



Full wwPDB EM Validation Report ⓘ

Sep 17, 2025 – 01:35 PM EDT

PDB ID : 9N8B / pdb_00009n8b
EMDB ID : EMD-49126
Title : In situ unsheathed flagellar filament of *Vibrio cholerae* resolved with helical reconstruction.
Authors : Wangbiao, G.; Jun, L.
Deposited on : 2025-02-08
Resolution : 2.45 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.dev126
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

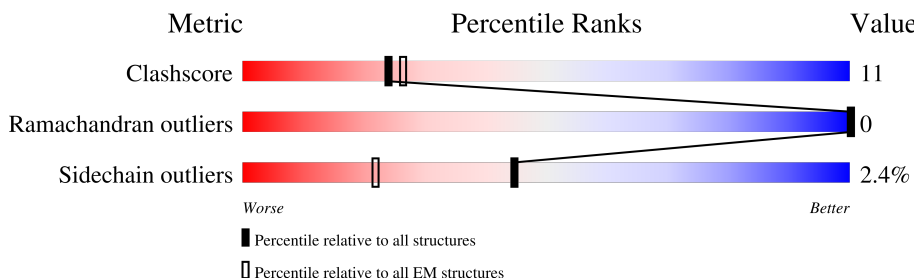
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.45 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	376	
1	B	376	
1	C	376	
1	D	376	
1	E	376	
1	F	376	
1	G	376	
1	H	376	

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Mol	Chain	Length	Quality of chain
1	I	376	
1	J	376	
1	K	376	
1	L	376	
1	M	376	
1	N	376	
1	O	376	
1	P	376	
1	Q	376	
1	R	376	
1	S	376	
1	T	376	
1	U	376	
1	V	376	
1	W	376	
1	X	376	
1	Y	376	
1	Z	376	
1	a	376	
1	b	376	
1	c	376	
1	d	376	
1	e	376	
1	f	376	
1	g	376	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 91905 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 Flagellin D.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	376	Total	C	N	O	S	0	0
			2785	1685	501	589	10		
1	B	376	Total	C	N	O	S	0	0
			2785	1685	501	589	10		
1	C	376	Total	C	N	O	S	0	0
			2785	1685	501	589	10		
1	D	376	Total	C	N	O	S	0	0
			2785	1685	501	589	10		
1	E	376	Total	C	N	O	S	0	0
			2785	1685	501	589	10		
1	F	376	Total	C	N	O	S	0	0
			2785	1685	501	589	10		
1	G	376	Total	C	N	O	S	0	0
			2785	1685	501	589	10		
1	H	376	Total	C	N	O	S	0	0
			2785	1685	501	589	10		
1	I	376	Total	C	N	O	S	0	0
			2785	1685	501	589	10		
1	J	376	Total	C	N	O	S	0	0
			2785	1685	501	589	10		
1	K	376	Total	C	N	O	S	0	0
			2785	1685	501	589	10		
1	L	376	Total	C	N	O	S	0	0
			2785	1685	501	589	10		
1	M	376	Total	C	N	O	S	0	0
			2785	1685	501	589	10		
1	N	376	Total	C	N	O	S	0	0
			2785	1685	501	589	10		
1	O	376	Total	C	N	O	S	0	0
			2785	1685	501	589	10		
1	P	376	Total	C	N	O	S	0	0
			2785	1685	501	589	10		
1	Q	376	Total	C	N	O	S	0	0
			2785	1685	501	589	10		

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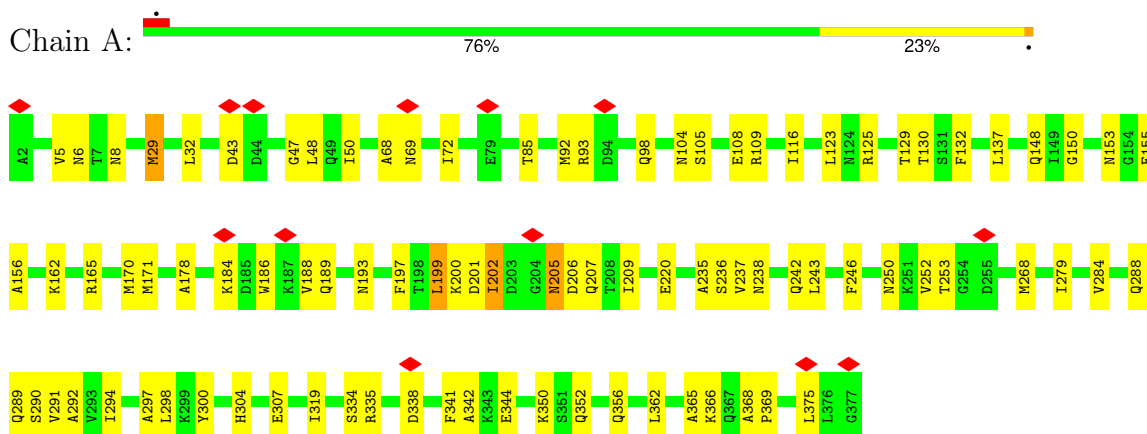
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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	376	Total 2785	C 1685	N 501	O 589	S 10	0	0
1	S	376	Total 2785	C 1685	N 501	O 589	S 10	0	0
1	T	376	Total 2785	C 1685	N 501	O 589	S 10	0	0
1	U	376	Total 2785	C 1685	N 501	O 589	S 10	0	0
1	V	376	Total 2785	C 1685	N 501	O 589	S 10	0	0
1	W	376	Total 2785	C 1685	N 501	O 589	S 10	0	0
1	X	376	Total 2785	C 1685	N 501	O 589	S 10	0	0
1	Y	376	Total 2785	C 1685	N 501	O 589	S 10	0	0
1	Z	376	Total 2785	C 1685	N 501	O 589	S 10	0	0
1	a	376	Total 2785	C 1685	N 501	O 589	S 10	0	0
1	b	376	Total 2785	C 1685	N 501	O 589	S 10	0	0
1	c	376	Total 2785	C 1685	N 501	O 589	S 10	0	0
1	d	376	Total 2785	C 1685	N 501	O 589	S 10	0	0
1	e	376	Total 2785	C 1685	N 501	O 589	S 10	0	0
1	f	376	Total 2785	C 1685	N 501	O 589	S 10	0	0
1	g	376	Total 2785	C 1685	N 501	O 589	S 10	0	0

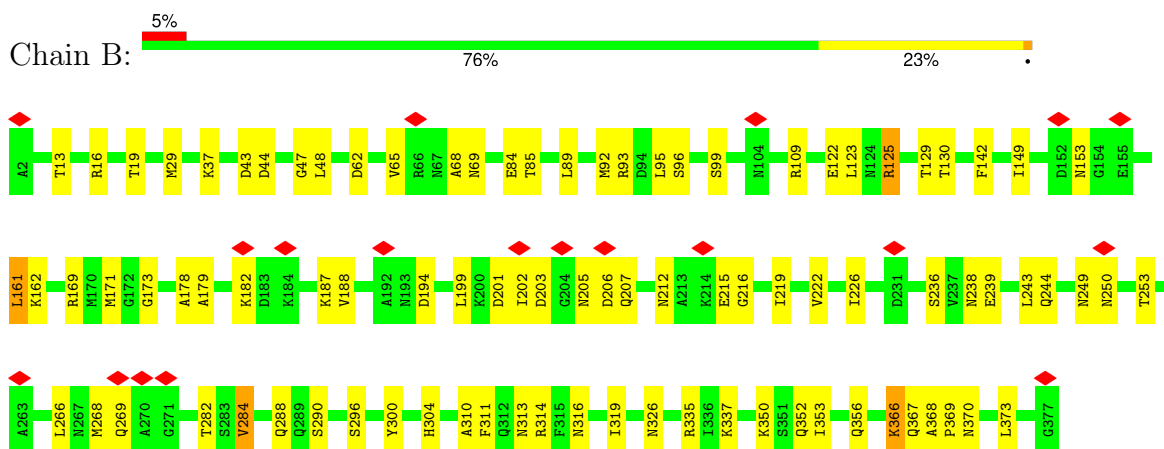
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

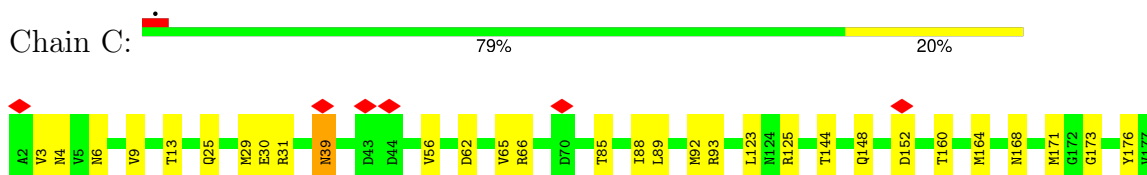
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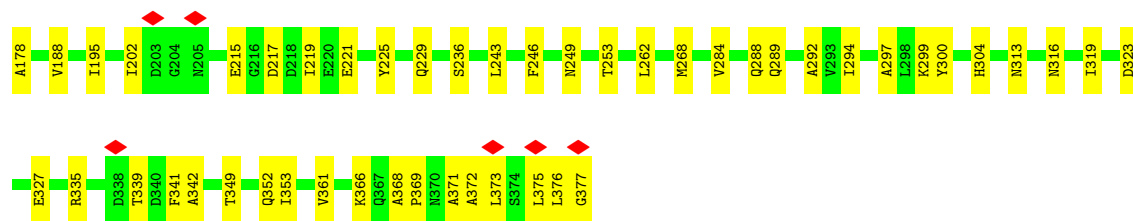


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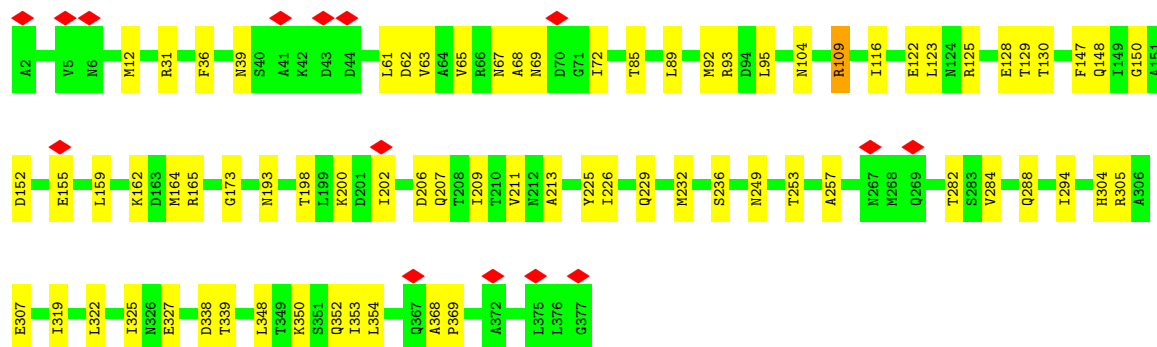
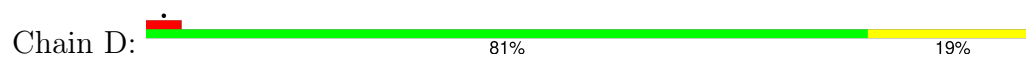


• Molecule 1: Flagellin D

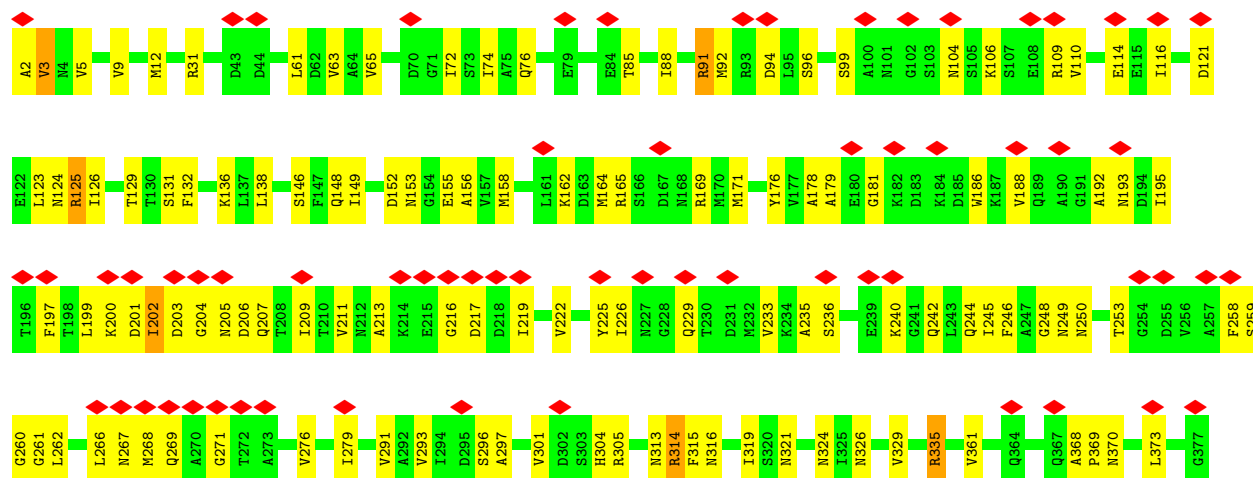




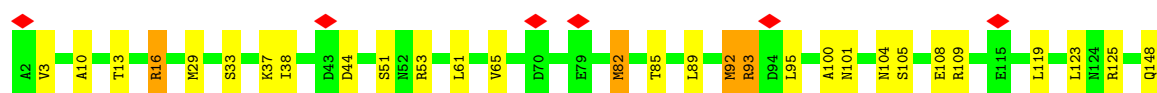
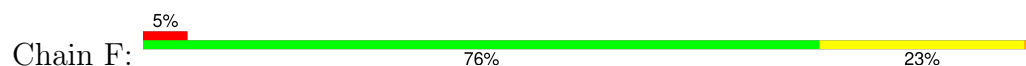
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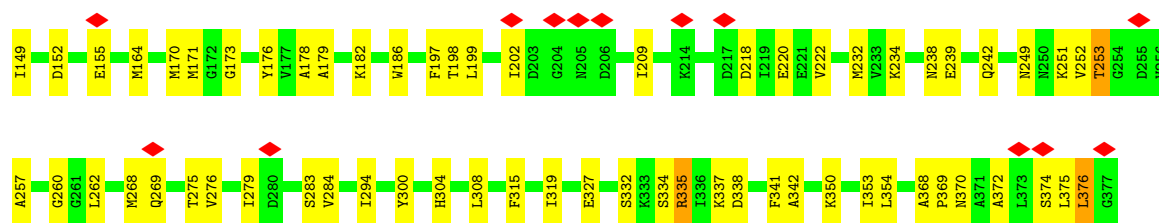


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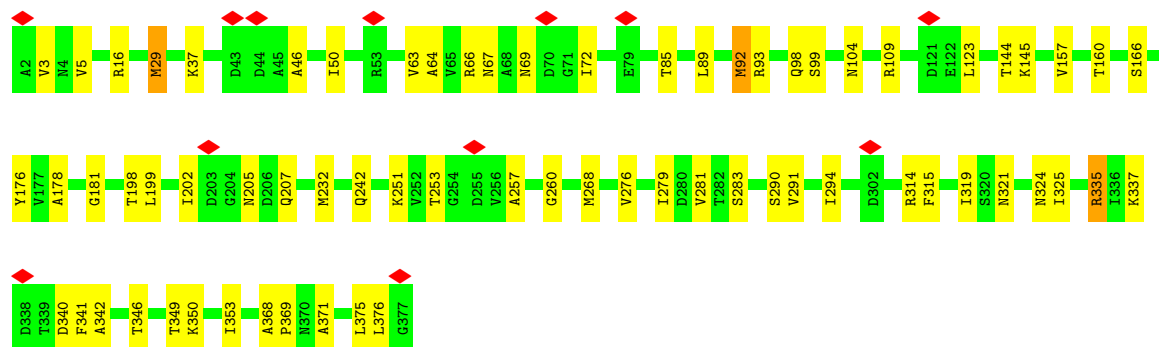
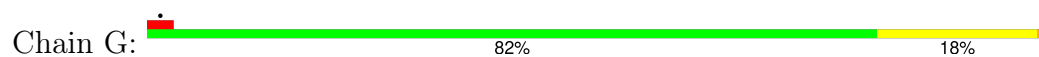


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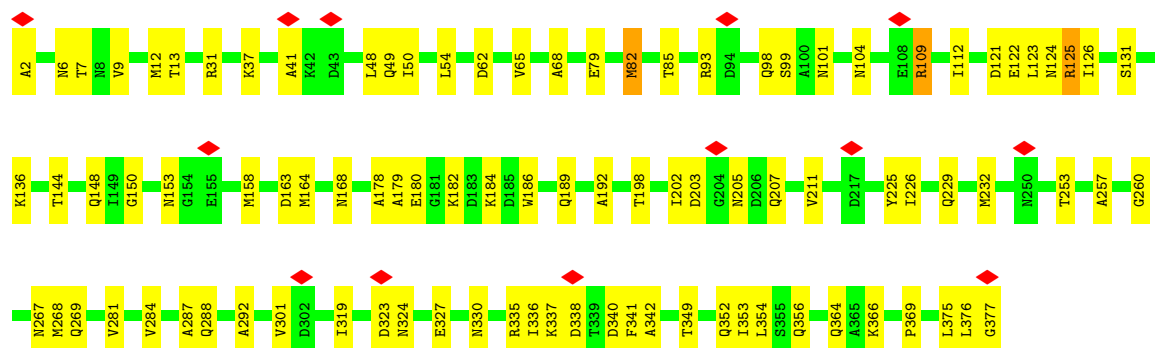
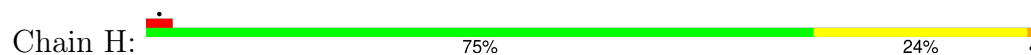




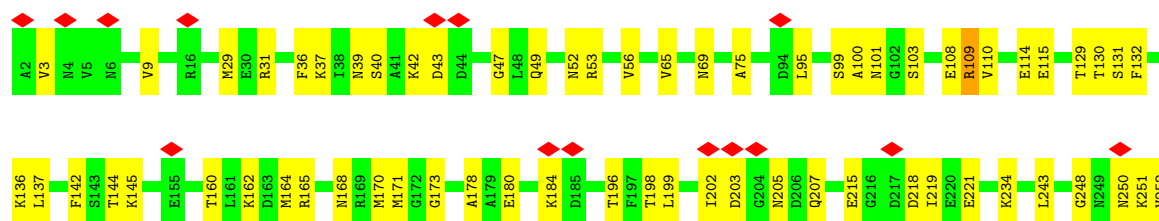
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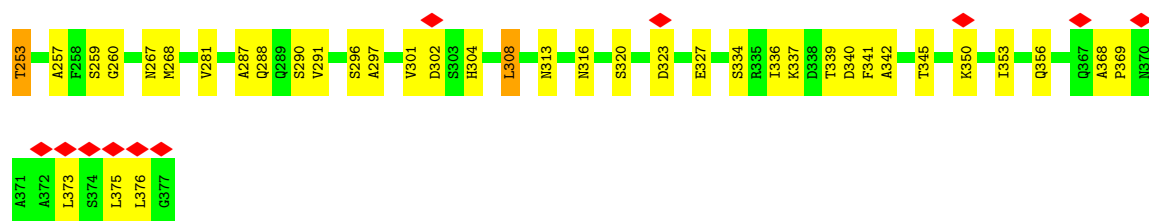


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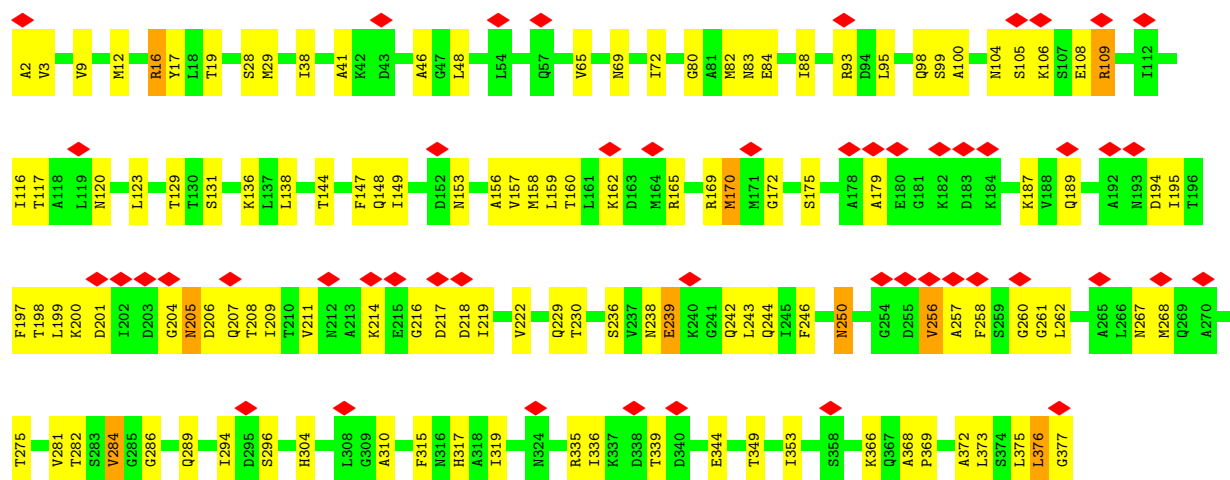


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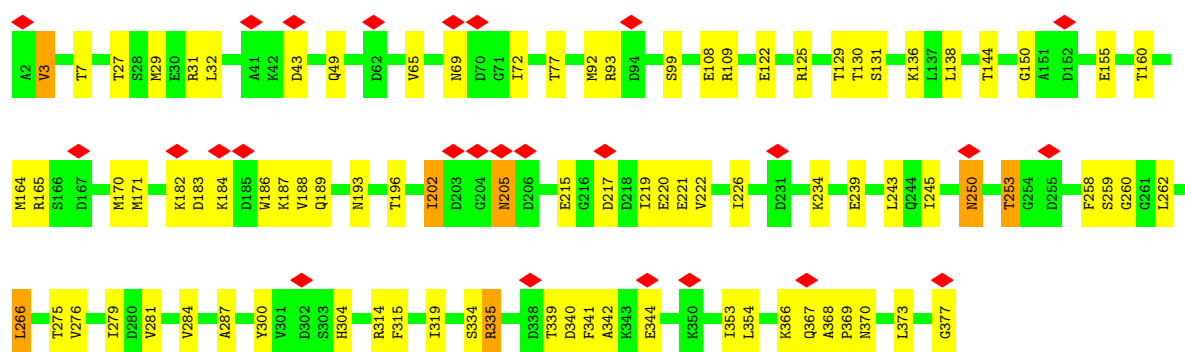




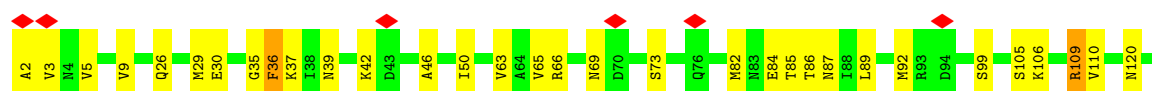
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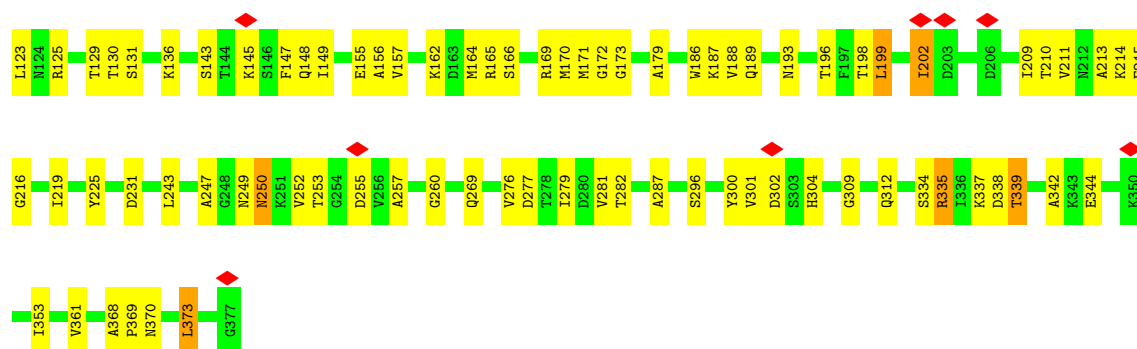


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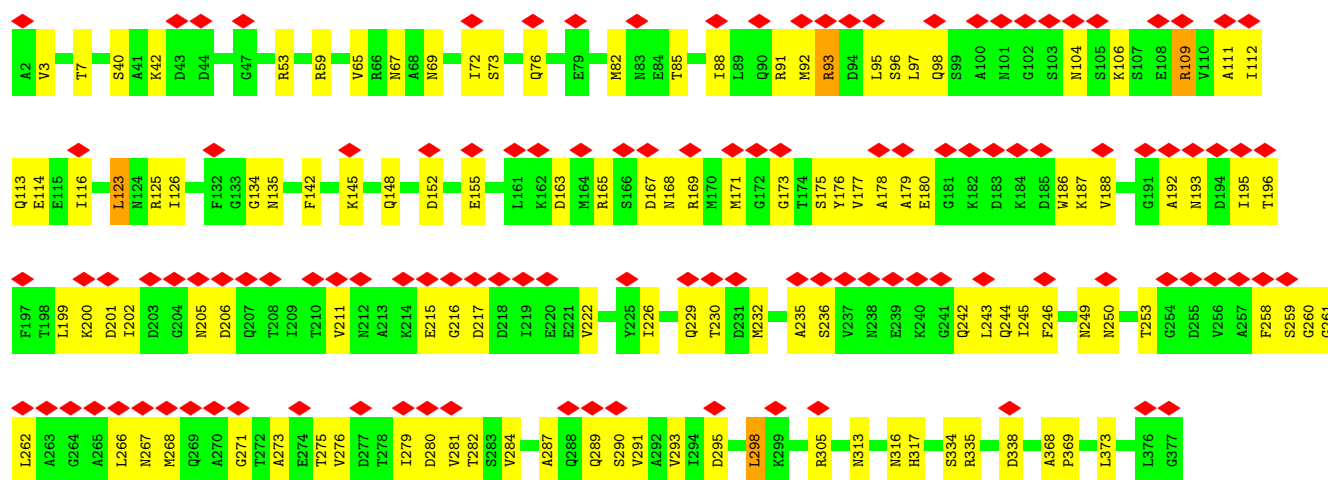


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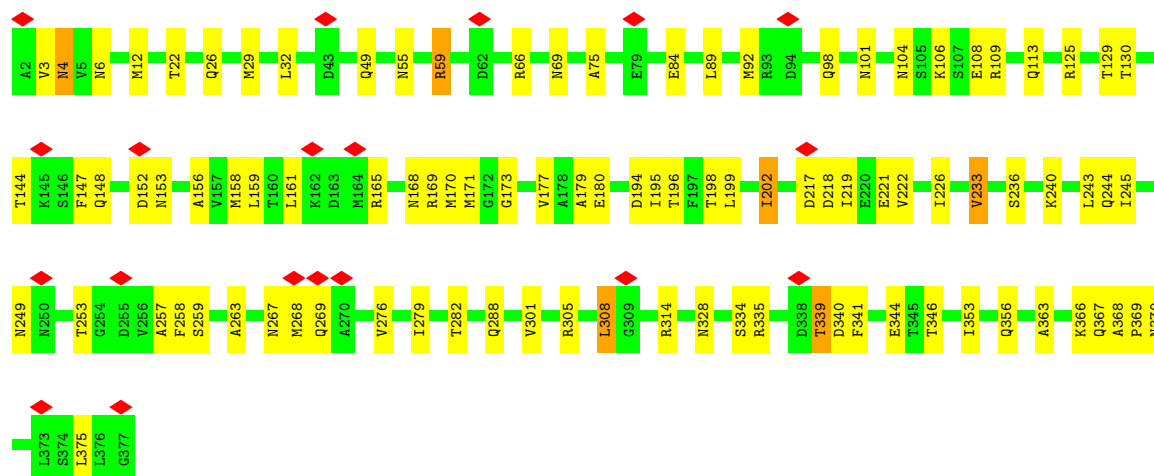





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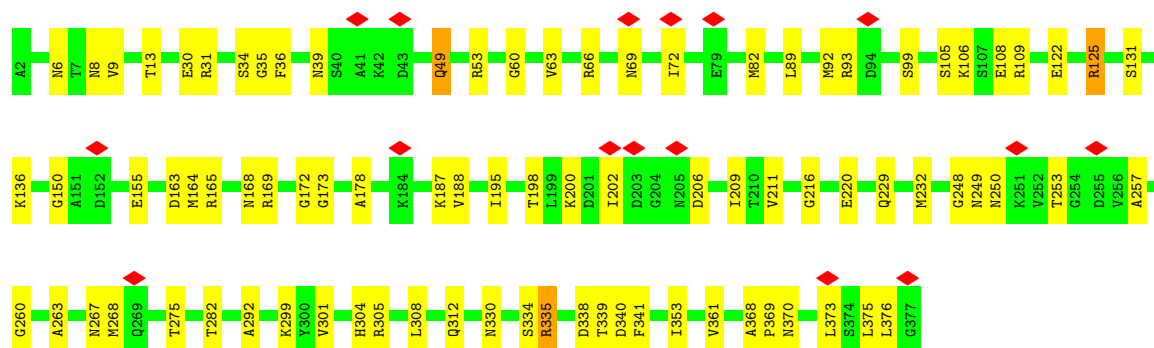


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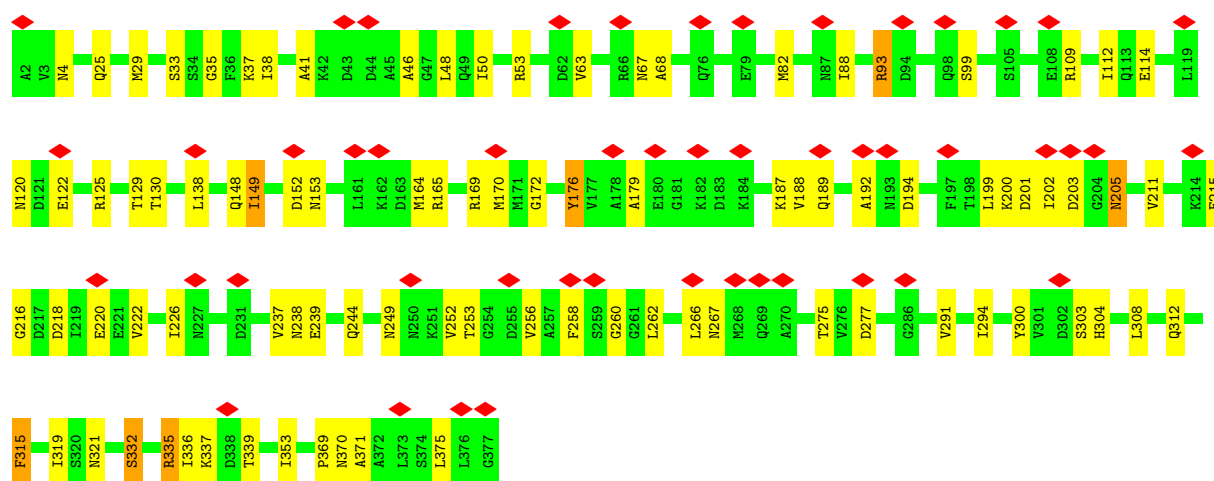
• Molecule 1: Flagellin D

Chain O:  77% 22%




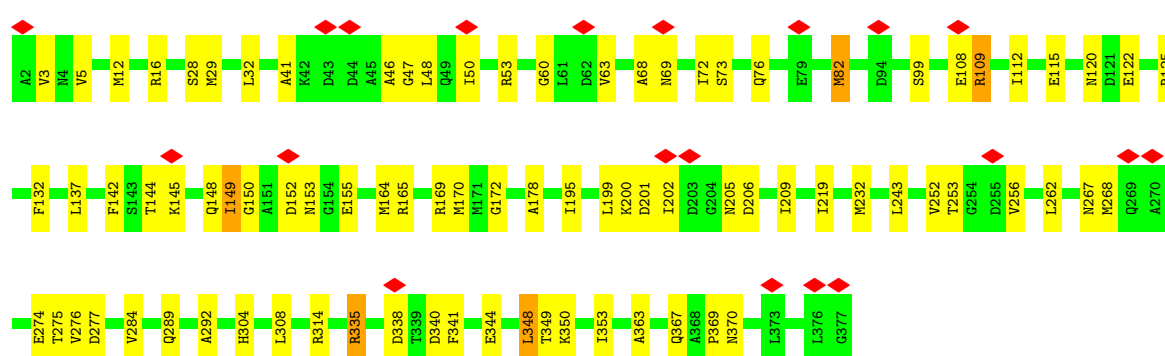
• Molecule 1: Flagellin D

Chain P:  13% 76% 23%




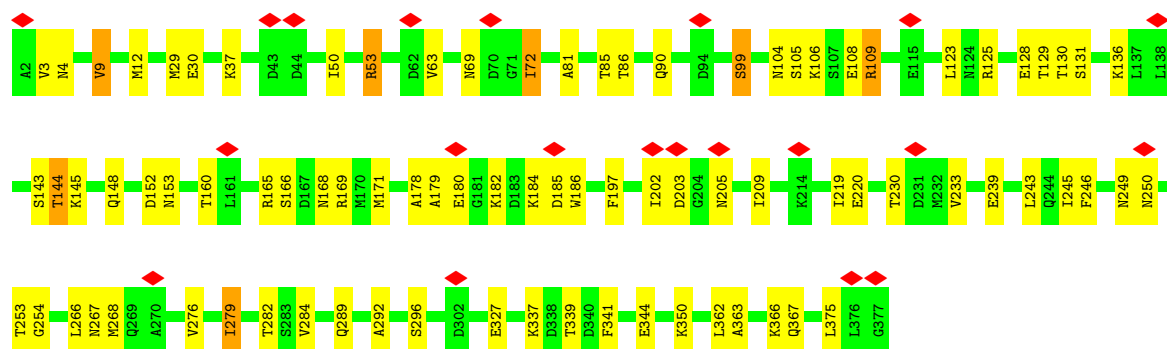
• Molecule 1: Flagellin D

Chain Q:  5% 77% 22%

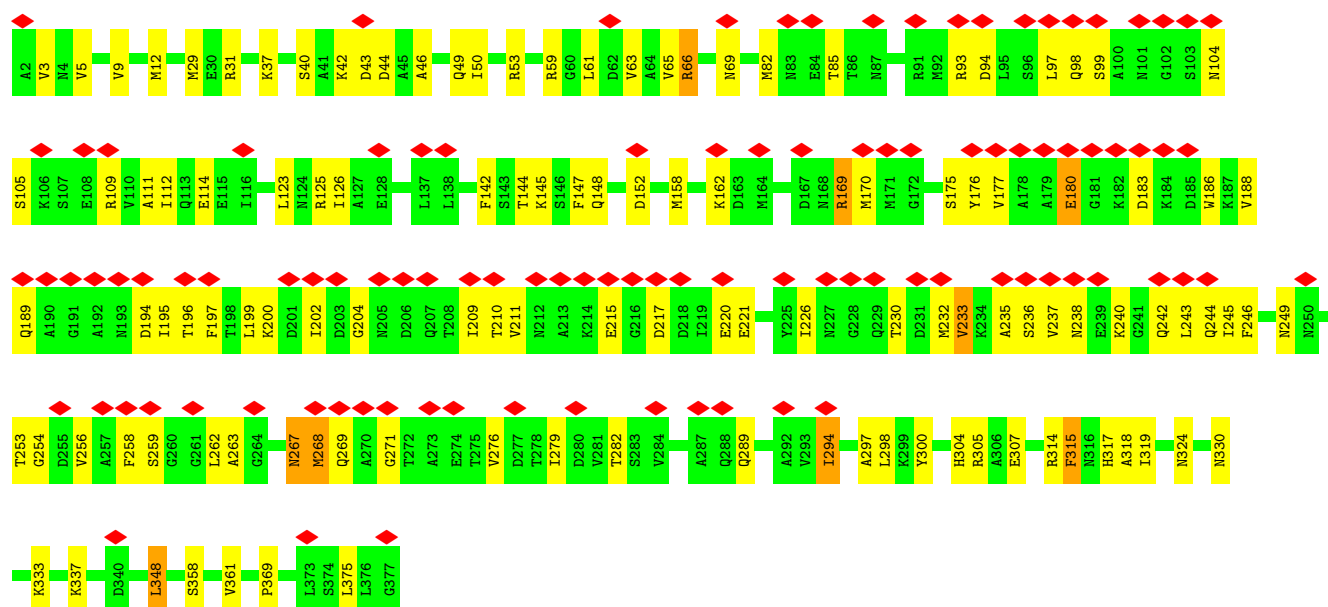


• Molecule 1: Flagellin D

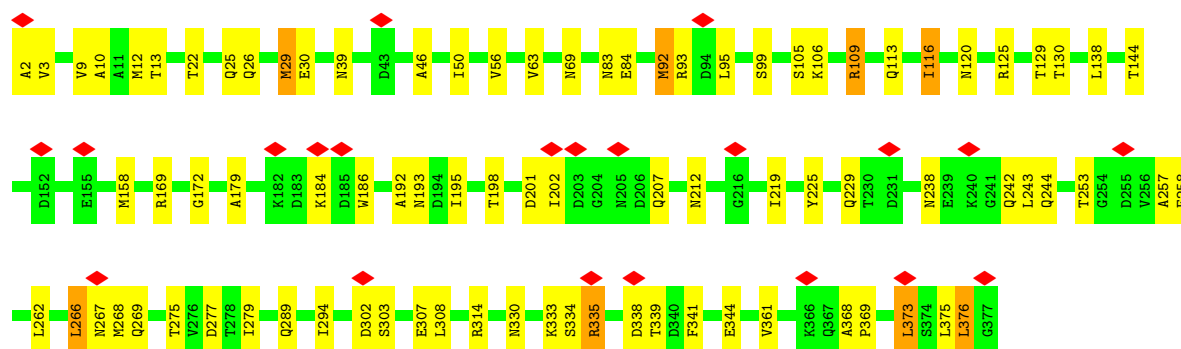
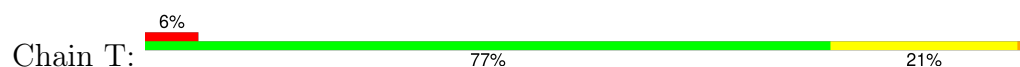
Chain R:  6% 77% 21%



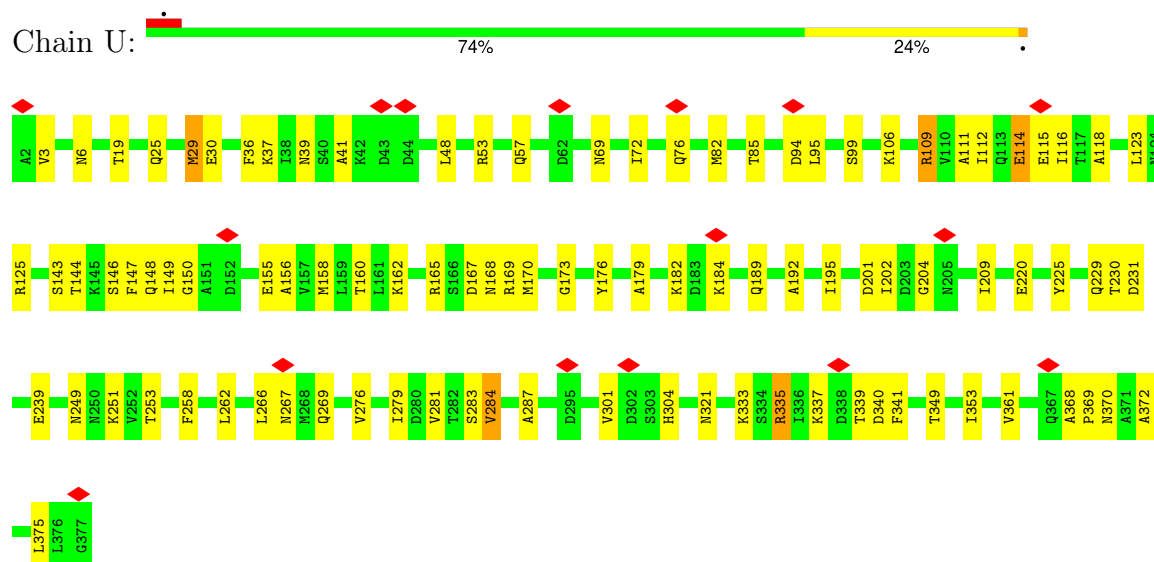
• Molecule 1: Flagellin D



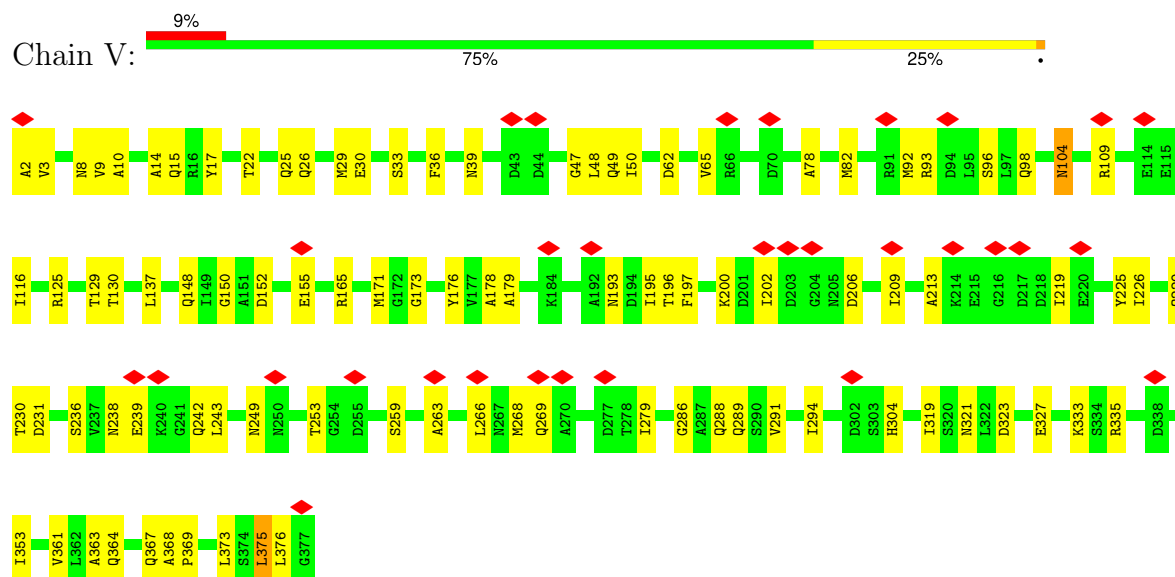
• Molecule 1: Flagellin D



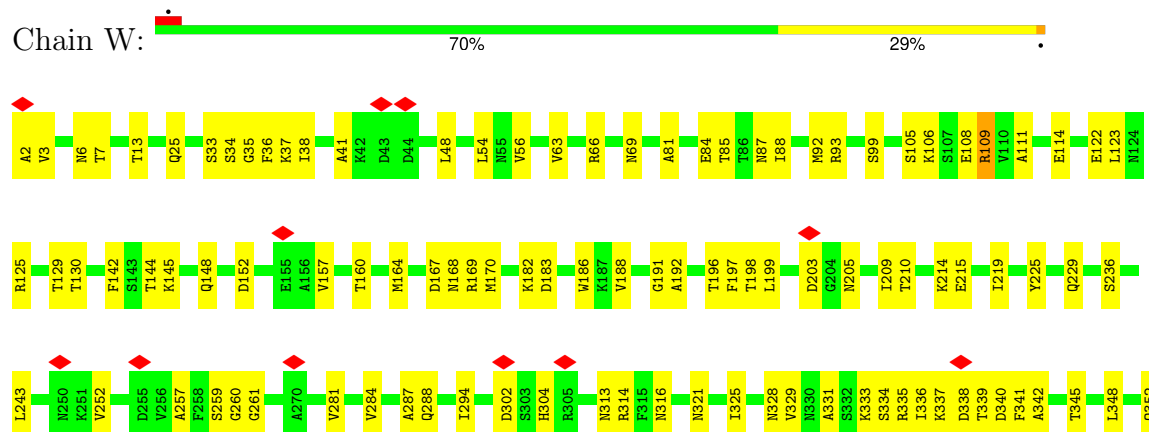
• Molecule 1: Flagellin D



• Molecule 1: Flagellin D



• Molecule 1: Flagellin D

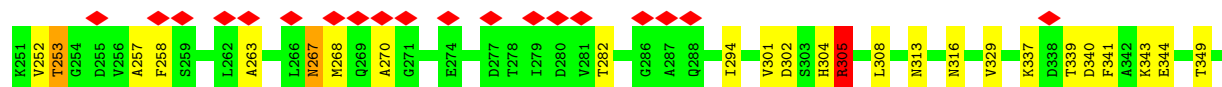
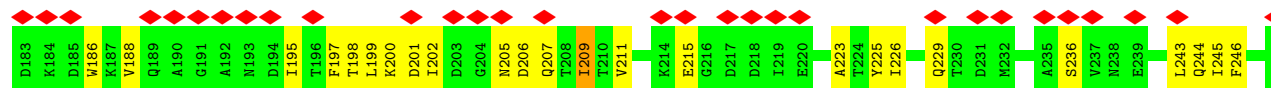
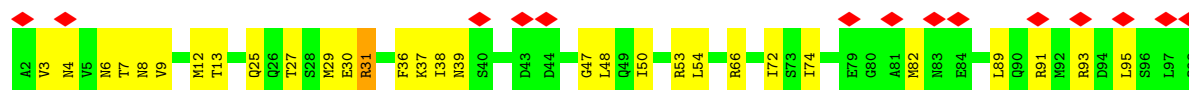




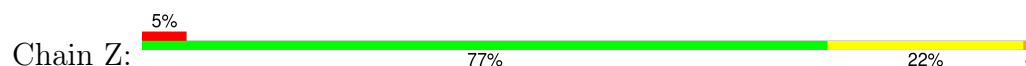
• Molecule 1: Flagellin D

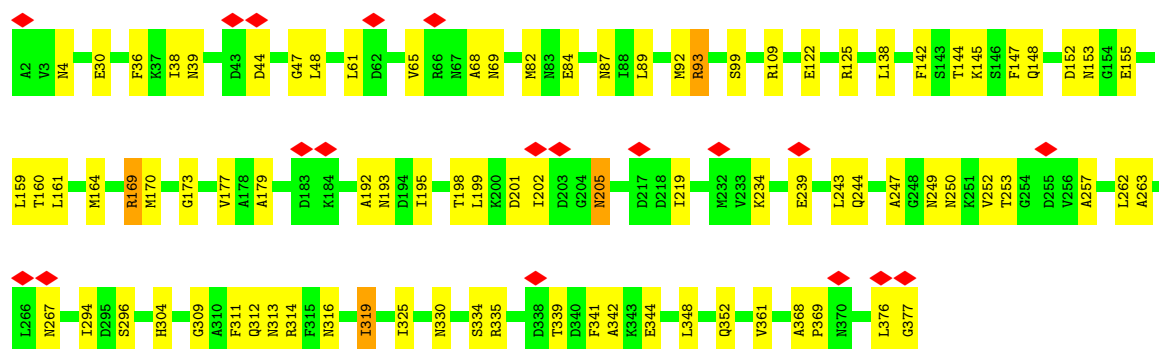


• Molecule 1: Flagellin D



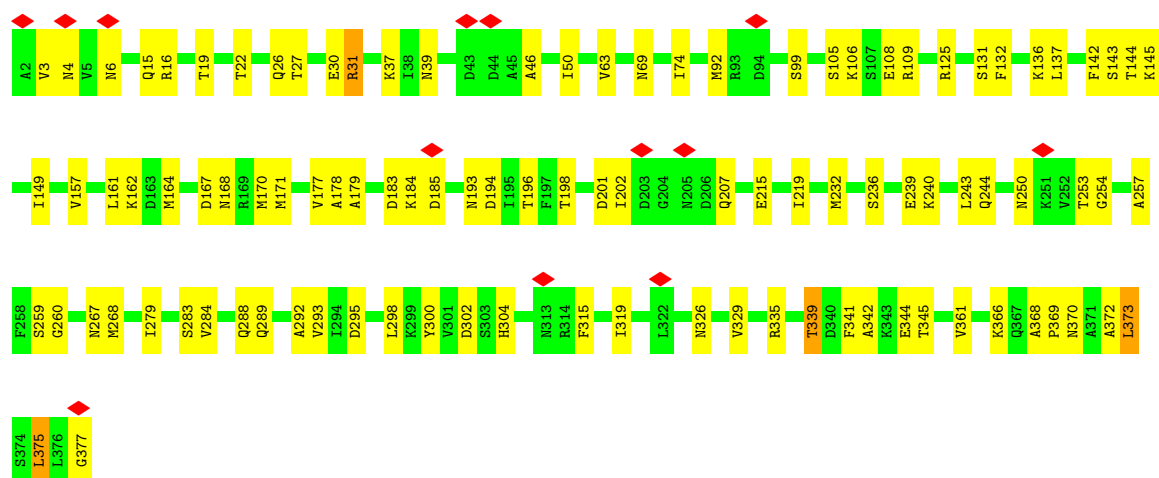
• Molecule 1: Flagellin D





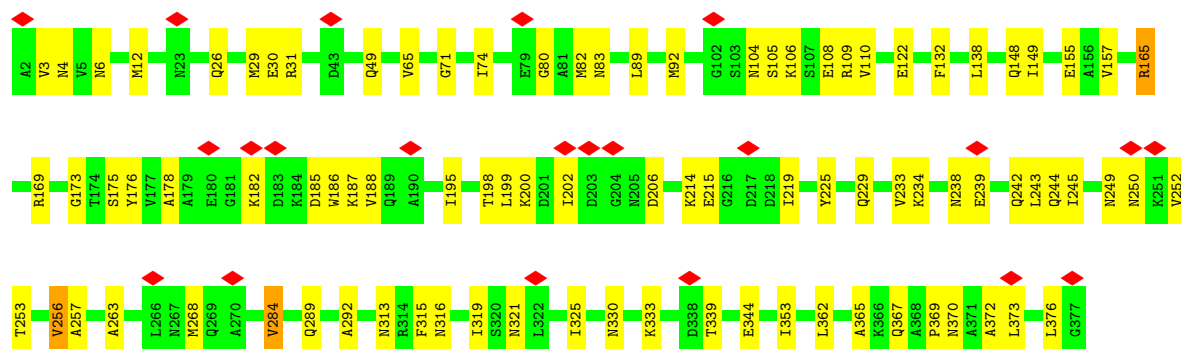
• Molecule 1: Flagellin D

Chain a: 73% 26%



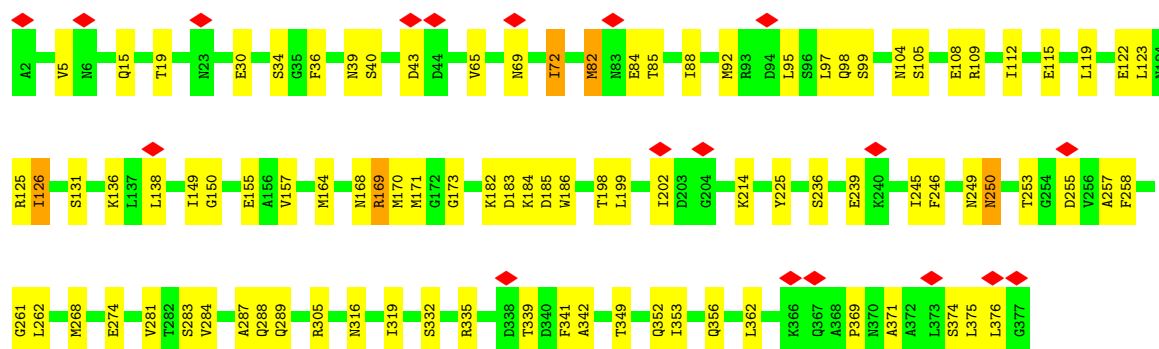
• Molecule 1: Flagellin D

Chain b: 6% 76% 23%



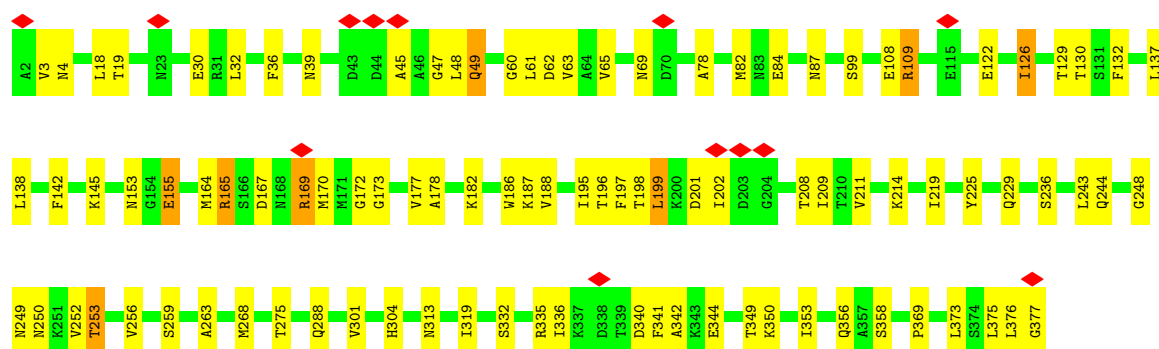
• Molecule 1: Flagellin D

Chain c: 5% 75% 23%



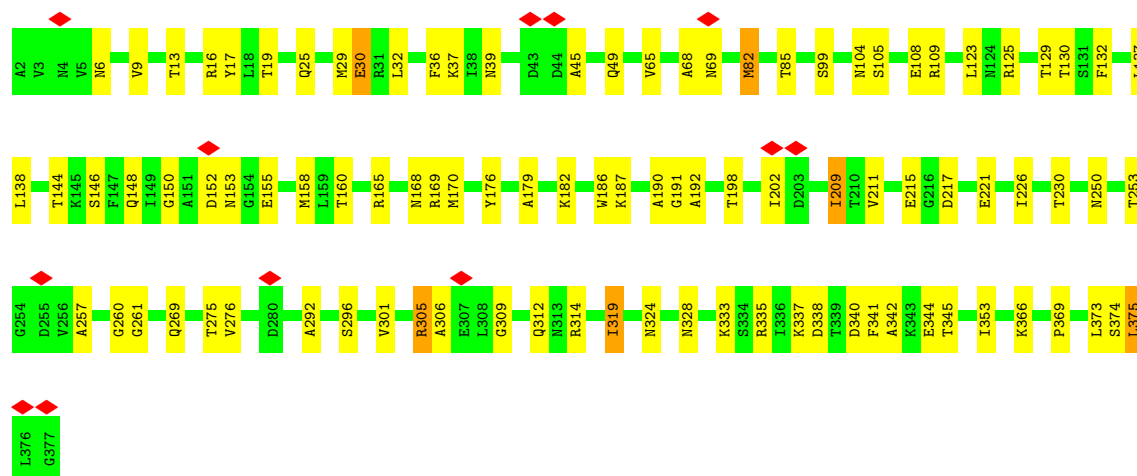
• Molecule 1: Flagellin D

Chain d: 74% 24%



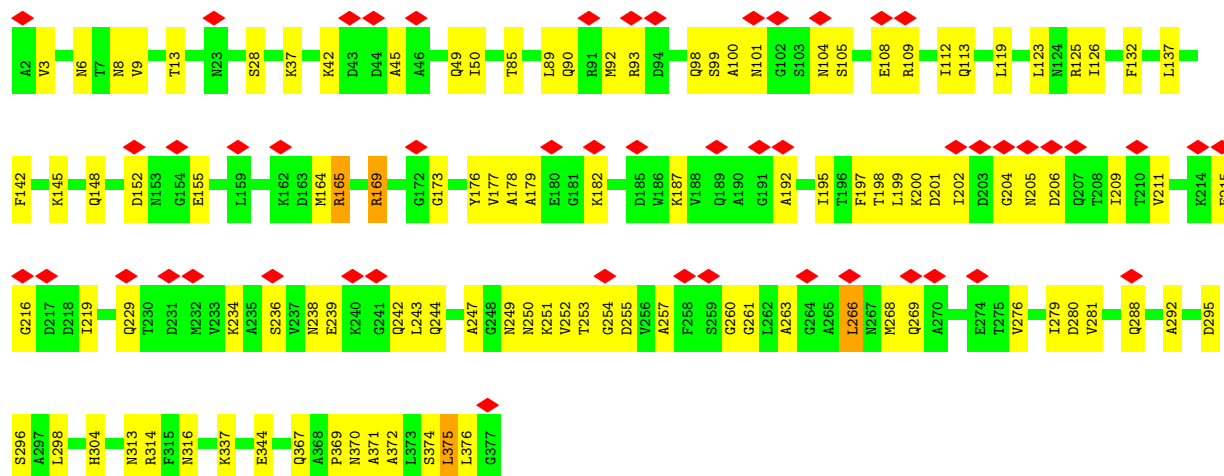
• Molecule 1: Flagellin D

Chain e: 74% 24%

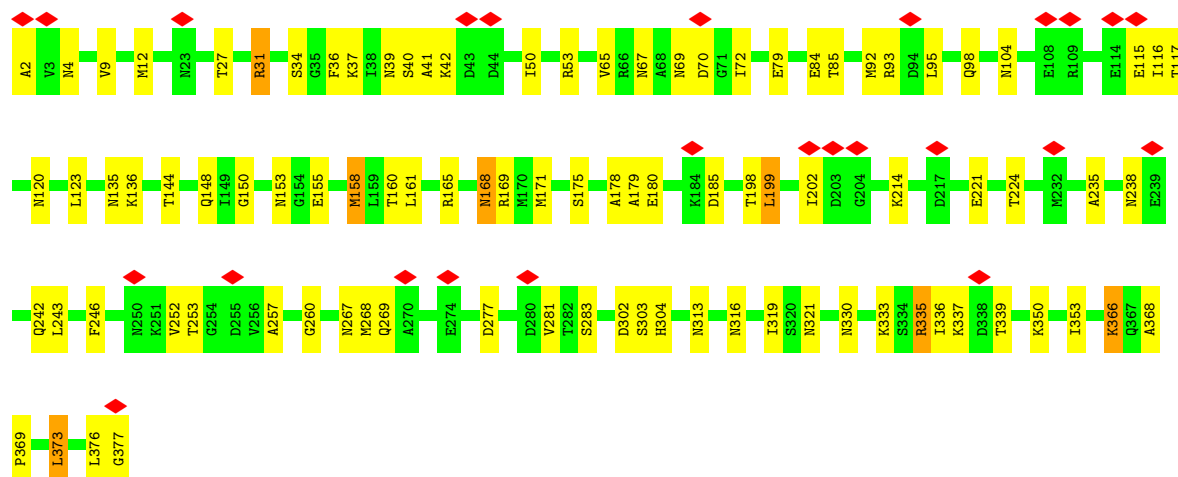
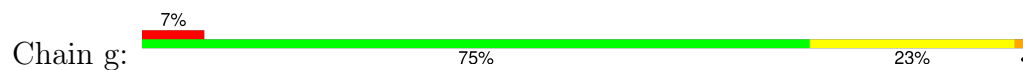


• Molecule 1: Flagellin D

Chain f: 14% 71% 28%



• Molecule 1: Flagellin D



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=65.41°, rise=4.74 Å, axial sym=C1	Depositor
Number of segments used	103479	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	70	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.580	Depositor
Minimum map value	-0.267	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.18	Depositor
Map size (Å)	478.464, 478.464, 478.464	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.068, 1.068, 1.068	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.89	0/2803	1.24	1/3783 (0.0%)
1	B	0.90	0/2803	1.24	0/3783
1	C	0.89	0/2803	1.24	0/3783
1	D	0.89	0/2803	1.25	1/3783 (0.0%)
1	E	0.91	1/2803 (0.0%)	1.25	1/3783 (0.0%)
1	F	0.90	0/2803	1.25	1/3783 (0.0%)
1	G	0.90	0/2803	1.24	1/3783 (0.0%)
1	H	0.90	0/2803	1.25	2/3783 (0.1%)
1	I	0.90	0/2803	1.23	1/3783 (0.0%)
1	J	0.90	0/2803	1.25	1/3783 (0.0%)
1	K	0.89	0/2803	1.25	1/3783 (0.0%)
1	L	0.90	0/2803	1.24	2/3783 (0.1%)
1	M	0.92	0/2803	1.24	1/3783 (0.0%)
1	N	0.90	0/2803	1.24	0/3783
1	O	0.90	0/2803	1.23	1/3783 (0.0%)
1	P	0.91	0/2803	1.25	2/3783 (0.1%)
1	Q	0.90	0/2803	1.24	0/3783
1	R	0.89	0/2803	1.23	1/3783 (0.0%)
1	S	0.91	0/2803	1.25	1/3783 (0.0%)
1	T	0.90	0/2803	1.25	0/3783
1	U	0.90	0/2803	1.25	0/3783
1	V	0.90	0/2803	1.25	1/3783 (0.0%)
1	W	0.90	0/2803	1.24	1/3783 (0.0%)
1	X	0.89	0/2803	1.24	0/3783
1	Y	0.90	0/2803	1.24	0/3783
1	Z	0.89	0/2803	1.24	0/3783
1	a	0.91	1/2803 (0.0%)	1.24	2/3783 (0.1%)
1	b	0.90	0/2803	1.24	0/3783
1	c	0.89	0/2803	1.23	0/3783
1	d	0.89	0/2803	1.24	1/3783 (0.0%)
1	e	0.89	0/2803	1.24	1/3783 (0.0%)
1	f	0.91	0/2803	1.24	0/3783
1	g	0.90	0/2803	1.24	1/3783 (0.0%)
All	All	0.90	2/92499 (0.0%)	1.24	25/124839 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
1	C	0	2
1	D	0	3
1	E	0	5
1	F	0	6
1	G	0	4
1	H	0	4
1	I	0	2
1	J	0	3
1	K	0	3
1	L	0	5
1	M	0	5
1	N	0	6
1	O	0	5
1	P	0	3
1	Q	0	6
1	R	0	2
1	S	0	4
1	T	0	4
1	U	0	5
1	V	0	3
1	W	0	2
1	X	0	5
1	Y	0	7
1	Z	0	3
1	a	0	2
1	b	0	3
1	c	0	2
1	d	0	3
1	e	0	6
1	f	0	5
1	g	0	5
All	All	0	128

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	6	ASN	C-N	-5.93	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	202	ILE	C-N	-5.00	1.27	1.33

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	254	GLY	CA-C-O	-6.28	118.14	122.22
1	J	260	GLY	CA-C-O	-6.25	118.16	122.22
1	R	254	GLY	CA-C-O	-6.23	117.93	122.23
1	g	260	GLY	CA-C-O	-6.16	118.22	122.22
1	S	254	GLY	CA-C-O	-6.08	117.93	122.37
1	P	260	GLY	CA-C-O	-5.99	118.33	122.22
1	K	260	GLY	CA-C-O	-5.95	118.13	122.23
1	O	260	GLY	CA-C-O	-5.81	118.12	122.37
1	H	260	GLY	CA-C-O	-5.81	118.44	122.22
1	V	231	ASP	N-CA-C	-5.80	107.19	114.56
1	F	260	GLY	CA-C-O	-5.68	118.36	122.45
1	a	260	GLY	CA-C-O	-5.64	118.34	122.23
1	H	150	GLY	CA-C-O	-5.60	117.79	122.33
1	G	260	GLY	CA-C-O	-5.55	118.32	122.37
1	M	260	GLY	CA-C-O	-5.55	118.45	122.45
1	d	155	GLU	N-CA-C	-5.53	106.37	114.39
1	E	260	GLY	CA-C-O	-5.48	118.37	122.37
1	W	260	GLY	CA-C-O	-5.41	118.42	122.37
1	I	260	GLY	CA-C-O	-5.41	118.50	122.23
1	D	39	ASN	N-CA-C	-5.34	106.93	113.50
1	e	260	GLY	CA-C-O	-5.21	118.56	122.37
1	P	38	ILE	CA-C-O	-5.15	118.15	122.63
1	L	260	GLY	CA-C-O	-5.07	118.22	122.33
1	A	5	VAL	N-CA-C	-5.04	108.59	113.53
1	L	231	ASP	N-CA-C	-5.04	107.52	113.97

There are no chirality outliers.

All (128) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109	ARG	Sidechain
1	A	125	ARG	Sidechain
1	A	165	ARG	Sidechain
1	B	125	ARG	Sidechain
1	B	93	ARG	Sidechain
1	C	125	ARG	Sidechain
1	C	66	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	D	109	ARG	Sidechain
1	D	125	ARG	Sidechain
1	D	305	ARG	Sidechain
1	E	125	ARG	Sidechain
1	E	31	ARG	Sidechain
1	E	314	ARG	Sidechain
1	E	335	ARG	Sidechain
1	E	91	ARG	Sidechain
1	F	109	ARG	Sidechain
1	F	125	ARG	Sidechain
1	F	16	ARG	Sidechain
1	F	335	ARG	Sidechain
1	F	53	ARG	Sidechain
1	F	93	ARG	Sidechain
1	G	109	ARG	Sidechain
1	G	16	ARG	Sidechain
1	G	335	ARG	Sidechain
1	G	66	ARG	Sidechain
1	H	109	ARG	Sidechain
1	H	125	ARG	Sidechain
1	H	31	ARG	Sidechain
1	H	93	ARG	Sidechain
1	I	109	ARG	Sidechain
1	I	165	ARG	Sidechain
1	J	109	ARG	Sidechain
1	J	16	ARG	Sidechain
1	J	165	ARG	Sidechain
1	K	125	ARG	Sidechain
1	K	335	ARG	Sidechain
1	K	93	ARG	Sidechain
1	L	109	ARG	Sidechain
1	L	125	ARG	Sidechain
1	L	165	ARG	Sidechain
1	L	169	ARG	Sidechain
1	L	335	ARG	Sidechain
1	M	109	ARG	Sidechain
1	M	125	ARG	Sidechain
1	M	53	ARG	Sidechain
1	M	59	ARG	Sidechain
1	M	93	ARG	Sidechain
1	N	109	ARG	Sidechain
1	N	125	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	N	165	ARG	Sidechain
1	N	169	ARG	Sidechain
1	N	59	ARG	Sidechain
1	N	66	ARG	Sidechain
1	O	125	ARG	Sidechain
1	O	165	ARG	Sidechain
1	O	335	ARG	Sidechain
1	O	66	ARG	Sidechain
1	O	93	ARG	Sidechain
1	P	125	ARG	Sidechain
1	P	165	ARG	Sidechain
1	P	93	ARG	Sidechain
1	Q	109	ARG	Sidechain
1	Q	125	ARG	Sidechain
1	Q	16	ARG	Sidechain
1	Q	165	ARG	Sidechain
1	Q	335	ARG	Sidechain
1	Q	53	ARG	Sidechain
1	R	109	ARG	Sidechain
1	R	125	ARG	Sidechain
1	S	125	ARG	Sidechain
1	S	169	ARG	Sidechain
1	S	59	ARG	Sidechain
1	S	66	ARG	Sidechain
1	T	109	ARG	Sidechain
1	T	125	ARG	Sidechain
1	T	169	ARG	Sidechain
1	T	335	ARG	Sidechain
1	U	109	ARG	Sidechain
1	U	125	ARG	Sidechain
1	U	169	ARG	Sidechain
1	U	335	ARG	Sidechain
1	U	53	ARG	Sidechain
1	V	109	ARG	Sidechain
1	V	125	ARG	Sidechain
1	V	165	ARG	Sidechain
1	W	109	ARG	Sidechain
1	W	169	ARG	Sidechain
1	X	169	ARG	Sidechain
1	X	314	ARG	Sidechain
1	X	53	ARG	Sidechain
1	X	59	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	X	93	ARG	Sidechain
1	Y	109	ARG	Sidechain
1	Y	125	ARG	Sidechain
1	Y	165	ARG	Sidechain
1	Y	305	ARG	Sidechain
1	Y	31	ARG	Sidechain
1	Y	66	ARG	Sidechain
1	Y	93	ARG	Sidechain
1	Z	125	ARG	Sidechain
1	Z	169	ARG	Sidechain
1	Z	93	ARG	Sidechain
1	a	16	ARG	Sidechain
1	a	31	ARG	Sidechain
1	b	109	ARG	Sidechain
1	b	165	ARG	Sidechain
1	b	31	ARG	Sidechain
1	c	125	ARG	Sidechain
1	c	169	ARG	Sidechain
1	d	109	ARG	Sidechain
1	d	165	ARG	Sidechain
1	d	169	ARG	Sidechain
1	e	109	ARG	Sidechain
1	e	125	ARG	Sidechain
1	e	16	ARG	Sidechain
1	e	165	ARG	Sidechain
1	e	169	ARG	Sidechain
1	e	305	ARG	Sidechain
1	f	109	ARG	Sidechain
1	f	125	ARG	Sidechain
1	f	165	ARG	Sidechain
1	f	169	ARG	Sidechain
1	f	93	ARG	Sidechain
1	g	169	ARG	Sidechain
1	g	31	ARG	Sidechain
1	g	335	ARG	Sidechain
1	g	53	ARG	Sidechain
1	g	93	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2785	0	2738	61	0
1	B	2785	0	2738	63	0
1	C	2785	0	2738	51	0
1	D	2785	0	2738	46	0
1	E	2785	0	2738	93	0
1	F	2785	0	2738	55	0
1	G	2785	0	2738	44	0
1	H	2785	0	2738	66	0
1	I	2785	0	2738	65	0
1	J	2785	0	2738	87	0
1	K	2785	0	2738	63	0
1	L	2785	0	2738	68	0
1	M	2785	0	2738	76	0
1	N	2785	0	2738	68	0
1	O	2785	0	2738	65	0
1	P	2785	0	2738	68	0
1	Q	2785	0	2738	53	0
1	R	2785	0	2738	52	0
1	S	2785	0	2738	93	0
1	T	2785	0	2738	58	0
1	U	2785	0	2738	67	0
1	V	2785	0	2738	57	0
1	W	2785	0	2738	80	0
1	X	2785	0	2738	67	0
1	Y	2785	0	2738	77	0
1	Z	2785	0	2738	59	0
1	a	2785	0	2738	72	0
1	b	2785	0	2738	58	0
1	c	2785	0	2738	58	0
1	d	2785	0	2738	72	0
1	e	2785	0	2738	63	0
1	f	2785	0	2738	76	0
1	g	2785	0	2738	61	0
All	All	91905	0	90354	1923	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 (1923) 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:f:178:ALA:HA	1:f:268:MET:HA	1.27	1.16
1:e:146:SER:HA	1:e:158:MET:HA	1.46	0.97
1:S:369:PRO:HB2	1:V:353:ILE:HD13	1.51	0.91
1:S:176:TYR:HA	1:S:271:GLY:HA2	1.55	0.88
1:M:177:VAL:HA	1:M:244:GLN:HA	1.54	0.88
1:f:200:LYS:HA	1:f:206:ASP:HA	1.56	0.88
1:M:177:VAL:HG13	1:M:244:GLN:HG2	1.55	0.87
1:B:353:ILE:HD13	1:Y:369:PRO:HB2	1.55	0.87
1:W:197:PHE:HB2	1:W:209:ILE:HG13	1.58	0.86
1:I:353:ILE:HD13	1:e:369:PRO:HB2	1.57	0.86
1:a:369:PRO:HB2	1:e:353:ILE:HD13	1.56	0.86
1:T:369:PRO:HB2	1:W:353:ILE:HD13	1.59	0.85
1:L:82:MET:HE1	1:L:304:HIS:HB3	1.59	0.85
1:P:202:ILE:HD11	1:P:249:ASN:O	1.76	0.84
1:V:82:MET:HE1	1:V:304:HIS:HB3	1.59	0.84
1:L:247:ALA:HB1	1:L:252:VAL:HG11	1.60	0.84
1:S:235:ALA:HA	1:S:245:ILE:HA	1.60	0.84
1:S:233:VAL:HB	1:S:245:ILE:HD11	1.59	0.83
1:V:178:ALA:HA	1:V:268:MET:HA	1.59	0.83
1:E:369:PRO:HB2	1:b:353:ILE:HD13	1.60	0.83
1:W:192:ALA:HA	1:W:261:GLY:HA3	1.58	0.83
1:J:369:PRO:HB2	1:N:353:ILE:HD13	1.58	0.83
1:T:238:ASN:HD21	1:T:242:GLN:HB2	1.41	0.83
1:L:339:THR:HG23	1:L:344:GLU:HG3	1.59	0.82
1:F:198:THR:HB	1:F:257:ALA:HB3	1.61	0.82
1:S:188:VAL:HB	1:S:215:GLU:HA	1.60	0.81
1:O:69:ASN:HB3	1:Q:335:ARG:HD3	1.63	0.81
1:H:353:ILE:HD13	1:d:369:PRO:HB2	1.62	0.81
1:S:375:LEU:HD11	1:T:341:PHE:HB3	1.62	0.81
1:f:179:ALA:HB2	1:f:269:GLN:HG2	1.63	0.81
1:A:148:GLN:HE22	1:A:155:GLU:HB3	1.47	0.80
1:b:238:ASN:HD21	1:b:242:GLN:HB2	1.45	0.80
1:Z:247:ALA:HB1	1:Z:252:VAL:HG21	1.62	0.80
1:f:260:GLY:H	1:f:263:ALA:HB3	1.46	0.80
1:a:3:VAL:HG21	1:c:341:PHE:HB2	1.62	0.79
1:e:192:ALA:HA	1:e:261:GLY:HA3	1.63	0.79
1:J:198:THR:HB	1:J:257:ALA:HB3	1.63	0.79
1:M:196:THR:HB	1:M:259:SER:HB2	1.63	0.79
1:b:178:ALA:HA	1:b:268:MET:HA	1.63	0.79
1:T:195:ILE:HD11	1:T:262:LEU:HD23	1.63	0.78
1:H:13:THR:HG21	1:e:30:GLU:HG2	1.66	0.78
1:Z:164:MET:HE3	1:Z:304:HIS:HD2	1.49	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:375:LEU:C	1:G:376:LEU:HD23	2.09	0.77
1:D:198:THR:HB	1:D:257:ALA:HB3	1.67	0.77
1:M:369:PRO:HB2	1:P:353:ILE:HD13	1.65	0.77
1:V:219:ILE:HD11	1:V:243:LEU:HB2	1.67	0.77
1:Z:339:THR:HG23	1:Z:344:GLU:HG3	1.65	0.77
1:H:184:LYS:HB3	1:g:144:THR:HG21	1.67	0.76
1:M:112:ILE:HG22	1:M:281:VAL:HG11	1.66	0.76
1:N:339:THR:HG23	1:N:344:GLU:HG3	1.66	0.76
1:O:202:ILE:HA	1:O:253:THR:HG23	1.67	0.76
1:c:69:ASN:HB3	1:e:335:ARG:HD3	1.68	0.76
1:U:146:SER:HB3	1:U:156:ALA:HB1	1.67	0.76
1:H:148:GLN:HE21	1:I:288:GLN:HE22	1.34	0.76
1:N:195:ILE:CD1	1:N:263:ALA:HB2	2.16	0.76
1:S:109:ARG:HB3	1:S:282:THR:HA	1.66	0.76
1:Y:188:VAL:HB	1:Y:215:GLU:HA	1.66	0.76
1:Y:223:ALA:HB2	1:Y:243:LEU:HD11	1.68	0.76
1:B:373:LEU:HB2	1:F:353:ILE:HD11	1.66	0.75
1:E:176:TYR:HA	1:E:271:GLY:HA2	1.67	0.75
1:d:19:THR:HG22	1:g:2:ALA:HB2	1.68	0.75
1:E:179:ALA:HA	1:E:269:GLN:HE21	1.52	0.75
1:E:211:VAL:HG11	1:E:226:ILE:HD13	1.69	0.75
1:S:93:ARG:HB2	1:S:294:ILE:HD11	1.69	0.75
1:V:8:ASN:HD21	1:V:369:PRO:HD3	1.52	0.74
1:E:236:SER:HB2	1:E:244:GLN:HB2	1.70	0.74
1:g:198:THR:HB	1:g:257:ALA:HB3	1.67	0.74
1:S:158:MET:HE3	1:T:184:LYS:HD2	1.70	0.74
1:T:202:ILE:HA	1:T:253:THR:HG23	1.70	0.74
1:I:69:ASN:HB3	1:L:335:ARG:HD2	1.69	0.73
1:M:168:ASN:HB3	1:M:171:MET:HG2	1.70	0.73
1:J:93:ARG:HB2	1:J:294:ILE:HG21	1.70	0.73
1:M:188:VAL:HB	1:M:215:GLU:HA	1.69	0.73
1:A:375:LEU:HD11	1:X:362:LEU:HD23	1.71	0.73
1:f:99:SER:HB2	1:f:112:ILE:HD12	1.70	0.73
1:W:198:THR:HB	1:W:257:ALA:HB3	1.70	0.73
1:P:88:ILE:HD11	1:S:317:HIS:HB3	1.71	0.73
1:V:202:ILE:HA	1:V:253:THR:HG23	1.69	0.73
1:J:41:ALA:HB2	1:J:48:LEU:HD22	1.71	0.73
1:A:93:ARG:HB2	1:A:294:ILE:HG21	1.70	0.72
1:f:202:ILE:HA	1:f:253:THR:HG23	1.71	0.72
1:N:195:ILE:HD11	1:N:263:ALA:HB2	1.71	0.72
1:Y:180:GLU:HG2	1:Y:267:ASN:HB2	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:69:ASN:HB3	1:N:335:ARG:HD3	1.69	0.72
1:C:171:MET:HE2	1:C:297:ALA:HB1	1.72	0.72
1:E:373:LEU:HD23	1:b:353:ILE:HG23	1.70	0.72
1:T:219:ILE:HD11	1:T:243:LEU:HB2	1.72	0.72
1:N:69:ASN:HB3	1:P:335:ARG:HE	1.53	0.72
1:b:89:LEU:HA	1:b:92:MET:HE2	1.71	0.72
1:Q:120:ASN:HD21	1:Q:277:ASP:HA	1.53	0.71
1:D:31:ARG:HB3	1:D:339:THR:HG21	1.72	0.71
1:C:89:LEU:HA	1:C:92:MET:HE2	1.73	0.71
1:C:353:ILE:HG13	1:Z:369:PRO:HB2	1.72	0.71
1:M:192:ALA:HA	1:M:261:GLY:HA3	1.71	0.71
1:S:144:THR:HG21	1:T:184:LYS:HB2	1.73	0.71
1:A:6:ASN:HA	1:D:350:LYS:HZ3	1.56	0.70
1:E:162:LYS:H	1:E:304:HIS:CE1	2.09	0.70
1:I:144:THR:HG22	1:I:160:THR:HB	1.72	0.70
1:T:172:GLY:HA3	1:T:275:THR:HA	1.73	0.70
1:E:211:VAL:HG13	1:E:229:GLN:HG3	1.72	0.70
1:J:197:PHE:HD2	1:J:209:ILE:HD11	1.56	0.70
1:C:178:ALA:HA	1:C:268:MET:HA	1.74	0.70
1:S:202:ILE:HD13	1:S:253:THR:HG23	1.74	0.70
1:L:131:SER:HB3	1:L:136:LYS:HD3	1.73	0.70
1:R:143:SER:H	1:R:145:LYS:HE3	1.56	0.70
1:a:339:THR:HG23	1:a:344:GLU:HG3	1.72	0.70
1:A:338:ASP:HB2	1:Z:4:ASN:ND2	2.07	0.69
1:J:3:VAL:HG22	1:K:341:PHE:HB2	1.74	0.69
1:C:30:GLU:HG2	1:C:39:ASN:HD22	1.57	0.69
1:e:202:ILE:HA	1:e:253:THR:HG23	1.72	0.69
1:Y:179:ALA:HB3	1:Y:267:ASN:HB3	1.74	0.69
1:e:65:VAL:HA	1:e:319:ILE:HD11	1.75	0.69
1:E:3:VAL:HG21	1:F:341:PHE:HB2	1.75	0.69
1:a:198:THR:HB	1:a:257:ALA:HB3	1.74	0.69
1:E:202:ILE:HA	1:E:253:THR:HG23	1.74	0.69
1:G:198:THR:HB	1:G:257:ALA:HB3	1.73	0.69
1:A:69:ASN:HB3	1:C:335:ARG:HD3	1.75	0.69
1:a:201:ASP:HB2	1:a:207:GLN:HE22	1.56	0.69
1:I:198:THR:HB	1:I:257:ALA:HB3	1.74	0.68
1:S:196:THR:HB	1:S:259:SER:HB2	1.75	0.68
1:I:171:MET:HE2	1:I:297:ALA:HB1	1.74	0.68
1:Z:219:ILE:HD11	1:Z:243:LEU:HB2	1.73	0.68
1:M:202:ILE:HA	1:M:253:THR:HG23	1.74	0.68
1:d:82:MET:HE3	1:d:301:VAL:HG13	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:PRO:HB2	1:D:353:ILE:HD13	1.76	0.68
1:I:350:LYS:HE3	1:e:6:ASN:HA	1.76	0.68
1:O:173:GLY:HA3	1:O:248:GLY:HA2	1.76	0.68
1:T:339:THR:HG23	1:T:344:GLU:HG3	1.75	0.68
1:T:92:MET:HA	1:T:95:LEU:HD12	1.75	0.68
1:L:143:SER:H	1:L:145:LYS:HZ3	1.42	0.68
1:B:202:ILE:HA	1:B:253:THR:HG23	1.75	0.68
1:O:375:LEU:HD23	1:O:376:LEU:HG	1.76	0.68
1:C:164:MET:HE1	1:C:304:HIS:HD2	1.58	0.67
1:S:195:ILE:HG23	1:S:263:ALA:HB2	1.76	0.67
1:U:95:LEU:HG	1:U:112:ILE:HG23	1.77	0.67
1:d:199:LEU:HB3	1:d:256:VAL:HG13	1.77	0.67
1:A:170:MET:HE1	1:A:250:ASN:HB3	1.75	0.67
1:X:200:LYS:HA	1:X:206:ASP:HA	1.77	0.66
1:Y:82:MET:HE1	1:Y:304:HIS:HB3	1.77	0.66
1:J:195:ILE:HG23	1:J:211:VAL:HB	1.76	0.66
1:L:202:ILE:HA	1:L:253:THR:HG23	1.78	0.66
1:U:69:ASN:HB3	1:W:335:ARG:HD3	1.78	0.66
1:P:192:ALA:HB1	1:P:262:LEU:HA	1.76	0.66
1:c:95:LEU:HG	1:c:112:ILE:HG23	1.76	0.66
1:e:309:GLY:HA2	1:e:312:GLN:HE21	1.60	0.66
1:G:178:ALA:HA	1:G:268:MET:HA	1.78	0.66
1:V:33:SER:HB3	1:Y:361:VAL:HG21	1.77	0.66
1:C:93:ARG:HB2	1:C:294:ILE:HG21	1.77	0.66
1:g:202:ILE:HA	1:g:253:THR:HG23	1.78	0.66
1:E:179:ALA:N	1:E:267:ASN:O	2.29	0.66
1:S:202:ILE:HA	1:S:253:THR:HG23	1.76	0.66
1:Y:99:SER:HB2	1:Y:112:ILE:HD12	1.78	0.65
1:G:144:THR:HG22	1:G:160:THR:HB	1.79	0.65
1:S:230:THR:HG22	1:S:232:MET:H	1.60	0.65
1:X:211:VAL:HG11	1:X:226:ILE:HD13	1.77	0.65
1:I:164:MET:HE1	1:I:301:VAL:HA	1.76	0.65
1:N:267:ASN:HB3	1:N:269:GLN:HE21	1.62	0.65
1:S:175:SER:HA	1:S:246:PHE:HA	1.77	0.65
1:d:219:ILE:HD11	1:d:243:LEU:HB2	1.78	0.65
1:P:202:ILE:HD13	1:P:253:THR:HG23	1.79	0.65
1:B:188:VAL:HB	1:B:215:GLU:HA	1.78	0.65
1:b:321:ASN:O	1:b:325:ILE:HG13	1.96	0.65
1:V:47:GLY:HA2	1:V:50:ILE:HG22	1.77	0.65
1:d:69:ASN:HB3	1:g:335:ARG:HD3	1.79	0.65
1:H:202:ILE:HA	1:H:253:THR:HG23	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:201:ASP:HB3	1:M:205:ASN:H	1.61	0.64
1:R:362:LEU:HD23	1:U:375:LEU:HD11	1.79	0.64
1:E:276:VAL:HA	1:E:279:ILE:HG23	1.80	0.64
1:L:84:GLU:HA	1:L:87:ASN:HD22	1.61	0.64
1:N:3:VAL:HG11	1:N:375:LEU:HD22	1.80	0.64
1:S:170:MET:HA	1:S:249:ASN:HD22	1.61	0.64
1:C:246:PHE:HB2	1:C:289:GLN:HE21	1.63	0.64
1:M:176:TYR:HB2	1:M:245:ILE:HB	1.79	0.64
1:b:198:THR:HB	1:b:257:ALA:HB3	1.78	0.64
1:F:148:GLN:NE2	1:F:152:ASP:O	2.31	0.64
1:S:65:VAL:HG12	1:S:69:ASN:HD21	1.63	0.64
1:a:244:GLN:HB3	1:a:289:GLN:HE22	1.62	0.64
1:M:373:LEU:HD23	1:P:353:ILE:HG23	1.80	0.63
1:A:148:GLN:NE2	1:A:155:GLU:HB3	2.14	0.63
1:F:171:MET:HG3	1:F:300:TYR:HD2	1.63	0.63
1:M:188:VAL:HG23	1:M:217:ASP:H	1.64	0.63
1:b:30:GLU:HG2	1:f:13:THR:HG21	1.81	0.63
1:N:177:VAL:HG13	1:N:244:GLN:HG2	1.81	0.63
1:V:286:GLY:HA2	1:V:289:GLN:HE21	1.64	0.63
1:B:350:LYS:HE2	1:Y:6:ASN:HA	1.80	0.63
1:E:99:SER:HA	1:E:104:ASN:HD21	1.63	0.63
1:M:276:VAL:HA	1:M:279:ILE:HG23	1.79	0.63
1:X:178:ALA:HA	1:X:268:MET:HA	1.80	0.62
1:T:46:ALA:O	1:T:50:ILE:HG13	1.99	0.62
1:H:369:PRO:HB2	1:L:353:ILE:HD13	1.80	0.62
1:S:245:ILE:HG12	1:S:258:PHE:HZ	1.64	0.62
1:T:69:ASN:HB3	1:V:335:ARG:HD3	1.81	0.62
1:W:36:PHE:HA	1:W:338:ASP:HA	1.80	0.62
1:d:48:LEU:HD21	1:e:305:ARG:HE	1.63	0.62
1:f:198:THR:HB	1:f:257:ALA:HB3	1.81	0.62
1:B:250:ASN:HD21	1:B:296:SER:HB3	1.64	0.62
1:L:368:ALA:HB3	1:L:369:PRO:HD3	1.82	0.62
1:Y:153:ASN:HD21	1:Z:234:LYS:HB3	1.64	0.62
1:d:4:ASN:ND2	1:e:338:ASP:HB3	2.14	0.62
1:E:92:MET:HG2	1:E:116:ILE:HG13	1.80	0.62
1:U:111:ALA:HA	1:U:114:GLU:HG3	1.81	0.62
1:A:6:ASN:HA	1:D:350:LYS:NZ	2.14	0.62
1:J:209:ILE:HD13	1:J:230:THR:HG21	1.81	0.62
1:D:93:ARG:HB2	1:D:294:ILE:HG21	1.81	0.62
1:O:163:ASP:HB3	1:O:168:ASN:HD22	1.64	0.62
1:S:31:ARG:HD2	1:S:37:LYS:HA	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:120:ASN:HD21	1:T:277:ASP:HA	1.65	0.62
1:Y:199:LEU:HD13	1:Y:252:VAL:HG13	1.80	0.62
1:S:238:ASN:HB3	1:S:244:GLN:NE2	2.14	0.62
1:b:74:ILE:HG12	1:b:132:PHE:CD2	2.35	0.62
1:A:162:LYS:H	1:A:304:HIS:CE1	2.18	0.62
1:f:250:ASN:HD21	1:f:296:SER:HB2	1.63	0.62
1:E:162:LYS:H	1:E:304:HIS:HE1	1.47	0.62
1:M:175:SER:O	1:M:271:GLY:HA2	2.00	0.62
1:E:192:ALA:HB1	1:E:261:GLY:HA3	1.81	0.61
1:S:236:SER:HB3	1:S:244:GLN:HB2	1.81	0.61
1:d:195:ILE:HD13	1:d:263:ALA:HB2	1.81	0.61
1:d:252:VAL:HG11	1:d:256:VAL:HG22	1.82	0.61
1:g:31:ARG:HE	1:g:37:LYS:HA	1.63	0.61
1:R:9:VAL:HA	1:R:12:MET:HE2	1.81	0.61
1:R:69:ASN:HB3	1:U:335:ARG:HD3	1.81	0.61
1:d:178:ALA:HA	1:d:268:MET:HA	1.82	0.61
1:V:375:LEU:HD11	1:W:342:ALA:HA	1.81	0.61
1:E:258:PHE:CD2	1:E:268:MET:HG3	2.35	0.61
1:X:168:ASN:HB3	1:X:171:MET:HG2	1.82	0.61
1:d:202:ILE:HD12	1:d:253:THR:HG23	1.81	0.61
1:N:173:GLY:HA2	1:N:249:ASN:ND2	2.16	0.61
1:V:361:VAL:HA	1:V:364:GLN:HE21	1.65	0.61
1:P:63:VAL:HG12	1:P:67:ASN:HD21	1.64	0.61
1:e:68:ALA:HB3	1:e:319:ILE:HD13	1.83	0.61
1:A:148:GLN:HA	1:A:156:ALA:HA	1.82	0.61
1:H:164:MET:HE1	1:H:301:VAL:HG22	1.83	0.61
1:D:162:LYS:H	1:D:304:HIS:CE1	2.18	0.61
1:I:202:ILE:HA	1:I:253:THR:HG23	1.82	0.61
1:K:219:ILE:HD11	1:K:243:LEU:HB2	1.82	0.61
1:P:41:ALA:HB2	1:P:48:LEU:HD22	1.82	0.61
1:a:171:MET:HG3	1:a:300:TYR:HD2	1.64	0.61
1:D:89:LEU:HA	1:D:92:MET:HE2	1.82	0.61
1:B:109:ARG:HB3	1:B:282:THR:HA	1.82	0.60
1:C:188:VAL:HB	1:C:215:GLU:HA	1.83	0.60
1:L:89:LEU:HA	1:L:92:MET:HE2	1.83	0.60
1:E:9:VAL:HA	1:E:12:MET:HE2	1.81	0.60
1:P:199:LEU:HB3	1:P:256:VAL:HG13	1.83	0.60
1:T:201:ASP:HB2	1:T:207:GLN:HE21	1.66	0.60
1:f:164:MET:HE3	1:f:304:HIS:HD2	1.66	0.60
1:P:332:SER:HA	1:P:335:ARG:HD2	1.83	0.60
1:T:373:LEU:HD21	1:W:353:ILE:HG23	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:197:PHE:HB2	1:f:209:ILE:HB	1.84	0.60
1:G:375:LEU:O	1:G:376:LEU:HD23	2.01	0.60
1:M:368:ALA:HB3	1:M:369:PRO:HD3	1.83	0.60
1:Z:368:ALA:HB3	1:Z:369:PRO:HD3	1.82	0.60
1:a:239:GLU:HG2	1:a:240:LYS:HD3	1.82	0.60
1:g:144:THR:HB	1:g:158:MET:HG3	1.83	0.60
1:F:92:MET:HG3	1:F:119:LEU:HD12	1.84	0.60
1:J:9:VAL:HA	1:J:12:MET:HE2	1.83	0.60
1:L:73:SER:HB3	1:O:335:ARG:HH21	1.67	0.60
1:P:252:VAL:HG11	1:P:256:VAL:HG22	1.83	0.60
1:c:202:ILE:HA	1:c:253:THR:HG23	1.84	0.60
1:O:178:ALA:HB2	1:O:268:MET:HE2	1.84	0.60
1:c:245:ILE:HD12	1:c:258:PHE:HE2	1.66	0.60
1:Q:153:ASN:ND2	1:R:292:ALA:HB2	2.17	0.60
1:g:27:THR:O	1:g:31:ARG:HG2	2.02	0.60
1:J:335:ARG:HD3	1:g:69:ASN:HB3	1.84	0.60
1:N:3:VAL:HG13	1:O:341:PHE:HB2	1.84	0.60
1:N:89:LEU:HA	1:N:92:MET:HE2	1.84	0.60
1:D:69:ASN:HB3	1:G:335:ARG:HD3	1.83	0.59
1:Q:178:ALA:HA	1:Q:268:MET:HA	1.84	0.59
1:E:200:LYS:HD2	1:E:204:GLY:HA2	1.84	0.59
1:K:92:MET:HE2	1:K:279:ILE:HD11	1.84	0.59
1:U:202:ILE:HA	1:U:253:THR:HB	1.84	0.59
1:X:198:THR:HB	1:X:257:ALA:HB3	1.84	0.59
1:X:217:ASP:HB3	1:X:221:GLU:HB2	1.84	0.59
1:E:181:GLY:HA2	1:E:242:GLN:HG2	1.84	0.59
1:Y:38:ILE:HG12	1:Y:337:LYS:HA	1.84	0.59
1:E:164:MET:HE1	1:E:301:VAL:HG22	1.83	0.59
1:M:175:SER:HA	1:M:246:PHE:HA	1.83	0.59
1:N:202:ILE:HA	1:N:253:THR:HG23	1.84	0.59
1:T:158:MET:HB2	1:U:220:GLU:OE1	2.02	0.59
1:V:93:ARG:HB2	1:V:294:ILE:HG21	1.84	0.59
1:Y:4:ASN:ND2	1:Y:7:THR:HB	2.18	0.59
1:K:131:SER:HB3	1:K:136:LYS:HD3	1.84	0.59
1:R:86:THR:HG22	1:R:90:GLN:HE21	1.68	0.59
1:V:22:THR:HA	1:V:25:GLN:HE21	1.66	0.59
1:V:30:GLU:HG2	1:Y:13:THR:HG21	1.85	0.59
1:Y:148:GLN:HE22	1:Y:155:GLU:H	1.50	0.59
1:D:109:ARG:HB3	1:D:282:THR:HA	1.83	0.59
1:H:41:ALA:HB2	1:H:48:LEU:HD22	1.84	0.59
1:P:199:LEU:HD13	1:P:252:VAL:HG22	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:85:THR:HG23	1:R:123:LEU:HD11	1.85	0.59
1:B:162:LYS:H	1:B:304:HIS:HE1	1.50	0.59
1:Y:47:GLY:HA2	1:Y:50:ILE:HG22	1.85	0.58
1:A:246:PHE:HB2	1:A:289:GLN:HE21	1.67	0.58
1:J:286:GLY:HA2	1:J:289:GLN:HE21	1.68	0.58
1:H:211:VAL:HG11	1:H:226:ILE:HG12	1.84	0.58
1:M:236:SER:HB2	1:M:244:GLN:HB2	1.84	0.58
1:a:27:THR:O	1:a:31:ARG:HG2	2.04	0.58
1:J:219:ILE:HD11	1:J:243:LEU:HB2	1.85	0.58
1:L:214:LYS:HE2	1:L:225:TYR:CE1	2.38	0.58
1:P:211:VAL:HG11	1:P:226:ILE:HD13	1.85	0.58
1:Y:182:LYS:HB3	1:Y:186:TRP:CD1	2.38	0.58
1:C:316:ASN:O	1:C:319:ILE:HG12	2.03	0.58
1:Y:195:ILE:HD13	1:Y:263:ALA:HB2	1.83	0.58
1:b:149:ILE:HD11	1:b:157:VAL:HG23	1.85	0.58
1:D:62:ASP:O	1:D:65:VAL:HG22	2.04	0.58
1:N:240:LYS:HD2	1:N:240:LYS:H	1.69	0.58
1:O:198:THR:HB	1:O:257:ALA:HB3	1.86	0.58
1:a:31:ARG:HH21	1:a:37:LYS:HG3	1.69	0.58
1:b:202:ILE:HA	1:b:253:THR:HG23	1.85	0.58
1:K:69:ASN:O	1:K:72:ILE:HG12	2.04	0.58
1:M:111:ALA:O	1:M:114:GLU:HG3	2.04	0.58
1:f:142:PHE:HA	1:f:145:LYS:HE3	1.85	0.58
1:F:164:MET:HE3	1:F:304:HIS:HD2	1.69	0.57
1:P:202:ILE:CD1	1:P:249:ASN:O	2.49	0.57
1:g:92:MET:HA	1:g:95:LEU:HD12	1.86	0.57
1:J:3:VAL:HG11	1:K:342:ALA:H	1.69	0.57
1:K:369:PRO:HB2	1:O:353:ILE:HD13	1.85	0.57
1:I:65:VAL:HG12	1:I:69:ASN:HD21	1.69	0.57
1:O:31:ARG:HB3	1:O:339:THR:HG21	1.85	0.57
1:A:47:GLY:HA2	1:A:50:ILE:HG22	1.86	0.57
1:A:200:LYS:HA	1:A:206:ASP:HA	1.86	0.57
1:D:68:ALA:HB3	1:D:319:ILE:HD11	1.87	0.57
1:P:33:SER:HB3	1:S:361:VAL:HG11	1.85	0.57
1:R:99:SER:HA	1:R:104:ASN:HD22	1.69	0.57
1:T:195:ILE:HG12	1:T:262:LEU:HB3	1.84	0.57
1:a:368:ALA:HB3	1:a:369:PRO:HD3	1.86	0.57
1:e:250:ASN:HD21	1:e:296:SER:HB2	1.69	0.57
1:N:198:THR:HB	1:N:257:ALA:HB3	1.86	0.57
1:V:196:THR:HB	1:V:259:SER:HB2	1.86	0.57
1:W:63:VAL:HA	1:W:66:ARG:HE	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:144:THR:HG22	1:g:160:THR:HB	1.85	0.57
1:b:369:PRO:HB2	1:d:353:ILE:HG13	1.86	0.57
1:c:246:PHE:HB2	1:c:289:GLN:HE21	1.69	0.57
1:G:368:ALA:HB3	1:G:369:PRO:HD3	1.87	0.57
1:J:156:ALA:HB3	1:K:220:GLU:OE2	2.03	0.57
1:E:88:ILE:HG22	1:E:92:MET:HE2	1.87	0.57
1:C:62:ASP:O	1:C:65:VAL:HG22	2.04	0.57
1:E:186:TRP:HD1	1:E:219:ILE:HB	1.70	0.57
1:E:203:ASP:HB2	1:E:205:ASN:HD21	1.69	0.57
1:Y:197:PHE:HB2	1:Y:209:ILE:HG23	1.86	0.57
1:J:99:SER:HA	1:J:104:ASN:HD22	1.70	0.57
1:Q:172:GLY:HA3	1:Q:275:THR:HA	1.87	0.56
1:T:9:VAL:HA	1:T:12:MET:HE2	1.87	0.56
1:F:199:LEU:HD13	1:F:252:VAL:HG22	1.87	0.56
1:f:195:ILE:HG13	1:f:263:ALA:HB2	1.85	0.56
1:A:184:LYS:HD3	1:Z:144:THR:HG22	1.85	0.56
1:B:125:ARG:NH1	1:E:155:GLU:OE2	2.37	0.56
1:H:281:VAL:HG12	1:H:287:ALA:HA	1.87	0.56
1:I:29:MET:HG2	1:L:361:VAL:HG13	1.87	0.56
1:T:113:GLN:HE22	1:T:116:ILE:HD11	1.70	0.56
1:d:142:PHE:CE1	1:d:145:LYS:HG3	2.40	0.56
1:L:370:ASN:HA	1:L:373:LEU:HD23	1.87	0.56
1:Q:150:GLY:HA3	1:Q:155:GLU:HB2	1.88	0.56
1:S:9:VAL:HA	1:S:12:MET:HE2	1.87	0.56
1:T:244:GLN:HB3	1:T:289:GLN:HE21	1.70	0.56
1:X:92:MET:HE2	1:X:279:ILE:HD11	1.86	0.56
1:Z:179:ALA:HB3	1:Z:267:ASN:HB3	1.88	0.56
1:e:190:ALA:HA	1:e:215:GLU:HG2	1.87	0.56
1:e:209:ILE:HG21	1:e:230:THR:HB	1.86	0.56
1:F:197:PHE:HD2	1:F:209:ILE:HB	1.71	0.56
1:K:196:THR:HB	1:K:259:SER:HB2	1.87	0.56
1:T:238:ASN:ND2	1:T:242:GLN:HB2	2.17	0.56
1:V:148:GLN:NE2	1:V:152:ASP:O	2.39	0.56
1:c:105:SER:H	1:c:108:GLU:CD	2.14	0.56
1:B:316:ASN:O	1:B:319:ILE:HG13	2.06	0.56
1:K:202:ILE:HA	1:K:253:THR:HG23	1.86	0.56
1:L:36:PHE:O	1:L:39:ASN:ND2	2.37	0.56
1:M:92:MET:HE2	1:M:279:ILE:HD11	1.86	0.56
1:R:182:LYS:HE2	1:R:266:LEU:HG	1.87	0.56
1:Y:207:GLN:HE22	1:Y:209:ILE:HG22	1.70	0.56
1:f:123:LEU:O	1:f:126:ILE:HG22	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:164:MET:HE3	1:O:304:HIS:HD2	1.71	0.56
1:D:36:PHE:C	1:D:339:THR:HG23	2.30	0.56
1:F:37:LYS:N	1:F:337:LYS:O	2.37	0.56
1:S:217:ASP:HB3	1:S:221:GLU:HB2	1.88	0.56
1:c:92:MET:HE2	1:c:119:LEU:HB3	1.87	0.56
1:b:173:GLY:HA2	1:b:249:ASN:CG	2.31	0.56
1:g:235:ALA:HB1	1:g:243:LEU:HD11	1.88	0.56
1:H:112:ILE:HG12	1:J:46:ALA:HB2	1.88	0.55
1:Q:199:LEU:HD13	1:Q:252:VAL:HG22	1.88	0.55
1:X:148:GLN:NE2	1:X:152:ASP:O	2.39	0.55
1:I:320:SER:HA	1:I:323:ASP:OD1	2.07	0.55
1:M:200:LYS:HD2	1:M:206:ASP:HA	1.87	0.55
1:T:179:ALA:HB2	1:T:269:GLN:CD	2.31	0.55
1:Y:349:THR:HA	1:Y:352:GLN:HE21	1.70	0.55
1:F:85:THR:HG23	1:F:123:LEU:HD22	1.88	0.55
1:H:198:THR:HB	1:H:257:ALA:HB3	1.88	0.55
1:J:368:ALA:HB3	1:J:369:PRO:HD3	1.88	0.55
1:O:34:SER:C	1:O:36:PHE:H	2.14	0.55
1:f:236:SER:HB3	1:f:288:GLN:HB3	1.87	0.55
1:D:148:GLN:NE2	1:D:152:ASP:O	2.39	0.55
1:D:200:LYS:HA	1:D:206:ASP:HA	1.89	0.55
1:K:205:ASN:OD1	1:K:205:ASN:N	2.40	0.55
1:e:170:MET:HE1	1:e:250:ASN:HB3	1.88	0.55
1:A:171:MET:HG3	1:A:300:TYR:CD2	2.42	0.55
1:H:101:ASN:HD21	1:g:70:ASP:HB2	1.71	0.55
1:K:171:MET:HG3	1:K:300:TYR:HD2	1.72	0.55
1:K:262:LEU:HG	1:K:266:LEU:HD23	1.87	0.55
1:N:106:LYS:NZ	1:N:282:THR:HB	2.21	0.55
1:a:105:SER:H	1:a:108:GLU:CD	2.14	0.55
1:d:84:GLU:HG2	1:g:321:ASN:HB2	1.88	0.55
1:X:219:ILE:HD11	1:X:243:LEU:HB2	1.88	0.55
1:Y:245:ILE:HG21	1:Y:258:PHE:CZ	2.41	0.55
1:A:307:GLU:HG2	1:X:114:GLU:HG3	1.89	0.55
1:Y:109:ARG:HB3	1:Y:282:THR:HA	1.88	0.55
1:b:195:ILE:HG13	1:b:263:ALA:HB2	1.88	0.55
1:R:250:ASN:HD21	1:R:296:SER:HB2	1.72	0.55
1:S:330:ASN:O	1:S:333:LYS:HG2	2.06	0.55
1:F:105:SER:H	1:F:108:GLU:CD	2.14	0.55
1:K:368:ALA:HB3	1:K:369:PRO:HD3	1.88	0.55
1:F:51:SER:HB2	1:F:337:LYS:HE2	1.89	0.55
1:Z:177:VAL:HG13	1:Z:244:GLN:HG2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:250:ASN:HD21	1:E:296:SER:HB2	1.70	0.54
1:a:170:MET:HE1	1:a:250:ASN:HB3	1.88	0.54
1:g:199:LEU:HD13	1:g:252:VAL:HG22	1.89	0.54
1:E:197:PHE:CD2	1:E:233:VAL:HG21	2.43	0.54
1:M:96:SER:HA	1:M:281:VAL:HG21	1.88	0.54
1:M:148:GLN:NE2	1:M:152:ASP:O	2.38	0.54
1:A:68:ALA:HB3	1:A:319:ILE:HD11	1.88	0.54
1:B:369:PRO:HB2	1:F:353:ILE:HG21	1.89	0.54
1:J:149:ILE:HD11	1:J:157:VAL:HG23	1.89	0.54
1:J:172:GLY:HA3	1:J:275:THR:HA	1.89	0.54
1:a:125:ARG:NH1	1:d:155:GLU:OE2	2.39	0.54
1:G:63:VAL:HG12	1:G:67:ASN:HD21	1.72	0.54
1:J:98:GLN:O	1:J:104:ASN:ND2	2.41	0.54
1:M:82:MET:HE3	1:M:305:ARG:HG2	1.89	0.54
1:X:201:ASP:HB3	1:X:205:ASN:OD1	2.08	0.54
1:D:85:THR:HG23	1:D:123:LEU:HD22	1.89	0.54
1:J:144:THR:HG22	1:J:160:THR:HG23	1.89	0.54
1:P:201:ASP:HB3	1:P:205:ASN:OD1	2.08	0.54
1:a:171:MET:HG3	1:a:300:TYR:CD2	2.42	0.54
1:b:182:LYS:HD2	1:b:186:TRP:CG	2.43	0.54
1:J:88:ILE:HD11	1:M:317:HIS:HB3	1.89	0.54
1:O:370:ASN:O	1:O:373:LEU:HG	2.08	0.54
1:J:195:ILE:HB	1:J:262:LEU:HB3	1.90	0.54
1:J:205:ASN:N	1:J:205:ASN:OD1	2.40	0.54
1:O:131:SER:HB3	1:O:136:LYS:HD3	1.90	0.54
1:H:163:ASP:HB3	1:H:168:ASN:HD22	1.72	0.54
1:M:179:ALA:HB3	1:M:267:ASN:HD22	1.73	0.54
1:V:65:VAL:HG13	1:V:319:ILE:HG23	1.90	0.54
1:a:131:SER:HB3	1:a:136:LYS:HD3	1.90	0.54
1:a:341:PHE:HB2	1:b:3:VAL:HG21	1.88	0.54
1:e:82:MET:HE3	1:e:301:VAL:HG13	1.89	0.54
1:H:68:ALA:HB3	1:H:319:ILE:HD11	1.90	0.54
1:N:267:ASN:O	1:N:269:GLN:HG2	2.08	0.54
1:T:22:THR:O	1:T:26:GLN:HG2	2.08	0.54
1:B:313:ASN:HA	1:B:316:ASN:HD22	1.72	0.54
1:F:178:ALA:HA	1:F:268:MET:HA	1.90	0.54
1:P:199:LEU:HB2	1:P:252:VAL:HG13	1.90	0.54
1:R:50:ILE:HD13	1:R:53:ARG:HH21	1.73	0.54
1:W:192:ALA:CA	1:W:261:GLY:HA3	2.35	0.54
1:a:366:LYS:HD3	1:e:345:THR:HG22	1.90	0.54
1:J:201:ASP:HB2	1:J:207:GLN:HE21	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:85:THR:HG23	1:L:123:LEU:HD22	1.89	0.53
1:V:150:GLY:HA3	1:V:155:GLU:HB2	1.90	0.53
1:b:373:LEU:HA	1:b:376:LEU:HD12	1.90	0.53
1:f:177:VAL:HG13	1:f:244:GLN:HB3	1.89	0.53
1:g:37:LYS:N	1:g:337:LYS:O	2.38	0.53
1:L:63:VAL:HA	1:L:66:ARG:HE	1.72	0.53
1:N:22:THR:O	1:N:26:GLN:HG2	2.08	0.53
1:c:198:THR:HB	1:c:257:ALA:HB3	1.90	0.53
1:f:192:ALA:HA	1:f:261:GLY:HA3	1.90	0.53
1:A:202:ILE:HA	1:A:253:THR:HG23	1.91	0.53
1:E:106:LYS:HA	1:E:109:ARG:HD2	1.90	0.53
1:K:122:GLU:HB2	1:N:314:ARG:HG3	1.90	0.53
1:O:122:GLU:HB2	1:Q:314:ARG:HG3	1.90	0.53
1:R:180:GLU:HG2	1:R:267:ASN:OD1	2.08	0.53
1:X:188:VAL:HB	1:X:215:GLU:HA	1.91	0.53
1:B:62:ASP:O	1:B:65:VAL:HG22	2.09	0.53
1:S:177:VAL:O	1:S:269:GLN:HB3	2.08	0.53
1:Y:31:ARG:HE	1:Y:37:LYS:HA	1.73	0.53
1:A:69:ASN:O	1:A:72:ILE:HG12	2.09	0.53
1:I:290:SER:O	1:I:291:VAL:C	2.51	0.53
1:K:245:ILE:HD12	1:K:258:PHE:HE1	1.72	0.53
1:M:91:ARG:HH22	1:M:95:LEU:HD21	1.74	0.53
1:Y:89:LEU:HD22	1:Y:294:ILE:HD11	1.91	0.53
1:J:187:LYS:O	1:J:189:GLN:HG2	2.08	0.53
1:M:258:PHE:HB2	1:M:268:MET:HE2	1.91	0.53
1:O:195:ILE:HG13	1:O:263:ALA:HB2	1.90	0.53
1:B:182:LYS:HE2	1:B:266:LEU:HD23	1.91	0.53
1:B:187:LYS:HB3	1:B:216:GLY:HA2	1.91	0.53
1:K:27:THR:O	1:K:31:ARG:HG2	2.09	0.53
1:K:164:MET:HE3	1:K:304:HIS:HD2	1.72	0.53
1:M:276:VAL:O	1:M:279:ILE:HG12	2.08	0.53
1:C:368:ALA:HB3	1:C:369:PRO:HD3	1.91	0.53
1:E:368:ALA:HB3	1:E:369:PRO:HD3	1.91	0.53
1:I:37:LYS:N	1:I:337:LYS:O	2.39	0.53
1:Y:211:VAL:HG11	1:Y:226:ILE:HG12	1.90	0.53
1:a:219:ILE:HD11	1:a:243:LEU:HB2	1.90	0.53
1:f:369:PRO:HB2	1:g:353:ILE:HD13	1.90	0.53
1:U:25:GLN:HG2	1:U:29:MET:HE2	1.90	0.53
1:Z:89:LEU:HA	1:Z:92:MET:HE2	1.90	0.53
1:b:238:ASN:ND2	1:b:242:GLN:HB2	2.20	0.53
1:B:84:GLU:HB3	1:E:321:ASN:HD22	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:ASN:HB3	1:B:244:GLN:NE2	2.24	0.52
1:Q:164:MET:HE3	1:Q:304:HIS:HD2	1.74	0.52
1:A:178:ALA:HA	1:A:268:MET:HA	1.91	0.52
1:F:334:SER:HB2	1:F:338:ASP:OD2	2.09	0.52
1:J:339:THR:OG1	1:J:344:GLU:HG3	2.09	0.52
1:K:49:GLN:HA	1:L:302:ASP:OD1	2.09	0.52
1:M:73:SER:O	1:M:76:GLN:HG3	2.09	0.52
1:M:180:GLU:HB3	1:M:266:LEU:HA	1.91	0.52
1:P:220:GLU:HG3	1:P:237:VAL:HG21	1.91	0.52
1:S:162:LYS:HB3	1:S:300:TYR:OH	2.09	0.52
1:E:202:ILE:HD12	1:E:253:THR:HG23	1.90	0.52
1:I:31:ARG:HA	1:I:39:ASN:HD21	1.75	0.52
1:I:47:GLY:HA2	1:I:336:ILE:HD11	1.90	0.52
1:L:309:GLY:HA2	1:L:312:GLN:HE21	1.74	0.52
1:O:125:ARG:HD2	1:Q:149:ILE:HD13	1.91	0.52
1:J:258:PHE:HD2	1:J:268:MET:HB3	1.73	0.52
1:L:281:VAL:HG12	1:L:287:ALA:HA	1.92	0.52
1:V:373:LEU:O	1:V:376:LEU:HG	2.09	0.52
1:c:202:ILE:HD12	1:c:250:ASN:HA	1.91	0.52
1:f:182:LYS:HG2	1:f:266:LEU:HD11	1.91	0.52
1:A:220:GLU:HA	1:A:237:VAL:HG21	1.90	0.52
1:J:82:MET:HG3	1:J:138:LEU:HD21	1.92	0.52
1:J:117:THR:HA	1:J:120:ASN:HD21	1.74	0.52
1:M:98:GLN:HG3	1:M:104:ASN:HD21	1.73	0.52
1:Q:148:GLN:NE2	1:Q:152:ASP:O	2.42	0.52
1:R:197:PHE:HE2	1:R:245:ILE:HD13	1.73	0.52
1:S:276:VAL:HA	1:S:279:ILE:HG23	1.92	0.52
1:X:68:ALA:HB3	1:X:319:ILE:HD11	1.91	0.52
1:Y:200:LYS:HA	1:Y:206:ASP:HA	1.92	0.52
1:g:179:ALA:HB2	1:g:269:GLN:HG2	1.91	0.52
1:I:173:GLY:HA3	1:I:248:GLY:HA2	1.92	0.52
1:b:252:VAL:HG11	1:b:256:VAL:HG22	1.92	0.52
1:A:201:ASP:O	1:A:253:THR:N	2.41	0.52
1:E:138:LEU:HB3	1:E:164:MET:HB2	1.91	0.52
1:O:6:ASN:HA	1:R:350:LYS:HE2	1.91	0.52
1:O:267:ASN:O	1:O:268:MET:HB2	2.09	0.52
1:P:205:ASN:OD1	1:P:205:ASN:N	2.41	0.52
1:Q:202:ILE:HA	1:Q:253:THR:CG2	2.40	0.52
1:W:84:GLU:HA	1:W:87:ASN:HD22	1.74	0.52
1:Y:4:ASN:ND2	1:Z:334:SER:HB2	2.24	0.52
1:C:85:THR:HG23	1:C:123:LEU:HD22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:353:ILE:HG23	1:g:373:LEU:HD21	1.92	0.52
1:H:62:ASP:O	1:H:65:VAL:HG22	2.09	0.51
1:L:162:LYS:HE2	1:L:300:TYR:HE1	1.75	0.51
1:T:330:ASN:O	1:T:333:LYS:HG2	2.10	0.51
1:U:19:THR:HG22	1:W:2:ALA:CB	2.40	0.51
1:U:95:LEU:HD21	1:U:115:GLU:HB3	1.90	0.51
1:X:37:LYS:N	1:X:337:LYS:O	2.40	0.51
1:f:178:ALA:O	1:f:242:GLN:HB3	2.10	0.51
1:A:197:PHE:HB2	1:A:209:ILE:HB	1.92	0.51
1:C:148:GLN:NE2	1:C:152:ASP:O	2.43	0.51
1:H:366:LYS:O	1:H:369:PRO:HD2	2.10	0.51
1:P:148:GLN:NE2	1:P:152:ASP:O	2.43	0.51
1:R:109:ARG:HB3	1:R:282:THR:HA	1.91	0.51
1:Y:142:PHE:HD2	1:Y:161:LEU:HB2	1.75	0.51
1:b:239:GLU:HB3	1:b:284:VAL:HG13	1.92	0.51
1:g:69:ASN:O	1:g:72:ILE:HG22	2.09	0.51
1:J:372:ALA:HB1	1:K:341:PHE:CD1	2.45	0.51
1:N:368:ALA:HB3	1:N:369:PRO:HD3	1.90	0.51
1:Q:252:VAL:HG11	1:Q:256:VAL:HG22	1.92	0.51
1:U:182:LYS:HE2	1:U:266:LEU:HD23	1.92	0.51
1:d:172:GLY:HA3	1:d:275:THR:HA	1.92	0.51
1:B:314:ARG:HG3	1:Z:122:GLU:HB2	1.92	0.51
1:E:276:VAL:O	1:E:279:ILE:HG12	2.10	0.51
1:E:301:VAL:O	1:E:305:ARG:HG3	2.11	0.51
1:I:250:ASN:HD21	1:I:296:SER:HB3	1.75	0.51
1:Y:236:SER:HB2	1:Y:244:GLN:HB2	1.91	0.51
1:a:92:MET:HE2	1:a:279:ILE:HD11	1.93	0.51
1:A:201:ASP:HB2	1:A:207:GLN:OE1	2.09	0.51
1:E:148:GLN:HA	1:E:156:ALA:HA	1.92	0.51
1:I:199:LEU:HD13	1:I:252:VAL:HG22	1.93	0.51
1:K:373:LEU:HD12	1:K:377:GLY:HA2	1.93	0.51
1:N:4:ASN:ND2	1:O:334:SER:OG	2.43	0.51
1:T:334:SER:HB2	1:T:338:ASP:OD2	2.11	0.51
1:U:30:GLU:HG3	1:W:13:THR:HG21	1.92	0.51
1:W:7:THR:HG21	1:X:334:SER:CB	2.41	0.51
1:W:125:ARG:NH1	1:Z:155:GLU:OE2	2.41	0.51
1:X:129:THR:O	1:X:130:THR:C	2.53	0.51
1:Y:36:PHE:C	1:Y:339:THR:HG23	2.36	0.51
1:b:165:ARG:HE	1:d:214:LYS:HE3	1.76	0.51
1:I:110:VAL:O	1:I:114:GLU:HG2	2.11	0.51
1:J:109:ARG:HD2	1:J:281:VAL:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:138:LEU:HD23	1:K:164:MET:HG3	1.91	0.51
1:N:98:GLN:HG2	1:N:104:ASN:HD21	1.74	0.51
1:O:30:GLU:HG2	1:O:39:ASN:HD22	1.75	0.51
1:Y:201:ASP:N	1:Y:205:ASN:O	2.43	0.51
1:H:338:ASP:OD2	1:g:4:ASN:HB2	2.10	0.51
1:K:171:MET:HG3	1:K:300:TYR:CD2	2.45	0.51
1:O:89:LEU:HA	1:O:92:MET:HE2	1.91	0.51
1:P:335:ARG:HG2	1:P:336:ILE:HG13	1.92	0.51
1:X:109:ARG:HB3	1:X:282:THR:HA	1.92	0.51
1:X:112:ILE:HG22	1:X:281:VAL:HG21	1.92	0.51
1:Y:225:TYR:O	1:Y:229:GLN:HG2	2.11	0.51
1:f:195:ILE:HA	1:f:260:GLY:HA3	1.91	0.51
1:F:368:ALA:HB3	1:F:369:PRO:HD3	1.93	0.51
1:J:376:LEU:O	1:J:377:GLY:C	2.53	0.51
1:L:199:LEU:HD13	1:L:252:VAL:HG23	1.93	0.51
1:Q:29:MET:HG2	1:T:361:VAL:HG13	1.92	0.51
1:S:148:GLN:NE2	1:S:152:ASP:O	2.43	0.51
1:f:367:GLN:O	1:f:370:ASN:HB2	2.10	0.51
1:B:335:ARG:HD3	1:Z:69:ASN:HB3	1.91	0.51
1:H:178:ALA:HA	1:H:268:MET:HA	1.92	0.51
1:L:37:LYS:N	1:L:337:LYS:O	2.43	0.51
1:c:375:LEU:HG	1:c:376:LEU:HG	1.92	0.51
1:E:131:SER:HB2	1:E:136:LYS:HD2	1.92	0.51
1:E:201:ASP:N	1:E:205:ASN:O	2.39	0.51
1:J:148:GLN:HA	1:J:156:ALA:HB2	1.92	0.51
1:J:197:PHE:CD2	1:J:209:ILE:HD11	2.40	0.51
1:T:225:TYR:O	1:T:229:GLN:HG2	2.11	0.51
1:U:85:THR:HG23	1:U:123:LEU:HD22	1.92	0.51
1:b:233:VAL:HB	1:b:245:ILE:HG23	1.92	0.51
1:A:171:MET:HG3	1:A:300:TYR:HD2	1.76	0.50
1:G:72:ILE:HG23	1:a:335:ARG:HH12	1.74	0.50
1:I:40:SER:HB3	1:I:42:LYS:HG2	1.92	0.50
1:I:131:SER:HB3	1:I:136:LYS:HD2	1.93	0.50
1:K:150:GLY:HA3	1:K:155:GLU:HB2	1.94	0.50
1:L:162:LYS:HE2	1:L:300:TYR:CE1	2.46	0.50
1:P:308:LEU:O	1:P:312:GLN:HG3	2.11	0.50
1:W:34:SER:C	1:W:36:PHE:H	2.20	0.50
1:Y:313:ASN:HA	1:Y:316:ASN:HD22	1.74	0.50
1:Z:142:PHE:HA	1:Z:145:LYS:HE3	1.92	0.50
1:Z:192:ALA:O	1:Z:262:LEU:HB2	2.11	0.50
1:Z:198:THR:HB	1:Z:257:ALA:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:146:SER:HA	1:E:158:MET:HA	1.92	0.50
1:W:41:ALA:HB2	1:W:48:LEU:HD22	1.94	0.50
1:D:63:VAL:HG12	1:D:67:ASN:HD21	1.76	0.50
1:E:197:PHE:HB2	1:E:209:ILE:HG13	1.93	0.50
1:H:49:GLN:HG2	1:I:302:ASP:HB3	1.92	0.50
1:J:198:THR:HA	1:J:208:THR:HA	1.94	0.50
1:U:36:PHE:C	1:U:339:THR:HG23	2.37	0.50
1:V:30:GLU:OE1	1:V:39:ASN:ND2	2.44	0.50
1:Y:178:ALA:HA	1:Y:268:MET:HA	1.93	0.50
1:B:236:SER:HB3	1:B:288:GLN:HB3	1.93	0.50
1:B:239:GLU:HB3	1:B:284:VAL:HG11	1.94	0.50
1:D:69:ASN:O	1:D:72:ILE:HG13	2.12	0.50
1:J:131:SER:HB3	1:J:136:LYS:HD2	1.93	0.50
1:M:69:ASN:O	1:M:72:ILE:HG12	2.11	0.50
1:P:82:MET:HE1	1:P:304:HIS:CD2	2.46	0.50
1:V:179:ALA:HB2	1:V:269:GLN:CD	2.37	0.50
1:X:3:VAL:HG22	1:X:372:ALA:HB2	1.92	0.50
1:a:99:SER:O	1:a:109:ARG:NH1	2.45	0.50
1:c:112:ILE:HG22	1:c:281:VAL:HG21	1.92	0.50
1:B:352:GLN:O	1:B:356:GLN:HG3	2.11	0.50
1:C:9:VAL:O	1:C:13:THR:HG23	2.11	0.50
1:K:353:ILE:HD13	1:g:369:PRO:HB2	1.94	0.50
1:L:202:ILE:HA	1:L:253:THR:CG2	2.42	0.50
1:N:194:ASP:N	1:N:194:ASP:OD1	2.45	0.50
1:T:63:VAL:HG21	1:U:94:ASP:HB2	1.93	0.50
1:U:148:GLN:HE22	1:U:155:GLU:H	1.59	0.50
1:X:189:GLN:O	1:X:215:GLU:HB2	2.12	0.50
1:Z:173:GLY:HA2	1:Z:249:ASN:CG	2.36	0.50
1:E:222:VAL:O	1:E:226:ILE:HG12	2.11	0.50
1:F:376:LEU:HD22	1:G:342:ALA:HA	1.94	0.50
1:H:2:ALA:HB2	1:e:19:THR:HG22	1.94	0.50
1:O:172:GLY:HA3	1:O:275:THR:HA	1.93	0.50
1:I:178:ALA:HA	1:I:268:MET:HA	1.93	0.50
1:P:179:ALA:HB3	1:P:267:ASN:HB3	1.93	0.50
1:U:150:GLY:HA3	1:U:155:GLU:HB2	1.93	0.50
1:X:205:ASN:OD1	1:X:205:ASN:N	2.45	0.50
1:Y:301:VAL:HG12	1:Y:305:ARG:HD2	1.94	0.50
1:a:105:SER:O	1:a:106:LYS:C	2.54	0.50
1:g:98:GLN:HG2	1:g:104:ASN:HD21	1.76	0.50
1:A:362:LEU:HG	1:A:366:LYS:HE2	1.94	0.50
1:Q:82:MET:HE1	1:Q:308:LEU:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:219:ILE:HD11	1:R:243:LEU:HB2	1.94	0.50
1:S:63:VAL:HA	1:S:66:ARG:HD3	1.94	0.50
1:W:313:ASN:HA	1:W:316:ASN:HD22	1.77	0.50
1:X:201:ASP:O	1:X:204:GLY:N	2.36	0.50
1:a:373:LEU:HD22	1:a:377:GLY:HA3	1.92	0.50
1:d:178:ALA:HB2	1:d:268:MET:HE2	1.94	0.50
1:A:47:GLY:O	1:A:48:LEU:C	2.54	0.50
1:K:340:ASP:O	1:K:341:PHE:C	2.54	0.50
1:M:334:SER:HA	1:M:338:ASP:OD1	2.12	0.50
1:N:84:GLU:HG2	1:P:321:ASN:HB2	1.93	0.50
1:C:376:LEU:O	1:C:377:GLY:C	2.55	0.49
1:E:148:GLN:NE2	1:E:152:ASP:O	2.40	0.49
1:E:188:VAL:HB	1:E:216:GLY:H	1.77	0.49
1:E:313:ASN:HA	1:E:316:ASN:HD22	1.77	0.49
1:J:239:GLU:CD	1:J:239:GLU:H	2.20	0.49
1:S:147:PHE:HB2	1:S:315:PHE:HZ	1.76	0.49
1:V:226:ILE:O	1:V:230:THR:HG22	2.12	0.49
1:X:169:ARG:NH1	1:X:170:MET:SD	2.85	0.49
1:c:169:ARG:HG2	1:c:249:ASN:ND2	2.27	0.49
1:f:179:ALA:HB2	1:f:269:GLN:CG	2.36	0.49
1:N:6:ASN:HA	1:Q:350:LYS:HE2	1.94	0.49
1:N:180:GLU:HG2	1:N:267:ASN:HB2	1.92	0.49
1:O:106:LYS:HZ2	1:O:282:THR:HB	1.76	0.49
1:T:10:ALA:O	1:T:13:THR:HG22	2.12	0.49
1:W:196:THR:HB	1:W:259:SER:HB2	1.95	0.49
1:Y:202:ILE:HA	1:Y:253:THR:HG23	1.93	0.49
1:C:164:MET:HE1	1:C:304:HIS:CD2	2.43	0.49
1:H:180:GLU:HG2	1:H:267:ASN:HB3	1.94	0.49
1:K:217:ASP:HB3	1:K:221:GLU:HB2	1.93	0.49
1:L:147:PHE:O	1:L:156:ALA:HA	2.12	0.49
1:T:83:ASN:OD1	1:T:84:GLU:N	2.45	0.49
1:a:63:VAL:HB	1:c:97:LEU:HD23	1.93	0.49
1:b:148:GLN:HE22	1:b:155:GLU:HB2	1.77	0.49
1:f:211:VAL:HG13	1:f:229:GLN:HG3	1.95	0.49
1:C:168:ASN:HB3	1:C:171:MET:HG3	1.94	0.49
1:M:85:THR:HG22	1:M:126:ILE:HG21	1.94	0.49
1:Q:150:GLY:HA3	1:Q:155:GLU:CB	2.43	0.49
1:R:108:GLU:CG	1:T:50:ILE:HG12	2.43	0.49
1:f:236:SER:O	1:f:244:GLN:N	2.44	0.49
1:B:153:ASN:HD21	1:C:292:ALA:HB2	1.78	0.49
1:C:373:LEU:HD11	1:G:353:ILE:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:368:ALA:HB3	1:D:369:PRO:HD3	1.95	0.49
1:L:30:GLU:HG3	1:O:13:THR:HG21	1.94	0.49
1:N:148:GLN:NE2	1:N:152:ASP:O	2.39	0.49
1:P:138:LEU:HB3	1:P:164:MET:HB2	1.93	0.49
1:P:153:ASN:ND2	1:Q:292:ALA:HB2	2.28	0.49
1:Q:112:ILE:HG12	1:S:46:ALA:HB2	1.93	0.49
1:X:226:ILE:O	1:X:230:THR:HG22	2.13	0.49
1:Y:144:THR:HB	1:Y:160:THR:HB	1.93	0.49
1:c:362:LEU:HD23	1:e:375:LEU:HD21	1.94	0.49
1:d:78:ALA:O	1:d:82:MET:HG2	2.13	0.49
1:J:148:GLN:O	1:J:149:ILE:C	2.56	0.49
1:P:194:ASP:N	1:P:194:ASP:OD1	2.45	0.49
1:R:202:ILE:HA	1:R:253:THR:HG23	1.94	0.49
1:U:37:LYS:N	1:U:337:LYS:O	2.45	0.49
1:U:82:MET:HE3	1:U:301:VAL:HG13	1.95	0.49
1:X:375:LEU:HG	1:X:376:LEU:HG	1.93	0.49
1:b:199:LEU:HB3	1:b:256:VAL:HG13	1.95	0.49
1:b:373:LEU:HD22	1:d:356:GLN:HE21	1.76	0.49
1:F:104:ASN:HB3	1:F:108:GLU:HG3	1.94	0.49
1:J:88:ILE:HB	1:J:123:LEU:HD21	1.95	0.49
1:K:186:TRP:CD1	1:K:189:GLN:HE22	2.31	0.49
1:R:203:ASP:HB2	1:R:205:ASN:OD1	2.12	0.49
1:X:250:ASN:HD21	1:X:296:SER:HB2	1.77	0.49
1:a:372:ALA:HA	1:a:375:LEU:HD23	1.94	0.49
1:c:15:GLN:O	1:c:19:THR:HG23	2.12	0.49
1:g:180:GLU:HG2	1:g:267:ASN:HB3	1.94	0.49
1:I:196:THR:HB	1:I:259:SER:HB2	1.95	0.49
1:L:173:GLY:HA2	1:L:249:ASN:CG	2.38	0.49
1:M:187:LYS:HB3	1:M:216:GLY:HA2	1.94	0.49
1:U:19:THR:HG22	1:W:2:ALA:HB2	1.94	0.49
1:V:2:ALA:HB1	1:W:340:ASP:OD1	2.12	0.49
1:Y:3:VAL:HG21	1:Y:372:ALA:HB2	1.94	0.49
1:A:205:ASN:OD1	1:A:205:ASN:N	2.46	0.49
1:D:173:GLY:HA2	1:D:249:ASN:ND2	2.27	0.49
1:D:193:ASN:O	1:D:213:ALA:N	2.43	0.49
1:G:37:LYS:N	1:G:337:LYS:O	2.43	0.49
1:G:46:ALA:O	1:G:50:ILE:HG12	2.12	0.49
1:H:189:GLN:HE21	1:H:192:ALA:HB3	1.77	0.49
1:N:196:THR:N	1:N:259:SER:O	2.46	0.49
1:O:308:LEU:O	1:O:312:GLN:HG3	2.13	0.49
1:V:195:ILE:HG13	1:V:263:ALA:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:47:GLY:O	1:Y:48:LEU:C	2.56	0.49
1:Z:205:ASN:N	1:Z:205:ASN:OD1	2.46	0.49
1:a:202:ILE:HA	1:a:253:THR:HG23	1.94	0.49
1:A:148:GLN:HE21	1:A:150:GLY:H	1.61	0.48
1:E:193:ASN:HB2	1:E:213:ALA:O	2.13	0.48
1:H:148:GLN:HE21	1:I:288:GLN:NE2	2.06	0.48
1:J:372:ALA:HB1	1:K:341:PHE:HD1	1.77	0.48
1:R:178:ALA:HA	1:R:268:MET:HA	1.95	0.48
1:W:144:THR:HG23	1:W:160:THR:HB	1.95	0.48
1:Y:198:THR:HB	1:Y:257:ALA:HB3	1.94	0.48
1:b:169:ARG:HG2	1:b:249:ASN:ND2	2.28	0.48
1:d:182:LYS:HD2	1:d:186:TRP:CG	2.48	0.48
1:d:195:ILE:HG23	1:d:211:VAL:HB	1.94	0.48
1:e:148:GLN:NE2	1:e:152:ASP:O	2.45	0.48
1:f:92:MET:HG3	1:f:119:LEU:HD12	1.95	0.48
1:A:32:LEU:HD21	1:A:344:GLU:HB3	1.96	0.48
1:B:205:ASN:HB3	1:B:207:GLN:HE21	1.78	0.48
1:C:202:ILE:HA	1:C:253:THR:HG23	1.95	0.48
1:I:215:GLU:H	1:I:215:GLU:CD	2.22	0.48
1:J:153:ASN:HD21	1:K:234:LYS:HB3	1.78	0.48
1:R:179:ALA:HB3	1:R:267:ASN:OD1	2.12	0.48
1:Z:84:GLU:HA	1:Z:87:ASN:HD22	1.78	0.48
1:a:142:PHE:HB3	1:a:161:LEU:HB2	1.95	0.48
1:A:366:LYS:O	1:A:369:PRO:HD2	2.14	0.48
1:H:353:ILE:CD1	1:d:369:PRO:HB2	2.37	0.48
1:M:179:ALA:HB3	1:M:267:ASN:ND2	2.28	0.48
1:e:186:TRP:O	1:e:187:LYS:HD2	2.13	0.48
1:f:152:ASP:N	1:f:152:ASP:OD1	2.44	0.48
1:f:369:PRO:HB2	1:g:353:ILE:CD1	2.42	0.48
1:E:181:GLY:CA	1:E:242:GLN:HG2	2.42	0.48
1:F:170:MET:HE2	1:F:170:MET:HA	1.95	0.48
1:H:98:GLN:O	1:H:104:ASN:ND2	2.47	0.48
1:J:187:LYS:HB3	1:J:216:GLY:HA2	1.95	0.48
1:L:46:ALA:O	1:L:50:ILE:HG22	2.13	0.48
1:Q:349:THR:O	1:Q:353:ILE:HG12	2.14	0.48
1:R:69:ASN:O	1:R:72:ILE:HG22	2.13	0.48
1:S:99:SER:HB2	1:S:112:ILE:HG13	1.95	0.48
1:S:195:ILE:O	1:S:210:THR:HA	2.14	0.48
1:T:116:ILE:HD13	1:T:279:ILE:HG13	1.94	0.48
1:W:148:GLN:NE2	1:W:152:ASP:O	2.39	0.48
1:E:195:ILE:HB	1:E:262:LEU:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:106:LYS:HD2	1:J:109:ARG:HH21	1.78	0.48
1:J:373:LEU:HD11	1:N:356:GLN:HB2	1.94	0.48
1:K:129:THR:O	1:K:130:THR:C	2.57	0.48
1:S:195:ILE:CG1	1:S:262:LEU:HB3	2.43	0.48
1:T:84:GLU:HG2	1:V:321:ASN:HB2	1.94	0.48
1:W:85:THR:HG23	1:W:123:LEU:HD22	1.93	0.48
1:b:30:GLU:HG2	1:f:13:THR:CG2	2.44	0.48
1:d:45:ALA:HB1	1:e:306:ALA:HA	1.95	0.48
1:d:313:ASN:OD1	1:f:42:LYS:HG3	2.13	0.48
1:f:234:LYS:HD2	1:f:292:ALA:HB2	1.95	0.48
1:g:50:ILE:HG23	1:g:336:ILE:HD12	1.94	0.48
1:E:248:GLY:C	1:E:250:ASN:H	2.22	0.48
1:I:36:PHE:C	1:I:339:THR:HG23	2.39	0.48
1:I:101:ASN:ND2	1:I:103:SER:OG	2.46	0.48
1:P:138:LEU:HD13	1:P:164:MET:HG3	1.95	0.48
1:P:238:ASN:HB3	1:P:244:GLN:CD	2.39	0.48
1:X:3:VAL:CG2	1:X:372:ALA:HB2	2.44	0.48
1:Y:91:ARG:O	1:Y:95:LEU:HG	2.14	0.48
1:D:31:ARG:HB3	1:D:339:THR:CG2	2.43	0.48
1:G:315:PHE:O	1:G:319:ILE:HG13	2.14	0.48
1:H:122:GLU:HB2	1:K:314:ARG:HG3	1.95	0.48
1:J:201:ASP:O	1:J:204:GLY:N	2.47	0.48
1:K:367:GLN:O	1:K:370:ASN:HB3	2.13	0.48
1:R:37:LYS:N	1:R:337:LYS:O	2.45	0.48
1:U:6:ASN:HA	1:X:350:LYS:HE2	1.94	0.48
1:V:368:ALA:N	1:V:369:PRO:HD2	2.28	0.48
1:a:369:PRO:O	1:a:370:ASN:C	2.57	0.48
1:d:62:ASP:OD1	1:d:63:VAL:N	2.46	0.48
1:d:236:SER:HB3	1:d:288:GLN:HB3	1.94	0.48
1:A:368:ALA:HB3	1:A:369:PRO:HD3	1.96	0.48
1:B:13:THR:HG21	1:Z:30:GLU:HG2	1.96	0.48
1:H:50:ILE:HG23	1:H:336:ILE:HD12	1.96	0.48
1:H:292:ALA:HB2	1:g:153:ASN:ND2	2.28	0.48
1:I:180:GLU:HG2	1:I:267:ASN:HB3	1.96	0.48
1:L:63:VAL:HG13	1:L:66:ARG:HH21	1.78	0.48
1:M:173:GLY:O	1:M:273:ALA:HA	2.14	0.48
1:S:37:LYS:N	1:S:337:LYS:O	2.38	0.48
1:X:340:ASP:O	1:X:341:PHE:C	2.56	0.48
1:b:122:GLU:HB2	1:f:314:ARG:HG3	1.95	0.48
1:H:189:GLN:CD	1:H:189:GLN:H	2.22	0.48
1:J:69:ASN:HB3	1:M:335:ARG:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:211:VAL:HG13	1:J:229:GLN:HG2	1.96	0.48
1:M:236:SER:O	1:M:244:GLN:N	2.36	0.48
1:N:219:ILE:HD11	1:N:243:LEU:HB2	1.96	0.48
1:O:301:VAL:O	1:O:305:ARG:HG3	2.14	0.48
1:P:4:ASN:HB2	1:Q:338:ASP:HB3	1.95	0.48
1:P:291:VAL:O	1:P:294:ILE:HG22	2.14	0.48
1:X:166:SER:HA	1:X:171:MET:HE2	1.95	0.48
1:a:27:THR:O	1:a:30:GLU:HG3	2.13	0.48
1:c:149:ILE:HD11	1:c:157:VAL:HG23	1.96	0.48
1:e:198:THR:HB	1:e:257:ALA:HB3	1.96	0.48
1:B:99:SER:O	1:B:109:ARG:NH1	2.47	0.48
1:P:188:VAL:HB	1:P:215:GLU:HA	1.96	0.48
1:Q:28:SER:HB2	1:Q:348:LEU:HD23	1.94	0.48
1:a:164:MET:HE3	1:a:304:HIS:ND1	2.28	0.48
1:d:197:PHE:HB2	1:d:209:ILE:HB	1.95	0.48
1:E:91:ARG:HA	1:E:94:ASP:OD2	2.14	0.47
1:E:96:SER:OG	1:E:291:VAL:HG22	2.14	0.47
1:J:373:LEU:HD11	1:N:356:GLN:CB	2.44	0.47
1:M:279:ILE:HB	1:M:290:SER:HB2	1.96	0.47
1:X:31:ARG:HA	1:X:39:ASN:HD21	1.78	0.47
1:H:99:SER:O	1:H:109:ARG:NH1	2.47	0.47
1:H:323:ASP:OD1	1:H:324:ASN:N	2.47	0.47
1:I:199:LEU:HG	1:I:207:GLN:HB2	1.96	0.47
1:W:152:ASP:HA	1:X:93:ARG:HH22	1.79	0.47
1:d:165:ARG:HB3	1:d:167:ASP:OD1	2.14	0.47
1:e:32:LEU:HD21	1:e:344:GLU:HB3	1.96	0.47
1:D:207:GLN:HG3	1:D:232:MET:HE3	1.96	0.47
1:H:85:THR:HG23	1:H:123:LEU:HD22	1.96	0.47
1:J:82:MET:HE1	1:J:304:HIS:HD2	1.80	0.47
1:P:114:GLU:OE1	1:S:307:GLU:HA	2.13	0.47
1:U:173:GLY:HA2	1:U:249:ASN:ND2	2.29	0.47
1:b:169:ARG:HG2	1:b:169:ARG:HH11	1.78	0.47
1:e:82:MET:HB2	1:e:305:ARG:HH11	1.80	0.47
1:f:85:THR:HG22	1:f:126:ILE:HG21	1.96	0.47
1:g:150:GLY:HA3	1:g:155:GLU:HB2	1.96	0.47
1:C:369:PRO:HB2	1:G:353:ILE:HG13	1.96	0.47
1:G:166:SER:HB2	1:G:276:VAL:HB	1.96	0.47
1:G:202:ILE:HA	1:G:253:THR:HG23	1.96	0.47
1:H:144:THR:HB	1:I:184:LYS:HD3	1.95	0.47
1:S:245:ILE:HG12	1:S:258:PHE:CZ	2.47	0.47
1:Y:352:GLN:O	1:Y:356:GLN:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:326:ASN:O	1:a:329:VAL:HG12	2.14	0.47
1:g:85:THR:HG23	1:g:123:LEU:HD22	1.95	0.47
1:H:144:THR:OG1	1:H:158:MET:HB3	2.15	0.47
1:H:375:LEU:O	1:I:345:THR:HG21	2.14	0.47
1:J:317:HIS:ND1	1:g:84:GLU:OE2	2.46	0.47
1:L:65:VAL:HG12	1:L:69:ASN:HD21	1.80	0.47
1:M:199:LEU:HD11	1:M:232:MET:HG2	1.96	0.47
1:P:149:ILE:HD13	1:P:315:PHE:CE1	2.48	0.47
1:Y:368:ALA:HB3	1:Y:369:PRO:HD3	1.97	0.47
1:Z:138:LEU:HB3	1:Z:164:MET:HB2	1.97	0.47
1:a:132:PHE:HB2	1:a:137:LEU:HD11	1.96	0.47
1:c:65:VAL:HG13	1:c:319:ILE:HG23	1.95	0.47
1:d:173:GLY:HA2	1:d:249:ASN:CG	2.40	0.47
1:B:37:LYS:N	1:B:337:LYS:O	2.42	0.47
1:D:122:GLU:HB2	1:G:314:ARG:HG3	1.96	0.47
1:J:84:GLU:O	1:J:88:ILE:HG12	2.15	0.47
1:K:65:VAL:HG13	1:K:319:ILE:HG23	1.97	0.47
1:R:230:THR:HG21	1:R:233:VAL:HG23	1.95	0.47
1:Y:123:LEU:O	1:Y:126:ILE:HG22	2.14	0.47
1:b:188:VAL:HB	1:b:215:GLU:HA	1.95	0.47
1:c:99:SER:O	1:c:109:ARG:NH1	2.48	0.47
1:g:120:ASN:HD21	1:g:277:ASP:HA	1.80	0.47
1:B:219:ILE:HD11	1:B:243:LEU:HB2	1.96	0.47
1:D:92:MET:HA	1:D:95:LEU:HD12	1.97	0.47
1:F:350:LYS:O	1:F:353:ILE:HG22	2.14	0.47
1:K:99:SER:O	1:K:109:ARG:NH1	2.48	0.47
1:S:195:ILE:HG12	1:S:262:LEU:HB3	1.97	0.47
1:V:14:ALA:O	1:V:15:GLN:C	2.57	0.47
1:W:199:LEU:HD13	1:W:252:VAL:HG22	1.97	0.47
1:Z:47:GLY:O	1:Z:48:LEU:C	2.56	0.47
1:Z:313:ASN:HA	1:Z:316:ASN:HD22	1.79	0.47
1:a:22:THR:HG22	1:a:26:GLN:HE21	1.79	0.47
1:d:153:ASN:ND2	1:e:292:ALA:HB2	2.30	0.47
1:d:196:THR:N	1:d:259:SER:O	2.42	0.47
1:f:372:ALA:HA	1:f:375:LEU:HD23	1.96	0.47
1:g:376:LEU:O	1:g:377:GLY:C	2.57	0.47
1:B:173:GLY:HA2	1:B:249:ASN:CG	2.40	0.47
1:C:313:ASN:HA	1:C:316:ASN:HD22	1.80	0.47
1:F:92:MET:HE1	1:F:123:LEU:HD11	1.96	0.47
1:P:122:GLU:HB2	1:S:314:ARG:HG3	1.96	0.47
1:U:239:GLU:HB3	1:U:284:VAL:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:193:ASN:HB2	1:V:213:ALA:O	2.14	0.47
1:V:239:GLU:H	1:V:239:GLU:CD	2.23	0.47
1:W:122:GLU:HB2	1:Z:314:ARG:HG3	1.97	0.47
1:d:225:TYR:O	1:d:229:GLN:HG2	2.15	0.47
1:A:105:SER:H	1:A:108:GLU:CD	2.23	0.47
1:B:366:LYS:O	1:B:367:GLN:HB2	2.15	0.47
1:E:176:TYR:HA	1:E:271:GLY:CA	2.40	0.47
1:G:89:LEU:HA	1:G:92:MET:HE3	1.96	0.47
1:T:303:SER:O	1:T:307:GLU:HG2	2.15	0.47
1:V:200:LYS:HA	1:V:206:ASP:HA	1.97	0.47
1:b:104:ASN:H	1:b:104:ASN:HD22	1.62	0.47
1:A:85:THR:HG23	1:A:123:LEU:HD22	1.96	0.47
1:B:122:GLU:OE1	1:E:314:ARG:HG2	2.15	0.47
1:I:313:ASN:HA	1:I:316:ASN:HD22	1.80	0.47
1:J:238:ASN:OD1	1:J:242:GLN:N	2.44	0.47
1:N:367:GLN:HA	1:N:370:ASN:HD22	1.79	0.47
1:O:209:ILE:HD11	1:O:232:MET:HG3	1.96	0.47
1:Q:142:PHE:HA	1:Q:145:LYS:HE3	1.96	0.47
1:X:44:ASP:O	1:X:45:ALA:C	2.58	0.47
1:Y:340:ASP:O	1:Y:341:PHE:C	2.58	0.47
1:b:6:ASN:HD22	1:d:350:LYS:HE2	1.79	0.47
1:c:122:GLU:HB2	1:e:314:ARG:HG3	1.96	0.47
1:c:168:ASN:HD21	1:c:170:MET:HB2	1.79	0.47
1:B:162:LYS:H	1:B:304:HIS:CE1	2.31	0.46
1:D:61:LEU:HD13	1:D:325:ILE:HG23	1.97	0.46
1:F:276:VAL:O	1:F:279:ILE:HG12	2.15	0.46
1:H:376:LEU:O	1:H:377:GLY:C	2.58	0.46
1:J:117:THR:HA	1:J:120:ASN:ND2	2.29	0.46
1:J:158:MET:HE1	1:K:219:ILE:HG22	1.97	0.46
1:M:113:GLN:O	1:M:116:ILE:HG13	2.15	0.46
1:P:189:GLN:HG3	1:P:192:ALA:H	1.80	0.46
1:Q:219:ILE:HD11	1:Q:243:LEU:HB2	1.96	0.46
1:U:179:ALA:HB3	1:U:267:ASN:HB2	1.96	0.46
1:W:111:ALA:O	1:W:114:GLU:HB3	2.15	0.46
1:A:341:PHE:O	1:A:342:ALA:C	2.58	0.46
1:F:239:GLU:OE2	1:F:283:SER:HB2	2.15	0.46
1:G:98:GLN:O	1:G:104:ASN:ND2	2.48	0.46
1:G:349:THR:O	1:G:353:ILE:HG12	2.15	0.46
1:M:235:ALA:HA	1:M:245:ILE:HD13	1.97	0.46
1:M:313:ASN:HA	1:M:316:ASN:HD22	1.80	0.46
1:S:194:ASP:HA	1:S:211:VAL:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:15:GLN:O	1:a:19:THR:HG23	2.15	0.46
1:b:219:ILE:HD11	1:b:243:LEU:HB2	1.97	0.46
1:b:373:LEU:HD22	1:d:356:GLN:NE2	2.31	0.46
1:C:219:ILE:HD11	1:C:243:LEU:HB2	1.97	0.46
1:H:288:GLN:HE22	1:g:148:GLN:HE21	1.63	0.46
1:I:218:ASP:CG	1:I:221:GLU:HG2	2.40	0.46
1:M:113:GLN:HE22	1:M:280:ASP:HA	1.80	0.46
1:S:202:ILE:HA	1:S:253:THR:CG2	2.43	0.46
1:U:281:VAL:HG12	1:U:287:ALA:HA	1.97	0.46
1:c:138:LEU:HB3	1:c:164:MET:HB2	1.97	0.46
1:A:188:VAL:CG1	1:A:193:ASN:HB3	2.46	0.46
1:B:171:MET:HG3	1:B:300:TYR:HD1	1.79	0.46
1:O:31:ARG:HB3	1:O:339:THR:CG2	2.46	0.46
1:P:120:ASN:HD21	1:P:277:ASP:HA	1.80	0.46
1:S:276:VAL:O	1:S:279:ILE:HG12	2.15	0.46
1:V:129:THR:O	1:V:130:THR:C	2.57	0.46
1:W:105:SER:O	1:W:106:LYS:C	2.59	0.46
1:E:169:ARG:CZ	1:E:249:ASN:HB3	2.46	0.46
1:G:340:ASP:O	1:G:341:PHE:C	2.59	0.46
1:H:79:GLU:OE2	1:g:41:ALA:N	2.37	0.46
1:J:375:LEU:HD11	1:g:366:LYS:HD3	1.97	0.46
1:K:182:LYS:HE2	1:K:266:LEU:HD13	1.98	0.46
1:L:198:THR:OG1	1:L:257:ALA:HB3	2.16	0.46
1:N:69:ASN:HB3	1:P:335:ARG:NE	2.25	0.46
1:O:99:SER:O	1:O:109:ARG:NH1	2.49	0.46
1:R:3:VAL:O	1:R:4:ASN:C	2.58	0.46
1:U:201:ASP:O	1:U:204:GLY:N	2.49	0.46
1:W:219:ILE:HD11	1:W:243:LEU:HB2	1.97	0.46
1:X:85:THR:HG23	1:X:123:LEU:HD22	1.97	0.46
1:Z:68:ALA:HB3	1:Z:319:ILE:HD13	1.97	0.46
1:e:99:SER:HA	1:e:104:ASN:HD22	1.81	0.46
1:e:129:THR:O	1:e:130:THR:C	2.59	0.46
1:E:85:THR:HG23	1:E:123:LEU:HG	1.98	0.46
1:F:202:ILE:HA	1:F:253:THR:HG23	1.98	0.46
1:L:196:THR:HA	1:L:210:THR:HA	1.97	0.46
1:V:236:SER:HB3	1:V:288:GLN:HB3	1.98	0.46
1:W:38:ILE:HD11	1:W:336:ILE:HG22	1.98	0.46
1:X:99:SER:O	1:X:109:ARG:NH1	2.48	0.46
1:X:162:LYS:H	1:X:304:HIS:CE1	2.33	0.46
1:Y:54:LEU:HD22	1:Y:329:VAL:HG13	1.98	0.46
1:d:201:ASP:O	1:d:202:ILE:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ASP:OD1	1:A:43:ASP:N	2.46	0.46
1:E:153:ASN:OD1	1:F:234:LYS:HG2	2.16	0.46
1:F:171:MET:HG3	1:F:300:TYR:CD2	2.47	0.46
1:H:323:ASP:O	1:H:327:GLU:HG3	2.16	0.46
1:K:77:THR:HG22	1:N:328:ASN:HB2	1.97	0.46
1:L:148:GLN:NE2	1:L:155:GLU:HB2	2.31	0.46
1:O:8:ASN:O	1:O:9:VAL:C	2.59	0.46
1:Q:202:ILE:HA	1:Q:253:THR:HG23	1.98	0.46
1:c:131:SER:HB3	1:c:136:LYS:HD2	1.97	0.46
1:B:194:ASP:HA	1:B:212:ASN:HA	1.98	0.46
1:C:217:ASP:HB3	1:C:221:GLU:HB2	1.98	0.46
1:E:176:TYR:CD1	1:E:271:GLY:HA3	2.51	0.46
1:I:75:ALA:HB1	1:I:308:LEU:HD12	1.98	0.46
1:J:38:ILE:HD13	1:J:336:ILE:O	2.16	0.46
1:N:108:GLU:OE1	1:N:108:GLU:N	2.46	0.46
1:P:187:LYS:HE2	1:P:216:GLY:HA2	1.97	0.46
1:R:148:GLN:NE2	1:R:152:ASP:O	2.47	0.46
1:U:276:VAL:HA	1:U:279:ILE:HG23	1.97	0.46
1:b:313:ASN:HA	1:b:316:ASN:HD22	1.81	0.46
1:c:341:PHE:O	1:c:342:ALA:C	2.58	0.46
1:I:375:LEU:HG	1:I:376:LEU:HG	1.97	0.46
1:K:187:LYS:O	1:K:188:VAL:C	2.57	0.46
1:M:40:SER:HB3	1:M:42:LYS:HG2	1.97	0.46
1:O:36:PHE:C	1:O:339:THR:HG23	2.40	0.46
1:Q:5:VAL:HG22	1:R:341:PHE:HE2	1.81	0.46
1:Q:46:ALA:O	1:Q:50:ILE:HG12	2.16	0.46
1:Q:108:GLU:HG2	1:S:50:ILE:HG12	1.98	0.46
1:W:157:VAL:HG21	1:W:314:ARG:NH1	2.31	0.46
1:Y:176:TYR:HA	1:Y:270:ALA:O	2.15	0.46
1:a:3:VAL:HB	1:a:372:ALA:HB2	1.98	0.46
1:a:162:LYS:H	1:a:304:HIS:CE1	2.34	0.46
1:c:36:PHE:O	1:c:39:ASN:ND2	2.49	0.46
1:c:123:LEU:O	1:c:126:ILE:HG22	2.16	0.46
1:d:373:LEU:HA	1:d:377:GLY:HA3	1.97	0.46
1:e:150:GLY:HA3	1:e:155:GLU:HB2	1.98	0.46
1:B:92:MET:HA	1:B:95:LEU:HD12	1.98	0.46
1:B:129:THR:O	1:B:130:THR:C	2.59	0.46
1:H:369:PRO:HB2	1:L:353:ILE:CD1	2.46	0.46
1:K:339:THR:OG1	1:K:344:GLU:HG3	2.16	0.46
1:M:287:ALA:O	1:M:291:VAL:HG23	2.16	0.46
1:O:250:ASN:ND2	1:O:299:LYS:HD2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:29:MET:HG2	1:U:361:VAL:HG13	1.96	0.46
1:V:22:THR:O	1:V:26:GLN:HG2	2.16	0.46
1:W:130:THR:HG22	1:Z:325:ILE:HD11	1.97	0.46
1:Y:150:GLY:HA3	1:Y:155:GLU:OE1	2.15	0.46
1:Y:339:THR:HB	1:Y:344:GLU:HG3	1.97	0.46
1:b:106:LYS:O	1:b:110:VAL:HG23	2.15	0.46
1:b:200:LYS:HD2	1:b:206:ASP:HA	1.98	0.46
1:b:330:ASN:O	1:b:333:LYS:HG2	2.16	0.46
1:d:198:THR:HG22	1:d:208:THR:HG22	1.98	0.46
1:d:199:LEU:HD13	1:d:252:VAL:HG22	1.97	0.46
1:A:29:MET:HG2	1:C:361:VAL:HG13	1.98	0.45
1:C:13:THR:HG22	1:D:327:GLU:CD	2.41	0.45
1:C:173:GLY:HA2	1:C:249:ASN:CG	2.41	0.45
1:I:132:PHE:HB2	1:I:137:LEU:HD11	1.98	0.45
1:N:144:THR:HG21	1:N:158:MET:HE2	1.96	0.45
1:O:369:PRO:O	1:O:370:ASN:C	2.59	0.45
1:P:37:LYS:N	1:P:337:LYS:O	2.46	0.45
1:S:211:VAL:HG11	1:S:226:ILE:HD13	1.99	0.45
1:U:267:ASN:C	1:U:269:GLN:H	2.24	0.45
1:W:99:SER:O	1:W:109:ARG:NH1	2.49	0.45
1:X:175:SER:HB2	1:X:274:GLU:HG3	1.98	0.45
1:C:29:MET:HE3	1:C:29:MET:HB3	1.81	0.45
1:D:225:TYR:O	1:D:229:GLN:HG2	2.16	0.45
1:F:149:ILE:N	1:F:155:GLU:OE2	2.49	0.45
1:J:179:ALA:HB3	1:J:267:ASN:HB3	1.97	0.45
1:J:315:PHE:O	1:J:319:ILE:HG13	2.16	0.45
1:M:109:ARG:HB3	1:M:282:THR:HA	1.98	0.45
1:Q:200:LYS:HA	1:Q:206:ASP:HA	1.99	0.45
1:V:36:PHE:O	1:V:39:ASN:ND2	2.49	0.45
1:W:373:LEU:HA	1:W:377:GLY:HA3	1.99	0.45
1:a:143:SER:O	1:a:144:THR:C	2.59	0.45
1:a:302:ASP:OD2	1:b:49:GLN:HA	2.17	0.45
1:c:352:GLN:O	1:c:356:GLN:HG3	2.16	0.45
1:B:47:GLY:O	1:B:48:LEU:C	2.59	0.45
1:E:240:LYS:HB2	1:E:242:GLN:HG3	1.98	0.45
1:G:232:MET:HE2	1:G:251:LYS:HE2	1.99	0.45
1:H:182:LYS:HD2	1:H:186:TRP:CD1	2.51	0.45
1:K:354:LEU:HD23	1:K:354:LEU:HA	1.75	0.45
1:L:69:ASN:HB3	1:O:335:ARG:HD2	1.98	0.45
1:M:295:ASP:O	1:M:298:LEU:HG	2.16	0.45
1:N:153:ASN:ND2	1:O:292:ALA:HB2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:37:LYS:N	1:W:337:LYS:O	2.48	0.45
1:W:81:ALA:CB	1:W:130:THR:HG21	2.47	0.45
1:Y:113:GLN:O	1:Y:116:ILE:HG13	2.16	0.45
1:C:366:LYS:HG2	1:G:346:THR:HG22	1.98	0.45
1:F:341:PHE:O	1:F:342:ALA:C	2.60	0.45
1:J:376:LEU:HD13	1:J:376:LEU:HA	1.83	0.45
1:O:105:SER:H	1:O:108:GLU:CD	2.24	0.45
1:O:368:ALA:HB3	1:O:369:PRO:HD3	1.99	0.45
1:P:129:THR:O	1:P:130:THR:C	2.60	0.45
1:T:105:SER:O	1:T:106:LYS:C	2.60	0.45
1:Z:202:ILE:HA	1:Z:253:THR:HG23	1.99	0.45
1:d:169:ARG:NH2	1:d:170:MET:SD	2.90	0.45
1:C:4:ASN:HB3	1:D:338:ASP:OD2	2.17	0.45
1:C:6:ASN:HA	1:G:350:LYS:HE3	1.98	0.45
1:G:181:GLY:HA2	1:G:242:GLN:HG2	1.99	0.45
1:J:175:SER:HB2	1:J:246:PHE:HD1	1.82	0.45
1:K:170:MET:HA	1:K:170:MET:HE2	1.99	0.45
1:L:105:SER:O	1:L:106:LYS:C	2.59	0.45
1:S:142:PHE:CE2	1:S:145:LYS:HD2	2.51	0.45
1:U:225:TYR:O	1:U:229:GLN:HG2	2.16	0.45
1:W:36:PHE:CD1	1:W:337:LYS:HG2	2.51	0.45
1:G:93:ARG:HB2	1:G:294:ILE:HG21	1.99	0.45
1:K:276:VAL:HA	1:K:279:ILE:HG23	1.99	0.45
1:P:218:ASP:O	1:P:222:VAL:HG23	2.17	0.45
1:T:30:GLU:OE1	1:T:39:ASN:ND2	2.50	0.45
1:W:7:THR:HG21	1:X:334:SER:HB2	1.98	0.45
1:B:178:ALA:HA	1:B:268:MET:HA	1.99	0.45
1:G:3:VAL:HG11	1:G:371:ALA:HB3	1.98	0.45
1:K:183:ASP:OD1	1:K:184:LYS:N	2.50	0.45
1:M:178:ALA:N	1:M:243:LEU:O	2.50	0.45
1:P:99:SER:HB2	1:P:112:ILE:HG21	1.98	0.45
1:S:50:ILE:HA	1:S:53:ARG:HH21	1.80	0.45
1:U:3:VAL:HG22	1:U:372:ALA:HB2	1.97	0.45
1:W:93:ARG:HB2	1:W:294:ILE:HG21	1.99	0.45
1:a:46:ALA:O	1:a:50:ILE:HG12	2.16	0.45
1:a:202:ILE:HA	1:a:253:THR:CG2	2.47	0.45
1:a:341:PHE:O	1:a:342:ALA:C	2.59	0.45
1:b:339:THR:OG1	1:b:344:GLU:HG3	2.16	0.45
1:d:248:GLY:C	1:d:250:ASN:H	2.24	0.45
1:A:236:SER:HB3	1:A:288:GLN:HB3	1.99	0.45
1:L:2:ALA:O	1:L:3:VAL:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:123:LEU:O	1:M:126:ILE:HG22	2.16	0.45
1:N:3:VAL:CG1	1:O:341:PHE:HB2	2.45	0.45
1:N:4:ASN:N	1:N:4:ASN:OD1	2.50	0.45
1:P:222:VAL:O	1:P:226:ILE:HG12	2.17	0.45
1:Q:60:GLY:O	1:Q:63:VAL:HG22	2.17	0.45
1:S:258:PHE:CB	1:S:268:MET:HG3	2.47	0.45
1:Y:82:MET:HE3	1:Y:164:MET:SD	2.57	0.45
1:b:71:GLY:HA3	1:b:315:PHE:HE2	1.81	0.45
1:e:82:MET:HE3	1:e:82:MET:HB3	1.74	0.45
1:B:68:ALA:HB2	1:B:149:ILE:HG22	1.99	0.45
1:E:12:MET:HE3	1:F:327:GLU:HG3	1.99	0.45
1:E:99:SER:HA	1:E:104:ASN:ND2	2.32	0.45
1:E:276:VAL:HA	1:E:279:ILE:CG2	2.46	0.45
1:F:105:SER:O	1:F:108:GLU:HG2	2.17	0.45
1:L:170:MET:C	1:L:172:GLY:H	2.25	0.45
1:U:118:ALA:HB1	1:W:314:ARG:HD2	1.98	0.45
1:V:49:GLN:HG2	1:W:302:ASP:HB3	1.99	0.45
1:V:323:ASP:O	1:V:327:GLU:HG3	2.16	0.45
1:Z:93:ARG:HB2	1:Z:294:ILE:HG21	1.97	0.45
1:e:374:SER:O	1:e:375:LEU:C	2.59	0.45
1:I:281:VAL:HG12	1:I:287:ALA:HA	1.99	0.45
1:K:245:ILE:HD12	1:K:258:PHE:CE1	2.52	0.45
1:V:47:GLY:O	1:V:48:LEU:C	2.60	0.45
1:V:197:PHE:HB2	1:V:209:ILE:HB	1.99	0.45
1:a:194:ASP:OD1	1:a:194:ASP:N	2.49	0.45
1:c:168:ASN:O	1:c:171:MET:HB2	2.17	0.45
1:d:30:GLU:OE1	1:d:39:ASN:ND2	2.50	0.45
1:d:349:THR:O	1:d:353:ILE:HG12	2.17	0.45
1:e:85:THR:HG23	1:e:123:LEU:HD22	1.99	0.45
1:e:217:ASP:HB3	1:e:221:GLU:HB2	1.99	0.45
1:I:31:ARG:HB3	1:I:339:THR:HG21	1.98	0.44
1:L:129:THR:O	1:L:130:THR:C	2.60	0.44
1:M:167:ASP:HA	1:M:275:THR:HG21	1.99	0.44
1:M:280:ASP:OD1	1:M:280:ASP:N	2.49	0.44
1:N:6:ASN:OD1	1:O:35:GLY:HA3	2.17	0.44
1:P:93:ARG:HB2	1:P:294:ILE:HG21	2.00	0.44
1:Q:153:ASN:HD21	1:R:292:ALA:HB2	1.82	0.44
1:S:315:PHE:O	1:S:319:ILE:HG13	2.16	0.44
1:T:26:GLN:HE22	1:V:10:ALA:HB2	1.82	0.44
1:Y:8:ASN:O	1:Y:9:VAL:C	2.59	0.44
1:b:82:MET:HG3	1:b:138:LEU:HD21	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:105:SER:H	1:e:108:GLU:CD	2.25	0.44
1:e:144:THR:H	1:e:160:THR:HA	1.81	0.44
1:f:28:SER:HA	1:f:344:GLU:OE2	2.17	0.44
1:B:89:LEU:HD11	1:B:171:MET:HE3	2.00	0.44
1:E:206:ASP:O	1:E:207:GLN:C	2.60	0.44
1:H:354:LEU:HD23	1:H:354:LEU:HA	1.89	0.44
1:J:147:PHE:HE1	1:J:159:LEU:HB3	1.83	0.44
1:P:68:ALA:HB2	1:P:149:ILE:HG22	1.99	0.44
1:R:276:VAL:O	1:R:279:ILE:HG13	2.17	0.44
1:Y:349:THR:O	1:Y:353:ILE:HG12	2.17	0.44
1:a:108:GLU:O	1:a:109:ARG:C	2.59	0.44
1:a:183:ASP:HB3	1:a:185:ASP:OD1	2.17	0.44
1:c:30:GLU:HG2	1:e:13:THR:HG21	1.99	0.44
1:d:84:GLU:HA	1:d:87:ASN:ND2	2.32	0.44
1:g:368:ALA:HB3	1:g:369:PRO:HD3	1.99	0.44
1:A:334:SER:O	1:A:335:ARG:C	2.60	0.44
1:P:172:GLY:HA3	1:P:275:THR:HA	1.98	0.44
1:P:370:ASN:O	1:P:371:ALA:C	2.60	0.44
1:R:131:SER:HB3	1:R:136:LYS:HD3	1.99	0.44
1:S:98:GLN:O	1:S:104:ASN:ND2	2.50	0.44
1:U:368:ALA:HB3	1:U:369:PRO:HD3	2.00	0.44
1:f:187:LYS:HB3	1:f:216:GLY:HA2	1.98	0.44
1:J:236:SER:O	1:J:244:GLN:N	2.46	0.44
1:L:219:ILE:HD11	1:L:243:LEU:HB2	2.00	0.44
1:P:300:TYR:O	1:P:303:SER:HB3	2.17	0.44
1:P:315:PHE:O	1:P:319:ILE:HG13	2.16	0.44
1:R:81:ALA:HA	1:U:321:ASN:ND2	2.33	0.44
1:S:244:GLN:NE2	1:S:289:GLN:OE1	2.50	0.44
1:T:198:THR:HB	1:T:257:ALA:HB3	2.00	0.44
1:W:34:SER:C	1:W:36:PHE:N	2.75	0.44
1:a:232:MET:HE2	1:a:232:MET:HA	2.00	0.44
1:C:372:ALA:O	1:C:373:LEU:C	2.60	0.44
1:D:147:PHE:HE1	1:D:159:LEU:HB3	1.83	0.44
1:D:162:LYS:HE2	1:D:162:LYS:HA	2.00	0.44
1:E:248:GLY:C	1:E:250:ASN:N	2.75	0.44
1:H:352:GLN:O	1:H:356:GLN:HG3	2.17	0.44
1:J:109:ARG:HB3	1:J:282:THR:HA	2.00	0.44
1:K:222:VAL:O	1:K:226:ILE:HG12	2.18	0.44
1:M:167:ASP:OD1	1:M:167:ASP:N	2.44	0.44
1:V:8:ASN:O	1:V:9:VAL:C	2.60	0.44
1:W:33:SER:HB3	1:Z:361:VAL:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:56:VAL:HG13	1:X:93:ARG:HD3	2.00	0.44
1:X:82:MET:HE3	1:X:305:ARG:HG2	1.99	0.44
1:Z:159:LEU:HD22	1:Z:311:PHE:CE2	2.52	0.44
1:a:179:ALA:HB3	1:a:267:ASN:HB3	1.99	0.44
1:d:99:SER:O	1:d:109:ARG:NH1	2.51	0.44
1:e:37:LYS:N	1:e:337:LYS:O	2.46	0.44
1:A:153:ASN:OD1	1:A:153:ASN:N	2.51	0.44
1:A:238:ASN:HD21	1:A:242:GLN:HB2	1.83	0.44
1:A:352:GLN:O	1:A:356:GLN:HG3	2.18	0.44
1:B:171:MET:HG3	1:B:300:TYR:CD1	2.52	0.44
1:B:179:ALA:HB2	1:B:269:GLN:CD	2.42	0.44
1:C:3:VAL:HG11	1:C:375:LEU:HD22	1.98	0.44
1:I:49:GLN:O	1:I:53:ARG:HG3	2.18	0.44
1:L:250:ASN:ND2	1:L:296:SER:OG	2.50	0.44
1:R:171:MET:HE3	1:R:171:MET:HB3	1.84	0.44
1:S:111:ALA:O	1:S:114:GLU:HB3	2.17	0.44
1:S:170:MET:HA	1:S:249:ASN:ND2	2.29	0.44
1:W:69:ASN:HB3	1:Z:335:ARG:HD3	2.00	0.44
1:W:108:GLU:CD	1:Y:53:ARG:HH22	2.25	0.44
1:b:65:VAL:HG13	1:b:319:ILE:HG23	2.00	0.44
1:c:173:GLY:HA2	1:c:249:ASN:OD1	2.18	0.44
1:e:340:ASP:O	1:e:341:PHE:C	2.59	0.44
1:f:148:GLN:NE2	1:f:152:ASP:O	2.51	0.44
1:f:376:LEU:HD23	1:f:376:LEU:HA	1.79	0.44
1:B:368:ALA:N	1:B:369:PRO:HD2	2.33	0.44
1:C:88:ILE:HB	1:C:123:LEU:HD21	1.99	0.44
1:F:38:ILE:HD13	1:F:44:ASP:HB3	1.99	0.44
1:H:341:PHE:O	1:H:342:ALA:C	2.61	0.44
1:J:100:ALA:HA	1:J:284:VAL:HG23	1.98	0.44
1:M:179:ALA:O	1:M:242:GLN:NE2	2.51	0.44
1:M:211:VAL:HG13	1:M:229:GLN:HG3	1.99	0.44
1:O:206:ASP:OD1	1:O:206:ASP:N	2.51	0.44
1:Q:201:ASP:N	1:Q:205:ASN:O	2.51	0.44
1:S:238:ASN:ND2	1:S:240:LYS:HD3	2.33	0.44
1:Y:142:PHE:HE2	1:Y:161:LEU:HD23	1.82	0.44
1:a:167:ASP:O	1:a:168:ASN:C	2.61	0.44
1:a:239:GLU:OE2	1:a:283:SER:HB2	2.18	0.44
1:B:367:GLN:O	1:B:370:ASN:HB2	2.18	0.44
1:D:348:LEU:HG	1:D:352:GLN:HE21	1.83	0.44
1:H:207:GLN:HG3	1:H:232:MET:HE3	1.99	0.44
1:H:330:ASN:ND2	1:g:12:MET:HE1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:169:ARG:HG2	1:R:249:ASN:HD22	1.83	0.44
1:U:95:LEU:HD23	1:U:116:ILE:HG13	1.99	0.44
1:U:179:ALA:CB	1:U:267:ASN:HB2	2.48	0.44
1:e:191:GLY:O	1:e:192:ALA:C	2.60	0.44
1:f:3:VAL:HG22	1:f:372:ALA:HB2	2.00	0.44
1:f:6:ASN:HA	1:g:350:LYS:HD2	1.99	0.44
1:f:165:ARG:NE	1:g:214:LYS:HE3	2.32	0.44
1:f:374:SER:O	1:f:375:LEU:C	2.60	0.44
1:g:221:GLU:O	1:g:224:THR:HG22	2.18	0.44
1:A:132:PHE:HB2	1:A:137:LEU:HD11	2.00	0.44
1:D:164:MET:HE3	1:D:304:HIS:ND1	2.33	0.44
1:E:165:ARG:HD3	1:b:214:LYS:HE3	2.00	0.44
1:E:171:MET:HE3	1:E:297:ALA:HB1	1.99	0.44
1:H:99:SER:HA	1:H:104:ASN:HD22	1.82	0.44
1:I:99:SER:O	1:I:109:ARG:NH1	2.51	0.44
1:M:93:ARG:NH1	1:M:97:LEU:HD11	2.33	0.44
1:N:363:ALA:HA	1:N:366:LYS:HE2	1.99	0.44
1:R:128:GLU:OE2	1:R:165:ARG:HD2	2.17	0.44
1:S:358:SER:HA	1:S:361:VAL:HG12	2.00	0.44
1:V:375:LEU:HD13	1:W:345:THR:HG21	2.00	0.44
1:X:334:SER:HA	1:X:338:ASP:OD2	2.17	0.44
1:c:72:ILE:HD12	1:c:316:ASN:OD1	2.18	0.44
1:e:45:ALA:O	1:e:49:GLN:HG2	2.17	0.44
1:A:8:ASN:HD21	1:A:365:ALA:C	2.26	0.43
1:F:202:ILE:N	1:F:251:LYS:O	2.51	0.43
1:G:99:SER:HA	1:G:104:ASN:HD22	1.82	0.43
1:H:54:LEU:HD23	1:H:54:LEU:HA	1.90	0.43
1:I:203:ASP:HB2	1:I:205:ASN:OD1	2.18	0.43
1:L:179:ALA:HB2	1:L:269:GLN:CD	2.42	0.43
1:O:49:GLN:O	1:O:53:ARG:HG3	2.18	0.43
1:O:69:ASN:O	1:O:72:ILE:HG22	2.18	0.43
1:S:186:TRP:CH2	1:S:262:LEU:HD11	2.52	0.43
1:V:225:TYR:O	1:V:229:GLN:HG2	2.18	0.43
1:X:165:ARG:HB3	1:X:167:ASP:OD1	2.18	0.43
1:Z:36:PHE:O	1:Z:39:ASN:ND2	2.51	0.43
1:d:187:LYS:O	1:d:188:VAL:C	2.61	0.43
1:e:340:ASP:OD1	1:e:340:ASP:N	2.50	0.43
1:f:37:LYS:N	1:f:337:LYS:O	2.50	0.43
1:f:152:ASP:OD1	1:f:155:GLU:HG2	2.18	0.43
1:f:247:ALA:HB1	1:f:252:VAL:HG21	2.00	0.43
1:B:62:ASP:OD1	1:B:326:ASN:ND2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:74:ILE:HG12	1:E:132:PHE:CD2	2.53	0.43
1:F:13:THR:HG23	1:F:16:ARG:HH21	1.83	0.43
1:K:144:THR:HG22	1:K:160:THR:HB	1.99	0.43
1:L:120:ASN:ND2	1:L:277:ASP:HA	2.33	0.43
1:L:166:SER:HA	1:L:171:MET:HE2	1.98	0.43
1:Q:108:GLU:OE1	1:Q:108:GLU:N	2.50	0.43
1:R:3:VAL:HG21	1:R:375:LEU:HD22	2.00	0.43
1:S:40:SER:HB2	1:S:42:LYS:HG2	2.01	0.43
1:S:267:ASN:N	1:S:267:ASN:OD1	2.51	0.43
1:V:14:ALA:O	1:V:17:TYR:N	2.51	0.43
1:W:183:ASP:OD1	1:W:183:ASP:N	2.50	0.43
1:Z:99:SER:O	1:Z:109:ARG:NH1	2.52	0.43
1:g:135:ASN:O	1:g:136:LYS:C	2.61	0.43
1:g:178:ALA:HA	1:g:268:MET:HA	1.99	0.43
1:A:292:ALA:HB2	1:Z:153:ASN:HD21	1.84	0.43
1:B:142:PHE:CE1	1:B:161:LEU:HD23	2.53	0.43
1:D:304:HIS:O	1:D:307:GLU:HG3	2.19	0.43
1:E:235:ALA:HA	1:E:245:ILE:HD13	2.01	0.43
1:F:100:ALA:O	1:F:101:ASN:C	2.61	0.43
1:F:182:LYS:HB3	1:F:186:TRP:CG	2.54	0.43
1:F:332:SER:HA	1:F:335:ARG:HH21	1.84	0.43
1:J:349:THR:O	1:J:353:ILE:HG12	2.18	0.43
1:L:35:GLY:C	1:L:339:THR:HB	2.44	0.43
1:M:134:GLY:O	1:M:135:ASN:C	2.60	0.43
1:N:179:ALA:HB3	1:N:267:ASN:HB3	2.01	0.43
1:P:239:GLU:H	1:P:239:GLU:CD	2.26	0.43
1:Q:275:THR:O	1:Q:276:VAL:C	2.60	0.43
1:Q:340:ASP:O	1:Q:341:PHE:C	2.61	0.43
1:S:183:ASP:OD1	1:S:186:TRP:HB2	2.18	0.43
1:S:220:GLU:HA	1:S:237:VAL:HG21	2.00	0.43
1:T:99:SER:O	1:T:109:ARG:NH1	2.51	0.43
1:U:349:THR:O	1:U:353:ILE:HG12	2.17	0.43
1:V:173:GLY:HA2	1:V:249:ASN:ND2	2.33	0.43
1:X:180:GLU:HG3	1:X:265:ALA:O	2.18	0.43
1:a:3:VAL:O	1:a:4:ASN:C	2.61	0.43
1:a:143:SER:O	1:a:145:LYS:HG3	2.18	0.43
1:f:164:MET:HE3	1:f:304:HIS:CD2	2.50	0.43
1:A:246:PHE:HB2	1:A:289:GLN:NE2	2.32	0.43
1:E:110:VAL:O	1:E:114:GLU:HG3	2.19	0.43
1:E:149:ILE:HD13	1:E:315:PHE:CE1	2.53	0.43
1:G:321:ASN:O	1:G:325:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:82:MET:HE3	1:H:82:MET:HB2	1.88	0.43
1:I:350:LYS:HA	1:I:353:ILE:HD12	2.01	0.43
1:J:16:ARG:O	1:J:19:THR:OG1	2.37	0.43
1:J:38:ILE:HD12	1:J:38:ILE:N	2.33	0.43
1:J:80:GLY:O	1:J:83:ASN:HB3	2.19	0.43
1:J:199:LEU:HB3	1:J:256:VAL:HG13	1.99	0.43
1:J:376:LEU:HB3	1:J:377:GLY:H	1.67	0.43
1:K:334:SER:O	1:K:335:ARG:C	2.61	0.43
1:L:162:LYS:HD3	1:L:304:HIS:CG	2.52	0.43
1:N:12:MET:HE1	1:O:330:ASN:ND2	2.34	0.43
1:S:297:ALA:O	1:S:298:LEU:C	2.60	0.43
1:X:193:ASN:HB2	1:X:213:ALA:O	2.19	0.43
1:c:183:ASP:CG	1:c:185:ASP:H	2.27	0.43
1:d:132:PHE:HB2	1:d:137:LEU:HD11	2.00	0.43
1:e:211:VAL:HG11	1:e:226:ILE:HG12	2.00	0.43
1:f:238:ASN:OD1	1:f:242:GLN:N	2.45	0.43
1:g:333:LYS:O	1:g:336:ILE:HG12	2.18	0.43
1:E:188:VAL:HB	1:E:216:GLY:N	2.33	0.43
1:O:211:VAL:HG13	1:O:229:GLN:HG3	2.01	0.43
1:P:46:ALA:O	1:P:50:ILE:HG22	2.17	0.43
1:Q:369:PRO:O	1:Q:370:ASN:C	2.62	0.43
1:T:368:ALA:HB3	1:T:369:PRO:HD3	2.01	0.43
1:W:331:ALA:O	1:W:334:SER:HB3	2.18	0.43
1:Y:113:GLN:NE2	1:Y:117:THR:OG1	2.51	0.43
1:Y:148:GLN:OE1	1:Y:155:GLU:HB2	2.18	0.43
1:Z:309:GLY:HA2	1:Z:312:GLN:HE21	1.83	0.43
1:a:236:SER:HB3	1:a:288:GLN:HB3	2.01	0.43
1:e:179:ALA:HB2	1:e:269:GLN:CD	2.43	0.43
1:G:321:ASN:HA	1:G:324:ASN:HD21	1.82	0.43
1:H:37:LYS:N	1:H:337:LYS:O	2.44	0.43
1:J:250:ASN:HD21	1:J:296:SER:HB2	1.84	0.43
1:L:276:VAL:HA	1:L:279:ILE:HG23	2.00	0.43
1:M:65:VAL:HG12	1:M:69:ASN:HD21	1.84	0.43
1:M:67:ASN:HB3	1:N:101:ASN:OD1	2.19	0.43
1:Q:32:LEU:HD21	1:Q:344:GLU:HB3	2.00	0.43
1:Q:69:ASN:HB3	1:T:335:ARG:HD3	2.01	0.43
1:T:93:ARG:HB2	1:T:294:ILE:HG21	2.00	0.43
1:U:144:THR:HG22	1:U:160:THR:HG23	2.00	0.43
1:Y:31:ARG:HH21	1:Y:37:LYS:HG3	1.83	0.43
1:Z:148:GLN:NE2	1:Z:152:ASP:O	2.47	0.43
1:a:196:THR:HB	1:a:259:SER:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:238:ASN:HB3	1:b:244:GLN:NE2	2.34	0.43
1:d:129:THR:O	1:d:130:THR:C	2.61	0.43
1:d:164:MET:HE3	1:d:304:HIS:HD2	1.83	0.43
1:A:238:ASN:ND2	1:A:242:GLN:HB2	2.33	0.43
1:B:239:GLU:OE1	1:B:239:GLU:N	2.51	0.43
1:I:170:MET:HE1	1:I:250:ASN:HB3	2.01	0.43
1:K:276:VAL:O	1:K:279:ILE:HG12	2.18	0.43
1:Q:99:SER:O	1:Q:109:ARG:NH1	2.52	0.43
1:R:209:ILE:HG21	1:R:230:THR:HB	2.01	0.43
1:W:167:ASP:OD1	1:W:167:ASP:N	2.52	0.43
1:X:297:ALA:O	1:X:298:LEU:C	2.62	0.43
1:Z:348:LEU:O	1:Z:352:GLN:HG3	2.19	0.43
1:b:225:TYR:O	1:b:229:GLN:HG2	2.19	0.43
1:c:34:SER:HB3	1:e:17:TYR:CZ	2.54	0.43
1:c:369:PRO:C	1:c:371:ALA:N	2.77	0.43
1:g:179:ALA:HB2	1:g:269:GLN:CG	2.47	0.43
1:A:98:GLN:O	1:A:104:ASN:ND2	2.51	0.43
1:A:184:LYS:HD2	1:Z:160:THR:HG21	2.01	0.43
1:C:236:SER:HB3	1:C:288:GLN:HB3	2.00	0.43
1:E:176:TYR:N	1:E:245:ILE:O	2.52	0.43
1:I:356:GLN:HB2	1:e:373:LEU:HD11	1.99	0.43
1:K:3:VAL:HG13	1:L:342:ALA:H	1.84	0.43
1:K:7:THR:HG21	1:L:334:SER:CB	2.48	0.43
1:L:36:PHE:HD2	1:L:36:PHE:HA	1.73	0.43
1:M:169:ARG:O	1:M:249:ASN:ND2	2.51	0.43
1:Q:274:GLU:HG3	1:Q:289:GLN:NE2	2.34	0.43
1:S:66:ARG:HA	1:S:69:ASN:HD22	1.84	0.43
1:S:123:LEU:O	1:S:126:ILE:HG22	2.18	0.43
1:S:199:LEU:HB3	1:S:256:VAL:HG13	2.00	0.43
1:T:193:ASN:O	1:T:212:ASN:HA	2.19	0.43
1:U:251:LYS:HA	1:U:251:LYS:HD2	1.83	0.43
1:Y:12:MET:HE1	1:Z:330:ASN:HD22	1.83	0.43
1:Y:176:TYR:O	1:Y:245:ILE:HG22	2.18	0.43
1:Y:197:PHE:HB2	1:Y:209:ILE:CG2	2.49	0.43
1:b:185:ASP:OD1	1:b:186:TRP:N	2.51	0.43
1:b:369:PRO:O	1:b:370:ASN:C	2.61	0.43
1:c:369:PRO:C	1:c:371:ALA:H	2.27	0.43
1:D:322:LEU:HA	1:D:325:ILE:HG22	2.00	0.43
1:G:29:MET:HG2	1:a:361:VAL:HG13	2.00	0.43
1:I:219:ILE:HD11	1:I:243:LEU:HB2	2.00	0.43
1:J:17:TYR:CZ	1:g:34:SER:HB3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:60:GLY:O	1:O:63:VAL:HG22	2.19	0.43
1:Q:68:ALA:HB2	1:Q:149:ILE:HG22	2.01	0.43
1:R:246:PHE:HB2	1:R:289:GLN:OE1	2.18	0.43
1:S:99:SER:O	1:S:109:ARG:NH1	2.52	0.43
1:S:200:LYS:HD3	1:S:204:GLY:HA2	2.00	0.43
1:S:235:ALA:HB1	1:S:243:LEU:HD11	2.00	0.43
1:V:96:SER:OG	1:V:291:VAL:HG22	2.18	0.43
1:Y:243:LEU:HB3	1:Y:268:MET:HE2	2.00	0.43
1:c:150:GLY:HA3	1:c:155:GLU:HB2	2.01	0.43
1:c:236:SER:HB3	1:c:288:GLN:HB3	2.00	0.43
1:d:36:PHE:HB2	1:d:39:ASN:OD1	2.19	0.43
1:d:340:ASP:O	1:d:341:PHE:C	2.60	0.43
1:e:36:PHE:O	1:e:39:ASN:ND2	2.51	0.43
1:C:25:GLN:OE1	1:C:352:GLN:HG2	2.19	0.43
1:D:129:THR:O	1:D:130:THR:C	2.61	0.43
1:E:5:VAL:HA	1:E:369:PRO:HB3	2.01	0.43
1:F:173:GLY:HA2	1:F:249:ASN:ND2	2.34	0.43
1:H:203:ASP:HB2	1:H:205:ASN:ND2	2.34	0.43
1:I:43:ASP:OD1	1:I:43:ASP:N	2.52	0.43
1:L:120:ASN:HD21	1:L:277:ASP:HA	1.82	0.43
1:O:105:SER:O	1:O:106:LYS:C	2.62	0.43
1:T:258:PHE:CG	1:T:268:MET:HG3	2.54	0.43
1:U:99:SER:O	1:U:109:ARG:NH1	2.49	0.43
1:U:202:ILE:HD12	1:U:253:THR:HB	2.00	0.43
1:X:276:VAL:O	1:X:279:ILE:HG23	2.19	0.43
1:Z:169:ARG:NH2	1:Z:170:MET:SD	2.92	0.43
1:a:315:PHE:O	1:a:319:ILE:HG13	2.18	0.43
1:d:45:ALA:O	1:d:48:LEU:HB3	2.19	0.43
1:f:100:ALA:O	1:f:101:ASN:C	2.60	0.43
1:B:16:ARG:HD3	1:C:323:ASP:OD1	2.18	0.42
1:C:171:MET:HG2	1:C:300:TYR:CD2	2.54	0.42
1:C:195:ILE:HB	1:C:262:LEU:HB3	2.01	0.42
1:E:236:SER:N	1:E:244:GLN:O	2.52	0.42
1:E:315:PHE:O	1:E:319:ILE:HG13	2.19	0.42
1:E:326:ASN:HA	1:E:329:VAL:HG22	2.00	0.42
1:F:92:MET:HA	1:F:95:LEU:HD12	2.01	0.42
1:I:108:GLU:OE1	1:I:108:GLU:N	2.52	0.42
1:N:222:VAL:O	1:N:226:ILE:HG12	2.18	0.42
1:O:34:SER:C	1:O:36:PHE:N	2.77	0.42
1:Q:73:SER:HA	1:Q:76:GLN:HG2	2.01	0.42
1:R:366:LYS:HG3	1:R:367:GLN:HE21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:29:MET:HG3	1:S:348:LEU:HD21	2.01	0.42
1:T:186:TRP:CH2	1:T:262:LEU:HD11	2.54	0.42
1:U:41:ALA:HB2	1:U:48:LEU:HD22	2.00	0.42
1:Y:173:GLY:H	1:Y:246:PHE:HZ	1.67	0.42
1:a:184:LYS:HG3	1:a:185:ASP:N	2.34	0.42
1:c:239:GLU:OE2	1:c:283:SER:HB2	2.19	0.42
1:d:84:GLU:HA	1:d:87:ASN:HD21	1.84	0.42
1:f:98:GLN:O	1:f:104:ASN:ND2	2.52	0.42
1:g:116:ILE:O	1:g:117:THR:C	2.62	0.42
1:A:92:MET:HE2	1:A:279:ILE:HD11	2.01	0.42
1:D:202:ILE:HA	1:D:253:THR:HG23	2.00	0.42
1:F:275:THR:O	1:F:276:VAL:C	2.60	0.42
1:J:105:SER:H	1:J:108:GLU:CD	2.27	0.42
1:J:218:ASP:O	1:J:222:VAL:HG23	2.19	0.42
1:O:108:GLU:CD	1:P:53:ARG:HH22	2.27	0.42
1:P:35:GLY:HA2	1:P:339:THR:HG22	2.01	0.42
1:Q:209:ILE:HD11	1:Q:232:MET:HG3	2.01	0.42
1:S:186:TRP:NE1	1:S:189:GLN:HE22	2.17	0.42
1:W:7:THR:HG21	1:X:334:SER:HB3	2.00	0.42
1:W:81:ALA:HB1	1:W:130:THR:HG21	2.01	0.42
1:W:191:GLY:O	1:W:192:ALA:C	2.61	0.42
1:X:88:ILE:HG23	1:X:119:LEU:HB3	2.00	0.42
1:Y:31:ARG:HB3	1:Y:339:THR:HG21	2.01	0.42
1:Z:82:MET:HE1	1:Z:304:HIS:CD2	2.54	0.42
1:Z:201:ASP:O	1:Z:253:THR:N	2.52	0.42
1:f:205:ASN:OD1	1:f:205:ASN:N	2.50	0.42
1:f:219:ILE:HD11	1:f:243:LEU:HB2	2.00	0.42
1:E:125:ARG:O	1:E:129:THR:N	2.52	0.42
1:E:205:ASN:HB2	1:E:207:GLN:HG2	2.01	0.42
1:G:64:ALA:HA	1:G:67:ASN:HD22	1.83	0.42
1:G:276:VAL:O	1:G:279:ILE:HG12	2.18	0.42
1:I:52:ASN:O	1:I:56:VAL:HG23	2.19	0.42
1:L:110:VAL:HA	1:L:282:THR:HG22	2.01	0.42
1:R:144:THR:H	1:R:160:THR:HA	1.83	0.42
1:S:43:ASP:O	1:S:44:ASP:C	2.62	0.42
1:X:22:THR:O	1:X:26:GLN:HG2	2.20	0.42
1:Y:202:ILE:HA	1:Y:253:THR:CG2	2.49	0.42
1:b:234:LYS:HD2	1:b:292:ALA:HB2	2.00	0.42
1:b:365:ALA:C	1:b:367:GLN:N	2.77	0.42
1:e:132:PHE:HB2	1:e:137:LEU:HD11	2.01	0.42
1:e:341:PHE:O	1:e:342:ALA:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:ARG:HH21	1:C:327:GLU:CD	2.26	0.42
1:B:236:SER:N	1:B:244:GLN:O	2.49	0.42
1:H:153:ASN:OD1	1:I:234:LYS:NZ	2.45	0.42
1:H:179:ALA:HB2	1:H:269:GLN:CD	2.45	0.42
1:I:65:VAL:HG12	1:I:69:ASN:ND2	2.32	0.42
1:K:32:LEU:HD21	1:K:344:GLU:HB2	2.00	0.42
1:N:202:ILE:HD12	1:N:253:THR:HG23	2.01	0.42
1:P:200:LYS:O	1:P:253:THR:N	2.41	0.42
1:Q:47:GLY:O	1:Q:48:LEU:C	2.63	0.42
1:Q:132:PHE:HB2	1:Q:137:LEU:HD11	2.01	0.42
1:U:30:GLU:HG2	1:U:39:ASN:HD22	1.84	0.42
1:Y:25:GLN:HG2	1:Y:29:MET:HE3	2.01	0.42
1:a:201:ASP:HB2	1:a:207:GLN:NE2	2.29	0.42
1:b:175:SER:OG	1:b:289:GLN:NE2	2.52	0.42
1:f:200:LYS:NZ	1:f:254:GLY:HA3	2.35	0.42
1:A:186:TRP:NE1	1:A:189:GLN:HE22	2.17	0.42
1:C:56:VAL:HG13	1:D:93:ARG:HD3	2.01	0.42
1:C:341:PHE:O	1:C:342:ALA:C	2.62	0.42
1:D:236:SER:HB3	1:D:288:GLN:HB3	2.00	0.42
1:E:321:ASN:HA	1:E:324:ASN:HD22	1.85	0.42
1:F:93:ARG:HB2	1:F:294:ILE:HG21	2.01	0.42
1:I:340:ASP:O	1:I:341:PHE:C	2.61	0.42
1:M:7:THR:HG21	1:N:334:SER:HB2	2.01	0.42
1:O:150:GLY:HA3	1:O:155:GLU:OE1	2.20	0.42
1:P:29:MET:HG2	1:S:361:VAL:HG23	2.00	0.42
1:Q:12:MET:HB3	1:R:327:GLU:HG2	2.01	0.42
1:T:129:THR:O	1:T:130:THR:C	2.62	0.42
1:T:376:LEU:HD13	1:T:376:LEU:HA	1.84	0.42
1:V:98:GLN:O	1:V:104:ASN:ND2	2.52	0.42
1:W:188:VAL:HB	1:W:215:GLU:HA	2.00	0.42
1:Z:159:LEU:HB2	1:Z:311:PHE:CE1	2.55	0.42
1:a:144:THR:HG21	1:c:184:LYS:HB3	2.02	0.42
1:e:319:ILE:HD12	1:e:319:ILE:HA	1.80	0.42
1:f:45:ALA:O	1:f:49:GLN:HG2	2.19	0.42
1:f:99:SER:O	1:f:100:ALA:C	2.62	0.42
1:f:173:GLY:HA2	1:f:249:ASN:CG	2.44	0.42
1:g:313:ASN:HA	1:g:316:ASN:HD22	1.84	0.42
1:E:201:ASP:HB2	1:E:207:GLN:CG	2.50	0.42
1:F:82:MET:HE1	1:F:308:LEU:HD12	2.02	0.42
1:H:131:SER:HB3	1:H:136:LYS:HD2	2.02	0.42
1:K:165:ARG:HE	1:K:165:ARG:HB3	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:193:ASN:O	1:M:262:LEU:HG	2.20	0.42
1:P:202:ILE:HA	1:P:253:THR:HG23	2.01	0.42
1:T:2:ALA:O	1:T:3:VAL:C	2.62	0.42
1:T:186:TRP:CZ2	1:T:262:LEU:HD11	2.54	0.42
1:U:72:ILE:O	1:U:76:GLN:HG2	2.20	0.42
1:U:189:GLN:CD	1:U:189:GLN:H	2.27	0.42
1:V:268:MET:HE3	1:V:268:MET:HB3	1.89	0.42
1:W:334:SER:C	1:W:336:ILE:N	2.77	0.42
1:Y:144:THR:HA	1:Y:160:THR:HA	2.00	0.42
1:Y:147:PHE:HE1	1:Y:159:LEU:HD23	1.84	0.42
1:c:85:THR:HG23	1:c:123:LEU:HD22	2.01	0.42
1:d:177:VAL:HG13	1:d:244:GLN:HG2	2.01	0.42
1:e:36:PHE:HB2	1:e:39:ASN:OD1	2.19	0.42
1:B:69:ASN:HB3	1:E:335:ARG:HD3	2.01	0.42
1:C:152:ASP:HA	1:D:93:ARG:HH22	1.84	0.42
1:G:202:ILE:HA	1:G:253:THR:CG2	2.49	0.42
1:I:142:PHE:CE1	1:I:145:LYS:HD2	2.55	0.42
1:J:170:MET:HE3	1:J:170:MET:HB2	1.80	0.42
1:L:82:MET:O	1:L:86:THR:HG23	2.20	0.42
1:L:187:LYS:HD3	1:L:216:GLY:HA2	2.01	0.42
1:O:82:MET:HE3	1:O:305:ARG:HG2	2.01	0.42
1:R:129:THR:O	1:R:130:THR:C	2.62	0.42
1:S:46:ALA:O	1:S:50:ILE:HG13	2.19	0.42
1:T:26:GLN:NE2	1:V:10:ALA:HB2	2.35	0.42
1:T:262:LEU:HG	1:T:266:LEU:HD23	2.01	0.42
1:U:162:LYS:H	1:U:304:HIS:CE1	2.38	0.42
1:V:171:MET:HB3	1:V:171:MET:HE3	1.80	0.42
1:W:88:ILE:HB	1:W:123:LEU:HD21	2.02	0.42
1:W:196:THR:HA	1:W:210:THR:HA	2.01	0.42
1:W:328:ASN:H	1:W:328:ASN:HD22	1.67	0.42
1:X:374:SER:O	1:X:375:LEU:C	2.62	0.42
1:Z:195:ILE:HG13	1:Z:263:ALA:HB2	2.02	0.42
1:c:261:GLY:O	1:c:262:LEU:C	2.62	0.42
1:d:32:LEU:HD21	1:d:344:GLU:HB3	2.01	0.42
1:d:45:ALA:O	1:d:49:GLN:HG2	2.20	0.42
1:f:276:VAL:O	1:f:279:ILE:HG12	2.20	0.42
1:F:89:LEU:HD23	1:F:89:LEU:HA	1.91	0.42
1:F:315:PHE:O	1:F:319:ILE:HG13	2.20	0.42
1:I:100:ALA:O	1:I:101:ASN:C	2.62	0.42
1:O:200:LYS:HB3	1:O:253:THR:O	2.20	0.42
1:O:340:ASP:O	1:O:341:PHE:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:61:LEU:HD23	1:S:61:LEU:HA	1.83	0.42
1:V:8:ASN:ND2	1:V:369:PRO:HD3	2.28	0.42
1:W:368:ALA:HB3	1:W:369:PRO:HD3	2.01	0.42
1:d:376:LEU:O	1:d:377:GLY:C	2.62	0.42
1:A:129:THR:O	1:A:130:THR:C	2.62	0.42
1:B:169:ARG:HG2	1:B:249:ASN:HD22	1.85	0.42
1:B:310:ALA:O	1:B:311:PHE:C	2.63	0.42
1:C:29:MET:HE1	1:F:10:ALA:HB1	2.01	0.42
1:E:121:ASP:HA	1:E:124:ASN:HD22	1.85	0.42
1:I:368:ALA:HB3	1:I:369:PRO:HD3	2.02	0.42
1:O:164:MET:HE3	1:O:304:HIS:CD2	2.53	0.42
1:O:187:LYS:O	1:O:188:VAL:C	2.62	0.42
1:P:266:LEU:O	1:P:267:ASN:C	2.62	0.42
1:Q:41:ALA:HB2	1:Q:48:LEU:HD22	2.01	0.42
1:R:166:SER:HA	1:R:171:MET:HE2	2.01	0.42
1:S:65:VAL:HG12	1:S:69:ASN:ND2	2.34	0.42
1:T:25:GLN:HG2	1:T:29:MET:HE2	2.02	0.42
1:W:182:LYS:HD2	1:W:186:TRP:CD1	2.54	0.42
1:X:275:THR:O	1:X:276:VAL:C	2.62	0.42
1:X:372:ALA:O	1:X:373:LEU:C	2.63	0.42
1:Y:302:ASP:O	1:Y:305:ARG:HB2	2.20	0.42
1:Z:376:LEU:O	1:Z:377:GLY:C	2.62	0.42
1:c:332:SER:HA	1:c:335:ARG:HD2	2.02	0.42
1:f:313:ASN:HA	1:f:316:ASN:HD22	1.85	0.42
1:g:69:ASN:HA	1:g:72:ILE:HG22	2.02	0.42
1:A:297:ALA:O	1:A:298:LEU:C	2.63	0.42
1:C:371:ALA:O	1:C:372:ALA:C	2.63	0.42
1:G:321:ASN:HA	1:G:324:ASN:ND2	2.35	0.42
1:J:200:LYS:HA	1:J:206:ASP:HA	2.02	0.42
1:K:366:LYS:O	1:K:369:PRO:HD2	2.20	0.42
1:M:195:ILE:HD12	1:M:259:SER:O	2.20	0.42
1:M:245:ILE:HG13	1:M:258:PHE:HE2	1.85	0.42
1:N:171:MET:HE3	1:N:171:MET:HB3	1.89	0.42
1:N:340:ASP:O	1:N:341:PHE:C	2.62	0.42
1:Q:169:ARG:HG3	1:Q:170:MET:N	2.35	0.42
1:Q:363:ALA:O	1:Q:367:GLN:HG2	2.19	0.42
1:R:131:SER:O	1:U:57:GLN:NE2	2.52	0.42
1:S:109:ARG:CB	1:S:282:THR:HA	2.45	0.42
1:U:340:ASP:O	1:U:341:PHE:C	2.62	0.42
1:V:92:MET:HE2	1:V:279:ILE:HD11	2.02	0.42
1:X:341:PHE:O	1:X:342:ALA:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:250:ASN:ND2	1:Z:296:SER:OG	2.50	0.42
1:a:69:ASN:HB3	1:d:335:ARG:HD3	2.02	0.42
1:d:122:GLU:O	1:d:126:ILE:HG23	2.20	0.42
1:f:295:ASP:HA	1:f:298:LEU:HD12	2.00	0.42
1:f:375:LEU:HD13	1:f:375:LEU:HA	1.85	0.42
1:g:36:PHE:O	1:g:39:ASN:ND2	2.53	0.42
1:B:29:MET:HG2	1:E:361:VAL:HG13	2.01	0.41
1:E:158:MET:HG3	1:F:220:GLU:HG3	2.01	0.41
1:G:290:SER:O	1:G:291:VAL:C	2.62	0.41
1:H:340:ASP:O	1:H:341:PHE:C	2.63	0.41
1:I:129:THR:O	1:I:130:THR:C	2.63	0.41
1:K:315:PHE:O	1:K:319:ILE:HG13	2.20	0.41
1:M:163:ASP:OD2	1:M:165:ARG:HB2	2.20	0.41
1:N:12:MET:HE1	1:O:330:ASN:HD22	1.84	0.41
1:N:129:THR:O	1:N:130:THR:C	2.63	0.41
1:N:301:VAL:O	1:N:305:ARG:HG3	2.20	0.41
1:S:238:ASN:OD1	1:S:242:GLN:N	2.53	0.41
1:T:179:ALA:HB3	1:T:267:ASN:HB2	2.02	0.41
1:T:201:ASP:O	1:T:253:THR:OG1	2.35	0.41
1:U:168:ASN:OD1	1:U:170:MET:HB2	2.20	0.41
1:W:168:ASN:OD1	1:W:170:MET:HB2	2.20	0.41
1:Y:376:LEU:O	1:Y:377:GLY:C	2.63	0.41
1:Z:30:GLU:OE1	1:Z:39:ASN:ND2	2.52	0.41
1:Z:319:ILE:HD12	1:Z:319:ILE:HA	1.73	0.41
1:a:341:PHE:O	1:a:345:THR:HG22	2.20	0.41
1:c:84:GLU:HB3	1:c:126:ILE:HD11	2.02	0.41
1:f:176:TYR:OH	1:f:255:ASP:HA	2.20	0.41
1:f:251:LYS:HE2	1:f:251:LYS:HB3	1.90	0.41
1:A:199:LEU:HB2	1:A:252:VAL:HG13	2.03	0.41
1:K:202:ILE:HD12	1:K:250:ASN:HA	2.02	0.41
1:L:171:MET:HE3	1:L:171:MET:HB3	1.73	0.41
1:Q:195:ILE:CG1	1:Q:262:LEU:HB3	2.50	0.41
1:R:108:GLU:OE1	1:R:108:GLU:N	2.53	0.41
1:R:171:MET:O	1:R:276:VAL:HG23	2.20	0.41
1:S:49:GLN:HG2	1:T:302:ASP:OD1	2.19	0.41
1:S:180:GLU:CB	1:S:267:ASN:HD21	2.33	0.41
1:U:370:ASN:ND2	1:X:353:ILE:HD11	2.35	0.41
1:c:95:LEU:HD21	1:c:115:GLU:HB3	2.01	0.41
1:f:239:GLU:H	1:f:239:GLU:CD	2.27	0.41
1:f:371:ALA:O	1:f:372:ALA:C	2.64	0.41
1:C:349:THR:O	1:C:353:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:129:THR:HG22	1:M:155:GLU:HG2	2.03	0.41
1:J:214:LYS:HB2	1:J:217:ASP:OD2	2.21	0.41
1:K:43:ASP:OD1	1:K:43:ASP:N	2.45	0.41
1:K:281:VAL:HG12	1:K:287:ALA:HA	2.02	0.41
1:L:188:VAL:HB	1:L:215:GLU:HA	2.02	0.41
1:N:75:ALA:HB1	1:N:308:LEU:HD12	2.02	0.41
1:N:258:PHE:CG	1:N:268:MET:HG3	2.55	0.41
1:R:363:ALA:O	1:R:366:LYS:HG2	2.21	0.41
1:S:82:MET:HE3	1:S:305:ARG:HG2	2.01	0.41
1:S:196:THR:N	1:S:259:SER:O	2.47	0.41
1:U:165:ARG:HB3	1:U:167:ASP:OD1	2.20	0.41
1:U:230:THR:OG1	1:U:231:ASP:N	2.54	0.41
1:X:159:LEU:HB2	1:X:311:PHE:CZ	2.54	0.41
1:Y:27:THR:O	1:Y:31:ARG:HG2	2.19	0.41
1:a:193:ASN:ND2	1:a:215:GLU:OE2	2.53	0.41
1:a:292:ALA:O	1:a:293:VAL:C	2.63	0.41
1:b:80:GLY:O	1:b:83:ASN:HB3	2.20	0.41
1:f:169:ARG:NH1	1:f:249:ASN:HB3	2.35	0.41
1:f:200:LYS:HG2	1:f:206:ASP:CG	2.45	0.41
1:g:175:SER:HB2	1:g:246:PHE:HD1	1.86	0.41
1:g:281:VAL:C	1:g:283:SER:N	2.77	0.41
1:B:85:THR:HG23	1:B:123:LEU:HD22	2.03	0.41
1:E:188:VAL:HG23	1:E:217:ASP:O	2.20	0.41
1:M:91:ARG:HD2	1:M:91:ARG:HA	1.95	0.41
1:P:199:LEU:HB2	1:P:252:VAL:CG1	2.49	0.41
1:R:105:SER:O	1:R:106:LYS:C	2.63	0.41
1:S:186:TRP:CZ2	1:S:262:LEU:HD11	2.56	0.41
1:W:352:GLN:O	1:W:356:GLN:HG2	2.20	0.41
1:X:38:ILE:HG23	1:X:43:ASP:HB2	2.02	0.41
1:Y:106:LYS:HD3	1:Y:106:LYS:H	1.85	0.41
1:Y:199:LEU:O	1:Y:207:GLN:N	2.50	0.41
1:d:332:SER:O	1:d:336:ILE:HG13	2.20	0.41
1:g:40:SER:C	1:g:42:LYS:N	2.76	0.41
1:A:235:ALA:HB1	1:A:243:LEU:HD11	2.02	0.41
1:D:128:GLU:OE2	1:D:165:ARG:HD2	2.21	0.41
1:E:61:LEU:O	1:E:65:VAL:HG23	2.21	0.41
1:E:125:ARG:O	1:E:126:ILE:C	2.64	0.41
1:F:3:VAL:HG22	1:F:372:ALA:HB2	2.02	0.41
1:H:7:THR:HG21	1:I:334:SER:CB	2.51	0.41
1:I:168:ASN:OD1	1:I:170:MET:HB2	2.21	0.41
1:J:2:ALA:O	1:J:3:VAL:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:169:ARG:HD2	1:J:169:ARG:HA	1.90	0.41
1:K:275:THR:O	1:K:276:VAL:C	2.63	0.41
1:L:29:MET:HG2	1:O:361:VAL:HG13	2.02	0.41
1:M:246:PHE:CZ	1:M:293:VAL:HG22	2.55	0.41
1:N:32:LEU:HD21	1:N:344:GLU:HB2	2.02	0.41
1:O:173:GLY:HA2	1:O:249:ASN:H	1.86	0.41
1:O:187:LYS:HE2	1:O:216:GLY:HA2	2.02	0.41
1:P:25:GLN:HG2	1:P:29:MET:HE2	2.03	0.41
1:S:318:ALA:O	1:S:319:ILE:C	2.62	0.41
1:U:167:ASP:OD2	1:X:214:LYS:HE2	2.21	0.41
1:W:54:LEU:HD22	1:W:329:VAL:HG13	2.03	0.41
1:W:203:ASP:HB2	1:W:205:ASN:OD1	2.20	0.41
1:W:225:TYR:O	1:W:229:GLN:HG2	2.20	0.41
1:X:367:GLN:O	1:X:370:ASN:ND2	2.53	0.41
1:d:108:GLU:OE1	1:d:108:GLU:N	2.51	0.41
1:d:236:SER:O	1:d:244:GLN:N	2.43	0.41
1:d:248:GLY:C	1:d:250:ASN:N	2.78	0.41
1:d:341:PHE:O	1:d:342:ALA:C	2.64	0.41
1:f:89:LEU:O	1:f:90:GLN:C	2.63	0.41
1:g:65:VAL:HG13	1:g:319:ILE:HG23	2.02	0.41
1:g:238:ASN:OD1	1:g:242:GLN:N	2.48	0.41
1:B:201:ASP:HB3	1:B:203:ASP:OD1	2.20	0.41
1:E:178:ALA:HB1	1:E:266:LEU:HB3	2.03	0.41
1:K:266:LEU:HD13	1:K:266:LEU:HA	1.87	0.41
1:M:186:TRP:CH2	1:M:188:VAL:HG22	2.56	0.41
1:N:195:ILE:HD13	1:N:263:ALA:H	1.85	0.41
1:N:218:ASP:O	1:N:222:VAL:HG23	2.21	0.41
1:O:202:ILE:HD12	1:O:253:THR:HG23	2.02	0.41
1:R:185:ASP:O	1:R:186:TRP:C	2.63	0.41
1:U:189:GLN:HE21	1:U:192:ALA:HB3	1.85	0.41
1:V:333:LYS:HE2	1:V:333:LYS:HB3	1.91	0.41
1:W:25:GLN:NE2	1:W:352:GLN:HG2	2.36	0.41
1:X:55:ASN:O	1:X:59:ARG:HG2	2.20	0.41
1:Z:38:ILE:HG21	1:Z:44:ASP:HB3	2.03	0.41
1:Z:82:MET:HE2	1:Z:138:LEU:HD22	2.02	0.41
1:Z:193:ASN:OD1	1:Z:193:ASN:N	2.48	0.41
1:a:375:LEU:HD13	1:a:375:LEU:HA	1.87	0.41
1:b:187:LYS:O	1:b:188:VAL:C	2.64	0.41
1:c:258:PHE:CD2	1:c:268:MET:HG3	2.55	0.41
1:f:369:PRO:O	1:f:370:ASN:C	2.62	0.41
1:B:43:ASP:O	1:B:44:ASP:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:ASP:O	1:B:207:GLN:C	2.64	0.41
1:E:72:ILE:O	1:E:76:GLN:HG3	2.20	0.41
1:F:376:LEU:CD2	1:G:342:ALA:HA	2.50	0.41
1:G:281:VAL:C	1:G:283:SER:N	2.78	0.41
1:H:101:ASN:ND2	1:g:67:ASN:HA	2.36	0.41
1:I:251:LYS:HE2	1:I:251:LYS:HB3	1.91	0.41
1:J:65:VAL:HG13	1:J:319:ILE:HG23	2.02	0.41
1:J:194:ASP:CG	1:J:261:GLY:H	2.28	0.41
1:N:236:SER:HB3	1:N:288:GLN:HB3	2.01	0.41
1:P:169:ARG:HG3	1:P:170:MET:N	2.35	0.41
1:P:369:PRO:O	1:P:370:ASN:C	2.62	0.41
1:Q:144:THR:HG22	1:R:184:LYS:HD3	2.02	0.41
1:U:30:GLU:HG2	1:U:39:ASN:ND2	2.36	0.41
1:U:147:PHE:O	1:U:148:GLN:C	2.63	0.41
1:W:35:GLY:O	1:W:339:THR:HG22	2.20	0.41
1:Z:147:PHE:HE1	1:Z:159:LEU:HD23	1.84	0.41
1:c:214:LYS:HE2	1:c:225:TYR:CE1	2.56	0.41
1:c:255:ASP:OD1	1:c:255:ASP:N	2.53	0.41
1:d:375:LEU:O	1:d:376:LEU:C	2.64	0.41
1:e:324:ASN:OD1	1:e:328:ASN:ND2	2.54	0.41
1:f:8:ASN:O	1:f:9:VAL:C	2.64	0.41
1:E:195:ILE:HD12	1:E:259:SER:O	2.21	0.41
1:E:246:PHE:CE1	1:E:293:VAL:HG22	2.56	0.41
1:E:370:ASN:O	1:E:373:LEU:HG	2.21	0.41
1:I:95:LEU:HD11	1:I:115:GLU:HG2	2.03	0.41
1:L:193:ASN:O	1:L:213:ALA:N	2.53	0.41
1:N:217:ASP:HB2	1:N:221:GLU:HB2	2.02	0.41
1:O:173:GLY:HA2	1:O:249:ASN:CG	2.46	0.41
1:O:334:SER:HA	1:O:338:ASP:OD1	2.20	0.41
1:P:63:VAL:HG12	1:P:67:ASN:ND2	2.35	0.41
1:V:178:ALA:HB1	1:V:266:LEU:O	2.21	0.41
1:V:363:ALA:O	1:V:367:GLN:HG2	2.21	0.41
1:W:142:PHE:O	1:W:145:LYS:NZ	2.54	0.41
1:X:275:THR:O	1:X:278:THR:N	2.49	0.41
1:a:177:VAL:HG13	1:a:244:GLN:HG2	2.02	0.41
1:c:30:GLU:OE2	1:c:39:ASN:ND2	2.54	0.41
1:c:168:ASN:ND2	1:c:170:MET:HB2	2.35	0.41
1:d:130:THR:HG21	1:d:138:LEU:HD13	2.03	0.41
1:f:201:ASP:O	1:f:204:GLY:N	2.43	0.41
1:f:370:ASN:O	1:f:371:ALA:C	2.63	0.41
1:g:168:ASN:O	1:g:171:MET:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:SER:O	1:B:244:GLN:N	2.44	0.41
1:C:225:TYR:O	1:C:229:GLN:HG2	2.20	0.41
1:D:211:VAL:HG11	1:D:226:ILE:HA	2.02	0.41
1:F:238:ASN:OD1	1:F:242:GLN:N	2.53	0.41
1:H:335:ARG:HH11	1:e:69:ASN:HB3	1.86	0.41
1:I:308:LEU:HD13	1:I:308:LEU:HA	1.87	0.41
1:K:193:ASN:ND2	1:K:215:GLU:OE2	2.54	0.41
1:L:42:LYS:H	1:L:42:LYS:HG3	1.68	0.41
1:L:186:TRP:CD1	1:L:189:GLN:HE22	2.39	0.41
1:N:156:ALA:HB3	1:O:220:GLU:OE2	2.21	0.41
1:N:366:LYS:NZ	1:P:375:LEU:O	2.54	0.41
1:O:200:LYS:HA	1:O:206:ASP:HA	2.02	0.41
1:R:168:ASN:O	1:R:171:MET:HB2	2.21	0.41
1:S:85:THR:HG22	1:S:126:ILE:HG21	2.02	0.41
1:S:105:SER:O	1:S:109:ARG:HG2	2.21	0.41
1:U:106:LYS:HE3	1:U:106:LYS:HB3	1.95	0.41
1:U:148:GLN:O	1:U:149:ILE:C	2.63	0.41
1:W:129:THR:O	1:W:130:THR:C	2.63	0.41
1:W:236:SER:HB3	1:W:288:GLN:HB3	2.03	0.41
1:Y:245:ILE:H	1:Y:268:MET:HE1	1.86	0.41
1:a:108:GLU:OE2	1:f:50:ILE:HD11	2.21	0.41
1:a:178:ALA:HA	1:a:268:MET:HA	2.03	0.41
1:b:105:SER:HB3	1:b:108:GLU:OE1	2.21	0.41
1:c:40:SER:O	1:c:43:ASP:N	2.46	0.41
1:e:158:MET:H	1:e:158:MET:HG2	1.61	0.41
1:e:168:ASN:ND2	1:e:170:MET:HB2	2.35	0.41
1:e:182:LYS:HB3	1:e:186:TRP:CG	2.56	0.41
1:e:333:LYS:HE2	1:e:333:LYS:HB3	1.96	0.41
1:f:113:GLN:OE1	1:f:280:ASP:HA	2.20	0.41
1:f:132:PHE:HB2	1:f:137:LEU:HD11	2.03	0.41
1:g:161:LEU:HD23	1:g:304:HIS:CE1	2.56	0.41
1:g:165:ARG:O	1:g:171:MET:HG3	2.21	0.41
1:A:334:SER:OG	1:A:335:ARG:N	2.54	0.41
1:D:104:ASN:HB2	1:D:109:ARG:NH1	2.35	0.41
1:G:92:MET:HE1	1:G:123:LEU:HD11	2.02	0.41
1:H:12:MET:HB3	1:I:327:GLU:HG2	2.03	0.41
1:H:349:THR:HG22	1:H:353:ILE:HD11	2.03	0.41
1:H:375:LEU:HD23	1:I:342:ALA:HA	2.03	0.41
1:J:310:ALA:HB2	1:g:115:GLU:HG2	2.01	0.41
1:L:214:LYS:HE2	1:L:225:TYR:CZ	2.56	0.41
1:M:165:ARG:HB3	1:M:167:ASP:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:176:TYR:CG	1:P:258:PHE:HE1	2.38	0.41
1:Q:267:ASN:O	1:Q:268:MET:HB2	2.21	0.41
1:S:94:ASP:O	1:S:97:LEU:HG	2.21	0.41
1:S:169:ARG:HH12	1:S:249:ASN:HD21	1.69	0.41
1:S:180:GLU:HB3	1:S:267:ASN:HD21	1.85	0.41
1:S:197:PHE:N	1:S:209:ILE:O	2.44	0.41
1:U:209:ILE:HG21	1:U:230:THR:HB	2.03	0.41
1:W:164:MET:HE3	1:W:304:HIS:HD2	1.86	0.41
1:W:354:LEU:HD23	1:W:354:LEU:HA	1.88	0.41
1:X:11:ALA:O	1:X:15:GLN:HG3	2.21	0.41
1:X:301:VAL:O	1:X:302:ASP:C	2.63	0.41
1:Z:61:LEU:HA	1:Z:61:LEU:HD23	1.76	0.41
1:Z:65:VAL:HA	1:Z:319:ILE:HD11	2.01	0.41
1:a:149:ILE:HD11	1:a:157:VAL:HG23	2.03	0.41
1:b:372:ALA:O	1:b:373:LEU:C	2.64	0.41
1:d:65:VAL:HG13	1:d:319:ILE:HG23	2.03	0.41
1:e:25:GLN:O	1:e:29:MET:HG3	2.21	0.41
1:f:50:ILE:HD13	1:f:50:ILE:HA	1.98	0.41
1:D:209:ILE:H	1:D:209:ILE:HG13	1.71	0.40
1:E:195:ILE:CG1	1:E:197:PHE:HE1	2.34	0.40
1:F:370:ASN:ND2	1:F:374:SER:OG	2.54	0.40
1:J:366:LYS:HG2	1:N:346:THR:HG22	2.03	0.40
1:L:99:SER:O	1:L:109:ARG:NH1	2.53	0.40
1:N:233:VAL:HG13	1:N:245:ILE:HG23	2.02	0.40
1:N:276:VAL:HA	1:N:279:ILE:HG23	2.02	0.40
1:T:192:ALA:O	1:T:262:LEU:HB2	2.21	0.40
1:W:341:PHE:O	1:W:342:ALA:C	2.64	0.40
1:a:31:ARG:HE	1:a:37:LYS:HA	1.85	0.40
1:d:49:GLN:NE2	1:e:306:ALA:HB2	2.36	0.40
1:e:275:THR:O	1:e:276:VAL:C	2.64	0.40
1:B:19:THR:HG22	1:E:2:ALA:HB2	2.03	0.40
1:B:222:VAL:O	1:B:226:ILE:HG13	2.21	0.40
1:F:218:ASP:O	1:F:222:VAL:HG23	2.21	0.40
1:G:69:ASN:HB3	1:a:335:ARG:HD3	2.02	0.40
1:G:157:VAL:HG21	1:G:314:ARG:NH1	2.36	0.40
1:G:205:ASN:OD1	1:G:207:GLN:NE2	2.54	0.40
1:H:225:TYR:O	1:H:229:GLN:HG2	2.21	0.40
1:I:162:LYS:H	1:I:304:HIS:CE1	2.39	0.40
1:J:95:LEU:HB2	1:J:116:ILE:HD11	2.02	0.40
1:L:209:ILE:HG22	1:L:211:VAL:HG23	2.03	0.40
1:M:142:PHE:CE1	1:M:145:LYS:HD3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:201:ASP:N	1:M:205:ASN:O	2.41	0.40
1:M:222:VAL:O	1:M:226:ILE:HG12	2.21	0.40
1:N:367:GLN:O	1:N:370:ASN:HB2	2.21	0.40
1:R:339:THR:OG1	1:R:344:GLU:HG3	2.22	0.40
1:S:196:THR:H	1:S:259:SER:C	2.29	0.40
1:V:78:ALA:HB2	1:V:137:LEU:HD23	2.03	0.40
1:V:238:ASN:OD1	1:V:242:GLN:N	2.50	0.40
1:W:105:SER:H	1:W:108:GLU:CD	2.29	0.40
1:W:199:LEU:HB2	1:W:252:VAL:HG13	2.02	0.40
1:Y:30:GLU:HG2	1:Y:39:ASN:ND2	2.36	0.40
1:Z:334:SER:O	1:Z:335:ARG:C	2.63	0.40
1:Z:341:PHE:O	1:Z:342:ALA:C	2.64	0.40
1:a:372:ALA:O	1:a:373:LEU:C	2.63	0.40
1:b:173:GLY:HA2	1:b:249:ASN:OD1	2.22	0.40
1:c:98:GLN:O	1:c:104:ASN:ND2	2.54	0.40
1:c:281:VAL:HG12	1:c:287:ALA:HA	2.03	0.40
1:c:349:THR:O	1:c:353:ILE:HG12	2.21	0.40
1:d:47:GLY:O	1:d:48:LEU:C	2.64	0.40
1:e:153:ASN:OD1	1:e:153:ASN:N	2.55	0.40
1:f:105:SER:O	1:f:108:GLU:HG2	2.21	0.40
1:A:155:GLU:OE2	1:X:125:ARG:NH1	2.54	0.40
1:D:354:LEU:HD23	1:D:354:LEU:HA	1.90	0.40
1:E:165:ARG:HE	1:E:165:ARG:HB3	1.79	0.40
1:F:179:ALA:HB2	1:F:269:GLN:CD	2.46	0.40
1:F:262:LEU:HD23	1:F:262:LEU:HA	1.83	0.40
1:G:85:THR:HG23	1:G:123:LEU:HD22	2.02	0.40
1:H:121:ASP:HA	1:H:124:ASN:HD22	1.86	0.40
1:J:28:SER:O	1:J:29:MET:C	2.65	0.40
1:L:149:ILE:HD11	1:L:157:VAL:HG23	2.03	0.40
1:L:334:SER:HA	1:L:338:ASP:HB2	2.03	0.40
1:N:168:ASN:ND2	1:N:170:MET:HB2	2.36	0.40
1:U:143:SER:OG	1:U:144:THR:N	2.55	0.40
1:U:239:GLU:OE2	1:U:283:SER:HB2	2.21	0.40
1:W:281:VAL:HG12	1:W:287:ALA:HA	2.03	0.40
1:W:321:ASN:O	1:W:325:ILE:HG12	2.21	0.40
1:a:30:GLU:OE1	1:a:39:ASN:ND2	2.54	0.40
1:a:295:ASP:O	1:a:298:LEU:HB2	2.21	0.40
1:b:3:VAL:O	1:b:4:ASN:C	2.65	0.40
1:c:88:ILE:HG22	1:c:92:MET:HE3	2.02	0.40
1:c:173:GLY:HA2	1:c:249:ASN:CG	2.46	0.40
1:d:18:LEU:HB2	1:d:358:SER:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:ARG:HA	1:C:39:ASN:HD21	1.85	0.40
1:D:150:GLY:HA3	1:D:155:GLU:HB2	2.02	0.40
1:E:225:TYR:O	1:E:229:GLN:HG2	2.21	0.40
1:F:61:LEU:O	1:F:65:VAL:HG23	2.21	0.40
1:H:125:ARG:O	1:H:126:ILE:C	2.65	0.40
1:H:292:ALA:HB2	1:g:153:ASN:HD21	1.86	0.40
1:M:246:PHE:HB2	1:M:289:GLN:NE2	2.35	0.40
1:S:162:LYS:H	1:S:304:HIS:CE1	2.40	0.40
1:S:240:LYS:H	1:S:240:LYS:HD2	1.86	0.40
1:U:173:GLY:HA2	1:U:249:ASN:HD22	1.86	0.40
1:U:176:TYR:CD2	1:U:258:PHE:HE2	2.40	0.40
1:U:201:ASP:O	1:U:202:ILE:C	2.63	0.40
1:W:6:ASN:OD1	1:X:35:GLY:HA3	2.21	0.40
1:X:234:LYS:HD2	1:X:292:ALA:HB1	2.04	0.40
1:Y:304:HIS:O	1:Y:308:LEU:HG	2.21	0.40
1:c:82:MET:HE3	1:c:305:ARG:HG2	2.04	0.40
1:c:182:LYS:HD2	1:c:186:TRP:CD1	2.56	0.40
1:g:302:ASP:O	1:g:303:SER:C	2.65	0.40
1:A:290:SER:O	1:A:291:VAL:C	2.64	0.40
1:B:96:SER:HB2	1:B:290:SER:OG	2.21	0.40
1:B:161:LEU:HD13	1:B:161:LEU:HA	1.86	0.40
1:C:299:LYS:O	1:C:300:TYR:C	2.65	0.40
1:F:209:ILE:HD11	1:F:232:MET:HB2	2.03	0.40
1:L:164:MET:HE1	1:L:301:VAL:HG22	2.03	0.40
1:N:55:ASN:O	1:N:59:ARG:HG3	2.21	0.40
1:N:147:PHE:HE1	1:N:159:LEU:HB3	1.87	0.40
1:P:99:SER:O	1:P:109:ARG:NH1	2.53	0.40
1:Q:122:GLU:HB2	1:T:314:ARG:HG3	2.04	0.40
1:U:82:MET:HE3	1:U:82:MET:HB3	1.79	0.40
1:U:195:ILE:HB	1:U:262:LEU:HB3	2.02	0.40
1:W:214:LYS:HE2	1:W:225:TYR:CE1	2.57	0.40
1:X:239:GLU:CD	1:X:284:VAL:HG12	2.47	0.40
1:b:178:ALA:N	1:b:268:MET:SD	2.95	0.40
1:c:374:SER:O	1:c:375:LEU:C	2.65	0.40
1:d:60:GLY:O	1:d:61:LEU:C	2.64	0.40
1:f:202:ILE:HD12	1:f:253:THR:HG23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	374/376 (100%)	357 (96%)	17 (4%)	0	100	100
1	B	374/376 (100%)	356 (95%)	18 (5%)	0	100	100
1	C	374/376 (100%)	360 (96%)	14 (4%)	0	100	100
1	D	374/376 (100%)	357 (96%)	17 (4%)	0	100	100
1	E	374/376 (100%)	361 (96%)	13 (4%)	0	100	100
1	F	374/376 (100%)	358 (96%)	16 (4%)	0	100	100
1	G	374/376 (100%)	354 (95%)	20 (5%)	0	100	100
1	H	374/376 (100%)	361 (96%)	13 (4%)	0	100	100
1	I	374/376 (100%)	363 (97%)	11 (3%)	0	100	100
1	J	374/376 (100%)	348 (93%)	26 (7%)	0	100	100
1	K	374/376 (100%)	358 (96%)	16 (4%)	0	100	100
1	L	374/376 (100%)	360 (96%)	14 (4%)	0	100	100
1	M	374/376 (100%)	357 (96%)	17 (4%)	0	100	100
1	N	374/376 (100%)	356 (95%)	18 (5%)	0	100	100
1	O	374/376 (100%)	355 (95%)	19 (5%)	0	100	100
1	P	374/376 (100%)	356 (95%)	18 (5%)	0	100	100
1	Q	374/376 (100%)	354 (95%)	20 (5%)	0	100	100
1	R	374/376 (100%)	356 (95%)	18 (5%)	0	100	100
1	S	374/376 (100%)	355 (95%)	19 (5%)	0	100	100
1	T	374/376 (100%)	356 (95%)	18 (5%)	0	100	100
1	U	374/376 (100%)	356 (95%)	18 (5%)	0	100	100
1	V	374/376 (100%)	362 (97%)	12 (3%)	0	100	100
1	W	374/376 (100%)	360 (96%)	14 (4%)	0	100	100
1	X	374/376 (100%)	353 (94%)	21 (6%)	0	100	100
1	Y	374/376 (100%)	351 (94%)	23 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Z	374/376 (100%)	355 (95%)	19 (5%)	0	100	100
1	a	374/376 (100%)	355 (95%)	19 (5%)	0	100	100
1	b	374/376 (100%)	356 (95%)	18 (5%)	0	100	100
1	c	374/376 (100%)	359 (96%)	15 (4%)	0	100	100
1	d	374/376 (100%)	352 (94%)	22 (6%)	0	100	100
1	e	374/376 (100%)	358 (96%)	16 (4%)	0	100	100
1	f	374/376 (100%)	356 (95%)	18 (5%)	0	100	100
1	g	374/376 (100%)	360 (96%)	14 (4%)	0	100	100
All	All	12342/12408 (100%)	11771 (95%)	571 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	298/298 (100%)	291 (98%)	7 (2%)	45	61
1	B	298/298 (100%)	294 (99%)	4 (1%)	65	78
1	C	298/298 (100%)	292 (98%)	6 (2%)	50	65
1	D	298/298 (100%)	295 (99%)	3 (1%)	73	83
1	E	298/298 (100%)	295 (99%)	3 (1%)	73	83
1	F	298/298 (100%)	288 (97%)	10 (3%)	32	46
1	G	298/298 (100%)	292 (98%)	6 (2%)	50	65
1	H	298/298 (100%)	293 (98%)	5 (2%)	56	70
1	I	298/298 (100%)	293 (98%)	5 (2%)	56	70
1	J	298/298 (100%)	289 (97%)	9 (3%)	36	51
1	K	298/298 (100%)	288 (97%)	10 (3%)	32	46
1	L	298/298 (100%)	288 (97%)	10 (3%)	32	46
1	M	298/298 (100%)	290 (97%)	8 (3%)	40	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	298/298 (100%)	288 (97%)	10 (3%)	32	46
1	O	298/298 (100%)	296 (99%)	2 (1%)	81	89
1	P	298/298 (100%)	291 (98%)	7 (2%)	45	61
1	Q	298/298 (100%)	291 (98%)	7 (2%)	45	61
1	R	298/298 (100%)	286 (96%)	12 (4%)	27	39
1	S	298/298 (100%)	288 (97%)	10 (3%)	32	46
1	T	298/298 (100%)	287 (96%)	11 (4%)	29	43
1	U	298/298 (100%)	292 (98%)	6 (2%)	50	65
1	V	298/298 (100%)	291 (98%)	7 (2%)	45	61
1	W	298/298 (100%)	292 (98%)	6 (2%)	50	65
1	X	298/298 (100%)	291 (98%)	7 (2%)	45	61
1	Y	298/298 (100%)	289 (97%)	9 (3%)	36	51
1	Z	298/298 (100%)	293 (98%)	5 (2%)	56	70
1	a	298/298 (100%)	293 (98%)	5 (2%)	56	70
1	b	298/298 (100%)	290 (97%)	8 (3%)	40	55
1	c	298/298 (100%)	289 (97%)	9 (3%)	36	51
1	d	298/298 (100%)	293 (98%)	5 (2%)	56	70
1	e	298/298 (100%)	289 (97%)	9 (3%)	36	51
1	f	298/298 (100%)	293 (98%)	5 (2%)	56	70
1	g	298/298 (100%)	288 (97%)	10 (3%)	32	46
All	All	9834/9834 (100%)	9598 (98%)	236 (2%)	45	60

All (236) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	MET
1	A	116	ILE
1	A	199	LEU
1	A	202	ILE
1	A	205	ASN
1	A	284	VAL
1	A	350	LYS
1	B	161	LEU
1	B	199	LEU
1	B	284	VAL

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Mol	Chain	Res	Type
1	B	366	LYS
1	C	39	ASN
1	C	144	THR
1	C	160	THR
1	C	176	TYR
1	C	284	VAL
1	C	339	THR
1	D	12	MET
1	D	116	ILE
1	D	284	VAL
1	E	3	VAL
1	E	63	VAL
1	E	199	LEU
1	F	29	MET
1	F	33	SER
1	F	82	MET
1	F	92	MET
1	F	176	TYR
1	F	253	THR
1	F	284	VAL
1	F	354	LEU
1	F	375	LEU
1	F	376	LEU
1	G	5	VAL
1	G	29	MET
1	G	92	MET
1	G	145	LYS
1	G	176	TYR
1	G	199	LEU
1	H	6	ASN
1	H	9	VAL
1	H	82	MET
1	H	284	VAL
1	H	364	GLN
1	I	3	VAL
1	I	9	VAL
1	I	253	THR
1	I	308	LEU
1	I	373	LEU
1	J	72	ILE
1	J	162	LYS
1	J	170	MET

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Mol	Chain	Res	Type
1	J	205	ASN
1	J	239	GLU
1	J	250	ASN
1	J	256	VAL
1	J	284	VAL
1	J	376	LEU
1	K	3	VAL
1	K	29	MET
1	K	108	GLU
1	K	202	ILE
1	K	205	ASN
1	K	239	GLU
1	K	250	ASN
1	K	253	THR
1	K	266	LEU
1	K	284	VAL
1	L	5	VAL
1	L	9	VAL
1	L	26	GLN
1	L	36	PHE
1	L	199	LEU
1	L	202	ILE
1	L	250	ASN
1	L	255	ASP
1	L	339	THR
1	L	373	LEU
1	M	3	VAL
1	M	88	ILE
1	M	106	LYS
1	M	123	LEU
1	M	230	THR
1	M	250	ASN
1	M	284	VAL
1	M	298	LEU
1	N	4	ASN
1	N	29	MET
1	N	49	GLN
1	N	113	GLN
1	N	161	LEU
1	N	199	LEU
1	N	202	ILE
1	N	233	VAL

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Mol	Chain	Res	Type
1	N	308	LEU
1	N	339	THR
1	O	49	GLN
1	O	169	ARG
1	P	149	ILE
1	P	176	TYR
1	P	203	ASP
1	P	205	ASN
1	P	315	PHE
1	P	332	SER
1	P	335	ARG
1	Q	3	VAL
1	Q	72	ILE
1	Q	82	MET
1	Q	115	GLU
1	Q	149	ILE
1	Q	284	VAL
1	Q	348	LEU
1	R	9	VAL
1	R	30	GLU
1	R	53	ARG
1	R	63	VAL
1	R	72	ILE
1	R	99	SER
1	R	144	THR
1	R	153	ASN
1	R	220	GLU
1	R	239	GLU
1	R	279	ILE
1	R	284	VAL
1	S	3	VAL
1	S	5	VAL
1	S	180	GLU
1	S	233	VAL
1	S	267	ASN
1	S	268	MET
1	S	294	ILE
1	S	315	PHE
1	S	324	ASN
1	S	348	LEU
1	T	29	MET
1	T	56	VAL

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Mol	Chain	Res	Type
1	T	92	MET
1	T	116	ILE
1	T	138	LEU
1	T	144	THR
1	T	266	LEU
1	T	308	LEU
1	T	373	LEU
1	T	375	LEU
1	T	376	LEU
1	U	29	MET
1	U	114	GLU
1	U	158	MET
1	U	184	LYS
1	U	284	VAL
1	U	333	LYS
1	V	3	VAL
1	V	29	MET
1	V	62	ASP
1	V	104	ASN
1	V	116	ILE
1	V	176	TYR
1	V	375	LEU
1	W	3	VAL
1	W	92	MET
1	W	284	VAL
1	W	333	LYS
1	W	348	LEU
1	W	373	LEU
1	X	5	VAL
1	X	9	VAL
1	X	82	MET
1	X	176	TYR
1	X	205	ASN
1	X	239	GLU
1	X	343	LYS
1	Y	72	ILE
1	Y	74	ILE
1	Y	158	MET
1	Y	209	ILE
1	Y	253	THR
1	Y	267	ASN
1	Y	305	ARG

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Mol	Chain	Res	Type
1	Y	343	LYS
1	Y	376	LEU
1	Z	161	LEU
1	Z	199	LEU
1	Z	205	ASN
1	Z	239	GLU
1	Z	319	ILE
1	a	74	ILE
1	a	284	VAL
1	a	339	THR
1	a	373	LEU
1	a	375	LEU
1	b	12	MET
1	b	26	GLN
1	b	29	MET
1	b	176	TYR
1	b	250	ASN
1	b	256	VAL
1	b	284	VAL
1	b	362	LEU
1	c	5	VAL
1	c	72	ILE
1	c	82	MET
1	c	126	ILE
1	c	199	LEU
1	c	250	ASN
1	c	274	GLU
1	c	284	VAL
1	c	339	THR
1	d	3	VAL
1	d	49	GLN
1	d	126	ILE
1	d	199	LEU
1	d	253	THR
1	e	9	VAL
1	e	30	GLU
1	e	82	MET
1	e	138	LEU
1	e	176	TYR
1	e	209	ILE
1	e	319	ILE
1	e	366	LYS

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Mol	Chain	Res	Type
1	e	375	LEU
1	f	199	LEU
1	f	215	GLU
1	f	266	LEU
1	f	281	VAL
1	f	375	LEU
1	g	9	VAL
1	g	79	GLU
1	g	158	MET
1	g	168	ASN
1	g	185	ASP
1	g	199	LEU
1	g	330	ASN
1	g	339	THR
1	g	366	LYS
1	g	373	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (365) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	67	ASN
1	A	69	ASN
1	A	101	ASN
1	A	148	GLN
1	A	244	GLN
1	A	304	HIS
1	A	321	ASN
1	A	330	ASN
1	B	69	ASN
1	B	135	ASN
1	B	205	ASN
1	B	207	GLN
1	B	304	HIS
1	B	316	ASN
1	B	326	ASN
1	B	328	ASN
1	B	356	GLN
1	C	6	ASN
1	C	39	ASN
1	C	69	ASN
1	C	101	ASN

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Mol	Chain	Res	Type
1	C	212	ASN
1	C	269	GLN
1	C	316	ASN
1	C	321	ASN
1	D	15	GLN
1	D	39	ASN
1	D	67	ASN
1	D	87	ASN
1	D	212	ASN
1	D	244	GLN
1	D	312	GLN
1	D	328	ASN
1	D	352	GLN
1	D	367	GLN
1	E	15	GLN
1	E	25	GLN
1	E	55	ASN
1	E	76	GLN
1	E	124	ASN
1	E	205	ASN
1	E	242	GLN
1	E	244	GLN
1	E	250	ASN
1	E	269	GLN
1	E	289	GLN
1	E	304	HIS
1	E	316	ASN
1	E	321	ASN
1	E	324	ASN
1	E	328	ASN
1	E	330	ASN
1	F	4	ASN
1	F	55	ASN
1	F	101	ASN
1	F	205	ASN
1	F	207	GLN
1	F	212	ASN
1	F	249	ASN
1	F	250	ASN
1	F	324	ASN
1	F	370	ASN
1	G	4	ASN

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Mol	Chain	Res	Type
1	G	26	GLN
1	G	39	ASN
1	G	55	ASN
1	G	67	ASN
1	G	69	ASN
1	G	212	ASN
1	G	250	ASN
1	G	324	ASN
1	H	25	GLN
1	H	39	ASN
1	H	55	ASN
1	H	76	GLN
1	H	124	ASN
1	H	148	GLN
1	H	289	GLN
1	H	316	ASN
1	H	330	ASN
1	I	25	GLN
1	I	39	ASN
1	I	49	GLN
1	I	69	ASN
1	I	101	ASN
1	I	104	ASN
1	I	148	GLN
1	I	244	GLN
1	I	250	ASN
1	I	316	ASN
1	I	328	ASN
1	I	330	ASN
1	J	8	ASN
1	J	26	GLN
1	J	55	ASN
1	J	104	ASN
1	J	148	GLN
1	J	269	GLN
1	J	289	GLN
1	J	304	HIS
1	J	328	ASN
1	J	330	ASN
1	J	356	GLN
1	K	25	GLN
1	K	39	ASN

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Mol	Chain	Res	Type
1	K	69	ASN
1	K	83	ASN
1	K	87	ASN
1	K	101	ASN
1	K	104	ASN
1	K	212	ASN
1	K	250	ASN
1	K	316	ASN
1	K	321	ASN
1	K	328	ASN
1	K	330	ASN
1	L	4	ASN
1	L	23	ASN
1	L	55	ASN
1	L	69	ASN
1	L	87	ASN
1	L	148	GLN
1	L	168	ASN
1	L	212	ASN
1	L	244	GLN
1	L	312	GLN
1	L	321	ASN
1	L	330	ASN
1	M	55	ASN
1	M	69	ASN
1	M	98	GLN
1	M	104	ASN
1	M	207	GLN
1	M	289	GLN
1	M	316	ASN
1	M	330	ASN
1	M	364	GLN
1	N	69	ASN
1	N	87	ASN
1	N	207	GLN
1	N	212	ASN
1	N	244	GLN
1	N	269	GLN
1	N	312	GLN
1	N	328	ASN
1	N	330	ASN
1	N	370	ASN

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Mol	Chain	Res	Type
1	O	4	ASN
1	O	25	GLN
1	O	26	GLN
1	O	83	ASN
1	O	104	ASN
1	O	212	ASN
1	O	249	ASN
1	O	330	ASN
1	O	370	ASN
1	P	25	GLN
1	P	67	ASN
1	P	69	ASN
1	P	104	ASN
1	P	120	ASN
1	P	124	ASN
1	P	168	ASN
1	P	207	GLN
1	P	212	ASN
1	P	249	ASN
1	P	316	ASN
1	P	330	ASN
1	P	370	ASN
1	Q	39	ASN
1	Q	124	ASN
1	Q	135	ASN
1	Q	212	ASN
1	Q	244	GLN
1	Q	316	ASN
1	Q	321	ASN
1	Q	330	ASN
1	R	23	ASN
1	R	67	ASN
1	R	83	ASN
1	R	87	ASN
1	R	90	GLN
1	R	101	ASN
1	R	104	ASN
1	R	153	ASN
1	R	269	GLN
1	R	312	GLN
1	R	328	ASN
1	R	330	ASN

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Mol	Chain	Res	Type
1	R	352	GLN
1	R	367	GLN
1	S	4	ASN
1	S	15	GLN
1	S	39	ASN
1	S	69	ASN
1	S	83	ASN
1	S	104	ASN
1	S	207	GLN
1	S	244	GLN
1	S	249	ASN
1	S	250	ASN
1	S	269	GLN
1	S	289	GLN
1	S	312	GLN
1	S	317	HIS
1	S	321	ASN
1	S	328	ASN
1	T	4	ASN
1	T	6	ASN
1	T	26	GLN
1	T	39	ASN
1	T	55	ASN
1	T	120	ASN
1	T	135	ASN
1	T	207	GLN
1	T	212	ASN
1	T	250	ASN
1	T	289	GLN
1	T	321	ASN
1	T	324	ASN
1	T	326	ASN
1	T	328	ASN
1	T	330	ASN
1	U	4	ASN
1	U	26	GLN
1	U	76	GLN
1	U	87	ASN
1	U	148	GLN
1	U	168	ASN
1	U	189	GLN
1	U	205	ASN

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Mol	Chain	Res	Type
1	U	244	GLN
1	U	249	ASN
1	U	269	GLN
1	U	289	GLN
1	U	321	ASN
1	U	364	GLN
1	U	370	ASN
1	V	23	ASN
1	V	25	GLN
1	V	39	ASN
1	V	55	ASN
1	V	168	ASN
1	V	244	GLN
1	V	289	GLN
1	V	312	GLN
1	V	330	ASN
1	V	364	GLN
1	W	4	ASN
1	W	8	ASN
1	W	25	GLN
1	W	69	ASN
1	W	87	ASN
1	W	189	GLN
1	W	212	ASN
1	W	244	GLN
1	W	289	GLN
1	W	316	ASN
1	W	328	ASN
1	X	69	ASN
1	X	101	ASN
1	X	244	GLN
1	X	269	GLN
1	X	289	GLN
1	X	304	HIS
1	X	312	GLN
1	X	326	ASN
1	X	328	ASN
1	X	352	GLN
1	Y	69	ASN
1	Y	101	ASN
1	Y	113	GLN
1	Y	207	GLN

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Mol	Chain	Res	Type
1	Y	316	ASN
1	Y	321	ASN
1	Y	330	ASN
1	Y	352	GLN
1	Y	367	GLN
1	Z	6	ASN
1	Z	69	ASN
1	Z	87	ASN
1	Z	168	ASN
1	Z	304	HIS
1	Z	312	GLN
1	Z	316	ASN
1	Z	321	ASN
1	Z	328	ASN
1	Z	330	ASN
1	a	26	GLN
1	a	55	ASN
1	a	76	GLN
1	a	135	ASN
1	a	207	GLN
1	a	244	GLN
1	a	249	ASN
1	a	250	ASN
1	a	288	GLN
1	a	312	GLN
1	a	326	ASN
1	a	328	ASN
1	a	330	ASN
1	a	356	GLN
1	b	6	ASN
1	b	39	ASN
1	b	69	ASN
1	b	76	GLN
1	b	104	ASN
1	b	148	GLN
1	b	205	ASN
1	b	207	GLN
1	b	250	ASN
1	b	316	ASN
1	b	328	ASN
1	b	370	ASN
1	c	4	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	c	25	GLN
1	c	69	ASN
1	c	104	ASN
1	c	168	ASN
1	c	207	GLN
1	c	212	ASN
1	c	250	ASN
1	c	328	ASN
1	c	330	ASN
1	d	205	ASN
1	d	207	GLN
1	d	244	GLN
1	d	267	ASN
1	d	289	GLN
1	d	328	ASN
1	d	330	ASN
1	d	356	GLN
1	e	49	GLN
1	e	67	ASN
1	e	124	ASN
1	e	250	ASN
1	e	289	GLN
1	e	312	GLN
1	e	316	ASN
1	e	321	ASN
1	e	328	ASN
1	e	352	GLN
1	f	4	ASN
1	f	6	ASN
1	f	104	ASN
1	f	207	GLN
1	f	250	ASN
1	f	269	GLN
1	f	316	ASN
1	f	326	ASN
1	f	328	ASN
1	f	367	GLN
1	g	4	ASN
1	g	6	ASN
1	g	69	ASN
1	g	83	ASN
1	g	104	ASN

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Mol	Chain	Res	Type
1	g	120	ASN
1	g	207	GLN
1	g	212	ASN
1	g	244	GLN
1	g	316	ASN
1	g	328	ASN
1	g	330	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.

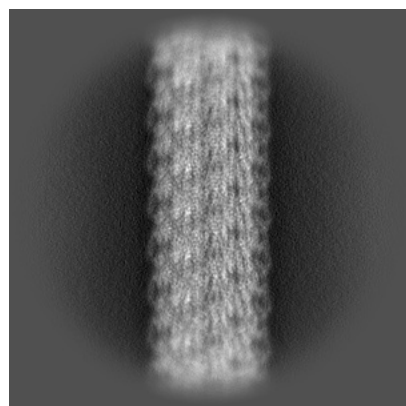
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49126. These allow visual inspection of the internal detail of the map and identification of artifacts.

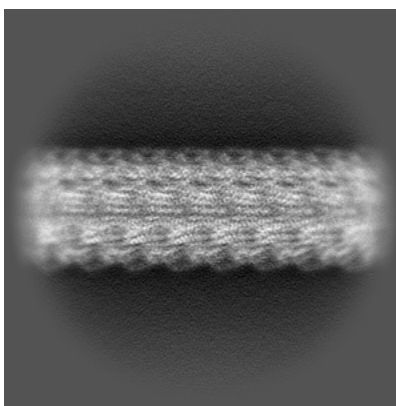
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

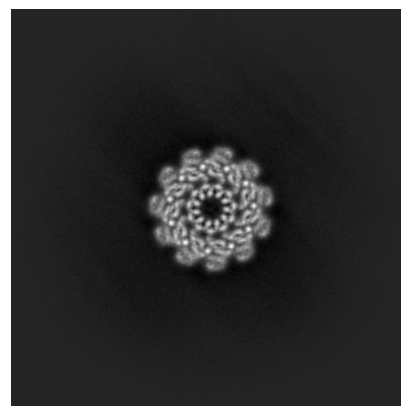
6.1.1 Primary map



X

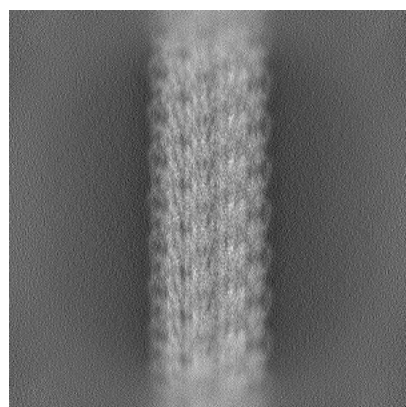


Y

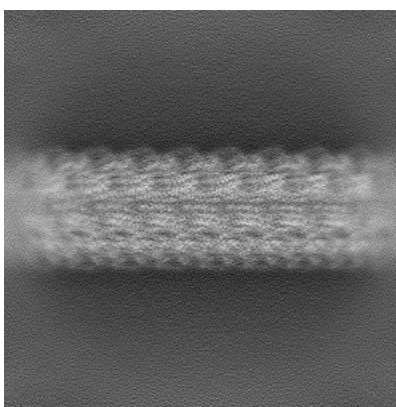


Z

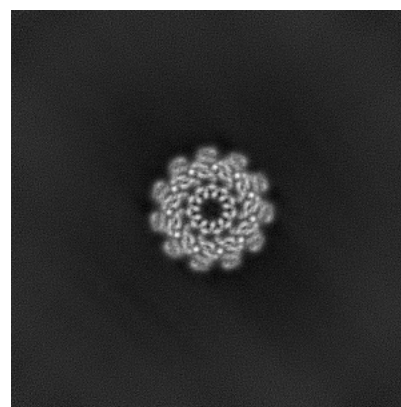
6.1.2 Raw map



X



Y

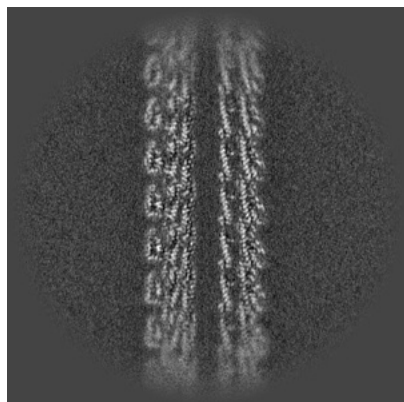


Z

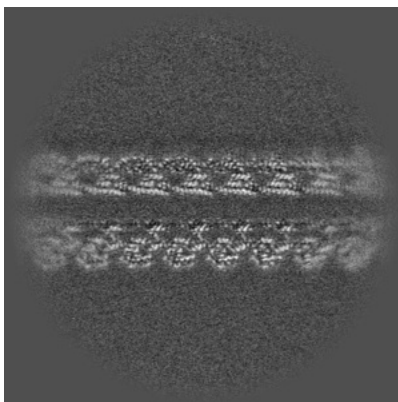
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

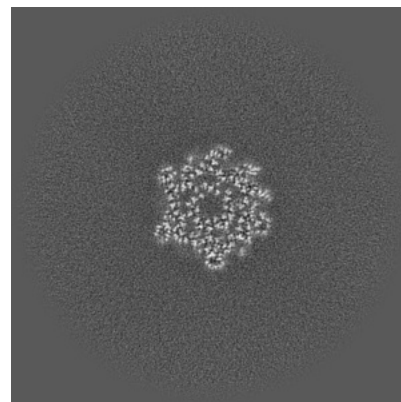
6.2.1 Primary map



X Index: 224

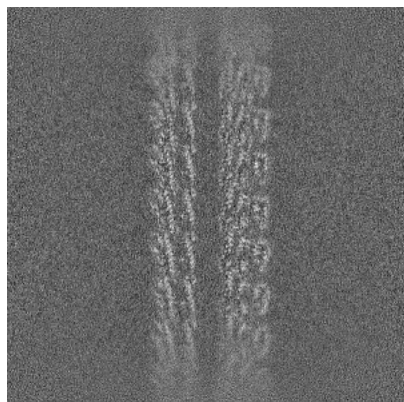


Y Index: 224

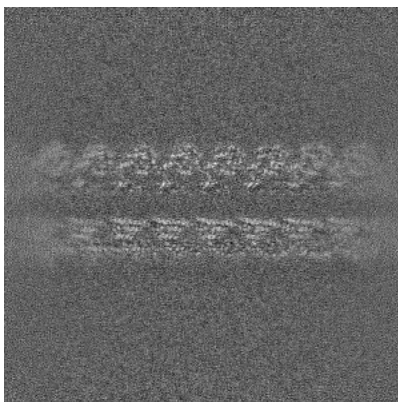


Z Index: 224

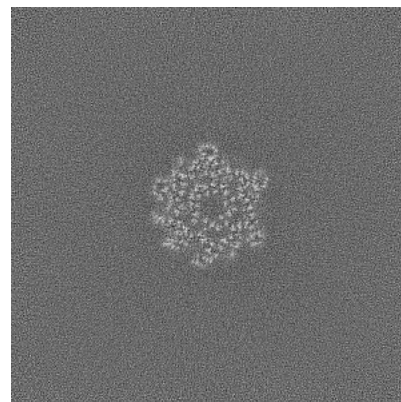
6.2.2 Raw map



X Index: 224



Y Index: 224

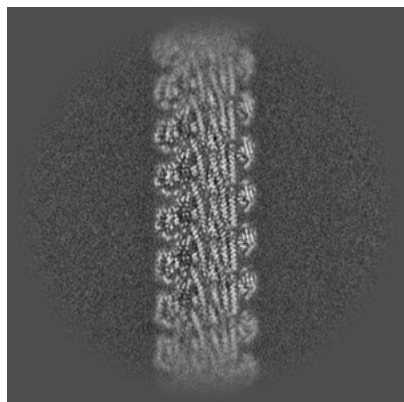


Z Index: 224

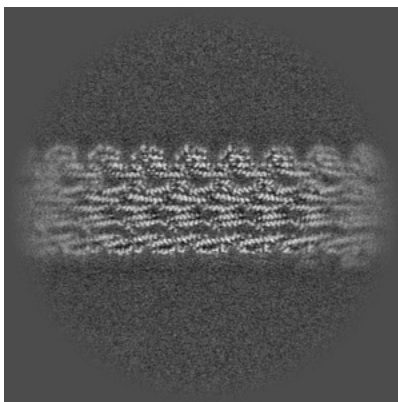
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

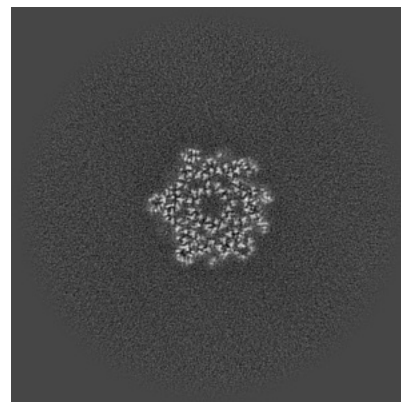
6.3.1 Primary map



X Index: 262

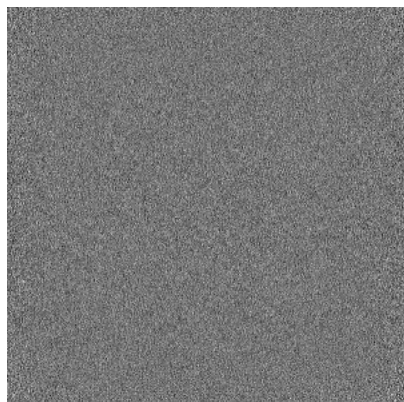


Y Index: 241

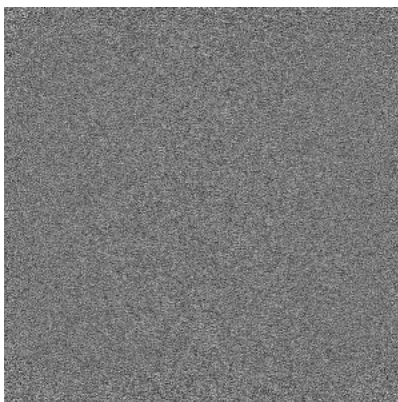


Z Index: 197

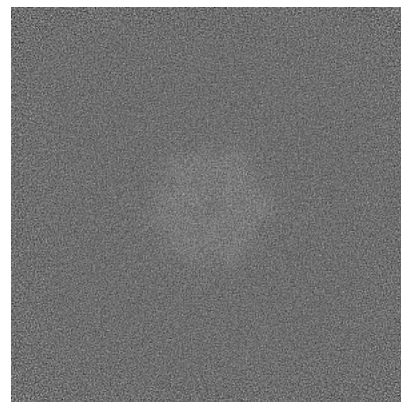
6.3.2 Raw map



X Index: 0



Y Index: 0

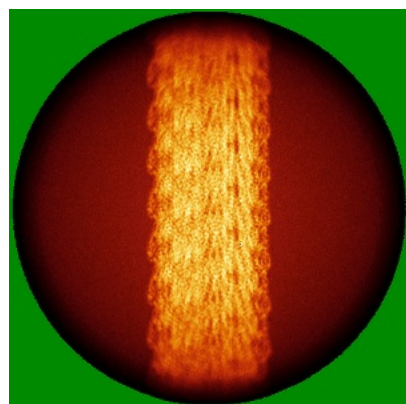


Z Index: 0

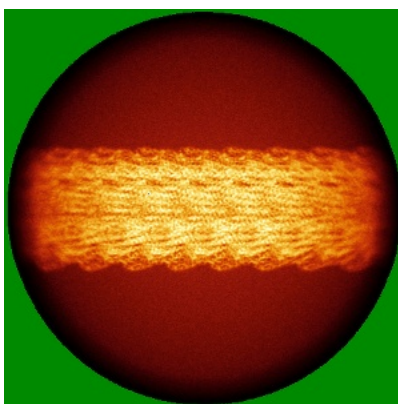
The images above show the largest variance slices of the map in three orthogonal directions.

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

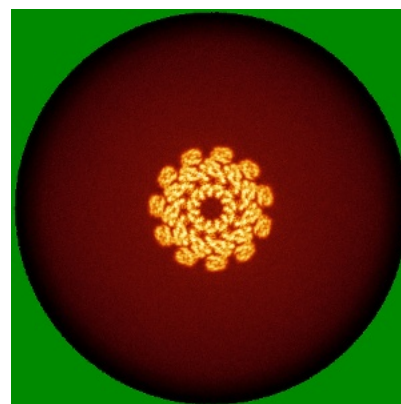
6.4.1 Primary map



X

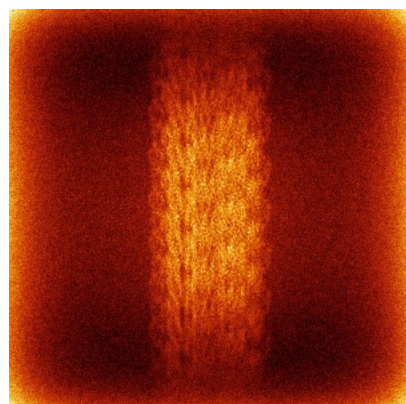


Y

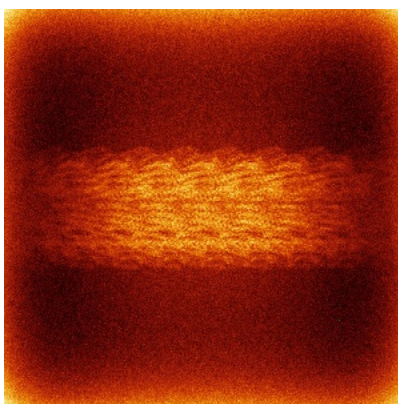


Z

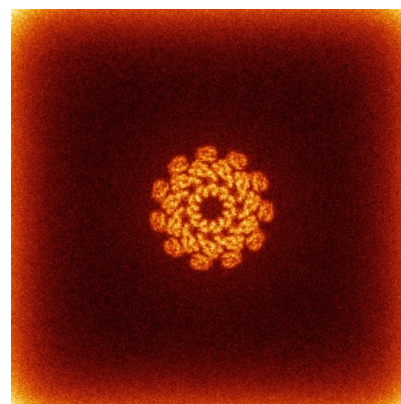
6.4.2 Raw map



X



Y



Z

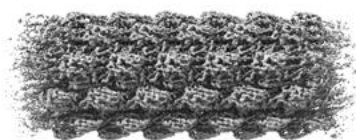
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

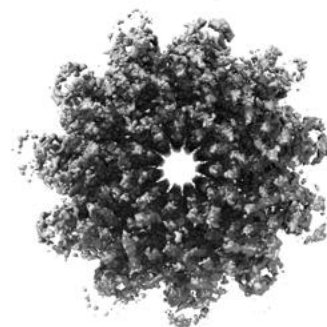
6.5.1 Primary map



X



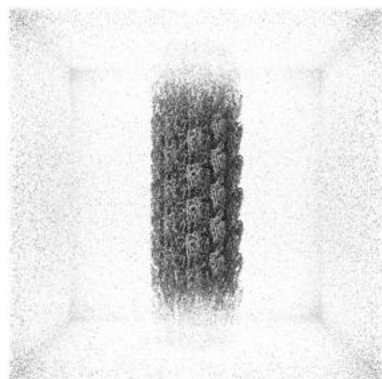
Y



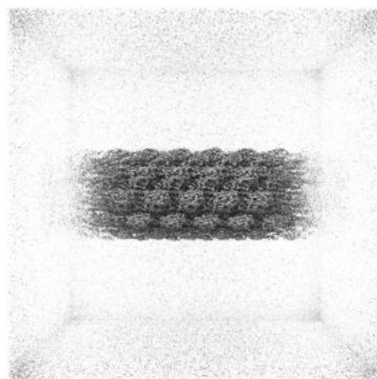
Z

The images above show the 3D surface view of the map at the recommended contour level 0.18. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

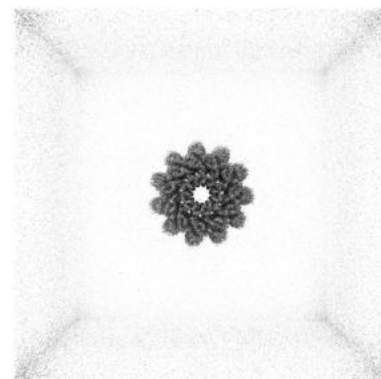
6.5.2 Raw map



X



Y



Z

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.

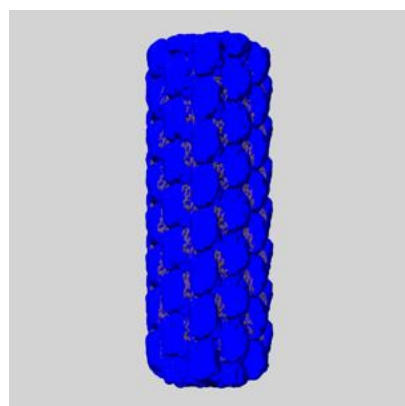
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

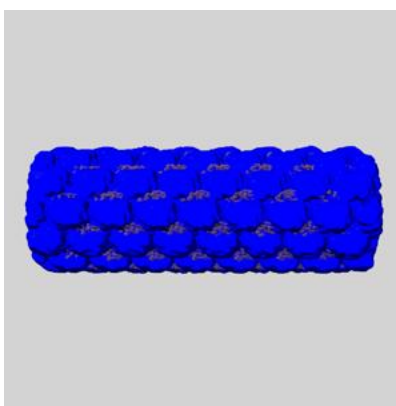
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

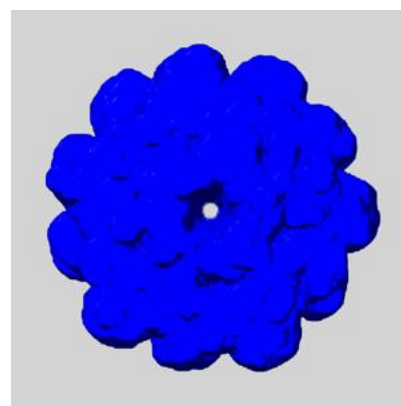
6.6.1 emd_49126_msk_1.map [i](#)



X



Y

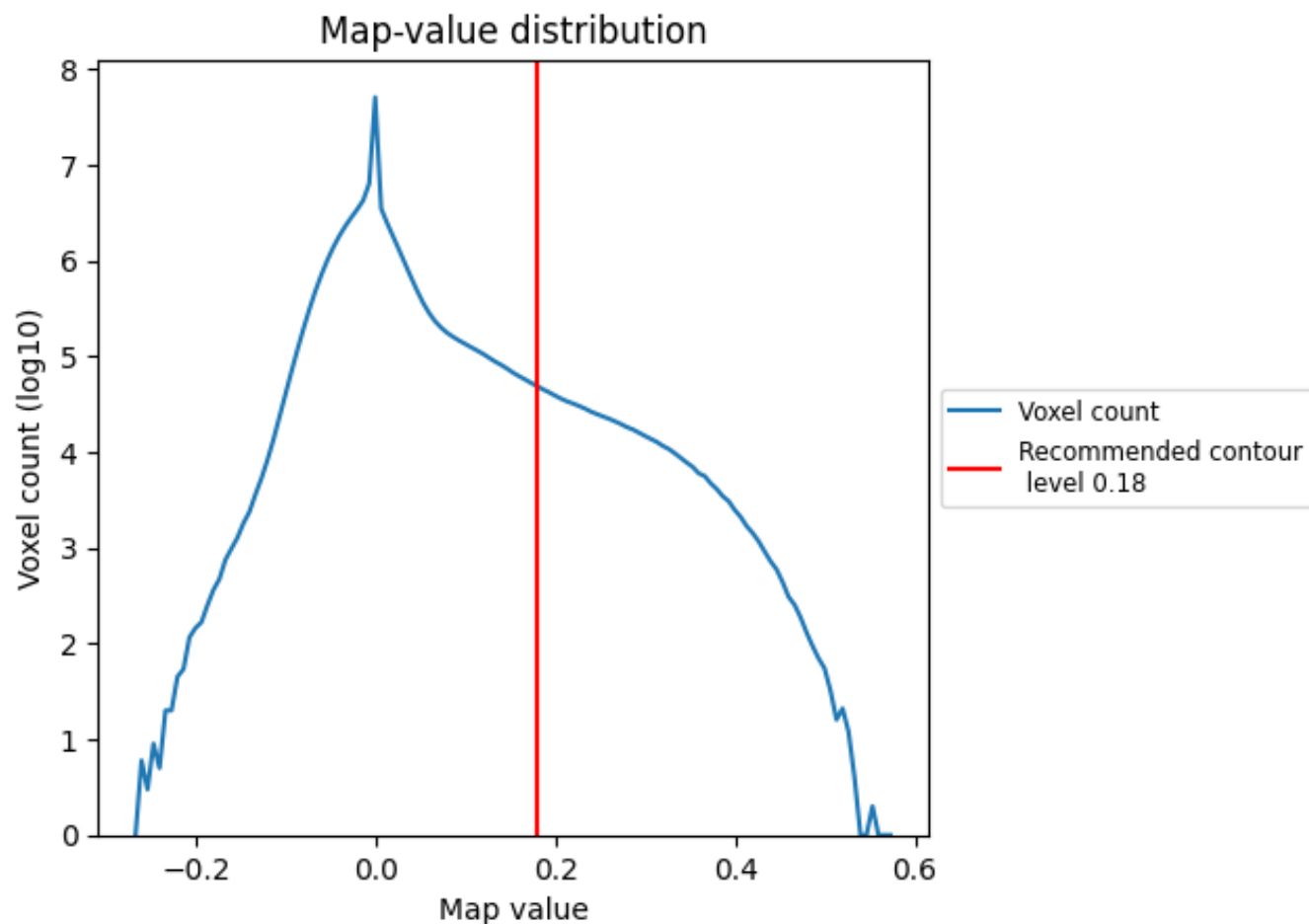


Z

7 Map analysis [i](#)

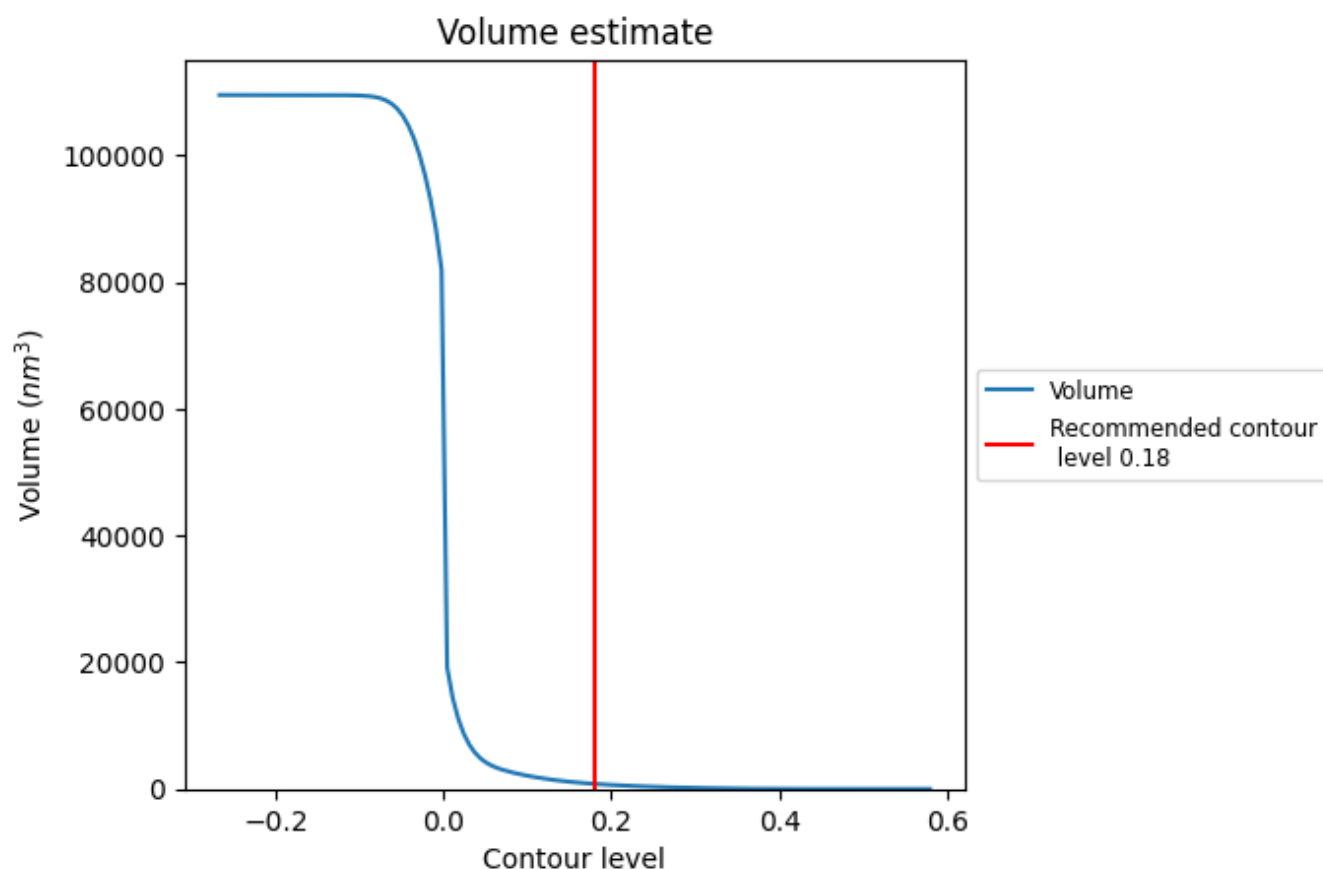
This section contains the results of statistical analysis of the map.

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.

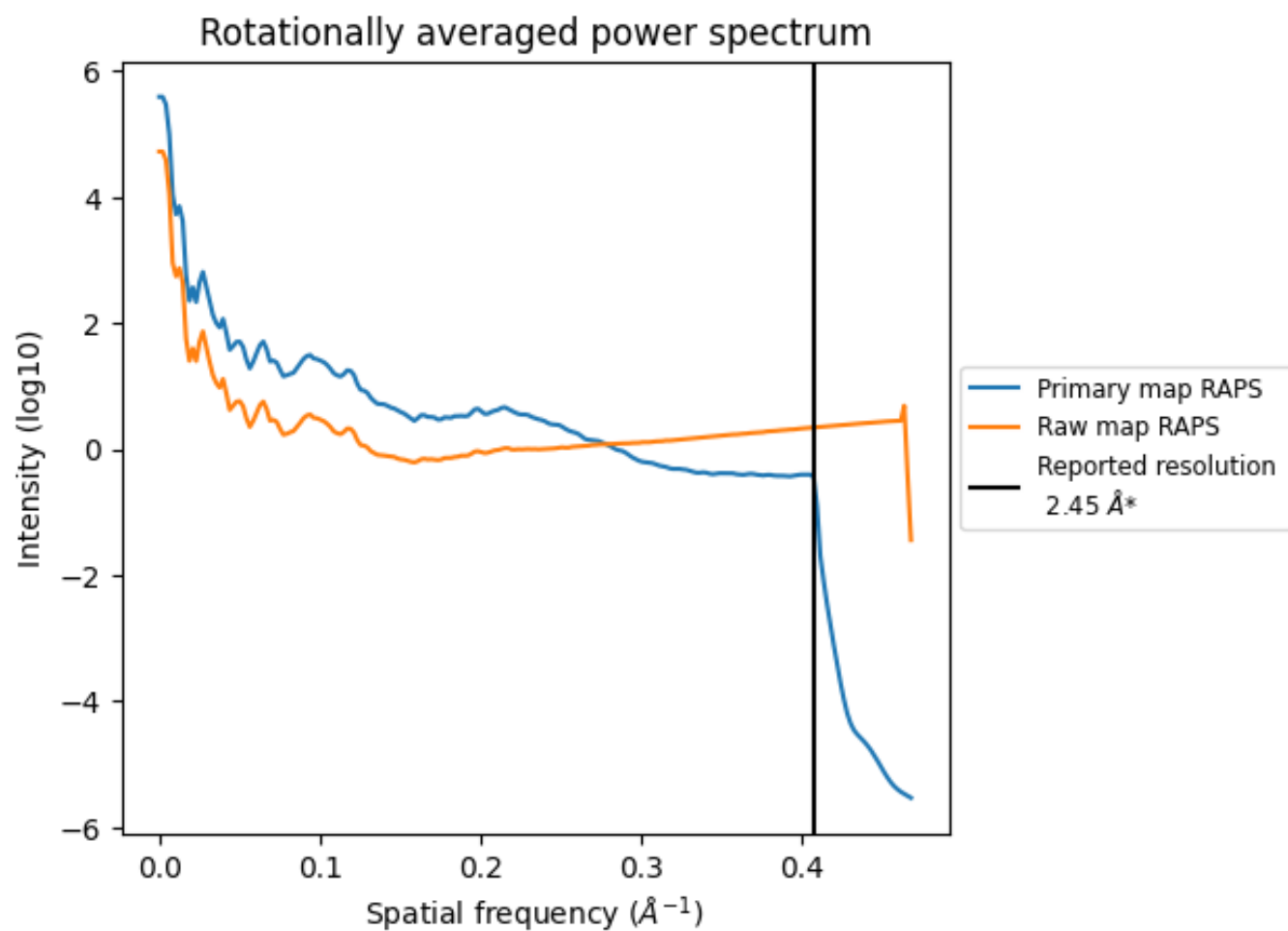
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 802 nm³; this corresponds to an approximate mass of 725 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 ⓘ

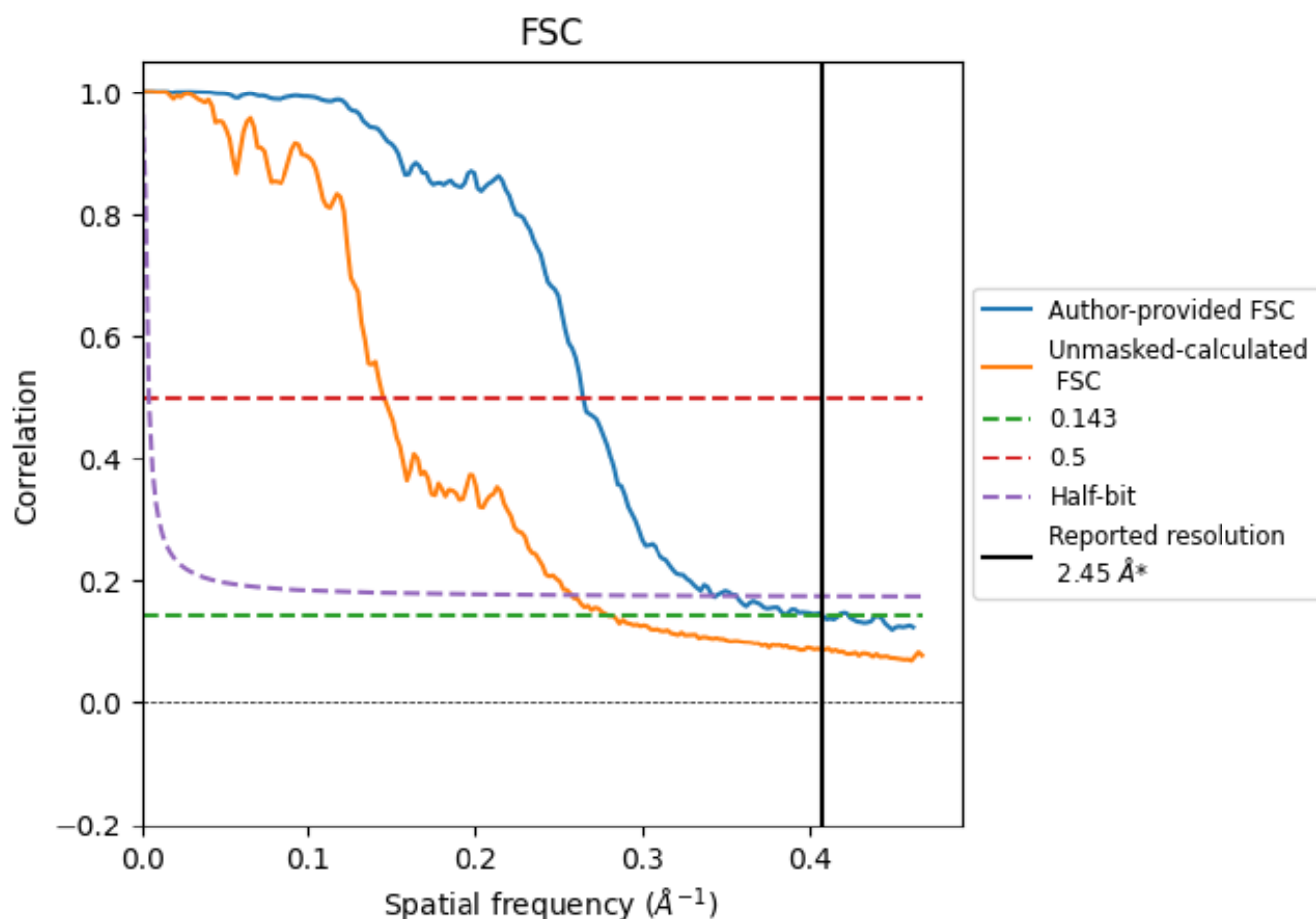


*Reported resolution corresponds to spatial frequency of 0.408 Å⁻¹

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 0.408 \AA^{-1}

8.2 Resolution estimates [i](#)

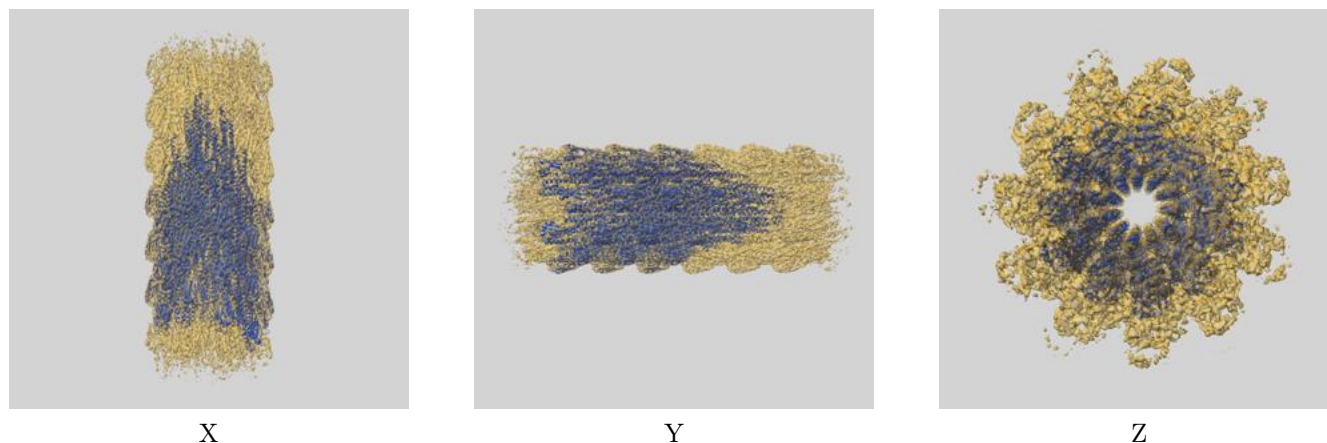
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.45	-	-
Author-provided FSC curve	2.45	3.78	2.92
Unmasked-calculated*	3.58	6.90	3.88

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.58 differs from the reported value 2.45 by more than 10 %

9 Map-model fit [i](#)

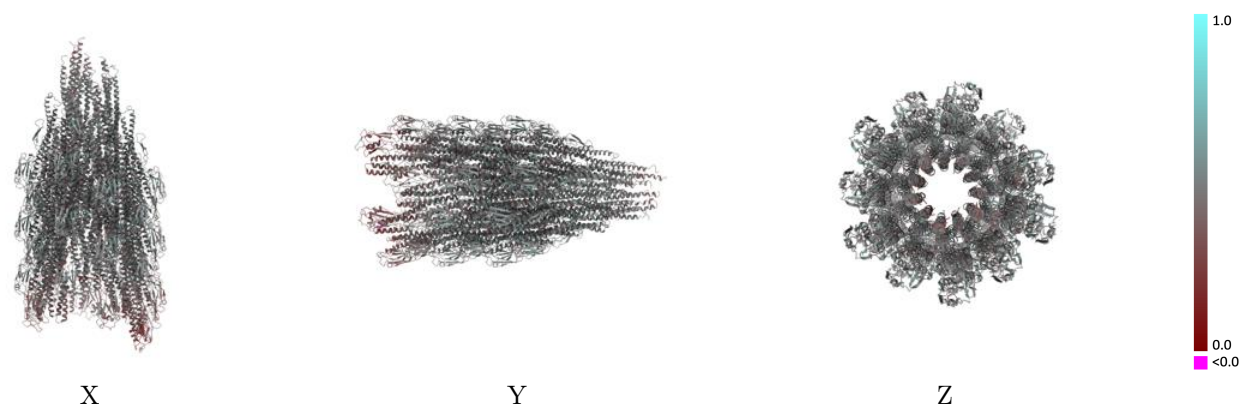
This section contains information regarding the fit between EMDB map EMD-49126 and PDB model 9N8B. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



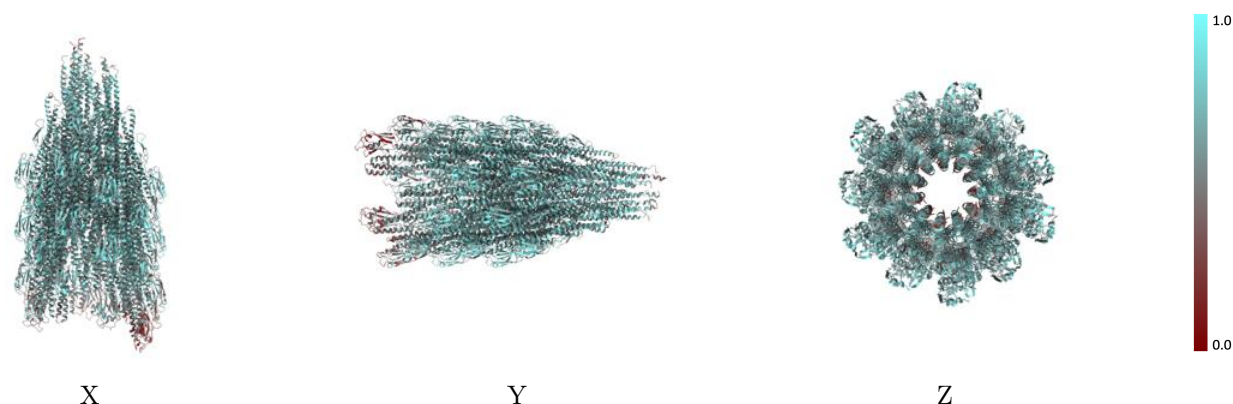
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



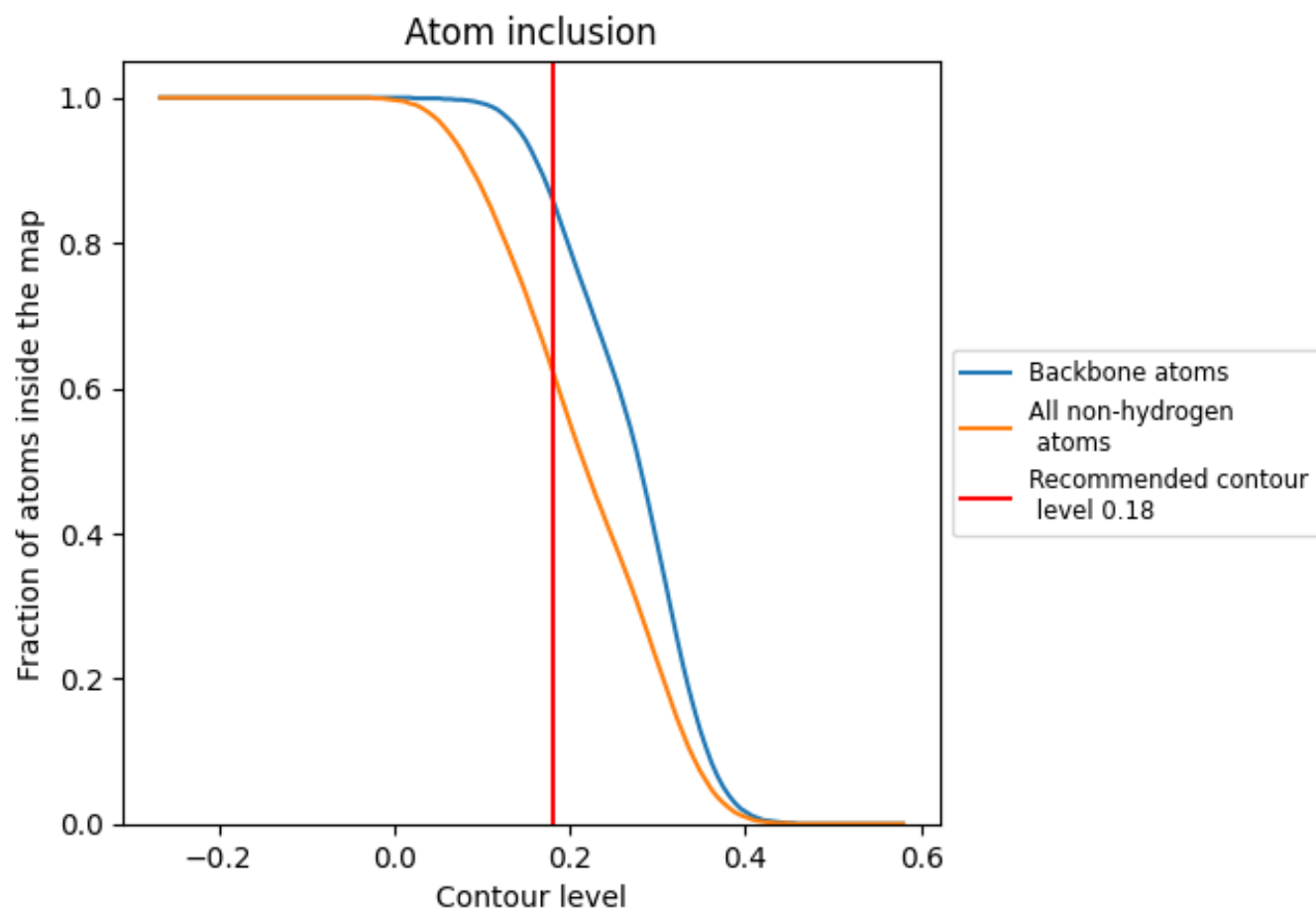
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.18).





































































9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 62% 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 (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6250	 0.4630
A	 0.6490	 0.4780
B	 0.6240	 0.4580
C	 0.6630	 0.4800
D	 0.6570	 0.4820
E	 0.5600	 0.4220
F	 0.6510	 0.4780
G	 0.6580	 0.4770
H	 0.6550	 0.4810
I	 0.6310	 0.4730
J	 0.5790	 0.4300
K	 0.6450	 0.4760
L	 0.6520	 0.4800
M	 0.4870	 0.3950
N	 0.6420	 0.4670
O	 0.6530	 0.4780
P	 0.5920	 0.4460
Q	 0.6470	 0.4820
R	 0.6480	 0.4840
S	 0.5150	 0.3970
T	 0.6460	 0.4740
U	 0.6510	 0.4830
V	 0.6180	 0.4570
W	 0.6540	 0.4870
X	 0.6530	 0.4820
Y	 0.5350	 0.4070
Z	 0.6460	 0.4730
a	 0.6590	 0.4830
b	 0.6240	 0.4640
c	 0.6430	 0.4730
d	 0.6410	 0.4710
e	 0.6560	 0.4770
f	 0.5730	 0.4240
g	 0.6190	 0.4620

