.18	119.78
1	J	1	MET	C-N-CA	7.18	127.18	119.78
1	T	43	GLY	CA-C-N	7.18	127.14	120.03
1	T	43	GLY	C-N-CA	7.18	127.14	120.03
2	c	56	LEU	N-CA-C	-7.15	100.41	110.50
2	e	56	LEU	N-CA-C	-7.13	100.45	110.50
1	J	9	VAL	N-CA-C	7.13	117.94	111.81
1	V	506	GLY	N-CA-C	-7.12	102.41	112.60
1	U	506	GLY	N-CA-C	-7.12	102.41	112.60
1	T	506	GLY	N-CA-C	-7.12	102.42	112.60
2	b	56	LEU	N-CA-C	-7.12	100.46	110.50
2	d	56	LEU	N-CA-C	-7.12	100.46	110.50
2	a	56	LEU	N-CA-C	-7.12	100.46	110.50
1	W	506	GLY	N-CA-C	-7.12	102.42	112.60
1	S	506	GLY	N-CA-C	-7.11	102.43	112.60
1	X	506	GLY	N-CA-C	-7.11	102.44	112.60
1	L	9	VAL	N-CA-C	7.10	117.92	111.81
2	f	56	LEU	N-CA-C	-7.10	100.49	110.50
1	K	9	VAL	N-CA-C	7.09	117.91	111.81
1	I	9	VAL	N-CA-C	7.09	117.90	111.81
1	H	9	VAL	N-CA-C	7.06	117.88	111.81
2	l	57	MET	CA-C-N	7.05	128.65	119.84
2	l	57	MET	C-N-CA	7.05	128.65	119.84
2	k	57	MET	CA-C-N	7.04	128.64	119.84
2	k	57	MET	C-N-CA	7.04	128.64	119.84
1	O	1	MET	CA-C-N	7.04	127.00	120.03
1	O	1	MET	C-N-CA	7.04	127.00	120.03
1	R	1	MET	CA-C-N	7.03	126.99	120.03
1	R	1	MET	C-N-CA	7.03	126.99	120.03
2	g	57	MET	CA-C-N	7.03	128.63	119.84
2	g	57	MET	C-N-CA	7.03	128.63	119.84
2	p	22	VAL	N-CA-C	7.03	117.82	110.72
1	P	1	MET	CA-C-N	7.03	126.99	120.03
1	P	1	MET	C-N-CA	7.03	126.99	120.03
1	F	46	ASN	N-CA-C	7.03	119.83	111.33
1	G	9	VAL	N-CA-C	7.02	117.85	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	ASN	N-CA-C	7.02	119.83	111.33
1	M	1	MET	CA-C-N	7.02	126.98	120.03
1	M	1	MET	C-N-CA	7.02	126.98	120.03
1	D	46	ASN	N-CA-C	7.01	119.82	111.33
2	h	57	MET	CA-C-N	7.01	128.60	119.84
2	h	57	MET	C-N-CA	7.01	128.60	119.84
1	B	46	ASN	N-CA-C	7.01	119.81	111.33
2	k	20	ASP	N-CA-C	7.00	120.52	109.39
2	r	22	VAL	N-CA-C	7.00	117.79	110.72
2	j	57	MET	CA-C-N	7.00	128.59	119.84
2	j	57	MET	C-N-CA	7.00	128.59	119.84
1	P	498	ASN	CA-C-N	7.00	127.58	120.38
1	P	498	ASN	C-N-CA	7.00	127.58	120.38
2	q	22	VAL	N-CA-C	6.99	117.78	110.72
1	N	1	MET	CA-C-N	6.99	126.95	120.03
1	N	1	MET	C-N-CA	6.99	126.95	120.03
2	n	22	VAL	N-CA-C	6.99	117.78	110.72
2	i	57	MET	CA-C-N	6.99	128.57	119.84
2	i	57	MET	C-N-CA	6.99	128.57	119.84
1	N	498	ASN	CA-C-N	6.98	127.57	120.38
1	N	498	ASN	C-N-CA	6.98	127.57	120.38
2	o	22	VAL	N-CA-C	6.98	117.77	110.72
2	j	20	ASP	N-CA-C	6.98	120.49	109.39
2	g	20	ASP	N-CA-C	6.98	120.48	109.39
2	h	20	ASP	N-CA-C	6.97	120.48	109.39
2	i	20	ASP	N-CA-C	6.97	120.48	109.39
1	R	498	ASN	CA-C-N	6.97	127.56	120.38
1	R	498	ASN	C-N-CA	6.97	127.56	120.38
2	l	20	ASP	N-CA-C	6.97	120.47	109.39
2	m	22	VAL	N-CA-C	6.96	117.75	110.72
1	M	498	ASN	CA-C-N	6.96	127.54	120.38
1	M	498	ASN	C-N-CA	6.96	127.54	120.38
1	Q	1	MET	CA-C-N	6.95	126.91	120.03
1	Q	1	MET	C-N-CA	6.95	126.91	120.03
1	Q	498	ASN	CA-C-N	6.95	127.53	120.38
1	Q	498	ASN	C-N-CA	6.95	127.53	120.38
1	O	498	ASN	CA-C-N	6.94	127.53	120.38
1	O	498	ASN	C-N-CA	6.94	127.53	120.38
1	I	318	VAL	CA-C-N	-6.94	110.29	120.28
1	I	318	VAL	C-N-CA	-6.94	110.29	120.28
1	G	6	SER	CA-C-N	6.92	126.62	119.56
1	G	6	SER	C-N-CA	6.92	126.62	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	318	VAL	CA-C-N	-6.92	110.31	120.28
1	K	318	VAL	C-N-CA	-6.92	110.31	120.28
1	H	318	VAL	CA-C-N	-6.92	110.31	120.28
1	H	318	VAL	C-N-CA	-6.92	110.31	120.28
1	J	318	VAL	CA-C-N	-6.92	110.32	120.28
1	J	318	VAL	C-N-CA	-6.92	110.32	120.28
1	K	6	SER	CA-C-N	6.91	126.61	119.56
1	K	6	SER	C-N-CA	6.91	126.61	119.56
1	L	318	VAL	CA-C-N	-6.91	110.33	120.28
1	L	318	VAL	C-N-CA	-6.91	110.33	120.28
1	G	318	VAL	CA-C-N	-6.91	110.33	120.28
1	G	318	VAL	C-N-CA	-6.91	110.33	120.28
1	I	6	SER	CA-C-N	6.89	126.59	119.56
1	I	6	SER	C-N-CA	6.89	126.59	119.56
1	C	6	SER	N-CA-C	6.88	114.41	108.22
1	E	6	SER	N-CA-C	6.87	114.40	108.22
1	H	6	SER	CA-C-N	6.87	126.57	119.56
1	H	6	SER	C-N-CA	6.87	126.57	119.56
1	V	238	PRO	N-CA-C	-6.86	101.14	111.57
1	X	238	PRO	N-CA-C	-6.86	101.15	111.57
1	A	6	SER	N-CA-C	6.85	114.38	108.22
1	U	238	PRO	N-CA-C	-6.85	101.16	111.57
1	L	6	SER	CA-C-N	6.84	126.54	119.56
1	L	6	SER	C-N-CA	6.84	126.54	119.56
1	W	238	PRO	N-CA-C	-6.84	101.17	111.57
1	T	238	PRO	N-CA-C	-6.84	101.17	111.57
1	J	6	SER	CA-C-N	6.84	126.53	119.56
1	J	6	SER	C-N-CA	6.84	126.53	119.56
1	B	6	SER	N-CA-C	6.83	114.36	108.22
1	T	308	PRO	CA-C-N	6.82	126.78	119.28
1	T	308	PRO	C-N-CA	6.82	126.78	119.28
1	W	308	PRO	CA-C-N	6.81	126.77	119.28
1	W	308	PRO	C-N-CA	6.81	126.77	119.28
1	P	248	SER	N-CA-C	-6.81	103.65	112.23
1	M	248	SER	N-CA-C	-6.80	103.66	112.23
1	N	248	SER	N-CA-C	-6.79	103.67	112.23
1	O	248	SER	N-CA-C	-6.79	103.67	112.23
1	S	308	PRO	CA-C-N	6.79	126.75	119.28
1	S	308	PRO	C-N-CA	6.79	126.75	119.28
1	F	6	SER	N-CA-C	6.79	114.33	108.22
1	V	308	PRO	CA-C-N	6.78	126.74	119.28
1	V	308	PRO	C-N-CA	6.78	126.74	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	6	SER	N-CA-C	6.78	114.33	108.22
1	U	308	PRO	CA-C-N	6.78	126.74	119.28
1	U	308	PRO	C-N-CA	6.78	126.74	119.28
1	X	308	PRO	CA-C-N	6.77	126.72	119.28
1	X	308	PRO	C-N-CA	6.77	126.72	119.28
1	R	248	SER	N-CA-C	-6.77	103.70	112.23
1	Q	248	SER	N-CA-C	-6.75	103.72	112.23
2	e	77	VAL	N-CA-C	6.71	116.86	110.42
2	f	77	VAL	N-CA-C	6.70	116.85	110.42
2	b	77	VAL	N-CA-C	6.69	116.84	110.42
2	a	77	VAL	N-CA-C	6.68	116.83	110.42
2	d	77	VAL	N-CA-C	6.66	116.81	110.42
1	T	306	ASP	CA-C-N	6.65	127.23	120.38
1	T	306	ASP	C-N-CA	6.65	127.23	120.38
2	c	77	VAL	N-CA-C	6.64	116.80	110.42
1	X	306	ASP	CA-C-N	6.64	127.22	120.38
1	X	306	ASP	C-N-CA	6.64	127.22	120.38
1	U	306	ASP	CA-C-N	6.62	127.20	120.38
1	U	306	ASP	C-N-CA	6.62	127.20	120.38
2	d	15	PHE	N-CA-C	6.62	120.29	109.24
2	b	15	PHE	N-CA-C	6.60	120.26	109.24
2	f	15	PHE	N-CA-C	6.59	120.25	109.24
1	I	498	ASN	CA-C-N	6.59	127.17	120.38
1	I	498	ASN	C-N-CA	6.59	127.17	120.38
1	S	306	ASP	CA-C-N	6.58	127.16	120.38
1	S	306	ASP	C-N-CA	6.58	127.16	120.38
2	a	15	PHE	N-CA-C	6.58	120.24	109.24
1	V	306	ASP	CA-C-N	6.58	127.16	120.38
1	V	306	ASP	C-N-CA	6.58	127.16	120.38
1	H	498	ASN	CA-C-N	6.58	127.16	120.38
1	H	498	ASN	C-N-CA	6.58	127.16	120.38
1	C	335	TYR	N-CA-C	6.57	121.42	112.55
2	c	15	PHE	N-CA-C	6.57	120.22	109.24
2	l	107	ASN	CA-C-N	6.57	126.19	119.56
2	l	107	ASN	C-N-CA	6.57	126.19	119.56
2	g	107	ASN	CA-C-N	6.57	126.19	119.56
2	g	107	ASN	C-N-CA	6.57	126.19	119.56
2	e	15	PHE	N-CA-C	6.56	120.20	109.24
1	L	498	ASN	CA-C-N	6.56	127.14	120.38
1	L	498	ASN	C-N-CA	6.56	127.14	120.38
1	K	498	ASN	CA-C-N	6.56	127.14	120.38
1	K	498	ASN	C-N-CA	6.56	127.14	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	498	ASN	CA-C-N	6.56	127.14	120.38
1	J	498	ASN	C-N-CA	6.56	127.14	120.38
1	B	335	TYR	N-CA-C	6.55	121.39	112.55
1	W	306	ASP	CA-C-N	6.55	127.12	120.38
1	W	306	ASP	C-N-CA	6.55	127.12	120.38
1	X	248	SER	N-CA-C	-6.55	105.11	113.23
1	G	498	ASN	CA-C-N	6.55	127.12	120.38
1	G	498	ASN	C-N-CA	6.55	127.12	120.38
2	k	107	ASN	CA-C-N	6.54	126.16	119.56
2	k	107	ASN	C-N-CA	6.54	126.16	119.56
1	D	335	TYR	N-CA-C	6.53	121.37	112.55
2	h	107	ASN	CA-C-N	6.53	126.16	119.56
2	h	107	ASN	C-N-CA	6.53	126.16	119.56
2	p	107	ASN	CA-C-N	6.53	126.15	119.56
2	p	107	ASN	C-N-CA	6.53	126.15	119.56
1	V	248	SER	N-CA-C	-6.52	105.14	113.23
1	S	248	SER	N-CA-C	-6.52	105.14	113.23
2	j	107	ASN	CA-C-N	6.52	126.15	119.56
2	j	107	ASN	C-N-CA	6.52	126.15	119.56
1	W	248	SER	N-CA-C	-6.52	105.15	113.23
1	E	335	TYR	N-CA-C	6.51	121.34	112.55
2	m	107	ASN	CA-C-N	6.51	126.14	119.56
2	m	107	ASN	C-N-CA	6.51	126.14	119.56
1	T	248	SER	N-CA-C	-6.50	105.17	113.23
2	n	107	ASN	CA-C-N	6.50	126.12	119.56
2	n	107	ASN	C-N-CA	6.50	126.12	119.56
1	E	267	VAL	CA-C-N	6.50	126.19	119.56
1	E	267	VAL	C-N-CA	6.50	126.19	119.56
1	U	248	SER	N-CA-C	-6.49	105.19	113.23
2	o	107	ASN	CA-C-N	6.48	126.11	119.56
2	o	107	ASN	C-N-CA	6.48	126.11	119.56
2	r	107	ASN	CA-C-N	6.48	126.11	119.56
2	r	107	ASN	C-N-CA	6.48	126.11	119.56
1	F	267	VAL	CA-C-N	6.48	126.17	119.56
1	F	267	VAL	C-N-CA	6.48	126.17	119.56
2	i	107	ASN	CA-C-N	6.48	126.10	119.56
2	i	107	ASN	C-N-CA	6.48	126.10	119.56
2	q	107	ASN	CA-C-N	6.47	126.10	119.56
2	q	107	ASN	C-N-CA	6.47	126.10	119.56
1	C	267	VAL	CA-C-N	6.47	126.16	119.56
1	C	267	VAL	C-N-CA	6.47	126.16	119.56
1	D	267	VAL	CA-C-N	6.46	126.15	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	267	VAL	C-N-CA	6.46	126.15	119.56
1	A	267	VAL	CA-C-N	6.46	126.14	119.56
1	A	267	VAL	C-N-CA	6.46	126.14	119.56
1	B	267	VAL	CA-C-N	6.43	126.12	119.56
1	B	267	VAL	C-N-CA	6.43	126.12	119.56
2	i	33	LEU	N-CA-C	6.36	119.27	108.90
2	v	57	MET	N-CA-C	6.36	120.93	108.21
2	j	33	LEU	N-CA-C	6.36	119.26	108.90
2	h	33	LEU	N-CA-C	6.35	119.25	108.90
2	x	57	MET	N-CA-C	6.35	120.90	108.21
2	u	57	MET	N-CA-C	6.35	120.90	108.21
2	k	33	LEU	N-CA-C	6.34	119.23	108.90
2	t	57	MET	N-CA-C	6.34	120.89	108.21
2	w	57	MET	N-CA-C	6.34	120.88	108.21
2	s	57	MET	N-CA-C	6.33	120.88	108.21
2	l	33	LEU	N-CA-C	6.33	119.22	108.90
1	E	1	MET	CA-C-N	6.32	126.29	120.03
1	E	1	MET	C-N-CA	6.32	126.29	120.03
2	g	33	LEU	N-CA-C	6.32	119.19	108.90
1	F	1	MET	CA-C-N	6.29	126.26	120.03
1	F	1	MET	C-N-CA	6.29	126.26	120.03
1	B	1	MET	CA-C-N	6.29	126.26	120.03
1	B	1	MET	C-N-CA	6.29	126.26	120.03
2	n	3	LEU	CA-C-N	6.29	125.91	119.56
2	n	3	LEU	C-N-CA	6.29	125.91	119.56
1	D	1	MET	CA-C-N	6.28	126.25	120.03
1	D	1	MET	C-N-CA	6.28	126.25	120.03
1	A	1	MET	CA-C-N	6.28	126.25	120.03
1	A	1	MET	C-N-CA	6.28	126.25	120.03
1	S	398	ASN	CA-C-N	6.28	125.97	119.82
1	S	398	ASN	C-N-CA	6.28	125.97	119.82
2	p	3	LEU	CA-C-N	6.27	125.90	119.56
2	p	3	LEU	C-N-CA	6.27	125.90	119.56
1	W	80	ASN	CA-C-N	-6.26	116.18	122.69
1	W	80	ASN	C-N-CA	-6.26	116.18	122.69
1	U	398	ASN	CA-C-N	6.26	125.95	119.82
1	U	398	ASN	C-N-CA	6.26	125.95	119.82
2	q	3	LEU	CA-C-N	6.26	125.88	119.56
2	q	3	LEU	C-N-CA	6.26	125.88	119.56
2	r	3	LEU	CA-C-N	6.25	125.87	119.56
2	r	3	LEU	C-N-CA	6.25	125.87	119.56
1	X	398	ASN	CA-C-N	6.25	125.94	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	398	ASN	C-N-CA	6.25	125.94	119.82
1	S	80	ASN	CA-C-N	-6.25	116.19	122.69
1	S	80	ASN	C-N-CA	-6.25	116.19	122.69
1	V	398	ASN	CA-C-N	6.24	125.94	119.82
1	V	398	ASN	C-N-CA	6.24	125.94	119.82
1	C	1	MET	CA-C-N	6.24	126.21	120.03
1	C	1	MET	C-N-CA	6.24	126.21	120.03
1	T	6	SER	CA-C-N	6.24	125.92	119.56
1	T	6	SER	C-N-CA	6.24	125.92	119.56
1	I	309	PRO	N-CA-C	6.24	122.20	113.53
1	W	6	SER	CA-C-N	6.23	125.91	119.56
1	W	6	SER	C-N-CA	6.23	125.91	119.56
1	T	398	ASN	CA-C-N	6.23	125.93	119.82
1	T	398	ASN	C-N-CA	6.23	125.93	119.82
1	W	398	ASN	CA-C-N	6.23	125.92	119.82
1	W	398	ASN	C-N-CA	6.23	125.92	119.82
2	o	3	LEU	CA-C-N	6.22	125.85	119.56
2	o	3	LEU	C-N-CA	6.22	125.85	119.56
1	K	309	PRO	N-CA-C	6.22	122.18	113.53
1	V	6	SER	CA-C-N	6.22	125.90	119.56
1	V	6	SER	C-N-CA	6.22	125.90	119.56
2	m	3	LEU	CA-C-N	6.22	125.84	119.56
2	m	3	LEU	C-N-CA	6.22	125.84	119.56
1	G	309	PRO	N-CA-C	6.22	122.17	113.53
2	n	11	VAL	N-CA-C	6.22	116.53	111.62
2	p	11	VAL	N-CA-C	6.21	116.53	111.62
1	S	6	SER	CA-C-N	6.21	125.89	119.56
1	S	6	SER	C-N-CA	6.21	125.89	119.56
1	J	309	PRO	N-CA-C	6.21	122.16	113.53
1	H	309	PRO	N-CA-C	6.20	122.15	113.53
2	u	22	VAL	N-CA-C	6.20	116.98	110.72
1	L	309	PRO	N-CA-C	6.20	122.14	113.53
2	w	22	VAL	N-CA-C	6.19	116.97	110.72
2	m	11	VAL	N-CA-C	6.19	116.51	111.62
1	G	484	SER	CA-C-N	6.18	126.64	119.47
1	G	484	SER	C-N-CA	6.18	126.64	119.47
2	q	11	VAL	N-CA-C	6.18	116.50	111.62
1	X	6	SER	CA-C-N	6.18	125.86	119.56
1	X	6	SER	C-N-CA	6.18	125.86	119.56
1	K	484	SER	CA-C-N	6.16	126.62	119.47
1	K	484	SER	C-N-CA	6.16	126.62	119.47
2	o	11	VAL	N-CA-C	6.16	116.49	111.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	6	SER	CA-C-N	6.16	125.84	119.56
1	U	6	SER	C-N-CA	6.16	125.84	119.56
2	t	22	VAL	N-CA-C	6.15	116.94	110.72
2	v	22	VAL	N-CA-C	6.15	116.93	110.72
1	J	484	SER	CA-C-N	6.15	126.61	119.47
1	J	484	SER	C-N-CA	6.15	126.61	119.47
2	x	22	VAL	N-CA-C	6.15	116.93	110.72
2	s	22	VAL	N-CA-C	6.14	116.92	110.72
1	U	242	GLN	N-CA-C	6.14	119.53	108.48
2	r	11	VAL	N-CA-C	6.13	116.47	111.62
1	I	484	SER	CA-C-N	6.13	126.59	119.47
1	I	484	SER	C-N-CA	6.13	126.59	119.47
1	T	242	GLN	N-CA-C	6.12	119.50	108.48
1	W	242	GLN	N-CA-C	6.12	119.49	108.48
1	X	242	GLN	N-CA-C	6.11	119.48	108.48
1	L	484	SER	CA-C-N	6.11	126.56	119.47
1	L	484	SER	C-N-CA	6.11	126.56	119.47
1	H	484	SER	CA-C-N	6.11	126.56	119.47
1	H	484	SER	C-N-CA	6.11	126.56	119.47
1	V	242	GLN	N-CA-C	6.10	119.46	108.48
2	e	107	ASN	CA-C-N	6.09	125.72	119.56
2	e	107	ASN	C-N-CA	6.09	125.72	119.56
1	D	238	PRO	N-CA-C	-6.09	107.67	114.92
1	S	242	GLN	N-CA-C	6.08	119.43	108.48
2	a	107	ASN	CA-C-N	6.08	125.70	119.56
2	a	107	ASN	C-N-CA	6.08	125.70	119.56
1	G	267	VAL	CA-C-N	6.07	125.96	119.28
1	G	267	VAL	C-N-CA	6.07	125.96	119.28
1	E	238	PRO	N-CA-C	-6.07	107.69	114.92
1	B	238	PRO	N-CA-C	-6.07	107.70	114.92
1	C	238	PRO	N-CA-C	-6.07	107.70	114.92
1	J	267	VAL	CA-C-N	6.07	125.95	119.28
1	J	267	VAL	C-N-CA	6.07	125.95	119.28
2	t	13	PRO	N-CA-C	-6.06	104.29	112.48
1	I	267	VAL	CA-C-N	6.06	125.94	119.28
1	I	267	VAL	C-N-CA	6.06	125.94	119.28
1	L	267	VAL	CA-C-N	6.05	125.94	119.28
1	L	267	VAL	C-N-CA	6.05	125.94	119.28
1	A	238	PRO	N-CA-C	-6.05	107.72	114.92
2	w	13	PRO	N-CA-C	-6.05	104.31	112.48
2	x	13	PRO	N-CA-C	-6.05	104.31	112.48
1	W	9	VAL	N-CA-C	6.05	117.08	111.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	r	69	GLU	N-CA-C	-6.05	101.33	110.28
2	o	69	GLU	N-CA-C	-6.05	101.33	110.28
1	X	9	VAL	N-CA-C	6.04	117.07	111.45
2	m	69	GLU	N-CA-C	-6.04	101.33	110.28
2	s	13	PRO	N-CA-C	-6.04	104.33	112.48
1	W	484	SER	CA-C-N	6.04	125.72	119.56
1	W	484	SER	C-N-CA	6.04	125.72	119.56
1	H	267	VAL	CA-C-N	6.04	125.92	119.28
1	H	267	VAL	C-N-CA	6.04	125.92	119.28
2	v	13	PRO	N-CA-C	-6.04	104.33	112.48
2	d	21	GLY	N-CA-C	-6.04	103.92	112.37
2	n	69	GLU	N-CA-C	-6.04	101.35	110.28
2	p	69	GLU	N-CA-C	-6.03	101.36	110.28
2	q	69	GLU	N-CA-C	-6.03	101.36	110.28
2	e	21	GLY	N-CA-C	-6.03	103.93	112.37
1	V	484	SER	CA-C-N	6.02	125.70	119.56
1	V	484	SER	C-N-CA	6.02	125.70	119.56
1	F	238	PRO	N-CA-C	-6.02	107.75	114.92
2	b	21	GLY	N-CA-C	-6.02	103.94	112.37
1	V	9	VAL	N-CA-C	6.02	117.05	111.45
2	f	21	GLY	N-CA-C	-6.01	103.95	112.37
1	T	9	VAL	N-CA-C	6.01	117.04	111.45
1	S	9	VAL	N-CA-C	6.01	117.04	111.45
2	u	13	PRO	N-CA-C	-6.01	104.37	112.48
1	E	347	GLN	N-CA-C	6.01	119.87	112.54
1	F	347	GLN	N-CA-C	6.01	119.87	112.54
1	T	80	ASN	CA-C-N	-6.01	116.44	122.69
1	T	80	ASN	C-N-CA	-6.01	116.44	122.69
2	a	21	GLY	N-CA-C	-6.00	103.96	112.37
1	T	484	SER	CA-C-N	6.00	125.69	119.56
1	T	484	SER	C-N-CA	6.00	125.69	119.56
1	K	267	VAL	CA-C-N	6.00	125.89	119.28
1	K	267	VAL	C-N-CA	6.00	125.89	119.28
1	S	484	SER	CA-C-N	6.00	125.68	119.56
1	S	484	SER	C-N-CA	6.00	125.68	119.56
1	B	347	GLN	N-CA-C	6.00	119.86	112.54
1	U	9	VAL	N-CA-C	5.99	117.02	111.45
2	c	21	GLY	N-CA-C	-5.99	103.98	112.37
2	j	15	PHE	N-CA-C	5.99	119.29	108.69
1	U	484	SER	CA-C-N	5.99	125.67	119.56
1	U	484	SER	C-N-CA	5.99	125.67	119.56
2	i	15	PHE	N-CA-C	5.99	119.29	108.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	484	SER	CA-C-N	5.98	125.66	119.56
1	X	484	SER	C-N-CA	5.98	125.66	119.56
1	X	80	ASN	CA-C-N	-5.98	116.47	122.69
1	X	80	ASN	C-N-CA	-5.98	116.47	122.69
2	h	15	PHE	N-CA-C	5.98	119.27	108.69
2	a	3	LEU	CA-C-N	5.97	125.59	119.56
2	a	3	LEU	C-N-CA	5.97	125.59	119.56
1	U	80	ASN	CA-C-N	-5.97	116.48	122.69
1	U	80	ASN	C-N-CA	-5.97	116.48	122.69
2	k	15	PHE	N-CA-C	5.97	119.26	108.69
1	C	347	GLN	N-CA-C	5.97	119.82	112.54
1	A	347	GLN	N-CA-C	5.97	119.82	112.54
2	l	15	PHE	N-CA-C	5.96	119.25	108.69
1	B	69	TYR	N-CA-C	5.96	117.86	111.36
1	C	69	TYR	N-CA-C	5.96	117.86	111.36
2	v	90	MET	N-CA-C	5.96	118.90	109.96
2	x	90	MET	N-CA-C	5.96	118.89	109.96
1	D	347	GLN	N-CA-C	5.95	119.80	112.54
2	g	15	PHE	N-CA-C	5.95	119.23	108.69
2	s	90	MET	N-CA-C	5.95	118.89	109.96
2	c	3	LEU	CA-C-N	5.95	125.56	119.56
2	c	3	LEU	C-N-CA	5.95	125.56	119.56
2	w	90	MET	N-CA-C	5.94	118.87	109.96
2	t	90	MET	N-CA-C	5.94	118.87	109.96
1	F	69	TYR	N-CA-C	5.94	117.83	111.36
1	V	80	ASN	CA-C-N	-5.94	116.51	122.69
1	V	80	ASN	C-N-CA	-5.94	116.51	122.69
2	k	3	LEU	CA-C-N	5.94	125.56	119.56
2	k	3	LEU	C-N-CA	5.94	125.56	119.56
2	u	90	MET	N-CA-C	5.94	118.86	109.96
2	j	3	LEU	CA-C-N	5.93	125.55	119.56
2	j	3	LEU	C-N-CA	5.93	125.55	119.56
2	g	3	LEU	CA-C-N	5.92	125.54	119.56
2	g	3	LEU	C-N-CA	5.92	125.54	119.56
1	D	69	TYR	N-CA-C	5.92	117.82	111.36
2	n	57	MET	CA-C-N	5.92	125.54	119.56
2	n	57	MET	C-N-CA	5.92	125.54	119.56
1	A	69	TYR	N-CA-C	5.92	117.81	111.36
2	i	3	LEU	CA-C-N	5.92	125.54	119.56
2	i	3	LEU	C-N-CA	5.92	125.54	119.56
2	h	3	LEU	CA-C-N	5.92	125.53	119.56
2	h	3	LEU	C-N-CA	5.92	125.53	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	o	57	MET	CA-C-N	5.91	125.53	119.56
2	o	57	MET	C-N-CA	5.91	125.53	119.56
2	e	3	LEU	CA-C-N	5.91	125.53	119.56
2	e	3	LEU	C-N-CA	5.91	125.53	119.56
1	Q	6	SER	CA-C-N	5.90	125.58	119.56
1	Q	6	SER	C-N-CA	5.90	125.58	119.56
1	A	6	SER	CA-C-N	5.90	125.58	119.56
1	A	6	SER	C-N-CA	5.90	125.58	119.56
1	N	6	SER	CA-C-N	5.90	125.58	119.56
1	N	6	SER	C-N-CA	5.90	125.58	119.56
2	q	57	MET	CA-C-N	5.90	125.52	119.56
2	q	57	MET	C-N-CA	5.90	125.52	119.56
1	J	52	THR	N-CA-C	5.89	116.34	108.38
1	C	6	SER	CA-C-N	5.89	125.57	119.56
1	C	6	SER	C-N-CA	5.89	125.57	119.56
1	M	52	THR	N-CA-C	5.89	118.65	109.52
1	P	6	SER	CA-C-N	5.89	125.57	119.56
1	P	6	SER	C-N-CA	5.89	125.57	119.56
1	R	52	THR	N-CA-C	5.89	118.65	109.52
2	m	57	MET	CA-C-N	5.89	125.51	119.56
2	m	57	MET	C-N-CA	5.89	125.51	119.56
2	r	57	MET	CA-C-N	5.89	125.51	119.56
2	r	57	MET	C-N-CA	5.89	125.51	119.56
2	l	3	LEU	CA-C-N	5.88	125.50	119.56
2	l	3	LEU	C-N-CA	5.88	125.50	119.56
1	F	6	SER	CA-C-N	5.88	125.56	119.56
1	F	6	SER	C-N-CA	5.88	125.56	119.56
1	E	6	SER	CA-C-N	5.88	125.56	119.56
1	E	6	SER	C-N-CA	5.88	125.56	119.56
1	L	398	ASN	CA-C-N	5.88	125.58	119.82
1	L	398	ASN	C-N-CA	5.88	125.58	119.82
1	I	398	ASN	CA-C-N	5.88	125.58	119.82
1	I	398	ASN	C-N-CA	5.88	125.58	119.82
1	N	52	THR	N-CA-C	5.88	118.63	109.52
1	R	6	SER	CA-C-N	5.88	125.55	119.56
1	R	6	SER	C-N-CA	5.88	125.55	119.56
1	K	398	ASN	CA-C-N	5.87	125.57	119.82
1	K	398	ASN	C-N-CA	5.87	125.57	119.82
2	b	3	LEU	CA-C-N	5.87	125.49	119.56
2	b	3	LEU	C-N-CA	5.87	125.49	119.56
2	p	57	MET	CA-C-N	5.87	125.49	119.56
2	p	57	MET	C-N-CA	5.87	125.49	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	j	26	TYR	N-CA-C	5.86	117.76	108.79
1	Q	52	THR	N-CA-C	5.86	118.61	109.52
1	M	6	SER	CA-C-N	5.86	125.54	119.56
1	M	6	SER	C-N-CA	5.86	125.54	119.56
1	O	6	SER	CA-C-N	5.86	125.54	119.56
1	O	6	SER	C-N-CA	5.86	125.54	119.56
1	P	52	THR	N-CA-C	5.86	118.60	109.52
1	I	52	THR	N-CA-C	5.86	116.29	108.38
1	G	398	ASN	CA-C-N	5.85	125.56	119.82
1	G	398	ASN	C-N-CA	5.85	125.56	119.82
1	D	6	SER	CA-C-N	5.85	125.53	119.56
1	D	6	SER	C-N-CA	5.85	125.53	119.56
2	k	26	TYR	N-CA-C	5.85	117.74	108.79
1	K	52	THR	N-CA-C	5.85	116.28	108.38
1	B	6	SER	CA-C-N	5.85	125.52	119.56
1	B	6	SER	C-N-CA	5.85	125.52	119.56
2	i	26	TYR	N-CA-C	5.84	117.73	108.79
1	J	398	ASN	CA-C-N	5.84	125.55	119.82
1	J	398	ASN	C-N-CA	5.84	125.55	119.82
2	l	26	TYR	N-CA-C	5.84	117.73	108.79
1	O	52	THR	N-CA-C	5.84	118.58	109.52
1	L	52	THR	N-CA-C	5.84	116.26	108.38
2	i	45	ASN	N-CA-C	5.84	123.23	110.80
2	h	26	TYR	N-CA-C	5.84	117.72	108.79
1	H	52	THR	N-CA-C	5.83	116.26	108.38
1	H	398	ASN	CA-C-N	5.83	125.54	119.82
1	H	398	ASN	C-N-CA	5.83	125.54	119.82
1	E	69	TYR	N-CA-C	5.82	117.71	111.36
1	G	52	THR	N-CA-C	5.82	116.24	108.38
1	X	235	SER	N-CA-C	5.82	118.41	110.55
1	T	40	ALA	CA-C-N	5.82	127.12	119.84
1	T	40	ALA	C-N-CA	5.82	127.12	119.84
1	V	235	SER	N-CA-C	5.81	118.39	110.55
1	X	40	ALA	CA-C-N	5.81	127.10	119.84
1	X	40	ALA	C-N-CA	5.81	127.10	119.84
2	g	26	TYR	N-CA-C	5.81	117.68	108.79
1	S	40	ALA	CA-C-N	5.80	127.09	119.84
1	S	40	ALA	C-N-CA	5.80	127.09	119.84
1	U	235	SER	N-CA-C	5.80	118.38	110.55
1	U	40	ALA	CA-C-N	5.79	127.08	119.84
1	U	40	ALA	C-N-CA	5.79	127.08	119.84
1	V	40	ALA	CA-C-N	5.79	127.08	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	40	ALA	C-N-CA	5.79	127.08	119.84
1	J	378	VAL	N-CA-C	5.79	116.53	108.89
1	H	378	VAL	N-CA-C	5.78	116.53	108.89
1	J	237	HIS	CA-C-N	5.78	126.24	120.52
1	J	237	HIS	C-N-CA	5.78	126.24	120.52
1	P	267	VAL	CA-C-N	5.78	125.25	119.24
1	P	267	VAL	C-N-CA	5.78	125.25	119.24
1	W	235	SER	N-CA-C	5.78	118.35	110.55
1	W	40	ALA	CA-C-N	5.77	127.06	119.84
1	W	40	ALA	C-N-CA	5.77	127.06	119.84
1	T	235	SER	N-CA-C	5.77	118.34	110.55
1	I	237	HIS	CA-C-N	5.76	126.22	120.52
1	I	237	HIS	C-N-CA	5.76	126.22	120.52
1	L	378	VAL	N-CA-C	5.76	116.49	108.89
1	W	342	ASP	CA-C-N	5.75	127.03	119.84
1	W	342	ASP	C-N-CA	5.75	127.03	119.84
1	I	378	VAL	N-CA-C	5.74	116.47	108.89
1	G	378	VAL	N-CA-C	5.74	116.46	108.89
1	K	378	VAL	N-CA-C	5.74	116.46	108.89
1	X	342	ASP	CA-C-N	5.73	127.01	119.84
1	X	342	ASP	C-N-CA	5.73	127.01	119.84
1	G	237	HIS	CA-C-N	5.73	126.20	120.52
1	G	237	HIS	C-N-CA	5.73	126.20	120.52
1	H	237	HIS	CA-C-N	5.73	126.19	120.52
1	H	237	HIS	C-N-CA	5.73	126.19	120.52
1	L	237	HIS	CA-C-N	5.73	126.19	120.52
1	L	237	HIS	C-N-CA	5.73	126.19	120.52
2	v	24	VAL	N-CA-C	5.72	116.54	108.36
1	U	342	ASP	CA-C-N	5.72	126.99	119.84
1	U	342	ASP	C-N-CA	5.72	126.99	119.84
1	S	342	ASP	CA-C-N	5.72	126.99	119.84
1	S	342	ASP	C-N-CA	5.72	126.99	119.84
1	T	342	ASP	CA-C-N	5.72	126.99	119.84
1	T	342	ASP	C-N-CA	5.72	126.99	119.84
1	V	342	ASP	CA-C-N	5.71	126.98	119.84
1	V	342	ASP	C-N-CA	5.71	126.98	119.84
2	x	24	VAL	N-CA-C	5.71	116.52	108.36
1	P	335	TYR	N-CA-C	5.71	120.25	112.55
2	w	24	VAL	N-CA-C	5.69	116.50	108.36
2	s	24	VAL	N-CA-C	5.69	116.50	108.36
1	D	514	ILE	N-CA-C	-5.69	100.03	107.88
2	u	24	VAL	N-CA-C	5.68	116.49	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	335	TYR	N-CA-C	5.68	120.22	112.55
1	K	237	HIS	CA-C-N	5.68	126.15	120.52
1	K	237	HIS	C-N-CA	5.68	126.15	120.52
1	I	347	GLN	N-CA-C	5.68	119.47	112.54
1	H	347	GLN	N-CA-C	5.68	119.46	112.54
1	O	335	TYR	N-CA-C	5.68	120.21	112.55
1	C	514	ILE	N-CA-C	-5.67	100.05	107.88
1	M	335	TYR	N-CA-C	5.67	120.20	112.55
2	t	24	VAL	N-CA-C	5.67	116.46	108.36
2	e	108	PRO	CA-C-N	-5.66	115.73	123.14
2	e	108	PRO	C-N-CA	-5.66	115.73	123.14
1	W	250	ARG	N-CA-C	5.66	118.65	111.69
2	c	108	PRO	CA-C-N	-5.66	115.73	123.14
2	c	108	PRO	C-N-CA	-5.66	115.73	123.14
1	F	514	ILE	N-CA-C	-5.66	100.08	107.88
1	T	378	VAL	N-CA-C	5.66	116.72	108.58
1	K	347	GLN	N-CA-C	5.65	119.44	112.54
2	b	108	PRO	CA-C-N	-5.65	115.74	123.14
2	b	108	PRO	C-N-CA	-5.65	115.74	123.14
1	A	514	ILE	N-CA-C	-5.65	100.09	107.88
1	J	347	GLN	N-CA-C	5.65	119.43	112.54
2	a	108	PRO	CA-C-N	-5.65	115.74	123.14
2	a	108	PRO	C-N-CA	-5.65	115.74	123.14
1	R	335	TYR	N-CA-C	5.64	120.17	112.55
2	j	44	GLN	N-CA-C	5.64	122.81	110.80
2	l	44	GLN	N-CA-C	5.64	122.82	110.80
1	X	250	ARG	N-CA-C	5.64	118.63	111.69
1	T	250	ARG	N-CA-C	5.64	118.62	111.69
1	N	335	TYR	N-CA-C	5.64	120.16	112.55
1	L	347	GLN	N-CA-C	5.64	119.42	112.54
2	f	108	PRO	CA-C-N	-5.64	115.75	123.14
2	f	108	PRO	C-N-CA	-5.64	115.75	123.14
1	E	514	ILE	N-CA-C	-5.63	100.11	107.88
2	g	44	GLN	N-CA-C	5.63	122.79	110.80
2	k	44	GLN	N-CA-C	5.63	122.79	110.80
1	G	347	GLN	N-CA-C	5.63	119.41	112.54
1	B	514	ILE	N-CA-C	-5.63	100.11	107.88
2	h	44	GLN	N-CA-C	5.62	122.78	110.80
1	W	378	VAL	N-CA-C	5.62	116.67	108.58
1	V	250	ARG	N-CA-C	5.62	118.60	111.69
1	S	378	VAL	N-CA-C	5.62	116.67	108.58
2	d	108	PRO	CA-C-N	-5.61	115.79	123.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	d	108	PRO	C-N-CA	-5.61	115.79	123.14
1	P	351	VAL	CA-C-N	5.61	126.16	120.38
1	P	351	VAL	C-N-CA	5.61	126.16	120.38
1	O	408	PHE	CA-C-N	5.61	126.85	119.84
1	O	408	PHE	C-N-CA	5.61	126.85	119.84
1	V	378	VAL	N-CA-C	5.61	116.66	108.58
1	X	378	VAL	N-CA-C	5.61	116.66	108.58
1	A	360	ILE	N-CA-C	-5.61	105.64	111.58
1	U	250	ARG	N-CA-C	5.61	118.59	111.69
1	N	408	PHE	CA-C-N	5.60	126.84	119.84
1	N	408	PHE	C-N-CA	5.60	126.84	119.84
1	U	378	VAL	N-CA-C	5.60	116.65	108.58
1	S	250	ARG	N-CA-C	5.60	118.58	111.69
2	v	11	VAL	N-CA-C	-5.60	106.75	111.56
1	M	351	VAL	CA-C-N	5.59	126.14	120.38
1	M	351	VAL	C-N-CA	5.59	126.14	120.38
1	R	408	PHE	CA-C-N	5.59	126.83	119.84
1	R	408	PHE	C-N-CA	5.59	126.83	119.84
1	M	408	PHE	CA-C-N	5.59	126.83	119.84
1	M	408	PHE	C-N-CA	5.59	126.83	119.84
2	u	11	VAL	N-CA-C	-5.59	106.75	111.56
2	w	11	VAL	N-CA-C	-5.59	106.75	111.56
1	P	408	PHE	CA-C-N	5.58	126.82	119.84
1	P	408	PHE	C-N-CA	5.58	126.82	119.84
1	Q	408	PHE	CA-C-N	5.58	126.82	119.84
1	Q	408	PHE	C-N-CA	5.58	126.82	119.84
1	N	351	VAL	CA-C-N	5.58	126.13	120.38
1	N	351	VAL	C-N-CA	5.58	126.13	120.38
1	B	360	ILE	N-CA-C	-5.58	105.67	111.58
1	Q	351	VAL	CA-C-N	5.57	126.11	120.38
1	Q	351	VAL	C-N-CA	5.57	126.11	120.38
1	F	360	ILE	N-CA-C	-5.57	105.68	111.58
1	O	351	VAL	CA-C-N	5.57	126.11	120.38
1	O	351	VAL	C-N-CA	5.57	126.11	120.38
1	R	351	VAL	CA-C-N	5.56	126.11	120.38
1	R	351	VAL	C-N-CA	5.56	126.11	120.38
2	s	11	VAL	N-CA-C	-5.56	106.78	111.56
1	E	360	ILE	N-CA-C	-5.54	105.71	111.58
2	t	11	VAL	N-CA-C	-5.54	106.79	111.56
2	e	33	LEU	N-CA-C	5.54	117.43	108.41
2	n	49	THR	N-CA-C	-5.53	103.39	110.53
2	d	20	ASP	N-CA-C	5.53	118.18	109.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	360	ILE	N-CA-C	-5.53	105.72	111.58
1	M	92	GLY	N-CA-C	5.53	119.54	112.13
2	p	49	THR	N-CA-C	-5.53	103.40	110.53
2	a	20	ASP	N-CA-C	5.53	118.17	109.39
2	a	33	LEU	N-CA-C	5.53	117.42	108.41
2	c	20	ASP	N-CA-C	5.53	118.17	109.39
1	Q	92	GLY	N-CA-C	5.52	119.53	112.13
2	q	49	THR	N-CA-C	-5.52	103.41	110.53
2	f	33	LEU	N-CA-C	5.52	117.41	108.41
1	D	360	ILE	N-CA-C	-5.52	105.73	111.58
2	x	11	VAL	N-CA-C	-5.52	106.82	111.56
2	r	49	THR	N-CA-C	-5.51	103.42	110.53
2	f	20	ASP	N-CA-C	5.51	118.15	109.39
2	b	20	ASP	N-CA-C	5.51	118.15	109.39
2	d	33	LEU	N-CA-C	5.51	117.39	108.41
2	e	20	ASP	N-CA-C	5.51	118.15	109.39
2	b	33	LEU	N-CA-C	5.50	117.38	108.41
1	N	92	GLY	N-CA-C	5.50	119.50	112.13
1	O	92	GLY	N-CA-C	5.50	119.50	112.13
2	m	49	THR	N-CA-C	-5.50	103.44	110.53
2	c	33	LEU	N-CA-C	5.50	117.37	108.41
2	o	49	THR	N-CA-C	-5.49	103.45	110.53
2	d	3	LEU	CA-C-N	5.47	125.56	119.87
2	d	3	LEU	C-N-CA	5.47	125.56	119.87
1	Q	306	ASP	CA-C-N	5.47	126.01	120.38
1	Q	306	ASP	C-N-CA	5.47	126.01	120.38
1	R	92	GLY	N-CA-C	5.47	119.46	112.13
2	f	21	GLY	CA-C-N	-5.46	117.37	123.16
2	f	21	GLY	C-N-CA	-5.46	117.37	123.16
1	P	306	ASP	CA-C-N	5.45	126.00	120.38
1	P	306	ASP	C-N-CA	5.45	126.00	120.38
1	F	424	ASP	CA-C-N	5.45	125.12	119.56
1	F	424	ASP	C-N-CA	5.45	125.12	119.56
1	O	306	ASP	CA-C-N	5.45	125.99	120.38
1	O	306	ASP	C-N-CA	5.45	125.99	120.38
1	P	92	GLY	N-CA-C	5.45	119.43	112.13
1	W	397	LEU	N-CA-C	5.44	119.09	112.23
1	E	424	ASP	CA-C-N	5.44	125.11	119.56
1	E	424	ASP	C-N-CA	5.44	125.11	119.56
2	d	21	GLY	CA-C-N	-5.44	117.40	123.16
2	d	21	GLY	C-N-CA	-5.44	117.40	123.16
2	f	3	LEU	CA-C-N	5.44	125.53	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	f	3	LEU	C-N-CA	5.44	125.53	119.87
2	n	33	LEU	N-CA-C	5.43	118.34	109.59
1	R	306	ASP	CA-C-N	5.43	125.97	120.38
1	R	306	ASP	C-N-CA	5.43	125.97	120.38
1	C	424	ASP	CA-C-N	5.43	125.10	119.56
1	C	424	ASP	C-N-CA	5.43	125.10	119.56
2	a	21	GLY	CA-C-N	-5.43	117.41	123.16
2	a	21	GLY	C-N-CA	-5.43	117.41	123.16
1	U	397	LEU	N-CA-C	5.42	119.06	112.23
1	D	424	ASP	CA-C-N	5.42	125.09	119.56
1	D	424	ASP	C-N-CA	5.42	125.09	119.56
1	M	306	ASP	CA-C-N	5.42	125.96	120.38
1	M	306	ASP	C-N-CA	5.42	125.96	120.38
1	D	254	GLY	N-CA-C	-5.41	104.18	111.54
2	e	21	GLY	CA-C-N	-5.41	117.42	123.16
2	e	21	GLY	C-N-CA	-5.41	117.42	123.16
1	A	254	GLY	N-CA-C	-5.41	104.18	111.54
1	S	397	LEU	N-CA-C	5.41	119.05	112.23
1	N	306	ASP	CA-C-N	5.41	125.95	120.38
1	N	306	ASP	C-N-CA	5.41	125.95	120.38
1	T	397	LEU	N-CA-C	5.41	119.05	112.23
2	t	26	TYR	N-CA-C	5.41	117.30	108.76
1	B	424	ASP	CA-C-N	5.41	125.08	119.56
1	B	424	ASP	C-N-CA	5.41	125.08	119.56
2	b	21	GLY	CA-C-N	-5.41	117.43	123.16
2	b	21	GLY	C-N-CA	-5.41	117.43	123.16
1	V	267	VAL	CA-C-N	5.40	125.74	119.47
1	V	267	VAL	C-N-CA	5.40	125.74	119.47
1	X	397	LEU	N-CA-C	5.40	119.04	112.23
2	s	26	TYR	N-CA-C	5.40	117.29	108.76
2	c	21	GLY	CA-C-N	-5.40	117.44	123.16
2	c	21	GLY	C-N-CA	-5.40	117.44	123.16
2	v	26	TYR	N-CA-C	5.40	117.29	108.76
1	V	397	LEU	N-CA-C	5.40	119.03	112.23
2	x	26	TYR	N-CA-C	5.40	117.29	108.76
1	U	267	VAL	CA-C-N	5.40	125.73	119.47
1	U	267	VAL	C-N-CA	5.40	125.73	119.47
2	g	135	LEU	N-CA-C	5.40	116.92	110.44
1	B	254	GLY	N-CA-C	-5.39	104.20	111.54
2	k	135	LEU	N-CA-C	5.39	116.91	110.44
1	X	267	VAL	CA-C-N	5.39	125.72	119.47
1	X	267	VAL	C-N-CA	5.39	125.72	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	m	108	PRO	CA-C-N	-5.39	116.08	123.14
2	m	108	PRO	C-N-CA	-5.39	116.08	123.14
2	i	135	LEU	N-CA-C	5.39	116.91	110.44
2	r	108	PRO	CA-C-N	-5.39	116.08	123.14
2	r	108	PRO	C-N-CA	-5.39	116.08	123.14
2	u	26	TYR	N-CA-C	5.39	117.27	108.76
1	W	267	VAL	CA-C-N	5.38	125.72	119.47
1	W	267	VAL	C-N-CA	5.38	125.72	119.47
1	E	254	GLY	N-CA-C	-5.38	104.22	111.54
1	A	424	ASP	CA-C-N	5.38	125.05	119.56
1	A	424	ASP	C-N-CA	5.38	125.05	119.56
2	h	135	LEU	N-CA-C	5.38	116.90	110.44
2	w	26	TYR	N-CA-C	5.38	117.27	108.76
1	T	267	VAL	CA-C-N	5.38	125.71	119.47
1	T	267	VAL	C-N-CA	5.38	125.71	119.47
2	l	108	PRO	CA-C-N	-5.37	115.52	122.99
2	l	108	PRO	C-N-CA	-5.37	115.52	122.99
1	S	267	VAL	CA-C-N	5.37	125.70	119.47
1	S	267	VAL	C-N-CA	5.37	125.70	119.47
1	C	254	GLY	N-CA-C	-5.37	104.24	111.54
2	h	108	PRO	CA-C-N	-5.36	115.53	122.99
2	h	108	PRO	C-N-CA	-5.36	115.53	122.99
2	j	108	PRO	CA-C-N	-5.36	115.54	122.99
2	j	108	PRO	C-N-CA	-5.36	115.54	122.99
2	g	108	PRO	CA-C-N	-5.36	115.54	122.99
2	g	108	PRO	C-N-CA	-5.36	115.54	122.99
2	n	108	PRO	CA-C-N	-5.36	116.12	123.14
2	n	108	PRO	C-N-CA	-5.36	116.12	123.14
2	q	108	PRO	CA-C-N	-5.35	116.13	123.14
2	q	108	PRO	C-N-CA	-5.35	116.13	123.14
1	F	254	GLY	N-CA-C	-5.35	104.26	111.54
2	i	108	PRO	CA-C-N	-5.35	115.55	122.99
2	i	108	PRO	C-N-CA	-5.35	115.55	122.99
2	k	108	PRO	CA-C-N	-5.35	115.56	122.99
2	k	108	PRO	C-N-CA	-5.35	115.56	122.99
2	p	108	PRO	CA-C-N	-5.35	116.14	123.14
2	p	108	PRO	C-N-CA	-5.35	116.14	123.14
2	o	108	PRO	CA-C-N	-5.34	116.14	123.14
2	o	108	PRO	C-N-CA	-5.34	116.14	123.14
2	r	33	LEU	N-CA-C	5.33	118.50	109.76
1	R	338	ILE	N-CA-C	5.33	116.25	108.53
2	l	135	LEU	N-CA-C	5.33	116.83	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	338	ILE	N-CA-C	5.32	116.25	108.53
2	j	135	LEU	N-CA-C	5.32	116.82	110.44
1	O	383	VAL	N-CA-C	-5.31	106.51	111.45
1	N	383	VAL	N-CA-C	-5.30	106.52	111.45
1	Q	383	VAL	N-CA-C	-5.30	106.52	111.45
1	M	383	VAL	N-CA-C	-5.30	106.52	111.45
1	O	338	ILE	N-CA-C	5.30	116.21	108.53
1	Q	338	ILE	N-CA-C	5.29	116.20	108.53
2	m	33	LEU	N-CA-C	5.28	118.42	109.76
2	p	33	LEU	N-CA-C	5.28	118.42	109.76
1	N	338	ILE	N-CA-C	5.28	116.19	108.53
1	B	516	PRO	CA-C-N	5.28	127.77	120.49
1	B	516	PRO	C-N-CA	5.28	127.77	120.49
1	P	338	ILE	N-CA-C	5.27	116.17	108.53
1	R	383	VAL	N-CA-C	-5.26	106.56	111.45
1	A	516	PRO	CA-C-N	5.26	127.75	120.49
1	A	516	PRO	C-N-CA	5.26	127.75	120.49
2	q	33	LEU	N-CA-C	5.26	118.39	109.76
1	F	516	PRO	CA-C-N	5.25	127.74	120.49
1	F	516	PRO	C-N-CA	5.25	127.74	120.49
1	E	516	PRO	CA-C-N	5.24	127.72	120.49
1	E	516	PRO	C-N-CA	5.24	127.72	120.49
1	N	267	VAL	CA-C-N	5.23	125.29	119.32
1	N	267	VAL	C-N-CA	5.23	125.29	119.32
1	Q	267	VAL	CA-C-N	5.23	125.28	119.32
1	Q	267	VAL	C-N-CA	5.23	125.28	119.32
1	A	335	TYR	N-CA-C	5.23	121.37	109.81
1	F	335	TYR	N-CA-C	5.23	121.36	109.81
1	R	267	VAL	CA-C-N	5.22	125.27	119.32
1	R	267	VAL	C-N-CA	5.22	125.27	119.32
1	I	284	VAL	CB-CA-C	-5.22	105.20	112.04
1	P	383	VAL	N-CA-C	-5.21	106.60	111.45
1	O	267	VAL	CA-C-N	5.21	125.26	119.32
1	O	267	VAL	C-N-CA	5.21	125.26	119.32
1	J	284	VAL	CB-CA-C	-5.20	105.22	112.04
1	D	516	PRO	CA-C-N	5.20	127.67	120.49
1	D	516	PRO	C-N-CA	5.20	127.67	120.49
1	R	378	VAL	N-CA-C	5.20	116.07	108.58
1	L	317	ARG	N-CA-C	-5.20	105.73	111.71
1	Q	378	VAL	N-CA-C	5.20	116.06	108.58
1	C	516	PRO	CA-C-N	5.20	127.66	120.49
1	C	516	PRO	C-N-CA	5.20	127.66	120.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	267	VAL	CA-C-N	5.19	125.24	119.32
1	M	267	VAL	C-N-CA	5.19	125.24	119.32
1	O	378	VAL	N-CA-C	5.19	116.06	108.58
1	I	317	ARG	N-CA-C	-5.19	105.74	111.71
1	M	378	VAL	N-CA-C	5.19	116.05	108.58
1	N	378	VAL	N-CA-C	5.18	116.05	108.58
1	J	317	ARG	N-CA-C	-5.18	105.75	111.71
1	G	317	ARG	N-CA-C	-5.18	105.76	111.71
1	P	378	VAL	N-CA-C	5.17	116.03	108.58
1	K	317	ARG	N-CA-C	-5.17	105.77	111.71
1	H	317	ARG	N-CA-C	-5.17	105.77	111.71
1	J	348	SER	N-CA-C	5.15	117.08	108.99
2	d	135	LEU	CA-C-N	-5.15	115.35	122.30
2	d	135	LEU	C-N-CA	-5.15	115.35	122.30
1	L	284	VAL	CB-CA-C	-5.14	105.19	111.92
1	B	335	TYR	CA-C-N	5.14	125.35	120.31
1	B	335	TYR	C-N-CA	5.14	125.35	120.31
1	K	455	ASN	N-CA-C	-5.14	102.30	109.96
1	M	327	ASP	N-CA-C	5.14	118.33	111.24
1	G	348	SER	N-CA-C	5.14	117.05	108.99
2	o	33	LEU	N-CA-C	5.13	118.18	109.76
1	K	348	SER	N-CA-C	5.13	117.04	108.99
1	I	348	SER	N-CA-C	5.13	117.04	108.99
1	H	348	SER	N-CA-C	5.13	117.04	108.99
2	e	135	LEU	CA-C-N	-5.12	115.39	122.30
2	e	135	LEU	C-N-CA	-5.12	115.39	122.30
2	a	6	PRO	N-CA-C	5.12	119.13	111.14
1	N	327	ASP	N-CA-C	5.12	118.31	111.24
2	f	135	LEU	CA-C-N	-5.12	115.39	122.30
2	f	135	LEU	C-N-CA	-5.12	115.39	122.30
1	G	455	ASN	N-CA-C	-5.12	102.34	109.96
2	c	135	LEU	CA-C-N	-5.12	115.39	122.30
2	c	135	LEU	C-N-CA	-5.12	115.39	122.30
1	D	335	TYR	CA-C-N	5.11	125.32	120.31
1	D	335	TYR	C-N-CA	5.11	125.32	120.31
1	L	348	SER	N-CA-C	5.11	117.02	108.99
1	H	455	ASN	N-CA-C	-5.11	102.34	109.96
2	e	6	PRO	N-CA-C	5.11	119.11	111.14
1	H	424	ASP	CA-C-N	5.11	125.40	119.47
1	H	424	ASP	C-N-CA	5.11	125.40	119.47
2	a	135	LEU	CA-C-N	-5.11	115.40	122.30
2	a	135	LEU	C-N-CA	-5.11	115.40	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	135	LEU	CA-C-N	-5.11	115.41	122.30
2	b	135	LEU	C-N-CA	-5.11	115.41	122.30
2	c	6	PRO	N-CA-C	5.11	119.11	111.14
2	b	6	PRO	N-CA-C	5.11	119.11	111.14
1	J	455	ASN	N-CA-C	-5.10	102.36	109.96
2	i	17	ILE	O-C-N	-5.10	118.53	122.97
1	Q	327	ASP	N-CA-C	5.10	118.28	111.24
2	e	29	SER	N-CA-C	5.10	118.66	111.52
2	u	96	ASN	N-CA-C	5.10	117.09	108.02
1	F	335	TYR	CA-C-N	5.09	125.30	120.31
1	F	335	TYR	C-N-CA	5.09	125.30	120.31
1	I	455	ASN	N-CA-C	-5.09	102.37	109.96
1	C	255	GLY	N-CA-C	-5.09	108.63	114.69
1	C	335	TYR	CA-C-N	5.09	125.30	120.31
1	C	335	TYR	C-N-CA	5.09	125.30	120.31
1	P	327	ASP	N-CA-C	5.09	118.26	111.24
2	d	29	SER	N-CA-C	5.09	118.64	111.52
2	x	96	ASN	N-CA-C	5.09	117.07	108.02
2	b	29	SER	N-CA-C	5.09	118.64	111.52
1	L	307	PRO	N-CA-C	-5.08	104.50	110.70
1	L	455	ASN	N-CA-C	-5.08	102.39	109.96
2	g	17	ILE	O-C-N	-5.08	118.55	122.97
1	G	424	ASP	CA-C-N	5.08	125.36	119.47
1	G	424	ASP	C-N-CA	5.08	125.36	119.47
1	E	378	VAL	N-CA-C	5.08	115.59	108.89
2	v	96	ASN	N-CA-C	5.08	117.06	108.02
1	L	64	PHE	CB-CA-C	-5.08	102.96	111.23
2	a	29	SER	N-CA-C	5.08	118.62	111.52
1	K	64	PHE	CB-CA-C	-5.07	102.96	111.23
1	L	424	ASP	CA-C-N	5.07	125.36	119.47
1	L	424	ASP	C-N-CA	5.07	125.36	119.47
2	t	96	ASN	N-CA-C	5.07	117.05	108.02
1	R	327	ASP	N-CA-C	5.07	118.24	111.24
1	O	327	ASP	N-CA-C	5.07	118.24	111.24
2	k	17	ILE	O-C-N	-5.07	118.56	122.97
2	h	17	ILE	O-C-N	-5.07	118.56	122.97
2	w	96	ASN	N-CA-C	5.07	117.04	108.02
1	E	47	GLU	N-CA-C	5.07	121.01	109.81
1	A	255	GLY	N-CA-C	-5.07	108.66	114.69
1	I	307	PRO	N-CA-C	-5.07	104.52	110.70
1	E	335	TYR	CA-C-N	5.06	125.27	120.31
1	E	335	TYR	C-N-CA	5.06	125.27	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	378	VAL	N-CA-C	5.06	115.58	108.89
2	f	29	SER	N-CA-C	5.06	118.61	111.52
1	A	47	GLU	N-CA-C	5.06	121.00	109.81
1	C	47	GLU	N-CA-C	5.06	121.00	109.81
1	H	64	PHE	CB-CA-C	-5.06	102.98	111.23
1	K	424	ASP	CA-C-N	5.06	125.34	119.47
1	K	424	ASP	C-N-CA	5.06	125.34	119.47
1	S	265	VAL	N-CA-C	5.06	117.11	108.86
1	F	378	VAL	N-CA-C	5.06	115.57	108.89
2	s	96	ASN	N-CA-C	5.06	117.02	108.02
1	B	255	GLY	N-CA-C	-5.06	108.67	114.69
1	I	424	ASP	CA-C-N	5.06	125.34	119.47
1	I	424	ASP	C-N-CA	5.06	125.34	119.47
1	J	307	PRO	N-CA-C	-5.06	104.53	110.70
1	V	265	VAL	N-CA-C	5.05	117.10	108.86
1	J	424	ASP	CA-C-N	5.05	125.33	119.47
1	J	424	ASP	C-N-CA	5.05	125.33	119.47
1	X	265	VAL	N-CA-C	5.05	117.10	108.86
1	B	47	GLU	N-CA-C	5.05	120.98	109.81
1	S	12	GLU	CA-C-N	5.05	128.69	120.60
1	S	12	GLU	C-N-CA	5.05	128.69	120.60
1	I	64	PHE	CB-CA-C	-5.05	103.00	111.23
1	C	378	VAL	N-CA-C	5.05	115.56	108.89
1	W	265	VAL	N-CA-C	5.05	117.09	108.86
1	K	307	PRO	N-CA-C	-5.05	104.54	110.70
1	A	378	VAL	N-CA-C	5.05	115.56	108.89
1	G	64	PHE	CB-CA-C	-5.05	103.00	111.23
2	h	108	PRO	N-CA-C	5.05	120.17	113.86
2	c	29	SER	N-CA-C	5.05	118.58	111.52
1	G	307	PRO	N-CA-C	-5.04	104.55	110.70
1	U	265	VAL	N-CA-C	5.04	117.08	108.86
2	j	17	ILE	O-C-N	-5.04	118.58	122.97
1	D	348	SER	N-CA-C	5.04	116.73	108.76
1	D	378	VAL	N-CA-C	5.04	115.55	108.89
1	F	47	GLU	N-CA-C	5.04	120.95	109.81
1	D	47	GLU	N-CA-C	5.04	120.94	109.81
1	W	12	GLU	CA-C-N	5.04	128.66	120.60
1	W	12	GLU	C-N-CA	5.04	128.66	120.60
1	E	348	SER	N-CA-C	5.04	116.72	108.76
1	C	348	SER	N-CA-C	5.04	116.72	108.76
1	J	64	PHE	CB-CA-C	-5.04	103.02	111.23
2	l	17	ILE	O-C-N	-5.03	118.59	122.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	12	GLU	CA-C-N	5.03	128.66	120.60
1	T	12	GLU	C-N-CA	5.03	128.66	120.60
1	T	265	VAL	N-CA-C	5.03	117.06	108.86
1	F	348	SER	N-CA-C	5.03	116.71	108.76
1	A	335	TYR	CA-C-N	5.03	125.24	120.31
1	A	335	TYR	C-N-CA	5.03	125.24	120.31
2	v	35	ILE	N-CA-C	5.03	115.98	108.54
1	M	398	ASN	CA-C-N	5.03	125.10	119.87
1	M	398	ASN	C-N-CA	5.03	125.10	119.87
1	G	239	GLY	CA-C-N	5.02	126.12	119.84
1	G	239	GLY	C-N-CA	5.02	126.12	119.84
1	V	401	GLY	CA-C-N	-5.02	116.59	123.12
1	V	401	GLY	C-N-CA	-5.02	116.59	123.12
1	P	398	ASN	CA-C-N	5.02	125.09	119.87
1	P	398	ASN	C-N-CA	5.02	125.09	119.87
1	D	398	ASN	CA-C-N	5.02	125.09	119.87
1	D	398	ASN	C-N-CA	5.02	125.09	119.87
1	Q	398	ASN	CA-C-N	5.02	125.09	119.87
1	Q	398	ASN	C-N-CA	5.02	125.09	119.87
1	A	348	SER	N-CA-C	5.02	116.69	108.76
1	U	12	GLU	CA-C-N	5.02	128.63	120.60
1	U	12	GLU	C-N-CA	5.02	128.63	120.60
1	R	398	ASN	CA-C-N	5.02	125.09	119.87
1	R	398	ASN	C-N-CA	5.02	125.09	119.87
1	H	307	PRO	N-CA-C	-5.02	104.58	110.70
1	O	398	ASN	CA-C-N	5.02	125.09	119.87
1	O	398	ASN	C-N-CA	5.02	125.09	119.87
2	t	35	ILE	N-CA-C	5.02	115.96	108.54
2	i	108	PRO	N-CA-C	5.01	120.13	113.86
1	N	398	ASN	CA-C-N	5.01	125.08	119.87
1	N	398	ASN	C-N-CA	5.01	125.08	119.87
1	V	432	ILE	CA-C-N	-5.01	113.57	120.28
1	V	432	ILE	C-N-CA	-5.01	113.57	120.28
1	T	432	ILE	CA-C-N	-5.01	113.57	120.28
1	T	432	ILE	C-N-CA	-5.01	113.57	120.28
2	k	108	PRO	N-CA-C	5.01	120.12	113.86
1	X	497	THR	N-CA-C	-5.01	107.72	113.88
2	j	108	PRO	N-CA-C	5.00	120.12	113.86
1	X	432	ILE	CA-C-N	-5.00	113.57	120.28
1	X	432	ILE	C-N-CA	-5.00	113.57	120.28
1	B	348	SER	N-CA-C	5.00	116.67	108.76
2	g	108	PRO	N-CA-C	5.00	120.11	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	401	GLY	CA-C-N	-5.00	116.62	123.12
1	W	401	GLY	C-N-CA	-5.00	116.62	123.12
1	M	369	GLY	CA-C-O	-5.00	118.06	122.16
1	U	497	THR	N-CA-C	-5.00	107.73	113.88

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2867	0	2761	46	0
1	B	2867	0	2761	63	0
1	C	2867	0	2761	47	0
1	D	2867	0	2761	45	0
1	E	2867	0	2761	49	0
1	F	2867	0	2761	47	0
1	G	2867	0	2761	59	0
1	H	2867	0	2761	49	0
1	I	2867	0	2761	47	0
1	J	2867	0	2761	48	0
1	K	2867	0	2761	54	0
1	L	2867	0	2761	53	0
1	M	2867	0	2761	46	0
1	N	2867	0	2761	41	0
1	O	2867	0	2761	41	0
1	P	2867	0	2761	37	0
1	Q	2867	0	2761	53	0
1	R	2867	0	2761	49	0
1	S	2867	0	2761	83	0
1	T	2867	0	2761	60	0
1	U	2867	0	2761	65	0
1	V	2867	0	2761	72	0
1	W	2867	0	2761	64	0
1	X	2867	0	2761	61	0
2	a	1152	0	1150	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	b	1152	0	1149	57	0
2	c	1152	0	1149	32	0
2	d	1152	0	1149	41	0
2	e	1152	0	1149	49	0
2	f	1152	0	1149	36	0
2	g	1152	0	1150	33	0
2	h	1152	0	1150	52	0
2	i	1152	0	1146	64	0
2	j	1152	0	1150	34	0
2	k	1152	0	1150	40	0
2	l	1152	0	1150	52	0
2	m	1152	0	1150	94	0
2	n	1152	0	1150	78	0
2	o	1152	0	1150	99	0
2	p	1152	0	1150	120	0
2	q	1152	0	1150	105	0
2	r	1152	0	1150	100	0
2	s	1152	0	1150	35	0
2	t	1152	0	1150	31	0
2	u	1152	0	1150	30	0
2	v	1152	0	1150	31	0
2	w	1152	0	1150	34	0
2	x	1152	0	1150	32	0
All	All	96456	0	93855	2060	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 11.

All (2060) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:452:PHE:CZ	1:W:507:ARG:HD3	1.32	1.63
1:U:452:PHE:CZ	1:U:507:ARG:HD3	1.31	1.62
1:T:452:PHE:CZ	1:T:507:ARG:HD3	1.33	1.60
1:X:452:PHE:CZ	1:X:507:ARG:HD3	1.34	1.60
1:S:452:PHE:CZ	1:S:507:ARG:HD3	1.31	1.57
1:V:452:PHE:CZ	1:V:507:ARG:HD3	1.33	1.56
1:V:452:PHE:HZ	1:V:507:ARG:CD	1.21	1.51
2:e:42:TYR:OH	2:l:12:ALA:CB	1.64	1.44
2:a:42:TYR:CE1	2:h:12:ALA:HA	1.53	1.43
2:p:22:VAL:C	2:i:44:GLN:HG2	1.18	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:42:TYR:OH	2:i:12:ALA:CB	1.67	1.41
2:e:42:TYR:CE1	2:l:12:ALA:HA	1.52	1.41
2:b:42:TYR:CE1	2:i:12:ALA:HA	1.53	1.39
2:a:42:TYR:OH	2:h:12:ALA:CB	1.70	1.36
1:V:453:GLU:HG2	1:V:454:PRO:CD	1.55	1.34
1:U:452:PHE:HZ	1:U:507:ARG:CD	1.40	1.33
1:T:453:GLU:HB3	1:T:454:PRO:CD	1.60	1.31
1:U:452:PHE:CZ	1:U:507:ARG:CD	2.14	1.30
2:e:42:TYR:OH	2:l:12:ALA:CA	1.78	1.30
1:X:453:GLU:HB3	1:X:454:PRO:CD	1.59	1.30
1:S:453:GLU:HB3	1:S:454:PRO:CD	1.60	1.30
1:W:453:GLU:HB3	1:W:454:PRO:CD	1.60	1.29
1:S:452:PHE:HZ	1:S:507:ARG:CD	1.45	1.29
2:e:42:TYR:OH	2:l:12:ALA:C	1.75	1.29
2:n:43:GLN:OE1	2:n:48:THR:HG21	1.31	1.29
2:e:42:TYR:OH	2:l:12:ALA:HB1	1.14	1.29
2:a:42:TYR:OH	2:h:12:ALA:HB1	1.15	1.29
2:b:42:TYR:OH	2:i:12:ALA:HB1	1.15	1.28
1:T:452:PHE:HZ	1:T:507:ARG:CD	1.45	1.28
2:b:42:TYR:OH	2:i:12:ALA:C	1.76	1.28
1:U:453:GLU:HB3	1:U:454:PRO:CD	1.63	1.27
2:b:42:TYR:OH	2:i:12:ALA:CA	1.82	1.27
1:X:452:PHE:HZ	1:X:507:ARG:CD	1.49	1.26
2:p:22:VAL:O	2:i:44:GLN:HG2	1.15	1.26
2:q:129:ALA:CA	2:i:42:TYR:CE1	2.17	1.26
1:K:453:GLU:CB	1:K:454:PRO:HD3	1.66	1.26
1:S:452:PHE:CZ	1:S:507:ARG:CD	2.17	1.26
1:W:452:PHE:HZ	1:W:507:ARG:CD	1.48	1.25
1:T:452:PHE:CZ	1:T:507:ARG:CD	2.18	1.25
1:I:453:GLU:CB	1:I:454:PRO:HD3	1.67	1.25
1:J:453:GLU:CB	1:J:454:PRO:HD3	1.66	1.25
2:o:43:GLN:OE1	2:o:48:THR:HG21	1.35	1.24
1:L:453:GLU:CB	1:L:454:PRO:HD3	1.67	1.24
1:W:452:PHE:CZ	1:W:507:ARG:CD	2.18	1.24
2:q:129:ALA:HA	2:i:42:TYR:CZ	1.73	1.23
2:q:129:ALA:N	2:i:42:TYR:HE1	1.37	1.23
1:X:452:PHE:CZ	1:X:507:ARG:CD	2.21	1.23
2:a:42:TYR:OH	2:h:12:ALA:CA	1.87	1.23
1:V:453:GLU:CG	1:V:454:PRO:HD3	1.68	1.22
2:m:43:GLN:OE1	2:m:48:THR:HG21	1.38	1.22
2:a:42:TYR:OH	2:h:12:ALA:C	1.80	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:453:GLU:CB	1:G:454:PRO:HD3	1.67	1.21
2:p:22:VAL:O	2:i:44:GLN:CG	1.87	1.21
2:p:43:GLN:OE1	2:p:48:THR:HG21	1.36	1.20
2:d:42:TYR:CE1	2:k:12:ALA:HA	1.51	1.20
2:q:129:ALA:HB2	2:i:42:TYR:CD1	1.75	1.20
1:H:453:GLU:CB	1:H:454:PRO:HD3	1.66	1.20
2:q:43:GLN:OE1	2:q:48:THR:HG21	1.37	1.19
2:p:22:VAL:C	2:i:44:GLN:CG	2.15	1.18
2:q:129:ALA:N	2:i:42:TYR:CE1	2.10	1.18
1:H:453:GLU:HB2	1:H:454:PRO:HD3	1.18	1.18
2:j:42:TYR:HE1	2:r:129:ALA:N	1.42	1.17
1:G:453:GLU:HB2	1:G:454:PRO:HD3	1.19	1.17
2:l:42:TYR:HE1	2:n:129:ALA:N	1.43	1.17
2:q:129:ALA:HB2	2:i:42:TYR:CE1	1.79	1.16
2:g:42:TYR:HE1	2:o:129:ALA:N	1.43	1.16
1:L:453:GLU:HB2	1:L:454:PRO:CD	1.75	1.15
1:H:453:GLU:HB2	1:H:454:PRO:CD	1.76	1.15
1:I:453:GLU:HB2	1:I:454:PRO:CD	1.76	1.15
2:l:42:TYR:CE1	2:n:129:ALA:CA	2.29	1.15
1:X:453:GLU:HG3	1:R:372:LYS:HD2	1.25	1.15
2:g:42:TYR:CE1	2:o:129:ALA:CA	2.30	1.15
1:K:453:GLU:HB2	1:K:454:PRO:CD	1.76	1.14
1:L:453:GLU:HB2	1:L:454:PRO:HD3	1.19	1.14
2:j:42:TYR:CE1	2:r:129:ALA:CA	2.29	1.14
2:k:42:TYR:HE1	2:m:129:ALA:N	1.46	1.14
1:G:453:GLU:HB2	1:G:454:PRO:CD	1.77	1.14
1:I:453:GLU:HB2	1:I:454:PRO:HD3	1.18	1.13
2:p:129:ALA:N	2:h:42:TYR:HE1	1.46	1.13
1:K:453:GLU:HB2	1:K:454:PRO:HD3	1.18	1.12
1:U:453:GLU:HB3	1:U:454:PRO:HD3	1.19	1.12
1:J:453:GLU:HB2	1:J:454:PRO:CD	1.77	1.12
2:p:129:ALA:CA	2:h:42:TYR:CE1	2.34	1.11
1:X:453:GLU:HB3	1:X:454:PRO:HD3	1.18	1.11
2:r:43:GLN:OE1	2:r:48:THR:HG21	1.48	1.10
2:l:42:TYR:CD1	2:n:129:ALA:HB2	1.85	1.10
2:q:129:ALA:CB	2:i:42:TYR:CE1	2.34	1.10
2:k:42:TYR:CE1	2:m:129:ALA:CA	2.33	1.10
2:g:42:TYR:CD1	2:o:129:ALA:HB2	1.86	1.10
2:j:42:TYR:CD1	2:r:129:ALA:HB2	1.85	1.10
1:T:453:GLU:HB3	1:T:454:PRO:HD3	1.21	1.09
1:V:452:PHE:HA	1:P:372:LYS:HE3	1.35	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:469:ALA:CB	2:p:94:ARG:HH22	1.65	1.09
1:J:453:GLU:HB2	1:J:454:PRO:HD3	1.17	1.09
1:V:453:GLU:CG	1:V:454:PRO:CD	2.29	1.09
1:U:453:GLU:HG3	1:O:372:LYS:HD2	1.34	1.09
2:p:85:SER:HB3	2:o:34:GLN:HE22	1.08	1.08
1:S:453:GLU:HB3	1:S:454:PRO:HD3	1.19	1.08
1:S:453:GLU:HG3	1:M:372:LYS:HD2	1.31	1.08
1:V:452:PHE:CZ	1:V:507:ARG:CD	2.07	1.07
2:a:42:TYR:CE1	2:h:12:ALA:CA	2.37	1.07
2:p:129:ALA:HB2	2:h:42:TYR:CD1	1.89	1.07
2:b:42:TYR:CE1	2:i:12:ALA:CA	2.37	1.07
1:W:453:GLU:HB3	1:W:454:PRO:HD3	1.16	1.07
1:T:453:GLU:HG3	1:N:372:LYS:HD2	1.30	1.07
2:j:42:TYR:CE1	2:r:129:ALA:N	2.23	1.06
2:d:42:TYR:CE1	2:k:12:ALA:CA	2.37	1.06
2:e:42:TYR:CE1	2:l:12:ALA:CA	2.37	1.06
2:f:42:TYR:CE1	2:g:13:PRO:HD2	1.91	1.06
2:k:42:TYR:CD1	2:m:129:ALA:HB2	1.89	1.05
2:l:42:TYR:CE1	2:n:129:ALA:N	2.23	1.05
2:g:42:TYR:CE1	2:o:129:ALA:N	2.24	1.05
2:j:13:PRO:HD2	2:c:42:TYR:CE1	1.91	1.05
2:e:42:TYR:CZ	2:l:12:ALA:CA	2.39	1.04
2:p:129:ALA:N	2:h:42:TYR:CE1	2.26	1.04
2:r:34:GLN:NE2	2:m:118:TRP:CH2	2.26	1.04
1:S:465:ARG:HH21	2:m:94:ARG:NH2	1.56	1.04
1:W:453:GLU:HG3	1:Q:372:LYS:HD2	1.34	1.03
2:m:35:ILE:HG21	2:t:132:THR:HG21	1.38	1.03
2:b:42:TYR:CZ	2:i:12:ALA:CA	2.41	1.03
1:S:489:TYR:HA	1:S:513:GLY:HA3	1.39	1.02
2:m:35:ILE:HG21	2:t:132:THR:CG2	1.88	1.02
2:k:42:TYR:CE1	2:m:129:ALA:N	2.26	1.02
2:r:35:ILE:HG21	2:s:132:THR:HG21	1.41	1.02
1:W:452:PHE:HA	1:Q:372:LYS:HE3	1.41	1.02
2:n:34:GLN:HE22	2:o:85:SER:HB3	1.24	1.02
2:b:11:VAL:HG21	2:b:102:MET:H	1.21	1.02
1:S:453:GLU:CB	1:S:454:PRO:CD	2.38	1.01
1:S:465:ARG:NH2	2:m:94:ARG:NH2	2.08	1.01
1:X:453:GLU:CB	1:X:454:PRO:CD	2.38	1.00
1:U:453:GLU:CB	1:U:454:PRO:CD	2.39	1.00
2:a:42:TYR:HH	2:h:12:ALA:C	1.66	1.00
1:T:453:GLU:CB	1:T:454:PRO:CD	2.39	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:453:GLU:HB3	1:C:454:PRO:CD	1.92	1.00
1:S:453:GLU:CG	1:M:372:LYS:HD2	1.93	0.99
1:X:469:ALA:HB2	2:r:94:ARG:HH22	1.25	0.99
2:r:35:ILE:HG21	2:s:132:THR:CG2	1.92	0.99
1:F:453:GLU:HB3	1:F:454:PRO:CD	1.92	0.99
2:a:42:TYR:CZ	2:h:12:ALA:CA	2.44	0.99
1:D:453:GLU:HB3	1:D:454:PRO:CD	1.93	0.98
1:W:469:ALA:HB2	2:q:94:ARG:HH22	1.24	0.98
1:U:469:ALA:HB2	2:o:94:ARG:HH22	1.27	0.98
1:W:453:GLU:CB	1:W:454:PRO:CD	2.37	0.98
2:b:42:TYR:CE1	2:i:13:PRO:HD2	1.99	0.98
2:d:42:TYR:CE1	2:k:13:PRO:HD2	1.99	0.98
2:p:35:ILE:HG21	2:w:132:THR:HG21	1.46	0.97
2:g:42:TYR:CE1	2:o:129:ALA:HB2	1.99	0.97
1:B:453:GLU:HB3	1:B:454:PRO:CD	1.93	0.97
2:j:42:TYR:CZ	2:r:129:ALA:HA	2.00	0.97
2:q:129:ALA:CA	2:i:42:TYR:CZ	2.43	0.97
1:X:453:GLU:CG	1:R:372:LYS:HD2	1.94	0.97
2:r:34:GLN:HE22	2:m:118:TRP:HH2	1.01	0.97
1:U:453:GLU:CG	1:O:372:LYS:HD2	1.92	0.97
2:l:42:TYR:CE1	2:n:129:ALA:HB2	1.98	0.97
2:j:42:TYR:CE1	2:r:129:ALA:HB2	1.98	0.97
2:l:42:TYR:CZ	2:n:129:ALA:HA	2.00	0.96
2:g:42:TYR:CZ	2:o:129:ALA:HA	2.00	0.96
2:e:42:TYR:CZ	2:l:12:ALA:C	2.43	0.96
1:T:453:GLU:CG	1:N:372:LYS:HD2	1.96	0.96
1:E:453:GLU:HB3	1:E:454:PRO:HD2	1.46	0.96
2:e:42:TYR:CE1	2:l:13:PRO:HD2	1.99	0.96
2:v:132:THR:HG21	2:o:35:ILE:HG21	1.48	0.96
1:G:453:GLU:CB	1:G:454:PRO:CD	2.40	0.96
1:U:452:PHE:HA	1:O:372:LYS:HE3	1.48	0.96
1:A:453:GLU:HB3	1:A:454:PRO:CD	1.94	0.95
1:H:453:GLU:CB	1:H:454:PRO:CD	2.39	0.95
2:m:94:ARG:HG2	2:m:115:ARG:HB3	1.49	0.95
2:b:42:TYR:CZ	2:i:12:ALA:C	2.44	0.95
1:L:453:GLU:CB	1:L:454:PRO:CD	2.39	0.94
2:j:6:PRO:HA	2:d:53:ASN:HD21	1.31	0.94
1:T:452:PHE:HA	1:N:372:LYS:HE3	1.48	0.94
2:p:35:ILE:HG21	2:w:132:THR:CG2	1.98	0.94
2:q:129:ALA:H	2:i:42:TYR:HE1	1.14	0.94
2:p:129:ALA:HB2	2:h:42:TYR:CE1	2.02	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:k:42:TYR:CE1	2:m:129:ALA:HB2	2.02	0.94
2:a:42:TYR:CZ	2:h:12:ALA:C	2.46	0.93
2:p:129:ALA:HA	2:h:42:TYR:CZ	2.03	0.93
1:S:452:PHE:HA	1:M:372:LYS:HE3	1.47	0.93
1:V:452:PHE:HA	1:P:372:LYS:CE	1.99	0.93
2:e:114:LEU:HD23	2:e:145:GLU:HB3	1.50	0.93
1:K:453:GLU:HB3	1:K:454:PRO:HD3	1.51	0.93
2:a:42:TYR:CE1	2:h:13:PRO:HD2	2.02	0.93
1:T:273:ALA:CA	1:T:276:ARG:HE	1.81	0.93
2:e:42:TYR:HE1	2:l:12:ALA:HA	0.90	0.93
1:T:273:ALA:CB	1:T:276:ARG:HE	1.80	0.93
2:j:42:TYR:CE1	2:r:129:ALA:CB	2.52	0.93
2:q:35:ILE:HG21	2:x:132:THR:HG21	1.50	0.92
2:g:6:PRO:HA	2:a:53:ASN:HD21	1.32	0.92
2:h:6:PRO:HA	2:b:53:ASN:HD21	1.33	0.92
1:S:4:TYR:HB3	1:S:509:VAL:HB	1.50	0.92
2:k:42:TYR:CZ	2:m:129:ALA:HA	2.03	0.92
1:F:453:GLU:HB3	1:F:454:PRO:HD2	1.51	0.92
1:S:514:ILE:HG22	1:S:516:PRO:HD2	1.52	0.92
2:v:132:THR:CG2	2:o:35:ILE:HG21	2.00	0.92
2:i:6:PRO:HA	2:c:53:ASN:HD21	1.33	0.92
1:Q:40:ALA:HB3	1:Q:89:ARG:HG3	1.49	0.92
2:l:42:TYR:CE1	2:n:129:ALA:CB	2.53	0.92
1:W:453:GLU:HG2	1:Q:372:LYS:HB2	1.52	0.92
2:l:6:PRO:HA	2:f:53:ASN:HD21	1.32	0.92
1:I:453:GLU:CB	1:I:454:PRO:CD	2.40	0.92
1:K:453:GLU:CB	1:K:454:PRO:CD	2.39	0.91
2:b:42:TYR:CZ	2:i:12:ALA:HA	2.03	0.91
1:W:452:PHE:HA	1:Q:372:LYS:CE	2.01	0.91
2:g:42:TYR:CE1	2:o:129:ALA:CB	2.53	0.91
2:k:6:PRO:HA	2:e:53:ASN:HD21	1.32	0.91
2:p:94:ARG:HH21	2:p:115:ARG:HD3	1.33	0.91
2:p:85:SER:HB3	2:o:34:GLN:NE2	1.85	0.91
1:C:453:GLU:HB3	1:C:454:PRO:HD2	1.51	0.90
1:J:54:TRP:CH2	1:J:75:TYR:OH	2.22	0.90
1:A:453:GLU:HB3	1:A:454:PRO:HD2	1.51	0.90
1:X:452:PHE:HA	1:R:372:LYS:HE3	1.51	0.90
1:D:453:GLU:HB3	1:D:454:PRO:HD2	1.51	0.90
1:L:453:GLU:HB3	1:L:454:PRO:HD3	1.53	0.90
2:l:42:TYR:CE1	2:n:129:ALA:HA	2.03	0.90
2:j:42:TYR:CE1	2:r:129:ALA:HA	2.03	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:42:TYR:CZ	2:l:12:ALA:HA	2.01	0.90
1:J:453:GLU:HB3	1:J:454:PRO:HD3	1.54	0.90
2:g:42:TYR:CE1	2:o:129:ALA:HA	2.04	0.90
1:S:1:MET:HA	1:S:518:LYS:HA	1.50	0.89
2:f:114:LEU:HD23	2:f:145:GLU:HB3	1.55	0.89
1:T:453:GLU:HB3	1:T:454:PRO:HD2	1.51	0.89
1:W:453:GLU:HB3	1:W:454:PRO:HD2	1.54	0.89
2:q:35:ILE:HG21	2:x:132:THR:CG2	2.03	0.89
2:a:42:TYR:CZ	2:h:12:ALA:HA	2.07	0.89
1:W:453:GLU:CG	1:Q:372:LYS:HD2	2.03	0.88
2:r:34:GLN:HE21	2:m:120:SER:HB2	1.37	0.88
1:B:453:GLU:HB3	1:B:454:PRO:HD2	1.52	0.88
1:I:453:GLU:HB3	1:I:454:PRO:HD3	1.54	0.88
1:K:61:PHE:CZ	1:K:87:VAL:HG11	2.08	0.88
1:X:453:GLU:HB3	1:X:454:PRO:HD2	1.52	0.88
1:G:453:GLU:HB3	1:G:454:PRO:HD3	1.53	0.88
1:H:453:GLU:HB3	1:H:454:PRO:HD3	1.52	0.88
1:V:469:ALA:HB3	2:p:94:ARG:HH22	1.35	0.88
2:n:35:ILE:HG21	2:u:132:THR:HG21	1.56	0.88
1:J:453:GLU:CB	1:J:454:PRO:CD	2.40	0.88
1:V:453:GLU:CB	1:V:454:PRO:CD	2.52	0.87
1:K:338:ILE:HD12	1:K:356:HIS:HE1	1.39	0.87
2:k:42:TYR:CE1	2:m:129:ALA:CB	2.57	0.87
1:S:453:GLU:HB3	1:S:454:PRO:HD2	1.52	0.87
2:a:42:TYR:HE1	2:h:12:ALA:HA	0.86	0.87
1:T:273:ALA:HA	1:T:276:ARG:HE	1.39	0.87
1:V:469:ALA:CB	2:p:94:ARG:NH2	2.37	0.87
2:a:114:LEU:HD23	2:a:145:GLU:HB3	1.55	0.87
2:b:42:TYR:HE1	2:i:12:ALA:HA	0.88	0.87
1:U:453:GLU:HB3	1:U:454:PRO:HD2	1.56	0.87
2:w:34:GLN:NE2	2:w:57:MET:SD	2.47	0.87
2:k:42:TYR:CE1	2:m:129:ALA:HA	2.06	0.87
1:J:54:TRP:CZ2	1:J:75:TYR:OH	2.27	0.87
1:N:270:LEU:CD1	1:N:284:VAL:HG13	2.04	0.87
2:p:129:ALA:CB	2:h:42:TYR:CE1	2.58	0.86
1:E:453:GLU:HB3	1:E:454:PRO:CD	2.04	0.86
2:p:129:ALA:HA	2:h:42:TYR:CE1	2.07	0.86
1:W:469:ALA:CB	2:q:94:ARG:NH2	2.38	0.86
1:I:338:ILE:HD12	1:I:356:HIS:HE1	1.39	0.86
1:W:453:GLU:CB	1:W:454:PRO:HD3	2.03	0.86
2:b:42:TYR:OH	2:i:12:ALA:O	1.92	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:452:PHE:HA	1:M:372:LYS:CE	2.06	0.85
2:m:44:GLN:O	2:m:46:GLN:HG2	1.77	0.85
2:d:42:TYR:HE1	2:k:12:ALA:HA	0.91	0.85
1:X:469:ALA:CB	2:r:94:ARG:NH2	2.39	0.85
1:U:452:PHE:HA	1:O:372:LYS:CE	2.06	0.85
1:U:469:ALA:CB	2:o:94:ARG:NH2	2.39	0.85
2:e:42:TYR:OH	2:l:12:ALA:O	1.93	0.84
2:r:44:GLN:O	2:r:46:GLN:HG2	1.77	0.84
1:A:307:PRO:HB2	1:A:311:GLN:HE22	1.40	0.84
2:n:44:GLN:O	2:n:46:GLN:HG2	1.78	0.84
2:o:44:GLN:O	2:o:46:GLN:HG2	1.77	0.84
2:x:7:GLU:OE2	2:s:70:ARG:HG2	1.77	0.84
1:G:338:ILE:HD12	1:G:356:HIS:HE1	1.41	0.84
2:n:94:ARG:HG2	2:n:115:ARG:HB3	1.60	0.84
2:p:44:GLN:O	2:p:46:GLN:HG2	1.76	0.84
2:q:44:GLN:O	2:q:46:GLN:HG2	1.77	0.83
2:n:35:ILE:HG21	2:u:132:THR:CG2	2.07	0.83
1:U:469:ALA:CB	2:o:94:ARG:HH22	1.91	0.83
1:G:61:PHE:CE2	1:G:87:VAL:HG11	2.13	0.83
1:U:466:ASN:HA	2:o:94:ARG:HH21	1.43	0.83
1:T:452:PHE:HA	1:N:372:LYS:CE	2.09	0.82
1:J:61:PHE:CE1	1:J:87:VAL:HG11	2.13	0.82
1:X:469:ALA:CB	2:r:94:ARG:HH22	1.92	0.82
1:W:469:ALA:CB	2:q:94:ARG:HH22	1.91	0.82
1:K:61:PHE:CE2	1:K:87:VAL:HG11	2.15	0.82
1:X:453:GLU:CB	1:X:454:PRO:HD3	2.05	0.82
1:N:270:LEU:HD11	1:N:284:VAL:HG13	1.61	0.81
2:q:128:LYS:C	2:i:42:TYR:OH	2.22	0.81
1:H:61:PHE:CE1	1:H:87:VAL:HG11	2.16	0.81
1:B:307:PRO:HB2	1:B:311:GLN:HE22	1.45	0.81
2:l:6:PRO:HA	2:f:53:ASN:ND2	1.95	0.81
2:a:42:TYR:CZ	2:h:12:ALA:HB1	2.15	0.81
1:C:237:HIS:CG	1:C:238:PRO:HD3	2.15	0.81
2:o:94:ARG:HB3	2:o:94:ARG:HH11	1.46	0.81
1:L:61:PHE:CE1	1:L:87:VAL:HG11	2.14	0.81
1:D:237:HIS:CG	1:D:238:PRO:HD3	2.15	0.81
2:r:94:ARG:HB3	2:r:94:ARG:HH11	1.45	0.81
1:B:237:HIS:CG	1:B:238:PRO:HD3	2.15	0.81
2:q:94:ARG:HB3	2:q:94:ARG:HH11	1.45	0.81
1:F:237:HIS:CG	1:F:238:PRO:HD3	2.15	0.81
2:e:42:TYR:CZ	2:l:12:ALA:HB1	2.15	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:94:ARG:HG2	2:m:115:ARG:CB	2.11	0.80
2:b:42:TYR:CZ	2:i:12:ALA:HB1	2.16	0.80
2:g:6:PRO:HA	2:a:53:ASN:ND2	1.95	0.80
2:h:6:PRO:HA	2:b:53:ASN:ND2	1.95	0.80
1:E:307:PRO:HB2	1:E:311:GLN:HE22	1.45	0.80
1:H:243:TYR:HB3	1:H:251:THR:O	1.81	0.80
2:i:6:PRO:HA	2:c:53:ASN:ND2	1.95	0.80
2:k:6:PRO:HA	2:e:53:ASN:ND2	1.95	0.80
2:j:6:PRO:HA	2:d:53:ASN:ND2	1.95	0.80
1:E:237:HIS:CG	1:E:238:PRO:HD3	2.15	0.80
1:W:469:ALA:HB2	2:q:94:ARG:NH2	1.97	0.80
2:p:34:GLN:OE1	2:q:118:TRP:HZ2	1.65	0.79
1:A:237:HIS:CG	1:A:238:PRO:HD3	2.15	0.79
2:r:34:GLN:CD	2:m:118:TRP:CZ2	2.60	0.79
1:V:453:GLU:HG2	1:V:454:PRO:HD3	0.82	0.79
1:X:452:PHE:HA	1:R:372:LYS:CE	2.11	0.79
1:B:80:ASN:HD21	1:B:380:ARG:HB2	1.47	0.79
1:S:512:ILE:HG22	1:S:513:GLY:H	1.47	0.79
2:r:34:GLN:CD	2:m:118:TRP:HZ2	1.91	0.79
1:S:465:ARG:HH21	2:m:94:ARG:HH21	1.28	0.79
1:T:273:ALA:HB2	1:T:276:ARG:HE	1.47	0.79
2:d:116:ASN:HD21	2:d:145:GLU:H	1.30	0.78
1:V:452:PHE:CZ	1:V:507:ARG:HD2	2.18	0.78
1:V:453:GLU:CG	1:V:454:PRO:HD2	2.11	0.78
1:X:466:ASN:HA	2:r:94:ARG:HH21	1.48	0.78
2:d:42:TYR:CZ	2:k:12:ALA:C	2.42	0.78
1:E:68:TYR:CE2	1:E:70:LEU:HD13	2.19	0.78
1:F:68:TYR:CE2	1:F:70:LEU:HD13	2.19	0.78
1:V:452:PHE:CE1	1:V:507:ARG:HD3	2.14	0.77
1:C:68:TYR:CE2	1:C:70:LEU:HD13	2.19	0.77
1:D:68:TYR:CE2	1:D:70:LEU:HD13	2.19	0.77
2:n:94:ARG:HG2	2:n:115:ARG:CB	2.15	0.77
1:B:68:TYR:CE2	1:B:70:LEU:HD13	2.19	0.77
1:A:68:TYR:CE2	1:A:70:LEU:HD13	2.19	0.77
2:p:34:GLN:HE21	2:q:82:ILE:HD11	1.50	0.77
2:j:42:TYR:HE1	2:r:129:ALA:H	1.33	0.76
2:q:129:ALA:HA	2:i:42:TYR:OH	1.85	0.76
1:W:466:ASN:HA	2:q:94:ARG:HH21	1.49	0.76
1:U:469:ALA:HB2	2:o:94:ARG:NH2	2.01	0.76
2:p:34:GLN:OE1	2:q:118:TRP:CZ2	2.39	0.76
2:l:42:TYR:HE1	2:n:129:ALA:H	1.33	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:236:ALA:HA	1:S:241:ALA:HB3	1.68	0.75
2:e:42:TYR:CZ	2:l:12:ALA:CB	2.66	0.75
2:m:34:GLN:HB3	2:n:120:SER:O	1.86	0.75
1:I:243:TYR:HB3	1:I:251:THR:O	1.86	0.75
2:r:34:GLN:NE2	2:m:118:TRP:CZ2	2.54	0.75
1:K:338:ILE:CD1	1:K:356:HIS:HE1	2.00	0.75
2:a:42:TYR:OH	2:h:12:ALA:O	1.94	0.75
1:K:243:TYR:HB3	1:K:251:THR:O	1.88	0.74
1:U:469:ALA:HB3	2:o:94:ARG:NH2	2.02	0.74
1:G:243:TYR:HB3	1:G:251:THR:O	1.86	0.74
1:I:338:ILE:CD1	1:I:356:HIS:HE1	2.00	0.74
1:V:4:TYR:HE1	1:V:443:ILE:HG21	1.52	0.74
1:T:452:PHE:CA	1:N:372:LYS:HE3	2.17	0.74
1:X:469:ALA:HB3	2:r:94:ARG:NH2	2.03	0.73
1:U:4:TYR:HE1	1:U:443:ILE:HG21	1.53	0.73
1:F:505:LEU:HD13	1:F:507:ARG:HH21	1.52	0.73
1:A:68:TYR:HE2	1:A:70:LEU:HD13	1.53	0.73
1:S:453:GLU:HG2	1:M:372:LYS:HB2	1.71	0.73
1:G:338:ILE:CD1	1:G:356:HIS:HE1	2.01	0.73
1:T:273:ALA:HB2	1:T:276:ARG:NE	2.02	0.73
2:q:94:ARG:NH1	2:q:115:ARG:HB3	2.04	0.73
1:T:234:GLU:O	1:T:279:ILE:HG21	1.89	0.73
2:r:94:ARG:HH11	2:r:115:ARG:HB3	1.53	0.73
2:r:94:ARG:NH1	2:r:115:ARG:HB3	2.03	0.73
2:d:100:ILE:HG21	2:d:104:TYR:HA	1.70	0.73
2:q:94:ARG:HH11	2:q:115:ARG:HB3	1.54	0.73
1:X:469:ALA:HB2	2:r:94:ARG:NH2	1.98	0.73
1:W:469:ALA:HB3	2:q:94:ARG:NH2	2.04	0.72
1:B:68:TYR:HE2	1:B:70:LEU:HD13	1.54	0.72
2:p:34:GLN:HE21	2:q:82:ILE:CD1	2.02	0.72
1:W:4:TYR:HE1	1:W:443:ILE:HG21	1.54	0.72
2:k:42:TYR:HE1	2:m:129:ALA:H	1.36	0.72
1:J:243:TYR:HB3	1:J:251:THR:O	1.90	0.72
2:o:94:ARG:NH1	2:o:115:ARG:HB3	2.05	0.72
1:U:452:PHE:HA	1:O:372:LYS:NZ	2.05	0.72
2:o:114:LEU:HD23	2:o:145:GLU:HB2	1.71	0.72
1:X:4:TYR:HE1	1:X:443:ILE:HG21	1.53	0.72
2:g:42:TYR:HE1	2:o:129:ALA:H	1.34	0.72
2:p:129:ALA:H	2:h:42:TYR:HE1	1.37	0.72
1:D:68:TYR:HE2	1:D:70:LEU:HD13	1.54	0.72
2:n:114:LEU:HD23	2:n:145:GLU:HB2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:o:94:ARG:HH11	2:o:115:ARG:HB3	1.55	0.72
1:Q:270:LEU:HD12	1:Q:284:VAL:HG13	1.72	0.71
2:c:100:ILE:HG21	2:c:104:TYR:HA	1.72	0.71
1:V:465:ARG:HG3	2:p:94:ARG:HH12	1.55	0.71
2:q:114:LEU:HD23	2:q:145:GLU:HB2	1.71	0.71
1:F:69:TYR:HA	1:F:72:HIS:ND1	2.05	0.71
2:m:114:LEU:HD23	2:m:145:GLU:HB2	1.71	0.71
1:T:4:TYR:HE1	1:T:443:ILE:HG21	1.54	0.71
1:H:453:GLU:HG2	1:B:372:LYS:HD2	1.72	0.71
1:B:69:TYR:HA	1:B:72:HIS:ND1	2.04	0.71
1:V:469:ALA:HB3	2:p:94:ARG:NH2	2.00	0.71
1:D:40:ALA:HB3	1:D:89:ARG:HD2	1.71	0.71
1:D:69:TYR:HA	1:D:72:HIS:ND1	2.05	0.71
1:B:463:ILE:HG21	1:B:509:VAL:HG21	1.72	0.71
2:b:116:ASN:HD21	2:b:145:GLU:HB3	1.55	0.71
1:D:454:PRO:O	1:D:456:ASP:N	2.24	0.71
1:K:338:ILE:HD12	1:K:356:HIS:CE1	2.25	0.71
1:S:469:ALA:CB	2:m:94:ARG:NH1	2.54	0.71
2:f:100:ILE:HG21	2:f:104:TYR:HA	1.70	0.71
1:G:46:ASN:HB2	1:G:251:THR:HG21	1.72	0.71
2:o:94:ARG:HD2	2:o:115:ARG:HB3	1.72	0.71
1:V:469:ALA:HB2	2:p:94:ARG:HH22	1.55	0.71
1:M:270:LEU:CD1	1:M:284:VAL:HG13	2.21	0.71
1:U:452:PHE:CA	1:O:372:LYS:HE3	2.21	0.71
1:O:270:LEU:CD1	1:O:284:VAL:HG13	2.21	0.71
1:Q:463:ILE:HD11	1:Q:507:ARG:CZ	2.21	0.71
1:E:69:TYR:HA	1:E:72:HIS:ND1	2.04	0.71
1:B:454:PRO:O	1:B:456:ASP:N	2.23	0.71
2:q:94:ARG:HD2	2:q:115:ARG:HB3	1.73	0.71
1:F:68:TYR:HE2	1:F:70:LEU:HD13	1.53	0.71
1:A:454:PRO:O	1:A:456:ASP:N	2.23	0.71
2:a:42:TYR:CZ	2:h:12:ALA:CB	2.69	0.71
2:r:114:LEU:HD23	2:r:145:GLU:HB2	1.71	0.71
1:L:243:TYR:HB3	1:L:251:THR:O	1.91	0.71
2:f:42:TYR:CE1	2:g:13:PRO:CD	2.73	0.71
2:p:114:LEU:HD23	2:p:145:GLU:HB2	1.71	0.70
1:W:452:PHE:HA	1:Q:372:LYS:NZ	2.05	0.70
1:S:452:PHE:HA	1:M:372:LYS:NZ	2.05	0.70
1:C:69:TYR:HA	1:C:72:HIS:ND1	2.06	0.70
1:F:454:PRO:O	1:F:456:ASP:N	2.23	0.70
1:V:72:HIS:HD2	1:V:351:VAL:HG11	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:453:GLU:HG2	1:E:372:LYS:HD2	1.72	0.70
2:r:34:GLN:NE2	2:m:120:SER:HB2	2.07	0.70
1:A:69:TYR:HA	1:A:72:HIS:ND1	2.06	0.70
1:R:270:LEU:HD12	1:R:284:VAL:HG13	1.73	0.70
1:I:453:GLU:HG2	1:C:372:LYS:HD2	1.73	0.70
1:E:68:TYR:HE2	1:E:70:LEU:HD13	1.53	0.70
1:K:338:ILE:CD1	1:K:356:HIS:CE1	2.74	0.70
2:r:94:ARG:HD2	2:r:115:ARG:HB3	1.73	0.70
1:W:72:HIS:HD2	1:W:351:VAL:HG11	1.56	0.70
2:q:129:ALA:N	2:i:42:TYR:CZ	2.58	0.70
1:X:72:HIS:HD2	1:X:351:VAL:HG11	1.56	0.70
1:X:452:PHE:CA	1:R:372:LYS:HE3	2.20	0.70
1:U:72:HIS:HD2	1:U:351:VAL:HG11	1.56	0.70
1:C:68:TYR:HE2	1:C:70:LEU:HD13	1.54	0.69
1:S:469:ALA:HB1	2:m:94:ARG:NH1	2.07	0.69
1:K:46:ASN:HB2	1:K:251:THR:HG21	1.74	0.69
1:V:453:GLU:HG2	1:V:454:PRO:HD2	1.67	0.69
1:P:274:TYR:HA	1:P:279:ILE:O	1.92	0.69
2:q:128:LYS:O	2:i:42:TYR:OH	2.09	0.69
1:C:454:PRO:O	1:C:456:ASP:N	2.23	0.69
1:J:46:ASN:HB2	1:J:251:THR:HG21	1.74	0.69
2:p:34:GLN:NE2	2:q:82:ILE:HD12	2.07	0.69
1:S:72:HIS:HD2	1:S:351:VAL:HG11	1.56	0.69
1:G:453:GLU:HG2	1:A:372:LYS:HD2	1.73	0.69
1:V:452:PHE:HZ	1:V:507:ARG:HD3	0.55	0.69
2:j:13:PRO:CD	2:c:42:TYR:CE1	2.73	0.69
1:S:465:ARG:NH2	2:m:94:ARG:HH22	1.90	0.69
1:N:274:TYR:HA	1:N:279:ILE:O	1.92	0.69
1:T:72:HIS:HD2	1:T:351:VAL:HG11	1.56	0.69
1:I:338:ILE:CD1	1:I:356:HIS:CE1	2.76	0.69
1:T:273:ALA:CB	1:T:276:ARG:NE	2.54	0.68
2:p:15:PHE:H	2:i:45:ASN:CG	2.00	0.68
1:Q:273:ALA:HB1	1:Q:279:ILE:HD12	1.76	0.68
2:f:57:MET:HG2	2:a:118:TRP:CZ2	2.29	0.68
1:S:452:PHE:CA	1:M:372:LYS:HE3	2.21	0.68
1:O:274:TYR:HA	1:O:279:ILE:O	1.94	0.68
1:J:453:GLU:HG2	1:D:372:LYS:HD2	1.73	0.68
1:L:453:GLU:HG2	1:F:372:LYS:HD2	1.73	0.68
2:w:34:GLN:CD	2:x:118:TRP:HZ3	2.02	0.68
1:L:46:ASN:HB2	1:L:251:THR:HG21	1.75	0.68
1:V:452:PHE:CA	1:P:372:LYS:HE3	2.19	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:476:ARG:O	2:i:43:GLN:OE1	2.12	0.68
2:t:5:LYS:HZ1	2:n:51:ARG:HH21	1.41	0.68
1:H:61:PHE:CZ	1:H:87:VAL:HG11	2.29	0.68
1:M:274:TYR:HA	1:M:279:ILE:O	1.93	0.67
1:G:61:PHE:CZ	1:G:87:VAL:HG11	2.29	0.67
1:W:453:GLU:HG3	1:Q:372:LYS:CD	2.19	0.67
2:p:118:TRP:HZ2	2:o:34:GLN:NE2	1.93	0.67
2:j:43:GLN:OE1	1:Q:476:ARG:O	2.12	0.67
2:d:100:ILE:CG2	2:d:104:TYR:HA	2.24	0.67
1:W:452:PHE:CA	1:Q:372:LYS:HE3	2.22	0.67
1:K:61:PHE:CZ	1:K:87:VAL:CG1	2.77	0.67
2:g:43:GLN:OE1	1:N:476:ARG:O	2.12	0.67
1:W:452:PHE:CE2	1:W:507:ARG:CD	2.78	0.67
1:S:5:LEU:HD13	1:S:508:VAL:HG22	1.76	0.67
1:C:41:PRO:HB3	1:C:94:ALA:O	1.95	0.67
2:r:84:ASP:HA	2:r:89:ARG:HH21	1.61	0.66
2:h:43:GLN:OE1	1:O:476:ARG:O	2.13	0.66
2:b:11:VAL:HG21	2:b:102:MET:N	2.03	0.66
1:I:46:ASN:HB2	1:I:251:THR:HG21	1.75	0.66
1:W:234:GLU:O	1:W:279:ILE:HG21	1.96	0.66
1:T:273:ALA:HA	1:T:276:ARG:NE	2.08	0.66
1:N:368:ARG:HB3	1:N:371:HIS:HE1	1.60	0.66
1:U:234:GLU:O	1:U:279:ILE:HG21	1.96	0.66
1:V:452:PHE:HA	1:P:372:LYS:NZ	2.09	0.66
1:Q:89:ARG:HB3	1:Q:89:ARG:HH11	1.61	0.66
1:G:338:ILE:CD1	1:G:356:HIS:CE1	2.78	0.66
2:a:114:LEU:HD22	2:a:146:LEU:HB3	1.77	0.66
2:b:42:TYR:CE1	2:i:13:PRO:CD	2.77	0.66
1:I:338:ILE:HD12	1:I:356:HIS:CE1	2.27	0.66
2:l:43:GLN:OE1	1:M:476:ARG:O	2.13	0.66
1:E:41:PRO:HB3	1:E:94:ALA:O	1.96	0.66
1:X:234:GLU:O	1:X:279:ILE:HG21	1.96	0.66
2:a:116:ASN:HD21	2:a:145:GLU:HB3	1.60	0.66
2:n:34:GLN:NE2	2:o:85:SER:HB3	2.06	0.66
2:p:120:SER:HB3	2:p:143:PHE:HE1	1.61	0.66
2:f:116:ASN:HD21	2:f:145:GLU:HB2	1.61	0.66
2:m:33:LEU:HD23	2:m:61:ALA:HB2	1.78	0.66
2:p:34:GLN:NE2	2:q:82:ILE:CD1	2.58	0.65
2:k:43:GLN:OE1	1:R:476:ARG:O	2.13	0.65
1:V:234:GLU:O	1:V:279:ILE:HG21	1.96	0.65
2:e:42:TYR:CE1	2:l:13:PRO:CD	2.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:273:ALA:HB1	1:R:279:ILE:HD12	1.78	0.65
2:b:92:THR:HB	2:b:115:ARG:O	1.96	0.65
1:U:453:GLU:HG2	1:O:372:LYS:HD2	1.78	0.65
1:D:80:ASN:HB3	1:D:359:GLY:HA3	1.77	0.65
1:L:244:LEU:HD12	1:L:249:ASP:HA	1.78	0.65
1:X:452:PHE:CE2	1:X:507:ARG:CD	2.79	0.65
1:P:329:LYS:HB3	1:P:433:ARG:HE	1.62	0.65
2:d:57:MET:HG2	2:e:118:TRP:CZ2	2.31	0.65
1:R:329:LYS:HB3	1:R:433:ARG:HE	1.61	0.65
2:d:42:TYR:OH	2:k:12:ALA:O	1.93	0.65
1:Q:329:LYS:HB3	1:Q:433:ARG:HE	1.61	0.65
2:e:57:MET:HG2	2:f:118:TRP:CZ2	2.31	0.65
2:m:93:ALA:O	2:m:117:ALA:HB3	1.97	0.65
2:p:22:VAL:O	2:i:44:GLN:HA	1.97	0.65
2:r:93:ALA:O	2:r:117:ALA:HB3	1.97	0.65
2:q:34:GLN:HE21	2:r:82:ILE:HD11	1.62	0.64
1:B:307:PRO:HB2	1:B:311:GLN:NE2	2.12	0.64
2:p:93:ALA:O	2:p:117:ALA:HB3	1.97	0.64
2:w:34:GLN:CD	2:x:118:TRP:CZ3	2.75	0.64
2:q:93:ALA:O	2:q:117:ALA:HB3	1.97	0.64
1:S:452:PHE:CE2	1:S:507:ARG:CD	2.79	0.64
2:m:120:SER:HB3	2:m:143:PHE:HE1	1.62	0.64
2:p:22:VAL:O	2:i:44:GLN:CA	2.45	0.64
2:d:116:ASN:HD21	2:d:145:GLU:N	1.95	0.64
1:S:453:GLU:CB	1:S:454:PRO:HD2	2.20	0.64
1:V:453:GLU:CB	1:V:454:PRO:HD2	2.26	0.64
1:U:453:GLU:HG2	1:O:372:LYS:HB2	1.78	0.64
2:o:93:ALA:O	2:o:117:ALA:HB3	1.97	0.64
2:q:34:GLN:OE1	2:r:85:SER:HB3	1.98	0.64
1:H:279:ILE:HG22	1:H:284:VAL:HG23	1.78	0.64
2:f:100:ILE:CG2	2:f:104:TYR:HA	2.27	0.64
2:a:42:TYR:CE1	2:h:13:PRO:CD	2.80	0.64
2:f:116:ASN:HD21	2:f:145:GLU:CB	2.11	0.64
1:A:41:PRO:HB3	1:A:94:ALA:O	1.98	0.64
1:W:453:GLU:OE2	1:Q:371:HIS:CD2	2.51	0.64
1:E:307:PRO:HB2	1:E:311:GLN:NE2	2.12	0.64
1:G:279:ILE:HG22	1:G:284:VAL:HG23	1.78	0.64
2:n:120:SER:HB3	2:n:143:PHE:HE1	1.62	0.64
2:p:22:VAL:O	2:i:44:GLN:CB	2.45	0.64
2:n:93:ALA:O	2:n:117:ALA:HB3	1.97	0.64
2:p:23:MET:HG3	2:i:44:GLN:HG3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:r:94:ARG:HB3	2:r:94:ARG:NH1	2.13	0.63
1:S:237:HIS:CD2	1:S:238:PRO:HD3	2.33	0.63
1:G:338:ILE:HD12	1:G:356:HIS:CE1	2.29	0.63
1:T:453:GLU:CB	1:T:454:PRO:HD2	2.22	0.63
1:N:329:LYS:HB3	1:N:433:ARG:HE	1.64	0.63
1:B:505:LEU:HD22	1:B:507:ARG:HH12	1.61	0.63
2:r:120:SER:HB3	2:r:143:PHE:HE1	1.63	0.63
1:S:235:SER:H	1:S:238:PRO:HG2	1.64	0.63
1:O:329:LYS:HB3	1:O:433:ARG:HE	1.64	0.63
1:D:68:TYR:OH	1:D:269:ASP:HB3	1.99	0.63
1:F:68:TYR:OH	1:F:269:ASP:HB3	1.98	0.63
1:S:515:ALA:HB3	1:S:516:PRO:HD3	1.80	0.63
2:m:35:ILE:HD13	2:t:132:THR:HG21	1.81	0.63
2:e:34:GLN:NE2	2:f:118:TRP:CZ2	2.67	0.63
1:T:452:PHE:C	1:N:372:LYS:HE3	2.24	0.63
1:N:271:MET:HG3	1:N:306:ASP:HB2	1.80	0.63
1:O:454:PRO:HA	1:O:507:ARG:HH12	1.63	0.63
2:p:15:PHE:N	2:i:45:ASN:OD1	2.25	0.63
2:p:85:SER:CB	2:o:34:GLN:HE22	1.98	0.63
2:d:42:TYR:CE1	2:k:13:PRO:CD	2.78	0.63
1:L:61:PHE:CZ	1:L:87:VAL:HG11	2.32	0.63
1:V:465:ARG:HG3	2:p:94:ARG:NH1	2.12	0.63
2:a:5:LYS:N	2:a:6:PRO:HD2	2.14	0.63
1:T:72:HIS:CD2	1:T:351:VAL:HG21	2.34	0.63
2:e:5:LYS:N	2:e:6:PRO:HD2	2.14	0.63
1:U:452:PHE:CE2	1:U:507:ARG:CD	2.80	0.63
2:d:34:GLN:NE2	2:e:86:MET:HA	2.14	0.63
2:b:5:LYS:N	2:b:6:PRO:HD2	2.14	0.63
1:G:243:TYR:O	1:G:250:ARG:HB3	1.99	0.62
2:f:34:GLN:NE2	2:a:118:TRP:CZ2	2.67	0.62
1:B:68:TYR:OH	1:B:269:ASP:HB3	1.98	0.62
2:q:94:ARG:HB3	2:q:94:ARG:NH1	2.13	0.62
1:A:68:TYR:OH	1:A:269:ASP:HB3	1.99	0.62
1:E:68:TYR:OH	1:E:269:ASP:HB3	1.99	0.62
1:M:329:LYS:HB3	1:M:433:ARG:HE	1.64	0.62
2:m:94:ARG:CG	2:m:115:ARG:HB3	2.27	0.62
1:C:237:HIS:ND1	1:C:238:PRO:HD3	2.14	0.62
1:V:72:HIS:CD2	1:V:351:VAL:HG21	2.34	0.62
1:A:307:PRO:HB2	1:A:311:GLN:NE2	2.12	0.62
2:d:118:TRP:CZ2	2:c:57:MET:HG2	2.33	0.62
2:o:120:SER:HG	2:o:143:PHE:HE1	1.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:5:LYS:N	2:c:6:PRO:HD2	2.14	0.62
2:e:116:ASN:HD21	2:e:145:GLU:CB	2.12	0.62
1:S:3:SER:H	1:S:518:LYS:HB3	1.65	0.62
1:T:452:PHE:CE2	1:T:507:ARG:CD	2.81	0.62
1:H:368:ARG:HG3	1:H:372:LYS:HD2	1.81	0.62
1:U:72:HIS:CD2	1:U:351:VAL:HG21	2.34	0.62
2:o:94:ARG:HB3	2:o:94:ARG:NH1	2.14	0.62
1:C:68:TYR:OH	1:C:269:ASP:HB3	1.99	0.62
1:F:237:HIS:ND1	1:F:238:PRO:HD3	2.15	0.62
1:A:517:VAL:O	1:A:518:LYS:C	2.43	0.62
1:V:450:VAL:O	1:V:451:VAL:C	2.43	0.61
2:b:42:TYR:CZ	2:i:12:ALA:CB	2.68	0.61
1:W:450:VAL:O	1:W:451:VAL:C	2.43	0.61
2:w:34:GLN:OE1	2:x:118:TRP:HZ3	1.84	0.61
2:q:120:SER:HB3	2:q:143:PHE:HE1	1.64	0.61
1:F:517:VAL:O	1:F:518:LYS:C	2.43	0.61
1:S:450:VAL:O	1:S:451:VAL:C	2.43	0.61
1:C:517:VAL:O	1:C:518:LYS:C	2.43	0.61
1:W:72:HIS:CD2	1:W:351:VAL:HG21	2.34	0.61
1:X:453:GLU:CB	1:X:454:PRO:HD2	2.22	0.61
2:m:44:GLN:HB2	2:t:22:VAL:HG23	1.83	0.61
1:U:69:TYR:HD1	1:U:276:ARG:HH22	1.49	0.61
1:V:69:TYR:HD1	1:V:276:ARG:HH22	1.48	0.61
2:j:5:LYS:O	2:d:41:ARG:NH1	2.33	0.61
1:S:72:HIS:CD2	1:S:351:VAL:HG21	2.34	0.61
1:P:270:LEU:CD1	1:P:284:VAL:HG13	2.31	0.61
2:p:118:TRP:CZ2	2:o:34:GLN:NE2	2.68	0.61
1:D:517:VAL:O	1:D:518:LYS:C	2.43	0.61
2:m:33:LEU:HD23	2:m:61:ALA:CB	2.30	0.61
1:X:72:HIS:CD2	1:X:351:VAL:HG21	2.34	0.61
1:F:309:PRO:HA	1:F:337:TRP:CE2	2.36	0.61
1:N:273:ALA:HB1	1:N:279:ILE:HD12	1.81	0.61
1:V:453:GLU:HB3	1:V:454:PRO:HD2	1.80	0.61
1:D:237:HIS:ND1	1:D:238:PRO:HD3	2.15	0.61
1:R:69:TYR:CD1	1:R:272:ALA:HB2	2.35	0.61
1:A:237:HIS:ND1	1:A:238:PRO:HD3	2.15	0.61
2:h:5:LYS:O	2:b:41:ARG:NH1	2.33	0.61
2:q:44:GLN:HB2	2:x:22:VAL:HG23	1.83	0.61
1:E:237:HIS:ND1	1:E:238:PRO:HD3	2.15	0.61
1:X:452:PHE:C	1:R:372:LYS:HE3	2.26	0.61
1:F:41:PRO:HB3	1:F:94:ALA:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:309:PRO:HA	1:D:337:TRP:CE2	2.36	0.60
1:X:450:VAL:O	1:X:451:VAL:C	2.43	0.60
2:c:92:THR:HB	2:c:115:ARG:O	2.00	0.60
2:c:100:ILE:CG2	2:c:104:TYR:HA	2.30	0.60
1:L:365:ASP:HA	1:L:369:GLY:HA2	1.83	0.60
2:a:116:ASN:HD21	2:a:145:GLU:CB	2.14	0.60
1:T:450:VAL:O	1:T:451:VAL:C	2.43	0.60
2:p:44:GLN:HB2	2:w:22:VAL:HG23	1.82	0.60
1:S:2:PRO:HD2	1:S:518:LYS:HG2	1.81	0.60
2:k:5:LYS:O	2:e:41:ARG:NH1	2.34	0.60
2:r:44:GLN:HB2	2:s:22:VAL:HG23	1.84	0.60
2:n:42:TYR:CE1	2:u:12:ALA:HB1	2.36	0.60
2:n:44:GLN:HB2	2:u:22:VAL:HG23	1.83	0.60
2:n:84:ASP:HA	2:n:89:ARG:HH21	1.66	0.60
1:B:517:VAL:O	1:B:518:LYS:C	2.43	0.60
2:v:22:VAL:HG23	2:o:44:GLN:HB2	1.83	0.60
1:Q:467:VAL:HG12	1:Q:489:TYR:HH	1.65	0.60
1:E:517:VAL:O	1:E:518:LYS:C	2.43	0.60
1:S:236:ALA:HA	1:S:241:ALA:CB	2.31	0.60
2:a:115:ARG:C	2:a:117:ALA:H	2.08	0.60
2:q:34:GLN:HE21	2:r:82:ILE:CD1	2.15	0.60
1:S:69:TYR:HD1	1:S:276:ARG:HH22	1.49	0.60
1:X:452:PHE:HZ	1:X:507:ARG:HD3	0.61	0.60
1:U:450:VAL:O	1:U:451:VAL:C	2.43	0.60
2:c:116:ASN:O	2:c:117:ALA:C	2.44	0.60
1:C:309:PRO:HA	1:C:337:TRP:CE2	2.36	0.60
2:p:42:TYR:CE1	2:w:12:ALA:HB1	2.37	0.60
1:P:270:LEU:C	1:P:272:ALA:H	2.10	0.59
1:K:61:PHE:HZ	1:K:87:VAL:CG1	2.15	0.59
1:X:69:TYR:HD1	1:X:276:ARG:HH22	1.49	0.59
2:r:35:ILE:HD13	2:s:132:THR:HG21	1.85	0.59
2:a:53:ASN:ND2	2:a:56:LEU:HD21	2.18	0.59
2:b:57:MET:HG2	2:c:118:TRP:CZ2	2.37	0.59
1:W:69:TYR:HD1	1:W:276:ARG:HH22	1.49	0.59
1:S:490:TYR:HB3	1:S:512:ILE:HB	1.85	0.59
2:o:27:LEU:HD12	2:o:66:VAL:O	2.03	0.59
1:Q:41:PRO:HG3	1:Q:66:GLY:HA3	1.84	0.59
1:R:368:ARG:HB3	1:R:371:HIS:HE1	1.67	0.59
2:l:5:LYS:O	2:f:41:ARG:NH1	2.34	0.59
1:M:467:VAL:HG12	1:M:489:TYR:HH	1.67	0.59
2:m:34:GLN:OE1	2:n:86:MET:HG2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:g:5:LYS:O	2:a:41:ARG:NH1	2.33	0.59
1:B:237:HIS:ND1	1:B:238:PRO:HD3	2.16	0.59
1:U:273:ALA:CB	1:U:276:ARG:HE	2.15	0.59
1:V:273:ALA:CB	1:V:276:ARG:HE	2.15	0.59
2:q:113:ASN:CG	2:q:144:GLU:HG2	2.28	0.59
1:X:273:ALA:CB	1:X:276:ARG:HE	2.16	0.59
2:r:9:VAL:O	2:r:11:VAL:HG23	2.03	0.59
1:S:273:ALA:HB2	1:S:276:ARG:HE	1.68	0.59
1:U:273:ALA:HB2	1:U:276:ARG:HE	1.67	0.59
2:q:9:VAL:O	2:q:11:VAL:HG23	2.03	0.59
2:f:53:ASN:ND2	2:f:56:LEU:HD21	2.18	0.59
2:v:5:LYS:HZ1	2:p:51:ARG:HH21	1.49	0.59
2:p:34:GLN:OE1	2:q:85:SER:HB3	2.01	0.59
1:X:273:ALA:HB2	1:X:276:ARG:HE	1.67	0.59
2:b:115:ARG:C	2:b:117:ALA:H	2.11	0.59
2:q:42:TYR:CE1	2:x:12:ALA:HB1	2.38	0.59
2:a:34:GLN:NE2	2:b:118:TRP:CZ2	2.69	0.59
1:B:501:GLU:HG3	1:B:503:VAL:H	1.67	0.59
2:b:34:GLN:NE2	2:c:118:TRP:CZ2	2.69	0.59
2:b:53:ASN:ND2	2:b:56:LEU:HD21	2.18	0.59
1:V:273:ALA:HB2	1:V:276:ARG:HE	1.67	0.59
2:v:5:LYS:NZ	2:p:51:ARG:HH21	1.99	0.59
2:p:113:ASN:CG	2:p:144:GLU:HG2	2.28	0.59
1:W:273:ALA:CB	1:W:276:ARG:HE	2.15	0.59
2:m:113:ASN:CG	2:m:144:GLU:HG2	2.28	0.59
1:T:453:GLU:CB	1:T:454:PRO:HD3	2.07	0.59
1:O:271:MET:HG3	1:O:306:ASP:HB2	1.85	0.59
2:v:12:ALA:HB1	2:o:42:TYR:CE1	2.38	0.59
1:D:77:PHE:CZ	1:D:82:GLY:HA3	2.38	0.59
2:r:113:ASN:CG	2:r:144:GLU:HG2	2.28	0.59
1:H:36:PHE:CE1	1:H:77:PHE:HE1	2.21	0.59
1:K:74:VAL:HG22	1:K:78:PHE:HE2	1.68	0.58
1:S:273:ALA:CB	1:S:276:ARG:HE	2.16	0.58
2:m:27:LEU:HD12	2:m:66:VAL:O	2.03	0.58
1:W:273:ALA:HB2	1:W:276:ARG:HE	1.67	0.58
1:R:316:ILE:O	1:R:320:ARG:HG3	2.03	0.58
2:t:5:LYS:NZ	2:n:51:ARG:HH21	1.99	0.58
2:n:113:ASN:CG	2:n:144:GLU:HG2	2.28	0.58
2:p:120:SER:O	2:o:34:GLN:HB3	2.03	0.58
1:J:74:VAL:HG22	1:J:78:PHE:HE2	1.69	0.58
1:S:453:GLU:HG2	1:M:372:LYS:HD2	1.82	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:n:9:VAL:O	2:n:11:VAL:HG23	2.03	0.58
2:n:27:LEU:HD12	2:n:66:VAL:O	2.04	0.58
1:I:36:PHE:CE1	1:I:77:PHE:HE1	2.22	0.58
2:c:53:ASN:ND2	2:c:56:LEU:HD21	2.18	0.58
1:R:41:PRO:HG3	1:R:66:GLY:HA3	1.86	0.58
1:G:453:GLU:CG	1:A:372:LYS:HD2	2.34	0.58
1:N:467:VAL:HG12	1:N:489:TYR:HH	1.68	0.58
2:o:113:ASN:CG	2:o:144:GLU:HG2	2.28	0.58
2:p:9:VAL:O	2:p:11:VAL:HG23	2.03	0.58
1:J:61:PHE:CZ	1:J:87:VAL:HG11	2.37	0.58
2:e:116:ASN:HD21	2:e:145:GLU:HB2	1.67	0.58
1:S:240:PRO:HB2	1:S:267:VAL:CG1	2.34	0.58
2:m:34:GLN:HB3	2:n:120:SER:CA	2.33	0.58
1:T:4:TYR:CE1	1:T:443:ILE:HG21	2.38	0.58
2:o:9:VAL:O	2:o:11:VAL:HG23	2.03	0.58
1:X:4:TYR:CD2	1:X:509:VAL:HB	2.39	0.58
2:m:9:VAL:O	2:m:11:VAL:HG23	2.02	0.58
2:q:34:GLN:NE2	2:r:82:ILE:HD12	2.19	0.58
2:e:53:ASN:ND2	2:e:56:LEU:HD21	2.18	0.58
2:m:42:TYR:CE1	2:t:12:ALA:HB1	2.38	0.58
1:U:4:TYR:CD2	1:U:509:VAL:HB	2.38	0.58
2:r:27:LEU:HD12	2:r:66:VAL:O	2.03	0.57
2:m:94:ARG:HA	2:m:115:ARG:HA	1.85	0.57
1:H:453:GLU:CG	1:B:372:LYS:HD2	2.34	0.57
2:o:94:ARG:HD2	2:o:115:ARG:CB	2.33	0.57
1:J:453:GLU:CG	1:D:372:LYS:HD2	2.33	0.57
1:N:41:PRO:HG3	1:N:66:GLY:HA3	1.86	0.57
1:C:453:GLU:CB	1:C:454:PRO:CD	2.73	0.57
1:V:452:PHE:HZ	1:V:507:ARG:NE	1.96	0.57
1:J:61:PHE:HE1	1:J:87:VAL:HG11	1.68	0.57
2:w:35:ILE:O	2:w:58:PRO:HD2	2.04	0.57
1:M:273:ALA:HB1	1:M:279:ILE:HD12	1.86	0.57
2:a:92:THR:HB	2:a:115:ARG:O	2.04	0.57
1:H:252:GLY:C	1:H:254:GLY:H	2.12	0.57
1:U:4:TYR:CE1	1:U:443:ILE:HG21	2.38	0.57
2:a:101:VAL:O	2:a:102:MET:C	2.47	0.57
2:d:118:TRP:CZ2	2:c:34:GLN:NE2	2.72	0.57
2:m:35:ILE:HG21	2:t:132:THR:HG22	1.81	0.57
1:I:243:TYR:O	1:I:250:ARG:HB3	2.05	0.57
1:W:4:TYR:CD2	1:W:509:VAL:HB	2.38	0.57
1:X:452:PHE:HA	1:R:372:LYS:NZ	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:453:GLU:HG2	1:R:372:LYS:HB2	1.85	0.57
2:m:34:GLN:CB	2:n:120:SER:O	2.53	0.57
1:T:273:ALA:HA	1:T:276:ARG:HG2	1.85	0.57
2:n:42:TYR:CE1	2:u:12:ALA:CB	2.88	0.57
2:i:5:LYS:O	2:c:41:ARG:NH1	2.34	0.57
2:q:27:LEU:HD12	2:q:66:VAL:O	2.04	0.57
1:W:453:GLU:CB	1:W:454:PRO:HD2	2.22	0.57
1:S:336:PRO:HB3	1:S:387:LEU:HB2	1.87	0.57
2:s:35:ILE:O	2:s:58:PRO:HD2	2.05	0.57
1:P:273:ALA:HB1	1:P:279:ILE:HD12	1.86	0.57
2:d:53:ASN:ND2	2:d:56:LEU:HD21	2.18	0.57
2:q:129:ALA:CA	2:i:42:TYR:OH	2.49	0.57
2:x:114:LEU:HD23	2:x:116:ASN:ND2	2.20	0.57
2:s:114:LEU:HD23	2:s:116:ASN:ND2	2.20	0.57
1:G:250:ARG:HH11	1:G:250:ARG:HA	1.69	0.57
1:A:505:LEU:HD21	1:A:507:ARG:HH21	1.69	0.57
1:T:4:TYR:CD2	1:T:509:VAL:HB	2.40	0.57
1:I:453:GLU:CG	1:C:372:LYS:HD2	2.35	0.57
2:f:114:LEU:HD12	2:f:115:ARG:H	1.70	0.56
2:a:100:ILE:HG21	2:a:104:TYR:HA	1.86	0.56
1:M:316:ILE:O	1:M:320:ARG:HG3	2.05	0.56
2:n:120:SER:CB	2:n:143:PHE:HE1	2.18	0.56
1:U:336:PRO:HB3	1:U:387:LEU:HB2	1.87	0.56
1:V:4:TYR:CD2	1:V:509:VAL:HB	2.39	0.56
1:V:4:TYR:CE1	1:V:443:ILE:HG21	2.37	0.56
1:V:449:TRP:C	1:V:452:PHE:CD2	2.83	0.56
2:v:35:ILE:O	2:v:58:PRO:HD2	2.05	0.56
2:v:114:LEU:HD23	2:v:116:ASN:ND2	2.19	0.56
2:p:120:SER:CB	2:p:143:PHE:HE1	2.17	0.56
2:e:114:LEU:HD12	2:e:115:ARG:H	1.71	0.56
1:L:74:VAL:HG22	1:L:78:PHE:HE2	1.70	0.56
1:M:271:MET:HG3	1:M:306:ASP:HB2	1.88	0.56
2:m:120:SER:CB	2:m:143:PHE:HE1	2.19	0.56
1:G:36:PHE:CE1	1:G:77:PHE:HE1	2.24	0.56
1:A:463:ILE:HG21	1:A:509:VAL:HG21	1.86	0.56
1:T:336:PRO:HB3	1:T:387:LEU:HB2	1.87	0.56
1:B:79:ASN:C	1:B:80:ASN:HD22	2.13	0.56
2:u:35:ILE:O	2:u:58:PRO:HD2	2.05	0.56
2:u:114:LEU:HD23	2:u:116:ASN:ND2	2.20	0.56
2:x:114:LEU:HD23	2:x:116:ASN:HD21	1.71	0.56
2:r:94:ARG:HD2	2:r:115:ARG:CB	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:452:PHE:HA	1:N:372:LYS:NZ	2.20	0.56
2:p:34:GLN:HB3	2:q:120:SER:O	2.04	0.56
2:p:94:ARG:HE	2:p:115:ARG:HB3	1.71	0.56
1:J:316:ILE:HD13	1:J:335:TYR:CD1	2.41	0.56
2:s:5:LYS:HZ1	2:m:51:ARG:HH21	1.54	0.56
2:r:120:SER:CB	2:r:143:PHE:HE1	2.19	0.56
1:H:316:ILE:HD13	1:H:335:TYR:CD1	2.41	0.56
2:b:116:ASN:HD21	2:b:145:GLU:CB	2.18	0.56
1:I:316:ILE:HD13	1:I:335:TYR:CD1	2.41	0.56
1:V:336:PRO:HB3	1:V:387:LEU:HB2	1.87	0.56
2:w:114:LEU:HD23	2:w:116:ASN:ND2	2.20	0.56
2:q:94:ARG:HD2	2:q:115:ARG:CB	2.35	0.56
1:H:74:VAL:HG22	1:H:78:PHE:HE2	1.70	0.56
1:V:453:GLU:HB3	1:V:454:PRO:CD	2.32	0.56
2:v:26:TYR:CZ	2:v:68:VAL:HG21	2.41	0.56
1:K:36:PHE:CE1	1:K:77:PHE:HE1	2.24	0.56
1:F:4:TYR:CD2	1:F:518:LYS:HD2	2.41	0.56
1:T:453:GLU:HG2	1:N:372:LYS:HB2	1.87	0.56
1:I:74:VAL:HG22	1:I:78:PHE:HE2	1.71	0.56
2:r:35:ILE:HG21	2:s:132:THR:HG22	1.81	0.56
2:s:26:TYR:CZ	2:s:68:VAL:HG21	2.41	0.56
2:t:26:TYR:CZ	2:t:68:VAL:HG21	2.41	0.56
1:N:454:PRO:HA	1:N:507:ARG:HH22	1.71	0.56
2:p:35:ILE:HG21	2:w:132:THR:HG22	1.86	0.56
2:w:114:LEU:HD23	2:w:116:ASN:HD21	1.71	0.56
2:a:42:TYR:CE1	2:h:12:ALA:C	2.78	0.56
2:u:26:TYR:CZ	2:u:68:VAL:HG21	2.40	0.56
2:v:114:LEU:HD23	2:v:116:ASN:HD21	1.71	0.55
1:J:497:THR:OG1	1:J:498:ASN:ND2	2.39	0.55
1:E:4:TYR:CD2	1:E:518:LYS:HD2	2.42	0.55
2:t:35:ILE:O	2:t:58:PRO:HD2	2.05	0.55
2:u:5:LYS:NZ	2:o:51:ARG:HH21	2.04	0.55
1:R:44:PRO:O	1:R:89:ARG:HG2	2.06	0.55
1:N:270:LEU:C	1:N:272:ALA:H	2.14	0.55
1:H:36:PHE:HE1	1:H:77:PHE:HE1	1.53	0.55
1:C:453:GLU:HB3	1:C:454:PRO:HD3	1.87	0.55
2:v:132:THR:HG21	2:o:35:ILE:HD13	1.87	0.55
2:p:35:ILE:HD13	2:w:132:THR:HG21	1.87	0.55
2:w:26:TYR:CZ	2:w:68:VAL:HG21	2.41	0.55
1:L:497:THR:OG1	1:L:498:ASN:ND2	2.39	0.55
1:G:316:ILE:HD13	1:G:335:TYR:CD1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:57:MET:HG2	2:b:118:TRP:CZ2	2.41	0.55
2:p:27:LEU:HD12	2:p:66:VAL:O	2.05	0.55
1:D:4:TYR:CD2	1:D:518:LYS:HD2	2.42	0.55
2:q:120:SER:CB	2:q:143:PHE:HE1	2.19	0.55
1:L:36:PHE:CE1	1:L:77:PHE:HE1	2.24	0.55
1:L:316:ILE:HD13	1:L:335:TYR:CD1	2.41	0.55
2:n:35:ILE:HG21	2:u:132:THR:HG22	1.88	0.55
1:P:12:GLU:OE2	1:P:505:LEU:HD23	2.07	0.55
1:K:316:ILE:HD13	1:K:335:TYR:CD1	2.41	0.55
1:K:497:THR:OG1	1:K:498:ASN:ND2	2.39	0.55
2:s:116:ASN:HD21	2:s:145:GLU:HB3	1.72	0.55
2:m:35:ILE:HB	2:m:59:GLY:O	2.06	0.55
2:t:116:ASN:HD21	2:t:145:GLU:HB3	1.72	0.55
2:n:25:GLU:HB3	2:n:68:VAL:HG13	1.89	0.55
1:B:80:ASN:ND2	1:B:380:ARG:HD3	2.21	0.55
2:o:25:GLU:HB3	2:o:68:VAL:HG13	1.89	0.55
2:p:34:GLN:CD	2:q:118:TRP:CZ2	2.84	0.55
2:x:26:TYR:CZ	2:x:68:VAL:HG21	2.41	0.55
1:I:497:THR:OG1	1:I:498:ASN:ND2	2.39	0.55
2:v:116:ASN:HD21	2:v:145:GLU:HB3	1.72	0.55
1:P:368:ARG:HB3	1:P:371:HIS:HE1	1.71	0.55
1:J:54:TRP:CH2	1:J:75:TYR:CZ	2.94	0.55
2:w:116:ASN:HD21	2:w:145:GLU:HB3	1.72	0.55
2:s:114:LEU:HD23	2:s:116:ASN:HD21	1.72	0.55
2:m:34:GLN:HB3	2:n:120:SER:HA	1.89	0.55
2:t:114:LEU:HD23	2:t:116:ASN:ND2	2.22	0.55
2:u:116:ASN:HD21	2:u:145:GLU:HB3	1.72	0.55
1:J:36:PHE:CE1	1:J:77:PHE:HE1	2.25	0.55
2:r:111:ARG:HH22	2:m:124:ALA:HB2	1.72	0.55
2:n:42:TYR:CZ	2:u:12:ALA:HB1	2.42	0.55
2:m:33:LEU:HB3	2:m:61:ALA:HB3	1.88	0.55
1:H:497:THR:OG1	1:H:498:ASN:ND2	2.39	0.55
1:D:68:TYR:O	1:D:72:HIS:CE1	2.60	0.55
1:Q:368:ARG:HB3	1:Q:371:HIS:HE1	1.72	0.55
2:x:116:ASN:HD21	2:x:145:GLU:HB3	1.72	0.55
2:r:42:TYR:CE1	2:s:12:ALA:HB1	2.42	0.55
2:r:120:SER:HB3	2:r:143:PHE:CE1	2.42	0.55
1:G:74:VAL:HG22	1:G:78:PHE:HE2	1.72	0.55
1:A:4:TYR:CD2	1:A:518:LYS:HD2	2.41	0.55
2:u:114:LEU:HD23	2:u:116:ASN:HD21	1.72	0.55
2:p:23:MET:HG3	2:i:44:GLN:CG	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:q:34:GLN:NE2	2:r:82:ILE:CD1	2.69	0.54
1:X:234:GLU:CG	1:X:277:GLY:HA3	2.37	0.54
2:n:35:ILE:HD13	2:u:132:THR:HG21	1.90	0.54
2:b:42:TYR:CE1	2:i:12:ALA:C	2.78	0.54
2:c:93:ALA:O	2:c:117:ALA:HB3	2.06	0.54
1:M:320:ARG:HE	1:M:333:LEU:HD13	1.73	0.54
2:m:120:SER:HB3	2:m:143:PHE:CE1	2.42	0.54
1:G:452:PHE:CZ	1:G:504:ASP:C	2.85	0.54
1:G:497:THR:OG1	1:G:498:ASN:ND2	2.39	0.54
1:B:4:TYR:CD2	1:B:518:LYS:HD2	2.41	0.54
1:B:501:GLU:HB2	1:B:503:VAL:HG23	1.90	0.54
1:U:234:GLU:CG	1:U:277:GLY:HA3	2.37	0.54
1:U:453:GLU:CB	1:U:454:PRO:HD2	2.23	0.54
1:C:4:TYR:CD2	1:C:518:LYS:HD2	2.42	0.54
2:p:25:GLU:HB3	2:p:68:VAL:HG13	1.89	0.54
2:p:124:ALA:HB2	2:o:111:ARG:HH12	1.73	0.54
2:d:116:ASN:O	2:d:117:ALA:C	2.50	0.54
1:Q:69:TYR:CD1	1:Q:272:ALA:HB2	2.42	0.54
1:F:453:GLU:CB	1:F:454:PRO:CD	2.73	0.54
1:B:493:CYS:SG	1:B:509:VAL:HG22	2.46	0.54
2:v:12:ALA:CB	2:o:42:TYR:CE1	2.91	0.54
1:E:68:TYR:O	1:E:72:HIS:CE1	2.61	0.54
1:X:4:TYR:CE1	1:X:443:ILE:HG21	2.38	0.54
1:X:307:PRO:HG2	1:X:337:TRP:HE1	1.73	0.54
1:F:68:TYR:O	1:F:72:HIS:CE1	2.61	0.54
1:M:270:LEU:C	1:M:272:ALA:H	2.15	0.54
1:H:490:TYR:HB3	1:H:512:ILE:HB	1.90	0.54
2:v:34:GLN:NE2	2:v:57:MET:SD	2.80	0.54
1:U:452:PHE:HZ	1:U:507:ARG:HD3	0.60	0.54
1:V:335:TYR:CB	1:V:336:PRO:HD3	2.38	0.54
2:d:101:VAL:HG23	2:d:103:ASP:H	1.73	0.54
1:W:4:TYR:CE1	1:W:443:ILE:HG21	2.39	0.54
2:m:26:TYR:CD2	2:m:68:VAL:HG11	2.42	0.54
1:V:449:TRP:O	1:V:452:PHE:CE2	2.60	0.54
1:J:490:TYR:HB3	1:J:512:ILE:HB	1.90	0.54
1:W:72:HIS:CD2	1:W:351:VAL:HG11	2.42	0.54
2:q:120:SER:HB3	2:q:143:PHE:CE1	2.43	0.54
1:S:465:ARG:CZ	2:m:94:ARG:NH2	2.70	0.54
2:n:120:SER:HB3	2:n:143:PHE:CE1	2.42	0.54
1:U:335:TYR:CB	1:U:336:PRO:HD3	2.38	0.54
1:C:68:TYR:O	1:C:72:HIS:CE1	2.61	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:101:VAL:O	2:c:102:MET:C	2.49	0.54
1:V:72:HIS:CD2	1:V:351:VAL:HG11	2.42	0.54
1:V:234:GLU:CG	1:V:277:GLY:HA3	2.38	0.54
1:W:234:GLU:CG	1:W:277:GLY:HA3	2.38	0.54
1:W:307:PRO:HG2	1:W:337:TRP:HE1	1.73	0.54
1:Q:459:LEU:HB3	1:Q:507:ARG:HH22	1.73	0.54
1:K:490:TYR:HB3	1:K:512:ILE:HB	1.90	0.54
1:M:368:ARG:HB3	1:M:371:HIS:HE1	1.73	0.54
1:G:490:TYR:HB3	1:G:512:ILE:HB	1.90	0.54
1:P:368:ARG:HB3	1:P:371:HIS:CE1	2.43	0.54
2:p:26:TYR:CD2	2:p:68:VAL:HG11	2.43	0.54
2:p:42:TYR:CE1	2:w:12:ALA:CB	2.90	0.54
1:J:452:PHE:CZ	1:J:504:ASP:C	2.86	0.54
2:k:34:GLN:HE22	2:l:85:SER:HB2	1.73	0.54
2:e:101:VAL:O	2:e:102:MET:C	2.51	0.54
2:n:26:TYR:CD2	2:n:68:VAL:HG11	2.43	0.54
1:Q:368:ARG:HB3	1:Q:371:HIS:CE1	2.43	0.54
1:R:467:VAL:HG12	1:R:489:TYR:OH	2.08	0.54
1:L:490:TYR:HB3	1:L:512:ILE:HB	1.90	0.54
2:l:34:GLN:HE22	2:g:85:SER:HB2	1.73	0.54
1:T:335:TYR:CB	1:T:336:PRO:HD3	2.38	0.54
2:o:26:TYR:CD2	2:o:68:VAL:HG11	2.43	0.54
1:P:467:VAL:HG12	1:P:489:TYR:OH	2.08	0.53
2:q:25:GLU:HB3	2:q:68:VAL:HG13	1.89	0.53
2:r:25:GLU:HB3	2:r:68:VAL:HG13	1.89	0.53
1:O:270:LEU:C	1:O:272:ALA:H	2.16	0.53
2:f:101:VAL:O	2:f:102:MET:C	2.50	0.53
1:S:335:TYR:CB	1:S:336:PRO:HD3	2.38	0.53
2:p:34:GLN:CD	2:q:118:TRP:HZ2	2.16	0.53
2:w:35:ILE:HB	2:w:58:PRO:HB2	1.90	0.53
1:K:74:VAL:HG22	1:K:78:PHE:CE2	2.44	0.53
1:K:338:ILE:HD13	1:K:356:HIS:CE1	2.43	0.53
1:X:335:TYR:CB	1:X:336:PRO:HD3	2.39	0.53
2:b:39:VAL:HG22	2:b:53:ASN:HB3	1.90	0.53
1:I:452:PHE:CZ	1:I:504:ASP:C	2.87	0.53
2:q:26:TYR:CD2	2:q:68:VAL:HG11	2.43	0.53
1:B:309:PRO:HA	1:B:337:TRP:CE2	2.43	0.53
2:b:115:ARG:HD3	2:b:116:ASN:N	2.24	0.53
2:v:132:THR:HG22	2:o:35:ILE:HG21	1.88	0.53
1:D:453:GLU:CB	1:D:454:PRO:CD	2.73	0.53
1:R:69:TYR:CE1	1:R:272:ALA:HB2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:25:GLU:HB3	2:m:68:VAL:HG13	1.90	0.53
1:A:68:TYR:O	1:A:72:HIS:CE1	2.61	0.53
2:h:34:GLN:HE22	2:i:85:SER:HB2	1.73	0.53
2:b:99:ILE:HD11	2:b:111:ARG:HH12	1.73	0.53
2:c:39:VAL:HG22	2:c:53:ASN:HB3	1.90	0.53
1:W:335:TYR:CB	1:W:336:PRO:HD3	2.39	0.53
2:q:94:ARG:HA	2:q:115:ARG:HA	1.90	0.53
2:k:114:LEU:HD12	2:k:115:ARG:H	1.74	0.53
2:e:39:VAL:HG22	2:e:53:ASN:HB3	1.90	0.53
2:j:44:GLN:HG2	2:q:22:VAL:HB	1.90	0.53
1:Q:467:VAL:HG12	1:Q:489:TYR:OH	2.08	0.53
2:e:116:ASN:O	2:e:117:ALA:C	2.51	0.53
2:n:111:ARG:HH12	2:o:124:ALA:HB2	1.74	0.53
1:H:243:TYR:O	1:H:250:ARG:HB3	2.09	0.53
1:B:68:TYR:O	1:B:72:HIS:CE1	2.61	0.53
2:j:85:SER:HB2	2:i:34:GLN:HE22	1.74	0.53
1:E:309:PRO:HA	1:E:337:TRP:CE2	2.43	0.53
2:l:114:LEU:HD12	2:l:115:ARG:H	1.74	0.53
1:M:467:VAL:HG12	1:M:489:TYR:OH	2.08	0.53
2:m:42:TYR:CE1	2:t:12:ALA:CB	2.92	0.53
2:a:42:TYR:HE1	2:h:12:ALA:CA	1.82	0.53
1:T:72:HIS:CD2	1:T:351:VAL:HG11	2.42	0.53
1:O:504:ASP:C	1:O:506:GLY:H	2.17	0.53
2:q:35:ILE:HD13	2:x:132:THR:HG21	1.90	0.53
1:X:4:TYR:OH	1:X:463:ILE:HD11	2.08	0.53
2:l:44:GLN:HG2	2:m:22:VAL:HB	1.90	0.53
1:S:72:HIS:CD2	1:S:351:VAL:HG11	2.41	0.53
1:T:466:ASN:OD1	2:n:94:ARG:HD2	2.08	0.53
1:U:72:HIS:CD2	1:U:351:VAL:HG11	2.41	0.53
1:J:74:VAL:HG22	1:J:78:PHE:CE2	2.44	0.53
1:Q:12:GLU:OE2	1:Q:505:LEU:HD23	2.08	0.53
2:q:42:TYR:CE1	2:x:12:ALA:CB	2.92	0.53
2:x:34:GLN:NE2	2:x:57:MET:SD	2.82	0.53
2:b:42:TYR:HE1	2:i:13:PRO:HD2	1.69	0.53
2:q:35:ILE:HG21	2:x:132:THR:HG22	1.88	0.52
1:R:320:ARG:HE	1:R:333:LEU:HD13	1.74	0.52
1:L:452:PHE:CZ	1:L:504:ASP:C	2.87	0.52
2:n:94:ARG:HA	2:n:115:ARG:HA	1.90	0.52
1:H:83:SER:OG	1:H:84:ALA:N	2.42	0.52
1:B:505:LEU:HD22	1:B:507:ARG:NH1	2.23	0.52
1:O:368:ARG:HB3	1:O:371:HIS:HE1	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:p:120:SER:HB3	2:p:143:PHE:CE1	2.41	0.52
2:e:95:LYS:HB2	2:e:113:ASN:HB2	1.91	0.52
1:L:370:VAL:HG12	1:L:434:ARG:NH2	2.24	0.52
2:f:7:GLU:HB3	2:a:71:GLY:HA3	1.91	0.52
2:g:114:LEU:HD12	2:g:115:ARG:H	1.74	0.52
2:j:114:LEU:HD12	2:j:115:ARG:H	1.74	0.52
1:Q:459:LEU:CB	1:Q:507:ARG:HH22	2.22	0.52
2:q:129:ALA:N	2:i:42:TYR:OH	2.40	0.52
2:r:26:TYR:CD2	2:r:68:VAL:HG11	2.43	0.52
2:r:35:ILE:CG2	2:s:132:THR:CG2	2.79	0.52
1:B:80:ASN:HD22	1:B:80:ASN:N	2.06	0.52
1:W:4:TYR:OH	1:W:463:ILE:HD11	2.08	0.52
2:h:114:LEU:HD12	2:h:115:ARG:H	1.74	0.52
1:O:467:VAL:HG12	1:O:489:TYR:OH	2.08	0.52
1:V:4:TYR:OH	1:V:463:ILE:HD11	2.09	0.52
1:K:244:LEU:HD12	1:K:249:ASP:HA	1.90	0.52
2:f:39:VAL:HG22	2:f:53:ASN:HB3	1.91	0.52
1:T:234:GLU:CG	1:T:277:GLY:HA3	2.39	0.52
1:U:4:TYR:OH	1:U:463:ILE:HD11	2.09	0.52
2:o:94:ARG:HA	2:o:115:ARG:HA	1.90	0.52
2:i:114:LEU:HD12	2:i:115:ARG:H	1.74	0.52
1:J:453:GLU:HB2	1:J:454:PRO:HD2	1.85	0.52
2:r:94:ARG:HA	2:r:115:ARG:HA	1.90	0.52
1:G:283:ALA:O	1:G:287:VAL:HG23	2.10	0.52
1:N:270:LEU:HD13	1:N:284:VAL:HG13	1.91	0.52
2:n:34:GLN:HE22	2:o:85:SER:CB	2.10	0.52
2:v:12:ALA:HB1	2:o:42:TYR:CZ	2.45	0.52
2:q:34:GLN:OE1	2:r:118:TRP:HZ2	1.92	0.52
1:K:453:GLU:CG	1:E:372:LYS:HD2	2.38	0.52
1:G:83:SER:OG	1:G:84:ALA:N	2.43	0.52
1:G:370:VAL:CG1	1:G:434:ARG:HB3	2.40	0.52
1:W:465:ARG:O	2:q:94:ARG:NH2	2.43	0.52
1:K:453:GLU:HB2	1:K:454:PRO:HD2	1.83	0.52
1:K:490:TYR:OH	1:K:492:LYS:HD2	2.10	0.52
1:R:467:VAL:HG12	1:R:489:TYR:HH	1.74	0.52
1:G:46:ASN:HD22	1:G:251:THR:CG2	2.23	0.52
2:b:92:THR:OG1	2:b:115:ARG:NH2	2.43	0.52
1:I:36:PHE:HE1	1:I:77:PHE:HE1	1.56	0.52
2:b:100:ILE:CG2	2:b:104:TYR:HA	2.40	0.52
1:I:338:ILE:HD13	1:I:356:HIS:CE1	2.44	0.52
1:J:490:TYR:OH	1:J:492:LYS:HD2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:453:GLU:CG	1:F:372:LYS:HD2	2.37	0.52
1:F:453:GLU:HB3	1:F:454:PRO:HD3	1.88	0.52
1:G:46:ASN:HD22	1:G:251:THR:HG23	1.75	0.52
2:g:44:GLN:HG2	2:n:22:VAL:HB	1.91	0.52
2:a:115:ARG:C	2:a:117:ALA:N	2.68	0.52
1:H:46:ASN:HB2	1:H:251:THR:HG21	1.91	0.52
1:B:236:ALA:O	1:B:241:ALA:HB2	2.10	0.52
1:B:306:ASP:OD2	1:B:352:PRO:HB2	2.10	0.52
1:D:453:GLU:HB3	1:D:454:PRO:HD3	1.89	0.51
2:d:101:VAL:O	2:d:102:MET:C	2.53	0.51
1:W:453:GLU:CG	1:Q:372:LYS:CD	2.84	0.51
1:E:236:ALA:O	1:E:241:ALA:HB2	2.10	0.51
1:X:465:ARG:O	2:r:94:ARG:NH2	2.43	0.51
1:C:236:ALA:O	1:C:241:ALA:HB2	2.10	0.51
1:L:490:TYR:OH	1:L:492:LYS:HD2	2.10	0.51
1:M:37:VAL:HA	1:M:88:VAL:HB	1.91	0.51
1:A:236:ALA:O	1:A:241:ALA:HB2	2.10	0.51
1:N:467:VAL:HG12	1:N:489:TYR:OH	2.08	0.51
1:H:74:VAL:HG22	1:H:78:PHE:CE2	2.46	0.51
1:U:452:PHE:C	1:O:372:LYS:HE3	2.35	0.51
1:C:463:ILE:HG21	1:C:509:VAL:HG21	1.93	0.51
2:p:94:ARG:HA	2:p:115:ARG:HA	1.91	0.51
1:J:54:TRP:CZ3	1:J:75:TYR:CZ	2.98	0.51
1:E:505:LEU:HD12	1:E:507:ARG:HB3	1.92	0.51
1:L:83:SER:OG	1:L:84:ALA:N	2.43	0.51
2:a:39:VAL:HG22	2:a:53:ASN:HB3	1.91	0.51
2:d:42:TYR:CE1	2:k:12:ALA:C	2.81	0.51
2:m:35:ILE:CG2	2:t:132:THR:CG2	2.77	0.51
1:T:4:TYR:OH	1:T:463:ILE:HD11	2.11	0.51
1:H:80:ASN:HB2	1:H:356:HIS:HD2	1.75	0.51
1:H:250:ARG:HG3	1:H:251:THR:N	2.25	0.51
2:u:5:LYS:HZ1	2:o:51:ARG:HH21	1.57	0.51
2:u:35:ILE:HB	2:u:58:PRO:HB2	1.93	0.51
2:v:35:ILE:HB	2:v:58:PRO:HB2	1.93	0.51
1:P:271:MET:HG3	1:P:306:ASP:HB2	1.92	0.51
2:f:116:ASN:O	2:f:117:ALA:C	2.52	0.51
2:s:5:LYS:NZ	2:m:51:ARG:HH21	2.08	0.51
1:G:338:ILE:HD13	1:G:356:HIS:CE1	2.45	0.51
1:A:306:ASP:OD2	1:A:352:PRO:HB2	2.11	0.51
2:t:114:LEU:HD23	2:t:116:ASN:HD21	1.74	0.51
1:H:490:TYR:OH	1:H:492:LYS:HD2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:46:ASN:HD22	1:K:251:THR:HG23	1.76	0.51
2:r:34:GLN:OE1	2:m:118:TRP:HZ2	1.93	0.51
1:L:46:ASN:HD22	1:L:251:THR:HG23	1.76	0.51
2:a:95:LYS:HB2	2:a:113:ASN:HB2	1.91	0.51
1:E:306:ASP:OD2	1:E:352:PRO:HB2	2.10	0.51
2:a:43:GLN:HG2	2:a:50:GLY:HA2	1.93	0.51
1:T:452:PHE:HZ	1:T:507:ARG:HD3	0.61	0.51
2:p:42:TYR:CZ	2:w:12:ALA:HB1	2.45	0.51
2:p:118:TRP:CZ2	2:o:34:GLN:CD	2.89	0.51
1:J:244:LEU:HD12	1:J:249:ASP:HA	1.92	0.51
2:d:94:ARG:HA	2:d:115:ARG:HA	1.92	0.51
1:F:236:ALA:O	1:F:241:ALA:HB2	2.10	0.51
1:G:46:ASN:HB2	1:G:251:THR:CG2	2.41	0.51
1:P:477:ASN:HD21	2:i:51:ARG:NH2	2.07	0.51
2:p:94:ARG:NE	2:p:115:ARG:HB3	2.26	0.51
1:H:283:ALA:O	1:H:287:VAL:HG23	2.10	0.51
1:U:273:ALA:HA	1:U:276:ARG:HG2	1.93	0.51
1:I:453:GLU:HB2	1:I:454:PRO:HD2	1.84	0.51
2:e:42:TYR:HE1	2:l:12:ALA:CA	1.85	0.51
1:S:452:PHE:HZ	1:S:507:ARG:HD3	0.61	0.51
1:G:490:TYR:OH	1:G:492:LYS:HD2	2.10	0.51
1:N:453:GLU:C	1:N:455:ASN:H	2.19	0.51
2:n:35:ILE:CD1	2:u:132:THR:HG21	2.40	0.51
1:U:465:ARG:O	2:o:94:ARG:NH2	2.43	0.51
2:d:39:VAL:HG22	2:d:53:ASN:HB3	1.91	0.50
1:K:83:SER:OG	1:K:84:ALA:N	2.42	0.50
1:O:453:GLU:C	1:O:455:ASN:H	2.19	0.50
1:V:273:ALA:HA	1:V:276:ARG:HG2	1.93	0.50
2:d:5:LYS:N	2:d:6:PRO:HD2	2.26	0.50
1:X:72:HIS:CD2	1:X:351:VAL:HG11	2.41	0.50
2:t:35:ILE:HB	2:t:58:PRO:HB2	1.93	0.50
1:L:453:GLU:HB2	1:L:454:PRO:HD2	1.81	0.50
1:F:463:ILE:HG21	1:F:509:VAL:HG21	1.93	0.50
1:T:453:GLU:HG2	1:N:372:LYS:HD2	1.90	0.50
2:o:120:SER:HB3	2:o:143:PHE:HE1	1.77	0.50
1:V:90:VAL:HG13	1:V:239:GLY:C	2.37	0.50
1:V:466:ASN:OD1	2:p:94:ARG:HD3	2.11	0.50
2:e:42:TYR:CE1	2:l:12:ALA:C	2.80	0.50
1:S:453:GLU:CB	1:S:454:PRO:HD3	2.06	0.50
2:m:42:TYR:CZ	2:t:12:ALA:HB1	2.47	0.50
1:D:236:ALA:O	1:D:241:ALA:HB2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:306:ASP:OD2	1:F:352:PRO:HB2	2.12	0.50
1:G:36:PHE:HE1	1:G:77:PHE:HE1	1.58	0.50
1:H:61:PHE:CZ	1:H:87:VAL:CG1	2.94	0.50
2:b:115:ARG:C	2:b:117:ALA:N	2.69	0.50
2:k:44:GLN:HG2	2:r:22:VAL:HB	1.93	0.50
2:e:100:ILE:HG21	2:e:104:TYR:HA	1.93	0.50
2:f:5:LYS:N	2:f:6:PRO:HD2	2.26	0.50
2:a:100:ILE:CG2	2:a:104:TYR:HA	2.41	0.50
1:C:306:ASP:OD2	1:C:352:PRO:HB2	2.12	0.50
1:K:36:PHE:HE1	1:K:77:PHE:HE1	1.60	0.50
1:X:90:VAL:HG13	1:X:239:GLY:C	2.37	0.50
1:X:273:ALA:HA	1:X:276:ARG:HG2	1.93	0.50
1:R:453:GLU:C	1:R:455:ASN:H	2.19	0.50
1:L:74:VAL:HG22	1:L:78:PHE:CE2	2.46	0.50
2:l:51:ARG:NH2	1:M:477:ASN:HD21	2.10	0.50
1:G:74:VAL:HG22	1:G:78:PHE:CE2	2.47	0.50
2:n:120:SER:HG	2:n:143:PHE:HE1	1.58	0.50
2:h:44:GLN:HG2	2:o:22:VAL:HB	1.94	0.50
1:J:83:SER:OG	1:J:84:ALA:N	2.42	0.50
1:K:370:VAL:CG1	1:K:434:ARG:HB3	2.42	0.50
1:O:270:LEU:HD12	1:O:284:VAL:HG13	1.93	0.50
2:v:120:SER:HB2	2:v:143:PHE:CE2	2.47	0.50
1:D:306:ASP:OD2	1:D:352:PRO:HB2	2.12	0.50
2:w:120:SER:HB2	2:w:143:PHE:CE2	2.47	0.50
2:r:120:SER:HG	2:r:143:PHE:HE1	1.59	0.50
1:G:314:ARG:O	1:G:318:VAL:HG23	2.12	0.50
2:g:42:TYR:CZ	2:o:129:ALA:CA	2.73	0.50
2:b:42:TYR:HE1	2:i:12:ALA:CA	1.84	0.50
2:d:70:ARG:HB3	2:c:7:GLU:CD	2.37	0.49
1:E:39:LEU:O	1:E:68:TYR:CE2	2.65	0.49
1:F:39:LEU:O	1:F:68:TYR:CE2	2.65	0.49
2:s:35:ILE:HB	2:s:58:PRO:HB2	1.93	0.49
1:G:61:PHE:CZ	1:G:87:VAL:CG1	2.94	0.49
1:A:335:TYR:HB3	1:A:336:PRO:HD3	1.94	0.49
2:u:120:SER:HB2	2:u:143:PHE:CE2	2.47	0.49
1:I:74:VAL:HG22	1:I:78:PHE:CE2	2.46	0.49
1:P:370:VAL:HG11	1:P:434:ARG:HB3	1.94	0.49
2:f:101:VAL:HG23	2:f:103:ASP:H	1.77	0.49
1:S:1:MET:CA	1:S:518:LYS:HA	2.33	0.49
1:T:90:VAL:HG13	1:T:239:GLY:C	2.37	0.49
1:U:90:VAL:HG13	1:U:239:GLY:C	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:452:PHE:HZ	1:U:507:ARG:NE	2.03	0.49
2:u:34:GLN:NE2	2:u:57:MET:SD	2.85	0.49
1:O:467:VAL:HG12	1:O:489:TYR:HH	1.77	0.49
1:I:490:TYR:HB3	1:I:512:ILE:HB	1.94	0.49
1:C:335:TYR:HB3	1:C:336:PRO:HD3	1.95	0.49
2:p:135:LEU:O	2:p:136:THR:C	2.56	0.49
2:j:51:ARG:NH2	1:Q:477:ASN:HD21	2.10	0.49
2:d:5:LYS:N	2:d:6:PRO:CD	2.76	0.49
1:E:455:ASN:ND2	1:E:506:GLY:H	2.09	0.49
1:M:37:VAL:HG22	1:M:88:VAL:HG21	1.93	0.49
2:a:7:GLU:CD	2:b:70:ARG:HB3	2.37	0.49
1:K:314:ARG:O	1:K:318:VAL:HG23	2.12	0.49
2:k:42:TYR:CZ	2:m:129:ALA:CA	2.76	0.49
1:M:504:ASP:C	1:M:506:GLY:H	2.20	0.49
1:A:39:LEU:O	1:A:68:TYR:CE2	2.65	0.49
2:t:120:SER:HB2	2:t:143:PHE:CE2	2.47	0.49
1:B:39:LEU:O	1:B:68:TYR:CE2	2.65	0.49
2:b:7:GLU:CD	2:c:70:ARG:HB3	2.37	0.49
1:O:273:ALA:HB1	1:O:279:ILE:HD12	1.94	0.49
2:o:120:SER:CB	2:o:143:PHE:HE1	2.25	0.49
1:I:83:SER:OG	1:I:84:ALA:N	2.43	0.49
1:J:314:ARG:O	1:J:318:VAL:HG23	2.12	0.49
1:D:335:TYR:HB3	1:D:336:PRO:HD3	1.95	0.49
1:W:90:VAL:HG13	1:W:239:GLY:C	2.37	0.49
1:K:46:ASN:HB2	1:K:251:THR:CG2	2.40	0.49
1:B:335:TYR:HB3	1:B:336:PRO:HD3	1.95	0.49
1:C:39:LEU:O	1:C:68:TYR:CE2	2.65	0.49
2:d:94:ARG:HB2	2:d:115:ARG:HG2	1.93	0.49
1:Q:453:GLU:C	1:Q:455:ASN:H	2.19	0.49
2:r:44:GLN:OE1	2:s:22:VAL:HA	2.13	0.49
2:f:5:LYS:N	2:f:6:PRO:CD	2.76	0.49
1:S:489:TYR:CA	1:S:513:GLY:HA3	2.28	0.49
1:H:370:VAL:HG21	1:H:438:TYR:CG	2.48	0.49
2:o:33:LEU:HB3	2:o:61:ALA:HB3	1.95	0.49
1:I:314:ARG:O	1:I:318:VAL:HG23	2.12	0.49
2:q:135:LEU:O	2:q:136:THR:C	2.56	0.49
1:M:503:VAL:HG12	1:M:505:LEU:H	1.78	0.49
1:H:314:ARG:O	1:H:318:VAL:HG23	2.13	0.49
1:I:46:ASN:HD22	1:I:251:THR:CG2	2.25	0.49
1:I:244:LEU:HD12	1:I:249:ASP:HA	1.94	0.49
2:p:43:GLN:CD	2:p:48:THR:HG21	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:q:41:ARG:HB3	2:x:70:ARG:HG3	1.95	0.49
2:x:120:SER:HB2	2:x:143:PHE:CE2	2.47	0.49
1:S:452:PHE:C	1:M:372:LYS:HE3	2.37	0.49
2:m:120:SER:HG	2:m:143:PHE:HE1	1.57	0.49
1:P:453:GLU:C	1:P:455:ASN:H	2.21	0.49
1:J:46:ASN:HD22	1:J:251:THR:HG23	1.78	0.49
2:j:13:PRO:O	2:c:42:TYR:CE2	2.66	0.49
1:K:46:ASN:HD22	1:K:251:THR:CG2	2.26	0.49
1:F:335:TYR:HB3	1:F:336:PRO:HD3	1.95	0.49
2:n:43:GLN:CD	2:n:48:THR:HG21	2.24	0.49
1:I:490:TYR:CE2	1:I:492:LYS:HB2	2.48	0.49
2:j:42:TYR:OH	2:r:128:LYS:C	2.56	0.49
1:E:335:TYR:HB3	1:E:336:PRO:HD3	1.94	0.49
2:f:42:TYR:CE2	2:g:13:PRO:O	2.66	0.49
2:m:41:ARG:HB3	2:t:70:ARG:HG3	1.95	0.49
1:T:273:ALA:HA	1:T:276:ARG:CG	2.42	0.49
2:r:135:LEU:O	2:r:136:THR:C	2.56	0.48
1:S:469:ALA:HB2	2:m:94:ARG:NH1	2.28	0.48
2:s:120:SER:HB2	2:s:143:PHE:CE2	2.47	0.48
1:G:398:ASN:N	1:G:399:PRO:CD	2.76	0.48
2:g:51:ARG:NH2	1:N:477:ASN:HD21	2.11	0.48
1:H:398:ASN:N	1:H:399:PRO:CD	2.76	0.48
1:O:45:LEU:O	1:O:48:PRO:HD2	2.13	0.48
1:J:46:ASN:HD22	1:J:251:THR:CG2	2.26	0.48
1:J:398:ASN:N	1:J:399:PRO:CD	2.76	0.48
1:H:452:PHE:CZ	1:H:504:ASP:C	2.91	0.48
1:B:41:PRO:HB3	1:B:94:ALA:O	2.13	0.48
1:W:273:ALA:HA	1:W:276:ARG:HG2	1.94	0.48
2:q:42:TYR:CZ	2:x:12:ALA:HB1	2.47	0.48
2:l:42:TYR:CZ	2:n:129:ALA:CA	2.73	0.48
2:d:113:ASN:O	2:d:114:LEU:C	2.55	0.48
2:k:51:ARG:NH2	1:R:477:ASN:HD21	2.11	0.48
1:L:46:ASN:HB2	1:L:251:THR:CG2	2.41	0.48
1:L:314:ARG:O	1:L:318:VAL:HG23	2.12	0.48
1:L:398:ASN:N	1:L:399:PRO:CD	2.76	0.48
1:S:273:ALA:HA	1:S:276:ARG:HG2	1.94	0.48
2:a:42:TYR:HE1	2:h:13:PRO:HD2	1.73	0.48
2:m:99:ILE:HB	2:m:109:VAL:HB	1.96	0.48
1:G:515:ALA:N	1:G:516:PRO:HD2	2.29	0.48
1:B:80:ASN:HB3	1:B:363:ARG:HD2	1.94	0.48
1:I:46:ASN:HB2	1:I:251:THR:CG2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:q:43:GLN:CD	2:q:48:THR:HG21	2.30	0.48
1:X:335:TYR:HB2	1:X:336:PRO:HD3	1.95	0.48
1:R:89:ARG:NH1	1:R:89:ARG:HB2	2.29	0.48
1:L:36:PHE:HE1	1:L:77:PHE:HE1	1.59	0.48
1:L:242:GLN:HG2	1:L:253:PHE:HD1	1.78	0.48
2:r:42:TYR:CE2	2:s:14:ASN:HA	2.48	0.48
1:H:515:ALA:N	1:H:516:PRO:HD2	2.29	0.48
1:I:52:THR:OG1	1:I:53:ASN:N	2.47	0.48
2:v:70:ARG:HG3	2:o:41:ARG:HB3	1.95	0.48
1:J:52:THR:OG1	1:J:53:ASN:N	2.47	0.48
1:D:328:SER:N	1:D:421:LEU:O	2.47	0.48
1:K:431:ASN:OD1	1:K:431:ASN:N	2.47	0.48
1:E:328:SER:N	1:E:421:LEU:O	2.47	0.48
1:X:453:GLU:HG2	1:R:372:LYS:HD2	1.91	0.48
2:l:42:TYR:OH	2:n:128:LYS:C	2.57	0.48
1:M:88:VAL:HG12	1:M:90:VAL:HG23	1.96	0.48
1:A:328:SER:N	1:A:421:LEU:O	2.47	0.48
1:I:398:ASN:N	1:I:399:PRO:CD	2.76	0.48
2:p:94:ARG:CA	2:p:115:ARG:HA	2.44	0.48
2:p:119:CYS:O	2:o:34:GLN:OE1	2.32	0.48
2:x:130:GLY:O	2:x:131:ASP:C	2.57	0.48
1:L:515:ALA:N	1:L:516:PRO:HD2	2.29	0.48
2:f:95:LYS:HB2	2:f:113:ASN:HB2	1.96	0.48
1:M:46:ASN:N	1:M:89:ARG:HD2	2.29	0.48
1:G:242:GLN:HG2	1:G:253:PHE:HD1	1.79	0.48
1:G:453:GLU:OE2	1:A:372:LYS:HD2	2.14	0.48
1:A:309:PRO:HA	1:A:337:TRP:CD1	2.48	0.48
2:t:130:GLY:O	2:t:131:ASP:C	2.57	0.48
1:H:453:GLU:HB2	1:H:454:PRO:HD2	1.83	0.48
1:I:46:ASN:HD22	1:I:251:THR:HG23	1.78	0.48
1:I:242:GLN:HG2	1:I:253:PHE:HD1	1.79	0.48
1:H:79:ASN:HB2	1:H:356:HIS:NE2	2.29	0.47
1:I:431:ASN:OD1	1:I:431:ASN:N	2.47	0.47
1:V:515:ALA:N	1:V:516:PRO:CD	2.78	0.47
2:d:1:MET:HE3	2:d:106:ASP:OD2	2.13	0.47
1:F:42:THR:N	1:F:95:GLU:OE2	2.41	0.47
2:s:130:GLY:O	2:s:131:ASP:C	2.57	0.47
1:B:269:ASP:N	1:B:269:ASP:OD1	2.45	0.47
2:b:42:TYR:CE2	2:i:13:PRO:O	2.67	0.47
1:V:466:ASN:OD1	2:p:94:ARG:NH1	2.47	0.47
1:P:54:TRP:CZ3	1:P:75:TYR:HB2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:42:TYR:CE2	2:k:13:PRO:O	2.68	0.47
2:q:34:GLN:CD	2:r:118:TRP:HZ2	2.22	0.47
1:K:52:THR:OG1	1:K:53:ASN:N	2.47	0.47
1:K:279:ILE:HG22	1:K:284:VAL:CG2	2.44	0.47
1:K:398:ASN:N	1:K:399:PRO:CD	2.76	0.47
1:E:453:GLU:CB	1:E:454:PRO:CD	2.79	0.47
1:R:40:ALA:HB3	1:R:89:ARG:HH12	1.79	0.47
1:R:500:PRO:C	1:R:502:SER:N	2.71	0.47
1:S:237:HIS:N	1:S:238:PRO:HD2	2.30	0.47
2:m:34:GLN:OE1	2:m:34:GLN:HA	2.15	0.47
1:U:515:ALA:N	1:U:516:PRO:CD	2.78	0.47
2:u:130:GLY:O	2:u:131:ASP:C	2.57	0.47
1:C:328:SER:N	1:C:421:LEU:O	2.47	0.47
2:p:118:TRP:HZ2	2:o:34:GLN:CD	2.22	0.47
1:Q:69:TYR:CE1	1:Q:272:ALA:HB2	2.50	0.47
1:G:431:ASN:OD1	1:G:431:ASN:N	2.47	0.47
1:B:328:SER:N	1:B:421:LEU:O	2.47	0.47
2:b:43:GLN:HG2	2:b:50:GLY:HA2	1.96	0.47
2:p:41:ARG:HB3	2:w:70:ARG:HG3	1.95	0.47
1:J:36:PHE:HE1	1:J:77:PHE:HE1	1.61	0.47
1:W:515:ALA:N	1:W:516:PRO:CD	2.78	0.47
1:R:274:TYR:CE1	1:R:275:GLN:HG3	2.49	0.47
2:r:111:ARG:HH22	2:m:124:ALA:CB	2.27	0.47
1:F:328:SER:N	1:F:421:LEU:O	2.47	0.47
1:A:269:ASP:OD1	1:A:269:ASP:N	2.45	0.47
1:T:515:ALA:N	1:T:516:PRO:CD	2.78	0.47
2:x:9:VAL:HG12	2:s:135:LEU:CD2	2.45	0.47
2:r:34:GLN:NE2	2:r:34:GLN:C	2.73	0.47
1:F:269:ASP:OD1	1:F:269:ASP:N	2.45	0.47
1:M:453:GLU:C	1:M:455:ASN:H	2.22	0.47
2:n:41:ARG:HB3	2:u:70:ARG:HG3	1.95	0.47
2:h:51:ARG:NH2	1:O:477:ASN:HD21	2.12	0.47
1:I:515:ALA:N	1:I:516:PRO:HD2	2.29	0.47
2:p:33:LEU:HB3	2:p:61:ALA:HB3	1.97	0.47
1:J:515:ALA:N	1:J:516:PRO:HD2	2.29	0.47
2:w:9:VAL:HG12	2:x:135:LEU:CD2	2.45	0.47
1:K:242:GLN:HG2	1:K:253:PHE:HD1	1.79	0.47
1:K:243:TYR:O	1:K:250:ARG:HB3	2.14	0.47
2:e:42:TYR:CE2	2:l:13:PRO:O	2.67	0.47
2:e:114:LEU:HD22	2:e:146:LEU:HB3	1.96	0.47
1:R:273:ALA:O	1:R:279:ILE:HB	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:r:99:ILE:HB	2:r:109:VAL:HB	1.96	0.47
1:L:61:PHE:HE1	1:L:87:VAL:HG11	1.74	0.47
1:L:80:ASN:HB2	1:L:356:HIS:HD2	1.79	0.47
1:F:237:HIS:CE1	1:F:238:PRO:HD3	2.50	0.47
2:f:7:GLU:CD	2:a:70:ARG:HB3	2.39	0.47
1:G:236:ALA:HB2	1:G:283:ALA:HB1	1.96	0.47
1:G:309:PRO:HA	1:G:337:TRP:CZ2	2.50	0.47
1:T:337:TRP:C	1:T:338:ILE:HG13	2.39	0.47
2:n:3:LEU:HB2	2:n:6:PRO:HD3	1.97	0.47
1:H:309:PRO:HA	1:H:337:TRP:CZ2	2.50	0.47
1:H:370:VAL:HG21	1:H:438:TYR:CB	2.45	0.47
1:U:452:PHE:CZ	1:U:507:ARG:NE	2.80	0.47
2:o:43:GLN:CD	2:o:48:THR:HG21	2.27	0.47
1:W:335:TYR:HB2	1:W:336:PRO:HD3	1.95	0.47
1:Q:273:ALA:O	1:Q:279:ILE:HB	2.15	0.47
1:K:515:ALA:N	1:K:516:PRO:HD2	2.29	0.47
1:L:52:THR:OG1	1:L:53:ASN:N	2.47	0.47
1:L:79:ASN:HB2	1:L:356:HIS:NE2	2.30	0.47
1:F:52:THR:OG1	1:F:53:ASN:N	2.48	0.47
2:m:3:LEU:HB2	2:m:6:PRO:HD3	1.97	0.47
2:g:42:TYR:OH	2:o:129:ALA:HA	2.14	0.47
1:A:237:HIS:CE1	1:A:238:PRO:HD3	2.50	0.47
1:T:273:ALA:HB2	1:T:276:ARG:CZ	2.45	0.47
2:n:99:ILE:HB	2:n:109:VAL:HB	1.96	0.47
1:I:309:PRO:HA	1:I:337:TRP:CZ2	2.50	0.47
2:c:101:VAL:HG23	2:c:103:ASP:H	1.79	0.47
2:v:9:VAL:HG12	2:w:135:LEU:CD2	2.45	0.47
1:J:242:GLN:HG2	1:J:253:PHE:HD1	1.79	0.47
1:J:309:PRO:HA	1:J:337:TRP:CZ2	2.50	0.47
2:w:34:GLN:OE1	2:x:118:TRP:CZ3	2.65	0.47
1:K:452:PHE:CZ	1:K:504:ASP:C	2.93	0.47
1:E:269:ASP:N	1:E:269:ASP:OD1	2.45	0.47
1:A:52:THR:OG1	1:A:53:ASN:N	2.48	0.47
1:B:453:GLU:HB3	1:B:454:PRO:HD3	1.89	0.47
2:j:42:TYR:OH	2:r:129:ALA:HA	2.14	0.47
1:X:515:ALA:N	1:X:516:PRO:CD	2.78	0.47
1:F:493:CYS:SG	1:F:509:VAL:HG22	2.55	0.47
2:s:9:VAL:HG12	2:t:135:LEU:CD2	2.45	0.47
2:g:42:TYR:OH	2:o:128:LYS:C	2.57	0.47
1:B:453:GLU:CB	1:B:454:PRO:CD	2.74	0.47
1:I:57:TYR:O	1:I:61:PHE:HD1	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:THR:OG1	1:C:53:ASN:N	2.48	0.47
1:E:40:ALA:HB3	1:E:89:ARG:HD2	1.97	0.46
1:F:471:LEU:HG	1:F:489:TYR:CZ	2.51	0.46
1:H:236:ALA:HB2	1:H:283:ALA:HB1	1.97	0.46
1:O:54:TRP:CZ3	1:O:75:TYR:HB2	2.50	0.46
1:V:337:TRP:C	1:V:338:ILE:HG13	2.40	0.46
2:v:130:GLY:O	2:v:131:ASP:C	2.57	0.46
1:P:365:ASP:CG	1:P:370:VAL:HG22	2.40	0.46
2:p:23:MET:CG	2:i:44:GLN:HG3	2.46	0.46
2:q:35:ILE:CD1	2:x:132:THR:HG21	2.45	0.46
2:q:99:ILE:HB	2:q:109:VAL:HB	1.96	0.46
1:E:45:LEU:HB2	1:E:48:PRO:CG	2.44	0.46
1:E:237:HIS:CE1	1:E:238:PRO:HD3	2.50	0.46
1:L:309:PRO:HA	1:L:337:TRP:CZ2	2.50	0.46
2:l:42:TYR:OH	2:n:129:ALA:HA	2.13	0.46
1:F:237:HIS:CD2	1:F:238:PRO:HD3	2.51	0.46
1:B:52:THR:OG1	1:B:53:ASN:N	2.48	0.46
2:j:42:TYR:CZ	2:r:129:ALA:CA	2.72	0.46
2:w:130:GLY:O	2:w:131:ASP:C	2.57	0.46
1:R:54:TRP:CZ3	1:R:75:TYR:HB2	2.50	0.46
2:n:135:LEU:O	2:n:136:THR:C	2.56	0.46
1:B:237:HIS:CD2	1:B:238:PRO:HD3	2.49	0.46
2:b:42:TYR:CD1	2:i:13:PRO:HD2	2.48	0.46
2:o:3:LEU:HB2	2:o:6:PRO:HD3	1.97	0.46
2:o:99:ILE:HB	2:o:109:VAL:HB	1.96	0.46
1:J:46:ASN:HB2	1:J:251:THR:CG2	2.43	0.46
1:D:52:THR:OG1	1:D:53:ASN:N	2.48	0.46
1:Q:54:TRP:CZ3	1:Q:75:TYR:HB2	2.50	0.46
1:Q:270:LEU:HD21	1:Q:287:VAL:HG21	1.96	0.46
2:r:3:LEU:HB2	2:r:6:PRO:HD3	1.97	0.46
2:r:33:LEU:HB3	2:r:61:ALA:HB3	1.96	0.46
1:L:46:ASN:HD22	1:L:251:THR:CG2	2.27	0.46
1:L:61:PHE:CZ	1:L:87:VAL:CG1	2.97	0.46
1:U:52:THR:OG1	1:U:53:ASN:N	2.46	0.46
1:U:337:TRP:C	1:U:338:ILE:HG13	2.40	0.46
1:C:45:LEU:HB2	1:C:48:PRO:CG	2.45	0.46
1:D:237:HIS:CD2	1:D:238:PRO:HD3	2.51	0.46
1:D:308:PRO:HD2	1:D:311:GLN:HE22	1.81	0.46
1:E:237:HIS:CD2	1:E:238:PRO:HD3	2.51	0.46
1:R:43:GLY:H	1:R:89:ARG:NH2	2.13	0.46
1:G:52:THR:OG1	1:G:53:ASN:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:t:9:VAL:HG12	2:u:135:LEU:CD2	2.45	0.46
1:B:505:LEU:HD13	1:B:507:ARG:NH2	2.30	0.46
2:v:135:LEU:CD2	2:u:9:VAL:HG12	2.45	0.46
1:P:270:LEU:C	1:P:272:ALA:N	2.74	0.46
2:p:99:ILE:HB	2:p:109:VAL:HB	1.96	0.46
1:D:471:LEU:HG	1:D:489:TYR:CZ	2.50	0.46
2:q:3:LEU:HB2	2:q:6:PRO:HD3	1.97	0.46
1:E:311:GLN:HG3	1:E:316:ILE:HD11	1.98	0.46
1:E:471:LEU:HG	1:E:489:TYR:CZ	2.50	0.46
2:j:13:PRO:HD2	2:c:42:TYR:HE1	1.67	0.46
2:d:114:LEU:HD23	2:d:145:GLU:HB3	1.97	0.46
2:w:5:LYS:NZ	2:q:51:ARG:HH21	2.13	0.46
1:K:309:PRO:HA	1:K:337:TRP:CZ2	2.50	0.46
2:r:34:GLN:HB3	2:m:120:SER:O	2.16	0.46
1:F:308:PRO:HD2	1:F:311:GLN:HE22	1.81	0.46
1:S:335:TYR:HB2	1:S:336:PRO:HD3	1.98	0.46
1:S:337:TRP:C	1:S:338:ILE:HG13	2.40	0.46
1:A:453:GLU:HB3	1:A:454:PRO:HD3	1.91	0.46
1:N:54:TRP:CZ3	1:N:75:TYR:HB2	2.50	0.46
1:B:82:GLY:O	1:B:84:ALA:N	2.49	0.46
2:b:115:ARG:O	2:b:117:ALA:N	2.48	0.46
1:C:237:HIS:CE1	1:C:238:PRO:HD3	2.49	0.46
2:c:1:MET:HE3	2:c:106:ASP:OD2	2.16	0.46
2:p:3:LEU:HB2	2:p:6:PRO:HD3	1.97	0.46
2:d:42:TYR:HE1	2:k:13:PRO:HD2	1.72	0.46
1:M:74:VAL:HA	1:M:77:PHE:CE2	2.50	0.46
2:m:135:LEU:O	2:m:136:THR:C	2.56	0.46
1:A:498:ASN:OD1	1:A:508:VAL:N	2.48	0.46
1:T:335:TYR:HB2	1:T:336:PRO:HD3	1.98	0.46
1:H:250:ARG:HG3	1:H:251:THR:H	1.80	0.46
1:B:237:HIS:CE1	1:B:238:PRO:HD3	2.50	0.46
2:b:100:ILE:HG21	2:b:104:TYR:HA	1.97	0.46
1:C:237:HIS:CD2	1:C:238:PRO:HD3	2.51	0.46
2:p:120:SER:HA	2:o:34:GLN:HB3	1.98	0.46
1:D:269:ASP:N	1:D:269:ASP:OD1	2.45	0.46
2:e:101:VAL:HG23	2:e:103:ASP:H	1.80	0.46
2:r:42:TYR:CE1	2:s:12:ALA:CB	2.99	0.46
1:S:52:THR:OG1	1:S:53:ASN:N	2.46	0.46
1:G:453:GLU:HB2	1:G:454:PRO:HD2	1.84	0.46
1:N:270:LEU:O	1:N:270:LEU:HD22	2.16	0.46
1:B:471:LEU:HG	1:B:489:TYR:CZ	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:243:TYR:O	1:J:250:ARG:HB3	2.16	0.46
1:J:453:GLU:OE2	1:D:372:LYS:HD2	2.15	0.46
1:D:237:HIS:CE1	1:D:238:PRO:HD3	2.50	0.46
1:Q:274:TYR:CE1	1:Q:275:GLN:HG3	2.51	0.46
2:e:42:TYR:CD1	2:l:13:PRO:HD2	2.49	0.46
1:M:274:TYR:HA	1:M:279:ILE:C	2.41	0.46
2:n:25:GLU:HB3	2:n:68:VAL:CG1	2.46	0.46
1:H:52:THR:OG1	1:H:53:ASN:N	2.47	0.46
1:B:78:PHE:HA	1:B:81:GLY:O	2.16	0.46
1:C:493:CYS:SG	1:C:509:VAL:HG22	2.55	0.46
1:V:280:ASP:O	1:V:281:LEU:HB2	2.16	0.45
1:P:370:VAL:HG11	1:P:434:ARG:CB	2.46	0.45
1:Q:370:VAL:HG11	1:Q:434:ARG:HB3	1.98	0.45
1:K:279:ILE:O	1:K:280:ASP:C	2.59	0.45
1:A:471:LEU:HG	1:A:489:TYR:CZ	2.51	0.45
2:a:42:TYR:CE2	2:h:13:PRO:O	2.68	0.45
1:B:493:CYS:SG	1:B:509:VAL:HG13	2.56	0.45
1:V:335:TYR:HB2	1:V:336:PRO:HD3	1.98	0.45
1:D:93:SER:OG	1:D:94:ALA:N	2.49	0.45
1:E:449:TRP:CD1	1:E:449:TRP:N	2.83	0.45
1:L:431:ASN:OD1	1:L:431:ASN:N	2.47	0.45
1:S:236:ALA:O	1:S:241:ALA:HB3	2.15	0.45
2:h:14:ASN:OD1	2:h:98:THR:HB	2.17	0.45
1:B:311:GLN:HG3	1:B:316:ILE:HD11	1.98	0.45
2:b:93:ALA:O	2:b:115:ARG:HA	2.17	0.45
1:C:471:LEU:HG	1:C:489:TYR:CZ	2.51	0.45
1:C:498:ASN:OD1	1:C:508:VAL:N	2.49	0.45
1:P:77:PHE:HB3	1:P:355:GLY:O	2.17	0.45
2:n:111:ARG:HH12	2:o:124:ALA:CB	2.29	0.45
2:o:135:LEU:O	2:o:136:THR:C	2.56	0.45
2:v:9:VAL:HB	2:p:37:GLN:HE22	1.82	0.45
2:p:34:GLN:NE2	2:q:120:SER:HA	2.32	0.45
2:l:38:ASP:C	2:l:38:ASP:OD1	2.58	0.45
2:l:44:GLN:HA	2:m:22:VAL:O	2.17	0.45
2:f:100:ILE:HG23	2:f:106:ASP:O	2.16	0.45
1:G:61:PHE:CE2	1:G:87:VAL:CG1	2.95	0.45
1:N:274:TYR:HA	1:N:279:ILE:C	2.41	0.45
2:u:95:LYS:HB2	2:u:113:ASN:HB3	1.99	0.45
2:o:25:GLU:HB3	2:o:68:VAL:CG1	2.46	0.45
1:C:40:ALA:HB3	1:C:89:ARG:HD2	1.98	0.45
2:v:26:TYR:HB3	2:w:128:LYS:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:v:95:LYS:HB2	2:v:113:ASN:HB3	1.99	0.45
2:p:36:GLU:HB3	2:q:118:TRP:CZ3	2.52	0.45
1:D:45:LEU:HB2	1:D:48:PRO:CG	2.46	0.45
1:W:452:PHE:HA	1:Q:372:LYS:HZ1	1.79	0.45
2:r:87:ALA:HB3	2:r:89:ARG:NE	2.32	0.45
2:g:38:ASP:C	2:g:38:ASP:OD1	2.58	0.45
1:V:452:PHE:CZ	1:V:507:ARG:NE	2.78	0.45
2:p:9:VAL:CG2	2:j:56:LEU:HD22	2.47	0.45
2:w:95:LYS:HB2	2:w:113:ASN:HB3	1.99	0.45
2:w:128:LYS:HB3	2:w:131:ASP:OD2	2.17	0.45
2:q:120:SER:HG	2:q:143:PHE:HE1	1.63	0.45
2:x:128:LYS:HB3	2:x:131:ASP:OD2	2.17	0.45
1:S:280:ASP:O	1:S:281:LEU:HB2	2.16	0.45
2:m:9:VAL:CG2	2:g:56:LEU:HD22	2.47	0.45
1:G:370:VAL:HG12	1:G:434:ARG:HB3	1.99	0.45
2:g:44:GLN:HA	2:n:22:VAL:O	2.17	0.45
1:N:501:GLU:CD	1:N:501:GLU:H	2.24	0.45
1:O:77:PHE:HB3	1:O:355:GLY:O	2.17	0.45
2:c:100:ILE:HG23	2:c:106:ASP:O	2.17	0.45
2:p:25:GLU:HB3	2:p:68:VAL:CG1	2.46	0.45
1:E:93:SER:OG	1:E:94:ALA:N	2.49	0.45
1:E:501:GLU:HG3	1:E:503:VAL:H	1.82	0.45
2:l:15:PHE:CE2	2:l:27:LEU:HD22	2.52	0.45
1:F:93:SER:OG	1:F:94:ALA:N	2.49	0.45
2:m:116:ASN:O	2:m:117:ALA:C	2.60	0.45
1:B:489:TYR:CD1	1:B:513:GLY:HA2	2.52	0.45
2:v:128:LYS:HB3	2:v:131:ASP:OD2	2.17	0.45
1:W:280:ASP:O	1:W:281:LEU:HB2	2.16	0.45
2:w:9:VAL:HB	2:q:37:GLN:HE22	1.82	0.45
1:E:489:TYR:CD1	1:E:513:GLY:HA2	2.52	0.45
2:l:5:LYS:N	2:l:6:PRO:HD2	2.32	0.45
1:F:237:HIS:CG	1:F:238:PRO:CD	2.95	0.45
2:s:9:VAL:HB	2:m:37:GLN:HE22	1.82	0.45
2:m:36:GLU:HB3	2:n:118:TRP:CZ3	2.52	0.45
2:t:95:LYS:HB2	2:t:113:ASN:HB3	1.99	0.45
2:n:116:ASN:O	2:n:117:ALA:C	2.60	0.45
2:h:38:ASP:C	2:h:38:ASP:OD1	2.58	0.45
1:B:308:PRO:HD2	1:B:311:GLN:HE22	1.82	0.45
1:U:335:TYR:HB2	1:U:336:PRO:HD3	1.98	0.45
1:O:414:ARG:HB2	1:O:416:TRP:CZ2	2.52	0.45
2:i:5:LYS:N	2:i:6:PRO:HD2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:i:38:ASP:C	2:i:38:ASP:OD1	2.58	0.45
1:C:308:PRO:HD2	1:C:311:GLN:HE22	1.81	0.45
2:p:82:ILE:HD12	2:o:34:GLN:OE1	2.17	0.45
2:q:94:ARG:CA	2:q:115:ARG:HA	2.47	0.45
2:k:38:ASP:C	2:k:38:ASP:OD1	2.58	0.45
1:R:414:ARG:HB2	1:R:416:TRP:CZ2	2.52	0.45
2:r:36:GLU:HB3	2:m:118:TRP:CZ3	2.52	0.45
1:L:370:VAL:CG2	1:L:435:TYR:HA	2.47	0.45
2:f:114:LEU:HD22	2:f:146:LEU:HB3	1.98	0.45
2:u:128:LYS:HB3	2:u:131:ASP:OD2	2.17	0.45
1:P:44:PRO:HD3	1:P:60:ALA:O	2.16	0.45
1:P:467:VAL:HG12	1:P:489:TYR:HH	1.79	0.45
2:j:5:LYS:N	2:j:6:PRO:HD2	2.32	0.45
2:k:42:TYR:OH	2:m:128:LYS:C	2.60	0.45
2:k:44:GLN:HA	2:r:22:VAL:O	2.17	0.45
2:e:34:GLN:HE22	2:f:118:TRP:HZ2	1.64	0.45
1:R:77:PHE:HB3	1:R:355:GLY:O	2.17	0.45
1:R:270:LEU:HD21	1:R:287:VAL:HG21	1.99	0.45
2:r:116:ASN:O	2:r:117:ALA:C	2.60	0.45
2:s:128:LYS:HB3	2:s:131:ASP:OD2	2.17	0.45
1:M:453:GLU:N	1:M:454:PRO:HD3	2.32	0.45
1:A:40:ALA:HB3	1:A:89:ARG:HD2	1.98	0.45
1:N:74:VAL:HA	1:N:77:PHE:CE2	2.52	0.45
2:b:114:LEU:HD12	2:b:115:ARG:H	1.81	0.45
2:p:118:TRP:CZ3	2:o:36:GLU:HB3	2.52	0.44
1:Q:74:VAL:HA	1:Q:77:PHE:CE2	2.52	0.44
1:K:370:VAL:HG12	1:K:434:ARG:HB3	1.99	0.44
2:x:95:LYS:HB2	2:x:113:ASN:HB3	1.99	0.44
1:S:234:GLU:OE1	1:S:239:GLY:HA2	2.16	0.44
2:g:5:LYS:N	2:g:6:PRO:HD2	2.32	0.44
2:t:116:ASN:HD21	2:t:145:GLU:CB	2.30	0.44
2:t:128:LYS:HB3	2:t:131:ASP:OD2	2.17	0.44
2:h:5:LYS:N	2:h:6:PRO:HD2	2.32	0.44
2:o:94:ARG:CA	2:o:115:ARG:HA	2.47	0.44
2:o:116:ASN:O	2:o:117:ALA:C	2.60	0.44
2:c:113:ASN:O	2:c:114:LEU:C	2.60	0.44
1:P:274:TYR:H	1:P:274:TYR:HD2	1.64	0.44
1:D:40:ALA:HB3	1:D:89:ARG:CD	2.43	0.44
2:w:26:TYR:HB3	2:x:128:LYS:HA	1.99	0.44
2:q:25:GLU:HB3	2:q:68:VAL:CG1	2.46	0.44
1:X:307:PRO:HG2	1:X:337:TRP:NE1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:r:9:VAL:CG2	2:l:56:LEU:HD22	2.47	0.44
2:r:94:ARG:CA	2:r:115:ARG:HA	2.47	0.44
1:L:90:VAL:HA	1:L:251:THR:HG21	1.99	0.44
2:f:93:ALA:O	2:f:117:ALA:HB3	2.16	0.44
2:n:9:VAL:CG2	2:h:56:LEU:HD22	2.47	0.44
1:H:431:ASN:OD1	1:H:431:ASN:N	2.47	0.44
2:o:9:VAL:CG2	2:i:56:LEU:HD22	2.47	0.44
1:C:93:SER:OG	1:C:94:ALA:N	2.49	0.44
1:V:449:TRP:O	1:V:452:PHE:CD2	2.69	0.44
2:q:116:ASN:O	2:q:117:ALA:C	2.60	0.44
2:k:5:LYS:N	2:k:6:PRO:HD2	2.32	0.44
2:k:14:ASN:OD1	2:k:98:THR:HB	2.18	0.44
2:k:15:PHE:CE2	2:k:27:LEU:HD22	2.52	0.44
1:X:280:ASP:O	1:X:281:LEU:HB2	2.16	0.44
2:l:42:TYR:CD1	2:n:129:ALA:CB	2.75	0.44
2:t:9:VAL:HB	2:n:37:GLN:HE22	1.82	0.44
1:N:77:PHE:HB3	1:N:355:GLY:O	2.17	0.44
2:h:15:PHE:CE2	2:h:27:LEU:HD22	2.52	0.44
1:U:72:HIS:CE1	1:U:340:SER:OG	2.71	0.44
2:p:116:ASN:O	2:p:117:ALA:C	2.60	0.44
1:J:431:ASN:OD1	1:J:431:ASN:N	2.47	0.44
2:j:14:ASN:OD1	2:j:98:THR:HB	2.17	0.44
1:Q:77:PHE:HB3	1:Q:355:GLY:O	2.17	0.44
1:R:69:TYR:HD1	1:R:272:ALA:HB2	1.81	0.44
2:r:35:ILE:HB	2:r:59:GLY:O	2.18	0.44
1:F:489:TYR:CD1	1:F:513:GLY:HA2	2.52	0.44
1:S:234:GLU:CG	1:S:277:GLY:HA3	2.48	0.44
1:A:237:HIS:CG	1:A:238:PRO:CD	2.95	0.44
2:b:34:GLN:HE22	2:c:118:TRP:HZ2	1.65	0.44
2:u:9:VAL:HB	2:o:37:GLN:HE22	1.82	0.44
2:o:35:ILE:HB	2:o:59:GLY:O	2.17	0.44
2:o:120:SER:OG	2:o:143:PHE:HE1	2.01	0.44
2:p:128:LYS:C	2:h:42:TYR:OH	2.61	0.44
2:j:38:ASP:C	2:j:38:ASP:OD1	2.58	0.44
1:D:506:GLY:O	1:D:508:VAL:HG23	2.18	0.44
1:Q:459:LEU:HB3	1:Q:507:ARG:HH12	1.83	0.44
1:E:45:LEU:O	1:E:48:PRO:HD2	2.18	0.44
2:e:93:ALA:O	2:e:117:ALA:HB3	2.17	0.44
2:r:35:ILE:CD1	2:s:132:THR:HG21	2.48	0.44
1:F:489:TYR:CE1	1:F:513:GLY:HA2	2.53	0.44
2:s:95:LYS:HB2	2:s:113:ASN:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:76:GLY:HA2	1:M:356:HIS:CE1	2.53	0.44
2:m:34:GLN:HB3	2:n:120:SER:C	2.43	0.44
1:G:282:GLU:O	1:G:283:ALA:C	2.61	0.44
1:I:453:GLU:OE2	1:C:372:LYS:HD2	2.17	0.44
2:i:14:ASN:OD1	2:i:98:THR:HB	2.17	0.44
2:p:124:ALA:CB	2:o:111:ARG:HH12	2.30	0.44
2:p:129:ALA:CA	2:h:42:TYR:CZ	2.76	0.44
1:X:72:HIS:CE1	1:X:340:SER:OG	2.71	0.44
2:x:26:TYR:HB3	2:s:128:LYS:HA	1.98	0.44
1:F:498:ASN:OD1	1:F:508:VAL:N	2.50	0.44
1:S:72:HIS:CE1	1:S:340:SER:OG	2.71	0.44
1:S:452:PHE:HA	1:M:372:LYS:HZ1	1.77	0.44
2:g:14:ASN:OD1	2:g:98:THR:HB	2.18	0.44
2:a:34:GLN:NE2	2:b:118:TRP:HZ2	2.15	0.44
2:a:114:LEU:HD12	2:a:115:ARG:H	1.82	0.44
1:T:72:HIS:CE1	1:T:340:SER:OG	2.71	0.44
1:I:371:HIS:O	1:I:431:ASN:HB2	2.17	0.44
1:I:453:GLU:HG2	1:C:372:LYS:CD	2.45	0.44
1:V:72:HIS:CE1	1:V:340:SER:OG	2.71	0.44
2:d:42:TYR:CD1	2:k:13:PRO:HD2	2.49	0.44
2:q:9:VAL:CG2	2:k:56:LEU:HD22	2.47	0.44
2:q:13:PRO:HG2	2:r:127:LEU:HB3	2.00	0.44
2:x:9:VAL:HB	2:r:37:GLN:HE22	1.82	0.44
1:R:320:ARG:HH21	1:R:333:LEU:HD13	1.83	0.44
2:s:116:ASN:HD21	2:s:145:GLU:CB	2.31	0.44
2:m:25:GLU:HB3	2:m:68:VAL:CG1	2.47	0.44
2:m:94:ARG:HG2	2:m:115:ARG:CA	2.48	0.44
1:A:352:PRO:HA	1:A:353:PRO:HD3	1.88	0.44
2:j:44:GLN:HA	2:q:22:VAL:O	2.17	0.44
1:W:307:PRO:HG2	1:W:337:TRP:NE1	2.32	0.44
1:Q:370:VAL:HG11	1:Q:434:ARG:CB	2.48	0.44
2:q:36:GLU:HB3	2:r:118:TRP:CZ3	2.52	0.44
1:K:279:ILE:HG22	1:K:284:VAL:HG23	2.00	0.44
2:e:43:GLN:HG2	2:e:50:GLY:HA2	1.99	0.44
2:e:100:ILE:HG23	2:e:106:ASP:O	2.18	0.44
1:F:489:TYR:CE2	1:F:491:VAL:HG23	2.53	0.44
1:M:316:ILE:HG12	1:M:320:ARG:HG3	2.00	0.44
1:T:280:ASP:O	1:T:281:LEU:HB2	2.16	0.44
2:n:13:PRO:HG2	2:o:127:LEU:HB3	2.00	0.44
1:U:234:GLU:HG2	1:U:277:GLY:HA3	1.99	0.44
1:V:390:THR:OG1	1:V:391:ARG:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:449:TRP:C	1:V:452:PHE:HD2	2.25	0.44
2:v:128:LYS:HA	2:u:26:TYR:HB3	2.00	0.44
1:D:489:TYR:CD1	1:D:513:GLY:HA2	2.53	0.44
1:R:453:GLU:C	1:R:455:ASN:N	2.76	0.44
2:r:25:GLU:HB3	2:r:68:VAL:CG1	2.46	0.44
1:O:74:VAL:HA	1:O:77:PHE:CE2	2.52	0.44
1:O:453:GLU:C	1:O:455:ASN:N	2.76	0.44
1:Q:365:ASP:O	1:Q:369:GLY:HA2	2.18	0.43
2:k:42:TYR:OH	2:m:129:ALA:HA	2.16	0.43
2:r:13:PRO:HG2	2:m:127:LEU:HB3	2.00	0.43
1:S:489:TYR:HA	1:S:513:GLY:CA	2.28	0.43
2:s:70:ARG:HD2	2:s:70:ARG:HA	1.75	0.43
2:n:36:GLU:HB3	2:o:118:TRP:CZ3	2.53	0.43
1:U:453:GLU:HG3	1:O:372:LYS:CD	2.26	0.43
2:u:116:ASN:HD21	2:u:145:GLU:CB	2.31	0.43
2:o:94:ARG:H	2:o:94:ARG:HG2	1.63	0.43
2:p:14:ASN:HB3	2:i:45:ASN:HA	2.01	0.43
2:d:101:VAL:C	2:d:103:ASP:N	2.74	0.43
1:W:72:HIS:CE1	1:W:340:SER:OG	2.71	0.43
1:W:390:THR:OG1	1:W:391:ARG:N	2.51	0.43
1:E:449:TRP:CZ3	1:E:459:LEU:HD22	2.52	0.43
1:E:489:TYR:CE1	1:E:513:GLY:HA2	2.53	0.43
1:B:489:TYR:CE1	1:B:513:GLY:HA2	2.53	0.43
1:P:74:VAL:HA	1:P:77:PHE:CE2	2.53	0.43
2:p:15:PHE:N	2:i:45:ASN:CG	2.72	0.43
2:p:127:LEU:HB3	2:o:13:PRO:HG2	2.00	0.43
2:d:100:ILE:HG23	2:d:106:ASP:O	2.17	0.43
1:X:234:GLU:HG2	1:X:277:GLY:HA3	2.00	0.43
1:S:235:SER:N	1:S:238:PRO:HG2	2.33	0.43
2:m:5:LYS:N	2:m:6:PRO:CD	2.82	0.43
1:A:453:GLU:CB	1:A:454:PRO:CD	2.74	0.43
1:A:489:TYR:CE2	1:A:491:VAL:HG23	2.54	0.43
2:h:44:GLN:HA	2:o:22:VAL:O	2.17	0.43
2:b:114:LEU:HD23	2:b:116:ASN:HD21	1.83	0.43
1:U:452:PHE:HA	1:O:372:LYS:HZ1	1.79	0.43
2:i:15:PHE:CE2	2:i:27:LEU:HD22	2.52	0.43
2:p:85:SER:HB3	2:p:118:TRP:HE1	1.83	0.43
2:p:120:SER:HA	2:o:34:GLN:OE1	2.17	0.43
1:Q:501:GLU:C	1:Q:503:VAL:N	2.76	0.43
2:r:34:GLN:OE1	2:m:118:TRP:CZ2	2.70	0.43
1:G:449:TRP:HE3	1:G:507:ARG:HH12	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:n:85:SER:HB3	2:n:118:TRP:HE1	1.83	0.43
1:U:390:THR:OG1	1:U:391:ARG:N	2.51	0.43
2:o:68:VAL:HG23	2:o:139:ILE:HD13	2.00	0.43
1:C:269:ASP:OD1	1:C:269:ASP:N	2.45	0.43
2:c:114:LEU:HD23	2:c:145:GLU:HB3	2.00	0.43
1:P:365:ASP:O	1:P:369:GLY:HA2	2.18	0.43
2:p:68:VAL:HG23	2:p:139:ILE:HD13	2.00	0.43
1:D:408:PHE:HB2	1:D:411:ARG:HB2	2.01	0.43
1:W:504:ASP:O	1:W:507:ARG:NH2	2.52	0.43
1:K:90:VAL:HA	1:K:251:THR:HG21	2.00	0.43
1:E:308:PRO:HD2	1:E:311:GLN:HE22	1.82	0.43
1:X:398:ASN:N	1:X:399:PRO:CD	2.82	0.43
1:R:74:VAL:HA	1:R:77:PHE:CE2	2.53	0.43
2:r:42:TYR:CZ	2:s:12:ALA:HB1	2.53	0.43
1:L:370:VAL:HG21	1:L:435:TYR:HA	2.00	0.43
2:s:38:ASP:OD2	2:t:62:LYS:NZ	2.39	0.43
1:A:408:PHE:HB2	1:A:411:ARG:HB2	2.01	0.43
1:A:489:TYR:CD1	1:A:513:GLY:HA2	2.53	0.43
2:t:26:TYR:HB3	2:u:128:LYS:HA	1.99	0.43
1:H:282:GLU:O	1:H:283:ALA:C	2.61	0.43
1:U:398:ASN:N	1:U:399:PRO:CD	2.82	0.43
2:p:34:GLN:HE22	2:q:82:ILE:HD12	1.81	0.43
2:j:15:PHE:CE2	2:j:27:LEU:HD22	2.52	0.43
1:E:309:PRO:HA	1:E:337:TRP:CD1	2.54	0.43
2:m:13:PRO:HG2	2:n:127:LEU:HB3	2.00	0.43
1:H:61:PHE:CE1	1:H:87:VAL:CG1	2.97	0.43
1:B:309:PRO:HA	1:B:337:TRP:CD1	2.54	0.43
1:C:408:PHE:HB2	1:C:411:ARG:HB2	2.01	0.43
2:p:5:LYS:N	2:p:6:PRO:CD	2.81	0.43
1:J:515:ALA:N	1:J:516:PRO:CD	2.82	0.43
1:W:234:GLU:HG2	1:W:277:GLY:HA3	2.00	0.43
1:W:452:PHE:HZ	1:W:507:ARG:HD3	0.63	0.43
2:q:33:LEU:HB3	2:q:61:ALA:HB3	2.00	0.43
2:q:51:ARG:HD2	2:q:51:ARG:HA	1.92	0.43
1:E:237:HIS:CG	1:E:238:PRO:CD	2.95	0.43
1:X:390:THR:OG1	1:X:391:ARG:N	2.51	0.43
2:r:5:LYS:N	2:r:6:PRO:CD	2.81	0.43
1:F:408:PHE:HB2	1:F:411:ARG:HB2	2.01	0.43
2:a:34:GLN:HE22	2:b:118:TRP:HZ2	1.67	0.43
1:B:408:PHE:HB2	1:B:411:ARG:HB2	2.01	0.43
1:W:398:ASN:N	1:W:399:PRO:CD	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:q:5:LYS:N	2:q:6:PRO:CD	2.82	0.43
2:k:15:PHE:HZ	2:k:27:LEU:HB2	1.84	0.43
1:E:408:PHE:HB2	1:E:411:ARG:HB2	2.01	0.43
1:E:489:TYR:CE2	1:E:491:VAL:HG23	2.54	0.43
1:R:454:PRO:HA	1:R:507:ARG:HH12	1.83	0.43
1:S:453:GLU:CG	1:M:372:LYS:CD	2.82	0.43
1:A:237:HIS:CD2	1:A:238:PRO:HD3	2.51	0.43
1:T:390:THR:OG1	1:T:391:ARG:N	2.51	0.43
1:N:45:LEU:O	1:N:48:PRO:HD2	2.19	0.43
1:B:489:TYR:CE2	1:B:491:VAL:HG23	2.53	0.43
1:V:504:ASP:O	1:V:507:ARG:NH2	2.52	0.43
2:v:116:ASN:HD21	2:v:145:GLU:CB	2.32	0.43
1:W:336:PRO:HB3	1:W:387:LEU:HB2	2.01	0.43
2:q:34:GLN:CD	2:r:118:TRP:CZ2	2.97	0.43
2:q:35:ILE:CG2	2:x:132:THR:CG2	2.87	0.43
2:l:15:PHE:HZ	2:l:27:LEU:HB2	1.84	0.43
1:G:469:ALA:HB3	2:a:115:ARG:NH2	2.34	0.43
2:a:42:TYR:CD1	2:h:13:PRO:HD2	2.50	0.43
1:T:398:ASN:N	1:T:399:PRO:CD	2.82	0.43
1:N:453:GLU:C	1:N:455:ASN:N	2.76	0.43
1:J:46:ASN:O	1:J:251:THR:HG22	2.19	0.43
1:J:371:HIS:O	1:J:431:ASN:HB2	2.18	0.43
1:K:515:ALA:N	1:K:516:PRO:CD	2.82	0.43
2:x:116:ASN:HD21	2:x:145:GLU:CB	2.32	0.43
2:s:26:TYR:HB3	2:t:128:LYS:HA	2.00	0.43
1:M:41:PRO:HG3	1:M:66:GLY:HA3	2.01	0.43
1:A:493:CYS:SG	1:A:509:VAL:HG22	2.59	0.43
1:N:368:ARG:HB3	1:N:371:HIS:CE1	2.46	0.43
2:n:5:LYS:N	2:n:6:PRO:CD	2.81	0.43
1:C:310:ASN:O	1:C:311:GLN:HB3	2.19	0.43
2:p:94:ARG:NH2	2:p:115:ARG:HD3	2.15	0.42
1:D:310:ASN:O	1:D:311:GLN:HB3	2.19	0.42
2:d:34:GLN:HE21	2:e:86:MET:HA	1.82	0.42
1:W:453:GLU:HG2	1:Q:372:LYS:CB	2.35	0.42
2:f:42:TYR:CD1	2:g:13:PRO:HD2	2.48	0.42
1:S:390:THR:OG1	1:S:391:ARG:N	2.51	0.42
1:M:89:ARG:CZ	1:M:91:GLY:HA2	2.49	0.42
1:T:335:TYR:CD1	1:T:402:VAL:HG12	2.54	0.42
1:B:80:ASN:HB3	1:B:363:ARG:CD	2.48	0.42
2:o:5:LYS:N	2:o:6:PRO:CD	2.81	0.42
1:I:515:ALA:N	1:I:516:PRO:CD	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:234:GLU:HG2	1:V:277:GLY:HA3	2.00	0.42
1:V:398:ASN:N	1:V:399:PRO:CD	2.82	0.42
1:P:501:GLU:H	1:P:501:GLU:CD	2.27	0.42
1:P:507:ARG:HE	1:P:507:ARG:N	2.17	0.42
2:p:13:PRO:HG2	2:q:127:LEU:HB3	2.00	0.42
2:j:15:PHE:HZ	2:j:27:LEU:HB2	1.84	0.42
1:R:76:GLY:HA2	1:R:356:HIS:CE1	2.55	0.42
2:r:51:ARG:HD2	2:r:51:ARG:HA	1.92	0.42
1:L:367:GLU:HG2	1:L:368:ARG:NH1	2.34	0.42
1:M:270:LEU:HD13	1:M:284:VAL:HG13	1.96	0.42
1:H:88:VAL:CG1	1:H:251:THR:HB	2.50	0.42
1:U:335:TYR:CD1	1:U:402:VAL:HG12	2.54	0.42
1:O:406:ARG:HB2	1:O:416:TRP:CD1	2.54	0.42
1:C:489:TYR:CD1	1:C:513:GLY:HA2	2.54	0.42
1:C:489:TYR:CE2	1:C:491:VAL:HG23	2.54	0.42
1:D:489:TYR:CE2	1:D:491:VAL:HG23	2.53	0.42
1:W:269:ASP:OD1	1:W:276:ARG:NH2	2.53	0.42
1:K:367:GLU:HG2	1:K:368:ARG:NH1	2.34	0.42
1:R:316:ILE:HG12	1:R:320:ARG:HG3	2.00	0.42
2:r:85:SER:HB3	2:r:118:TRP:HE1	1.84	0.42
1:L:453:GLU:HG2	1:F:372:LYS:CD	2.46	0.42
2:f:1:MET:HE3	2:f:106:ASP:OD2	2.20	0.42
2:f:101:VAL:C	2:f:103:ASP:N	2.77	0.42
1:S:504:ASP:O	1:S:507:ARG:NH2	2.52	0.42
1:M:74:VAL:HA	1:M:77:PHE:CD2	2.54	0.42
1:N:270:LEU:C	1:N:272:ALA:N	2.77	0.42
2:n:68:VAL:HG23	2:n:139:ILE:HD13	2.00	0.42
1:B:237:HIS:CG	1:B:238:PRO:CD	2.96	0.42
1:U:504:ASP:O	1:U:507:ARG:NH2	2.52	0.42
1:O:503:VAL:HG12	1:O:505:LEU:H	1.84	0.42
2:p:35:ILE:CG2	2:w:132:THR:CG2	2.84	0.42
1:R:40:ALA:HB3	1:R:89:ARG:NH1	2.34	0.42
1:R:406:ARG:HB2	1:R:416:TRP:CD1	2.55	0.42
2:r:68:VAL:HG23	2:r:139:ILE:HD13	2.00	0.42
1:F:69:TYR:O	1:F:70:LEU:C	2.62	0.42
2:f:114:LEU:HD12	2:f:115:ARG:N	2.33	0.42
2:n:113:ASN:OD1	2:n:114:LEU:N	2.52	0.42
1:O:269:ASP:O	1:O:272:ALA:HB3	2.20	0.42
2:i:15:PHE:HZ	2:i:27:LEU:HB2	1.84	0.42
1:V:63:ASP:O	1:V:64:PHE:HB2	2.20	0.42
1:Q:89:ARG:HB3	1:Q:89:ARG:NH1	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:449:TRP:HZ3	1:E:459:LEU:HD22	1.84	0.42
2:g:15:PHE:HZ	2:g:27:LEU:HB2	1.84	0.42
1:O:43:GLY:O	1:O:89:ARG:NH1	2.53	0.42
1:P:76:GLY:HA2	1:P:356:HIS:CE1	2.55	0.42
2:w:116:ASN:HD21	2:w:145:GLU:CB	2.32	0.42
1:Q:41:PRO:HG3	1:Q:66:GLY:CA	2.50	0.42
1:E:69:TYR:O	1:E:70:LEU:C	2.62	0.42
1:L:515:ALA:N	1:L:516:PRO:CD	2.82	0.42
1:S:398:ASN:N	1:S:399:PRO:CD	2.82	0.42
1:G:244:LEU:HD12	1:G:249:ASP:HA	2.02	0.42
1:G:453:GLU:CD	1:A:372:LYS:HD2	2.45	0.42
1:H:515:ALA:N	1:H:516:PRO:CD	2.82	0.42
2:q:68:VAL:HG23	2:q:139:ILE:HD13	2.00	0.42
2:q:113:ASN:OD1	2:q:114:LEU:N	2.52	0.42
1:K:282:GLU:OE1	1:K:285:LYS:HD3	2.19	0.42
1:F:310:ASN:O	1:F:311:GLN:HB3	2.19	0.42
1:S:335:TYR:CD1	1:S:402:VAL:HG12	2.54	0.42
1:A:311:GLN:HG3	1:A:316:ILE:HD11	2.01	0.42
2:h:15:PHE:HZ	2:h:27:LEU:HB2	1.84	0.42
2:b:115:ARG:HD3	2:b:116:ASN:H	1.84	0.42
2:o:85:SER:HB3	2:o:118:TRP:HE1	1.85	0.42
1:C:45:LEU:O	1:C:48:PRO:HD2	2.19	0.42
2:p:113:ASN:OD1	2:p:114:LEU:N	2.52	0.42
1:X:63:ASP:O	1:X:64:PHE:HB2	2.20	0.42
2:r:113:ASN:OD1	2:r:114:LEU:N	2.52	0.42
1:G:515:ALA:N	1:G:516:PRO:CD	2.82	0.42
1:U:269:ASP:OD1	1:U:276:ARG:NH2	2.51	0.42
2:o:3:LEU:O	2:o:6:PRO:HD2	2.20	0.42
2:o:33:LEU:HD23	2:o:61:ALA:HB2	2.02	0.42
1:V:269:ASP:OD1	1:V:276:ARG:NH2	2.51	0.42
1:P:274:TYR:HA	1:P:279:ILE:C	2.45	0.42
1:J:453:GLU:CD	1:D:372:LYS:HD2	2.44	0.42
1:D:489:TYR:CE1	1:D:513:GLY:HA2	2.54	0.42
1:W:465:ARG:HG3	2:q:94:ARG:NH2	2.35	0.42
2:q:85:SER:HB3	2:q:118:TRP:HE1	1.84	0.42
1:X:504:ASP:O	1:X:507:ARG:NH2	2.52	0.42
1:S:512:ILE:HG22	1:S:513:GLY:N	2.23	0.42
1:M:77:PHE:HB3	1:M:355:GLY:O	2.20	0.42
1:N:269:ASP:OD1	1:N:269:ASP:N	2.53	0.42
2:n:94:ARG:CA	2:n:115:ARG:HA	2.50	0.42
1:B:32:SER:O	1:B:83:SER:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:307:PRO:HG2	1:U:337:TRP:HE1	1.85	0.42
2:p:35:ILE:HB	2:p:59:GLY:O	2.20	0.42
2:p:85:SER:CB	2:o:34:GLN:NE2	2.70	0.42
1:Q:244:LEU:HG	1:Q:247:SER:H	1.85	0.42
2:f:34:GLN:HE22	2:a:118:TRP:HZ2	1.66	0.42
2:m:85:SER:HB3	2:m:118:TRP:HE1	1.85	0.42
1:N:46:ASN:N	1:N:89:ARG:HD2	2.34	0.42
1:O:274:TYR:HA	1:O:279:ILE:C	2.45	0.42
2:o:51:ARG:HD2	2:o:51:ARG:HA	1.93	0.42
1:I:490:TYR:OH	1:I:492:LYS:HD2	2.20	0.42
1:W:408:PHE:HB2	1:W:411:ARG:HB2	2.02	0.41
1:Q:365:ASP:CG	1:Q:370:VAL:HG22	2.44	0.41
1:Q:453:GLU:C	1:Q:455:ASN:N	2.78	0.41
2:q:34:GLN:HB3	2:r:120:SER:O	2.19	0.41
1:K:369:GLY:HA3	1:K:371:HIS:NE2	2.35	0.41
1:X:408:PHE:HB2	1:X:411:ARG:HB2	2.02	0.41
1:G:367:GLU:HG2	1:G:368:ARG:NH1	2.35	0.41
2:g:15:PHE:CE2	2:g:27:LEU:HD22	2.55	0.41
1:A:489:TYR:CE1	1:A:513:GLY:HA2	2.54	0.41
1:B:76:GLY:O	1:B:79:ASN:HB3	2.19	0.41
1:X:336:PRO:HB3	1:X:387:LEU:HB2	2.01	0.41
1:S:307:PRO:HG2	1:S:337:TRP:NE1	2.35	0.41
1:M:244:LEU:HG	1:M:247:SER:H	1.85	0.41
2:m:94:ARG:HG2	2:m:115:ARG:HA	2.03	0.41
2:g:114:LEU:HD23	2:g:145:GLU:CD	2.45	0.41
2:h:114:LEU:HD23	2:h:145:GLU:CD	2.45	0.41
2:v:5:LYS:NZ	2:p:51:ARG:NH2	2.67	0.41
2:v:132:THR:HG21	2:o:35:ILE:CD1	2.49	0.41
2:p:3:LEU:O	2:p:6:PRO:HD2	2.20	0.41
2:p:34:GLN:HB3	2:q:120:SER:HA	2.02	0.41
1:Q:463:ILE:HD11	1:Q:507:ARG:NH1	2.35	0.41
2:e:44:GLN:HG2	2:l:22:VAL:HG12	2.03	0.41
1:S:307:PRO:HG2	1:S:337:TRP:HE1	1.85	0.41
2:s:70:ARG:HH21	2:s:135:LEU:HD13	1.85	0.41
1:T:307:PRO:HG2	1:T:337:TRP:HE1	1.85	0.41
2:n:3:LEU:O	2:n:6:PRO:HD2	2.20	0.41
2:n:87:ALA:HB3	2:n:89:ARG:NE	2.35	0.41
1:V:52:THR:OG1	1:V:53:ASN:N	2.46	0.41
1:V:335:TYR:CD1	1:V:402:VAL:HG12	2.54	0.41
2:q:34:GLN:OE1	2:r:118:TRP:CZ2	2.72	0.41
1:K:466:ASN:O	2:e:115:ARG:NH2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:499:PRO:HA	1:K:500:PRO:HD3	1.92	0.41
1:E:52:THR:OG1	1:E:53:ASN:N	2.48	0.41
1:F:69:TYR:HA	1:F:72:HIS:CE1	2.56	0.41
2:m:42:TYR:CE2	2:t:14:ASN:HA	2.56	0.41
1:A:69:TYR:O	1:A:70:LEU:C	2.62	0.41
1:T:63:ASP:O	1:T:64:PHE:HB2	2.20	0.41
1:N:244:LEU:HG	1:N:247:SER:H	1.85	0.41
1:B:69:TYR:O	1:B:70:LEU:C	2.62	0.41
1:P:500:PRO:C	1:P:502:SER:N	2.79	0.41
2:q:94:ARG:H	2:q:94:ARG:HG2	1.63	0.41
2:r:35:ILE:O	2:r:58:PRO:HD2	2.21	0.41
1:L:46:ASN:OD1	1:L:46:ASN:N	2.50	0.41
2:l:14:ASN:OD1	2:l:98:THR:HB	2.21	0.41
1:F:506:GLY:O	1:F:508:VAL:HG23	2.20	0.41
1:S:63:ASP:O	1:S:64:PHE:HB2	2.20	0.41
2:m:113:ASN:OD1	2:m:114:LEU:N	2.52	0.41
2:u:9:VAL:O	2:u:11:VAL:HG23	2.20	0.41
2:o:113:ASN:OD1	2:o:114:LEU:N	2.52	0.41
1:I:243:TYR:CE2	1:I:250:ARG:HD2	2.55	0.41
1:V:408:PHE:HB2	1:V:411:ARG:HB2	2.02	0.41
2:v:9:VAL:O	2:v:11:VAL:HG23	2.20	0.41
2:p:43:GLN:HB2	2:p:48:THR:OG1	2.21	0.41
1:Q:40:ALA:HB3	1:Q:89:ARG:CG	2.37	0.41
1:R:244:LEU:HG	1:R:247:SER:H	1.85	0.41
2:r:3:LEU:O	2:r:6:PRO:HD2	2.20	0.41
2:l:114:LEU:HD23	2:l:145:GLU:CD	2.45	0.41
2:a:115:ARG:O	2:a:117:ALA:N	2.53	0.41
1:T:234:GLU:HG2	1:T:277:GLY:HA3	2.01	0.41
1:B:9:VAL:HA	1:B:505:LEU:CD1	2.51	0.41
1:U:54:TRP:HH2	1:U:64:PHE:CE1	2.39	0.41
1:U:307:PRO:HG2	1:U:337:TRP:NE1	2.35	0.41
1:O:89:ARG:O	1:O:90:VAL:HB	2.20	0.41
1:W:63:ASP:O	1:W:64:PHE:HB2	2.20	0.41
1:L:47:GLU:N	1:L:48:PRO:HD2	2.36	0.41
2:l:53:ASN:OD1	2:l:53:ASN:C	2.64	0.41
1:S:269:ASP:OD1	1:S:276:ARG:NH2	2.51	0.41
1:S:408:PHE:HB2	1:S:411:ARG:HB2	2.02	0.41
1:H:90:VAL:HA	1:H:251:THR:HG21	2.01	0.41
1:H:368:ARG:HG3	1:H:372:LYS:CD	2.48	0.41
1:B:69:TYR:HA	1:B:72:HIS:CE1	2.54	0.41
1:V:451:VAL:HB	1:P:375:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:p:129:ALA:HA	2:h:42:TYR:OH	2.17	0.41
2:j:13:PRO:HD2	2:c:42:TYR:CD1	2.48	0.41
2:j:53:ASN:OD1	2:j:53:ASN:C	2.64	0.41
2:w:9:VAL:O	2:w:11:VAL:HG23	2.21	0.41
1:K:47:GLU:N	1:K:48:PRO:HD2	2.36	0.41
2:k:114:LEU:HD23	2:k:145:GLU:CD	2.45	0.41
1:X:465:ARG:HG3	2:r:94:ARG:NH2	2.36	0.41
2:s:9:VAL:O	2:s:11:VAL:HG23	2.20	0.41
2:m:3:LEU:O	2:m:6:PRO:HD2	2.20	0.41
1:T:307:PRO:HG2	1:T:337:TRP:NE1	2.35	0.41
2:b:115:ARG:NH1	2:b:116:ASN:HB3	2.36	0.41
1:U:63:ASP:O	1:U:64:PHE:HB2	2.21	0.41
1:P:237:HIS:HB2	1:P:238:PRO:HD3	2.03	0.41
1:P:342:ASP:OD1	1:P:342:ASP:C	2.64	0.41
2:p:35:ILE:CD1	2:w:132:THR:HG21	2.49	0.41
1:J:61:PHE:CZ	1:J:87:VAL:CG1	3.01	0.41
1:J:273:ALA:O	1:J:274:TYR:C	2.64	0.41
1:J:453:GLU:HG2	1:D:372:LYS:CD	2.45	0.41
1:D:352:PRO:HA	1:D:353:PRO:HD3	1.88	0.41
1:Q:342:ASP:OD1	1:Q:342:ASP:C	2.64	0.41
2:e:69:GLU:HB3	2:e:138:THR:OG1	2.21	0.41
1:R:368:ARG:HB3	1:R:371:HIS:CE1	2.53	0.41
1:R:452:PHE:CD2	1:R:452:PHE:O	2.74	0.41
1:L:46:ASN:O	1:L:251:THR:HG22	2.20	0.41
1:L:61:PHE:CE1	1:L:87:VAL:CG1	2.95	0.41
1:L:243:TYR:O	1:L:250:ARG:HB2	2.21	0.41
1:F:41:PRO:O	1:F:42:THR:C	2.64	0.41
1:S:54:TRP:HH2	1:S:64:PHE:CE1	2.39	0.41
2:a:69:GLU:HB3	2:a:138:THR:OG1	2.21	0.41
1:T:54:TRP:HH2	1:T:64:PHE:CE1	2.39	0.41
1:T:408:PHE:HB2	1:T:411:ARG:HB2	2.02	0.41
2:t:9:VAL:O	2:t:11:VAL:HG23	2.21	0.41
1:N:342:ASP:C	1:N:342:ASP:OD1	2.64	0.41
2:n:35:ILE:O	2:n:58:PRO:HD2	2.21	0.41
1:H:253:PHE:CE2	1:H:291:LEU:HD13	2.55	0.41
1:H:453:GLU:HG2	1:B:372:LYS:CD	2.45	0.41
2:b:85:SER:OG	2:b:118:TRP:NE1	2.54	0.41
1:U:408:PHE:HB2	1:U:411:ARG:HB2	2.02	0.41
1:O:244:LEU:HG	1:O:247:SER:H	1.85	0.41
1:I:46:ASN:O	1:I:251:THR:HG22	2.21	0.41
2:c:5:LYS:N	2:c:6:PRO:CD	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:101:VAL:C	2:c:103:ASP:N	2.78	0.41
1:V:307:PRO:HG2	1:V:337:TRP:HE1	1.86	0.41
2:p:82:ILE:CD1	2:o:34:GLN:OE1	2.69	0.41
2:j:114:LEU:HD23	2:j:145:GLU:CD	2.45	0.41
2:d:101:VAL:O	2:d:103:ASP:N	2.54	0.41
1:Q:45:LEU:O	1:Q:48:PRO:HD2	2.21	0.41
1:E:309:PRO:HA	1:E:337:TRP:NE1	2.35	0.41
1:R:45:LEU:C	1:R:89:ARG:HG2	2.46	0.41
1:L:248:SER:HB2	1:L:250:ARG:HG3	2.02	0.41
1:S:453:GLU:HG3	1:M:372:LYS:CD	2.23	0.41
1:N:270:LEU:C	1:N:270:LEU:HD13	2.46	0.41
2:b:5:LYS:N	2:b:6:PRO:CD	2.83	0.41
2:q:3:LEU:O	2:q:6:PRO:HD2	2.20	0.40
2:q:43:GLN:HB2	2:q:48:THR:OG1	2.21	0.40
1:X:269:ASP:OD1	1:X:276:ARG:NH2	2.51	0.40
1:S:451:VAL:HB	1:M:375:ALA:HB3	2.03	0.40
1:A:6:SER:HB2	1:A:507:ARG:NH2	2.35	0.40
2:h:53:ASN:OD1	2:h:53:ASN:C	2.64	0.40
2:b:69:GLU:HB3	2:b:138:THR:OG1	2.21	0.40
1:U:72:HIS:CG	1:U:351:VAL:HG21	2.56	0.40
1:I:282:GLU:HA	1:I:285:LYS:HB3	2.03	0.40
1:I:453:GLU:CD	1:C:372:LYS:HD2	2.46	0.40
2:i:114:LEU:HD23	2:i:145:GLU:CD	2.45	0.40
1:V:307:PRO:HG2	1:V:337:TRP:NE1	2.36	0.40
2:p:69:GLU:O	2:p:70:ARG:C	2.65	0.40
2:p:120:SER:CA	2:o:34:GLN:HB3	2.50	0.40
2:d:43:GLN:HG2	2:d:50:GLY:HA2	2.03	0.40
1:W:452:PHE:CZ	1:W:507:ARG:NE	2.85	0.40
1:X:54:TRP:HH2	1:X:64:PHE:CE1	2.39	0.40
1:X:72:HIS:CG	1:X:351:VAL:HG21	2.56	0.40
1:L:246:ASP:O	1:L:247:SER:HB2	2.21	0.40
1:M:45:LEU:O	1:M:48:PRO:HD2	2.22	0.40
1:G:42:THR:OG1	1:G:43:GLY:N	2.54	0.40
1:T:504:ASP:O	1:T:507:ARG:NH2	2.52	0.40
1:B:93:SER:OG	1:B:94:ALA:N	2.49	0.40
2:o:43:GLN:HB2	2:o:48:THR:OG1	2.21	0.40
1:C:506:GLY:O	1:C:508:VAL:HG23	2.21	0.40
2:c:69:GLU:HB3	2:c:138:THR:OG1	2.21	0.40
1:P:244:LEU:HG	1:P:247:SER:H	1.85	0.40
2:p:34:GLN:NE2	2:q:119:CYS:O	2.55	0.40
2:q:35:ILE:O	2:q:58:PRO:HD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:44:GLN:HG2	2:l:22:VAL:CG1	2.52	0.40
1:L:453:GLU:OE2	1:F:372:LYS:HD2	2.21	0.40
2:f:42:TYR:HE1	2:g:13:PRO:HD2	1.67	0.40
1:S:452:PHE:HZ	1:S:507:ARG:NE	2.11	0.40
2:m:68:VAL:HG23	2:m:139:ILE:HD13	2.01	0.40
1:G:46:ASN:O	1:G:251:THR:HG22	2.21	0.40
2:a:5:LYS:N	2:a:6:PRO:CD	2.83	0.40
1:V:54:TRP:HH2	1:V:64:PHE:CE1	2.39	0.40
1:V:72:HIS:CG	1:V:351:VAL:HG21	2.57	0.40
1:V:335:TYR:CB	1:V:336:PRO:CD	3.00	0.40
2:p:120:SER:HG	2:p:143:PHE:HE1	1.69	0.40
1:D:46:ASN:HA	1:D:89:ARG:HB3	2.04	0.40
1:W:335:TYR:CD1	1:W:402:VAL:HG12	2.56	0.40
1:Q:515:ALA:N	1:Q:516:PRO:CD	2.85	0.40
2:k:51:ARG:HH22	1:R:477:ASN:HD21	1.69	0.40
1:X:335:TYR:CD1	1:X:402:VAL:HG12	2.56	0.40
1:R:89:ARG:HG3	1:R:90:VAL:N	2.37	0.40
1:S:72:HIS:CG	1:S:351:VAL:HG21	2.57	0.40
1:M:342:ASP:C	1:M:342:ASP:OD1	2.64	0.40
1:G:61:PHE:HE2	1:G:87:VAL:HG11	1.73	0.40
2:a:44:GLN:HG2	2:h:22:VAL:HG12	2.03	0.40
1:T:451:VAL:HB	1:N:375:ALA:HB3	2.03	0.40
2:h:51:ARG:HH22	1:O:477:ASN:HD21	1.69	0.40
1:U:234:GLU:HG2	1:U:277:GLY:CA	2.52	0.40
1:C:80:ASN:OD1	1:C:380:ARG:HD3	2.22	0.40
1:J:282:GLU:HA	1:J:285:LYS:HB3	2.03	0.40
1:D:69:TYR:O	1:D:70:LEU:C	2.62	0.40
2:d:69:GLU:HB3	2:d:138:THR:OG1	2.21	0.40
1:W:451:VAL:HB	1:Q:375:ALA:HB3	2.03	0.40
2:q:42:TYR:CE2	2:x:14:ASN:HA	2.56	0.40
1:E:43:GLY:H	1:E:89:ARG:CZ	2.34	0.40
2:e:94:ARG:HA	2:e:115:ARG:HA	2.03	0.40
2:m:34:GLN:HB2	2:n:82:ILE:HD11	2.03	0.40
1:G:47:GLU:N	1:G:48:PRO:HD2	2.36	0.40
1:G:367:GLU:HG2	1:G:368:ARG:HG2	2.03	0.40
2:n:44:GLN:OE1	2:n:44:GLN:HA	2.21	0.40
1:B:46:ASN:HA	1:B:89:ARG:HB3	2.04	0.40
1:B:309:PRO:HA	1:B:337:TRP:NE1	2.36	0.40
1:O:342:ASP:OD1	1:O:342:ASP:C	2.64	0.40
1:C:46:ASN:HA	1:C:89:ARG:HB3	2.04	0.40
1:C:68:TYR:CZ	1:C:70:LEU:HD13	2.57	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	365/539 (68%)	343 (94%)	20 (6%)	2 (0%)	24	59
1	B	365/539 (68%)	341 (93%)	21 (6%)	3 (1%)	16	50
1	C	365/539 (68%)	344 (94%)	19 (5%)	2 (0%)	24	59
1	D	365/539 (68%)	343 (94%)	20 (6%)	2 (0%)	24	59
1	E	365/539 (68%)	345 (94%)	20 (6%)	0	100	100
1	F	365/539 (68%)	344 (94%)	19 (5%)	2 (0%)	24	59
1	G	365/539 (68%)	339 (93%)	23 (6%)	3 (1%)	16	50
1	H	365/539 (68%)	335 (92%)	26 (7%)	4 (1%)	11	43
1	I	365/539 (68%)	340 (93%)	22 (6%)	3 (1%)	16	50
1	J	365/539 (68%)	340 (93%)	22 (6%)	3 (1%)	16	50
1	K	365/539 (68%)	341 (93%)	21 (6%)	3 (1%)	16	50
1	L	365/539 (68%)	339 (93%)	23 (6%)	3 (1%)	16	50
1	M	365/539 (68%)	339 (93%)	22 (6%)	4 (1%)	11	43
1	N	365/539 (68%)	342 (94%)	19 (5%)	4 (1%)	11	43
1	O	365/539 (68%)	339 (93%)	22 (6%)	4 (1%)	11	43
1	P	365/539 (68%)	339 (93%)	22 (6%)	4 (1%)	11	43
1	Q	365/539 (68%)	340 (93%)	21 (6%)	4 (1%)	11	43
1	R	365/539 (68%)	342 (94%)	20 (6%)	3 (1%)	16	50
1	S	365/539 (68%)	328 (90%)	35 (10%)	2 (0%)	24	59
1	T	365/539 (68%)	331 (91%)	29 (8%)	5 (1%)	9	38
1	U	365/539 (68%)	331 (91%)	27 (7%)	7 (2%)	6	33
1	V	365/539 (68%)	331 (91%)	29 (8%)	5 (1%)	9	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	W	365/539 (68%)	331 (91%)	28 (8%)	6 (2%)	7	36
1	X	365/539 (68%)	331 (91%)	29 (8%)	5 (1%)	9	38
2	a	147/149 (99%)	135 (92%)	11 (8%)	1 (1%)	18	53
2	b	147/149 (99%)	133 (90%)	13 (9%)	1 (1%)	18	53
2	c	147/149 (99%)	135 (92%)	11 (8%)	1 (1%)	18	53
2	d	147/149 (99%)	134 (91%)	12 (8%)	1 (1%)	18	53
2	e	147/149 (99%)	135 (92%)	12 (8%)	0	100	100
2	f	147/149 (99%)	135 (92%)	12 (8%)	0	100	100
2	g	147/149 (99%)	142 (97%)	4 (3%)	1 (1%)	18	53
2	h	147/149 (99%)	142 (97%)	4 (3%)	1 (1%)	18	53
2	i	147/149 (99%)	142 (97%)	4 (3%)	1 (1%)	18	53
2	j	147/149 (99%)	142 (97%)	4 (3%)	1 (1%)	18	53
2	k	147/149 (99%)	142 (97%)	4 (3%)	1 (1%)	18	53
2	l	147/149 (99%)	142 (97%)	4 (3%)	1 (1%)	18	53
2	m	147/149 (99%)	138 (94%)	8 (5%)	1 (1%)	18	53
2	n	147/149 (99%)	138 (94%)	7 (5%)	2 (1%)	9	38
2	o	147/149 (99%)	138 (94%)	8 (5%)	1 (1%)	18	53
2	p	147/149 (99%)	138 (94%)	8 (5%)	1 (1%)	18	53
2	q	147/149 (99%)	138 (94%)	7 (5%)	2 (1%)	9	38
2	r	147/149 (99%)	138 (94%)	8 (5%)	1 (1%)	18	53
2	s	147/149 (99%)	143 (97%)	4 (3%)	0	100	100
2	t	147/149 (99%)	142 (97%)	5 (3%)	0	100	100
2	u	147/149 (99%)	143 (97%)	4 (3%)	0	100	100
2	v	147/149 (99%)	143 (97%)	4 (3%)	0	100	100
2	w	147/149 (99%)	143 (97%)	4 (3%)	0	100	100
2	x	147/149 (99%)	143 (97%)	4 (3%)	0	100	100
All	All	12288/16512 (74%)	11462 (93%)	725 (6%)	101 (1%)	18	50

All (101) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	V	4	TYR
1	P	515	ALA

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Mol	Chain	Res	Type
2	p	45	ASN
1	J	453	GLU
2	j	44	GLN
1	D	455	ASN
1	W	4	TYR
1	W	453	GLU
1	Q	515	ALA
2	q	45	ASN
1	K	453	GLU
2	k	44	GLN
1	X	4	TYR
1	X	453	GLU
1	R	515	ALA
2	r	45	ASN
1	L	453	GLU
2	l	44	GLN
1	F	455	ASN
1	S	453	GLU
1	M	515	ALA
2	m	45	ASN
1	G	453	GLU
2	g	44	GLN
1	A	455	ASN
1	T	4	TYR
1	T	453	GLU
1	N	515	ALA
2	n	45	ASN
1	H	453	GLU
2	h	44	GLN
1	B	455	ASN
1	U	4	TYR
1	U	453	GLU
1	O	515	ALA
2	o	45	ASN
1	I	453	GLU
2	i	45	ASN
1	C	455	ASN
1	P	514	ILE
1	Q	514	ILE
1	R	514	ILE
1	M	514	ILE
1	N	514	ILE

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Mol	Chain	Res	Type
1	B	83	SER
1	O	514	ILE
1	P	271	MET
1	J	454	PRO
1	D	451	VAL
1	K	454	PRO
1	L	454	PRO
1	F	451	VAL
1	M	271	MET
1	G	454	PRO
1	A	451	VAL
2	a	116	ASN
1	H	454	PRO
1	B	451	VAL
2	b	116	ASN
1	O	271	MET
1	I	454	PRO
1	C	451	VAL
2	c	117	ALA
1	V	237	HIS
1	V	453	GLU
1	W	237	HIS
1	X	237	HIS
1	T	237	HIS
1	N	271	MET
1	U	237	HIS
1	J	451	VAL
2	d	114	LEU
1	K	451	VAL
1	L	451	VAL
1	M	454	PRO
1	G	451	VAL
1	H	451	VAL
1	U	281	LEU
1	O	505	LEU
1	I	451	VAL
1	W	504	ASP
2	q	44	GLN
2	n	44	GLN
1	H	253	PHE
1	U	504	ASP
1	V	451	VAL

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Mol	Chain	Res	Type
1	V	514	ILE
1	W	451	VAL
1	W	514	ILE
1	X	451	VAL
1	X	514	ILE
1	S	451	VAL
1	T	451	VAL
1	T	514	ILE
1	U	451	VAL
1	U	514	ILE
1	P	454	PRO
1	R	90	VAL
1	N	90	VAL
1	Q	454	PRO
1	Q	90	VAL

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	295/417 (71%)	295 (100%)	0	100	100
1	B	295/417 (71%)	294 (100%)	1 (0%)	86	85
1	C	295/417 (71%)	295 (100%)	0	100	100
1	D	295/417 (71%)	295 (100%)	0	100	100
1	E	295/417 (71%)	294 (100%)	1 (0%)	86	85
1	F	295/417 (71%)	295 (100%)	0	100	100
1	G	295/417 (71%)	295 (100%)	0	100	100
1	H	295/417 (71%)	294 (100%)	1 (0%)	86	85
1	I	295/417 (71%)	295 (100%)	0	100	100
1	J	295/417 (71%)	295 (100%)	0	100	100
1	K	295/417 (71%)	295 (100%)	0	100	100
1	L	295/417 (71%)	295 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	295/417 (71%)	291 (99%)	4 (1%)	59	71
1	N	295/417 (71%)	291 (99%)	4 (1%)	59	71
1	O	295/417 (71%)	292 (99%)	3 (1%)	68	75
1	P	295/417 (71%)	290 (98%)	5 (2%)	53	68
1	Q	295/417 (71%)	291 (99%)	4 (1%)	59	71
1	R	295/417 (71%)	291 (99%)	4 (1%)	59	71
1	S	295/417 (71%)	292 (99%)	3 (1%)	68	75
1	T	295/417 (71%)	293 (99%)	2 (1%)	76	78
1	U	295/417 (71%)	293 (99%)	2 (1%)	76	78
1	V	295/417 (71%)	293 (99%)	2 (1%)	76	78
1	W	295/417 (71%)	293 (99%)	2 (1%)	76	78
1	X	295/417 (71%)	293 (99%)	2 (1%)	76	78
2	a	129/129 (100%)	129 (100%)	0	100	100
2	b	129/129 (100%)	128 (99%)	1 (1%)	73	77
2	c	129/129 (100%)	129 (100%)	0	100	100
2	d	129/129 (100%)	129 (100%)	0	100	100
2	e	129/129 (100%)	129 (100%)	0	100	100
2	f	129/129 (100%)	128 (99%)	1 (1%)	73	77
2	g	129/129 (100%)	129 (100%)	0	100	100
2	h	129/129 (100%)	129 (100%)	0	100	100
2	i	129/129 (100%)	129 (100%)	0	100	100
2	j	129/129 (100%)	129 (100%)	0	100	100
2	k	129/129 (100%)	129 (100%)	0	100	100
2	l	129/129 (100%)	129 (100%)	0	100	100
2	m	129/129 (100%)	129 (100%)	0	100	100
2	n	129/129 (100%)	129 (100%)	0	100	100
2	o	129/129 (100%)	128 (99%)	1 (1%)	73	77
2	p	129/129 (100%)	128 (99%)	1 (1%)	73	77
2	q	129/129 (100%)	128 (99%)	1 (1%)	73	77
2	r	129/129 (100%)	128 (99%)	1 (1%)	73	77
2	s	129/129 (100%)	129 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	t	129/129 (100%)	129 (100%)	0	100	100
2	u	129/129 (100%)	129 (100%)	0	100	100
2	v	129/129 (100%)	129 (100%)	0	100	100
2	w	129/129 (100%)	129 (100%)	0	100	100
2	x	129/129 (100%)	129 (100%)	0	100	100
All	All	10176/13104 (78%)	10130 (100%)	46 (0%)	78	82

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	V	451	VAL
1	V	475	TRP
1	P	89	ARG
1	P	269	ASP
1	P	271	MET
1	P	471	LEU
1	P	507	ARG
2	p	94	ARG
1	W	451	VAL
1	W	475	TRP
1	Q	269	ASP
1	Q	270	LEU
1	Q	471	LEU
1	Q	503	VAL
2	q	94	ARG
1	E	505	LEU
1	X	451	VAL
1	X	475	TRP
1	R	89	ARG
1	R	269	ASP
1	R	270	LEU
1	R	471	LEU
2	r	94	ARG
2	f	7	GLU
1	S	237	HIS
1	S	451	VAL
1	S	475	TRP
1	M	269	ASP
1	M	271	MET
1	M	471	LEU

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Mol	Chain	Res	Type
1	M	507	ARG
1	T	451	VAL
1	T	475	TRP
1	N	269	ASP
1	N	270	LEU
1	N	271	MET
1	N	471	LEU
1	H	370	VAL
1	B	508	VAL
2	b	115	ARG
1	U	451	VAL
1	U	475	TRP
1	O	269	ASP
1	O	271	MET
1	O	471	LEU
2	o	94	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (131) such sidechains are listed below:

Mol	Chain	Res	Type
1	V	72	HIS
1	V	80	ASN
1	V	371	HIS
1	V	473	ASN
2	v	34	GLN
2	v	44	GLN
2	v	46	GLN
2	v	116	ASN
1	P	311	GLN
1	P	477	ASN
2	p	18	GLN
2	p	34	GLN
2	p	37	GLN
1	J	237	HIS
1	J	288	GLN
1	J	294	HIS
1	J	321	GLN
1	D	311	GLN
2	d	53	ASN
2	d	116	ASN
1	W	72	HIS
1	W	371	HIS

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Mol	Chain	Res	Type
1	W	473	ASN
2	w	44	GLN
2	w	46	GLN
2	w	116	ASN
1	Q	311	GLN
1	Q	477	ASN
2	q	18	GLN
2	q	34	GLN
1	K	237	HIS
1	K	288	GLN
1	K	294	HIS
1	K	321	GLN
1	K	356	HIS
2	k	34	GLN
1	E	311	GLN
1	E	455	ASN
2	e	34	GLN
2	e	53	ASN
1	X	72	HIS
1	X	80	ASN
1	X	371	HIS
1	X	473	ASN
2	x	46	GLN
2	x	116	ASN
1	R	288	GLN
1	R	311	GLN
1	R	371	HIS
1	R	477	ASN
2	r	14	ASN
2	r	18	GLN
2	r	34	GLN
2	r	37	GLN
1	L	237	HIS
1	L	288	GLN
1	L	294	HIS
2	l	34	GLN
1	F	311	GLN
2	f	34	GLN
2	f	53	ASN
1	S	72	HIS
1	S	232	GLN
1	S	371	HIS

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Mol	Chain	Res	Type
2	s	44	GLN
2	s	46	GLN
2	s	116	ASN
1	M	294	HIS
1	M	311	GLN
1	M	371	HIS
1	M	477	ASN
2	m	14	ASN
2	m	18	GLN
2	m	37	GLN
1	G	237	HIS
1	G	288	GLN
1	G	294	HIS
1	G	321	GLN
1	G	356	HIS
1	A	311	GLN
2	a	34	GLN
2	a	53	ASN
1	T	72	HIS
1	T	80	ASN
1	T	371	HIS
1	T	473	ASN
2	t	44	GLN
2	t	46	GLN
2	t	116	ASN
1	N	311	GLN
1	N	371	HIS
1	N	477	ASN
2	n	14	ASN
2	n	18	GLN
2	n	37	GLN
1	H	237	HIS
1	H	288	GLN
1	H	321	GLN
1	H	371	HIS
2	h	34	GLN
1	B	79	ASN
1	B	80	ASN
1	B	311	GLN
2	b	34	GLN
2	b	53	ASN
2	b	116	ASN

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Mol	Chain	Res	Type
1	U	72	HIS
1	U	80	ASN
1	U	371	HIS
1	U	473	ASN
2	u	34	GLN
2	u	44	GLN
2	u	46	GLN
2	u	116	ASN
1	O	294	HIS
1	O	311	GLN
1	O	477	ASN
2	o	14	ASN
2	o	18	GLN
2	o	34	GLN
2	o	37	GLN
1	I	237	HIS
1	I	288	GLN
1	I	294	HIS
1	I	321	GLN
1	I	356	HIS
2	i	34	GLN
1	C	311	GLN
2	c	34	GLN
2	c	53	ASN
2	c	116	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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.

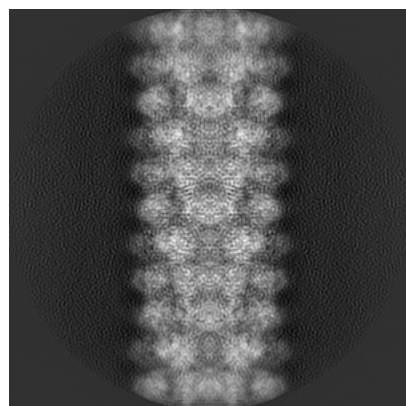
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16101. These allow visual inspection of the internal detail of the map and identification of artifacts.

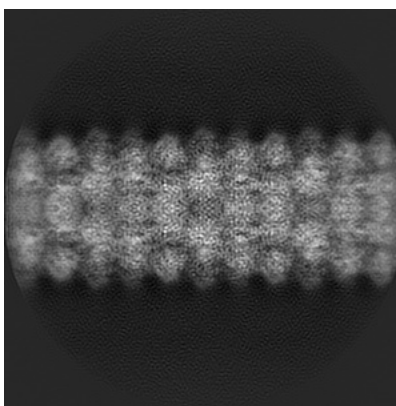
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

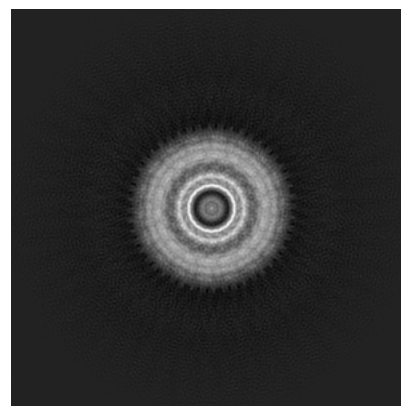
6.1.1 Primary map



X

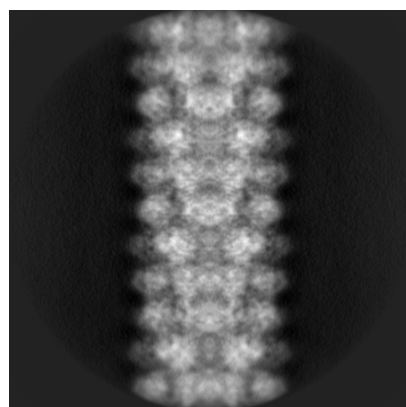


Y

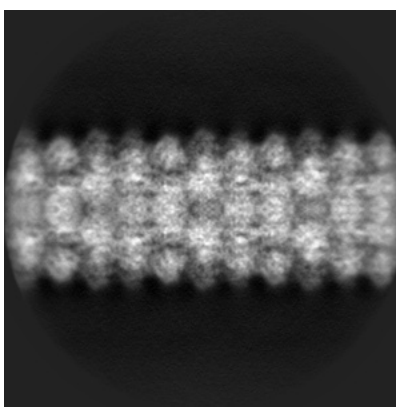


Z

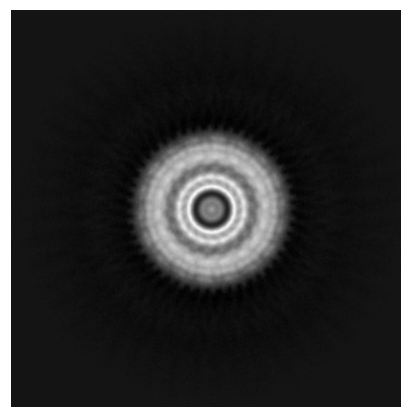
6.1.2 Raw map



X



Y

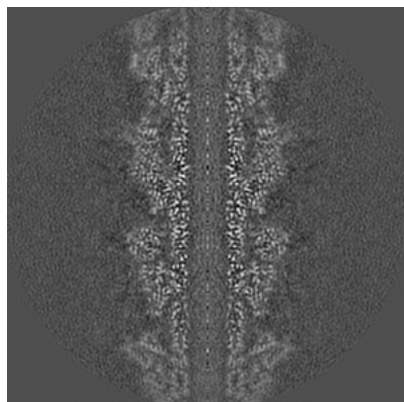


Z

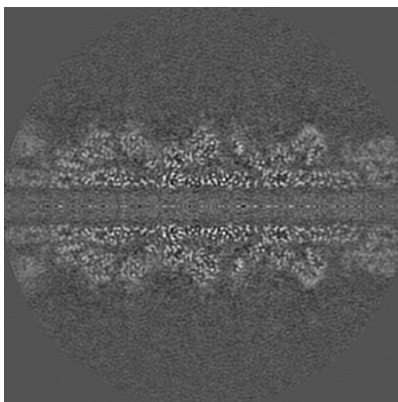
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

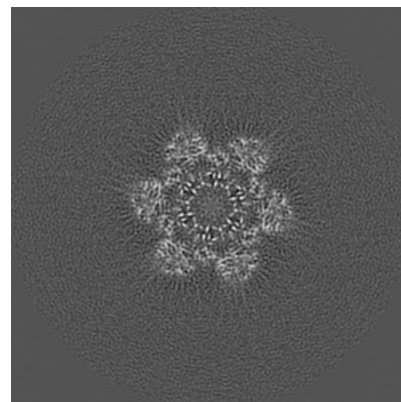
6.2.1 Primary map



X Index: 160

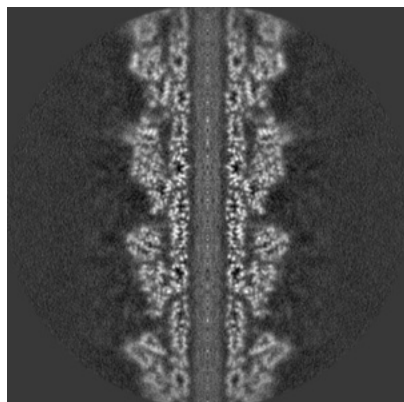


Y Index: 160

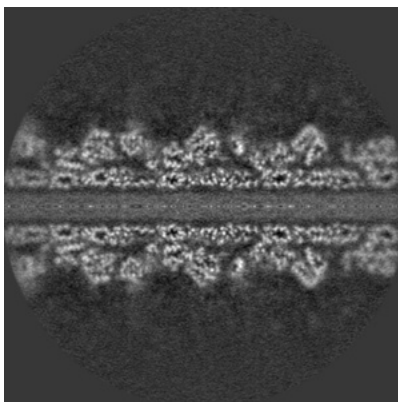


Z Index: 160

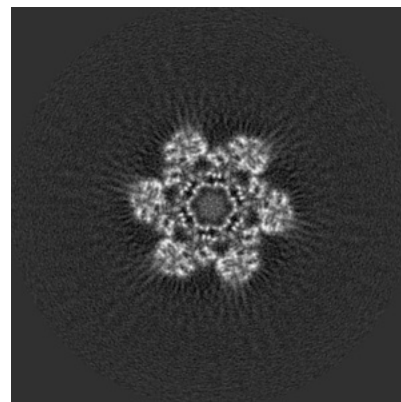
6.2.2 Raw map



X Index: 160



Y Index: 160

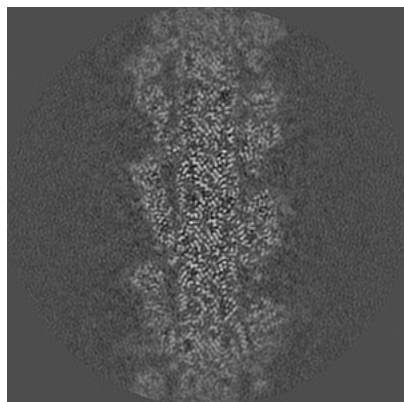


Z Index: 160

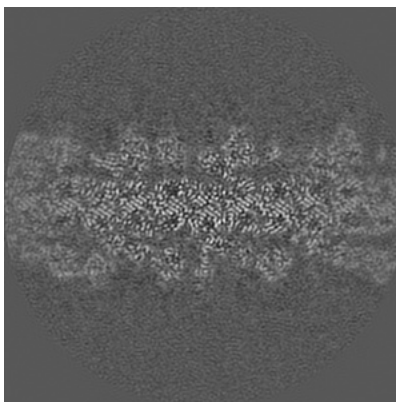
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

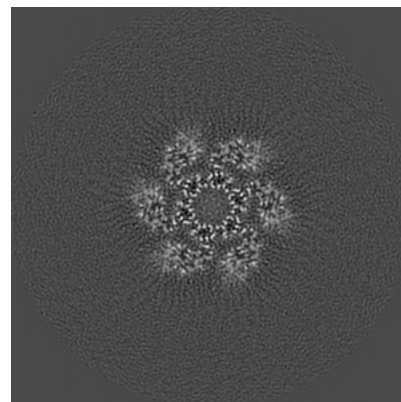
6.3.1 Primary map



X Index: 143

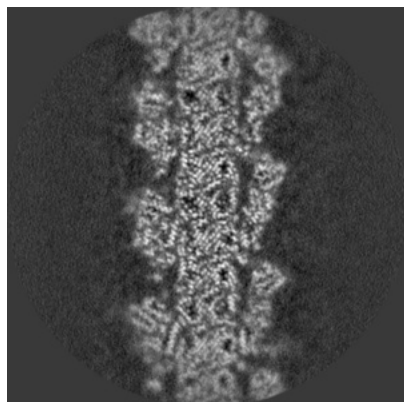


Y Index: 178

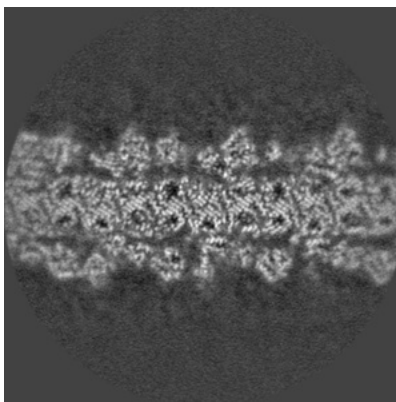


Z Index: 163

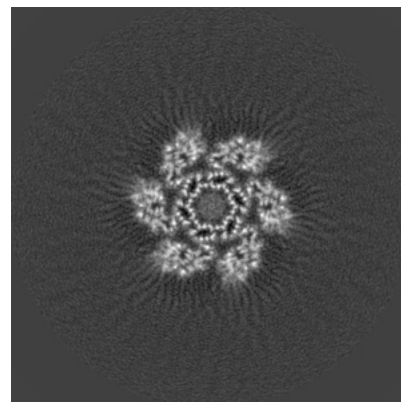
6.3.2 Raw map



X Index: 177



Y Index: 178

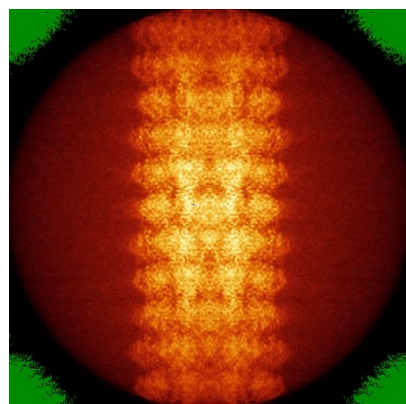


Z Index: 163

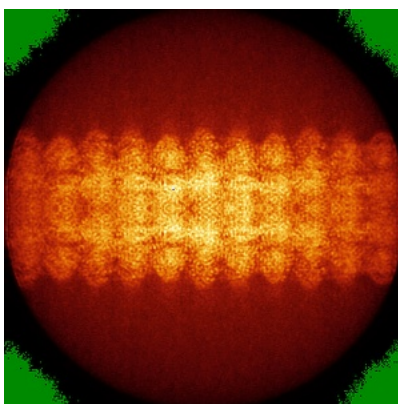
The images above show the largest variance slices of the map in three orthogonal directions.

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

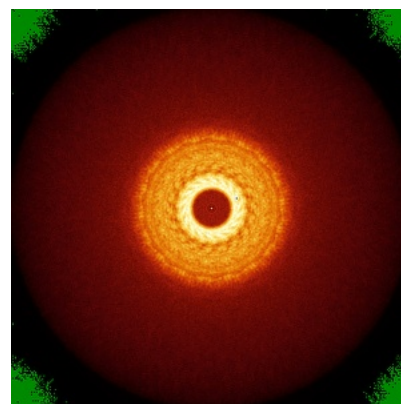
6.4.1 Primary map



X

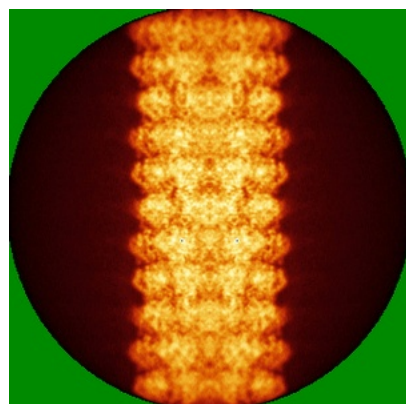


Y

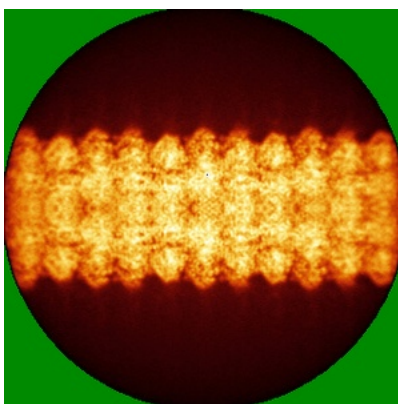


Z

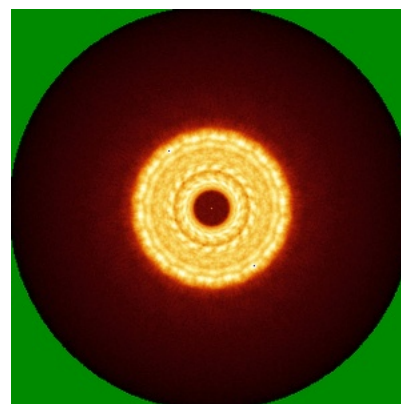
6.4.2 Raw map



X



Y

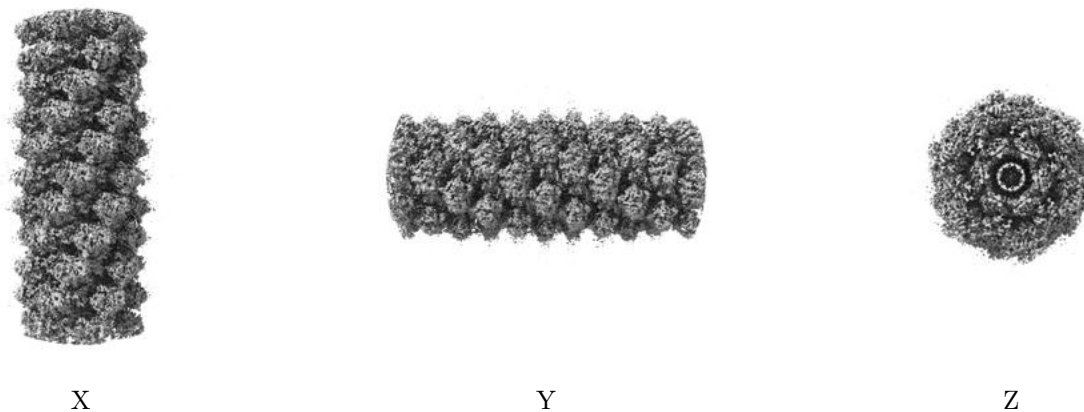


Z

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.

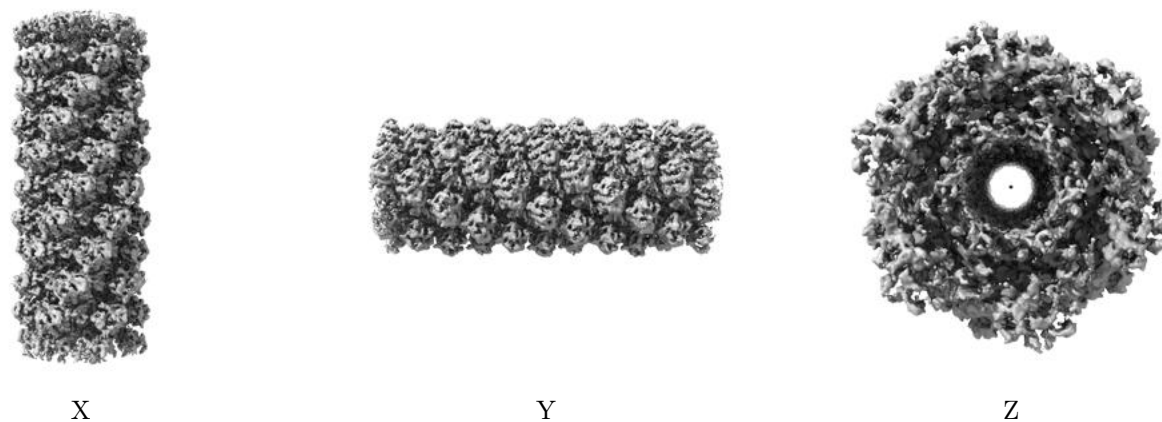
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

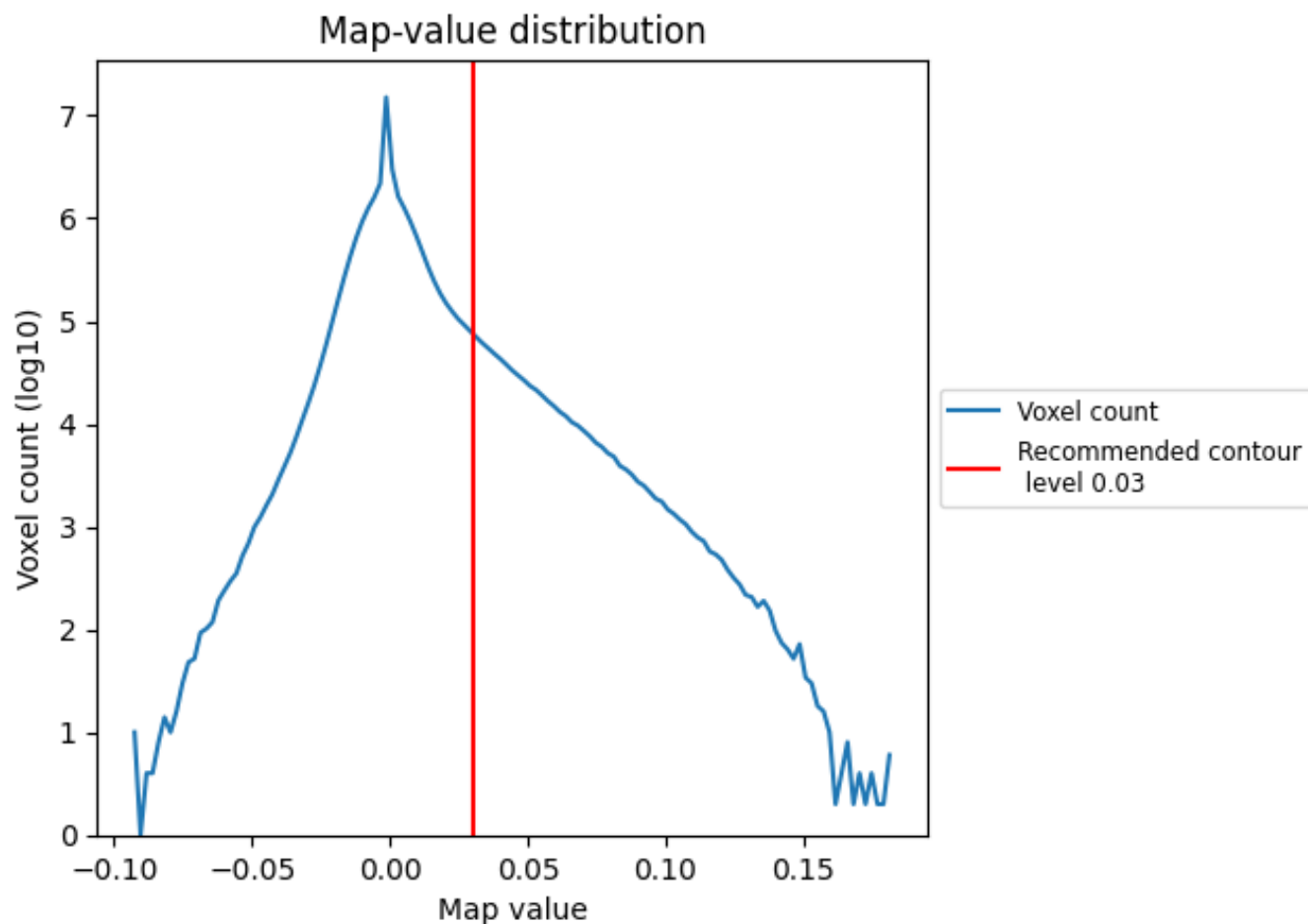
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

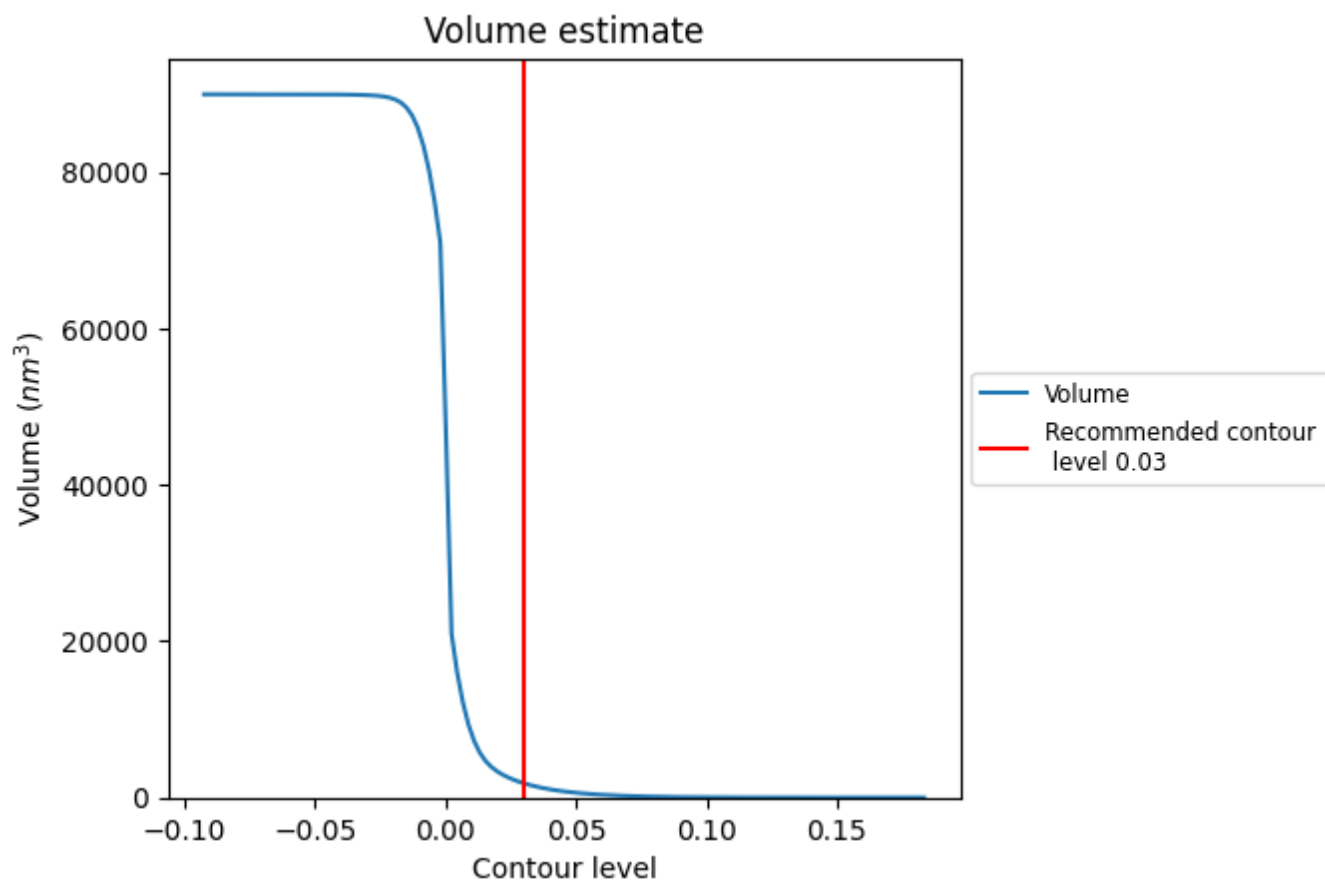
This section contains the results of statistical analysis of the map.

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.

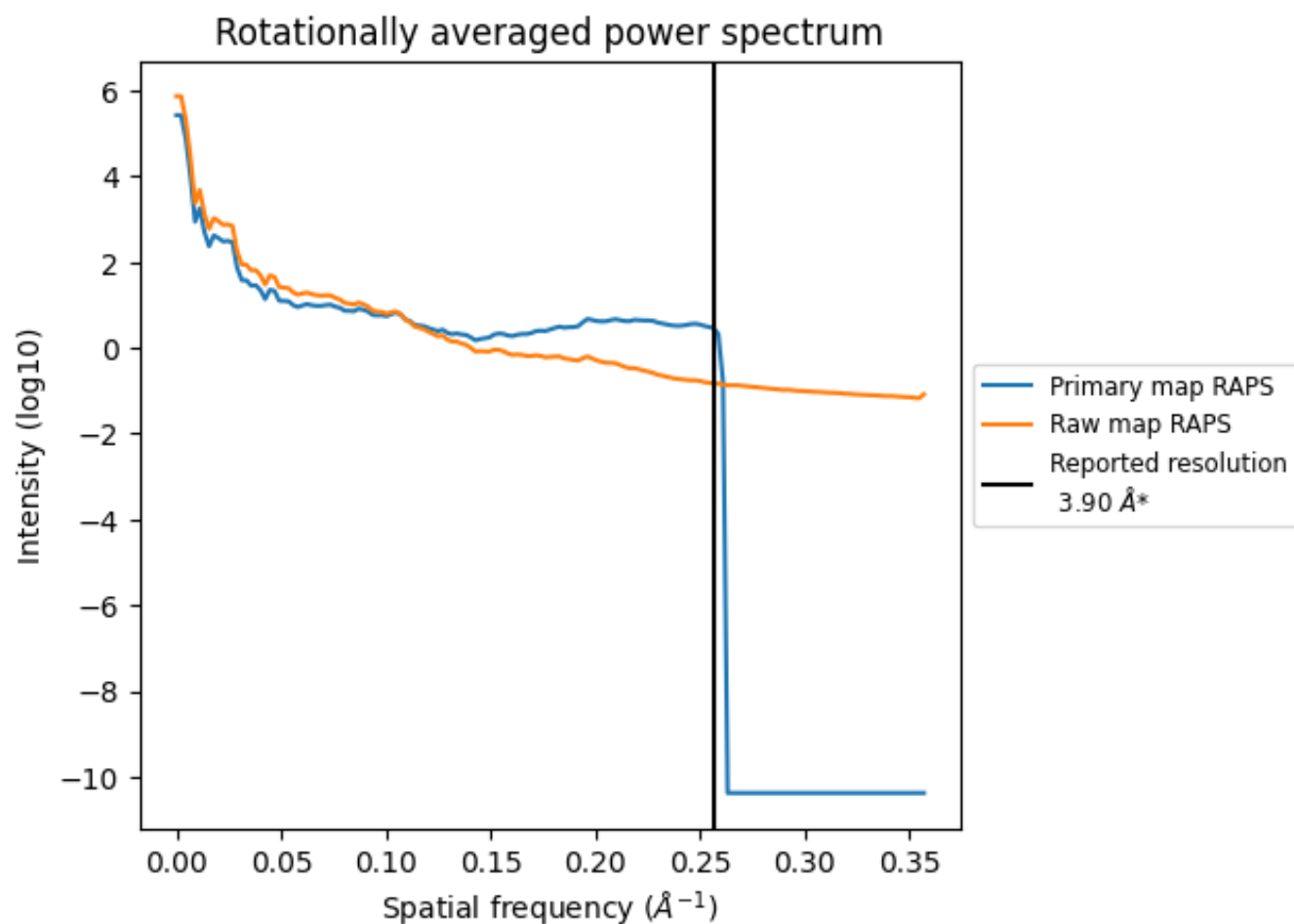
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1828 nm³; this corresponds to an approximate mass of 1651 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 ⓘ

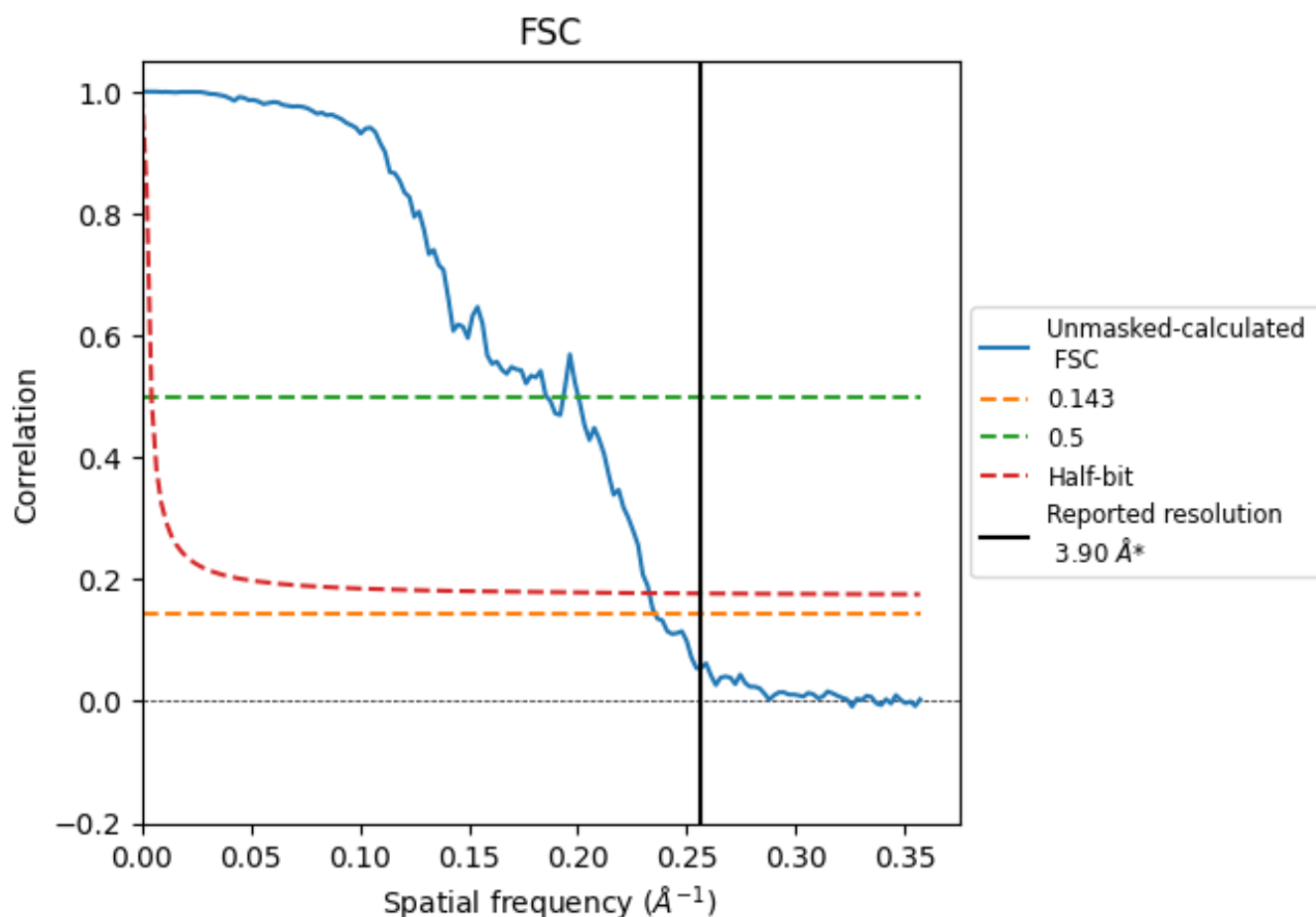


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.256 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

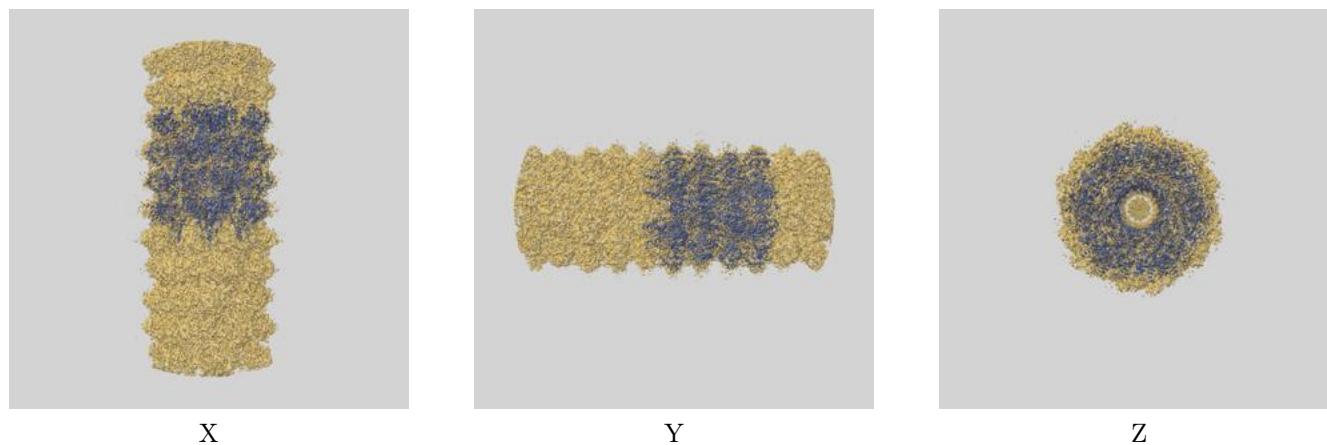
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.24	5.39	4.29

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

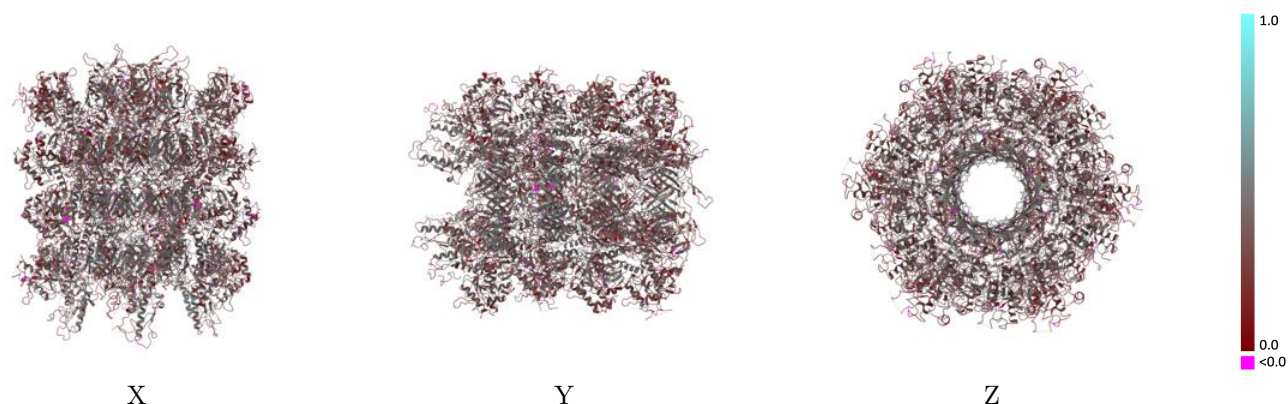
This section contains information regarding the fit between EMDB map EMD-16101 and PDB model 8BL4. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



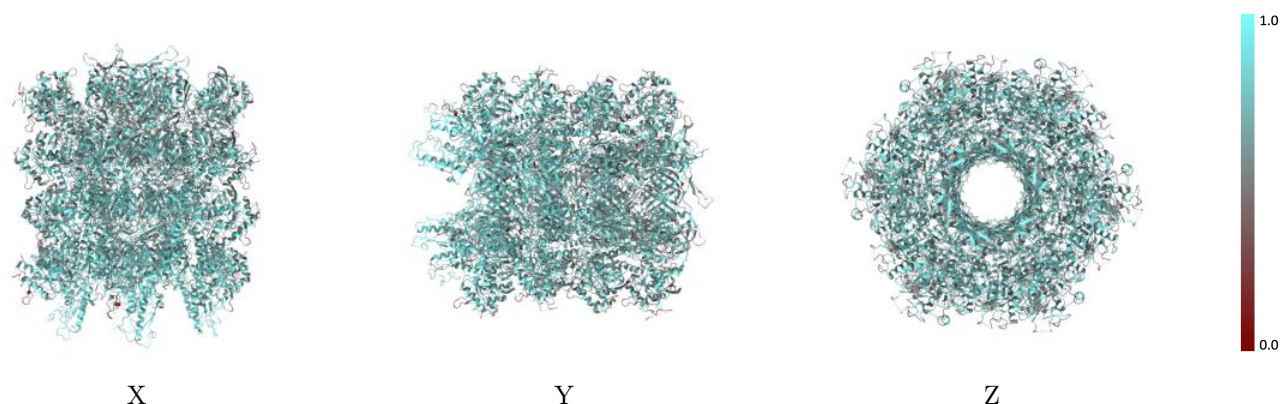
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



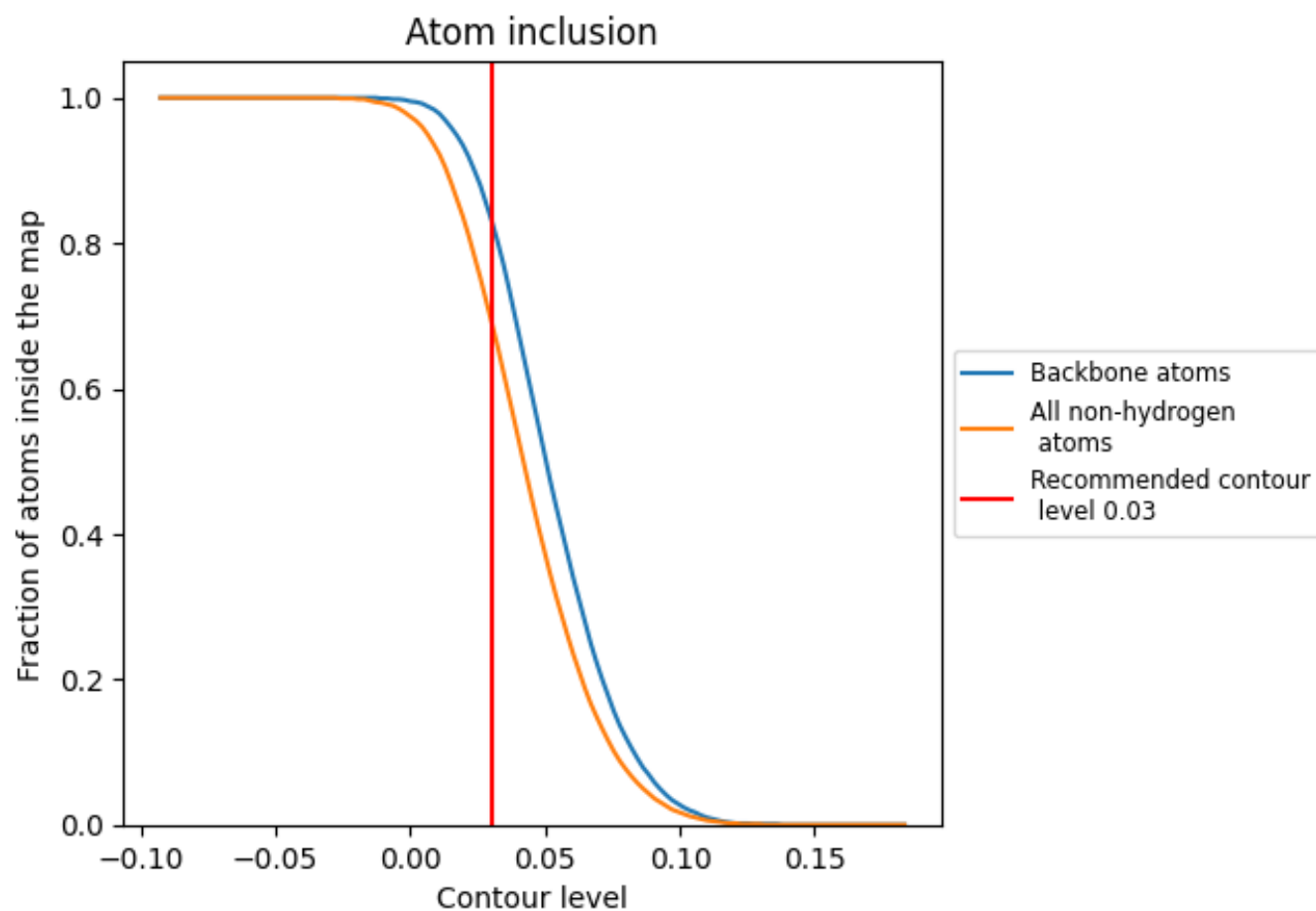
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 70% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6950	 0.3350
A	 0.7310	 0.3450
B	 0.7310	 0.3390
C	 0.7380	 0.3420
D	 0.7310	 0.3440
E	 0.7260	 0.3390
F	 0.7410	 0.3450
G	 0.7140	 0.3290
H	 0.7160	 0.3260
I	 0.7180	 0.3300
J	 0.7150	 0.3300
K	 0.7190	 0.3260
L	 0.7170	 0.3260
M	 0.6920	 0.3200
N	 0.6920	 0.3220
O	 0.6900	 0.3200
P	 0.6900	 0.3210
Q	 0.6910	 0.3230
R	 0.6920	 0.3230
S	 0.6460	 0.3050
T	 0.6550	 0.3090
U	 0.6530	 0.3110
V	 0.6500	 0.3120
W	 0.6490	 0.3120
X	 0.6510	 0.3110
a	 0.7240	 0.3750
b	 0.7130	 0.3710
c	 0.7210	 0.3730
d	 0.7300	 0.3750
e	 0.7270	 0.3740
f	 0.7300	 0.3730
g	 0.7090	 0.3600
h	 0.7100	 0.3630
i	 0.7220	 0.3640
j	 0.7100	 0.3620



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Chain	Atom inclusion	Q-score
k	 0.7150	 0.3640
l	 0.7140	 0.3620
m	 0.6650	 0.3540
n	 0.6690	 0.3550
o	 0.6620	 0.3510
p	 0.6650	 0.3500
q	 0.6700	 0.3560
r	 0.6630	 0.3510
s	 0.6580	 0.3520
t	 0.6510	 0.3490
u	 0.6540	 0.3500
v	 0.6540	 0.3500
w	 0.6490	 0.3510
x	 0.6550	 0.3500