



## Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 06:35 am GMT

PDB ID : 6H7W  
EMDB ID : EMD-0154  
Title : Model of retromer-Vps5 complex assembled on membrane.  
Authors : Kovtun, O.; Leneva, N.; Ariotti, N.; Rohan, T.S.; Owen, D.J.; Briggs, J.A.G.;  
Collins, B.M.  
Deposited on : 2018-07-31  
Resolution : 11.40 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

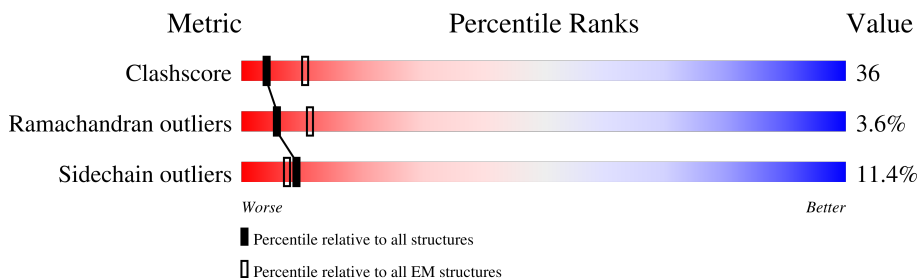
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 11.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	C	292	
1	J	292	
2	A	368	
2	B	368	
2	E	368	
2	F	368	
2	G	368	
2	H	368	

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Mol	Chain	Length	Quality of chain
2	N	368	
2	P	368	
3	D	129	
3	K	129	
3	L	129	
3	V	129	
4	M	220	
4	O	220	
5	S	193	
5	T	193	
6	Q	846	
6	R	846	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 95648 atoms, of which 45448 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 Vacuolar protein sorting-associated protein 26-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	J	292	Total	C	N	O	S	0	0
			2417	1550	416	442	9		
1	C	292	Total	C	N	O	S	0	0
			2417	1550	416	442	9		

- Molecule 2 is a protein called Putative vacuolar protein sorting-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	B	349	Total	C	H	N	O	S	0	0
			5688	1796	2845	507	533	7		
2	A	349	Total	C	H	N	O	S	0	0
			5688	1796	2845	507	533	7		
2	G	349	Total	C	H	N	O	S	0	0
			5688	1796	2845	507	533	7		
2	E	349	Total	C	H	N	O	S	0	0
			5688	1796	2845	507	533	7		
2	P	349	Total	C	H	N	O	S	0	0
			5688	1796	2845	507	533	7		
2	N	349	Total	C	H	N	O	S	0	0
			5688	1796	2845	507	533	7		
2	H	349	Total	C	H	N	O	S	0	0
			5688	1796	2845	507	533	7		
2	F	349	Total	C	H	N	O	S	0	0
			5688	1796	2845	507	533	7		

- Molecule 3 is a protein called Putative vacuolar protein sorting-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	D	129	Total	C	H	N	O	S	0	0
			2112	671	1059	190	191	1		
3	K	129	Total	C	H	N	O	S	0	0
			2112	671	1059	190	191	1		
3	V	129	Total	C	H	N	O	S	0	0
			2112	671	1059	190	191	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	L	129	2112	671	1059	190	191	1	0	0

- Molecule 4 is a protein called Putative vacuolar protein sorting-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	O	220	3579	1125	1788	317	343	6	0	0
4	M	220	3579	1125	1788	317	343	6	0	0

- Molecule 5 is a protein called Vacuolar protein sorting-associated protein 29.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
5	S	184	2893	925	1457	235	268	8	0	0
5	T	184	2893	925	1457	235	268	8	0	0

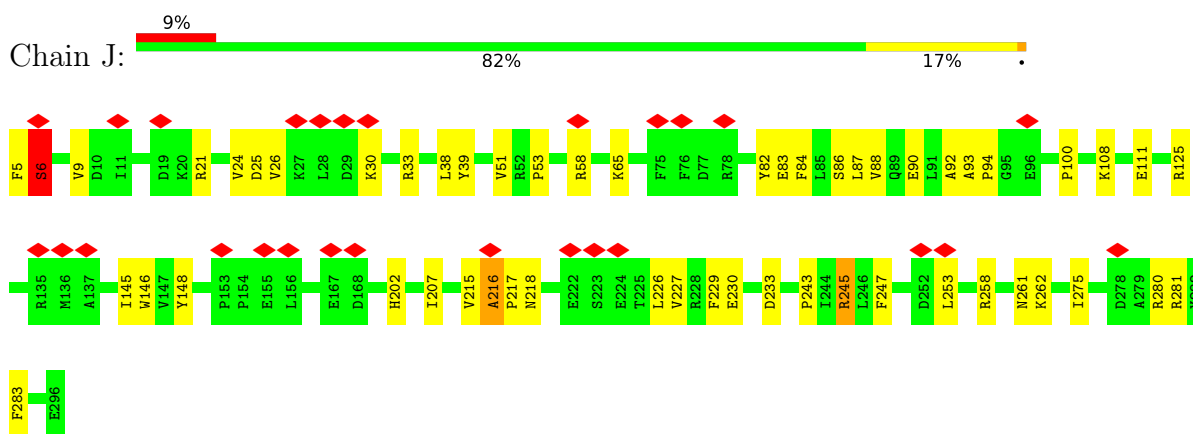
- Molecule 6 is a protein called Vacuolar protein sorting-associated protein 35.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
6	Q	744	11959	3785	5981	1047	1115	31	0	0
6	R	744	11959	3785	5981	1047	1115	31	0	0

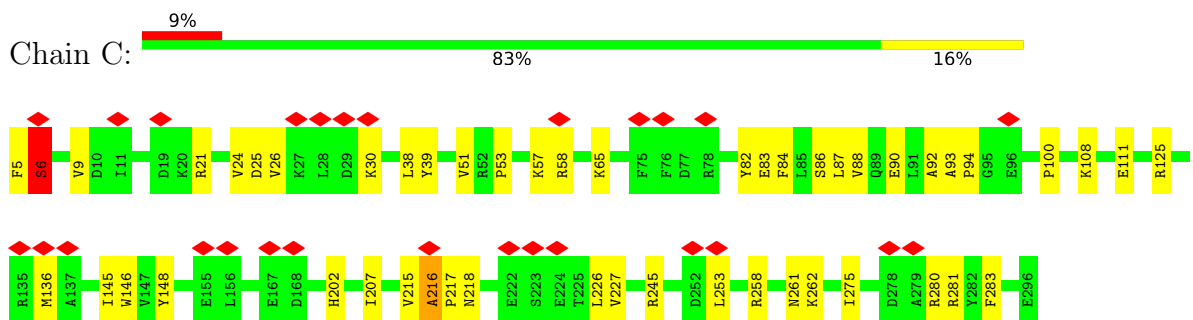
### 3 Residue-property plots [i](#)

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.

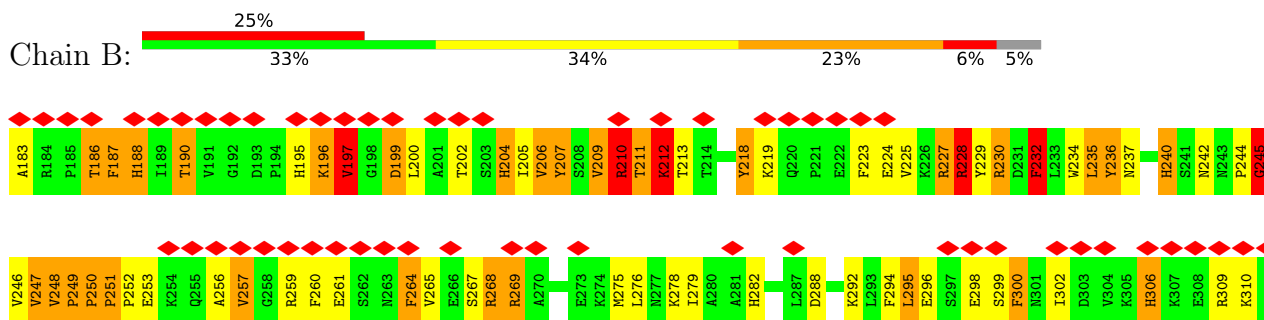
- Molecule 1: Vacuolar protein sorting-associated protein 26-like protein

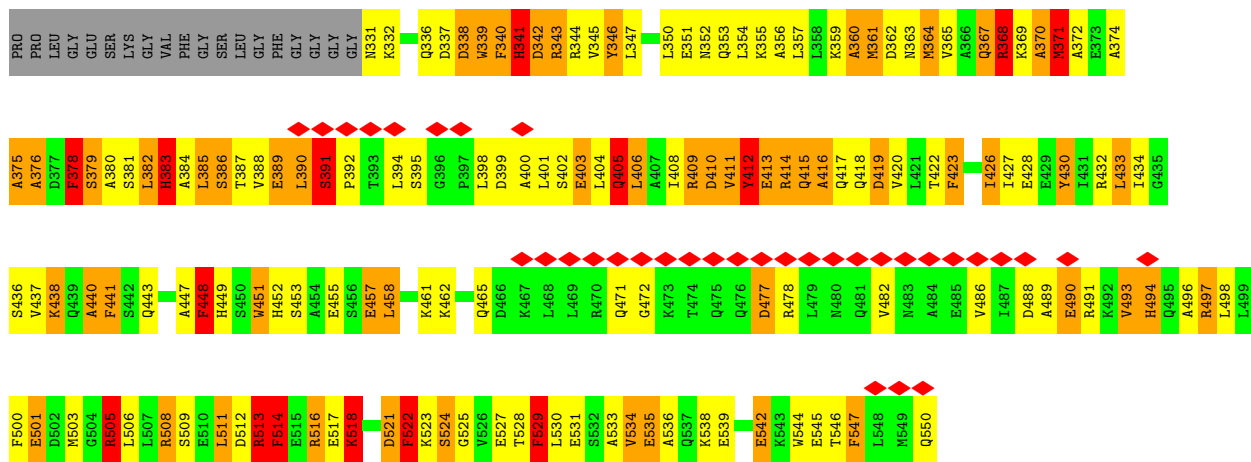


- Molecule 1: Vacuolar protein sorting-associated protein 26-like protein

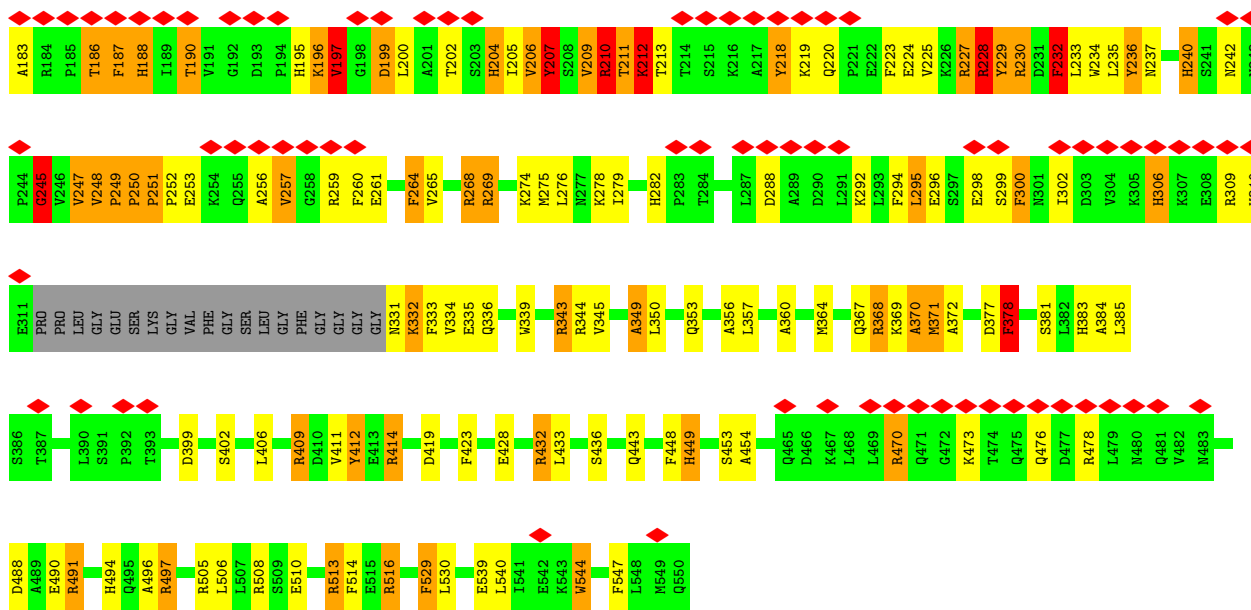


- Molecule 2: Putative vacuolar protein sorting-associated protein

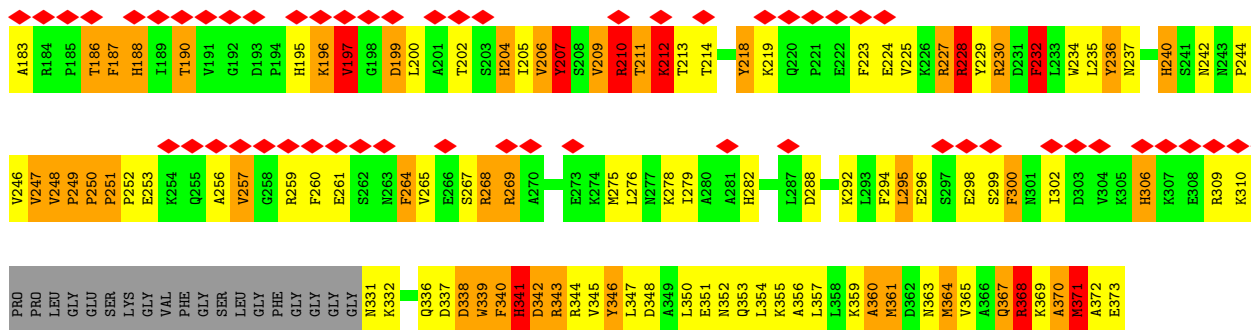


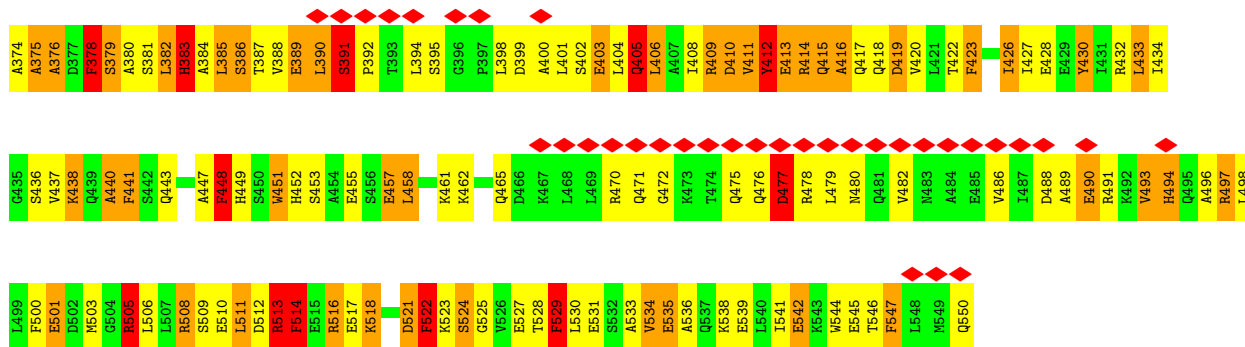


● Molecule 2: Putative vacuolar protein sorting-associated protein

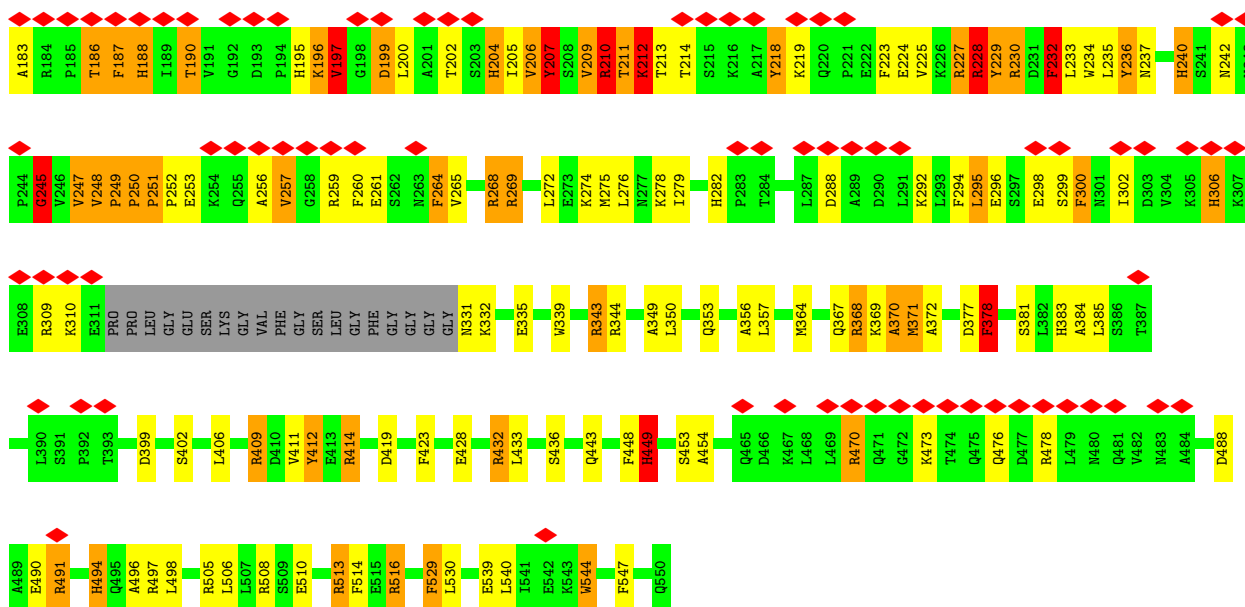


● Molecule 2: Putative vacuolar protein sorting-associated protein

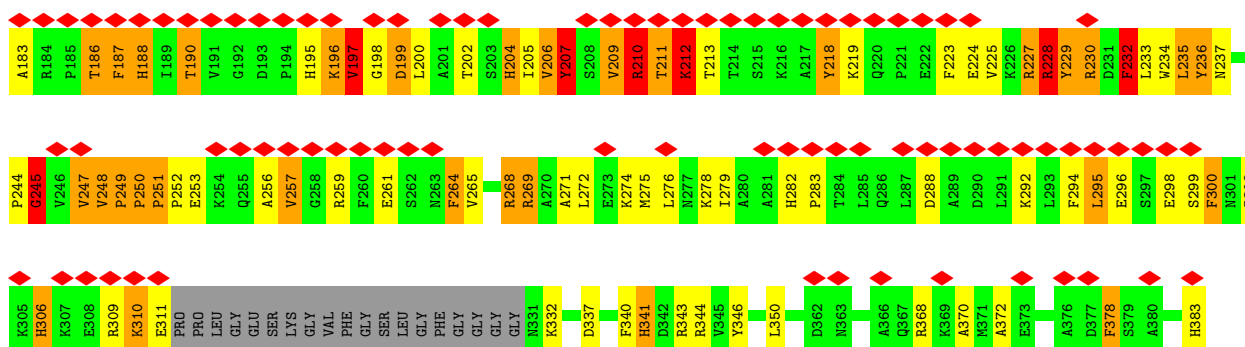




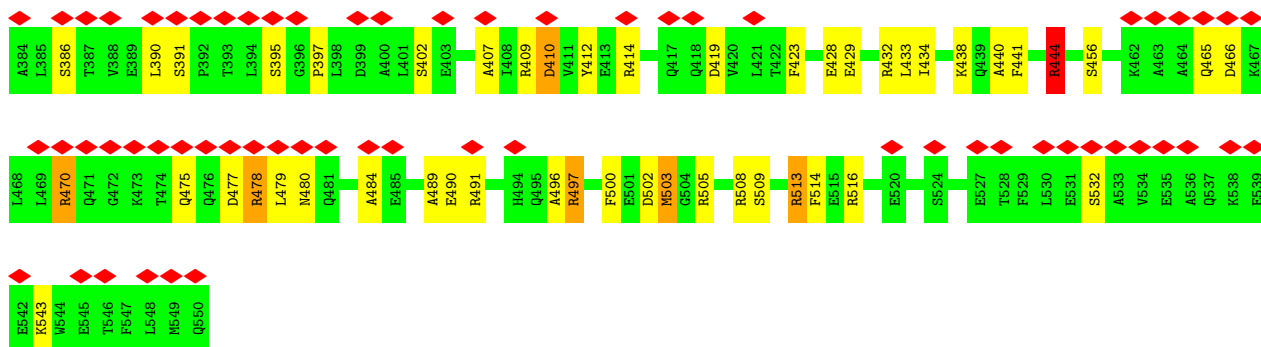
• Molecule 2: Putative vacuolar protein sorting-associated protein



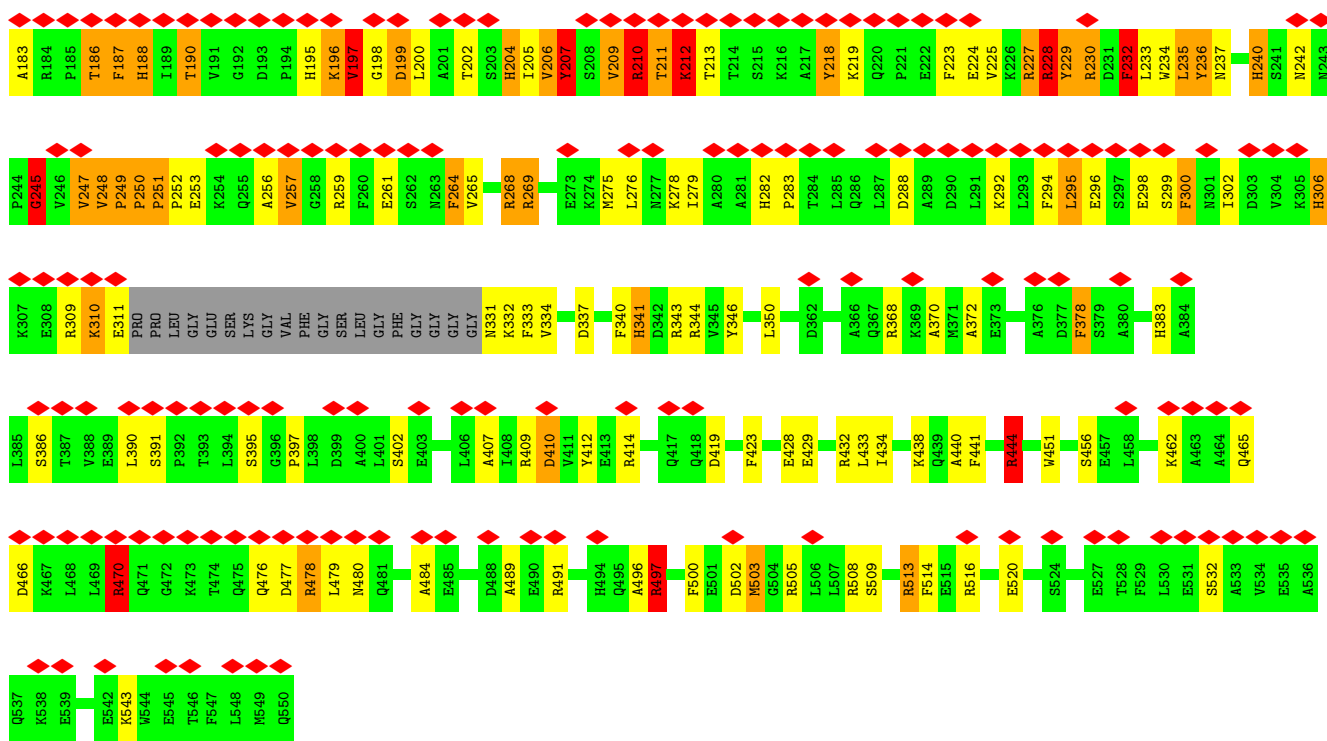
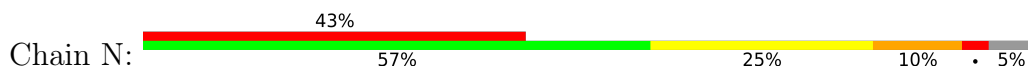
• Molecule 2: Putative vacuolar protein sorting-associated protein



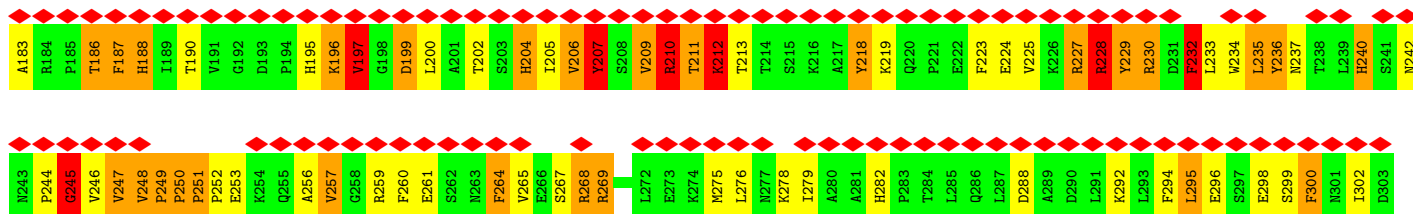


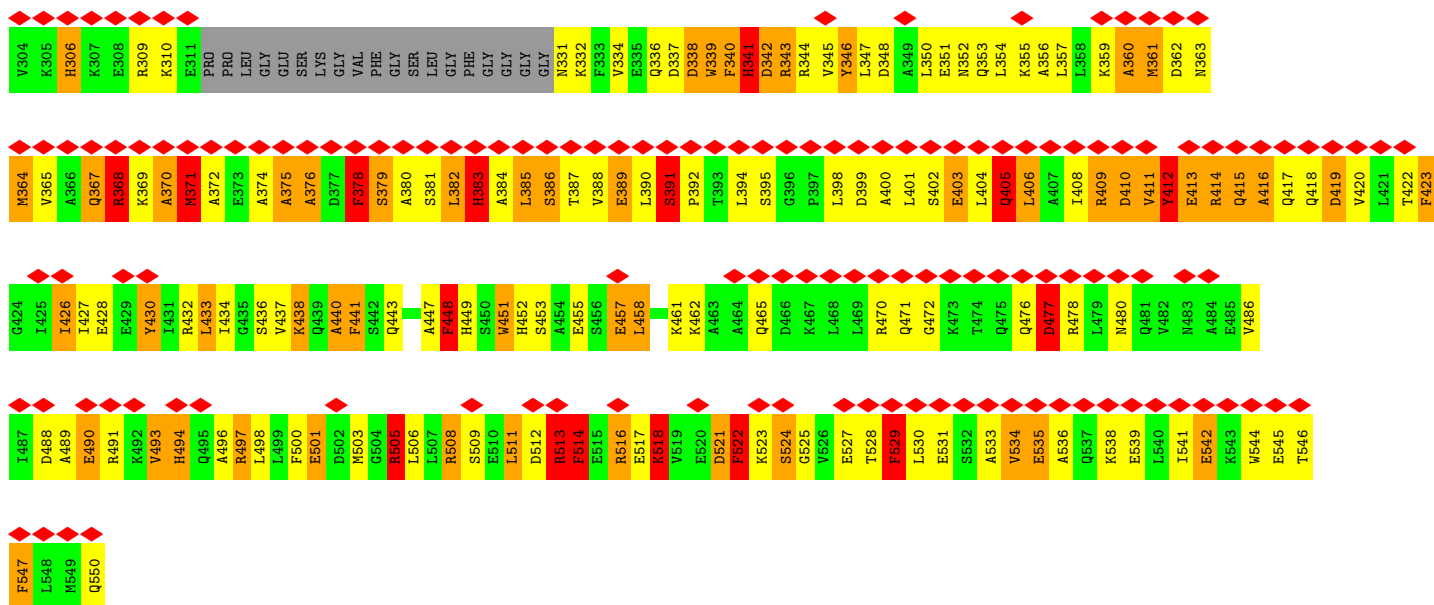


● Molecule 2: Putative vacuolar protein sorting-associated protein

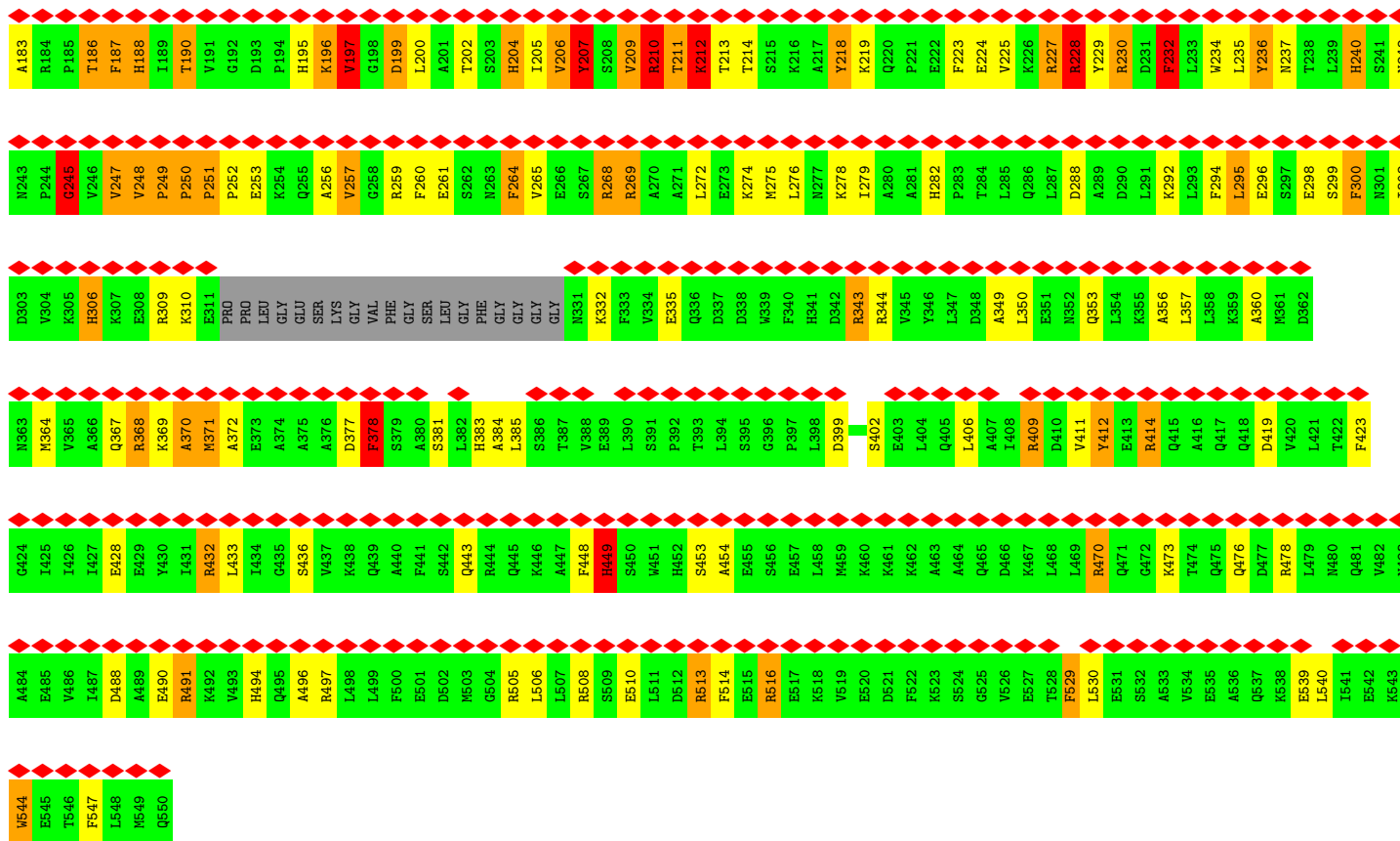
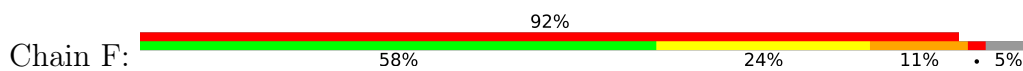


● Molecule 2: Putative vacuolar protein sorting-associated protein

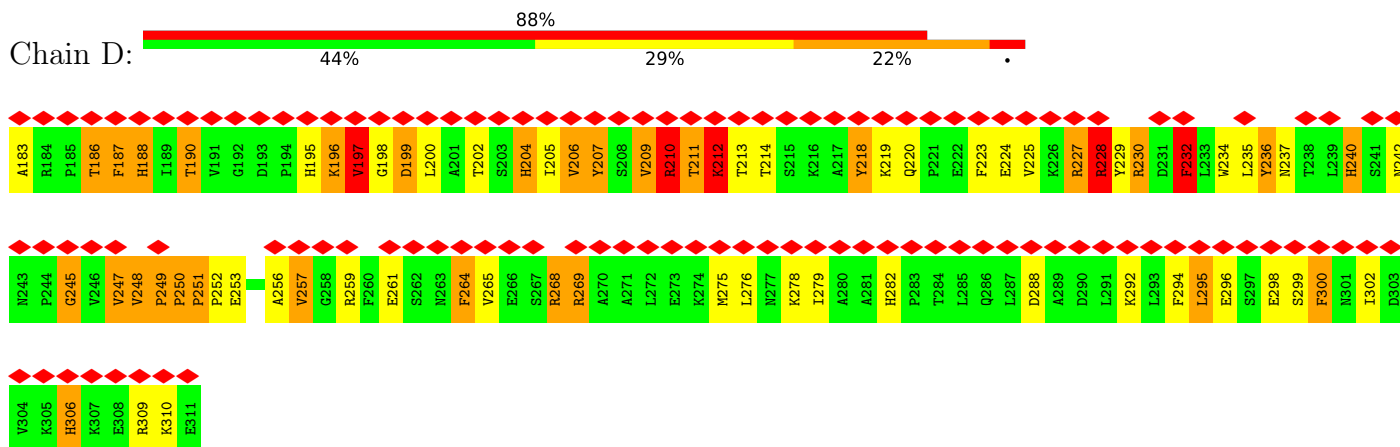




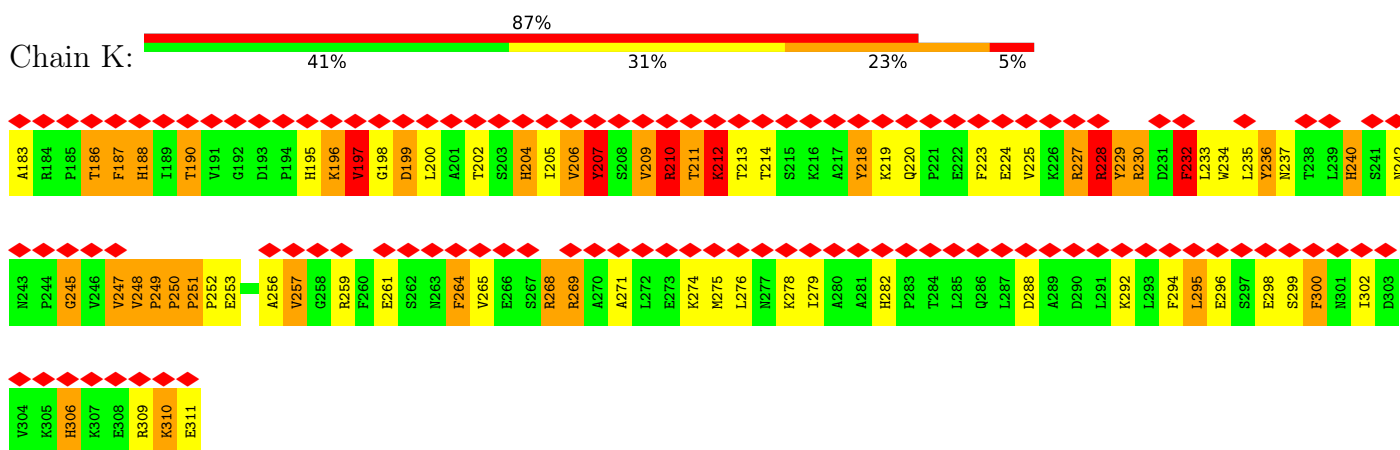
• Molecule 2: Putative vacuolar protein sorting-associated protein



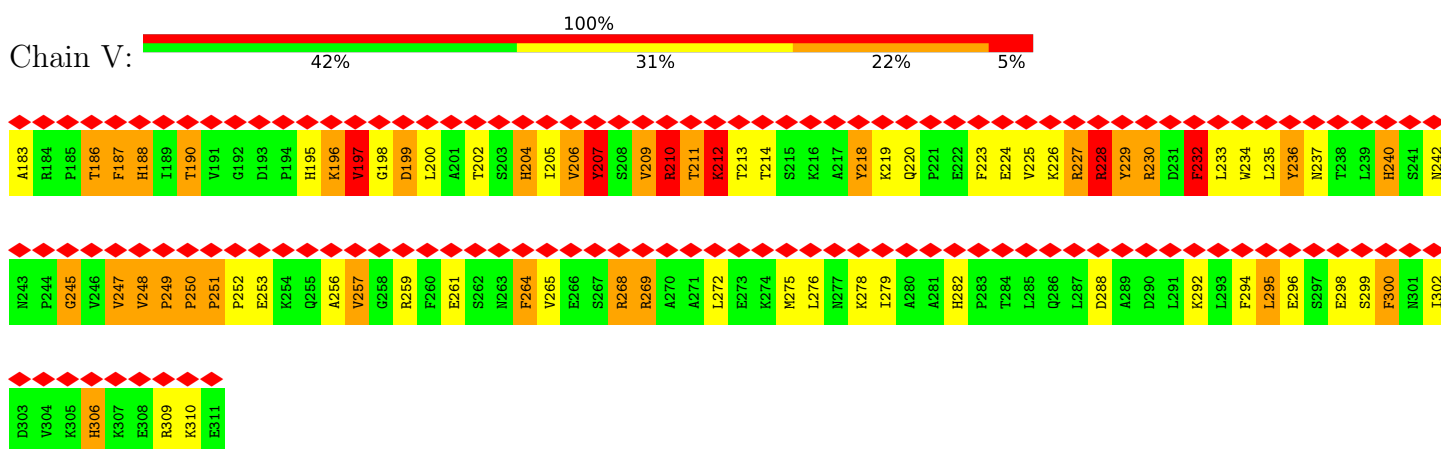
• Molecule 3: Putative vacuolar protein sorting-associated protein



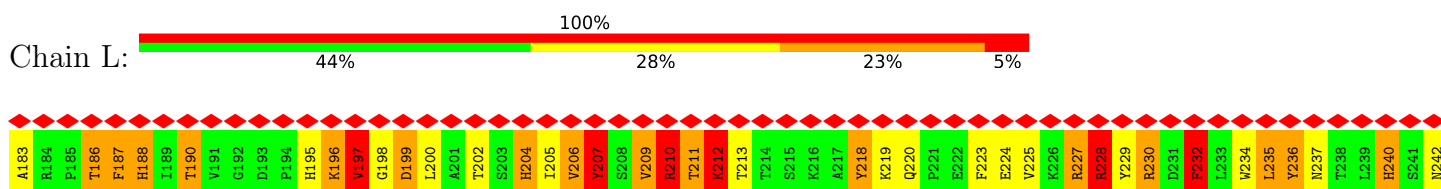
- Molecule 3: Putative vacuolar protein sorting-associated protein

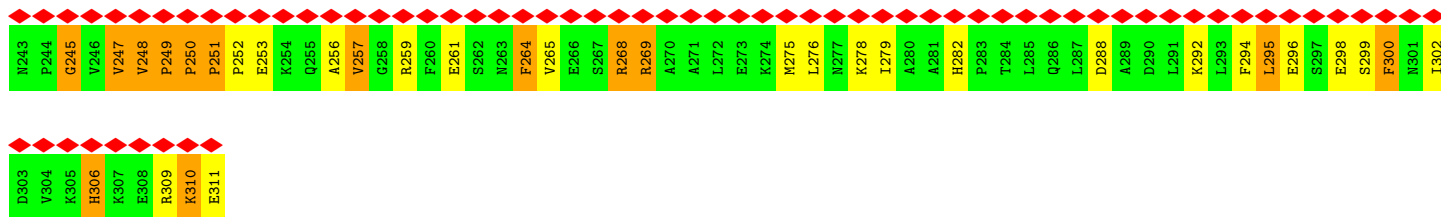


- Molecule 3: Putative vacuolar protein sorting-associated protein

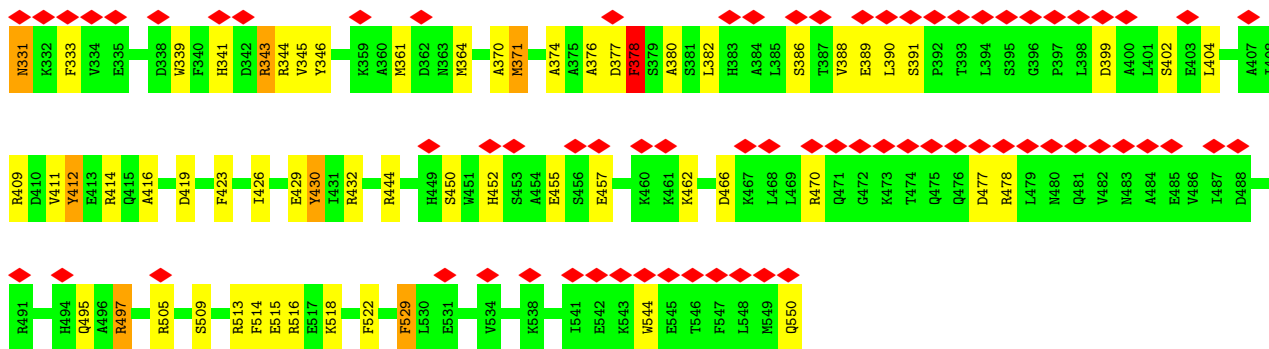
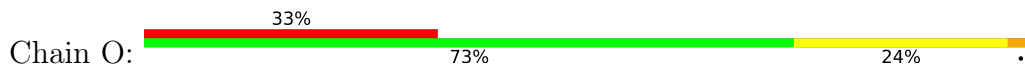


- Molecule 3: Putative vacuolar protein sorting-associated protein

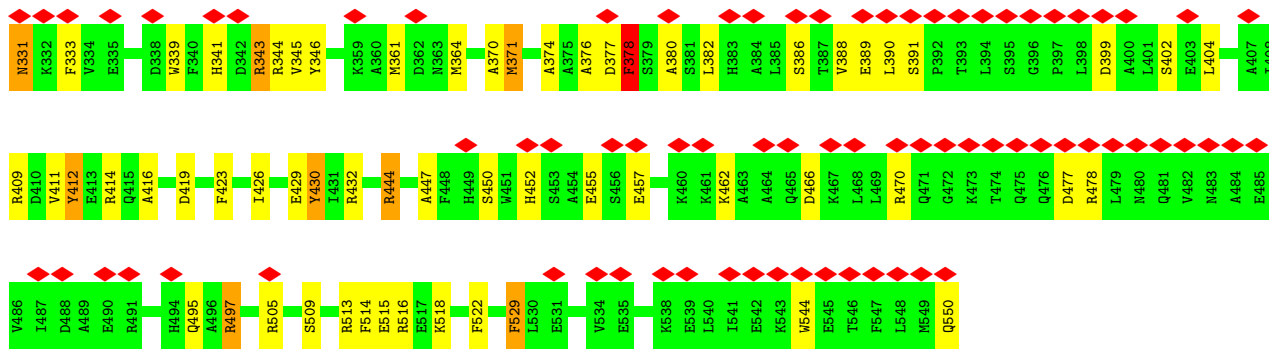
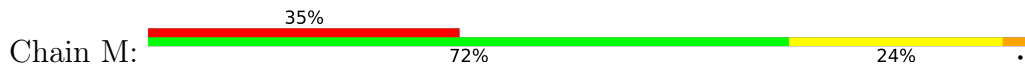




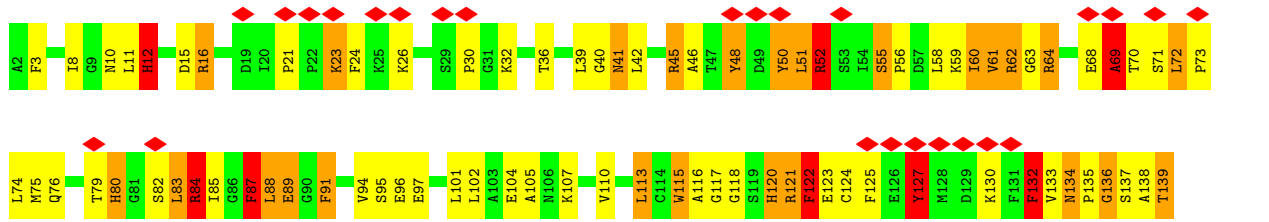
• Molecule 4: Putative vacuolar protein sorting-associated protein

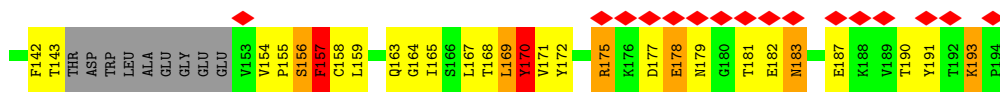


• Molecule 4: Putative vacuolar protein sorting-associated protein

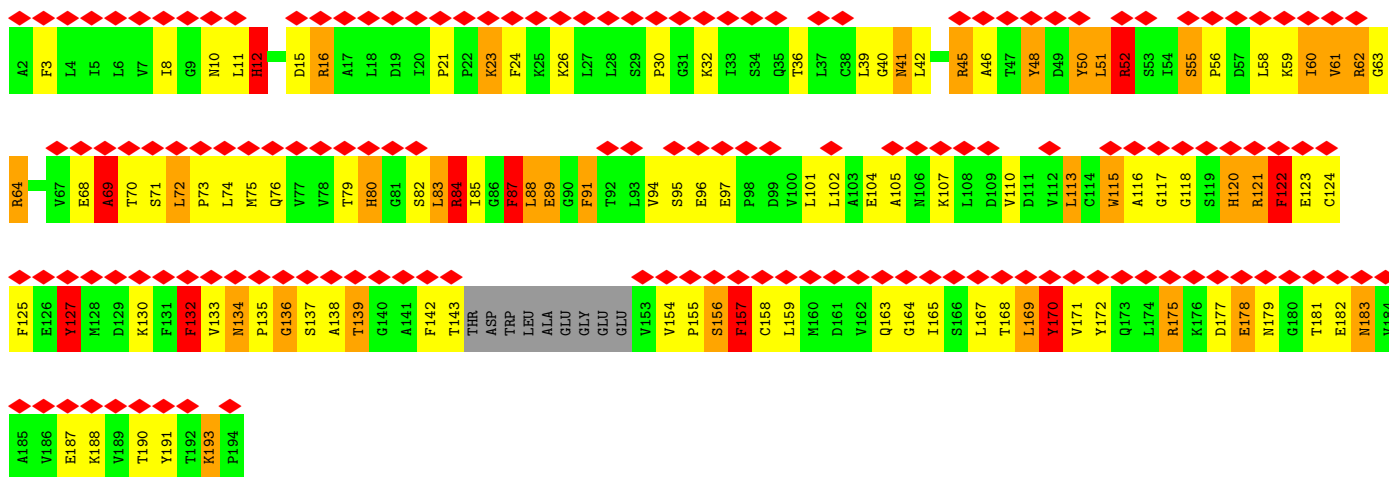
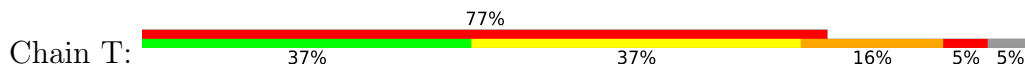


• Molecule 5: Vacuolar protein sorting-associated protein 29

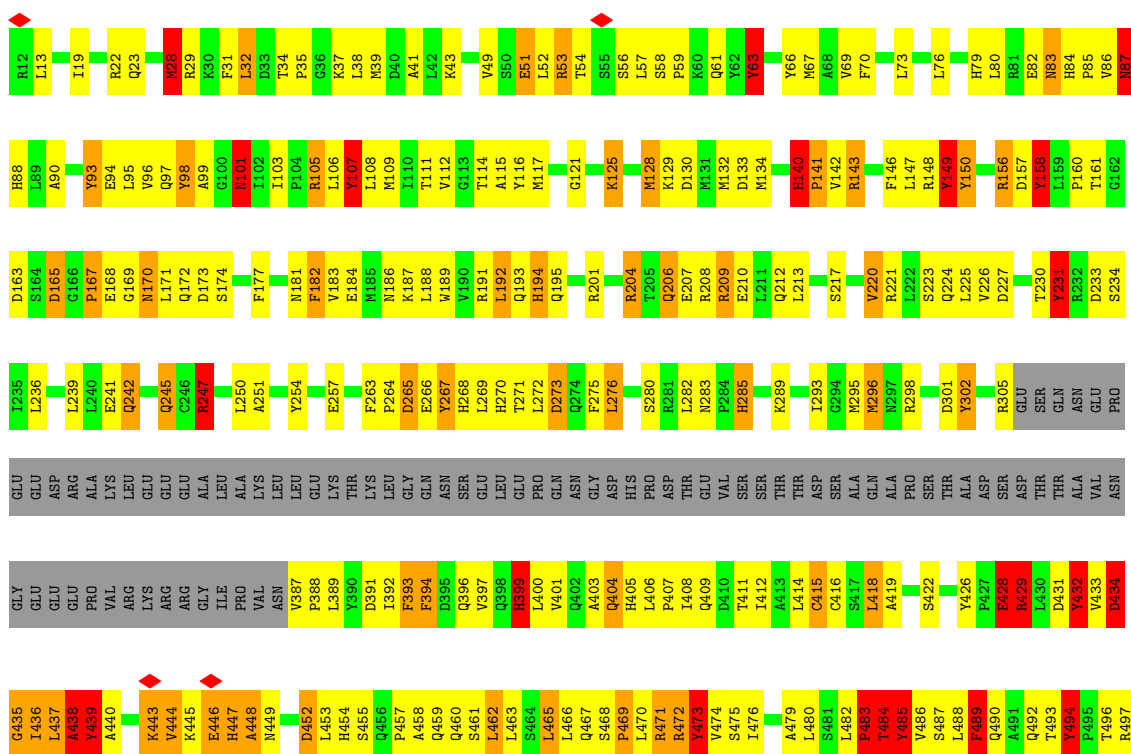


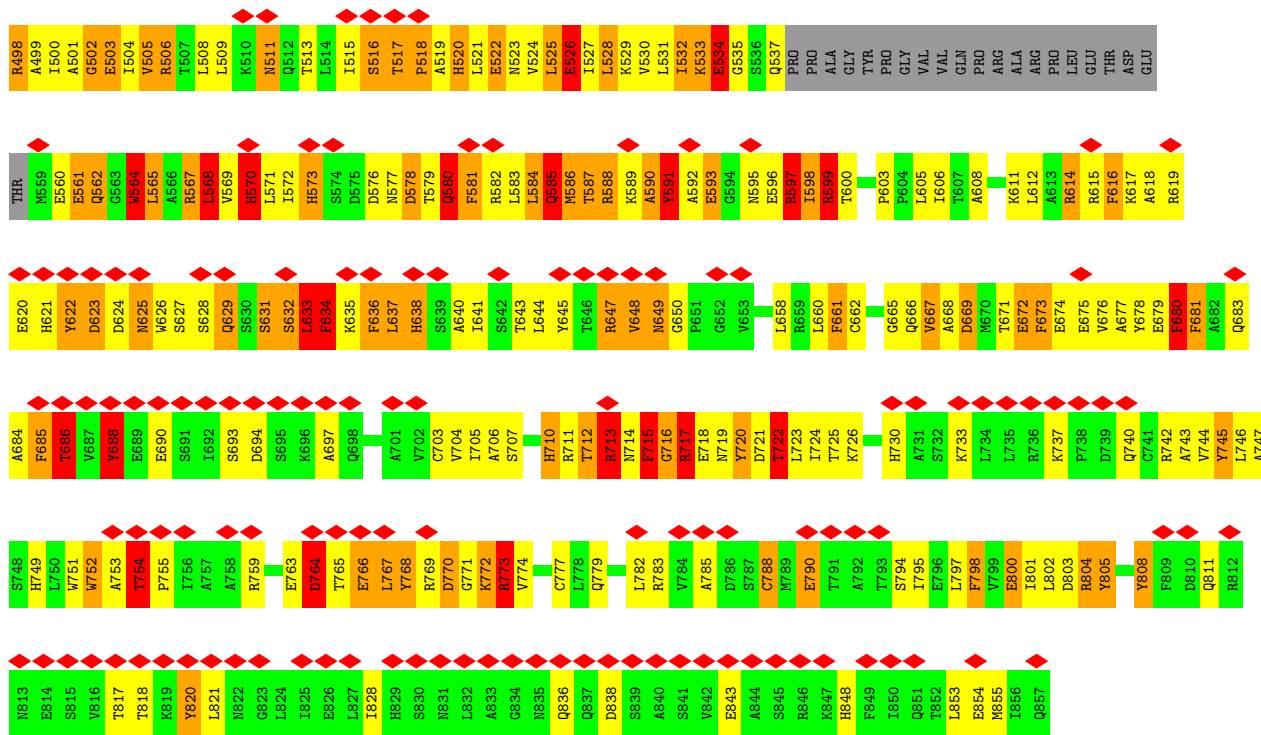


• Molecule 5: Vacuolar protein sorting-associated protein 29

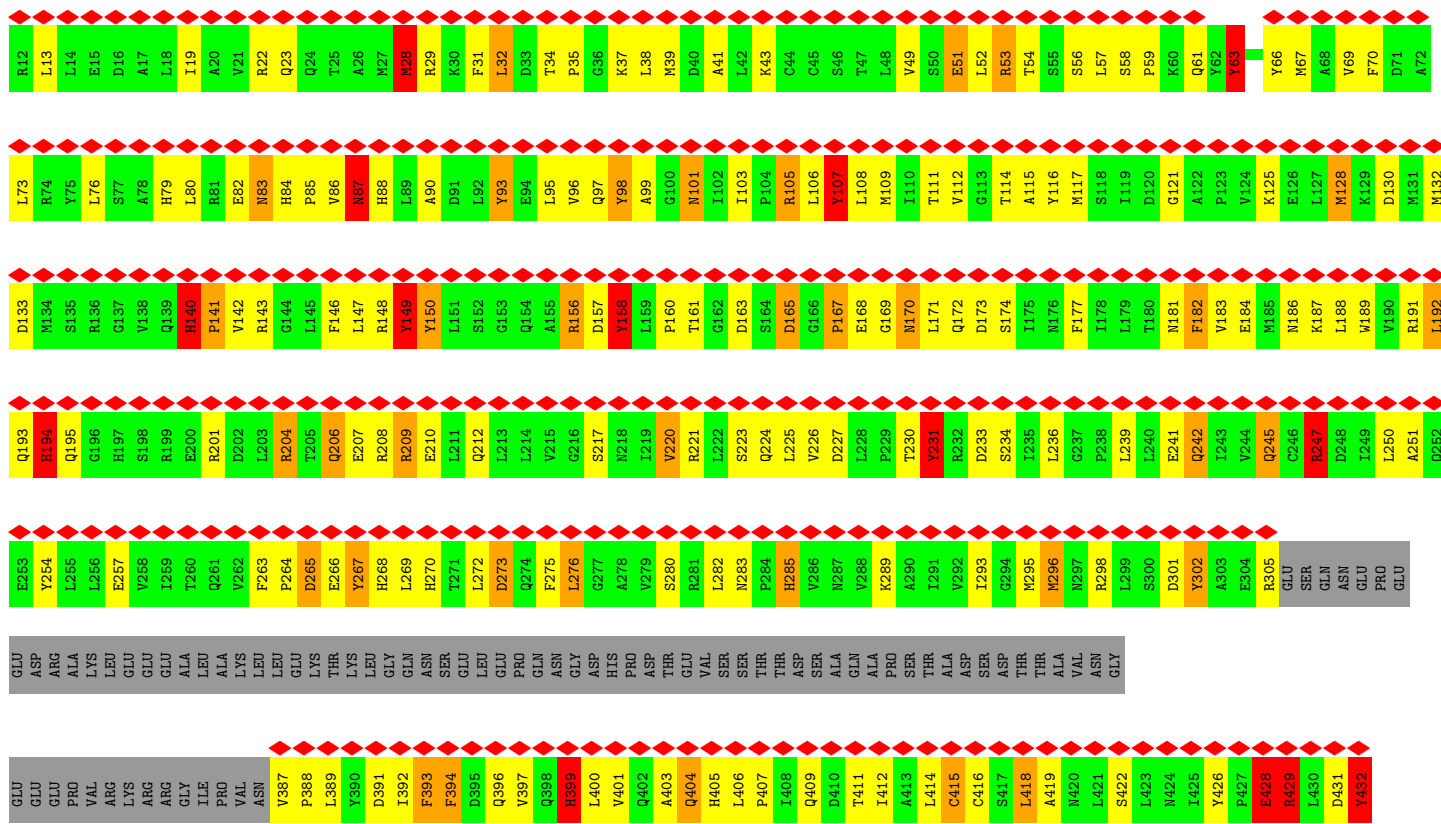
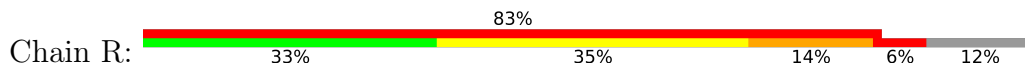


• Molecule 6: Vacuolar protein sorting-associated protein 35





• Molecule 6: Vacuolar protein sorting-associated protein 35





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of subtomograms used	16037	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF correction was performed with ctfphaseflip IMOD command using defocus values measured by CTFFIND4 on non-dose-filtered images.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	3.17	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	6500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.765	Depositor
Minimum map value	-0.535	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.058	Depositor
Recommended contour level	0.15	Depositor
Map size ( $\text{\AA}$ )	388.80002, 388.80002, 388.80002	wwPDB
Map dimensions	144, 144, 144	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	2.7, 2.7, 2.7	Depositor



## 5 Model quality i

### 5.1 Standard geometry i

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	C	0.73	0/2469	1.08	10/3327 (0.3%)
1	J	0.74	0/2469	1.08	10/3327 (0.3%)
2	A	1.94	35/2896 (1.2%)	1.78	62/3898 (1.6%)
2	B	1.87	19/2896 (0.7%)	1.77	84/3898 (2.2%)
2	E	1.94	36/2896 (1.2%)	1.78	60/3898 (1.5%)
2	F	1.94	36/2896 (1.2%)	1.78	61/3898 (1.6%)
2	G	1.88	18/2896 (0.6%)	1.77	84/3898 (2.2%)
2	H	1.87	18/2896 (0.6%)	1.77	83/3898 (2.1%)
2	N	1.93	31/2896 (1.1%)	1.87	68/3898 (1.7%)
2	P	1.93	31/2896 (1.1%)	1.87	68/3898 (1.7%)
3	D	2.18	8/1080 (0.7%)	1.74	25/1460 (1.7%)
3	K	2.18	8/1080 (0.7%)	1.74	25/1460 (1.7%)
3	L	2.18	8/1080 (0.7%)	1.74	25/1460 (1.7%)
3	V	2.18	8/1080 (0.7%)	1.74	25/1460 (1.7%)
4	M	1.77	23/1817 (1.3%)	1.85	43/2438 (1.8%)
4	O	1.77	22/1817 (1.2%)	1.85	42/2438 (1.7%)
5	S	1.32	1/1465 (0.1%)	1.77	32/1986 (1.6%)
5	T	1.32	1/1465 (0.1%)	1.77	32/1986 (1.6%)
6	Q	1.50	22/6092 (0.4%)	1.71	127/8255 (1.5%)
6	R	1.50	22/6092 (0.4%)	1.71	127/8255 (1.5%)
All	All	1.72	347/51174 (0.7%)	1.72	1093/69036 (1.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	J	0	1
2	A	0	15
2	B	0	27
2	E	0	16

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	F	0	16
2	G	0	27
2	H	0	27
2	N	0	16
2	P	0	16
3	D	0	11
3	K	0	11
3	L	0	11
3	V	0	11
4	M	0	7
4	O	0	7
5	S	0	12
5	T	0	12
6	Q	1	56
6	R	1	57
All	All	2	357

All (347) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	250	PRO	N-CD	32.85	1.93	1.47
2	H	250	PRO	N-CD	32.84	1.93	1.47
2	F	250	PRO	N-CD	32.83	1.93	1.47
3	D	250	PRO	N-CD	32.81	1.93	1.47
2	P	250	PRO	N-CD	32.79	1.93	1.47
3	K	250	PRO	N-CD	32.78	1.93	1.47
2	G	250	PRO	N-CD	32.78	1.93	1.47
2	A	250	PRO	N-CD	32.76	1.93	1.47
3	V	250	PRO	N-CD	32.76	1.93	1.47
3	L	250	PRO	N-CD	32.74	1.93	1.47
2	E	250	PRO	N-CD	32.74	1.93	1.47
2	B	250	PRO	N-CD	32.73	1.93	1.47
2	P	250	PRO	CA-CB	29.93	2.13	1.53
3	K	250	PRO	CA-CB	29.92	2.13	1.53
2	B	250	PRO	CA-CB	29.91	2.13	1.53
2	A	250	PRO	CA-CB	29.90	2.13	1.53
2	H	250	PRO	CA-CB	29.90	2.13	1.53
2	N	250	PRO	CA-CB	29.89	2.13	1.53
2	G	250	PRO	CA-CB	29.89	2.13	1.53
3	V	250	PRO	CA-CB	29.89	2.13	1.53
2	E	250	PRO	CA-CB	29.88	2.13	1.53
3	D	250	PRO	CA-CB	29.86	2.13	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	250	PRO	CA-CB	29.82	2.13	1.53
3	L	250	PRO	CA-CB	29.82	2.13	1.53
3	L	250	PRO	N-CA	26.35	1.92	1.47
2	P	250	PRO	N-CA	26.34	1.92	1.47
2	B	250	PRO	N-CA	26.34	1.92	1.47
2	G	250	PRO	N-CA	26.32	1.92	1.47
2	N	250	PRO	N-CA	26.32	1.92	1.47
3	D	250	PRO	N-CA	26.32	1.92	1.47
3	V	250	PRO	N-CA	26.28	1.92	1.47
2	F	250	PRO	N-CA	26.27	1.92	1.47
2	H	250	PRO	N-CA	26.27	1.92	1.47
3	K	250	PRO	N-CA	26.25	1.91	1.47
2	A	250	PRO	N-CA	26.21	1.91	1.47
2	E	250	PRO	N-CA	26.17	1.91	1.47
3	K	250	PRO	CG-CD	15.93	2.03	1.50
2	A	250	PRO	CG-CD	15.89	2.03	1.50
2	B	250	PRO	CG-CD	15.87	2.03	1.50
2	P	250	PRO	CG-CD	15.87	2.03	1.50
2	H	250	PRO	CG-CD	15.87	2.03	1.50
3	L	250	PRO	CG-CD	15.87	2.03	1.50
3	D	250	PRO	CG-CD	15.86	2.02	1.50
2	F	250	PRO	CG-CD	15.86	2.02	1.50
3	V	250	PRO	CG-CD	15.86	2.02	1.50
2	G	250	PRO	CG-CD	15.85	2.02	1.50
2	E	250	PRO	CG-CD	15.85	2.02	1.50
2	N	250	PRO	CG-CD	15.84	2.02	1.50
3	V	250	PRO	CB-CG	10.96	2.04	1.50
3	L	250	PRO	CB-CG	10.95	2.04	1.50
2	N	250	PRO	CB-CG	10.95	2.04	1.50
2	G	250	PRO	CB-CG	10.95	2.04	1.50
2	B	250	PRO	CB-CG	10.95	2.04	1.50
2	H	250	PRO	CB-CG	10.95	2.04	1.50
3	D	250	PRO	CB-CG	10.94	2.04	1.50
2	P	250	PRO	CB-CG	10.93	2.04	1.50
2	F	250	PRO	CB-CG	10.93	2.04	1.50
2	E	250	PRO	CB-CG	10.93	2.04	1.50
2	A	250	PRO	CB-CG	10.93	2.04	1.50
3	K	250	PRO	CB-CG	10.90	2.04	1.50
2	N	532	SER	CA-CB	7.82	1.64	1.52
2	P	532	SER	CA-CB	7.80	1.64	1.52
2	B	406	LEU	N-CA	-7.35	1.31	1.46
2	G	406	LEU	N-CA	-7.33	1.31	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	406	LEU	N-CA	-7.33	1.31	1.46
2	E	343	ARG	NE-CZ	7.33	1.42	1.33
2	F	343	ARG	NE-CZ	7.18	1.42	1.33
2	A	343	ARG	NE-CZ	7.18	1.42	1.33
6	Q	716	GLY	N-CA	-6.96	1.35	1.46
2	N	434	ILE	C-N	6.80	1.45	1.33
6	R	716	GLY	N-CA	-6.80	1.35	1.46
2	G	405	GLN	CA-C	-6.78	1.35	1.52
2	A	448	PHE	CG-CD2	6.74	1.48	1.38
6	R	502	GLY	CA-C	-6.74	1.41	1.51
6	Q	716	GLY	CA-C	-6.74	1.41	1.51
2	B	405	GLN	CA-C	-6.73	1.35	1.52
2	F	448	PHE	CG-CD2	6.72	1.48	1.38
6	Q	502	GLY	CA-C	-6.72	1.41	1.51
2	P	434	ILE	C-N	6.71	1.45	1.33
2	H	405	GLN	CA-C	-6.71	1.35	1.52
6	R	716	GLY	CA-C	-6.69	1.41	1.51
2	E	448	PHE	CG-CD2	6.69	1.48	1.38
4	M	380	ALA	CA-CB	6.64	1.66	1.52
4	O	380	ALA	CA-CB	6.63	1.66	1.52
4	O	409	ARG	CZ-NH2	6.61	1.41	1.33
4	M	409	ARG	CZ-NH2	6.56	1.41	1.33
2	E	378	PHE	CE2-CZ	6.50	1.49	1.37
2	F	378	PHE	CE2-CZ	6.48	1.49	1.37
2	A	378	PHE	CE2-CZ	6.47	1.49	1.37
4	O	509	SER	CA-CB	6.39	1.62	1.52
2	P	344	ARG	CZ-NH2	6.39	1.41	1.33
4	M	509	SER	CA-CB	6.37	1.62	1.52
2	N	344	ARG	CZ-NH2	6.37	1.41	1.33
2	E	539	GLU	CD-OE2	6.33	1.32	1.25
2	E	513	ARG	CZ-NH2	6.26	1.41	1.33
2	N	456	SER	CA-CB	6.25	1.62	1.52
2	P	456	SER	CA-CB	6.24	1.62	1.52
2	F	539	GLU	CD-OE2	6.23	1.32	1.25
2	A	539	GLU	CD-OE2	6.20	1.32	1.25
2	F	412	TYR	CE2-CZ	6.19	1.46	1.38
4	M	432	ARG	CD-NE	6.18	1.56	1.46
2	A	513	ARG	CZ-NH2	6.16	1.41	1.33
2	A	412	TYR	CE2-CZ	6.15	1.46	1.38
2	F	513	ARG	CZ-NH2	6.15	1.41	1.33
4	M	432	ARG	NE-CZ	6.14	1.41	1.33
2	B	382	LEU	CA-C	-6.12	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	O	432	ARG	CD-NE	6.12	1.56	1.46
2	G	382	LEU	CA-C	-6.12	1.37	1.52
2	H	382	LEU	CA-C	-6.12	1.37	1.52
4	O	430	TYR	CG-CD1	6.11	1.47	1.39
4	M	429	GLU	CG-CD	6.10	1.61	1.51
6	Q	634	PHE	CA-C	-6.09	1.37	1.52
4	O	432	ARG	NE-CZ	6.07	1.41	1.33
6	Q	631	SER	CA-C	-6.07	1.37	1.52
4	M	450	SER	CA-CB	6.07	1.62	1.52
2	B	522	PHE	CA-C	-6.06	1.37	1.52
6	R	631	SER	CA-C	-6.06	1.37	1.52
2	P	508	ARG	CD-NE	6.05	1.56	1.46
6	R	634	PHE	CA-C	-6.04	1.37	1.52
2	G	522	PHE	CA-C	-6.04	1.37	1.52
4	M	430	TYR	CG-CD1	6.03	1.47	1.39
2	H	522	PHE	CA-C	-6.02	1.37	1.52
2	N	508	ARG	CD-NE	6.02	1.56	1.46
4	O	429	GLU	CG-CD	6.01	1.60	1.51
2	N	508	ARG	CZ-NH2	6.00	1.40	1.33
4	O	450	SER	CA-CB	6.00	1.61	1.52
5	S	136	GLY	CA-C	-5.99	1.42	1.51
2	E	412	TYR	CE2-CZ	5.99	1.46	1.38
2	P	508	ARG	CZ-NH2	5.99	1.40	1.33
5	T	136	GLY	CA-C	-5.95	1.42	1.51
2	H	410	ASP	CA-C	-5.92	1.37	1.52
6	Q	435	GLY	CA-C	-5.89	1.42	1.51
2	G	410	ASP	CA-C	-5.88	1.37	1.52
6	R	435	GLY	CA-C	-5.87	1.42	1.51
2	B	410	ASP	CA-C	-5.86	1.37	1.52
2	E	508	ARG	CD-NE	5.85	1.56	1.46
2	A	470	ARG	CD-NE	5.83	1.56	1.46
4	M	389	GLU	CG-CD	5.83	1.60	1.51
3	V	250	PRO	CA-C	5.82	1.64	1.52
2	N	368	ARG	CZ-NH1	5.82	1.40	1.33
2	E	490	GLU	CG-CD	5.82	1.60	1.51
2	A	508	ARG	CD-NE	5.81	1.56	1.46
2	F	490	GLU	CG-CD	5.80	1.60	1.51
4	O	389	GLU	CG-CD	5.79	1.60	1.51
6	Q	527	ILE	N-CA	-5.78	1.34	1.46
2	P	368	ARG	CZ-NH1	5.78	1.40	1.33
2	N	250	PRO	CA-C	5.78	1.64	1.52
2	E	250	PRO	CA-C	5.76	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	490	GLU	CG-CD	5.76	1.60	1.51
2	G	250	PRO	CA-C	5.75	1.64	1.52
2	P	250	PRO	CA-C	5.75	1.64	1.52
2	F	508	ARG	CD-NE	5.75	1.56	1.46
2	F	470	ARG	CD-NE	5.75	1.56	1.46
4	M	402	SER	CA-CB	5.73	1.61	1.52
4	M	515	GLU	CD-OE1	5.73	1.31	1.25
4	M	331	ASN	CB-CG	5.72	1.64	1.51
2	E	470	ARG	CD-NE	5.72	1.56	1.46
2	A	250	PRO	CA-C	5.71	1.64	1.52
2	N	513	ARG	CZ-NH2	5.71	1.40	1.33
4	M	457	GLU	CB-CG	5.70	1.62	1.52
2	N	249	PRO	C-N	-5.70	1.23	1.34
6	R	527	ILE	N-CA	-5.70	1.34	1.46
4	O	457	GLU	CB-CG	5.69	1.62	1.52
4	O	515	GLU	CD-OE1	5.69	1.31	1.25
4	O	402	SER	CA-CB	5.69	1.61	1.52
2	F	250	PRO	CA-C	5.69	1.64	1.52
2	P	513	ARG	CZ-NH2	5.69	1.40	1.33
3	D	249	PRO	C-N	-5.68	1.23	1.34
2	B	250	PRO	CA-C	5.68	1.64	1.52
4	O	331	ASN	CB-CG	5.67	1.64	1.51
2	H	249	PRO	C-N	-5.67	1.23	1.34
2	A	249	PRO	C-N	-5.67	1.23	1.34
2	F	249	PRO	C-N	-5.67	1.23	1.34
3	L	250	PRO	CA-C	5.67	1.64	1.52
3	K	250	PRO	CA-C	5.67	1.64	1.52
2	P	344	ARG	CZ-NH1	5.67	1.40	1.33
6	R	629	GLN	CA-C	-5.67	1.38	1.52
3	K	249	PRO	C-N	-5.66	1.23	1.34
2	E	249	PRO	C-N	-5.66	1.23	1.34
2	H	250	PRO	CA-C	5.66	1.64	1.52
3	D	250	PRO	CA-C	5.66	1.64	1.52
2	N	344	ARG	CZ-NH1	5.66	1.40	1.33
6	Q	633	LEU	N-CA	-5.65	1.35	1.46
4	M	346	TYR	CE2-CZ	5.64	1.45	1.38
2	F	516	ARG	CD-NE	5.64	1.56	1.46
6	R	633	LEU	N-CA	-5.63	1.35	1.46
4	O	346	TYR	CE2-CZ	5.63	1.45	1.38
2	P	249	PRO	C-N	-5.63	1.23	1.34
2	P	378	PHE	CB-CG	-5.62	1.41	1.51
2	G	249	PRO	C-N	-5.62	1.23	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	514	PHE	CG-CD2	5.61	1.47	1.38
3	V	249	PRO	C-N	-5.61	1.23	1.34
2	N	514	PHE	CG-CD2	5.61	1.47	1.38
6	R	525	LEU	N-CA	-5.61	1.35	1.46
2	B	249	PRO	C-N	-5.60	1.23	1.34
3	L	249	PRO	C-N	-5.60	1.23	1.34
2	N	378	PHE	CB-CG	-5.59	1.41	1.51
6	Q	629	GLN	CA-C	-5.59	1.38	1.52
2	A	491	ARG	CD-NE	5.57	1.55	1.46
6	Q	633	LEU	CA-C	-5.57	1.38	1.52
2	E	516	ARG	CD-NE	5.56	1.55	1.46
2	A	516	ARG	CD-NE	5.56	1.55	1.46
2	P	484	ALA	N-CA	-5.55	1.35	1.46
6	Q	525	LEU	N-CA	-5.54	1.35	1.46
2	F	491	ARG	CD-NE	5.53	1.55	1.46
6	R	633	LEU	CA-C	-5.53	1.38	1.52
2	E	491	ARG	CD-NE	5.53	1.55	1.46
2	G	379	SER	N-CA	-5.52	1.35	1.46
2	B	379	SER	N-CA	-5.52	1.35	1.46
2	N	478	ARG	CD-NE	5.52	1.55	1.46
2	H	379	SER	N-CA	-5.52	1.35	1.46
2	A	491	ARG	CZ-NH1	5.49	1.40	1.33
2	E	491	ARG	CZ-NH1	5.49	1.40	1.33
2	A	432	ARG	CZ-NH2	5.48	1.40	1.33
2	E	505	ARG	NE-CZ	5.48	1.40	1.33
2	N	470	ARG	NE-CZ	5.47	1.40	1.33
2	P	484	ALA	CA-CB	5.47	1.64	1.52
2	E	335	GLU	CB-CG	5.47	1.62	1.52
2	N	484	ALA	N-CA	-5.47	1.35	1.46
2	P	478	ARG	CD-NE	5.46	1.55	1.46
2	F	335	GLU	CB-CG	5.46	1.62	1.52
2	A	335	GLU	CB-CG	5.46	1.62	1.52
2	E	432	ARG	CZ-NH2	5.45	1.40	1.33
4	O	478	ARG	CZ-NH2	5.44	1.40	1.33
2	F	432	ARG	CZ-NH2	5.43	1.40	1.33
2	F	491	ARG	CZ-NH1	5.43	1.40	1.33
6	R	637	LEU	N-CA	-5.42	1.35	1.46
2	N	484	ALA	CA-CB	5.42	1.63	1.52
6	R	469	PRO	CA-C	-5.42	1.42	1.52
6	Q	469	PRO	CA-C	-5.42	1.42	1.52
4	O	391	SER	CA-CB	5.41	1.61	1.52
6	R	635	LYS	N-CA	-5.40	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	505	ARG	NE-CZ	5.40	1.40	1.33
2	P	509	SER	CA-CB	5.39	1.61	1.52
6	Q	432	TYR	CB-CG	-5.38	1.43	1.51
6	R	585	GLN	N-CA	-5.37	1.35	1.46
6	Q	585	GLN	N-CA	-5.37	1.35	1.46
2	A	505	ARG	NE-CZ	5.35	1.40	1.33
4	M	478	ARG	CZ-NH2	5.35	1.40	1.33
2	N	509	SER	CA-CB	5.35	1.60	1.52
4	M	391	SER	CA-CB	5.34	1.60	1.52
6	Q	635	LYS	N-CA	-5.34	1.35	1.46
2	F	516	ARG	CZ-NH2	5.34	1.40	1.33
6	R	730	HIS	CB-CG	-5.34	1.40	1.50
6	Q	730	HIS	CB-CG	-5.34	1.40	1.50
4	O	505	ARG	CZ-NH2	5.33	1.40	1.33
6	R	432	TYR	CB-CG	-5.33	1.43	1.51
2	N	444	ARG	CD-NE	5.33	1.55	1.46
2	P	470	ARG	NE-CZ	5.32	1.40	1.33
2	P	412	TYR	CB-CG	5.32	1.59	1.51
6	Q	637	LEU	N-CA	-5.31	1.35	1.46
2	A	516	ARG	CZ-NH2	5.30	1.40	1.33
2	E	516	ARG	CZ-NH2	5.28	1.40	1.33
2	P	343	ARG	CZ-NH1	5.28	1.40	1.33
4	M	505	ARG	CZ-NH2	5.28	1.40	1.33
4	M	414	ARG	CD-NE	5.26	1.55	1.46
4	M	497	ARG	CZ-NH2	5.26	1.39	1.33
2	A	372	ALA	N-CA	-5.26	1.35	1.46
2	A	436	SER	CA-CB	5.25	1.60	1.52
2	N	428	GLU	CD-OE1	5.25	1.31	1.25
6	Q	587	THR	N-CA	-5.24	1.35	1.46
6	R	632	SER	CA-C	-5.24	1.39	1.52
2	E	436	SER	CA-CB	5.23	1.60	1.52
6	R	587	THR	N-CA	-5.23	1.35	1.46
2	F	436	SER	CA-CB	5.23	1.60	1.52
2	F	372	ALA	N-CA	-5.23	1.35	1.46
4	O	414	ARG	CD-NE	5.22	1.55	1.46
2	F	544	TRP	CB-CG	5.22	1.59	1.50
2	P	444	ARG	CD-NE	5.22	1.55	1.46
2	N	343	ARG	CZ-NH1	5.20	1.39	1.33
6	Q	632	SER	CA-C	-5.20	1.39	1.52
2	N	412	TYR	CB-CG	5.19	1.59	1.51
2	A	544	TRP	CB-CG	5.18	1.59	1.50
2	F	510	GLU	CB-CG	5.18	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	478	ARG	CG-CD	5.18	1.65	1.51
2	E	510	GLU	CB-CG	5.18	1.61	1.52
2	A	478	ARG	CG-CD	5.17	1.64	1.51
2	E	372	ALA	N-CA	-5.17	1.36	1.46
2	E	544	TRP	CB-CG	5.16	1.59	1.50
2	A	344	ARG	CZ-NH1	5.16	1.39	1.33
2	A	510	GLU	CB-CG	5.16	1.61	1.52
2	H	339	TRP	CA-C	-5.15	1.39	1.52
4	O	344	ARG	CZ-NH2	5.15	1.39	1.33
4	O	497	ARG	CZ-NH2	5.15	1.39	1.33
2	E	478	ARG	CG-CD	5.15	1.64	1.51
4	M	344	ARG	CZ-NH2	5.13	1.39	1.33
2	P	428	GLU	CD-OE1	5.13	1.31	1.25
2	A	343	ARG	CD-NE	5.13	1.55	1.46
6	Q	580	GLN	N-CA	-5.13	1.36	1.46
2	G	339	TRP	CA-C	-5.12	1.39	1.52
2	N	236	TYR	CB-CG	-5.12	1.44	1.51
2	A	236	TYR	CB-CG	-5.12	1.44	1.51
2	F	344	ARG	CD-NE	5.11	1.55	1.46
2	P	343	ARG	CD-NE	5.11	1.55	1.46
2	N	505	ARG	CZ-NH2	5.11	1.39	1.33
3	D	236	TYR	CB-CG	-5.11	1.44	1.51
3	V	236	TYR	CB-CG	-5.10	1.44	1.51
2	B	339	TRP	CA-C	-5.10	1.39	1.52
2	F	343	ARG	CD-NE	5.10	1.55	1.46
4	O	455	GLU	CB-CG	5.09	1.61	1.52
2	P	236	TYR	CB-CG	-5.09	1.44	1.51
4	M	515	GLU	CB-CG	5.09	1.61	1.52
6	R	580	GLN	N-CA	-5.09	1.36	1.46
2	B	340	PHE	CA-C	-5.09	1.39	1.52
2	E	344	ARG	CZ-NH1	5.09	1.39	1.33
2	N	343	ARG	CD-NE	5.09	1.55	1.46
6	Q	444	VAL	N-CA	-5.09	1.36	1.46
6	R	580	GLN	CA-C	-5.09	1.39	1.52
2	E	470	ARG	NE-CZ	5.08	1.39	1.33
2	F	344	ARG	CZ-NH1	5.08	1.39	1.33
6	Q	580	GLN	CA-C	-5.08	1.39	1.52
2	F	236	TYR	CB-CG	-5.08	1.44	1.51
2	G	236	TYR	CB-CG	-5.08	1.44	1.51
2	P	505	ARG	CZ-NH2	5.08	1.39	1.33
3	L	236	TYR	CB-CG	-5.08	1.44	1.51
2	P	414	ARG	CZ-NH2	5.08	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	453	SER	N-CA	-5.08	1.36	1.46
2	A	344	ARG	CD-NE	5.08	1.55	1.46
2	A	453	SER	N-CA	-5.08	1.36	1.46
3	K	236	TYR	CB-CG	-5.08	1.44	1.51
2	E	344	ARG	CD-NE	5.07	1.55	1.46
2	H	340	PHE	CA-C	-5.07	1.39	1.52
2	G	340	PHE	CA-C	-5.07	1.39	1.52
2	F	470	ARG	NE-CZ	5.07	1.39	1.33
2	A	470	ARG	NE-CZ	5.06	1.39	1.33
2	H	518	LYS	N-CA	-5.06	1.36	1.46
4	O	515	GLU	CB-CG	5.05	1.61	1.52
2	F	368	ARG	CZ-NH1	5.05	1.39	1.33
4	M	455	GLU	CB-CG	5.04	1.61	1.52
2	E	368	ARG	CZ-NH1	5.04	1.39	1.33
2	E	236	TYR	CB-CG	-5.04	1.44	1.51
2	B	522	PHE	CB-CG	-5.04	1.42	1.51
2	B	383	HIS	N-CA	-5.03	1.36	1.46
4	M	343	ARG	CZ-NH1	5.03	1.39	1.33
2	H	522	PHE	CB-CG	-5.03	1.42	1.51
2	E	453	SER	N-CA	-5.03	1.36	1.46
2	G	383	HIS	N-CA	-5.03	1.36	1.46
2	E	343	ARG	CD-NE	5.03	1.54	1.46
2	F	383	HIS	CB-CG	5.02	1.59	1.50
2	A	383	HIS	CB-CG	5.02	1.59	1.50
2	H	383	HIS	N-CA	-5.02	1.36	1.46
2	B	236	TYR	CB-CG	-5.02	1.44	1.51
2	B	518	LYS	N-CA	-5.01	1.36	1.46
2	G	339	TRP	N-CA	-5.01	1.36	1.46
2	N	520	GLU	CD-OE2	5.01	1.31	1.25
2	E	383	HIS	CB-CG	5.01	1.59	1.50
6	R	444	VAL	N-CA	-5.00	1.36	1.46

All (1093) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	470	ARG	NE-CZ-NH1	-14.31	113.14	120.30
6	Q	98	TYR	CB-CG-CD2	-14.31	112.42	121.00
6	R	98	TYR	CB-CG-CD2	-14.21	112.48	121.00
2	N	470	ARG	NE-CZ-NH1	-14.20	113.20	120.30
4	O	516	ARG	NE-CZ-NH2	14.00	127.30	120.30
4	M	516	ARG	NE-CZ-NH2	13.92	127.26	120.30
5	S	87	PHE	CB-CG-CD1	13.18	130.03	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	T	87	PHE	CB-CG-CD1	13.12	129.98	120.80
6	Q	98	TYR	CB-CG-CD1	12.63	128.58	121.00
6	R	98	TYR	CB-CG-CD1	12.62	128.57	121.00
2	P	513	ARG	NE-CZ-NH2	-12.45	114.07	120.30
2	N	513	ARG	NE-CZ-NH2	-12.38	114.11	120.30
2	P	470	ARG	NE-CZ-NH2	12.36	126.48	120.30
4	M	514	PHE	CB-CG-CD1	12.28	129.40	120.80
4	O	514	PHE	CB-CG-CD1	12.27	129.39	120.80
2	E	412	TYR	CB-CG-CD2	12.06	128.24	121.00
2	N	470	ARG	NE-CZ-NH2	12.05	126.32	120.30
2	A	412	TYR	CB-CG-CD2	11.89	128.14	121.00
2	F	412	TYR	CB-CG-CD2	11.89	128.13	121.00
2	P	505	ARG	NE-CZ-NH2	11.76	126.18	120.30
2	N	505	ARG	NE-CZ-NH2	11.65	126.12	120.30
2	N	346	TYR	CB-CG-CD2	-11.07	114.36	121.00
5	S	87	PHE	CB-CG-CD2	-11.06	113.06	120.80
5	T	87	PHE	CB-CG-CD2	-11.01	113.09	120.80
2	P	346	TYR	CB-CG-CD2	-11.00	114.40	121.00
2	P	441	PHE	CB-CG-CD1	-10.84	113.21	120.80
2	N	441	PHE	CB-CG-CD1	-10.83	113.22	120.80
4	M	444	ARG	NE-CZ-NH1	10.69	125.65	120.30
2	H	376	ALA	CB-CA-C	-10.56	94.26	110.10
2	G	376	ALA	CB-CA-C	-10.55	94.28	110.10
2	B	376	ALA	CB-CA-C	-10.53	94.31	110.10
4	O	444	ARG	NE-CZ-NH1	10.53	125.56	120.30
6	Q	485	TYR	CB-CG-CD1	10.38	127.23	121.00
6	R	485	TYR	CB-CG-CD1	10.38	127.23	121.00
2	N	497	ARG	NE-CZ-NH1	-10.31	115.14	120.30
6	Q	688	TYR	CB-CG-CD1	10.31	127.19	121.00
4	M	412	TYR	CB-CG-CD2	-10.14	114.92	121.00
6	R	688	TYR	CB-CG-CD1	10.12	127.07	121.00
6	R	485	TYR	CB-CG-CD2	-10.09	114.95	121.00
2	P	497	ARG	NE-CZ-NH1	-10.03	115.28	120.30
4	O	412	TYR	CB-CG-CD2	-10.03	114.98	121.00
6	Q	485	TYR	CB-CG-CD2	-9.99	115.01	121.00
4	O	514	PHE	CB-CG-CD2	-9.93	113.85	120.80
4	M	514	PHE	CB-CG-CD2	-9.91	113.86	120.80
6	R	432	TYR	CB-CA-C	-9.67	91.06	110.40
6	R	267	TYR	CB-CG-CD1	9.66	126.80	121.00
2	B	378	PHE	CB-CG-CD2	-9.64	114.05	120.80
6	Q	432	TYR	CB-CA-C	-9.63	91.14	110.40
6	Q	267	TYR	CB-CG-CD1	9.61	126.77	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	378	PHE	CB-CG-CD2	-9.61	114.07	120.80
2	G	378	PHE	CB-CG-CD2	-9.59	114.09	120.80
1	C	245	ARG	NE-CZ-NH1	9.41	125.00	120.30
2	G	412	TYR	CB-CG-CD2	-9.38	115.37	121.00
1	J	245	ARG	NE-CZ-NH1	9.37	124.98	120.30
2	A	514	PHE	CB-CG-CD1	9.26	127.28	120.80
2	B	412	TYR	CB-CG-CD2	-9.26	115.45	121.00
2	F	514	PHE	CB-CG-CD1	9.24	127.27	120.80
4	O	529	PHE	CB-CG-CD1	9.22	127.26	120.80
2	E	514	PHE	CB-CG-CD1	9.21	127.25	120.80
4	M	529	PHE	CB-CG-CD1	9.19	127.23	120.80
6	Q	63	TYR	CB-CG-CD2	-9.15	115.51	121.00
2	H	412	TYR	CB-CG-CD2	-9.14	115.51	121.00
6	R	63	TYR	CB-CG-CD2	-9.08	115.55	121.00
6	R	616	PHE	CB-CG-CD2	-9.02	114.49	120.80
5	S	191	TYR	CB-CG-CD1	-9.00	115.60	121.00
6	Q	616	PHE	CB-CG-CD2	-8.97	114.52	120.80
6	R	149	TYR	CB-CG-CD1	-8.97	115.62	121.00
6	Q	149	TYR	CB-CG-CD1	-8.96	115.62	121.00
5	T	191	TYR	CB-CG-CD1	-8.96	115.63	121.00
6	Q	688	TYR	CB-CG-CD2	-8.88	115.67	121.00
6	R	688	TYR	CB-CG-CD2	-8.84	115.69	121.00
2	N	340	PHE	CB-CG-CD1	8.79	126.95	120.80
2	A	414	ARG	NE-CZ-NH2	8.75	124.67	120.30
2	B	375	ALA	CB-CA-C	8.72	123.17	110.10
2	H	375	ALA	CB-CA-C	8.69	123.14	110.10
2	G	375	ALA	CB-CA-C	8.69	123.13	110.10
2	P	340	PHE	CB-CG-CD1	8.68	126.88	120.80
2	F	414	ARG	NE-CZ-NH2	8.68	124.64	120.30
6	Q	590	ALA	CB-CA-C	8.66	123.09	110.10
2	E	414	ARG	NE-CZ-NH2	8.65	124.63	120.30
6	R	590	ALA	CB-CA-C	8.64	123.06	110.10
2	N	343	ARG	NE-CZ-NH1	-8.63	115.98	120.30
2	P	343	ARG	NE-CZ-NH1	-8.62	115.99	120.30
2	A	516	ARG	NE-CZ-NH2	8.61	124.61	120.30
2	N	502	ASP	CB-CG-OD2	-8.56	110.60	118.30
6	R	485	TYR	N-CA-CB	-8.55	95.22	110.60
6	Q	485	TYR	N-CA-CB	-8.54	95.23	110.60
2	F	516	ARG	NE-CZ-NH2	8.53	124.57	120.30
2	P	502	ASP	CB-CG-OD2	-8.49	110.66	118.30
2	B	386	SER	CB-CA-C	-8.45	94.04	110.10
4	O	346	TYR	CB-CG-CD1	-8.45	115.93	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	494	TYR	CB-CG-CD2	-8.45	115.93	121.00
2	B	368	ARG	NE-CZ-NH2	8.44	124.52	120.30
2	E	412	TYR	CB-CG-CD1	-8.44	115.94	121.00
2	E	516	ARG	NE-CZ-NH2	8.44	124.52	120.30
4	M	346	TYR	CB-CG-CD1	-8.44	115.94	121.00
2	H	386	SER	CB-CA-C	-8.44	94.07	110.10
2	G	386	SER	CB-CA-C	-8.41	94.11	110.10
2	H	368	ARG	NE-CZ-NH2	8.41	124.50	120.30
2	G	368	ARG	NE-CZ-NH2	8.41	124.50	120.30
6	Q	715	PHE	CB-CG-CD2	-8.39	114.92	120.80
2	G	440	ALA	CB-CA-C	-8.37	97.55	110.10
6	Q	494	TYR	CB-CG-CD2	-8.35	115.99	121.00
2	G	340	PHE	CB-CG-CD2	-8.34	114.96	120.80
2	H	440	ALA	CB-CA-C	-8.32	97.63	110.10
6	R	715	PHE	CB-CG-CD2	-8.30	114.99	120.80
2	H	340	PHE	CB-CG-CD2	-8.30	114.99	120.80
2	B	340	PHE	CB-CG-CD2	-8.29	115.00	120.80
2	B	440	ALA	CB-CA-C	-8.29	97.66	110.10
2	A	412	TYR	CB-CG-CD1	-8.28	116.03	121.00
6	Q	848	HIS	CA-CB-CG	8.26	127.64	113.60
2	F	412	TYR	CB-CG-CD1	-8.25	116.05	121.00
6	R	848	HIS	CA-CB-CG	8.19	127.53	113.60
6	Q	591	TYR	CB-CG-CD2	-8.11	116.14	121.00
6	R	591	TYR	CB-CG-CD2	-8.10	116.14	121.00
2	H	451	TRP	CB-CG-CD2	-8.09	116.09	126.60
6	R	581	PHE	CB-CG-CD1	8.06	126.44	120.80
6	Q	28	MET	CG-SD-CE	-8.04	87.33	100.20
6	R	28	MET	CG-SD-CE	-8.04	87.34	100.20
2	B	451	TRP	CB-CG-CD2	-8.03	116.16	126.60
6	Q	581	PHE	CB-CG-CD1	8.03	126.42	120.80
2	G	451	TRP	CB-CG-CD2	-8.00	116.20	126.60
4	M	478	ARG	NE-CZ-NH1	-7.98	116.31	120.30
5	S	121	ARG	NE-CZ-NH2	-7.94	116.33	120.30
6	R	116	TYR	CB-CG-CD1	7.93	125.76	121.00
2	N	378	PHE	CB-CG-CD2	-7.92	115.26	120.80
2	E	269	ARG	NE-CZ-NH1	7.91	124.25	120.30
5	T	121	ARG	NE-CZ-NH2	-7.89	116.35	120.30
4	M	343	ARG	NE-CZ-NH1	-7.86	116.37	120.30
2	P	378	PHE	CB-CG-CD2	-7.85	115.30	120.80
6	Q	116	TYR	CB-CG-CD1	7.83	125.70	121.00
5	S	121	ARG	NE-CZ-NH1	7.81	124.20	120.30
2	H	269	ARG	NE-CZ-NH1	7.81	124.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	451	TRP	CB-CG-CD1	-7.80	116.86	127.00
4	O	478	ARG	NE-CZ-NH1	-7.79	116.40	120.30
2	P	269	ARG	NE-CZ-NH1	7.77	124.19	120.30
3	L	269	ARG	NE-CZ-NH1	7.77	124.19	120.30
2	E	378	PHE	CB-CG-CD1	7.76	126.23	120.80
2	N	491	ARG	NE-CZ-NH2	-7.76	116.42	120.30
2	G	451	TRP	CB-CG-CD1	-7.75	116.92	127.00
2	P	491	ARG	NE-CZ-NH2	-7.75	116.42	120.30
5	T	121	ARG	NE-CZ-NH1	7.74	124.17	120.30
2	G	430	TYR	CB-CG-CD2	-7.74	116.36	121.00
1	J	21	ARG	NE-CZ-NH1	7.73	124.17	120.30
2	F	378	PHE	CB-CG-CD1	7.73	126.21	120.80
4	O	343	ARG	NE-CZ-NH1	-7.73	116.44	120.30
2	B	430	TYR	CB-CG-CD2	-7.72	116.36	121.00
2	B	451	TRP	CB-CG-CD1	-7.70	116.99	127.00
4	O	529	PHE	CB-CG-CD2	-7.69	115.42	120.80
1	C	21	ARG	NE-CZ-NH1	7.69	124.14	120.30
3	D	269	ARG	NE-CZ-NH1	7.68	124.14	120.30
2	A	378	PHE	CB-CG-CD1	7.67	126.17	120.80
3	K	269	ARG	NE-CZ-NH1	7.67	124.13	120.30
2	B	269	ARG	NE-CZ-NH1	7.66	124.13	120.30
2	N	269	ARG	NE-CZ-NH1	7.66	124.13	120.30
2	H	430	TYR	CB-CG-CD2	-7.64	116.42	121.00
6	R	591	TYR	CA-CB-CG	-7.62	98.92	113.40
2	P	412	TYR	CB-CG-CD2	-7.62	116.43	121.00
2	A	269	ARG	NE-CZ-NH1	7.61	124.11	120.30
6	R	267	TYR	CB-CG-CD2	-7.61	116.43	121.00
6	Q	591	TYR	CA-CB-CG	-7.60	98.96	113.40
2	N	412	TYR	CB-CG-CD2	-7.59	116.45	121.00
4	M	529	PHE	CB-CG-CD2	-7.58	115.49	120.80
2	F	269	ARG	NE-CZ-NH1	7.57	124.08	120.30
2	H	405	GLN	CB-CA-C	-7.57	95.27	110.40
2	G	269	ARG	NE-CZ-NH1	7.56	124.08	120.30
3	V	269	ARG	NE-CZ-NH1	7.55	124.07	120.30
6	Q	597	ARG	C-N-CA	7.55	140.56	121.70
2	B	405	GLN	CB-CA-C	-7.54	95.32	110.40
6	R	597	ARG	C-N-CA	7.54	140.55	121.70
1	J	245	ARG	NE-CZ-NH2	-7.52	116.54	120.30
6	Q	267	TYR	CB-CG-CD2	-7.52	116.49	121.00
6	R	449	ASN	N-CA-C	-7.49	90.79	111.00
6	Q	449	ASN	N-CA-C	-7.48	90.80	111.00
2	G	405	GLN	CB-CA-C	-7.48	95.44	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	681	PHE	CB-CA-C	7.46	125.33	110.40
6	Q	505	VAL	CB-CA-C	-7.42	97.29	111.40
6	R	505	VAL	CB-CA-C	-7.42	97.30	111.40
1	C	245	ARG	NE-CZ-NH2	-7.40	116.60	120.30
2	P	212	LYS	N-CA-C	-7.40	91.03	111.00
2	B	368	ARG	NE-CZ-NH1	-7.39	116.61	120.30
2	A	212	LYS	N-CA-C	-7.38	91.07	111.00
3	V	212	LYS	N-CA-C	-7.38	91.08	111.00
6	Q	681	PHE	CB-CA-C	7.38	125.16	110.40
2	H	212	LYS	N-CA-C	-7.37	91.09	111.00
2	H	433	LEU	CB-CA-C	-7.37	96.19	110.20
2	B	412	TYR	CB-CG-CD1	-7.37	116.58	121.00
2	N	212	LYS	N-CA-C	-7.37	91.10	111.00
5	T	83	LEU	N-CA-C	-7.37	91.09	111.00
2	G	212	LYS	N-CA-C	-7.37	91.10	111.00
2	B	433	LEU	CB-CA-C	-7.37	96.21	110.20
5	S	83	LEU	N-CA-C	-7.37	91.11	111.00
3	K	212	LYS	N-CA-C	-7.36	91.13	111.00
2	B	212	LYS	N-CA-C	-7.36	91.13	111.00
2	E	212	LYS	N-CA-C	-7.36	91.13	111.00
2	F	212	LYS	N-CA-C	-7.36	91.14	111.00
2	G	433	LEU	CB-CA-C	-7.35	96.23	110.20
3	L	212	LYS	N-CA-C	-7.35	91.15	111.00
3	D	212	LYS	N-CA-C	-7.35	91.15	111.00
2	H	412	TYR	CB-CG-CD1	-7.34	116.60	121.00
2	G	412	TYR	CB-CG-CD1	-7.33	116.60	121.00
2	H	368	ARG	NE-CZ-NH1	-7.32	116.64	120.30
6	Q	489	PHE	CB-CA-C	-7.30	95.80	110.40
5	S	170	TYR	N-CA-C	-7.29	91.32	111.00
5	T	170	TYR	N-CA-C	-7.29	91.32	111.00
6	Q	720	TYR	CB-CG-CD2	-7.28	116.63	121.00
6	R	616	PHE	CB-CG-CD1	7.28	125.90	120.80
6	Q	614	ARG	NE-CZ-NH2	-7.27	116.67	120.30
6	Q	616	PHE	CB-CG-CD1	7.27	125.89	120.80
6	R	489	PHE	CB-CA-C	-7.25	95.90	110.40
6	R	720	TYR	CB-CG-CD2	-7.24	116.66	121.00
2	G	368	ARG	NE-CZ-NH1	-7.23	116.68	120.30
2	H	346	TYR	CB-CG-CD2	-7.22	116.67	121.00
2	B	522	PHE	CA-CB-CG	-7.14	96.75	113.90
2	H	522	PHE	CA-CB-CG	-7.14	96.76	113.90
2	B	339	TRP	CB-CG-CD2	-7.14	117.32	126.60
2	G	522	PHE	CA-CB-CG	-7.14	96.77	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	339	TRP	CB-CG-CD2	-7.13	117.33	126.60
6	Q	149	TYR	CB-CG-CD2	-7.09	116.75	121.00
6	R	614	ARG	NE-CZ-NH2	-7.08	116.76	120.30
2	G	346	TYR	CB-CG-CD2	-7.07	116.76	121.00
2	H	339	TRP	CB-CG-CD2	-7.06	117.42	126.60
6	Q	494	TYR	CB-CG-CD1	7.06	125.23	121.00
2	H	236	TYR	CB-CG-CD1	-7.04	116.78	121.00
6	R	149	TYR	CB-CG-CD2	-7.04	116.78	121.00
3	V	236	TYR	CB-CG-CD1	-7.03	116.78	121.00
2	B	236	TYR	CB-CG-CD1	-7.02	116.79	121.00
6	R	494	TYR	CB-CG-CD1	7.00	125.20	121.00
3	L	236	TYR	CB-CG-CD1	-7.00	116.80	121.00
2	G	236	TYR	CB-CG-CD1	-7.00	116.80	121.00
2	F	409	ARG	NE-CZ-NH2	-6.99	116.81	120.30
6	R	661	PHE	CB-CA-C	-6.97	96.45	110.40
2	A	364	MET	CG-SD-CE	-6.97	89.05	100.20
6	Q	661	PHE	CB-CA-C	-6.96	96.47	110.40
6	R	38	LEU	N-CA-CB	-6.96	96.47	110.40
2	B	346	TYR	CB-CG-CD2	-6.96	116.82	121.00
3	K	236	TYR	CB-CG-CD1	-6.96	116.82	121.00
6	Q	730	HIS	CB-CA-C	-6.96	96.49	110.40
6	Q	439	TYR	CB-CG-CD1	6.95	125.17	121.00
1	C	280	ARG	NE-CZ-NH2	-6.95	116.83	120.30
2	E	454	ALA	N-CA-CB	6.94	119.82	110.10
6	Q	38	LEU	N-CA-CB	-6.94	96.51	110.40
3	D	236	TYR	CB-CG-CD1	-6.94	116.84	121.00
2	F	529	PHE	CB-CG-CD1	-6.93	115.94	120.80
2	E	409	ARG	NE-CZ-NH2	-6.93	116.83	120.30
2	E	364	MET	CG-SD-CE	-6.93	89.12	100.20
1	C	25	ASP	CB-CG-OD2	-6.93	112.07	118.30
2	A	454	ALA	N-CA-CB	6.93	119.80	110.10
6	R	584	LEU	CB-CA-C	-6.92	97.05	110.20
4	O	416	ALA	N-CA-CB	-6.92	100.41	110.10
4	M	416	ALA	N-CA-CB	-6.92	100.41	110.10
2	A	529	PHE	CB-CG-CD1	-6.92	115.96	120.80
5	S	125	PHE	CB-CG-CD2	-6.92	115.96	120.80
6	Q	584	LEU	CB-CA-C	-6.91	97.06	110.20
5	T	125	PHE	CB-CG-CD2	-6.91	115.96	120.80
6	R	730	HIS	CB-CA-C	-6.91	96.58	110.40
2	B	370	ALA	C-N-CA	6.91	138.97	121.70
2	G	370	ALA	C-N-CA	6.91	138.97	121.70
2	H	370	ALA	C-N-CA	6.91	138.97	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	364	MET	CG-SD-CE	-6.91	89.14	100.20
6	R	673	PHE	CB-CG-CD1	6.91	125.64	120.80
6	R	439	TYR	CB-CG-CD1	6.91	125.14	121.00
4	M	466	ASP	CB-CG-OD1	6.90	124.51	118.30
2	E	236	TYR	CB-CG-CD1	-6.90	116.86	121.00
2	F	236	TYR	CB-CG-CD1	-6.90	116.86	121.00
2	H	448	PHE	CB-CG-CD1	-6.89	115.97	120.80
2	P	236	TYR	CB-CG-CD2	-6.89	116.87	121.00
1	J	280	ARG	NE-CZ-NH2	-6.88	116.86	120.30
2	F	454	ALA	N-CA-CB	6.88	119.74	110.10
2	P	236	TYR	CB-CG-CD1	-6.88	116.87	121.00
5	S	84	ARG	N-CA-C	-6.88	92.43	111.00
2	N	229	TYR	CB-CG-CD2	-6.88	116.88	121.00
2	P	229	TYR	CB-CG-CD2	-6.87	116.88	121.00
2	N	370	ALA	C-N-CA	6.87	138.87	121.70
5	T	84	ARG	N-CA-C	-6.87	92.46	111.00
2	P	370	ALA	C-N-CA	6.86	138.84	121.70
6	Q	680	PHE	CB-CG-CD2	-6.86	116.00	120.80
4	O	466	ASP	CB-CG-OD1	6.85	124.47	118.30
1	J	25	ASP	CB-CG-OD2	-6.85	112.13	118.30
2	N	236	TYR	CB-CG-CD1	-6.85	116.89	121.00
2	A	409	ARG	NE-CZ-NH2	-6.85	116.88	120.30
6	Q	712	THR	N-CA-C	-6.85	92.51	111.00
2	B	448	PHE	CB-CG-CD1	-6.84	116.01	120.80
2	G	448	PHE	CB-CG-CD1	-6.84	116.01	120.80
6	Q	673	PHE	CB-CG-CD1	6.84	125.59	120.80
6	Q	140	HIS	CA-CB-CG	-6.84	101.97	113.60
6	R	680	PHE	CB-CG-CD2	-6.84	116.01	120.80
6	R	93	TYR	CB-CG-CD1	-6.84	116.90	121.00
6	R	712	THR	N-CA-C	-6.83	92.55	111.00
4	O	412	TYR	N-CA-CB	6.83	122.90	110.60
6	R	140	HIS	CA-CB-CG	-6.83	101.99	113.60
2	A	236	TYR	CB-CG-CD1	-6.82	116.91	121.00
2	G	340	PHE	CB-CG-CD1	6.82	125.57	120.80
6	Q	432	TYR	CB-CG-CD2	-6.81	116.92	121.00
4	M	412	TYR	N-CA-CB	6.81	122.85	110.60
3	V	236	TYR	CB-CG-CD2	-6.81	116.92	121.00
6	Q	93	TYR	CB-CG-CD1	-6.81	116.92	121.00
2	H	236	TYR	CB-CG-CD2	-6.80	116.92	121.00
2	E	529	PHE	CB-CG-CD1	-6.80	116.04	120.80
2	N	236	TYR	CB-CG-CD2	-6.80	116.92	121.00
3	D	236	TYR	CB-CG-CD2	-6.79	116.92	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	412	TYR	CB-CG-CD1	6.79	125.07	121.00
2	B	236	TYR	CB-CG-CD2	-6.78	116.93	121.00
2	P	423	PHE	CB-CG-CD1	6.78	125.55	120.80
2	B	378	PHE	CB-CG-CD1	6.78	125.54	120.80
2	G	229	TYR	CB-CG-CD2	-6.78	116.93	121.00
3	L	229	TYR	CB-CG-CD2	-6.78	116.94	121.00
2	B	368	ARG	CG-CD-NE	6.77	126.01	111.80
2	B	340	PHE	CB-CG-CD1	6.76	125.53	120.80
6	R	800	GLU	CA-CB-CG	-6.76	98.52	113.40
2	N	428	GLU	OE1-CD-OE2	-6.76	115.19	123.30
2	B	387	THR	CA-CB-CG2	-6.76	102.94	112.40
2	G	236	TYR	CB-CG-CD2	-6.75	116.95	121.00
2	G	387	THR	CA-CB-CG2	-6.75	102.95	112.40
6	Q	800	GLU	CA-CB-CG	-6.75	98.54	113.40
2	H	378	PHE	CB-CG-CD1	6.75	125.53	120.80
2	E	229	TYR	CB-CG-CD2	-6.75	116.95	121.00
2	F	236	TYR	CB-CG-CD2	-6.75	116.95	121.00
2	H	368	ARG	CG-CD-NE	6.75	125.97	111.80
6	R	149	TYR	CA-CB-CG	-6.75	100.58	113.40
6	Q	672	GLU	N-CA-CB	6.74	122.73	110.60
2	H	387	THR	CA-CB-CG2	-6.74	102.97	112.40
2	A	236	TYR	CB-CG-CD2	-6.73	116.96	121.00
2	G	368	ARG	CG-CD-NE	6.73	125.94	111.80
2	B	229	TYR	CB-CG-CD2	-6.73	116.96	121.00
2	F	229	TYR	CB-CG-CD2	-6.73	116.96	121.00
6	R	432	TYR	CB-CG-CD2	-6.72	116.97	121.00
6	R	672	GLU	N-CA-CB	6.72	122.70	110.60
6	Q	149	TYR	CA-CB-CG	-6.72	100.64	113.40
2	P	428	GLU	OE1-CD-OE2	-6.71	115.24	123.30
2	H	340	PHE	CB-CG-CD1	6.71	125.49	120.80
3	L	236	TYR	CB-CG-CD2	-6.71	116.98	121.00
2	E	236	TYR	CB-CG-CD2	-6.69	116.99	121.00
6	R	820	TYR	CA-CB-CG	-6.69	100.69	113.40
3	D	229	TYR	CB-CG-CD2	-6.69	116.99	121.00
6	Q	820	TYR	CA-CB-CG	-6.68	100.71	113.40
2	N	423	PHE	CB-CG-CD1	6.68	125.47	120.80
2	H	229	TYR	CB-CG-CD2	-6.67	117.00	121.00
6	Q	158	TYR	CB-CG-CD2	-6.67	117.00	121.00
4	O	412	TYR	CB-CG-CD1	6.65	124.99	121.00
2	N	386	SER	O-C-N	-6.65	112.06	122.70
2	A	229	TYR	CB-CG-CD2	-6.65	117.01	121.00
6	Q	564	TRP	CB-CG-CD1	-6.65	118.36	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	229	TYR	CB-CG-CD2	-6.64	117.01	121.00
2	P	211	THR	N-CA-C	-6.64	93.08	111.00
3	V	211	THR	N-CA-C	-6.64	93.08	111.00
2	E	377	ASP	CB-CG-OD2	-6.63	112.33	118.30
6	R	32	LEU	CB-CA-C	-6.63	97.59	110.20
2	N	211	THR	N-CA-C	-6.63	93.09	111.00
3	L	211	THR	N-CA-C	-6.63	93.11	111.00
6	Q	32	LEU	CB-CA-C	-6.63	97.61	110.20
2	E	211	THR	N-CA-C	-6.62	93.12	111.00
2	B	211	THR	N-CA-C	-6.62	93.13	111.00
3	K	211	THR	N-CA-C	-6.62	93.13	111.00
2	A	377	ASP	CB-CG-OD2	-6.61	112.35	118.30
3	D	211	THR	N-CA-C	-6.61	93.14	111.00
6	R	564	TRP	CB-CG-CD1	-6.61	118.40	127.00
2	G	211	THR	N-CA-C	-6.61	93.15	111.00
2	F	211	THR	N-CA-C	-6.61	93.16	111.00
2	H	211	THR	N-CA-C	-6.60	93.17	111.00
2	G	378	PHE	CB-CG-CD1	6.60	125.42	120.80
3	V	229	TYR	CB-CG-CD2	-6.59	117.04	121.00
2	P	386	SER	O-C-N	-6.59	112.15	122.70
2	F	218	TYR	CB-CG-CD2	-6.58	117.05	121.00
2	F	377	ASP	CB-CG-OD2	-6.58	112.37	118.30
3	K	236	TYR	CB-CG-CD2	-6.58	117.05	121.00
3	V	197	VAL	CG1-CB-CG2	-6.58	100.37	110.90
2	A	211	THR	N-CA-C	-6.57	93.25	111.00
2	B	197	VAL	CG1-CB-CG2	-6.56	100.40	110.90
2	B	361	MET	CB-CA-C	-6.56	97.28	110.40
3	D	197	VAL	CG1-CB-CG2	-6.56	100.40	110.90
2	E	197	VAL	CG1-CB-CG2	-6.56	100.40	110.90
2	N	378	PHE	CB-CG-CD1	6.56	125.39	120.80
4	O	346	TYR	CB-CG-CD2	6.56	124.94	121.00
2	P	197	VAL	CG1-CB-CG2	-6.56	100.41	110.90
2	A	197	VAL	CG1-CB-CG2	-6.55	100.41	110.90
2	B	416	ALA	CB-CA-C	-6.55	100.27	110.10
2	F	197	VAL	CG1-CB-CG2	-6.55	100.42	110.90
3	L	197	VAL	CG1-CB-CG2	-6.55	100.42	110.90
6	R	158	TYR	CB-CG-CD2	-6.55	117.07	121.00
6	R	534	GLU	N-CA-CB	6.54	122.37	110.60
3	K	197	VAL	CG1-CB-CG2	-6.54	100.44	110.90
4	M	346	TYR	CB-CG-CD2	6.54	124.92	121.00
2	H	416	ALA	CB-CA-C	-6.53	100.30	110.10
2	G	361	MET	CB-CA-C	-6.53	97.34	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	197	VAL	CG1-CB-CG2	-6.53	100.46	110.90
6	Q	534	GLU	N-CA-CB	6.53	122.35	110.60
5	T	69	ALA	N-CA-CB	6.53	119.24	110.10
2	H	361	MET	CB-CA-C	-6.52	97.36	110.40
2	H	197	VAL	CG1-CB-CG2	-6.52	100.47	110.90
2	N	497	ARG	NE-CZ-NH2	6.51	123.56	120.30
2	G	197	VAL	CG1-CB-CG2	-6.51	100.48	110.90
5	S	69	ALA	N-CA-CB	6.51	119.22	110.10
2	P	497	ARG	NE-CZ-NH2	6.51	123.56	120.30
2	G	218	TYR	CB-CG-CD2	-6.51	117.09	121.00
6	R	247	ARG	NE-CZ-NH2	-6.50	117.05	120.30
2	P	378	PHE	CB-CG-CD1	6.48	125.33	120.80
2	H	218	TYR	CB-CG-CD2	-6.47	117.12	121.00
2	E	218	TYR	CB-CG-CD2	-6.47	117.12	121.00
2	N	346	TYR	CB-CG-CD1	6.46	124.88	121.00
2	G	416	ALA	CB-CA-C	-6.46	100.41	110.10
5	T	102	LEU	N-CA-CB	-6.45	97.50	110.40
2	N	508	ARG	NE-CZ-NH1	-6.44	117.08	120.30
3	K	218	TYR	CB-CG-CD2	-6.43	117.14	121.00
2	P	508	ARG	NE-CZ-NH1	-6.43	117.08	120.30
2	A	218	TYR	CB-CG-CD2	-6.42	117.15	121.00
2	P	211	THR	CA-CB-CG2	-6.42	103.41	112.40
2	F	211	THR	CA-CB-CG2	-6.42	103.41	112.40
5	S	102	LEU	N-CA-CB	-6.41	97.57	110.40
2	N	218	TYR	CB-CG-CD2	-6.41	117.15	121.00
6	R	716	GLY	CA-C-N	-6.41	103.10	117.20
2	A	497	ARG	NE-CZ-NH2	6.40	123.50	120.30
3	D	211	THR	CA-CB-CG2	-6.40	103.44	112.40
3	V	211	THR	CA-CB-CG2	-6.39	103.45	112.40
4	O	378	PHE	CB-CG-CD1	6.39	125.27	120.80
2	E	211	THR	CA-CB-CG2	-6.39	103.46	112.40
3	K	211	THR	CA-CB-CG2	-6.38	103.46	112.40
2	F	343	ARG	NE-CZ-NH1	-6.38	117.11	120.30
2	N	211	THR	CA-CB-CG2	-6.38	103.47	112.40
2	B	426	ILE	CB-CA-C	6.38	124.35	111.60
2	B	211	THR	CA-CB-CG2	-6.37	103.48	112.40
3	D	218	TYR	CB-CG-CD2	-6.37	117.18	121.00
2	B	218	TYR	CB-CG-CD2	-6.37	117.18	121.00
2	H	426	ILE	CB-CA-C	6.36	124.32	111.60
4	M	444	ARG	NE-CZ-NH2	-6.36	117.12	120.30
3	L	211	THR	CA-CB-CG2	-6.36	103.50	112.40
3	L	218	TYR	CB-CG-CD2	-6.36	117.19	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	T	51	LEU	CB-CA-C	-6.36	98.12	110.20
5	S	132	PHE	N-CA-C	-6.35	93.85	111.00
2	E	343	ARG	NE-CZ-NH1	-6.34	117.13	120.30
4	M	378	PHE	CB-CG-CD1	6.34	125.24	120.80
2	G	426	ILE	CB-CA-C	6.34	124.27	111.60
2	E	419	ASP	CB-CG-OD1	6.33	124.00	118.30
5	S	51	LEU	CB-CA-C	-6.33	98.17	110.20
6	Q	716	GLY	CA-C-N	-6.33	103.28	117.20
2	P	218	TYR	CB-CG-CD2	-6.33	117.20	121.00
2	G	211	THR	CA-CB-CG2	-6.32	103.55	112.40
6	Q	170	ASN	N-CA-CB	6.32	121.98	110.60
2	A	211	THR	CA-CB-CG2	-6.32	103.55	112.40
2	A	478	ARG	NE-CZ-NH2	-6.32	117.14	120.30
2	A	343	ARG	NE-CZ-NH1	-6.32	117.14	120.30
2	F	207	TYR	CB-CG-CD2	-6.31	117.21	121.00
2	H	211	THR	CA-CB-CG2	-6.31	103.56	112.40
5	T	132	PHE	N-CA-C	-6.31	93.97	111.00
2	E	478	ARG	NE-CZ-NH2	-6.31	117.15	120.30
2	P	346	TYR	CB-CG-CD1	6.31	124.78	121.00
2	F	419	ASP	CB-CG-OD1	6.30	123.97	118.30
2	G	493	VAL	CA-CB-CG2	-6.30	101.45	110.90
3	V	218	TYR	CB-CG-CD2	-6.30	117.22	121.00
6	Q	438	ALA	N-CA-CB	6.30	118.92	110.10
6	R	438	ALA	N-CA-CB	6.30	118.92	110.10
2	B	493	VAL	CA-CB-CG2	-6.29	101.46	110.90
4	O	404	LEU	CB-CG-CD1	6.29	121.69	111.00
2	H	493	VAL	CA-CB-CG2	-6.29	101.46	110.90
6	R	393	PHE	CB-CG-CD2	-6.29	116.40	120.80
4	O	444	ARG	NE-CZ-NH2	-6.28	117.16	120.30
6	Q	434	ASP	CB-CA-C	6.28	122.96	110.40
2	E	497	ARG	NE-CZ-NH2	6.28	123.44	120.30
4	O	361	MET	CB-CA-C	-6.26	97.87	110.40
4	M	404	LEU	CB-CG-CD1	6.26	121.65	111.00
6	R	170	ASN	N-CA-CB	6.26	121.87	110.60
2	A	414	ARG	NE-CZ-NH1	-6.26	117.17	120.30
6	Q	393	PHE	CB-CG-CD2	-6.26	116.42	120.80
2	A	419	ASP	CB-CG-OD1	6.26	123.93	118.30
2	E	414	ARG	NE-CZ-NH1	-6.26	117.17	120.30
6	Q	247	ARG	NE-CZ-NH2	-6.26	117.17	120.30
6	R	434	ASP	CB-CA-C	6.25	122.90	110.40
4	M	361	MET	CB-CA-C	-6.24	97.92	110.40
2	H	415	GLN	CA-CB-CG	-6.23	99.69	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	415	GLN	CA-CB-CG	-6.23	99.70	113.40
2	G	415	GLN	CA-CB-CG	-6.22	99.71	113.40
2	E	473	LYS	N-CA-C	-6.22	94.21	111.00
2	B	207	TYR	CB-CG-CD2	-6.21	117.27	121.00
2	F	473	LYS	N-CA-C	-6.21	94.23	111.00
3	D	207	TYR	CB-CG-CD2	-6.20	117.28	121.00
4	O	370	ALA	O-C-N	-6.20	112.78	122.70
4	M	370	ALA	O-C-N	-6.19	112.80	122.70
6	R	404	GLN	N-CA-C	-6.19	94.29	111.00
5	S	170	TYR	N-CA-CB	6.18	121.73	110.60
6	Q	207	GLU	CB-CA-C	6.18	122.77	110.40
2	A	207	TYR	CB-CG-CD2	-6.18	117.29	121.00
4	M	550	GLN	N-CA-CB	6.18	121.72	110.60
2	F	478	ARG	NE-CZ-NH2	-6.18	117.21	120.30
3	V	207	TYR	CB-CG-CD2	-6.17	117.30	121.00
2	A	473	LYS	N-CA-C	-6.17	94.35	111.00
5	T	170	TYR	N-CA-CB	6.17	121.70	110.60
3	K	207	TYR	CB-CG-CD2	-6.16	117.30	121.00
6	Q	404	GLN	N-CA-C	-6.16	94.36	111.00
2	F	414	ARG	NE-CZ-NH1	-6.16	117.22	120.30
2	N	207	TYR	CB-CG-CD2	-6.15	117.31	121.00
3	L	207	TYR	CB-CG-CD2	-6.15	117.31	121.00
2	E	207	TYR	CB-CG-CD2	-6.15	117.31	121.00
4	O	550	GLN	N-CA-CB	6.15	121.66	110.60
2	F	370	ALA	N-CA-C	6.14	127.58	111.00
2	A	370	ALA	N-CA-C	6.14	127.57	111.00
2	F	497	ARG	NE-CZ-NH2	6.13	123.37	120.30
2	H	438	LYS	CB-CA-C	6.13	122.67	110.40
6	R	207	GLU	CB-CA-C	6.13	122.66	110.40
2	N	412	TYR	CB-CG-CD1	6.12	124.67	121.00
2	F	378	PHE	CB-CG-CD2	-6.12	116.51	120.80
2	E	370	ALA	N-CA-C	6.12	127.53	111.00
2	P	207	TYR	CB-CG-CD2	-6.11	117.33	121.00
2	P	503	MET	CG-SD-CE	-6.11	90.42	100.20
2	H	521	ASP	CB-CA-C	-6.11	98.18	110.40
2	G	438	LYS	CB-CA-C	6.11	122.61	110.40
2	H	207	TYR	CB-CG-CD2	-6.10	117.34	121.00
2	G	521	ASP	CB-CA-C	-6.09	98.21	110.40
2	B	438	LYS	CB-CA-C	6.09	122.59	110.40
2	N	503	MET	CG-SD-CE	-6.09	90.45	100.20
5	S	170	TYR	CB-CG-CD2	-6.09	117.35	121.00
2	H	513	ARG	N-CA-CB	-6.08	99.65	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	209	VAL	N-CA-C	-6.08	94.59	111.00
2	E	209	VAL	N-CA-C	-6.08	94.59	111.00
2	P	368	ARG	NE-CZ-NH2	6.08	123.34	120.30
3	L	209	VAL	N-CA-C	-6.08	94.59	111.00
2	A	209	VAL	N-CA-C	-6.07	94.60	111.00
2	B	521	ASP	CB-CA-C	-6.07	98.25	110.40
2	G	209	VAL	N-CA-C	-6.07	94.61	111.00
3	V	209	VAL	N-CA-C	-6.07	94.62	111.00
2	H	209	VAL	N-CA-C	-6.06	94.64	111.00
2	B	209	VAL	N-CA-C	-6.06	94.64	111.00
3	K	209	VAL	N-CA-C	-6.06	94.65	111.00
2	B	513	ARG	N-CA-CB	-6.05	99.70	110.60
3	D	209	VAL	N-CA-C	-6.05	94.66	111.00
2	P	209	VAL	N-CA-C	-6.05	94.66	111.00
2	F	209	VAL	N-CA-C	-6.05	94.66	111.00
2	E	378	PHE	CB-CG-CD2	-6.04	116.57	120.80
5	T	170	TYR	CB-CG-CD2	-6.04	117.37	121.00
2	G	406	LEU	N-CA-CB	-6.04	98.32	110.40
5	T	80	HIS	CA-CB-CG	-6.04	103.34	113.60
2	G	207	TYR	CB-CG-CD2	-6.03	117.38	121.00
5	S	91	PHE	CB-CG-CD2	-6.03	116.58	120.80
2	H	472	GLY	N-CA-C	-6.03	98.03	113.10
6	Q	194	HIS	CA-CB-CG	-6.03	103.35	113.60
2	G	513	ARG	N-CA-CB	-6.03	99.75	110.60
5	S	80	HIS	CA-CB-CG	-6.03	103.35	113.60
2	H	406	LEU	N-CA-CB	-6.03	98.35	110.40
2	B	472	GLY	N-CA-C	-6.03	98.04	113.10
2	G	472	GLY	N-CA-C	-6.02	98.05	113.10
2	A	378	PHE	CB-CG-CD2	-6.02	116.59	120.80
2	B	406	LEU	N-CA-CB	-6.02	98.37	110.40
6	Q	484	THR	CA-CB-CG2	-6.01	103.99	112.40
6	Q	296	MET	CG-SD-CE	-6.00	90.60	100.20
2	P	412	TYR	CB-CG-CD1	6.00	124.60	121.00
5	T	127	TYR	N-CA-C	-5.99	94.82	111.00
6	R	296	MET	CG-SD-CE	-5.99	90.62	100.20
1	C	125	ARG	NE-CZ-NH1	5.99	123.29	120.30
6	R	484	THR	CA-CB-CG2	-5.98	104.02	112.40
6	R	805	TYR	CB-CG-CD2	-5.98	117.41	121.00
2	A	505	ARG	NE-CZ-NH2	-5.98	117.31	120.30
2	F	508	ARG	CD-NE-CZ	-5.98	115.23	123.60
5	S	127	TYR	N-CA-C	-5.98	94.86	111.00
6	R	688	TYR	CA-CB-CG	5.98	124.75	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	O	339	TRP	CD2-CE2-CZ2	-5.97	115.14	122.30
4	M	470	ARG	NE-CZ-NH2	5.96	123.28	120.30
3	L	212	LYS	N-CA-CB	5.96	121.33	110.60
6	R	194	HIS	CA-CB-CG	-5.96	103.47	113.60
6	Q	805	TYR	CB-CG-CD2	-5.95	117.43	121.00
4	O	399	ASP	CB-CG-OD1	5.95	123.66	118.30
4	M	339	TRP	CD2-CE2-CZ2	-5.95	115.16	122.30
2	A	508	ARG	CD-NE-CZ	-5.95	115.28	123.60
4	M	376	ALA	CB-CA-C	-5.94	101.19	110.10
2	N	212	LYS	N-CA-CB	5.94	121.30	110.60
6	R	568	LEU	N-CA-CB	-5.94	98.52	110.40
4	O	376	ALA	CB-CA-C	-5.94	101.19	110.10
5	T	91	PHE	CB-CG-CD2	-5.94	116.64	120.80
6	Q	688	TYR	CA-CB-CG	5.93	124.67	113.40
6	Q	808	TYR	CA-CB-CG	-5.93	102.14	113.40
6	R	432	TYR	N-CA-CB	5.93	121.27	110.60
2	B	212	LYS	N-CA-CB	5.92	121.26	110.60
3	V	212	LYS	N-CA-CB	5.92	121.26	110.60
3	D	212	LYS	N-CA-CB	5.92	121.25	110.60
2	P	505	ARG	NE-CZ-NH1	-5.92	117.34	120.30
2	E	368	ARG	NE-CZ-NH1	-5.92	117.34	120.30
2	E	508	ARG	CD-NE-CZ	-5.92	115.32	123.60
2	G	212	LYS	N-CA-CB	5.92	121.25	110.60
4	M	399	ASP	CB-CG-OD1	5.92	123.62	118.30
2	F	212	LYS	N-CA-CB	5.92	121.25	110.60
2	A	212	LYS	N-CA-CB	5.91	121.24	110.60
2	P	212	LYS	N-CA-CB	5.91	121.24	110.60
3	K	212	LYS	N-CA-CB	5.91	121.24	110.60
2	E	212	LYS	N-CA-CB	5.91	121.23	110.60
2	E	402	SER	N-CA-CB	5.90	119.36	110.50
6	Q	568	LEU	N-CA-CB	-5.90	98.59	110.40
5	T	122	PHE	N-CA-C	-5.90	95.06	111.00
2	H	212	LYS	N-CA-CB	5.90	121.22	110.60
6	Q	432	TYR	N-CA-CB	5.90	121.21	110.60
2	A	206	VAL	N-CA-C	-5.89	95.10	111.00
2	N	466	ASP	CB-CG-OD2	-5.89	113.00	118.30
5	S	122	PHE	N-CA-C	-5.88	95.11	111.00
2	F	402	SER	N-CA-CB	5.88	119.32	110.50
6	R	146	PHE	CB-CG-CD1	5.88	124.92	120.80
2	A	402	SER	N-CA-CB	5.88	119.32	110.50
2	G	206	VAL	N-CA-C	-5.88	95.13	111.00
2	E	206	VAL	N-CA-C	-5.88	95.13	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	530	LEU	CB-CG-CD1	5.88	120.99	111.00
3	K	206	VAL	N-CA-C	-5.88	95.13	111.00
2	F	206	VAL	N-CA-C	-5.88	95.13	111.00
2	P	206	VAL	N-CA-C	-5.88	95.14	111.00
2	F	505	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	J	125	ARG	NE-CZ-NH1	5.88	123.24	120.30
6	R	515	ILE	C-N-CA	5.88	136.39	121.70
2	G	196	LYS	N-CA-C	-5.87	95.14	111.00
2	H	206	VAL	N-CA-C	-5.87	95.15	111.00
3	D	206	VAL	N-CA-C	-5.87	95.15	111.00
2	H	522	PHE	CB-CA-C	-5.87	98.66	110.40
6	Q	515	ILE	C-N-CA	5.87	136.37	121.70
6	Q	146	PHE	CB-CG-CD1	5.87	124.91	120.80
5	T	170	TYR	CA-CB-CG	-5.87	102.26	113.40
6	R	808	TYR	CA-CB-CG	-5.87	102.26	113.40
5	S	170	TYR	CA-CB-CG	-5.86	102.26	113.40
2	A	530	LEU	CB-CG-CD1	5.86	120.96	111.00
2	P	466	ASP	CB-CG-OD2	-5.86	113.03	118.30
2	B	522	PHE	CB-CA-C	-5.86	98.68	110.40
3	V	206	VAL	N-CA-C	-5.86	95.19	111.00
3	L	196	LYS	N-CA-C	-5.86	95.19	111.00
6	Q	393	PHE	CB-CG-CD1	5.86	124.90	120.80
3	K	196	LYS	N-CA-C	-5.85	95.19	111.00
2	N	206	VAL	N-CA-C	-5.85	95.19	111.00
2	G	522	PHE	CB-CA-C	-5.85	98.69	110.40
2	P	407	ALA	CB-CA-C	-5.85	101.33	110.10
2	N	368	ARG	NE-CZ-NH2	5.85	123.22	120.30
2	H	382	LEU	CA-CB-CG	-5.85	101.85	115.30
2	B	206	VAL	N-CA-C	-5.85	95.21	111.00
2	E	196	LYS	N-CA-C	-5.85	95.21	111.00
3	L	206	VAL	N-CA-C	-5.85	95.21	111.00
2	G	382	LEU	CA-CB-CG	-5.85	101.85	115.30
2	B	196	LYS	N-CA-C	-5.84	95.22	111.00
2	A	196	LYS	N-CA-C	-5.84	95.22	111.00
3	D	196	LYS	N-CA-C	-5.84	95.22	111.00
2	H	196	LYS	N-CA-C	-5.84	95.23	111.00
2	F	196	LYS	N-CA-C	-5.83	95.25	111.00
2	B	382	LEU	CA-CB-CG	-5.83	101.89	115.30
2	P	196	LYS	N-CA-C	-5.83	95.26	111.00
2	F	530	LEU	CB-CG-CD1	5.83	120.91	111.00
3	V	196	LYS	N-CA-C	-5.82	95.27	111.00
6	R	393	PHE	CB-CG-CD1	5.82	124.88	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	196	LYS	N-CA-C	-5.82	95.28	111.00
2	N	407	ALA	CB-CA-C	-5.82	101.38	110.10
2	F	368	ARG	NE-CZ-NH1	-5.81	117.39	120.30
6	R	415	CYS	CA-CB-SG	-5.81	103.54	114.00
6	Q	156	ARG	NE-CZ-NH2	-5.81	117.39	120.30
5	T	183	ASN	CA-CB-CG	-5.81	100.62	113.40
5	S	183	ASN	CA-CB-CG	-5.80	100.63	113.40
6	Q	415	CYS	CA-CB-SG	-5.80	103.55	114.00
4	O	470	ARG	NE-CZ-NH2	5.80	123.20	120.30
2	G	371	MET	CG-SD-CE	-5.79	90.93	100.20
2	B	371	MET	CG-SD-CE	-5.79	90.94	100.20
6	R	673	PHE	CB-CG-CD2	-5.79	116.75	120.80
2	H	371	MET	CG-SD-CE	-5.79	90.94	100.20
2	E	514	PHE	CB-CG-CD2	-5.78	116.76	120.80
2	N	419	ASP	CB-CG-OD1	-5.77	113.11	118.30
6	Q	210	GLU	CB-CA-C	-5.77	98.86	110.40
2	A	514	PHE	CB-CG-CD2	-5.76	116.77	120.80
5	T	85	ILE	N-CA-C	-5.76	95.44	111.00
5	T	23	LYS	CB-CA-C	-5.76	98.88	110.40
2	E	505	ARG	NE-CZ-NH2	-5.76	117.42	120.30
6	R	210	GLU	CB-CA-C	-5.76	98.89	110.40
6	Q	439	TYR	CA-CB-CG	5.75	124.33	113.40
2	H	465	GLN	CB-CG-CD	-5.75	96.65	111.60
2	B	465	GLN	CB-CG-CD	-5.75	96.65	111.60
2	N	264	PHE	CB-CG-CD2	-5.74	116.78	120.80
5	S	23	LYS	CB-CA-C	-5.74	98.92	110.40
6	R	439	TYR	CA-CB-CG	5.74	124.31	113.40
4	O	341	HIS	N-CA-CB	5.74	120.92	110.60
2	A	370	ALA	C-N-CA	5.73	136.04	121.70
5	S	85	ILE	N-CA-C	-5.73	95.52	111.00
2	F	488	ASP	CB-CG-OD1	5.73	123.46	118.30
2	E	411	VAL	CA-CB-CG2	-5.72	102.31	110.90
2	P	414	ARG	NE-CZ-NH2	5.72	123.16	120.30
2	A	411	VAL	CA-CB-CG2	-5.72	102.32	110.90
2	A	488	ASP	CB-CG-OD1	5.72	123.45	118.30
2	E	349	ALA	N-CA-CB	5.71	118.10	110.10
4	M	341	HIS	N-CA-CB	5.71	120.89	110.60
2	G	465	GLN	CB-CG-CD	-5.71	96.75	111.60
2	P	441	PHE	CB-CG-CD2	5.71	124.80	120.80
2	H	232	PHE	CB-CA-C	-5.71	98.97	110.40
2	F	370	ALA	C-N-CA	5.71	135.98	121.70
6	Q	598	ILE	N-CA-C	5.71	126.41	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	371	MET	CG-SD-CE	-5.71	91.07	100.20
2	F	349	ALA	N-CA-CB	5.70	118.08	110.10
2	E	370	ALA	C-N-CA	5.70	135.95	121.70
6	Q	485	TYR	CA-CB-CG	5.70	124.22	113.40
5	T	135	PRO	C-N-CA	5.69	134.25	122.30
2	N	441	PHE	CB-CG-CD2	5.69	124.78	120.80
2	F	411	VAL	CA-CB-CG2	-5.69	102.36	110.90
2	B	232	PHE	CB-CA-C	-5.69	99.02	110.40
2	G	522	PHE	CB-CG-CD2	-5.69	116.82	120.80
6	Q	573	HIS	N-CA-C	5.69	126.36	111.00
2	H	264	PHE	CB-CG-CD2	-5.69	116.82	120.80
6	R	790	GLU	C-N-CA	5.69	135.92	121.70
6	R	598	ILE	N-CA-C	5.68	126.34	111.00
6	Q	790	GLU	C-N-CA	5.68	135.90	121.70
2	A	349	ALA	N-CA-CB	5.68	118.05	110.10
3	D	232	PHE	CB-CA-C	-5.68	99.04	110.40
2	N	232	PHE	CB-CA-C	-5.68	99.04	110.40
6	R	156	ARG	NE-CZ-NH2	-5.68	117.46	120.30
4	O	371	MET	CG-SD-CE	-5.67	91.12	100.20
2	F	232	PHE	CB-CA-C	-5.67	99.05	110.40
2	P	264	PHE	CB-CG-CD2	-5.67	116.83	120.80
2	F	514	PHE	CB-CG-CD2	-5.66	116.84	120.80
4	O	423	PHE	CB-CG-CD2	-5.66	116.84	120.80
2	A	232	PHE	CB-CA-C	-5.66	99.08	110.40
5	S	135	PRO	C-N-CA	5.66	134.18	122.30
2	B	522	PHE	CB-CG-CD2	-5.66	116.84	120.80
6	R	485	TYR	CA-CB-CG	5.66	124.14	113.40
2	G	232	PHE	CB-CA-C	-5.65	99.10	110.40
2	E	232	PHE	CB-CA-C	-5.65	99.09	110.40
6	Q	768	TYR	CB-CG-CD1	5.65	124.39	121.00
3	V	232	PHE	CB-CA-C	-5.65	99.10	110.40
2	G	347	LEU	CB-CA-C	-5.65	99.47	110.20
2	E	488	ASP	CB-CG-OD1	5.65	123.38	118.30
6	R	573	HIS	N-CA-C	5.65	126.25	111.00
2	A	368	ARG	NE-CZ-NH1	-5.64	117.48	120.30
2	A	377	ASP	CB-CG-OD1	5.64	123.38	118.30
6	R	752	TRP	CB-CG-CD2	-5.64	119.27	126.60
2	G	430	TYR	CA-CB-CG	-5.64	102.69	113.40
3	K	232	PHE	CB-CA-C	-5.64	99.13	110.40
2	N	505	ARG	NE-CZ-NH1	-5.64	117.48	120.30
2	B	430	TYR	CA-CB-CG	-5.63	102.69	113.40
2	H	347	LEU	CB-CA-C	-5.63	99.50	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	529	PHE	CB-CG-CD1	-5.63	116.86	120.80
2	P	419	ASP	CB-CG-OD1	-5.63	113.23	118.30
2	B	389	GLU	CB-CG-CD	-5.63	99.00	114.20
3	K	264	PHE	CB-CG-CD2	-5.63	116.86	120.80
3	L	232	PHE	CB-CA-C	-5.63	99.14	110.40
6	R	717	ARG	NE-CZ-NH1	5.62	123.11	120.30
2	B	347	LEU	CB-CA-C	-5.62	99.52	110.20
2	P	232	PHE	CB-CA-C	-5.62	99.15	110.40
2	G	389	GLU	CB-CG-CD	-5.62	99.03	114.20
2	H	430	TYR	CA-CB-CG	-5.62	102.73	113.40
6	Q	715	PHE	CB-CG-CD1	5.62	124.73	120.80
2	E	496	ALA	N-CA-CB	5.62	117.96	110.10
6	R	768	TYR	CB-CG-CD1	5.62	124.37	121.00
6	Q	672	GLU	CB-CA-C	-5.61	99.18	110.40
2	H	389	GLU	CB-CG-CD	-5.61	99.06	114.20
6	Q	673	PHE	CB-CG-CD2	-5.61	116.88	120.80
1	C	6	SER	N-CA-CB	5.61	118.91	110.50
4	M	377	ASP	N-CA-CB	5.60	120.68	110.60
6	R	672	GLU	CB-CA-C	-5.60	99.21	110.40
2	E	377	ASP	CB-CG-OD1	5.60	123.34	118.30
2	N	500	PHE	CB-CG-CD2	-5.59	116.88	120.80
1	J	125	ARG	NE-CZ-NH2	-5.59	117.51	120.30
6	R	623	ASP	N-CA-CB	5.59	120.66	110.60
2	N	414	ARG	NE-CZ-NH2	5.59	123.09	120.30
2	F	264	PHE	CB-CG-CD2	-5.59	116.89	120.80
2	F	496	ALA	N-CA-CB	5.59	117.92	110.10
2	F	377	ASP	CB-CG-OD1	5.58	123.33	118.30
6	Q	717	ARG	NE-CZ-NH1	5.58	123.09	120.30
4	O	377	ASP	N-CA-CB	5.58	120.64	110.60
6	Q	623	ASP	N-CA-CB	5.58	120.64	110.60
2	H	522	PHE	CB-CG-CD2	-5.58	116.90	120.80
3	D	264	PHE	CB-CG-CD2	-5.57	116.90	120.80
1	J	6	SER	N-CA-CB	5.57	118.85	110.50
2	A	496	ALA	N-CA-CB	5.57	117.89	110.10
6	Q	586	MET	CG-SD-CE	-5.57	91.29	100.20
2	G	264	PHE	CB-CG-CD2	-5.56	116.91	120.80
2	H	529	PHE	CB-CG-CD1	-5.56	116.91	120.80
2	P	500	PHE	CB-CG-CD2	-5.55	116.91	120.80
2	H	360	ALA	CB-CA-C	5.54	118.41	110.10
2	A	264	PHE	CB-CG-CD2	-5.54	116.92	120.80
6	Q	752	TRP	CB-CG-CD2	-5.54	119.41	126.60
2	B	264	PHE	CB-CG-CD2	-5.53	116.93	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	489	ALA	N-CA-CB	5.53	117.84	110.10
4	M	423	PHE	CB-CG-CD2	-5.53	116.93	120.80
3	L	264	PHE	CB-CG-CD2	-5.52	116.93	120.80
2	B	529	PHE	CB-CG-CD1	-5.52	116.94	120.80
3	D	197	VAL	CB-CA-C	5.52	121.88	111.40
6	R	586	MET	CG-SD-CE	-5.52	91.37	100.20
6	Q	722	THR	CA-CB-CG2	-5.51	104.68	112.40
6	R	715	PHE	CB-CG-CD1	5.51	124.66	120.80
2	N	197	VAL	CB-CA-C	5.51	121.88	111.40
6	R	526	GLU	CB-CA-C	-5.51	99.37	110.40
3	L	197	VAL	CB-CA-C	5.51	121.87	111.40
2	G	411	VAL	CA-CB-CG2	-5.51	102.64	110.90
2	G	197	VAL	CB-CA-C	5.51	121.86	111.40
2	B	411	VAL	CA-CB-CG2	-5.50	102.64	110.90
2	E	197	VAL	CB-CA-C	5.50	121.85	111.40
2	B	197	VAL	CB-CA-C	5.50	121.84	111.40
3	K	197	VAL	CB-CA-C	5.50	121.84	111.40
2	N	489	ALA	N-CA-CB	5.49	117.79	110.10
2	H	411	VAL	CA-CB-CG2	-5.49	102.66	110.90
6	Q	645	TYR	CA-CB-CG	-5.49	102.96	113.40
6	Q	422	SER	N-CA-CB	5.49	118.73	110.50
2	E	264	PHE	CB-CG-CD2	-5.48	116.96	120.80
2	G	360	ALA	CB-CA-C	5.48	118.33	110.10
2	P	197	VAL	CB-CA-C	5.48	121.82	111.40
4	M	382	LEU	CB-CG-CD2	5.48	120.32	111.00
2	H	197	VAL	CB-CA-C	5.48	121.82	111.40
2	F	197	VAL	CB-CA-C	5.48	121.82	111.40
6	Q	686	THR	CA-CB-CG2	-5.48	104.72	112.40
6	R	686	THR	CA-CB-CG2	-5.48	104.72	112.40
2	G	245	GLY	N-CA-C	-5.48	99.40	113.10
2	P	372	ALA	N-CA-CB	5.48	117.77	110.10
4	O	382	LEU	CB-CG-CD2	5.48	120.31	111.00
3	V	245	GLY	N-CA-C	-5.48	99.40	113.10
2	B	245	GLY	N-CA-C	-5.48	99.41	113.10
2	A	197	VAL	CB-CA-C	5.48	121.81	111.40
6	R	764	ASP	N-CA-CB	5.48	120.46	110.60
2	N	337	ASP	CB-CG-OD1	-5.47	113.38	118.30
3	V	264	PHE	CB-CG-CD2	-5.47	116.97	120.80
2	A	245	GLY	N-CA-C	-5.47	99.42	113.10
6	R	645	TYR	CA-CB-CG	-5.47	103.01	113.40
2	P	337	ASP	CB-CG-OD1	-5.47	113.38	118.30
2	F	245	GLY	N-CA-C	-5.47	99.43	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Q	517	THR	N-CA-C	-5.47	96.24	111.00
6	Q	526	GLU	CB-CA-C	-5.47	99.47	110.40
3	L	245	GLY	N-CA-C	-5.46	99.44	113.10
6	R	484	THR	N-CA-C	-5.46	96.26	111.00
2	E	356	ALA	CB-CA-C	-5.46	101.91	110.10
2	G	345	VAL	CA-CB-CG2	-5.46	102.71	110.90
2	P	245	GLY	N-CA-C	-5.46	99.46	113.10
2	N	245	GLY	N-CA-C	-5.46	99.46	113.10
2	H	345	VAL	CA-CB-CG2	-5.45	102.72	110.90
2	F	356	ALA	CB-CA-C	-5.45	101.92	110.10
3	D	245	GLY	N-CA-C	-5.45	99.47	113.10
2	A	356	ALA	CB-CA-C	-5.45	101.92	110.10
6	R	448	ALA	N-CA-CB	5.45	117.73	110.10
4	M	522	PHE	CD1-CE1-CZ	-5.45	113.56	120.10
6	R	227	ASP	N-CA-C	-5.45	96.29	111.00
6	R	722	THR	CA-CB-CG2	-5.45	104.77	112.40
3	K	245	GLY	N-CA-C	-5.44	99.49	113.10
2	H	245	GLY	N-CA-C	-5.44	99.49	113.10
6	Q	448	ALA	N-CA-CB	5.44	117.72	110.10
6	Q	484	THR	N-CA-C	-5.44	96.31	111.00
2	E	245	GLY	N-CA-C	-5.44	99.50	113.10
1	C	125	ARG	NE-CZ-NH2	-5.44	117.58	120.30
6	Q	764	ASP	N-CA-CB	5.44	120.39	110.60
2	B	345	VAL	CA-CB-CG2	-5.43	102.75	110.90
5	S	12	HIS	N-CA-C	-5.43	96.33	111.00
6	Q	116	TYR	CB-CG-CD2	-5.43	117.74	121.00
3	V	197	VAL	CB-CA-C	5.43	121.72	111.40
6	R	517	THR	N-CA-C	-5.43	96.33	111.00
2	N	503	MET	CA-CB-CG	-5.43	104.07	113.30
2	B	360	ALA	CB-CA-C	5.43	118.24	110.10
5	T	12	HIS	N-CA-C	-5.43	96.34	111.00
6	R	720	TYR	CB-CG-CD1	5.43	124.26	121.00
2	N	372	ALA	N-CA-CB	5.42	117.69	110.10
6	Q	720	TYR	CB-CG-CD1	5.42	124.25	121.00
2	H	501	GLU	CB-CA-C	-5.42	99.56	110.40
5	T	16	ARG	N-CA-CB	5.42	120.36	110.60
2	B	501	GLU	CB-CA-C	-5.42	99.56	110.40
3	D	295	LEU	CB-CA-C	-5.42	99.90	110.20
2	P	295	LEU	CB-CA-C	-5.42	99.90	110.20
6	Q	227	ASP	N-CA-C	-5.42	96.37	111.00
2	E	295	LEU	CB-CA-C	-5.42	99.91	110.20
3	V	295	LEU	CB-CA-C	-5.42	99.91	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	295	LEU	CB-CA-C	-5.41	99.92	110.20
5	S	16	ARG	N-CA-CB	5.41	120.34	110.60
6	R	116	TYR	CB-CG-CD2	-5.41	117.75	121.00
2	F	295	LEU	CB-CA-C	-5.41	99.92	110.20
3	L	295	LEU	CB-CA-C	-5.41	99.92	110.20
2	G	501	GLU	CB-CA-C	-5.41	99.58	110.40
6	R	422	SER	N-CA-CB	5.41	118.61	110.50
6	R	503	GLU	N-CA-CB	5.41	120.33	110.60
2	N	340	PHE	CB-CG-CD2	-5.40	117.02	120.80
2	N	295	LEU	CB-CA-C	-5.40	99.94	110.20
2	B	295	LEU	CB-CA-C	-5.39	99.95	110.20
2	P	503	MET	CA-CB-CG	-5.39	104.13	113.30
2	G	524	SER	N-CA-CB	-5.39	102.42	110.50
2	G	206	VAL	CG1-CB-CG2	5.38	119.50	110.90
3	K	295	LEU	CB-CA-C	-5.38	99.98	110.20
4	M	478	ARG	CB-CA-C	-5.38	99.64	110.40
4	O	522	PHE	CD1-CE1-CZ	-5.38	113.65	120.10
2	G	295	LEU	CB-CA-C	-5.38	99.99	110.20
2	B	524	SER	N-CA-CB	-5.37	102.44	110.50
4	O	478	ARG	CB-CA-C	-5.37	99.67	110.40
5	T	125	PHE	CB-CG-CD1	5.37	124.56	120.80
2	A	295	LEU	CB-CA-C	-5.36	100.01	110.20
3	K	206	VAL	CG1-CB-CG2	5.36	119.48	110.90
6	Q	101	ASN	CA-C-N	-5.36	105.41	117.20
2	P	206	VAL	CG1-CB-CG2	5.35	119.45	110.90
3	L	206	VAL	CG1-CB-CG2	5.34	119.45	110.90
2	N	206	VAL	CG1-CB-CG2	5.34	119.45	110.90
3	V	206	VAL	CG1-CB-CG2	5.34	119.45	110.90
1	C	258	ARG	NE-CZ-NH1	5.34	122.97	120.30
3	D	206	VAL	CG1-CB-CG2	5.34	119.44	110.90
5	T	187	GLU	N-CA-C	-5.34	96.58	111.00
6	Q	503	GLU	N-CA-CB	5.34	120.21	110.60
6	R	101	ASN	CA-C-N	-5.34	105.46	117.20
2	B	206	VAL	CG1-CB-CG2	5.33	119.44	110.90
2	F	206	VAL	CG1-CB-CG2	5.33	119.43	110.90
2	H	524	SER	N-CA-CB	-5.33	102.50	110.50
2	A	206	VAL	CG1-CB-CG2	5.33	119.42	110.90
5	S	182	GLU	N-CA-C	-5.33	96.62	111.00
4	O	516	ARG	NE-CZ-NH1	-5.32	117.64	120.30
4	O	518	LYS	N-CA-CB	5.32	120.17	110.60
6	R	669	ASP	N-CA-CB	5.31	120.17	110.60
2	E	206	VAL	CG1-CB-CG2	5.31	119.40	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	350	LEU	CB-CG-CD2	5.31	120.03	111.00
2	P	350	LEU	CB-CG-CD2	5.31	120.03	111.00
5	T	182	GLU	N-CA-C	-5.31	96.66	111.00
5	S	125	PHE	CB-CG-CD1	5.31	124.52	120.80
6	Q	572	ILE	N-CA-C	5.31	125.33	111.00
2	H	206	VAL	CG1-CB-CG2	5.30	119.38	110.90
5	S	187	GLU	N-CA-C	-5.30	96.68	111.00
6	R	169	GLY	N-CA-C	-5.30	99.85	113.10
6	R	227	ASP	CA-CB-CG	-5.30	101.73	113.40
4	M	544	TRP	CA-CB-CG	5.30	123.77	113.70
2	H	427	ILE	CB-CA-C	-5.29	101.01	111.60
2	B	427	ILE	CB-CA-C	-5.29	101.02	111.60
2	G	427	ILE	CB-CA-C	-5.29	101.02	111.60
6	Q	227	ASP	CA-CB-CG	-5.28	101.78	113.40
6	Q	669	ASP	N-CA-CB	5.28	120.11	110.60
6	Q	169	GLY	N-CA-C	-5.28	99.90	113.10
6	R	572	ILE	N-CA-C	5.28	125.25	111.00
4	O	544	TRP	CA-CB-CG	5.28	123.73	113.70
6	Q	187	LYS	CB-CA-C	-5.28	99.85	110.40
2	B	423	PHE	CA-CB-CG	-5.27	101.26	113.90
4	M	518	LYS	N-CA-CB	5.26	120.07	110.60
3	K	206	VAL	CA-CB-CG2	-5.26	103.01	110.90
3	D	206	VAL	CA-CB-CG2	-5.26	103.01	110.90
6	R	204	ARG	NE-CZ-NH1	5.25	122.93	120.30
2	P	210	ARG	N-CA-C	-5.25	96.83	111.00
2	G	423	PHE	CA-CB-CG	-5.25	101.31	113.90
3	K	210	ARG	N-CA-C	-5.25	96.83	111.00
2	G	210	ARG	N-CA-C	-5.24	96.84	111.00
6	R	187	LYS	CB-CA-C	-5.24	99.92	110.40
2	P	206	VAL	CA-CB-CG2	-5.24	103.04	110.90
2	H	423	PHE	CA-CB-CG	-5.24	101.32	113.90
3	V	206	VAL	CA-CB-CG2	-5.24	103.04	110.90
3	L	210	ARG	N-CA-C	-5.24	96.85	111.00
6	R	428	GLU	C-N-CA	5.24	134.80	121.70
2	B	514	PHE	CB-CG-CD1	5.24	124.47	120.80
3	D	210	ARG	N-CA-C	-5.24	96.86	111.00
2	F	419	ASP	CB-CG-OD2	-5.24	113.59	118.30
2	P	340	PHE	CB-CG-CD2	-5.23	117.14	120.80
2	H	206	VAL	CA-CB-CG2	-5.23	103.05	110.90
4	M	516	ARG	NE-CZ-NH1	-5.23	117.68	120.30
3	L	206	VAL	CA-CB-CG2	-5.23	103.05	110.90
2	B	210	ARG	N-CA-C	-5.23	96.88	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	210	ARG	N-CA-C	-5.23	96.89	111.00
6	R	128	MET	CG-SD-CE	-5.23	91.84	100.20
2	A	210	ARG	N-CA-C	-5.23	96.89	111.00
6	R	465	LEU	N-CA-CB	-5.22	99.95	110.40
2	E	210	ARG	N-CA-C	-5.22	96.90	111.00
2	E	419	ASP	CB-CG-OD2	-5.22	113.60	118.30
2	N	210	ARG	N-CA-C	-5.22	96.90	111.00
6	Q	465	LEU	N-CA-CB	-5.22	99.96	110.40
2	H	477	ASP	N-CA-CB	-5.22	101.21	110.60
2	G	477	ASP	N-CA-CB	-5.21	101.22	110.60
2	N	206	VAL	CA-CB-CG2	-5.21	103.08	110.90
2	B	477	ASP	N-CA-CB	-5.21	101.23	110.60
2	G	206	VAL	CA-CB-CG2	-5.21	103.09	110.90
2	F	423	PHE	CB-CG-CD2	5.21	124.45	120.80
2	B	511	LEU	CB-CA-C	-5.21	100.31	110.20
2	F	206	VAL	CA-CB-CG2	-5.21	103.09	110.90
2	F	210	ARG	N-CA-C	-5.21	96.94	111.00
6	Q	428	GLU	C-N-CA	5.21	134.71	121.70
2	G	514	PHE	CB-CG-CD1	5.20	124.44	120.80
6	R	737	LYS	N-CA-C	5.20	125.05	111.00
4	M	426	ILE	CA-CB-CG2	-5.20	100.50	110.90
6	R	439	TYR	N-CA-CB	5.20	119.96	110.60
4	M	432	ARG	NE-CZ-NH2	5.20	122.90	120.30
3	V	210	ARG	N-CA-C	-5.20	96.96	111.00
2	B	206	VAL	CA-CB-CG2	-5.20	103.10	110.90
6	Q	128	MET	CG-SD-CE	-5.19	91.90	100.20
2	A	206	VAL	CA-CB-CG2	-5.18	103.12	110.90
2	E	206	VAL	CA-CB-CG2	-5.18	103.13	110.90
6	Q	703	CYS	CB-CA-C	-5.18	100.04	110.40
6	R	703	CYS	CB-CA-C	-5.18	100.04	110.40
4	O	364	MET	CG-SD-CE	5.18	108.49	100.20
1	J	258	ARG	NE-CZ-NH1	5.18	122.89	120.30
2	H	511	LEU	CB-CA-C	-5.17	100.37	110.20
2	N	496	ALA	N-CA-CB	5.17	117.34	110.10
4	O	477	ASP	CB-CG-OD1	-5.17	113.65	118.30
2	H	390	LEU	N-CA-C	-5.17	97.05	111.00
2	E	423	PHE	CB-CG-CD2	5.17	124.42	120.80
4	O	426	ILE	CA-CB-CG2	-5.17	100.57	110.90
2	G	390	LEU	N-CA-C	-5.16	97.06	111.00
2	H	514	PHE	CB-CG-CD1	5.16	124.42	120.80
2	B	390	LEU	N-CA-C	-5.16	97.06	111.00
2	G	511	LEU	CB-CA-C	-5.16	100.39	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	798	PHE	CB-CG-CD2	-5.16	117.19	120.80
4	M	364	MET	CG-SD-CE	5.16	108.45	100.20
6	Q	439	TYR	N-CA-CB	5.16	119.89	110.60
6	R	528	LEU	CB-CG-CD1	5.16	119.77	111.00
2	G	493	VAL	CA-CB-CG1	5.16	118.63	110.90
6	Q	737	LYS	N-CA-C	5.16	124.92	111.00
4	M	345	VAL	CA-CB-CG1	5.15	118.63	110.90
6	R	647	ARG	N-CA-C	-5.15	97.09	111.00
2	P	496	ALA	N-CA-CB	5.15	117.31	110.10
5	T	159	LEU	N-CA-C	-5.15	97.10	111.00
5	S	159	LEU	N-CA-C	-5.14	97.11	111.00
1	J	33	ARG	NE-CZ-NH2	5.14	122.87	120.30
6	R	754	THR	N-CA-C	-5.14	97.13	111.00
2	N	390	LEU	N-CA-C	-5.14	97.13	111.00
2	A	419	ASP	CB-CG-OD2	-5.13	113.68	118.30
2	A	423	PHE	CB-CG-CD2	5.13	124.39	120.80
6	Q	528	LEU	CB-CG-CD1	5.13	119.73	111.00
2	H	493	VAL	CA-CB-CG1	5.13	118.60	110.90
6	Q	647	ARG	N-CA-C	-5.13	97.14	111.00
6	Q	754	THR	N-CA-C	-5.13	97.15	111.00
2	P	390	LEU	N-CA-C	-5.13	97.16	111.00
2	G	385	LEU	N-CA-CB	5.12	120.65	110.40
6	Q	107	TYR	CB-CG-CD1	5.12	124.08	121.00
5	S	134	ASN	CA-CB-CG	-5.12	102.13	113.40
5	T	134	ASN	CA-CB-CG	-5.12	102.13	113.40
2	N	341	HIS	CB-CA-C	5.12	120.64	110.40
2	B	493	VAL	CA-CB-CG1	5.12	118.57	110.90
4	M	477	ASP	CB-CG-OD1	-5.11	113.70	118.30
4	M	388	VAL	CG1-CB-CG2	-5.11	102.73	110.90
2	P	341	HIS	CB-CA-C	5.10	120.61	110.40
6	R	768	TYR	CB-CG-CD2	-5.10	117.94	121.00
4	O	388	VAL	CG1-CB-CG2	-5.10	102.74	110.90
6	R	107	TYR	CB-CG-CD1	5.10	124.06	121.00
2	G	542	GLU	N-CA-CB	5.10	119.78	110.60
2	H	542	GLU	N-CA-CB	5.09	119.77	110.60
6	Q	204	ARG	NE-CZ-NH1	5.09	122.84	120.30
6	R	273	ASP	N-CA-CB	-5.09	101.44	110.60
2	B	542	GLU	N-CA-CB	5.08	119.75	110.60
2	F	344	ARG	CD-NE-CZ	5.08	130.72	123.60
6	Q	584	LEU	CA-CB-CG	5.08	126.99	115.30
2	N	410	ASP	N-CA-CB	5.08	119.74	110.60
2	B	341	HIS	CB-CA-C	5.08	120.55	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	385	LEU	N-CA-CB	5.08	120.55	110.40
2	A	344	ARG	CD-NE-CZ	5.07	130.70	123.60
4	M	339	TRP	CH2-CZ2-CE2	5.07	122.47	117.40
6	R	511	ASN	N-CA-CB	5.07	119.72	110.60
6	Q	109	MET	CB-CA-C	-5.07	100.27	110.40
2	N	500	PHE	CB-CG-CD1	5.06	124.34	120.80
6	R	109	MET	CB-CA-C	-5.06	100.27	110.40
6	R	584	LEU	CA-CB-CG	5.06	126.94	115.30
5	S	122	PHE	CB-CG-CD2	-5.06	117.26	120.80
6	Q	798	PHE	CB-CG-CD2	-5.06	117.26	120.80
3	K	190	THR	N-CA-C	-5.05	97.36	111.00
4	O	345	VAL	CA-CB-CG1	5.05	118.48	110.90
3	L	187	PHE	N-CA-C	-5.05	97.35	111.00
2	A	190	THR	N-CA-C	-5.05	97.36	111.00
6	R	434	ASP	CA-CB-CG	-5.05	102.28	113.40
5	T	122	PHE	CB-CG-CD2	-5.05	117.26	120.80
3	D	190	THR	N-CA-C	-5.05	97.36	111.00
2	E	344	ARG	CD-NE-CZ	5.05	130.67	123.60
3	K	187	PHE	N-CA-C	-5.05	97.37	111.00
2	H	187	PHE	N-CA-C	-5.05	97.37	111.00
2	F	190	THR	N-CA-C	-5.05	97.37	111.00
6	Q	271	THR	CA-CB-CG2	-5.05	105.33	112.40
3	D	310	LYS	N-CA-CB	5.05	119.69	110.60
2	P	543	LYS	CB-CA-C	-5.05	100.30	110.40
2	P	187	PHE	N-CA-C	-5.05	97.38	111.00
2	N	543	LYS	CB-CA-C	-5.05	100.31	110.40
3	D	187	PHE	N-CA-C	-5.04	97.38	111.00
2	P	190	THR	N-CA-C	-5.04	97.38	111.00
2	G	187	PHE	N-CA-C	-5.04	97.39	111.00
2	H	341	HIS	CB-CA-C	5.04	120.48	110.40
2	A	491	ARG	NE-CZ-NH2	5.04	122.82	120.30
2	E	310	LYS	N-CA-CB	5.04	119.67	110.60
3	K	310	LYS	N-CA-CB	5.04	119.67	110.60
2	P	500	PHE	CB-CG-CD1	5.04	124.33	120.80
2	F	332	LYS	N-CA-CB	5.04	119.67	110.60
3	V	187	PHE	N-CA-C	-5.04	97.39	111.00
6	R	680	PHE	CB-CA-C	-5.04	100.32	110.40
2	B	385	LEU	N-CA-CB	5.04	120.47	110.40
2	G	441	PHE	N-CA-CB	-5.04	101.53	110.60
2	N	310	LYS	N-CA-CB	5.04	119.67	110.60
6	Q	489	PHE	N-CA-CB	5.04	119.67	110.60
2	F	310	LYS	N-CA-CB	5.04	119.66	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	187	PHE	N-CA-C	-5.03	97.41	111.00
2	B	310	LYS	N-CA-CB	5.03	119.66	110.60
2	A	332	LYS	N-CA-CB	5.03	119.66	110.60
2	E	187	PHE	N-CA-C	-5.03	97.41	111.00
3	V	310	LYS	N-CA-CB	5.03	119.66	110.60
6	Q	511	ASN	N-CA-CB	5.03	119.66	110.60
4	O	339	TRP	CH2-CZ2-CE2	5.03	122.43	117.40
3	L	190	THR	N-CA-C	-5.03	97.42	111.00
2	H	310	LYS	N-CA-CB	5.03	119.65	110.60
6	Q	768	TYR	CB-CG-CD2	-5.03	117.98	121.00
2	G	341	HIS	CB-CA-C	5.03	120.45	110.40
2	A	310	LYS	N-CA-CB	5.03	119.65	110.60
4	O	333	PHE	O-C-N	-5.03	114.66	122.70
2	P	410	ASP	N-CA-CB	5.03	119.65	110.60
3	L	310	LYS	N-CA-CB	5.03	119.65	110.60
6	R	443	LYS	CB-CA-C	-5.02	100.35	110.40
2	P	310	LYS	N-CA-CB	5.02	119.64	110.60
2	A	187	PHE	N-CA-C	-5.02	97.44	111.00
3	V	190	THR	N-CA-C	-5.02	97.44	111.00
6	R	622	TYR	N-CA-C	-5.02	97.45	111.00
4	M	333	PHE	O-C-N	-5.02	114.67	122.70
2	N	190	THR	N-CA-C	-5.02	97.45	111.00
2	E	190	THR	N-CA-C	-5.02	97.46	111.00
6	R	489	PHE	N-CA-CB	5.02	119.63	110.60
2	N	187	PHE	N-CA-C	-5.01	97.46	111.00
2	F	187	PHE	N-CA-C	-5.01	97.46	111.00
6	Q	680	PHE	CB-CA-C	-5.01	100.37	110.40
2	B	190	THR	N-CA-C	-5.01	97.47	111.00
2	G	310	LYS	N-CA-CB	5.01	119.62	110.60
6	Q	273	ASP	N-CA-CB	-5.01	101.58	110.60
2	B	441	PHE	N-CA-CB	-5.01	101.58	110.60
6	Q	434	ASP	CA-CB-CG	-5.01	102.38	113.40
2	G	190	THR	N-CA-C	-5.01	97.48	111.00
2	H	441	PHE	N-CA-CB	-5.00	101.59	110.60
6	Q	443	LYS	CB-CA-C	-5.00	100.39	110.40
1	C	280	ARG	NE-CZ-NH1	5.00	122.80	120.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	Q	87	ASN	CA
6	R	87	ASN	CA

All (357) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	207	TYR	Sidechain
2	A	210	ARG	Sidechain
2	A	227	ARG	Sidechain
2	A	228	ARG	Sidechain
2	A	230	ARG	Sidechain
2	A	232	PHE	Sidechain
2	A	236	TYR	Sidechain
2	A	251	PRO	Peptide
2	A	264	PHE	Sidechain
2	A	268	ARG	Sidechain
2	A	306	HIS	Sidechain
2	A	409	ARG	Sidechain
2	A	470	ARG	Peptide
2	A	491	ARG	Sidechain
2	A	494	HIS	Sidechain
2	B	207	TYR	Sidechain
2	B	210	ARG	Sidechain
2	B	227	ARG	Sidechain
2	B	228	ARG	Sidechain
2	B	230	ARG	Sidechain
2	B	232	PHE	Sidechain
2	B	236	TYR	Sidechain
2	B	251	PRO	Peptide
2	B	264	PHE	Sidechain
2	B	268	ARG	Sidechain
2	B	306	HIS	Sidechain
2	B	341	HIS	Sidechain
2	B	367	GLN	Peptide
2	B	368	ARG	Sidechain
2	B	383	HIS	Sidechain
2	B	391	SER	Peptide
2	B	412	TYR	Sidechain
2	B	448	PHE	Sidechain
2	B	478	ARG	Sidechain
2	B	494	HIS	Sidechain
2	B	497	ARG	Sidechain
2	B	505	ARG	Sidechain
2	B	508	ARG	Sidechain
2	B	513	ARG	Sidechain
2	B	522	PHE	Sidechain
2	B	529	PHE	Sidechain
2	B	547	PHE	Sidechain

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
1	C	148	TYR	Sidechain
3	D	207	TYR	Sidechain
3	D	210	ARG	Sidechain
3	D	227	ARG	Sidechain
3	D	228	ARG	Sidechain
3	D	230	ARG	Sidechain
3	D	232	PHE	Sidechain
3	D	236	TYR	Sidechain
3	D	251	PRO	Peptide
3	D	264	PHE	Sidechain
3	D	268	ARG	Sidechain
3	D	306	HIS	Sidechain
2	E	207	TYR	Sidechain
2	E	210	ARG	Sidechain
2	E	227	ARG	Sidechain
2	E	228	ARG	Sidechain
2	E	230	ARG	Sidechain
2	E	232	PHE	Sidechain
2	E	236	TYR	Sidechain
2	E	251	PRO	Peptide
2	E	264	PHE	Sidechain
2	E	268	ARG	Sidechain
2	E	306	HIS	Sidechain
2	E	409	ARG	Sidechain
2	E	449	HIS	Sidechain
2	E	470	ARG	Peptide
2	E	491	ARG	Sidechain
2	E	494	HIS	Sidechain
2	F	207	TYR	Sidechain
2	F	210	ARG	Sidechain
2	F	227	ARG	Sidechain
2	F	228	ARG	Sidechain
2	F	230	ARG	Sidechain
2	F	232	PHE	Sidechain
2	F	236	TYR	Sidechain
2	F	251	PRO	Peptide
2	F	264	PHE	Sidechain
2	F	268	ARG	Sidechain
2	F	306	HIS	Sidechain
2	F	409	ARG	Sidechain
2	F	449	HIS	Sidechain
2	F	470	ARG	Peptide

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
2	F	491	ARG	Sidechain
2	F	494	HIS	Sidechain
2	G	207	TYR	Sidechain
2	G	210	ARG	Sidechain
2	G	227	ARG	Sidechain
2	G	228	ARG	Sidechain
2	G	230	ARG	Sidechain
2	G	232	PHE	Sidechain
2	G	236	TYR	Sidechain
2	G	251	PRO	Peptide
2	G	264	PHE	Sidechain
2	G	268	ARG	Sidechain
2	G	306	HIS	Sidechain
2	G	341	HIS	Sidechain
2	G	367	GLN	Peptide
2	G	368	ARG	Sidechain
2	G	383	HIS	Sidechain
2	G	391	SER	Peptide
2	G	412	TYR	Sidechain
2	G	448	PHE	Sidechain
2	G	478	ARG	Sidechain
2	G	494	HIS	Sidechain
2	G	497	ARG	Sidechain
2	G	505	ARG	Sidechain
2	G	508	ARG	Sidechain
2	G	513	ARG	Sidechain
2	G	522	PHE	Sidechain
2	G	529	PHE	Sidechain
2	G	547	PHE	Sidechain
2	H	207	TYR	Sidechain
2	H	210	ARG	Sidechain
2	H	227	ARG	Sidechain
2	H	228	ARG	Sidechain
2	H	230	ARG	Sidechain
2	H	232	PHE	Sidechain
2	H	236	TYR	Sidechain
2	H	251	PRO	Peptide
2	H	264	PHE	Sidechain
2	H	268	ARG	Sidechain
2	H	306	HIS	Sidechain
2	H	341	HIS	Sidechain
2	H	367	GLN	Peptide

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
2	H	368	ARG	Sidechain
2	H	383	HIS	Sidechain
2	H	391	SER	Peptide
2	H	412	TYR	Sidechain
2	H	448	PHE	Sidechain
2	H	478	ARG	Sidechain
2	H	494	HIS	Sidechain
2	H	497	ARG	Sidechain
2	H	505	ARG	Sidechain
2	H	508	ARG	Sidechain
2	H	513	ARG	Sidechain
2	H	522	PHE	Sidechain
2	H	529	PHE	Sidechain
2	H	547	PHE	Sidechain
1	J	148	TYR	Sidechain
3	K	207	TYR	Sidechain
3	K	210	ARG	Sidechain
3	K	227	ARG	Sidechain
3	K	228	ARG	Sidechain
3	K	230	ARG	Sidechain
3	K	232	PHE	Sidechain
3	K	236	TYR	Sidechain
3	K	251	PRO	Peptide
3	K	264	PHE	Sidechain
3	K	268	ARG	Sidechain
3	K	306	HIS	Sidechain
3	L	207	TYR	Sidechain
3	L	210	ARG	Sidechain
3	L	227	ARG	Sidechain
3	L	228	ARG	Sidechain
3	L	230	ARG	Sidechain
3	L	232	PHE	Sidechain
3	L	236	TYR	Sidechain
3	L	251	PRO	Peptide
3	L	264	PHE	Sidechain
3	L	268	ARG	Sidechain
3	L	306	HIS	Sidechain
4	M	343	ARG	Sidechain
4	M	378	PHE	Sidechain
4	M	412	TYR	Sidechain
4	M	430	TYR	Sidechain
4	M	452	HIS	Sidechain

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
4	M	497	ARG	Sidechain
4	M	513	ARG	Sidechain
2	N	207	TYR	Sidechain
2	N	210	ARG	Sidechain
2	N	227	ARG	Sidechain
2	N	228	ARG	Sidechain
2	N	230	ARG	Sidechain
2	N	232	PHE	Sidechain
2	N	236	TYR	Sidechain
2	N	251	PRO	Peptide
2	N	264	PHE	Sidechain
2	N	268	ARG	Sidechain
2	N	306	HIS	Sidechain
2	N	378	PHE	Sidechain
2	N	391	SER	Peptide
2	N	470	ARG	Peptide
2	N	497	ARG	Sidechain
2	N	516	ARG	Sidechain
4	O	343	ARG	Sidechain
4	O	378	PHE	Sidechain
4	O	412	TYR	Sidechain
4	O	430	TYR	Sidechain
4	O	452	HIS	Sidechain
4	O	497	ARG	Sidechain
4	O	513	ARG	Sidechain
2	P	207	TYR	Sidechain
2	P	210	ARG	Sidechain
2	P	227	ARG	Sidechain
2	P	228	ARG	Sidechain
2	P	230	ARG	Sidechain
2	P	232	PHE	Sidechain
2	P	236	TYR	Sidechain
2	P	251	PRO	Peptide
2	P	264	PHE	Sidechain
2	P	268	ARG	Sidechain
2	P	306	HIS	Sidechain
2	P	378	PHE	Sidechain
2	P	391	SER	Peptide
2	P	470	ARG	Peptide
2	P	497	ARG	Sidechain
2	P	516	ARG	Sidechain
6	Q	101	ASN	Mainchain,Peptide

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
6	Q	105	ARG	Sidechain
6	Q	107	TYR	Sidechain
6	Q	140	HIS	Sidechain
6	Q	149	TYR	Sidechain
6	Q	158	TYR	Sidechain
6	Q	231	TYR	Sidechain
6	Q	233	ASP	Peptide
6	Q	285	HIS	Sidechain
6	Q	302	TYR	Sidechain
6	Q	399	HIS	Sidechain
6	Q	407	PRO	Mainchain
6	Q	426	TYR	Sidechain
6	Q	429	ARG	Sidechain
6	Q	432	TYR	Mainchain,Sidechain
6	Q	438	ALA	Mainchain,Peptide
6	Q	439	TYR	Sidechain
6	Q	471	ARG	Sidechain
6	Q	473	TYR	Sidechain
6	Q	484	THR	Mainchain,Peptide
6	Q	489	PHE	Sidechain
6	Q	494	TYR	Sidechain
6	Q	498	ARG	Sidechain
6	Q	506	ARG	Sidechain
6	Q	53	ARG	Sidechain
6	Q	561	GLU	Mainchain
6	Q	570	HIS	Peptide
6	Q	591	TYR	Sidechain
6	Q	597	ARG	Sidechain
6	Q	599	ARG	Sidechain
6	Q	622	TYR	Sidechain
6	Q	63	TYR	Sidechain
6	Q	634	PHE	Sidechain
6	Q	638	HIS	Sidechain
6	Q	647	ARG	Peptide
6	Q	650	GLY	Peptide
6	Q	678	TYR	Sidechain
6	Q	680	PHE	Sidechain
6	Q	688	TYR	Sidechain
6	Q	690	GLU	Peptide
6	Q	713	ARG	Sidechain
6	Q	715	PHE	Sidechain
6	Q	717	ARG	Sidechain

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
6	Q	742	ARG	Sidechain
6	Q	745	TYR	Sidechain
6	Q	768	TYR	Sidechain
6	Q	771	GLY	Mainchain
6	Q	773	ARG	Sidechain
6	Q	805	TYR	Sidechain
6	Q	808	TYR	Sidechain
6	Q	820	TYR	Sidechain
6	Q	93	TYR	Sidechain
6	R	101	ASN	Mainchain,Peptide
6	R	105	ARG	Sidechain
6	R	107	TYR	Sidechain
6	R	140	HIS	Sidechain
6	R	149	TYR	Sidechain
6	R	158	TYR	Sidechain
6	R	194	HIS	Sidechain
6	R	231	TYR	Sidechain
6	R	233	ASP	Peptide
6	R	285	HIS	Sidechain
6	R	302	TYR	Sidechain
6	R	399	HIS	Sidechain
6	R	407	PRO	Mainchain
6	R	426	TYR	Sidechain
6	R	429	ARG	Sidechain
6	R	432	TYR	Mainchain,Sidechain
6	R	438	ALA	Mainchain,Peptide
6	R	439	TYR	Sidechain
6	R	471	ARG	Sidechain
6	R	473	TYR	Sidechain
6	R	484	THR	Mainchain,Peptide
6	R	489	PHE	Sidechain
6	R	494	TYR	Sidechain
6	R	498	ARG	Sidechain
6	R	506	ARG	Sidechain
6	R	53	ARG	Sidechain
6	R	561	GLU	Mainchain
6	R	570	HIS	Peptide
6	R	591	TYR	Sidechain
6	R	597	ARG	Sidechain
6	R	599	ARG	Sidechain
6	R	622	TYR	Sidechain
6	R	63	TYR	Sidechain

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
6	R	634	PHE	Sidechain
6	R	638	HIS	Sidechain
6	R	647	ARG	Peptide
6	R	650	GLY	Peptide
6	R	678	TYR	Sidechain
6	R	680	PHE	Sidechain
6	R	688	TYR	Sidechain
6	R	690	GLU	Peptide
6	R	713	ARG	Sidechain
6	R	715	PHE	Sidechain
6	R	717	ARG	Sidechain
6	R	742	ARG	Sidechain
6	R	745	TYR	Sidechain
6	R	768	TYR	Sidechain
6	R	771	GLY	Mainchain
6	R	773	ARG	Sidechain
6	R	805	TYR	Sidechain
6	R	808	TYR	Sidechain
6	R	820	TYR	Sidechain
6	R	93	TYR	Sidechain
5	S	120	HIS	Sidechain
5	S	122	PHE	Sidechain
5	S	127	TYR	Sidechain
5	S	132	PHE	Sidechain
5	S	157	PHE	Sidechain
5	S	170	TYR	Sidechain
5	S	48	TYR	Sidechain
5	S	50	TYR	Sidechain
5	S	52	ARG	Sidechain
5	S	64	ARG	Sidechain
5	S	80	HIS	Sidechain
5	S	84	ARG	Sidechain
5	T	120	HIS	Sidechain
5	T	122	PHE	Sidechain
5	T	127	TYR	Sidechain
5	T	132	PHE	Sidechain
5	T	157	PHE	Sidechain
5	T	170	TYR	Sidechain
5	T	48	TYR	Sidechain
5	T	50	TYR	Sidechain
5	T	52	ARG	Sidechain
5	T	64	ARG	Sidechain

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Mol	Chain	Res	Type	Group
5	T	80	HIS	Sidechain
5	T	84	ARG	Sidechain
3	V	207	TYR	Sidechain
3	V	210	ARG	Sidechain
3	V	227	ARG	Sidechain
3	V	228	ARG	Sidechain
3	V	230	ARG	Sidechain
3	V	232	PHE	Sidechain
3	V	236	TYR	Sidechain
3	V	251	PRO	Peptide
3	V	264	PHE	Sidechain
3	V	268	ARG	Sidechain
3	V	306	HIS	Sidechain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2417	0	2432	218	0
1	J	2417	0	2430	249	0
2	A	2843	2845	2835	317	0
2	B	2843	2845	2836	449	0
2	E	2843	2845	2835	275	0
2	F	2843	2845	2835	231	0
2	G	2843	2845	2834	503	0
2	H	2843	2845	2833	437	0
2	N	2843	2845	2833	297	0
2	P	2843	2845	2834	223	0
3	D	1053	1059	1056	112	0
3	K	1053	1059	1055	129	0
3	L	1053	1059	1054	140	0
3	V	1053	1059	1056	109	0
4	M	1791	1788	1785	2	0
4	O	1791	1788	1785	1	0
5	S	1436	1457	1453	83	0
5	T	1436	1457	1453	78	0
6	Q	5978	5981	5974	454	0
6	R	5978	5981	5976	417	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	50200	45448	50184	3648	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 36.

All (3648) 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:B:350:LEU:HD22	2:A:385:LEU:CG	1.21	1.65
2:G:350:LEU:HD22	2:E:385:LEU:CG	1.21	1.61
2:H:350:LEU:HD22	2:F:385:LEU:CG	1.21	1.59
1:J:217:PRO:CB	2:G:390:LEU:HD12	1.25	1.59
1:J:217:PRO:CD	2:G:390:LEU:HG	1.16	1.58
2:G:248:VAL:CG2	2:G:443:GLN:HE22	0.97	1.58
2:H:248:VAL:CG2	2:H:443:GLN:HE22	0.98	1.57
2:B:248:VAL:CG2	2:B:443:GLN:HE22	0.98	1.55
1:C:217:PRO:CD	2:B:390:LEU:HG	1.37	1.54
2:A:250:PRO:CG	2:A:433:LEU:HG	1.36	1.52
2:F:250:PRO:CG	2:F:433:LEU:HG	1.37	1.52
2:E:250:PRO:CG	2:E:433:LEU:HG	1.36	1.51
2:H:530:LEU:HD21	2:F:544:TRP:CD1	1.47	1.49
1:J:217:PRO:HD2	2:G:390:LEU:CG	1.41	1.49
2:G:530:LEU:HD21	2:E:544:TRP:CD1	1.47	1.49
2:A:333:PHE:CG	2:N:333:PHE:HD1	1.28	1.48
2:P:475:GLN:CD	2:N:311:GLU:HA	1.27	1.48
2:B:246:VAL:HG22	2:B:503:MET:CE	1.41	1.47
2:B:246:VAL:CG2	2:B:503:MET:HE3	1.44	1.47
1:J:261:ASN:ND2	1:C:90:GLU:CG	1.74	1.47
1:C:217:PRO:CB	2:B:390:LEU:HD12	1.42	1.47
2:B:530:LEU:HD21	2:A:544:TRP:CD1	1.47	1.47
2:A:196:LYS:NZ	3:D:196:LYS:HZ2	1.08	1.47
2:H:350:LEU:CD2	2:F:385:LEU:CG	1.92	1.47
2:G:350:LEU:CD2	2:E:385:LEU:CG	1.92	1.47
1:J:90:GLU:CG	1:C:261:ASN:ND2	1.74	1.46
2:H:246:VAL:HG22	2:H:503:MET:CE	1.41	1.46
1:J:247:PHE:CB	6:Q:98:TYR:CE1	1.96	1.46
2:B:350:LEU:CD2	2:A:385:LEU:CG	1.92	1.46
2:F:274:LYS:NZ	2:F:432:ARG:NH1	1.62	1.46
2:G:246:VAL:HG22	2:G:503:MET:CE	1.41	1.45
2:A:274:LYS:NZ	2:A:432:ARG:NH1	1.62	1.43
2:G:248:VAL:CG2	2:G:443:GLN:NE2	1.82	1.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:196:LYS:NZ	2:P:196:LYS:NZ	1.66	1.43
2:B:350:LEU:HD22	2:A:385:LEU:CD2	1.47	1.43
2:H:350:LEU:HD22	2:F:385:LEU:CD2	1.47	1.42
2:A:196:LYS:NZ	3:D:196:LYS:NZ	1.66	1.41
2:G:196:LYS:NZ	2:N:196:LYS:NZ	1.66	1.41
1:J:90:GLU:CG	1:C:261:ASN:CG	1.89	1.41
2:G:350:LEU:HD22	2:E:385:LEU:CD2	1.47	1.41
1:J:90:GLU:HG3	1:C:261:ASN:CG	1.41	1.41
2:B:246:VAL:CG2	2:B:503:MET:CE	1.97	1.41
2:E:274:LYS:NZ	2:E:432:ARG:NH1	1.62	1.41
2:F:196:LYS:NZ	3:L:196:LYS:HZ2	1.03	1.41
2:A:332:LYS:HG2	2:N:331:ASN:N	1.36	1.40
2:H:248:VAL:CG2	2:H:443:GLN:NE2	1.82	1.40
2:P:477:ASP:C	2:N:310:LYS:CE	1.75	1.40
2:N:249:PRO:CA	2:N:433:LEU:HD21	1.52	1.40
2:H:246:VAL:CG2	2:H:503:MET:HE3	1.50	1.40
1:J:88:VAL:CG1	1:C:82:TYR:OH	1.70	1.39
2:H:196:LYS:NZ	3:V:196:LYS:NZ	1.66	1.39
2:H:246:VAL:CG2	2:H:503:MET:CE	1.97	1.39
2:B:248:VAL:CG2	2:B:443:GLN:NE2	1.82	1.39
2:G:246:VAL:CG2	2:G:503:MET:CE	1.97	1.39
1:J:82:TYR:OH	1:C:88:VAL:CG1	1.70	1.38
2:P:475:GLN:CD	2:N:311:GLU:CA	1.92	1.38
2:N:250:PRO:CA	2:N:429:GLU:OE2	1.66	1.38
1:J:261:ASN:CG	1:C:90:GLU:CG	1.89	1.38
2:P:310:LYS:CD	2:N:480:ASN:HB2	1.27	1.38
2:E:196:LYS:NZ	3:K:196:LYS:NZ	1.66	1.37
1:J:217:PRO:HB2	2:G:390:LEU:CD1	1.52	1.37
2:G:250:PRO:CD	2:G:250:PRO:CG	2.03	1.37
2:E:245:GLY:HA2	2:E:443:GLN:NE2	1.05	1.37
2:P:475:GLN:OE1	2:N:311:GLU:CA	1.68	1.37
2:F:196:LYS:NZ	3:L:196:LYS:NZ	1.66	1.37
3:V:250:PRO:CG	3:V:250:PRO:CD	2.03	1.37
1:J:247:PHE:HB2	6:Q:98:TYR:CD1	1.58	1.37
2:H:250:PRO:CG	2:H:250:PRO:CD	2.03	1.37
6:Q:721:ASP:CG	6:R:721:ASP:OD2	1.63	1.37
3:D:250:PRO:CD	3:D:250:PRO:CG	2.03	1.37
1:C:217:PRO:HD2	2:B:390:LEU:CG	1.54	1.36
2:A:250:PRO:CG	2:A:250:PRO:CD	2.03	1.36
2:B:196:LYS:NZ	2:P:196:LYS:HZ2	1.17	1.36
2:G:350:LEU:HD22	2:E:385:LEU:CD1	1.54	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:250:PRO:CG	2:N:250:PRO:CD	2.02	1.36
2:H:250:PRO:CB	2:H:436:SER:HB3	1.56	1.36
2:H:350:LEU:HD22	2:F:385:LEU:CD1	1.54	1.36
3:L:250:PRO:CD	3:L:250:PRO:CG	2.03	1.36
2:P:250:PRO:CG	2:P:250:PRO:CD	2.03	1.36
1:J:88:VAL:HG11	1:C:82:TYR:OH	1.19	1.36
2:E:250:PRO:CG	2:E:250:PRO:CD	2.03	1.35
3:K:250:PRO:CG	3:K:250:PRO:CB	2.04	1.35
2:B:250:PRO:CB	2:B:250:PRO:CG	2.04	1.35
2:A:250:PRO:CG	2:A:250:PRO:CB	2.04	1.35
3:K:250:PRO:CG	3:K:250:PRO:CD	2.03	1.35
2:B:250:PRO:CG	2:B:250:PRO:CD	2.03	1.35
2:E:250:PRO:CG	2:E:250:PRO:CB	2.04	1.35
3:K:311:GLU:O	2:H:476:GLN:CB	1.73	1.35
2:G:250:PRO:CB	2:G:436:SER:HB3	1.56	1.35
6:Q:721:ASP:OD2	6:R:721:ASP:CG	1.63	1.35
2:B:248:VAL:HG21	2:B:443:GLN:NE2	1.38	1.34
3:D:250:PRO:CG	3:D:250:PRO:CB	2.04	1.34
2:F:250:PRO:CG	2:F:250:PRO:CD	2.03	1.34
3:V:250:PRO:CG	3:V:250:PRO:CB	2.04	1.34
2:A:333:PHE:CG	2:N:333:PHE:CD1	2.14	1.34
2:P:475:GLN:NE2	2:N:311:GLU:CA	1.87	1.34
2:B:350:LEU:HD22	2:A:385:LEU:CD1	1.54	1.34
1:J:261:ASN:CG	1:C:90:GLU:HG3	1.41	1.34
2:B:250:PRO:CB	2:B:436:SER:HB3	1.56	1.34
2:A:245:GLY:CA	2:A:443:GLN:HE21	1.41	1.33
2:N:250:PRO:CA	2:N:250:PRO:N	1.92	1.33
2:G:250:PRO:CG	2:G:250:PRO:CB	2.04	1.33
2:E:250:PRO:N	2:E:250:PRO:CA	1.91	1.33
3:K:250:PRO:N	3:K:250:PRO:CA	1.91	1.33
2:N:250:PRO:CD	2:N:429:GLU:OE2	1.76	1.33
2:H:250:PRO:N	2:H:250:PRO:CA	1.91	1.33
3:V:250:PRO:N	3:V:250:PRO:CA	1.91	1.33
2:G:250:PRO:N	2:G:250:PRO:CA	1.92	1.33
2:F:245:GLY:CA	2:F:443:GLN:HE21	1.41	1.33
3:L:250:PRO:N	3:L:250:PRO:CA	1.92	1.33
2:H:250:PRO:CG	2:H:250:PRO:CB	2.04	1.33
2:F:250:PRO:CG	2:F:250:PRO:CB	2.04	1.33
2:A:245:GLY:HA2	2:A:443:GLN:NE2	1.04	1.33
2:P:310:LYS:CE	2:N:477:ASP:O	1.74	1.33
2:H:267:SER:HB3	2:H:432:ARG:NH1	1.01	1.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:245:GLY:HA2	2:F:443:GLN:NE2	1.05	1.33
2:B:250:PRO:N	2:B:250:PRO:CA	1.92	1.32
2:P:250:PRO:N	2:P:250:PRO:CA	1.92	1.32
3:L:250:PRO:CG	3:L:250:PRO:CB	2.04	1.32
2:B:267:SER:HB3	2:B:432:ARG:NH1	1.01	1.32
2:G:267:SER:HB3	2:G:432:ARG:NH1	1.01	1.32
2:E:245:GLY:CA	2:E:443:GLN:HE21	1.41	1.32
2:F:250:PRO:N	2:F:250:PRO:CA	1.91	1.31
3:V:250:PRO:CD	3:V:250:PRO:N	1.93	1.31
1:J:90:GLU:OE2	1:C:82:TYR:CE2	1.81	1.31
2:A:250:PRO:CD	2:A:250:PRO:N	1.93	1.31
3:K:250:PRO:CD	3:K:250:PRO:N	1.93	1.31
3:D:250:PRO:CD	3:D:250:PRO:N	1.93	1.31
2:N:250:PRO:CD	2:N:250:PRO:N	1.93	1.31
2:B:250:PRO:CD	2:B:250:PRO:N	1.93	1.30
2:H:248:VAL:HG21	2:H:443:GLN:NE2	1.38	1.30
3:D:250:PRO:N	3:D:250:PRO:CA	1.92	1.30
2:H:250:PRO:CD	2:H:250:PRO:N	1.93	1.30
1:J:82:TYR:CE2	1:C:90:GLU:OE2	1.81	1.30
2:A:250:PRO:N	2:A:250:PRO:CA	1.91	1.30
2:E:250:PRO:CD	2:E:250:PRO:N	1.93	1.30
2:G:250:PRO:CD	2:G:250:PRO:N	1.93	1.30
1:J:217:PRO:CD	2:G:390:LEU:CG	2.00	1.30
1:J:230:GLU:HB3	6:Q:101:ASN:OD1	1.21	1.29
2:F:250:PRO:CD	2:F:250:PRO:N	1.93	1.29
6:Q:725:THR:OG1	6:R:722:THR:CG2	1.79	1.29
2:P:250:PRO:CD	2:P:250:PRO:N	1.93	1.29
3:L:250:PRO:CD	3:L:250:PRO:N	1.93	1.29
1:J:261:ASN:ND2	1:C:90:GLU:HG2	0.96	1.29
2:G:267:SER:CB	2:G:432:ARG:HH12	1.46	1.29
2:H:267:SER:CB	2:H:432:ARG:NH1	1.95	1.29
2:B:267:SER:CB	2:B:432:ARG:HH12	1.46	1.28
6:Q:683:GLN:CG	6:R:733:LYS:NZ	1.96	1.28
1:C:5:PHE:CB	2:E:331:ASN:OD1	1.78	1.28
2:B:267:SER:CB	2:B:432:ARG:NH1	1.95	1.28
2:G:248:VAL:HG21	2:G:443:GLN:NE2	1.38	1.28
6:Q:722:THR:CG2	6:R:725:THR:OG1	1.79	1.28
1:J:6:SER:O	2:A:331:ASN:N	1.66	1.27
1:J:90:GLU:HG2	1:C:261:ASN:ND2	0.96	1.27
6:Q:683:GLN:CG	6:R:733:LYS:HZ1	1.45	1.27
2:E:196:LYS:NZ	3:K:196:LYS:HZ2	1.20	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:250:PRO:CB	2:H:250:PRO:CA	2.13	1.27
2:H:267:SER:CB	2:H:432:ARG:HH12	1.46	1.27
3:L:250:PRO:CA	3:L:250:PRO:CB	2.13	1.27
1:J:217:PRO:CB	2:G:390:LEU:CD1	2.10	1.27
2:B:250:PRO:CB	2:B:250:PRO:CA	2.13	1.27
2:F:250:PRO:CB	2:F:250:PRO:CA	2.13	1.27
3:D:250:PRO:CB	3:D:250:PRO:CA	2.13	1.26
2:G:267:SER:CB	2:G:432:ARG:NH1	1.95	1.26
2:P:250:PRO:CA	2:P:250:PRO:CB	2.13	1.26
6:Q:733:LYS:NZ	6:R:683:GLN:CG	1.96	1.26
2:G:250:PRO:CB	2:G:250:PRO:CA	2.13	1.26
2:P:310:LYS:HE2	2:N:477:ASP:C	1.50	1.26
2:B:350:LEU:CD2	2:A:385:LEU:CD1	2.13	1.26
2:E:250:PRO:CB	2:E:250:PRO:CA	2.13	1.26
2:P:310:LYS:HE2	2:N:477:ASP:O	1.19	1.26
2:A:250:PRO:CB	2:A:250:PRO:CA	2.13	1.25
2:N:250:PRO:CA	2:N:250:PRO:CB	2.13	1.25
3:K:250:PRO:CB	3:K:250:PRO:CA	2.13	1.25
3:V:250:PRO:CB	3:V:250:PRO:CA	2.13	1.25
2:H:371:MET:HE2	2:F:371:MET:CE	1.67	1.25
2:A:333:PHE:CD2	2:N:333:PHE:CD1	2.25	1.25
2:P:310:LYS:CE	2:N:477:ASP:C	1.99	1.25
6:Q:722:THR:HG21	6:R:725:THR:CG2	1.67	1.24
6:Q:725:THR:CG2	6:R:722:THR:HG21	1.67	1.24
2:P:249:PRO:HA	2:P:433:LEU:CD2	1.67	1.24
2:F:250:PRO:HB3	2:F:432:ARG:CB	1.68	1.24
2:G:370:ALA:N	2:E:367:GLN:OE1	1.69	1.24
2:P:475:GLN:NE2	2:N:311:GLU:HA	0.92	1.24
2:G:350:LEU:CD2	2:E:385:LEU:HG	1.58	1.23
1:C:217:PRO:HB2	2:B:390:LEU:CD1	1.67	1.23
2:A:245:GLY:CA	2:A:443:GLN:NE2	1.99	1.23
2:H:370:ALA:N	2:F:367:GLN:OE1	1.70	1.23
2:A:250:PRO:HB3	2:A:432:ARG:CB	1.68	1.23
2:N:250:PRO:CD	2:N:429:GLU:CG	2.14	1.23
1:J:82:TYR:OH	1:C:88:VAL:HG11	1.20	1.23
2:B:370:ALA:N	2:A:367:GLN:OE1	1.70	1.23
2:H:350:LEU:CD2	2:F:385:LEU:CD1	2.13	1.23
2:G:196:LYS:NZ	2:N:196:LYS:HZ2	1.20	1.22
2:E:406:LEU:CD2	3:K:220:GLN:HE22	1.53	1.22
2:E:250:PRO:HB3	2:E:432:ARG:CB	1.68	1.21
1:J:88:VAL:HG11	1:C:82:TYR:CZ	1.75	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:PHE:HB3	2:E:331:ASN:OD1	1.30	1.21
2:P:475:GLN:HE22	2:N:311:GLU:CA	1.51	1.21
2:A:336:GLN:HB2	2:N:332:LYS:NZ	1.55	1.21
2:G:350:LEU:CD2	2:E:385:LEU:CD1	2.13	1.21
2:P:478:ARG:N	2:N:310:LYS:HE2	1.55	1.21
1:J:82:TYR:CZ	1:C:88:VAL:HG11	1.75	1.21
2:G:250:PRO:CB	2:G:436:SER:CB	2.18	1.21
2:F:406:LEU:CD2	3:L:220:GLN:HE22	1.53	1.21
2:A:406:LEU:CD2	3:D:220:GLN:HE22	1.53	1.20
2:H:250:PRO:CB	2:H:436:SER:CB	2.18	1.20
6:Q:683:GLN:HA	6:R:733:LYS:NZ	1.55	1.20
2:B:199:ASP:HB2	2:P:198:GLY:O	1.39	1.20
2:B:250:PRO:CB	2:B:436:SER:CB	2.18	1.20
2:A:199:ASP:HB2	3:D:198:GLY:O	1.39	1.20
1:J:247:PHE:CG	6:Q:98:TYR:HE1	1.60	1.20
2:E:245:GLY:CA	2:E:443:GLN:NE2	1.99	1.20
2:P:310:LYS:CD	2:N:480:ASN:CB	2.18	1.20
2:P:475:GLN:OE1	2:N:311:GLU:C	1.78	1.20
1:C:217:PRO:N	2:B:392:PRO:HG3	1.57	1.19
2:B:350:LEU:CD2	2:A:385:LEU:HD11	1.71	1.19
2:N:250:PRO:CD	2:N:429:GLU:CD	2.08	1.19
2:H:350:LEU:CD2	2:F:385:LEU:HD11	1.72	1.19
1:J:217:PRO:CA	2:G:390:LEU:HD12	1.73	1.19
2:A:333:PHE:CD2	2:N:333:PHE:HD1	1.61	1.19
2:G:199:ASP:HB2	2:N:198:GLY:O	1.39	1.19
2:P:477:ASP:C	2:N:310:LYS:HE2	0.95	1.19
1:J:30:LYS:CE	2:N:283:PRO:HG2	1.73	1.19
2:H:199:ASP:HB2	3:V:198:GLY:O	1.39	1.19
2:B:350:LEU:CD2	2:A:385:LEU:HG	1.58	1.18
2:N:248:VAL:O	2:N:433:LEU:HD23	1.35	1.18
6:Q:733:LYS:HZ1	6:R:683:GLN:CG	1.52	1.18
2:H:530:LEU:CD2	2:F:544:TRP:CD1	2.25	1.18
2:F:199:ASP:HB2	3:L:198:GLY:O	1.39	1.18
1:C:5:PHE:CG	2:E:331:ASN:OD1	1.97	1.18
2:B:530:LEU:CD2	2:A:544:TRP:CD1	2.25	1.18
2:G:371:MET:HE2	2:E:371:MET:CE	1.73	1.18
2:E:199:ASP:HB2	3:K:198:GLY:O	1.39	1.18
2:H:350:LEU:CD2	2:F:385:LEU:HG	1.57	1.18
6:Q:733:LYS:NZ	6:R:683:GLN:CA	2.07	1.18
2:H:384:ALA:HB1	2:F:353:GLN:NE2	1.59	1.18
2:G:530:LEU:CD2	2:E:544:TRP:CD1	2.25	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:274:LYS:NZ	2:P:429:GLU:OE1	1.77	1.18
2:F:245:GLY:CA	2:F:443:GLN:NE2	1.99	1.17
1:C:58:ARG:NH2	2:E:339:TRP:CH2	2.11	1.17
2:G:246:VAL:CG2	2:G:503:MET:HE3	1.62	1.17
2:P:475:GLN:OE1	2:N:311:GLU:O	1.60	1.17
6:Q:733:LYS:NZ	6:R:683:GLN:HA	1.56	1.17
2:B:250:PRO:HG3	2:B:433:LEU:HA	1.27	1.17
2:B:371:MET:HE2	2:A:371:MET:CE	1.75	1.17
6:Q:733:LYS:HZ1	6:R:683:GLN:CA	1.57	1.17
2:B:384:ALA:HB1	2:A:353:GLN:NE2	1.59	1.16
2:A:333:PHE:CE2	2:N:333:PHE:CE1	2.33	1.16
2:G:350:LEU:CD2	2:E:385:LEU:HD11	1.72	1.16
2:A:250:PRO:CG	2:A:433:LEU:CG	2.24	1.16
2:G:384:ALA:HB1	2:E:353:GLN:NE2	1.58	1.16
6:Q:683:GLN:CA	6:R:733:LYS:NZ	2.07	1.16
1:C:5:PHE:HB3	2:E:331:ASN:CG	1.66	1.16
2:G:248:VAL:HG22	2:G:443:GLN:HE22	1.06	1.16
2:P:475:GLN:OE1	2:N:311:GLU:N	1.79	1.16
2:G:350:LEU:HD21	2:E:385:LEU:HG	1.17	1.16
2:E:250:PRO:CG	2:E:433:LEU:CG	2.24	1.15
2:F:250:PRO:HB3	2:F:432:ARG:HB3	1.22	1.15
1:C:58:ARG:NH2	2:E:339:TRP:HH2	1.43	1.15
2:N:249:PRO:HA	2:N:433:LEU:CD2	1.74	1.15
2:N:250:PRO:CD	2:N:429:GLU:HG3	1.70	1.15
2:B:381:SER:HB3	2:A:357:LEU:HD21	1.19	1.15
2:G:371:MET:CE	2:E:371:MET:HE1	1.76	1.15
2:F:250:PRO:CG	2:F:433:LEU:CG	2.24	1.15
1:J:5:PHE:N	2:N:332:LYS:CB	2.11	1.14
2:B:530:LEU:CD2	2:A:544:TRP:NE1	2.10	1.14
2:H:196:LYS:NZ	3:V:196:LYS:HZ2	1.25	1.14
1:J:247:PHE:HB2	6:Q:98:TYR:CE1	1.68	1.14
1:C:6:SER:O	2:E:331:ASN:N	1.78	1.14
2:H:250:PRO:CA	2:H:436:SER:HB2	1.78	1.14
2:A:250:PRO:HB3	2:A:432:ARG:HB3	1.22	1.14
2:G:250:PRO:HG3	2:G:433:LEU:HA	1.27	1.14
2:H:248:VAL:HG22	2:H:443:GLN:HE22	1.06	1.14
2:H:357:LEU:HD21	2:F:381:SER:CB	1.78	1.14
2:G:530:LEU:CD2	2:E:544:TRP:NE1	2.10	1.13
2:P:249:PRO:HA	2:P:433:LEU:HD21	1.16	1.13
1:J:5:PHE:CB	2:N:332:LYS:HB2	1.79	1.13
2:B:357:LEU:HD21	2:A:381:SER:CB	1.78	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:357:LEU:HD21	2:E:381:SER:CB	1.78	1.13
2:P:250:PRO:HD3	2:P:433:LEU:CG	1.78	1.13
2:H:530:LEU:CD2	2:F:544:TRP:NE1	2.10	1.13
2:N:250:PRO:CA	2:N:429:GLU:CD	2.16	1.13
6:Q:683:GLN:HG3	6:R:733:LYS:HZ1	1.04	1.13
2:G:250:PRO:CA	2:G:436:SER:HB2	1.78	1.12
2:P:310:LYS:HE3	2:N:476:GLN:O	1.47	1.12
2:N:250:PRO:HA	2:N:432:ARG:HD2	1.26	1.12
2:B:250:PRO:CA	2:B:436:SER:HB2	1.78	1.12
2:G:246:VAL:CG2	2:G:503:MET:HE1	1.67	1.12
1:J:247:PHE:HB3	6:Q:98:TYR:CE1	1.75	1.12
1:C:5:PHE:CD1	2:E:331:ASN:OD1	2.01	1.12
1:J:217:PRO:CG	2:G:390:LEU:HG	1.54	1.11
2:H:381:SER:HB3	2:F:357:LEU:HD21	1.19	1.11
2:A:250:PRO:HG3	2:A:433:LEU:HG	1.17	1.11
2:G:479:LEU:HD23	3:L:310:LYS:HE3	1.31	1.11
2:E:250:PRO:HG3	2:E:433:LEU:HG	1.17	1.11
2:H:250:PRO:HG3	2:H:433:LEU:HA	1.28	1.11
2:A:332:LYS:HA	2:N:331:ASN:C	1.68	1.11
2:B:246:VAL:HG22	2:B:503:MET:HE1	1.12	1.10
2:B:248:VAL:HG22	2:B:443:GLN:HE22	1.07	1.10
2:B:371:MET:HE2	2:A:371:MET:HE1	1.25	1.10
1:J:230:GLU:HB3	6:Q:101:ASN:CG	1.71	1.10
1:C:217:PRO:CD	2:B:392:PRO:HG3	1.80	1.10
2:H:381:SER:CB	2:F:357:LEU:HD21	1.81	1.10
6:Q:725:THR:HG21	6:R:722:THR:HG21	1.31	1.10
2:G:381:SER:HB3	2:E:357:LEU:HD21	1.19	1.10
2:N:248:VAL:O	2:N:433:LEU:CD2	1.99	1.10
2:B:381:SER:CB	2:A:357:LEU:HD21	1.81	1.10
2:H:250:PRO:HB3	2:H:436:SER:HB3	1.20	1.10
2:G:246:VAL:HG23	2:G:503:MET:HE3	1.12	1.09
2:G:350:LEU:HD22	2:E:385:LEU:HD21	1.32	1.09
2:G:250:PRO:HB3	2:G:436:SER:HB3	1.20	1.09
2:G:381:SER:CB	2:E:357:LEU:HD21	1.81	1.09
2:H:350:LEU:HD21	2:F:385:LEU:HG	1.17	1.09
6:Q:722:THR:HG21	6:R:725:THR:HG21	1.31	1.09
2:B:250:PRO:HB3	2:B:436:SER:HB3	1.20	1.09
6:Q:722:THR:HG22	6:R:725:THR:OG1	1.46	1.09
1:C:216:ALA:C	2:B:392:PRO:HG3	1.73	1.08
2:P:310:LYS:CD	2:N:477:ASP:O	1.85	1.08
6:Q:733:LYS:HZ1	6:R:683:GLN:CB	1.65	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:247:PHE:CD1	6:Q:94:GLU:OE2	1.98	1.08
2:B:350:LEU:HD21	2:A:385:LEU:HG	1.17	1.08
2:P:310:LYS:HD2	2:N:480:ASN:HB2	1.17	1.08
1:J:86:SER:HB3	1:C:86:SER:HB3	1.33	1.08
2:G:365:VAL:HG22	2:G:416:ALA:HB1	1.35	1.08
2:H:371:MET:HE2	2:F:371:MET:HE1	1.17	1.08
6:Q:725:THR:OG1	6:R:722:THR:HG22	1.45	1.08
2:G:476:GLN:H	3:L:311:GLU:C	1.45	1.08
2:E:250:PRO:HB3	2:E:432:ARG:HB3	1.22	1.08
2:H:350:LEU:HD22	2:F:385:LEU:HD21	1.32	1.08
1:J:92:ALA:CA	1:C:262:LYS:HD3	1.82	1.07
2:B:350:LEU:HD22	2:A:385:LEU:HD21	1.32	1.07
2:A:333:PHE:CD1	2:N:333:PHE:CD1	2.40	1.07
1:J:6:SER:N	2:A:331:ASN:N	2.02	1.07
1:J:262:LYS:HD3	1:C:92:ALA:CA	1.82	1.07
2:P:310:LYS:HD2	2:N:480:ASN:CB	1.82	1.07
1:J:6:SER:O	2:A:331:ASN:CA	2.02	1.07
1:C:217:PRO:CD	2:B:390:LEU:CG	2.20	1.07
2:B:367:GLN:OE1	2:A:370:ALA:O	1.73	1.07
2:H:367:GLN:OE1	2:F:370:ALA:O	1.73	1.07
1:C:30:LYS:CE	2:P:283:PRO:HG2	1.84	1.06
1:J:243:PRO:CG	6:Q:134:MET:HA	1.84	1.06
2:A:253:GLU:OE2	2:A:428:GLU:OE1	1.74	1.06
2:G:367:GLN:OE1	2:E:370:ALA:O	1.73	1.06
2:H:350:LEU:CD2	2:F:385:LEU:CD2	2.28	1.06
2:H:199:ASP:OD2	3:V:200:LEU:CD2	2.04	1.06
2:F:253:GLU:OE2	2:F:428:GLU:OE1	1.74	1.06
1:C:6:SER:O	2:E:331:ASN:CA	2.04	1.06
2:E:199:ASP:CB	3:K:198:GLY:O	2.04	1.06
2:F:199:ASP:OD2	3:L:200:LEU:CD2	2.04	1.05
1:C:5:PHE:CG	2:E:331:ASN:CG	2.30	1.05
2:A:199:ASP:OD2	3:D:200:LEU:CD2	2.04	1.05
2:G:199:ASP:OD2	2:N:200:LEU:CD2	2.04	1.05
2:G:371:MET:HE2	2:E:371:MET:HE1	1.09	1.05
2:E:199:ASP:OD2	3:K:200:LEU:CD2	2.04	1.05
2:F:250:PRO:HG2	2:F:433:LEU:HG	1.38	1.05
2:F:250:PRO:HG3	2:F:433:LEU:HG	1.17	1.05
1:C:283:PHE:HE1	2:B:545:GLU:HB3	1.14	1.05
2:P:250:PRO:CD	2:P:429:GLU:OE2	2.02	1.05
6:Q:733:LYS:NZ	6:R:683:GLN:CB	2.20	1.05
2:E:253:GLU:OE2	2:E:428:GLU:OE1	1.74	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:250:PRO:CA	2:B:436:SER:CB	2.35	1.05
2:G:350:LEU:CD2	2:E:385:LEU:CD2	2.28	1.05
2:H:199:ASP:CB	3:V:198:GLY:O	2.04	1.05
2:H:250:PRO:CA	2:H:436:SER:CB	2.35	1.05
2:H:365:VAL:HG22	2:H:416:ALA:HB1	1.35	1.05
6:Q:733:LYS:CE	6:R:683:GLN:HA	1.86	1.05
2:B:199:ASP:OD2	2:P:200:LEU:CD2	2.04	1.04
2:A:199:ASP:CB	3:D:198:GLY:O	2.04	1.04
2:G:250:PRO:CA	2:G:436:SER:CB	2.35	1.04
2:H:357:LEU:CD2	2:F:381:SER:HB2	1.87	1.04
6:Q:683:GLN:HA	6:R:733:LYS:CE	1.85	1.04
1:J:217:PRO:N	2:G:392:PRO:HG3	1.70	1.04
2:G:199:ASP:CB	2:N:198:GLY:O	2.04	1.04
2:P:310:LYS:HD3	2:N:480:ASN:HB2	1.06	1.04
2:F:199:ASP:CB	3:L:198:GLY:O	2.04	1.04
2:B:199:ASP:CB	2:P:198:GLY:O	2.04	1.04
2:G:530:LEU:HD22	2:E:544:TRP:NE1	1.73	1.04
6:Q:683:GLN:CB	6:R:733:LYS:NZ	2.20	1.04
2:B:365:VAL:HG22	2:B:416:ALA:HB1	1.35	1.04
1:J:5:PHE:N	2:N:332:LYS:HB3	1.73	1.03
2:G:350:LEU:CD2	2:E:385:LEU:HD21	1.89	1.03
2:G:357:LEU:CD2	2:E:381:SER:HB2	1.87	1.03
2:A:333:PHE:CD1	2:N:333:PHE:HB2	1.93	1.03
2:B:350:LEU:CD2	2:A:385:LEU:HD21	1.89	1.03
2:B:357:LEU:CD2	2:A:381:SER:HB2	1.87	1.03
1:J:283:PHE:HE1	2:G:545:GLU:HB3	1.18	1.02
2:B:350:LEU:CD2	2:A:385:LEU:CD2	2.28	1.02
6:Q:733:LYS:HZ1	6:R:683:GLN:HG3	1.22	1.02
2:H:246:VAL:HG23	2:H:503:MET:HE3	1.04	1.02
2:B:260:PHE:CD2	2:P:198:GLY:HA3	1.95	1.02
2:E:250:PRO:HG2	2:E:433:LEU:HG	1.37	1.02
2:H:371:MET:CE	2:F:367:GLN:O	2.08	1.02
2:B:384:ALA:HB1	2:A:353:GLN:HE21	1.25	1.01
2:A:260:PHE:CD2	3:D:198:GLY:HA3	1.95	1.01
2:E:260:PHE:CD2	3:K:198:GLY:HA3	1.95	1.01
2:N:250:PRO:HD3	2:N:433:LEU:HD11	1.41	1.01
2:H:260:PHE:CD2	3:V:198:GLY:HA3	1.95	1.01
6:Q:725:THR:CB	6:R:722:THR:HG21	1.89	1.01
2:G:350:LEU:HD23	2:E:385:LEU:HD11	1.42	1.01
2:P:249:PRO:CA	2:P:433:LEU:HD21	1.88	1.01
2:N:250:PRO:HB3	2:N:429:GLU:HA	1.37	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:92:ALA:C	1:C:262:LYS:HD3	1.81	1.01
1:C:283:PHE:CE1	2:B:545:GLU:HB3	1.94	1.01
2:B:371:MET:CE	2:A:371:MET:HE1	1.90	1.01
2:A:250:PRO:HG2	2:A:433:LEU:HG	1.37	1.01
2:A:406:LEU:HD23	3:D:220:GLN:HE22	1.21	1.01
2:B:530:LEU:HD22	2:A:544:TRP:NE1	1.73	1.01
2:P:250:PRO:CD	2:P:433:LEU:HD21	1.91	1.01
2:H:246:VAL:HG22	2:H:503:MET:HE1	1.06	1.01
1:J:216:ALA:C	2:G:392:PRO:HG3	1.80	1.01
1:J:261:ASN:OD1	1:C:90:GLU:HG3	1.59	1.01
6:Q:722:THR:HG21	6:R:725:THR:CB	1.89	1.01
2:G:476:GLN:N	3:L:311:GLU:C	2.03	1.00
6:Q:722:THR:HG21	6:R:725:THR:OG1	1.58	1.00
1:J:243:PRO:HG3	6:Q:134:MET:HA	1.38	1.00
1:J:262:LYS:HD3	1:C:92:ALA:C	1.81	1.00
1:C:217:PRO:CB	2:B:390:LEU:CD1	2.30	1.00
2:F:406:LEU:HD23	3:L:220:GLN:HE22	1.21	1.00
6:Q:725:THR:OG1	6:R:722:THR:HG21	1.58	1.00
2:G:371:MET:CE	2:E:367:GLN:O	2.08	1.00
2:H:245:GLY:C	2:H:503:MET:HG3	1.82	1.00
2:B:371:MET:CE	2:A:367:GLN:O	2.08	1.00
2:F:260:PHE:CD2	3:L:198:GLY:HA3	1.95	1.00
1:J:230:GLU:CB	6:Q:101:ASN:OD1	2.08	0.99
1:J:90:GLU:HG3	1:C:261:ASN:OD1	1.59	0.99
2:E:406:LEU:HD23	3:K:220:GLN:HE22	1.21	0.99
2:N:250:PRO:CA	2:N:429:GLU:OE1	2.09	0.99
2:G:260:PHE:CD2	2:N:198:GLY:HA3	1.95	0.99
1:C:217:PRO:CG	2:B:390:LEU:HG	1.75	0.99
2:P:250:PRO:HD3	2:P:433:LEU:CD1	1.91	0.99
2:H:370:ALA:CA	2:F:367:GLN:OE1	2.11	0.99
2:H:530:LEU:HD22	2:F:544:TRP:NE1	1.73	0.99
2:H:350:LEU:CD2	2:F:385:LEU:HD21	1.89	0.99
2:H:371:MET:CE	2:F:371:MET:HE1	1.93	0.99
2:H:372:ALA:HB1	2:H:409:ARG:HH11	1.28	0.99
2:G:196:LYS:NZ	2:N:196:LYS:HZ3	1.52	0.98
1:J:83:GLU:O	1:C:88:VAL:HG21	1.63	0.98
2:B:371:MET:HE3	2:A:367:GLN:O	1.61	0.98
1:J:6:SER:C	2:A:331:ASN:N	2.16	0.98
2:B:245:GLY:C	2:B:503:MET:HG3	1.83	0.98
2:B:246:VAL:HG23	2:B:503:MET:HE3	1.01	0.98
2:B:196:LYS:NZ	2:P:196:LYS:HZ3	1.55	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:384:ALA:HB1	2:E:353:GLN:HE21	1.25	0.98
2:N:250:PRO:CB	2:N:432:ARG:HH21	1.76	0.98
2:B:370:ALA:CA	2:A:367:GLN:OE1	2.11	0.98
2:A:333:PHE:CE1	2:N:333:PHE:CD1	2.51	0.98
1:J:5:PHE:HB2	2:N:332:LYS:HB2	1.42	0.98
2:G:245:GLY:C	2:G:503:MET:HG3	1.82	0.98
2:H:350:LEU:HD23	2:F:385:LEU:HD11	1.42	0.98
1:J:88:VAL:HG21	1:C:83:GLU:O	1.63	0.97
2:G:196:LYS:HZ3	2:N:196:LYS:NZ	1.44	0.97
1:J:247:PHE:CB	6:Q:98:TYR:HE1	1.56	0.97
2:G:371:MET:HE3	2:E:367:GLN:O	1.63	0.97
1:J:247:PHE:CG	6:Q:98:TYR:CE1	2.44	0.97
2:G:250:PRO:CG	2:G:433:LEU:HA	1.94	0.97
2:G:370:ALA:CA	2:E:367:GLN:OE1	2.11	0.97
6:Q:683:GLN:HA	6:R:733:LYS:HZ2	1.25	0.97
1:J:90:GLU:HG2	1:C:261:ASN:CG	1.64	0.97
2:B:250:PRO:CG	2:B:433:LEU:HA	1.94	0.97
2:B:350:LEU:HD23	2:A:385:LEU:HD11	1.42	0.97
2:A:332:LYS:CG	2:N:331:ASN:N	2.28	0.97
2:A:406:LEU:HD21	3:D:220:GLN:NE2	1.80	0.97
2:A:406:LEU:HD21	3:D:220:GLN:HE22	1.30	0.97
2:H:196:LYS:HZ3	3:V:196:LYS:NZ	1.43	0.97
2:P:250:PRO:HD3	2:P:433:LEU:HD11	1.46	0.96
2:P:477:ASP:O	2:N:310:LYS:HE2	1.62	0.96
2:G:372:ALA:HB1	2:G:409:ARG:HH11	1.28	0.96
2:H:196:LYS:NZ	3:V:196:LYS:HZ3	1.47	0.96
2:F:406:LEU:HD21	3:L:220:GLN:NE2	1.80	0.96
2:E:406:LEU:HD21	3:K:220:GLN:NE2	1.80	0.96
1:J:82:TYR:CZ	1:C:90:GLU:OE2	2.19	0.96
6:Q:733:LYS:NZ	6:R:683:GLN:HG3	1.77	0.96
1:J:90:GLU:OE2	1:C:82:TYR:CZ	2.18	0.96
2:H:246:VAL:CG2	2:H:503:MET:HE1	1.80	0.96
1:C:217:PRO:CA	2:B:390:LEU:HD12	1.94	0.95
2:B:350:LEU:CG	2:A:385:LEU:HD21	1.95	0.95
1:J:217:PRO:CG	2:G:390:LEU:CG	2.11	0.95
1:J:261:ASN:OD1	1:C:90:GLU:CG	2.11	0.95
2:G:350:LEU:CG	2:E:385:LEU:HD21	1.95	0.95
2:E:196:LYS:HZ3	3:K:196:LYS:NZ	1.43	0.95
2:P:250:PRO:CB	2:P:432:ARG:HD2	1.96	0.95
2:H:250:PRO:CG	2:H:433:LEU:HA	1.95	0.95
2:H:350:LEU:CG	2:F:385:LEU:HD21	1.95	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:372:ALA:HB1	2:B:409:ARG:HH11	1.28	0.95
2:E:406:LEU:HD21	3:K:220:GLN:HE22	1.30	0.94
1:J:217:PRO:CD	2:G:390:LEU:CD1	2.44	0.94
1:J:30:LYS:HE2	2:N:283:PRO:HG2	1.44	0.94
2:G:248:VAL:HG21	2:G:443:GLN:HE22	0.79	0.94
2:A:336:GLN:HB2	2:N:332:LYS:HZ1	1.31	0.94
1:J:261:ASN:CG	1:C:90:GLU:HG2	1.64	0.94
2:G:357:LEU:HD21	2:E:381:SER:HB2	0.95	0.94
2:E:196:LYS:NZ	3:K:196:LYS:HZ3	1.52	0.94
1:C:217:PRO:CG	2:B:390:LEU:CG	2.33	0.94
2:B:371:MET:SD	2:A:367:GLN:HB3	2.08	0.94
2:G:371:MET:SD	2:E:367:GLN:HB3	2.08	0.94
2:P:250:PRO:HD3	2:P:433:LEU:CD2	1.98	0.94
2:H:371:MET:SD	2:F:367:GLN:HB3	2.08	0.94
2:F:406:LEU:HD21	3:L:220:GLN:HE22	1.30	0.94
2:A:245:GLY:HA2	2:A:443:GLN:HE22	1.32	0.94
1:J:90:GLU:CG	1:C:261:ASN:OD1	2.11	0.94
2:G:470:ARG:HH11	2:H:352:ASN:HD21	1.14	0.94
2:G:530:LEU:HD22	2:E:544:TRP:CE2	2.03	0.94
2:B:530:LEU:HD22	2:A:544:TRP:CE2	2.03	0.93
6:Q:683:GLN:HG2	6:R:733:LYS:NZ	1.83	0.93
1:J:58:ARG:NH2	2:A:339:TRP:CH2	2.36	0.93
2:H:530:LEU:HD22	2:F:544:TRP:CE2	2.03	0.93
2:F:196:LYS:HZ3	3:L:196:LYS:NZ	1.43	0.93
1:J:247:PHE:HD1	6:Q:94:GLU:OE2	1.39	0.93
2:E:245:GLY:HA2	2:E:443:GLN:HE22	1.32	0.93
2:E:406:LEU:CD2	3:K:220:GLN:NE2	2.32	0.93
2:P:247:VAL:HG11	2:P:513:ARG:HH11	1.33	0.93
1:C:5:PHE:CB	2:E:331:ASN:CG	2.30	0.93
2:B:357:LEU:HD21	2:A:381:SER:HB2	0.95	0.93
2:B:371:MET:CE	2:A:371:MET:CE	2.46	0.93
2:F:406:LEU:CD2	3:L:220:GLN:NE2	2.32	0.93
1:C:6:SER:C	2:E:331:ASN:N	2.22	0.93
2:B:248:VAL:HG21	2:B:443:GLN:HE22	0.78	0.93
2:N:247:VAL:HG12	2:N:513:ARG:HH11	1.33	0.93
2:H:371:MET:CE	2:F:371:MET:CE	2.46	0.93
1:J:5:PHE:CG	2:A:331:ASN:ND2	2.33	0.92
2:A:333:PHE:CD2	2:N:333:PHE:CE1	2.53	0.92
2:P:475:GLN:CD	2:N:311:GLU:N	2.19	0.92
2:A:333:PHE:CZ	2:N:333:PHE:CD1	2.56	0.92
2:A:333:PHE:CZ	2:N:333:PHE:CE1	2.57	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:246:VAL:HG22	2:G:503:MET:HE1	0.94	0.92
1:J:283:PHE:CE1	2:G:545:GLU:HB3	2.05	0.92
2:A:333:PHE:CE2	2:N:333:PHE:CD1	2.54	0.92
2:P:251:PRO:HD2	2:P:432:ARG:CD	2.00	0.92
1:J:6:SER:O	2:A:331:ASN:HA	1.70	0.92
2:A:406:LEU:CD2	3:D:220:GLN:NE2	2.32	0.92
2:P:250:PRO:HB3	2:P:432:ARG:HD2	1.50	0.92
2:N:250:PRO:CA	2:N:432:ARG:HD2	1.99	0.92
2:E:199:ASP:CB	3:K:200:LEU:HG	2.00	0.91
2:H:357:LEU:HD21	2:F:381:SER:HB2	0.95	0.91
2:H:199:ASP:CB	3:V:200:LEU:HG	2.00	0.91
2:B:199:ASP:CB	2:P:200:LEU:HG	2.00	0.91
2:G:530:LEU:CD1	2:E:544:TRP:HE1	1.84	0.91
2:H:248:VAL:HG21	2:H:443:GLN:HE22	0.79	0.91
2:F:245:GLY:HA2	2:F:443:GLN:HE22	1.32	0.91
2:N:250:PRO:HA	2:N:432:ARG:CD	2.01	0.91
6:Q:733:LYS:NZ	6:R:683:GLN:HG2	1.83	0.91
1:J:58:ARG:NH2	2:A:339:TRP:HH2	1.67	0.91
2:A:332:LYS:HD3	2:N:497:ARG:HD3	1.52	0.90
2:G:240:HIS:CG	2:G:248:VAL:HG21	2.07	0.90
2:N:251:PRO:HD3	2:N:432:ARG:HD3	1.50	0.90
2:A:199:ASP:CB	3:D:200:LEU:HG	2.00	0.90
2:E:250:PRO:HB3	2:E:432:ARG:HB2	1.53	0.90
2:H:530:LEU:CD1	2:F:544:TRP:HE1	1.84	0.90
1:J:82:TYR:HH	1:C:88:VAL:CG1	1.84	0.90
2:H:384:ALA:HB1	2:F:353:GLN:HE21	1.25	0.90
2:G:267:SER:HB3	2:G:432:ARG:HH11	1.08	0.90
3:K:240:HIS:CG	3:K:248:VAL:HG21	2.07	0.90
1:J:88:VAL:HG13	1:C:82:TYR:OH	1.71	0.90
2:F:199:ASP:CB	3:L:200:LEU:HG	2.00	0.90
2:F:240:HIS:CG	2:F:248:VAL:HG21	2.07	0.90
2:F:250:PRO:HB3	2:F:432:ARG:HB2	1.53	0.90
1:C:217:PRO:HD3	2:B:392:PRO:HG3	1.52	0.90
2:E:196:LYS:HZ1	3:K:196:LYS:NZ	1.67	0.90
2:G:199:ASP:CB	2:N:200:LEU:HG	2.00	0.90
1:C:5:PHE:N	2:P:332:LYS:HB2	1.86	0.90
2:B:530:LEU:CD1	2:A:544:TRP:HE1	1.84	0.90
2:B:196:LYS:HZ2	2:P:196:LYS:NZ	1.69	0.90
2:A:336:GLN:CB	2:N:332:LYS:NZ	2.35	0.90
2:E:240:HIS:CG	2:E:248:VAL:HG21	2.06	0.90
2:A:331:ASN:HD21	2:N:332:LYS:CE	1.84	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:334:VAL:HG22	2:N:451:TRP:CZ2	2.06	0.89
2:N:240:HIS:CG	2:N:248:VAL:HG21	2.07	0.89
2:H:196:LYS:HZ2	3:V:196:LYS:NZ	1.67	0.89
3:L:240:HIS:CG	3:L:248:VAL:HG21	2.07	0.89
2:G:196:LYS:HZ1	2:N:196:LYS:NZ	1.65	0.89
2:H:240:HIS:CG	2:H:248:VAL:HG21	2.07	0.89
2:B:240:HIS:CG	2:B:248:VAL:HG21	2.07	0.89
3:D:240:HIS:CG	3:D:248:VAL:HG21	2.06	0.89
1:J:217:PRO:HD2	2:G:390:LEU:CD2	2.03	0.89
2:A:250:PRO:HB3	2:A:432:ARG:HB2	1.53	0.89
2:B:353:GLN:HE22	2:A:384:ALA:HB3	1.34	0.89
2:A:196:LYS:HZ3	3:D:196:LYS:NZ	1.43	0.89
2:A:196:LYS:HZ1	3:D:196:LYS:NZ	1.68	0.89
2:A:240:HIS:CG	2:A:248:VAL:HG21	2.07	0.89
2:P:240:HIS:CG	2:P:248:VAL:HG21	2.07	0.89
1:J:92:ALA:CA	1:C:262:LYS:CD	2.47	0.89
2:B:250:PRO:CD	2:B:436:SER:OG	2.21	0.89
3:V:240:HIS:CG	3:V:248:VAL:HG21	2.06	0.89
1:C:58:ARG:NH2	2:E:339:TRP:CZ2	2.40	0.89
2:H:371:MET:HE3	2:F:367:GLN:O	1.70	0.89
1:J:217:PRO:CD	2:G:392:PRO:HG3	2.02	0.89
2:G:353:GLN:HE22	2:E:384:ALA:HB3	1.34	0.89
2:G:470:ARG:HH11	2:H:352:ASN:ND2	1.70	0.89
1:J:82:TYR:OH	1:C:88:VAL:HG13	1.71	0.88
2:A:334:VAL:HG21	2:N:451:TRP:HE1	1.37	0.88
2:H:250:PRO:CD	2:H:436:SER:OG	2.21	0.88
2:P:477:ASP:O	2:N:310:LYS:CE	2.17	0.88
2:N:250:PRO:CB	2:N:429:GLU:HA	1.99	0.88
6:Q:733:LYS:HE3	6:R:683:GLN:HA	1.54	0.88
2:A:196:LYS:NZ	3:D:196:LYS:HZ3	1.64	0.88
2:G:250:PRO:CD	2:G:436:SER:OG	2.21	0.88
2:P:310:LYS:CE	2:N:476:GLN:O	2.21	0.88
2:H:353:GLN:HE22	2:F:384:ALA:HB3	1.34	0.88
2:E:196:LYS:HZ2	3:K:196:LYS:NZ	1.69	0.88
6:Q:683:GLN:CB	6:R:733:LYS:HZ1	1.81	0.88
2:B:371:MET:CE	2:A:367:GLN:HB3	2.04	0.88
2:P:475:GLN:HE22	2:N:311:GLU:CB	1.86	0.88
2:H:199:ASP:HB3	3:V:200:LEU:HG	1.56	0.88
1:J:5:PHE:CG	2:N:332:LYS:HB2	2.09	0.88
1:J:217:PRO:CA	2:G:390:LEU:CD1	2.47	0.88
2:G:199:ASP:HB3	2:N:200:LEU:HG	1.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:371:MET:HE2	2:F:371:MET:HE2	1.56	0.88
2:F:196:LYS:HZ2	3:L:196:LYS:NZ	1.67	0.88
2:B:267:SER:HB3	2:B:432:ARG:HH11	1.08	0.87
2:N:250:PRO:HB3	2:N:432:ARG:HH21	1.39	0.87
1:C:216:ALA:C	2:B:392:PRO:CG	2.42	0.87
2:F:199:ASP:HB3	3:L:200:LEU:HG	1.56	0.87
2:G:371:MET:CE	2:E:367:GLN:HB3	2.04	0.87
2:B:250:PRO:HG3	2:B:433:LEU:CA	2.04	0.87
2:B:196:LYS:HZ1	2:P:196:LYS:NZ	1.67	0.87
2:F:196:LYS:NZ	3:L:196:LYS:HZ3	1.69	0.87
1:J:88:VAL:HB	1:C:84:PHE:HA	1.57	0.86
2:B:199:ASP:HB3	2:P:200:LEU:HG	1.56	0.86
2:H:250:PRO:HG3	2:H:433:LEU:CA	2.04	0.86
2:F:196:LYS:HZ1	3:L:196:LYS:NZ	1.69	0.86
6:Q:683:GLN:HA	6:R:733:LYS:HE3	1.54	0.86
2:A:196:LYS:HZ2	3:D:196:LYS:NZ	1.69	0.86
2:G:196:LYS:HZ2	2:N:196:LYS:NZ	1.72	0.86
2:B:260:PHE:HD2	2:P:198:GLY:HA3	1.40	0.86
2:H:196:LYS:HZ1	3:V:196:LYS:NZ	1.70	0.86
2:N:251:PRO:HD3	2:N:432:ARG:CD	2.04	0.86
2:H:260:PHE:HD2	3:V:198:GLY:HA3	1.40	0.86
2:H:371:MET:CE	2:F:367:GLN:HB3	2.04	0.86
1:J:30:LYS:NZ	2:N:283:PRO:HG2	1.91	0.86
1:J:82:TYR:HE1	1:C:65:LYS:HZ2	0.87	0.86
1:J:262:LYS:CD	1:C:92:ALA:CA	2.47	0.86
6:Q:722:THR:CG2	6:R:721:ASP:O	2.24	0.86
2:G:479:LEU:CD2	3:L:310:LYS:HE3	2.05	0.85
2:H:267:SER:HB3	2:H:432:ARG:HH11	1.08	0.85
2:B:250:PRO:N	2:B:436:SER:HB2	1.91	0.85
1:J:65:LYS:HZ2	1:C:82:TYR:HE1	0.87	0.85
2:G:250:PRO:HG3	2:G:433:LEU:CA	2.04	0.85
2:G:530:LEU:HD21	2:E:544:TRP:NE1	1.85	0.85
2:H:250:PRO:N	2:H:436:SER:HB2	1.91	0.85
2:P:251:PRO:CD	2:P:432:ARG:HD3	2.06	0.85
1:C:6:SER:N	2:E:331:ASN:N	2.25	0.85
2:A:199:ASP:HB3	3:D:200:LEU:HG	1.56	0.85
2:B:196:LYS:HZ3	2:P:196:LYS:NZ	1.43	0.85
2:A:250:PRO:HB2	2:A:432:ARG:NE	1.92	0.85
2:G:250:PRO:N	2:G:436:SER:HB2	1.92	0.85
2:E:250:PRO:HB2	2:E:432:ARG:NE	1.92	0.85
6:Q:683:GLN:CA	6:R:733:LYS:HZ2	1.79	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:5:PHE:CD2	2:N:332:LYS:CB	2.58	0.84
2:E:199:ASP:HB3	3:K:200:LEU:HG	1.56	0.84
6:Q:721:ASP:O	6:R:722:THR:CG2	2.24	0.84
1:J:84:PHE:HA	1:C:88:VAL:HB	1.57	0.84
2:A:260:PHE:HD2	3:D:198:GLY:HA3	1.40	0.84
2:G:260:PHE:HD2	2:N:198:GLY:HA3	1.40	0.84
3:K:311:GLU:O	2:H:476:GLN:HB2	1.77	0.84
2:F:260:PHE:HD2	3:L:198:GLY:HA3	1.40	0.84
2:P:247:VAL:HG11	2:P:513:ARG:NH1	1.92	0.84
2:B:384:ALA:CB	2:A:353:GLN:NE2	2.41	0.84
1:C:6:SER:O	2:E:331:ASN:HA	1.76	0.84
2:P:250:PRO:HD3	2:P:433:LEU:HD21	1.56	0.84
1:J:88:VAL:CG1	1:C:82:TYR:HH	1.84	0.84
1:J:82:TYR:HE1	1:C:65:LYS:NZ	1.74	0.84
2:H:246:VAL:HG23	2:H:503:MET:CE	1.84	0.84
2:H:371:MET:HE1	2:F:367:GLN:O	1.74	0.84
2:H:384:ALA:CB	2:F:353:GLN:NE2	2.41	0.84
1:J:88:VAL:HG11	1:C:82:TYR:CE2	2.13	0.84
2:B:246:VAL:HG23	2:B:503:MET:CE	1.84	0.83
1:C:217:PRO:CD	2:B:390:LEU:CD1	2.55	0.83
2:P:249:PRO:CA	2:P:433:LEU:CD2	2.49	0.83
2:F:250:PRO:HB2	2:F:432:ARG:NE	1.92	0.83
1:C:217:PRO:HD2	2:B:390:LEU:HG	0.85	0.83
1:C:217:PRO:HB2	2:B:390:LEU:HD12	0.84	0.83
2:B:350:LEU:HD22	2:A:385:LEU:HD11	1.39	0.83
2:P:250:PRO:CA	2:P:429:GLU:OE2	2.25	0.83
1:J:58:ARG:HH21	2:A:339:TRP:HH2	0.88	0.83
1:C:30:LYS:HE2	2:P:283:PRO:HG2	1.59	0.83
2:G:246:VAL:H	2:G:503:MET:HE3	1.43	0.82
2:N:250:PRO:HD3	2:N:433:LEU:CD1	2.08	0.82
1:J:82:TYR:CE2	1:C:88:VAL:HG11	2.13	0.82
2:A:331:ASN:ND2	2:N:332:LYS:CE	2.43	0.82
2:N:251:PRO:CD	2:N:432:ARG:CD	2.58	0.82
6:Q:733:LYS:HZ3	6:R:683:GLN:CG	1.87	0.82
1:J:94:PRO:O	1:C:215:VAL:CG1	2.27	0.82
2:N:247:VAL:CG1	2:N:513:ARG:HH11	1.92	0.82
2:N:249:PRO:CA	2:N:433:LEU:CD2	2.44	0.82
6:Q:722:THR:HA	6:R:722:THR:HA	1.61	0.82
3:K:310:LYS:HG3	2:H:480:ASN:HB2	1.60	0.82
2:H:350:LEU:HD22	2:F:385:LEU:HD11	1.39	0.82
1:J:65:LYS:NZ	1:C:82:TYR:HE1	1.75	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:250:PRO:CB	2:A:432:ARG:NE	2.43	0.82
2:G:384:ALA:CB	2:E:353:GLN:NE2	2.41	0.82
2:P:477:ASP:OD1	2:N:310:LYS:HG2	1.79	0.82
2:B:371:MET:HE2	2:A:371:MET:HE2	1.60	0.82
2:G:455:GLU:OE1	2:H:334:VAL:HG11	1.80	0.82
2:H:384:ALA:CB	2:F:353:GLN:HE21	1.93	0.82
2:H:530:LEU:HD21	2:F:544:TRP:NE1	1.85	0.82
2:F:250:PRO:CB	2:F:432:ARG:NE	2.43	0.81
2:E:260:PHE:HD2	3:K:198:GLY:HA3	1.40	0.81
2:P:310:LYS:HD3	2:N:480:ASN:CB	1.98	0.81
2:B:530:LEU:HD21	2:A:544:TRP:NE1	1.85	0.81
2:A:333:PHE:CD1	2:N:333:PHE:CG	2.68	0.81
6:Q:683:GLN:CB	6:R:733:LYS:HZ2	1.88	0.81
2:E:250:PRO:CB	2:E:432:ARG:NE	2.43	0.81
2:A:250:PRO:CB	2:A:432:ARG:HB3	2.09	0.81
2:G:248:VAL:HG22	2:G:443:GLN:NE2	1.74	0.81
2:A:334:VAL:CG2	2:N:451:TRP:HE1	1.94	0.80
2:G:338:ASP:HA	2:G:341:HIS:CE1	2.17	0.80
6:R:107:TYR:CE1	6:R:147:LEU:HD13	2.17	0.80
2:B:384:ALA:CB	2:A:353:GLN:HE21	1.93	0.80
2:G:352:ASN:HD21	2:H:470:ARG:NH1	1.77	0.80
2:N:250:PRO:HB3	2:N:432:ARG:NH2	1.96	0.80
1:C:30:LYS:NZ	2:P:283:PRO:HG2	1.95	0.80
1:J:5:PHE:N	2:N:332:LYS:HB2	1.96	0.80
1:J:82:TYR:OH	1:C:65:LYS:HD2	1.81	0.80
1:J:215:VAL:CG1	1:C:94:PRO:O	2.27	0.80
6:Q:107:TYR:CE1	6:Q:147:LEU:HD13	2.16	0.80
2:G:371:MET:HE1	2:E:367:GLN:O	1.82	0.80
2:G:384:ALA:CB	2:E:353:GLN:HE21	1.93	0.80
2:B:338:ASP:HA	2:B:341:HIS:CE1	2.17	0.80
3:K:311:GLU:O	2:H:476:GLN:HB3	1.13	0.80
1:J:217:PRO:HD2	2:G:390:LEU:HG	0.81	0.80
2:H:244:PRO:O	2:H:447:ALA:HB2	1.82	0.80
2:A:331:ASN:HD21	2:N:332:LYS:NZ	1.79	0.79
2:G:244:PRO:O	2:G:447:ALA:HB2	1.82	0.79
6:Q:683:GLN:CA	6:R:733:LYS:HZ1	1.80	0.79
1:J:65:LYS:HD2	1:C:82:TYR:OH	1.81	0.79
2:G:476:GLN:N	3:L:311:GLU:O	2.09	0.79
1:J:86:SER:O	1:C:86:SER:O	1.99	0.79
1:J:229:PHE:CE1	6:Q:105:ARG:NH1	2.50	0.79
2:P:480:ASN:HB2	2:N:310:LYS:HD3	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:251:PRO:HD2	2:N:432:ARG:NH2	1.97	0.79
6:R:447:HIS:CE1	6:R:448:ALA:HB2	2.17	0.79
1:J:217:PRO:N	2:G:390:LEU:CD1	2.46	0.79
2:B:244:PRO:O	2:B:447:ALA:HB2	1.82	0.79
2:E:250:PRO:CB	2:E:432:ARG:HB3	2.09	0.79
2:E:250:PRO:CB	2:E:432:ARG:HE	1.95	0.79
2:A:331:ASN:O	2:N:331:ASN:HA	1.83	0.79
2:G:253:GLU:H	2:G:268:ARG:HA	1.48	0.79
2:A:199:ASP:OD2	3:D:200:LEU:HG	1.83	0.79
2:G:352:ASN:HD21	2:H:470:ARG:HH11	1.29	0.79
2:N:245:GLY:HA2	2:N:440:ALA:HB2	1.64	0.79
2:H:338:ASP:HA	2:H:341:HIS:CE1	2.16	0.79
3:D:253:GLU:H	3:D:268:ARG:HA	1.48	0.79
2:B:199:ASP:OD2	2:P:200:LEU:HG	1.83	0.79
2:A:199:ASP:OD2	3:D:200:LEU:HD21	1.83	0.79
2:A:250:PRO:HG3	2:A:433:LEU:CG	2.02	0.79
2:N:250:PRO:HB3	2:N:429:GLU:CA	2.12	0.79
2:P:253:GLU:H	2:P:268:ARG:HA	1.48	0.79
1:J:217:PRO:HB2	2:G:390:LEU:HD12	0.79	0.78
1:C:5:PHE:HB3	2:E:331:ASN:CA	2.12	0.78
2:A:250:PRO:CB	2:A:432:ARG:HE	1.95	0.78
2:N:249:PRO:HA	2:N:433:LEU:HD21	0.80	0.78
2:F:199:ASP:OD2	3:L:200:LEU:HG	1.83	0.78
2:E:199:ASP:CA	3:K:198:GLY:O	2.30	0.78
2:B:253:GLU:H	2:B:268:ARG:HA	1.48	0.78
2:G:199:ASP:OD2	2:N:200:LEU:HD21	1.83	0.78
2:A:199:ASP:CA	3:D:198:GLY:O	2.30	0.78
2:G:199:ASP:OD2	2:N:200:LEU:HG	1.83	0.78
1:J:5:PHE:CD2	2:A:331:ASN:ND2	2.51	0.78
1:C:5:PHE:CG	2:E:331:ASN:ND2	2.50	0.78
2:E:253:GLU:H	2:E:268:ARG:HA	1.48	0.78
2:P:247:VAL:CG1	2:P:513:ARG:HH11	1.96	0.78
2:F:250:PRO:CB	2:F:432:ARG:HB3	2.09	0.78
3:L:253:GLU:H	3:L:268:ARG:HA	1.48	0.78
6:Q:733:LYS:HZ3	6:R:683:GLN:HG2	1.44	0.78
2:A:253:GLU:H	2:A:268:ARG:HA	1.48	0.78
2:G:530:LEU:HD13	2:E:544:TRP:HE1	1.46	0.78
2:E:199:ASP:OD2	3:K:200:LEU:HG	1.83	0.78
2:H:199:ASP:OD2	3:V:200:LEU:HD21	1.83	0.78
1:J:5:PHE:HB3	2:A:331:ASN:CA	2.13	0.78
2:B:530:LEU:HD13	2:A:544:TRP:HE1	1.46	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:455:GLU:OE1	2:H:334:VAL:CG1	2.32	0.78
2:E:199:ASP:OD2	3:K:200:LEU:HD21	1.83	0.78
6:Q:733:LYS:HZ2	6:R:683:GLN:HA	1.47	0.78
2:B:371:MET:HE1	2:A:367:GLN:O	1.84	0.78
2:A:333:PHE:CE2	2:N:333:PHE:HE1	1.99	0.78
2:H:199:ASP:CA	3:V:198:GLY:O	2.30	0.78
1:J:217:PRO:CB	2:G:390:LEU:CG	2.56	0.77
2:N:247:VAL:HG12	2:N:513:ARG:NH1	1.99	0.77
2:H:253:GLU:H	2:H:268:ARG:HA	1.48	0.77
2:F:253:GLU:H	2:F:268:ARG:HA	1.48	0.77
6:Q:447:HIS:CE1	6:Q:448:ALA:HB2	2.17	0.77
2:E:250:PRO:HB2	2:E:432:ARG:HE	1.48	0.77
2:H:530:LEU:HD13	2:F:544:TRP:HE1	1.47	0.77
2:F:250:PRO:HG3	2:F:433:LEU:CG	2.02	0.77
6:Q:438:ALA:HB2	6:Q:484:THR:HG21	1.67	0.77
3:K:253:GLU:H	3:K:268:ARG:HA	1.48	0.77
6:R:438:ALA:HB2	6:R:484:THR:HG21	1.67	0.77
2:B:199:ASP:OD2	2:P:200:LEU:HD21	1.83	0.77
2:B:199:ASP:CA	2:P:198:GLY:O	2.30	0.77
2:H:350:LEU:CB	2:F:385:LEU:HD21	2.14	0.77
2:F:250:PRO:CB	2:F:432:ARG:HE	1.95	0.77
3:V:253:GLU:H	3:V:268:ARG:HA	1.48	0.77
2:F:199:ASP:CA	3:L:198:GLY:O	2.30	0.77
2:G:350:LEU:CB	2:E:385:LEU:HD21	2.14	0.77
2:B:246:VAL:CG2	2:B:503:MET:HE1	1.86	0.77
2:G:480:ASN:HB2	3:L:310:LYS:CG	2.14	0.77
2:N:250:PRO:CB	2:N:432:ARG:NH2	2.48	0.77
2:A:333:PHE:CD1	2:N:333:PHE:CB	2.67	0.77
2:G:480:ASN:HB2	3:L:310:LYS:HG3	1.67	0.77
1:J:30:LYS:HE2	2:N:283:PRO:CG	2.15	0.77
1:C:217:PRO:HD3	2:B:392:PRO:CG	2.15	0.77
2:B:246:VAL:H	2:B:503:MET:HE3	1.49	0.77
2:B:248:VAL:HG22	2:B:443:GLN:NE2	1.74	0.77
2:G:250:PRO:CA	2:G:436:SER:HB3	2.14	0.77
2:H:246:VAL:H	2:H:503:MET:HE3	1.46	0.77
1:J:243:PRO:HG2	6:Q:134:MET:HA	1.67	0.76
2:B:350:LEU:CB	2:A:385:LEU:HD21	2.14	0.76
2:G:199:ASP:CA	2:N:198:GLY:O	2.30	0.76
2:N:253:GLU:H	2:N:268:ARG:HA	1.48	0.76
2:B:250:PRO:CA	2:B:436:SER:HB3	2.14	0.76
2:G:245:GLY:CA	2:G:503:MET:HG3	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:199:ASP:OD2	3:L:200:LEU:HD21	1.83	0.76
2:B:384:ALA:HB1	2:A:353:GLN:HE22	1.50	0.76
3:K:311:GLU:C	2:H:476:GLN:N	2.32	0.76
2:A:199:ASP:CG	3:D:200:LEU:HG	2.06	0.76
2:G:246:VAL:HG23	2:G:503:MET:CE	1.84	0.76
2:H:250:PRO:CA	2:H:436:SER:HB3	2.14	0.76
6:Q:435:GLY:HA2	6:Q:439:TYR:CD2	2.21	0.76
2:G:470:ARG:HH12	2:H:348:ASP:CB	1.99	0.76
2:E:199:ASP:CG	3:K:200:LEU:HG	2.06	0.76
2:P:250:PRO:HB3	2:P:429:GLU:HA	1.66	0.76
2:P:251:PRO:HD3	2:P:432:ARG:HD3	1.66	0.76
2:H:199:ASP:OD2	3:V:200:LEU:HG	1.83	0.76
1:J:217:PRO:HD2	2:G:390:LEU:CD1	2.15	0.76
1:J:247:PHE:HB2	6:Q:98:TYR:HD1	1.48	0.76
2:B:199:ASP:CG	2:P:200:LEU:HG	2.06	0.76
2:B:199:ASP:OD2	2:P:200:LEU:CG	2.34	0.75
2:A:199:ASP:OD2	3:D:200:LEU:CG	2.33	0.75
2:H:245:GLY:CA	2:H:503:MET:HG3	2.15	0.75
6:R:435:GLY:HA2	6:R:439:TYR:CD2	2.21	0.75
2:A:250:PRO:HB2	2:A:432:ARG:HE	1.49	0.75
6:Q:683:GLN:HG2	6:R:733:LYS:HZ3	1.48	0.75
2:B:245:GLY:CA	2:B:503:MET:HG3	2.15	0.75
2:P:250:PRO:CB	2:P:432:ARG:HH21	1.98	0.75
2:H:250:PRO:CB	2:H:436:SER:OG	2.34	0.75
2:F:199:ASP:OD2	3:L:200:LEU:CG	2.33	0.75
1:J:216:ALA:C	2:G:392:PRO:CG	2.55	0.75
2:B:250:PRO:CB	2:B:436:SER:OG	2.34	0.75
2:G:199:ASP:OD2	2:N:200:LEU:CG	2.34	0.75
2:P:477:ASP:OD1	2:N:310:LYS:CG	2.24	0.75
2:H:199:ASP:OD2	3:V:200:LEU:CG	2.34	0.75
2:F:250:PRO:HB2	2:F:432:ARG:HE	1.48	0.75
1:J:5:PHE:HB3	2:A:331:ASN:N	2.02	0.75
2:B:267:SER:CA	2:B:432:ARG:HH12	2.00	0.75
2:G:196:LYS:HZ2	2:N:196:LYS:HZ3	1.29	0.75
2:E:199:ASP:OD2	3:K:200:LEU:CG	2.33	0.75
2:H:199:ASP:CG	3:V:200:LEU:HG	2.06	0.75
2:H:248:VAL:HG22	2:H:443:GLN:NE2	1.74	0.74
2:H:260:PHE:CE2	3:V:198:GLY:HA3	2.22	0.74
2:F:199:ASP:CG	3:L:200:LEU:HG	2.06	0.74
1:J:230:GLU:HB3	6:Q:101:ASN:ND2	2.01	0.74
2:P:251:PRO:HD2	2:P:432:ARG:HD3	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:250:PRO:CD	2:P:433:LEU:CD2	2.61	0.74
2:H:267:SER:CA	2:H:432:ARG:HH12	2.00	0.74
2:G:199:ASP:CG	2:N:200:LEU:HG	2.06	0.74
2:H:384:ALA:HB1	2:F:353:GLN:HE22	1.50	0.74
1:J:230:GLU:CB	6:Q:101:ASN:ND2	2.51	0.74
2:G:384:ALA:HB1	2:E:353:GLN:HE22	1.50	0.74
3:K:311:GLU:HB2	2:H:477:ASP:HB2	1.67	0.74
2:A:333:PHE:CE1	2:N:333:PHE:CG	2.75	0.74
1:C:5:PHE:HB3	2:E:331:ASN:CB	2.17	0.74
2:G:250:PRO:CB	2:G:436:SER:OG	2.34	0.74
2:E:260:PHE:CE2	3:K:198:GLY:HA3	2.22	0.74
2:F:260:PHE:CE2	3:L:198:GLY:HA3	2.23	0.73
1:J:218:ASN:H	2:G:390:LEU:HD11	1.52	0.73
2:B:260:PHE:CE2	2:P:198:GLY:HA3	2.22	0.73
2:E:250:PRO:HG3	2:E:433:LEU:CG	2.02	0.73
2:P:310:LYS:HE2	2:N:478:ARG:N	2.01	0.73
6:Q:683:GLN:CG	6:R:733:LYS:HZ3	1.99	0.73
2:G:371:MET:CE	2:E:371:MET:CE	2.46	0.73
2:H:370:ALA:CB	2:F:367:GLN:OE1	2.36	0.73
2:A:260:PHE:CE2	3:D:198:GLY:HA3	2.23	0.73
2:G:267:SER:CA	2:G:432:ARG:HH12	2.00	0.73
2:H:196:LYS:HZ1	3:V:196:LYS:HZ3	1.27	0.73
2:H:357:LEU:CD2	2:F:381:SER:CB	2.58	0.73
6:R:84:HIS:CD2	6:R:115:ALA:HB1	2.23	0.73
2:G:260:PHE:CE2	2:N:198:GLY:HA3	2.22	0.73
2:A:334:VAL:CG2	2:N:451:TRP:CZ2	2.71	0.73
2:A:345:VAL:HG21	2:N:462:LYS:CE	2.18	0.73
6:Q:686:THR:OG1	6:R:733:LYS:HE3	1.89	0.73
2:P:250:PRO:HD3	2:P:433:LEU:HG	1.69	0.73
1:J:5:PHE:N	2:N:332:LYS:CG	2.52	0.73
2:H:250:PRO:HA	2:H:436:SER:HB2	1.71	0.73
6:Q:84:HIS:CD2	6:Q:115:ALA:HB1	2.23	0.73
2:B:370:ALA:CB	2:A:367:GLN:OE1	2.36	0.72
2:G:357:LEU:HD11	2:E:381:SER:HB3	1.71	0.72
2:G:370:ALA:CB	2:E:367:GLN:OE1	2.36	0.72
1:J:230:GLU:CB	6:Q:101:ASN:CG	2.54	0.72
2:B:357:LEU:HD11	2:A:381:SER:HB3	1.71	0.72
2:P:310:LYS:HD2	2:N:480:ASN:CG	2.08	0.72
2:N:251:PRO:HD2	2:N:432:ARG:CZ	2.19	0.72
2:H:199:ASP:HB3	3:V:200:LEU:CG	2.19	0.72
1:C:217:PRO:HG3	2:B:392:PRO:N	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:250:PRO:CD	2:P:433:LEU:HD11	2.18	0.72
1:J:262:LYS:HB3	1:C:93:ALA:CA	2.20	0.72
2:B:199:ASP:HB3	2:P:200:LEU:CG	2.19	0.72
2:B:372:ALA:HB1	2:B:409:ARG:NH1	2.05	0.72
2:A:199:ASP:HB3	3:D:200:LEU:CG	2.19	0.72
2:G:250:PRO:HB3	2:G:436:SER:CB	2.04	0.72
2:F:199:ASP:HB3	3:L:200:LEU:CG	2.19	0.72
3:K:311:GLU:C	2:H:476:GLN:H	1.92	0.72
2:H:357:LEU:HD11	2:F:381:SER:HB3	1.71	0.72
2:G:199:ASP:HB3	2:N:200:LEU:CG	2.19	0.71
2:E:199:ASP:HB3	3:K:200:LEU:CG	2.19	0.71
1:J:90:GLU:CB	1:C:261:ASN:ND2	2.53	0.71
2:B:382:LEU:HD13	2:B:401:LEU:C	2.11	0.71
2:P:245:GLY:HA2	2:P:440:ALA:HB2	1.72	0.71
1:J:247:PHE:CB	6:Q:98:TYR:CD1	2.42	0.71
2:B:458:LEU:HB2	2:B:489:ALA:HB1	1.73	0.71
2:G:458:LEU:HB2	2:G:489:ALA:HB1	1.73	0.71
2:H:382:LEU:HD13	2:H:401:LEU:C	2.11	0.71
6:Q:733:LYS:HE3	6:R:686:THR:OG1	1.89	0.71
6:R:141:PRO:HD3	6:R:191:ARG:HE	1.55	0.71
1:J:261:ASN:ND2	1:C:90:GLU:CB	2.53	0.71
2:G:382:LEU:HD13	2:G:401:LEU:C	2.11	0.71
6:Q:683:GLN:HG3	6:R:733:LYS:NZ	1.77	0.71
2:N:247:VAL:CG1	2:N:513:ARG:NH1	2.53	0.71
6:Q:666:GLN:HE22	6:Q:711:ARG:HB2	1.55	0.71
1:J:217:PRO:C	2:G:390:LEU:HD12	2.10	0.71
2:A:334:VAL:CG2	2:N:451:TRP:NE1	2.54	0.71
1:C:217:PRO:CD	2:B:392:PRO:CG	2.65	0.71
2:G:470:ARG:NH1	2:H:352:ASN:HD21	1.86	0.71
2:P:310:LYS:HE3	2:N:476:GLN:C	2.09	0.71
1:J:281:ARG:O	2:G:545:GLU:OE1	2.08	0.70
1:J:93:ALA:CA	1:C:262:LYS:HB3	2.20	0.70
1:C:217:PRO:HD2	2:B:390:LEU:CD1	2.17	0.70
6:Q:141:PRO:HD3	6:Q:191:ARG:HE	1.55	0.70
6:R:58:SER:H	6:R:61:GLN:HE21	1.38	0.70
2:F:199:ASP:OD2	3:L:200:LEU:HD23	1.91	0.70
6:R:397:VAL:O	6:R:401:VAL:HG23	1.91	0.70
1:J:5:PHE:N	2:N:332:LYS:HG2	2.07	0.70
2:A:334:VAL:HG22	2:N:451:TRP:HZ2	1.54	0.70
2:G:370:ALA:HB3	2:E:367:GLN:OE1	1.92	0.70
6:Q:397:VAL:O	6:Q:401:VAL:HG23	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:245:GLY:HA2	2:P:440:ALA:CB	2.21	0.70
1:C:58:ARG:CZ	2:E:339:TRP:CH2	2.75	0.70
2:E:199:ASP:OD2	3:K:200:LEU:HD23	1.91	0.70
2:P:250:PRO:HB3	2:P:432:ARG:HH21	1.55	0.70
2:H:458:LEU:HB2	2:H:489:ALA:HB1	1.73	0.69
2:P:310:LYS:CG	2:N:477:ASP:OD1	2.38	0.69
3:D:306:HIS:HA	3:D:309:ARG:HH21	1.58	0.69
2:P:310:LYS:HG2	2:N:477:ASP:OD1	1.92	0.69
2:F:250:PRO:CB	2:F:432:ARG:CB	2.61	0.69
6:Q:58:SER:H	6:Q:61:GLN:HE21	1.38	0.69
2:H:370:ALA:HB3	2:F:367:GLN:OE1	1.92	0.69
6:Q:726:LYS:HE3	6:R:722:THR:O	1.92	0.69
2:N:306:HIS:HA	2:N:309:ARG:HH21	1.58	0.69
2:H:306:HIS:HA	2:H:309:ARG:HH21	1.58	0.69
2:F:250:PRO:HG3	2:F:433:LEU:N	2.08	0.69
1:J:94:PRO:O	1:C:215:VAL:HG12	1.92	0.69
6:Q:437:LEU:HD11	6:Q:485:TYR:HB2	1.73	0.69
2:B:199:ASP:OD2	2:P:200:LEU:HD23	1.91	0.69
2:B:381:SER:CB	2:A:357:LEU:CD2	2.68	0.69
2:A:250:PRO:HG3	2:A:433:LEU:N	2.08	0.69
3:V:306:HIS:HA	3:V:309:ARG:HH21	1.58	0.69
6:R:666:GLN:HE22	6:R:711:ARG:HB2	1.55	0.69
1:C:5:PHE:CD1	2:E:331:ASN:CG	2.61	0.69
2:A:306:HIS:HA	2:A:309:ARG:HH21	1.58	0.69
6:Q:722:THR:O	6:R:726:LYS:HE3	1.92	0.69
2:G:372:ALA:HB1	2:G:409:ARG:NH1	2.05	0.69
2:P:310:LYS:HE3	2:N:477:ASP:C	2.12	0.69
2:F:306:HIS:HA	2:F:309:ARG:HH21	1.58	0.69
1:J:6:SER:CA	2:A:331:ASN:N	2.56	0.68
2:B:361:MET:HA	2:B:364:MET:SD	2.33	0.68
2:G:253:GLU:OE2	2:G:432:ARG:NH1	2.26	0.68
3:K:306:HIS:HA	3:K:309:ARG:HH21	1.58	0.68
2:G:470:ARG:HH22	2:H:348:ASP:HB2	1.58	0.68
1:J:243:PRO:HG3	6:Q:134:MET:CA	2.20	0.68
2:G:361:MET:HA	2:G:364:MET:SD	2.33	0.68
6:R:437:LEU:HD11	6:R:485:TYR:HB2	1.74	0.68
2:A:333:PHE:HD2	2:N:451:TRP:HH2	1.39	0.68
2:E:250:PRO:CG	2:E:433:LEU:CD2	2.71	0.68
3:K:310:LYS:N	2:H:476:GLN:CD	2.39	0.68
2:H:361:MET:HA	2:H:364:MET:SD	2.33	0.68
2:A:199:ASP:HB3	3:D:200:LEU:CB	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:199:ASP:OD2	3:V:200:LEU:HD23	1.91	0.68
2:B:306:HIS:HA	2:B:309:ARG:HH21	1.58	0.68
2:B:370:ALA:HB3	2:A:367:GLN:OE1	1.92	0.68
2:A:199:ASP:OD2	3:D:200:LEU:HD23	1.91	0.68
2:A:334:VAL:HG21	2:N:451:TRP:NE1	2.08	0.68
2:G:200:LEU:HG	2:N:199:ASP:OD2	1.94	0.68
2:G:470:ARG:HH12	2:H:348:ASP:HB3	1.59	0.68
2:B:253:GLU:OE2	2:B:432:ARG:NH1	2.26	0.68
2:G:357:LEU:O	2:G:360:ALA:HB3	1.93	0.68
2:H:372:ALA:HB1	2:H:409:ARG:NH1	2.05	0.68
2:F:250:PRO:CG	2:F:433:LEU:CD2	2.71	0.68
1:J:5:PHE:CG	2:N:332:LYS:CB	2.73	0.68
2:B:200:LEU:HG	2:P:199:ASP:OD2	1.94	0.68
2:G:250:PRO:HA	2:G:436:SER:HB2	1.71	0.68
2:H:199:ASP:HB3	3:V:200:LEU:CB	2.24	0.68
2:H:200:LEU:HG	3:V:199:ASP:OD2	1.94	0.68
2:H:253:GLU:OE2	2:H:432:ARG:NH1	2.26	0.68
6:Q:733:LYS:HZ2	6:R:683:GLN:CA	2.04	0.68
2:B:357:LEU:O	2:B:360:ALA:HB3	1.93	0.68
2:B:433:LEU:HD13	2:B:514:PHE:CZ	2.29	0.68
2:G:246:VAL:HG22	2:G:503:MET:SD	2.34	0.68
2:E:250:PRO:HG3	2:E:433:LEU:N	2.08	0.68
2:H:357:LEU:O	2:H:360:ALA:HB3	1.93	0.68
6:Q:483:PRO:HA	6:Q:486:VAL:H	1.59	0.68
6:R:483:PRO:HA	6:R:486:VAL:H	1.59	0.68
1:J:217:PRO:HD3	2:G:392:PRO:HG3	1.74	0.67
2:B:350:LEU:HB3	2:A:385:LEU:HD21	1.75	0.67
2:H:250:PRO:HB3	2:H:436:SER:CB	2.03	0.67
5:S:52:ARG:HE	5:S:58:LEU:H	1.40	0.67
1:J:84:PHE:HA	1:C:88:VAL:CB	2.25	0.67
2:B:367:GLN:CD	2:A:370:ALA:O	2.33	0.67
2:G:357:LEU:CD2	2:E:381:SER:CB	2.58	0.67
2:E:200:LEU:HG	3:K:199:ASP:OD2	1.94	0.67
2:P:475:GLN:HE22	2:N:311:GLU:HA	0.85	0.67
2:F:200:LEU:HG	3:L:199:ASP:OD2	1.94	0.67
1:C:5:PHE:HB3	2:E:331:ASN:N	2.08	0.67
2:A:200:LEU:HG	3:D:199:ASP:OD2	1.94	0.67
2:A:250:PRO:CG	2:A:433:LEU:CD2	2.71	0.67
2:P:306:HIS:HA	2:P:309:ARG:HH21	1.58	0.67
2:H:350:LEU:HB3	2:F:385:LEU:HD21	1.75	0.67
2:F:199:ASP:HB3	3:L:200:LEU:CB	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:246:VAL:HG22	2:B:503:MET:SD	2.34	0.67
2:A:334:VAL:HG22	2:N:451:TRP:CE2	2.29	0.67
2:G:433:LEU:HD13	2:G:514:PHE:CZ	2.29	0.67
2:G:449:HIS:CD2	2:G:452:HIS:CE1	2.83	0.67
2:P:480:ASN:HB2	2:N:310:LYS:CD	2.23	0.67
2:H:379:SER:HA	2:H:402:SER:HA	1.76	0.67
1:J:247:PHE:CZ	6:Q:94:GLU:HA	2.30	0.67
1:C:30:LYS:HZ1	2:P:283:PRO:HG2	1.58	0.67
2:B:253:GLU:OE2	2:B:432:ARG:NE	2.28	0.67
2:G:199:ASP:HB3	2:N:200:LEU:CB	2.24	0.67
2:G:306:HIS:HA	2:G:309:ARG:HH21	1.57	0.67
2:G:379:SER:HA	2:G:402:SER:HA	1.76	0.67
2:E:250:PRO:CB	2:E:432:ARG:CB	2.61	0.67
2:E:306:HIS:HA	2:E:309:ARG:HH21	1.58	0.67
2:H:253:GLU:OE2	2:H:432:ARG:NE	2.28	0.67
6:Q:389:LEU:HA	6:Q:392:ILE:HD12	1.77	0.67
5:T:52:ARG:HE	5:T:58:LEU:H	1.40	0.67
2:B:370:ALA:HB3	2:A:367:GLN:CD	2.15	0.67
2:H:433:LEU:HD13	2:H:514:PHE:CZ	2.29	0.67
3:L:306:HIS:HA	3:L:309:ARG:HH21	1.58	0.67
2:B:250:PRO:HA	2:B:436:SER:HB2	1.71	0.67
2:G:350:LEU:HB3	2:E:385:LEU:HD21	1.75	0.67
2:H:367:GLN:CD	2:F:370:ALA:O	2.33	0.67
1:J:5:PHE:C	2:A:331:ASN:N	2.47	0.67
1:J:215:VAL:HG12	1:C:94:PRO:O	1.92	0.67
6:Q:32:LEU:HD13	6:Q:76:LEU:HB2	1.76	0.67
1:J:58:ARG:NH2	2:A:339:TRP:CZ2	2.62	0.67
1:J:261:ASN:HD21	1:C:90:GLU:CG	1.71	0.67
2:B:199:ASP:HB3	2:P:200:LEU:CB	2.24	0.67
2:G:477:ASP:HB2	3:L:311:GLU:CD	2.16	0.67
2:H:449:HIS:CD2	2:H:452:HIS:CE1	2.83	0.67
2:B:449:HIS:CD2	2:B:452:HIS:CE1	2.83	0.67
2:A:334:VAL:CG2	2:N:451:TRP:HZ2	2.08	0.67
2:G:367:GLN:CD	2:E:370:ALA:O	2.33	0.67
2:E:250:PRO:HB2	2:E:432:ARG:CZ	2.25	0.67
5:S:16:ARG:CZ	5:S:120:HIS:CE1	2.78	0.67
6:R:389:LEU:HA	6:R:392:ILE:HD12	1.77	0.67
2:B:379:SER:HA	2:B:402:SER:HA	1.76	0.66
2:G:370:ALA:HB3	2:E:367:GLN:CD	2.15	0.66
2:H:370:ALA:HB3	2:F:367:GLN:CD	2.15	0.66
2:H:381:SER:CB	2:F:357:LEU:CD2	2.68	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:530:LEU:CD1	2:F:544:TRP:NE1	2.58	0.66
1:J:5:PHE:CD1	2:A:331:ASN:ND2	2.63	0.66
2:H:246:VAL:HG22	2:H:503:MET:SD	2.34	0.66
6:R:435:GLY:HA2	6:R:439:TYR:CG	2.30	0.66
2:E:199:ASP:HB3	3:K:200:LEU:CB	2.24	0.66
6:Q:509:LEU:HD13	6:Q:567:ARG:HH11	1.61	0.66
6:Q:722:THR:CG2	6:R:725:THR:CG2	2.61	0.66
2:G:199:ASP:OD2	2:N:200:LEU:HD23	1.91	0.66
6:Q:435:GLY:HA2	6:Q:439:TYR:CG	2.30	0.66
5:T:123:GLU:H	5:T:134:ASN:HB3	1.61	0.66
6:R:32:LEU:HD13	6:R:76:LEU:HB2	1.76	0.66
2:G:253:GLU:OE2	2:G:432:ARG:NE	2.28	0.66
2:G:260:PHE:CE2	2:N:198:GLY:CA	2.79	0.66
5:S:123:GLU:H	5:S:134:ASN:HB3	1.61	0.66
6:Q:733:LYS:HZ1	6:R:683:GLN:N	1.92	0.66
1:J:247:PHE:CZ	6:Q:94:GLU:CA	2.78	0.66
2:A:250:PRO:HB2	2:A:432:ARG:CZ	2.25	0.66
2:N:251:PRO:HD2	2:N:432:ARG:CD	2.25	0.66
1:J:5:PHE:CD2	2:N:332:LYS:HB2	2.27	0.66
1:C:58:ARG:NE	2:E:339:TRP:CH2	2.64	0.66
2:A:332:LYS:HA	2:N:332:LYS:N	2.10	0.66
2:A:260:PHE:CE2	3:D:198:GLY:CA	2.79	0.65
6:R:509:LEU:HD13	6:R:567:ARG:HH11	1.61	0.65
2:B:385:LEU:HD21	2:A:350:LEU:HD13	1.79	0.65
2:H:488:ASP:HA	2:H:491:ARG:HE	1.61	0.65
2:F:260:PHE:CE2	3:L:198:GLY:CA	2.79	0.65
1:J:5:PHE:CA	2:N:332:LYS:HB2	2.25	0.65
1:C:5:PHE:N	2:P:332:LYS:CB	2.57	0.65
2:P:477:ASP:O	2:N:310:LYS:CD	2.41	0.65
5:T:16:ARG:CZ	5:T:120:HIS:CE1	2.78	0.65
2:B:488:ASP:HA	2:B:491:ARG:HE	1.61	0.65
2:A:345:VAL:HG21	2:N:462:LYS:NZ	2.11	0.65
2:G:488:ASP:HA	2:G:491:ARG:HE	1.62	0.65
2:E:260:PHE:CE2	3:K:198:GLY:CA	2.79	0.65
6:Q:725:THR:HG1	6:R:722:THR:HG22	1.61	0.65
2:B:406:LEU:CD1	2:B:409:ARG:HH21	2.10	0.65
2:G:530:LEU:CD1	2:E:544:TRP:NE1	2.58	0.65
1:J:88:VAL:CB	1:C:84:PHE:HA	2.25	0.65
2:B:250:PRO:HA	2:B:436:SER:CB	2.26	0.65
2:F:250:PRO:HD3	2:F:433:LEU:HA	1.79	0.65
2:G:248:VAL:CG2	2:G:443:GLN:CD	2.64	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:406:LEU:CD1	2:G:409:ARG:HH21	2.10	0.65
2:P:250:PRO:HB3	2:P:432:ARG:CD	2.24	0.65
2:H:385:LEU:HD21	2:F:350:LEU:HD13	1.79	0.65
2:F:211:THR:HG21	2:F:295:LEU:HB3	1.79	0.65
6:Q:722:THR:HG22	6:R:721:ASP:O	1.96	0.65
6:Q:722:THR:HG22	6:R:725:THR:HG1	1.57	0.65
2:B:211:THR:HG21	2:B:295:LEU:HB3	1.79	0.65
2:B:245:GLY:HA3	2:B:503:MET:HG3	1.79	0.65
2:H:248:VAL:CG2	2:H:443:GLN:CD	2.64	0.65
1:J:230:GLU:O	6:Q:105:ARG:NH2	2.29	0.65
2:G:367:GLN:HE22	2:E:370:ALA:C	2.01	0.65
2:G:368:ARG:HD2	2:G:416:ALA:H	1.62	0.65
2:H:260:PHE:CE2	3:V:198:GLY:CA	2.79	0.65
2:H:267:SER:HB3	2:H:432:ARG:HH12	0.82	0.65
2:G:196:LYS:HZ3	2:N:196:LYS:HZ2	0.67	0.64
2:E:209:VAL:HB	2:E:225:VAL:HG22	1.80	0.64
2:N:251:PRO:CD	2:N:432:ARG:HD2	2.26	0.64
2:H:211:THR:HG21	2:H:295:LEU:HB3	1.79	0.64
6:R:264:PRO:HB2	6:R:267:TYR:H	1.62	0.64
2:B:260:PHE:CE2	2:P:198:GLY:CA	2.79	0.64
2:H:209:VAL:HB	2:H:225:VAL:HG22	1.80	0.64
2:F:250:PRO:HB2	2:F:432:ARG:CZ	2.25	0.64
6:Q:103:ILE:HG23	6:Q:107:TYR:CE1	2.33	0.64
1:C:217:PRO:CA	2:B:390:LEU:CD1	2.70	0.64
2:B:267:SER:HB3	2:B:432:ARG:HH12	0.82	0.64
2:B:380:ALA:O	2:B:383:HIS:CD2	2.51	0.64
2:G:380:ALA:O	2:G:383:HIS:CD2	2.51	0.64
2:P:211:THR:HG21	2:P:295:LEU:HB3	1.79	0.64
6:R:96:VAL:HG23	6:R:97:GLN:OE1	1.98	0.64
1:J:217:PRO:CG	2:G:390:LEU:CD1	2.59	0.64
2:B:368:ARG:HD2	2:B:416:ALA:H	1.62	0.64
2:B:370:ALA:HB3	2:A:367:GLN:NE2	2.13	0.64
2:H:375:ALA:CB	2:H:409:ARG:HB2	2.28	0.64
2:H:380:ALA:O	2:H:383:HIS:CD2	2.51	0.64
3:L:209:VAL:HB	3:L:225:VAL:HG22	1.80	0.64
6:R:103:ILE:HG23	6:R:107:TYR:CE1	2.33	0.64
2:A:209:VAL:HB	2:A:225:VAL:HG22	1.80	0.64
2:A:250:PRO:HD3	2:A:433:LEU:HA	1.79	0.64
2:E:211:THR:HG21	2:E:295:LEU:HB3	1.79	0.64
2:E:250:PRO:HB2	2:E:432:ARG:NH1	2.13	0.64
3:K:211:THR:HG21	3:K:295:LEU:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:350:LEU:CG	2:F:385:LEU:CD2	2.69	0.64
2:H:367:GLN:HE22	2:F:370:ALA:C	2.01	0.64
6:Q:721:ASP:O	6:R:722:THR:HG22	1.96	0.64
2:A:211:THR:HG21	2:A:295:LEU:HB3	1.79	0.64
3:D:234:TRP:CZ3	3:D:237:ASN:HB2	2.33	0.64
2:G:375:ALA:CB	2:G:409:ARG:HB2	2.28	0.64
2:G:385:LEU:HD21	2:E:350:LEU:HD13	1.79	0.64
2:P:251:PRO:HD2	2:P:432:ARG:HD2	1.80	0.64
2:H:245:GLY:HA3	2:H:503:MET:HG3	1.79	0.64
2:F:250:PRO:HB2	2:F:432:ARG:NH1	2.13	0.64
2:G:245:GLY:HA3	2:G:503:MET:HG3	1.79	0.64
2:P:234:TRP:CZ3	2:P:237:ASN:HB2	2.33	0.64
6:Q:264:PRO:HB2	6:Q:267:TYR:H	1.63	0.64
2:G:267:SER:HB3	2:G:432:ARG:HH12	0.82	0.64
2:P:475:GLN:CD	2:N:310:LYS:C	2.55	0.64
2:N:234:TRP:CZ3	2:N:237:ASN:HB2	2.33	0.64
3:V:211:THR:HG21	3:V:295:LEU:HB3	1.79	0.64
3:L:211:THR:HG21	3:L:295:LEU:HB3	1.79	0.64
6:Q:96:VAL:HG23	6:Q:97:GLN:OE1	1.98	0.64
2:B:227:ARG:HB2	2:B:232:PHE:CZ	2.33	0.64
2:B:248:VAL:CG2	2:B:443:GLN:CD	2.64	0.64
2:G:211:THR:HG21	2:G:295:LEU:HB3	1.79	0.64
2:P:227:ARG:HB2	2:P:232:PHE:CZ	2.33	0.64
2:N:209:VAL:HB	2:N:225:VAL:HG22	1.80	0.64
2:H:406:LEU:CD1	2:H:409:ARG:HH21	2.10	0.64
3:V:209:VAL:HB	3:V:225:VAL:HG22	1.79	0.64
3:L:234:TRP:CZ3	3:L:237:ASN:HB2	2.33	0.64
6:Q:438:ALA:HB3	6:Q:439:TYR:HD1	1.63	0.64
1:J:82:TYR:HE2	1:C:90:GLU:OE2	1.75	0.64
2:B:234:TRP:CZ3	2:B:237:ASN:HB2	2.33	0.64
2:A:234:TRP:CZ3	2:A:237:ASN:HB2	2.33	0.64
3:D:227:ARG:HB2	3:D:232:PHE:CZ	2.33	0.64
2:E:234:TRP:CZ3	2:E:237:ASN:HB2	2.33	0.64
2:E:250:PRO:HD3	2:E:433:LEU:HA	1.79	0.64
2:G:209:VAL:HB	2:G:225:VAL:HG22	1.79	0.63
3:K:209:VAL:HB	3:K:225:VAL:HG22	1.80	0.63
3:K:309:ARG:N	2:H:476:GLN:OE1	2.31	0.63
2:F:209:VAL:HB	2:F:225:VAL:HG22	1.80	0.63
6:Q:80:LEU:HD21	6:Q:111:THR:O	1.98	0.63
6:Q:725:THR:CG2	6:R:722:THR:CG2	2.61	0.63
1:C:5:PHE:CD1	2:E:331:ASN:ND2	2.67	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:209:VAL:HB	2:B:225:VAL:HG22	1.79	0.63
3:K:234:TRP:CZ3	3:K:237:ASN:HB2	2.33	0.63
1:J:5:PHE:HB2	2:A:331:ASN:C	2.19	0.63
1:J:217:PRO:N	2:G:390:LEU:HD11	2.12	0.63
2:B:350:LEU:CG	2:A:385:LEU:CD2	2.70	0.63
2:B:367:GLN:HE22	2:A:370:ALA:C	2.00	0.63
2:G:350:LEU:HD22	2:E:385:LEU:HD11	1.39	0.63
2:G:370:ALA:C	2:E:367:GLN:OE1	2.36	0.63
2:N:249:PRO:C	2:N:433:LEU:HD21	2.16	0.63
2:H:246:VAL:HA	2:H:503:MET:SD	2.39	0.63
6:Q:471:ARG:HH21	6:Q:472:ARG:HH22	1.47	0.63
2:B:530:LEU:CD1	2:A:544:TRP:NE1	2.58	0.63
2:A:250:PRO:HB2	2:A:432:ARG:NH1	2.13	0.63
2:G:371:MET:HE2	2:E:371:MET:HE2	1.73	0.63
2:G:430:TYR:CE2	2:G:522:PHE:CZ	2.87	0.63
2:H:357:LEU:HD22	2:F:378:PHE:CD1	2.34	0.63
2:H:368:ARG:HD2	2:H:416:ALA:H	1.62	0.63
2:F:234:TRP:CZ3	2:F:237:ASN:HB2	2.33	0.63
3:V:227:ARG:HB2	3:V:232:PHE:CZ	2.33	0.63
6:Q:752:TRP:CZ2	6:Q:811:GLN:HB3	2.33	0.63
6:R:438:ALA:HB3	6:R:439:TYR:HD1	1.63	0.63
6:R:631:SER:HA	6:R:634:PHE:CE2	2.34	0.63
6:R:752:TRP:CZ2	6:R:811:GLN:HB3	2.33	0.63
2:B:357:LEU:HD22	2:A:378:PHE:CD1	2.34	0.63
2:B:430:TYR:CE2	2:B:522:PHE:CZ	2.87	0.63
3:D:211:THR:HG21	3:D:295:LEU:HB3	1.79	0.63
2:G:234:TRP:CZ3	2:G:237:ASN:HB2	2.33	0.63
2:G:246:VAL:N	2:G:503:MET:HE3	2.12	0.63
2:G:449:HIS:HA	2:G:452:HIS:CE1	2.34	0.63
2:E:227:ARG:HB2	2:E:232:PHE:CZ	2.33	0.63
2:N:250:PRO:CB	2:N:429:GLU:CA	2.61	0.63
2:A:227:ARG:HB2	2:A:232:PHE:CZ	2.33	0.63
2:G:370:ALA:HB3	2:E:367:GLN:NE2	2.13	0.63
2:N:227:ARG:HB2	2:N:232:PHE:CZ	2.33	0.63
2:H:234:TRP:CZ3	2:H:237:ASN:HB2	2.33	0.63
6:R:471:ARG:HH21	6:R:472:ARG:HH22	1.47	0.63
3:K:311:GLU:HB2	2:H:477:ASP:CB	1.80	0.63
2:P:209:VAL:HB	2:P:225:VAL:HG22	1.79	0.63
2:P:250:PRO:CD	2:P:433:LEU:CG	2.68	0.63
2:H:250:PRO:HA	2:H:436:SER:CB	2.26	0.63
6:Q:683:GLN:CA	6:R:733:LYS:CE	2.66	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:80:LEU:HD21	6:R:111:THR:O	1.99	0.63
2:B:375:ALA:CB	2:B:409:ARG:HB2	2.28	0.63
3:L:227:ARG:HB2	3:L:232:PHE:CZ	2.34	0.63
1:C:30:LYS:HE2	2:P:283:PRO:CG	2.27	0.63
2:B:449:HIS:HA	2:B:452:HIS:CE1	2.34	0.63
2:G:227:ARG:HB2	2:G:232:PHE:CZ	2.33	0.63
2:G:246:VAL:HA	2:G:503:MET:SD	2.39	0.63
2:H:370:ALA:C	2:F:367:GLN:OE1	2.36	0.63
6:Q:108:LEU:O	6:Q:112:VAL:HG23	1.99	0.63
6:Q:435:GLY:HA2	6:Q:439:TYR:CE2	2.34	0.63
6:R:435:GLY:HA2	6:R:439:TYR:CE2	2.34	0.63
2:A:332:LYS:HA	2:N:331:ASN:O	1.97	0.62
2:E:196:LYS:HZ2	3:K:196:LYS:HZ3	1.34	0.62
3:K:227:ARG:HB2	3:K:232:PHE:CZ	2.33	0.62
2:P:250:PRO:HG3	2:P:429:GLU:C	2.18	0.62
2:H:227:ARG:HB2	2:H:232:PHE:CZ	2.33	0.62
2:F:227:ARG:HB2	2:F:232:PHE:CZ	2.33	0.62
2:A:206:VAL:HG21	2:A:228:ARG:CZ	2.30	0.62
2:N:206:VAL:HG21	2:N:228:ARG:CZ	2.30	0.62
6:Q:733:LYS:HZ2	6:R:683:GLN:CB	2.06	0.62
1:C:5:PHE:HB2	2:E:331:ASN:C	2.20	0.62
2:P:204:HIS:CE1	2:P:230:ARG:HE	2.17	0.62
2:H:370:ALA:HB3	2:F:367:GLN:NE2	2.13	0.62
3:V:234:TRP:CZ3	3:V:237:ASN:HB2	2.33	0.62
3:L:206:VAL:HG21	3:L:228:ARG:CZ	2.30	0.62
6:Q:631:SER:HA	6:Q:634:PHE:CE2	2.34	0.62
1:J:218:ASN:N	2:G:390:LEU:CD1	2.63	0.62
2:A:250:PRO:CB	2:A:432:ARG:CB	2.62	0.62
2:G:382:LEU:HD12	2:G:405:GLN:HG3	1.82	0.62
3:K:206:VAL:HG21	3:K:228:ARG:CZ	2.30	0.62
3:V:204:HIS:CE1	3:V:230:ARG:HE	2.17	0.62
1:C:217:PRO:HD2	2:B:390:LEU:CD2	2.27	0.62
3:D:206:VAL:HG21	3:D:228:ARG:CZ	2.30	0.62
2:F:204:HIS:CE1	2:F:230:ARG:HE	2.18	0.62
5:S:138:ALA:HB1	5:S:157:PHE:CD2	2.35	0.62
6:R:564:TRP:CH2	6:R:568:LEU:HD22	2.34	0.62
2:B:246:VAL:HA	2:B:503:MET:SD	2.39	0.62
3:D:209:VAL:HB	3:D:225:VAL:HG22	1.80	0.62
2:G:204:HIS:CE1	2:G:230:ARG:HE	2.18	0.62
2:E:204:HIS:CE1	2:E:230:ARG:HE	2.17	0.62
2:P:206:VAL:HG21	2:P:228:ARG:CZ	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:211:THR:HG21	2:N:295:LEU:HB3	1.79	0.62
3:V:206:VAL:HG21	3:V:228:ARG:CZ	2.30	0.62
2:B:250:PRO:HB3	2:B:436:SER:CB	2.04	0.62
2:G:415:GLN:HG3	2:G:418:GLN:NE2	2.15	0.62
3:K:204:HIS:CE1	3:K:230:ARG:HE	2.18	0.62
2:P:310:LYS:HD3	2:N:477:ASP:O	1.93	0.62
3:L:204:HIS:CE1	3:L:230:ARG:HE	2.18	0.62
1:C:218:ASN:H	2:B:390:LEU:HD11	1.65	0.62
2:B:494:HIS:CE1	2:B:498:LEU:HB2	2.35	0.62
2:A:331:ASN:ND2	2:N:332:LYS:NZ	2.47	0.62
2:A:497:ARG:HD3	2:N:334:VAL:HG21	1.80	0.62
3:D:204:HIS:CE1	3:D:230:ARG:HE	2.18	0.62
2:G:206:VAL:HG21	2:G:228:ARG:CZ	2.30	0.62
2:H:246:VAL:N	2:H:503:MET:HE3	2.14	0.62
2:H:449:HIS:HA	2:H:452:HIS:CE1	2.34	0.62
2:F:250:PRO:CB	2:F:432:ARG:HB2	2.30	0.62
1:J:88:VAL:HB	1:C:84:PHE:CA	2.30	0.62
2:E:206:VAL:HG21	2:E:228:ARG:CZ	2.30	0.62
2:H:196:LYS:HZ3	3:V:196:LYS:HZ2	0.63	0.62
6:Q:429:ARG:HB2	6:Q:432:TYR:CZ	2.35	0.62
5:T:138:ALA:HB1	5:T:157:PHE:CD2	2.35	0.62
6:R:429:ARG:HB2	6:R:432:TYR:CZ	2.35	0.62
6:R:508:LEU:HD22	6:R:513:THR:H	1.65	0.62
1:J:218:ASN:N	2:G:390:LEU:HD11	2.15	0.62
2:P:250:PRO:CA	2:P:432:ARG:HD2	2.30	0.62
2:H:196:LYS:HZ2	3:V:196:LYS:HZ3	1.33	0.62
2:H:206:VAL:HG21	2:H:228:ARG:CZ	2.30	0.62
2:G:357:LEU:HD22	2:E:378:PHE:CD1	2.34	0.61
2:H:415:GLN:HG3	2:H:418:GLN:NE2	2.15	0.61
2:H:430:TYR:CE2	2:H:522:PHE:CZ	2.87	0.61
2:F:206:VAL:HG21	2:F:228:ARG:CZ	2.30	0.61
6:Q:516:SER:HA	6:Q:520:HIS:CD2	2.35	0.61
6:Q:564:TRP:CH2	6:Q:568:LEU:HD22	2.34	0.61
2:B:206:VAL:HG21	2:B:228:ARG:CZ	2.30	0.61
2:B:357:LEU:CD2	2:A:381:SER:CB	2.58	0.61
2:A:204:HIS:CE1	2:A:230:ARG:HE	2.18	0.61
2:H:204:HIS:CE1	2:H:230:ARG:HE	2.18	0.61
2:H:494:HIS:CE1	2:H:498:LEU:HB2	2.35	0.61
6:R:516:SER:HA	6:R:520:HIS:CD2	2.35	0.61
2:B:415:GLN:HG3	2:B:418:GLN:NE2	2.15	0.61
2:F:250:PRO:HB3	2:F:432:ARG:NE	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:564:TRP:CZ2	6:R:568:LEU:HD22	2.35	0.61
1:J:90:GLU:CG	1:C:261:ASN:HD21	1.71	0.61
1:C:217:PRO:HG3	2:B:391:SER:C	2.16	0.61
2:G:250:PRO:HA	2:G:436:SER:CB	2.26	0.61
2:H:199:ASP:O	3:V:199:ASP:CG	2.39	0.61
2:B:370:ALA:C	2:A:367:GLN:OE1	2.36	0.61
2:A:199:ASP:O	3:D:199:ASP:CG	2.39	0.61
2:G:476:GLN:HB3	3:L:306:HIS:O	1.99	0.61
2:G:479:LEU:HG	3:L:310:LYS:HE2	1.81	0.61
6:Q:564:TRP:CZ2	6:Q:568:LEU:HD22	2.35	0.61
1:C:217:PRO:HD3	2:B:392:PRO:CD	2.31	0.61
2:G:494:HIS:CE1	2:G:498:LEU:HB2	2.35	0.61
2:H:382:LEU:HD12	2:H:405:GLN:HG3	1.82	0.61
6:Q:562:GLN:CD	6:Q:562:GLN:H	2.04	0.61
6:R:108:LEU:O	6:R:112:VAL:HG23	1.99	0.61
1:C:216:ALA:HA	2:B:392:PRO:HG2	1.83	0.61
2:N:204:HIS:CE1	2:N:230:ARG:HE	2.18	0.61
6:Q:494:TYR:HA	6:Q:497:ARG:HE	1.65	0.61
6:Q:508:LEU:HD22	6:Q:513:THR:H	1.65	0.61
6:R:562:GLN:H	6:R:562:GLN:CD	2.04	0.61
2:B:196:LYS:HZ1	2:P:196:LYS:HZ3	1.36	0.61
2:B:204:HIS:CE1	2:B:230:ARG:HE	2.18	0.61
2:A:349:ALA:HB2	2:N:470:ARG:HH21	1.66	0.61
6:R:473:TYR:CE2	6:R:476:ILE:HA	2.36	0.61
2:B:410:ASP:HB3	2:B:414:ARG:HH11	1.66	0.61
2:B:534:VAL:HG13	2:B:535:GLU:OE2	2.01	0.61
2:G:381:SER:CB	2:E:357:LEU:CD2	2.69	0.61
2:E:250:PRO:HB3	2:E:432:ARG:NE	2.15	0.61
2:N:251:PRO:HD2	2:N:432:ARG:HD2	1.81	0.61
2:G:337:ASP:O	2:G:341:HIS:CD2	2.54	0.60
2:H:337:ASP:O	2:H:341:HIS:CD2	2.54	0.60
2:A:334:VAL:CG2	2:N:451:TRP:CE2	2.84	0.60
2:H:534:VAL:HG13	2:H:535:GLU:OE2	2.01	0.60
2:B:199:ASP:O	2:P:199:ASP:CG	2.39	0.60
2:G:199:ASP:O	2:N:199:ASP:CG	2.39	0.60
2:P:250:PRO:CB	2:P:429:GLU:HA	2.30	0.60
2:H:385:LEU:HD12	2:H:388:VAL:HG21	1.84	0.60
2:F:199:ASP:O	3:L:199:ASP:CG	2.39	0.60
1:J:30:LYS:HZ1	2:N:283:PRO:HG2	1.67	0.60
2:B:382:LEU:HD12	2:B:405:GLN:HG3	1.82	0.60
2:H:408:ILE:HD13	2:F:529:PHE:CZ	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:410:ASP:HB3	2:G:414:ARG:HH11	1.66	0.60
2:E:199:ASP:O	3:K:199:ASP:CG	2.39	0.60
1:J:5:PHE:CB	2:A:331:ASN:N	2.64	0.60
2:B:408:ILE:HD13	2:A:529:PHE:CZ	2.36	0.60
2:B:337:ASP:O	2:B:341:HIS:CD2	2.54	0.60
2:H:382:LEU:HD13	2:H:401:LEU:O	2.01	0.60
6:Q:579:THR:HA	6:Q:582:ARG:CZ	2.32	0.60
1:J:5:PHE:CB	2:A:331:ASN:CA	2.79	0.60
1:C:217:PRO:N	2:B:390:LEU:CD1	2.64	0.60
1:C:283:PHE:HE1	2:B:545:GLU:CB	2.04	0.60
2:G:225:VAL:HG23	2:G:227:ARG:HG2	1.84	0.60
2:G:385:LEU:HD12	2:G:388:VAL:HG21	1.84	0.60
2:G:480:ASN:HA	3:L:310:LYS:HD3	1.82	0.60
2:E:250:PRO:CB	2:E:432:ARG:HB2	2.30	0.60
3:K:311:GLU:O	2:H:476:GLN:N	2.32	0.60
6:R:795:ILE:HA	6:R:798:PHE:CD2	2.37	0.60
2:G:382:LEU:HD13	2:G:401:LEU:O	2.01	0.60
6:R:494:TYR:HA	6:R:497:ARG:HE	1.65	0.60
2:B:225:VAL:HG23	2:B:227:ARG:HG2	1.84	0.59
2:B:246:VAL:N	2:B:503:MET:HE3	2.15	0.59
2:G:352:ASN:ND2	2:H:470:ARG:HH11	1.97	0.59
2:G:408:ILE:HD13	2:E:529:PHE:CZ	2.36	0.59
6:R:579:THR:HA	6:R:582:ARG:CZ	2.32	0.59
2:B:382:LEU:HD13	2:B:401:LEU:O	2.01	0.59
2:A:250:PRO:HB3	2:A:432:ARG:NE	2.15	0.59
2:P:250:PRO:HA	2:P:432:ARG:CD	2.32	0.59
1:C:58:ARG:HH21	2:E:339:TRP:HH2	0.70	0.59
2:P:310:LYS:CE	2:N:479:LEU:N	2.65	0.59
6:Q:579:THR:HG22	6:Q:583:LEU:HD12	1.84	0.59
2:G:451:TRP:CD1	2:G:493:VAL:O	2.56	0.59
2:G:480:ASN:HB2	3:L:310:LYS:HG2	1.84	0.59
2:G:534:VAL:HG13	2:G:535:GLU:OE2	2.01	0.59
2:H:451:TRP:CD1	2:H:493:VAL:O	2.56	0.59
1:J:111:GLU:HG2	1:C:108:LYS:HB3	1.85	0.59
1:C:217:PRO:N	2:B:392:PRO:CG	2.49	0.59
2:A:225:VAL:HG23	2:A:227:ARG:HG2	1.84	0.59
2:G:477:ASP:HB2	3:L:311:GLU:OE1	2.02	0.59
2:E:225:VAL:HG23	2:E:227:ARG:HG2	1.84	0.59
2:B:204:HIS:HE1	2:B:230:ARG:HE	1.51	0.59
2:B:382:LEU:HD22	2:B:401:LEU:HB2	1.84	0.59
2:G:343:ARG:HA	2:G:346:TYR:CZ	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:204:HIS:HE1	3:K:230:ARG:HE	1.51	0.59
2:H:410:ASP:HB3	2:H:414:ARG:HH11	1.66	0.59
2:B:343:ARG:HA	2:B:346:TYR:CZ	2.38	0.59
2:H:204:HIS:HE1	2:H:230:ARG:HE	1.51	0.59
2:H:343:ARG:HA	2:H:346:TYR:CZ	2.38	0.59
3:V:204:HIS:HE1	3:V:230:ARG:HE	1.51	0.59
6:Q:721:ASP:O	6:R:722:THR:HG23	2.03	0.59
6:R:715:PHE:HB2	6:R:720:TYR:CE1	2.38	0.59
2:B:240:HIS:N	2:B:248:VAL:HG11	2.18	0.59
2:G:479:LEU:C	3:L:310:LYS:HE2	2.23	0.59
3:K:204:HIS:CE1	3:K:228:ARG:HD3	2.38	0.59
2:N:225:VAL:HG23	2:N:227:ARG:HG2	1.84	0.59
6:Q:189:TRP:CZ3	6:Q:251:ALA:HA	2.38	0.59
6:Q:473:TYR:CE2	6:Q:476:ILE:HA	2.36	0.59
6:R:579:THR:HG22	6:R:583:LEU:HD12	1.84	0.59
6:R:587:THR:O	6:R:591:TYR:CE2	2.56	0.59
6:R:715:PHE:HB2	6:R:720:TYR:CZ	2.38	0.59
1:J:245:ARG:NH1	6:Q:130:ASP:OD2	2.36	0.59
3:D:204:HIS:CE1	3:D:228:ARG:HD3	2.38	0.59
2:G:240:HIS:N	2:G:248:VAL:HG11	2.18	0.59
2:G:480:ASN:CB	3:L:310:LYS:HG3	2.33	0.59
2:N:240:HIS:N	2:N:248:VAL:HG11	2.18	0.59
2:H:382:LEU:HD22	2:H:401:LEU:HB2	1.84	0.59
2:F:225:VAL:HG23	2:F:227:ARG:HG2	1.84	0.59
6:Q:587:THR:O	6:Q:591:TYR:CE2	2.56	0.59
5:T:12:HIS:HB2	5:T:16:ARG:H	1.68	0.59
2:B:451:TRP:CD1	2:B:493:VAL:O	2.55	0.59
2:A:250:PRO:CB	2:A:432:ARG:HB2	2.30	0.59
2:G:204:HIS:HE1	2:G:230:ARG:HE	1.51	0.59
2:B:385:LEU:HD12	2:B:388:VAL:HG21	1.84	0.58
2:G:382:LEU:HD22	2:G:401:LEU:HB2	1.84	0.58
2:E:240:HIS:N	2:E:248:VAL:HG11	2.18	0.58
2:P:204:HIS:CE1	2:P:228:ARG:HD3	2.38	0.58
2:H:386:SER:HA	2:H:398:LEU:HD23	1.84	0.58
2:H:538:LYS:HZ1	2:H:542:GLU:HG3	1.68	0.58
3:V:204:HIS:CE1	3:V:228:ARG:HD3	2.38	0.58
6:Q:795:ILE:HA	6:Q:798:PHE:CD2	2.37	0.58
2:A:204:HIS:CE1	2:A:228:ARG:HD3	2.38	0.58
2:G:386:SER:HA	2:G:398:LEU:HD23	1.85	0.58
2:N:204:HIS:HE1	2:N:230:ARG:HE	1.51	0.58
3:L:240:HIS:N	3:L:248:VAL:HG11	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:528:LEU:HD23	6:Q:586:MET:SD	2.43	0.58
2:B:449:HIS:CD2	2:B:452:HIS:HE1	2.21	0.58
2:H:225:VAL:HG23	2:H:227:ARG:HG2	1.84	0.58
6:Q:715:PHE:HB2	6:Q:720:TYR:CZ	2.38	0.58
1:J:92:ALA:C	1:C:262:LYS:CD	2.67	0.58
1:J:108:LYS:HB3	1:C:111:GLU:HG2	1.85	0.58
1:C:58:ARG:CZ	2:E:339:TRP:CZ2	2.86	0.58
2:E:204:HIS:CE1	2:E:228:ARG:HD3	2.38	0.58
2:H:246:VAL:CA	2:H:503:MET:SD	2.92	0.58
2:H:367:GLN:NE2	2:F:369:LYS:O	2.36	0.58
2:F:240:HIS:N	2:F:248:VAL:HG11	2.18	0.58
5:S:12:HIS:HB2	5:S:16:ARG:H	1.68	0.58
5:T:107:LYS:HZ2	6:R:800:GLU:HB3	1.68	0.58
6:R:480:LEU:HD23	6:R:485:TYR:HE1	1.68	0.58
3:D:240:HIS:N	3:D:248:VAL:HG11	2.18	0.58
2:G:246:VAL:CA	2:G:503:MET:SD	2.92	0.58
2:P:240:HIS:N	2:P:248:VAL:HG11	2.18	0.58
2:H:204:HIS:CE1	2:H:228:ARG:HD3	2.38	0.58
3:L:204:HIS:CE1	3:L:228:ARG:HD3	2.38	0.58
6:R:264:PRO:HD2	6:R:267:TYR:CD2	2.39	0.58
6:R:528:LEU:HD23	6:R:586:MET:SD	2.44	0.58
2:A:240:HIS:N	2:A:248:VAL:HG11	2.18	0.58
2:G:479:LEU:HD23	3:L:310:LYS:CE	2.19	0.58
2:N:204:HIS:CE1	2:N:228:ARG:HD3	2.38	0.58
2:F:199:ASP:O	3:L:199:ASP:OD2	2.22	0.58
6:Q:733:LYS:CE	6:R:683:GLN:CA	2.66	0.58
2:A:199:ASP:O	3:D:199:ASP:OD2	2.22	0.58
3:D:225:VAL:HG23	3:D:227:ARG:HG2	1.84	0.58
2:G:204:HIS:CE1	2:G:228:ARG:HD3	2.38	0.58
2:G:246:VAL:N	2:G:503:MET:SD	2.77	0.58
2:G:470:ARG:NH1	2:H:352:ASN:ND2	2.48	0.58
3:K:240:HIS:N	3:K:248:VAL:HG11	2.18	0.58
2:F:204:HIS:CE1	2:F:228:ARG:HD3	2.38	0.58
3:V:225:VAL:HG23	3:V:227:ARG:HG2	1.84	0.58
5:S:52:ARG:HE	5:S:58:LEU:N	2.02	0.58
6:Q:264:PRO:HD2	6:Q:267:TYR:CD2	2.39	0.58
6:Q:722:THR:O	6:R:726:LYS:CE	2.51	0.58
1:C:5:PHE:C	2:E:331:ASN:N	2.56	0.58
2:A:406:LEU:HD23	3:D:220:GLN:NE2	2.06	0.58
2:H:240:HIS:N	2:H:248:VAL:HG11	2.18	0.58
6:Q:715:PHE:HB2	6:Q:720:TYR:CE1	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:722:THR:HG23	6:R:721:ASP:O	2.03	0.58
2:B:196:LYS:HZ3	2:P:196:LYS:HZ2	0.60	0.58
2:B:246:VAL:N	2:B:503:MET:SD	2.77	0.58
2:G:367:GLN:NE2	2:E:369:LYS:O	2.36	0.58
2:G:449:HIS:CD2	2:G:452:HIS:HE1	2.21	0.58
2:G:538:LYS:HZ1	2:G:542:GLU:HG3	1.69	0.58
3:K:310:LYS:H	2:H:476:GLN:CD	2.07	0.58
6:Q:725:THR:HG21	6:R:722:THR:CG2	2.20	0.58
5:T:52:ARG:HE	5:T:58:LEU:N	2.02	0.58
1:J:93:ALA:HB2	1:C:262:LYS:HB3	1.85	0.58
2:B:367:GLN:NE2	2:A:369:LYS:O	2.36	0.58
2:E:196:LYS:HZ3	3:K:196:LYS:HZ2	0.61	0.58
2:E:199:ASP:O	3:K:199:ASP:OD2	2.22	0.58
3:K:225:VAL:HG23	3:K:227:ARG:HG2	1.84	0.58
2:P:250:PRO:N	2:P:433:LEU:HD21	2.18	0.58
2:H:199:ASP:O	3:V:199:ASP:OD2	2.22	0.58
6:Q:480:LEU:HD23	6:Q:485:TYR:HE1	1.68	0.58
6:R:189:TRP:CZ3	6:R:251:ALA:HA	2.38	0.58
1:C:5:PHE:HD1	2:E:331:ASN:OD1	1.78	0.57
1:C:202:HIS:CE1	1:C:275:ILE:HD12	2.39	0.57
2:B:199:ASP:O	2:P:199:ASP:OD2	2.22	0.57
3:L:225:VAL:HG23	3:L:227:ARG:HG2	1.84	0.57
1:J:217:PRO:C	2:G:390:LEU:CD1	2.72	0.57
1:J:262:LYS:HB3	1:C:93:ALA:HB2	1.85	0.57
2:B:204:HIS:CE1	2:B:228:ARG:HD3	2.38	0.57
6:R:184:GLU:O	6:R:188:LEU:HD12	2.04	0.57
6:R:247:ARG:HH22	6:R:282:LEU:HA	1.69	0.57
1:J:261:ASN:HD21	1:C:90:GLU:HG2	0.75	0.57
2:B:246:VAL:CA	2:B:503:MET:SD	2.92	0.57
2:P:225:VAL:HG23	2:P:227:ARG:HG2	1.84	0.57
3:L:204:HIS:HE1	3:L:230:ARG:HE	1.51	0.57
5:S:61:VAL:HG22	5:S:87:PHE:CD2	2.40	0.57
6:R:193:GLN:HB2	6:R:208:ARG:HH11	1.69	0.57
2:H:449:HIS:CD2	2:H:452:HIS:HE1	2.21	0.57
5:S:107:LYS:HZ2	6:Q:800:GLU:HB3	1.70	0.57
6:Q:247:ARG:HH22	6:Q:282:LEU:HA	1.70	0.57
2:H:343:ARG:HE	2:H:344:ARG:HA	1.69	0.57
1:J:90:GLU:HG2	1:C:261:ASN:HD21	0.75	0.57
1:J:202:HIS:CE1	1:J:275:ILE:HD12	2.40	0.57
2:B:386:SER:HA	2:B:398:LEU:HD23	1.85	0.57
2:H:246:VAL:N	2:H:503:MET:SD	2.77	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:240:HIS:N	3:V:248:VAL:HG11	2.18	0.57
5:T:61:VAL:HG22	5:T:87:PHE:CD2	2.39	0.57
1:C:136:MET:SD	2:P:490:GLU:OE2	2.63	0.57
2:E:204:HIS:HE1	2:E:230:ARG:HE	1.51	0.57
2:P:204:HIS:HE1	2:P:230:ARG:HE	1.51	0.57
6:Q:193:GLN:HB2	6:Q:208:ARG:HH11	1.69	0.57
6:Q:722:THR:CG2	6:R:725:THR:HG21	2.20	0.57
2:B:408:ILE:HD13	2:A:529:PHE:CE2	2.40	0.57
2:B:430:TYR:CD1	2:B:518:LYS:HE2	2.40	0.57
2:A:497:ARG:HD3	2:N:334:VAL:CG2	2.35	0.57
2:G:253:GLU:CD	2:G:432:ARG:HH11	2.08	0.57
2:P:247:VAL:CG1	2:P:513:ARG:NH1	2.63	0.57
2:B:253:GLU:OE2	2:B:432:ARG:CZ	2.53	0.57
2:G:343:ARG:HE	2:G:344:ARG:HA	1.69	0.57
2:G:430:TYR:CD1	2:G:518:LYS:HE2	2.40	0.57
5:S:130:LYS:HB2	5:S:132:PHE:CE2	2.40	0.57
2:B:379:SER:HB3	2:B:406:LEU:HB2	1.87	0.56
2:A:204:HIS:HE1	2:A:230:ARG:HE	1.51	0.56
2:G:199:ASP:O	2:N:199:ASP:OD2	2.22	0.56
2:H:408:ILE:HD13	2:F:529:PHE:CE2	2.40	0.56
6:Q:148:ARG:HH11	6:Q:181:ASN:HA	1.70	0.56
6:Q:726:LYS:CE	6:R:722:THR:O	2.52	0.56
6:R:148:ARG:HH11	6:R:181:ASN:HA	1.70	0.56
2:B:538:LYS:HZ1	2:B:542:GLU:HG3	1.69	0.56
2:G:416:ALA:HB3	2:G:417:GLN:OE1	2.05	0.56
2:H:379:SER:HB3	2:H:406:LEU:HB2	1.87	0.56
2:F:204:HIS:HE1	2:F:230:ARG:HE	1.51	0.56
6:Q:184:GLU:O	6:Q:188:LEU:HD12	2.04	0.56
6:Q:401:VAL:HG22	6:Q:406:LEU:HD12	1.87	0.56
1:J:39:TYR:CD1	1:J:145:ILE:HG23	2.40	0.56
2:A:345:VAL:HG21	2:N:462:LYS:HE2	1.87	0.56
2:G:350:LEU:CG	2:E:385:LEU:CD2	2.70	0.56
2:G:379:SER:HB3	2:G:402:SER:O	2.06	0.56
2:G:408:ILE:HD13	2:E:529:PHE:CE2	2.40	0.56
2:H:371:MET:HE1	2:F:367:GLN:HB3	1.83	0.56
2:H:416:ALA:HB3	2:H:417:GLN:OE1	2.05	0.56
2:H:430:TYR:CD1	2:H:518:LYS:HE2	2.40	0.56
6:Q:578:ASP:O	6:Q:582:ARG:HG3	2.05	0.56
5:T:130:LYS:HB2	5:T:132:PHE:CE2	2.40	0.56
6:R:570:HIS:CE1	6:R:571:LEU:HA	2.40	0.56
6:R:578:ASP:O	6:R:582:ARG:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:86:SER:N	1:C:86:SER:O	2.35	0.56
2:P:249:PRO:C	2:P:433:LEU:HD21	2.25	0.56
1:J:84:PHE:CA	1:C:88:VAL:HB	2.30	0.56
2:B:343:ARG:HE	2:B:344:ARG:HA	1.69	0.56
3:D:204:HIS:HE1	3:D:230:ARG:HE	1.51	0.56
6:Q:570:HIS:CE1	6:Q:571:LEU:HA	2.40	0.56
6:R:632:SER:O	6:R:636:PHE:HB3	2.06	0.56
2:G:253:GLU:OE2	2:G:432:ARG:CZ	2.54	0.56
2:G:479:LEU:HG	3:L:310:LYS:CE	2.35	0.56
2:H:253:GLU:CD	2:H:432:ARG:HH11	2.09	0.56
6:R:740:GLN:O	6:R:744:VAL:HG23	2.06	0.56
2:B:253:GLU:CD	2:B:432:ARG:HH11	2.08	0.56
2:P:240:HIS:CD2	2:P:248:VAL:HG21	2.41	0.56
3:V:240:HIS:CD2	3:V:248:VAL:HG21	2.41	0.56
6:Q:28:MET:HE3	6:Q:32:LEU:HD11	1.88	0.56
6:Q:683:GLN:N	6:R:733:LYS:HZ1	2.04	0.56
1:C:217:PRO:CG	2:B:390:LEU:CD1	2.72	0.56
5:S:105:ALA:HA	5:S:110:VAL:HG23	1.88	0.56
6:Q:579:THR:HA	6:Q:582:ARG:NE	2.21	0.56
1:J:247:PHE:CE2	6:Q:94:GLU:O	2.58	0.56
1:C:217:PRO:HD3	2:B:392:PRO:HD3	1.86	0.56
6:Q:429:ARG:HA	6:Q:429:ARG:CZ	2.36	0.56
6:R:401:VAL:HG22	6:R:406:LEU:HD12	1.87	0.56
2:N:245:GLY:HA2	2:N:440:ALA:CB	2.36	0.56
2:H:367:GLN:NE2	2:F:370:ALA:O	2.39	0.56
5:S:61:VAL:HG22	5:S:87:PHE:CE2	2.41	0.56
5:T:105:ALA:HA	5:T:110:VAL:HG23	1.88	0.56
2:B:367:GLN:NE2	2:A:370:ALA:O	2.39	0.55
2:B:426:ILE:O	2:B:430:TYR:CE2	2.59	0.55
3:K:240:HIS:CD2	3:K:248:VAL:HG21	2.41	0.55
2:H:253:GLU:OE2	2:H:432:ARG:CZ	2.53	0.55
2:F:196:LYS:HZ1	3:L:196:LYS:HZ3	1.42	0.55
6:Q:632:SER:O	6:Q:636:PHE:HB3	2.06	0.55
5:T:52:ARG:CZ	5:T:52:ARG:HA	2.36	0.55
6:R:438:ALA:CB	6:R:484:THR:HG21	2.36	0.55
6:R:590:ALA:HA	6:R:593:GLU:OE2	2.06	0.55
2:G:379:SER:HB3	2:G:406:LEU:HB2	1.87	0.55
2:G:422:THR:HG21	2:G:528:THR:HG21	1.88	0.55
2:G:426:ILE:O	2:G:430:TYR:CE2	2.59	0.55
6:R:579:THR:HA	6:R:582:ARG:NE	2.21	0.55
1:J:262:LYS:HB3	1:C:93:ALA:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:TYR:CD1	1:C:145:ILE:HG23	2.40	0.55
2:P:310:LYS:HE2	2:N:478:ARG:CA	2.36	0.55
2:H:426:ILE:O	2:H:430:TYR:CE2	2.59	0.55
2:F:240:HIS:CD2	2:F:248:VAL:HG21	2.41	0.55
6:Q:438:ALA:CB	6:Q:484:THR:HG21	2.35	0.55
5:T:61:VAL:HG22	5:T:87:PHE:CE2	2.41	0.55
6:R:476:ILE:O	6:R:479:ALA:HB3	2.06	0.55
6:R:526:GLU:HA	6:R:529:LYS:HD2	1.88	0.55
6:R:429:ARG:CZ	6:R:429:ARG:HA	2.36	0.55
1:J:217:PRO:HB2	2:G:390:LEU:CG	2.23	0.55
1:C:58:ARG:NE	2:E:339:TRP:CZ2	2.75	0.55
6:Q:99:ALA:HB3	6:Q:105:ARG:HA	1.89	0.55
6:R:603:PRO:HA	6:R:606:ILE:HG12	1.89	0.55
2:B:379:SER:HB3	2:B:402:SER:O	2.06	0.55
2:B:406:LEU:O	2:B:409:ARG:HB3	2.06	0.55
2:H:437:VAL:HA	2:H:440:ALA:HB2	1.88	0.55
2:B:422:THR:HG21	2:B:528:THR:HG21	1.88	0.55
6:Q:32:LEU:O	6:Q:79:HIS:CD2	2.60	0.55
6:Q:428:GLU:CG	6:Q:429:ARG:H	2.18	0.55
6:Q:603:PRO:HA	6:Q:606:ILE:HG12	1.89	0.55
6:R:428:GLU:CG	6:R:429:ARG:H	2.18	0.55
6:R:532:ILE:HG21	6:R:590:ALA:HB1	1.89	0.55
3:D:240:HIS:CD2	3:D:248:VAL:HG21	2.41	0.55
2:G:367:GLN:NE2	2:E:370:ALA:O	2.39	0.55
2:H:406:LEU:O	2:H:409:ARG:HB3	2.07	0.55
2:H:516:ARG:HH11	2:H:517:GLU:HB2	1.72	0.55
5:S:52:ARG:HA	5:S:52:ARG:CZ	2.36	0.55
6:Q:476:ILE:O	6:Q:479:ALA:HB3	2.06	0.55
6:R:32:LEU:O	6:R:79:HIS:CD2	2.60	0.55
1:J:261:ASN:O	1:C:90:GLU:HG3	2.07	0.55
2:A:196:LYS:HZ3	3:D:196:LYS:HZ2	0.55	0.55
2:E:240:HIS:CD2	2:E:248:VAL:HG21	2.41	0.55
2:H:371:MET:CE	2:F:371:MET:HE2	2.26	0.55
6:R:99:ALA:HB3	6:R:105:ARG:HA	1.89	0.55
2:B:195:HIS:CD2	2:B:197:VAL:HG22	2.42	0.55
2:B:416:ALA:HB3	2:B:417:GLN:OE1	2.05	0.55
2:H:372:ALA:HB2	2:H:413:GLU:CD	2.28	0.55
3:L:240:HIS:CD2	3:L:248:VAL:HG21	2.41	0.55
6:Q:590:ALA:HA	6:Q:593:GLU:OE2	2.06	0.55
2:B:372:ALA:HB2	2:B:413:GLU:CD	2.28	0.54
2:A:406:LEU:HD21	3:D:220:GLN:CD	2.27	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:437:VAL:HA	2:G:440:ALA:HB2	1.89	0.54
2:H:379:SER:HB3	2:H:402:SER:O	2.06	0.54
1:J:93:ALA:N	1:C:262:LYS:HB3	2.21	0.54
2:N:195:HIS:CD2	2:N:197:VAL:HG22	2.42	0.54
6:R:587:THR:HA	6:R:590:ALA:HB3	1.90	0.54
2:B:437:VAL:HA	2:B:440:ALA:HB2	1.89	0.54
2:B:451:TRP:HE1	2:B:493:VAL:HG13	1.72	0.54
2:A:406:LEU:HD11	3:D:223:PHE:HE1	1.73	0.54
2:H:195:HIS:CD2	2:H:197:VAL:HG22	2.42	0.54
2:F:406:LEU:HD21	3:L:220:GLN:CD	2.27	0.54
6:Q:740:GLN:O	6:Q:744:VAL:HG23	2.06	0.54
2:B:516:ARG:HH11	2:B:517:GLU:HB2	1.72	0.54
2:A:240:HIS:CD2	2:A:248:VAL:HG21	2.41	0.54
2:A:250:PRO:HG3	2:A:433:LEU:H	1.73	0.54
2:A:331:ASN:HD21	2:N:332:LYS:HE3	1.70	0.54
2:G:195:HIS:CD2	2:G:197:VAL:HG22	2.42	0.54
2:P:195:HIS:CD2	2:P:197:VAL:HG22	2.42	0.54
2:P:310:LYS:CD	2:N:476:GLN:O	2.54	0.54
2:H:422:THR:HG21	2:H:528:THR:HG21	1.88	0.54
3:V:195:HIS:CD2	3:V:197:VAL:HG22	2.42	0.54
6:Q:526:GLU:HA	6:Q:529:LYS:HD2	1.89	0.54
6:R:32:LEU:HD23	6:R:41:ALA:HB1	1.89	0.54
3:D:195:HIS:CD2	3:D:197:VAL:HG22	2.42	0.54
2:G:199:ASP:O	2:N:199:ASP:CB	2.53	0.54
2:E:406:LEU:HD11	3:K:223:PHE:HE1	1.73	0.54
2:F:195:HIS:CD2	2:F:197:VAL:HG22	2.42	0.54
6:Q:32:LEU:HD23	6:Q:41:ALA:HB1	1.89	0.54
5:T:69:ALA:HA	5:T:72:LEU:HD12	1.90	0.54
1:J:90:GLU:HG3	1:C:261:ASN:O	2.07	0.54
2:E:406:LEU:HD21	3:K:220:GLN:CD	2.28	0.54
2:N:240:HIS:CD2	2:N:248:VAL:HG21	2.41	0.54
6:Q:584:LEU:HD12	6:Q:585:GLN:HE22	1.72	0.54
2:B:357:LEU:CG	2:A:381:SER:CB	2.86	0.54
2:G:470:ARG:HH12	2:H:348:ASP:HB2	1.73	0.54
2:N:248:VAL:C	2:N:433:LEU:CD2	2.76	0.54
6:R:584:LEU:HD12	6:R:585:GLN:HE22	1.72	0.54
6:R:707:SER:HA	6:R:710:HIS:CD2	2.43	0.54
2:G:361:MET:O	2:G:365:VAL:HG23	2.08	0.54
2:G:516:ARG:HH11	2:G:517:GLU:HB2	1.72	0.54
5:S:58:LEU:HD11	5:S:60:ILE:HG23	1.89	0.54
2:G:406:LEU:O	2:G:409:ARG:HB3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:195:HIS:CD2	2:E:197:VAL:HG22	2.42	0.54
2:H:451:TRP:HE1	2:H:493:VAL:HG13	1.72	0.54
5:T:169:LEU:HD23	5:T:169:LEU:O	2.08	0.54
1:J:217:PRO:HG3	2:G:392:PRO:N	2.23	0.54
1:C:217:PRO:C	2:B:390:LEU:HD12	2.27	0.54
2:A:195:HIS:CD2	2:A:197:VAL:HG22	2.42	0.54
2:F:196:LYS:HZ3	3:L:196:LYS:HZ2	0.54	0.54
3:L:195:HIS:CD2	3:L:197:VAL:HG22	2.42	0.54
2:B:375:ALA:HB3	2:B:409:ARG:HB2	1.90	0.53
2:B:400:ALA:CB	2:B:550:GLN:HE22	2.21	0.53
2:G:357:LEU:CG	2:E:381:SER:CB	2.86	0.53
2:G:375:ALA:HB3	2:G:409:ARG:HB2	1.90	0.53
2:E:250:PRO:HG3	2:E:433:LEU:H	1.73	0.53
2:P:250:PRO:CD	2:P:433:LEU:HG	2.37	0.53
2:H:361:MET:O	2:H:365:VAL:HG23	2.08	0.53
1:J:5:PHE:HD2	2:N:332:LYS:HA	1.73	0.53
1:J:108:LYS:O	1:C:111:GLU:OE2	2.26	0.53
1:C:5:PHE:CB	2:E:331:ASN:C	2.76	0.53
2:G:451:TRP:HE1	2:G:493:VAL:HG13	1.72	0.53
2:G:470:ARG:NH2	2:H:348:ASP:HB2	2.21	0.53
2:G:480:ASN:N	3:L:310:LYS:HG3	2.23	0.53
3:K:195:HIS:CD2	3:K:197:VAL:HG22	2.42	0.53
2:H:357:LEU:CG	2:F:381:SER:CB	2.86	0.53
1:J:243:PRO:HG3	6:Q:133:ASP:O	2.08	0.53
2:H:368:ARG:HD2	2:H:413:GLU:O	2.09	0.53
6:Q:193:GLN:HB3	6:Q:194:HIS:CE1	2.43	0.53
6:Q:707:SER:HA	6:Q:710:HIS:CD2	2.43	0.53
6:R:193:GLN:HB3	6:R:194:HIS:CE1	2.43	0.53
1:J:93:ALA:CB	1:C:262:LYS:HB3	2.39	0.53
1:C:217:PRO:HA	2:B:392:PRO:HA	1.90	0.53
3:K:310:LYS:HG3	2:H:480:ASN:CB	2.33	0.53
2:P:250:PRO:HB2	2:P:432:ARG:HH21	1.70	0.53
2:P:477:ASP:O	2:N:310:LYS:HD3	2.07	0.53
6:Q:587:THR:HA	6:Q:590:ALA:HB3	1.90	0.53
6:Q:641:ILE:HA	6:Q:644:LEU:HG	1.91	0.53
1:J:243:PRO:HB2	6:Q:134:MET:CE	2.38	0.53
2:G:368:ARG:HD2	2:G:413:GLU:O	2.09	0.53
2:P:251:PRO:CD	2:P:432:ARG:CD	2.70	0.53
2:P:475:GLN:NE2	2:N:310:LYS:O	2.40	0.53
3:L:228:ARG:HG3	3:L:300:PHE:CE1	2.44	0.53
6:Q:779:GLN:HB2	6:Q:783:ARG:HH21	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:58:LEU:HD11	5:T:60:ILE:HG23	1.89	0.53
1:J:111:GLU:OE2	1:C:108:LYS:O	2.26	0.53
1:C:226:LEU:HD13	1:C:253:LEU:HD22	1.89	0.53
2:B:361:MET:O	2:B:365:VAL:HG23	2.08	0.53
2:P:310:LYS:HE2	2:N:478:ARG:C	2.28	0.53
2:F:274:LYS:CE	2:F:432:ARG:NH1	2.66	0.53
5:S:69:ALA:HA	5:S:72:LEU:HD12	1.90	0.53
5:S:169:LEU:O	5:S:169:LEU:HD23	2.08	0.53
6:Q:532:ILE:HG21	6:Q:590:ALA:HB1	1.89	0.53
6:Q:586:MET:HA	6:Q:589:LYS:HD2	1.91	0.53
5:T:120:HIS:HB2	5:T:143:THR:HA	1.90	0.53
2:B:228:ARG:HG3	2:B:300:PHE:CE1	2.44	0.53
2:B:240:HIS:ND1	2:B:248:VAL:HG21	2.24	0.53
2:B:368:ARG:HD2	2:B:413:GLU:O	2.09	0.53
2:G:228:ARG:HG3	2:G:300:PHE:CE1	2.44	0.53
2:G:400:ALA:CB	2:G:550:GLN:HE22	2.21	0.53
2:G:479:LEU:CD2	3:L:310:LYS:CE	2.82	0.53
2:E:274:LYS:CE	2:E:432:ARG:NH1	2.66	0.53
2:H:400:ALA:CB	2:H:550:GLN:HE22	2.21	0.53
2:F:228:ARG:HG3	2:F:300:PHE:CE1	2.44	0.53
2:F:250:PRO:HG3	2:F:433:LEU:H	1.73	0.53
2:F:406:LEU:HD11	3:L:223:PHE:HE1	1.73	0.53
3:V:228:ARG:HG3	3:V:300:PHE:CE1	2.44	0.53
1:J:262:LYS:CD	1:C:92:ALA:C	2.67	0.53
2:B:370:ALA:CB	2:A:367:GLN:NE2	2.71	0.53
2:G:372:ALA:HB2	2:G:413:GLU:CD	2.28	0.53
5:S:115:TRP:CH2	5:S:134:ASN:HB2	2.44	0.53
6:Q:751:TRP:CZ3	6:Q:774:VAL:HA	2.44	0.53
1:J:226:LEU:HD13	1:J:253:LEU:HD22	1.89	0.53
2:G:232:PHE:HB2	2:G:252:PRO:HG3	1.92	0.53
2:E:196:LYS:HZ1	3:K:196:LYS:HZ3	1.35	0.53
5:T:96:GLU:HB3	5:T:121:ARG:HH22	1.74	0.53
6:R:480:LEU:HA	6:R:485:TYR:CE1	2.44	0.53
1:J:86:SER:O	1:C:86:SER:N	2.34	0.52
2:B:232:PHE:HB2	2:B:252:PRO:HG3	1.92	0.52
2:B:244:PRO:O	2:B:447:ALA:CB	2.56	0.52
2:G:479:LEU:CG	3:L:310:LYS:HE2	2.39	0.52
2:N:240:HIS:ND1	2:N:248:VAL:HG21	2.24	0.52
6:Q:480:LEU:HA	6:Q:485:TYR:CE1	2.44	0.52
1:J:217:PRO:HD3	2:G:392:PRO:CG	2.39	0.52
2:G:406:LEU:HA	2:G:409:ARG:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:497:ARG:HH22	2:G:501:GLU:HB2	1.75	0.52
6:R:429:ARG:HB2	6:R:432:TYR:CE1	2.44	0.52
6:R:749:HIS:CE1	6:R:754:THR:O	2.63	0.52
2:A:253:GLU:OE2	2:A:428:GLU:CD	2.48	0.52
2:A:274:LYS:CE	2:A:432:ARG:NH1	2.66	0.52
3:D:228:ARG:HG3	3:D:300:PHE:CE1	2.44	0.52
2:G:437:VAL:O	2:G:440:ALA:HB3	2.09	0.52
2:E:240:HIS:ND1	2:E:248:VAL:HG21	2.24	0.52
2:P:240:HIS:ND1	2:P:248:VAL:HG21	2.24	0.52
2:N:232:PHE:HB2	2:N:252:PRO:HG3	1.91	0.52
6:Q:429:ARG:HB2	6:Q:432:TYR:CE1	2.44	0.52
5:T:62:ARG:HH12	6:R:697:ALA:HA	1.73	0.52
1:C:6:SER:CA	2:E:331:ASN:N	2.71	0.52
2:E:228:ARG:HG3	2:E:300:PHE:CE1	2.44	0.52
2:H:375:ALA:HB3	2:H:409:ARG:HB2	1.90	0.52
3:V:232:PHE:HB2	3:V:252:PRO:HG3	1.92	0.52
6:Q:633:LEU:HA	6:Q:636:PHE:HB3	1.92	0.52
1:J:262:LYS:HB3	1:C:93:ALA:CB	2.39	0.52
2:B:356:ALA:HA	2:B:359:LYS:HZ2	1.75	0.52
3:D:240:HIS:ND1	3:D:248:VAL:HG21	2.24	0.52
2:G:419:ASP:O	2:G:423:PHE:CD2	2.63	0.52
2:P:232:PHE:HB2	2:P:252:PRO:HG3	1.92	0.52
3:L:204:HIS:CD2	3:L:204:HIS:O	2.63	0.52
5:S:96:GLU:HB3	5:S:121:ARG:HH22	1.74	0.52
6:Q:58:SER:HB2	6:Q:61:GLN:H	1.74	0.52
5:T:115:TRP:CH2	5:T:134:ASN:HB2	2.44	0.52
6:R:641:ILE:HA	6:R:644:LEU:HG	1.91	0.52
2:B:406:LEU:HA	2:B:409:ARG:HB3	1.91	0.52
2:B:497:ARG:HH22	2:B:501:GLU:HB2	1.75	0.52
2:G:370:ALA:CB	2:E:367:GLN:NE2	2.71	0.52
2:P:228:ARG:HG3	2:P:300:PHE:CE1	2.44	0.52
2:N:228:ARG:HG3	2:N:300:PHE:CE1	2.44	0.52
2:H:415:GLN:HG3	2:H:418:GLN:HE21	1.75	0.52
2:F:199:ASP:O	3:L:199:ASP:CB	2.52	0.52
3:L:232:PHE:HB2	3:L:252:PRO:HG3	1.92	0.52
5:S:120:HIS:HB2	5:S:143:THR:HA	1.90	0.52
6:Q:638:HIS:CD2	6:Q:638:HIS:C	2.82	0.52
6:R:606:ILE:HG21	6:R:660:LEU:HD22	1.91	0.52
6:R:779:GLN:HB2	6:R:783:ARG:HH21	1.74	0.52
1:J:84:PHE:HA	1:C:88:VAL:CG2	2.40	0.52
1:J:88:VAL:CG2	1:C:84:PHE:HA	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:228:ARG:HG3	2:A:300:PHE:CE1	2.44	0.52
2:E:260:PHE:CD2	3:K:198:GLY:CA	2.84	0.52
2:H:228:ARG:HG3	2:H:300:PHE:CE1	2.44	0.52
2:H:356:ALA:HA	2:H:359:LYS:HZ2	1.75	0.52
2:H:406:LEU:HA	2:H:409:ARG:HB3	1.90	0.52
3:V:240:HIS:ND1	3:V:248:VAL:HG21	2.24	0.52
6:R:28:MET:HE3	6:R:32:LEU:HD11	1.92	0.52
6:R:188:LEU:HD23	6:R:191:ARG:NH2	2.24	0.52
6:R:586:MET:HA	6:R:589:LYS:HD2	1.91	0.52
2:A:196:LYS:NZ	3:D:196:LYS:CE	2.68	0.52
2:E:199:ASP:O	3:K:199:ASP:CB	2.53	0.52
3:K:204:HIS:CD2	3:K:204:HIS:O	2.63	0.52
3:K:228:ARG:HG3	3:K:300:PHE:CE1	2.44	0.52
2:H:419:ASP:O	2:H:423:PHE:CD2	2.63	0.52
3:V:218:TYR:CE1	3:V:295:LEU:HD12	2.45	0.52
6:Q:468:SER:HA	6:Q:471:ARG:HE	1.75	0.52
6:Q:480:LEU:HD23	6:Q:485:TYR:CE1	2.44	0.52
2:B:218:TYR:CE1	2:B:295:LEU:HD12	2.45	0.52
2:B:458:LEU:HD22	2:B:490:GLU:HA	1.92	0.52
2:A:204:HIS:O	2:A:204:HIS:CD2	2.63	0.52
2:A:240:HIS:ND1	2:A:248:VAL:HG21	2.24	0.52
3:D:204:HIS:CD2	3:D:204:HIS:O	2.63	0.52
2:H:199:ASP:O	3:V:199:ASP:CB	2.53	0.52
2:F:218:TYR:CE1	2:F:295:LEU:HD12	2.45	0.52
5:S:62:ARG:HH12	6:Q:697:ALA:HA	1.74	0.52
6:Q:722:THR:HA	6:R:722:THR:HG22	1.91	0.52
6:R:415:CYS:HA	6:R:418:LEU:HB2	1.91	0.52
6:R:640:ALA:O	6:R:644:LEU:HG	2.10	0.52
6:R:751:TRP:CZ3	6:R:774:VAL:HA	2.44	0.52
2:B:357:LEU:HD11	2:A:381:SER:CB	2.40	0.52
2:B:385:LEU:HD12	2:B:388:VAL:CG2	2.40	0.52
2:G:513:ARG:HG2	2:G:513:ARG:HH21	1.75	0.52
2:P:218:TYR:CE1	2:P:295:LEU:HD12	2.45	0.52
3:V:204:HIS:CD2	3:V:204:HIS:O	2.63	0.52
5:S:138:ALA:O	5:S:139:THR:HG23	2.10	0.52
6:Q:394:PHE:CE1	6:Q:436:ILE:HD13	2.45	0.52
6:R:208:ARG:HH22	6:R:251:ALA:HB2	1.74	0.52
6:Q:97:GLN:HE22	6:Q:106:LEU:HA	1.75	0.51
6:Q:188:LEU:HD23	6:Q:191:ARG:NH2	2.24	0.51
2:G:356:ALA:HA	2:G:359:LYS:HZ2	1.75	0.51
2:G:480:ASN:CA	3:L:310:LYS:HG3	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:232:PHE:HB2	2:H:252:PRO:HG3	1.91	0.51
2:H:240:HIS:ND1	2:H:248:VAL:HG21	2.24	0.51
2:H:244:PRO:O	2:H:447:ALA:CB	2.56	0.51
2:H:513:ARG:HH21	2:H:513:ARG:HG2	1.75	0.51
5:S:79:THR:HG23	5:S:84:ARG:HH12	1.75	0.51
6:R:97:GLN:HE22	6:R:106:LEU:HA	1.75	0.51
6:R:468:SER:HA	6:R:471:ARG:HE	1.75	0.51
1:C:24:VAL:HG21	1:C:38:LEU:HD13	1.92	0.51
2:A:332:LYS:CA	2:N:331:ASN:C	2.61	0.51
2:P:250:PRO:N	2:P:429:GLU:OE2	2.43	0.51
2:N:204:HIS:O	2:N:204:HIS:CD2	2.63	0.51
2:H:437:VAL:O	2:H:440:ALA:HB3	2.09	0.51
2:F:240:HIS:ND1	2:F:248:VAL:HG21	2.24	0.51
3:L:240:HIS:ND1	3:L:248:VAL:HG21	2.24	0.51
6:Q:396:GLN:O	6:Q:399:HIS:CD2	2.63	0.51
6:Q:665:GLY:O	6:Q:668:ALA:HB3	2.10	0.51
6:R:58:SER:HB2	6:R:61:GLN:H	1.74	0.51
6:R:80:LEU:HD11	6:R:115:ALA:HB2	1.92	0.51
6:R:749:HIS:HA	6:R:752:TRP:HB2	1.93	0.51
1:C:207:ILE:HB	1:C:227:VAL:HG12	1.92	0.51
2:B:204:HIS:CD2	2:B:204:HIS:O	2.63	0.51
2:B:437:VAL:O	2:B:440:ALA:HB3	2.09	0.51
2:A:218:TYR:CE1	2:A:295:LEU:HD12	2.45	0.51
2:G:218:TYR:CE1	2:G:295:LEU:HD12	2.45	0.51
2:G:371:MET:HE1	2:E:367:GLN:HB3	1.90	0.51
2:E:204:HIS:CD2	2:E:204:HIS:O	2.63	0.51
2:H:204:HIS:CD2	2:H:204:HIS:O	2.63	0.51
2:H:497:ARG:HH22	2:H:501:GLU:HB2	1.75	0.51
6:Q:749:HIS:HA	6:Q:752:TRP:HB2	1.92	0.51
5:T:79:THR:HG23	5:T:84:ARG:HH12	1.75	0.51
6:R:396:GLN:O	6:R:399:HIS:CD2	2.63	0.51
1:J:207:ILE:HB	1:J:227:VAL:HG12	1.92	0.51
2:G:352:ASN:ND2	2:H:470:ARG:NH1	2.53	0.51
2:P:204:HIS:CD2	2:P:204:HIS:O	2.63	0.51
2:F:204:HIS:O	2:F:204:HIS:CD2	2.63	0.51
5:S:138:ALA:HA	5:S:156:SER:H	1.76	0.51
6:Q:570:HIS:CE1	6:Q:571:LEU:HD23	2.46	0.51
6:Q:640:ALA:O	6:Q:644:LEU:HG	2.10	0.51
5:T:138:ALA:O	5:T:139:THR:HG23	2.10	0.51
6:R:401:VAL:HG22	6:R:406:LEU:CD1	2.41	0.51
6:R:597:ARG:H	6:R:598:ILE:HG23	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:638:HIS:C	6:R:638:HIS:CD2	2.82	0.51
6:R:749:HIS:CE1	6:R:754:THR:HB	2.45	0.51
2:G:240:HIS:ND1	2:G:248:VAL:HG21	2.24	0.51
2:G:458:LEU:HB2	2:G:489:ALA:CB	2.40	0.51
2:G:518:LYS:HA	2:G:521:ASP:OD1	2.11	0.51
2:E:218:TYR:CE1	2:E:295:LEU:HD12	2.45	0.51
2:H:196:LYS:NZ	3:V:196:LYS:CE	2.68	0.51
2:H:518:LYS:HA	2:H:521:ASP:OD1	2.11	0.51
6:Q:208:ARG:HH22	6:Q:251:ALA:HB2	1.74	0.51
6:Q:401:VAL:HG22	6:Q:406:LEU:CD1	2.41	0.51
6:Q:722:THR:HG22	6:R:722:THR:HA	1.91	0.51
6:R:570:HIS:CE1	6:R:571:LEU:HD23	2.46	0.51
2:B:415:GLN:HG3	2:B:418:GLN:HE21	1.75	0.51
2:B:419:ASP:O	2:B:423:PHE:CD2	2.63	0.51
2:G:357:LEU:HD11	2:E:381:SER:CB	2.40	0.51
3:K:218:TYR:CE1	3:K:295:LEU:HD12	2.45	0.51
2:H:457:GLU:HB3	2:H:461:LYS:HZ1	1.76	0.51
3:L:249:PRO:C	3:L:250:PRO:CA	2.73	0.51
6:Q:749:HIS:CE1	6:Q:754:THR:O	2.63	0.51
2:B:513:ARG:HG2	2:B:513:ARG:HH21	1.75	0.51
2:B:518:LYS:HA	2:B:521:ASP:OD1	2.11	0.51
2:B:544:TRP:CZ3	2:B:545:GLU:HG2	2.46	0.51
2:G:204:HIS:CD2	2:G:204:HIS:O	2.63	0.51
2:G:530:LEU:HD11	2:E:544:TRP:HE1	1.73	0.51
2:P:249:PRO:C	2:P:433:LEU:CD2	2.77	0.51
2:N:218:TYR:CE1	2:N:295:LEU:HD12	2.45	0.51
2:H:458:LEU:HB2	2:H:489:ALA:CB	2.40	0.51
6:Q:415:CYS:HA	6:Q:418:LEU:HB2	1.92	0.51
6:R:509:LEU:HD13	6:R:567:ARG:NH1	2.26	0.51
1:J:30:LYS:NZ	2:N:283:PRO:CG	2.70	0.51
1:J:217:PRO:HG2	2:G:390:LEU:HG	1.50	0.51
1:C:216:ALA:HB1	1:C:217:PRO:CD	2.41	0.51
2:B:196:LYS:NZ	2:P:196:LYS:CE	2.68	0.51
2:A:232:PHE:HB2	2:A:252:PRO:HG3	1.92	0.51
2:H:385:LEU:HD12	2:H:388:VAL:CG2	2.40	0.51
3:V:228:ARG:HG3	3:V:230:ARG:HH21	1.76	0.51
3:L:218:TYR:CE1	3:L:295:LEU:HD12	2.45	0.51
1:J:247:PHE:HB3	6:Q:98:TYR:CZ	2.41	0.51
3:D:232:PHE:HB2	3:D:252:PRO:HG3	1.92	0.51
2:G:244:PRO:O	2:G:447:ALA:CB	2.56	0.51
2:G:476:GLN:CB	3:L:311:GLU:O	2.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:633:LEU:HA	6:R:636:PHE:HB3	1.91	0.51
1:J:247:PHE:CD2	6:Q:94:GLU:O	2.64	0.50
3:D:218:TYR:CE1	3:D:295:LEU:HD12	2.45	0.50
2:E:190:THR:HB	2:E:210:ARG:HE	1.76	0.50
2:E:232:PHE:HB2	2:E:252:PRO:HG3	1.92	0.50
2:H:218:TYR:CE1	2:H:295:LEU:HD12	2.45	0.50
2:F:232:PHE:HB2	2:F:252:PRO:HG3	1.91	0.50
3:L:228:ARG:HG3	3:L:230:ARG:HH21	1.77	0.50
6:Q:749:HIS:CE1	6:Q:754:THR:HB	2.45	0.50
5:T:61:VAL:O	5:T:61:VAL:HG23	2.12	0.50
6:R:394:PHE:CE1	6:R:436:ILE:HD13	2.45	0.50
6:R:399:HIS:CG	6:R:400:LEU:N	2.79	0.50
6:R:625:ASN:HD22	6:R:629:GLN:NE2	2.10	0.50
2:B:433:LEU:HD13	2:B:514:PHE:HZ	1.75	0.50
2:G:371:MET:HE1	2:E:371:MET:HE1	1.84	0.50
2:H:433:LEU:HD13	2:H:514:PHE:HZ	1.75	0.50
2:P:311:GLU:HB3	2:N:477:ASP:OD2	2.10	0.50
2:H:370:ALA:CB	2:F:367:GLN:NE2	2.71	0.50
6:R:665:GLY:O	6:R:668:ALA:HB3	2.10	0.50
1:J:30:LYS:CE	2:N:283:PRO:CG	2.66	0.50
1:C:281:ARG:O	2:B:545:GLU:OE1	2.28	0.50
2:B:228:ARG:HG3	2:B:230:ARG:HH21	1.77	0.50
2:B:385:LEU:HD21	2:A:350:LEU:CD1	2.41	0.50
2:G:458:LEU:HD22	2:G:490:GLU:HA	1.92	0.50
3:K:232:PHE:HB2	3:K:252:PRO:HG3	1.92	0.50
2:P:249:PRO:HA	2:P:433:LEU:HD22	1.82	0.50
2:H:246:VAL:N	2:H:503:MET:HG3	2.27	0.50
2:H:385:LEU:HD21	2:F:350:LEU:CD1	2.41	0.50
2:H:544:TRP:CZ3	2:H:545:GLU:HG2	2.46	0.50
6:Q:264:PRO:O	6:Q:268:HIS:CG	2.64	0.50
6:Q:533:LYS:CE	6:Q:537:GLN:HA	2.42	0.50
6:Q:597:ARG:H	6:Q:598:ILE:HG23	1.76	0.50
6:R:212:GLN:HB2	6:R:254:TYR:CD2	2.46	0.50
1:J:216:ALA:HB1	1:J:217:PRO:CD	2.41	0.50
1:C:226:LEU:HD13	1:C:253:LEU:CD2	2.42	0.50
2:P:190:THR:HB	2:P:210:ARG:HE	1.77	0.50
2:H:458:LEU:HD22	2:H:490:GLU:HA	1.93	0.50
2:H:518:LYS:O	2:H:522:PHE:CD2	2.65	0.50
5:S:55:SER:HB2	5:S:56:PRO:HD2	1.93	0.50
6:Q:80:LEU:HD11	6:Q:115:ALA:HB2	1.92	0.50
6:Q:189:TRP:CZ2	6:Q:212:GLN:HB3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:606:ILE:HG21	6:Q:660:LEU:HD22	1.92	0.50
6:R:189:TRP:CZ2	6:R:212:GLN:HB3	2.46	0.50
6:R:264:PRO:O	6:R:268:HIS:CG	2.65	0.50
1:J:24:VAL:HG21	1:J:38:LEU:HD13	1.92	0.50
1:C:5:PHE:CA	2:E:331:ASN:OD1	2.55	0.50
3:D:190:THR:HB	3:D:210:ARG:HE	1.77	0.50
2:G:514:PHE:O	2:G:517:GLU:HB3	2.11	0.50
2:G:544:TRP:CZ3	2:G:545:GLU:HG2	2.46	0.50
3:K:310:LYS:N	2:H:476:GLN:OE1	2.43	0.50
2:P:228:ARG:HG3	2:P:230:ARG:HH21	1.76	0.50
2:P:265:VAL:HG23	2:P:269:ARG:NH2	2.27	0.50
2:N:190:THR:HB	2:N:210:ARG:HE	1.76	0.50
2:N:247:VAL:HG11	2:N:513:ARG:NH1	2.27	0.50
2:N:250:PRO:CD	2:N:433:LEU:HD11	2.28	0.50
2:F:265:VAL:HG23	2:F:269:ARG:NH2	2.27	0.50
6:Q:399:HIS:CG	6:Q:400:LEU:N	2.79	0.50
6:R:533:LYS:CE	6:R:537:GLN:HA	2.42	0.50
1:C:5:PHE:CB	2:E:331:ASN:CA	2.88	0.50
2:B:518:LYS:O	2:B:522:PHE:CD2	2.65	0.50
2:G:246:VAL:N	2:G:503:MET:HG3	2.26	0.50
2:G:518:LYS:O	2:G:522:PHE:CD2	2.65	0.50
3:K:228:ARG:HG3	3:K:230:ARG:HH21	1.77	0.50
3:K:240:HIS:ND1	3:K:248:VAL:HG21	2.24	0.50
2:P:205:ILE:CD1	2:P:269:ARG:HH21	2.25	0.50
2:H:365:VAL:CG2	2:H:416:ALA:HB1	2.26	0.50
2:F:190:THR:HB	2:F:210:ARG:HE	1.77	0.50
2:F:196:LYS:NZ	3:L:196:LYS:CE	2.68	0.50
6:Q:447:HIS:CG	6:Q:448:ALA:N	2.80	0.50
2:B:430:TYR:HE2	2:B:522:PHE:CZ	2.29	0.50
2:A:345:VAL:CG2	2:N:462:LYS:NZ	2.74	0.50
2:G:199:ASP:O	2:N:200:LEU:CA	2.55	0.50
2:G:385:LEU:HD21	2:E:350:LEU:CD1	2.41	0.50
3:V:190:THR:HB	3:V:210:ARG:HE	1.77	0.50
6:Q:188:LEU:HD23	6:Q:191:ARG:HH22	1.77	0.50
6:R:447:HIS:CG	6:R:448:ALA:N	2.80	0.50
6:R:480:LEU:HD23	6:R:485:TYR:CE1	2.44	0.50
6:R:483:PRO:CA	6:R:486:VAL:H	2.25	0.50
2:B:190:THR:HB	2:B:210:ARG:HE	1.77	0.50
2:A:199:ASP:O	3:D:199:ASP:CB	2.52	0.50
3:D:228:ARG:HG3	3:D:230:ARG:HH21	1.77	0.50
2:G:457:GLU:HB3	2:G:461:LYS:HZ1	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:479:LEU:CG	3:L:310:LYS:CE	2.90	0.50
2:N:228:ARG:HG3	2:N:230:ARG:HH21	1.76	0.50
2:N:265:VAL:HG23	2:N:269:ARG:NH2	2.27	0.50
6:Q:508:LEU:HB2	6:Q:567:ARG:NH2	2.27	0.50
5:T:138:ALA:HA	5:T:156:SER:H	1.76	0.50
6:R:706:ALA:O	6:R:710:HIS:CG	2.65	0.50
2:A:349:ALA:HA	2:N:470:ARG:NH2	2.27	0.49
3:D:265:VAL:HG23	3:D:269:ARG:NH2	2.27	0.49
2:G:190:THR:HB	2:G:210:ARG:HE	1.77	0.49
2:G:205:ILE:CD1	2:G:269:ARG:HH21	2.25	0.49
2:G:415:GLN:HG3	2:G:418:GLN:HE21	1.75	0.49
3:K:265:VAL:HG23	3:K:269:ARG:NH2	2.27	0.49
2:F:228:ARG:HG3	2:F:230:ARG:HH21	1.77	0.49
3:V:205:ILE:CD1	3:V:269:ARG:HH21	2.25	0.49
3:V:265:VAL:HG23	3:V:269:ARG:NH2	2.27	0.49
5:S:61:VAL:HG23	5:S:61:VAL:O	2.11	0.49
5:T:117:GLY:HA3	5:T:121:ARG:H	1.77	0.49
6:R:508:LEU:HB2	6:R:567:ARG:NH2	2.27	0.49
1:J:217:PRO:HG3	2:G:391:SER:C	2.31	0.49
2:B:365:VAL:CG2	2:B:416:ALA:HB1	2.25	0.49
2:A:205:ILE:CD1	2:A:269:ARG:HH21	2.25	0.49
2:G:265:VAL:HG23	2:G:269:ARG:NH2	2.27	0.49
2:G:385:LEU:HD12	2:G:388:VAL:CG2	2.40	0.49
2:F:253:GLU:OE2	2:F:428:GLU:CD	2.48	0.49
3:L:205:ILE:CD1	3:L:269:ARG:HH21	2.25	0.49
3:L:265:VAL:HG23	3:L:269:ARG:NH2	2.27	0.49
5:S:60:ILE:O	5:S:61:VAL:HG13	2.12	0.49
1:C:5:PHE:CD2	2:E:331:ASN:ND2	2.79	0.49
2:B:196:LYS:HZ2	2:P:196:LYS:HZ3	1.37	0.49
2:B:353:GLN:HE22	2:A:384:ALA:CB	2.17	0.49
2:B:514:PHE:O	2:B:517:GLU:HB3	2.11	0.49
2:A:334:VAL:HG22	2:N:451:TRP:NE1	2.24	0.49
2:G:430:TYR:HE2	2:G:522:PHE:CZ	2.29	0.49
2:G:458:LEU:HA	2:G:461:LYS:HD2	1.94	0.49
2:H:228:ARG:HG3	2:H:230:ARG:HH21	1.77	0.49
2:H:365:VAL:HG23	2:H:420:VAL:HG11	1.94	0.49
2:F:406:LEU:HD23	3:L:220:GLN:NE2	2.06	0.49
6:Q:212:GLN:HB2	6:Q:254:TYR:CD2	2.46	0.49
6:Q:508:LEU:HD21	6:Q:513:THR:HG22	1.95	0.49
6:Q:533:LYS:HE2	6:Q:537:GLN:HA	1.94	0.49
6:Q:803:ASP:HB2	6:Q:804:ARG:NH1	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:188:LEU:HD23	6:R:191:ARG:HH22	1.77	0.49
6:R:192:LEU:HA	6:R:195:GLN:HB2	1.95	0.49
6:R:565:LEU:HD11	6:R:605:LEU:CD1	2.42	0.49
1:J:5:PHE:CD2	2:N:332:LYS:HA	2.47	0.49
1:J:90:GLU:HB2	1:C:261:ASN:HA	1.94	0.49
1:J:261:ASN:HA	1:C:90:GLU:HB2	1.94	0.49
2:B:458:LEU:HB2	2:B:489:ALA:CB	2.40	0.49
2:A:228:ARG:HG3	2:A:230:ARG:HH21	1.77	0.49
3:D:205:ILE:CD1	3:D:269:ARG:HH21	2.25	0.49
3:L:190:THR:HB	3:L:210:ARG:HE	1.77	0.49
6:Q:499:ALA:O	6:Q:503:GLU:HB2	2.12	0.49
6:Q:509:LEU:HD13	6:Q:567:ARG:NH1	2.26	0.49
5:T:60:ILE:O	5:T:61:VAL:HG13	2.12	0.49
2:B:205:ILE:CD1	2:B:269:ARG:HH21	2.25	0.49
2:G:409:ARG:C	2:G:409:ARG:HD3	2.33	0.49
2:H:430:TYR:HE2	2:H:522:PHE:CZ	2.29	0.49
6:Q:624:ASP:HA	6:Q:626:TRP:CD1	2.48	0.49
1:J:226:LEU:HD13	1:J:253:LEU:CD2	2.42	0.49
2:A:332:LYS:CA	2:N:331:ASN:O	2.60	0.49
2:G:250:PRO:N	2:G:436:SER:CB	2.73	0.49
2:G:365:VAL:HG23	2:G:420:VAL:HG11	1.94	0.49
2:H:190:THR:HB	2:H:210:ARG:HE	1.77	0.49
2:H:376:ALA:HA	2:H:406:LEU:HD13	1.94	0.49
2:F:205:ILE:CD1	2:F:269:ARG:HH21	2.25	0.49
5:S:59:LYS:HZ2	5:S:76:GLN:HB3	1.77	0.49
6:Q:625:ASN:HD22	6:Q:629:GLN:NE2	2.09	0.49
6:R:51:GLU:O	6:R:54:THR:HG22	2.12	0.49
6:R:285:HIS:CD2	6:R:285:HIS:H	2.31	0.49
6:R:469:PRO:HB2	6:R:473:TYR:CD2	2.47	0.49
6:R:533:LYS:HE2	6:R:537:GLN:HA	1.94	0.49
2:B:451:TRP:HA	2:B:496:ALA:HB3	1.95	0.49
2:E:228:ARG:HG3	2:E:230:ARG:HH21	1.77	0.49
3:K:190:THR:HB	3:K:210:ARG:HE	1.77	0.49
3:K:205:ILE:CD1	3:K:269:ARG:HH21	2.25	0.49
2:H:409:ARG:C	2:H:409:ARG:HD3	2.33	0.49
5:S:11:LEU:O	5:S:16:ARG:HB2	2.12	0.49
6:Q:53:ARG:HH12	6:Q:103:ILE:HG12	1.77	0.49
6:Q:295:MET:HA	6:Q:298:ARG:HH11	1.77	0.49
6:Q:469:PRO:HB2	6:Q:473:TYR:CE2	2.48	0.49
6:R:295:MET:HA	6:R:298:ARG:HH11	1.77	0.49
6:R:469:PRO:HB2	6:R:473:TYR:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:803:ASP:HB2	6:R:804:ARG:NH1	2.28	0.49
2:B:371:MET:HB3	2:B:412:TYR:CE2	2.48	0.49
2:A:190:THR:HB	2:A:210:ARG:HE	1.77	0.49
2:A:333:PHE:HD1	2:N:333:PHE:HB2	1.66	0.49
2:N:249:PRO:C	2:N:250:PRO:CA	2.73	0.49
2:F:196:LYS:HZ2	3:L:196:LYS:CE	2.26	0.49
6:Q:141:PRO:HD2	6:Q:195:GLN:HG2	1.94	0.49
5:T:11:LEU:O	5:T:16:ARG:HB2	2.12	0.49
5:T:55:SER:HB2	5:T:56:PRO:HD2	1.94	0.49
6:R:573:HIS:CE1	6:R:612:LEU:HA	2.48	0.49
2:B:265:VAL:HG23	2:B:269:ARG:NH2	2.27	0.49
2:B:365:VAL:HG23	2:B:420:VAL:HG11	1.94	0.49
2:B:409:ARG:C	2:B:409:ARG:HD3	2.33	0.49
2:A:265:VAL:HG23	2:A:269:ARG:NH2	2.27	0.49
2:E:209:VAL:O	2:E:224:GLU:HA	2.13	0.49
2:E:265:VAL:HG23	2:E:269:ARG:NH2	2.27	0.49
2:H:514:PHE:O	2:H:517:GLU:HB3	2.12	0.49
6:Q:483:PRO:CA	6:Q:486:VAL:H	2.25	0.49
6:Q:565:LEU:HD11	6:Q:605:LEU:CD1	2.42	0.49
5:T:59:LYS:HZ2	5:T:76:GLN:HB3	1.77	0.49
6:R:428:GLU:HG3	6:R:429:ARG:H	1.78	0.49
3:D:209:VAL:O	3:D:224:GLU:HA	2.13	0.49
2:G:228:ARG:HG3	2:G:230:ARG:HH21	1.76	0.49
2:H:458:LEU:HA	2:H:461:LYS:HD2	1.94	0.49
3:V:209:VAL:O	3:V:224:GLU:HA	2.13	0.49
5:S:117:GLY:HA3	5:S:121:ARG:H	1.77	0.49
6:Q:497:ARG:HD2	6:Q:530:VAL:HG13	1.95	0.49
6:R:95:LEU:HD12	6:R:98:TYR:CE2	2.48	0.49
6:R:141:PRO:HD2	6:R:195:GLN:HG2	1.94	0.49
6:R:457:PRO:HA	6:R:460:GLN:CD	2.34	0.49
2:B:530:LEU:HD11	2:A:544:TRP:HE1	1.73	0.48
2:N:205:ILE:CD1	2:N:269:ARG:HH21	2.25	0.48
2:H:336:GLN:HG3	2:H:340:PHE:CZ	2.48	0.48
2:H:371:MET:HB3	2:H:412:TYR:CE2	2.48	0.48
2:H:426:ILE:HB	2:H:430:TYR:OH	2.13	0.48
6:Q:469:PRO:HB2	6:Q:473:TYR:CD2	2.47	0.48
5:T:83:LEU:HB2	5:T:164:GLY:O	2.13	0.48
5:T:154:VAL:HG22	5:T:175:ARG:HG3	1.95	0.48
6:R:53:ARG:HH12	6:R:103:ILE:HG12	1.77	0.48
6:R:624:ASP:HA	6:R:626:TRP:CD1	2.48	0.48
2:G:267:SER:CA	2:G:432:ARG:NH1	2.69	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:451:TRP:HA	2:G:496:ALA:HB3	1.95	0.48
2:E:205:ILE:CD1	2:E:269:ARG:HH21	2.25	0.48
3:K:209:VAL:O	3:K:224:GLU:HA	2.13	0.48
2:P:477:ASP:OD1	2:N:309:ARG:O	2.30	0.48
6:Q:51:GLU:O	6:Q:54:THR:HG22	2.12	0.48
6:Q:266:GLU:O	6:Q:270:HIS:CD2	2.66	0.48
6:Q:581:PHE:CZ	6:Q:633:LEU:HD21	2.48	0.48
6:Q:706:ALA:O	6:Q:710:HIS:CG	2.65	0.48
5:T:104:GLU:OE2	5:T:113:LEU:HD23	2.13	0.48
6:R:266:GLU:O	6:R:270:HIS:CD2	2.66	0.48
6:R:499:ALA:O	6:R:503:GLU:HB2	2.12	0.48
6:R:617:LYS:CE	6:R:671:THR:HG22	2.42	0.48
1:C:218:ASN:N	2:B:390:LEU:CD1	2.76	0.48
2:B:199:ASP:O	2:P:199:ASP:CB	2.52	0.48
2:G:209:VAL:O	2:G:224:GLU:HA	2.13	0.48
2:G:430:TYR:CD1	2:G:430:TYR:N	2.79	0.48
2:N:209:VAL:O	2:N:224:GLU:HA	2.13	0.48
2:H:419:ASP:HB3	2:H:529:PHE:HA	1.95	0.48
2:H:451:TRP:CZ2	2:H:452:HIS:HA	2.49	0.48
2:H:451:TRP:HA	2:H:496:ALA:HB3	1.95	0.48
6:Q:95:LEU:HD12	6:Q:98:TYR:CE2	2.48	0.48
6:Q:617:LYS:CE	6:Q:671:THR:HG22	2.43	0.48
6:R:508:LEU:HD21	6:R:513:THR:HG22	1.95	0.48
2:B:376:ALA:HA	2:B:406:LEU:HD13	1.94	0.48
2:G:371:MET:HB3	2:G:412:TYR:CE2	2.47	0.48
6:R:95:LEU:HA	6:R:98:TYR:CZ	2.49	0.48
6:R:782:LEU:O	6:R:785:ALA:HB3	2.13	0.48
2:B:433:LEU:HD22	2:B:514:PHE:CE2	2.49	0.48
2:B:451:TRP:CZ2	2:B:452:HIS:HA	2.49	0.48
2:G:451:TRP:CZ2	2:G:452:HIS:HA	2.49	0.48
6:Q:32:LEU:HD22	6:Q:76:LEU:HD22	1.95	0.48
6:Q:192:LEU:HA	6:Q:195:GLN:HB2	1.95	0.48
2:G:426:ILE:HB	2:G:430:TYR:OH	2.13	0.48
2:G:433:LEU:HD22	2:G:514:PHE:CE2	2.49	0.48
2:E:199:ASP:O	3:K:200:LEU:CA	2.55	0.48
2:P:245:GLY:HA2	2:P:440:ALA:HB1	1.95	0.48
2:H:265:VAL:HG23	2:H:269:ARG:NH2	2.27	0.48
6:R:497:ARG:HD2	6:R:530:VAL:HG13	1.95	0.48
2:B:458:LEU:HA	2:B:461:LYS:HD2	1.94	0.48
2:H:433:LEU:HD22	2:H:514:PHE:CE2	2.49	0.48
5:S:104:GLU:OE2	5:S:113:LEU:HD23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:605:LEU:H	6:Q:605:LEU:HD12	1.79	0.48
6:R:130:ASP:HA	6:R:133:ASP:OD2	2.14	0.48
2:B:336:GLN:HG3	2:B:340:PHE:CZ	2.49	0.48
2:B:536:ALA:HA	2:B:539:GLU:CD	2.34	0.48
2:A:209:VAL:O	2:A:224:GLU:HA	2.13	0.48
2:G:302:ILE:O	2:G:306:HIS:CE1	2.67	0.48
2:G:536:ALA:HA	2:G:539:GLU:CD	2.34	0.48
2:E:227:ARG:HH21	2:E:294:PHE:HA	1.79	0.48
2:E:253:GLU:OE2	2:E:428:GLU:CD	2.48	0.48
2:E:406:LEU:HD23	3:K:220:GLN:NE2	2.06	0.48
3:K:302:ILE:O	3:K:306:HIS:CE1	2.67	0.48
3:L:227:ARG:HH21	3:L:294:PHE:HA	1.79	0.48
5:S:168:THR:HG23	5:S:190:THR:HG22	1.96	0.48
6:Q:428:GLU:HG3	6:Q:429:ARG:H	1.78	0.48
6:Q:525:LEU:HD22	6:Q:586:MET:HG3	1.96	0.48
6:Q:561:GLU:O	6:Q:564:TRP:HE3	1.97	0.48
6:Q:725:THR:OG1	6:R:722:THR:CB	2.56	0.48
5:T:113:LEU:HD22	5:T:130:LYS:HZ1	1.79	0.48
6:R:32:LEU:HD22	6:R:76:LEU:HD22	1.95	0.48
6:R:523:ASN:HA	6:R:526:GLU:HG3	1.96	0.48
6:R:605:LEU:H	6:R:605:LEU:HD12	1.79	0.48
1:J:58:ARG:NE	2:A:339:TRP:CH2	2.81	0.48
2:B:426:ILE:HB	2:B:430:TYR:OH	2.13	0.48
2:B:462:LYS:HA	2:B:486:VAL:HG21	1.96	0.48
2:G:376:ALA:HA	2:G:406:LEU:HD13	1.95	0.48
2:G:423:PHE:CZ	2:G:525:GLY:O	2.67	0.48
2:G:426:ILE:O	2:G:430:TYR:CZ	2.67	0.48
2:G:533:ALA:HB1	2:E:540:LEU:CD2	2.43	0.48
3:K:227:ARG:HH21	3:K:294:PHE:HA	1.79	0.48
2:H:227:ARG:HH21	2:H:294:PHE:HA	1.79	0.48
2:H:426:ILE:O	2:H:430:TYR:CZ	2.67	0.48
2:H:430:TYR:CG	2:H:518:LYS:HD2	2.49	0.48
2:F:209:VAL:O	2:F:224:GLU:HA	2.13	0.48
5:S:45:ARG:HA	5:S:48:TYR:HB2	1.95	0.48
6:Q:49:VAL:HG11	6:Q:103:ILE:HG22	1.95	0.48
6:Q:95:LEU:HA	6:Q:98:TYR:CZ	2.49	0.48
6:Q:289:LYS:HG3	6:Q:414:LEU:HD11	1.95	0.48
6:Q:500:ILE:HG23	6:Q:501:ALA:N	2.29	0.48
6:Q:573:HIS:CE1	6:Q:612:LEU:HA	2.48	0.48
6:Q:688:TYR:CD2	6:Q:705:ILE:HD13	2.49	0.48
6:Q:782:LEU:O	6:Q:785:ALA:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:521:LEU:O	6:R:524:VAL:HB	2.14	0.48
2:G:260:PHE:CD2	2:N:198:GLY:CA	2.84	0.48
2:G:336:GLN:HG3	2:G:340:PHE:CZ	2.48	0.48
2:G:430:TYR:CG	2:G:518:LYS:HD2	2.49	0.48
2:G:433:LEU:HD13	2:G:514:PHE:HZ	1.75	0.48
2:H:205:ILE:CD1	2:H:269:ARG:HH21	2.25	0.48
2:H:209:VAL:O	2:H:224:GLU:HA	2.13	0.48
2:H:368:ARG:NH2	2:H:416:ALA:HB2	2.29	0.48
2:F:302:ILE:O	2:F:306:HIS:CE1	2.67	0.48
5:S:83:LEU:HB2	5:S:164:GLY:O	2.13	0.48
6:Q:201:ARG:HA	6:Q:204:ARG:HE	1.79	0.48
6:Q:457:PRO:HA	6:Q:460:GLN:CD	2.34	0.48
6:R:49:VAL:HG11	6:R:103:ILE:HG22	1.95	0.48
6:R:434:ASP:HA	6:R:437:LEU:HB2	1.96	0.48
6:R:581:PHE:CZ	6:R:633:LEU:HD21	2.48	0.48
6:R:803:ASP:HB2	6:R:804:ARG:HH12	1.79	0.48
2:B:426:ILE:O	2:B:430:TYR:CZ	2.67	0.47
2:B:533:ALA:HB1	2:A:540:LEU:CD2	2.43	0.47
2:A:227:ARG:HH21	2:A:294:PHE:HA	1.79	0.47
2:P:209:VAL:O	2:P:224:GLU:HA	2.13	0.47
2:H:462:LYS:HA	2:H:486:VAL:HG21	1.96	0.47
2:H:533:ALA:HB1	2:F:540:LEU:CD2	2.43	0.47
6:Q:467:GLN:HE22	6:Q:500:ILE:HG13	1.79	0.47
6:Q:505:VAL:O	6:Q:509:LEU:HB2	2.14	0.47
6:Q:521:LEU:O	6:Q:524:VAL:HB	2.14	0.47
1:J:90:GLU:HG3	1:C:261:ASN:CB	2.36	0.47
2:B:368:ARG:NH2	2:B:416:ALA:HB2	2.29	0.47
2:B:430:TYR:CG	2:B:518:LYS:HD2	2.49	0.47
3:D:247:VAL:HG22	3:D:248:VAL:N	2.29	0.47
2:G:368:ARG:NH2	2:G:416:ALA:HB2	2.29	0.47
2:G:409:ARG:HE	2:G:413:GLU:HG2	1.80	0.47
2:E:302:ILE:O	2:E:306:HIS:CE1	2.67	0.47
2:H:423:PHE:CZ	2:H:525:GLY:O	2.67	0.47
2:H:536:ALA:HA	2:H:539:GLU:CD	2.34	0.47
3:V:227:ARG:HH21	3:V:294:PHE:HA	1.79	0.47
3:V:302:ILE:O	3:V:306:HIS:CE1	2.67	0.47
5:T:64:ARG:CZ	5:T:91:PHE:HA	2.45	0.47
5:T:168:THR:HG23	5:T:190:THR:HG22	1.96	0.47
6:R:561:GLU:O	6:R:564:TRP:HE3	1.97	0.47
6:R:688:TYR:CD2	6:R:705:ILE:HD13	2.49	0.47
3:D:225:VAL:HA	3:D:298:GLU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:196:LYS:HZ3	2:N:196:LYS:CE	2.25	0.47
2:H:247:VAL:HG22	2:H:248:VAL:N	2.29	0.47
5:S:64:ARG:CZ	5:S:91:PHE:HA	2.45	0.47
6:Q:28:MET:HE1	6:Q:73:LEU:HG	1.96	0.47
6:Q:453:LEU:HD22	6:Q:459:GLN:HA	1.96	0.47
6:Q:523:ASN:HA	6:Q:526:GLU:HG3	1.96	0.47
6:Q:564:TRP:CZ3	6:Q:565:LEU:HD22	2.49	0.47
6:R:289:LYS:HG3	6:R:414:LEU:HD11	1.95	0.47
2:N:227:ARG:HH21	2:N:294:PHE:HA	1.79	0.47
2:H:302:ILE:O	2:H:306:HIS:CE1	2.67	0.47
3:L:209:VAL:O	3:L:224:GLU:HA	2.13	0.47
5:S:170:TYR:HB2	5:S:172:TYR:CE1	2.50	0.47
6:Q:434:ASP:HA	6:Q:437:LEU:HB2	1.96	0.47
6:Q:528:LEU:CD2	6:Q:586:MET:SD	3.03	0.47
6:R:505:VAL:O	6:R:509:LEU:HB2	2.15	0.47
6:R:661:PHE:CE2	6:R:684:ALA:HA	2.50	0.47
1:J:82:TYR:CE1	1:C:65:LYS:CD	2.98	0.47
1:J:215:VAL:HG13	1:C:94:PRO:O	2.13	0.47
1:J:262:LYS:CD	1:C:92:ALA:HA	2.29	0.47
1:C:216:ALA:CA	2:B:392:PRO:HG3	2.44	0.47
2:B:225:VAL:HA	2:B:298:GLU:HB2	1.96	0.47
2:B:227:ARG:HH21	2:B:294:PHE:HA	1.79	0.47
2:G:389:GLU:OE2	2:G:395:SER:HA	2.14	0.47
2:G:419:ASP:HB3	2:G:529:PHE:HA	1.95	0.47
2:P:302:ILE:O	2:P:306:HIS:CE1	2.67	0.47
3:L:306:HIS:HA	3:L:309:ARG:NH2	2.29	0.47
5:S:154:VAL:HG22	5:S:175:ARG:HG3	1.95	0.47
6:Q:570:HIS:CD2	6:Q:570:HIS:O	2.67	0.47
5:T:45:ARG:HA	5:T:48:TYR:HB2	1.95	0.47
5:T:61:VAL:HG12	5:T:75:MET:HA	1.96	0.47
5:T:170:TYR:HB2	5:T:172:TYR:CE1	2.49	0.47
6:R:201:ARG:HA	6:R:204:ARG:HE	1.79	0.47
6:R:802:LEU:HB2	6:R:828:ILE:HD11	1.97	0.47
2:B:209:VAL:O	2:B:224:GLU:HA	2.13	0.47
2:B:409:ARG:HE	2:B:413:GLU:HG2	1.79	0.47
3:D:227:ARG:HH21	3:D:294:PHE:HA	1.79	0.47
2:G:247:VAL:HG22	2:G:248:VAL:N	2.29	0.47
2:H:357:LEU:HD11	2:F:381:SER:CB	2.40	0.47
3:L:302:ILE:O	3:L:306:HIS:CE1	2.67	0.47
6:Q:280:SER:HB3	6:Q:399:HIS:CE1	2.50	0.47
6:Q:479:ALA:HB1	6:Q:485:TYR:HE2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:661:PHE:CE2	6:Q:684:ALA:HA	2.50	0.47
6:Q:802:LEU:HB2	6:Q:828:ILE:HD11	1.97	0.47
6:R:570:HIS:CD2	6:R:570:HIS:O	2.68	0.47
1:J:26:VAL:HG22	1:J:146:TRP:CE3	2.50	0.47
1:J:65:LYS:CD	1:C:82:TYR:CE1	2.98	0.47
1:J:87:LEU:HD21	1:C:87:LEU:HD21	1.96	0.47
1:J:247:PHE:CE2	6:Q:97:GLN:HB2	2.49	0.47
2:B:247:VAL:HG22	2:B:248:VAL:N	2.29	0.47
2:B:423:PHE:CZ	2:B:525:GLY:O	2.67	0.47
2:G:344:ARG:HH22	2:G:441:PHE:HB3	1.80	0.47
2:G:368:ARG:CD	2:G:413:GLU:O	2.63	0.47
2:G:371:MET:HE1	2:E:371:MET:CE	2.42	0.47
2:G:383:HIS:HA	2:G:399:ASP:OD1	2.14	0.47
3:K:247:VAL:HG22	3:K:248:VAL:N	2.29	0.47
4:M:371:MET:O	4:M:374:ALA:HB3	2.15	0.47
2:N:306:HIS:HA	2:N:309:ARG:NH2	2.29	0.47
2:H:225:VAL:HA	2:H:298:GLU:HB2	1.96	0.47
2:H:375:ALA:HB1	2:H:409:ARG:HB2	1.95	0.47
2:F:249:PRO:C	2:F:250:PRO:CA	2.73	0.47
3:V:249:PRO:C	3:V:250:PRO:CA	2.73	0.47
3:L:225:VAL:HA	3:L:298:GLU:HB2	1.96	0.47
6:Q:285:HIS:CD2	6:Q:285:HIS:H	2.31	0.47
6:Q:462:LEU:HD21	6:Q:492:GLN:HE21	1.79	0.47
6:Q:773:ARG:H	6:Q:773:ARG:CD	2.26	0.47
6:R:462:LEU:HD21	6:R:492:GLN:HE21	1.79	0.47
6:R:500:ILE:HG23	6:R:501:ALA:N	2.29	0.47
6:R:525:LEU:HD22	6:R:586:MET:HG3	1.96	0.47
6:R:564:TRP:CZ3	6:R:565:LEU:HD22	2.49	0.47
6:R:759:ARG:HE	6:R:767:LEU:CD2	2.28	0.47
6:R:773:ARG:CD	6:R:773:ARG:H	2.26	0.47
2:B:302:ILE:O	2:B:306:HIS:CE1	2.67	0.47
2:B:368:ARG:CD	2:B:413:GLU:O	2.63	0.47
2:B:389:GLU:OE2	2:B:395:SER:HA	2.14	0.47
2:A:332:LYS:HB3	2:N:331:ASN:O	2.15	0.47
2:G:227:ARG:HH21	2:G:294:PHE:HA	1.79	0.47
2:G:339:TRP:HA	2:G:339:TRP:CE3	2.50	0.47
2:G:357:LEU:CD1	2:E:381:SER:HB3	2.44	0.47
2:E:196:LYS:NZ	3:K:196:LYS:CE	2.68	0.47
2:E:225:VAL:HA	2:E:298:GLU:HB2	1.96	0.47
2:P:225:VAL:HA	2:P:298:GLU:HB2	1.96	0.47
2:P:227:ARG:HH21	2:P:294:PHE:HA	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:267:SER:CB	2:H:432:ARG:HH11	1.95	0.47
2:H:409:ARG:HE	2:H:413:GLU:HG2	1.79	0.47
2:H:448:PHE:HB2	2:H:500:PHE:CZ	2.50	0.47
2:H:451:TRP:HE1	2:H:493:VAL:CA	2.28	0.47
6:Q:172:GLN:CD	6:Q:172:GLN:H	2.18	0.47
6:Q:273:ASP:HA	6:Q:276:LEU:HD12	1.97	0.47
6:R:463:LEU:HA	6:R:466:LEU:HD12	1.97	0.47
6:R:493:THR:HG23	6:R:496:THR:H	1.80	0.47
1:J:111:GLU:CG	1:C:108:LYS:HB3	2.45	0.47
1:C:26:VAL:HG22	1:C:146:TRP:CE3	2.50	0.47
2:A:247:VAL:O	2:A:248:VAL:HG13	2.15	0.47
2:A:497:ARG:CD	2:N:334:VAL:CG2	2.92	0.47
2:G:267:SER:CB	2:G:432:ARG:HH11	1.95	0.47
3:K:225:VAL:HA	3:K:298:GLU:HB2	1.97	0.47
3:K:311:GLU:O	2:H:476:GLN:CA	2.49	0.47
2:P:247:VAL:O	2:P:248:VAL:HG13	2.15	0.47
2:N:247:VAL:HG22	2:N:248:VAL:N	2.30	0.47
2:H:389:GLU:OE2	2:H:395:SER:HA	2.14	0.47
2:F:225:VAL:HA	2:F:298:GLU:HB2	1.96	0.47
2:F:227:ARG:HH21	2:F:294:PHE:HA	1.79	0.47
3:V:247:VAL:HG22	3:V:248:VAL:N	2.30	0.47
6:Q:161:THR:HB	6:Q:171:LEU:HA	1.96	0.47
6:Q:468:SER:N	6:Q:469:PRO:HD2	2.30	0.47
6:Q:528:LEU:HG	6:Q:586:MET:HE1	1.96	0.47
5:T:158:CYS:SG	5:T:171:VAL:HA	2.55	0.47
6:R:161:THR:HB	6:R:171:LEU:HA	1.96	0.47
6:R:263:PHE:HB2	6:R:268:HIS:CE1	2.50	0.47
6:R:273:ASP:HA	6:R:276:LEU:HD12	1.97	0.47
6:R:467:GLN:HE22	6:R:500:ILE:HG13	1.79	0.47
6:R:468:SER:N	6:R:469:PRO:HD2	2.30	0.47
6:R:528:LEU:CD2	6:R:586:MET:SD	3.03	0.47
1:J:9:VAL:CG2	1:J:51:VAL:HG13	2.45	0.47
2:B:246:VAL:N	2:B:503:MET:HG3	2.27	0.47
2:B:344:ARG:HH22	2:B:441:PHE:HB3	1.80	0.47
2:B:375:ALA:HB1	2:B:409:ARG:HB2	1.95	0.47
2:B:457:GLU:HB3	2:B:461:LYS:HZ1	1.79	0.47
2:G:250:PRO:HG2	2:G:433:LEU:HA	1.90	0.47
2:G:448:PHE:HB2	2:G:500:PHE:CZ	2.50	0.47
2:G:462:LYS:HA	2:G:486:VAL:HG21	1.96	0.47
2:G:475:GLN:C	3:L:311:GLU:HA	1.97	0.47
2:E:247:VAL:HG22	2:E:248:VAL:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:478:ARG:N	2:N:310:LYS:CE	2.47	0.47
2:H:383:HIS:HA	2:H:399:ASP:OD1	2.15	0.47
5:S:63:GLY:HA2	5:S:89:GLU:HB3	1.97	0.47
6:Q:583:LEU:O	6:Q:587:THR:HG23	2.15	0.47
6:R:66:TYR:O	6:R:70:PHE:CB	2.63	0.47
6:R:280:SER:HB3	6:R:399:HIS:CE1	2.50	0.47
6:R:583:LEU:O	6:R:587:THR:HG23	2.15	0.47
1:C:9:VAL:CG2	1:C:51:VAL:HG13	2.45	0.46
2:B:339:TRP:CE3	2:B:339:TRP:HA	2.50	0.46
2:B:371:MET:CE	2:A:371:MET:HE2	2.29	0.46
2:B:448:PHE:HB2	2:B:500:PHE:CZ	2.50	0.46
3:D:302:ILE:O	3:D:306:HIS:CE1	2.67	0.46
2:G:375:ALA:HB1	2:G:409:ARG:HB2	1.95	0.46
2:P:306:HIS:HA	2:P:309:ARG:NH2	2.29	0.46
2:N:247:VAL:O	2:N:248:VAL:HG13	2.15	0.46
2:N:302:ILE:O	2:N:306:HIS:CE1	2.67	0.46
2:H:339:TRP:HA	2:H:339:TRP:CE3	2.50	0.46
6:Q:194:HIS:CD2	6:Q:201:ARG:HH12	2.33	0.46
6:Q:444:VAL:HA	6:Q:447:HIS:HD2	1.80	0.46
6:Q:722:THR:CB	6:R:725:THR:OG1	2.56	0.46
1:J:5:PHE:CB	2:N:332:LYS:CB	2.72	0.46
1:J:108:LYS:HB3	1:C:111:GLU:CG	2.45	0.46
1:J:243:PRO:HB2	6:Q:134:MET:HE3	1.97	0.46
2:B:247:VAL:O	2:B:248:VAL:HG13	2.16	0.46
2:B:371:MET:HE1	2:A:367:GLN:HB3	1.93	0.46
2:B:383:HIS:HA	2:B:399:ASP:OD1	2.14	0.46
2:B:419:ASP:HB3	2:B:529:PHE:HA	1.96	0.46
2:B:498:LEU:O	2:B:501:GLU:HB3	2.16	0.46
2:A:302:ILE:O	2:A:306:HIS:CE1	2.67	0.46
3:K:247:VAL:O	3:K:248:VAL:HG13	2.15	0.46
2:H:196:LYS:HZ2	3:V:196:LYS:CE	2.26	0.46
2:H:247:VAL:O	2:H:248:VAL:HG13	2.15	0.46
2:H:372:ALA:HA	2:H:409:ARG:NE	2.31	0.46
3:L:223:PHE:CB	3:L:296:GLU:HA	2.46	0.46
3:L:247:VAL:O	3:L:248:VAL:HG13	2.15	0.46
5:S:61:VAL:HG12	5:S:75:MET:HA	1.97	0.46
6:Q:66:TYR:O	6:Q:70:PHE:CB	2.63	0.46
6:Q:148:ARG:NH1	6:Q:181:ASN:HA	2.29	0.46
6:Q:479:ALA:HB1	6:Q:485:TYR:CE2	2.50	0.46
5:T:24:PHE:CE1	5:T:157:PHE:CE1	3.04	0.46
6:R:148:ARG:NH1	6:R:181:ASN:HA	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:194:HIS:CD2	6:R:201:ARG:HH12	2.33	0.46
1:C:218:ASN:N	2:B:390:LEU:HD11	2.30	0.46
2:A:225:VAL:HA	2:A:298:GLU:HB2	1.97	0.46
2:A:260:PHE:HE2	3:D:198:GLY:CA	2.29	0.46
2:G:223:PHE:CB	2:G:296:GLU:HA	2.46	0.46
2:G:227:ARG:HD2	2:G:294:PHE:CE1	2.50	0.46
2:E:227:ARG:HD2	2:E:294:PHE:CE1	2.50	0.46
2:H:368:ARG:CD	2:H:413:GLU:O	2.63	0.46
2:H:498:LEU:O	2:H:501:GLU:HB3	2.16	0.46
2:F:247:VAL:O	2:F:248:VAL:HG13	2.16	0.46
5:S:107:LYS:HZ1	6:Q:804:ARG:NH1	2.13	0.46
6:Q:130:ASP:HA	6:Q:133:ASP:OD2	2.14	0.46
6:Q:443:LYS:N	6:Q:443:LYS:HE2	2.30	0.46
6:Q:468:SER:HA	6:Q:471:ARG:NE	2.30	0.46
6:Q:483:PRO:HA	6:Q:486:VAL:HG23	1.97	0.46
6:Q:625:ASN:HD22	6:Q:629:GLN:HE22	1.62	0.46
6:R:88:HIS:CE1	6:R:90:ALA:HA	2.50	0.46
6:R:401:VAL:O	6:R:405:HIS:HA	2.15	0.46
6:R:483:PRO:HA	6:R:486:VAL:HG23	1.97	0.46
2:B:391:SER:CB	2:B:394:LEU:HD12	2.46	0.46
2:B:400:ALA:HB1	2:B:550:GLN:HE22	1.81	0.46
2:E:223:PHE:CG	2:E:296:GLU:HA	2.51	0.46
2:E:247:VAL:O	2:E:248:VAL:HG13	2.15	0.46
2:P:223:PHE:CB	2:P:296:GLU:HA	2.46	0.46
2:H:223:PHE:CG	2:H:296:GLU:HA	2.51	0.46
5:S:110:VAL:HG23	5:S:113:LEU:HD11	1.98	0.46
6:Q:528:LEU:HD12	6:Q:531:LEU:HB3	1.98	0.46
5:T:63:GLY:HA2	5:T:89:GLU:HB3	1.97	0.46
5:T:107:LYS:HZ1	6:R:804:ARG:NH1	2.14	0.46
6:R:28:MET:CE	6:R:32:LEU:HD11	2.46	0.46
6:R:132:MET:HG2	6:R:177:PHE:CZ	2.50	0.46
6:R:528:LEU:HD12	6:R:531:LEU:HB3	1.98	0.46
6:R:573:HIS:NE2	6:R:612:LEU:HA	2.30	0.46
2:B:246:VAL:N	2:B:503:MET:CE	2.79	0.46
2:B:375:ALA:HA	2:B:378:PHE:CB	2.46	0.46
2:B:455:GLU:HG3	2:B:493:VAL:HG21	1.97	0.46
2:A:227:ARG:HD2	2:A:294:PHE:CE1	2.50	0.46
3:D:247:VAL:O	3:D:248:VAL:HG13	2.15	0.46
2:G:225:VAL:HA	2:G:298:GLU:HB2	1.96	0.46
2:G:247:VAL:O	2:G:248:VAL:HG13	2.15	0.46
2:G:498:LEU:O	2:G:501:GLU:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:249:PRO:C	2:H:250:PRO:CA	2.73	0.46
2:H:455:GLU:HG3	2:H:493:VAL:HG21	1.97	0.46
2:F:223:PHE:CB	2:F:296:GLU:HA	2.46	0.46
3:V:227:ARG:HD2	3:V:294:PHE:CE1	2.50	0.46
3:L:227:ARG:HD2	3:L:294:PHE:CE1	2.51	0.46
5:S:24:PHE:CE1	5:S:157:PHE:CE1	3.04	0.46
6:Q:28:MET:CE	6:Q:32:LEU:HD11	2.46	0.46
6:Q:759:ARG:HE	6:Q:767:LEU:CD2	2.28	0.46
5:T:88:LEU:HB2	5:T:91:PHE:CE1	2.51	0.46
5:T:110:VAL:HG23	5:T:113:LEU:HD11	1.98	0.46
6:R:468:SER:HA	6:R:471:ARG:NE	2.30	0.46
6:R:617:LYS:HE3	6:R:671:THR:HG22	1.98	0.46
2:B:451:TRP:HE1	2:B:493:VAL:CA	2.28	0.46
2:A:223:PHE:CB	2:A:296:GLU:HA	2.46	0.46
2:G:353:GLN:HE22	2:E:384:ALA:CB	2.17	0.46
2:G:455:GLU:HG3	2:G:493:VAL:HG21	1.97	0.46
2:F:247:VAL:HG22	2:F:248:VAL:N	2.30	0.46
3:V:223:PHE:CB	3:V:296:GLU:HA	2.46	0.46
3:V:225:VAL:HA	3:V:298:GLU:HB2	1.97	0.46
3:L:247:VAL:HG22	3:L:248:VAL:N	2.29	0.46
5:S:113:LEU:HD22	5:S:130:LYS:HZ1	1.79	0.46
5:S:158:CYS:SG	5:S:171:VAL:HA	2.55	0.46
6:Q:565:LEU:O	6:Q:569:VAL:HG23	2.15	0.46
1:J:262:LYS:HE3	1:C:92:ALA:HA	1.36	0.46
3:D:227:ARG:HD2	3:D:294:PHE:CE1	2.51	0.46
2:E:249:PRO:C	2:E:250:PRO:CA	2.73	0.46
3:K:227:ARG:HD2	3:K:294:PHE:CE1	2.51	0.46
2:P:187:PHE:CD1	2:P:218:TYR:CD2	3.04	0.46
2:P:247:VAL:HG22	2:P:248:VAL:N	2.29	0.46
2:N:223:PHE:CG	2:N:296:GLU:HA	2.51	0.46
2:N:223:PHE:CB	2:N:296:GLU:HA	2.46	0.46
2:N:227:ARG:HD2	2:N:294:PHE:CE1	2.51	0.46
2:F:223:PHE:CG	2:F:296:GLU:HA	2.51	0.46
5:S:30:PRO:C	5:S:32:LYS:H	2.19	0.46
5:S:46:ALA:O	5:S:50:TYR:CD2	2.69	0.46
6:Q:263:PHE:HB2	6:Q:268:HIS:CE1	2.50	0.46
6:Q:265:ASP:HA	6:Q:268:HIS:CD2	2.51	0.46
6:Q:667:VAL:O	6:Q:671:THR:HG23	2.16	0.46
6:R:479:ALA:HB1	6:R:485:TYR:CE2	2.51	0.46
1:C:57:LYS:HZ3	2:E:331:ASN:ND2	2.14	0.46
2:B:227:ARG:HD2	2:B:294:PHE:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:250:PRO:HG2	2:B:433:LEU:HA	1.90	0.46
2:A:223:PHE:CG	2:A:296:GLU:HA	2.51	0.46
2:A:247:VAL:HG22	2:A:248:VAL:N	2.30	0.46
2:A:306:HIS:HA	2:A:309:ARG:NH2	2.29	0.46
2:G:246:VAL:N	2:G:503:MET:CE	2.79	0.46
2:N:204:HIS:CE1	2:N:228:ARG:CD	2.99	0.46
2:H:223:PHE:CB	2:H:296:GLU:HA	2.46	0.46
2:H:250:PRO:HG2	2:H:433:LEU:HA	1.90	0.46
6:Q:88:HIS:CE1	6:Q:90:ALA:HA	2.50	0.46
6:Q:399:HIS:CE1	6:Q:403:ALA:CB	2.99	0.46
6:Q:401:VAL:O	6:Q:405:HIS:HA	2.15	0.46
6:R:399:HIS:CE1	6:R:403:ALA:CB	2.99	0.46
6:R:453:LEU:HD22	6:R:459:GLN:HA	1.96	0.46
2:B:204:HIS:CE1	2:B:228:ARG:CD	2.99	0.46
2:B:223:PHE:CG	2:B:296:GLU:HA	2.51	0.46
2:B:357:LEU:CD1	2:A:381:SER:HB3	2.44	0.46
2:B:372:ALA:HA	2:B:409:ARG:NE	2.31	0.46
2:B:382:LEU:HD22	2:B:401:LEU:CB	2.46	0.46
3:D:187:PHE:CD1	3:D:218:TYR:CD2	3.04	0.46
3:D:223:PHE:CB	3:D:296:GLU:HA	2.46	0.46
3:D:306:HIS:HA	3:D:309:ARG:NH2	2.29	0.46
2:G:391:SER:CB	2:G:394:LEU:HD12	2.46	0.46
2:E:306:HIS:HA	2:E:309:ARG:NH2	2.29	0.46
3:K:223:PHE:CB	3:K:296:GLU:HA	2.46	0.46
2:P:227:ARG:HH12	2:P:299:SER:N	2.14	0.46
2:H:375:ALA:HA	2:H:378:PHE:CB	2.46	0.46
3:V:223:PHE:CG	3:V:296:GLU:HA	2.51	0.46
6:Q:132:MET:HG2	6:Q:177:PHE:CZ	2.50	0.46
6:Q:463:LEU:HA	6:Q:466:LEU:HD12	1.97	0.46
6:Q:532:ILE:HB	6:Q:593:GLU:OE2	2.16	0.46
5:T:12:HIS:CE1	5:T:16:ARG:HE	2.34	0.46
6:R:172:GLN:CD	6:R:172:GLN:H	2.18	0.46
6:R:565:LEU:O	6:R:569:VAL:HG23	2.15	0.46
2:B:227:ARG:HH12	2:B:299:SER:N	2.14	0.46
2:G:196:LYS:HZ1	2:N:196:LYS:HZ3	1.41	0.46
2:G:451:TRP:HE1	2:G:493:VAL:CA	2.28	0.46
2:E:227:ARG:HH12	2:E:299:SER:N	2.14	0.46
3:K:204:HIS:CE1	3:K:228:ARG:CD	2.99	0.46
2:P:227:ARG:HD2	2:P:294:PHE:CE1	2.50	0.46
2:P:250:PRO:N	2:P:433:LEU:CD2	2.78	0.46
2:N:225:VAL:HA	2:N:298:GLU:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:430:TYR:CD1	2:H:430:TYR:N	2.79	0.46
3:L:204:HIS:CE1	3:L:228:ARG:CD	2.99	0.46
6:Q:573:HIS:NE2	6:Q:612:LEU:HA	2.30	0.46
6:R:444:VAL:HA	6:R:447:HIS:HD2	1.80	0.46
1:J:5:PHE:HZ	2:A:336:GLN:HG2	1.81	0.45
2:G:187:PHE:CD1	2:G:218:TYR:CD2	3.04	0.45
2:E:187:PHE:CD1	2:E:218:TYR:CD2	3.04	0.45
3:K:223:PHE:CG	3:K:296:GLU:HA	2.51	0.45
3:K:227:ARG:HH12	3:K:299:SER:N	2.14	0.45
2:P:204:HIS:CE1	2:P:228:ARG:CD	2.99	0.45
2:H:187:PHE:CD1	2:H:218:TYR:CD2	3.04	0.45
2:H:227:ARG:HD2	2:H:294:PHE:CE1	2.51	0.45
2:H:382:LEU:HD22	2:H:401:LEU:CB	2.46	0.45
3:L:227:ARG:HH12	3:L:299:SER:N	2.14	0.45
6:Q:66:TYR:O	6:Q:70:PHE:HB3	2.16	0.45
6:Q:404:GLN:O	6:Q:405:HIS:CG	2.69	0.45
6:Q:493:THR:HG23	6:Q:496:THR:H	1.80	0.45
6:R:265:ASP:HA	6:R:268:HIS:CD2	2.51	0.45
6:R:404:GLN:O	6:R:405:HIS:CG	2.69	0.45
1:J:58:ARG:CZ	2:A:339:TRP:CH2	2.98	0.45
1:J:233:ASP:OD2	6:Q:143:ARG:NE	2.49	0.45
2:A:332:LYS:HA	2:N:331:ASN:CA	2.44	0.45
3:D:227:ARG:HH12	3:D:299:SER:N	2.14	0.45
2:G:400:ALA:HB1	2:G:550:GLN:HE22	1.81	0.45
4:O:371:MET:O	4:O:374:ALA:HB3	2.15	0.45
2:P:223:PHE:CG	2:P:296:GLU:HA	2.51	0.45
2:H:227:ARG:HH12	2:H:299:SER:N	2.14	0.45
2:F:227:ARG:HD2	2:F:294:PHE:CE1	2.50	0.45
2:F:227:ARG:HH12	2:F:299:SER:N	2.14	0.45
3:V:247:VAL:O	3:V:248:VAL:HG13	2.15	0.45
5:S:12:HIS:CE1	5:S:16:ARG:HE	2.34	0.45
5:S:118:GLY:C	5:S:120:HIS:H	2.19	0.45
6:Q:461:SER:O	6:Q:465:LEU:HB2	2.16	0.45
6:Q:525:LEU:HD21	6:Q:583:LEU:HD23	1.98	0.45
5:T:118:GLY:C	5:T:120:HIS:H	2.18	0.45
5:T:175:ARG:HH21	5:T:183:ASN:C	2.20	0.45
2:E:223:PHE:CB	2:E:296:GLU:HA	2.46	0.45
2:P:249:PRO:C	2:P:250:PRO:CA	2.73	0.45
6:Q:565:LEU:O	6:Q:568:LEU:HD23	2.17	0.45
5:T:30:PRO:C	5:T:32:LYS:H	2.19	0.45
5:T:46:ALA:O	5:T:50:TYR:CD2	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:399:HIS:CE1	6:R:403:ALA:HB2	2.51	0.45
6:R:479:ALA:HB1	6:R:485:TYR:HE2	1.80	0.45
6:R:565:LEU:O	6:R:568:LEU:HD23	2.17	0.45
6:R:625:ASN:HD22	6:R:629:GLN:HE22	1.62	0.45
2:G:227:ARG:HH12	2:G:299:SER:N	2.14	0.45
2:G:369:LYS:O	2:G:372:ALA:HB3	2.16	0.45
2:G:372:ALA:HA	2:G:409:ARG:NE	2.31	0.45
3:K:187:PHE:CD1	3:K:218:TYR:CD2	3.04	0.45
3:K:249:PRO:C	3:K:250:PRO:CA	2.73	0.45
2:H:372:ALA:HB2	2:H:413:GLU:OE1	2.17	0.45
2:H:391:SER:CB	2:H:394:LEU:HD12	2.46	0.45
2:F:260:PHE:CD2	3:L:198:GLY:CA	2.84	0.45
5:S:88:LEU:HB2	5:S:91:PHE:CE1	2.51	0.45
1:J:94:PRO:O	1:C:215:VAL:HG13	2.13	0.45
2:B:278:LYS:HB3	2:B:282:HIS:CE1	2.52	0.45
2:B:352:ASN:HA	2:B:355:LYS:HE3	1.98	0.45
3:D:204:HIS:CE1	3:D:228:ARG:CD	2.99	0.45
3:D:251:PRO:HA	3:D:275:MET:SD	2.57	0.45
2:G:204:HIS:CE1	2:G:228:ARG:CD	2.99	0.45
2:G:375:ALA:HA	2:G:378:PHE:CB	2.46	0.45
2:G:382:LEU:HD22	2:G:401:LEU:CB	2.46	0.45
2:E:250:PRO:HG2	2:E:433:LEU:CG	2.22	0.45
2:P:278:LYS:HB3	2:P:282:HIS:CE1	2.52	0.45
2:H:204:HIS:CE1	2:H:228:ARG:CD	2.99	0.45
2:H:278:LYS:HB3	2:H:282:HIS:CE1	2.52	0.45
2:H:352:ASN:HA	2:H:355:LYS:HE3	1.99	0.45
3:V:187:PHE:CD1	3:V:218:TYR:CD2	3.04	0.45
5:S:168:THR:CG2	5:S:190:THR:HG22	2.46	0.45
6:Q:621:HIS:HB2	6:Q:622:TYR:CZ	2.51	0.45
6:R:443:LYS:HE2	6:R:443:LYS:N	2.30	0.45
6:R:667:VAL:O	6:R:671:THR:HG23	2.16	0.45
1:J:90:GLU:OE2	1:C:82:TYR:HE2	1.75	0.45
1:J:92:ALA:HA	1:C:262:LYS:HE3	1.36	0.45
1:J:229:PHE:CE1	6:Q:105:ARG:HD3	2.52	0.45
2:B:187:PHE:CD1	2:B:218:TYR:CD2	3.04	0.45
2:B:251:PRO:HA	2:B:275:MET:SD	2.57	0.45
2:A:349:ALA:CB	2:N:470:ARG:HH21	2.27	0.45
2:G:251:PRO:HA	2:G:275:MET:SD	2.57	0.45
2:G:352:ASN:HA	2:G:355:LYS:HE3	1.99	0.45
2:G:376:ALA:HB2	2:G:409:ARG:NH2	2.32	0.45
2:G:380:ALA:O	2:G:383:HIS:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:278:LYS:HB3	3:K:282:HIS:CE1	2.52	0.45
2:P:206:VAL:HA	2:P:227:ARG:O	2.17	0.45
2:P:310:LYS:CE	2:N:478:ARG:N	2.68	0.45
2:N:187:PHE:CD1	2:N:218:TYR:CD2	3.04	0.45
2:N:227:ARG:HH12	2:N:299:SER:N	2.14	0.45
2:H:251:PRO:HA	2:H:275:MET:SD	2.57	0.45
3:V:278:LYS:HB3	3:V:282:HIS:CE1	2.52	0.45
3:L:187:PHE:CD1	3:L:218:TYR:CD2	3.04	0.45
6:Q:565:LEU:HA	6:Q:568:LEU:HD23	1.99	0.45
5:T:12:HIS:HA	5:T:41:ASN:O	2.16	0.45
6:R:621:HIS:HB2	6:R:622:TYR:CZ	2.52	0.45
1:C:30:LYS:NZ	2:P:283:PRO:CG	2.75	0.45
2:A:227:ARG:HH12	2:A:299:SER:N	2.14	0.45
3:D:223:PHE:CG	3:D:296:GLU:HA	2.51	0.45
2:G:206:VAL:HA	2:G:227:ARG:O	2.17	0.45
2:E:278:LYS:HB3	2:E:282:HIS:CE1	2.52	0.45
2:P:310:LYS:HD2	2:N:480:ASN:ND2	2.31	0.45
2:H:406:LEU:HD12	2:H:409:ARG:HH21	1.81	0.45
2:F:187:PHE:CD1	2:F:218:TYR:CD2	3.04	0.45
2:F:204:HIS:CE1	2:F:228:ARG:CD	2.99	0.45
3:V:204:HIS:CE1	3:V:228:ARG:CD	2.99	0.45
6:Q:428:GLU:OE1	6:Q:433:VAL:HG21	2.17	0.45
5:T:168:THR:CG2	5:T:190:THR:HG22	2.46	0.45
6:R:428:GLU:OE1	6:R:433:VAL:HG21	2.17	0.45
6:R:525:LEU:HD21	6:R:583:LEU:HD23	1.98	0.45
1:J:5:PHE:CD2	2:N:332:LYS:CA	3.00	0.45
1:C:216:ALA:CA	2:B:392:PRO:CG	2.94	0.45
2:A:204:HIS:CE1	2:A:228:ARG:CD	2.99	0.45
2:A:206:VAL:HA	2:A:227:ARG:O	2.17	0.45
2:A:278:LYS:HB3	2:A:282:HIS:CE1	2.52	0.45
2:E:204:HIS:CE1	2:E:228:ARG:CD	2.99	0.45
2:E:251:PRO:HA	2:E:275:MET:SD	2.57	0.45
2:H:344:ARG:HH22	2:H:441:PHE:HB3	1.80	0.45
2:F:206:VAL:HA	2:F:227:ARG:O	2.17	0.45
5:T:51:LEU:HD13	5:T:58:LEU:CD1	2.47	0.45
6:R:532:ILE:HB	6:R:593:GLU:OE2	2.16	0.45
1:J:92:ALA:HA	1:C:262:LYS:CD	2.28	0.45
2:B:372:ALA:HB2	2:B:413:GLU:OE1	2.17	0.45
2:B:414:ARG:HB3	2:B:418:GLN:HE21	1.82	0.45
2:B:535:GLU:OE1	2:B:535:GLU:HA	2.17	0.45
2:A:187:PHE:CD1	2:A:218:TYR:CD2	3.04	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:249:PRO:C	2:A:250:PRO:CA	2.73	0.45
2:A:260:PHE:CD2	3:D:198:GLY:CA	2.84	0.45
3:K:251:PRO:HA	3:K:275:MET:SD	2.57	0.45
2:P:383:HIS:CD2	2:P:402:SER:HB3	2.52	0.45
2:H:376:ALA:HB2	2:H:409:ARG:NH2	2.32	0.45
3:V:306:HIS:HA	3:V:309:ARG:NH2	2.29	0.45
3:L:251:PRO:HA	3:L:275:MET:SD	2.57	0.45
5:S:127:TYR:CE2	5:S:132:PHE:CE2	3.04	0.45
6:Q:399:HIS:CE1	6:Q:403:ALA:HB2	2.51	0.45
6:Q:498:ARG:HH11	6:Q:506:ARG:HH11	1.65	0.45
6:Q:719:ASN:O	6:Q:723:LEU:HG	2.17	0.45
6:R:486:VAL:HA	6:R:489:PHE:CE1	2.52	0.45
6:R:631:SER:HA	6:R:634:PHE:CZ	2.52	0.45
2:A:250:PRO:HG2	2:A:433:LEU:CG	2.22	0.45
3:D:249:PRO:C	3:D:250:PRO:CA	2.73	0.45
2:G:223:PHE:CG	2:G:296:GLU:HA	2.51	0.45
2:G:434:ILE:O	2:G:438:LYS:HG3	2.17	0.45
2:G:514:PHE:CZ	2:G:518:LYS:NZ	2.81	0.45
3:K:209:VAL:HB	3:K:225:VAL:CG2	2.47	0.45
2:H:400:ALA:HB1	2:H:550:GLN:HE22	1.81	0.45
2:H:414:ARG:HB3	2:H:418:GLN:HE21	1.82	0.45
3:V:251:PRO:HA	3:V:275:MET:SD	2.57	0.45
3:L:278:LYS:HB3	3:L:282:HIS:CE1	2.52	0.45
5:S:175:ARG:HH21	5:S:183:ASN:C	2.20	0.45
6:Q:617:LYS:HE3	6:Q:671:THR:HG22	1.98	0.45
6:Q:803:ASP:HB2	6:Q:804:ARG:HH12	1.79	0.45
5:T:124:CYS:SG	5:T:133:VAL:HG13	2.57	0.45
5:T:127:TYR:CE2	5:T:132:PHE:CE2	3.04	0.45
6:R:66:TYR:O	6:R:70:PHE:HB3	2.16	0.45
6:R:87:ASN:CG	6:R:88:HIS:H	2.21	0.45
6:R:416:CYS:O	6:R:419:ALA:HB3	2.16	0.45
6:R:461:SER:O	6:R:465:LEU:HB2	2.16	0.45
6:R:588:ARG:HH21	6:R:591:TYR:HB2	1.82	0.45
6:R:612:LEU:HD11	6:R:616:PHE:CE1	2.52	0.45
6:R:676:VAL:HB	6:R:680:PHE:CZ	2.52	0.45
1:J:30:LYS:HZ3	2:N:283:PRO:HD2	1.81	0.44
2:B:223:PHE:CB	2:B:296:GLU:HA	2.46	0.44
2:B:367:GLN:HA	2:B:369:LYS:HB2	1.99	0.44
3:D:278:LYS:HB3	3:D:282:HIS:CE1	2.52	0.44
2:E:206:VAL:HA	2:E:227:ARG:O	2.17	0.44
2:N:278:LYS:HB3	2:N:282:HIS:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:206:VAL:HA	3:L:227:ARG:O	2.17	0.44
5:S:124:CYS:SG	5:S:133:VAL:HG13	2.57	0.44
6:Q:276:LEU:HD21	6:Q:393:PHE:CD1	2.52	0.44
6:Q:416:CYS:SG	6:Q:465:LEU:HB2	2.58	0.44
6:R:97:GLN:HA	6:R:105:ARG:HG3	1.99	0.44
6:R:473:TYR:CD2	6:R:476:ILE:HG22	2.52	0.44
6:R:626:TRP:CD2	6:R:627:SER:N	2.85	0.44
6:R:677:ALA:O	6:R:681:PHE:CD2	2.70	0.44
2:G:365:VAL:CG2	2:G:416:ALA:HB1	2.26	0.44
2:G:372:ALA:HB2	2:G:413:GLU:OE1	2.17	0.44
2:P:479:LEU:N	2:N:310:LYS:NZ	2.65	0.44
2:H:246:VAL:N	2:H:503:MET:CE	2.79	0.44
6:Q:34:THR:HB	6:Q:37:LYS:HB2	1.99	0.44
6:Q:59:PRO:O	6:Q:63:TYR:HB2	2.17	0.44
6:Q:206:GLN:HA	6:Q:209:ARG:CZ	2.47	0.44
6:Q:416:CYS:O	6:Q:419:ALA:HB3	2.16	0.44
6:Q:486:VAL:HA	6:Q:489:PHE:CE1	2.52	0.44
2:B:369:LYS:O	2:B:372:ALA:HB3	2.16	0.44
2:B:376:ALA:HB2	2:B:409:ARG:NH2	2.32	0.44
2:B:433:LEU:HD22	2:B:514:PHE:CZ	2.53	0.44
2:A:251:PRO:HA	2:A:275:MET:SD	2.57	0.44
2:G:368:ARG:HG3	2:G:416:ALA:HB2	1.99	0.44
2:G:538:LYS:HZ2	2:G:541:ILE:HB	1.82	0.44
3:K:206:VAL:HA	3:K:227:ARG:O	2.17	0.44
2:H:434:ILE:O	2:H:438:LYS:HG3	2.17	0.44
2:F:278:LYS:HB3	2:F:282:HIS:CE1	2.52	0.44
2:F:306:HIS:HA	2:F:309:ARG:NH2	2.29	0.44
3:V:227:ARG:HH12	3:V:299:SER:N	2.14	0.44
3:L:223:PHE:CG	3:L:296:GLU:HA	2.51	0.44
6:Q:494:TYR:CD2	6:Q:535:GLY:HA3	2.53	0.44
6:Q:612:LEU:HD11	6:Q:616:PHE:CE1	2.52	0.44
6:Q:715:PHE:HB3	6:Q:719:ASN:HB2	2.00	0.44
1:C:5:PHE:CB	2:E:331:ASN:N	2.78	0.44
2:B:385:LEU:CD2	2:A:350:LEU:HD13	2.46	0.44
3:D:206:VAL:HA	3:D:227:ARG:O	2.17	0.44
2:G:250:PRO:CD	2:G:436:SER:CB	2.96	0.44
2:G:470:ARG:NH1	2:H:348:ASP:HB2	2.32	0.44
2:H:206:VAL:HA	2:H:227:ARG:O	2.17	0.44
2:H:357:LEU:CD2	2:F:378:PHE:CD1	3.01	0.44
2:H:406:LEU:O	2:H:410:ASP:CG	2.56	0.44
2:F:197:VAL:HG23	2:F:204:HIS:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:206:VAL:HA	3:V:227:ARG:O	2.17	0.44
5:S:12:HIS:HA	5:S:41:ASN:O	2.17	0.44
6:Q:263:PHE:HB2	6:Q:268:HIS:HE1	1.83	0.44
6:Q:409:GLN:HG2	6:Q:458:ALA:HA	1.99	0.44
6:Q:471:ARG:HB2	6:Q:472:ARG:HH12	1.83	0.44
6:Q:626:TRP:CD2	6:Q:627:SER:N	2.86	0.44
5:T:117:GLY:N	5:T:134:ASN:HD21	2.15	0.44
6:R:59:PRO:O	6:R:63:TYR:HB2	2.17	0.44
6:R:276:LEU:HD21	6:R:393:PHE:CD1	2.52	0.44
6:R:494:TYR:CD2	6:R:535:GLY:HA3	2.53	0.44
6:R:525:LEU:C	6:R:529:LYS:HZ2	2.21	0.44
6:R:565:LEU:HA	6:R:568:LEU:HD23	1.99	0.44
1:J:24:VAL:CG2	1:J:38:LEU:HD13	2.48	0.44
2:B:246:VAL:H	2:B:503:MET:CE	2.27	0.44
2:B:249:PRO:C	2:B:250:PRO:CA	2.73	0.44
2:A:260:PHE:CE2	3:D:198:GLY:HA2	2.53	0.44
2:G:278:LYS:HB3	2:G:282:HIS:CE1	2.52	0.44
2:P:251:PRO:HA	2:P:275:MET:SD	2.57	0.44
2:H:369:LYS:O	2:H:372:ALA:HB3	2.16	0.44
2:F:251:PRO:HA	2:F:275:MET:SD	2.57	0.44
6:Q:479:ALA:O	6:Q:485:TYR:CE2	2.71	0.44
6:Q:677:ALA:O	6:Q:681:PHE:CD2	2.70	0.44
6:R:675:GLU:CD	6:R:675:GLU:H	2.21	0.44
1:J:261:ASN:CB	1:C:90:GLU:HG3	2.36	0.44
1:C:216:ALA:HB1	1:C:217:PRO:HD3	2.00	0.44
1:C:217:PRO:N	2:B:390:LEU:HD11	2.33	0.44
2:B:260:PHE:HE2	2:P:198:GLY:CA	2.29	0.44
2:B:434:ILE:O	2:B:438:LYS:HG3	2.17	0.44
2:A:349:ALA:CA	2:N:470:ARG:NH2	2.81	0.44
2:P:244:PRO:O	2:P:444:ARG:NH2	2.39	0.44
2:N:197:VAL:HG23	2:N:204:HIS:O	2.18	0.44
2:N:302:ILE:HD12	2:N:302:ILE:H	1.83	0.44
2:H:391:SER:HA	2:H:392:PRO:HD3	1.82	0.44
6:Q:560:GLU:HA	6:Q:562:GLN:HE22	1.83	0.44
6:Q:588:ARG:HH21	6:Q:591:TYR:HB2	1.82	0.44
6:Q:631:SER:HA	6:Q:634:PHE:CZ	2.52	0.44
6:R:440:ALA:O	6:R:444:VAL:HG23	2.18	0.44
6:R:498:ARG:HH11	6:R:506:ARG:HH11	1.65	0.44
6:R:582:ARG:HG3	6:R:582:ARG:H	1.54	0.44
2:B:242:ASN:HD22	2:B:288:ASP:CG	2.21	0.44
2:B:337:ASP:O	2:B:341:HIS:CG	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:523:LYS:HA	2:B:523:LYS:HE2	2.00	0.44
2:A:242:ASN:HD22	2:A:288:ASP:CG	2.21	0.44
3:D:242:ASN:HD22	3:D:288:ASP:CG	2.21	0.44
2:P:240:HIS:CA	2:P:248:VAL:HG11	2.48	0.44
2:N:383:HIS:CD2	2:N:402:SER:HB3	2.52	0.44
5:S:8:ILE:HD12	5:S:157:PHE:CE2	2.53	0.44
6:Q:31:PHE:HB2	6:Q:41:ALA:HA	2.00	0.44
6:Q:87:ASN:CG	6:Q:88:HIS:H	2.21	0.44
6:Q:676:VAL:HB	6:Q:680:PHE:CZ	2.52	0.44
6:Q:717:ARG:HA	6:Q:720:TYR:HB2	1.99	0.44
6:R:31:PHE:HB2	6:R:41:ALA:HA	2.00	0.44
6:R:114:THR:HA	6:R:117:MET:SD	2.58	0.44
6:R:206:GLN:HA	6:R:209:ARG:CZ	2.47	0.44
6:R:479:ALA:O	6:R:485:TYR:CE2	2.71	0.44
1:C:30:LYS:HZ1	2:P:283:PRO:CG	2.27	0.44
2:B:206:VAL:HA	2:B:227:ARG:O	2.17	0.44
2:B:380:ALA:O	2:B:383:HIS:HD2	1.99	0.44
2:B:406:LEU:O	2:B:410:ASP:CG	2.56	0.44
2:B:451:TRP:CH2	2:B:452:HIS:HA	2.53	0.44
3:D:197:VAL:HG23	3:D:204:HIS:O	2.18	0.44
2:G:209:VAL:HB	2:G:225:VAL:CG2	2.47	0.44
2:G:406:LEU:CD1	2:G:409:ARG:NH2	2.81	0.44
2:G:414:ARG:HB3	2:G:418:GLN:HE21	1.82	0.44
2:G:451:TRP:HE1	2:G:493:VAL:HA	1.83	0.44
2:E:240:HIS:CA	2:E:248:VAL:HG11	2.48	0.44
2:N:251:PRO:HA	2:N:275:MET:SD	2.57	0.44
2:H:337:ASP:O	2:H:341:HIS:CG	2.71	0.44
2:F:240:HIS:CA	2:F:248:VAL:HG11	2.48	0.44
2:F:242:ASN:HD22	2:F:288:ASP:CG	2.21	0.44
5:S:51:LEU:HD13	5:S:58:LEU:CD1	2.47	0.44
6:Q:648:VAL:HG23	6:Q:649:ASN:H	1.82	0.44
6:Q:675:GLU:H	6:Q:675:GLU:CD	2.21	0.44
6:R:141:PRO:CD	6:R:191:ARG:HE	2.27	0.44
6:R:409:GLN:HG2	6:R:458:ALA:HA	1.99	0.44
6:R:416:CYS:SG	6:R:465:LEU:HB2	2.58	0.44
1:C:24:VAL:CG2	1:C:38:LEU:HD13	2.48	0.44
2:B:240:HIS:CA	2:B:248:VAL:HG11	2.48	0.44
2:B:260:PHE:CE2	2:P:198:GLY:HA2	2.53	0.44
2:B:371:MET:HE1	2:A:371:MET:CE	2.40	0.44
2:B:379:SER:CB	2:B:402:SER:O	2.66	0.44
2:B:530:LEU:CD2	2:A:544:TRP:CG	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:240:HIS:CA	3:K:248:VAL:HG11	2.48	0.44
2:H:433:LEU:HD22	2:H:514:PHE:CZ	2.53	0.44
3:V:197:VAL:HG23	3:V:204:HIS:O	2.18	0.44
5:S:79:THR:HG23	5:S:82:SER:HA	2.00	0.44
5:S:88:LEU:HD12	5:S:91:PHE:CD1	2.53	0.44
6:Q:97:GLN:HA	6:Q:105:ARG:HG3	1.99	0.44
6:Q:440:ALA:O	6:Q:444:VAL:HG23	2.17	0.44
6:Q:471:ARG:HB2	6:Q:472:ARG:NH1	2.33	0.44
6:Q:580:GLN:O	6:Q:584:LEU:HG	2.17	0.44
5:T:88:LEU:HD12	5:T:91:PHE:CD1	2.53	0.44
6:R:471:ARG:HB2	6:R:472:ARG:NH1	2.33	0.44
6:R:680:PHE:HA	6:R:683:GLN:CD	2.38	0.44
1:J:217:PRO:HA	2:G:392:PRO:HA	2.00	0.43
2:B:250:PRO:CD	2:B:436:SER:CB	2.96	0.43
2:B:368:ARG:HG3	2:B:416:ALA:HB2	1.99	0.43
3:D:240:HIS:CA	3:D:248:VAL:HG11	2.48	0.43
2:G:302:ILE:H	2:G:302:ILE:HD12	1.83	0.43
2:G:433:LEU:HD22	2:G:514:PHE:CZ	2.53	0.43
2:E:206:VAL:HG13	2:E:228:ARG:HG2	2.00	0.43
2:H:260:PHE:HE2	3:V:198:GLY:CA	2.29	0.43
2:H:353:GLN:HE22	2:F:384:ALA:CB	2.17	0.43
5:S:117:GLY:N	5:S:134:ASN:HD21	2.15	0.43
6:Q:114:THR:HA	6:Q:117:MET:SD	2.58	0.43
6:Q:266:GLU:O	6:Q:269:LEU:HB3	2.18	0.43
6:R:565:LEU:HD11	6:R:605:LEU:HG	2.00	0.43
6:R:611:LYS:HG3	6:R:612:LEU:N	2.33	0.43
6:R:648:VAL:HG23	6:R:649:ASN:H	1.82	0.43
6:R:717:ARG:HA	6:R:720:TYR:HB2	1.99	0.43
2:A:449:HIS:CD2	2:A:449:HIS:C	2.92	0.43
2:G:357:LEU:CD2	2:E:378:PHE:CD1	3.01	0.43
2:G:379:SER:CB	2:G:402:SER:O	2.66	0.43
2:G:538:LYS:HD2	2:G:538:LYS:HA	1.86	0.43
2:E:209:VAL:HB	2:E:225:VAL:CG2	2.47	0.43
2:P:242:ASN:HD22	2:P:288:ASP:CG	2.21	0.43
2:P:302:ILE:H	2:P:302:ILE:HD12	1.83	0.43
2:N:206:VAL:HA	2:N:227:ARG:O	2.17	0.43
2:H:276:LEU:HA	2:H:279:ILE:HG12	2.00	0.43
2:H:302:ILE:H	2:H:302:ILE:HD12	1.83	0.43
2:H:530:LEU:CD2	2:F:544:TRP:CG	2.95	0.43
2:H:535:GLU:OE1	2:H:535:GLU:HA	2.17	0.43
2:F:253:GLU:CD	2:F:428:GLU:OE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:240:HIS:CA	3:V:248:VAL:HG11	2.48	0.43
3:L:206:VAL:HG13	3:L:228:ARG:HG2	2.00	0.43
3:L:242:ASN:HD22	3:L:288:ASP:CG	2.21	0.43
3:L:276:LEU:HA	3:L:279:ILE:HG12	2.00	0.43
6:Q:84:HIS:HB3	6:Q:85:PRO:HD3	2.00	0.43
6:Q:520:HIS:HA	6:Q:523:ASN:HD22	1.83	0.43
6:Q:525:LEU:C	6:Q:529:LYS:HZ2	2.21	0.43
6:Q:569:VAL:HG13	6:Q:608:ALA:HB2	1.99	0.43
6:Q:611:LYS:HG3	6:Q:612:LEU:N	2.33	0.43
5:T:60:ILE:H	5:T:60:ILE:HD12	1.82	0.43
6:R:468:SER:HA	6:R:471:ARG:CZ	2.48	0.43
6:R:560:GLU:HA	6:R:562:GLN:HE22	1.83	0.43
6:R:569:VAL:HG13	6:R:608:ALA:HB2	1.99	0.43
2:B:451:TRP:HE1	2:B:493:VAL:HA	1.82	0.43
2:A:333:PHE:CD2	2:N:451:TRP:HH2	2.28	0.43
2:G:242:ASN:HD22	2:G:288:ASP:CG	2.21	0.43
2:G:260:PHE:CE2	2:N:198:GLY:HA2	2.53	0.43
3:K:242:ASN:HD22	3:K:288:ASP:CG	2.21	0.43
2:H:197:VAL:HG23	2:H:204:HIS:O	2.18	0.43
2:H:206:VAL:HG13	2:H:228:ARG:HG2	2.00	0.43
2:H:368:ARG:HG3	2:H:416:ALA:HB2	1.99	0.43
3:V:209:VAL:HB	3:V:225:VAL:CG2	2.47	0.43
5:S:60:ILE:HD12	5:S:60:ILE:H	1.82	0.43
6:Q:473:TYR:CD2	6:Q:476:ILE:HG22	2.52	0.43
5:T:79:THR:HG23	5:T:82:SER:HA	2.00	0.43
6:R:785:ALA:HA	6:R:788:CYS:SG	2.59	0.43
2:B:199:ASP:O	2:P:200:LEU:CA	2.55	0.43
2:B:227:ARG:HA	2:B:300:PHE:HE1	1.83	0.43
2:G:197:VAL:HG23	2:G:204:HIS:O	2.18	0.43
2:G:206:VAL:HG13	2:G:228:ARG:HG2	2.00	0.43
2:G:406:LEU:O	2:G:410:ASP:CG	2.56	0.43
2:G:423:PHE:HA	2:G:426:ILE:HG12	2.01	0.43
2:E:197:VAL:HG23	2:E:204:HIS:O	2.18	0.43
2:P:197:VAL:HG23	2:P:204:HIS:O	2.18	0.43
2:N:240:HIS:CA	2:N:248:VAL:HG11	2.48	0.43
2:H:250:PRO:CD	2:H:436:SER:CB	2.96	0.43
2:H:250:PRO:N	2:H:436:SER:CB	2.72	0.43
2:H:451:TRP:CH2	2:H:452:HIS:HA	2.53	0.43
6:R:580:GLN:O	6:R:584:LEU:HG	2.18	0.43
6:R:719:ASN:O	6:R:723:LEU:HG	2.17	0.43
1:J:93:ALA:HA	1:C:262:LYS:HB3	1.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:216:ALA:HB1	1:J:217:PRO:HD3	2.00	0.43
1:C:216:ALA:HA	2:B:392:PRO:CG	2.48	0.43
1:C:217:PRO:HA	2:B:392:PRO:HB3	1.99	0.43
2:B:197:VAL:HG23	2:B:204:HIS:O	2.18	0.43
2:A:332:LYS:CB	2:N:331:ASN:O	2.67	0.43
3:D:302:ILE:H	3:D:302:ILE:HD12	1.83	0.43
2:G:260:PHE:HE2	2:N:198:GLY:CA	2.29	0.43
2:G:306:HIS:HA	2:G:309:ARG:NH2	2.28	0.43
2:G:505:ARG:NE	2:G:505:ARG:HA	2.34	0.43
2:G:523:LYS:HA	2:G:523:LYS:HE2	2.00	0.43
3:K:197:VAL:HG23	3:K:204:HIS:O	2.18	0.43
2:N:209:VAL:HB	2:N:225:VAL:CG2	2.47	0.43
2:F:227:ARG:HA	2:F:300:PHE:HE1	1.84	0.43
3:L:302:ILE:H	3:L:302:ILE:HD12	1.83	0.43
6:Q:443:LYS:HA	6:Q:446:GLU:OE2	2.18	0.43
6:Q:473:TYR:CD2	6:Q:476:ILE:HA	2.54	0.43
6:Q:564:TRP:HZ3	6:Q:565:LEU:HD22	1.83	0.43
6:Q:573:HIS:CD2	6:Q:615:ARG:HG2	2.53	0.43
6:Q:753:ALA:HA	6:Q:767:LEU:HD13	2.00	0.43
5:T:178:GLU:H	5:T:178:GLU:CD	2.22	0.43
6:R:517:THR:HB	6:R:518:PRO:HD2	2.01	0.43
2:B:391:SER:HB2	2:B:394:LEU:HD12	2.01	0.43
2:B:423:PHE:HA	2:B:426:ILE:HG12	2.01	0.43
3:D:206:VAL:HG13	3:D:228:ARG:HG2	2.00	0.43
3:D:276:LEU:HA	3:D:279:ILE:HG12	2.00	0.43
2:G:227:ARG:HA	2:G:300:PHE:HE1	1.84	0.43
2:G:352:ASN:HA	2:G:355:LYS:HZ2	1.83	0.43
2:E:227:ARG:HA	2:E:300:PHE:HE1	1.84	0.43
2:E:260:PHE:CE2	3:K:198:GLY:HA2	2.53	0.43
3:K:306:HIS:HA	3:K:309:ARG:NH2	2.29	0.43
2:H:451:TRP:HE1	2:H:493:VAL:HA	1.83	0.43
2:H:518:LYS:HA	2:H:518:LYS:HE3	2.01	0.43
2:F:199:ASP:O	3:L:200:LEU:CA	2.55	0.43
3:V:242:ASN:HD22	3:V:288:ASP:CG	2.21	0.43
6:Q:53:ARG:NH1	6:Q:103:ILE:H	2.17	0.43
6:Q:242:GLN:HA	6:Q:245:GLN:NE2	2.33	0.43
6:Q:293:ILE:HA	6:Q:296:MET:SD	2.59	0.43
6:Q:570:HIS:CG	6:Q:571:LEU:N	2.86	0.43
6:Q:580:GLN:O	6:Q:584:LEU:N	2.48	0.43
6:Q:747:ALA:O	6:Q:751:TRP:CZ3	2.71	0.43
6:R:53:ARG:NH1	6:R:103:ILE:H	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:443:LYS:HA	6:R:446:GLU:OE2	2.17	0.43
6:R:743:ALA:HA	6:R:746:LEU:HB2	2.00	0.43
2:B:302:ILE:H	2:B:302:ILE:HD12	1.83	0.43
2:B:505:ARG:NE	2:B:505:ARG:HA	2.34	0.43
2:G:337:ASP:O	2:G:341:HIS:CG	2.71	0.43
2:E:276:LEU:HA	2:E:279:ILE:HG12	2.00	0.43
2:P:276:LEU:HA	2:P:279:ILE:HG12	2.01	0.43
2:N:227:ARG:HA	2:N:300:PHE:HE1	1.83	0.43
2:H:199:ASP:O	3:V:200:LEU:CA	2.55	0.43
2:H:379:SER:CB	2:H:402:SER:O	2.65	0.43
2:H:530:LEU:HD11	2:F:544:TRP:HE1	1.73	0.43
3:V:227:ARG:HA	3:V:300:PHE:HE1	1.84	0.43
3:V:302:ILE:HD12	3:V:302:ILE:H	1.83	0.43
5:S:137:SER:C	5:S:155:PRO:HA	2.39	0.43
6:Q:565:LEU:HD11	6:Q:605:LEU:HG	2.00	0.43
6:Q:638:HIS:CE1	6:Q:638:HIS:O	2.72	0.43
6:Q:662:CYS:SG	6:Q:704:VAL:HG11	2.59	0.43
6:Q:680:PHE:HA	6:Q:683:GLN:CD	2.38	0.43
5:T:51:LEU:HB2	5:T:58:LEU:HD22	2.01	0.43
5:T:137:SER:C	5:T:155:PRO:HA	2.39	0.43
6:R:34:THR:HB	6:R:37:LYS:HB2	1.99	0.43
6:R:236:LEU:HA	6:R:239:LEU:HG	2.01	0.43
6:R:662:CYS:SG	6:R:704:VAL:HG11	2.59	0.43
2:B:451:TRP:CD2	2:B:451:TRP:C	2.92	0.43
2:A:227:ARG:HA	2:A:300:PHE:HE1	1.84	0.43
2:G:367:GLN:HA	2:G:369:LYS:HB2	1.99	0.43
2:G:385:LEU:HD11	2:E:350:LEU:HD11	1.53	0.43
2:N:276:LEU:HA	2:N:279:ILE:HG12	2.01	0.43
2:H:391:SER:HB2	2:H:394:LEU:HD12	2.01	0.43
2:F:449:HIS:C	2:F:449:HIS:CD2	2.92	0.43
3:L:197:VAL:HG23	3:L:204:HIS:O	2.18	0.43
6:Q:212:GLN:HG3	6:Q:254:TYR:CE1	2.53	0.43
5:T:8:ILE:HD12	5:T:157:PHE:CE2	2.53	0.43
5:T:52:ARG:HA	5:T:52:ARG:NE	2.34	0.43
6:R:84:HIS:HB3	6:R:85:PRO:HD3	2.00	0.43
6:R:293:ILE:HA	6:R:296:MET:SD	2.59	0.43
6:R:484:THR:O	6:R:488:LEU:HG	2.18	0.43
6:R:520:HIS:HA	6:R:523:ASN:HD22	1.84	0.43
6:R:573:HIS:CD2	6:R:615:ARG:HG2	2.53	0.43
6:R:615:ARG:HG3	6:R:619:ARG:HH21	1.84	0.43
6:R:747:ALA:O	6:R:751:TRP:CZ3	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:217:PRO:CD	2:G:392:PRO:CG	2.87	0.43
2:A:197:VAL:HG23	2:A:204:HIS:O	2.18	0.43
2:A:302:ILE:H	2:A:302:ILE:HD12	1.83	0.43
2:G:276:LEU:HA	2:G:279:ILE:HG12	2.00	0.43
2:G:368:ARG:HH21	2:G:416:ALA:HB2	1.84	0.43
2:E:242:ASN:HD22	2:E:288:ASP:CG	2.21	0.43
2:E:302:ILE:H	2:E:302:ILE:HD12	1.83	0.43
2:H:188:HIS:HB2	2:H:212:LYS:HG2	2.01	0.43
2:H:367:GLN:HA	2:H:369:LYS:HB2	1.99	0.43
2:F:260:PHE:CE2	3:L:198:GLY:HA2	2.53	0.43
3:L:240:HIS:CA	3:L:248:VAL:HG11	2.48	0.43
6:Q:79:HIS:CE1	6:Q:83:ASN:HD22	2.37	0.43
6:Q:236:LEU:HA	6:Q:239:LEU:HG	2.01	0.43
6:Q:462:LEU:O	6:Q:466:LEU:HG	2.19	0.43
6:Q:468:SER:HA	6:Q:471:ARG:CZ	2.48	0.43
6:Q:484:THR:O	6:Q:488:LEU:HG	2.18	0.43
5:T:94:VAL:HG22	6:R:746:LEU:HD22	1.99	0.43
6:R:263:PHE:HB2	6:R:268:HIS:HE1	1.83	0.43
2:G:404:LEU:HD13	2:G:547:PHE:HE2	1.84	0.43
2:G:451:TRP:CH2	2:G:452:HIS:HA	2.53	0.43
2:G:476:GLN:HB3	3:L:311:GLU:O	2.15	0.43
2:G:535:GLU:OE1	2:G:535:GLU:HA	2.17	0.43
3:K:188:HIS:HB2	3:K:212:LYS:HG2	2.01	0.43
3:K:302:ILE:HD12	3:K:302:ILE:H	1.83	0.43
2:H:227:ARG:HA	2:H:300:PHE:HE1	1.83	0.43
2:H:240:HIS:CA	2:H:248:VAL:HG11	2.48	0.43
2:H:368:ARG:HH21	2:H:416:ALA:HB2	1.84	0.43
2:H:413:GLU:HB3	2:H:414:ARG:NH2	2.34	0.43
2:H:451:TRP:CD2	2:H:451:TRP:C	2.92	0.43
5:S:177:ASP:C	5:S:179:ASN:H	2.22	0.43
5:S:178:GLU:CD	5:S:178:GLU:H	2.22	0.43
6:Q:107:TYR:CD2	6:Q:150:TYR:CE2	3.07	0.43
6:Q:160:PRO:HA	6:Q:167:PRO:HG2	2.00	0.43
6:Q:517:THR:HB	6:Q:518:PRO:HD2	2.01	0.43
5:T:177:ASP:C	5:T:179:ASN:H	2.22	0.43
6:R:160:PRO:HA	6:R:167:PRO:HG2	2.00	0.43
6:R:266:GLU:O	6:R:269:LEU:HB3	2.18	0.43
6:R:564:TRP:HZ3	6:R:565:LEU:HD22	1.83	0.43
1:C:217:PRO:HA	2:B:392:PRO:CB	2.49	0.42
2:B:188:HIS:HB2	2:B:212:LYS:HG2	2.01	0.42
2:B:267:SER:CA	2:B:432:ARG:NH1	2.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:276:LEU:HA	2:B:279:ILE:HG12	2.00	0.42
2:A:349:ALA:CA	2:N:470:ARG:HH21	2.32	0.42
2:A:368:ARG:HD3	2:A:412:TYR:CE2	2.54	0.42
2:G:391:SER:HA	2:G:392:PRO:HD3	1.82	0.42
2:H:260:PHE:CE2	3:V:198:GLY:HA2	2.53	0.42
2:H:423:PHE:HA	2:H:426:ILE:HG12	2.01	0.42
3:L:227:ARG:HA	3:L:300:PHE:HE1	1.84	0.42
5:S:23:LYS:HA	5:S:26:LYS:HZ2	1.84	0.42
6:Q:140:HIS:CE1	6:Q:142:VAL:H	2.37	0.42
6:Q:615:ARG:HG3	6:Q:619:ARG:HH21	1.84	0.42
6:Q:688:TYR:CD2	6:Q:705:ILE:CD1	3.02	0.42
6:R:28:MET:HE1	6:R:73:LEU:HG	2.01	0.42
6:R:471:ARG:HB2	6:R:472:ARG:HH12	1.83	0.42
6:R:638:HIS:O	6:R:638:HIS:CE1	2.72	0.42
6:R:715:PHE:HB3	6:R:719:ASN:HB2	2.00	0.42
6:R:753:ALA:HA	6:R:767:LEU:HD13	2.00	0.42
1:J:5:PHE:CB	2:A:331:ASN:C	2.86	0.42
2:B:368:ARG:HH21	2:B:416:ALA:HB2	1.84	0.42
2:B:391:SER:HA	2:B:392:PRO:HD3	1.82	0.42
2:G:379:SER:CB	2:G:406:LEU:HB2	2.48	0.42
2:G:391:SER:HB2	2:G:394:LEU:HD12	2.01	0.42
2:G:413:GLU:HB3	2:G:414:ARG:NH2	2.34	0.42
2:E:253:GLU:N	2:E:268:ARG:HA	2.27	0.42
3:K:206:VAL:HG13	3:K:228:ARG:HG2	2.01	0.42
3:K:227:ARG:HA	3:K:300:PHE:HE1	1.84	0.42
2:N:242:ASN:HD22	2:N:288:ASP:CG	2.21	0.42
2:H:267:SER:CA	2:H:432:ARG:NH1	2.69	0.42
2:H:338:ASP:O	2:H:342:ASP:HB3	2.19	0.42
2:H:380:ALA:O	2:H:383:HIS:HD2	1.99	0.42
2:H:508:ARG:O	2:H:511:LEU:HB2	2.19	0.42
3:L:209:VAL:HB	3:L:225:VAL:CG2	2.47	0.42
3:L:247:VAL:HG22	3:L:248:VAL:H	1.84	0.42
5:S:51:LEU:HB2	5:S:58:LEU:HD22	2.01	0.42
6:Q:280:SER:CB	6:Q:399:HIS:CE1	3.02	0.42
6:R:242:GLN:HA	6:R:245:GLN:NE2	2.33	0.42
6:R:577:ASN:O	6:R:581:PHE:CD1	2.72	0.42
1:J:38:LEU:CD1	1:J:146:TRP:HD1	2.33	0.42
1:J:65:LYS:HD2	1:C:82:TYR:CZ	2.54	0.42
2:B:306:HIS:HA	2:B:309:ARG:NH2	2.29	0.42
2:B:353:GLN:O	2:B:357:LEU:HG	2.19	0.42
2:B:372:ALA:HB2	2:B:413:GLU:CG	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:379:SER:CB	2:B:406:LEU:HB2	2.48	0.42
2:A:206:VAL:HG13	2:A:228:ARG:HG2	2.00	0.42
3:D:188:HIS:HB2	3:D:212:LYS:HG2	2.01	0.42
2:G:249:PRO:C	2:G:250:PRO:CA	2.73	0.42
2:G:338:ASP:O	2:G:342:ASP:HB3	2.19	0.42
2:E:188:HIS:HB2	2:E:212:LYS:HG2	2.01	0.42
2:P:250:PRO:HG3	2:P:429:GLU:O	2.20	0.42
2:N:250:PRO:HD3	2:N:433:LEU:CG	2.49	0.42
2:H:242:ASN:HD22	2:H:288:ASP:CG	2.21	0.42
3:V:220:GLN:H	3:V:220:GLN:HG2	1.60	0.42
5:S:52:ARG:HA	5:S:52:ARG:NE	2.34	0.42
6:Q:182:PHE:CD1	6:Q:182:PHE:C	2.93	0.42
6:Q:189:TRP:CZ2	6:Q:250:LEU:HD22	2.54	0.42
6:Q:223:SER:C	6:Q:225:LEU:H	2.22	0.42
6:Q:743:ALA:HA	6:Q:746:LEU:HB2	2.00	0.42
6:Q:753:ALA:HA	6:Q:767:LEU:HD22	2.01	0.42
1:C:26:VAL:HG22	1:C:146:TRP:CZ3	2.55	0.42
2:B:406:LEU:HD12	2:B:409:ARG:HH21	1.81	0.42
2:G:205:ILE:HG22	2:G:268:ARG:HH11	1.85	0.42
2:G:385:LEU:CD2	2:E:350:LEU:HD13	2.46	0.42
2:G:451:TRP:C	2:G:451:TRP:CD2	2.92	0.42
2:G:518:LYS:HA	2:G:518:LYS:HE3	2.01	0.42
2:H:385:LEU:CD2	2:F:350:LEU:HD13	2.46	0.42
2:H:423:PHE:CE1	2:H:525:GLY:C	2.93	0.42
2:H:523:LYS:HE2	2:H:523:LYS:HA	2.00	0.42
2:F:276:LEU:HA	2:F:279:ILE:HG12	2.00	0.42
5:S:61:VAL:CG2	5:S:87:PHE:CD2	3.02	0.42
6:Q:19:ILE:HG13	6:Q:22:ARG:HH21	1.85	0.42
6:Q:480:LEU:HD22	6:Q:526:GLU:OE2	2.19	0.42
6:Q:532:ILE:H	6:Q:532:ILE:HG13	1.63	0.42
6:Q:577:ASN:O	6:Q:581:PHE:CD1	2.72	0.42
5:T:23:LYS:HA	5:T:26:LYS:HZ2	1.84	0.42
5:T:45:ARG:HA	5:T:48:TYR:CB	2.50	0.42
5:T:120:HIS:HB2	5:T:143:THR:CA	2.50	0.42
6:R:212:GLN:HG3	6:R:254:TYR:CE1	2.53	0.42
6:R:280:SER:CB	6:R:399:HIS:CE1	3.02	0.42
6:R:528:LEU:HD12	6:R:528:LEU:O	2.20	0.42
2:B:205:ILE:HG22	2:B:268:ARG:HH11	1.85	0.42
2:B:423:PHE:CE1	2:B:525:GLY:C	2.93	0.42
2:B:430:TYR:CD1	2:B:430:TYR:N	2.79	0.42
2:B:518:LYS:HA	2:B:518:LYS:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:205:ILE:HG22	2:A:268:ARG:HH11	1.85	0.42
2:G:196:LYS:NZ	2:N:196:LYS:CE	2.68	0.42
2:G:353:GLN:NE2	2:E:384:ALA:HB3	2.17	0.42
2:G:404:LEU:HG	2:G:408:ILE:HD12	2.02	0.42
2:G:489:ALA:O	2:G:493:VAL:HG23	2.19	0.42
2:P:227:ARG:HA	2:P:300:PHE:HE1	1.84	0.42
2:P:253:GLU:N	2:P:268:ARG:HA	2.27	0.42
2:N:247:VAL:HG22	2:N:248:VAL:H	1.85	0.42
2:H:404:LEU:HD13	2:H:547:PHE:HE2	1.84	0.42
2:H:489:ALA:O	2:H:493:VAL:HG23	2.19	0.42
5:S:16:ARG:HA	5:S:142:PHE:CZ	2.54	0.42
5:S:94:VAL:HG22	6:Q:746:LEU:HD22	1.99	0.42
5:S:120:HIS:HB2	5:S:143:THR:CA	2.50	0.42
6:Q:264:PRO:O	6:Q:268:HIS:CD2	2.72	0.42
6:Q:479:ALA:O	6:Q:482:LEU:HB2	2.20	0.42
6:Q:570:HIS:CD2	6:Q:570:HIS:C	2.92	0.42
6:R:140:HIS:CD2	6:R:195:GLN:HE21	2.37	0.42
1:J:262:LYS:HB3	1:C:93:ALA:HA	1.97	0.42
1:C:57:LYS:NZ	2:E:331:ASN:CG	2.73	0.42
2:B:209:VAL:HB	2:B:225:VAL:CG2	2.47	0.42
2:B:413:GLU:HB3	2:B:414:ARG:NH2	2.34	0.42
2:B:489:ALA:O	2:B:493:VAL:HG23	2.19	0.42
2:A:220:GLN:H	2:A:220:GLN:HG2	1.60	0.42
2:G:204:HIS:NE2	2:G:228:ARG:HD3	2.35	0.42
2:G:292:LYS:O	2:G:296:GLU:HB2	2.20	0.42
2:G:372:ALA:HB2	2:G:413:GLU:CG	2.50	0.42
3:K:204:HIS:NE2	3:K:228:ARG:HD3	2.35	0.42
2:P:183:ALA:N	2:P:186:THR:HG1	2.18	0.42
2:P:206:VAL:HG13	2:P:228:ARG:HG2	2.00	0.42
2:N:302:ILE:HG22	2:N:306:HIS:HE1	1.85	0.42
2:H:379:SER:CB	2:H:406:LEU:HB2	2.48	0.42
2:H:546:THR:HB	2:H:547:PHE:CE1	2.55	0.42
2:F:302:ILE:HD12	2:F:302:ILE:H	1.83	0.42
3:V:205:ILE:HG22	3:V:268:ARG:HH11	1.85	0.42
6:Q:84:HIS:HD2	6:Q:115:ALA:HB1	1.80	0.42
6:Q:785:ALA:HA	6:Q:788:CYS:SG	2.59	0.42
5:T:16:ARG:HA	5:T:142:PHE:CZ	2.54	0.42
6:R:389:LEU:HB3	6:R:393:PHE:CE2	2.55	0.42
6:R:580:GLN:O	6:R:584:LEU:N	2.48	0.42
6:R:673:PHE:CD1	6:R:675:GLU:OE1	2.73	0.42
1:J:111:GLU:CD	1:C:108:LYS:HB3	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:PHE:HB2	2:E:331:ASN:O	2.18	0.42
2:B:339:TRP:O	2:B:343:ARG:HB3	2.20	0.42
2:B:346:TYR:O	2:B:350:LEU:HG	2.20	0.42
2:B:352:ASN:HA	2:B:355:LYS:HZ2	1.84	0.42
2:B:368:ARG:CZ	2:B:416:ALA:N	2.83	0.42
2:B:494:HIS:CD2	2:B:494:HIS:C	2.93	0.42
2:B:508:ARG:O	2:B:511:LEU:HB2	2.19	0.42
2:A:276:LEU:HA	2:A:279:ILE:HG12	2.00	0.42
3:D:183:ALA:N	3:D:186:THR:HG1	2.18	0.42
2:G:188:HIS:HB2	2:G:212:LYS:HG2	2.01	0.42
2:G:240:HIS:CA	2:G:248:VAL:HG11	2.48	0.42
2:G:247:VAL:HG22	2:G:248:VAL:H	1.84	0.42
2:G:368:ARG:CZ	2:G:416:ALA:N	2.83	0.42
2:G:423:PHE:CE1	2:G:525:GLY:C	2.93	0.42
2:E:247:VAL:HG22	2:E:248:VAL:H	1.85	0.42
2:E:449:HIS:CD2	2:E:449:HIS:C	2.92	0.42
3:K:276:LEU:HA	3:K:279:ILE:HG12	2.00	0.42
2:N:251:PRO:HD2	2:N:432:ARG:HH21	1.83	0.42
2:H:353:GLN:O	2:H:357:LEU:HG	2.19	0.42
2:H:372:ALA:HB2	2:H:413:GLU:CG	2.50	0.42
2:H:505:ARG:NE	2:H:505:ARG:HA	2.34	0.42
2:F:206:VAL:HG13	2:F:228:ARG:HG2	2.00	0.42
6:Q:683:GLN:N	6:R:733:LYS:CE	2.83	0.42
6:R:107:TYR:CD2	6:R:150:TYR:CE2	3.07	0.42
6:R:140:HIS:CE1	6:R:142:VAL:H	2.37	0.42
6:R:473:TYR:CD2	6:R:476:ILE:HA	2.54	0.42
6:R:753:ALA:HA	6:R:767:LEU:HD22	2.00	0.42
1:J:217:PRO:HD3	2:G:392:PRO:HD3	2.02	0.42
2:B:206:VAL:HG13	2:B:228:ARG:HG2	2.00	0.42
2:B:451:TRP:NE1	2:B:493:VAL:HA	2.35	0.42
2:A:240:HIS:CA	2:A:248:VAL:HG11	2.48	0.42
3:D:302:ILE:HG22	3:D:306:HIS:HE1	1.85	0.42
2:G:248:VAL:HG23	2:G:443:GLN:OE1	2.20	0.42
2:E:368:ARG:HD3	2:E:412:TYR:CE2	2.54	0.42
3:K:220:GLN:H	3:K:220:GLN:HG2	1.60	0.42
2:N:206:VAL:HG13	2:N:228:ARG:HG2	2.01	0.42
2:H:406:LEU:CD1	2:H:409:ARG:NH2	2.81	0.42
2:F:205:ILE:HG22	2:F:268:ARG:HH11	1.85	0.42
2:F:292:LYS:O	2:F:296:GLU:HB2	2.20	0.42
3:L:205:ILE:HG22	3:L:268:ARG:HH11	1.85	0.42
3:L:234:TRP:CZ3	3:L:237:ASN:CB	3.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:101:LEU:HB3	5:S:132:PHE:CD1	2.55	0.42
6:Q:673:PHE:CD1	6:Q:675:GLU:OE1	2.73	0.42
5:T:61:VAL:CG2	5:T:87:PHE:CD2	3.02	0.42
6:R:189:TRP:CZ2	6:R:250:LEU:HD22	2.54	0.42
6:R:480:LEU:HD22	6:R:526:GLU:OE2	2.19	0.42
6:R:688:TYR:CD2	6:R:705:ILE:CD1	3.02	0.42
1:J:26:VAL:HG22	1:J:146:TRP:CZ3	2.55	0.42
2:B:338:ASP:O	2:B:342:ASP:HB3	2.19	0.42
2:B:404:LEU:HD13	2:B:547:PHE:HE2	1.84	0.42
2:B:539:GLU:HA	2:B:542:GLU:OE1	2.20	0.42
2:A:302:ILE:HG22	2:A:306:HIS:HE1	1.85	0.42
3:D:227:ARG:HA	3:D:300:PHE:HE1	1.84	0.42
2:G:353:GLN:O	2:G:357:LEU:HG	2.19	0.42
2:E:183:ALA:N	2:E:186:THR:HG1	2.18	0.42
2:E:302:ILE:HG22	2:E:306:HIS:HE1	1.85	0.42
2:P:188:HIS:HB2	2:P:212:LYS:HG2	2.01	0.42
2:H:253:GLU:N	2:H:268:ARG:HA	2.27	0.42
2:H:265:VAL:HG23	2:H:269:ARG:HH22	1.85	0.42
2:H:339:TRP:O	2:H:343:ARG:HB3	2.20	0.42
2:H:368:ARG:CZ	2:H:416:ALA:N	2.83	0.42
2:F:183:ALA:N	2:F:186:THR:HG1	2.18	0.42
2:F:204:HIS:NE2	2:F:228:ARG:HD3	2.35	0.42
2:F:265:VAL:HG23	2:F:269:ARG:HH22	1.85	0.42
2:F:513:ARG:HG2	2:F:516:ARG:HH22	1.85	0.42
3:V:276:LEU:HA	3:V:279:ILE:HG12	2.01	0.42
3:L:302:ILE:HG22	3:L:306:HIS:HE1	1.85	0.42
6:Q:140:HIS:CD2	6:Q:195:GLN:HE21	2.37	0.42
6:Q:759:ARG:HH21	6:Q:767:LEU:HD21	1.85	0.42
6:R:182:PHE:CD1	6:R:182:PHE:C	2.93	0.42
6:R:264:PRO:O	6:R:268:HIS:CD2	2.72	0.42
6:R:561:GLU:O	6:R:564:TRP:HB3	2.20	0.42
1:J:90:GLU:CB	1:C:261:ASN:O	2.68	0.42
1:C:38:LEU:CD1	1:C:146:TRP:HD1	2.32	0.42
2:B:204:HIS:NE2	2:B:228:ARG:HD3	2.35	0.42
2:B:265:VAL:HG23	2:B:269:ARG:HH22	1.85	0.42
2:B:302:ILE:HG22	2:B:306:HIS:HE1	1.85	0.42
2:A:292:LYS:O	2:A:296:GLU:HB2	2.20	0.42
3:D:204:HIS:NE2	3:D:228:ARG:HD3	2.35	0.42
2:G:183:ALA:N	2:G:186:THR:HG1	2.18	0.42
2:G:346:TYR:O	2:G:350:LEU:HG	2.20	0.42
2:G:348:ASP:HA	2:G:438:LYS:HZ3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:452:HIS:CD2	2:G:453:SER:N	2.88	0.42
2:H:247:VAL:HG22	2:H:248:VAL:H	1.85	0.42
2:H:404:LEU:HG	2:H:408:ILE:HD12	2.01	0.42
2:H:452:HIS:CD2	2:H:453:SER:N	2.88	0.42
2:F:302:ILE:HG22	2:F:306:HIS:HE1	1.85	0.42
3:V:187:PHE:CE1	3:V:218:TYR:CD2	3.08	0.42
3:V:292:LYS:O	3:V:296:GLU:HB2	2.20	0.42
3:L:188:HIS:HB2	3:L:212:LYS:HG2	2.01	0.42
6:Q:389:LEU:HB3	6:Q:393:PHE:CE2	2.55	0.42
6:Q:528:LEU:HD12	6:Q:528:LEU:O	2.19	0.42
6:R:19:ILE:HG13	6:R:22:ARG:HH21	1.85	0.42
6:R:462:LEU:O	6:R:466:LEU:HG	2.19	0.42
2:B:183:ALA:N	2:B:186:THR:HG1	2.18	0.41
2:B:367:GLN:C	2:B:369:LYS:H	2.24	0.41
2:B:375:ALA:HA	2:B:378:PHE:HB2	2.02	0.41
2:B:406:LEU:CD1	2:B:409:ARG:NH2	2.81	0.41
2:B:406:LEU:HD11	2:B:409:ARG:HH21	1.84	0.41
2:A:196:LYS:HZ2	3:D:196:LYS:CE	2.30	0.41
2:A:265:VAL:HG23	2:A:269:ARG:HH22	1.85	0.41
2:A:513:ARG:HG2	2:A:516:ARG:HH22	1.85	0.41
3:D:265:VAL:HG23	3:D:269:ARG:HH22	1.85	0.41
2:G:411:VAL:HG22	2:G:539:GLU:OE2	2.20	0.41
2:G:458:LEU:CB	2:G:489:ALA:HB1	2.48	0.41
2:G:508:ARG:O	2:G:511:LEU:HB2	2.19	0.41
2:E:279:ILE:O	2:E:282:HIS:O	2.38	0.41
3:K:187:PHE:CE1	3:K:218:TYR:CD2	3.08	0.41
3:K:234:TRP:CZ3	3:K:237:ASN:CB	3.03	0.41
2:P:187:PHE:CE1	2:P:218:TYR:CD2	3.08	0.41
2:N:188:HIS:HB2	2:N:212:LYS:HG2	2.01	0.41
2:F:247:VAL:HG22	2:F:248:VAL:H	1.85	0.41
2:F:368:ARG:HD3	2:F:412:TYR:CE2	2.54	0.41
3:V:227:ARG:NH1	3:V:298:GLU:HA	2.35	0.41
3:V:302:ILE:HG22	3:V:306:HIS:HE1	1.85	0.41
3:L:265:VAL:HG23	3:L:269:ARG:HH22	1.85	0.41
5:S:97:GLU:OE2	6:Q:749:HIS:CE1	2.73	0.41
5:S:165:ILE:HD12	5:S:193:LYS:O	2.20	0.41
6:Q:302:TYR:CE1	6:Q:305:ARG:HB3	2.55	0.41
6:Q:483:PRO:C	6:Q:486:VAL:H	2.24	0.41
5:T:188:LYS:HZ3	5:T:190:THR:HG23	1.84	0.41
6:R:223:SER:C	6:R:225:LEU:H	2.22	0.41
6:R:530:VAL:HA	6:R:534:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:461:LYS:HZ3	2:B:489:ALA:HB2	1.85	0.41
2:A:199:ASP:O	3:D:200:LEU:CA	2.55	0.41
2:A:204:HIS:NE2	2:A:228:ARG:HD3	2.35	0.41
2:G:279:ILE:O	2:G:282:HIS:O	2.38	0.41
2:G:339:TRP:O	2:G:343:ARG:HB3	2.20	0.41
2:G:476:GLN:OE1	3:L:306:HIS:O	2.37	0.41
2:E:205:ILE:HG22	2:E:268:ARG:HH11	1.85	0.41
2:P:247:VAL:HG22	2:P:248:VAL:H	1.85	0.41
2:P:292:LYS:O	2:P:296:GLU:HB2	2.20	0.41
2:N:204:HIS:NE2	2:N:228:ARG:HD3	2.35	0.41
2:H:302:ILE:HG22	2:H:306:HIS:HE1	1.85	0.41
2:H:367:GLN:C	2:H:369:LYS:H	2.24	0.41
2:F:260:PHE:HE2	3:L:198:GLY:CA	2.29	0.41
3:V:188:HIS:HB2	3:V:212:LYS:HG2	2.01	0.41
3:V:206:VAL:HG13	3:V:228:ARG:HG2	2.00	0.41
3:V:234:TRP:CZ3	3:V:237:ASN:CB	3.03	0.41
6:Q:519:ALA:O	6:Q:522:GLU:HB2	2.20	0.41
6:Q:569:VAL:HG22	6:Q:608:ALA:HB2	2.02	0.41
5:T:116:ALA:CA	5:T:134:ASN:HD21	2.33	0.41
5:T:165:ILE:HD12	5:T:193:LYS:O	2.20	0.41
6:R:479:ALA:O	6:R:482:LEU:HB2	2.20	0.41
1:C:5:PHE:HD2	2:E:332:LYS:C	2.24	0.41
2:B:374:ALA:O	2:B:378:PHE:HB2	2.21	0.41
2:B:451:TRP:HE1	2:B:493:VAL:CG1	2.34	0.41
2:A:209:VAL:HB	2:A:225:VAL:CG2	2.47	0.41
3:D:227:ARG:NH1	3:D:298:GLU:HA	2.35	0.41
3:D:292:LYS:O	3:D:296:GLU:HB2	2.20	0.41
2:G:350:LEU:CD1	2:E:385:LEU:CD2	2.98	0.41
2:G:406:LEU:HD12	2:G:409:ARG:HH21	1.81	0.41
2:G:546:THR:HB	2:G:547:PHE:CE1	2.55	0.41
3:K:279:ILE:O	3:K:282:HIS:O	2.39	0.41
3:K:292:LYS:O	3:K:296:GLU:HB2	2.20	0.41
2:P:279:ILE:O	2:P:282:HIS:O	2.38	0.41
2:P:302:ILE:HG22	2:P:306:HIS:HE1	1.85	0.41
2:H:209:VAL:HB	2:H:225:VAL:CG2	2.47	0.41
3:V:265:VAL:HG23	3:V:269:ARG:HH22	1.85	0.41
3:L:279:ILE:O	3:L:282:HIS:O	2.39	0.41
6:Q:63:TYR:O	6:Q:66:TYR:HB3	2.20	0.41
6:Q:412:ILE:HB	6:Q:461:SER:CB	2.50	0.41
6:Q:726:LYS:HE3	6:R:726:LYS:HE3	1.16	0.41
5:T:101:LEU:HB3	5:T:132:PHE:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:63:TYR:O	6:R:66:TYR:HB3	2.20	0.41
6:R:79:HIS:CE1	6:R:83:ASN:HD22	2.37	0.41
6:R:519:ALA:O	6:R:522:GLU:HB2	2.20	0.41
6:R:712:THR:HG22	6:R:713:ARG:N	2.36	0.41
2:B:292:LYS:O	2:B:296:GLU:HB2	2.20	0.41
2:A:187:PHE:CE1	2:A:218:TYR:CD2	3.08	0.41
2:G:350:LEU:CD1	2:E:385:LEU:HD21	2.50	0.41
2:G:451:TRP:NE1	2:G:493:VAL:HA	2.35	0.41
2:E:265:VAL:HG23	2:E:269:ARG:HH22	1.85	0.41
2:E:513:ARG:HG2	2:E:516:ARG:HH22	1.85	0.41
3:K:253:GLU:N	3:K:268:ARG:HA	2.27	0.41
2:P:234:TRP:CZ3	2:P:237:ASN:CB	3.03	0.41
6:Q:561:GLU:O	6:Q:564:TRP:HB3	2.20	0.41
6:Q:599:ARG:NE	6:Q:599:ARG:H	2.19	0.41
5:T:97:GLU:OE2	6:R:749:HIS:CE1	2.73	0.41
6:R:759:ARG:HH21	6:R:767:LEU:HD21	1.85	0.41
1:J:86:SER:HB3	1:C:86:SER:CB	2.25	0.41
2:B:546:THR:HB	2:B:547:PHE:CE1	2.55	0.41
2:G:365:VAL:HA	2:G:416:ALA:HB2	2.02	0.41
2:G:539:GLU:HA	2:G:542:GLU:OE1	2.20	0.41
2:P:227:ARG:NH1	2:P:298:GLU:HA	2.36	0.41
2:N:444:ARG:HE	2:N:503:MET:HB3	1.85	0.41
2:H:227:ARG:HA	2:H:227:ARG:HD3	1.87	0.41
2:H:248:VAL:HG23	2:H:443:GLN:OE1	2.20	0.41
2:H:346:TYR:O	2:H:350:LEU:HG	2.20	0.41
3:L:187:PHE:CE1	3:L:218:TYR:CD2	3.08	0.41
5:S:105:ALA:HA	5:S:110:VAL:CG2	2.51	0.41
6:Q:29:ARG:HA	6:Q:32:LEU:HG	2.03	0.41
6:Q:182:PHE:CG	6:Q:183:VAL:N	2.89	0.41
6:Q:408:ILE:HG12	6:Q:447:HIS:CE1	2.56	0.41
6:Q:473:TYR:CE1	6:Q:475:SER:O	2.73	0.41
6:Q:482:LEU:HA	6:Q:483:PRO:HD3	1.90	0.41
6:Q:487:SER:HA	6:Q:490:GLN:HE21	1.86	0.41
6:Q:759:ARG:HD3	6:Q:766:GLU:HA	2.02	0.41
5:T:8:ILE:HD12	5:T:157:PHE:CD2	2.55	0.41
6:R:302:TYR:CE1	6:R:305:ARG:HB3	2.55	0.41
6:R:473:TYR:CE1	6:R:475:SER:O	2.73	0.41
6:R:525:LEU:HD11	6:R:583:LEU:HD23	2.03	0.41
1:J:53:PRO:HD3	1:J:100:PRO:HA	2.02	0.41
1:J:216:ALA:HA	2:G:392:PRO:HG2	2.01	0.41
1:J:261:ASN:O	1:C:90:GLU:CB	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:PRO:HD3	1:C:100:PRO:HA	2.02	0.41
2:B:187:PHE:CE1	2:B:218:TYR:CD2	3.08	0.41
2:B:248:VAL:HG23	2:B:443:GLN:OE1	2.20	0.41
2:B:279:ILE:O	2:B:282:HIS:O	2.38	0.41
2:B:363:ASN:HB3	2:B:367:GLN:OE1	2.21	0.41
2:B:365:VAL:HA	2:B:416:ALA:HB2	2.02	0.41
2:A:188:HIS:HB2	2:A:212:LYS:HG2	2.01	0.41
2:G:227:ARG:NH1	2:G:298:GLU:HA	2.36	0.41
2:G:302:ILE:HG22	2:G:306:HIS:HE1	1.85	0.41
2:G:494:HIS:CD2	2:G:494:HIS:C	2.93	0.41
2:P:444:ARG:HE	2:P:503:MET:HB3	1.86	0.41
2:N:187:PHE:CE1	2:N:218:TYR:CD2	3.08	0.41
2:H:187:PHE:CE1	2:H:218:TYR:CD2	3.08	0.41
2:H:357:LEU:CD1	2:F:381:SER:HB3	2.44	0.41
2:H:400:ALA:HA	2:H:403:GLU:HG3	2.03	0.41
2:H:538:LYS:HZ2	2:H:541:ILE:HB	1.85	0.41
3:V:183:ALA:N	3:V:186:THR:HG1	2.18	0.41
3:L:227:ARG:NH1	3:L:298:GLU:HA	2.35	0.41
5:S:8:ILE:HD12	5:S:157:PHE:CD2	2.55	0.41
6:Q:733:LYS:HD3	6:Q:733:LYS:HA	1.98	0.41
6:R:569:VAL:HG22	6:R:608:ALA:HB2	2.02	0.41
6:R:745:TYR:CE2	6:R:801:ILE:HG12	2.56	0.41
1:C:6:SER:O	2:E:331:ASN:C	2.58	0.41
2:B:227:ARG:NH1	2:B:298:GLU:HA	2.36	0.41
2:B:350:LEU:CD1	2:A:385:LEU:CD2	2.98	0.41
2:B:452:HIS:CD2	2:B:453:SER:N	2.88	0.41
3:D:187:PHE:CE1	3:D:218:TYR:CD2	3.08	0.41
2:G:367:GLN:C	2:G:369:LYS:H	2.24	0.41
2:G:375:ALA:HA	2:G:378:PHE:HB2	2.02	0.41
2:G:400:ALA:HA	2:G:403:GLU:HG3	2.03	0.41
2:G:530:LEU:CD2	2:E:544:TRP:CG	2.95	0.41
2:E:205:ILE:HD13	2:E:207:TYR:CE1	2.56	0.41
2:E:292:LYS:O	2:E:296:GLU:HB2	2.20	0.41
3:K:205:ILE:HD13	3:K:207:TYR:CE1	2.56	0.41
2:N:205:ILE:HG22	2:N:268:ARG:HH11	1.85	0.41
2:N:227:ARG:NH1	2:N:298:GLU:HA	2.35	0.41
2:H:205:ILE:HD13	2:H:207:TYR:CE1	2.56	0.41
2:H:451:TRP:NE1	2:H:493:VAL:HA	2.36	0.41
2:F:250:PRO:HG2	2:F:433:LEU:CG	2.22	0.41
3:L:204:HIS:NE2	3:L:228:ARG:HD3	2.35	0.41
5:S:116:ALA:CA	5:S:134:ASN:HD21	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:772:LYS:HG2	6:Q:773:ARG:HE	1.86	0.41
6:R:462:LEU:HD23	6:R:463:LEU:N	2.36	0.41
6:R:716:GLY:HA3	6:R:763:GLU:OE2	2.21	0.41
6:R:800:GLU:HA	6:R:803:ASP:CG	2.41	0.41
1:J:229:PHE:CD1	6:Q:105:ARG:NH1	2.89	0.41
1:J:261:ASN:OD1	1:C:90:GLU:CD	2.59	0.41
2:B:404:LEU:HG	2:B:408:ILE:HD12	2.02	0.41
2:B:451:TRP:CZ3	2:B:452:HIS:HB3	2.56	0.41
2:B:455:GLU:N	2:B:493:VAL:HG22	2.36	0.41
2:A:279:ILE:O	2:A:282:HIS:O	2.38	0.41
2:G:374:ALA:O	2:G:378:PHE:HB2	2.21	0.41
3:K:227:ARG:NH1	3:K:298:GLU:HA	2.36	0.41
4:M:444:ARG:O	4:M:447:ALA:HB3	2.21	0.41
2:H:234:TRP:CZ3	2:H:237:ASN:CB	3.03	0.41
2:F:188:HIS:HB2	2:F:212:LYS:HG2	2.01	0.41
2:F:279:ILE:O	2:F:282:HIS:O	2.38	0.41
3:V:204:HIS:NE2	3:V:228:ARG:HD3	2.35	0.41
3:V:227:ARG:HA	3:V:227:ARG:HD3	1.87	0.41
5:S:45:ARG:HA	5:S:48:TYR:CB	2.50	0.41
5:S:83:LEU:HD13	5:S:193:LYS:HB3	2.02	0.41
6:Q:112:VAL:O	6:Q:115:ALA:HB3	2.21	0.41
6:Q:498:ARG:O	6:Q:502:GLY:HA3	2.21	0.41
6:Q:503:GLU:HA	6:Q:506:ARG:NE	2.36	0.41
5:T:16:ARG:NE	5:T:120:HIS:CE1	2.89	0.41
5:T:83:LEU:HD13	5:T:193:LYS:HB3	2.02	0.41
6:R:182:PHE:CE2	6:R:183:VAL:HG13	2.56	0.41
6:R:498:ARG:O	6:R:502:GLY:HA3	2.21	0.41
6:R:808:TYR:CE1	6:R:811:GLN:HG3	2.56	0.41
2:B:250:PRO:N	2:B:436:SER:CB	2.72	0.41
2:B:357:LEU:CD2	2:A:378:PHE:CD1	3.01	0.41
2:B:400:ALA:HA	2:B:403:GLU:HG3	2.03	0.41
2:A:183:ALA:N	2:A:186:THR:HG1	2.18	0.41
2:A:196:LYS:HZ1	3:D:196:LYS:HZ3	1.41	0.41
2:A:205:ILE:HD13	2:A:207:TYR:CE1	2.56	0.41
2:A:227:ARG:HA	2:A:227:ARG:HD3	1.87	0.41
2:A:227:ARG:NH1	2:A:298:GLU:HA	2.36	0.41
2:A:247:VAL:HG22	2:A:248:VAL:H	1.85	0.41
2:A:357:LEU:O	2:A:360:ALA:HB3	2.21	0.41
3:D:205:ILE:HG22	3:D:268:ARG:HH11	1.85	0.41
3:D:227:ARG:HA	3:D:227:ARG:HD3	1.87	0.41
3:D:247:VAL:HG22	3:D:248:VAL:H	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:205:ILE:HD13	2:G:207:TYR:CE1	2.56	0.41
2:G:449:HIS:HA	2:G:452:HIS:ND1	2.36	0.41
2:E:188:HIS:CE1	2:E:214:THR:H	2.39	0.41
2:E:252:PRO:HB3	2:E:272:LEU:HG	2.03	0.41
3:K:183:ALA:N	3:K:186:THR:HG1	2.18	0.41
3:K:265:VAL:HG23	3:K:269:ARG:HH22	1.85	0.41
2:P:204:HIS:NE2	2:P:228:ARG:HD3	2.35	0.41
2:P:209:VAL:HB	2:P:225:VAL:CG2	2.47	0.41
2:N:183:ALA:N	2:N:186:THR:HG1	2.18	0.41
2:N:223:PHE:HB3	2:N:296:GLU:HA	2.03	0.41
2:N:292:LYS:O	2:N:296:GLU:HB2	2.20	0.41
2:H:204:HIS:NE2	2:H:228:ARG:HD3	2.35	0.41
2:H:292:LYS:O	2:H:296:GLU:HB2	2.20	0.41
2:H:350:LEU:CD1	2:F:385:LEU:CD2	2.98	0.41
2:H:374:ALA:O	2:H:378:PHE:HB2	2.21	0.41
2:H:434:ILE:HA	2:H:437:VAL:HG22	2.03	0.41
2:H:539:GLU:HA	2:H:542:GLU:OE1	2.20	0.41
2:F:205:ILE:HD13	2:F:207:TYR:CE1	2.56	0.41
2:F:227:ARG:NH1	2:F:298:GLU:HA	2.35	0.41
3:L:292:LYS:O	3:L:296:GLU:HB2	2.20	0.41
6:Q:156:ARG:HH22	6:Q:217:SER:C	2.25	0.41
6:Q:182:PHE:CE2	6:Q:183:VAL:HG13	2.56	0.41
6:Q:269:LEU:HA	6:Q:272:LEU:HG	2.03	0.41
6:Q:412:ILE:O	6:Q:416:CYS:SG	2.79	0.41
6:Q:530:VAL:HA	6:Q:534:GLU:OE1	2.20	0.41
6:Q:599:ARG:H	6:Q:599:ARG:HE	1.67	0.41
6:Q:800:GLU:HA	6:Q:803:ASP:CG	2.41	0.41
5:T:105:ALA:HA	5:T:110:VAL:CG2	2.50	0.41
6:R:231:TYR:CZ	6:R:267:TYR:HB3	2.56	0.41
6:R:269:LEU:HA	6:R:272:LEU:HG	2.03	0.41
6:R:412:ILE:O	6:R:416:CYS:SG	2.79	0.41
6:R:412:ILE:HB	6:R:461:SER:CB	2.50	0.41
6:R:470:LEU:HD13	6:R:504:ILE:HD11	2.02	0.41
6:R:483:PRO:C	6:R:486:VAL:H	2.24	0.41
6:R:498:ARG:HG3	6:R:506:ARG:HH12	1.86	0.41
6:R:503:GLU:HA	6:R:506:ARG:NE	2.36	0.41
6:R:568:LEU:HG	6:R:569:VAL:N	2.36	0.41
6:R:570:HIS:CE1	6:R:571:LEU:HG	2.56	0.41
6:R:599:ARG:HE	6:R:599:ARG:H	1.67	0.41
6:R:633:LEU:O	6:R:637:LEU:HG	2.21	0.41
6:R:719:ASN:H	6:R:719:ASN:ND2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:411:VAL:HG22	2:B:539:GLU:OE2	2.20	0.41
3:D:209:VAL:HB	3:D:225:VAL:CG2	2.47	0.41
3:D:223:PHE:HB3	3:D:296:GLU:HA	2.03	0.41
2:G:187:PHE:CE1	2:G:218:TYR:CD2	3.08	0.41
2:G:412:TYR:CD2	2:G:412:TYR:C	2.94	0.41
2:G:451:TRP:CZ3	2:G:452:HIS:HB3	2.56	0.41
2:E:187:PHE:CE1	2:E:218:TYR:CD2	3.08	0.41
3:K:188:HIS:CE1	3:K:214:THR:H	2.39	0.41
3:K:247:VAL:HG22	3:K:248:VAL:H	1.84	0.41
2:H:183:ALA:N	2:H:186:THR:HG1	2.18	0.41
2:H:235:LEU:HD22	2:H:235:LEU:O	2.21	0.41
2:H:279:ILE:O	2:H:282:HIS:O	2.39	0.41
2:H:365:VAL:HA	2:H:416:ALA:HB2	2.02	0.41
2:H:451:TRP:CZ3	2:H:452:HIS:HB3	2.56	0.41
2:F:187:PHE:CE1	2:F:218:TYR:CD2	3.09	0.41
2:F:250:PRO:HD3	2:F:433:LEU:CA	2.50	0.41
5:S:130:LYS:NZ	5:S:132:PHE:CE1	2.82	0.41
6:Q:733:LYS:CE	6:R:683:GLN:N	2.83	0.41
6:R:35:PRO:CB	6:R:83:ASN:HD21	2.33	0.41
6:R:759:ARG:HD3	6:R:766:GLU:HA	2.02	0.41
2:B:440:ALA:HA	2:B:443:GLN:OE1	2.22	0.40
2:B:513:ARG:NH2	2:B:514:PHE:HA	2.37	0.40
2:G:368:ARG:CD	2:G:416:ALA:H	2.32	0.40
2:G:385:LEU:O	2:G:385:LEU:HG	2.21	0.40
2:G:513:ARG:NH2	2:G:514:PHE:HA	2.37	0.40
2:G:533:ALA:CB	2:E:540:LEU:HD21	2.51	0.40
3:K:205:ILE:HG22	3:K:268:ARG:HH11	1.85	0.40
2:N:229:TYR:CZ	2:N:233:LEU:HD11	2.56	0.40
2:N:235:LEU:HD22	2:N:235:LEU:O	2.22	0.40
2:H:205:ILE:HG22	2:H:268:ARG:HH11	1.85	0.40
2:H:411:VAL:HG22	2:H:539:GLU:OE2	2.20	0.40
2:H:440:ALA:HA	2:H:443:GLN:OE1	2.21	0.40
3:V:279:ILE:O	3:V:282:HIS:O	2.39	0.40
3:L:223:PHE:HB3	3:L:296:GLU:HA	2.04	0.40
5:S:16:ARG:NE	5:S:120:HIS:CE1	2.89	0.40
5:S:165:ILE:O	5:S:193:LYS:HB3	2.21	0.40
6:Q:480:LEU:HD13	6:Q:523:ASN:HB3	2.03	0.40
6:Q:498:ARG:HG3	6:Q:506:ARG:HH12	1.86	0.40
6:Q:525:LEU:HD11	6:Q:583:LEU:HD23	2.03	0.40
6:Q:603:PRO:HA	6:Q:606:ILE:CG1	2.50	0.40
6:Q:716:GLY:HA3	6:Q:763:GLU:OE2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:52:LEU:HD13	6:R:69:VAL:HG21	2.02	0.40
6:R:83:ASN:HA	6:R:86:VAL:HG22	2.03	0.40
6:R:156:ARG:HH22	6:R:217:SER:C	2.24	0.40
6:R:599:ARG:H	6:R:599:ARG:NE	2.19	0.40
6:R:599:ARG:CG	6:R:600:THR:HG23	2.51	0.40
1:J:30:LYS:NZ	2:N:283:PRO:HD2	2.35	0.40
1:C:5:PHE:CD2	2:E:332:LYS:C	2.94	0.40
2:B:227:ARG:HA	2:B:227:ARG:HD3	1.87	0.40
2:B:247:VAL:HG22	2:B:248:VAL:H	1.85	0.40
2:B:359:LYS:HA	2:B:362:ASP:OD2	2.22	0.40
2:B:414:ARG:HB3	2:B:418:GLN:NE2	2.37	0.40
3:D:225:VAL:HG21	3:D:294:PHE:O	2.21	0.40
3:D:234:TRP:CZ3	3:D:237:ASN:CB	3.03	0.40
2:G:188:HIS:CE1	2:G:214:THR:H	2.39	0.40
2:G:225:VAL:HG21	2:G:294:PHE:O	2.22	0.40
2:G:351:GLU:HA	2:G:354:LEU:HD12	2.04	0.40
2:E:227:ARG:NH1	2:E:298:GLU:HA	2.36	0.40
3:K:302:ILE:HG22	3:K:306:HIS:HE1	1.85	0.40
2:P:265:VAL:HG23	2:P:269:ARG:HH22	1.85	0.40
2:P:274:LYS:NZ	2:P:429:GLU:CD	2.66	0.40
2:N:225:VAL:HG21	2:N:294:PHE:O	2.21	0.40
2:N:279:ILE:O	2:N:282:HIS:O	2.39	0.40
2:H:227:ARG:NH1	2:H:298:GLU:HA	2.36	0.40
2:H:229:TYR:CZ	2:H:233:LEU:HD11	2.56	0.40
2:H:306:HIS:HA	2:H:309:ARG:NH2	2.29	0.40
2:H:351:GLU:HA	2:H:354:LEU:HD12	2.04	0.40
2:H:400:ALA:HB2	2:H:550:GLN:HE22	1.86	0.40
2:H:523:LYS:HA	2:H:523:LYS:CE	2.51	0.40
2:H:533:ALA:CB	2:F:540:LEU:HD21	2.51	0.40
2:F:234:TRP:CZ3	2:F:237:ASN:CB	3.03	0.40
3:V:188:HIS:CE1	3:V:214:THR:H	2.40	0.40
3:V:252:PRO:HB3	3:V:272:LEU:HG	2.04	0.40
3:L:183:ALA:N	3:L:186:THR:HG1	2.18	0.40
3:L:205:ILE:HD13	3:L:207:TYR:CE1	2.56	0.40
3:L:235:LEU:O	3:L:235:LEU:HD22	2.22	0.40
5:S:138:ALA:HA	5:S:156:SER:N	2.35	0.40
6:Q:35:PRO:CB	6:Q:83:ASN:HD21	2.33	0.40
6:Q:52:LEU:HD13	6:Q:69:VAL:HG21	2.02	0.40
6:Q:83:ASN:HA	6:Q:86:VAL:HG22	2.03	0.40
6:Q:470:LEU:HD13	6:Q:504:ILE:HD11	2.02	0.40
6:Q:633:LEU:O	6:Q:637:LEU:HG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:712:THR:HG22	6:Q:713:ARG:N	2.36	0.40
6:R:182:PHE:CG	6:R:183:VAL:N	2.89	0.40
6:R:220:VAL:CG1	6:R:224:GLN:HE21	2.35	0.40
6:R:503:GLU:HA	6:R:506:ARG:HE	1.86	0.40
1:J:5:PHE:CD1	2:A:331:ASN:CG	2.55	0.40
2:B:235:LEU:O	2:B:235:LEU:HD22	2.21	0.40
2:B:267:SER:CB	2:B:432:ARG:HH11	1.95	0.40
2:A:229:TYR:CZ	2:A:233:LEU:HD11	2.57	0.40
2:A:332:LYS:CD	2:N:497:ARG:HD3	2.37	0.40
2:G:223:PHE:HB3	2:G:296:GLU:HA	2.03	0.40
2:G:363:ASN:HB3	2:G:367:GLN:OE1	2.21	0.40
2:G:480:ASN:HA	3:L:310:LYS:CD	2.48	0.40
2:G:510:GLU:CD	2:G:510:GLU:C	2.80	0.40
2:E:234:TRP:CZ3	2:E:237:ASN:CB	3.03	0.40
3:K:271:ALA:HA	3:K:274:LYS:HE2	2.04	0.40
2:P:205:ILE:HG22	2:P:268:ARG:HH11	1.85	0.40
2:P:229:TYR:CZ	2:P:233:LEU:HD11	2.56	0.40
2:H:359:LYS:HA	2:H:362:ASP:OD2	2.22	0.40
2:H:458:LEU:HA	2:H:461:LYS:HZ2	1.87	0.40
2:F:188:HIS:CE1	2:F:214:THR:H	2.39	0.40
2:F:209:VAL:HB	2:F:225:VAL:CG2	2.48	0.40
2:F:357:LEU:O	2:F:360:ALA:HB3	2.21	0.40
6:Q:220:VAL:HG13	6:Q:224:GLN:HE21	1.86	0.40
6:Q:231:TYR:CZ	6:Q:267:TYR:HB3	2.56	0.40
6:Q:685:PHE:O	6:Q:688:TYR:HB3	2.21	0.40
6:Q:719:ASN:H	6:Q:719:ASN:ND2	2.19	0.40
6:R:561:GLU:CD	6:R:561:GLU:N	2.75	0.40
6:R:631:SER:HA	6:R:634:PHE:CD2	2.57	0.40
1:J:30:LYS:HE3	2:N:283:PRO:HG2	1.88	0.40
1:J:108:LYS:HB3	1:C:111:GLU:CD	2.40	0.40
2:B:351:GLU:HA	2:B:354:LEU:HD12	2.04	0.40
2:G:350:LEU:HD13	2:E:385:LEU:CD2	2.52	0.40
2:G:372:ALA:HB3	2:G:373:GLU:OE2	2.22	0.40
2:G:455:GLU:N	2:G:493:VAL:HG22	2.36	0.40
2:E:204:HIS:NE2	2:E:228:ARG:HD3	2.35	0.40
2:E:229:TYR:CZ	2:E:233:LEU:HD11	2.56	0.40
3:K:229:TYR:CZ	3:K:233:LEU:HD11	2.57	0.40
2:P:205:ILE:HD13	2:P:207:TYR:CE1	2.56	0.40
2:P:235:LEU:HD22	2:P:235:LEU:O	2.22	0.40
2:P:252:PRO:HB3	2:P:272:LEU:HG	2.04	0.40
2:H:363:ASN:HB3	2:H:367:GLN:OE1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:449:HIS:HA	2:H:452:HIS:ND1	2.36	0.40
2:F:252:PRO:HB3	2:F:272:LEU:HG	2.03	0.40
2:F:253:GLU:N	2:F:268:ARG:HA	2.27	0.40
3:V:229:TYR:CZ	3:V:233:LEU:HD11	2.57	0.40
3:V:247:VAL:HG22	3:V:248:VAL:H	1.85	0.40
3:L:220:GLN:H	3:L:220:GLN:HG2	1.60	0.40
5:S:23:LYS:HA	5:S:26:LYS:HD2	2.04	0.40
5:S:105:ALA:HB2	5:S:113:LEU:HD21	2.03	0.40
5:S:122:PHE:C	5:S:122:PHE:CD1	2.94	0.40
6:Q:213:LEU:H	6:Q:213:LEU:HG	1.59	0.40
6:Q:462:LEU:HD23	6:Q:463:LEU:N	2.36	0.40
6:Q:570:HIS:CE1	6:Q:571:LEU:HG	2.56	0.40
6:Q:582:ARG:HG3	6:Q:582:ARG:H	1.54	0.40
6:R:49:VAL:CG1	6:R:103:ILE:HG22	2.51	0.40
6:R:117:MET:SD	6:R:158:TYR:CD2	3.14	0.40
6:R:467:GLN:NE2	6:R:470:LEU:HD12	2.37	0.40
6:R:480:LEU:HD13	6:R:523:ASN:HB3	2.03	0.40
6:R:570:HIS:CE1	6:R:571:LEU:CD2	3.05	0.40
6:R:584:LEU:HB3	6:R:585:GLN:OE1	2.21	0.40
6:R:798:PHE:CB	6:R:828:ILE:HG12	2.52	0.40
2:B:368:ARG:HA	2:B:412:TYR:OH	2.22	0.40
2:B:400:ALA:HB2	2:B:550:GLN:HE22	1.86	0.40
2:A:225:VAL:HG21	2:A:294:PHE:O	2.21	0.40
2:A:250:PRO:HG3	2:A:433:LEU:CB	2.52	0.40
3:D:188:HIS:CE1	3:D:214:THR:H	2.40	0.40
2:G:227:ARG:HA	2:G:227:ARG:HD3	1.87	0.40
2:G:368:ARG:HA	2:G:412:TYR:OH	2.22	0.40
2:G:409:ARG:HD3	2:G:410:ASP:HA	2.04	0.40
2:G:434:ILE:HA	2:G:437:VAL:HG22	2.03	0.40
2:G:451:TRP:CD1	2:G:451:TRP:C	2.92	0.40
2:E:494:HIS:CE1	2:E:498:LEU:HD22	2.57	0.40
2:P:271:ALA:HA	2:P:274:LYS:HE2	2.04	0.40
2:N:205:ILE:HD13	2:N:207:TYR:CE1	2.56	0.40
2:N:227:ARG:NH2	2:N:300:PHE:H	2.20	0.40
2:H:412:TYR:CD2	2:H:412:TYR:C	2.94	0.40
2:H:447:ALA:HB3	2:H:500:PHE:CD1	2.57	0.40
2:H:514:PHE:CZ	2:H:518:LYS:NZ	2.81	0.40
3:V:207:TYR:O	3:V:226:LYS:HA	2.22	0.40
3:V:223:PHE:HB3	3:V:296:GLU:HA	2.03	0.40
3:V:225:VAL:HG21	3:V:294:PHE:O	2.22	0.40
6:Q:117:MET:SD	6:Q:158:TYR:CD2	3.14	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:125:LYS:O	6:Q:129:LYS:HG2	2.21	0.40
6:Q:633:LEU:HA	6:Q:633:LEU:HD12	1.96	0.40
6:Q:745:TYR:CE2	6:Q:801:ILE:HG12	2.56	0.40
6:R:29:ARG:HA	6:R:32:LEU:HG	2.03	0.40
6:R:603:PRO:HA	6:R:606:ILE:CG1	2.50	0.40
6:R:749:HIS:HE1	6:R:754:THR:HB	1.86	0.40
6:R:772:LYS:HG2	6:R:773:ARG:HE	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	290/292 (99%)	280 (97%)	8 (3%)	2 (1%)	22 63
1	J	290/292 (99%)	280 (97%)	8 (3%)	2 (1%)	22 63
2	A	345/368 (94%)	321 (93%)	15 (4%)	9 (3%)	5 31
2	B	345/368 (94%)	314 (91%)	21 (6%)	10 (3%)	4 29
2	E	345/368 (94%)	321 (93%)	15 (4%)	9 (3%)	5 31
2	F	345/368 (94%)	321 (93%)	15 (4%)	9 (3%)	5 31
2	G	345/368 (94%)	313 (91%)	22 (6%)	10 (3%)	4 29
2	H	345/368 (94%)	313 (91%)	22 (6%)	10 (3%)	4 29
2	N	345/368 (94%)	318 (92%)	19 (6%)	8 (2%)	6 34
2	P	345/368 (94%)	318 (92%)	19 (6%)	8 (2%)	6 34
3	D	127/129 (98%)	105 (83%)	14 (11%)	8 (6%)	1 17
3	K	127/129 (98%)	105 (83%)	14 (11%)	8 (6%)	1 17
3	L	127/129 (98%)	105 (83%)	14 (11%)	8 (6%)	1 17
3	V	127/129 (98%)	105 (83%)	14 (11%)	8 (6%)	1 17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	M	218/220 (99%)	215 (99%)	2 (1%)	1 (0%)	29	69
4	O	218/220 (99%)	215 (99%)	2 (1%)	1 (0%)	29	69
5	S	180/193 (93%)	145 (81%)	19 (11%)	16 (9%)	1	11
5	T	180/193 (93%)	145 (81%)	19 (11%)	16 (9%)	1	11
6	Q	738/846 (87%)	666 (90%)	32 (4%)	40 (5%)	2	19
6	R	738/846 (87%)	666 (90%)	32 (4%)	40 (5%)	2	19
All	All	6120/6562 (93%)	5571 (91%)	326 (5%)	223 (4%)	6	25

All (223) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	6	SER
1	J	216	ALA
1	C	6	SER
1	C	216	ALA
2	B	247	VAL
2	B	332	LYS
2	A	247	VAL
3	D	247	VAL
2	G	247	VAL
2	G	332	LYS
2	E	247	VAL
3	K	247	VAL
2	P	247	VAL
2	N	247	VAL
2	H	247	VAL
2	H	332	LYS
2	F	247	VAL
3	V	247	VAL
3	L	247	VAL
5	S	10	ASN
5	S	62	ARG
6	Q	56	SER
6	Q	57	LEU
6	Q	87	ASN
6	Q	170	ASN
6	Q	428	GLU
6	Q	429	ARG
6	Q	452	ASP
6	Q	454	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	Q	483	PRO
6	Q	516	SER
6	Q	534	GLU
6	Q	595	ASN
6	Q	649	ASN
6	Q	672	GLU
6	Q	755	PRO
6	Q	764	ASP
6	Q	770	ASP
5	T	10	ASN
5	T	62	ARG
6	R	56	SER
6	R	57	LEU
6	R	87	ASN
6	R	170	ASN
6	R	428	GLU
6	R	429	ARG
6	R	452	ASP
6	R	454	HIS
6	R	483	PRO
6	R	516	SER
6	R	534	GLU
6	R	595	ASN
6	R	649	ASN
6	R	672	GLU
6	R	755	PRO
6	R	764	ASP
6	R	770	ASP
2	B	199	ASP
2	B	256	ALA
2	A	199	ASP
2	A	256	ALA
3	D	199	ASP
3	D	256	ALA
2	G	199	ASP
2	G	256	ALA
2	E	199	ASP
2	E	256	ALA
3	K	199	ASP
3	K	256	ALA
2	P	199	ASP
2	P	256	ALA

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	N	199	ASP
2	N	256	ALA
2	H	199	ASP
2	H	256	ALA
2	F	199	ASP
2	F	256	ALA
3	V	199	ASP
3	V	256	ALA
3	L	199	ASP
3	L	256	ALA
5	S	40	GLY
5	S	41	ASN
5	S	69	ALA
5	S	71	SER
5	S	74	LEU
5	S	136	GLY
6	Q	167	PRO
6	Q	226	VAL
6	Q	455	SER
6	Q	713	ARG
6	Q	767	LEU
5	T	40	GLY
5	T	41	ASN
5	T	69	ALA
5	T	71	SER
5	T	74	LEU
5	T	136	GLY
6	R	167	PRO
6	R	226	VAL
6	R	455	SER
6	R	713	ARG
6	R	767	LEU
2	B	202	THR
2	A	202	THR
2	A	371	MET
3	D	202	THR
2	G	202	THR
2	E	202	THR
2	E	371	MET
3	K	202	THR
4	O	390	LEU
2	P	202	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	M	390	LEU
2	N	202	THR
2	H	202	THR
2	F	202	THR
2	F	371	MET
3	V	202	THR
3	L	202	THR
6	Q	165	ASP
6	Q	388	PRO
6	Q	473	TYR
6	Q	485	TYR
6	Q	511	ASN
6	Q	618	ALA
6	Q	710	HIS
6	Q	765	THR
6	Q	769	ARG
6	Q	788	CYS
6	R	165	ASP
6	R	388	PRO
6	R	473	TYR
6	R	485	TYR
6	R	511	ASN
6	R	618	ALA
6	R	710	HIS
6	R	765	THR
6	R	769	ARG
6	R	788	CYS
2	B	300	PHE
2	A	300	PHE
3	D	300	PHE
2	G	300	PHE
2	E	300	PHE
3	K	300	PHE
2	P	300	PHE
2	N	300	PHE
2	H	300	PHE
2	F	300	PHE
3	V	300	PHE
3	L	300	PHE
5	S	61	VAL
5	S	73	PRO
5	S	139	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	Q	168	GLU
6	Q	474	VAL
6	Q	592	ALA
6	Q	766	GLU
5	T	61	VAL
5	T	73	PRO
5	T	139	THR
6	R	168	GLU
6	R	474	VAL
6	R	592	ALA
6	R	766	GLU
2	B	219	LYS
2	B	245	GLY
2	B	391	SER
2	A	219	LYS
2	A	245	GLY
3	D	219	LYS
3	D	245	GLY
2	G	245	GLY
2	G	391	SER
2	E	219	LYS
2	E	245	GLY
3	K	245	GLY
2	P	245	GLY
2	N	245	GLY
2	H	245	GLY
2	H	391	SER
2	F	219	LYS
2	F	245	GLY
3	V	219	LYS
3	V	245	GLY
3	L	245	GLY
5	S	42	LEU
5	S	55	SER
6	Q	121	GLY
6	Q	576	ASP
6	Q	693	SER
6	Q	838	ASP
5	T	42	LEU
5	T	55	SER
6	R	121	GLY
6	R	576	ASP

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Mol	Chain	Res	Type
6	R	693	SER
6	R	838	ASP
2	G	219	LYS
3	K	219	LYS
2	P	219	LYS
2	N	219	LYS
2	H	219	LYS
3	L	219	LYS
5	S	12	HIS
5	S	68	GLU
5	S	72	LEU
5	T	12	HIS
5	T	68	GLU
5	T	72	LEU
2	B	257	VAL
2	A	257	VAL
3	D	257	VAL
2	G	257	VAL
2	E	257	VAL
3	K	257	VAL
2	P	257	VAL
2	N	257	VAL
2	H	257	VAL
2	F	257	VAL
3	V	257	VAL
3	L	257	VAL

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	269/269 (100%)	269 (100%)	0	100	100
1	J	269/269 (100%)	269 (100%)	0	100	100
2	A	306/317 (96%)	285 (93%)	21 (7%)	15	40
2	B	306/317 (96%)	257 (84%)	49 (16%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	306/317 (96%)	285 (93%)	21 (7%)	15	40
2	F	306/317 (96%)	285 (93%)	21 (7%)	15	40
2	G	306/317 (96%)	257 (84%)	49 (16%)	2	13
2	H	306/317 (96%)	258 (84%)	48 (16%)	2	14
2	N	306/317 (96%)	285 (93%)	21 (7%)	15	40
2	P	306/317 (96%)	285 (93%)	21 (7%)	15	40
3	D	116/116 (100%)	103 (89%)	13 (11%)	6	22
3	K	116/116 (100%)	103 (89%)	13 (11%)	6	22
3	L	116/116 (100%)	103 (89%)	13 (11%)	6	22
3	V	116/116 (100%)	103 (89%)	13 (11%)	6	22
4	M	190/190 (100%)	182 (96%)	8 (4%)	30	54
4	O	190/190 (100%)	182 (96%)	8 (4%)	30	54
5	S	161/168 (96%)	133 (83%)	28 (17%)	2	11
5	T	161/168 (96%)	133 (83%)	28 (17%)	2	11
6	Q	656/743 (88%)	531 (81%)	125 (19%)	1	8
6	R	656/743 (88%)	532 (81%)	124 (19%)	1	8
All	All	5464/5740 (95%)	4840 (89%)	624 (11%)	9	21

All (624) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	186	THR
2	B	188	HIS
2	B	197	VAL
2	B	204	HIS
2	B	212	LYS
2	B	213	THR
2	B	228	ARG
2	B	235	LEU
2	B	240	HIS
2	B	248	VAL
2	B	257	VAL
2	B	259	ARG
2	B	261	GLU
2	B	331	ASN
2	B	338	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	342	ASP
2	B	343	ARG
2	B	364	MET
2	B	368	ARG
2	B	371	MET
2	B	378	PHE
2	B	383	HIS
2	B	403	GLU
2	B	405	GLN
2	B	409	ARG
2	B	413	GLU
2	B	414	ARG
2	B	419	ASP
2	B	428	GLU
2	B	448	PHE
2	B	457	GLU
2	B	458	LEU
2	B	471	GLN
2	B	477	ASP
2	B	482	VAL
2	B	490	GLU
2	B	505	ARG
2	B	506	LEU
2	B	509	SER
2	B	512	ASP
2	B	513	ARG
2	B	514	PHE
2	B	516	ARG
2	B	518	LYS
2	B	524	SER
2	B	527	GLU
2	B	531	GLU
2	B	534	VAL
2	B	535	GLU
2	A	186	THR
2	A	188	HIS
2	A	197	VAL
2	A	204	HIS
2	A	212	LYS
2	A	213	THR
2	A	228	ARG
2	A	235	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	A	240	HIS
2	A	248	VAL
2	A	257	VAL
2	A	259	ARG
2	A	261	GLU
2	A	343	ARG
2	A	378	PHE
2	A	399	ASP
2	A	414	ARG
2	A	449	HIS
2	A	476	GLN
2	A	506	LEU
2	A	547	PHE
3	D	186	THR
3	D	188	HIS
3	D	197	VAL
3	D	204	HIS
3	D	212	LYS
3	D	213	THR
3	D	228	ARG
3	D	235	LEU
3	D	240	HIS
3	D	248	VAL
3	D	257	VAL
3	D	259	ARG
3	D	261	GLU
2	G	186	THR
2	G	188	HIS
2	G	197	VAL
2	G	204	HIS
2	G	212	LYS
2	G	213	THR
2	G	228	ARG
2	G	235	LEU
2	G	240	HIS
2	G	248	VAL
2	G	257	VAL
2	G	259	ARG
2	G	261	GLU
2	G	331	ASN
2	G	338	ASP
2	G	342	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	G	343	ARG
2	G	364	MET
2	G	368	ARG
2	G	371	MET
2	G	378	PHE
2	G	383	HIS
2	G	403	GLU
2	G	405	GLN
2	G	409	ARG
2	G	413	GLU
2	G	414	ARG
2	G	419	ASP
2	G	428	GLU
2	G	448	PHE
2	G	457	GLU
2	G	458	LEU
2	G	471	GLN
2	G	477	ASP
2	G	482	VAL
2	G	490	GLU
2	G	505	ARG
2	G	506	LEU
2	G	509	SER
2	G	512	ASP
2	G	513	ARG
2	G	514	PHE
2	G	516	ARG
2	G	518	LYS
2	G	524	SER
2	G	527	GLU
2	G	531	GLU
2	G	534	VAL
2	G	535	GLU
2	E	186	THR
2	E	188	HIS
2	E	197	VAL
2	E	204	HIS
2	E	212	LYS
2	E	213	THR
2	E	228	ARG
2	E	235	LEU
2	E	240	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	E	248	VAL
2	E	257	VAL
2	E	259	ARG
2	E	261	GLU
2	E	343	ARG
2	E	378	PHE
2	E	399	ASP
2	E	414	ARG
2	E	449	HIS
2	E	476	GLN
2	E	506	LEU
2	E	547	PHE
3	K	186	THR
3	K	188	HIS
3	K	197	VAL
3	K	204	HIS
3	K	212	LYS
3	K	213	THR
3	K	228	ARG
3	K	235	LEU
3	K	240	HIS
3	K	248	VAL
3	K	257	VAL
3	K	259	ARG
3	K	261	GLU
4	O	331	ASN
4	O	378	PHE
4	O	386	SER
4	O	411	VAL
4	O	419	ASP
4	O	462	LYS
4	O	495	GLN
4	O	529	PHE
2	P	186	THR
2	P	188	HIS
2	P	197	VAL
2	P	204	HIS
2	P	212	LYS
2	P	213	THR
2	P	228	ARG
2	P	235	LEU
2	P	240	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	P	248	VAL
2	P	257	VAL
2	P	259	ARG
2	P	261	GLU
2	P	341	HIS
2	P	395	SER
2	P	397	PRO
2	P	409	ARG
2	P	410	ASP
2	P	438	LYS
2	P	444	ARG
2	P	465	GLN
4	M	331	ASN
4	M	378	PHE
4	M	386	SER
4	M	411	VAL
4	M	419	ASP
4	M	462	LYS
4	M	495	GLN
4	M	529	PHE
2	N	186	THR
2	N	188	HIS
2	N	197	VAL
2	N	204	HIS
2	N	212	LYS
2	N	213	THR
2	N	228	ARG
2	N	235	LEU
2	N	240	HIS
2	N	248	VAL
2	N	257	VAL
2	N	259	ARG
2	N	261	GLU
2	N	341	HIS
2	N	395	SER
2	N	397	PRO
2	N	409	ARG
2	N	410	ASP
2	N	438	LYS
2	N	444	ARG
2	N	465	GLN
2	H	186	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	H	188	HIS
2	H	197	VAL
2	H	204	HIS
2	H	212	LYS
2	H	213	THR
2	H	228	ARG
2	H	235	LEU
2	H	240	HIS
2	H	248	VAL
2	H	257	VAL
2	H	259	ARG
2	H	261	GLU
2	H	331	ASN
2	H	338	ASP
2	H	342	ASP
2	H	343	ARG
2	H	364	MET
2	H	368	ARG
2	H	371	MET
2	H	378	PHE
2	H	383	HIS
2	H	403	GLU
2	H	405	GLN
2	H	409	ARG
2	H	413	GLU
2	H	414	ARG
2	H	419	ASP
2	H	428	GLU
2	H	448	PHE
2	H	457	GLU
2	H	458	LEU
2	H	471	GLN
2	H	477	ASP
2	H	490	GLU
2	H	505	ARG
2	H	506	LEU
2	H	509	SER
2	H	512	ASP
2	H	513	ARG
2	H	514	PHE
2	H	516	ARG
2	H	518	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	H	524	SER
2	H	527	GLU
2	H	531	GLU
2	H	534	VAL
2	H	535	GLU
2	F	186	THR
2	F	188	HIS
2	F	197	VAL
2	F	204	HIS
2	F	212	LYS
2	F	213	THR
2	F	228	ARG
2	F	235	LEU
2	F	240	HIS
2	F	248	VAL
2	F	257	VAL
2	F	259	ARG
2	F	261	GLU
2	F	343	ARG
2	F	378	PHE
2	F	399	ASP
2	F	414	ARG
2	F	449	HIS
2	F	476	GLN
2	F	506	LEU
2	F	547	PHE
3	V	186	THR
3	V	188	HIS
3	V	197	VAL
3	V	204	HIS
3	V	212	LYS
3	V	213	THR
3	V	228	ARG
3	V	235	LEU
3	V	240	HIS
3	V	248	VAL
3	V	257	VAL
3	V	259	ARG
3	V	261	GLU
3	L	186	THR
3	L	188	HIS
3	L	197	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	L	204	HIS
3	L	212	LYS
3	L	213	THR
3	L	228	ARG
3	L	235	LEU
3	L	240	HIS
3	L	248	VAL
3	L	257	VAL
3	L	259	ARG
3	L	261	GLU
5	S	3	PHE
5	S	15	ASP
5	S	21	PRO
5	S	36	THR
5	S	39	LEU
5	S	45	ARG
5	S	52	ARG
5	S	60	ILE
5	S	70	THR
5	S	84	ARG
5	S	87	PHE
5	S	88	LEU
5	S	89	GLU
5	S	95	SER
5	S	113	LEU
5	S	115	TRP
5	S	122	PHE
5	S	127	TYR
5	S	156	SER
5	S	157	PHE
5	S	163	GLN
5	S	167	LEU
5	S	169	LEU
5	S	170	TYR
5	S	175	ARG
5	S	178	GLU
5	S	181	THR
5	S	193	LYS
6	Q	13	LEU
6	Q	23	GLN
6	Q	28	MET
6	Q	39	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	Q	43	LYS
6	Q	51	GLU
6	Q	67	MET
6	Q	82	GLU
6	Q	83	ASN
6	Q	87	ASN
6	Q	125	LYS
6	Q	128	MET
6	Q	141	PRO
6	Q	143	ARG
6	Q	149	TYR
6	Q	150	TYR
6	Q	157	ASP
6	Q	163	ASP
6	Q	165	ASP
6	Q	173	ASP
6	Q	174	SER
6	Q	182	PHE
6	Q	186	ASN
6	Q	192	LEU
6	Q	206	GLN
6	Q	209	ARG
6	Q	220	VAL
6	Q	221	ARG
6	Q	230	THR
6	Q	231	TYR
6	Q	234	SER
6	Q	241	GLU
6	Q	242	GLN
6	Q	245	GLN
6	Q	247	ARG
6	Q	257	GLU
6	Q	265	ASP
6	Q	275	PHE
6	Q	276	LEU
6	Q	283	ASN
6	Q	301	ASP
6	Q	387	VAL
6	Q	391	ASP
6	Q	394	PHE
6	Q	399	HIS
6	Q	411	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	Q	418	LEU
6	Q	428	GLU
6	Q	431	ASP
6	Q	434	ASP
6	Q	436	ILE
6	Q	437	LEU
6	Q	439	TYR
6	Q	445	LYS
6	Q	446	GLU
6	Q	447	HIS
6	Q	452	ASP
6	Q	462	LEU
6	Q	472	ARG
6	Q	473	TYR
6	Q	483	PRO
6	Q	484	THR
6	Q	485	TYR
6	Q	494	TYR
6	Q	518	PRO
6	Q	520	HIS
6	Q	522	GLU
6	Q	526	GLU
6	Q	532	ILE
6	Q	533	LYS
6	Q	562	GLN
6	Q	564	TRP
6	Q	565	LEU
6	Q	567	ARG
6	Q	568	LEU
6	Q	570	HIS
6	Q	578	ASP
6	Q	580	GLN
6	Q	585	GLN
6	Q	588	ARG
6	Q	593	GLU
6	Q	596	GLU
6	Q	599	ARG
6	Q	600	THR
6	Q	614	ARG
6	Q	620	GLU
6	Q	623	ASP
6	Q	625	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	Q	628	SER
6	Q	633	LEU
6	Q	636	PHE
6	Q	643	THR
6	Q	648	VAL
6	Q	658	LEU
6	Q	667	VAL
6	Q	669	ASP
6	Q	674	GLU
6	Q	679	GLU
6	Q	685	PHE
6	Q	686	THR
6	Q	688	TYR
6	Q	694	ASP
6	Q	713	ARG
6	Q	714	ASN
6	Q	718	GLU
6	Q	722	THR
6	Q	724	ILE
6	Q	754	THR
6	Q	764	ASP
6	Q	770	ASP
6	Q	772	LYS
6	Q	773	ARG
6	Q	777	CYS
6	Q	790	GLU
6	Q	794	SER
6	Q	797	LEU
6	Q	804	ARG
6	Q	817	THR
6	Q	818	THR
6	Q	821	LEU
6	Q	836	GLN
6	Q	843	GLU
6	Q	853	LEU
6	Q	854	GLU
6	Q	855	MET
5	T	3	PHE
5	T	15	ASP
5	T	21	PRO
5	T	36	THR
5	T	39	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	T	45	ARG
5	T	52	ARG
5	T	60	ILE
5	T	70	THR
5	T	84	ARG
5	T	87	PHE
5	T	88	LEU
5	T	89	GLU
5	T	95	SER
5	T	113	LEU
5	T	115	TRP
5	T	122	PHE
5	T	127	TYR
5	T	156	SER
5	T	157	PHE
5	T	163	GLN
5	T	167	LEU
5	T	169	LEU
5	T	170	TYR
5	T	175	ARG
5	T	178	GLU
5	T	181	THR
5	T	193	LYS
6	R	13	LEU
6	R	23	GLN
6	R	28	MET
6	R	39	MET
6	R	43	LYS
6	R	51	GLU
6	R	67	MET
6	R	82	GLU
6	R	83	ASN
6	R	87	ASN
6	R	125	LYS
6	R	128	MET
6	R	141	PRO
6	R	143	ARG
6	R	149	TYR
6	R	150	TYR
6	R	157	ASP
6	R	163	ASP
6	R	165	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	R	173	ASP
6	R	174	SER
6	R	182	PHE
6	R	186	ASN
6	R	192	LEU
6	R	206	GLN
6	R	209	ARG
6	R	220	VAL
6	R	221	ARG
6	R	230	THR
6	R	231	TYR
6	R	234	SER
6	R	241	GLU
6	R	242	GLN
6	R	245	GLN
6	R	247	ARG
6	R	257	GLU
6	R	265	ASP
6	R	275	PHE
6	R	276	LEU
6	R	283	ASN
6	R	301	ASP
6	R	387	VAL
6	R	391	ASP
6	R	394	PHE
6	R	399	HIS
6	R	411	THR
6	R	418	LEU
6	R	428	GLU
6	R	431	ASP
6	R	434	ASP
6	R	436	ILE
6	R	437	LEU
6	R	439	TYR
6	R	445	LYS
6	R	446	GLU
6	R	447	HIS
6	R	452	ASP
6	R	462	LEU
6	R	472	ARG
6	R	483	PRO
6	R	484	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	R	485	TYR
6	R	494	TYR
6	R	518	PRO
6	R	520	HIS
6	R	522	GLU
6	R	526	GLU
6	R	532	ILE
6	R	533	LYS
6	R	562	GLN
6	R	564	TRP
6	R	565	LEU
6	R	567	ARG
6	R	568	LEU
6	R	570	HIS
6	R	578	ASP
6	R	580	GLN
6	R	585	GLN
6	R	588	ARG
6	R	593	GLU
6	R	596	GLU
6	R	599	ARG
6	R	600	THR
6	R	614	ARG
6	R	620	GLU
6	R	623	ASP
6	R	625	ASN
6	R	628	SER
6	R	633	LEU
6	R	636	PHE
6	R	643	THR
6	R	648	VAL
6	R	658	LEU
6	R	667	VAL
6	R	669	ASP
6	R	674	GLU
6	R	679	GLU
6	R	685	PHE
6	R	686	THR
6	R	688	TYR
6	R	694	ASP
6	R	713	ARG
6	R	714	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	R	718	GLU
6	R	722	THR
6	R	724	ILE
6	R	754	THR
6	R	764	ASP
6	R	770	ASP
6	R	772	LYS
6	R	773	ARG
6	R	777	CYS
6	R	790	GLU
6	R	794	SER
6	R	797	LEU
6	R	804	ARG
6	R	817	THR
6	R	818	THR
6	R	821	LEU
6	R	836	GLN
6	R	843	GLU
6	R	853	LEU
6	R	854	GLU
6	R	855	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (165) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	195	HIS
2	B	204	HIS
2	B	220	GLN
2	B	242	ASN
2	B	243	ASN
2	B	282	HIS
2	B	306	HIS
2	B	331	ASN
2	B	341	HIS
2	B	353	GLN
2	B	367	GLN
2	B	383	HIS
2	B	418	GLN
2	B	445	GLN
2	B	449	HIS
2	B	483	ASN
2	B	494	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	550	GLN
2	A	204	HIS
2	A	220	GLN
2	A	242	ASN
2	A	282	HIS
2	A	306	HIS
2	A	331	ASN
2	A	336	GLN
2	A	341	HIS
2	A	353	GLN
2	A	443	GLN
2	A	449	HIS
2	A	494	HIS
3	D	195	HIS
3	D	204	HIS
3	D	220	GLN
3	D	242	ASN
3	D	282	HIS
3	D	306	HIS
2	G	204	HIS
2	G	220	GLN
2	G	242	ASN
2	G	282	HIS
2	G	306	HIS
2	G	331	ASN
2	G	341	HIS
2	G	352	ASN
2	G	353	GLN
2	G	367	GLN
2	G	383	HIS
2	G	418	GLN
2	G	445	GLN
2	G	449	HIS
2	G	483	ASN
2	G	494	HIS
2	G	550	GLN
2	E	204	HIS
2	E	220	GLN
2	E	242	ASN
2	E	282	HIS
2	E	306	HIS
2	E	336	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	E	353	GLN
2	E	443	GLN
2	E	449	HIS
2	E	494	HIS
3	K	195	HIS
3	K	204	HIS
3	K	220	GLN
3	K	242	ASN
3	K	282	HIS
3	K	306	HIS
2	P	195	HIS
2	P	204	HIS
2	P	220	GLN
2	P	240	HIS
2	P	242	ASN
2	P	282	HIS
2	P	306	HIS
2	P	452	HIS
2	N	204	HIS
2	N	220	GLN
2	N	240	HIS
2	N	242	ASN
2	N	282	HIS
2	N	306	HIS
2	N	452	HIS
2	H	195	HIS
2	H	204	HIS
2	H	220	GLN
2	H	242	ASN
2	H	282	HIS
2	H	306	HIS
2	H	331	ASN
2	H	341	HIS
2	H	352	ASN
2	H	353	GLN
2	H	367	GLN
2	H	383	HIS
2	H	418	GLN
2	H	445	GLN
2	H	449	HIS
2	H	480	ASN
2	H	483	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	H	494	HIS
2	H	550	GLN
2	F	195	HIS
2	F	204	HIS
2	F	220	GLN
2	F	242	ASN
2	F	282	HIS
2	F	306	HIS
2	F	353	GLN
2	F	443	GLN
2	F	449	HIS
2	F	494	HIS
3	V	195	HIS
3	V	204	HIS
3	V	220	GLN
3	V	242	ASN
3	V	282	HIS
3	V	306	HIS
3	L	195	HIS
3	L	204	HIS
3	L	220	GLN
3	L	242	ASN
3	L	282	HIS
3	L	306	HIS
5	S	10	ASN
5	S	120	HIS
5	S	173	GLN
6	Q	61	GLN
6	Q	79	HIS
6	Q	83	ASN
6	Q	88	HIS
6	Q	193	GLN
6	Q	212	GLN
6	Q	268	HIS
6	Q	399	HIS
6	Q	447	HIS
6	Q	570	HIS
6	Q	629	GLN
6	Q	719	ASN
6	Q	749	HIS
6	Q	779	GLN
6	Q	836	GLN

*Continued on next page...*

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Mol	Chain	Res	Type
5	T	10	ASN
5	T	120	HIS
5	T	173	GLN
6	R	61	GLN
6	R	79	HIS
6	R	83	ASN
6	R	88	HIS
6	R	101	ASN
6	R	139	GLN
6	R	193	GLN
6	R	212	GLN
6	R	268	HIS
6	R	399	HIS
6	R	447	HIS
6	R	460	GLN
6	R	523	ASN
6	R	570	HIS
6	R	629	GLN
6	R	719	ASN
6	R	749	HIS
6	R	779	GLN
6	R	836	GLN

### 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 monosaccharides 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-0154. These allow visual inspection of the internal detail of the map and identification of artifacts.

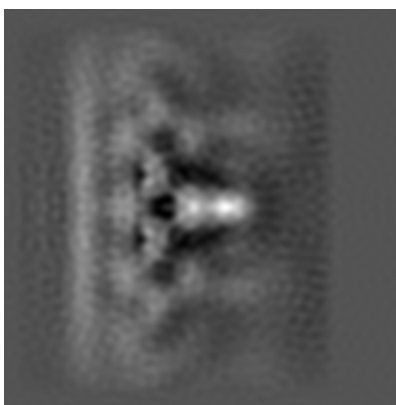
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

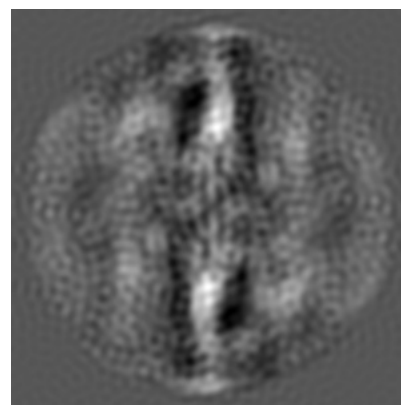
#### 6.1.1 Primary map



X



Y

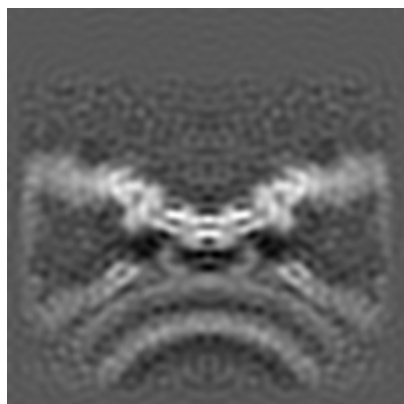


Z

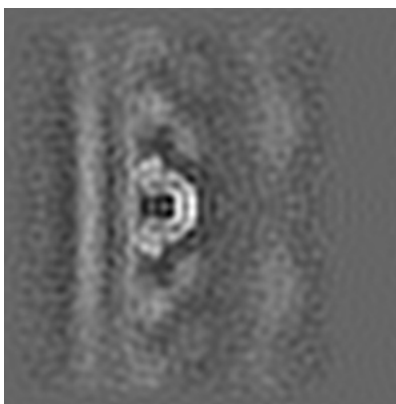
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

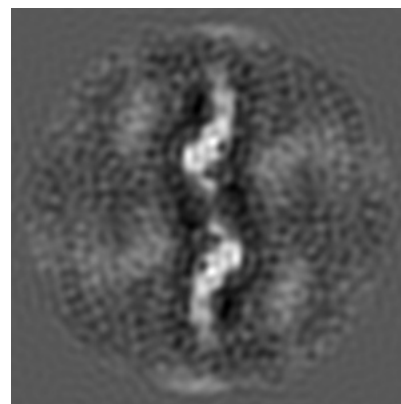
#### 6.2.1 Primary map



X Index: 72



Y Index: 72

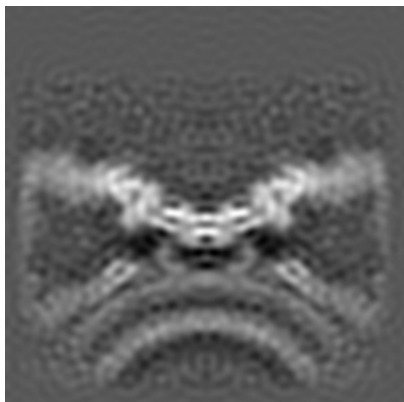


Z Index: 72

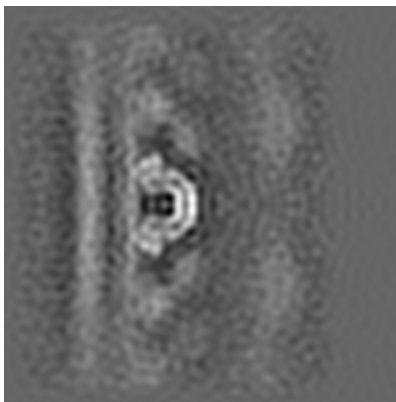
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

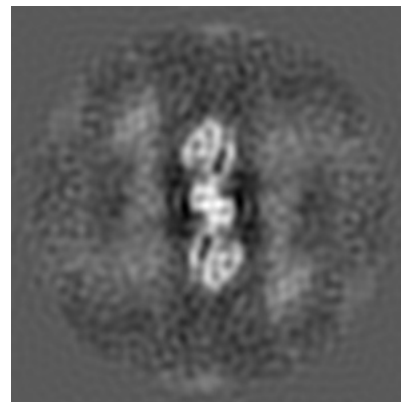
### 6.3.1 Primary map



X Index: 72



Y Index: 72



Z Index: 67

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

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

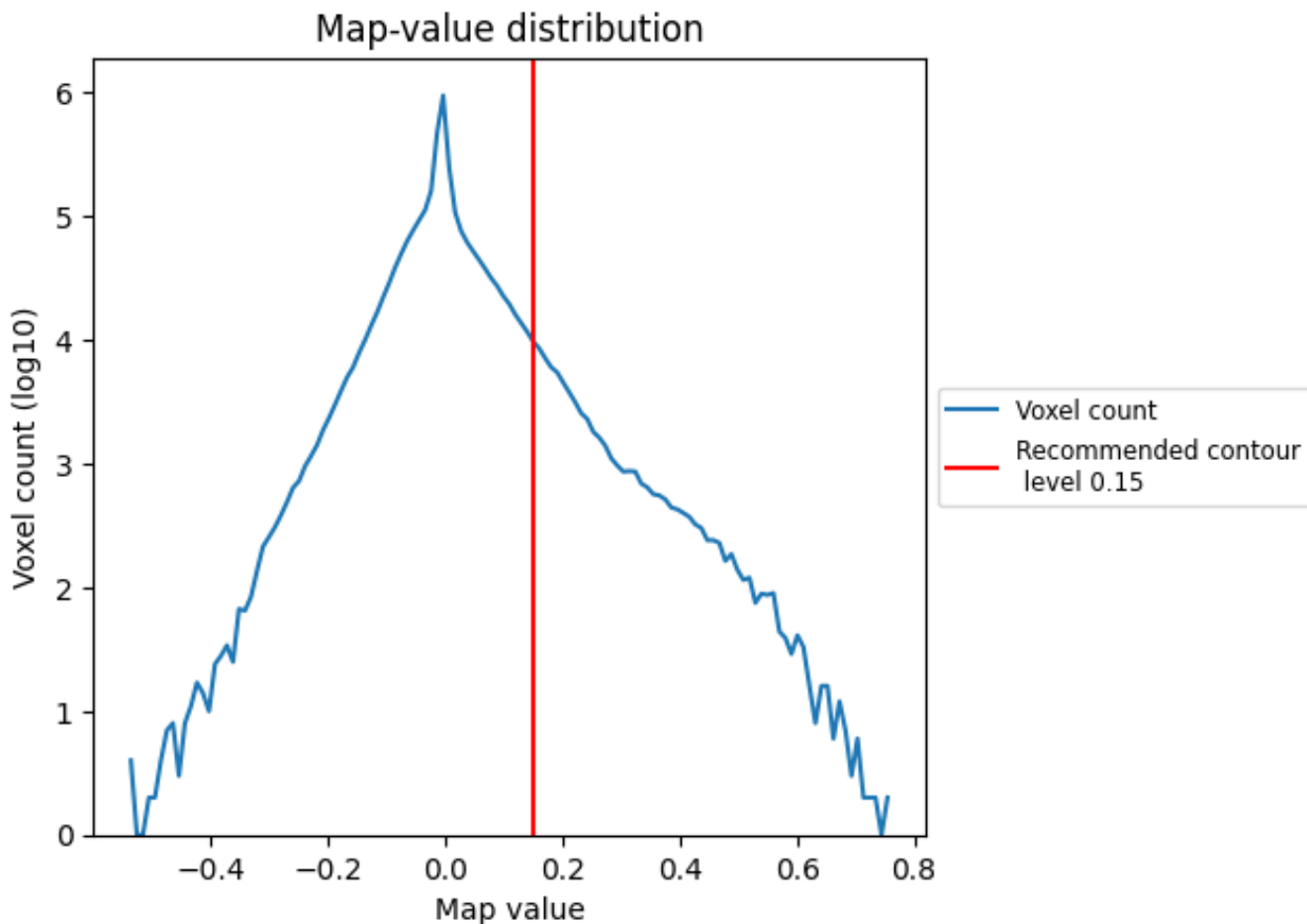
## 6.5 Mask visualisation

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.

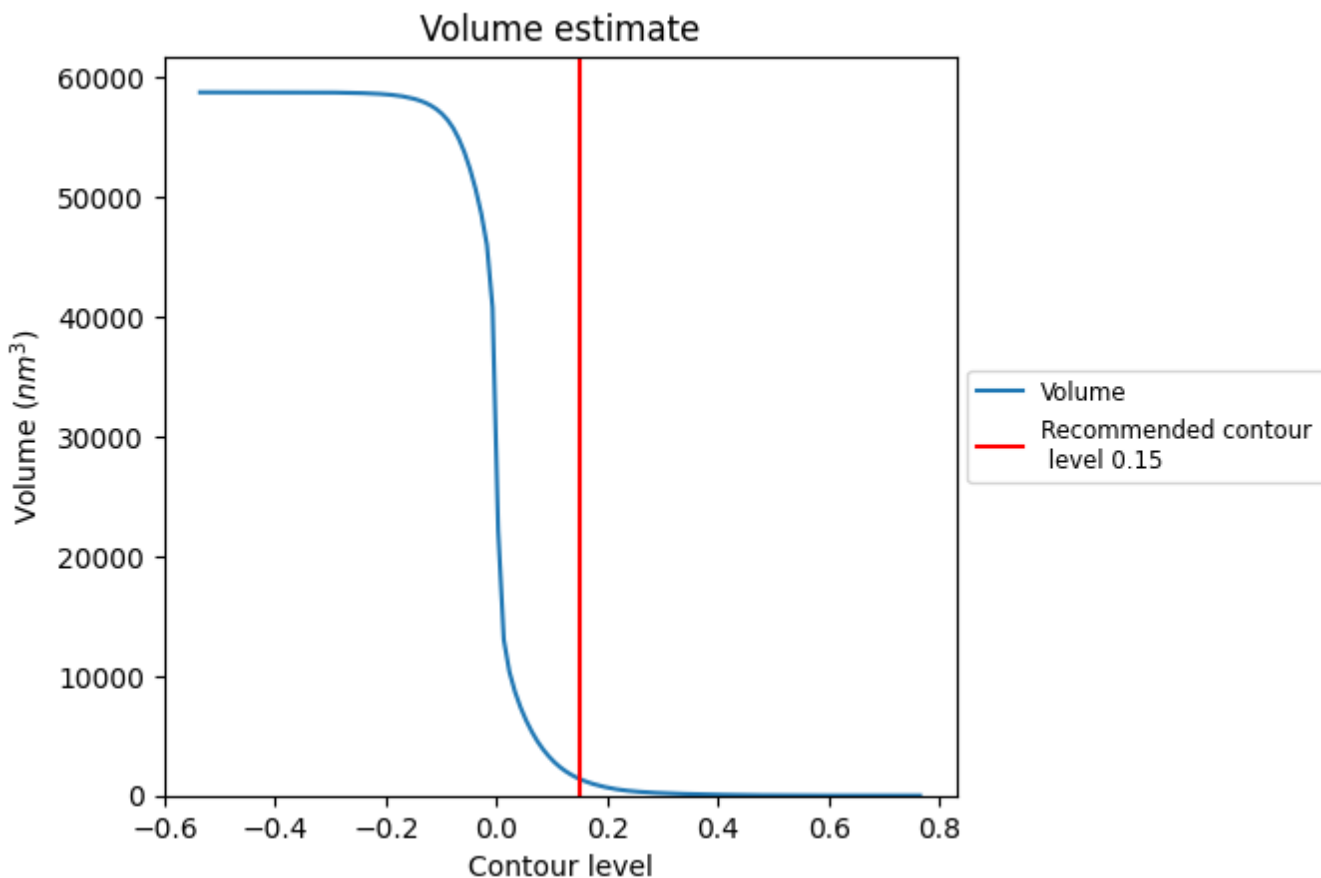
### 7.1 Map-value distribution [i](#)



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.



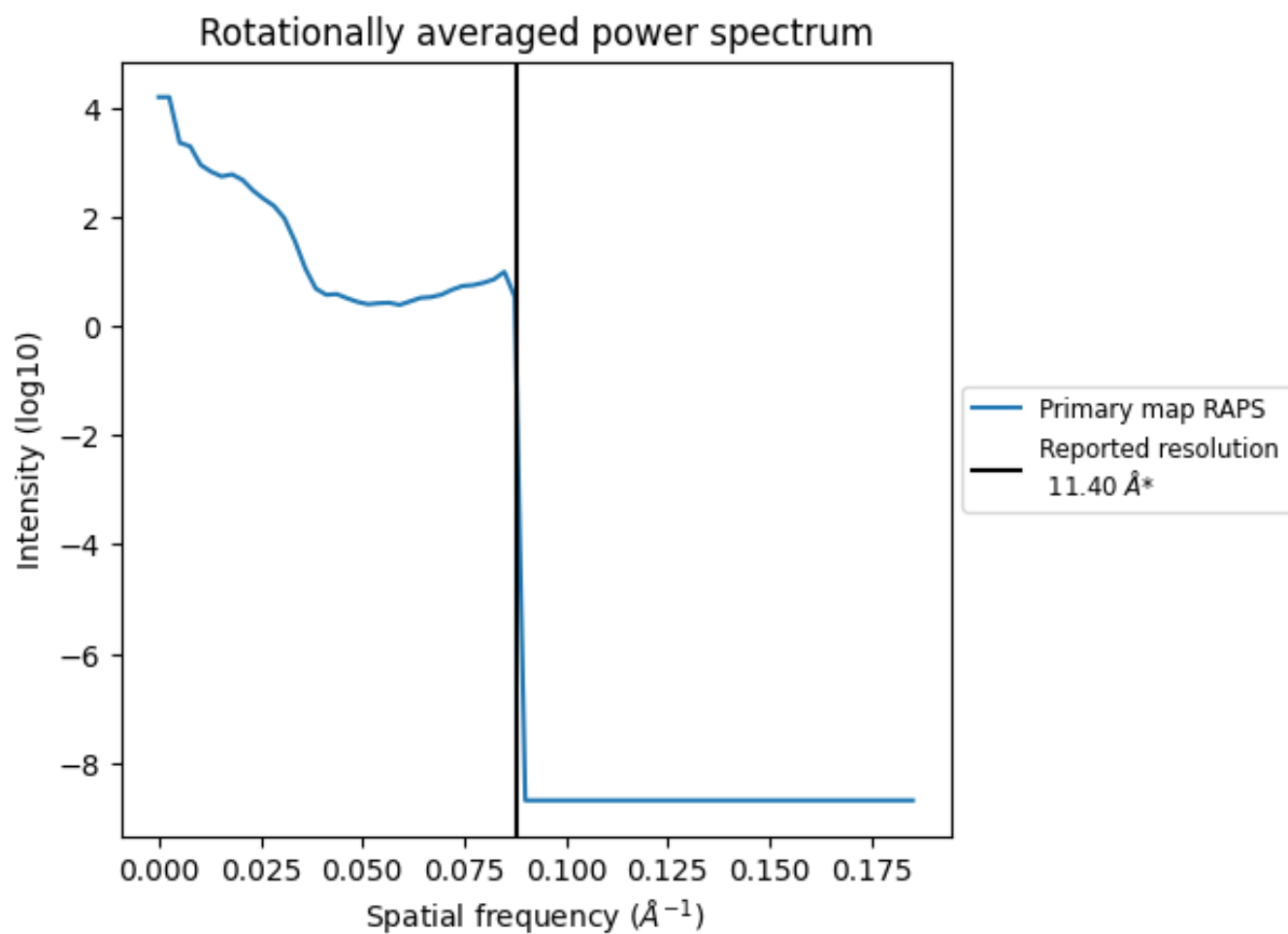
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1393 nm<sup>3</sup>; this corresponds to an approximate mass of 1259 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 [i](#)



\*Reported resolution corresponds to spatial frequency of 0.088 Å<sup>-1</sup>

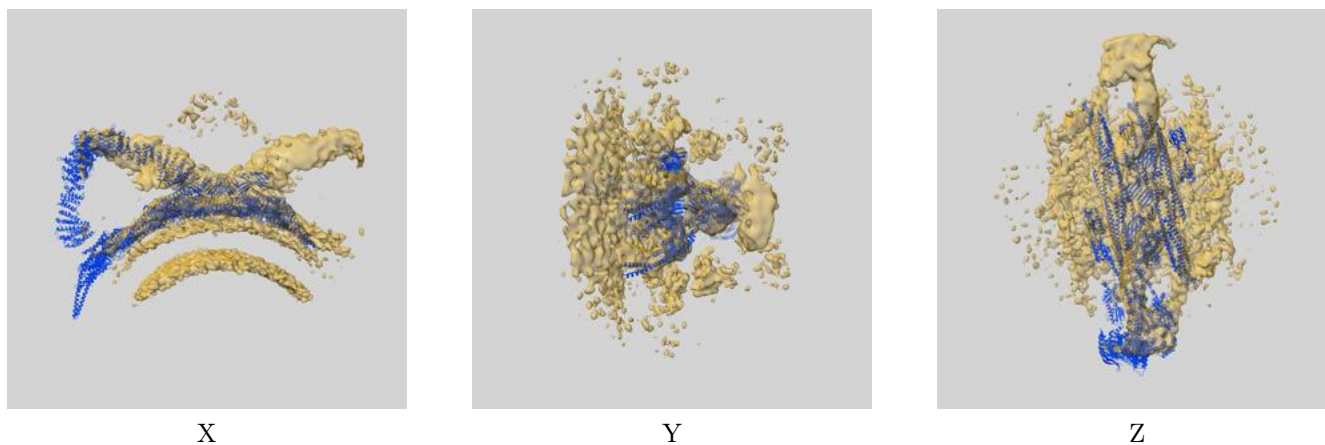
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

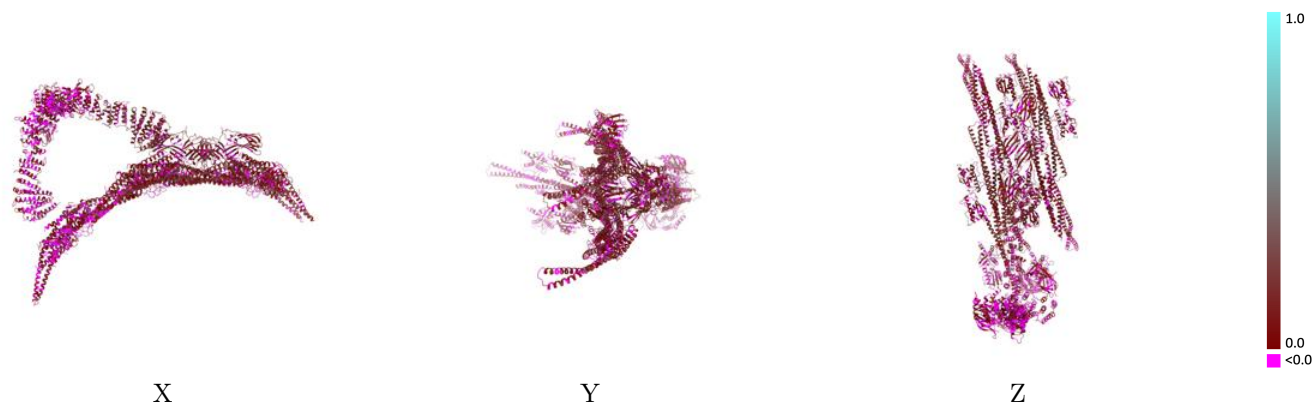
This section contains information regarding the fit between EMDB map EMD-0154 and PDB model 6H7W. Per-residue inclusion information can be found in section [3](#) on page [6](#).

### 9.1 Map-model overlay [i](#)



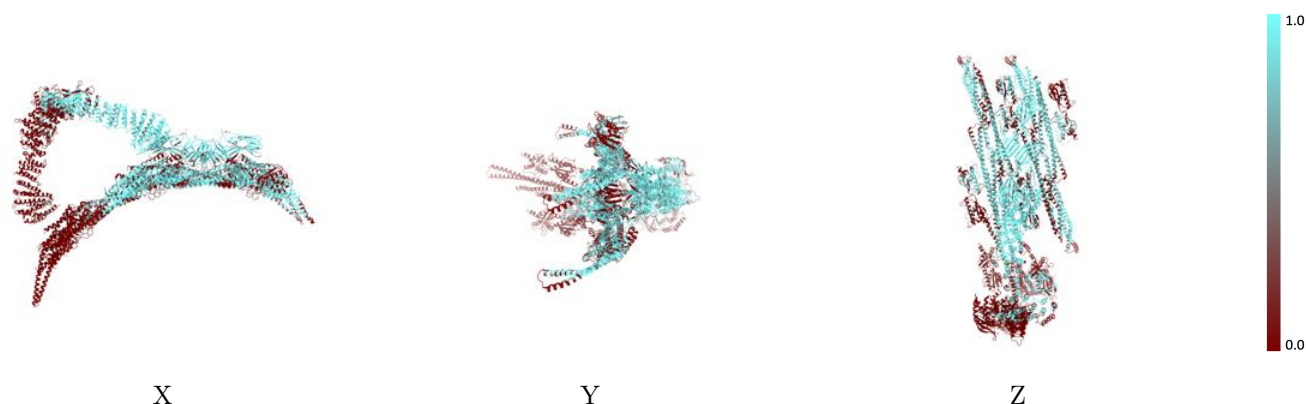
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



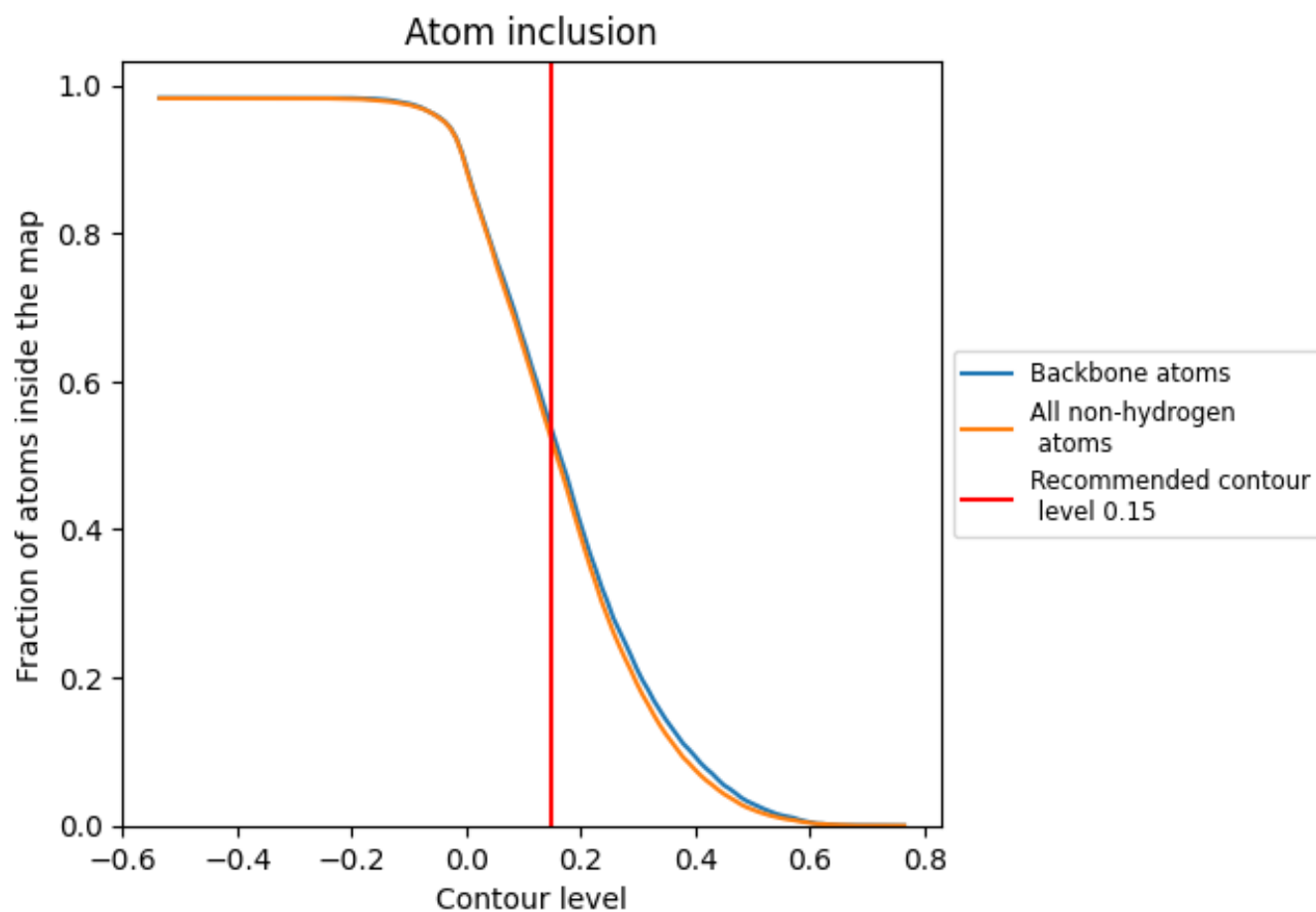
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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 (0.15).











































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 53% of all backbone atoms, 52% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5181	 0.0760
A	 0.6864	 0.1290
B	 0.7055	 0.1310
C	 0.8177	 0.0990
D	 0.1320	 0.0330
E	 0.6879	 0.1310
F	 0.0266	 0.0280
G	 0.7047	 0.1280
H	 0.2866	 0.0720
J	 0.8177	 0.1000
K	 0.1320	 0.0320
L	 0.0019	 0.0320
M	 0.6114	 0.0750
N	 0.5208	 0.0980
O	 0.6182	 0.0740
P	 0.5330	 0.0910
Q	 0.8019	 0.0880
R	 0.0564	 0.0140
S	 0.7282	 0.0490
T	 0.1635	 0.0130
V	 0.0000	 -0.0110

