



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 04:57 PM UTC

PDB ID : 5N8N / pdb_00005n8n
EMDB ID : EMD-3600
Title : Contracted sheath of a Pseudomonas aeruginosa type six secretion system consisting of TssB1 and TssC1
Authors : Salih, O.; He, S.; Stach, L.; Macdonald, J.T.; Planamente, S.; Manoli, E.; Scheres, S.; Filloux, A.; Freemont, P.S.
Deposited on : 2017-02-23
Resolution : 3.28 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

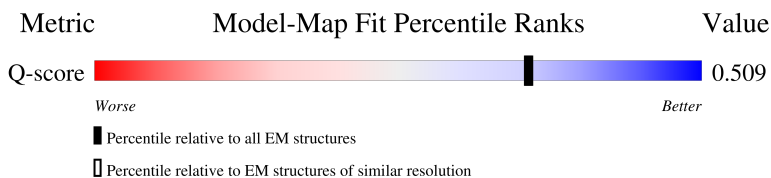
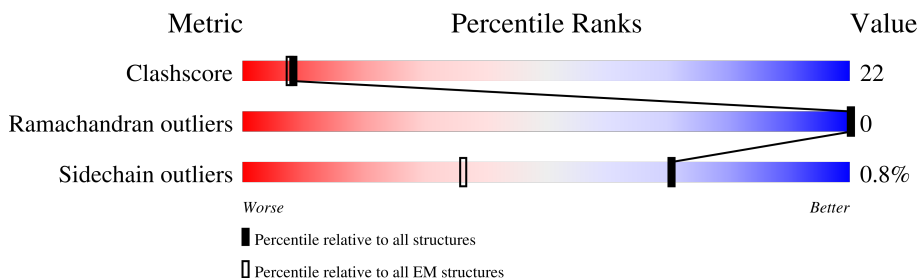
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.28 Å.

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



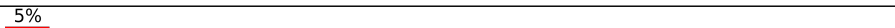
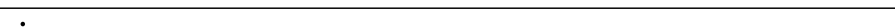
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14492 (2.78 - 3.78)

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	132	
1	C	132	
1	E	132	
1	G	132	

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Mol	Chain	Length	Quality of chain
1	I	132	 64%33%.
1	K	132	 64%33%.
1	M	132	 65%32%.
1	O	132	 64%33%.
1	Q	132	 71%27%.
1	S	132	 69%29%.
1	U	132	 68%30%.
1	W	132	 70%28%.
1	Y	132	 70%27%.
1	a	132	 65%33%.
1	c	132	 67%32%.
2	B	461	 5%65%34%.
2	D	461	 5%64%35%.
2	F	461	 5%66%33%.
2	H	461	 5%66%33%.
2	J	461	 5%66%33%.
2	L	461	 5%66%33%.
2	N	461	 5%64%34%.
2	P	461	 5%63%36%.
2	R	461	 5%63%36%.
2	T	461	 5%65%34%.
2	V	461	 5%65%34%.
2	X	461	 5%64%34%.
2	Z	461	 5%65%34%.
2	b	461	 5%64%35%.

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Mol	Chain	Length	Quality of chain
2	d	461	64% 35%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 70035 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 Type VI secretion protein, family.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	132	Total	C	N	O	S	0	0
			1027	651	177	195	4		
1	C	132	Total	C	N	O	S	0	0
			1027	651	177	195	4		
1	E	132	Total	C	N	O	S	0	0
			1027	651	177	195	4		
1	G	132	Total	C	N	O	S	0	0
			1027	651	177	195	4		
1	I	132	Total	C	N	O	S	0	0
			1027	651	177	195	4		
1	K	132	Total	C	N	O	S	0	0
			1027	651	177	195	4		
1	M	132	Total	C	N	O	S	0	0
			1027	651	177	195	4		
1	O	132	Total	C	N	O	S	0	0
			1027	651	177	195	4		
1	Q	132	Total	C	N	O	S	0	0
			1027	651	177	195	4		
1	S	132	Total	C	N	O	S	0	0
			1027	651	177	195	4		
1	U	132	Total	C	N	O	S	0	0
			1027	651	177	195	4		
1	W	132	Total	C	N	O	S	0	0
			1027	651	177	195	4		
1	Y	132	Total	C	N	O	S	0	0
			1027	651	177	195	4		
1	a	132	Total	C	N	O	S	0	0
			1027	651	177	195	4		
1	c	132	Total	C	N	O	S	0	0
			1027	651	177	195	4		

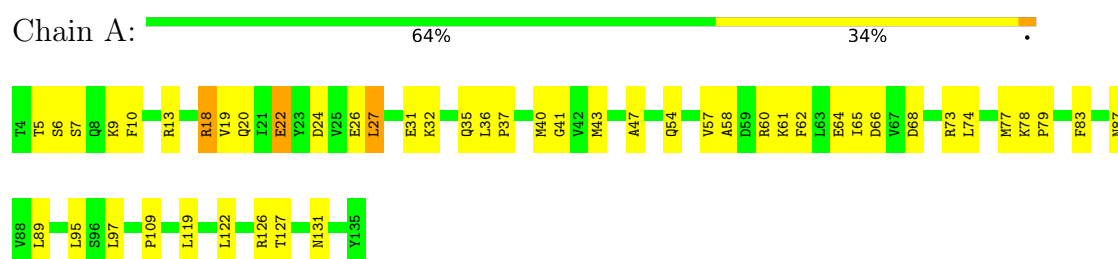
- Molecule 2 is a protein called EvpB family type VI secretion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	461	Total	C	N	O	S	0	0
			3642	2313	616	698	15		
2	D	461	Total	C	N	O	S	0	0
			3642	2313	616	698	15		
2	F	461	Total	C	N	O	S	0	0
			3642	2313	616	698	15		
2	H	461	Total	C	N	O	S	0	0
			3642	2313	616	698	15		
2	J	461	Total	C	N	O	S	0	0
			3642	2313	616	698	15		
2	L	461	Total	C	N	O	S	0	0
			3642	2313	616	698	15		
2	N	461	Total	C	N	O	S	0	0
			3642	2313	616	698	15		
2	P	461	Total	C	N	O	S	0	0
			3642	2313	616	698	15		
2	R	461	Total	C	N	O	S	0	0
			3642	2313	616	698	15		
2	T	461	Total	C	N	O	S	0	0
			3642	2313	616	698	15		
2	V	461	Total	C	N	O	S	0	0
			3642	2313	616	698	15		
2	X	461	Total	C	N	O	S	0	0
			3642	2313	616	698	15		
2	Z	461	Total	C	N	O	S	0	0
			3642	2313	616	698	15		
2	b	461	Total	C	N	O	S	0	0
			3642	2313	616	698	15		
2	d	461	Total	C	N	O	S	0	0
			3642	2313	616	698	15		

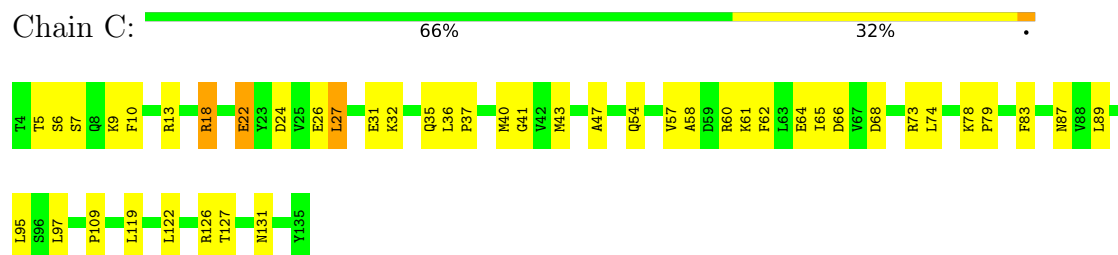
3 Residue-property plots [i](#)

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

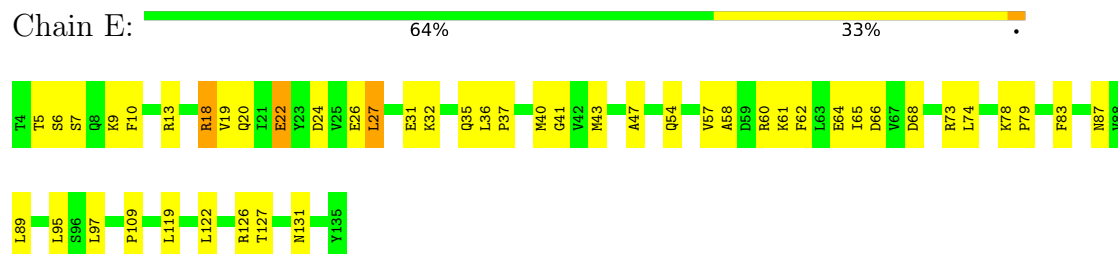
- Molecule 1: Type VI secretion protein, family



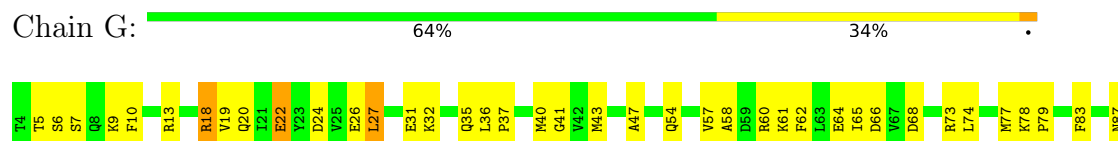
- Molecule 1: Type VI secretion protein, family



- Molecule 1: Type VI secretion protein, family



- Molecule 1: Type VI secretion protein, family





- Molecule 1: Type VI secretion protein, family

Chain I: 64% 33% .



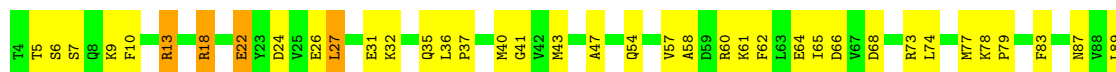
- Molecule 1: Type VI secretion protein, family

Chain K: 64% 33% .



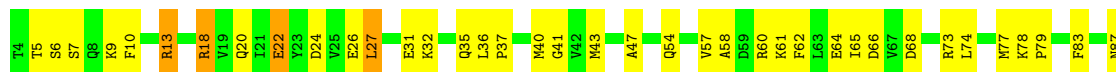
- Molecule 1: Type VI secretion protein, family

Chain M: 65% 32% .



- Molecule 1: Type VI secretion protein, family

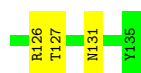
Chain O: 64% 33% .



- Molecule 1: Type VI secretion protein, family

Chain Q: 71% 27% .





- Molecule 1: Type VI secretion protein, family

Chain S: 69% 29% .



- Molecule 1: Type VI secretion protein, family

Chain U: 68% 30% .



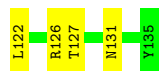
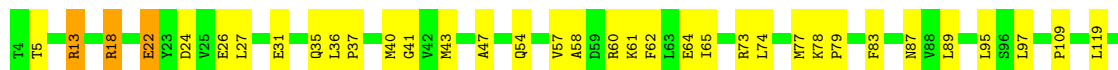
- Molecule 1: Type VI secretion protein, family

Chain W: 70% 28% .



- Molecule 1: Type VI secretion protein, family

Chain Y: 70% 27% .



- Molecule 1: Type VI secretion protein, family

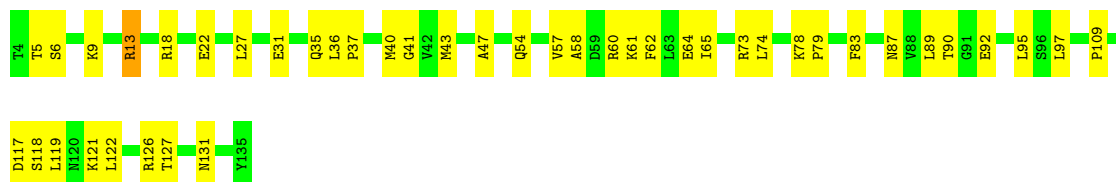
Chain a: 65% 33% .





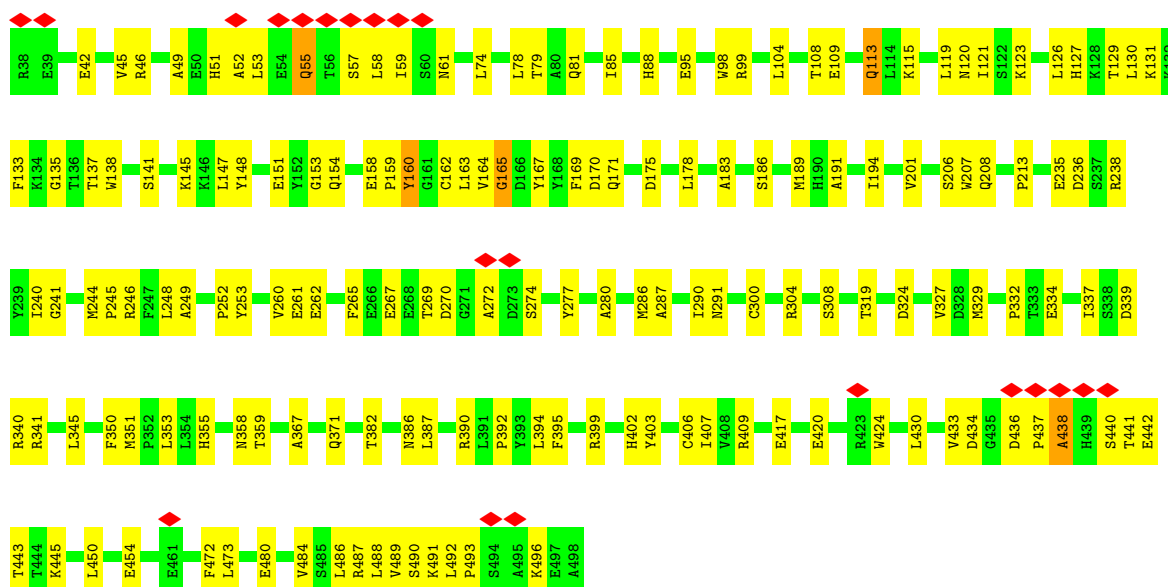
- Molecule 1: Type VI secretion protein, family

Chain c: 67% 32%



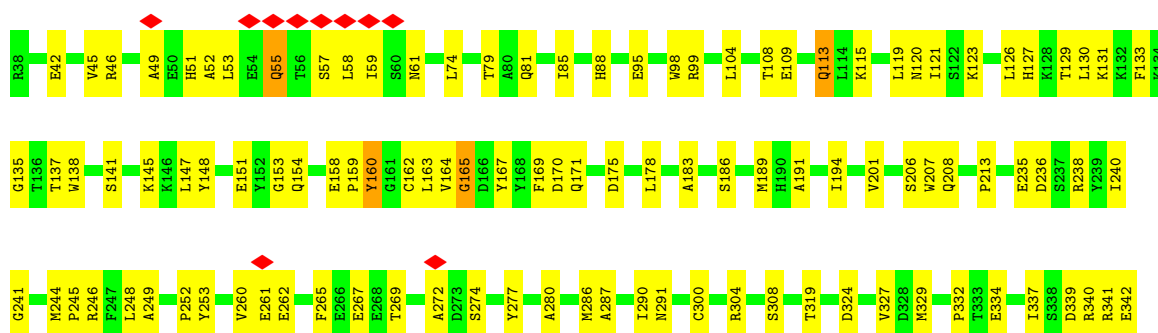
- Molecule 2: EvpB family type VI secretion protein

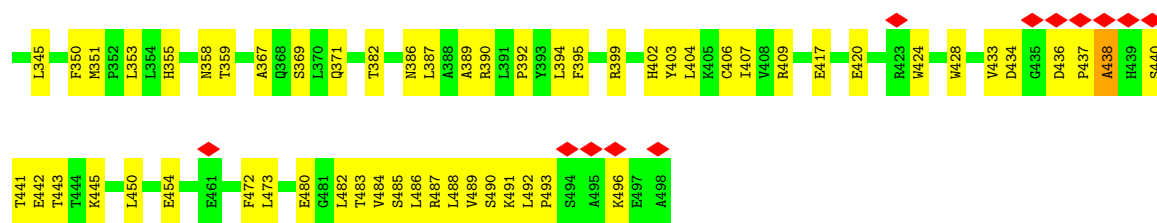
Chain B: 5% 65% 34%



- Molecule 2: EvpB family type VI secretion protein

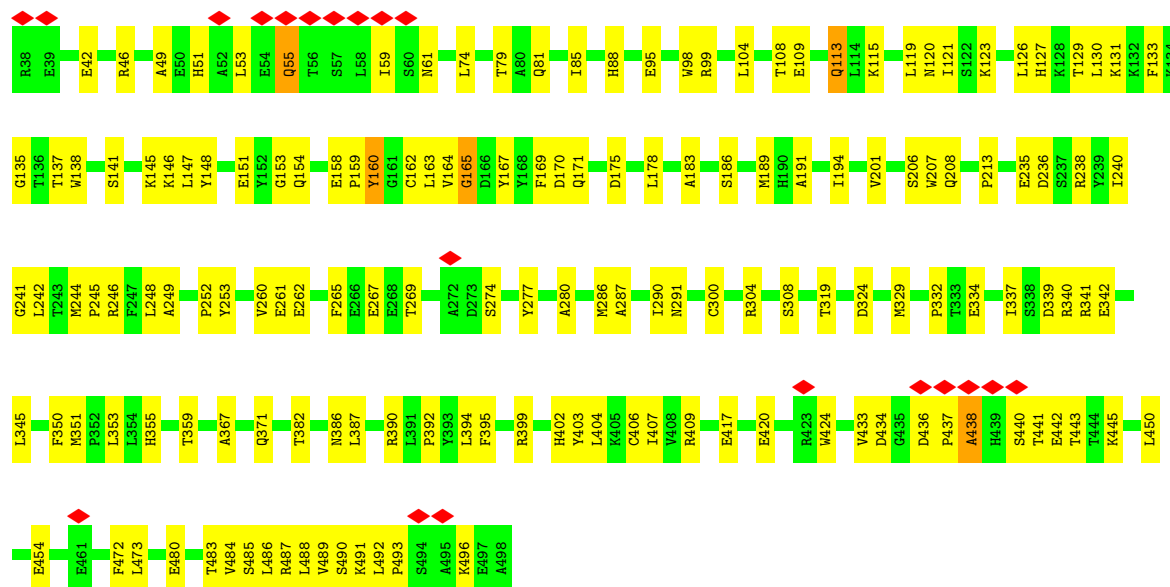
Chain D: 5% 64% 35%





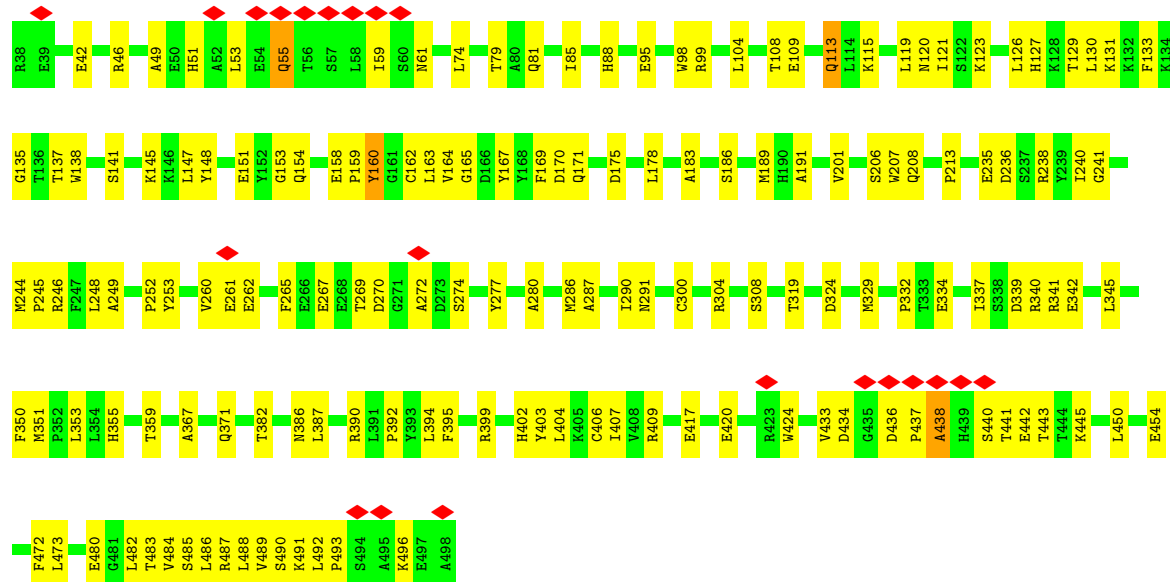
• Molecule 2: EvpB family type VI secretion protein

Chain F: 66% 33%

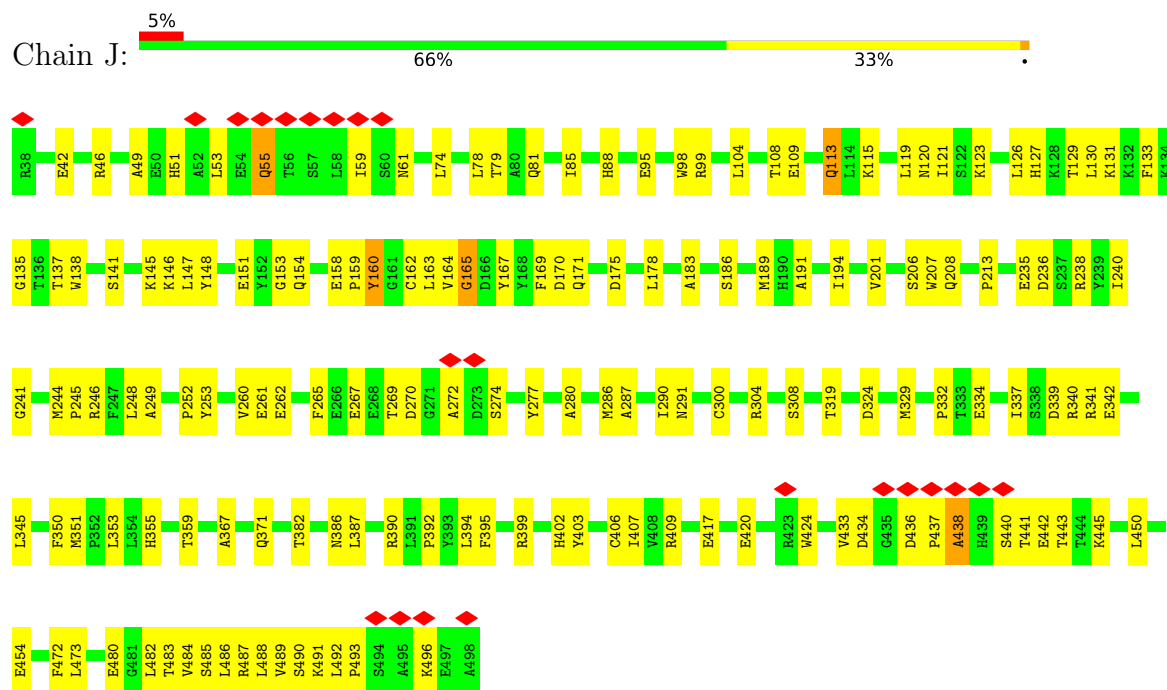


• Molecule 2: EvpB family type VI secretion protein

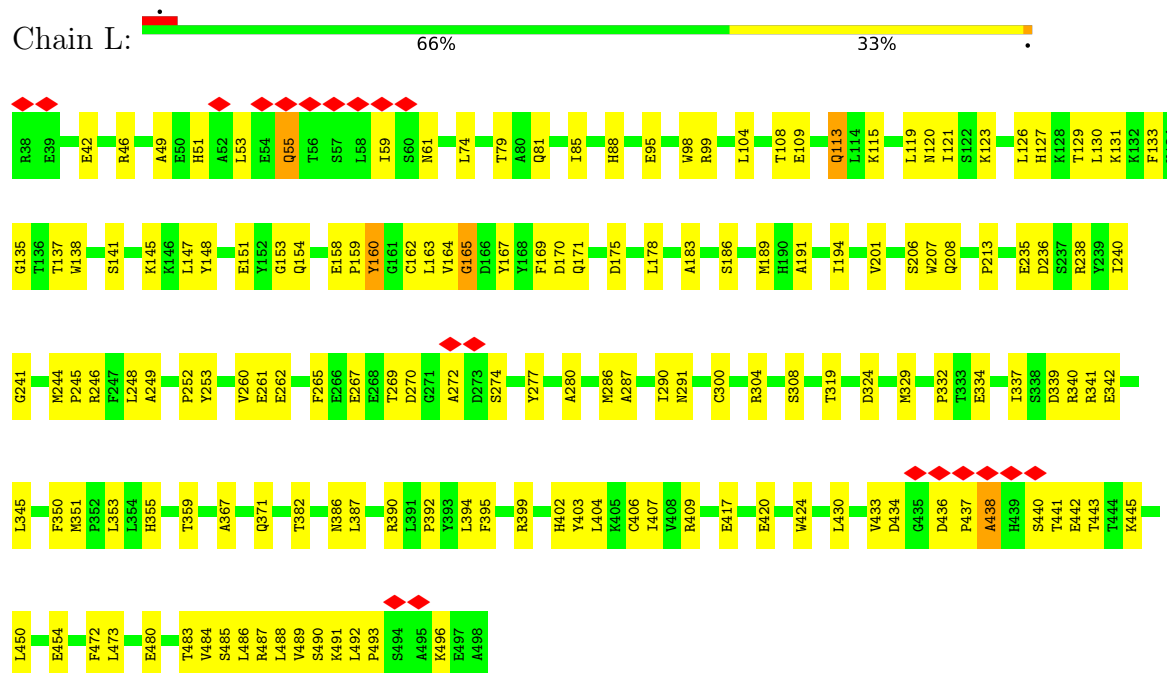
Chain H: 5% 66% 33%



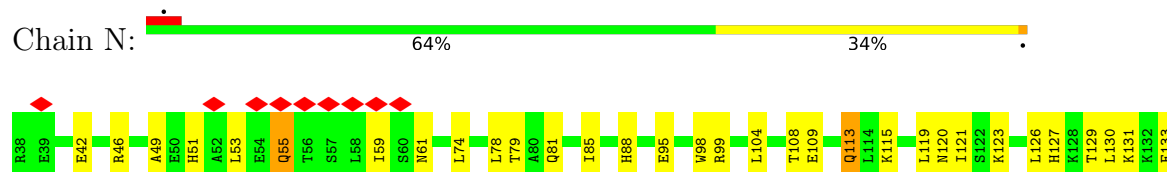
- Molecule 2: EvpB family type VI secretion protein



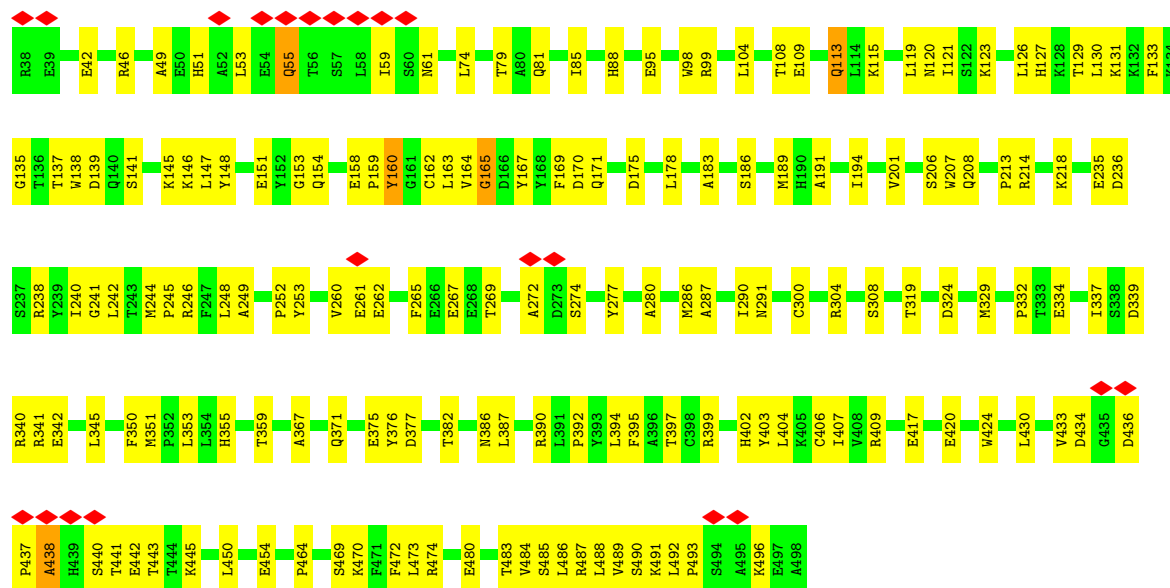
- Molecule 2: EvpB family type VI secretion protein



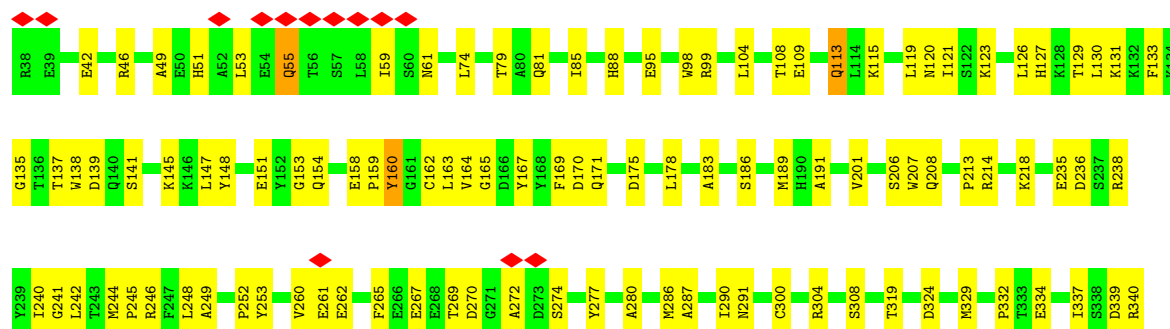
- Molecule 2: EvpB family type VI secretion protein

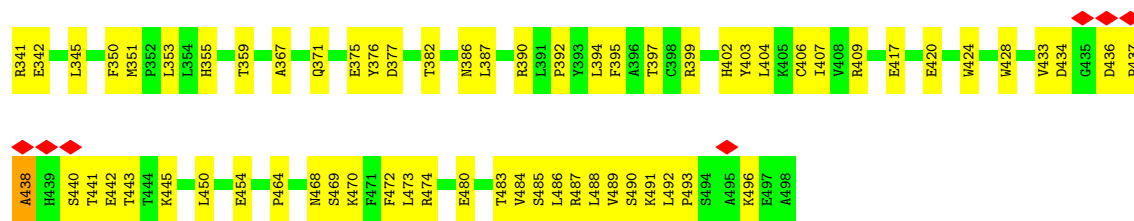


- Molecule 2: EvpB family type VI secretion protein



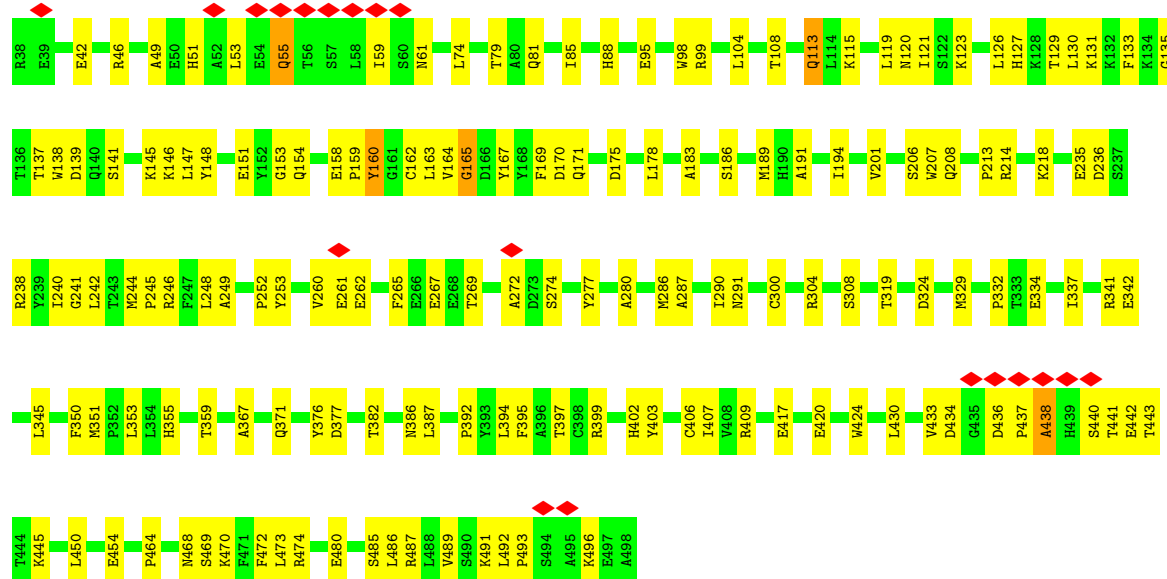
- Molecule 2: EvpB family type VI secretion protein





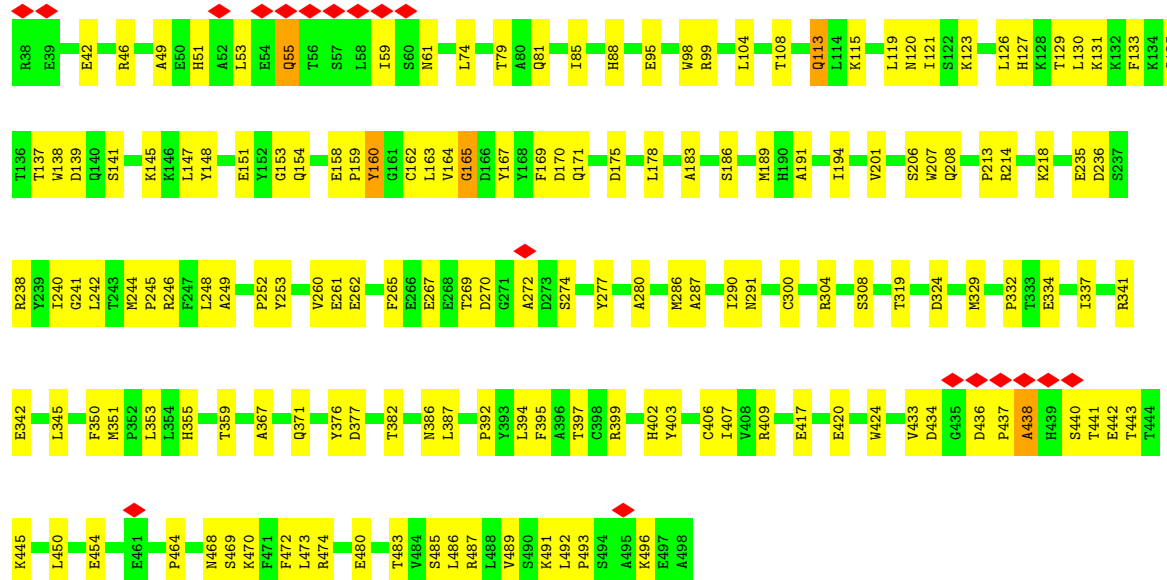
• Molecule 2: EvpB family type VI secretion protein

Chain T: 65% 34%

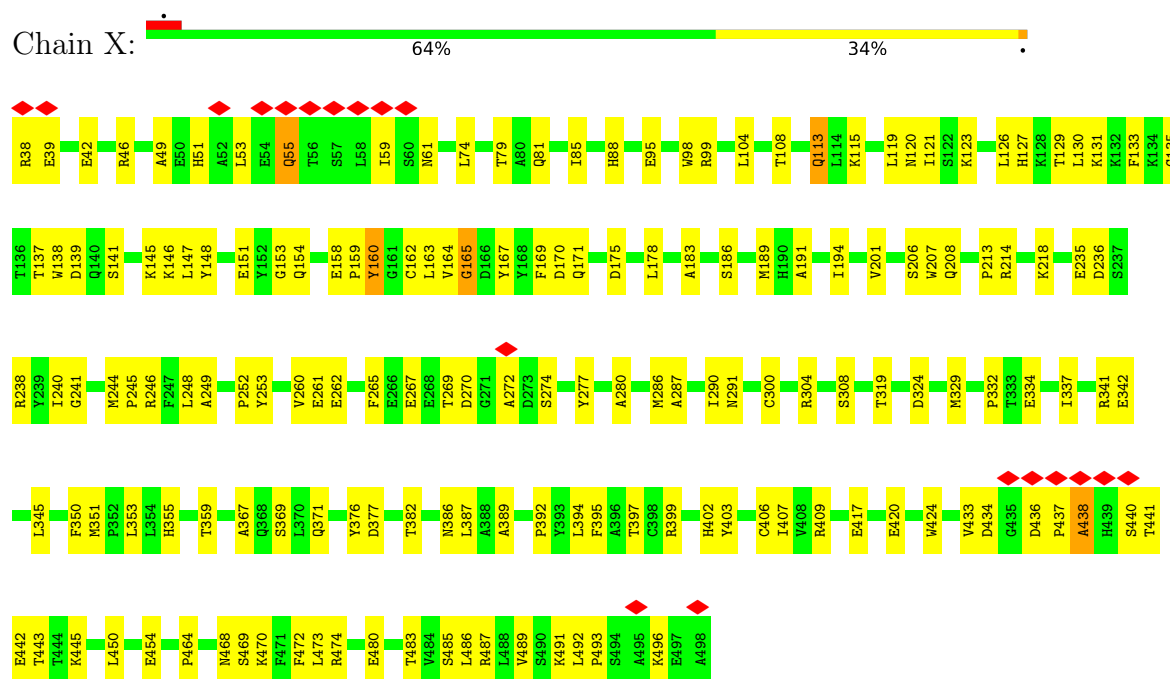


• Molecule 2: EvpB family type VI secretion protein

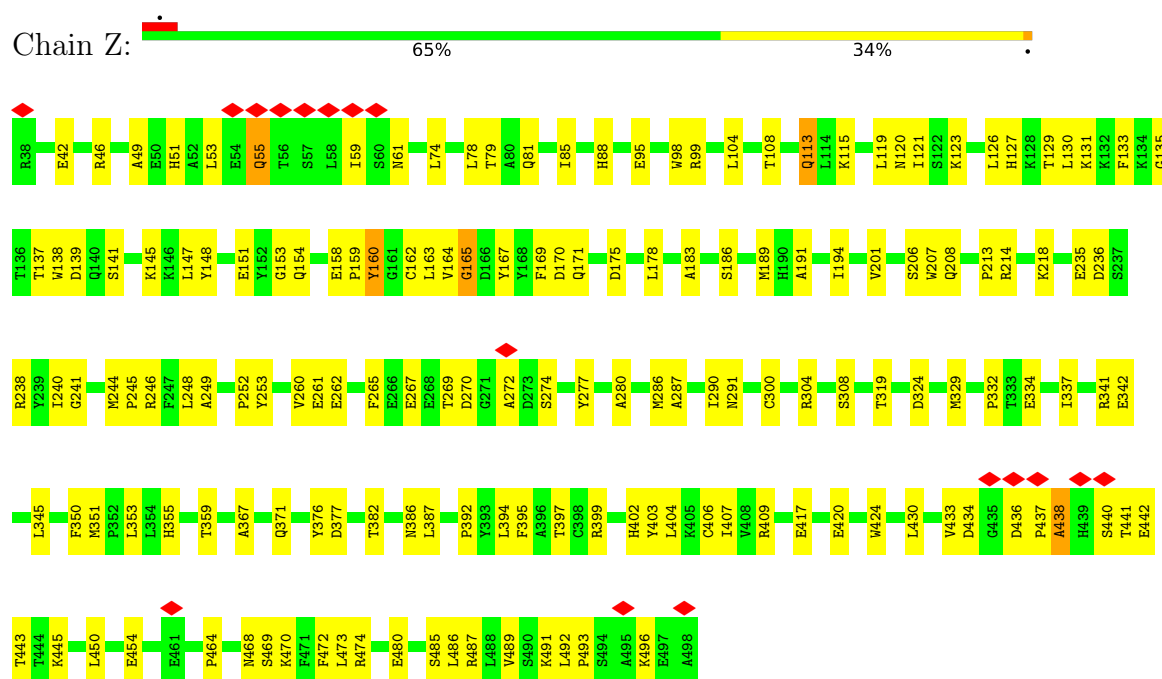
Chain V: 65% 34%



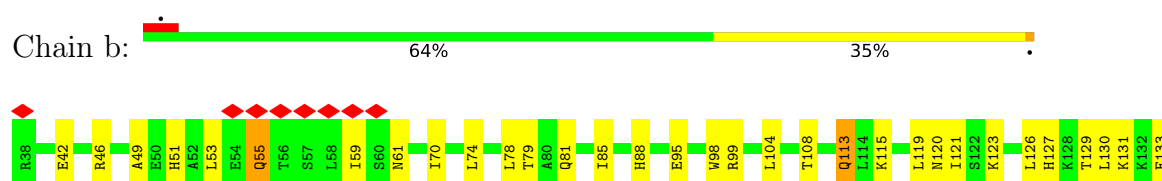
- Molecule 2: EvpB family type VI secretion protein

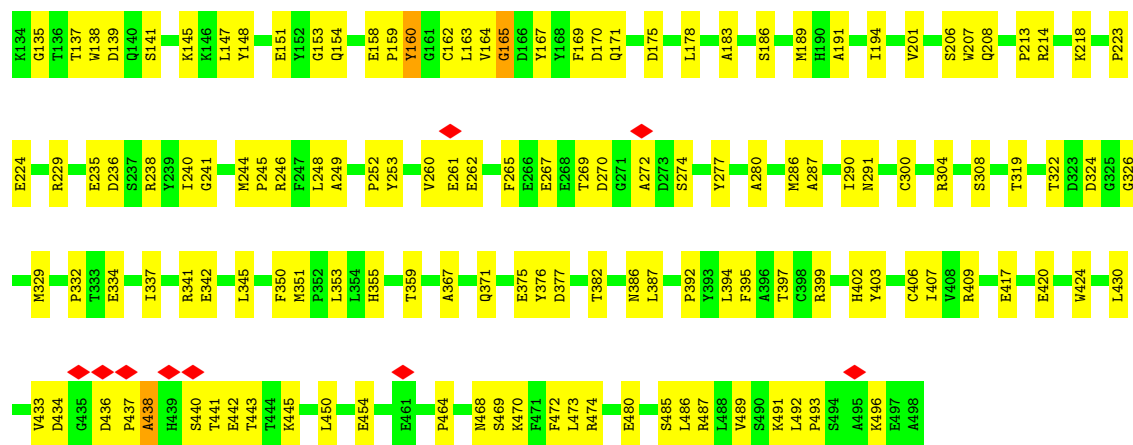


- Molecule 2: EvpB family type VI secretion protein

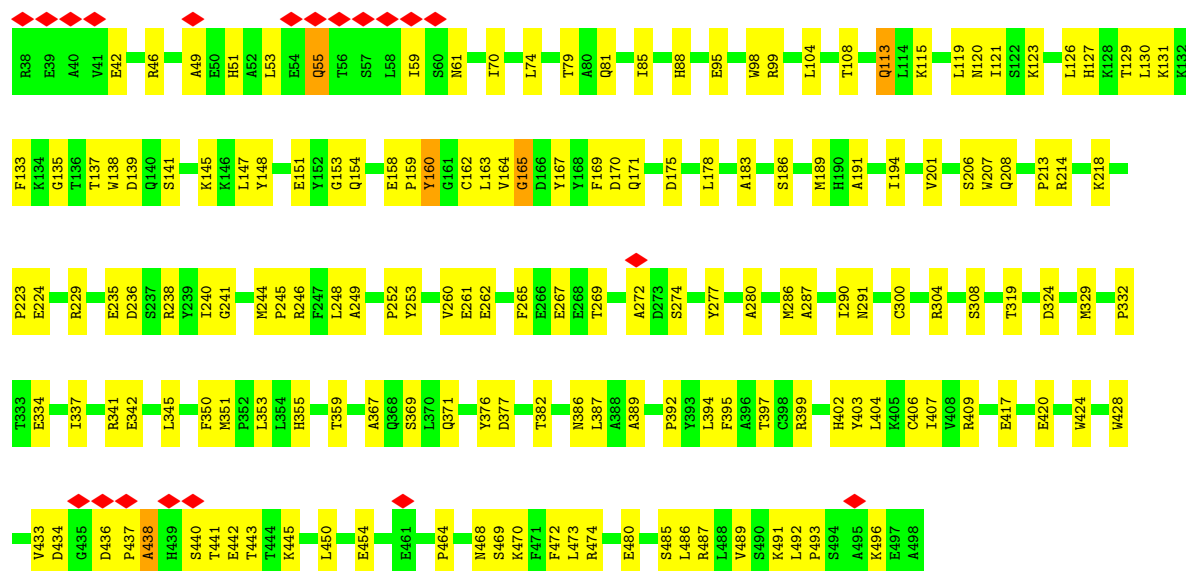


- Molecule 2: EvpB family type VI secretion protein





• Molecule 2: EvpB family type VI secretion protein



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=27.7°, rise=20.2 Å, axial sym=C1	Depositor
Number of segments used	71264	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.512	Depositor
Minimum map value	-0.286	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.0385	Depositor
Map size (Å)	335.0, 335.0, 335.0	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.12	2/1043 (0.2%)	0.91	2/1411 (0.1%)
1	C	1.12	2/1043 (0.2%)	0.91	2/1411 (0.1%)
1	E	1.12	2/1043 (0.2%)	0.91	2/1411 (0.1%)
1	G	1.12	2/1043 (0.2%)	0.91	2/1411 (0.1%)
1	I	1.12	2/1043 (0.2%)	0.91	2/1411 (0.1%)
1	K	1.13	2/1043 (0.2%)	0.91	2/1411 (0.1%)
1	M	1.12	2/1043 (0.2%)	0.91	2/1411 (0.1%)
1	O	1.12	2/1043 (0.2%)	0.91	2/1411 (0.1%)
1	Q	1.12	2/1043 (0.2%)	0.91	2/1411 (0.1%)
1	S	1.12	2/1043 (0.2%)	0.91	2/1411 (0.1%)
1	U	1.12	2/1043 (0.2%)	0.91	2/1411 (0.1%)
1	W	1.12	2/1043 (0.2%)	0.91	2/1411 (0.1%)
1	Y	1.12	2/1043 (0.2%)	0.91	2/1411 (0.1%)
1	a	1.12	2/1043 (0.2%)	0.91	2/1411 (0.1%)
1	c	1.12	2/1043 (0.2%)	0.91	2/1411 (0.1%)
2	B	1.11	2/3732 (0.1%)	0.81	5/5061 (0.1%)
2	D	1.11	2/3732 (0.1%)	0.81	5/5061 (0.1%)
2	F	1.11	2/3732 (0.1%)	0.81	5/5061 (0.1%)
2	H	1.11	2/3732 (0.1%)	0.81	5/5061 (0.1%)
2	J	1.11	2/3732 (0.1%)	0.81	5/5061 (0.1%)
2	L	1.11	2/3732 (0.1%)	0.81	5/5061 (0.1%)
2	N	1.11	2/3732 (0.1%)	0.81	5/5061 (0.1%)
2	P	1.11	2/3732 (0.1%)	0.81	5/5061 (0.1%)
2	R	1.11	2/3732 (0.1%)	0.81	5/5061 (0.1%)
2	T	1.11	2/3732 (0.1%)	0.81	5/5061 (0.1%)
2	V	1.11	2/3732 (0.1%)	0.81	5/5061 (0.1%)
2	X	1.11	2/3732 (0.1%)	0.81	5/5061 (0.1%)
2	Z	1.11	2/3732 (0.1%)	0.81	5/5061 (0.1%)
2	b	1.11	2/3732 (0.1%)	0.81	5/5061 (0.1%)
2	d	1.11	2/3732 (0.1%)	0.81	5/5061 (0.1%)
All	All	1.11	60/71625 (0.1%)	0.83	105/97080 (0.1%)

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	W	78	LYS	C-O	-7.30	1.20	1.23
1	S	78	LYS	C-O	-7.28	1.20	1.23
1	C	78	LYS	C-O	-7.25	1.20	1.23
1	U	78	LYS	C-O	-7.18	1.20	1.23
1	K	78	LYS	C-O	-7.16	1.20	1.23
1	Y	78	LYS	C-O	-7.16	1.20	1.23
1	G	78	LYS	C-O	-7.13	1.20	1.23
1	I	78	LYS	C-O	-7.13	1.20	1.23
1	A	78	LYS	C-O	-7.11	1.20	1.23
1	E	78	LYS	C-O	-7.11	1.20	1.23
1	O	78	LYS	C-O	-7.09	1.20	1.23
1	a	78	LYS	C-O	-7.09	1.20	1.23
1	c	78	LYS	C-O	-7.05	1.20	1.23
1	Q	78	LYS	C-O	-7.03	1.20	1.23
1	M	78	LYS	C-O	-6.90	1.20	1.23
2	T	337	ILE	C-O	5.37	1.30	1.24
2	N	337	ILE	C-O	5.34	1.30	1.24
2	D	337	ILE	C-O	5.33	1.30	1.24
2	F	337	ILE	C-O	5.33	1.30	1.24
2	V	337	ILE	C-O	5.33	1.30	1.24
2	d	337	ILE	C-O	5.32	1.30	1.24
2	L	337	ILE	C-O	5.32	1.30	1.24
2	X	337	ILE	C-O	5.31	1.30	1.24
2	Z	337	ILE	C-O	5.31	1.30	1.24
2	D	486	LEU	C-O	5.28	1.30	1.23
2	b	337	ILE	C-O	5.28	1.30	1.24
2	B	337	ILE	C-O	5.27	1.30	1.24
2	R	486	LEU	C-O	5.27	1.30	1.23
2	H	337	ILE	C-O	5.26	1.30	1.24
2	J	337	ILE	C-O	5.26	1.30	1.24
2	J	486	LEU	C-O	5.26	1.30	1.23
2	P	337	ILE	C-O	5.25	1.29	1.24
2	d	486	LEU	C-O	5.24	1.30	1.23
2	R	337	ILE	C-O	5.24	1.29	1.24
2	H	486	LEU	C-O	5.23	1.30	1.23
2	X	486	LEU	C-O	5.23	1.30	1.23
2	V	486	LEU	C-O	5.23	1.30	1.23
2	F	486	LEU	C-O	5.22	1.30	1.23
2	b	486	LEU	C-O	5.22	1.30	1.23
2	Z	486	LEU	C-O	5.22	1.30	1.23
2	N	486	LEU	C-O	5.22	1.30	1.23
2	L	486	LEU	C-O	5.20	1.30	1.23
1	K	13	ARG	CZ-NH1	5.20	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	486	LEU	C-O	5.20	1.30	1.23
1	W	13	ARG	CZ-NH1	5.19	1.40	1.32
1	M	13	ARG	CZ-NH1	5.18	1.40	1.32
1	Q	13	ARG	CZ-NH1	5.18	1.40	1.32
2	P	486	LEU	C-O	5.18	1.30	1.23
1	C	13	ARG	CZ-NH1	5.18	1.40	1.32
1	O	13	ARG	CZ-NH1	5.18	1.40	1.32
1	A	13	ARG	CZ-NH1	5.18	1.40	1.32
1	S	13	ARG	CZ-NH1	5.17	1.40	1.32
1	I	13	ARG	CZ-NH1	5.17	1.40	1.32
1	Y	13	ARG	CZ-NH1	5.17	1.40	1.32
1	E	13	ARG	CZ-NH1	5.16	1.40	1.32
2	B	486	LEU	C-O	5.16	1.30	1.23
1	U	13	ARG	CZ-NH1	5.15	1.40	1.32
1	c	13	ARG	CZ-NH1	5.14	1.40	1.32
1	a	13	ARG	CZ-NH1	5.13	1.40	1.32
1	G	13	ARG	CZ-NH1	5.12	1.40	1.32

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	165	GLY	N-CA-C	7.55	122.44	112.77
2	R	165	GLY	N-CA-C	7.55	122.43	112.77
2	N	165	GLY	N-CA-C	7.54	122.43	112.77
2	Z	165	GLY	N-CA-C	7.54	122.42	112.77
2	T	165	GLY	N-CA-C	7.53	122.41	112.77
2	V	165	GLY	N-CA-C	7.53	122.41	112.77
2	b	165	GLY	N-CA-C	7.53	122.41	112.77
2	X	165	GLY	N-CA-C	7.53	122.41	112.77
2	B	165	GLY	N-CA-C	7.53	122.40	112.77
2	F	165	GLY	N-CA-C	7.53	122.40	112.77
2	H	165	GLY	N-CA-C	7.53	122.40	112.77
2	d	165	GLY	N-CA-C	7.53	122.40	112.77
2	D	165	GLY	N-CA-C	7.52	122.40	112.77
2	J	165	GLY	N-CA-C	7.52	122.40	112.77
2	L	165	GLY	N-CA-C	7.51	122.38	112.77
2	N	113	GLN	N-CA-C	6.39	118.32	111.36
2	D	113	GLN	N-CA-C	6.38	118.32	111.36
2	L	113	GLN	N-CA-C	6.36	118.30	111.36
2	Z	113	GLN	N-CA-C	6.35	118.29	111.36
2	d	113	GLN	N-CA-C	6.35	118.29	111.36
2	B	113	GLN	N-CA-C	6.35	118.28	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	113	GLN	N-CA-C	6.35	118.28	111.36
2	X	113	GLN	N-CA-C	6.35	118.28	111.36
2	J	113	GLN	N-CA-C	6.35	118.28	111.36
2	R	113	GLN	N-CA-C	6.34	118.27	111.36
2	b	113	GLN	N-CA-C	6.33	118.26	111.36
2	P	113	GLN	N-CA-C	6.33	118.26	111.36
2	H	113	GLN	N-CA-C	6.33	118.25	111.36
2	T	113	GLN	N-CA-C	6.31	118.24	111.36
2	F	113	GLN	N-CA-C	6.29	118.22	111.36
2	T	55	GLN	N-CA-C	5.91	117.73	111.28
2	F	55	GLN	N-CA-C	5.91	117.72	111.28
2	H	55	GLN	N-CA-C	5.91	117.72	111.28
2	P	55	GLN	N-CA-C	5.91	117.72	111.28
2	J	55	GLN	N-CA-C	5.90	117.71	111.28
2	Z	55	GLN	N-CA-C	5.88	117.69	111.28
2	L	55	GLN	N-CA-C	5.87	117.68	111.28
2	d	55	GLN	N-CA-C	5.87	117.68	111.28
2	R	55	GLN	N-CA-C	5.87	117.68	111.28
2	N	55	GLN	N-CA-C	5.86	117.67	111.28
2	B	55	GLN	N-CA-C	5.86	117.67	111.28
2	V	55	GLN	N-CA-C	5.85	117.66	111.28
2	b	55	GLN	N-CA-C	5.85	117.66	111.28
2	D	55	GLN	N-CA-C	5.84	117.65	111.28
2	X	55	GLN	N-CA-C	5.84	117.65	111.28
1	Y	13	ARG	NE-CZ-NH2	-5.41	114.33	119.20
1	a	13	ARG	NE-CZ-NH2	-5.41	114.33	119.20
1	G	13	ARG	NE-CZ-NH2	-5.41	114.33	119.20
1	S	13	ARG	NE-CZ-NH2	-5.40	114.34	119.20
1	O	13	ARG	NE-CZ-NH2	-5.39	114.35	119.20
1	A	13	ARG	NE-CZ-NH2	-5.38	114.35	119.20
1	U	13	ARG	NE-CZ-NH2	-5.38	114.35	119.20
1	W	13	ARG	NE-CZ-NH2	-5.38	114.36	119.20
1	c	13	ARG	NE-CZ-NH2	-5.38	114.36	119.20
1	I	13	ARG	NE-CZ-NH2	-5.34	114.39	119.20
1	C	13	ARG	NE-CZ-NH2	-5.34	114.39	119.20
1	E	13	ARG	NE-CZ-NH2	-5.34	114.40	119.20
1	K	13	ARG	NE-CZ-NH2	-5.33	114.40	119.20
1	Q	13	ARG	NE-CZ-NH2	-5.32	114.41	119.20
1	M	13	ARG	NE-CZ-NH2	-5.32	114.42	119.20
1	A	18	ARG	NH1-CZ-NH2	5.12	125.96	119.30
1	a	18	ARG	NH1-CZ-NH2	5.12	125.95	119.30
1	C	18	ARG	NH1-CZ-NH2	5.11	125.94	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	18	ARG	NH1-CZ-NH2	5.11	125.94	119.30
1	K	18	ARG	NH1-CZ-NH2	5.11	125.94	119.30
1	S	18	ARG	NH1-CZ-NH2	5.10	125.93	119.30
1	Y	18	ARG	NH1-CZ-NH2	5.10	125.93	119.30
1	W	18	ARG	NH1-CZ-NH2	5.09	125.92	119.30
2	V	438	ALA	N-CA-C	5.09	117.49	111.33
1	G	18	ARG	NH1-CZ-NH2	5.09	125.91	119.30
2	B	438	ALA	N-CA-C	5.08	117.48	111.33
1	Q	18	ARG	NH1-CZ-NH2	5.08	125.90	119.30
1	c	18	ARG	NH1-CZ-NH2	5.08	125.90	119.30
1	O	18	ARG	NH1-CZ-NH2	5.07	125.89	119.30
1	U	18	ARG	NH1-CZ-NH2	5.07	125.89	119.30
1	E	18	ARG	NH1-CZ-NH2	5.06	125.88	119.30
2	P	324	ASP	CB-CA-C	-5.06	110.35	117.23
2	L	324	ASP	CB-CA-C	-5.06	110.35	117.23
2	b	438	ALA	N-CA-C	5.06	117.45	111.33
2	F	438	ALA	N-CA-C	5.06	117.45	111.33
1	I	18	ARG	NH1-CZ-NH2	5.06	125.88	119.30
2	J	438	ALA	N-CA-C	5.06	117.45	111.33
2	R	324	ASP	CB-CA-C	-5.06	110.35	117.23
2	R	438	ALA	N-CA-C	5.05	117.45	111.33
2	X	324	ASP	CB-CA-C	-5.05	110.36	117.23
2	d	438	ALA	N-CA-C	5.05	117.44	111.33
2	D	438	ALA	N-CA-C	5.05	117.44	111.33
2	F	324	ASP	CB-CA-C	-5.05	110.36	117.23
2	L	438	ALA	N-CA-C	5.05	117.44	111.33
2	P	438	ALA	N-CA-C	5.05	117.44	111.33
2	V	324	ASP	CB-CA-C	-5.05	110.36	117.23
2	H	438	ALA	N-CA-C	5.04	117.43	111.33
2	T	438	ALA	N-CA-C	5.04	117.43	111.33
2	d	324	ASP	CB-CA-C	-5.04	110.38	117.23
2	T	324	ASP	CB-CA-C	-5.04	110.38	117.23
2	Z	324	ASP	CB-CA-C	-5.04	110.38	117.23
2	X	438	ALA	N-CA-C	5.04	117.42	111.33
2	D	324	ASP	CB-CA-C	-5.03	110.39	117.23
2	H	324	ASP	CB-CA-C	-5.03	110.39	117.23
2	N	324	ASP	CB-CA-C	-5.03	110.39	117.23
2	b	324	ASP	CB-CA-C	-5.03	110.40	117.23
2	Z	438	ALA	N-CA-C	5.02	117.40	111.33
2	B	324	ASP	CB-CA-C	-5.01	110.41	117.23
2	J	324	ASP	CB-CA-C	-5.01	110.42	117.23
2	N	438	ALA	N-CA-C	5.00	117.38	111.33

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1027	0	1043	72	0
1	C	1027	0	1043	69	0
1	E	1027	0	1043	74	0
1	G	1027	0	1043	72	0
1	I	1027	0	1043	72	0
1	K	1027	0	1043	72	0
1	M	1027	0	1043	73	0
1	O	1027	0	1043	74	0
1	Q	1027	0	1043	59	0
1	S	1027	0	1043	63	0
1	U	1027	0	1043	61	0
1	W	1027	0	1043	60	0
1	Y	1027	0	1043	60	0
1	a	1027	0	1043	72	0
1	c	1027	0	1043	65	0
2	B	3642	0	3539	191	0
2	D	3642	0	3539	201	0
2	F	3642	0	3539	177	0
2	H	3642	0	3539	181	0
2	J	3642	0	3539	182	0
2	L	3642	0	3539	178	0
2	N	3642	0	3539	196	0
2	P	3642	0	3539	205	0
2	R	3642	0	3539	206	0
2	T	3642	0	3539	189	0
2	V	3642	0	3539	189	0
2	X	3642	0	3539	191	0
2	Z	3642	0	3539	190	0
2	b	3642	0	3539	196	0
2	d	3642	0	3539	198	0
All	All	70035	0	68730	2999	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 22.

All (2999) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:244:MET:CG	2:V:245:PRO:HD3	1.72	1.20
2:B:244:MET:CG	2:B:245:PRO:HD3	1.72	1.19
2:X:244:MET:CG	2:X:245:PRO:HD3	1.72	1.19
2:b:244:MET:CG	2:b:245:PRO:HD3	1.72	1.19
2:d:244:MET:CG	2:d:245:PRO:HD3	1.72	1.19
2:D:244:MET:CG	2:D:245:PRO:HD3	1.72	1.19
2:N:441:THR:OG1	2:N:445:LYS:NZ	1.76	1.19
2:Z:244:MET:CG	2:Z:245:PRO:HD3	1.72	1.19
2:Z:441:THR:OG1	2:Z:445:LYS:NZ	1.76	1.19
2:T:244:MET:CG	2:T:245:PRO:HD3	1.72	1.19
2:F:244:MET:CG	2:F:245:PRO:HD3	1.72	1.19
2:L:441:THR:OG1	2:L:445:LYS:NZ	1.76	1.19
2:N:244:MET:CG	2:N:245:PRO:HD3	1.72	1.19
2:R:441:THR:OG1	2:R:445:LYS:NZ	1.76	1.19
2:V:441:THR:OG1	2:V:445:LYS:NZ	1.75	1.19
2:B:441:THR:OG1	2:B:445:LYS:NZ	1.76	1.19
2:b:441:THR:OG1	2:b:445:LYS:NZ	1.76	1.19
2:H:441:THR:OG1	2:H:445:LYS:NZ	1.76	1.18
2:D:441:THR:OG1	2:D:445:LYS:NZ	1.76	1.18
2:L:244:MET:CG	2:L:245:PRO:HD3	1.72	1.18
2:d:441:THR:OG1	2:d:445:LYS:NZ	1.76	1.18
2:H:244:MET:CG	2:H:245:PRO:HD3	1.72	1.18
2:P:244:MET:CG	2:P:245:PRO:HD3	1.72	1.18
2:X:441:THR:OG1	2:X:445:LYS:NZ	1.76	1.18
2:J:244:MET:CG	2:J:245:PRO:HD3	1.72	1.18
2:D:45:VAL:HG13	2:d:70:ILE:HD11	1.20	1.17
2:F:441:THR:OG1	2:F:445:LYS:NZ	1.76	1.17
2:J:441:THR:OG1	2:J:445:LYS:NZ	1.76	1.17
2:R:244:MET:CG	2:R:245:PRO:HD3	1.72	1.17
2:P:441:THR:OG1	2:P:445:LYS:NZ	1.76	1.17
2:T:441:THR:OG1	2:T:445:LYS:NZ	1.76	1.16
2:B:45:VAL:HG13	2:b:70:ILE:HD11	1.19	1.16
2:D:58:LEU:HD22	1:c:95:LEU:HD11	1.29	1.10
2:B:58:LEU:HD22	1:a:95:LEU:HD11	1.30	1.07
2:d:244:MET:HG3	2:d:245:PRO:HD3	1.38	1.06
2:D:244:MET:HG3	2:D:245:PRO:HD3	1.38	1.06
2:B:244:MET:HG3	2:B:245:PRO:HD3	1.38	1.05
2:T:244:MET:HG3	2:T:245:PRO:HD3	1.38	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:244:MET:HG3	2:b:245:PRO:HD3	1.38	1.05
2:R:244:MET:HG3	2:R:245:PRO:HD3	1.38	1.04
2:N:244:MET:HG3	2:N:245:PRO:HD3	1.38	1.04
1:O:43:MET:CE	2:P:163:LEU:HD21	1.88	1.04
1:C:43:MET:CE	2:D:163:LEU:HD21	1.88	1.04
1:A:43:MET:CE	2:B:163:LEU:HD21	1.88	1.03
1:I:43:MET:CE	2:J:163:LEU:HD21	1.88	1.03
1:U:43:MET:CE	2:V:163:LEU:HD21	1.88	1.03
1:a:43:MET:CE	2:b:163:LEU:HD21	1.88	1.03
1:c:43:MET:CE	2:d:163:LEU:HD21	1.88	1.03
2:F:244:MET:HG3	2:F:245:PRO:HD3	1.38	1.03
1:W:43:MET:CE	2:X:163:LEU:HD21	1.88	1.03
1:G:43:MET:CE	2:H:163:LEU:HD21	1.88	1.03
1:Q:43:MET:CE	2:R:163:LEU:HD21	1.88	1.03
1:M:43:MET:CE	2:N:163:LEU:HD21	1.88	1.03
2:Z:244:MET:HG2	2:Z:245:PRO:HD3	1.40	1.03
2:L:244:MET:HG2	2:L:245:PRO:HD3	1.40	1.02
1:S:43:MET:CE	2:T:163:LEU:HD21	1.88	1.02
1:K:43:MET:CE	2:L:163:LEU:HD21	1.88	1.02
2:X:244:MET:HG2	2:X:245:PRO:HD3	1.40	1.02
2:d:244:MET:HG2	2:d:245:PRO:HD3	1.40	1.02
2:D:244:MET:HG2	2:D:245:PRO:HD3	1.40	1.02
2:N:244:MET:HG2	2:N:245:PRO:HD3	1.40	1.02
2:P:244:MET:HG2	2:P:245:PRO:HD3	1.40	1.02
2:R:244:MET:HG2	2:R:245:PRO:HD3	1.40	1.02
2:B:244:MET:HG2	2:B:245:PRO:HD3	1.40	1.02
1:E:43:MET:CE	2:F:163:LEU:HD21	1.88	1.02
2:H:244:MET:HG3	2:H:245:PRO:HD3	1.38	1.02
2:b:244:MET:HG2	2:b:245:PRO:HD3	1.40	1.02
2:P:244:MET:HG3	2:P:245:PRO:HD3	1.38	1.02
1:Y:43:MET:CE	2:Z:163:LEU:HD21	1.88	1.02
2:J:244:MET:HG2	2:J:245:PRO:HD3	1.40	1.01
2:F:244:MET:HG2	2:F:245:PRO:HD3	1.40	1.01
2:J:244:MET:HG3	2:J:245:PRO:HD3	1.38	1.01
2:X:244:MET:HG3	2:X:245:PRO:HD3	1.38	1.01
1:Y:18:ARG:NH1	2:b:342:GLU:OE2	1.94	1.01
2:L:244:MET:HG3	2:L:245:PRO:HD3	1.38	1.00
1:W:18:ARG:NH1	2:Z:342:GLU:OE2	1.95	1.00
2:V:244:MET:HG2	2:V:245:PRO:HD3	1.40	1.00
2:Z:244:MET:HG3	2:Z:245:PRO:HD3	1.38	1.00
2:V:244:MET:HG3	2:V:245:PRO:HD3	1.38	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:18:ARG:NH1	2:V:342:GLU:OE2	1.95	0.99
2:T:244:MET:HG2	2:T:245:PRO:HD3	1.40	0.99
2:H:244:MET:HG2	2:H:245:PRO:HD3	1.40	0.99
1:a:18:ARG:NH1	2:d:342:GLU:OE2	1.94	0.99
1:C:18:ARG:NH1	2:F:342:GLU:OE2	1.95	0.98
1:Q:18:ARG:NH1	2:T:342:GLU:OE2	1.96	0.98
1:U:18:ARG:NH1	2:X:342:GLU:OE2	1.96	0.98
2:H:340:ARG:NH2	2:T:139:ASP:OD2	1.97	0.98
1:K:18:ARG:NH1	2:N:342:GLU:OE2	1.97	0.98
2:L:244:MET:HE1	2:L:345:LEU:HD22	1.46	0.98
1:I:18:ARG:NH1	2:L:342:GLU:OE2	1.97	0.97
2:J:340:ARG:NH2	2:V:139:ASP:OD2	1.97	0.97
1:M:18:ARG:NH1	2:P:342:GLU:OE2	1.97	0.97
2:Z:244:MET:HE1	2:Z:345:LEU:HD22	1.46	0.97
2:B:340:ARG:NH2	2:N:139:ASP:OD2	1.97	0.97
2:D:340:ARG:NH2	2:P:139:ASP:OD2	1.97	0.97
2:X:244:MET:HE1	2:X:345:LEU:HD22	1.46	0.96
1:O:18:ARG:NH1	2:R:342:GLU:OE2	1.96	0.96
1:G:18:ARG:NH1	2:J:342:GLU:OE2	1.98	0.96
1:E:18:ARG:NH1	2:H:342:GLU:OE2	1.98	0.96
2:N:244:MET:HE1	2:N:345:LEU:HD22	1.46	0.96
2:N:340:ARG:NH2	2:Z:139:ASP:OD2	1.97	0.96
2:L:340:ARG:NH2	2:X:139:ASP:OD2	1.98	0.96
2:F:340:ARG:NH2	2:R:139:ASP:OD2	1.99	0.95
1:A:18:ARG:NH1	2:D:342:GLU:OE2	1.98	0.95
2:H:244:MET:HE1	2:H:345:LEU:HD22	1.46	0.95
2:Z:244:MET:CG	2:Z:245:PRO:CD	2.45	0.95
2:T:244:MET:HE1	2:T:345:LEU:HD22	1.46	0.95
2:X:244:MET:CG	2:X:245:PRO:CD	2.45	0.95
2:V:244:MET:HE1	2:V:345:LEU:HD22	1.46	0.95
2:B:244:MET:CG	2:B:245:PRO:CD	2.45	0.95
2:J:244:MET:HE1	2:J:345:LEU:HD22	1.46	0.95
2:b:244:MET:CG	2:b:245:PRO:CD	2.45	0.95
2:R:244:MET:HE1	2:R:345:LEU:HD22	1.46	0.94
2:R:340:ARG:NH2	2:d:139:ASP:OD2	1.98	0.94
2:B:244:MET:HE1	2:B:345:LEU:HD22	1.46	0.94
2:F:244:MET:CG	2:F:245:PRO:CD	2.45	0.94
2:F:244:MET:HE1	2:F:345:LEU:HD22	1.46	0.94
2:D:244:MET:HE1	2:D:345:LEU:HD22	1.46	0.94
2:J:244:MET:CG	2:J:245:PRO:CD	2.45	0.94
2:d:244:MET:HE1	2:d:345:LEU:HD22	1.46	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:66:ASP:OD2	2:X:218:LYS:NZ	2.01	0.94
2:V:244:MET:CG	2:V:245:PRO:CD	2.45	0.94
2:b:244:MET:HE1	2:b:345:LEU:HD22	1.46	0.94
2:L:244:MET:CG	2:L:245:PRO:CD	2.45	0.94
2:N:244:MET:CG	2:N:245:PRO:CD	2.45	0.94
2:P:340:ARG:NH2	2:b:139:ASP:OD2	1.99	0.93
2:T:244:MET:CG	2:T:245:PRO:CD	2.45	0.93
1:M:66:ASP:OD2	2:b:218:LYS:NZ	2.02	0.93
2:H:244:MET:CG	2:H:245:PRO:CD	2.45	0.93
2:P:244:MET:CG	2:P:245:PRO:CD	2.45	0.93
2:D:244:MET:CG	2:D:245:PRO:CD	2.45	0.93
2:d:244:MET:CG	2:d:245:PRO:CD	2.45	0.93
2:R:244:MET:CG	2:R:245:PRO:CD	2.45	0.93
1:K:66:ASP:OD2	2:Z:218:LYS:NZ	2.02	0.93
2:P:244:MET:HE1	2:P:345:LEU:HD22	1.46	0.93
1:C:66:ASP:OD2	2:R:218:LYS:NZ	2.02	0.92
1:O:66:ASP:OD2	2:d:218:LYS:NZ	2.02	0.91
2:H:244:MET:HG2	2:H:245:PRO:CD	2.01	0.91
1:G:66:ASP:OD2	2:V:218:LYS:NZ	2.02	0.91
2:T:244:MET:HG2	2:T:245:PRO:CD	2.01	0.91
1:A:66:ASP:OD2	2:P:218:LYS:NZ	2.04	0.91
1:E:66:ASP:OD2	2:T:218:LYS:NZ	2.02	0.91
2:V:244:MET:HG2	2:V:245:PRO:CD	2.01	0.91
2:B:123:LYS:NZ	2:B:175:ASP:OD1	2.04	0.90
2:b:123:LYS:NZ	2:b:175:ASP:OD1	2.04	0.90
1:C:43:MET:HE1	2:D:163:LEU:HD21	1.54	0.90
2:H:123:LYS:NZ	2:H:175:ASP:OD1	2.04	0.90
2:V:123:LYS:NZ	2:V:175:ASP:OD1	2.04	0.90
1:C:43:MET:HE2	2:D:163:LEU:HD21	1.54	0.90
2:N:244:MET:HG2	2:N:245:PRO:CD	2.01	0.90
2:T:123:LYS:NZ	2:T:175:ASP:OD1	2.04	0.90
2:b:244:MET:HG2	2:b:245:PRO:CD	2.01	0.90
1:c:43:MET:HE1	2:d:163:LEU:HD21	1.54	0.90
1:c:43:MET:HE2	2:d:163:LEU:HD21	1.54	0.90
2:B:244:MET:HG2	2:B:245:PRO:CD	2.01	0.90
1:O:43:MET:HE2	2:P:163:LEU:HD21	1.54	0.90
2:P:123:LYS:NZ	2:P:175:ASP:OD1	2.04	0.90
2:Z:244:MET:HG2	2:Z:245:PRO:CD	2.01	0.90
2:D:244:MET:HG2	2:D:245:PRO:CD	2.01	0.90
2:J:123:LYS:NZ	2:J:175:ASP:OD1	2.04	0.90
2:N:123:LYS:NZ	2:N:175:ASP:OD1	2.04	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:244:MET:HG2	2:X:245:PRO:CD	2.01	0.90
1:Y:43:MET:HE2	2:Z:163:LEU:HD21	1.54	0.90
2:d:244:MET:HG2	2:d:245:PRO:CD	2.01	0.90
2:F:123:LYS:NZ	2:F:175:ASP:OD1	2.04	0.90
2:L:244:MET:HG2	2:L:245:PRO:CD	2.01	0.89
2:P:244:MET:HG2	2:P:245:PRO:CD	2.01	0.89
2:F:244:MET:HG2	2:F:245:PRO:CD	2.01	0.89
2:X:123:LYS:NZ	2:X:175:ASP:OD1	2.04	0.89
1:O:43:MET:HE1	2:P:163:LEU:HD21	1.54	0.89
1:Q:43:MET:HE1	2:R:163:LEU:HD21	1.54	0.89
2:R:123:LYS:NZ	2:R:175:ASP:OD1	2.04	0.89
2:L:123:LYS:NZ	2:L:175:ASP:OD1	2.04	0.89
2:J:244:MET:HG2	2:J:245:PRO:CD	2.01	0.89
1:S:43:MET:HE2	2:T:163:LEU:HD21	1.54	0.89
2:Z:123:LYS:NZ	2:Z:175:ASP:OD1	2.04	0.89
2:D:123:LYS:NZ	2:D:175:ASP:OD1	2.04	0.88
1:K:43:MET:HE2	2:L:163:LEU:HD21	1.54	0.88
2:d:123:LYS:NZ	2:d:175:ASP:OD1	2.04	0.88
1:M:43:MET:HE2	2:N:163:LEU:HD21	1.54	0.88
1:G:43:MET:HE1	2:H:163:LEU:HD21	1.54	0.88
1:A:43:MET:HE2	2:B:163:LEU:HD21	1.54	0.88
1:Q:43:MET:HE2	2:R:163:LEU:HD21	1.54	0.88
1:Y:43:MET:HE1	2:Z:163:LEU:HD21	1.54	0.88
1:a:43:MET:HE2	2:b:163:LEU:HD21	1.54	0.88
1:E:43:MET:HE2	2:F:163:LEU:HD21	1.54	0.88
1:I:43:MET:HE2	2:J:163:LEU:HD21	1.54	0.88
1:S:43:MET:HE1	2:T:163:LEU:HD21	1.54	0.88
1:M:43:MET:HE1	2:N:163:LEU:HD21	1.54	0.87
1:K:43:MET:HE1	2:L:163:LEU:HD21	1.54	0.87
1:U:43:MET:HE1	2:V:163:LEU:HD21	1.54	0.87
1:E:43:MET:HE1	2:F:163:LEU:HD21	1.54	0.87
2:R:244:MET:HG2	2:R:245:PRO:CD	2.01	0.87
1:a:43:MET:HE1	2:b:163:LEU:HD21	1.54	0.87
1:A:43:MET:HE1	2:B:163:LEU:HD21	1.54	0.87
2:F:441:THR:HG1	2:F:445:LYS:HZ3	1.20	0.87
1:U:43:MET:HE2	2:V:163:LEU:HD21	1.54	0.87
1:G:43:MET:HE2	2:H:163:LEU:HD21	1.54	0.86
1:W:43:MET:HE2	2:X:163:LEU:HD21	1.54	0.86
1:W:43:MET:HE1	2:X:163:LEU:HD21	1.54	0.86
1:I:43:MET:HE1	2:J:163:LEU:HD21	1.54	0.85
2:Z:441:THR:HG1	2:Z:445:LYS:NZ	1.73	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:441:THR:HG1	2:X:445:LYS:HZ3	1.21	0.84
2:H:441:THR:HG1	2:H:445:LYS:HZ3	1.25	0.84
2:B:45:VAL:HG13	2:b:70:ILE:CD1	2.05	0.84
2:D:45:VAL:HG13	2:d:70:ILE:CD1	2.06	0.84
2:R:238:ARG:HB3	2:R:371:GLN:OE1	1.78	0.84
2:V:238:ARG:HB3	2:V:371:GLN:OE1	1.78	0.84
2:H:238:ARG:HB3	2:H:371:GLN:OE1	1.78	0.83
2:D:440:SER:O	2:D:441:THR:HG23	1.78	0.83
2:F:238:ARG:HB3	2:F:371:GLN:OE1	1.78	0.83
2:X:440:SER:O	2:X:441:THR:HG23	1.79	0.83
2:d:440:SER:O	2:d:441:THR:HG23	1.79	0.83
2:H:440:SER:O	2:H:441:THR:HG23	1.78	0.83
2:T:440:SER:O	2:T:441:THR:HG23	1.79	0.83
2:N:440:SER:O	2:N:441:THR:HG23	1.79	0.83
2:L:440:SER:O	2:L:441:THR:HG23	1.79	0.83
2:B:440:SER:O	2:B:441:THR:HG23	1.79	0.83
2:Z:440:SER:O	2:Z:441:THR:HG23	1.78	0.83
2:b:440:SER:O	2:b:441:THR:HG23	1.79	0.83
2:R:440:SER:O	2:R:441:THR:HG23	1.79	0.82
2:P:440:SER:O	2:P:441:THR:HG23	1.79	0.82
2:J:440:SER:O	2:J:441:THR:HG23	1.79	0.82
2:V:440:SER:O	2:V:441:THR:HG23	1.79	0.82
2:F:440:SER:O	2:F:441:THR:HG23	1.78	0.82
2:d:441:THR:HG1	2:d:445:LYS:NZ	1.73	0.82
2:D:441:THR:HG1	2:D:445:LYS:NZ	1.73	0.82
2:T:238:ARG:HB3	2:T:371:GLN:OE1	1.78	0.82
2:P:238:ARG:HB3	2:P:371:GLN:OE1	1.78	0.82
2:B:238:ARG:HB3	2:B:371:GLN:OE1	1.78	0.82
2:D:238:ARG:HB3	2:D:371:GLN:OE1	1.78	0.82
2:N:238:ARG:HB3	2:N:371:GLN:OE1	1.78	0.82
2:X:238:ARG:HB3	2:X:371:GLN:OE1	1.78	0.82
2:Z:238:ARG:HB3	2:Z:371:GLN:OE1	1.78	0.82
2:b:238:ARG:HB3	2:b:371:GLN:OE1	1.78	0.82
2:d:238:ARG:HB3	2:d:371:GLN:OE1	1.78	0.82
2:J:238:ARG:HB3	2:J:371:GLN:OE1	1.78	0.82
2:L:238:ARG:HB3	2:L:371:GLN:OE1	1.78	0.82
2:F:441:THR:HG1	2:F:445:LYS:NZ	1.72	0.81
2:V:441:THR:HG1	2:V:445:LYS:HZ3	1.28	0.81
2:D:441:THR:HG1	2:D:445:LYS:HZ3	1.22	0.81
2:B:441:THR:HG1	2:B:445:LYS:NZ	1.78	0.80
1:A:60:ARG:O	1:A:61:LYS:CG	2.30	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:487:ARG:NH1	2:X:470:LYS:HE2	1.97	0.80
1:O:60:ARG:O	1:O:61:LYS:CG	2.30	0.80
1:M:60:ARG:O	1:M:61:LYS:CG	2.30	0.80
1:U:60:ARG:O	1:U:61:LYS:CG	2.30	0.80
1:a:60:ARG:O	1:a:61:LYS:CG	2.30	0.80
1:C:60:ARG:O	1:C:61:LYS:CG	2.30	0.80
1:K:60:ARG:O	1:K:61:LYS:CG	2.30	0.80
2:L:441:THR:HG1	2:L:445:LYS:NZ	1.80	0.80
1:c:60:ARG:O	1:c:61:LYS:CG	2.30	0.80
1:S:60:ARG:O	1:S:61:LYS:CG	2.30	0.80
2:Z:442:GLU:HG2	2:Z:443:THR:H	1.47	0.80
2:d:441:THR:HG1	2:d:445:LYS:HZ3	1.24	0.80
1:G:60:ARG:O	1:G:61:LYS:CG	2.30	0.80
1:E:60:ARG:O	1:E:61:LYS:CG	2.30	0.80
2:H:183:ALA:HB2	2:H:240:ILE:HD11	1.64	0.80
1:I:60:ARG:O	1:I:61:LYS:CG	2.30	0.80
2:B:183:ALA:HB2	2:B:240:ILE:HD11	1.64	0.79
2:F:183:ALA:HB2	2:F:240:ILE:HD11	1.64	0.79
2:J:441:THR:HG1	2:J:445:LYS:HZ3	1.28	0.79
1:W:60:ARG:O	1:W:61:LYS:CG	2.30	0.79
2:L:183:ALA:HB2	2:L:240:ILE:HD11	1.65	0.79
2:N:183:ALA:HB2	2:N:240:ILE:HD11	1.64	0.79
2:R:183:ALA:HB2	2:R:240:ILE:HD11	1.64	0.79
2:b:183:ALA:HB2	2:b:240:ILE:HD11	1.64	0.79
2:J:487:ARG:NH1	2:V:470:LYS:HE2	1.97	0.79
2:Z:183:ALA:HB2	2:Z:240:ILE:HD11	1.64	0.79
2:J:183:ALA:HB2	2:J:240:ILE:HD11	1.64	0.79
2:N:442:GLU:HG2	2:N:443:THR:H	1.47	0.79
2:V:442:GLU:HG2	2:V:443:THR:H	1.47	0.79
2:L:260:VAL:O	2:L:261:GLU:HG2	1.83	0.79
1:Q:60:ARG:O	1:Q:61:LYS:CG	2.30	0.79
2:T:183:ALA:HB2	2:T:240:ILE:HD11	1.64	0.79
2:b:441:THR:HG1	2:b:445:LYS:NZ	1.80	0.79
2:B:260:VAL:O	2:B:261:GLU:HG2	1.83	0.79
2:D:487:ARG:NH1	2:P:470:LYS:HE2	1.98	0.79
2:F:442:GLU:HG2	2:F:443:THR:H	1.47	0.79
2:H:260:VAL:O	2:H:261:GLU:HG2	1.83	0.79
2:P:183:ALA:HB2	2:P:240:ILE:HD11	1.64	0.79
2:V:183:ALA:HB2	2:V:240:ILE:HD11	1.64	0.79
2:b:260:VAL:O	2:b:261:GLU:HG2	1.83	0.79
2:F:260:VAL:O	2:F:261:GLU:HG2	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:260:VAL:O	2:J:261:GLU:HG2	1.83	0.79
2:J:442:GLU:HG2	2:J:443:THR:H	1.47	0.79
2:R:442:GLU:HG2	2:R:443:THR:H	1.47	0.79
1:Y:60:ARG:O	1:Y:61:LYS:CG	2.30	0.79
2:D:58:LEU:CD2	1:c:95:LEU:HD11	2.12	0.79
2:T:442:GLU:HG2	2:T:443:THR:H	1.47	0.79
2:D:183:ALA:HB2	2:D:240:ILE:HD11	1.65	0.79
2:D:437:PRO:HB2	2:D:441:THR:CG2	2.13	0.79
2:N:260:VAL:O	2:N:261:GLU:HG2	1.83	0.79
2:P:437:PRO:HB2	2:P:441:THR:CG2	2.13	0.79
2:P:487:ARG:NH1	2:b:470:LYS:HE2	1.97	0.79
2:Z:441:THR:HG1	2:Z:445:LYS:HZ3	1.23	0.79
2:d:437:PRO:HB2	2:d:441:THR:CG2	2.13	0.79
2:D:442:GLU:HG2	2:D:443:THR:H	1.47	0.79
2:R:260:VAL:O	2:R:261:GLU:HG2	1.83	0.79
2:R:441:THR:HG1	2:R:445:LYS:NZ	1.78	0.79
2:d:183:ALA:HB2	2:d:240:ILE:HD11	1.65	0.79
2:L:442:GLU:HG2	2:L:443:THR:H	1.47	0.78
2:X:183:ALA:HB2	2:X:240:ILE:HD11	1.64	0.78
2:H:442:GLU:HG2	2:H:443:THR:H	1.47	0.78
2:T:260:VAL:O	2:T:261:GLU:HG2	1.83	0.78
2:B:437:PRO:HB2	2:B:441:THR:CG2	2.13	0.78
2:F:487:ARG:NH1	2:R:470:LYS:HE2	1.97	0.78
2:H:487:ARG:NH1	2:T:470:LYS:HE2	1.98	0.78
2:P:260:VAL:O	2:P:261:GLU:HG2	1.83	0.78
2:b:437:PRO:HB2	2:b:441:THR:CG2	2.13	0.78
2:d:442:GLU:HG2	2:d:443:THR:H	1.47	0.78
2:P:442:GLU:HG2	2:P:443:THR:H	1.47	0.78
2:R:437:PRO:HB2	2:R:441:THR:CG2	2.13	0.78
2:R:487:ARG:NH1	2:d:470:LYS:HE2	1.98	0.78
2:V:437:PRO:HB2	2:V:441:THR:CG2	2.13	0.78
1:W:43:MET:CE	2:X:163:LEU:CD2	2.62	0.78
2:H:437:PRO:HB2	2:H:441:THR:CG2	2.13	0.78
2:J:437:PRO:HB2	2:J:441:THR:CG2	2.13	0.78
1:K:43:MET:CE	2:L:163:LEU:CD2	2.62	0.78
2:X:442:GLU:HG2	2:X:443:THR:H	1.47	0.78
1:I:43:MET:CE	2:J:163:LEU:CD2	2.62	0.78
2:B:487:ARG:NH1	2:N:470:LYS:HE2	1.98	0.78
2:D:244:MET:CE	2:D:345:LEU:HD22	2.14	0.78
2:R:244:MET:CE	2:R:345:LEU:HD22	2.14	0.78
2:X:437:PRO:HB2	2:X:441:THR:CG2	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:244:MET:CE	2:d:345:LEU:HD22	2.14	0.78
2:D:260:VAL:O	2:D:261:GLU:HG2	1.83	0.78
1:E:43:MET:CE	2:F:163:LEU:CD2	2.62	0.78
2:F:244:MET:CE	2:F:345:LEU:HD22	2.14	0.78
2:L:437:PRO:HB2	2:L:441:THR:CG2	2.13	0.78
2:N:437:PRO:HB2	2:N:441:THR:CG2	2.13	0.78
2:N:441:THR:HG1	2:N:445:LYS:NZ	1.78	0.78
2:T:437:PRO:HB2	2:T:441:THR:CG2	2.13	0.78
1:U:43:MET:CE	2:V:163:LEU:CD2	2.62	0.78
2:V:260:VAL:O	2:V:261:GLU:HG2	1.83	0.78
1:Y:43:MET:CE	2:Z:163:LEU:CD2	2.62	0.78
2:d:260:VAL:O	2:d:261:GLU:HG2	1.83	0.78
1:Q:43:MET:CE	2:R:163:LEU:CD2	2.62	0.77
2:F:437:PRO:HB2	2:F:441:THR:CG2	2.13	0.77
2:V:441:THR:HG1	2:V:445:LYS:NZ	1.76	0.77
2:Z:437:PRO:HB2	2:Z:441:THR:CG2	2.13	0.77
2:B:442:GLU:HG2	2:B:443:THR:H	1.47	0.77
2:N:487:ARG:NH1	2:Z:470:LYS:HE2	1.98	0.77
2:P:244:MET:CE	2:P:345:LEU:HD22	2.14	0.77
1:S:43:MET:CE	2:T:163:LEU:CD2	2.62	0.77
2:Z:260:VAL:O	2:Z:261:GLU:HG2	1.83	0.77
2:b:442:GLU:HG2	2:b:443:THR:H	1.47	0.77
1:C:43:MET:CE	2:D:163:LEU:CD2	2.62	0.77
2:P:151:GLU:HB3	2:P:158:GLU:O	1.85	0.77
2:T:244:MET:CE	2:T:345:LEU:HD22	2.14	0.77
2:X:260:VAL:O	2:X:261:GLU:HG2	1.83	0.77
2:b:151:GLU:HB3	2:b:158:GLU:O	1.85	0.77
2:B:151:GLU:HB3	2:B:158:GLU:O	1.85	0.77
2:H:151:GLU:HB3	2:H:158:GLU:O	1.85	0.77
2:L:151:GLU:HB3	2:L:158:GLU:O	1.85	0.77
2:N:151:GLU:HB3	2:N:158:GLU:O	1.85	0.77
2:Z:151:GLU:HB3	2:Z:158:GLU:O	1.85	0.77
1:c:43:MET:CE	2:d:163:LEU:CD2	2.62	0.77
2:d:151:GLU:HB3	2:d:158:GLU:O	1.85	0.77
2:D:151:GLU:HB3	2:D:158:GLU:O	1.85	0.77
2:T:151:GLU:HB3	2:T:158:GLU:O	1.85	0.77
1:G:43:MET:CE	2:H:163:LEU:CD2	2.62	0.77
2:P:487:ARG:HH11	2:b:470:LYS:HE2	1.49	0.77
2:F:487:ARG:HH11	2:R:470:LYS:HE2	1.49	0.77
2:R:151:GLU:HB3	2:R:158:GLU:O	1.85	0.77
2:X:151:GLU:HB3	2:X:158:GLU:O	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:43:MET:CE	2:P:163:LEU:CD2	2.62	0.77
2:J:244:MET:CE	2:J:345:LEU:HD22	2.14	0.77
1:M:43:MET:CE	2:N:163:LEU:CD2	2.62	0.77
2:V:244:MET:CE	2:V:345:LEU:HD22	2.14	0.77
1:A:43:MET:CE	2:B:163:LEU:CD2	2.62	0.76
2:B:244:MET:CE	2:B:345:LEU:HD22	2.13	0.76
2:J:441:THR:HG1	2:J:445:LYS:NZ	1.77	0.76
1:a:43:MET:CE	2:b:163:LEU:CD2	2.62	0.76
2:P:441:THR:HG1	2:P:445:LYS:NZ	1.78	0.76
2:R:487:ARG:HH11	2:d:470:LYS:HE2	1.50	0.76
2:b:244:MET:CE	2:b:345:LEU:HD22	2.14	0.76
2:N:244:MET:CE	2:N:345:LEU:HD22	2.14	0.76
2:Z:244:MET:CE	2:Z:345:LEU:HD22	2.14	0.76
2:H:441:THR:HG1	2:H:445:LYS:NZ	1.78	0.76
2:L:244:MET:CE	2:L:345:LEU:HD22	2.14	0.76
2:F:244:MET:HG3	2:F:245:PRO:CD	2.13	0.76
2:H:244:MET:CE	2:H:345:LEU:HD22	2.14	0.76
2:V:151:GLU:HB3	2:V:158:GLU:O	1.85	0.76
2:X:244:MET:CE	2:X:345:LEU:HD22	2.14	0.76
2:F:151:GLU:HB3	2:F:158:GLU:O	1.85	0.76
1:A:60:ARG:C	1:A:61:LYS:HG2	2.11	0.76
2:J:151:GLU:HB3	2:J:158:GLU:O	1.85	0.76
2:D:487:ARG:HH11	2:P:470:LYS:HE2	1.51	0.76
2:B:45:VAL:CG1	2:b:70:ILE:HD11	2.10	0.76
1:I:60:ARG:C	1:I:61:LYS:HG2	2.11	0.76
2:X:244:MET:HG3	2:X:245:PRO:CD	2.13	0.76
1:a:60:ARG:C	1:a:61:LYS:HG2	2.11	0.76
2:L:487:ARG:HH11	2:X:470:LYS:HE2	1.49	0.75
2:P:244:MET:HG3	2:P:245:PRO:CD	2.13	0.75
1:U:60:ARG:C	1:U:61:LYS:HG2	2.11	0.75
2:D:53:LEU:HD13	1:c:90:THR:OG1	1.86	0.75
2:T:441:THR:HG1	2:T:445:LYS:HZ3	1.33	0.75
1:M:60:ARG:C	1:M:61:LYS:HG2	2.11	0.75
1:O:60:ARG:C	1:O:61:LYS:HG2	2.11	0.75
1:W:60:ARG:C	1:W:61:LYS:HG2	2.11	0.75
2:T:441:THR:HG1	2:T:445:LYS:NZ	1.81	0.75
1:E:60:ARG:C	1:E:61:LYS:HG2	2.11	0.74
2:N:244:MET:HG3	2:N:245:PRO:CD	2.13	0.74
2:D:45:VAL:CG1	2:d:70:ILE:HD11	2.10	0.74
1:C:60:ARG:C	1:C:61:LYS:HG2	2.11	0.74
2:F:109:GLU:OE2	1:Q:13:ARG:NH1	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:60:ARG:C	1:Y:61:LYS:HG2	2.11	0.74
1:K:60:ARG:C	1:K:61:LYS:HG2	2.11	0.74
1:c:60:ARG:C	1:c:61:LYS:HG2	2.12	0.74
2:B:487:ARG:HH11	2:N:470:LYS:HE2	1.51	0.74
2:H:487:ARG:HH11	2:T:470:LYS:HE2	1.50	0.74
1:G:60:ARG:C	1:G:61:LYS:HG2	2.11	0.74
2:L:244:MET:HG3	2:L:245:PRO:CD	2.13	0.74
1:Q:60:ARG:C	1:Q:61:LYS:HG2	2.12	0.74
2:R:109:GLU:OE2	1:c:13:ARG:NH1	2.20	0.74
2:N:487:ARG:HH11	2:Z:470:LYS:HE2	1.51	0.74
1:S:60:ARG:C	1:S:61:LYS:HG2	2.11	0.74
2:P:109:GLU:OE2	1:a:13:ARG:NH1	2.21	0.74
2:R:151:GLU:HG3	2:R:160:TYR:CE2	2.23	0.74
2:X:441:THR:HG1	2:X:445:LYS:NZ	1.78	0.74
2:B:53:LEU:HD13	1:a:90:THR:OG1	1.87	0.74
2:D:151:GLU:HG3	2:D:160:TYR:CE2	2.23	0.74
2:J:304:ARG:HH12	2:J:480:GLU:CD	1.96	0.74
2:N:441:THR:HG1	2:N:445:LYS:HZ3	1.28	0.74
2:X:151:GLU:HG3	2:X:160:TYR:CE2	2.23	0.74
2:d:151:GLU:HG3	2:d:160:TYR:CE2	2.23	0.74
2:F:151:GLU:HG3	2:F:160:TYR:CE2	2.23	0.73
2:H:304:ARG:HH12	2:H:480:GLU:CD	1.96	0.73
2:N:213:PRO:O	2:N:341:ARG:NH2	2.21	0.73
2:R:304:ARG:HH12	2:R:480:GLU:CD	1.96	0.73
2:T:304:ARG:HH12	2:T:480:GLU:CD	1.96	0.73
2:J:151:GLU:HG3	2:J:160:TYR:CE2	2.23	0.73
2:J:487:ARG:HH11	2:V:470:LYS:HE2	1.50	0.73
2:B:442:GLU:HG2	2:B:443:THR:N	2.03	0.73
2:L:304:ARG:NH1	2:L:480:GLU:OE2	2.22	0.73
2:R:304:ARG:NH1	2:R:480:GLU:OE2	2.22	0.73
2:b:442:GLU:HG2	2:b:443:THR:N	2.03	0.73
2:D:304:ARG:NH1	2:D:480:GLU:OE2	2.22	0.73
2:N:442:GLU:HG2	2:N:443:THR:N	2.03	0.73
2:P:442:GLU:HG2	2:P:443:THR:N	2.03	0.73
2:Z:213:PRO:O	2:Z:341:ARG:NH2	2.21	0.73
2:Z:304:ARG:NH1	2:Z:480:GLU:OE2	2.22	0.73
2:H:244:MET:HG3	2:H:245:PRO:CD	2.13	0.73
2:b:151:GLU:HG3	2:b:160:TYR:CE2	2.23	0.73
2:d:304:ARG:NH1	2:d:480:GLU:OE2	2.22	0.73
2:B:151:GLU:HG3	2:B:160:TYR:CE2	2.23	0.73
2:F:304:ARG:HH12	2:F:480:GLU:CD	1.96	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:442:GLU:HG2	2:J:443:THR:N	2.03	0.73
2:L:151:GLU:HG3	2:L:160:TYR:CE2	2.23	0.73
2:N:109:GLU:OE2	1:Y:13:ARG:NH1	2.22	0.73
2:N:151:GLU:HG3	2:N:160:TYR:CE2	2.23	0.73
2:R:253:TYR:N	2:R:267:GLU:OE1	2.22	0.73
2:V:442:GLU:HG2	2:V:443:THR:N	2.03	0.73
2:D:442:GLU:HG2	2:D:443:THR:N	2.03	0.73
2:N:253:TYR:N	2:N:267:GLU:OE1	2.22	0.73
2:V:304:ARG:HH12	2:V:480:GLU:CD	1.96	0.73
2:L:109:GLU:OE2	1:W:13:ARG:NH1	2.21	0.73
2:L:213:PRO:O	2:L:341:ARG:NH2	2.21	0.73
2:L:304:ARG:HH12	2:L:480:GLU:CD	1.96	0.73
2:P:151:GLU:HG3	2:P:160:TYR:CE2	2.23	0.73
2:Z:442:GLU:HG2	2:Z:443:THR:N	2.03	0.73
2:d:442:GLU:HG2	2:d:443:THR:N	2.03	0.73
2:D:253:TYR:N	2:D:267:GLU:OE1	2.22	0.73
2:H:109:GLU:OE2	1:S:13:ARG:NH1	2.22	0.73
2:H:442:GLU:HG2	2:H:443:THR:N	2.03	0.73
2:P:304:ARG:HH12	2:P:480:GLU:CD	1.96	0.73
2:V:244:MET:HG3	2:V:245:PRO:CD	2.13	0.73
2:d:253:TYR:N	2:d:267:GLU:OE1	2.22	0.73
2:N:304:ARG:NH1	2:N:480:GLU:OE2	2.22	0.73
2:P:304:ARG:NH1	2:P:480:GLU:OE2	2.22	0.73
2:R:442:GLU:HG2	2:R:443:THR:N	2.03	0.73
2:V:151:GLU:HG3	2:V:160:TYR:CE2	2.23	0.73
2:B:58:LEU:CD2	1:a:95:LEU:HD11	2.13	0.72
2:F:304:ARG:NH1	2:F:480:GLU:OE2	2.22	0.72
2:Z:304:ARG:HH12	2:Z:480:GLU:CD	1.96	0.72
2:B:304:ARG:HH12	2:B:480:GLU:CD	1.96	0.72
2:T:151:GLU:HG3	2:T:160:TYR:CE2	2.23	0.72
2:T:442:GLU:HG2	2:T:443:THR:N	2.03	0.72
2:X:213:PRO:O	2:X:341:ARG:NH2	2.21	0.72
2:X:304:ARG:NH1	2:X:480:GLU:OE2	2.22	0.72
2:X:442:GLU:HG2	2:X:443:THR:N	2.03	0.72
2:Z:151:GLU:HG3	2:Z:160:TYR:CE2	2.23	0.72
2:b:304:ARG:HH12	2:b:480:GLU:CD	1.96	0.72
2:F:442:GLU:HG2	2:F:443:THR:N	2.03	0.72
2:V:304:ARG:NH1	2:V:480:GLU:OE2	2.22	0.72
2:H:304:ARG:NH1	2:H:480:GLU:OE2	2.22	0.72
2:R:244:MET:HG3	2:R:245:PRO:CD	2.13	0.72
2:T:253:TYR:N	2:T:267:GLU:OE1	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:358:ASN:O	2:b:229:ARG:NH2	2.22	0.72
2:D:244:MET:HG3	2:D:245:PRO:CD	2.13	0.72
2:H:151:GLU:HG3	2:H:160:TYR:CE2	2.23	0.72
2:P:213:PRO:O	2:P:341:ARG:NH2	2.21	0.72
2:X:304:ARG:HH12	2:X:480:GLU:CD	1.96	0.72
2:B:244:MET:HG3	2:B:245:PRO:CD	2.13	0.72
2:D:304:ARG:HH12	2:D:480:GLU:CD	1.96	0.72
2:L:442:GLU:HG2	2:L:443:THR:N	2.03	0.72
2:B:304:ARG:NH1	2:B:480:GLU:OE2	2.22	0.72
2:J:109:GLU:OE2	1:U:13:ARG:NH1	2.22	0.72
2:d:244:MET:HG3	2:d:245:PRO:CD	2.13	0.72
2:d:304:ARG:HH12	2:d:480:GLU:CD	1.96	0.72
2:D:358:ASN:O	2:d:229:ARG:NH2	2.22	0.72
2:b:244:MET:HG3	2:b:245:PRO:CD	2.13	0.72
2:b:304:ARG:NH1	2:b:480:GLU:OE2	2.22	0.72
2:D:109:GLU:OE2	1:O:13:ARG:NH1	2.23	0.72
2:J:213:PRO:O	2:J:341:ARG:NH2	2.21	0.72
2:X:253:TYR:N	2:X:267:GLU:OE1	2.22	0.72
2:B:109:GLU:OE2	1:M:13:ARG:NH1	2.22	0.71
2:Z:253:TYR:N	2:Z:267:GLU:OE1	2.22	0.71
1:A:31:GLU:HB3	2:P:377:ASP:OD2	1.89	0.71
2:J:304:ARG:NH1	2:J:480:GLU:OE2	2.22	0.71
2:P:253:TYR:N	2:P:267:GLU:OE1	2.22	0.71
2:B:441:THR:HG1	2:B:445:LYS:HZ3	1.29	0.71
2:T:304:ARG:NH1	2:T:480:GLU:OE2	2.22	0.71
2:V:253:TYR:N	2:V:267:GLU:OE1	2.22	0.71
2:F:213:PRO:O	2:F:341:ARG:NH2	2.21	0.71
2:N:304:ARG:HH12	2:N:480:GLU:CD	1.96	0.71
2:F:253:TYR:N	2:F:267:GLU:OE1	2.22	0.71
2:J:244:MET:HG3	2:J:245:PRO:CD	2.13	0.70
1:E:31:GLU:HB3	2:T:377:ASP:OD2	1.90	0.70
1:E:40:MET:HE1	2:F:104:LEU:HD11	1.73	0.70
1:O:31:GLU:HB3	2:d:377:ASP:OD2	1.91	0.70
1:Q:40:MET:HE1	2:R:104:LEU:HD11	1.73	0.70
1:A:27:LEU:HD22	2:P:376:TYR:CE2	2.26	0.70
2:B:213:PRO:O	2:B:341:ARG:NH2	2.21	0.70
1:C:40:MET:HE1	2:D:104:LEU:HD11	1.73	0.70
1:O:40:MET:HE1	2:P:104:LEU:HD11	1.73	0.70
1:c:40:MET:HE1	2:d:104:LEU:HD11	1.73	0.70
1:C:31:GLU:HB3	2:R:377:ASP:OD2	1.90	0.70
2:b:213:PRO:O	2:b:341:ARG:NH2	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:31:GLU:HB3	2:V:377:ASP:OD2	1.91	0.70
1:K:31:GLU:HB3	2:Z:377:ASP:OD2	1.91	0.70
1:S:40:MET:HE1	2:T:104:LEU:HD11	1.73	0.70
1:S:60:ARG:O	1:S:61:LYS:HG3	1.92	0.70
1:M:60:ARG:O	1:M:61:LYS:HG3	1.92	0.70
2:V:213:PRO:O	2:V:341:ARG:NH2	2.21	0.70
1:A:40:MET:HE1	2:B:104:LEU:HD11	1.73	0.70
2:B:436:ASP:HB2	2:B:437:PRO:HD3	1.74	0.70
1:a:40:MET:HE1	2:b:104:LEU:HD11	1.73	0.70
2:d:436:ASP:HB2	2:d:437:PRO:HD3	1.74	0.70
1:C:60:ARG:O	1:C:61:LYS:HG3	1.92	0.70
2:D:436:ASP:HB2	2:D:437:PRO:HD3	1.74	0.70
1:M:31:GLU:HB3	2:b:377:ASP:OD2	1.90	0.70
2:N:436:ASP:HB2	2:N:437:PRO:HD3	1.74	0.70
2:P:436:ASP:HB2	2:P:437:PRO:HD3	1.74	0.70
2:b:436:ASP:HB2	2:b:437:PRO:HD3	1.74	0.70
1:c:60:ARG:O	1:c:61:LYS:HG3	1.92	0.70
2:B:340:ARG:NH1	2:N:139:ASP:OD1	2.24	0.70
2:D:441:THR:OG1	2:D:445:LYS:CE	2.40	0.70
2:F:441:THR:OG1	2:F:445:LYS:CE	2.40	0.70
2:R:436:ASP:HB2	2:R:437:PRO:HD3	1.74	0.70
2:Z:244:MET:HG3	2:Z:245:PRO:CD	2.13	0.70
2:d:441:THR:OG1	2:d:445:LYS:CE	2.40	0.70
1:G:27:LEU:HD22	2:V:376:TYR:CE2	2.28	0.69
1:M:27:LEU:HD22	2:b:376:TYR:CE2	2.27	0.69
1:A:60:ARG:O	1:A:61:LYS:HG3	1.92	0.69
1:K:60:ARG:O	1:K:61:LYS:HG3	1.92	0.69
1:a:60:ARG:O	1:a:61:LYS:HG3	1.92	0.69
2:F:340:ARG:NH1	2:R:139:ASP:OD1	2.25	0.69
2:F:436:ASP:HB2	2:F:437:PRO:HD3	1.74	0.69
2:H:441:THR:OG1	2:H:445:LYS:CE	2.40	0.69
1:I:60:ARG:O	1:I:61:LYS:HG3	1.92	0.69
2:J:253:TYR:N	2:J:267:GLU:OE1	2.22	0.69
2:R:441:THR:OG1	2:R:445:LYS:CE	2.40	0.69
1:W:40:MET:HE1	2:X:104:LEU:HD11	1.73	0.69
2:Z:441:THR:OG1	2:Z:445:LYS:CE	2.40	0.69
2:D:61:ASN:CG	1:c:92:GLU:OE2	2.35	0.69
1:S:43:MET:HE2	2:T:163:LEU:CD2	2.23	0.69
2:X:441:THR:OG1	2:X:445:LYS:CE	2.40	0.69
2:Z:436:ASP:HB2	2:Z:437:PRO:HD3	1.74	0.69
1:C:27:LEU:HD22	2:R:376:TYR:CE2	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:40:MET:HE1	2:H:104:LEU:HD11	1.73	0.69
1:K:40:MET:HE1	2:L:104:LEU:HD11	1.73	0.69
2:N:437:PRO:O	2:N:441:THR:HG23	1.93	0.69
2:T:441:THR:OG1	2:T:445:LYS:CE	2.40	0.69
1:U:60:ARG:O	1:U:61:LYS:HG3	1.92	0.69
2:B:253:TYR:N	2:B:267:GLU:OE1	2.22	0.69
1:E:43:MET:HE2	2:F:163:LEU:CD2	2.23	0.69
1:G:43:MET:HE2	2:H:163:LEU:CD2	2.23	0.69
2:H:253:TYR:N	2:H:267:GLU:OE1	2.22	0.69
1:M:40:MET:HE1	2:N:104:LEU:HD11	1.73	0.69
1:Q:60:ARG:O	1:Q:61:LYS:HG3	1.92	0.69
2:V:437:PRO:O	2:V:441:THR:HG23	1.93	0.69
2:b:253:TYR:N	2:b:267:GLU:OE1	2.22	0.69
2:B:61:ASN:CG	1:a:92:GLU:OE2	2.36	0.69
2:B:441:THR:OG1	2:B:445:LYS:CE	2.40	0.69
2:D:244:MET:HE1	2:D:345:LEU:HB3	1.75	0.69
2:D:340:ARG:NH1	2:P:139:ASP:OD1	2.24	0.69
2:F:244:MET:HE1	2:F:345:LEU:HB3	1.75	0.69
2:F:437:PRO:O	2:F:441:THR:HG23	1.93	0.69
1:G:60:ARG:O	1:G:61:LYS:HG3	1.92	0.69
2:H:340:ARG:NH1	2:T:139:ASP:OD1	2.24	0.69
1:I:31:GLU:HB3	2:X:377:ASP:OD2	1.92	0.69
1:K:27:LEU:HD22	2:Z:376:TYR:CE2	2.28	0.69
2:L:441:THR:HG1	2:L:445:LYS:HZ3	1.34	0.69
1:M:43:MET:HE2	2:N:163:LEU:CD2	2.23	0.69
1:O:60:ARG:O	1:O:61:LYS:HG3	1.92	0.69
2:P:441:THR:OG1	2:P:445:LYS:CE	2.40	0.69
2:P:441:THR:HG1	2:P:445:LYS:HZ3	1.30	0.69
2:R:213:PRO:O	2:R:341:ARG:NH2	2.21	0.69
2:R:244:MET:HE1	2:R:345:LEU:HB3	1.75	0.69
1:U:40:MET:HE1	2:V:104:LEU:HD11	1.73	0.69
2:X:244:MET:HE1	2:X:345:LEU:HB3	1.75	0.69
1:Y:43:MET:HE2	2:Z:163:LEU:CD2	2.23	0.69
2:Z:244:MET:HE1	2:Z:345:LEU:HB3	1.75	0.69
2:b:441:THR:OG1	2:b:445:LYS:CE	2.40	0.69
2:d:244:MET:HE1	2:d:345:LEU:HB3	1.75	0.69
1:E:27:LEU:HD22	2:T:376:TYR:CE2	2.28	0.69
1:E:60:ARG:O	1:E:61:LYS:HG3	1.92	0.69
2:J:340:ARG:NH1	2:V:139:ASP:OD1	2.25	0.69
1:O:27:LEU:HD22	2:d:376:TYR:CE2	2.28	0.69
2:P:437:PRO:O	2:P:441:THR:HG23	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:436:ASP:HB2	2:T:437:PRO:HD3	1.74	0.69
1:U:43:MET:HE2	2:V:163:LEU:CD2	2.23	0.69
2:b:244:MET:HE1	2:b:345:LEU:HB3	1.75	0.69
2:B:244:MET:HE1	2:B:345:LEU:HB3	1.75	0.69
2:D:437:PRO:O	2:D:441:THR:HG23	1.93	0.69
2:H:436:ASP:HB2	2:H:437:PRO:HD3	1.74	0.69
2:L:253:TYR:N	2:L:267:GLU:OE1	2.22	0.69
1:Y:40:MET:HE1	2:Z:104:LEU:HD11	1.73	0.69
1:a:43:MET:HE2	2:b:163:LEU:CD2	2.23	0.69
1:A:43:MET:HE2	2:B:163:LEU:CD2	2.23	0.68
2:D:58:LEU:HD22	1:c:95:LEU:CD1	2.18	0.68
2:H:170:ASP:HA	2:H:201:VAL:HG22	1.75	0.68
2:H:437:PRO:O	2:H:441:THR:HG23	1.93	0.68
2:J:441:THR:OG1	2:J:445:LYS:CE	2.40	0.68
2:R:437:PRO:O	2:R:441:THR:HG23	1.93	0.68
2:T:244:MET:HG3	2:T:245:PRO:CD	2.13	0.68
2:V:170:ASP:HA	2:V:201:VAL:HG22	1.75	0.68
2:V:244:MET:HE1	2:V:345:LEU:HB3	1.75	0.68
2:d:437:PRO:O	2:d:441:THR:HG23	1.93	0.68
1:I:43:MET:HE2	2:J:163:LEU:CD2	2.23	0.68
2:L:436:ASP:HB2	2:L:437:PRO:HD3	1.74	0.68
2:T:170:ASP:HA	2:T:201:VAL:HG22	1.75	0.68
2:T:213:PRO:O	2:T:341:ARG:NH2	2.21	0.68
2:T:244:MET:HE1	2:T:345:LEU:HB3	1.75	0.68
2:V:436:ASP:HB2	2:V:437:PRO:HD3	1.74	0.68
2:J:244:MET:HE1	2:J:345:LEU:HB3	1.75	0.68
2:J:436:ASP:HB2	2:J:437:PRO:HD3	1.74	0.68
2:N:244:MET:HE1	2:N:345:LEU:HB3	1.75	0.68
2:P:244:MET:HE1	2:P:345:LEU:HB3	1.75	0.68
2:X:437:PRO:O	2:X:441:THR:HG23	1.93	0.68
2:Z:437:PRO:O	2:Z:441:THR:HG23	1.93	0.68
2:H:244:MET:HE1	2:H:345:LEU:HB3	1.75	0.68
1:I:27:LEU:HD22	2:X:376:TYR:CE2	2.29	0.68
2:L:244:MET:HE1	2:L:345:LEU:HB3	1.75	0.68
2:L:441:THR:OG1	2:L:445:LYS:CE	2.40	0.68
1:W:60:ARG:O	1:W:61:LYS:HG3	1.92	0.68
2:D:213:PRO:O	2:D:341:ARG:NH2	2.21	0.68
2:N:441:THR:OG1	2:N:445:LYS:CE	2.40	0.68
2:V:441:THR:OG1	2:V:445:LYS:CE	2.40	0.68
2:d:213:PRO:O	2:d:341:ARG:NH2	2.21	0.68
2:F:170:ASP:HA	2:F:201:VAL:HG22	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:43:MET:HE2	2:P:163:LEU:CD2	2.23	0.68
2:X:436:ASP:HB2	2:X:437:PRO:HD3	1.74	0.68
2:J:170:ASP:HA	2:J:201:VAL:HG22	1.75	0.68
2:J:437:PRO:O	2:J:441:THR:HG23	1.93	0.68
2:L:437:PRO:O	2:L:441:THR:HG23	1.93	0.68
2:N:340:ARG:NH1	2:Z:139:ASP:OD1	2.24	0.68
1:I:40:MET:HE1	2:J:104:LEU:HD11	1.73	0.68
1:O:43:MET:HE1	2:P:163:LEU:CD2	2.24	0.68
1:Y:60:ARG:O	1:Y:61:LYS:HG3	1.92	0.68
1:W:43:MET:HE2	2:X:163:LEU:CD2	2.23	0.68
1:C:43:MET:HE1	2:D:163:LEU:CD2	2.23	0.68
2:R:340:ARG:NH1	2:d:139:ASP:OD1	2.24	0.68
2:T:437:PRO:O	2:T:441:THR:HG23	1.93	0.68
1:c:43:MET:HE1	2:d:163:LEU:CD2	2.24	0.68
2:B:437:PRO:O	2:B:441:THR:HG23	1.93	0.67
2:H:213:PRO:O	2:H:341:ARG:NH2	2.21	0.67
2:Z:170:ASP:HA	2:Z:201:VAL:HG22	1.75	0.67
2:F:207:TRP:CZ2	2:F:244:MET:HB2	2.30	0.67
1:Q:119:LEU:HD11	2:R:81:GLN:HG2	1.76	0.67
1:S:119:LEU:HD11	2:T:81:GLN:HG2	1.76	0.67
2:T:207:TRP:CZ2	2:T:244:MET:HB2	2.30	0.67
2:X:170:ASP:HA	2:X:201:VAL:HG22	1.75	0.67
2:b:437:PRO:O	2:b:441:THR:HG23	1.93	0.67
1:E:60:ARG:C	1:E:61:LYS:CG	2.68	0.67
2:N:170:ASP:HA	2:N:201:VAL:HG22	1.75	0.67
2:R:170:ASP:HA	2:R:201:VAL:HG22	1.75	0.67
2:R:207:TRP:CZ2	2:R:244:MET:HB2	2.30	0.67
1:A:43:MET:HE1	2:B:163:LEU:CD2	2.24	0.67
1:C:32:LYS:HA	2:R:376:TYR:HA	1.77	0.67
1:C:43:MET:HE2	2:D:163:LEU:CD2	2.23	0.67
1:a:43:MET:HE1	2:b:163:LEU:CD2	2.23	0.67
1:c:43:MET:HE2	2:d:163:LEU:CD2	2.23	0.67
1:A:32:LYS:HA	2:P:376:TYR:HA	1.77	0.67
2:L:170:ASP:HA	2:L:201:VAL:HG22	1.75	0.67
1:Y:18:ARG:HH11	2:b:342:GLU:CD	2.03	0.67
2:d:207:TRP:CZ2	2:d:244:MET:HB2	2.30	0.67
1:A:60:ARG:C	1:A:61:LYS:CG	2.68	0.67
2:D:207:TRP:CZ2	2:D:244:MET:HB2	2.30	0.67
2:H:207:TRP:CZ2	2:H:244:MET:HB2	2.30	0.67
1:K:60:ARG:C	1:K:61:LYS:CG	2.68	0.67
2:P:207:TRP:CZ2	2:P:244:MET:HB2	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:60:ARG:C	1:W:61:LYS:CG	2.68	0.67
1:a:60:ARG:C	1:a:61:LYS:CG	2.68	0.67
2:b:207:TRP:CZ2	2:b:244:MET:HB2	2.30	0.67
2:B:207:TRP:CZ2	2:B:244:MET:HB2	2.30	0.67
1:E:119:LEU:HD11	2:F:81:GLN:HG2	1.76	0.67
2:N:207:TRP:CZ2	2:N:244:MET:HB2	2.30	0.67
1:U:60:ARG:C	1:U:61:LYS:CG	2.68	0.67
1:K:43:MET:HE2	2:L:163:LEU:CD2	2.23	0.67
1:M:60:ARG:C	1:M:61:LYS:CG	2.68	0.67
2:P:340:ARG:NH1	2:b:139:ASP:OD1	2.25	0.67
2:b:170:ASP:HA	2:b:201:VAL:HG22	1.75	0.67
1:c:119:LEU:HD11	2:d:81:GLN:HG2	1.76	0.67
2:B:170:ASP:HA	2:B:201:VAL:HG22	1.75	0.67
1:C:119:LEU:HD11	2:D:81:GLN:HG2	1.76	0.67
1:G:119:LEU:HD11	2:H:81:GLN:HG2	1.77	0.67
1:U:119:LEU:HD11	2:V:81:GLN:HG2	1.77	0.67
1:W:43:MET:HE1	2:X:163:LEU:CD2	2.24	0.67
1:O:119:LEU:HD11	2:P:81:GLN:HG2	1.76	0.67
2:Z:207:TRP:CZ2	2:Z:244:MET:HB2	2.30	0.67
2:L:340:ARG:NH1	2:X:139:ASP:OD1	2.25	0.66
1:a:18:ARG:HH11	2:d:342:GLU:CD	2.03	0.66
1:Q:60:ARG:C	1:Q:61:LYS:CG	2.68	0.66
2:V:207:TRP:CZ2	2:V:244:MET:HB2	2.30	0.66
2:d:170:ASP:HA	2:d:201:VAL:HG22	1.75	0.66
2:D:170:ASP:HA	2:D:201:VAL:HG22	1.75	0.66
1:O:32:LYS:HA	2:d:376:TYR:HA	1.77	0.66
2:R:441:THR:HG1	2:R:445:LYS:HZ3	1.30	0.66
2:b:441:THR:HG1	2:b:445:LYS:HZ3	1.32	0.66
2:B:58:LEU:HD22	1:a:95:LEU:CD1	2.19	0.66
1:E:43:MET:HE1	2:F:163:LEU:CD2	2.23	0.66
1:I:60:ARG:C	1:I:61:LYS:CG	2.68	0.66
1:Q:43:MET:HE2	2:R:163:LEU:CD2	2.23	0.66
1:S:43:MET:HE1	2:T:163:LEU:CD2	2.24	0.66
1:Y:60:ARG:C	1:Y:61:LYS:CG	2.68	0.66
1:W:18:ARG:HH11	2:Z:342:GLU:CD	2.03	0.66
1:G:60:ARG:C	1:G:61:LYS:CG	2.68	0.66
2:L:207:TRP:CZ2	2:L:244:MET:HB2	2.30	0.66
2:P:170:ASP:HA	2:P:201:VAL:HG22	1.75	0.66
2:X:207:TRP:CZ2	2:X:244:MET:HB2	2.30	0.66
2:J:207:TRP:CZ2	2:J:244:MET:HB2	2.30	0.66
1:K:43:MET:HE1	2:L:163:LEU:CD2	2.23	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:119:LEU:HD11	2:Z:81:GLN:HG2	1.76	0.66
1:I:119:LEU:HD11	2:J:81:GLN:HG2	1.76	0.66
1:M:43:MET:HE1	2:N:163:LEU:CD2	2.24	0.66
1:G:43:MET:HE1	2:H:163:LEU:CD2	2.23	0.66
1:M:119:LEU:HD11	2:N:81:GLN:HG2	1.76	0.66
1:A:119:LEU:HD11	2:B:81:GLN:HG2	1.77	0.66
1:E:32:LYS:HA	2:T:376:TYR:HA	1.78	0.66
1:I:43:MET:HE1	2:J:163:LEU:CD2	2.24	0.66
1:K:119:LEU:HD11	2:L:81:GLN:HG2	1.77	0.66
1:M:32:LYS:HA	2:b:376:TYR:HA	1.78	0.66
1:a:119:LEU:HD11	2:b:81:GLN:HG2	1.77	0.66
1:K:32:LYS:HA	2:Z:376:TYR:HA	1.78	0.65
1:W:119:LEU:HD11	2:X:81:GLN:HG2	1.76	0.65
1:Q:18:ARG:HH11	2:T:342:GLU:CD	2.04	0.65
2:B:340:ARG:HH12	2:N:139:ASP:CG	2.04	0.65
2:L:340:ARG:HH12	2:X:139:ASP:CG	2.04	0.65
1:Q:43:MET:HE1	2:R:163:LEU:CD2	2.23	0.65
1:K:60:ARG:O	1:K:61:LYS:HG2	1.97	0.65
1:C:60:ARG:C	1:C:61:LYS:CG	2.68	0.65
2:H:137:THR:O	2:H:137:THR:HG22	1.97	0.65
1:S:18:ARG:HH11	2:V:342:GLU:CD	2.04	0.65
1:c:60:ARG:C	1:c:61:LYS:CG	2.68	0.65
1:C:18:ARG:HH11	2:F:342:GLU:CD	2.04	0.65
1:I:32:LYS:HA	2:X:376:TYR:HA	1.78	0.65
1:M:60:ARG:O	1:M:61:LYS:HG2	1.97	0.65
2:R:244:MET:HE2	2:R:350:PHE:HB3	1.79	0.65
2:F:244:MET:HE2	2:F:350:PHE:HB3	1.79	0.65
1:O:18:ARG:HH11	2:R:342:GLU:CD	2.05	0.65
2:D:244:MET:HE2	2:D:350:PHE:HB3	1.79	0.65
2:D:340:ARG:HH12	2:P:139:ASP:CG	2.04	0.65
2:H:340:ARG:HH12	2:T:139:ASP:CG	2.04	0.65
2:J:137:THR:O	2:J:137:THR:HG22	1.97	0.65
2:N:340:ARG:HH12	2:Z:139:ASP:CG	2.04	0.65
2:d:244:MET:HE2	2:d:350:PHE:HB3	1.79	0.65
2:H:130:LEU:HD12	2:H:178:LEU:CD1	2.27	0.65
2:P:244:MET:HE2	2:P:350:PHE:HB3	1.79	0.64
2:T:130:LEU:HD12	2:T:178:LEU:CD1	2.27	0.64
2:T:244:MET:HE2	2:T:350:PHE:HB3	1.79	0.64
1:U:60:ARG:O	1:U:61:LYS:HG2	1.97	0.64
2:F:340:ARG:HH12	2:R:139:ASP:CG	2.05	0.64
1:W:60:ARG:O	1:W:61:LYS:HG2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:137:THR:O	2:X:137:THR:HG22	1.97	0.64
2:F:137:THR:HG22	2:F:137:THR:O	1.97	0.64
2:V:130:LEU:HD12	2:V:178:LEU:CD1	2.27	0.64
1:A:60:ARG:O	1:A:61:LYS:HG2	1.97	0.64
2:B:244:MET:HE2	2:B:350:PHE:HB3	1.79	0.64
1:I:18:ARG:HH11	2:L:342:GLU:CD	2.06	0.64
1:I:60:ARG:O	1:I:61:LYS:HG2	1.97	0.64
2:L:244:MET:HE2	2:L:350:PHE:HB3	1.79	0.64
1:M:18:ARG:HH11	2:P:342:GLU:CD	2.05	0.64
2:R:340:ARG:HH12	2:d:139:ASP:CG	2.04	0.64
2:X:244:MET:HE2	2:X:350:PHE:HB3	1.79	0.64
2:Z:130:LEU:HD12	2:Z:178:LEU:CD1	2.27	0.64
2:F:130:LEU:HD12	2:F:178:LEU:CD1	2.27	0.64
2:L:130:LEU:HD12	2:L:178:LEU:CD1	2.28	0.64
1:a:60:ARG:O	1:a:61:LYS:HG2	1.97	0.64
2:b:244:MET:HE2	2:b:350:PHE:HB3	1.79	0.64
1:E:60:ARG:O	1:E:61:LYS:HG2	1.97	0.64
1:U:43:MET:HE1	2:V:163:LEU:CD2	2.24	0.64
2:V:137:THR:HG22	2:V:137:THR:O	1.97	0.64
2:H:244:MET:HE2	2:H:350:PHE:HB3	1.79	0.64
2:H:244:MET:SD	2:H:345:LEU:HD22	2.38	0.64
2:H:438:ALA:O	2:H:445:LYS:NZ	2.28	0.64
2:J:244:MET:HE2	2:J:350:PHE:HB3	1.79	0.64
2:N:244:MET:HE2	2:N:350:PHE:HB3	1.78	0.64
2:R:130:LEU:HD12	2:R:178:LEU:CD1	2.27	0.64
1:S:60:ARG:C	1:S:61:LYS:CG	2.68	0.64
2:T:244:MET:SD	2:T:345:LEU:HD22	2.38	0.64
2:B:137:THR:O	2:B:137:THR:HG22	1.97	0.64
2:J:340:ARG:HH12	2:V:139:ASP:CG	2.05	0.64
2:b:137:THR:O	2:b:137:THR:HG22	1.97	0.64
2:D:130:LEU:HD12	2:D:178:LEU:CD1	2.27	0.64
2:J:130:LEU:HD12	2:J:178:LEU:CD1	2.27	0.64
2:V:244:MET:SD	2:V:345:LEU:HD22	2.38	0.64
1:Y:43:MET:HE1	2:Z:163:LEU:CD2	2.24	0.64
2:d:130:LEU:HD12	2:d:178:LEU:CD1	2.27	0.64
1:G:18:ARG:HH11	2:J:342:GLU:CD	2.06	0.64
2:H:304:ARG:O	2:H:308:SER:OG	2.16	0.64
2:Z:137:THR:O	2:Z:137:THR:HG22	1.97	0.64
1:C:60:ARG:O	1:C:61:LYS:HG2	1.97	0.63
1:G:32:LYS:HA	2:V:376:TYR:HA	1.79	0.63
2:J:244:MET:SD	2:J:345:LEU:HD22	2.38	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:130:LEU:HD12	2:X:178:LEU:CD1	2.27	0.63
1:Y:60:ARG:O	1:Y:61:LYS:HG2	1.97	0.63
2:Z:244:MET:HE2	2:Z:350:PHE:HB3	1.79	0.63
1:c:60:ARG:O	1:c:61:LYS:HG2	1.97	0.63
2:D:61:ASN:CB	1:c:92:GLU:OE2	2.47	0.63
2:D:137:THR:O	2:D:137:THR:HG22	1.97	0.63
2:F:304:ARG:O	2:F:308:SER:OG	2.16	0.63
2:N:130:LEU:HD12	2:N:178:LEU:CD1	2.27	0.63
2:N:244:MET:SD	2:N:345:LEU:HD22	2.38	0.63
2:N:387:LEU:CD2	2:Z:464:PRO:HG3	2.28	0.63
1:O:60:ARG:O	1:O:61:LYS:HG2	1.97	0.63
2:J:304:ARG:O	2:J:308:SER:OG	2.16	0.63
2:X:304:ARG:O	2:X:308:SER:OG	2.16	0.63
2:d:137:THR:HG22	2:d:137:THR:O	1.97	0.63
2:B:130:LEU:HD12	2:B:178:LEU:CD1	2.27	0.63
2:B:387:LEU:CD2	2:N:464:PRO:HG3	2.29	0.63
1:Q:60:ARG:O	1:Q:61:LYS:HG2	1.97	0.63
2:R:137:THR:O	2:R:137:THR:HG22	1.97	0.63
1:S:60:ARG:O	1:S:61:LYS:HG2	1.97	0.63
1:U:18:ARG:HH11	2:X:342:GLU:CD	2.05	0.63
2:b:130:LEU:HD12	2:b:178:LEU:CD1	2.27	0.63
2:b:244:MET:SD	2:b:345:LEU:HD22	2.38	0.63
2:B:244:MET:SD	2:B:345:LEU:HD22	2.38	0.63
1:K:18:ARG:HH11	2:N:342:GLU:CD	2.06	0.63
2:L:137:THR:O	2:L:137:THR:HG22	1.97	0.63
2:P:130:LEU:HD12	2:P:178:LEU:CD1	2.28	0.63
2:T:137:THR:O	2:T:137:THR:HG22	1.97	0.63
2:V:244:MET:HE2	2:V:350:PHE:HB3	1.79	0.63
2:V:304:ARG:O	2:V:308:SER:OG	2.16	0.63
2:X:244:MET:SD	2:X:345:LEU:HD22	2.38	0.63
2:P:137:THR:O	2:P:137:THR:HG22	1.97	0.63
2:P:340:ARG:HH12	2:b:139:ASP:CG	2.05	0.63
2:T:492:LEU:H	2:T:496:LYS:HD2	1.64	0.63
2:N:137:THR:HG22	2:N:137:THR:O	1.97	0.63
2:D:244:MET:SD	2:D:345:LEU:HD22	2.38	0.63
2:d:244:MET:SD	2:d:345:LEU:HD22	2.38	0.63
2:F:244:MET:SD	2:F:345:LEU:HD22	2.38	0.62
2:H:340:ARG:HH22	2:T:139:ASP:CG	2.06	0.62
2:H:387:LEU:CD2	2:T:464:PRO:HG3	2.28	0.62
2:L:492:LEU:H	2:L:496:LYS:HD2	1.64	0.62
2:N:340:ARG:HH22	2:Z:139:ASP:CG	2.06	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:244:MET:SD	2:R:345:LEU:HD22	2.38	0.62
2:Z:304:ARG:O	2:Z:308:SER:OG	2.16	0.62
2:F:95:GLU:O	2:F:99:ARG:HB2	2.00	0.62
2:P:492:LEU:H	2:P:496:LYS:HD2	1.64	0.62
2:T:262:GLU:OE1	2:T:262:GLU:HA	1.99	0.62
2:X:95:GLU:O	2:X:99:ARG:HB2	1.99	0.62
2:Z:244:MET:SD	2:Z:345:LEU:HD22	2.38	0.62
2:b:492:LEU:H	2:b:496:LYS:HD2	1.64	0.62
2:d:304:ARG:O	2:d:308:SER:OG	2.16	0.62
1:A:18:ARG:HH11	2:D:342:GLU:CD	2.07	0.62
2:B:492:LEU:H	2:B:496:LYS:HD2	1.64	0.62
2:D:304:ARG:O	2:D:308:SER:OG	2.16	0.62
1:E:18:ARG:HH11	2:H:342:GLU:CD	2.07	0.62
2:F:162:CYS:HB2	2:F:395:PHE:HE1	1.64	0.62
2:F:492:LEU:H	2:F:496:LYS:HD2	1.64	0.62
2:H:262:GLU:OE1	2:H:262:GLU:HA	1.99	0.62
2:J:262:GLU:HA	2:J:262:GLU:OE1	2.00	0.62
2:L:244:MET:SD	2:L:345:LEU:HD22	2.38	0.62
2:L:304:ARG:O	2:L:308:SER:OG	2.16	0.62
2:P:262:GLU:OE1	2:P:262:GLU:HA	1.99	0.62
2:R:492:LEU:H	2:R:496:LYS:HD2	1.64	0.62
2:J:492:LEU:H	2:J:496:LYS:HD2	1.64	0.62
2:P:244:MET:SD	2:P:345:LEU:HD22	2.38	0.62
2:R:262:GLU:HA	2:R:262:GLU:OE1	2.00	0.62
2:V:95:GLU:O	2:V:99:ARG:HB2	1.99	0.62
2:Z:492:LEU:H	2:Z:496:LYS:HD2	1.64	0.62
2:B:61:ASN:CB	1:a:92:GLU:OE2	2.47	0.62
2:B:95:GLU:O	2:B:99:ARG:HB2	1.99	0.62
2:J:387:LEU:CD2	2:V:464:PRO:HG3	2.30	0.62
2:R:95:GLU:O	2:R:99:ARG:HB2	1.99	0.62
2:R:387:LEU:CD2	2:d:464:PRO:HG3	2.28	0.62
2:T:162:CYS:HB2	2:T:395:PHE:HE1	1.64	0.62
2:T:304:ARG:O	2:T:308:SER:OG	2.16	0.62
2:X:438:ALA:O	2:X:445:LYS:NZ	2.28	0.62
2:b:95:GLU:O	2:b:99:ARG:HB2	1.99	0.62
2:D:244:MET:HE1	2:D:345:LEU:CD2	2.27	0.62
2:H:162:CYS:HB2	2:H:395:PHE:HE1	1.64	0.62
2:L:95:GLU:O	2:L:99:ARG:HB2	1.99	0.62
2:N:95:GLU:O	2:N:99:ARG:HB2	2.00	0.62
2:P:387:LEU:CD2	2:b:464:PRO:HG3	2.29	0.62
2:R:162:CYS:HB2	2:R:395:PHE:HE1	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:492:LEU:H	2:V:496:LYS:HD2	1.64	0.62
2:d:244:MET:HE1	2:d:345:LEU:CD2	2.27	0.62
2:d:492:LEU:H	2:d:496:LYS:HD2	1.64	0.62
2:D:492:LEU:H	2:D:496:LYS:HD2	1.64	0.62
2:F:262:GLU:OE1	2:F:262:GLU:HA	1.99	0.62
1:G:60:ARG:O	1:G:61:LYS:HG2	1.97	0.62
2:H:95:GLU:O	2:H:99:ARG:HB2	2.00	0.62
2:b:304:ARG:O	2:b:308:SER:OG	2.16	0.62
2:B:304:ARG:O	2:B:308:SER:OG	2.16	0.62
2:D:162:CYS:HB2	2:D:395:PHE:HE1	1.64	0.62
2:L:438:ALA:O	2:L:445:LYS:NZ	2.28	0.62
2:L:262:GLU:OE1	2:L:262:GLU:HA	2.00	0.62
1:a:89:LEU:HD11	2:b:81:GLN:HB2	1.82	0.62
1:A:89:LEU:HD11	2:B:81:GLN:HB2	1.82	0.62
2:D:95:GLU:O	2:D:99:ARG:HB2	1.99	0.62
2:L:387:LEU:CD2	2:X:464:PRO:HG3	2.30	0.62
2:N:262:GLU:OE1	2:N:262:GLU:HA	2.00	0.62
2:N:304:ARG:O	2:N:308:SER:OG	2.16	0.62
2:N:492:LEU:H	2:N:496:LYS:HD2	1.64	0.62
2:d:95:GLU:O	2:d:99:ARG:HB2	1.99	0.62
2:d:162:CYS:HB2	2:d:395:PHE:HE1	1.64	0.62
2:R:304:ARG:O	2:R:308:SER:OG	2.16	0.61
2:R:438:ALA:O	2:R:445:LYS:NZ	2.28	0.61
2:T:438:ALA:O	2:T:445:LYS:NZ	2.28	0.61
2:Z:244:MET:HE1	2:Z:345:LEU:CD2	2.27	0.61
2:D:387:LEU:CD2	2:P:464:PRO:HG3	2.29	0.61
2:J:95:GLU:O	2:J:99:ARG:HB2	2.00	0.61
2:P:304:ARG:O	2:P:308:SER:OG	2.16	0.61
2:T:95:GLU:O	2:T:99:ARG:HB2	2.00	0.61
2:D:262:GLU:OE1	2:D:262:GLU:HA	2.00	0.61
2:P:95:GLU:O	2:P:99:ARG:HB2	2.00	0.61
1:Y:89:LEU:HD11	2:Z:81:GLN:HB2	1.82	0.61
2:B:169:PHE:HE1	2:B:178:LEU:HD23	1.66	0.61
1:M:89:LEU:HD11	2:N:81:GLN:HB2	1.82	0.61
1:O:5:THR:HG23	1:O:5:THR:O	2.01	0.61
1:O:89:LEU:HD11	2:P:81:GLN:HB2	1.82	0.61
2:Z:169:PHE:HE1	2:Z:178:LEU:HD23	1.66	0.61
2:d:262:GLU:OE1	2:d:262:GLU:HA	2.00	0.61
1:C:89:LEU:HD11	2:D:81:GLN:HB2	1.82	0.61
2:D:433:VAL:HG22	2:D:450:LEU:HB2	1.83	0.61
2:F:387:LEU:CD2	2:R:464:PRO:HG3	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:5:THR:HG23	1:M:5:THR:O	2.01	0.61
1:O:60:ARG:C	1:O:61:LYS:CG	2.68	0.61
2:P:162:CYS:HB2	2:P:395:PHE:HE1	1.64	0.61
1:Y:5:THR:O	1:Y:5:THR:HG23	2.01	0.61
2:b:169:PHE:HE1	2:b:178:LEU:HD23	1.66	0.61
1:c:89:LEU:HD11	2:d:81:GLN:HB2	1.82	0.61
2:d:433:VAL:HG22	2:d:450:LEU:HB2	1.83	0.61
2:B:162:CYS:HB2	2:B:395:PHE:HE1	1.64	0.61
2:D:438:ALA:O	2:D:445:LYS:NZ	2.28	0.61
2:H:492:LEU:H	2:H:496:LYS:HD2	1.64	0.61
2:R:387:LEU:HD23	2:d:464:PRO:HG3	1.82	0.61
1:S:26:GLU:OE1	2:V:487:ARG:NH2	2.34	0.61
2:V:162:CYS:HB2	2:V:395:PHE:HE1	1.64	0.61
2:V:262:GLU:OE1	2:V:262:GLU:HA	2.00	0.61
2:Z:95:GLU:O	2:Z:99:ARG:HB2	2.00	0.61
2:J:438:ALA:O	2:J:445:LYS:NZ	2.28	0.61
2:R:244:MET:HE1	2:R:345:LEU:CD2	2.27	0.61
2:T:169:PHE:HE1	2:T:178:LEU:HD23	1.66	0.61
2:X:169:PHE:HE1	2:X:178:LEU:HD23	1.66	0.61
2:b:162:CYS:HB2	2:b:395:PHE:HE1	1.64	0.61
2:b:433:VAL:HG22	2:b:450:LEU:HB2	1.82	0.61
2:B:433:VAL:HG22	2:B:450:LEU:HB2	1.83	0.61
1:C:5:THR:HG23	1:C:5:THR:O	2.01	0.61
2:L:162:CYS:HB2	2:L:395:PHE:HE1	1.64	0.61
2:N:387:LEU:HD23	2:Z:464:PRO:HG3	1.83	0.61
2:P:433:VAL:HG22	2:P:450:LEU:HB2	1.83	0.61
2:V:244:MET:HE1	2:V:345:LEU:CD2	2.27	0.61
2:X:162:CYS:HB2	2:X:395:PHE:HE1	1.64	0.61
2:Z:162:CYS:HB2	2:Z:395:PHE:HE1	1.64	0.61
1:c:5:THR:HG23	1:c:5:THR:O	2.00	0.61
2:F:244:MET:HE1	2:F:345:LEU:CD2	2.27	0.61
2:F:433:VAL:HG22	2:F:450:LEU:HB2	1.83	0.61
2:N:162:CYS:HB2	2:N:395:PHE:HE1	1.64	0.61
2:P:387:LEU:HD23	2:b:464:PRO:HG3	1.83	0.61
2:R:169:PHE:HE1	2:R:178:LEU:HD23	1.66	0.61
2:R:433:VAL:HG22	2:R:450:LEU:HB2	1.82	0.61
2:J:169:PHE:HE1	2:J:178:LEU:HD23	1.66	0.61
1:U:89:LEU:HD11	2:V:81:GLN:HB2	1.82	0.61
2:Z:262:GLU:HA	2:Z:262:GLU:OE1	2.00	0.61
2:B:387:LEU:HD23	2:N:464:PRO:HG3	1.83	0.60
2:D:436:ASP:HB2	2:D:437:PRO:CD	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:340:ARG:HH22	2:R:139:ASP:CG	2.07	0.60
1:G:5:THR:HG23	1:G:5:THR:O	2.01	0.60
1:G:89:LEU:HD11	2:H:81:GLN:HB2	1.82	0.60
1:Q:89:LEU:HD11	2:R:81:GLN:HB2	1.82	0.60
1:S:89:LEU:HD11	2:T:81:GLN:HB2	1.82	0.60
1:U:5:THR:HG23	1:U:5:THR:O	2.01	0.60
1:Y:26:GLU:OE1	2:b:487:ARG:NH2	2.34	0.60
2:Z:436:ASP:HB2	2:Z:437:PRO:CD	2.31	0.60
2:d:436:ASP:HB2	2:d:437:PRO:CD	2.31	0.60
2:B:262:GLU:HA	2:B:262:GLU:OE1	2.00	0.60
2:D:169:PHE:HE1	2:D:178:LEU:HD23	1.66	0.60
1:W:5:THR:HG23	1:W:5:THR:O	2.01	0.60
2:b:262:GLU:OE1	2:b:262:GLU:HA	2.00	0.60
2:d:169:PHE:HE1	2:d:178:LEU:HD23	1.66	0.60
1:E:5:THR:HG23	1:E:5:THR:O	2.01	0.60
2:F:169:PHE:HE1	2:F:178:LEU:HD23	1.66	0.60
2:J:162:CYS:HB2	2:J:395:PHE:HE1	1.64	0.60
1:K:89:LEU:HD11	2:L:81:GLN:HB2	1.82	0.60
2:L:387:LEU:HD23	2:X:464:PRO:HG3	1.84	0.60
2:H:387:LEU:HD23	2:T:464:PRO:HG3	1.83	0.60
2:H:436:ASP:HB2	2:H:437:PRO:CD	2.31	0.60
2:N:433:VAL:HG22	2:N:450:LEU:HB2	1.82	0.60
2:N:436:ASP:HB2	2:N:437:PRO:CD	2.31	0.60
2:P:169:PHE:HE1	2:P:178:LEU:HD23	1.66	0.60
2:R:340:ARG:HH22	2:d:139:ASP:CG	2.07	0.60
2:R:436:ASP:HB2	2:R:437:PRO:CD	2.32	0.60
2:X:492:LEU:H	2:X:496:LYS:HD2	1.64	0.60
2:H:169:PHE:HE1	2:H:178:LEU:HD23	1.66	0.60
2:J:433:VAL:HG22	2:J:450:LEU:HB2	1.83	0.60
1:O:26:GLU:OE1	2:R:487:ARG:NH2	2.34	0.60
1:S:5:THR:HG23	1:S:5:THR:O	2.01	0.60
1:W:89:LEU:HD11	2:X:81:GLN:HB2	1.82	0.60
2:X:262:GLU:OE1	2:X:262:GLU:HA	2.00	0.60
2:D:340:ARG:HH22	2:P:139:ASP:CG	2.06	0.60
1:I:5:THR:O	1:I:5:THR:HG23	2.01	0.60
1:I:89:LEU:HD11	2:J:81:GLN:HB2	1.82	0.60
2:L:169:PHE:HE1	2:L:178:LEU:HD23	1.66	0.60
2:L:436:ASP:HB2	2:L:437:PRO:CD	2.31	0.60
2:P:436:ASP:HB2	2:P:437:PRO:CD	2.31	0.60
1:Q:5:THR:O	1:Q:5:THR:HG23	2.01	0.60
1:Q:41:GLY:O	2:R:163:LEU:HD12	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:436:ASP:HB2	2:V:437:PRO:CD	2.31	0.60
2:B:327:VAL:HG13	2:b:224:GLU:HB2	1.83	0.60
1:E:89:LEU:HD11	2:F:81:GLN:HB2	1.82	0.60
1:K:41:GLY:O	2:L:163:LEU:HD12	2.02	0.60
1:O:41:GLY:O	2:P:163:LEU:HD12	2.02	0.60
2:T:244:MET:HE1	2:T:345:LEU:CD2	2.27	0.60
2:X:433:VAL:HG22	2:X:450:LEU:HB2	1.83	0.60
2:X:436:ASP:HB2	2:X:437:PRO:CD	2.31	0.60
1:a:5:THR:HG23	1:a:5:THR:O	2.00	0.60
1:A:5:THR:O	1:A:5:THR:HG23	2.01	0.60
2:D:387:LEU:HD23	2:P:464:PRO:HG3	1.84	0.60
2:N:244:MET:HE1	2:N:345:LEU:CD2	2.27	0.60
2:P:438:ALA:O	2:P:445:LYS:NZ	2.28	0.60
2:T:433:VAL:HG22	2:T:450:LEU:HB2	1.82	0.60
2:T:436:ASP:HB2	2:T:437:PRO:CD	2.31	0.60
1:K:5:THR:HG23	1:K:5:THR:O	2.01	0.60
2:L:433:VAL:HG22	2:L:450:LEU:HB2	1.83	0.60
2:N:169:PHE:HE1	2:N:178:LEU:HD23	1.66	0.60
2:N:438:ALA:O	2:N:445:LYS:NZ	2.28	0.60
1:Y:41:GLY:O	2:Z:163:LEU:HD12	2.02	0.60
1:G:41:GLY:O	2:H:163:LEU:HD12	2.02	0.60
2:H:433:VAL:HG22	2:H:450:LEU:HB2	1.82	0.60
1:M:26:GLU:OE1	2:P:487:ARG:NH2	2.35	0.60
2:V:433:VAL:HG22	2:V:450:LEU:HB2	1.83	0.60
2:Z:433:VAL:HG22	2:Z:450:LEU:HB2	1.83	0.60
2:F:387:LEU:HD23	2:R:464:PRO:HG3	1.84	0.59
2:F:436:ASP:HB2	2:F:437:PRO:CD	2.31	0.59
2:J:436:ASP:HB2	2:J:437:PRO:CD	2.31	0.59
1:U:41:GLY:O	2:V:163:LEU:HD12	2.01	0.59
2:D:488:LEU:HG	2:P:397:THR:HG21	1.83	0.59
2:J:387:LEU:HD23	2:V:464:PRO:HG3	1.84	0.59
1:W:41:GLY:O	2:X:163:LEU:HD12	2.02	0.59
1:S:41:GLY:O	2:T:163:LEU:HD12	2.02	0.59
2:B:436:ASP:HB2	2:B:437:PRO:CD	2.31	0.59
2:B:438:ALA:O	2:B:445:LYS:NZ	2.28	0.59
2:b:436:ASP:HB2	2:b:437:PRO:CD	2.31	0.59
2:b:438:ALA:O	2:b:445:LYS:NZ	2.28	0.59
1:M:41:GLY:O	2:N:163:LEU:HD12	2.02	0.59
2:D:327:VAL:HG13	2:d:224:GLU:HB2	1.83	0.59
2:H:244:MET:HE1	2:H:345:LEU:CD2	2.27	0.59
2:J:488:LEU:HG	2:V:397:THR:HG21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:26:GLU:OE1	2:Z:487:ARG:NH2	2.35	0.59
2:B:488:LEU:HG	2:N:397:THR:HG21	1.84	0.59
2:Z:438:ALA:O	2:Z:445:LYS:NZ	2.28	0.59
1:C:26:GLU:OE1	2:F:487:ARG:NH2	2.36	0.59
2:L:141:SER:O	2:L:145:LYS:HG2	2.03	0.59
2:N:488:LEU:HG	2:Z:397:THR:HG21	1.85	0.59
2:V:169:PHE:HE1	2:V:178:LEU:HD23	1.66	0.59
2:L:340:ARG:HH22	2:X:139:ASP:CG	2.07	0.59
1:I:41:GLY:O	2:J:163:LEU:HD12	2.02	0.58
1:a:26:GLU:OE1	2:d:487:ARG:NH2	2.35	0.58
1:A:41:GLY:O	2:B:163:LEU:HD12	2.01	0.58
1:C:41:GLY:O	2:D:163:LEU:HD12	2.02	0.58
1:E:26:GLU:OE1	2:H:487:ARG:NH2	2.36	0.58
1:E:41:GLY:O	2:F:163:LEU:HD12	2.02	0.58
1:Q:64:GLU:OE1	2:R:115:LYS:HD2	2.04	0.58
1:a:41:GLY:O	2:b:163:LEU:HD12	2.02	0.58
1:c:41:GLY:O	2:d:163:LEU:HD12	2.02	0.58
2:J:244:MET:HE1	2:J:345:LEU:CD2	2.27	0.58
1:U:26:GLU:OE1	2:X:487:ARG:NH2	2.36	0.58
2:V:438:ALA:O	2:V:445:LYS:NZ	2.28	0.58
2:X:141:SER:O	2:X:145:LYS:HG2	2.03	0.58
2:Z:141:SER:O	2:Z:145:LYS:HG2	2.03	0.58
1:C:64:GLU:OE1	2:D:115:LYS:HD2	2.04	0.58
2:N:170:ASP:OD1	2:N:175:ASP:OD2	2.22	0.58
2:R:141:SER:O	2:R:145:LYS:HG2	2.03	0.58
2:B:170:ASP:OD1	2:B:175:ASP:OD2	2.22	0.58
1:I:26:GLU:OE1	2:L:487:ARG:NH2	2.35	0.58
2:J:170:ASP:OD1	2:J:175:ASP:OD2	2.22	0.58
1:K:64:GLU:OE1	2:L:115:LYS:HD2	2.04	0.58
1:Q:26:GLU:OE1	2:T:487:ARG:NH2	2.36	0.58
2:b:170:ASP:OD1	2:b:175:ASP:OD2	2.22	0.58
1:c:64:GLU:OE1	2:d:115:LYS:HD2	2.04	0.58
1:E:64:GLU:OE1	2:F:115:LYS:HD2	2.04	0.58
1:G:26:GLU:OE1	2:J:487:ARG:NH2	2.37	0.58
2:H:79:THR:HG22	2:H:265:PHE:HD1	1.69	0.58
2:P:170:ASP:OD1	2:P:175:ASP:OD2	2.22	0.58
1:W:64:GLU:OE1	2:X:115:LYS:HD2	2.04	0.58
2:Z:170:ASP:OD1	2:Z:175:ASP:OD2	2.22	0.58
2:B:244:MET:HE1	2:B:345:LEU:CD2	2.27	0.58
2:D:79:THR:HG22	2:D:265:PHE:HD1	1.69	0.58
2:F:79:THR:HG22	2:F:265:PHE:HD1	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:488:LEU:HG	2:T:397:THR:HG21	1.85	0.58
2:L:170:ASP:OD1	2:L:175:ASP:OD2	2.22	0.58
1:O:64:GLU:OE1	2:P:115:LYS:HD2	2.04	0.58
2:P:488:LEU:HG	2:b:397:THR:HG21	1.85	0.58
2:V:170:ASP:OD1	2:V:175:ASP:OD2	2.22	0.58
2:X:170:ASP:OD1	2:X:175:ASP:OD2	2.22	0.58
2:d:438:ALA:O	2:d:445:LYS:NZ	2.28	0.58
1:A:64:GLU:OE1	2:B:115:LYS:HD2	2.04	0.58
2:F:438:ALA:O	2:F:445:LYS:NZ	2.28	0.58
2:H:141:SER:O	2:H:145:LYS:HG2	2.03	0.58
2:d:79:THR:HG22	2:d:265:PHE:HD1	1.69	0.58
2:H:170:ASP:OD1	2:H:175:ASP:OD2	2.22	0.58
1:I:64:GLU:OE1	2:J:115:LYS:HD2	2.04	0.58
2:J:141:SER:O	2:J:145:LYS:HG2	2.03	0.58
1:M:64:GLU:OE1	2:N:115:LYS:HD2	2.04	0.58
2:P:79:THR:HG22	2:P:265:PHE:HD1	1.69	0.58
2:T:79:THR:HG22	2:T:265:PHE:HD1	1.69	0.58
2:V:79:THR:HG22	2:V:265:PHE:HD1	1.69	0.58
1:Y:36:LEU:O	2:Z:399:ARG:NH2	2.37	0.58
1:Y:64:GLU:OE1	2:Z:115:LYS:HD2	2.04	0.58
2:b:244:MET:HE1	2:b:345:LEU:CD2	2.27	0.58
1:A:36:LEU:O	2:B:399:ARG:NH2	2.37	0.58
2:D:170:ASP:OD1	2:D:175:ASP:OD2	2.22	0.58
1:K:36:LEU:O	2:L:399:ARG:NH2	2.37	0.58
2:T:141:SER:O	2:T:145:LYS:HG2	2.03	0.58
2:V:141:SER:O	2:V:145:LYS:HG2	2.03	0.58
1:W:36:LEU:O	1:W:36:LEU:HD23	2.04	0.58
1:W:36:LEU:O	2:X:399:ARG:NH2	2.37	0.58
1:a:36:LEU:O	2:b:399:ARG:NH2	2.37	0.58
1:a:64:GLU:OE1	2:b:115:LYS:HD2	2.04	0.58
2:b:79:THR:HG22	2:b:265:PHE:HD1	1.69	0.58
2:d:170:ASP:OD1	2:d:175:ASP:OD2	2.22	0.58
2:B:79:THR:HG22	2:B:265:PHE:HD1	1.69	0.57
2:D:141:SER:O	2:D:145:LYS:HG2	2.03	0.57
1:G:31:GLU:HA	1:G:31:GLU:OE1	2.04	0.57
2:L:488:LEU:HG	2:X:397:THR:HG21	1.85	0.57
2:N:141:SER:O	2:N:145:LYS:HG2	2.03	0.57
2:d:141:SER:O	2:d:145:LYS:HG2	2.03	0.57
1:I:36:LEU:O	2:J:399:ARG:NH2	2.37	0.57
1:K:36:LEU:O	1:K:36:LEU:HD23	2.04	0.57
1:M:36:LEU:O	1:M:36:LEU:HD23	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:79:THR:HG22	2:N:265:PHE:HD1	1.69	0.57
1:O:36:LEU:O	2:P:399:ARG:NH2	2.37	0.57
2:P:141:SER:O	2:P:145:LYS:HG2	2.03	0.57
2:R:79:THR:HG22	2:R:265:PHE:HD1	1.69	0.57
2:R:170:ASP:OD1	2:R:175:ASP:OD2	2.22	0.57
2:T:170:ASP:OD1	2:T:175:ASP:OD2	2.22	0.57
1:A:36:LEU:O	1:A:36:LEU:HD23	2.05	0.57
2:F:170:ASP:OD1	2:F:175:ASP:OD2	2.22	0.57
1:I:36:LEU:O	1:I:36:LEU:HD23	2.05	0.57
1:K:26:GLU:OE1	2:N:487:ARG:NH2	2.36	0.57
1:S:64:GLU:OE1	2:T:115:LYS:HD2	2.04	0.57
1:U:31:GLU:OE1	1:U:31:GLU:HA	2.04	0.57
1:Y:36:LEU:O	1:Y:36:LEU:HD23	2.05	0.57
1:a:36:LEU:O	1:a:36:LEU:HD23	2.05	0.57
1:O:36:LEU:O	1:O:36:LEU:HD23	2.04	0.57
1:Q:36:LEU:O	2:R:399:ARG:NH2	2.37	0.57
1:U:36:LEU:O	1:U:36:LEU:HD23	2.05	0.57
2:J:79:THR:HG22	2:J:265:PHE:HD1	1.69	0.57
2:b:141:SER:O	2:b:145:LYS:HG2	2.03	0.57
2:B:141:SER:O	2:B:145:LYS:HG2	2.03	0.57
2:F:488:LEU:HG	2:R:397:THR:HG21	1.85	0.57
1:G:36:LEU:O	2:H:399:ARG:NH2	2.37	0.57
1:U:64:GLU:OE1	2:V:115:LYS:HD2	2.04	0.57
2:P:340:ARG:HH22	2:b:139:ASP:CG	2.07	0.57
1:S:31:GLU:OE1	1:S:31:GLU:HA	2.04	0.57
1:A:31:GLU:OE1	1:A:31:GLU:HA	2.04	0.57
1:G:64:GLU:OE1	2:H:115:LYS:HD2	2.04	0.57
2:J:340:ARG:HH22	2:V:139:ASP:CG	2.07	0.57
1:M:36:LEU:O	2:N:399:ARG:NH2	2.37	0.57
1:a:31:GLU:OE1	1:a:31:GLU:HA	2.04	0.57
2:F:141:SER:O	2:F:145:LYS:HG2	2.03	0.57
1:G:36:LEU:O	1:G:36:LEU:HD23	2.05	0.57
1:K:68:ASP:OD1	2:Z:214:ARG:HD3	2.05	0.57
1:M:31:GLU:OE1	1:M:31:GLU:HA	2.04	0.57
1:O:68:ASP:OD1	2:d:214:ARG:HD3	2.05	0.57
1:C:36:LEU:HD23	1:C:36:LEU:O	2.05	0.57
1:C:36:LEU:O	2:D:399:ARG:NH2	2.37	0.57
2:Z:79:THR:HG22	2:Z:265:PHE:HD1	1.69	0.57
1:c:36:LEU:O	1:c:36:LEU:HD23	2.05	0.57
1:I:31:GLU:OE1	1:I:31:GLU:HA	2.04	0.56
1:Q:36:LEU:O	1:Q:36:LEU:HD23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:36:LEU:O	2:d:399:ARG:NH2	2.37	0.56
2:B:340:ARG:HH22	2:N:139:ASP:CG	2.06	0.56
1:E:68:ASP:OD1	2:T:214:ARG:HD3	2.04	0.56
2:X:79:THR:HG22	2:X:265:PHE:HD1	1.69	0.56
1:E:36:LEU:O	2:F:399:ARG:NH2	2.37	0.56
2:L:151:GLU:HG3	2:L:160:TYR:HE2	1.70	0.56
1:S:36:LEU:O	2:T:399:ARG:NH2	2.37	0.56
1:U:36:LEU:O	2:V:399:ARG:NH2	2.37	0.56
2:V:434:ASP:OD1	2:V:434:ASP:O	2.24	0.56
2:L:79:THR:HG22	2:L:265:PHE:HD1	1.69	0.56
1:Y:31:GLU:OE1	1:Y:31:GLU:HA	2.04	0.56
2:Z:151:GLU:HG3	2:Z:160:TYR:HE2	1.70	0.56
1:E:36:LEU:O	1:E:36:LEU:HD23	2.04	0.56
1:K:31:GLU:OE1	1:K:31:GLU:HA	2.04	0.56
1:O:31:GLU:HA	1:O:31:GLU:OE1	2.04	0.56
1:Y:127:THR:O	1:Y:131:ASN:HB2	2.06	0.56
2:d:133:PHE:HD2	2:d:137:THR:CG2	2.19	0.56
2:D:133:PHE:HD2	2:D:137:THR:CG2	2.19	0.56
1:O:127:THR:O	1:O:131:ASN:HB2	2.06	0.56
2:P:133:PHE:HD2	2:P:137:THR:CG2	2.19	0.56
2:R:133:PHE:HD2	2:R:137:THR:CG2	2.19	0.56
2:R:488:LEU:HG	2:d:397:THR:HG21	1.86	0.56
1:W:127:THR:O	1:W:131:ASN:HB2	2.06	0.56
2:Z:133:PHE:HD2	2:Z:137:THR:CG2	2.19	0.56
1:c:31:GLU:OE1	1:c:31:GLU:HA	2.04	0.56
2:B:133:PHE:HD2	2:B:137:THR:CG2	2.19	0.56
1:C:31:GLU:OE1	1:C:31:GLU:HA	2.04	0.56
1:E:31:GLU:OE1	1:E:31:GLU:HA	2.04	0.56
1:S:36:LEU:O	1:S:36:LEU:HD23	2.05	0.56
1:S:127:THR:O	1:S:131:ASN:HB2	2.06	0.56
1:U:127:THR:O	1:U:131:ASN:HB2	2.06	0.56
2:V:151:GLU:HG3	2:V:160:TYR:HE2	1.70	0.56
2:X:434:ASP:OD1	2:X:434:ASP:O	2.24	0.56
2:b:133:PHE:HD2	2:b:137:THR:CG2	2.19	0.56
1:A:127:THR:O	1:A:131:ASN:HB2	2.06	0.56
1:E:127:THR:O	1:E:131:ASN:HB2	2.06	0.56
2:H:151:GLU:HG3	2:H:160:TYR:HE2	1.70	0.56
2:L:434:ASP:OD1	2:L:434:ASP:O	2.24	0.56
2:N:133:PHE:HD2	2:N:137:THR:CG2	2.19	0.56
1:Q:31:GLU:OE1	1:Q:31:GLU:HA	2.04	0.56
1:Q:61:LYS:O	2:R:119:LEU:HD13	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:434:ASP:OD1	2:T:434:ASP:O	2.24	0.56
1:a:127:THR:O	1:a:131:ASN:HB2	2.06	0.56
1:G:127:THR:O	1:G:131:ASN:HB2	2.06	0.56
1:I:68:ASP:OD1	2:X:214:ARG:HD3	2.04	0.56
2:F:133:PHE:HD2	2:F:137:THR:CG2	2.19	0.56
1:G:61:LYS:O	2:H:119:LEU:HD13	2.06	0.56
1:A:68:ASP:OD1	2:P:214:ARG:HD3	2.06	0.55
2:B:440:SER:O	2:B:441:THR:CG2	2.53	0.55
2:D:489:VAL:HG11	2:D:493:PRO:HD3	1.88	0.55
2:P:244:MET:HE1	2:P:345:LEU:CD2	2.27	0.55
2:R:489:VAL:HG11	2:R:493:PRO:HD3	1.88	0.55
2:T:489:VAL:HG11	2:T:493:PRO:HD3	1.88	0.55
1:W:31:GLU:HA	1:W:31:GLU:OE1	2.04	0.55
2:X:151:GLU:HG3	2:X:160:TYR:HE2	1.70	0.55
1:a:61:LYS:O	2:b:119:LEU:HD13	2.06	0.55
2:b:440:SER:O	2:b:441:THR:CG2	2.53	0.55
1:A:61:LYS:O	2:B:119:LEU:HD13	2.06	0.55
2:D:327:VAL:HG12	2:d:223:PRO:HG2	1.88	0.55
2:F:489:VAL:HG11	2:F:493:PRO:HD3	1.89	0.55
2:J:434:ASP:O	2:J:434:ASP:OD1	2.24	0.55
2:L:133:PHE:HD2	2:L:137:THR:CG2	2.19	0.55
2:R:355:HIS:NE2	2:R:359:THR:O	2.38	0.55
1:S:61:LYS:O	2:T:119:LEU:HD13	2.06	0.55
2:Z:440:SER:O	2:Z:441:THR:CG2	2.53	0.55
2:d:489:VAL:HG11	2:d:493:PRO:HD3	1.89	0.55
1:C:68:ASP:OD1	2:R:214:ARG:HD3	2.06	0.55
1:C:127:THR:O	1:C:131:ASN:HB2	2.06	0.55
1:E:61:LYS:O	2:F:119:LEU:HD13	2.06	0.55
2:F:434:ASP:OD1	2:F:434:ASP:O	2.24	0.55
1:U:61:LYS:O	2:V:119:LEU:HD13	2.06	0.55
1:c:127:THR:O	1:c:131:ASN:HB2	2.06	0.55
2:H:434:ASP:OD1	2:H:434:ASP:O	2.24	0.55
1:I:127:THR:O	1:I:131:ASN:HB2	2.06	0.55
2:P:489:VAL:HG11	2:P:493:PRO:HD3	1.88	0.55
2:X:244:MET:HE1	2:X:345:LEU:CD2	2.27	0.55
1:c:61:LYS:O	2:d:119:LEU:HD13	2.06	0.55
1:C:61:LYS:O	2:D:119:LEU:HD13	2.06	0.55
1:I:61:LYS:O	2:J:119:LEU:HD13	2.06	0.55
2:N:434:ASP:OD1	2:N:434:ASP:O	2.24	0.55
2:N:440:SER:O	2:N:441:THR:CG2	2.53	0.55
2:V:133:PHE:HD2	2:V:137:THR:CG2	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:355:HIS:NE2	2:B:359:THR:O	2.38	0.55
1:G:68:ASP:OD1	2:V:214:ARG:HD3	2.06	0.55
1:K:127:THR:O	1:K:131:ASN:HB2	2.06	0.55
1:M:68:ASP:OD1	2:b:214:ARG:HD3	2.06	0.55
2:P:434:ASP:OD1	2:P:434:ASP:O	2.24	0.55
2:B:57:SER:HB2	1:a:117:ASP:OD2	2.07	0.55
2:B:434:ASP:O	2:B:434:ASP:OD1	2.24	0.55
2:D:57:SER:HB2	1:c:117:ASP:OD2	2.07	0.55
2:H:489:VAL:HG11	2:H:493:PRO:HD3	1.89	0.55
2:J:133:PHE:HD2	2:J:137:THR:CG2	2.19	0.55
1:O:61:LYS:O	2:P:119:LEU:HD13	2.06	0.55
1:Q:127:THR:O	1:Q:131:ASN:HB2	2.06	0.55
1:W:61:LYS:O	2:X:119:LEU:HD13	2.06	0.55
1:a:47:ALA:HA	1:a:79:PRO:HA	1.89	0.55
2:b:355:HIS:NE2	2:b:359:THR:O	2.38	0.55
1:A:47:ALA:HA	1:A:79:PRO:HA	1.89	0.55
2:H:133:PHE:HD2	2:H:137:THR:CG2	2.19	0.55
2:X:108:THR:HG21	2:X:291:ASN:HD22	1.72	0.55
2:b:434:ASP:O	2:b:434:ASP:OD1	2.24	0.55
1:A:26:GLU:OE1	2:D:487:ARG:NH2	2.39	0.55
2:B:327:VAL:HG12	2:b:223:PRO:HG2	1.88	0.55
2:B:489:VAL:HG11	2:B:493:PRO:HD3	1.88	0.55
2:D:434:ASP:OD1	2:D:434:ASP:O	2.24	0.55
1:K:47:ALA:HA	1:K:79:PRO:HA	1.89	0.55
1:K:61:LYS:O	2:L:119:LEU:HD13	2.06	0.55
1:M:47:ALA:HA	1:M:79:PRO:HA	1.89	0.55
2:P:108:THR:HG21	2:P:291:ASN:HD22	1.72	0.55
2:P:440:SER:O	2:P:441:THR:CG2	2.53	0.55
1:Y:47:ALA:HA	1:Y:79:PRO:HA	1.89	0.55
2:b:489:VAL:HG11	2:b:493:PRO:HD3	1.88	0.55
2:d:434:ASP:OD1	2:d:434:ASP:O	2.24	0.55
2:D:440:SER:O	2:D:441:THR:CG2	2.53	0.55
2:N:108:THR:HG21	2:N:291:ASN:HD22	1.72	0.55
2:V:108:THR:HG21	2:V:291:ASN:HD22	1.72	0.55
1:Y:61:LYS:O	2:Z:119:LEU:HD13	2.06	0.55
1:M:43:MET:HE2	2:N:163:LEU:CG	2.38	0.54
2:R:108:THR:HG21	2:R:291:ASN:HD22	1.72	0.54
2:Z:434:ASP:O	2:Z:434:ASP:OD1	2.24	0.54
1:a:43:MET:HE2	2:b:163:LEU:CG	2.38	0.54
2:d:440:SER:O	2:d:441:THR:CG2	2.53	0.54
1:A:43:MET:HE2	2:B:163:LEU:CG	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:108:THR:HG21	2:D:291:ASN:HD22	1.72	0.54
2:F:108:THR:HG21	2:F:291:ASN:HD22	1.72	0.54
2:T:151:GLU:HG3	2:T:160:TYR:HE2	1.70	0.54
2:V:489:VAL:HG11	2:V:493:PRO:HD3	1.88	0.54
1:A:36:LEU:HB3	2:B:403:TYR:HE1	1.73	0.54
2:L:440:SER:O	2:L:441:THR:CG2	2.53	0.54
1:M:61:LYS:O	2:N:119:LEU:HD13	2.06	0.54
1:M:127:THR:O	1:M:131:ASN:HB2	2.06	0.54
2:N:489:VAL:HG11	2:N:493:PRO:HD3	1.88	0.54
1:O:43:MET:HE2	2:P:163:LEU:CG	2.38	0.54
2:P:151:GLU:HG3	2:P:160:TYR:HE2	1.70	0.54
1:S:47:ALA:HA	1:S:79:PRO:HA	1.89	0.54
1:Y:43:MET:HE2	2:Z:163:LEU:CG	2.38	0.54
1:a:36:LEU:HB3	2:b:403:TYR:HE1	1.73	0.54
2:d:108:THR:HG21	2:d:291:ASN:HD22	1.72	0.54
1:G:47:ALA:HA	1:G:79:PRO:HA	1.89	0.54
1:O:47:ALA:HA	1:O:79:PRO:HA	1.89	0.54
2:P:244:MET:HE2	2:P:350:PHE:CB	2.38	0.54
2:R:434:ASP:O	2:R:434:ASP:OD1	2.24	0.54
2:Z:108:THR:HG21	2:Z:291:ASN:HD22	1.72	0.54
1:G:43:MET:HE2	2:H:163:LEU:CG	2.38	0.54
2:J:126:LEU:HG	2:J:178:LEU:HD11	1.90	0.54
2:T:133:PHE:HD2	2:T:137:THR:CG2	2.19	0.54
2:X:355:HIS:NE2	2:X:359:THR:O	2.38	0.54
1:C:43:MET:HE2	2:D:163:LEU:CG	2.38	0.54
2:D:151:GLU:HG3	2:D:160:TYR:HE2	1.70	0.54
2:H:108:THR:HG21	2:H:291:ASN:HD22	1.72	0.54
2:J:108:THR:HG21	2:J:291:ASN:HD22	1.72	0.54
2:J:355:HIS:NE2	2:J:359:THR:O	2.38	0.54
1:M:36:LEU:HB3	2:N:403:TYR:HE1	1.73	0.54
2:R:390:ARG:NH1	2:d:464:PRO:HG2	2.23	0.54
1:S:43:MET:HE2	2:T:163:LEU:CG	2.38	0.54
1:W:47:ALA:HA	1:W:79:PRO:HA	1.89	0.54
2:X:126:LEU:HG	2:X:178:LEU:HD11	1.90	0.54
2:X:133:PHE:HD2	2:X:137:THR:CG2	2.19	0.54
1:c:43:MET:HE2	2:d:163:LEU:CG	2.38	0.54
2:d:151:GLU:HG3	2:d:160:TYR:HE2	1.70	0.54
2:D:126:LEU:HG	2:D:178:LEU:HD11	1.90	0.54
2:D:244:MET:HE2	2:D:350:PHE:CB	2.38	0.54
1:E:36:LEU:HB3	2:F:403:TYR:HE1	1.73	0.54
1:I:36:LEU:HB3	2:J:403:TYR:HE1	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:126:LEU:HG	2:L:178:LEU:HD11	1.90	0.54
2:L:355:HIS:NE2	2:L:359:THR:O	2.38	0.54
2:R:126:LEU:HG	2:R:178:LEU:HD11	1.90	0.54
2:T:108:THR:HG21	2:T:291:ASN:HD22	1.72	0.54
2:T:244:MET:HE2	2:T:350:PHE:CB	2.38	0.54
1:W:36:LEU:HB3	2:X:403:TYR:HE1	1.73	0.54
2:Z:126:LEU:HG	2:Z:178:LEU:HD11	1.90	0.54
2:Z:489:VAL:HG11	2:Z:493:PRO:HD3	1.88	0.54
2:d:126:LEU:HG	2:d:178:LEU:HD11	1.90	0.54
2:d:244:MET:HE2	2:d:350:PHE:CB	2.38	0.54
2:F:390:ARG:NH1	2:R:464:PRO:HG2	2.23	0.54
1:K:43:MET:HE2	2:L:163:LEU:CG	2.38	0.54
2:L:390:ARG:NH1	2:X:464:PRO:HG2	2.23	0.54
2:L:489:VAL:HG11	2:L:493:PRO:HD3	1.88	0.54
1:S:36:LEU:HB3	2:T:403:TYR:HE1	1.73	0.54
1:U:36:LEU:HB3	2:V:403:TYR:HE1	1.73	0.54
1:U:43:MET:HE2	2:V:163:LEU:CG	2.38	0.54
2:V:126:LEU:HG	2:V:178:LEU:HD11	1.90	0.54
2:X:440:SER:O	2:X:441:THR:CG2	2.53	0.54
2:F:244:MET:HE2	2:F:350:PHE:CB	2.38	0.54
1:G:36:LEU:HB3	2:H:403:TYR:HE1	1.73	0.54
1:K:36:LEU:HB3	2:L:403:TYR:HE1	1.73	0.54
2:N:126:LEU:HG	2:N:178:LEU:HD11	1.90	0.54
1:O:36:LEU:HB3	2:P:403:TYR:HE1	1.73	0.54
2:P:126:LEU:HG	2:P:178:LEU:HD11	1.90	0.54
1:Q:36:LEU:HB3	2:R:403:TYR:HE1	1.73	0.54
2:V:121:ILE:O	2:V:167:TYR:OH	2.24	0.54
2:B:126:LEU:HG	2:B:178:LEU:HD11	1.90	0.54
2:B:244:MET:HE2	2:B:350:PHE:CB	2.38	0.54
2:F:126:LEU:HG	2:F:178:LEU:HD11	1.90	0.54
2:J:489:VAL:HG11	2:J:493:PRO:HD3	1.88	0.54
1:Q:47:ALA:HA	1:Q:79:PRO:HA	1.89	0.54
2:Z:244:MET:HE2	2:Z:350:PHE:CB	2.38	0.54
2:b:126:LEU:HG	2:b:178:LEU:HD11	1.90	0.54
2:b:151:GLU:HG3	2:b:160:TYR:HE2	1.70	0.54
2:b:244:MET:HE2	2:b:350:PHE:CB	2.38	0.54
2:B:151:GLU:HG3	2:B:160:TYR:HE2	1.70	0.53
1:C:36:LEU:HB3	2:D:403:TYR:HE1	1.73	0.53
1:E:22:GLU:O	2:H:485:SER:HA	2.08	0.53
2:H:126:LEU:HG	2:H:178:LEU:HD11	1.90	0.53
1:I:43:MET:HE2	2:J:163:LEU:CG	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:108:THR:HG21	2:L:291:ASN:HD22	1.72	0.53
1:Q:43:MET:HE2	2:R:163:LEU:CG	2.38	0.53
2:X:489:VAL:HG11	2:X:493:PRO:HD3	1.89	0.53
1:E:43:MET:HE2	2:F:163:LEU:CG	2.38	0.53
2:F:355:HIS:NE2	2:F:359:THR:O	2.38	0.53
2:V:355:HIS:NE2	2:V:359:THR:O	2.38	0.53
1:Y:36:LEU:HB3	2:Z:403:TYR:HE1	1.73	0.53
2:b:108:THR:HG21	2:b:291:ASN:HD22	1.72	0.53
1:c:36:LEU:HB3	2:d:403:TYR:HE1	1.73	0.53
2:B:108:THR:HG21	2:B:291:ASN:HD22	1.72	0.53
1:C:47:ALA:HA	1:C:79:PRO:HA	1.89	0.53
2:R:151:GLU:HG3	2:R:160:TYR:HE2	1.71	0.53
2:T:126:LEU:HG	2:T:178:LEU:HD11	1.90	0.53
2:B:53:LEU:HD11	1:a:87:ASN:HD21	1.72	0.53
2:F:121:ILE:O	2:F:167:TYR:OH	2.24	0.53
1:I:47:ALA:HA	1:I:79:PRO:HA	1.89	0.53
2:Z:355:HIS:NE2	2:Z:359:THR:O	2.38	0.53
1:c:47:ALA:HA	1:c:79:PRO:HA	1.89	0.53
2:H:390:ARG:NH1	2:T:464:PRO:HG2	2.24	0.53
2:J:151:GLU:HG3	2:J:160:TYR:HE2	1.71	0.53
2:P:390:ARG:NH1	2:b:464:PRO:HG2	2.23	0.53
1:W:43:MET:HE2	2:X:163:LEU:CG	2.38	0.53
1:E:47:ALA:HA	1:E:79:PRO:HA	1.89	0.53
2:J:244:MET:HE2	2:J:350:PHE:CB	2.38	0.53
1:K:22:GLU:O	2:N:485:SER:HA	2.09	0.53
2:L:244:MET:HE2	2:L:350:PHE:CB	2.38	0.53
2:N:244:MET:HE2	2:N:350:PHE:CB	2.38	0.53
2:N:390:ARG:NH1	2:Z:464:PRO:HG2	2.24	0.53
2:R:244:MET:HE2	2:R:350:PHE:CB	2.38	0.53
2:R:440:SER:O	2:R:441:THR:CG2	2.53	0.53
2:H:244:MET:HE2	2:H:350:PHE:CB	2.38	0.53
2:X:121:ILE:O	2:X:167:TYR:OH	2.24	0.53
2:D:53:LEU:HD11	1:c:87:ASN:HD21	1.72	0.53
2:H:148:TYR:O	2:H:153:GLY:N	2.42	0.53
2:F:440:SER:O	2:F:441:THR:CG2	2.53	0.53
2:J:148:TYR:O	2:J:153:GLY:N	2.42	0.53
2:J:440:SER:O	2:J:441:THR:CG2	2.53	0.53
1:U:47:ALA:HA	1:U:79:PRO:HA	1.89	0.53
2:V:244:MET:HE2	2:V:350:PHE:CB	2.38	0.53
2:Z:148:TYR:O	2:Z:153:GLY:N	2.42	0.53
1:A:22:GLU:O	2:D:485:SER:HA	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:148:TYR:O	2:F:153:GLY:N	2.42	0.52
2:P:121:ILE:O	2:P:167:TYR:OH	2.24	0.52
2:B:148:TYR:O	2:B:153:GLY:N	2.42	0.52
2:N:355:HIS:NE2	2:N:359:THR:O	2.38	0.52
2:P:355:HIS:NE2	2:P:359:THR:O	2.38	0.52
1:U:22:GLU:O	2:X:485:SER:HA	2.10	0.52
2:b:148:TYR:O	2:b:153:GLY:N	2.42	0.52
1:O:122:LEU:HD22	2:P:74:LEU:HD11	1.91	0.52
2:H:355:HIS:NE2	2:H:359:THR:O	2.38	0.52
1:I:22:GLU:O	2:L:485:SER:HA	2.10	0.52
1:M:122:LEU:HD22	2:N:74:LEU:HD11	1.91	0.52
2:B:390:ARG:NH1	2:N:464:PRO:HG2	2.25	0.52
2:F:151:GLU:HG3	2:F:160:TYR:HE2	1.70	0.52
1:Y:122:LEU:HD22	2:Z:74:LEU:HD11	1.91	0.52
2:X:244:MET:HE2	2:X:350:PHE:CB	2.38	0.52
1:G:122:LEU:HD22	2:H:74:LEU:HD11	1.91	0.52
2:H:42:GLU:O	2:H:46:ARG:NE	2.40	0.52
2:L:244:MET:HE1	2:L:345:LEU:CD2	2.27	0.52
2:N:42:GLU:O	2:N:46:ARG:NE	2.40	0.52
2:N:151:GLU:HG3	2:N:160:TYR:HE2	1.70	0.52
2:X:148:TYR:O	2:X:153:GLY:N	2.42	0.52
2:H:440:SER:O	2:H:441:THR:CG2	2.53	0.52
2:J:390:ARG:NH1	2:V:464:PRO:HG2	2.24	0.52
2:N:437:PRO:HB2	2:N:441:THR:HG21	1.92	0.52
1:O:22:GLU:O	2:R:485:SER:HA	2.10	0.52
2:B:367:ALA:HB3	2:B:392:PRO:HD3	1.92	0.52
2:F:437:PRO:HB2	2:F:441:THR:HG21	1.92	0.52
2:P:367:ALA:HB3	2:P:392:PRO:HD3	1.92	0.52
1:S:122:LEU:HD22	2:T:74:LEU:HD11	1.91	0.52
1:U:122:LEU:HD22	2:V:74:LEU:HD11	1.91	0.52
2:V:437:PRO:HB2	2:V:441:THR:HG21	1.92	0.52
2:V:440:SER:O	2:V:441:THR:CG2	2.53	0.52
2:Z:437:PRO:HB2	2:Z:441:THR:HG21	1.92	0.52
1:A:122:LEU:HD22	2:B:74:LEU:HD11	1.91	0.52
1:C:122:LEU:HD22	2:D:74:LEU:HD11	1.91	0.52
1:K:37:PRO:HB3	2:L:113:GLN:HA	1.92	0.52
2:L:121:ILE:O	2:L:167:TYR:OH	2.24	0.52
2:R:437:PRO:HB2	2:R:441:THR:HG21	1.92	0.52
1:a:122:LEU:HD22	2:b:74:LEU:HD11	1.91	0.52
2:b:367:ALA:HB3	2:b:392:PRO:HD3	1.92	0.52
2:D:367:ALA:HB3	2:D:392:PRO:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:390:ARG:NH1	2:P:464:PRO:HG2	2.25	0.51
1:G:22:GLU:O	2:J:485:SER:HA	2.10	0.51
1:M:37:PRO:HB3	2:N:113:GLN:HA	1.92	0.51
2:N:367:ALA:HB3	2:N:392:PRO:HD3	1.92	0.51
2:T:367:ALA:HB3	2:T:392:PRO:HD3	1.92	0.51
1:c:122:LEU:HD22	2:d:74:LEU:HD11	1.91	0.51
2:H:367:ALA:HB3	2:H:392:PRO:HD3	1.92	0.51
1:I:37:PRO:HB3	2:J:113:GLN:HA	1.92	0.51
1:I:54:GLN:NE2	2:J:120:ASN:HD21	2.09	0.51
1:I:122:LEU:HD22	2:J:74:LEU:HD11	1.91	0.51
2:R:367:ALA:HB3	2:R:392:PRO:HD3	1.92	0.51
2:V:148:TYR:O	2:V:153:GLY:N	2.42	0.51
1:W:54:GLN:NE2	2:X:120:ASN:HD21	2.09	0.51
2:d:367:ALA:HB3	2:d:392:PRO:HD3	1.92	0.51
2:B:52:ALA:HB1	1:a:121:LYS:HB2	1.92	0.51
2:F:367:ALA:HB3	2:F:392:PRO:HD3	1.92	0.51
1:Q:122:LEU:HD22	2:R:74:LEU:HD11	1.91	0.51
1:S:22:GLU:O	2:V:485:SER:HA	2.11	0.51
1:U:54:GLN:NE2	2:V:120:ASN:HD21	2.09	0.51
1:Y:37:PRO:HB3	2:Z:113:GLN:HA	1.92	0.51
1:E:122:LEU:HD22	2:F:74:LEU:HD11	1.91	0.51
1:Q:22:GLU:O	2:T:485:SER:HA	2.11	0.51
1:S:54:GLN:NE2	2:T:120:ASN:HD21	2.09	0.51
2:V:367:ALA:HB3	2:V:392:PRO:HD3	1.92	0.51
1:W:37:PRO:HB3	2:X:113:GLN:HA	1.92	0.51
2:b:437:PRO:HB2	2:b:441:THR:HG21	1.92	0.51
2:B:437:PRO:HB2	2:B:441:THR:HG21	1.92	0.51
1:W:122:LEU:HD22	2:X:74:LEU:HD11	1.91	0.51
2:Z:121:ILE:O	2:Z:167:TYR:OH	2.24	0.51
2:Z:367:ALA:HB3	2:Z:392:PRO:HD3	1.92	0.51
1:K:54:GLN:NE2	2:L:120:ASN:HD21	2.09	0.51
2:J:367:ALA:HB3	2:J:392:PRO:HD3	1.92	0.51
2:T:440:SER:O	2:T:441:THR:CG2	2.53	0.51
1:A:37:PRO:HB3	2:B:113:GLN:HA	1.92	0.51
2:D:437:PRO:HB2	2:D:441:THR:HG21	1.92	0.51
2:H:437:PRO:HB2	2:H:441:THR:HG21	1.92	0.51
2:T:148:TYR:O	2:T:153:GLY:N	2.42	0.51
1:a:37:PRO:HB3	2:b:113:GLN:HA	1.92	0.51
2:d:437:PRO:HB2	2:d:441:THR:HG21	1.92	0.51
1:M:22:GLU:O	2:P:485:SER:HA	2.10	0.51
1:S:36:LEU:HD12	2:T:406:CYS:SG	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:355:HIS:NE2	2:T:359:THR:O	2.38	0.51
1:Y:54:GLN:NE2	2:Z:120:ASN:HD21	2.09	0.51
1:c:36:LEU:HD12	2:d:406:CYS:SG	2.51	0.51
1:A:54:GLN:NE2	2:B:120:ASN:HD21	2.09	0.51
1:C:36:LEU:HD12	2:D:406:CYS:SG	2.51	0.51
2:D:121:ILE:O	2:D:167:TYR:OH	2.24	0.51
1:E:54:GLN:NE2	2:F:120:ASN:HD21	2.09	0.51
2:H:121:ILE:O	2:H:167:TYR:OH	2.24	0.51
2:L:367:ALA:HB3	2:L:392:PRO:HD3	1.92	0.51
1:O:37:PRO:HB3	2:P:113:GLN:HA	1.92	0.51
1:C:54:GLN:NE2	2:D:120:ASN:HD21	2.09	0.50
1:M:54:GLN:NE2	2:N:120:ASN:HD21	2.09	0.50
1:U:37:PRO:HB3	2:V:113:GLN:HA	1.92	0.50
1:a:54:GLN:NE2	2:b:120:ASN:HD21	2.09	0.50
1:A:27:LEU:HD22	2:P:376:TYR:CZ	2.47	0.50
2:L:437:PRO:HB2	2:L:441:THR:HG21	1.92	0.50
2:X:367:ALA:HB3	2:X:392:PRO:HD3	1.92	0.50
2:X:382:THR:O	2:X:386:ASN:ND2	2.38	0.50
1:c:54:GLN:NE2	2:d:120:ASN:HD21	2.09	0.50
1:E:37:PRO:HB3	2:F:113:GLN:HA	1.92	0.50
1:I:36:LEU:HD12	2:J:406:CYS:SG	2.51	0.50
1:K:122:LEU:HD22	2:L:74:LEU:HD11	1.91	0.50
1:O:36:LEU:HD12	2:P:406:CYS:SG	2.51	0.50
1:Q:37:PRO:HB3	2:R:113:GLN:HA	1.92	0.50
1:G:37:PRO:HB3	2:H:113:GLN:HA	1.92	0.50
1:G:54:GLN:NE2	2:H:120:ASN:HD21	2.09	0.50
1:Q:54:GLN:NE2	2:R:120:ASN:HD21	2.09	0.50
1:S:37:PRO:HB3	2:T:113:GLN:HA	1.92	0.50
2:d:382:THR:O	2:d:386:ASN:ND2	2.38	0.50
2:D:382:THR:O	2:D:386:ASN:ND2	2.38	0.50
1:G:36:LEU:HD12	2:H:406:CYS:SG	2.51	0.50
2:P:148:TYR:O	2:P:153:GLY:N	2.42	0.50
1:Q:36:LEU:HD12	2:R:406:CYS:SG	2.51	0.50
2:R:42:GLU:O	2:R:46:ARG:NE	2.40	0.50
2:R:148:TYR:O	2:R:153:GLY:N	2.42	0.50
2:V:42:GLU:O	2:V:46:ARG:NE	2.40	0.50
1:Y:36:LEU:HD12	2:Z:406:CYS:SG	2.51	0.50
1:C:22:GLU:O	2:F:485:SER:HA	2.12	0.50
2:D:52:ALA:HB1	1:c:121:LYS:HB2	1.93	0.50
2:J:382:THR:O	2:J:386:ASN:ND2	2.38	0.50
2:N:148:TYR:O	2:N:153:GLY:N	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:36:LEU:HD12	2:X:406:CYS:SG	2.51	0.50
1:A:36:LEU:HD12	2:B:406:CYS:SG	2.51	0.50
2:B:332:PRO:HD2	2:B:355:HIS:CD2	2.47	0.50
1:K:36:LEU:HD12	2:L:406:CYS:SG	2.51	0.50
2:N:332:PRO:HD2	2:N:355:HIS:CD2	2.47	0.50
2:V:332:PRO:HD2	2:V:355:HIS:CD2	2.47	0.50
1:a:36:LEU:HD12	2:b:406:CYS:SG	2.51	0.50
2:b:332:PRO:HD2	2:b:355:HIS:CD2	2.47	0.50
1:C:37:PRO:HB3	2:D:113:GLN:HA	1.92	0.50
2:D:490:SER:OG	2:P:387:LEU:HD11	2.12	0.50
1:E:36:LEU:HD12	2:F:406:CYS:SG	2.51	0.50
1:M:27:LEU:HD22	2:b:376:TYR:CZ	2.47	0.50
1:E:24:ASP:OD2	2:H:487:ARG:NH1	2.45	0.50
2:F:332:PRO:HD2	2:F:355:HIS:CD2	2.47	0.50
1:I:109:PRO:HD3	2:J:253:TYR:CE2	2.47	0.50
2:J:79:THR:HG22	2:J:265:PHE:HA	1.94	0.50
2:L:382:THR:O	2:L:386:ASN:ND2	2.38	0.50
2:R:121:ILE:O	2:R:167:TYR:OH	2.24	0.50
2:R:332:PRO:HD2	2:R:355:HIS:CD2	2.47	0.50
1:U:36:LEU:HD12	2:V:406:CYS:SG	2.51	0.50
2:V:79:THR:HG22	2:V:265:PHE:HA	1.94	0.50
1:a:22:GLU:O	2:d:485:SER:HA	2.12	0.50
1:c:37:PRO:HB3	2:d:113:GLN:HA	1.92	0.50
2:H:332:PRO:HD2	2:H:355:HIS:CD2	2.47	0.49
2:L:79:THR:HG22	2:L:265:PHE:HA	1.94	0.49
1:W:109:PRO:HD3	2:X:253:TYR:CE2	2.48	0.49
2:X:79:THR:HG22	2:X:265:PHE:HA	1.94	0.49
1:A:109:PRO:HD3	2:B:253:TYR:CE2	2.47	0.49
2:B:490:SER:OG	2:N:387:LEU:HD11	2.12	0.49
2:D:355:HIS:NE2	2:D:359:THR:O	2.38	0.49
1:E:109:PRO:HD3	2:F:253:TYR:CE2	2.47	0.49
2:J:332:PRO:HD2	2:J:355:HIS:CD2	2.47	0.49
2:V:382:THR:O	2:V:386:ASN:ND2	2.38	0.49
1:a:109:PRO:HD3	2:b:253:TYR:CE2	2.47	0.49
2:b:42:GLU:O	2:b:46:ARG:NE	2.40	0.49
2:d:148:TYR:O	2:d:153:GLY:N	2.42	0.49
2:D:148:TYR:O	2:D:153:GLY:N	2.42	0.49
1:G:27:LEU:HD22	2:V:376:TYR:CZ	2.48	0.49
1:K:109:PRO:HD3	2:L:253:TYR:CE2	2.47	0.49
2:L:147:LEU:HB3	2:L:189:MET:SD	2.53	0.49
1:M:18:ARG:HD2	2:P:342:GLU:OE1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:109:PRO:HD3	2:P:253:TYR:CE2	2.47	0.49
2:P:332:PRO:HD2	2:P:355:HIS:CD2	2.47	0.49
1:Q:109:PRO:HD3	2:R:253:TYR:CE2	2.48	0.49
1:W:36:LEU:HD11	2:X:159:PRO:HG2	1.95	0.49
1:Y:22:GLU:O	2:b:485:SER:HA	2.11	0.49
2:d:355:HIS:NE2	2:d:359:THR:O	2.38	0.49
1:A:24:ASP:OD2	2:D:487:ARG:NH1	2.45	0.49
2:B:42:GLU:O	2:B:46:ARG:NE	2.40	0.49
2:B:121:ILE:O	2:B:167:TYR:OH	2.24	0.49
2:H:79:THR:HG22	2:H:265:PHE:HA	1.94	0.49
2:L:148:TYR:O	2:L:153:GLY:N	2.42	0.49
1:O:54:GLN:NE2	2:P:120:ASN:HD21	2.09	0.49
2:P:437:PRO:HB2	2:P:441:THR:HG21	1.92	0.49
1:S:109:PRO:HD3	2:T:253:TYR:CE2	2.47	0.49
1:U:109:PRO:HD3	2:V:253:TYR:CE2	2.47	0.49
2:d:79:THR:HG22	2:d:265:PHE:HA	1.94	0.49
1:C:27:LEU:HD22	2:R:376:TYR:CZ	2.47	0.49
2:D:79:THR:HG22	2:D:265:PHE:HA	1.94	0.49
2:D:147:LEU:HB3	2:D:189:MET:SD	2.53	0.49
1:I:36:LEU:HD11	2:J:159:PRO:HG2	1.95	0.49
2:X:208:GLN:OE1	2:X:274:SER:OG	2.28	0.49
2:Z:79:THR:HG22	2:Z:265:PHE:HA	1.94	0.49
2:b:121:ILE:O	2:b:167:TYR:OH	2.24	0.49
2:D:208:GLN:OE1	2:D:274:SER:OG	2.28	0.49
2:F:147:LEU:HB3	2:F:189:MET:SD	2.53	0.49
2:J:130:LEU:HD12	2:J:178:LEU:HD11	1.94	0.49
2:N:147:LEU:HB3	2:N:189:MET:SD	2.53	0.49
2:P:79:THR:HG22	2:P:265:PHE:HA	1.94	0.49
2:R:183:ALA:HB2	2:R:240:ILE:CD1	2.41	0.49
2:T:332:PRO:HD2	2:T:355:HIS:CD2	2.47	0.49
2:Z:332:PRO:HD2	2:Z:355:HIS:CD2	2.47	0.49
2:Z:382:THR:O	2:Z:386:ASN:ND2	2.38	0.49
2:d:147:LEU:HB3	2:d:189:MET:SD	2.53	0.49
2:d:208:GLN:OE1	2:d:274:SER:OG	2.28	0.49
1:E:36:LEU:HD11	2:F:159:PRO:HG2	1.95	0.49
2:J:241:GLY:HA3	2:J:351:MET:HE2	1.95	0.49
1:K:36:LEU:HD11	2:L:159:PRO:HG2	1.95	0.49
1:M:36:LEU:HD12	2:N:406:CYS:SG	2.51	0.49
2:P:147:LEU:HB3	2:P:189:MET:SD	2.53	0.49
2:T:147:LEU:HB3	2:T:189:MET:SD	2.53	0.49
2:T:437:PRO:HB2	2:T:441:THR:HG21	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:130:LEU:HD12	2:V:178:LEU:HD11	1.94	0.49
2:D:332:PRO:HD2	2:D:355:HIS:CD2	2.47	0.49
2:F:79:THR:HG22	2:F:265:PHE:HA	1.94	0.49
2:J:147:LEU:HB3	2:J:189:MET:SD	2.53	0.49
2:L:484:VAL:HG22	2:X:469:SER:OG	2.13	0.49
1:M:109:PRO:HD3	2:N:253:TYR:CE2	2.48	0.49
2:P:241:GLY:HA3	2:P:351:MET:HE2	1.95	0.49
1:W:22:GLU:O	2:Z:485:SER:HA	2.12	0.49
2:X:332:PRO:HD2	2:X:355:HIS:CD2	2.47	0.49
2:B:147:LEU:HB3	2:B:189:MET:SD	2.53	0.49
2:F:208:GLN:OE1	2:F:274:SER:OG	2.28	0.49
1:G:18:ARG:HD2	2:J:342:GLU:OE1	2.13	0.49
2:H:183:ALA:HB2	2:H:240:ILE:CD1	2.41	0.49
1:K:24:ASP:OD2	2:N:487:ARG:NH1	2.46	0.49
2:L:208:GLN:OE1	2:L:274:SER:OG	2.28	0.49
2:L:436:ASP:CB	2:L:437:PRO:CD	2.91	0.49
2:N:241:GLY:HA3	2:N:351:MET:HE2	1.95	0.49
1:Q:36:LEU:HD11	2:R:159:PRO:HG2	1.95	0.49
1:U:36:LEU:HD11	2:V:159:PRO:HG2	1.95	0.49
2:d:241:GLY:HA3	2:d:351:MET:HE2	1.95	0.49
2:d:332:PRO:HD2	2:d:355:HIS:CD2	2.47	0.49
1:C:109:PRO:HD3	2:D:253:TYR:CE2	2.47	0.49
2:D:241:GLY:HA3	2:D:351:MET:HE2	1.95	0.49
2:F:130:LEU:HD12	2:F:178:LEU:HD11	1.94	0.49
2:F:484:VAL:HG22	2:R:469:SER:OG	2.13	0.49
1:G:109:PRO:HD3	2:H:253:TYR:CE2	2.48	0.49
2:H:79:THR:HG22	2:H:265:PHE:CD1	2.48	0.49
1:K:126:ARG:HB2	2:L:74:LEU:HD23	1.95	0.49
2:L:241:GLY:HA3	2:L:351:MET:HE2	1.95	0.49
1:O:27:LEU:HD22	2:d:376:TYR:CZ	2.48	0.49
2:R:484:VAL:HG22	2:d:469:SER:OG	2.13	0.49
2:T:241:GLY:HA3	2:T:351:MET:HE2	1.95	0.49
2:X:130:LEU:HD12	2:X:178:LEU:HD11	1.94	0.49
2:Z:436:ASP:CB	2:Z:437:PRO:CD	2.91	0.49
1:a:18:ARG:HD2	2:d:342:GLU:OE1	2.12	0.49
2:b:147:LEU:HB3	2:b:189:MET:SD	2.53	0.49
1:c:109:PRO:HD3	2:d:253:TYR:CE2	2.47	0.49
1:G:65:ILE:HG13	1:G:73:ARG:HG3	1.95	0.48
2:H:241:GLY:HA3	2:H:351:MET:HE2	1.95	0.48
1:I:126:ARG:HB2	2:J:74:LEU:HD23	1.95	0.48
2:R:147:LEU:HB3	2:R:189:MET:SD	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:126:ARG:HB2	2:V:74:LEU:HD23	1.95	0.48
2:V:79:THR:HG22	2:V:265:PHE:CD1	2.48	0.48
2:V:241:GLY:HA3	2:V:351:MET:HE2	1.95	0.48
1:W:126:ARG:HB2	2:X:74:LEU:HD23	1.95	0.48
1:c:36:LEU:HD11	2:d:159:PRO:HG2	1.95	0.48
2:B:208:GLN:OE1	2:B:274:SER:OG	2.28	0.48
1:C:36:LEU:HD11	2:D:159:PRO:HG2	1.95	0.48
1:E:65:ILE:HG13	1:E:73:ARG:HG3	1.95	0.48
2:F:241:GLY:HA3	2:F:351:MET:HE2	1.95	0.48
1:G:36:LEU:HD11	2:H:402:HIS:HB3	1.95	0.48
2:J:490:SER:OG	2:V:387:LEU:HD11	2.13	0.48
2:L:332:PRO:HD2	2:L:355:HIS:CD2	2.47	0.48
2:N:436:ASP:CB	2:N:437:PRO:CD	2.91	0.48
1:S:36:LEU:HD11	2:T:159:PRO:HG2	1.95	0.48
1:S:36:LEU:HD11	2:T:402:HIS:HB3	1.95	0.48
1:S:65:ILE:HG13	1:S:73:ARG:HG3	1.95	0.48
2:T:79:THR:HG22	2:T:265:PHE:CD1	2.48	0.48
2:T:79:THR:HG22	2:T:265:PHE:HA	1.94	0.48
2:V:147:LEU:HB3	2:V:189:MET:SD	2.53	0.48
2:X:147:LEU:HB3	2:X:189:MET:SD	2.53	0.48
2:X:437:PRO:HB2	2:X:441:THR:HG21	1.92	0.48
2:Z:147:LEU:HB3	2:Z:189:MET:SD	2.53	0.48
1:A:6:SER:O	1:A:9:LYS:N	2.44	0.48
2:B:241:GLY:HA3	2:B:351:MET:HE2	1.95	0.48
1:E:27:LEU:HD22	2:T:376:TYR:CZ	2.48	0.48
2:J:79:THR:HG22	2:J:265:PHE:CD1	2.48	0.48
2:J:121:ILE:O	2:J:167:TYR:OH	2.24	0.48
2:N:79:THR:HG22	2:N:265:PHE:HA	1.94	0.48
2:N:490:SER:OG	2:Z:387:LEU:HD11	2.13	0.48
1:S:18:ARG:HD2	2:V:342:GLU:OE1	2.12	0.48
1:U:65:ILE:HG13	1:U:73:ARG:HG3	1.95	0.48
1:W:18:ARG:HD2	2:Z:342:GLU:OE1	2.13	0.48
2:X:241:GLY:HA3	2:X:351:MET:HE2	1.95	0.48
1:Y:109:PRO:HD3	2:Z:253:TYR:CE2	2.48	0.48
2:Z:241:GLY:HA3	2:Z:351:MET:HE2	1.95	0.48
1:I:18:ARG:HD2	2:L:342:GLU:OE1	2.13	0.48
2:J:42:GLU:O	2:J:46:ARG:NE	2.40	0.48
1:K:74:LEU:CD1	2:L:98:TRP:CZ3	2.97	0.48
2:L:183:ALA:HB2	2:L:240:ILE:CD1	2.41	0.48
2:R:241:GLY:HA3	2:R:351:MET:HE2	1.95	0.48
2:T:130:LEU:HD12	2:T:178:LEU:HD11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:36:LEU:HD11	2:V:402:HIS:HB3	1.95	0.48
1:a:6:SER:O	1:a:9:LYS:N	2.44	0.48
2:b:208:GLN:OE1	2:b:274:SER:OG	2.28	0.48
2:b:241:GLY:HA3	2:b:351:MET:HE2	1.95	0.48
2:H:147:LEU:HB3	2:H:189:MET:SD	2.53	0.48
1:K:27:LEU:HD22	2:Z:376:TYR:CZ	2.48	0.48
1:S:126:ARG:HB2	2:T:74:LEU:HD23	1.95	0.48
1:W:74:LEU:CD1	2:X:98:TRP:CZ3	2.97	0.48
1:Y:18:ARG:HD2	2:b:342:GLU:OE1	2.12	0.48
1:Y:126:ARG:HB2	2:Z:74:LEU:HD23	1.95	0.48
1:A:36:LEU:HD11	2:B:402:HIS:HB3	1.95	0.48
1:C:74:LEU:CD1	2:D:98:TRP:CZ3	2.97	0.48
1:E:36:LEU:HD11	2:F:402:HIS:HB3	1.95	0.48
1:G:126:ARG:HB2	2:H:74:LEU:HD23	1.95	0.48
1:I:65:ILE:HG13	1:I:73:ARG:HG3	1.95	0.48
1:O:24:ASP:OD2	2:R:487:ARG:NH1	2.47	0.48
1:O:36:LEU:HD11	2:P:159:PRO:HG2	1.95	0.48
2:P:130:LEU:HD12	2:P:178:LEU:HD11	1.94	0.48
2:R:79:THR:HG22	2:R:265:PHE:HA	1.94	0.48
2:X:79:THR:HG22	2:X:265:PHE:CD1	2.48	0.48
1:Y:36:LEU:HD11	2:Z:159:PRO:HG2	1.95	0.48
1:c:74:LEU:CD1	2:d:98:TRP:CZ3	2.97	0.48
1:A:57:VAL:HG21	2:B:129:THR:HG21	1.96	0.48
2:H:171:GLN:OE1	2:H:201:VAL:HA	2.14	0.48
2:H:208:GLN:OE1	2:H:274:SER:OG	2.28	0.48
2:H:382:THR:O	2:H:386:ASN:ND2	2.38	0.48
1:M:126:ARG:HB2	2:N:74:LEU:HD23	1.95	0.48
1:Q:65:ILE:HG13	1:Q:73:ARG:HG3	1.95	0.48
1:c:40:MET:HE3	2:d:104:LEU:HD21	1.96	0.48
2:B:79:THR:HG22	2:B:265:PHE:HA	1.94	0.48
2:B:436:ASP:CB	2:B:437:PRO:CD	2.91	0.48
1:C:40:MET:HE3	2:D:104:LEU:HD21	1.96	0.48
2:J:171:GLN:OE1	2:J:201:VAL:HA	2.14	0.48
2:L:130:LEU:HD12	2:L:178:LEU:HD11	1.94	0.48
2:L:171:GLN:OE1	2:L:201:VAL:HA	2.14	0.48
1:O:74:LEU:CD1	2:P:98:TRP:CZ3	2.97	0.48
2:P:260:VAL:O	2:P:261:GLU:CG	2.60	0.48
1:Q:40:MET:HE3	2:R:104:LEU:HD21	1.96	0.48
2:T:171:GLN:OE1	2:T:201:VAL:HA	2.14	0.48
2:V:171:GLN:OE1	2:V:201:VAL:HA	2.14	0.48
2:X:171:GLN:OE1	2:X:201:VAL:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:74:LEU:CD1	2:Z:98:TRP:CZ3	2.97	0.48
1:a:36:LEU:HD11	2:b:402:HIS:HB3	1.96	0.48
2:b:79:THR:HG22	2:b:265:PHE:HA	1.94	0.48
1:A:40:MET:HE3	2:B:104:LEU:HD21	1.96	0.48
2:H:490:SER:OG	2:T:387:LEU:HD11	2.14	0.48
1:I:74:LEU:CD1	2:J:98:TRP:CZ3	2.97	0.48
1:M:36:LEU:HD11	2:N:402:HIS:HB3	1.95	0.48
1:O:36:LEU:HD11	2:P:402:HIS:HB3	1.95	0.48
1:O:40:MET:HE3	2:P:104:LEU:HD21	1.96	0.48
2:P:484:VAL:HG22	2:b:469:SER:OG	2.13	0.48
2:P:490:SER:OG	2:b:387:LEU:HD11	2.14	0.48
1:Q:18:ARG:HD2	2:T:342:GLU:OE1	2.13	0.48
1:Q:74:LEU:CD1	2:R:98:TRP:CZ3	2.97	0.48
1:U:24:ASP:OD2	2:X:487:ARG:NH1	2.46	0.48
2:Z:171:GLN:OE1	2:Z:201:VAL:HA	2.14	0.48
1:a:57:VAL:HG21	2:b:129:THR:HG21	1.96	0.48
2:b:436:ASP:CB	2:b:437:PRO:CD	2.91	0.48
1:A:74:LEU:CD1	2:B:98:TRP:CZ3	2.97	0.48
2:B:339:ASP:OD2	2:N:409:ARG:NH1	2.46	0.48
1:I:24:ASP:OD2	2:L:487:ARG:NH1	2.47	0.48
1:M:57:VAL:HG21	2:N:129:THR:HG21	1.96	0.48
2:R:130:LEU:HD12	2:R:178:LEU:HD11	1.94	0.48
1:W:65:ILE:HG13	1:W:73:ARG:HG3	1.95	0.48
1:a:36:LEU:HD11	2:b:159:PRO:HG2	1.95	0.48
1:a:40:MET:HE3	2:b:104:LEU:HD21	1.96	0.48
1:a:74:LEU:CD1	2:b:98:TRP:CZ3	2.97	0.48
2:d:130:LEU:HD12	2:d:178:LEU:HD11	1.94	0.48
1:A:36:LEU:HD11	2:B:159:PRO:HG2	1.95	0.47
1:C:18:ARG:HD2	2:F:342:GLU:OE1	2.13	0.47
2:D:130:LEU:HD12	2:D:178:LEU:HD11	1.94	0.47
2:D:339:ASP:OD2	2:P:409:ARG:NH1	2.46	0.47
2:F:171:GLN:OE1	2:F:201:VAL:HA	2.14	0.47
1:G:36:LEU:HD11	2:H:159:PRO:HG2	1.95	0.47
2:H:127:HIS:O	2:H:131:LYS:HB2	2.15	0.47
1:K:65:ILE:HG13	1:K:73:ARG:HG3	1.95	0.47
1:M:74:LEU:CD1	2:N:98:TRP:CZ3	2.97	0.47
2:N:171:GLN:OE1	2:N:201:VAL:HA	2.14	0.47
1:Q:36:LEU:HD11	2:R:402:HIS:HB3	1.95	0.47
1:Q:57:VAL:HG21	2:R:129:THR:HG21	1.96	0.47
2:R:127:HIS:O	2:R:131:LYS:HB2	2.15	0.47
1:U:74:LEU:CD1	2:V:98:TRP:CZ3	2.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:57:VAL:HG21	2:X:129:THR:HG21	1.96	0.47
1:c:65:ILE:HG13	1:c:73:ARG:HG3	1.95	0.47
1:E:40:MET:HE3	2:F:104:LEU:HD21	1.96	0.47
2:L:79:THR:HG22	2:L:265:PHE:CD1	2.48	0.47
2:N:382:THR:O	2:N:386:ASN:ND2	2.38	0.47
1:O:18:ARG:HD2	2:R:342:GLU:OE1	2.13	0.47
1:U:18:ARG:HD2	2:X:342:GLU:OE1	2.14	0.47
1:c:126:ARG:HB2	2:d:74:LEU:HD23	1.95	0.47
2:B:260:VAL:O	2:B:261:GLU:CG	2.60	0.47
1:C:65:ILE:HG13	1:C:73:ARG:HG3	1.95	0.47
1:C:126:ARG:HB2	2:D:74:LEU:HD23	1.95	0.47
1:G:74:LEU:CD1	2:H:98:TRP:CZ3	2.97	0.47
1:I:36:LEU:HD11	2:J:402:HIS:HB3	1.96	0.47
2:J:260:VAL:O	2:J:261:GLU:CG	2.60	0.47
1:K:57:VAL:HG21	2:L:129:THR:HG21	1.96	0.47
2:N:244:MET:HG2	2:N:245:PRO:HD2	1.94	0.47
2:P:183:ALA:HB2	2:P:240:ILE:CD1	2.41	0.47
1:Y:36:LEU:HD11	2:Z:402:HIS:HB3	1.95	0.47
2:b:260:VAL:O	2:b:261:GLU:CG	2.60	0.47
2:B:171:GLN:OE1	2:B:201:VAL:HA	2.14	0.47
2:B:484:VAL:HG22	2:N:469:SER:OG	2.15	0.47
1:C:97:LEU:HD21	2:D:85:ILE:HG23	1.97	0.47
1:E:57:VAL:HG21	2:F:129:THR:HG21	1.96	0.47
1:E:126:ARG:HB2	2:F:74:LEU:HD23	1.95	0.47
2:F:490:SER:OG	2:R:387:LEU:HD11	2.15	0.47
1:I:27:LEU:HD22	2:X:376:TYR:CZ	2.49	0.47
2:J:436:ASP:CB	2:J:437:PRO:CD	2.91	0.47
1:M:24:ASP:OD2	2:P:487:ARG:NH1	2.48	0.47
1:M:40:MET:HE3	2:N:104:LEU:HD21	1.96	0.47
2:N:484:VAL:HG22	2:Z:469:SER:OG	2.14	0.47
1:O:57:VAL:HG21	2:P:129:THR:HG21	1.96	0.47
1:Q:24:ASP:OD2	2:T:487:ARG:NH1	2.47	0.47
2:X:260:VAL:O	2:X:261:GLU:CG	2.60	0.47
2:b:171:GLN:OE1	2:b:201:VAL:HA	2.14	0.47
1:A:126:ARG:HB2	2:B:74:LEU:HD23	1.95	0.47
1:C:36:LEU:HD11	2:D:402:HIS:HB3	1.95	0.47
2:D:496:LYS:NZ	2:P:474:ARG:HD2	2.30	0.47
1:E:74:LEU:CD1	2:F:98:TRP:CZ3	2.97	0.47
1:M:36:LEU:HD11	2:N:159:PRO:HG2	1.95	0.47
1:M:97:LEU:HD21	2:N:85:ILE:HG23	1.97	0.47
2:P:436:ASP:N	2:P:437:PRO:HD2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:87:ASN:HD22	1:Q:95:LEU:HD22	1.80	0.47
2:V:260:VAL:O	2:V:261:GLU:CG	2.60	0.47
1:Y:65:ILE:HG13	1:Y:73:ARG:HG3	1.95	0.47
1:a:87:ASN:HD22	1:a:95:LEU:HD22	1.80	0.47
1:a:126:ARG:HB2	2:b:74:LEU:HD23	1.95	0.47
2:b:130:LEU:HD12	2:b:178:LEU:HD11	1.94	0.47
1:c:36:LEU:HD11	2:d:402:HIS:HB3	1.95	0.47
1:c:97:LEU:HD21	2:d:85:ILE:HG23	1.97	0.47
1:A:87:ASN:HD22	1:A:95:LEU:HD22	1.80	0.47
2:B:130:LEU:HD12	2:B:178:LEU:HD11	1.94	0.47
1:E:18:ARG:HD2	2:H:342:GLU:OE1	2.15	0.47
1:E:87:ASN:HD22	1:E:95:LEU:HD22	1.80	0.47
2:J:127:HIS:O	2:J:131:LYS:HB2	2.15	0.47
2:P:127:HIS:O	2:P:131:LYS:HB2	2.15	0.47
1:Q:126:ARG:HB2	2:R:74:LEU:HD23	1.95	0.47
2:R:171:GLN:OE1	2:R:201:VAL:HA	2.14	0.47
1:S:6:SER:O	1:S:9:LYS:N	2.44	0.47
1:S:74:LEU:CD1	2:T:98:TRP:CZ3	2.97	0.47
2:V:208:GLN:OE1	2:V:274:SER:OG	2.28	0.47
2:Z:436:ASP:N	2:Z:437:PRO:HD2	2.30	0.47
1:c:87:ASN:HD22	1:c:95:LEU:HD22	1.80	0.47
2:d:121:ILE:O	2:d:167:TYR:OH	2.24	0.47
1:C:6:SER:O	1:C:9:LYS:N	2.44	0.47
1:C:24:ASP:OD2	2:F:487:ARG:NH1	2.48	0.47
1:C:87:ASN:HD22	1:C:95:LEU:HD22	1.80	0.47
2:D:327:VAL:CG1	2:d:224:GLU:HB2	2.45	0.47
2:F:127:HIS:O	2:F:131:LYS:HB2	2.15	0.47
2:F:436:ASP:N	2:F:437:PRO:HD2	2.30	0.47
1:G:24:ASP:OD2	2:J:487:ARG:NH1	2.47	0.47
1:G:57:VAL:HG21	2:H:129:THR:HG21	1.96	0.47
2:H:244:MET:HG2	2:H:245:PRO:HD2	1.94	0.47
2:H:484:VAL:HG22	2:T:469:SER:OG	2.13	0.47
2:J:484:VAL:HG22	2:V:469:SER:OG	2.14	0.47
1:K:40:MET:HE3	2:L:104:LEU:HD21	1.96	0.47
2:L:135:GLY:O	2:L:138:TRP:HD1	1.98	0.47
2:L:260:VAL:O	2:L:261:GLU:CG	2.60	0.47
2:L:436:ASP:N	2:L:437:PRO:HD2	2.30	0.47
2:L:490:SER:OG	2:X:387:LEU:HD11	2.15	0.47
1:M:65:ILE:HG13	1:M:73:ARG:HG3	1.95	0.47
2:N:260:VAL:O	2:N:261:GLU:CG	2.60	0.47
2:N:436:ASP:N	2:N:437:PRO:HD2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:87:ASN:HD22	1:O:95:LEU:HD22	1.80	0.47
1:O:126:ARG:HB2	2:P:74:LEU:HD23	1.95	0.47
2:R:436:ASP:N	2:R:437:PRO:HD2	2.30	0.47
1:S:40:MET:HE3	2:T:104:LEU:HD21	1.96	0.47
1:S:87:ASN:HD22	1:S:95:LEU:HD22	1.80	0.47
2:V:300:CYS:HB2	2:V:395:PHE:HB3	1.97	0.47
2:V:436:ASP:CB	2:V:437:PRO:CD	2.91	0.47
1:W:40:MET:HE3	2:X:104:LEU:HD21	1.96	0.47
2:X:42:GLU:O	2:X:46:ARG:NE	2.40	0.47
2:Z:79:THR:HG22	2:Z:265:PHE:CD1	2.48	0.47
2:Z:130:LEU:HD12	2:Z:178:LEU:HD11	1.94	0.47
2:Z:260:VAL:O	2:Z:261:GLU:CG	2.60	0.47
1:A:97:LEU:HD21	2:B:85:ILE:HG23	1.97	0.47
2:D:484:VAL:HG22	2:P:469:SER:OG	2.15	0.47
2:F:42:GLU:O	2:F:46:ARG:NE	2.40	0.47
2:H:130:LEU:HD12	2:H:178:LEU:HD11	1.94	0.47
2:H:246:ARG:HB2	2:H:280:ALA:O	2.15	0.47
2:H:300:CYS:HB2	2:H:395:PHE:HB3	1.97	0.47
2:J:135:GLY:O	2:J:138:TRP:HD1	1.98	0.47
1:O:65:ILE:HG13	1:O:73:ARG:HG3	1.95	0.47
2:P:246:ARG:HB2	2:P:280:ALA:O	2.15	0.47
1:S:24:ASP:OD2	2:V:487:ARG:NH1	2.47	0.47
2:T:127:HIS:O	2:T:131:LYS:HB2	2.15	0.47
2:T:382:THR:O	2:T:386:ASN:ND2	2.38	0.47
2:V:246:ARG:HB2	2:V:280:ALA:O	2.15	0.47
1:a:65:ILE:HG13	1:a:73:ARG:HG3	1.95	0.47
2:b:244:MET:HG2	2:b:245:PRO:HD2	1.94	0.47
1:c:6:SER:O	1:c:9:LYS:N	2.44	0.47
2:d:171:GLN:OE1	2:d:201:VAL:HA	2.14	0.47
1:A:65:ILE:HG13	1:A:73:ARG:HG3	1.95	0.47
2:B:244:MET:HG2	2:B:245:PRO:HD2	1.94	0.47
2:D:171:GLN:OE1	2:D:201:VAL:HA	2.14	0.47
2:D:246:ARG:HB2	2:D:280:ALA:O	2.15	0.47
2:J:300:CYS:HB2	2:J:395:PHE:HB3	1.97	0.47
2:R:490:SER:OG	2:d:387:LEU:HD11	2.15	0.47
2:T:135:GLY:O	2:T:138:TRP:HD1	1.98	0.47
1:U:57:VAL:HG21	2:V:129:THR:HG21	1.96	0.47
2:V:135:GLY:O	2:V:138:TRP:HD1	1.98	0.47
1:Y:40:MET:HE3	2:Z:104:LEU:HD21	1.96	0.47
2:Z:183:ALA:HB2	2:Z:240:ILE:CD1	2.41	0.47
1:a:97:LEU:HD21	2:b:85:ILE:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:246:ARG:HB2	2:b:280:ALA:O	2.15	0.47
2:B:135:GLY:O	2:B:138:TRP:HD1	1.98	0.47
2:B:246:ARG:HB2	2:B:280:ALA:O	2.15	0.47
1:C:57:VAL:HG21	2:D:129:THR:HG21	1.96	0.47
1:G:40:MET:HE3	2:H:104:LEU:HD21	1.96	0.47
2:H:436:ASP:CB	2:H:437:PRO:CD	2.91	0.47
1:K:36:LEU:HD11	2:L:402:HIS:HB3	1.95	0.47
1:O:97:LEU:HD21	2:P:85:ILE:HG23	1.97	0.47
2:R:246:ARG:HB2	2:R:280:ALA:O	2.15	0.47
2:T:165:GLY:N	2:T:194:ILE:O	2.33	0.47
2:Z:135:GLY:O	2:Z:138:TRP:HD1	1.98	0.47
1:a:24:ASP:OD2	2:d:487:ARG:NH1	2.48	0.47
1:c:57:VAL:HG21	2:d:129:THR:HG21	1.96	0.47
2:d:246:ARG:HB2	2:d:280:ALA:O	2.15	0.47
2:B:327:VAL:CG1	2:b:224:GLU:HB2	2.45	0.46
2:B:496:LYS:NZ	2:N:474:ARG:HD2	2.30	0.46
2:F:246:ARG:HB2	2:F:280:ALA:O	2.15	0.46
1:G:87:ASN:HD22	1:G:95:LEU:HD22	1.80	0.46
1:K:18:ARG:HD2	2:N:342:GLU:OE1	2.14	0.46
1:K:97:LEU:HD21	2:L:85:ILE:HG23	1.97	0.46
2:L:246:ARG:HB2	2:L:280:ALA:O	2.15	0.46
1:M:87:ASN:HD22	1:M:95:LEU:HD22	1.80	0.46
2:P:135:GLY:O	2:P:138:TRP:HD1	1.98	0.46
2:P:171:GLN:OE1	2:P:201:VAL:HA	2.14	0.46
2:T:42:GLU:O	2:T:46:ARG:NE	2.40	0.46
2:T:246:ARG:HB2	2:T:280:ALA:O	2.15	0.46
2:V:127:HIS:O	2:V:131:LYS:HB2	2.15	0.46
2:X:127:HIS:O	2:X:131:LYS:HB2	2.14	0.46
2:X:246:ARG:HB2	2:X:280:ALA:O	2.15	0.46
1:Y:57:VAL:HG21	2:Z:129:THR:HG21	1.96	0.46
2:b:135:GLY:O	2:b:138:TRP:HD1	1.98	0.46
2:B:127:HIS:O	2:B:131:LYS:HB2	2.15	0.46
2:D:127:HIS:O	2:D:131:LYS:HB2	2.15	0.46
2:F:135:GLY:O	2:F:138:TRP:HD1	1.98	0.46
2:H:135:GLY:O	2:H:138:TRP:HD1	1.98	0.46
1:I:6:SER:O	1:I:9:LYS:N	2.44	0.46
2:J:246:ARG:HB2	2:J:280:ALA:O	2.15	0.46
2:J:436:ASP:N	2:J:437:PRO:HD2	2.30	0.46
2:N:135:GLY:O	2:N:138:TRP:HD1	1.98	0.46
2:V:436:ASP:N	2:V:437:PRO:HD2	2.30	0.46
2:Z:208:GLN:OE1	2:Z:274:SER:OG	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:127:HIS:O	2:b:131:LYS:HB2	2.15	0.46
2:d:127:HIS:O	2:d:131:LYS:HB2	2.15	0.46
1:A:77:MET:HE3	1:A:77:MET:HB2	1.88	0.46
2:H:260:VAL:O	2:H:261:GLU:CG	2.60	0.46
1:I:57:VAL:HG21	2:J:129:THR:HG21	1.96	0.46
2:L:127:HIS:O	2:L:131:LYS:HB2	2.15	0.46
2:L:339:ASP:OD2	2:X:409:ARG:NH1	2.48	0.46
2:N:79:THR:HG22	2:N:265:PHE:CD1	2.48	0.46
2:N:127:HIS:O	2:N:131:LYS:HB2	2.15	0.46
2:R:135:GLY:O	2:R:138:TRP:HD1	1.98	0.46
1:S:97:LEU:HD21	2:T:85:ILE:HG23	1.97	0.46
2:T:300:CYS:HB2	2:T:395:PHE:HB3	1.97	0.46
1:W:36:LEU:HD11	2:X:402:HIS:HB3	1.95	0.46
1:W:97:LEU:HD21	2:X:85:ILE:HG23	1.97	0.46
1:Y:24:ASP:OD2	2:b:487:ARG:NH1	2.48	0.46
1:a:77:MET:HE3	1:a:77:MET:HB2	1.88	0.46
2:b:436:ASP:N	2:b:437:PRO:HD2	2.30	0.46
2:B:436:ASP:N	2:B:437:PRO:HD2	2.30	0.46
2:D:436:ASP:N	2:D:437:PRO:HD2	2.30	0.46
1:E:97:LEU:HD21	2:F:85:ILE:HG23	1.97	0.46
1:I:87:ASN:HD22	1:I:95:LEU:HD22	1.80	0.46
2:J:183:ALA:HB2	2:J:240:ILE:CD1	2.41	0.46
2:V:183:ALA:HB2	2:V:240:ILE:CD1	2.41	0.46
1:W:24:ASP:OD2	2:Z:487:ARG:NH1	2.48	0.46
1:W:87:ASN:HD22	1:W:95:LEU:HD22	1.80	0.46
2:X:135:GLY:O	2:X:138:TRP:HD1	1.98	0.46
2:Z:127:HIS:O	2:Z:131:LYS:HB2	2.15	0.46
2:d:436:ASP:N	2:d:437:PRO:HD2	2.30	0.46
2:B:79:THR:HG22	2:B:265:PHE:CD1	2.48	0.46
2:D:79:THR:HG22	2:D:265:PHE:CD1	2.48	0.46
2:F:454:GLU:HB3	2:F:472:PHE:HB2	1.98	0.46
1:I:40:MET:HE3	2:J:104:LEU:HD21	1.96	0.46
2:J:437:PRO:HB2	2:J:441:THR:HG21	1.92	0.46
2:L:454:GLU:HB3	2:L:472:PHE:HB2	1.98	0.46
2:N:246:ARG:HB2	2:N:280:ALA:O	2.15	0.46
1:Q:97:LEU:HD21	2:R:85:ILE:HG23	1.97	0.46
2:T:454:GLU:HB3	2:T:472:PHE:HB2	1.98	0.46
1:U:40:MET:HE3	2:V:104:LEU:HD21	1.96	0.46
2:X:244:MET:HG2	2:X:245:PRO:HD2	1.94	0.46
2:X:300:CYS:HB2	2:X:395:PHE:HB3	1.97	0.46
2:Z:454:GLU:HB3	2:Z:472:PHE:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:382:THR:O	2:b:386:ASN:ND2	2.38	0.46
2:B:382:THR:O	2:B:386:ASN:ND2	2.39	0.46
2:F:339:ASP:OD2	2:R:409:ARG:NH1	2.47	0.46
2:N:454:GLU:HB3	2:N:472:PHE:HB2	1.98	0.46
2:T:121:ILE:O	2:T:167:TYR:OH	2.24	0.46
2:T:436:ASP:CB	2:T:437:PRO:HD3	2.46	0.46
2:b:79:THR:HG22	2:b:265:PHE:CD1	2.48	0.46
2:d:79:THR:HG22	2:d:265:PHE:CD1	2.48	0.46
2:F:183:ALA:HB2	2:F:240:ILE:CD1	2.41	0.46
2:P:260:VAL:C	2:P:261:GLU:HG2	2.41	0.46
2:P:436:ASP:CB	2:P:437:PRO:CD	2.91	0.46
2:T:436:ASP:CB	2:T:437:PRO:CD	2.91	0.46
2:T:436:ASP:N	2:T:437:PRO:HD2	2.30	0.46
2:X:130:LEU:HD12	2:X:178:LEU:HD12	1.98	0.46
2:X:436:ASP:N	2:X:437:PRO:HD2	2.30	0.46
2:B:130:LEU:HD12	2:B:178:LEU:HD12	1.98	0.46
2:B:260:VAL:C	2:B:261:GLU:HG2	2.41	0.46
2:D:58:LEU:HD11	1:c:118:SER:HB3	1.98	0.46
2:D:260:VAL:C	2:D:261:GLU:HG2	2.41	0.46
2:F:51:HIS:NE2	2:F:55:GLN:OE1	2.49	0.46
2:F:417:GLU:H	2:F:420:GLU:HB2	1.81	0.46
2:H:454:GLU:HB3	2:H:472:PHE:HB2	1.98	0.46
2:J:339:ASP:OD2	2:V:409:ARG:NH1	2.47	0.46
2:N:496:LYS:NZ	2:Z:474:ARG:HD2	2.31	0.46
2:P:42:GLU:O	2:P:46:ARG:NE	2.40	0.46
2:P:404:LEU:HD12	2:P:404:LEU:HA	1.80	0.46
2:T:208:GLN:OE1	2:T:274:SER:OG	2.28	0.46
1:U:87:ASN:HD22	1:U:95:LEU:HD22	1.80	0.46
1:W:74:LEU:N	1:W:74:LEU:HD12	2.31	0.46
1:Y:97:LEU:HD21	2:Z:85:ILE:HG23	1.97	0.46
2:b:130:LEU:HD12	2:b:178:LEU:HD12	1.98	0.46
2:b:260:VAL:C	2:b:261:GLU:HG2	2.41	0.46
2:d:135:GLY:O	2:d:138:TRP:HD1	1.98	0.46
2:d:260:VAL:C	2:d:261:GLU:HG2	2.41	0.46
1:C:62:PHE:CZ	2:D:147:LEU:HD21	2.51	0.46
2:D:135:GLY:O	2:D:138:TRP:HD1	1.98	0.46
2:H:436:ASP:N	2:H:437:PRO:HD2	2.30	0.46
1:K:62:PHE:CZ	2:L:147:LEU:HD21	2.51	0.46
2:N:165:GLY:N	2:N:194:ILE:O	2.33	0.46
1:Q:62:PHE:CZ	2:R:147:LEU:HD21	2.51	0.46
2:T:417:GLU:H	2:T:420:GLU:HB2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:154:GLN:O	2:X:409:ARG:NH1	2.49	0.46
1:Y:62:PHE:CZ	2:Z:147:LEU:HD21	2.51	0.46
1:Y:87:ASN:HD22	1:Y:95:LEU:HD22	1.80	0.46
1:A:62:PHE:CZ	2:B:147:LEU:HD21	2.51	0.46
1:A:74:LEU:HD12	1:A:74:LEU:N	2.31	0.46
2:D:51:HIS:NE2	2:D:55:GLN:OE1	2.49	0.46
2:D:417:GLU:H	2:D:420:GLU:HB2	1.81	0.46
2:D:436:ASP:CB	2:D:437:PRO:CD	2.91	0.46
1:G:97:LEU:HD21	2:H:85:ILE:HG23	1.97	0.46
2:H:137:THR:O	2:H:137:THR:CG2	2.63	0.46
2:H:154:GLN:O	2:H:409:ARG:NH1	2.49	0.46
2:H:339:ASP:OD2	2:T:409:ARG:NH1	2.47	0.46
1:I:97:LEU:HD21	2:J:85:ILE:HG23	1.97	0.46
1:K:87:ASN:HD22	1:K:95:LEU:HD22	1.80	0.46
2:L:442:GLU:CG	2:L:443:THR:H	2.25	0.46
1:M:62:PHE:CZ	2:N:147:LEU:HD21	2.51	0.46
2:N:121:ILE:O	2:N:167:TYR:OH	2.24	0.46
2:N:130:LEU:HD12	2:N:178:LEU:HD11	1.94	0.46
1:O:62:PHE:CZ	2:P:147:LEU:HD21	2.51	0.46
2:R:454:GLU:HB3	2:R:472:PHE:HB2	1.98	0.46
1:S:57:VAL:HG21	2:T:129:THR:HG21	1.96	0.46
1:a:62:PHE:CZ	2:b:147:LEU:HD21	2.51	0.46
1:a:74:LEU:HD12	1:a:74:LEU:N	2.31	0.46
1:c:62:PHE:CZ	2:d:147:LEU:HD21	2.51	0.46
2:d:51:HIS:NE2	2:d:55:GLN:OE1	2.49	0.46
2:d:417:GLU:H	2:d:420:GLU:HB2	1.81	0.46
2:B:454:GLU:HB3	2:B:472:PHE:HB2	1.98	0.45
2:H:417:GLU:H	2:H:420:GLU:HB2	1.82	0.45
2:L:51:HIS:NE2	2:L:55:GLN:OE1	2.49	0.45
2:L:130:LEU:HD12	2:L:178:LEU:HD12	1.98	0.45
2:R:79:THR:HG22	2:R:265:PHE:CD1	2.48	0.45
2:T:137:THR:O	2:T:137:THR:CG2	2.63	0.45
2:V:51:HIS:NE2	2:V:55:GLN:OE1	2.49	0.45
2:V:154:GLN:O	2:V:409:ARG:NH1	2.49	0.45
2:V:417:GLU:H	2:V:420:GLU:HB2	1.81	0.45
1:W:62:PHE:CZ	2:X:147:LEU:HD21	2.51	0.45
2:X:51:HIS:NE2	2:X:55:GLN:OE1	2.49	0.45
2:Z:246:ARG:HB2	2:Z:280:ALA:O	2.15	0.45
2:d:436:ASP:CB	2:d:437:PRO:CD	2.91	0.45
2:B:51:HIS:NE2	2:B:55:GLN:OE1	2.49	0.45
2:B:58:LEU:HD11	1:a:118:SER:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:62:PHE:CZ	2:F:147:LEU:HD21	2.51	0.45
2:F:154:GLN:O	2:F:409:ARG:NH1	2.49	0.45
2:F:300:CYS:HB2	2:F:395:PHE:HB3	1.97	0.45
2:H:436:ASP:CB	2:H:437:PRO:HD3	2.46	0.45
2:J:208:GLN:OE1	2:J:274:SER:OG	2.28	0.45
2:J:496:LYS:NZ	2:V:474:ARG:HD2	2.31	0.45
2:N:51:HIS:NE2	2:N:55:GLN:OE1	2.49	0.45
2:N:130:LEU:HD12	2:N:178:LEU:HD12	1.98	0.45
2:N:260:VAL:C	2:N:261:GLU:HG2	2.41	0.45
2:P:417:GLU:H	2:P:420:GLU:HB2	1.81	0.45
2:R:417:GLU:H	2:R:420:GLU:HB2	1.82	0.45
2:b:51:HIS:NE2	2:b:55:GLN:OE1	2.49	0.45
2:H:51:HIS:NE2	2:H:55:GLN:OE1	2.49	0.45
2:J:130:LEU:HD12	2:J:178:LEU:HD12	1.98	0.45
2:J:442:GLU:CG	2:J:443:THR:H	2.25	0.45
1:K:6:SER:O	1:K:9:LYS:N	2.44	0.45
1:O:74:LEU:N	1:O:74:LEU:HD12	2.31	0.45
2:P:51:HIS:NE2	2:P:55:GLN:OE1	2.49	0.45
2:P:79:THR:HG22	2:P:265:PHE:CD1	2.48	0.45
2:P:130:LEU:HD12	2:P:178:LEU:HD12	1.98	0.45
2:R:154:GLN:O	2:R:409:ARG:NH1	2.49	0.45
2:R:260:VAL:C	2:R:261:GLU:HG2	2.41	0.45
2:R:442:GLU:CG	2:R:443:THR:H	2.24	0.45
2:R:496:LYS:NZ	2:d:474:ARG:HD2	2.32	0.45
2:T:154:GLN:O	2:T:409:ARG:NH1	2.49	0.45
2:X:454:GLU:HB3	2:X:472:PHE:HB2	1.98	0.45
2:b:165:GLY:N	2:b:194:ILE:O	2.33	0.45
2:b:238:ARG:HD2	2:b:394:LEU:HD11	1.99	0.45
2:b:454:GLU:HB3	2:b:472:PHE:HB2	1.98	0.45
2:B:154:GLN:O	2:B:409:ARG:NH1	2.49	0.45
2:B:165:GLY:N	2:B:194:ILE:O	2.33	0.45
2:B:238:ARG:HD2	2:B:394:LEU:HD11	1.99	0.45
2:D:442:GLU:CG	2:D:443:THR:H	2.24	0.45
2:H:260:VAL:C	2:H:261:GLU:HG2	2.41	0.45
2:J:417:GLU:H	2:J:420:GLU:HB2	1.81	0.45
1:K:40:MET:HE2	2:L:291:ASN:HD21	1.82	0.45
2:L:42:GLU:O	2:L:46:ARG:NE	2.40	0.45
2:L:300:CYS:HB2	2:L:395:PHE:HB3	1.97	0.45
2:N:238:ARG:HD2	2:N:394:LEU:HD11	1.99	0.45
1:S:40:MET:HE2	2:T:291:ASN:HD21	1.82	0.45
2:T:260:VAL:C	2:T:261:GLU:HG2	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:154:GLN:O	2:b:409:ARG:NH1	2.49	0.45
2:d:454:GLU:HB3	2:d:472:PHE:HB2	1.98	0.45
2:B:300:CYS:HB2	2:B:395:PHE:HB3	1.97	0.45
2:H:394:LEU:HD23	2:H:394:LEU:HA	1.77	0.45
2:J:206:SER:O	2:J:207:TRP:HB2	2.17	0.45
1:K:74:LEU:HD12	1:K:74:LEU:N	2.31	0.45
2:L:154:GLN:O	2:L:409:ARG:NH1	2.49	0.45
1:M:40:MET:HE2	2:N:291:ASN:HD21	1.82	0.45
2:N:154:GLN:O	2:N:409:ARG:NH1	2.49	0.45
2:N:442:GLU:CG	2:N:443:THR:H	2.25	0.45
1:O:97:LEU:C	1:O:97:LEU:HD12	2.42	0.45
2:P:382:THR:O	2:P:386:ASN:ND2	2.38	0.45
2:P:407:ILE:HG12	2:P:424:TRP:HZ2	1.82	0.45
2:R:51:HIS:NE2	2:R:55:GLN:OE1	2.49	0.45
2:R:208:GLN:OE1	2:R:274:SER:OG	2.28	0.45
2:V:137:THR:O	2:V:137:THR:CG2	2.63	0.45
2:V:206:SER:O	2:V:207:TRP:HB2	2.17	0.45
2:V:454:GLU:HB3	2:V:472:PHE:HB2	1.98	0.45
2:Z:165:GLY:N	2:Z:194:ILE:O	2.33	0.45
2:Z:238:ARG:HD2	2:Z:394:LEU:HD11	1.99	0.45
1:c:97:LEU:C	1:c:97:LEU:HD12	2.42	0.45
2:B:407:ILE:HG12	2:B:424:TRP:HZ2	1.82	0.45
1:C:97:LEU:C	1:C:97:LEU:HD12	2.42	0.45
2:D:206:SER:O	2:D:207:TRP:HB2	2.17	0.45
2:D:238:ARG:HD2	2:D:394:LEU:HD11	1.99	0.45
2:D:407:ILE:HG12	2:D:424:TRP:HZ2	1.82	0.45
2:D:454:GLU:HB3	2:D:472:PHE:HB2	1.98	0.45
1:I:40:MET:HE2	2:J:291:ASN:HD21	1.82	0.45
1:I:62:PHE:CZ	2:J:147:LEU:HD21	2.51	0.45
1:I:74:LEU:HD12	1:I:74:LEU:N	2.31	0.45
2:J:252:PRO:HB3	2:J:269:THR:HG21	1.99	0.45
2:N:252:PRO:HB3	2:N:269:THR:HG21	1.99	0.45
2:N:407:ILE:HG12	2:N:424:TRP:HZ2	1.82	0.45
2:P:154:GLN:O	2:P:409:ARG:NH1	2.49	0.45
2:P:206:SER:O	2:P:207:TRP:HB2	2.17	0.45
2:P:300:CYS:HB2	2:P:395:PHE:HB3	1.97	0.45
2:R:206:SER:O	2:R:207:TRP:HB2	2.17	0.45
2:V:252:PRO:HB3	2:V:269:THR:HG21	1.98	0.45
2:V:260:VAL:C	2:V:261:GLU:HG2	2.41	0.45
2:Z:300:CYS:HB2	2:Z:395:PHE:HB3	1.97	0.45
2:b:300:CYS:HB2	2:b:395:PHE:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:394:LEU:HD23	2:b:394:LEU:HA	1.77	0.45
2:d:238:ARG:HD2	2:d:394:LEU:HD11	1.99	0.45
2:d:407:ILE:HG12	2:d:424:TRP:HZ2	1.82	0.45
2:d:442:GLU:CG	2:d:443:THR:H	2.25	0.45
1:A:97:LEU:C	1:A:97:LEU:HD12	2.42	0.45
2:B:394:LEU:HD23	2:B:394:LEU:HA	1.77	0.45
2:D:154:GLN:O	2:D:409:ARG:NH1	2.49	0.45
2:F:260:VAL:C	2:F:261:GLU:HG2	2.41	0.45
1:G:74:LEU:N	1:G:74:LEU:HD12	2.31	0.45
2:N:206:SER:O	2:N:207:TRP:HB2	2.17	0.45
2:P:238:ARG:HD2	2:P:394:LEU:HD11	1.99	0.45
2:P:244:MET:HG2	2:P:245:PRO:HD2	1.94	0.45
1:Q:40:MET:HE2	2:R:291:ASN:HD21	1.82	0.45
1:Q:97:LEU:C	1:Q:97:LEU:HD12	2.42	0.45
2:R:238:ARG:HD2	2:R:394:LEU:HD11	1.99	0.45
2:R:407:ILE:HG12	2:R:424:TRP:HZ2	1.82	0.45
1:S:74:LEU:HD12	1:S:74:LEU:N	2.31	0.45
2:T:260:VAL:O	2:T:261:GLU:CG	2.60	0.45
2:X:235:GLU:HG2	2:X:238:ARG:NH2	2.32	0.45
2:X:440:SER:C	2:X:441:THR:HG23	2.42	0.45
1:Y:40:MET:HE2	2:Z:291:ASN:HD21	1.82	0.45
2:Z:154:GLN:O	2:Z:409:ARG:NH1	2.49	0.45
2:Z:206:SER:O	2:Z:207:TRP:HB2	2.17	0.45
2:Z:235:GLU:HG2	2:Z:238:ARG:NH2	2.32	0.45
2:Z:260:VAL:C	2:Z:261:GLU:HG2	2.41	0.45
2:Z:417:GLU:H	2:Z:420:GLU:HB2	1.81	0.45
1:a:97:LEU:C	1:a:97:LEU:HD12	2.42	0.45
2:b:206:SER:O	2:b:207:TRP:HB2	2.17	0.45
2:b:407:ILE:HG12	2:b:424:TRP:HZ2	1.82	0.45
2:b:417:GLU:H	2:b:420:GLU:HB2	1.81	0.45
1:c:89:LEU:N	1:c:89:LEU:HD12	2.32	0.45
2:d:206:SER:O	2:d:207:TRP:HB2	2.17	0.45
2:B:206:SER:O	2:B:207:TRP:HB2	2.17	0.45
2:B:417:GLU:H	2:B:420:GLU:HB2	1.82	0.45
1:C:89:LEU:N	1:C:89:LEU:HD12	2.32	0.45
2:F:244:MET:HG2	2:F:245:PRO:HD2	1.94	0.45
2:F:382:THR:O	2:F:386:ASN:ND2	2.38	0.45
1:G:10:PHE:HE1	2:V:139:ASP:HB2	1.81	0.45
2:H:206:SER:O	2:H:207:TRP:HB2	2.17	0.45
2:H:496:LYS:NZ	2:T:474:ARG:HD2	2.31	0.45
1:M:74:LEU:N	1:M:74:LEU:HD12	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:394:LEU:HD23	2:P:394:LEU:HA	1.77	0.45
1:Q:89:LEU:HD12	1:Q:89:LEU:N	2.32	0.45
2:R:300:CYS:HB2	2:R:395:PHE:HB3	1.97	0.45
2:R:436:ASP:CB	2:R:437:PRO:CD	2.91	0.45
2:T:235:GLU:HG2	2:T:238:ARG:NH2	2.32	0.45
1:U:97:LEU:HD21	2:V:85:ILE:HG23	1.97	0.45
2:X:260:VAL:HG13	2:X:261:GLU:N	2.32	0.45
2:d:154:GLN:O	2:d:409:ARG:NH1	2.49	0.45
2:d:404:LEU:HD12	2:d:404:LEU:HA	1.80	0.45
1:A:40:MET:CE	2:B:104:LEU:HD21	2.47	0.45
1:A:40:MET:HE2	2:B:291:ASN:HD21	1.82	0.45
2:B:252:PRO:HB3	2:B:269:THR:HG21	1.99	0.45
1:C:74:LEU:HD12	1:C:74:LEU:N	2.31	0.45
2:D:404:LEU:HD12	2:D:404:LEU:HA	1.80	0.45
1:E:74:LEU:N	1:E:74:LEU:HD12	2.31	0.45
2:F:137:THR:O	2:F:137:THR:CG2	2.63	0.45
2:H:235:GLU:HG2	2:H:238:ARG:NH2	2.32	0.45
2:H:442:GLU:CG	2:H:443:THR:H	2.25	0.45
1:I:89:LEU:HD12	1:I:89:LEU:N	2.32	0.45
2:J:154:GLN:O	2:J:409:ARG:NH1	2.49	0.45
2:J:260:VAL:HG13	2:J:261:GLU:N	2.32	0.45
1:K:10:PHE:HE1	2:Z:139:ASP:HB2	1.82	0.45
2:L:238:ARG:HD2	2:L:394:LEU:HD11	1.99	0.45
2:L:440:SER:C	2:L:441:THR:HG23	2.42	0.45
1:M:97:LEU:C	1:M:97:LEU:HD12	2.42	0.45
2:N:300:CYS:HB2	2:N:395:PHE:HB3	1.97	0.45
2:N:417:GLU:H	2:N:420:GLU:HB2	1.81	0.45
1:S:62:PHE:CZ	2:T:147:LEU:HD21	2.51	0.45
2:T:206:SER:O	2:T:207:TRP:HB2	2.17	0.45
1:U:40:MET:HE2	2:V:291:ASN:HD21	1.82	0.45
2:V:436:ASP:CB	2:V:437:PRO:HD3	2.46	0.45
1:W:89:LEU:HD12	1:W:89:LEU:N	2.32	0.45
2:X:137:THR:O	2:X:137:THR:CG2	2.63	0.45
2:X:206:SER:O	2:X:207:TRP:HB2	2.17	0.45
2:X:238:ARG:HD2	2:X:394:LEU:HD11	1.99	0.45
2:Z:252:PRO:HB3	2:Z:269:THR:HG21	1.99	0.45
2:Z:407:ILE:HG12	2:Z:424:TRP:HZ2	1.82	0.45
1:a:40:MET:HE2	2:b:291:ASN:HD21	1.82	0.45
2:b:252:PRO:HB3	2:b:269:THR:HG21	1.99	0.45
1:A:89:LEU:HD12	1:A:89:LEU:N	2.32	0.45
2:D:300:CYS:HB2	2:D:395:PHE:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:89:LEU:N	1:E:89:LEU:HD12	2.32	0.45
2:F:206:SER:O	2:F:207:TRP:HB2	2.17	0.45
2:F:436:ASP:CB	2:F:437:PRO:CD	2.91	0.45
1:I:40:MET:CE	2:J:104:LEU:HD21	2.47	0.45
2:J:260:VAL:C	2:J:261:GLU:HG2	2.41	0.45
2:L:235:GLU:HG2	2:L:238:ARG:NH2	2.32	0.45
1:M:10:PHE:HE1	2:b:139:ASP:HB2	1.82	0.45
1:O:40:MET:CE	2:P:104:LEU:HD21	2.47	0.45
1:O:89:LEU:HD12	1:O:89:LEU:N	2.32	0.45
2:P:133:PHE:HD2	2:P:137:THR:HG22	1.82	0.45
2:R:382:THR:O	2:R:386:ASN:ND2	2.38	0.45
2:R:442:GLU:CG	2:R:443:THR:N	2.79	0.45
2:T:130:LEU:HD12	2:T:178:LEU:HD12	1.98	0.45
2:T:260:VAL:HG13	2:T:261:GLU:N	2.32	0.45
2:T:437:PRO:HB2	2:T:441:THR:HG23	1.98	0.45
1:Y:74:LEU:HD12	1:Y:74:LEU:N	2.31	0.45
1:a:40:MET:CE	2:b:104:LEU:HD21	2.47	0.45
1:c:74:LEU:HD12	1:c:74:LEU:N	2.31	0.45
1:A:18:ARG:HD2	2:D:342:GLU:OE1	2.17	0.44
2:F:79:THR:HG22	2:F:265:PHE:CD1	2.48	0.44
2:F:130:LEU:HD12	2:F:178:LEU:HD12	1.98	0.44
2:H:260:VAL:HG13	2:H:261:GLU:N	2.32	0.44
2:J:51:HIS:NE2	2:J:55:GLN:OE1	2.49	0.44
2:J:137:THR:O	2:J:137:THR:CG2	2.63	0.44
1:K:97:LEU:C	1:K:97:LEU:HD12	2.42	0.44
2:L:49:ALA:O	2:L:53:LEU:HB2	2.18	0.44
2:L:137:THR:O	2:L:137:THR:CG2	2.63	0.44
2:L:260:VAL:HG13	2:L:261:GLU:N	2.32	0.44
2:L:260:VAL:C	2:L:261:GLU:HG2	2.41	0.44
1:M:6:SER:O	1:M:9:LYS:N	2.44	0.44
2:N:235:GLU:HG2	2:N:238:ARG:NH2	2.32	0.44
1:O:40:MET:HE2	2:P:291:ASN:HD21	1.82	0.44
2:P:454:GLU:HB3	2:P:472:PHE:HB2	1.98	0.44
1:U:40:MET:CE	2:V:104:LEU:HD21	2.47	0.44
2:V:49:ALA:O	2:V:53:LEU:HB2	2.18	0.44
2:V:260:VAL:HG13	2:V:261:GLU:N	2.32	0.44
2:Z:51:HIS:NE2	2:Z:55:GLN:OE1	2.49	0.44
2:d:42:GLU:O	2:d:46:ARG:NE	2.40	0.44
2:d:133:PHE:HD2	2:d:137:THR:HG22	1.82	0.44
2:d:300:CYS:HB2	2:d:395:PHE:HB3	1.97	0.44
2:B:133:PHE:HD2	2:B:137:THR:HG22	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:MET:CE	2:D:104:LEU:HD21	2.47	0.44
2:D:42:GLU:O	2:D:46:ARG:NE	2.40	0.44
1:E:97:LEU:C	1:E:97:LEU:HD12	2.42	0.44
2:F:407:ILE:HG12	2:F:424:TRP:HZ2	1.82	0.44
1:K:89:LEU:N	1:K:89:LEU:HD12	2.32	0.44
1:S:97:LEU:C	1:S:97:LEU:HD12	2.42	0.44
1:U:62:PHE:CZ	2:V:147:LEU:HD21	2.51	0.44
1:U:74:LEU:N	1:U:74:LEU:HD12	2.31	0.44
1:W:40:MET:CE	2:X:104:LEU:HD21	2.47	0.44
2:X:252:PRO:HB3	2:X:269:THR:HG21	1.99	0.44
2:X:260:VAL:C	2:X:261:GLU:HG2	2.41	0.44
2:X:417:GLU:H	2:X:420:GLU:HB2	1.81	0.44
1:c:40:MET:CE	2:d:104:LEU:HD21	2.47	0.44
1:c:40:MET:HE2	2:d:291:ASN:HD21	1.82	0.44
1:C:40:MET:HE2	2:D:291:ASN:HD21	1.82	0.44
2:D:133:PHE:HD2	2:D:137:THR:HG22	1.83	0.44
1:E:40:MET:HE2	2:F:291:ASN:HD21	1.82	0.44
2:F:238:ARG:HD2	2:F:394:LEU:HD11	1.99	0.44
1:I:10:PHE:HE1	2:X:139:ASP:HB2	1.82	0.44
2:J:235:GLU:HG2	2:J:238:ARG:NH2	2.32	0.44
2:J:238:ARG:HD2	2:J:394:LEU:HD11	1.99	0.44
1:K:74:LEU:HD11	2:L:98:TRP:CZ3	2.53	0.44
2:L:407:ILE:HG12	2:L:424:TRP:HZ2	1.82	0.44
2:N:260:VAL:HG13	2:N:261:GLU:N	2.32	0.44
2:T:51:HIS:NE2	2:T:55:GLN:OE1	2.49	0.44
1:U:89:LEU:N	1:U:89:LEU:HD12	2.32	0.44
1:Y:97:LEU:C	1:Y:97:LEU:HD12	2.42	0.44
2:Z:130:LEU:HD12	2:Z:178:LEU:HD12	1.98	0.44
2:Z:440:SER:C	2:Z:441:THR:HG23	2.42	0.44
1:a:89:LEU:HD12	1:a:89:LEU:N	2.32	0.44
2:b:133:PHE:HD2	2:b:137:THR:HG22	1.83	0.44
2:B:133:PHE:HD2	2:B:137:THR:HG21	1.82	0.44
2:F:49:ALA:O	2:F:53:LEU:HB2	2.18	0.44
2:F:496:LYS:NZ	2:R:474:ARG:HD2	2.33	0.44
2:H:49:ALA:O	2:H:53:LEU:HB2	2.18	0.44
2:H:130:LEU:HD12	2:H:178:LEU:HD12	1.98	0.44
2:H:164:VAL:HG21	2:H:287:ALA:HB2	1.99	0.44
2:H:252:PRO:HB3	2:H:269:THR:HG21	1.99	0.44
1:I:77:MET:HE3	1:I:77:MET:HB2	1.88	0.44
2:J:442:GLU:CG	2:J:443:THR:N	2.79	0.44
2:J:454:GLU:HB3	2:J:472:PHE:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:165:GLY:N	2:L:194:ILE:O	2.33	0.44
2:L:206:SER:O	2:L:207:TRP:HB2	2.17	0.44
2:L:417:GLU:H	2:L:420:GLU:HB2	1.81	0.44
1:M:40:MET:CE	2:N:104:LEU:HD21	2.47	0.44
2:R:137:THR:O	2:R:137:THR:CG2	2.63	0.44
1:S:89:LEU:N	1:S:89:LEU:HD12	2.32	0.44
2:T:164:VAL:HG21	2:T:287:ALA:HB2	1.99	0.44
2:V:133:PHE:HD2	2:V:137:THR:HG22	1.82	0.44
2:V:235:GLU:HG2	2:V:238:ARG:NH2	2.32	0.44
1:W:74:LEU:HD11	2:X:98:TRP:CZ3	2.53	0.44
1:W:97:LEU:C	1:W:97:LEU:HD12	2.42	0.44
2:Z:42:GLU:O	2:Z:46:ARG:NE	2.40	0.44
2:b:133:PHE:HD2	2:b:137:THR:HG21	1.82	0.44
1:C:74:LEU:HD11	2:D:98:TRP:CZ3	2.53	0.44
1:E:6:SER:O	1:E:9:LYS:N	2.44	0.44
1:G:40:MET:HE2	2:H:291:ASN:HD21	1.82	0.44
1:G:97:LEU:C	1:G:97:LEU:HD12	2.42	0.44
1:I:97:LEU:C	1:I:97:LEU:HD12	2.42	0.44
2:J:133:PHE:HD2	2:J:137:THR:HG22	1.83	0.44
2:J:407:ILE:HG12	2:J:424:TRP:HZ2	1.82	0.44
2:N:164:VAL:HG21	2:N:287:ALA:HB2	1.99	0.44
2:N:394:LEU:HD23	2:N:394:LEU:HA	1.77	0.44
2:N:437:PRO:HB2	2:N:441:THR:HG23	1.97	0.44
2:P:496:LYS:NZ	2:b:474:ARG:HD2	2.33	0.44
1:Q:40:MET:CE	2:R:104:LEU:HD21	2.47	0.44
1:Q:74:LEU:HD11	2:R:98:TRP:CZ3	2.53	0.44
2:R:133:PHE:HD2	2:R:137:THR:HG22	1.82	0.44
2:T:238:ARG:HD2	2:T:394:LEU:HD11	1.99	0.44
2:V:238:ARG:HD2	2:V:394:LEU:HD11	1.99	0.44
2:b:260:VAL:HG13	2:b:261:GLU:N	2.32	0.44
1:c:74:LEU:HD11	2:d:98:TRP:CZ3	2.53	0.44
2:d:235:GLU:HG2	2:d:238:ARG:NH2	2.32	0.44
2:D:130:LEU:HD12	2:D:178:LEU:HD12	1.98	0.44
2:D:137:THR:O	2:D:137:THR:CG2	2.63	0.44
2:D:235:GLU:HG2	2:D:238:ARG:NH2	2.32	0.44
2:F:164:VAL:HG21	2:F:287:ALA:HB2	1.99	0.44
1:G:62:PHE:CZ	2:H:147:LEU:HD21	2.51	0.44
2:H:133:PHE:HD2	2:H:137:THR:HG21	1.82	0.44
1:Q:74:LEU:HD12	1:Q:74:LEU:N	2.31	0.44
2:R:130:LEU:HD12	2:R:178:LEU:HD12	1.98	0.44
2:V:165:GLY:N	2:V:194:ILE:O	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:137:THR:O	2:d:137:THR:CG2	2.63	0.44
2:B:260:VAL:HG13	2:B:261:GLU:N	2.32	0.44
1:C:10:PHE:HE1	2:R:139:ASP:HB2	1.81	0.44
2:D:133:PHE:HD2	2:D:137:THR:HG21	1.82	0.44
2:D:252:PRO:HB3	2:D:269:THR:HG21	1.99	0.44
2:D:260:VAL:HG13	2:D:261:GLU:N	2.32	0.44
1:E:40:MET:CE	2:F:104:LEU:HD21	2.47	0.44
2:F:252:PRO:HB3	2:F:269:THR:HG21	1.99	0.44
2:J:133:PHE:HD2	2:J:137:THR:HG21	1.82	0.44
2:J:436:ASP:CB	2:J:437:PRO:HD3	2.46	0.44
2:L:252:PRO:HB3	2:L:269:THR:HG21	1.99	0.44
1:M:89:LEU:N	1:M:89:LEU:HD12	2.32	0.44
2:N:49:ALA:O	2:N:53:LEU:HB2	2.17	0.44
2:N:133:PHE:HD2	2:N:137:THR:HG22	1.83	0.44
2:N:137:THR:O	2:N:137:THR:CG2	2.63	0.44
1:O:74:LEU:HD11	2:P:98:TRP:CZ3	2.53	0.44
2:P:208:GLN:OE1	2:P:274:SER:OG	2.28	0.44
2:P:252:PRO:HB3	2:P:269:THR:HG21	1.99	0.44
2:R:235:GLU:HG2	2:R:238:ARG:NH2	2.32	0.44
2:R:491:LYS:HE2	2:R:496:LYS:O	2.18	0.44
1:Y:40:MET:CE	2:Z:104:LEU:HD21	2.47	0.44
1:Y:74:LEU:HD11	2:Z:98:TRP:CZ3	2.53	0.44
1:Y:89:LEU:HD12	1:Y:89:LEU:N	2.32	0.44
2:b:49:ALA:O	2:b:53:LEU:HB2	2.18	0.44
2:b:137:THR:O	2:b:137:THR:CG2	2.63	0.44
2:d:130:LEU:HD12	2:d:178:LEU:HD12	1.98	0.44
2:d:133:PHE:HD2	2:d:137:THR:HG21	1.82	0.44
2:d:252:PRO:HB3	2:d:269:THR:HG21	1.99	0.44
2:d:441:THR:HG1	2:d:445:LYS:HZ2	1.61	0.44
1:A:74:LEU:HD11	2:B:98:TRP:CZ3	2.53	0.44
2:B:49:ALA:O	2:B:53:LEU:HB2	2.18	0.44
2:B:137:THR:O	2:B:137:THR:CG2	2.63	0.44
1:E:74:LEU:HD11	2:F:98:TRP:CZ3	2.53	0.44
2:F:235:GLU:HG2	2:F:238:ARG:NH2	2.32	0.44
2:F:246:ARG:NH1	2:F:334:GLU:OE2	2.51	0.44
2:H:133:PHE:HD2	2:H:137:THR:HG22	1.83	0.44
1:I:74:LEU:HD11	2:J:98:TRP:CZ3	2.53	0.44
2:L:244:MET:HG2	2:L:245:PRO:HD2	1.94	0.44
2:P:133:PHE:HD2	2:P:137:THR:HG21	1.82	0.44
2:P:137:THR:O	2:P:137:THR:CG2	2.63	0.44
2:P:165:GLY:N	2:P:194:ILE:O	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:235:GLU:HG2	2:P:238:ARG:NH2	2.32	0.44
2:R:252:PRO:HB3	2:R:269:THR:HG21	1.99	0.44
2:T:246:ARG:NH1	2:T:334:GLU:OE2	2.51	0.44
2:V:407:ILE:HG12	2:V:424:TRP:HZ2	1.82	0.44
2:V:437:PRO:HB2	2:V:441:THR:HG23	1.98	0.44
1:W:40:MET:HE2	2:X:291:ASN:HD21	1.82	0.44
2:X:49:ALA:O	2:X:53:LEU:HB2	2.18	0.44
2:X:407:ILE:HG12	2:X:424:TRP:HZ2	1.82	0.44
1:a:74:LEU:HD11	2:b:98:TRP:CZ3	2.53	0.44
2:d:260:VAL:HG13	2:d:261:GLU:N	2.32	0.44
2:D:491:LYS:HE2	2:D:496:LYS:O	2.18	0.44
1:G:40:MET:CE	2:H:104:LEU:HD21	2.47	0.44
2:H:238:ARG:HD2	2:H:394:LEU:HD11	1.99	0.44
2:L:491:LYS:HE2	2:L:496:LYS:O	2.18	0.44
1:M:74:LEU:HD11	2:N:98:TRP:CZ3	2.53	0.44
1:M:77:MET:HE3	1:M:77:MET:HB2	1.88	0.44
2:N:440:SER:C	2:N:441:THR:HG23	2.42	0.44
2:R:260:VAL:HG13	2:R:261:GLU:N	2.32	0.44
2:T:183:ALA:HB2	2:T:240:ILE:CD1	2.41	0.44
2:T:407:ILE:HG12	2:T:424:TRP:HZ2	1.82	0.44
1:U:6:SER:O	1:U:9:LYS:N	2.44	0.44
2:X:246:ARG:NH1	2:X:334:GLU:OE2	2.51	0.44
2:Z:49:ALA:O	2:Z:53:LEU:HB2	2.18	0.44
2:Z:133:PHE:HD2	2:Z:137:THR:HG21	1.82	0.44
2:d:491:LYS:HE2	2:d:496:LYS:O	2.18	0.44
2:F:260:VAL:O	2:F:261:GLU:CG	2.60	0.43
1:G:7:SER:HB2	2:V:138:TRP:CZ2	2.53	0.43
1:G:77:MET:HE3	1:G:77:MET:HB2	1.88	0.43
1:G:89:LEU:HD12	1:G:89:LEU:N	2.32	0.43
2:J:246:ARG:NH1	2:J:334:GLU:OE2	2.51	0.43
2:L:246:ARG:NH1	2:L:334:GLU:OE2	2.51	0.43
2:L:249:ALA:HB2	2:L:280:ALA:HB2	2.00	0.43
2:N:59:ILE:C	2:N:61:ASN:H	2.26	0.43
2:N:246:ARG:NH1	2:N:334:GLU:OE2	2.51	0.43
2:N:441:THR:OG1	2:N:445:LYS:CG	2.66	0.43
2:R:246:ARG:NH1	2:R:334:GLU:OE2	2.51	0.43
1:S:40:MET:CE	2:T:104:LEU:HD21	2.47	0.43
2:T:441:THR:OG1	2:T:445:LYS:CG	2.66	0.43
2:T:491:LYS:HE2	2:T:496:LYS:O	2.18	0.43
1:U:97:LEU:C	1:U:97:LEU:HD12	2.42	0.43
2:X:133:PHE:HD2	2:X:137:THR:HG22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:207:TRP:CE3	2:X:207:TRP:HA	2.53	0.43
2:Z:246:ARG:NH1	2:Z:334:GLU:OE2	2.51	0.43
2:d:49:ALA:O	2:d:53:LEU:HB2	2.18	0.43
2:d:441:THR:OG1	2:d:445:LYS:CG	2.66	0.43
2:B:183:ALA:HB2	2:B:240:ILE:CD1	2.41	0.43
2:B:246:ARG:NH1	2:B:334:GLU:OE2	2.51	0.43
2:D:49:ALA:O	2:D:53:LEU:HB2	2.18	0.43
2:D:441:THR:OG1	2:D:445:LYS:CG	2.66	0.43
2:H:59:ILE:C	2:H:61:ASN:H	2.26	0.43
2:J:49:ALA:O	2:J:53:LEU:HB2	2.17	0.43
2:J:207:TRP:HA	2:J:207:TRP:CE3	2.53	0.43
2:J:249:ALA:HB2	2:J:280:ALA:HB2	2.00	0.43
2:L:164:VAL:HG21	2:L:287:ALA:HB2	1.99	0.43
2:L:207:TRP:HA	2:L:207:TRP:CE3	2.54	0.43
2:L:286:MET:O	2:L:290:ILE:HG13	2.19	0.43
2:N:339:ASP:OD2	2:Z:409:ARG:NH1	2.47	0.43
1:O:10:PHE:HE1	2:d:139:ASP:HB2	1.82	0.43
2:P:246:ARG:NH1	2:P:334:GLU:OE2	2.51	0.43
2:V:59:ILE:C	2:V:61:ASN:H	2.26	0.43
2:V:164:VAL:HG21	2:V:287:ALA:HB2	1.99	0.43
2:V:244:MET:HG2	2:V:245:PRO:HD2	1.94	0.43
2:V:249:ALA:HB2	2:V:280:ALA:HB2	2.00	0.43
1:W:6:SER:O	1:W:9:LYS:N	2.44	0.43
2:X:441:THR:OG1	2:X:445:LYS:CG	2.66	0.43
2:Z:59:ILE:C	2:Z:61:ASN:H	2.27	0.43
2:Z:133:PHE:HD2	2:Z:137:THR:HG22	1.83	0.43
2:Z:137:THR:O	2:Z:137:THR:CG2	2.63	0.43
2:Z:249:ALA:HB2	2:Z:280:ALA:HB2	2.00	0.43
2:Z:491:LYS:HE2	2:Z:496:LYS:O	2.18	0.43
2:b:246:ARG:NH1	2:b:334:GLU:OE2	2.51	0.43
1:A:10:PHE:HE1	2:P:139:ASP:HB2	1.82	0.43
2:B:286:MET:O	2:B:290:ILE:HG13	2.19	0.43
2:B:437:PRO:HB2	2:B:441:THR:HG23	1.98	0.43
2:D:183:ALA:HB2	2:D:240:ILE:CD1	2.41	0.43
2:D:394:LEU:HD23	2:D:394:LEU:HA	1.77	0.43
2:F:133:PHE:HD2	2:F:137:THR:HG21	1.82	0.43
2:F:491:LYS:HE2	2:F:496:LYS:O	2.18	0.43
2:H:246:ARG:NH1	2:H:334:GLU:OE2	2.51	0.43
2:J:164:VAL:HG21	2:J:287:ALA:HB2	1.99	0.43
1:K:40:MET:CE	2:L:104:LEU:HD21	2.47	0.43
2:L:441:THR:OG1	2:L:445:LYS:CG	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:133:PHE:HD2	2:N:137:THR:HG21	1.82	0.43
2:R:133:PHE:HD2	2:R:137:THR:HG21	1.82	0.43
2:R:164:VAL:HG21	2:R:287:ALA:HB2	1.99	0.43
1:S:74:LEU:HD11	2:T:98:TRP:CZ3	2.53	0.43
2:T:59:ILE:C	2:T:61:ASN:H	2.26	0.43
2:T:133:PHE:HD2	2:T:137:THR:HG21	1.82	0.43
2:T:252:PRO:HB3	2:T:269:THR:HG21	1.99	0.43
2:T:442:GLU:CG	2:T:443:THR:H	2.25	0.43
2:X:249:ALA:HB2	2:X:280:ALA:HB2	2.00	0.43
2:b:183:ALA:HB2	2:b:240:ILE:CD1	2.41	0.43
2:b:286:MET:O	2:b:290:ILE:HG13	2.19	0.43
2:b:437:PRO:HB2	2:b:441:THR:HG23	1.98	0.43
2:d:183:ALA:HB2	2:d:240:ILE:CD1	2.41	0.43
2:D:246:ARG:NH1	2:D:334:GLU:OE2	2.51	0.43
2:D:286:MET:O	2:D:290:ILE:HG13	2.19	0.43
2:F:260:VAL:HG13	2:F:261:GLU:N	2.32	0.43
2:H:249:ALA:HB2	2:H:280:ALA:HB2	2.00	0.43
2:J:441:THR:OG1	2:J:445:LYS:CG	2.66	0.43
2:J:491:LYS:HE2	2:J:496:LYS:O	2.18	0.43
1:K:31:GLU:CB	2:Z:377:ASP:OD2	2.65	0.43
2:L:248:LEU:HD11	2:L:277:TYR:HB3	2.01	0.43
2:N:183:ALA:HB2	2:N:240:ILE:CD1	2.41	0.43
2:N:286:MET:O	2:N:290:ILE:HG13	2.19	0.43
2:P:286:MET:O	2:P:290:ILE:HG13	2.19	0.43
2:P:339:ASP:OD2	2:b:409:ARG:NH1	2.47	0.43
2:P:442:GLU:CG	2:P:443:THR:H	2.25	0.43
2:T:49:ALA:O	2:T:53:LEU:HB2	2.18	0.43
2:V:246:ARG:NH1	2:V:334:GLU:OE2	2.51	0.43
2:V:286:MET:O	2:V:290:ILE:HG13	2.19	0.43
2:Z:207:TRP:HA	2:Z:207:TRP:CE3	2.54	0.43
2:Z:260:VAL:HG13	2:Z:261:GLU:N	2.32	0.43
2:d:246:ARG:NH1	2:d:334:GLU:OE2	2.51	0.43
2:d:286:MET:O	2:d:290:ILE:HG13	2.19	0.43
2:d:394:LEU:HD23	2:d:394:LEU:HA	1.77	0.43
1:A:27:LEU:CD2	2:P:376:TYR:CZ	3.01	0.43
2:B:59:ILE:C	2:B:61:ASN:H	2.26	0.43
2:B:164:VAL:HG21	2:B:287:ALA:HB2	1.99	0.43
2:B:235:GLU:HG2	2:B:238:ARG:NH2	2.32	0.43
2:D:164:VAL:HG21	2:D:287:ALA:HB2	1.99	0.43
1:E:10:PHE:HE1	2:T:139:ASP:HB2	1.83	0.43
2:F:59:ILE:C	2:F:61:ASN:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:437:PRO:HB2	2:H:441:THR:HG23	1.98	0.43
2:J:59:ILE:C	2:J:61:ASN:H	2.26	0.43
2:J:123:LYS:HD2	2:J:167:TYR:HB3	2.01	0.43
2:J:437:PRO:HB2	2:J:441:THR:HG23	1.97	0.43
2:L:59:ILE:C	2:L:61:ASN:H	2.26	0.43
2:N:491:LYS:HE2	2:N:496:LYS:O	2.18	0.43
2:P:245:PRO:HG2	2:P:353:LEU:HB3	2.00	0.43
2:R:245:PRO:HG2	2:R:353:LEU:HB3	2.00	0.43
2:R:441:THR:OG1	2:R:445:LYS:CG	2.66	0.43
2:T:133:PHE:HD2	2:T:137:THR:HG22	1.82	0.43
2:T:286:MET:O	2:T:290:ILE:HG13	2.19	0.43
2:V:130:LEU:HD12	2:V:178:LEU:HD12	1.98	0.43
2:V:441:THR:OG1	2:V:445:LYS:CG	2.66	0.43
2:V:442:GLU:CG	2:V:443:THR:H	2.25	0.43
2:X:164:VAL:HG21	2:X:287:ALA:HB2	1.99	0.43
2:X:248:LEU:HD11	2:X:277:TYR:HB3	2.01	0.43
2:Z:248:LEU:HD11	2:Z:277:TYR:HB3	2.01	0.43
2:b:440:SER:C	2:b:441:THR:HG23	2.42	0.43
2:d:164:VAL:HG21	2:d:287:ALA:HB2	1.99	0.43
2:B:440:SER:C	2:B:441:THR:HG23	2.42	0.43
2:B:441:THR:OG1	2:B:445:LYS:CG	2.66	0.43
2:F:441:THR:OG1	2:F:445:LYS:CG	2.66	0.43
2:H:123:LYS:HD2	2:H:167:TYR:HB3	2.01	0.43
2:H:407:ILE:HG12	2:H:424:TRP:HZ2	1.82	0.43
2:J:248:LEU:HD11	2:J:277:TYR:HB3	2.01	0.43
1:M:27:LEU:CD2	2:b:376:TYR:CZ	3.02	0.43
2:N:207:TRP:HA	2:N:207:TRP:CE3	2.53	0.43
2:P:260:VAL:HG13	2:P:261:GLU:N	2.32	0.43
2:R:286:MET:O	2:R:290:ILE:HG13	2.19	0.43
2:T:123:LYS:HD2	2:T:167:TYR:HB3	2.01	0.43
2:V:207:TRP:HA	2:V:207:TRP:CE3	2.53	0.43
2:V:248:LEU:HD11	2:V:277:TYR:HB3	2.01	0.43
2:X:123:LYS:HD2	2:X:167:TYR:HB3	2.01	0.43
2:X:436:ASP:CB	2:X:437:PRO:HD3	2.46	0.43
2:b:59:ILE:C	2:b:61:ASN:H	2.26	0.43
2:b:164:VAL:HG21	2:b:287:ALA:HB2	1.99	0.43
2:b:235:GLU:HG2	2:b:238:ARG:NH2	2.32	0.43
2:b:441:THR:OG1	2:b:445:LYS:CG	2.67	0.43
1:C:27:LEU:CD2	2:R:376:TYR:CZ	3.02	0.43
2:F:133:PHE:HD2	2:F:137:THR:HG22	1.83	0.43
2:F:245:PRO:HG2	2:F:353:LEU:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:248:LEU:HD11	2:H:277:TYR:HB3	2.01	0.43
2:N:248:LEU:HD11	2:N:277:TYR:HB3	2.01	0.43
2:P:164:VAL:HG21	2:P:287:ALA:HB2	1.99	0.43
1:U:74:LEU:HD11	2:V:98:TRP:CZ3	2.53	0.43
2:X:491:LYS:HE2	2:X:496:LYS:O	2.18	0.43
2:D:58:LEU:HD13	1:c:95:LEU:HD13	2.00	0.43
2:D:369:SER:OG	2:D:389:ALA:O	2.22	0.43
2:J:286:MET:O	2:J:290:ILE:HG13	2.19	0.43
2:L:133:PHE:HD2	2:L:137:THR:HG22	1.83	0.43
2:L:245:PRO:HG2	2:L:353:LEU:HB3	2.00	0.43
2:L:496:LYS:NZ	2:X:474:ARG:HD2	2.33	0.43
2:N:319:THR:HG22	2:N:329:MET:HB3	2.01	0.43
2:P:49:ALA:O	2:P:53:LEU:HB2	2.17	0.43
2:R:404:LEU:HD12	2:R:404:LEU:HA	1.80	0.43
2:V:123:LYS:HD2	2:V:167:TYR:HB3	2.01	0.43
2:V:442:GLU:CG	2:V:443:THR:N	2.79	0.43
2:V:491:LYS:HE2	2:V:496:LYS:O	2.18	0.43
2:X:245:PRO:HG2	2:X:353:LEU:HB3	2.00	0.43
2:Z:286:MET:O	2:Z:290:ILE:HG13	2.19	0.43
2:D:127:HIS:HA	2:D:178:LEU:HD13	2.01	0.43
1:E:7:SER:HB2	2:T:138:TRP:CZ2	2.54	0.43
2:F:286:MET:O	2:F:290:ILE:HG13	2.19	0.43
1:G:27:LEU:CD2	2:V:376:TYR:CZ	3.02	0.43
1:G:74:LEU:HD11	2:H:98:TRP:CZ3	2.53	0.43
2:H:441:THR:OG1	2:H:445:LYS:CG	2.66	0.43
2:H:491:LYS:HE2	2:H:496:LYS:O	2.18	0.43
2:L:127:HIS:HA	2:L:178:LEU:HD13	2.01	0.43
2:L:133:PHE:HD2	2:L:137:THR:HG21	1.82	0.43
1:M:7:SER:HB2	2:b:138:TRP:CZ2	2.53	0.43
2:P:127:HIS:HA	2:P:178:LEU:HD13	2.01	0.43
2:P:441:THR:OG1	2:P:445:LYS:CG	2.67	0.43
2:R:49:ALA:O	2:R:53:LEU:HB2	2.18	0.43
2:T:248:LEU:HD11	2:T:277:TYR:HB3	2.01	0.43
2:X:59:ILE:C	2:X:61:ASN:H	2.27	0.43
2:X:133:PHE:HD2	2:X:137:THR:HG21	1.82	0.43
2:Z:127:HIS:HA	2:Z:178:LEU:HD13	2.01	0.43
2:Z:164:VAL:HG21	2:Z:287:ALA:HB2	1.99	0.43
2:Z:441:THR:OG1	2:Z:445:LYS:CG	2.66	0.43
2:d:127:HIS:HA	2:d:178:LEU:HD13	2.01	0.43
1:C:83:PHE:CE2	2:D:88:HIS:CG	3.07	0.43
2:F:248:LEU:HD11	2:F:277:TYR:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:61:LYS:HB3	1:G:61:LYS:HE2	1.81	0.43
2:L:483:THR:OG1	2:X:468:ASN:OD1	2.37	0.43
1:O:6:SER:O	1:O:9:LYS:N	2.44	0.43
2:P:430:LEU:HD12	2:P:430:LEU:HA	1.90	0.43
1:Q:83:PHE:CE2	2:R:88:HIS:CG	3.07	0.43
2:R:127:HIS:HA	2:R:178:LEU:HD13	2.01	0.43
2:R:242:LEU:O	2:R:351:MET:N	2.46	0.43
2:T:249:ALA:HB2	2:T:280:ALA:HB2	2.00	0.43
1:c:83:PHE:CE2	2:d:88:HIS:CG	3.07	0.43
2:B:58:LEU:HD13	1:a:95:LEU:HD13	2.00	0.42
2:B:248:LEU:HD11	2:B:277:TYR:HB3	2.01	0.42
2:B:319:THR:HG22	2:B:329:MET:HB3	2.01	0.42
2:D:207:TRP:HA	2:D:207:TRP:CE3	2.53	0.42
1:E:68:ASP:OD1	2:T:214:ARG:CD	2.67	0.42
1:I:7:SER:HB2	2:X:138:TRP:CZ2	2.53	0.42
1:K:27:LEU:CD2	2:Z:376:TYR:CZ	3.02	0.42
2:L:123:LYS:HD2	2:L:167:TYR:HB3	2.01	0.42
2:N:127:HIS:HA	2:N:178:LEU:HD13	2.01	0.42
2:N:249:ALA:HB2	2:N:280:ALA:HB2	2.00	0.42
1:S:57:VAL:HG12	1:S:58:ALA:N	2.34	0.42
2:V:394:LEU:HD23	2:V:394:LEU:HA	1.77	0.42
2:X:127:HIS:HA	2:X:178:LEU:HD13	2.01	0.42
2:Z:394:LEU:HD23	2:Z:394:LEU:HA	1.77	0.42
2:b:207:TRP:HA	2:b:207:TRP:CE3	2.53	0.42
2:b:491:LYS:HE2	2:b:496:LYS:O	2.18	0.42
2:d:207:TRP:HA	2:d:207:TRP:CE3	2.54	0.42
2:B:127:HIS:HA	2:B:178:LEU:HD13	2.01	0.42
2:B:207:TRP:HA	2:B:207:TRP:CE3	2.53	0.42
2:B:319:THR:HG21	2:b:224:GLU:HA	2.01	0.42
2:B:491:LYS:HE2	2:B:496:LYS:O	2.18	0.42
1:E:83:PHE:CE2	2:F:88:HIS:CG	3.07	0.42
2:F:483:THR:OG1	2:R:468:ASN:OD1	2.37	0.42
1:K:7:SER:HB2	2:Z:138:TRP:CZ2	2.54	0.42
1:M:61:LYS:HB3	1:M:61:LYS:HE2	1.81	0.42
1:O:83:PHE:CE2	2:P:88:HIS:CG	3.07	0.42
2:R:248:LEU:HD11	2:R:277:TYR:HB3	2.01	0.42
2:X:165:GLY:N	2:X:194:ILE:O	2.33	0.42
2:X:272:ALA:C	2:X:274:SER:H	2.28	0.42
2:Z:272:ALA:C	2:Z:274:SER:H	2.28	0.42
2:Z:319:THR:HG22	2:Z:329:MET:HB3	2.01	0.42
2:b:248:LEU:HD11	2:b:277:TYR:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:319:THR:HG22	2:b:329:MET:HB3	2.01	0.42
1:A:20:GLN:HB3	2:D:483:THR:HG22	2.01	0.42
2:B:249:ALA:HB2	2:B:280:ALA:HB2	2.00	0.42
1:C:7:SER:HB2	2:R:138:TRP:CZ2	2.54	0.42
2:D:248:LEU:HD11	2:D:277:TYR:HB3	2.01	0.42
2:D:441:THR:HG1	2:D:445:LYS:HZ2	1.63	0.42
1:E:20:GLN:HB3	2:H:483:THR:HG22	2.00	0.42
1:E:27:LEU:CD2	2:T:376:TYR:CZ	3.03	0.42
1:E:31:GLU:CB	2:T:377:ASP:OD2	2.64	0.42
2:F:127:HIS:HA	2:F:178:LEU:HD13	2.01	0.42
2:F:249:ALA:HB2	2:F:280:ALA:HB2	2.00	0.42
1:G:57:VAL:HG12	1:G:58:ALA:N	2.34	0.42
1:I:83:PHE:CE2	2:J:88:HIS:CG	3.07	0.42
2:J:272:ALA:C	2:J:274:SER:H	2.28	0.42
1:K:57:VAL:HG12	1:K:58:ALA:N	2.34	0.42
1:M:57:VAL:HG12	1:M:58:ALA:N	2.35	0.42
1:O:7:SER:HB2	2:d:138:TRP:CZ2	2.54	0.42
2:P:249:ALA:HB2	2:P:280:ALA:HB2	2.00	0.42
2:P:440:SER:C	2:P:441:THR:HG23	2.42	0.42
2:R:249:ALA:HB2	2:R:280:ALA:HB2	2.00	0.42
1:S:83:PHE:CE2	2:T:88:HIS:CG	3.07	0.42
2:T:207:TRP:HA	2:T:207:TRP:CE3	2.54	0.42
2:T:319:THR:HG22	2:T:329:MET:HB3	2.01	0.42
1:W:83:PHE:CE2	2:X:88:HIS:CG	3.07	0.42
2:X:369:SER:OG	2:X:389:ALA:O	2.22	0.42
2:Z:123:LYS:HD2	2:Z:167:TYR:HB3	2.01	0.42
2:Z:245:PRO:HG2	2:Z:353:LEU:HB3	2.00	0.42
2:b:249:ALA:HB2	2:b:280:ALA:HB2	2.00	0.42
2:d:248:LEU:HD11	2:d:277:TYR:HB3	2.01	0.42
2:B:52:ALA:HB1	1:a:121:LYS:CB	2.49	0.42
2:B:245:PRO:HG2	2:B:353:LEU:HB3	2.00	0.42
1:C:31:GLU:CB	2:R:377:ASP:OD2	2.64	0.42
2:H:245:PRO:HG2	2:H:353:LEU:HB3	2.00	0.42
2:P:437:PRO:HB2	2:P:441:THR:HG23	1.97	0.42
2:R:339:ASP:OD2	2:d:409:ARG:NH1	2.47	0.42
2:T:430:LEU:HD12	2:T:430:LEU:HA	1.90	0.42
1:U:57:VAL:HG12	1:U:58:ALA:N	2.35	0.42
1:U:77:MET:HE3	1:U:77:MET:HB2	1.88	0.42
1:U:83:PHE:CE2	2:V:88:HIS:CG	3.07	0.42
2:V:245:PRO:HG2	2:V:353:LEU:HB3	2.00	0.42
2:X:286:MET:O	2:X:290:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:441:THR:HG1	2:Z:445:LYS:HZ2	1.61	0.42
2:b:245:PRO:HG2	2:b:353:LEU:HB3	2.00	0.42
1:A:83:PHE:CE2	2:B:88:HIS:CG	3.07	0.42
2:D:52:ALA:HB1	1:c:121:LYS:CB	2.50	0.42
2:F:123:LYS:HD2	2:F:167:TYR:HB3	2.01	0.42
2:F:165:GLY:N	2:F:194:ILE:O	2.33	0.42
1:G:83:PHE:CE2	2:H:88:HIS:CG	3.07	0.42
2:H:183:ALA:HB1	2:H:236:ASP:O	2.20	0.42
2:H:186:SER:HB2	2:H:191:ALA:O	2.19	0.42
2:H:286:MET:O	2:H:290:ILE:HG13	2.19	0.42
2:J:127:HIS:HA	2:J:178:LEU:HD13	2.01	0.42
2:J:186:SER:HB2	2:J:191:ALA:O	2.19	0.42
2:J:245:PRO:HG2	2:J:353:LEU:HB3	2.00	0.42
2:L:186:SER:HB2	2:L:191:ALA:O	2.19	0.42
2:L:272:ALA:C	2:L:274:SER:H	2.28	0.42
2:L:319:THR:HG22	2:L:329:MET:HB3	2.01	0.42
2:L:436:ASP:CB	2:L:437:PRO:HD3	2.46	0.42
2:P:248:LEU:HD11	2:P:277:TYR:HB3	2.01	0.42
2:P:491:LYS:HE2	2:P:496:LYS:O	2.18	0.42
2:R:123:LYS:HD2	2:R:167:TYR:HB3	2.01	0.42
1:W:57:VAL:HG12	1:W:58:ALA:N	2.34	0.42
2:X:436:ASP:CB	2:X:437:PRO:CD	2.91	0.42
2:Z:186:SER:HB2	2:Z:191:ALA:O	2.19	0.42
1:a:83:PHE:CE2	2:b:88:HIS:CG	3.07	0.42
2:b:127:HIS:HA	2:b:178:LEU:HD13	2.01	0.42
2:b:272:ALA:C	2:b:274:SER:H	2.27	0.42
2:B:272:ALA:C	2:B:274:SER:H	2.28	0.42
2:D:165:GLY:N	2:D:194:ILE:O	2.33	0.42
2:F:183:ALA:HB1	2:F:236:ASP:O	2.20	0.42
2:F:186:SER:HB2	2:F:191:ALA:O	2.19	0.42
2:F:207:TRP:HA	2:F:207:TRP:CE3	2.53	0.42
2:H:207:TRP:CE3	2:H:207:TRP:HA	2.54	0.42
2:H:272:ALA:C	2:H:274:SER:H	2.27	0.42
2:H:404:LEU:HD12	2:H:404:LEU:HA	1.80	0.42
2:H:442:GLU:CG	2:H:443:THR:N	2.79	0.42
1:I:35:GLN:HE21	2:J:113:GLN:HE22	1.68	0.42
1:I:57:VAL:HG12	1:I:58:ALA:N	2.34	0.42
2:N:272:ALA:C	2:N:274:SER:H	2.27	0.42
1:O:57:VAL:HG12	1:O:58:ALA:N	2.34	0.42
2:P:59:ILE:C	2:P:61:ASN:H	2.26	0.42
2:P:207:TRP:CE3	2:P:207:TRP:HA	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:127:HIS:HA	2:T:178:LEU:HD13	2.01	0.42
2:T:186:SER:HB2	2:T:191:ALA:O	2.19	0.42
1:U:35:GLN:HE21	2:V:113:GLN:HE22	1.68	0.42
2:V:186:SER:HB2	2:V:191:ALA:O	2.19	0.42
2:X:183:ALA:HB2	2:X:240:ILE:CD1	2.41	0.42
2:X:183:ALA:HB1	2:X:236:ASP:O	2.20	0.42
2:X:186:SER:HB2	2:X:191:ALA:O	2.19	0.42
2:d:165:GLY:N	2:d:194:ILE:O	2.33	0.42
2:d:245:PRO:HG2	2:d:353:LEU:HB3	2.00	0.42
2:F:442:GLU:CG	2:F:443:THR:H	2.25	0.42
2:H:127:HIS:HA	2:H:178:LEU:HD13	2.01	0.42
2:J:483:THR:OG1	2:V:468:ASN:OD1	2.37	0.42
1:K:83:PHE:CE2	2:L:88:HIS:CG	3.07	0.42
1:M:35:GLN:HE21	2:N:113:GLN:HE22	1.68	0.42
2:N:123:LYS:HD2	2:N:167:TYR:HB3	2.01	0.42
2:N:208:GLN:OE1	2:N:274:SER:OG	2.28	0.42
2:V:183:ALA:HB1	2:V:236:ASP:O	2.20	0.42
2:V:272:ALA:C	2:V:274:SER:H	2.28	0.42
2:X:38:ARG:HB3	2:X:39:GLU:H	1.65	0.42
2:X:319:THR:HG22	2:X:329:MET:HB3	2.01	0.42
2:b:430:LEU:HD12	2:b:430:LEU:HA	1.90	0.42
1:A:35:GLN:HE21	2:B:113:GLN:HE22	1.68	0.42
2:B:430:LEU:HD12	2:B:430:LEU:HA	1.90	0.42
2:D:245:PRO:HG2	2:D:353:LEU:HB3	2.00	0.42
1:E:61:LYS:HB3	1:E:61:LYS:HE2	1.81	0.42
1:G:20:GLN:HB3	2:J:483:THR:HG22	2.02	0.42
1:G:35:GLN:HE21	2:H:113:GLN:HE22	1.68	0.42
2:J:183:ALA:HB1	2:J:236:ASP:O	2.20	0.42
2:N:186:SER:HB2	2:N:191:ALA:O	2.19	0.42
2:P:272:ALA:C	2:P:274:SER:H	2.28	0.42
2:P:319:THR:HG22	2:P:329:MET:HB3	2.01	0.42
2:R:483:THR:OG1	2:d:468:ASN:OD1	2.38	0.42
2:T:394:LEU:HD23	2:T:394:LEU:HA	1.77	0.42
2:V:127:HIS:HA	2:V:178:LEU:HD13	2.01	0.42
1:W:35:GLN:HE21	2:X:113:GLN:HE22	1.68	0.42
1:Y:35:GLN:HE21	2:Z:113:GLN:HE22	1.68	0.42
2:Z:404:LEU:HD12	2:Z:404:LEU:HA	1.80	0.42
2:D:319:THR:HG22	2:D:329:MET:HB3	2.01	0.42
2:D:440:SER:C	2:D:441:THR:HG23	2.42	0.42
2:F:404:LEU:HD12	2:F:404:LEU:HA	1.80	0.42
1:K:35:GLN:HE21	2:L:113:GLN:HE22	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:78:LEU:HD23	2:N:78:LEU:HA	1.85	0.42
2:N:404:LEU:HD12	2:N:404:LEU:HA	1.80	0.42
1:O:27:LEU:CD2	2:d:376:TYR:CZ	3.03	0.42
2:R:186:SER:HB2	2:R:191:ALA:O	2.19	0.42
2:R:207:TRP:HA	2:R:207:TRP:CE3	2.54	0.42
2:T:245:PRO:HG2	2:T:353:LEU:HB3	2.00	0.42
1:Y:57:VAL:HG12	1:Y:58:ALA:N	2.35	0.42
2:Z:183:ALA:HB1	2:Z:236:ASP:O	2.20	0.42
2:d:319:THR:HG22	2:d:329:MET:HB3	2.01	0.42
2:d:440:SER:C	2:d:441:THR:HG23	2.42	0.42
1:M:83:PHE:CE2	2:N:88:HIS:CG	3.07	0.42
2:N:245:PRO:HG2	2:N:353:LEU:HB3	2.00	0.42
2:P:186:SER:HB2	2:P:191:ALA:O	2.19	0.42
2:X:437:PRO:HB2	2:X:441:THR:HG23	1.97	0.42
2:X:442:GLU:CG	2:X:443:THR:H	2.24	0.42
1:a:35:GLN:HE21	2:b:113:GLN:HE22	1.68	0.42
2:D:123:LYS:HD2	2:D:167:TYR:HB3	2.01	0.41
2:H:319:THR:HG22	2:H:329:MET:HB3	2.01	0.41
1:I:20:GLN:HB3	2:L:483:THR:HG22	2.02	0.41
1:K:20:GLN:HB3	2:N:483:THR:HG22	2.01	0.41
1:K:77:MET:HE3	1:K:77:MET:HB2	1.88	0.41
2:P:242:LEU:O	2:P:351:MET:N	2.46	0.41
2:V:319:THR:HG22	2:V:329:MET:HB3	2.01	0.41
2:b:123:LYS:HD2	2:b:167:TYR:HB3	2.01	0.41
2:d:123:LYS:HD2	2:d:167:TYR:HB3	2.01	0.41
1:A:19:VAL:HA	2:D:482:LEU:O	2.19	0.41
2:B:123:LYS:HD2	2:B:167:TYR:HB3	2.01	0.41
2:D:319:THR:HG21	2:d:224:GLU:HA	2.02	0.41
2:J:270:ASP:OD1	2:J:270:ASP:N	2.54	0.41
1:O:35:GLN:HE21	2:P:113:GLN:HE22	1.68	0.41
2:P:123:LYS:HD2	2:P:167:TYR:HB3	2.01	0.41
2:R:319:THR:HG22	2:R:329:MET:HB3	2.01	0.41
1:S:35:GLN:HE21	2:T:113:GLN:HE22	1.68	0.41
2:T:242:LEU:O	2:T:351:MET:N	2.46	0.41
1:Y:83:PHE:CE2	2:Z:88:HIS:CG	3.07	0.41
2:Z:244:MET:HG2	2:Z:245:PRO:HD2	1.94	0.41
1:A:31:GLU:CB	2:P:377:ASP:OD2	2.63	0.41
2:B:78:LEU:HA	2:B:78:LEU:HD23	1.84	0.41
2:D:183:ALA:HB1	2:D:236:ASP:O	2.20	0.41
2:D:244:MET:HG2	2:D:245:PRO:HD2	1.94	0.41
2:D:249:ALA:HB2	2:D:280:ALA:HB2	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:394:LEU:HD23	2:L:394:LEU:HA	1.77	0.41
2:N:430:LEU:HD12	2:N:430:LEU:HA	1.90	0.41
1:O:20:GLN:HB3	2:R:483:THR:HG22	2.02	0.41
1:O:68:ASP:OD1	2:d:214:ARG:CD	2.69	0.41
2:T:183:ALA:HB1	2:T:236:ASP:O	2.20	0.41
2:T:442:GLU:CG	2:T:443:THR:N	2.79	0.41
2:V:270:ASP:OD1	2:V:270:ASP:N	2.54	0.41
2:Z:436:ASP:CB	2:Z:437:PRO:HD3	2.46	0.41
2:d:183:ALA:HB1	2:d:236:ASP:O	2.20	0.41
2:d:244:MET:HG2	2:d:245:PRO:HD2	1.94	0.41
2:B:186:SER:HB2	2:B:191:ALA:O	2.19	0.41
2:B:270:ASP:OD1	2:B:270:ASP:N	2.54	0.41
2:D:59:ILE:C	2:D:61:ASN:H	2.26	0.41
2:F:394:LEU:HD23	2:F:394:LEU:HA	1.77	0.41
1:G:6:SER:O	1:G:9:LYS:N	2.44	0.41
2:J:319:THR:HG22	2:J:329:MET:HB3	2.01	0.41
2:J:394:LEU:HD23	2:J:394:LEU:HA	1.77	0.41
1:U:20:GLN:HB3	2:X:483:THR:HG22	2.02	0.41
2:V:151:GLU:HG3	2:V:160:TYR:CD2	2.56	0.41
2:X:270:ASP:N	2:X:270:ASP:OD1	2.54	0.41
2:b:186:SER:HB2	2:b:191:ALA:O	2.19	0.41
2:b:270:ASP:OD1	2:b:270:ASP:N	2.54	0.41
2:d:59:ILE:C	2:d:61:ASN:H	2.26	0.41
2:d:151:GLU:HG3	2:d:160:TYR:CD2	2.56	0.41
2:L:430:LEU:HD12	2:L:430:LEU:HA	1.90	0.41
1:M:89:LEU:HD23	1:M:122:LEU:HD11	2.02	0.41
2:R:151:GLU:HG3	2:R:160:TYR:CD2	2.56	0.41
2:R:272:ALA:C	2:R:274:SER:H	2.28	0.41
2:R:440:SER:C	2:R:441:THR:HG23	2.42	0.41
2:b:78:LEU:HA	2:b:78:LEU:HD23	1.85	0.41
2:d:249:ALA:HB2	2:d:280:ALA:HB2	2.00	0.41
1:C:35:GLN:HE21	2:D:113:GLN:HE22	1.68	0.41
2:D:186:SER:HB2	2:D:191:ALA:O	2.19	0.41
1:E:19:VAL:HA	2:H:482:LEU:O	2.21	0.41
1:G:43:MET:HE2	2:H:163:LEU:HD11	2.03	0.41
1:G:89:LEU:HD23	1:G:122:LEU:HD11	2.02	0.41
2:T:272:ALA:C	2:T:274:SER:H	2.28	0.41
1:Y:89:LEU:HD23	1:Y:122:LEU:HD11	2.02	0.41
2:Z:430:LEU:HD12	2:Z:430:LEU:HA	1.90	0.41
2:b:183:ALA:HB1	2:b:236:ASP:O	2.20	0.41
1:c:35:GLN:HE21	2:d:113:GLN:HE22	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:186:SER:HB2	2:d:191:ALA:O	2.19	0.41
1:A:57:VAL:HG12	1:A:58:ALA:N	2.34	0.41
2:B:183:ALA:HB1	2:B:236:ASP:O	2.20	0.41
1:C:32:LYS:HB2	2:R:375:GLU:O	2.21	0.41
1:C:57:VAL:HG12	1:C:58:ALA:N	2.34	0.41
1:E:35:GLN:HE21	2:F:113:GLN:HE22	1.68	0.41
2:F:319:THR:HG22	2:F:329:MET:HB3	2.01	0.41
1:G:54:GLN:NE2	2:H:120:ASN:ND2	2.69	0.41
2:H:483:THR:OG1	2:T:468:ASN:OD1	2.38	0.41
1:I:54:GLN:NE2	2:J:120:ASN:ND2	2.69	0.41
1:K:43:MET:HE2	2:L:163:LEU:HD11	2.03	0.41
2:L:183:ALA:HB1	2:L:236:ASP:O	2.20	0.41
2:L:270:ASP:OD1	2:L:270:ASP:N	2.54	0.41
1:Q:57:VAL:HG12	1:Q:58:ALA:N	2.35	0.41
1:Q:89:LEU:HD23	1:Q:122:LEU:HD11	2.02	0.41
2:R:394:LEU:HD23	2:R:394:LEU:HA	1.77	0.41
1:U:43:MET:HE2	2:V:163:LEU:HD11	2.03	0.41
1:Y:43:MET:HE2	2:Z:163:LEU:HD11	2.03	0.41
2:Z:442:GLU:CG	2:Z:443:THR:H	2.24	0.41
1:a:57:VAL:HG12	1:a:58:ALA:N	2.35	0.41
1:c:57:VAL:HG12	1:c:58:ALA:N	2.34	0.41
2:D:272:ALA:C	2:D:274:SER:H	2.27	0.41
1:I:43:MET:HE2	2:J:163:LEU:HD11	2.03	0.41
1:K:68:ASP:OD1	2:Z:214:ARG:CD	2.68	0.41
1:K:89:LEU:HD23	1:K:122:LEU:HD11	2.02	0.41
1:M:43:MET:HE2	2:N:163:LEU:HD11	2.03	0.41
2:N:270:ASP:OD1	2:N:270:ASP:N	2.54	0.41
1:Q:43:MET:HE2	2:R:163:LEU:HD11	2.03	0.41
2:R:437:PRO:HB2	2:R:441:THR:HG23	1.98	0.41
2:X:394:LEU:HD23	2:X:394:LEU:HA	1.77	0.41
2:Z:78:LEU:HD23	2:Z:78:LEU:HA	1.85	0.41
1:A:43:MET:HE2	2:B:163:LEU:HD11	2.03	0.41
1:A:89:LEU:HD23	1:A:122:LEU:HD11	2.02	0.41
1:C:43:MET:HE2	2:D:163:LEU:HD11	2.03	0.41
2:D:260:VAL:O	2:D:261:GLU:CG	2.60	0.41
1:E:43:MET:HE2	2:F:163:LEU:HD11	2.03	0.41
1:E:57:VAL:HG12	1:E:58:ALA:N	2.34	0.41
1:E:89:LEU:HD23	1:E:122:LEU:HD11	2.02	0.41
2:F:151:GLU:HG3	2:F:160:TYR:CD2	2.56	0.41
2:F:403:TYR:HD1	2:F:403:TYR:HA	1.78	0.41
2:F:440:SER:C	2:F:441:THR:HG23	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:270:ASP:OD1	2:H:270:ASP:N	2.54	0.41
2:J:151:GLU:HG3	2:J:160:TYR:CD2	2.56	0.41
2:J:340:ARG:CZ	2:V:139:ASP:OD2	2.67	0.41
2:N:151:GLU:HG3	2:N:160:TYR:CD2	2.56	0.41
2:N:436:ASP:CB	2:N:437:PRO:HD3	2.45	0.41
1:O:31:GLU:CB	2:d:377:ASP:OD2	2.65	0.41
1:O:77:MET:HE3	1:O:77:MET:HB2	1.88	0.41
2:P:183:ALA:HB1	2:P:236:ASP:O	2.20	0.41
2:P:483:THR:OG1	2:b:468:ASN:OD1	2.37	0.41
1:Q:35:GLN:HE21	2:R:113:GLN:HE22	1.68	0.41
2:R:59:ILE:C	2:R:61:ASN:H	2.26	0.41
2:R:270:ASP:OD1	2:R:270:ASP:N	2.54	0.41
1:S:43:MET:HE2	2:T:163:LEU:HD11	2.03	0.41
2:T:434:ASP:HB2	2:T:437:PRO:HG2	2.03	0.41
2:T:440:SER:C	2:T:441:THR:HG23	2.42	0.41
1:W:43:MET:HE2	2:X:163:LEU:HD11	2.03	0.41
2:Z:151:GLU:HG3	2:Z:160:TYR:CD2	2.56	0.41
1:a:43:MET:HE2	2:b:163:LEU:HD11	2.03	0.41
1:a:89:LEU:HD23	1:a:122:LEU:HD11	2.02	0.41
1:c:43:MET:HE2	2:d:163:LEU:HD11	2.03	0.41
2:d:272:ALA:C	2:d:274:SER:H	2.28	0.41
2:D:437:PRO:HB2	2:D:441:THR:HG23	1.98	0.41
1:I:27:LEU:CD2	2:X:376:TYR:CZ	3.04	0.41
2:J:78:LEU:HA	2:J:78:LEU:HD23	1.84	0.41
2:L:404:LEU:HD12	2:L:404:LEU:HA	1.80	0.41
1:U:89:LEU:HD23	1:U:122:LEU:HD11	2.02	0.41
2:X:434:ASP:HB2	2:X:437:PRO:HG2	2.03	0.41
2:d:260:VAL:O	2:d:261:GLU:CG	2.60	0.41
2:d:369:SER:OG	2:d:389:ALA:O	2.22	0.41
2:d:437:PRO:HB2	2:d:441:THR:HG23	1.97	0.41
1:E:54:GLN:NE2	2:F:120:ASN:ND2	2.69	0.40
1:G:19:VAL:HA	2:J:482:LEU:O	2.21	0.40
2:H:440:SER:C	2:H:441:THR:HG23	2.42	0.40
2:N:483:THR:OG1	2:Z:468:ASN:OD1	2.38	0.40
1:O:43:MET:HE2	2:P:163:LEU:HD11	2.03	0.40
2:R:183:ALA:HB1	2:R:236:ASP:O	2.20	0.40
2:R:260:VAL:O	2:R:261:GLU:CG	2.60	0.40
1:S:61:LYS:HB3	1:S:61:LYS:HE2	1.81	0.40
1:A:7:SER:HB2	2:P:138:TRP:CZ2	2.55	0.40
1:A:32:LYS:HB2	2:P:375:GLU:O	2.21	0.40
1:E:61:LYS:HA	2:F:146:LYS:HZ2	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:434:ASP:HB2	2:H:437:PRO:HG2	2.03	0.40
1:I:31:GLU:CB	2:X:377:ASP:OD2	2.66	0.40
1:K:54:GLN:NE2	2:L:120:ASN:ND2	2.69	0.40
1:M:68:ASP:OD1	2:b:214:ARG:CD	2.69	0.40
2:N:183:ALA:HB1	2:N:236:ASP:O	2.20	0.40
2:N:403:TYR:HD1	2:N:403:TYR:HA	1.78	0.40
1:Q:54:GLN:NE2	2:R:120:ASN:ND2	2.69	0.40
2:R:441:THR:HG1	2:R:445:LYS:HZ2	1.63	0.40
1:S:20:GLN:HB3	2:V:483:THR:HG22	2.03	0.40
1:S:89:LEU:HD23	1:S:122:LEU:HD11	2.02	0.40
1:W:89:LEU:HD23	1:W:122:LEU:HD11	2.02	0.40
1:Y:77:MET:HE3	1:Y:77:MET:HB2	1.88	0.40
2:d:434:ASP:HB2	2:d:437:PRO:HG2	2.03	0.40
1:C:35:GLN:HB3	1:C:36:LEU:H	1.69	0.40
2:D:332:PRO:HD2	2:D:355:HIS:CG	2.57	0.40
2:D:434:ASP:HB2	2:D:437:PRO:HG2	2.03	0.40
1:I:61:LYS:HA	2:J:146:LYS:HZ2	1.87	0.40
1:O:54:GLN:HE22	2:P:120:ASN:ND2	2.20	0.40
2:P:332:PRO:HD2	2:P:355:HIS:CG	2.57	0.40
1:S:54:GLN:NE2	2:T:120:ASN:ND2	2.69	0.40
2:V:332:PRO:HD2	2:V:355:HIS:CG	2.57	0.40
2:Z:270:ASP:N	2:Z:270:ASP:OD1	2.54	0.40
2:d:332:PRO:HD2	2:d:355:HIS:CG	2.57	0.40
2:B:151:GLU:HG3	2:B:160:TYR:CD2	2.56	0.40
2:B:436:ASP:CB	2:B:437:PRO:HD3	2.46	0.40
2:D:403:TYR:HB3	2:D:428:TRP:HZ2	1.87	0.40
2:D:488:LEU:HG	2:P:397:THR:CG2	2.50	0.40
2:F:242:LEU:O	2:F:351:MET:N	2.46	0.40
2:J:165:GLY:N	2:J:194:ILE:O	2.33	0.40
2:J:434:ASP:HB2	2:J:437:PRO:HG2	2.03	0.40
1:O:89:LEU:HD23	1:O:122:LEU:HD11	2.02	0.40
1:S:61:LYS:HA	2:T:146:LYS:HZ2	1.86	0.40
2:V:133:PHE:HD2	2:V:137:THR:HG21	1.82	0.40
1:W:61:LYS:HA	2:X:146:LYS:HZ2	1.87	0.40
2:b:151:GLU:HG3	2:b:160:TYR:CD2	2.56	0.40
2:b:436:ASP:CB	2:b:437:PRO:HD3	2.46	0.40
1:c:35:GLN:HB3	1:c:36:LEU:H	1.69	0.40
2:B:332:PRO:HD2	2:B:355:HIS:CG	2.57	0.40
2:H:332:PRO:HD2	2:H:355:HIS:CG	2.57	0.40
1:I:7:SER:HB2	2:X:138:TRP:CH2	2.57	0.40
1:M:32:LYS:HB2	2:b:375:GLU:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:54:GLN:HE22	2:N:120:ASN:ND2	2.20	0.40
1:O:61:LYS:HA	2:P:146:LYS:HZ2	1.85	0.40
2:R:403:TYR:HB3	2:R:428:TRP:HZ2	1.87	0.40
2:V:242:LEU:O	2:V:351:MET:N	2.46	0.40
2:V:440:SER:C	2:V:441:THR:HG23	2.42	0.40
2:X:332:PRO:HD2	2:X:355:HIS:CG	2.57	0.40
1:Y:54:GLN:NE2	2:Z:120:ASN:ND2	2.69	0.40
2:b:322:THR:HG22	2:b:326:GLY:HA2	2.04	0.40
2:d:403:TYR:HB3	2:d:428:TRP:HZ2	1.87	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	130/132 (98%)	121 (93%)	9 (7%)	0	100	100
1	C	130/132 (98%)	121 (93%)	9 (7%)	0	100	100
1	E	130/132 (98%)	121 (93%)	9 (7%)	0	100	100
1	G	130/132 (98%)	121 (93%)	9 (7%)	0	100	100
1	I	130/132 (98%)	121 (93%)	9 (7%)	0	100	100
1	K	130/132 (98%)	121 (93%)	9 (7%)	0	100	100
1	M	130/132 (98%)	121 (93%)	9 (7%)	0	100	100
1	O	130/132 (98%)	121 (93%)	9 (7%)	0	100	100
1	Q	130/132 (98%)	121 (93%)	9 (7%)	0	100	100
1	S	130/132 (98%)	121 (93%)	9 (7%)	0	100	100
1	U	130/132 (98%)	121 (93%)	9 (7%)	0	100	100
1	W	130/132 (98%)	121 (93%)	9 (7%)	0	100	100
1	Y	130/132 (98%)	121 (93%)	9 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	130/132 (98%)	121 (93%)	9 (7%)	0	100	100
1	c	130/132 (98%)	121 (93%)	9 (7%)	0	100	100
2	B	459/461 (100%)	442 (96%)	17 (4%)	0	100	100
2	D	459/461 (100%)	442 (96%)	17 (4%)	0	100	100
2	F	459/461 (100%)	442 (96%)	17 (4%)	0	100	100
2	H	459/461 (100%)	442 (96%)	17 (4%)	0	100	100
2	J	459/461 (100%)	442 (96%)	17 (4%)	0	100	100
2	L	459/461 (100%)	442 (96%)	17 (4%)	0	100	100
2	N	459/461 (100%)	442 (96%)	17 (4%)	0	100	100
2	P	459/461 (100%)	442 (96%)	17 (4%)	0	100	100
2	R	459/461 (100%)	442 (96%)	17 (4%)	0	100	100
2	T	459/461 (100%)	442 (96%)	17 (4%)	0	100	100
2	V	459/461 (100%)	442 (96%)	17 (4%)	0	100	100
2	X	459/461 (100%)	442 (96%)	17 (4%)	0	100	100
2	Z	459/461 (100%)	442 (96%)	17 (4%)	0	100	100
2	b	459/461 (100%)	442 (96%)	17 (4%)	0	100	100
2	d	459/461 (100%)	442 (96%)	17 (4%)	0	100	100
All	All	8835/8895 (99%)	8445 (96%)	390 (4%)	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	110/110 (100%)	108 (98%)	2 (2%)	51	70
1	C	110/110 (100%)	108 (98%)	2 (2%)	51	70
1	E	110/110 (100%)	108 (98%)	2 (2%)	51	70
1	G	110/110 (100%)	108 (98%)	2 (2%)	51	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	110/110 (100%)	108 (98%)	2 (2%)	51	70
1	K	110/110 (100%)	108 (98%)	2 (2%)	51	70
1	M	110/110 (100%)	108 (98%)	2 (2%)	51	70
1	O	110/110 (100%)	108 (98%)	2 (2%)	51	70
1	Q	110/110 (100%)	108 (98%)	2 (2%)	51	70
1	S	110/110 (100%)	108 (98%)	2 (2%)	51	70
1	U	110/110 (100%)	108 (98%)	2 (2%)	51	70
1	W	110/110 (100%)	108 (98%)	2 (2%)	51	70
1	Y	110/110 (100%)	108 (98%)	2 (2%)	51	70
1	a	110/110 (100%)	108 (98%)	2 (2%)	51	70
1	c	110/110 (100%)	108 (98%)	2 (2%)	51	70
2	B	384/384 (100%)	382 (100%)	2 (0%)	81	83
2	D	384/384 (100%)	382 (100%)	2 (0%)	81	83
2	F	384/384 (100%)	382 (100%)	2 (0%)	81	83
2	H	384/384 (100%)	382 (100%)	2 (0%)	81	83
2	J	384/384 (100%)	382 (100%)	2 (0%)	81	83
2	L	384/384 (100%)	382 (100%)	2 (0%)	81	83
2	N	384/384 (100%)	382 (100%)	2 (0%)	81	83
2	P	384/384 (100%)	382 (100%)	2 (0%)	81	83
2	R	384/384 (100%)	382 (100%)	2 (0%)	81	83
2	T	384/384 (100%)	382 (100%)	2 (0%)	81	83
2	V	384/384 (100%)	382 (100%)	2 (0%)	81	83
2	X	384/384 (100%)	382 (100%)	2 (0%)	81	83
2	Z	384/384 (100%)	382 (100%)	2 (0%)	81	83
2	b	384/384 (100%)	382 (100%)	2 (0%)	81	83
2	d	384/384 (100%)	382 (100%)	2 (0%)	81	83
All	All	7410/7410 (100%)	7350 (99%)	60 (1%)	70	79

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLU
1	A	27	LEU

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Mol	Chain	Res	Type
2	B	160	TYR
2	B	473	LEU
1	C	22	GLU
1	C	27	LEU
2	D	160	TYR
2	D	473	LEU
1	E	22	GLU
1	E	27	LEU
2	F	160	TYR
2	F	473	LEU
1	G	22	GLU
1	G	27	LEU
2	H	160	TYR
2	H	473	LEU
1	I	22	GLU
1	I	27	LEU
2	J	160	TYR
2	J	473	LEU
1	K	22	GLU
1	K	27	LEU
2	L	160	TYR
2	L	473	LEU
1	M	22	GLU
1	M	27	LEU
2	N	160	TYR
2	N	473	LEU
1	O	22	GLU
1	O	27	LEU
2	P	160	TYR
2	P	473	LEU
1	Q	22	GLU
1	Q	27	LEU
2	R	160	TYR
2	R	473	LEU
1	S	22	GLU
1	S	27	LEU
2	T	160	TYR
2	T	473	LEU
1	U	22	GLU
1	U	27	LEU
2	V	160	TYR
2	V	473	LEU

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Mol	Chain	Res	Type
1	W	22	GLU
1	W	27	LEU
2	X	160	TYR
2	X	473	LEU
1	Y	22	GLU
1	Y	27	LEU
2	Z	160	TYR
2	Z	473	LEU
1	a	22	GLU
1	a	27	LEU
2	b	160	TYR
2	b	473	LEU
1	c	22	GLU
1	c	27	LEU
2	d	160	TYR
2	d	473	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (105) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	87	ASN
2	B	87	HIS
2	B	102	HIS
2	B	113	GLN
2	B	127	HIS
2	B	291	ASN
1	C	54	GLN
1	C	87	ASN
2	D	87	HIS
2	D	102	HIS
2	D	113	GLN
2	D	127	HIS
2	D	291	ASN
1	E	54	GLN
1	E	87	ASN
2	F	87	HIS
2	F	102	HIS
2	F	113	GLN
2	F	127	HIS
2	F	291	ASN
1	G	54	GLN

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Mol	Chain	Res	Type
1	G	87	ASN
2	H	87	HIS
2	H	102	HIS
2	H	113	GLN
2	H	127	HIS
2	H	291	ASN
1	I	54	GLN
1	I	87	ASN
2	J	87	HIS
2	J	102	HIS
2	J	113	GLN
2	J	127	HIS
2	J	291	ASN
1	K	54	GLN
1	K	87	ASN
2	L	87	HIS
2	L	102	HIS
2	L	113	GLN
2	L	127	HIS
2	L	291	ASN
1	M	54	GLN
1	M	87	ASN
2	N	87	HIS
2	N	102	HIS
2	N	113	GLN
2	N	127	HIS
2	N	291	ASN
1	O	54	GLN
1	O	87	ASN
2	P	87	HIS
2	P	102	HIS
2	P	113	GLN
2	P	127	HIS
2	P	291	ASN
1	Q	54	GLN
1	Q	87	ASN
2	R	87	HIS
2	R	102	HIS
2	R	113	GLN
2	R	127	HIS
2	R	291	ASN
1	S	54	GLN

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Mol	Chain	Res	Type
1	S	87	ASN
2	T	87	HIS
2	T	102	HIS
2	T	113	GLN
2	T	127	HIS
2	T	291	ASN
1	U	54	GLN
1	U	87	ASN
2	V	87	HIS
2	V	102	HIS
2	V	113	GLN
2	V	127	HIS
2	V	291	ASN
1	W	54	GLN
1	W	87	ASN
2	X	87	HIS
2	X	102	HIS
2	X	113	GLN
2	X	127	HIS
2	X	291	ASN
1	Y	54	GLN
1	Y	87	ASN
2	Z	87	HIS
2	Z	102	HIS
2	Z	113	GLN
2	Z	127	HIS
2	Z	291	ASN
1	a	54	GLN
1	a	87	ASN
2	b	87	HIS
2	b	102	HIS
2	b	113	GLN
2	b	127	HIS
2	b	291	ASN
1	c	54	GLN
1	c	87	ASN
2	d	87	HIS
2	d	102	HIS
2	d	113	GLN
2	d	127	HIS
2	d	291	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.

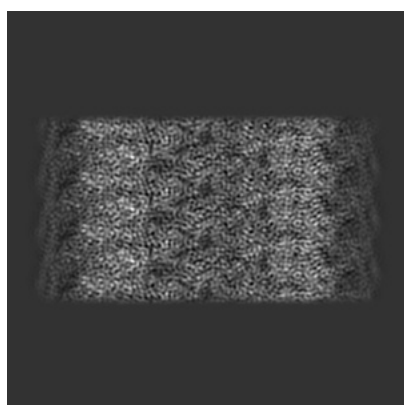
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3600. These allow visual inspection of the internal detail of the map and identification of artifacts.

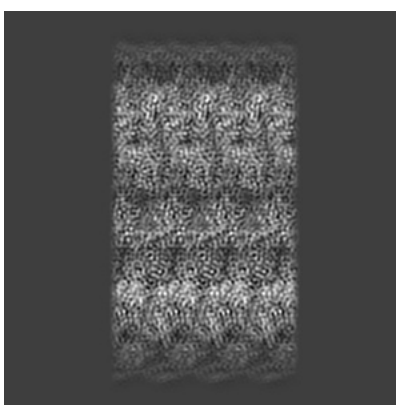
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

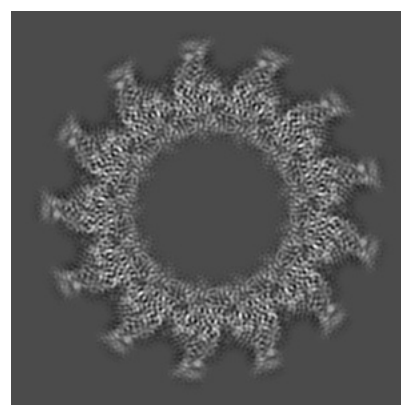
6.1.1 Primary map



X



Y

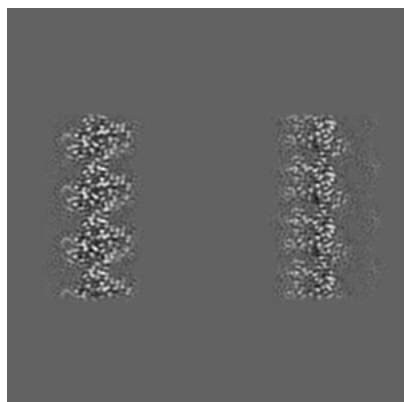


Z

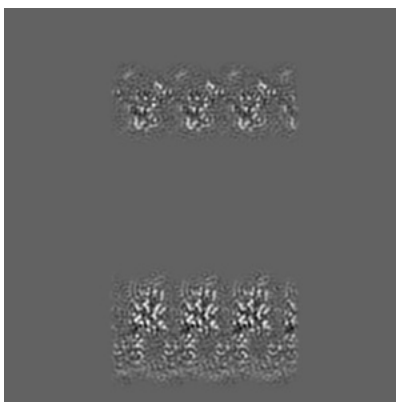
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

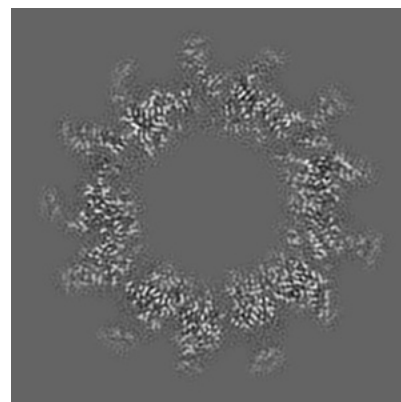
6.2.1 Primary map



X Index: 125



Y Index: 125

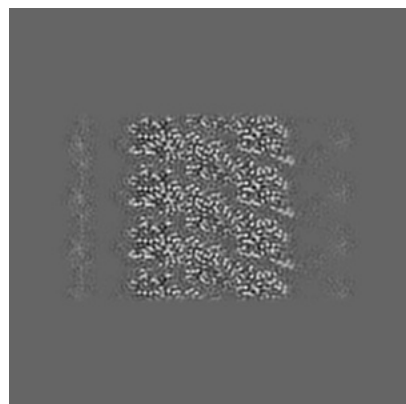


Z Index: 125

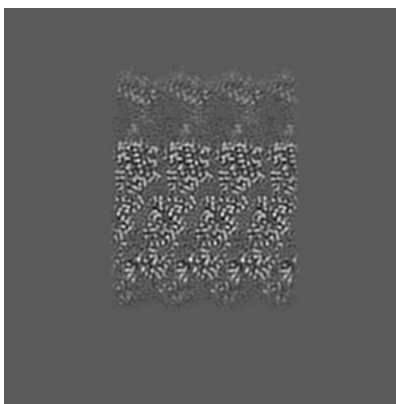
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

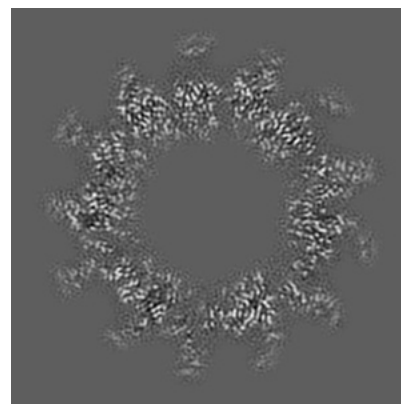
6.3.1 Primary map



X Index: 60



Y Index: 59

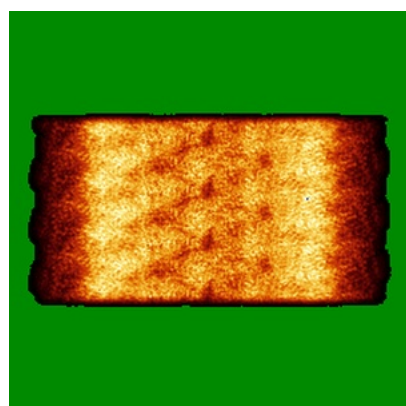


Z Index: 117

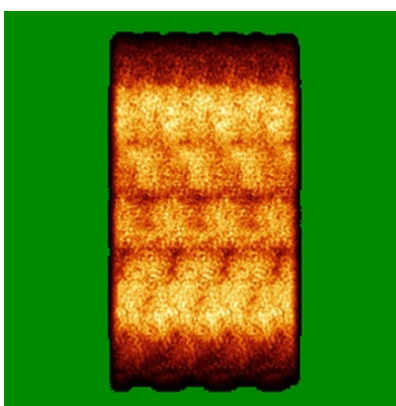
The images above show the largest variance slices of the map in three orthogonal directions.

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

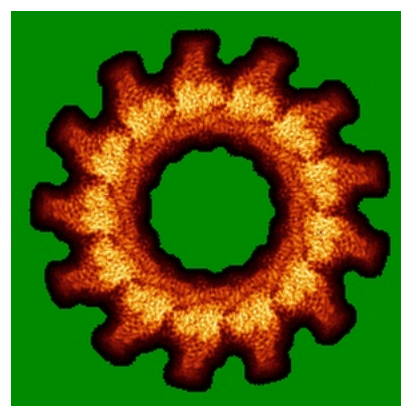
6.4.1 Primary map



X



Y

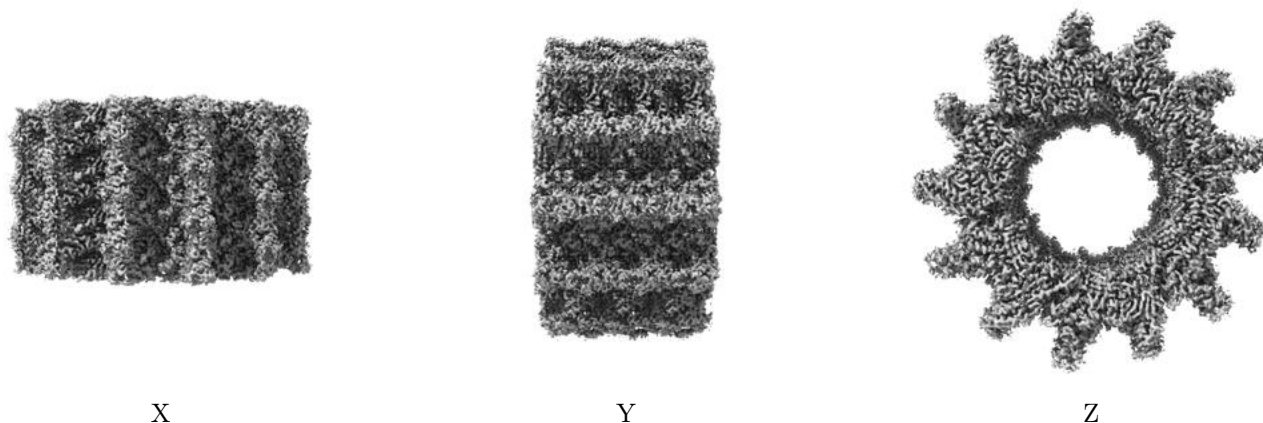


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0385. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

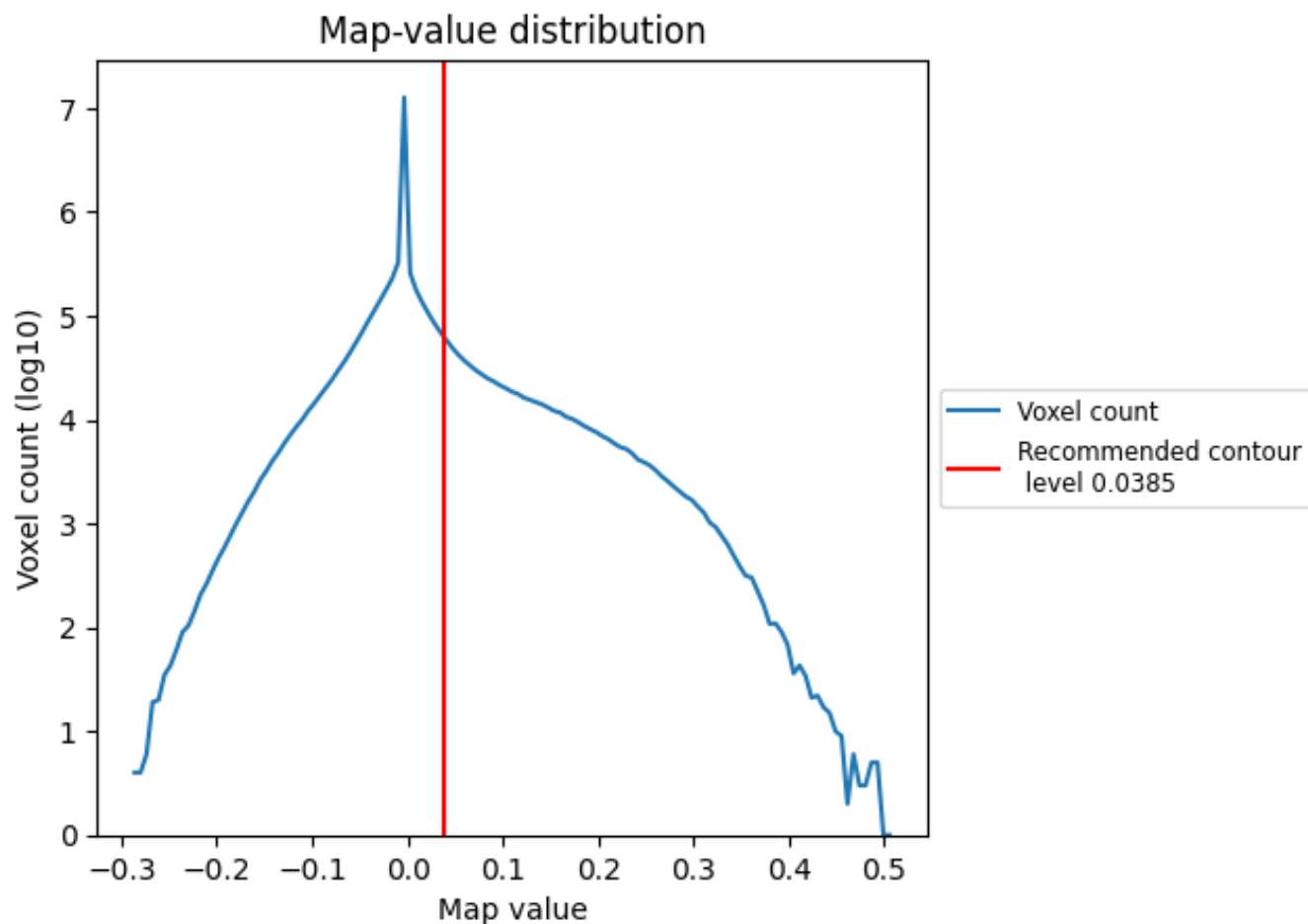
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

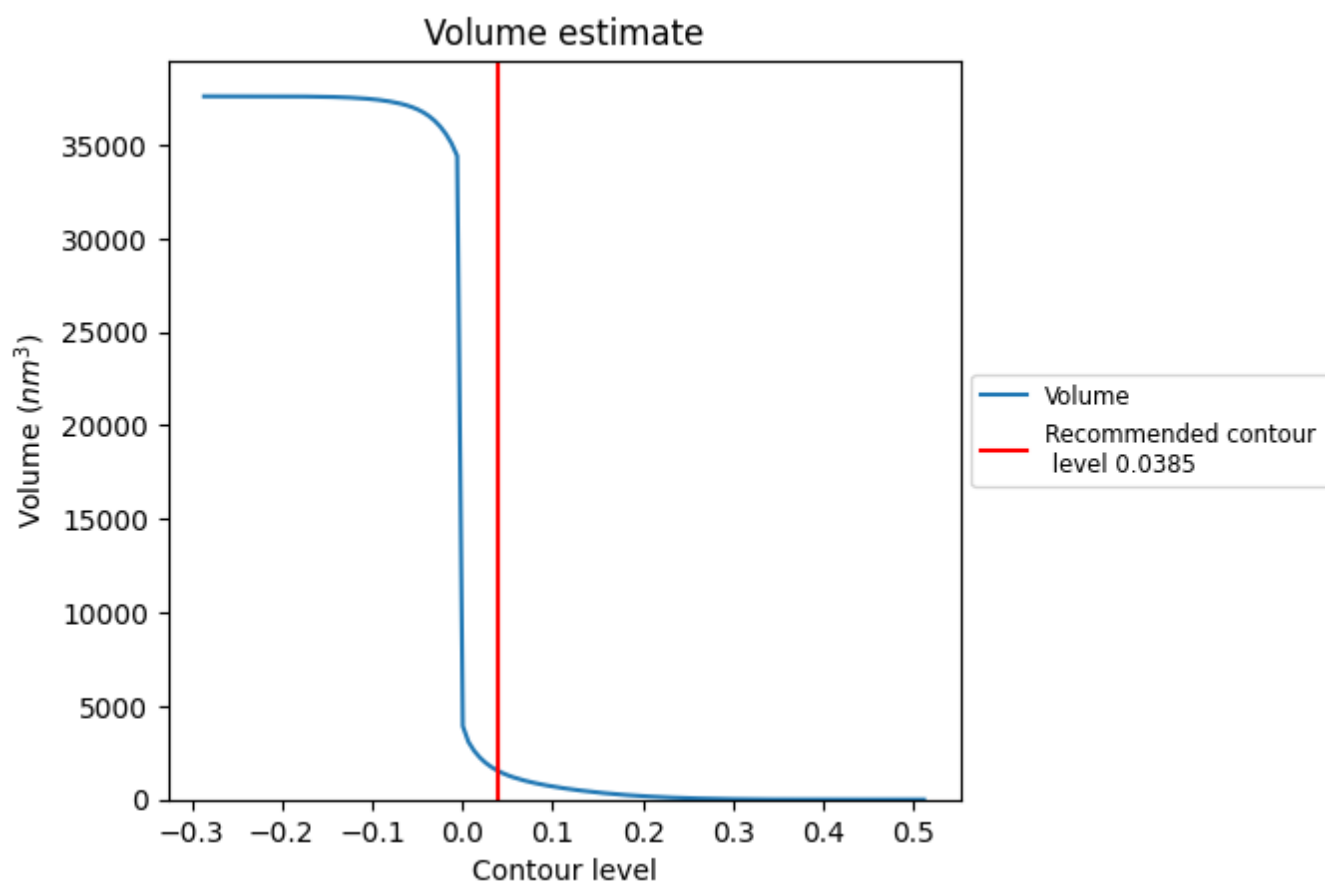
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

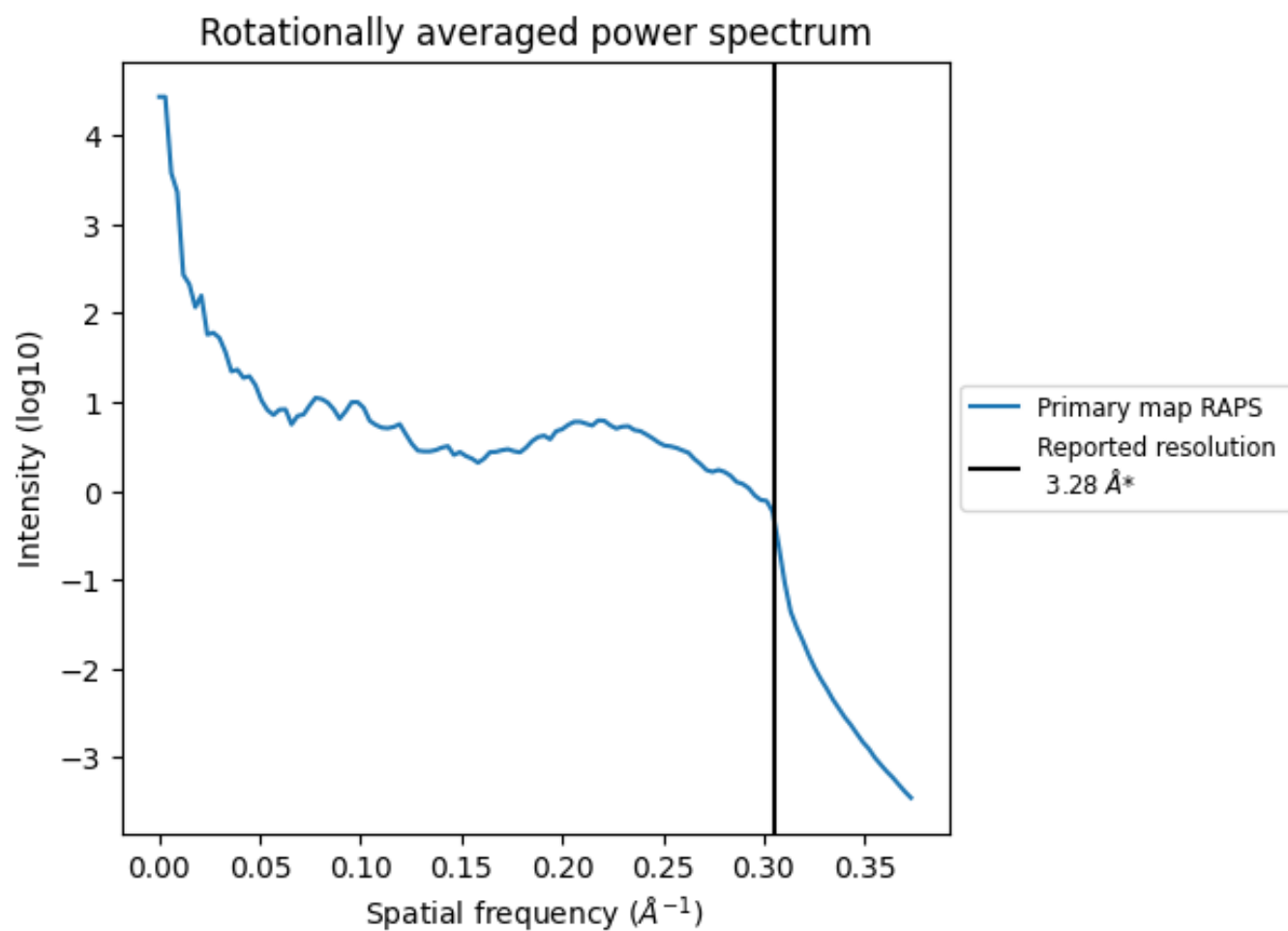
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1563 nm³; this corresponds to an approximate mass of 1412 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 0.305 Å⁻¹

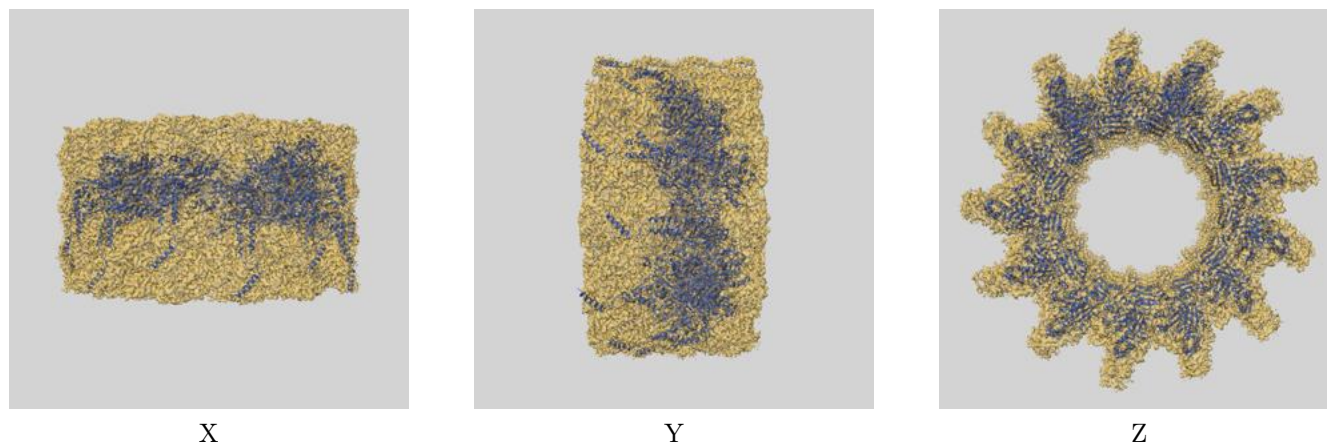
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

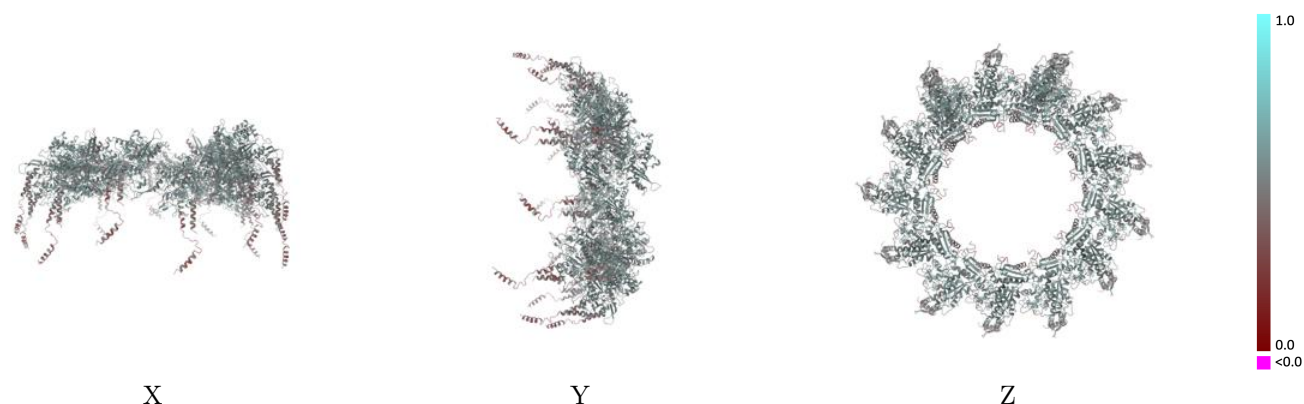
This section contains information regarding the fit between EMDB map EMD-3600 and PDB model 5N8N. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



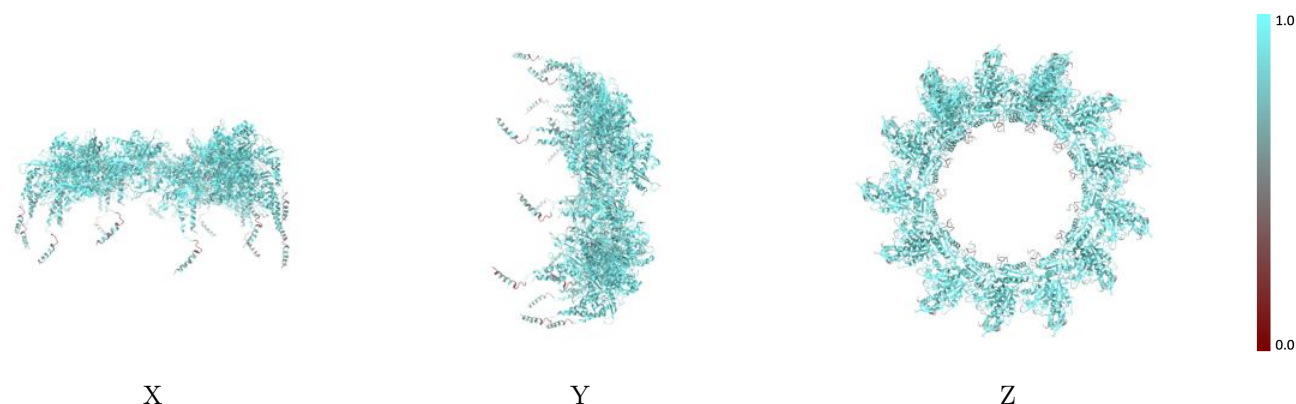
The images above show the 3D surface view of the map at the recommended contour level 0.0385 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



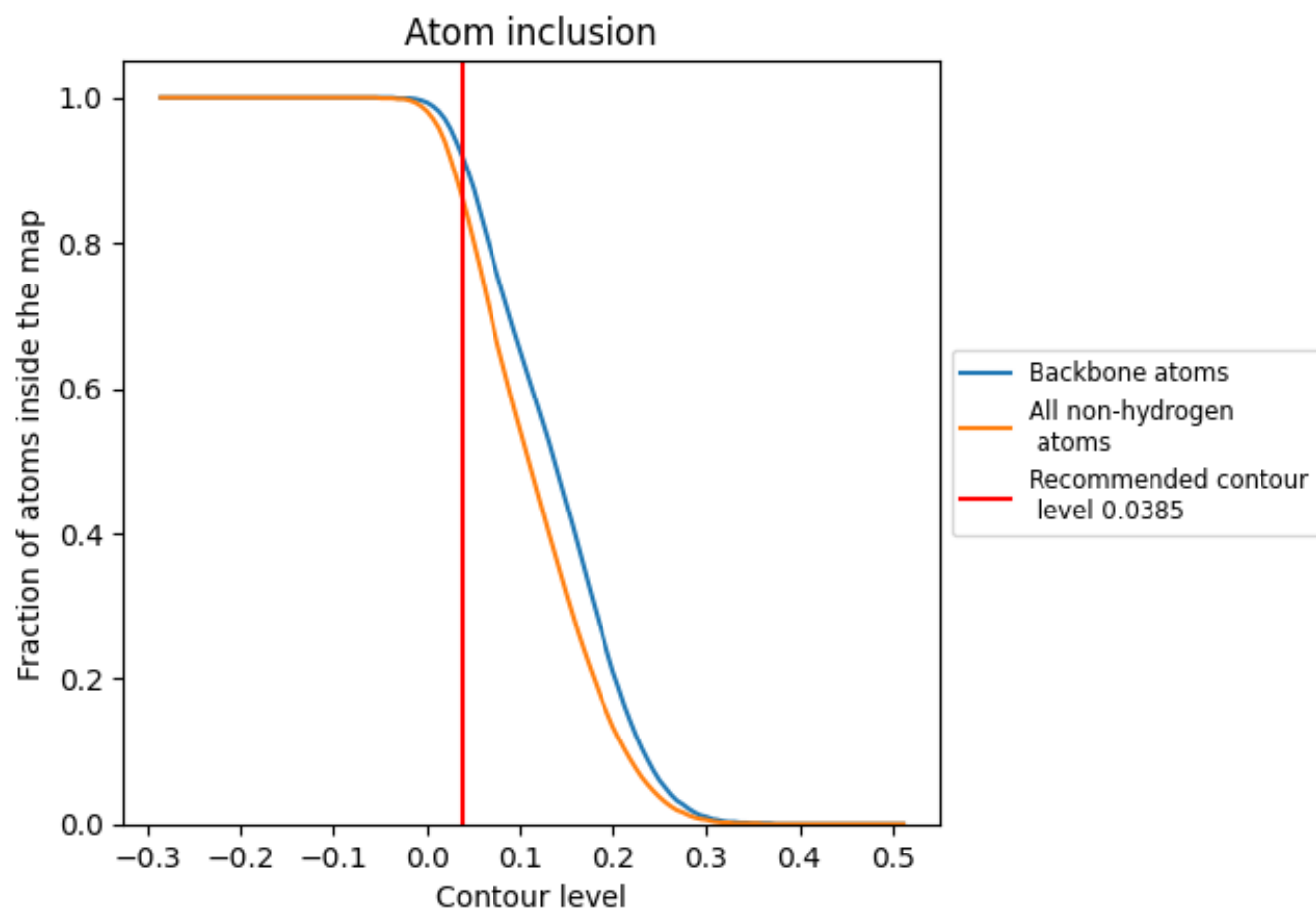
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0385).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 86% 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 (0.0385) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8600	 0.5090
A	 0.8530	 0.5010
B	 0.8530	 0.5080
C	 0.8550	 0.5040
D	 0.8550	 0.5080
E	 0.8580	 0.4990
F	 0.8610	 0.5110
G	 0.8600	 0.5000
H	 0.8590	 0.5110
I	 0.8530	 0.5030
J	 0.8610	 0.5120
K	 0.8590	 0.5050
L	 0.8560	 0.5120
M	 0.8580	 0.5050
N	 0.8640	 0.5130
O	 0.8680	 0.5060
P	 0.8610	 0.5130
Q	 0.8630	 0.5050
R	 0.8590	 0.5100
S	 0.8580	 0.5020
T	 0.8600	 0.5130
U	 0.8540	 0.5030
V	 0.8670	 0.5120
W	 0.8640	 0.5050
X	 0.8630	 0.5100
Y	 0.8510	 0.5030
Z	 0.8650	 0.5100
a	 0.8590	 0.5050
b	 0.8590	 0.5100
c	 0.8640	 0.5060
d	 0.8630	 0.5090

