



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 02:24 PM UTC

PDB ID : 5VY4 / pdb_00005vy4
EMDB ID : EMD-8742
Title : Thermoplasma acidophilum 20S Proteasome using 200keV with image shift
Authors : Herzik Jr., M.A.; Wu, M.; Lander, G.C.
Deposited on : 2017-05-24
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

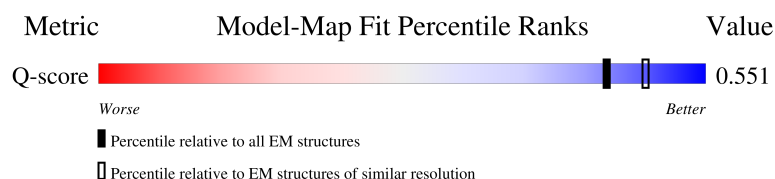
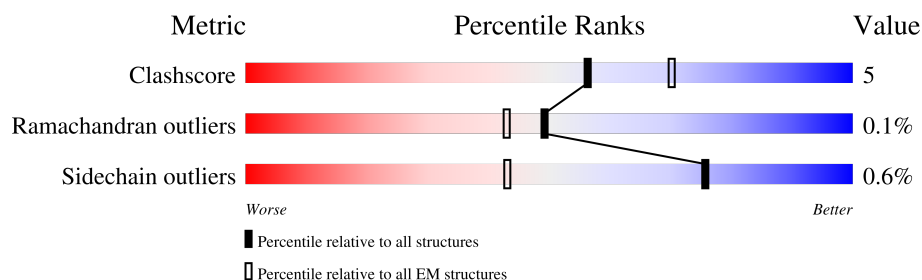
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

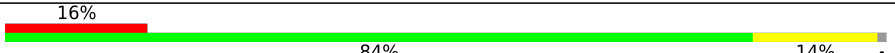
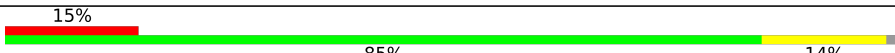
The reported resolution of this entry is 3.30 Å.

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



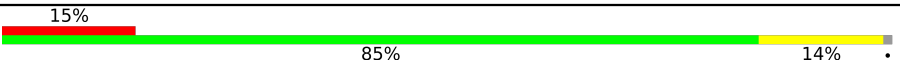
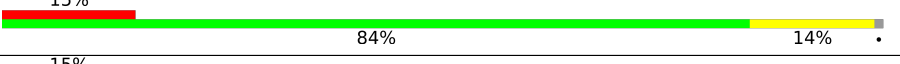
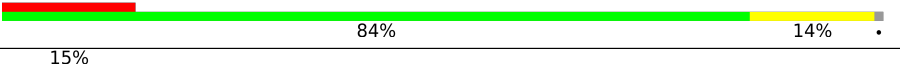
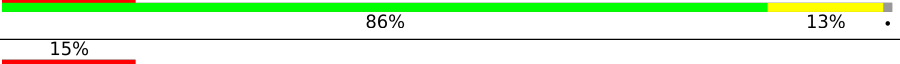
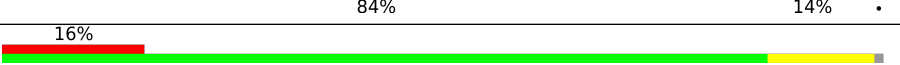
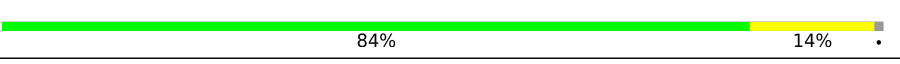
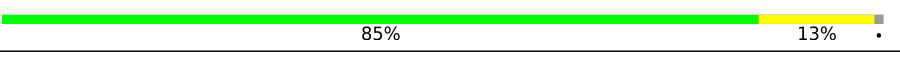
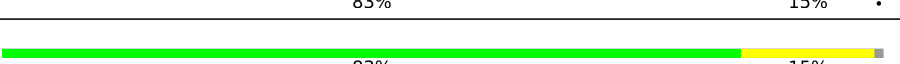
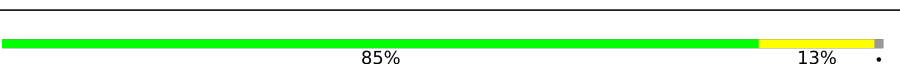
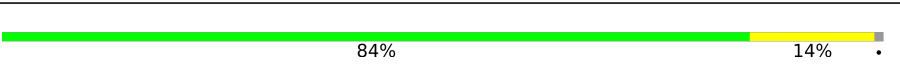
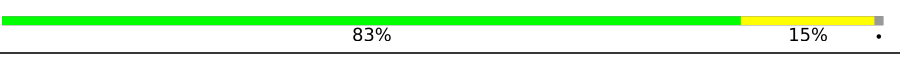
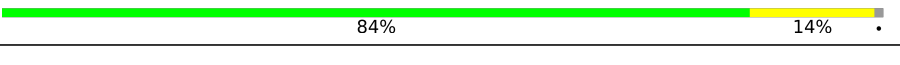
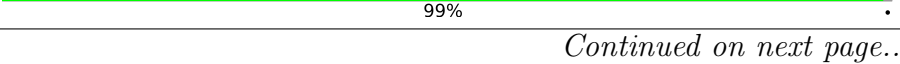
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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

Mol	Chain	Length	Quality of chain
1	1-0	224	
1	1-A	224	
1	1-C	224	
1	1-E	224	

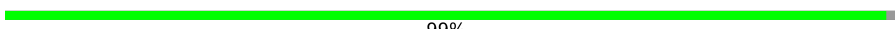
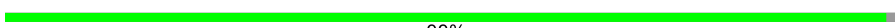
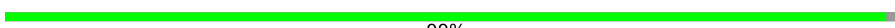
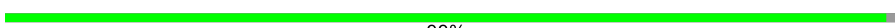
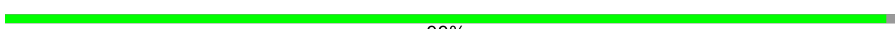
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Mol	Chain	Length	Quality of chain
1	1-G	224	
1	1-I	224	
1	1-K	224	
1	1-M	224	
1	1-O	224	
1	1-Q	224	
1	1-S	224	
1	1-U	224	
1	1-W	224	
1	1-Y	224	
1	10-0	224	
1	10-A	224	
1	10-C	224	
1	10-E	224	
1	10-G	224	
1	10-I	224	
1	10-K	224	
1	10-M	224	
1	10-O	224	
1	10-Q	224	
1	10-S	224	
1	10-U	224	
1	10-W	224	
1	10-Y	224	
1	2-0	224	

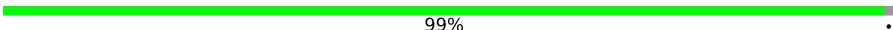
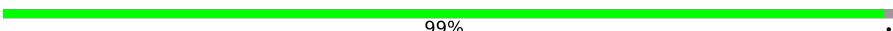
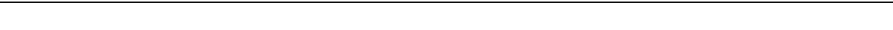
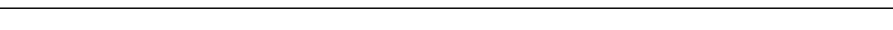
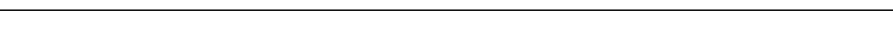
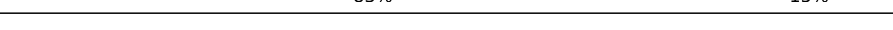
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Mol	Chain	Length	Quality of chain
1	2-A	224	 86% 13% .
1	2-C	224	 85% 14% .
1	2-E	224	 85% 14% .
1	2-G	224	 83% 13% .
1	2-I	224	 84% 14% .
1	2-K	224	 84% 14% .
1	2-M	224	 84% 14% .
1	2-O	224	 86% 12% .
1	2-Q	224	 84% 15% .
1	2-S	224	 84% 14% .
1	2-U	224	 84% 14% .
1	2-W	224	 85% 13% .
1	2-Y	224	 87% 12% .
1	3-0	224	 99% .
1	3-A	224	 86% 13% .
1	3-C	224	 84% 14% .
1	3-E	224	 86% 13% .
1	3-G	224	 99% .
1	3-I	224	 99% .
1	3-K	224	 99% .
1	3-M	224	 99% .
1	3-O	224	 99% .
1	3-Q	224	 99% .
1	3-S	224	 99% .
1	3-U	224	 99% .

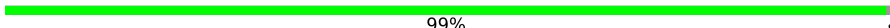
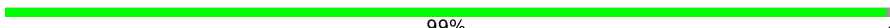
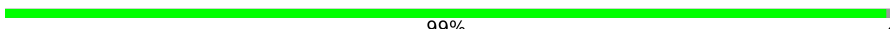
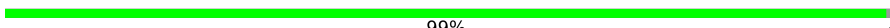
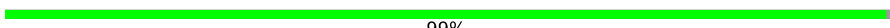
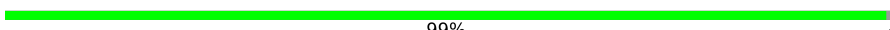
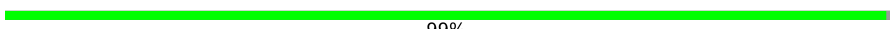
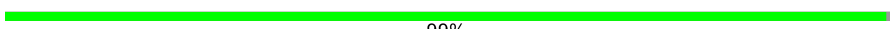
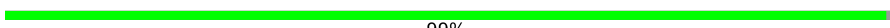
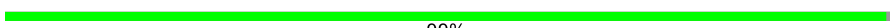
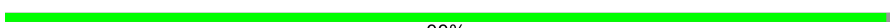
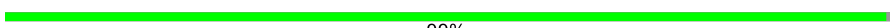
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Mol	Chain	Length	Quality of chain
1	3-W	224	 99% .
1	3-Y	224	 99% .
1	4-O	224	 84% 14% .
1	4-A	224	 80% 14% 6% .
1	4-C	224	 84% 15% .
1	4-E	224	 85% 14% .
1	4-G	224	 84% 14% .
1	4-I	224	 83% 16% .
1	4-K	224	 84% 14% .
1	4-M	224	 84% 14% .
1	4-O	224	 76% 12% 12% .
1	4-Q	224	 86% 13% .
1	4-S	224	 84% 14% .
1	4-U	224	 83% 15% .
1	4-W	224	 84% 14% .
1	4-Y	224	 85% 13% .
1	5-O	224	 83% 15% .
1	5-A	224	 85% 13% .
1	5-C	224	 84% 15% .
1	5-E	224	 84% 14% .
1	5-G	224	 85% 13% .
1	5-I	224	 84% 14% .
1	5-K	224	 84% 14% .
1	5-M	224	 84% 14% .
1	5-O	224	 85% 13% .

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Mol	Chain	Length	Quality of chain
1	5-Q	224	 84% 14%
1	5-S	224	 83% 15%
1	5-U	224	 84% 14%
1	5-W	224	 84% 14%
1	5-Y	224	 84% 14%
1	6-0	224	 99%
1	6-A	224	 83% 15%
1	6-C	224	 84% 15%
1	6-E	224	 99%
1	6-G	224	 99%
1	6-I	224	 99%
1	6-K	224	 99%
1	6-M	224	 99%
1	6-O	224	 99%
1	6-Q	224	 99%
1	6-S	224	 99%
1	6-U	224	 99%
1	6-W	224	 99%
1	6-Y	224	 99%
1	7-0	224	 86% 13%
1	7-A	224	 86% 13%
1	7-C	224	 87% 12%
1	7-E	224	 87% 12%
1	7-G	224	 87% 12%
1	7-I	224	 87% 12%

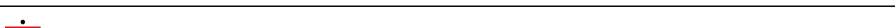
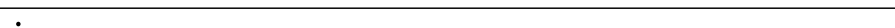
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Mol	Chain	Length	Quality of chain
1	7-K	224	 86% 12% .
1	7-M	224	 86% 13% .
1	7-O	224	 86% 13% .
1	7-Q	224	 87% 12% .
1	7-S	224	 86% 12% .
1	7-U	224	 87% 12% .
1	7-W	224	 87% 12% .
1	7-Y	224	 87% 12% .
1	8-0	224	 88% 11% .
1	8-A	224	 87% 12% .
1	8-C	224	 87% 12% .
1	8-E	224	 87% 12% .
1	8-G	224	 86% 12% .
1	8-I	224	 85% 14% .
1	8-K	224	 86% 12% .
1	8-M	224	 88% 11% .
1	8-O	224	 88% 11% .
1	8-Q	224	 88% 11% .
1	8-S	224	 86% 12% .
1	8-U	224	 85% 14% .
1	8-W	224	 86% 12% .
1	8-Y	224	 86% 13% .
1	9-0	224	 85% 13% .
1	9-A	224	 85% 13% .
1	9-C	224	 86% 13% .

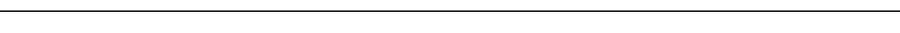
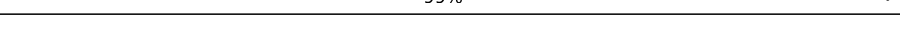
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Mol	Chain	Length	Quality of chain
1	9-E	224	 87% 12%
1	9-G	224	 83% 15%
1	9-I	224	 83% 16%
1	9-K	224	 85% 14%
1	9-M	224	 84% 15%
1	9-O	224	 85% 13%
1	9-Q	224	 85% 14%
1	9-S	224	 84% 15%
1	9-U	224	 83% 16%
1	9-W	224	 83% 15%
1	9-Y	224	 86% 12%
2	1-1	203	 5% 87% 12%
2	1-B	203	 1% 86% 13%
2	1-D	203	 1% 87% 13%
2	1-F	203	 1% 87% 13%
2	1-H	203	 5% 88% 12%
2	1-J	203	 1% 87% 12%
2	1-L	203	 1% 88% 12%
2	1-N	203	 1% 87% 13%
2	1-P	203	 1% 86% 13%
2	1-R	203	 1% 87% 13%
2	1-T	203	 1% 88% 12%
2	1-V	203	 1% 86% 13%
2	1-X	203	 1% 88% 12%
2	1-Z	203	 5% 87% 13%

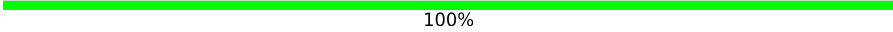
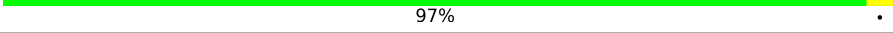
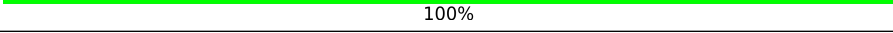
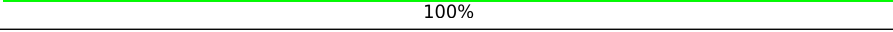
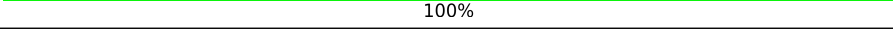
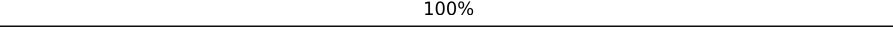
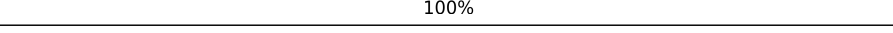
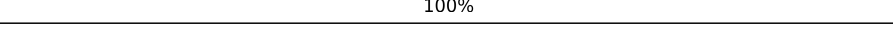
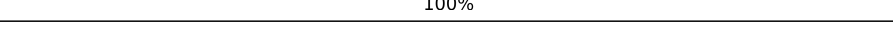
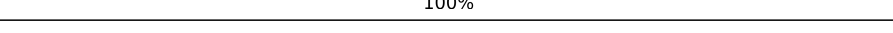
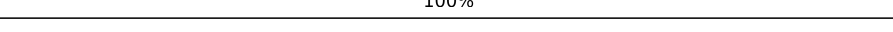
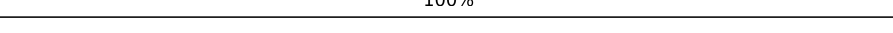
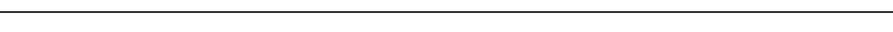
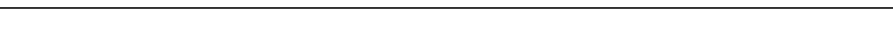
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Mol	Chain	Length	Quality of chain
2	10-1	203	 87% 13%
2	10-B	203	 86% 14%
2	10-D	203	 86% 13%
2	10-F	203	 86% 14%
2	10-H	203	 86% 14%
2	10-J	203	 88% 12%
2	10-L	203	 87% 13%
2	10-N	203	 87% 13%
2	10-P	203	 85% 14%
2	10-R	203	 87% 13%
2	10-T	203	 86% 13%
2	10-V	203	 85% 14%
2	10-X	203	 86% 13%
2	10-Z	203	 85% 14%
2	2-1	203	 99% 1%
2	2-B	203	 86% 14%
2	2-D	203	 88% 12%
2	2-F	203	 85% 15%
2	2-H	203	 84% 16%
2	2-J	203	 88% 12%
2	2-L	203	 87% 13%
2	2-N	203	 88% 12%
2	2-P	203	 86% 14%
2	2-R	203	 87% 13%
2	2-T	203	 87% 13%

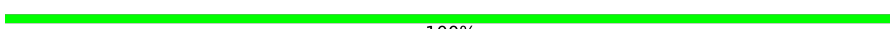
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Mol	Chain	Length	Quality of chain
2	2-V	203	 87% 13%
2	2-X	203	 84% 16%
2	2-Z	203	 90% 10%
2	3-1	203	 100%
2	3-B	203	 86% 11% .
2	3-D	203	 89% 11%
2	3-F	203	 97% .
2	3-H	203	 100%
2	3-J	203	 100%
2	3-L	203	 100%
2	3-N	203	 100%
2	3-P	203	 100%
2	3-R	203	 100%
2	3-T	203	 100%
2	3-V	203	 100%
2	3-X	203	 100%
2	3-Z	203	 100%
2	4-1	203	 89% 11%
2	4-B	203	 90% 10%
2	4-D	203	 90% 10%
2	4-F	203	 90% 10%
2	4-H	203	 90% 9%
2	4-J	203	 90% 9%
2	4-L	203	 90% 10%
2	4-N	203	 89% 10%

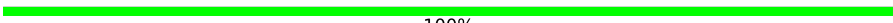
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Mol	Chain	Length	Quality of chain
2	4-P	203	 90% 9%
2	4-R	203	 90% 10%
2	4-T	203	 90% 9%
2	4-V	203	 90% 9%
2	4-X	203	 90% 10%
2	4-Z	203	 90% 9%
2	5-1	203	 85% 14%
2	5-B	203	 86% 13%
2	5-D	203	 85% 14%
2	5-F	203	 85% 14%
2	5-H	203	 86% 14%
2	5-J	203	 86% 14%
2	5-L	203	 86% 14%
2	5-N	203	 85% 15%
2	5-P	203	 85% 14%
2	5-R	203	 85% 15%
2	5-T	203	 86% 14%
2	5-V	203	 86% 14%
2	5-X	203	 86% 14%
2	5-Z	203	 85% 14%
2	6-1	203	 100%
2	6-B	203	 88% 12%
2	6-D	203	 100%
2	6-F	203	 100%
2	6-H	203	 100%

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Mol	Chain	Length	Quality of chain
2	6-J	203	 100%
2	6-L	203	 100%
2	6-N	203	 100%
2	6-P	203	 100%
2	6-R	203	 100%
2	6-T	203	 100%
2	6-V	203	 100%
2	6-X	203	 100%
2	6-Z	203	 100%
2	7-1	203	 82% 18%
2	7-B	203	 80% 20%
2	7-D	203	 81% 19%
2	7-F	203	 82% 18%
2	7-H	203	 81% 19%
2	7-J	203	 80% 20%
2	7-L	203	 81% 19%
2	7-N	203	 81% 19%
2	7-P	203	 80% 20%
2	7-R	203	 82% 18%
2	7-T	203	 81% 19%
2	7-V	203	 80% 20%
2	7-X	203	 81% 19%
2	7-Z	203	 81% 19%
2	8-1	203	 85% 15%
2	8-B	203	 84% 15%

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Mol	Chain	Length	Quality of chain
2	8-D	203	 85% 15%
2	8-F	203	 85% 15%
2	8-H	203	 84% 16%
2	8-J	203	 84% 15%
2	8-L	203	 84% 15%
2	8-N	203	 85% 15%
2	8-P	203	 84% 16%
2	8-R	203	 85% 15%
2	8-T	203	 83% 16%
2	8-V	203	 85% 14%
2	8-X	203	 84% 16%
2	8-Z	203	 85% 15%
2	9-1	203	 85% 14% .
2	9-B	203	 85% 14% .
2	9-D	203	 85% 14% .
2	9-F	203	 85% 14% .
2	9-H	203	 85% 14% .
2	9-J	203	 85% 14% .
2	9-L	203	 85% 14% .
2	9-N	203	 85% 14% .
2	9-P	203	 85% 14% .
2	9-R	203	 85% 14% .
2	9-T	203	 85% 14% .
2	9-V	203	 85% 14% .
2	9-X	203	 85% 14% .

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Mol	Chain	Length	Quality of chain
2	9-Z	203	85% 14%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 458560 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1-A	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	2-A	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	3-A	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	4-A	210	Total	C	N	O	S	0	1
			1630	1036	275	316	3		
1	5-A	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	6-A	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	7-A	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	8-A	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	9-A	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	10-A	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	1-C	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	2-C	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	3-C	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	4-C	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	5-C	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	6-C	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	7-C	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	8-C	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	9-C	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	10-C	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	1-E	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	2-E	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	3-E	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	4-E	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	5-E	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	6-E	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	7-E	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	8-E	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	9-E	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	10-E	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	1-G	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	2-G	216	Total 1675	C 1063	N 284	O 325	S 3	0	1
1	3-G	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	4-G	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	5-G	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	6-G	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	7-G	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	8-G	221	Total 1720	C 1092	N 290	O 335	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	9-G	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	10-G	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	1-I	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	2-I	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	3-I	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	4-I	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	5-I	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	6-I	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	7-I	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	8-I	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	9-I	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	10-I	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	1-K	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	2-K	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	3-K	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	4-K	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	5-K	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	6-K	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	7-K	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	8-K	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	9-K	221	Total 1720	C 1092	N 290	O 335	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	10-K	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	1-M	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	2-M	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	3-M	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	4-M	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	5-M	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	6-M	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	7-M	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	8-M	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	9-M	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	10-M	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	1-O	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	2-O	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	3-O	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	4-O	198	Total	C	N	O	S	0	0
			1540	979	262	296	3		
1	5-O	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	6-O	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	7-O	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	8-O	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	9-O	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	10-O	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	1-Q	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	2-Q	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	3-Q	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	4-Q	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	5-Q	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	6-Q	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	7-Q	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	8-Q	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	9-Q	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	10-Q	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	1-S	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	2-S	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	3-S	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	4-S	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	5-S	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	6-S	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	7-S	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	8-S	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	9-S	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	10-S	221	Total 1720	C 1092	N 290	O 335	S 3	0	0
1	1-U	221	Total 1720	C 1092	N 290	O 335	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	2-U	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	3-U	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	4-U	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	5-U	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	6-U	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	7-U	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	8-U	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	9-U	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	10-U	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	1-W	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	2-W	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	3-W	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	4-W	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	5-W	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	6-W	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	7-W	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	8-W	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	9-W	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	10-W	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	1-Y	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	2-Y	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	3-Y	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	4-Y	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	5-Y	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	6-Y	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	7-Y	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	8-Y	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	9-Y	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	10-Y	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	1-0	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	2-0	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	3-0	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	4-0	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	5-0	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	6-0	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	7-0	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	8-0	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	9-0	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	10-0	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		

- Molecule 2 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1-B	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	2-B	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	3-B	197	Total	C	N	O	S	0	0
			1513	958	258	286	11		
2	4-B	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	5-B	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	6-B	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	7-B	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	8-B	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	9-B	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	10-B	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	1-D	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	2-D	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	3-D	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	4-D	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	5-D	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	6-D	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	7-D	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	8-D	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	9-D	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	10-D	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	1-F	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	2-F	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	3-F	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	4-F	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	5-F	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	6-F	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	7-F	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	8-F	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	9-F	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	10-F	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	1-H	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	2-H	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	3-H	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	4-H	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	5-H	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	6-H	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	7-H	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	8-H	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	9-H	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	10-H	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	1-J	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	2-J	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	3-J	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	4-J	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	5-J	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	6-J	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	7-J	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	8-J	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	9-J	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	10-J	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	1-L	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	2-L	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	3-L	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	4-L	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	5-L	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	6-L	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	7-L	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	8-L	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	9-L	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	10-L	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	1-N	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	2-N	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	3-N	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	4-N	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	5-N	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	6-N	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	7-N	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	8-N	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	9-N	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	10-N	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	1-P	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	2-P	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	3-P	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	4-P	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	5-P	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	6-P	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	7-P	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	8-P	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	9-P	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	10-P	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	1-R	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	2-R	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	3-R	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	4-R	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	5-R	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	6-R	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	7-R	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	8-R	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	9-R	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	10-R	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	1-T	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	2-T	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	3-T	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	4-T	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	5-T	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	6-T	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	7-T	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	8-T	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	9-T	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	10-T	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	1-V	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	2-V	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	3-V	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	4-V	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	5-V	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	6-V	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	7-V	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	8-V	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	9-V	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	10-V	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	1-X	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	2-X	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	3-X	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	4-X	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	5-X	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	6-X	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	7-X	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	8-X	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	9-X	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	10-X	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	1-Z	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	2-Z	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	3-Z	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	4-Z	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	5-Z	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	6-Z	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	7-Z	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		

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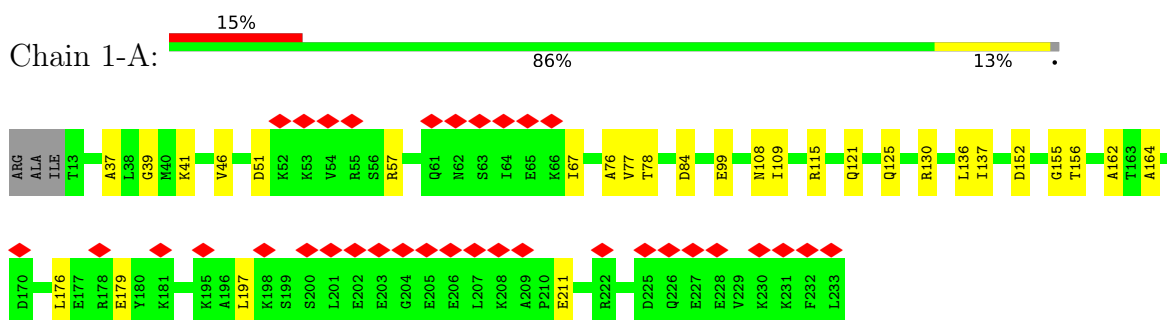
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Mol	Chain	Residues	Atoms					AltConf	Trace
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			1558	985	264	298	11		
2	9-Z	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	10-Z	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	1-1	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	2-1	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	3-1	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	4-1	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	5-1	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	6-1	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	7-1	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	8-1	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	9-1	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
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			1558	985	264	298	11		

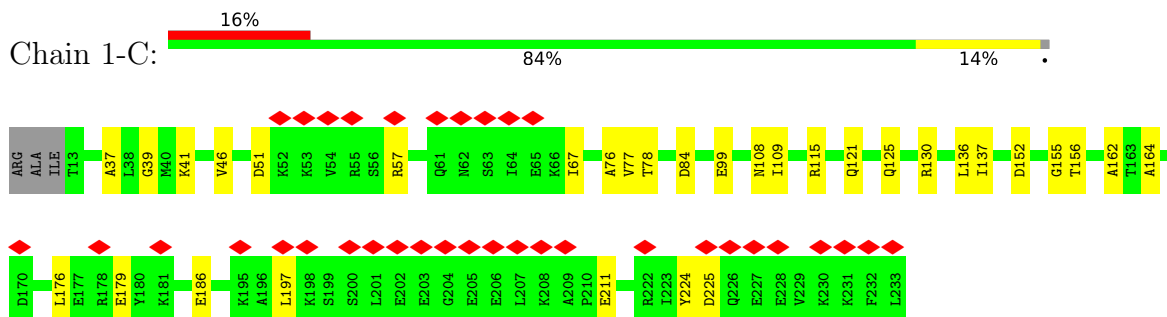
3 Residue-property plots [i](#)

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.

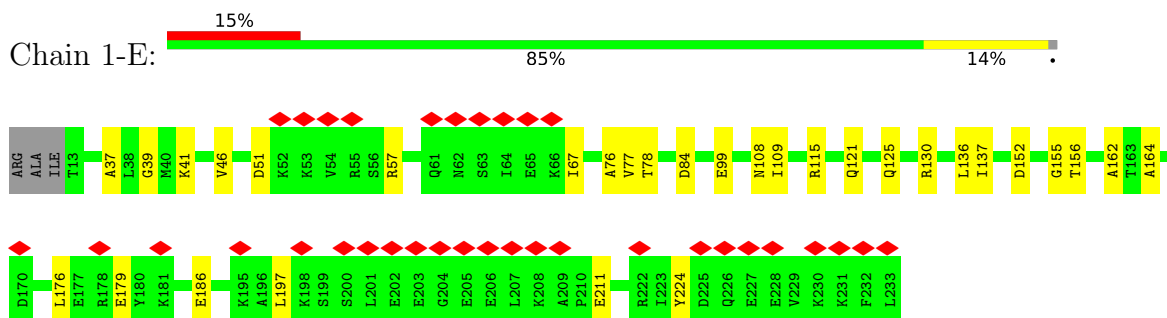
- Molecule 1: Proteasome subunit alpha



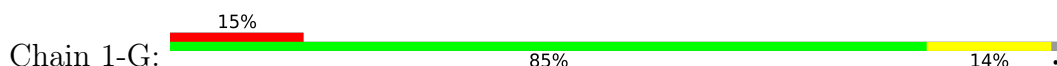
- Molecule 1: Proteasome subunit alpha

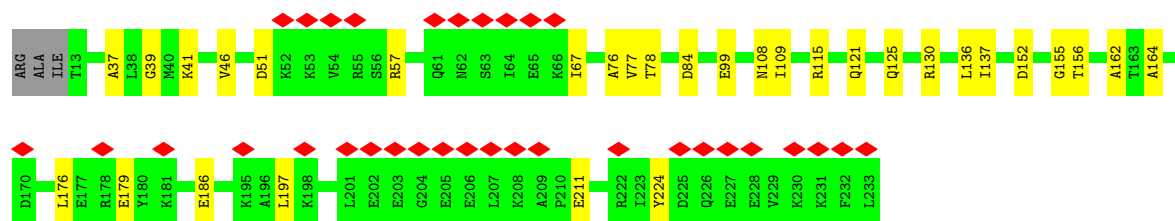


- Molecule 1: Proteasome subunit alpha

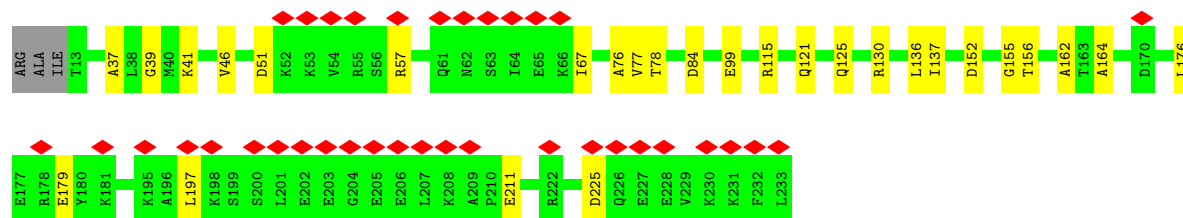
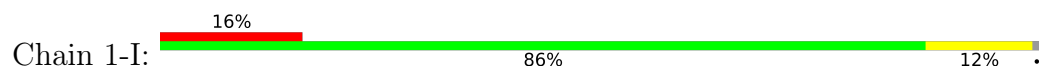


- Molecule 1: Proteasome subunit alpha

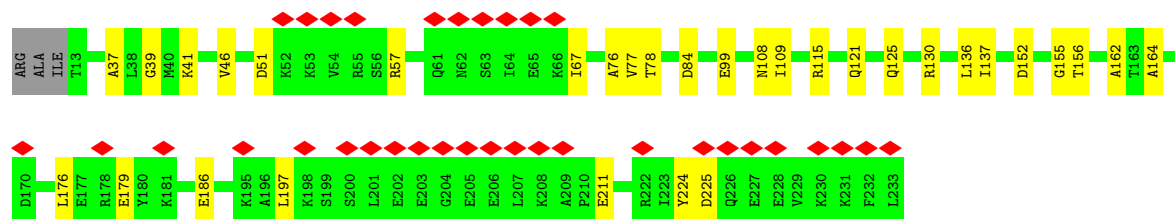
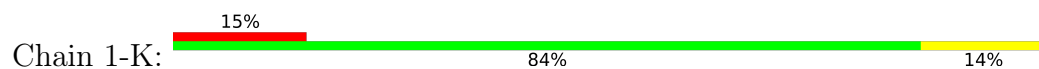




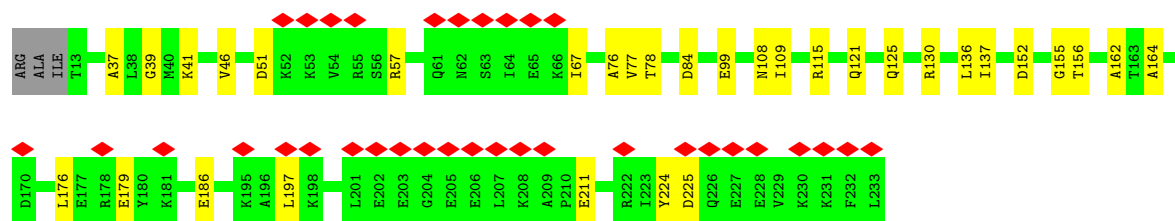
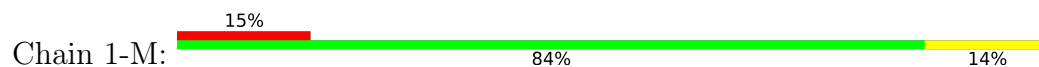
• Molecule 1: Proteasome subunit alpha



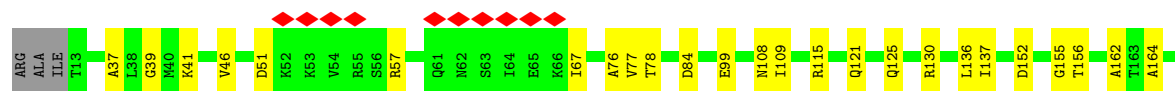
• Molecule 1: Proteasome subunit alpha

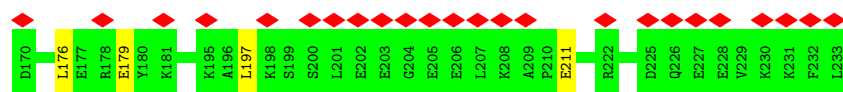


• Molecule 1: Proteasome subunit alpha

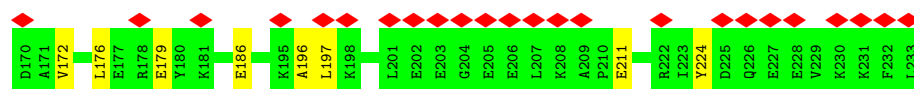
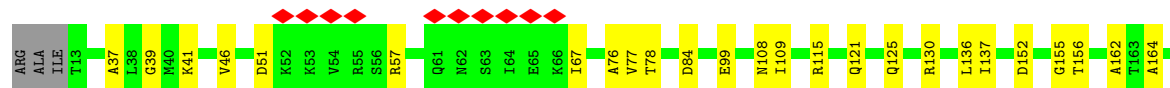
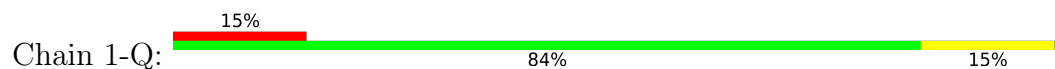


• Molecule 1: Proteasome subunit alpha

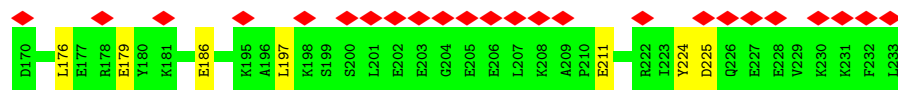
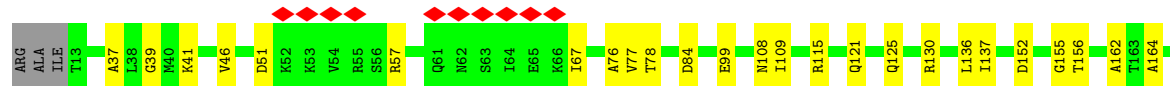
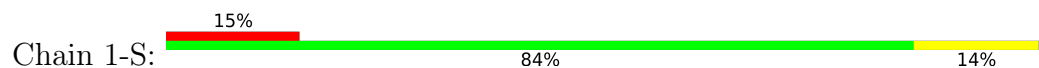




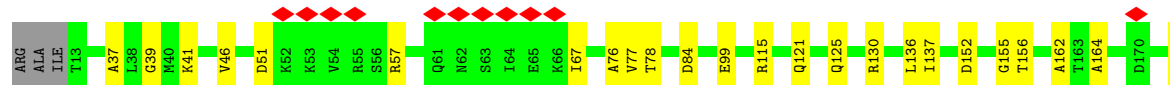
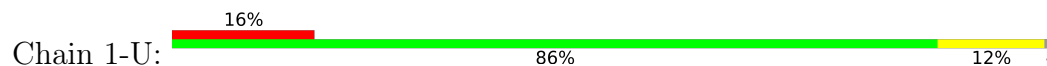
• Molecule 1: Proteasome subunit alpha



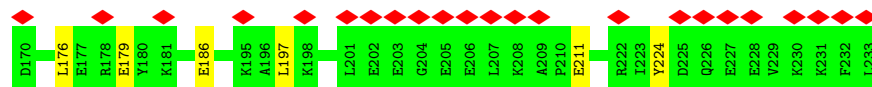
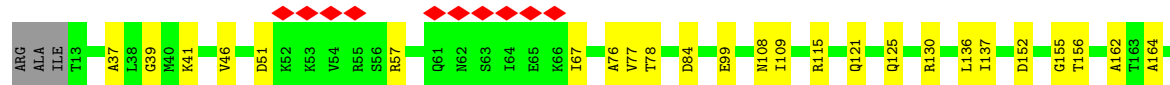
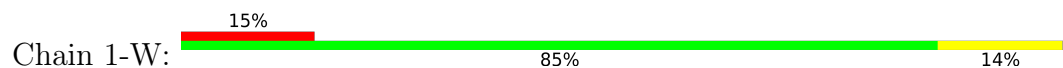
• Molecule 1: Proteasome subunit alpha



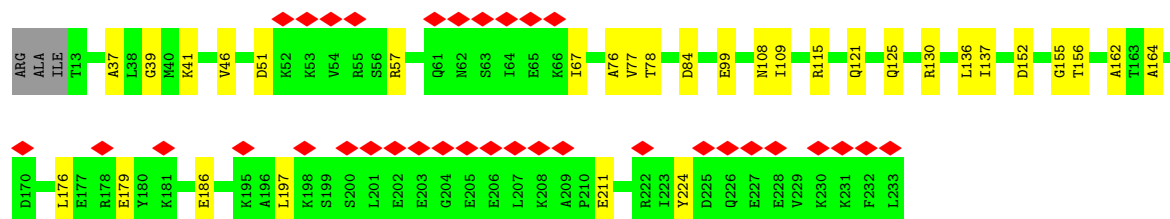
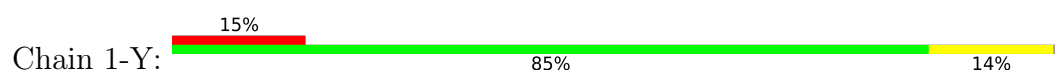
• Molecule 1: Proteasome subunit alpha



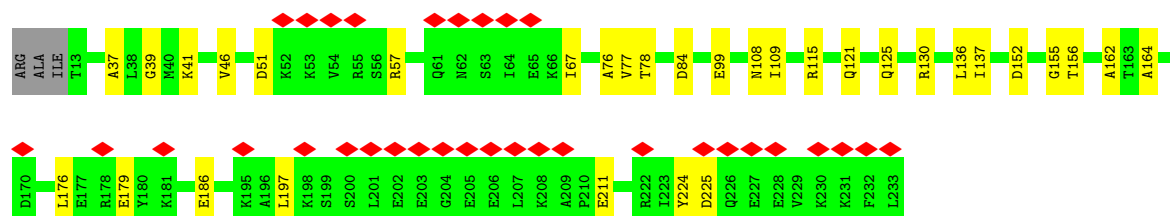
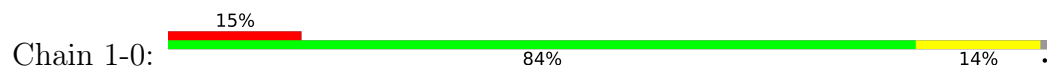
• Molecule 1: Proteasome subunit alpha



• Molecule 1: Proteasome subunit alpha



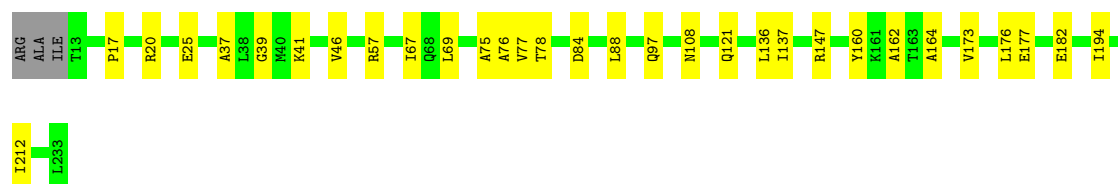
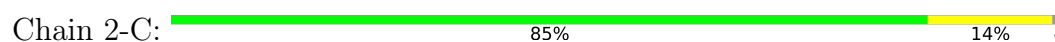
- Molecule 1: Proteasome subunit alpha



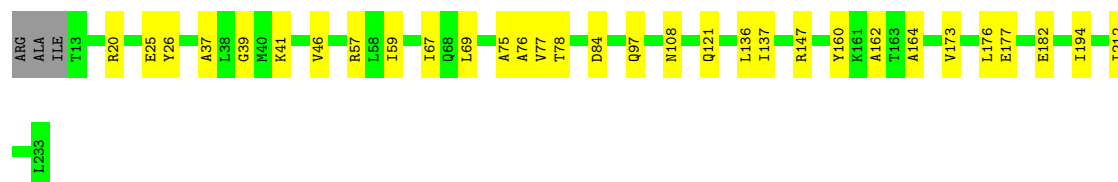
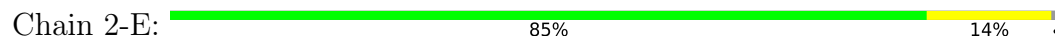
- Molecule 1: Proteasome subunit alpha



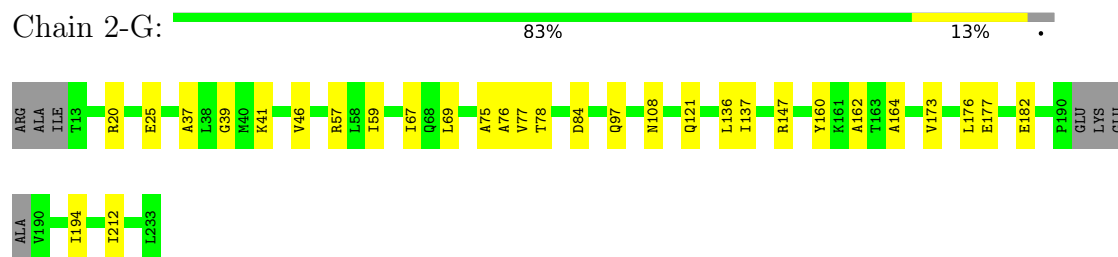
- Molecule 1: Proteasome subunit alpha



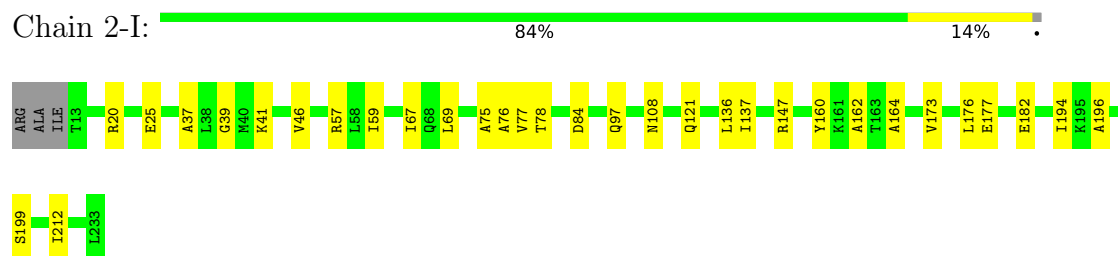
- Molecule 1: Proteasome subunit alpha



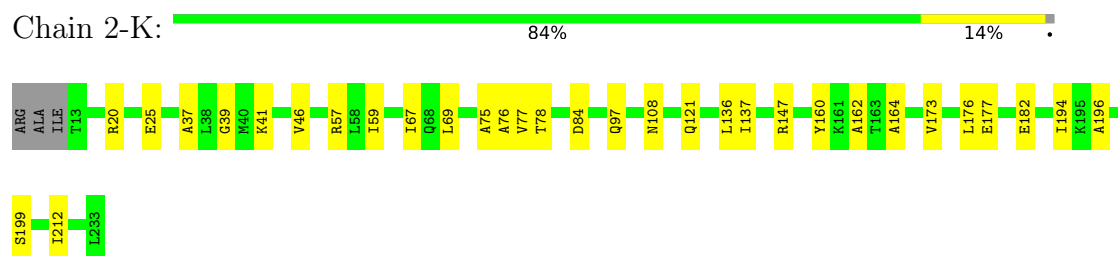
- Molecule 1: Proteasome subunit alpha



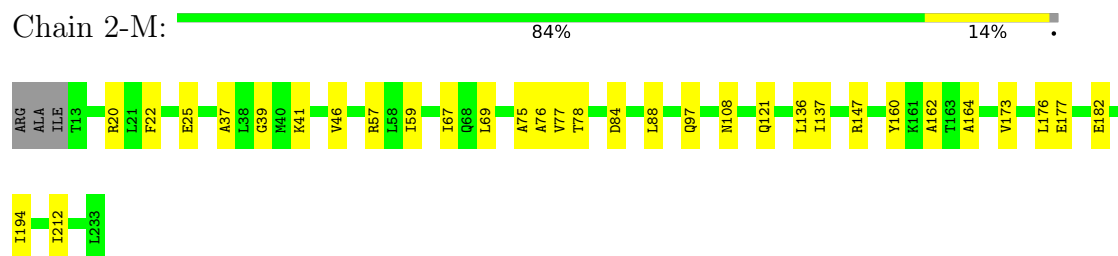
- Molecule 1: Proteasome subunit alpha



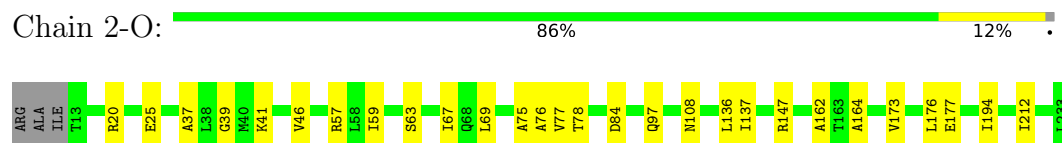
- Molecule 1: Proteasome subunit alpha



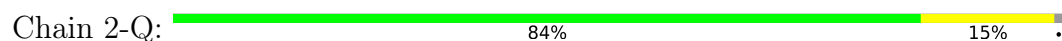
- Molecule 1: Proteasome subunit alpha

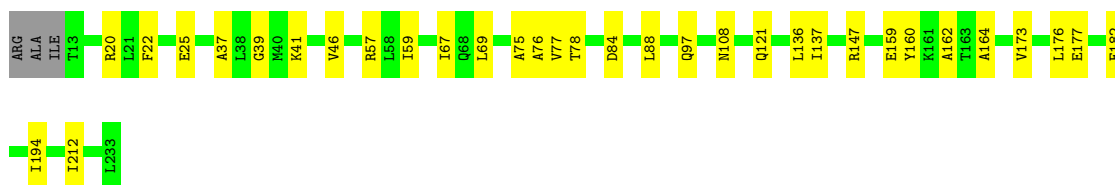


- Molecule 1: Proteasome subunit alpha



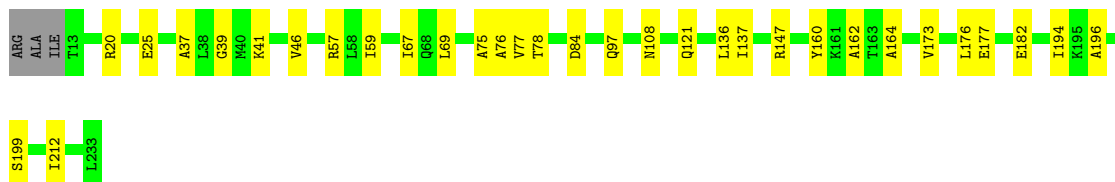
- Molecule 1: Proteasome subunit alpha





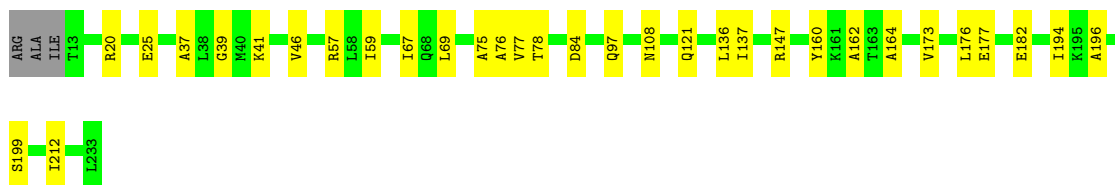
- Molecule 1: Proteasome subunit alpha

Chain 2-S: 84% 14%



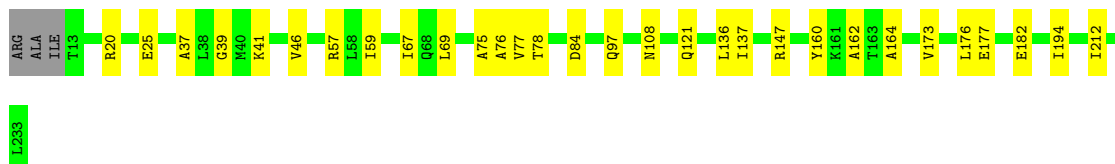
- Molecule 1: Proteasome subunit alpha

Chain 2-U: 84% 14%



- Molecule 1: Proteasome subunit alpha

Chain 2-W: 85% 13%



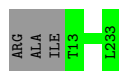
- Molecule 1: Proteasome subunit alpha

Chain 2-Y: 87% 12%



- Molecule 1: Proteasome subunit alpha

Chain 2-0: 99%



● Molecule 1: Proteasome subunit alpha

Chain 3-A:  86% 13%

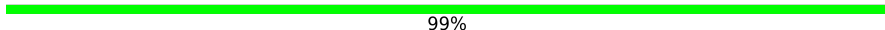
● Molecule 1: Proteasome subunit alpha

Chain 3-C:  84% 14%

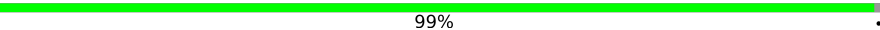
● Molecule 1: Proteasome subunit alpha

Chain 3-E:  86% 13%

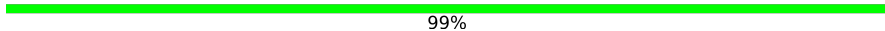
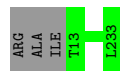
● Molecule 1: Proteasome subunit alpha

Chain 3-G:  99%

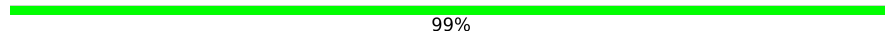
● Molecule 1: Proteasome subunit alpha

Chain 3-I:  99%

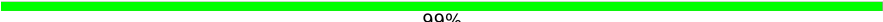
● Molecule 1: Proteasome subunit alpha

Chain 3-K:  99%

● Molecule 1: Proteasome subunit alpha

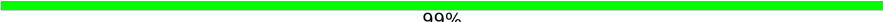
Chain 3-M:  99%

● Molecule 1: Proteasome subunit alpha

Chain 3-O:  99%

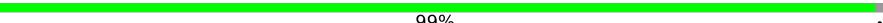


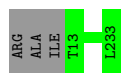
- Molecule 1: Proteasome subunit alpha

Chain 3-Q:  99%

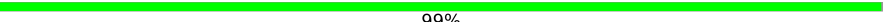


- Molecule 1: Proteasome subunit alpha

Chain 3-S:  99%



- Molecule 1: Proteasome subunit alpha

Chain 3-U:  99%

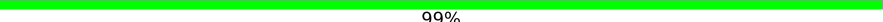


- Molecule 1: Proteasome subunit alpha

Chain 3-W:  99%

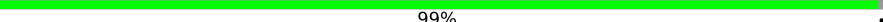


- Molecule 1: Proteasome subunit alpha

Chain 3-Y:  99%



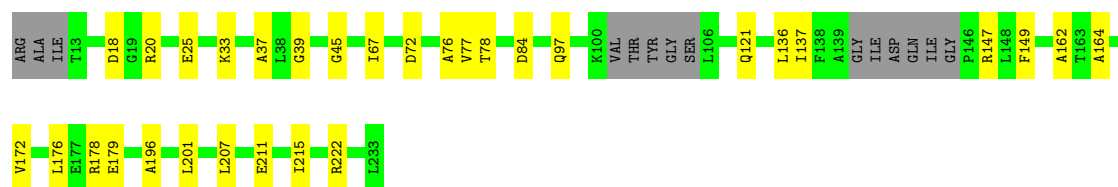
- Molecule 1: Proteasome subunit alpha

Chain 3-0:  99%



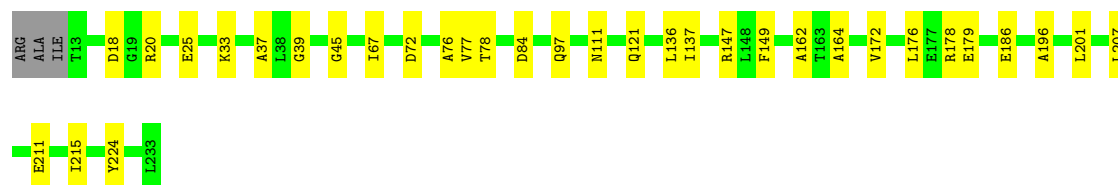
- Molecule 1: Proteasome subunit alpha

Chain 4-A:  80% 14% 6%



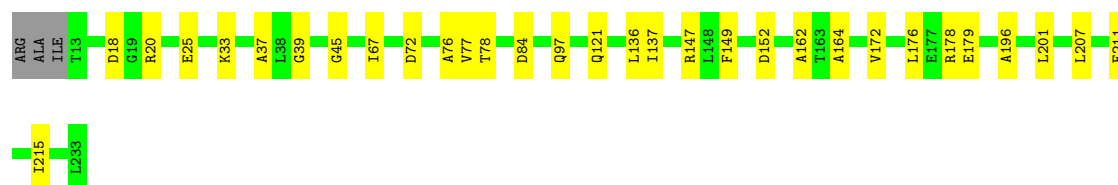
- Molecule 1: Proteasome subunit alpha

Chain 4-C:  84% 15% .



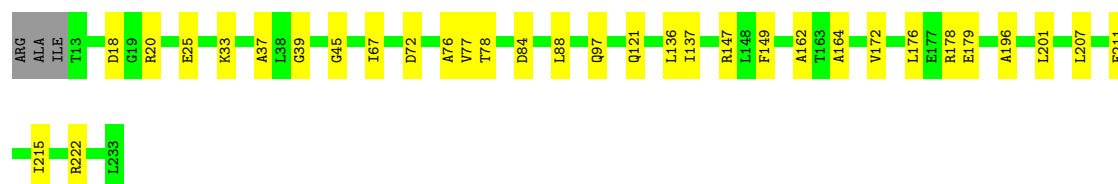
- Molecule 1: Proteasome subunit alpha

Chain 4-E:  85% 14% .



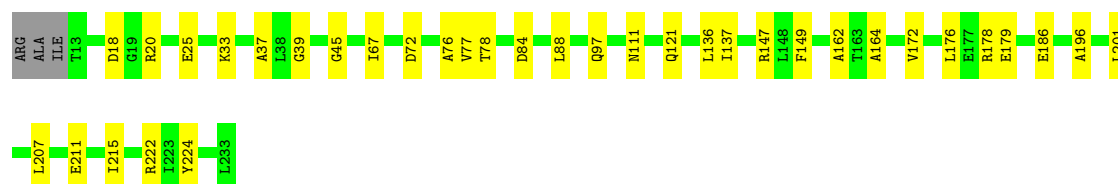
- Molecule 1: Proteasome subunit alpha

Chain 4-G:  84% 14% .

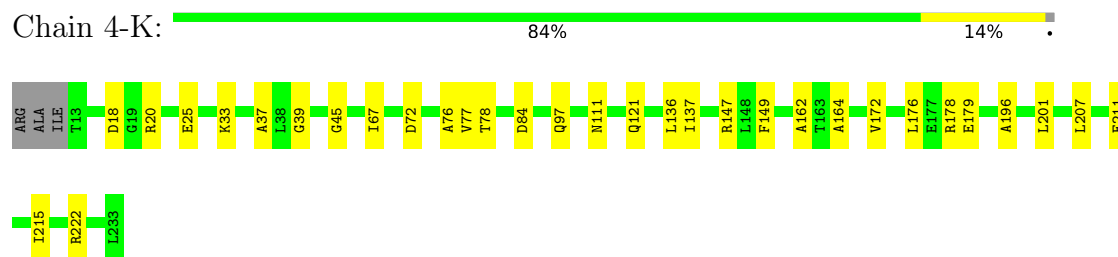


- Molecule 1: Proteasome subunit alpha

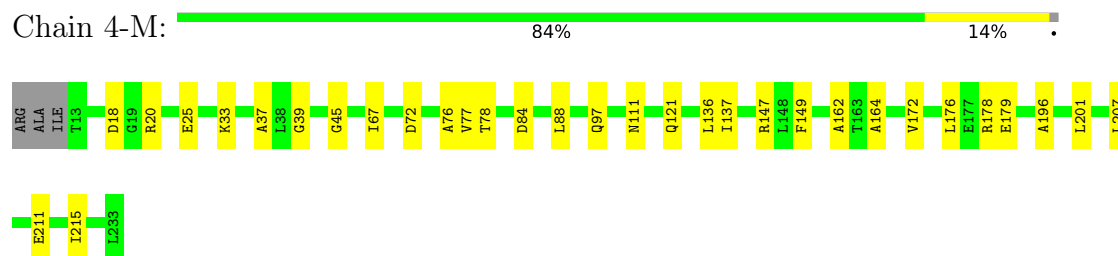
Chain 4-I:  83% 16% .



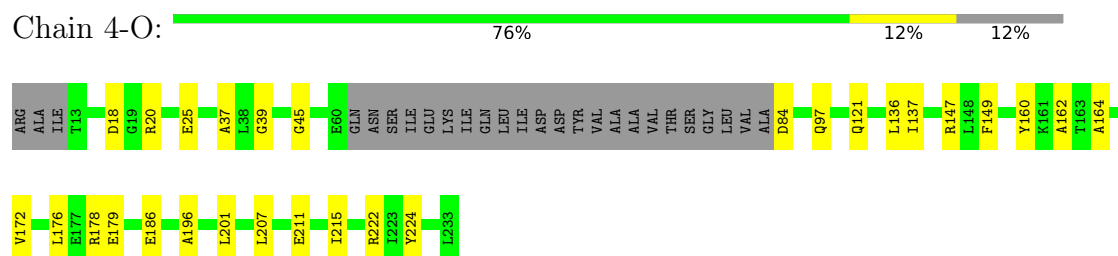
- Molecule 1: Proteasome subunit alpha



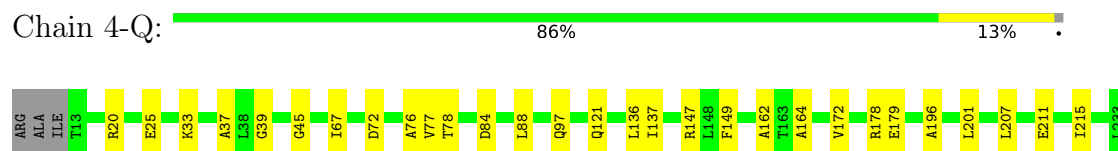
- Molecule 1: Proteasome subunit alpha



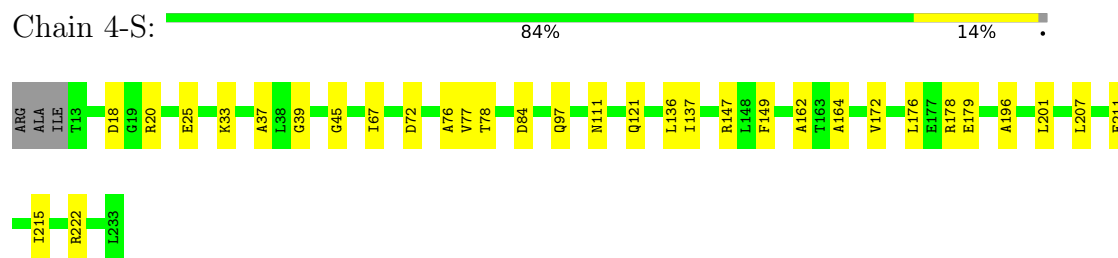
- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha

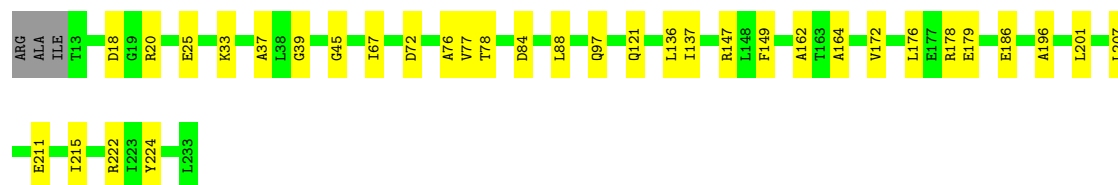


- Molecule 1: Proteasome subunit alpha



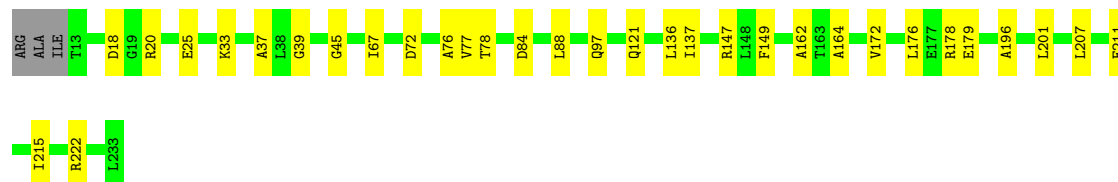
- Molecule 1: Proteasome subunit alpha





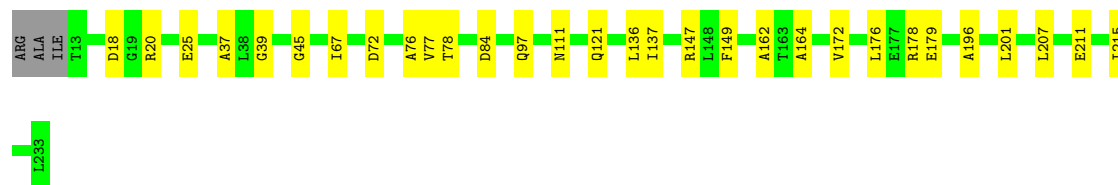
- Molecule 1: Proteasome subunit alpha

Chain 4-W: 84% 14%



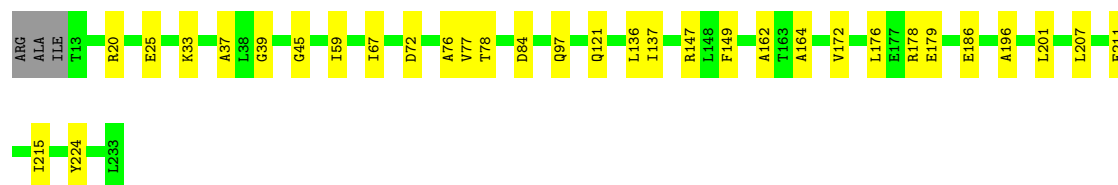
- Molecule 1: Proteasome subunit alpha

Chain 4-Y: 85% 13%



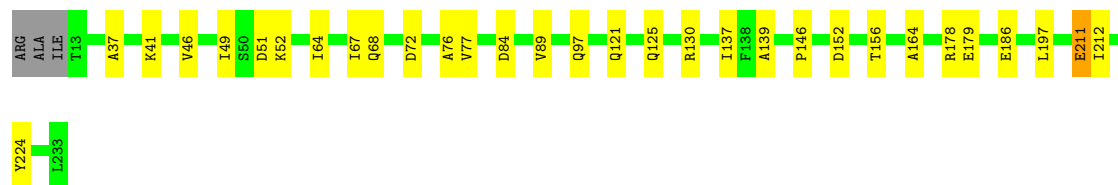
- Molecule 1: Proteasome subunit alpha

Chain 4-0: 84% 14%



- Molecule 1: Proteasome subunit alpha

Chain 5-A: 85% 13%



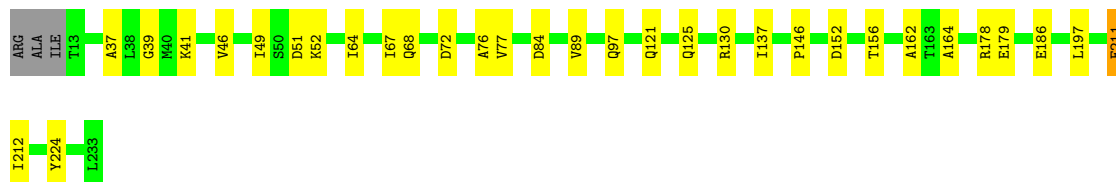
- Molecule 1: Proteasome subunit alpha

Chain 5-C: 84% 15%



- Molecule 1: Proteasome subunit alpha

Chain 5-E: 84% 14%



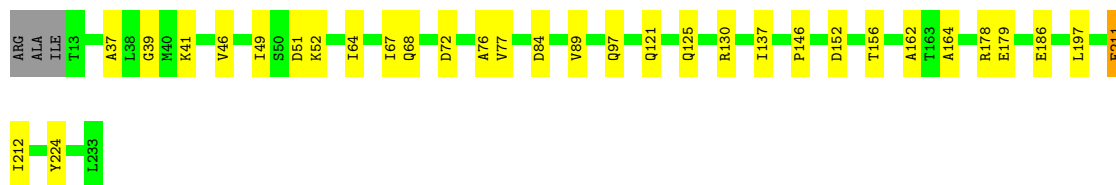
- Molecule 1: Proteasome subunit alpha

Chain 5-G: 85% 13%



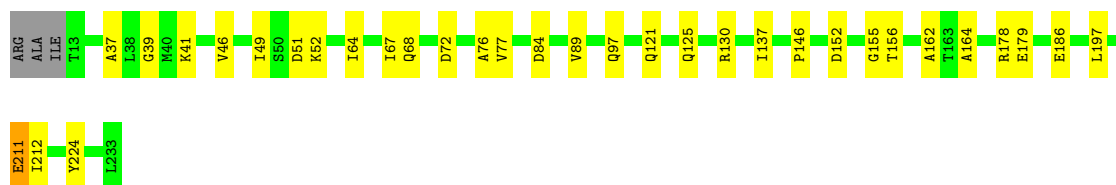
- Molecule 1: Proteasome subunit alpha

Chain 5-I: 84% 14%



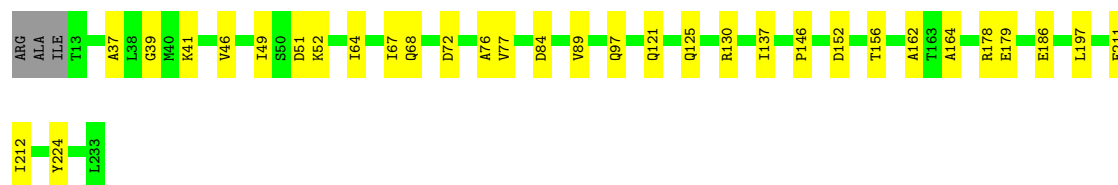
- Molecule 1: Proteasome subunit alpha

Chain 5-K: 84% 14%



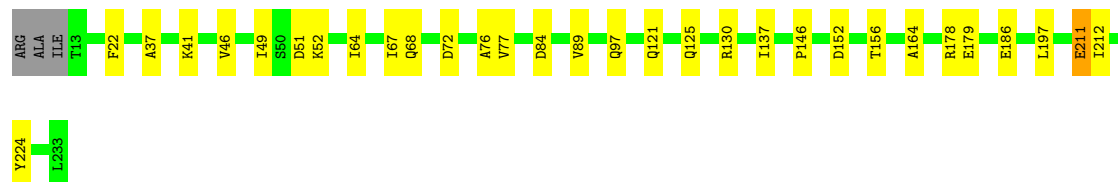
- Molecule 1: Proteasome subunit alpha

Chain 5-M: 84% 14%



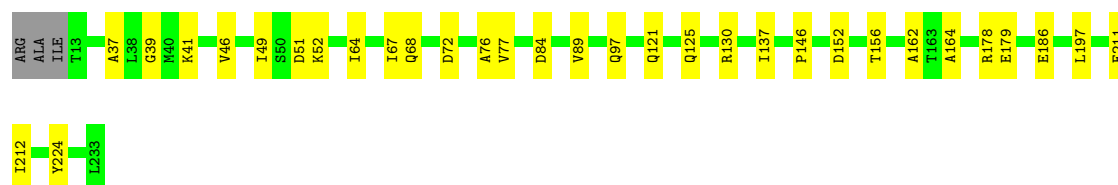
- Molecule 1: Proteasome subunit alpha

Chain 5-O: .



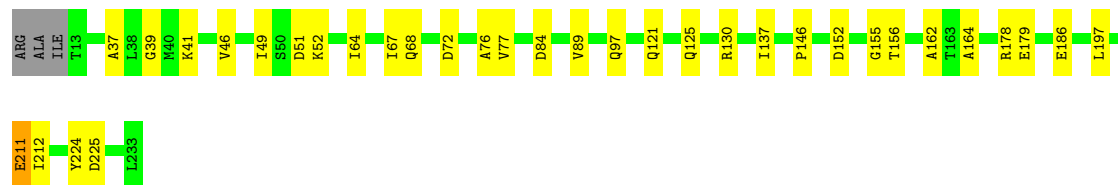
- Molecule 1: Proteasome subunit alpha

Chain 5-Q: .



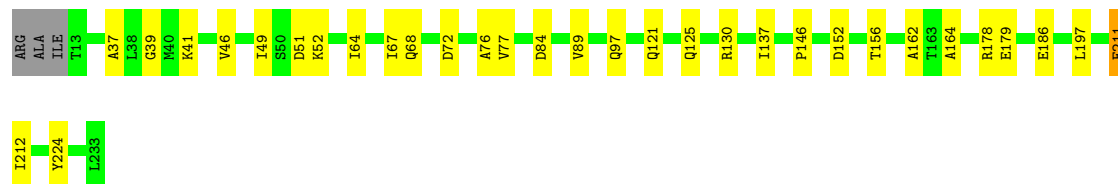
- Molecule 1: Proteasome subunit alpha

Chain 5-S: .



- Molecule 1: Proteasome subunit alpha

Chain 5-U: .



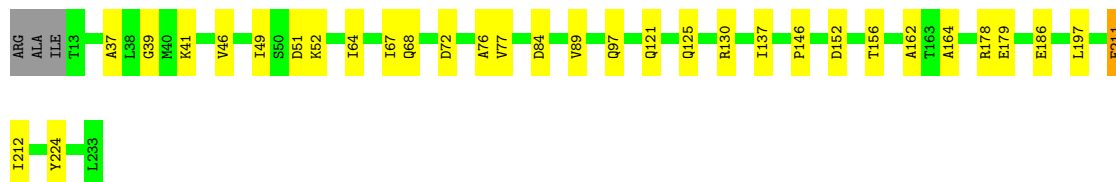
- Molecule 1: Proteasome subunit alpha

Chain 5-W: .



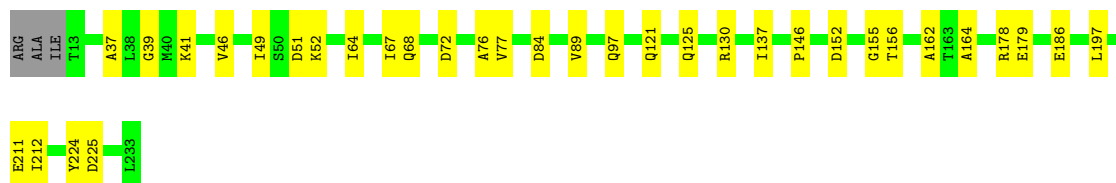
- Molecule 1: Proteasome subunit alpha

Chain 5-Y: 84% 14% .



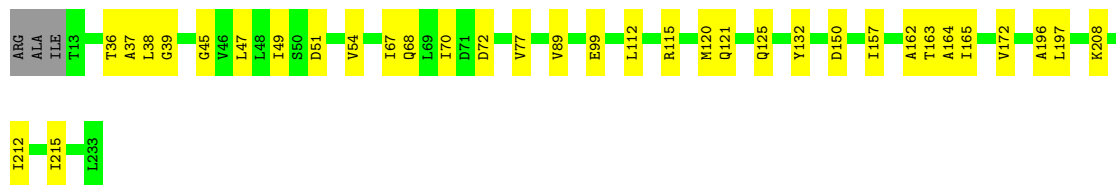
- Molecule 1: Proteasome subunit alpha

Chain 5-0: 83% 15% .



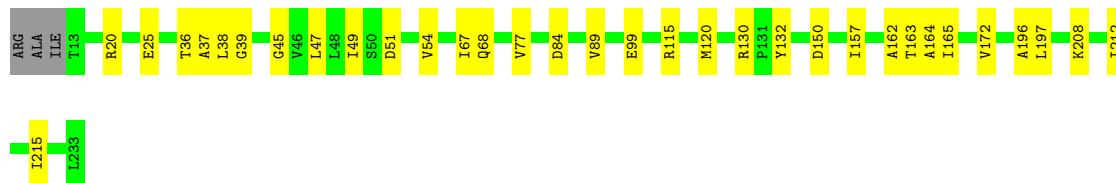
- Molecule 1: Proteasome subunit alpha

Chain 6-A: 83% 15% .



- Molecule 1: Proteasome subunit alpha

Chain 6-C: 84% 15% .

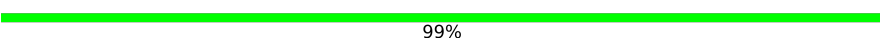


- Molecule 1: Proteasome subunit alpha

Chain 6-E: 99% .

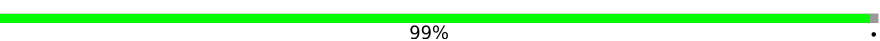


- Molecule 1: Proteasome subunit alpha

Chain 6-G:  99%

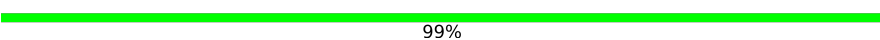


- Molecule 1: Proteasome subunit alpha

Chain 6-I:  99%

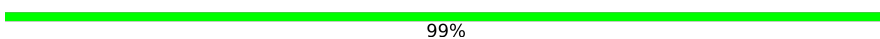


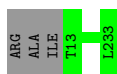
- Molecule 1: Proteasome subunit alpha

Chain 6-K:  99%

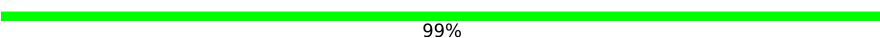


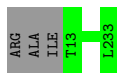
- Molecule 1: Proteasome subunit alpha

Chain 6-M:  99%

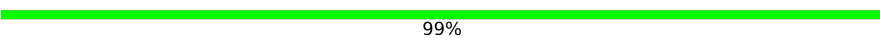


- Molecule 1: Proteasome subunit alpha

Chain 6-O:  99%

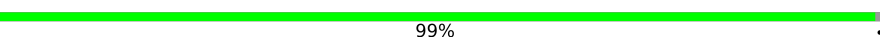


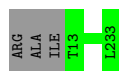
- Molecule 1: Proteasome subunit alpha

Chain 6-Q:  99%



- Molecule 1: Proteasome subunit alpha

Chain 6-S:  99%



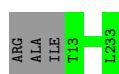
- Molecule 1: Proteasome subunit alpha

Chain 6-U: 99% .



- Molecule 1: Proteasome subunit alpha

Chain 6-W: 99% .



- Molecule 1: Proteasome subunit alpha

Chain 6-Y: 99% .



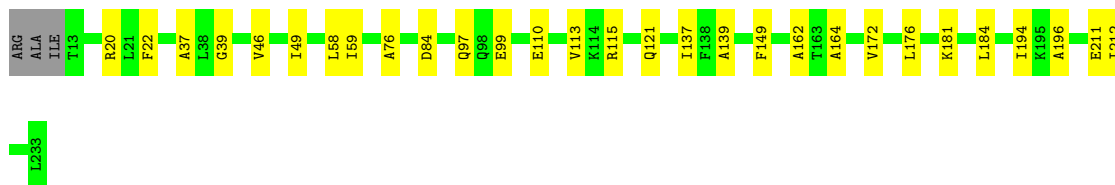
- Molecule 1: Proteasome subunit alpha

Chain 6-0: 99% .



- Molecule 1: Proteasome subunit alpha

Chain 7-A: 86% 13% .

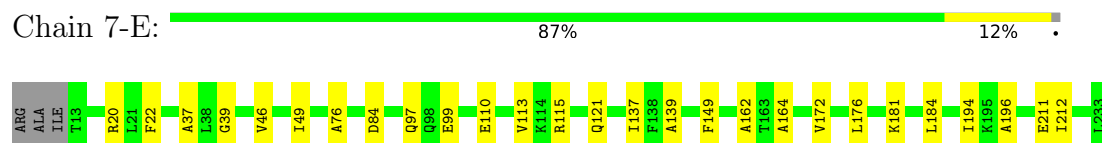


- Molecule 1: Proteasome subunit alpha

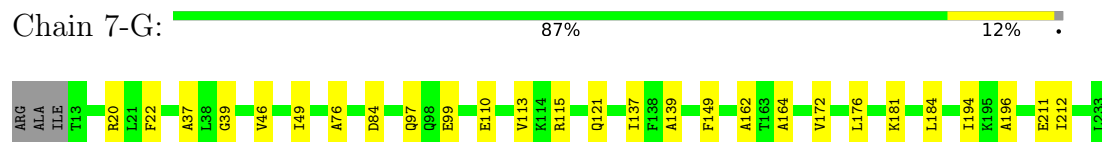
Chain 7-C: 87% 12% .



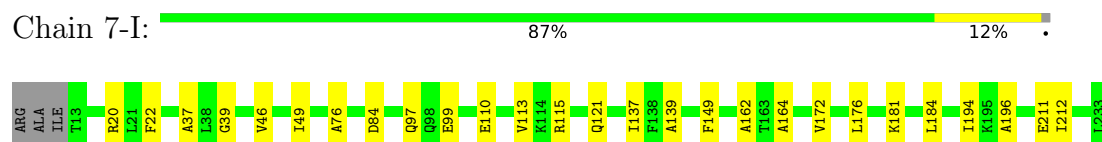
- Molecule 1: Proteasome subunit alpha



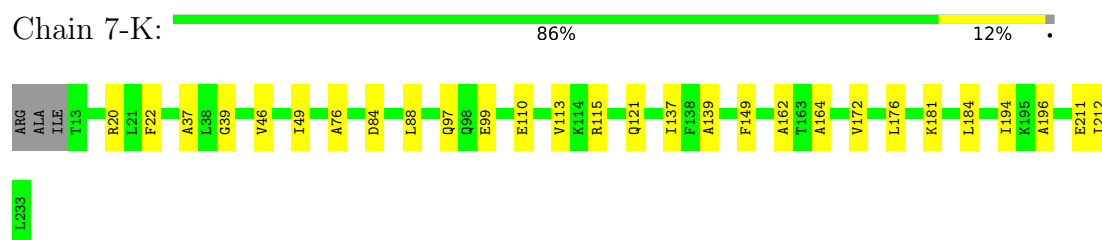
- Molecule 1: Proteasome subunit alpha



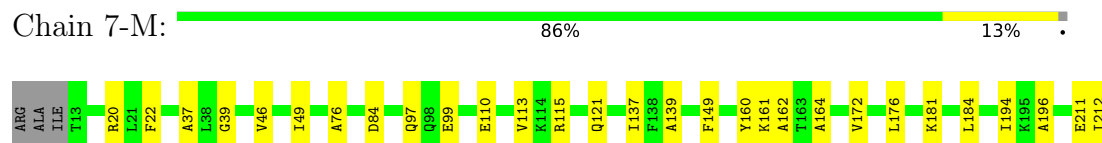
- Molecule 1: Proteasome subunit alpha



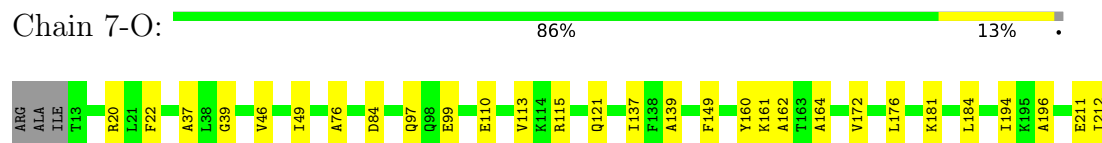
- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha

Chain 7-Q:  87% 12% .



- Molecule 1: Proteasome subunit alpha

Chain 7-S:  86% 12% .



- Molecule 1: Proteasome subunit alpha

Chain 7-U:  87% 12% .



- Molecule 1: Proteasome subunit alpha

Chain 7-W:  87% 12% .



- Molecule 1: Proteasome subunit alpha

Chain 7-Y:  87% 12% .



- Molecule 1: Proteasome subunit alpha

Chain 7-O:  86% 13% .



- Molecule 1: Proteasome subunit alpha

Chain 8-A:  87% 12% .



- Molecule 1: Proteasome subunit alpha

Chain 8-C: 87% 12%



- Molecule 1: Proteasome subunit alpha

Chain 8-E: 87% 12%



- Molecule 1: Proteasome subunit alpha

Chain 8-G: 86% 12%



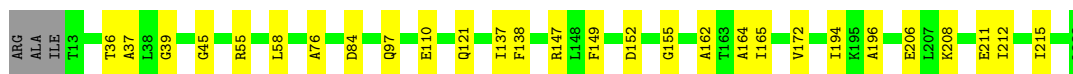
- Molecule 1: Proteasome subunit alpha

Chain 8-I: 85% 14%



- Molecule 1: Proteasome subunit alpha

Chain 8-K: 86% 12%



- Molecule 1: Proteasome subunit alpha

Chain 8-M: 88% 11%



- Molecule 1: Proteasome subunit alpha

Chain 8-O:  88% 11% .



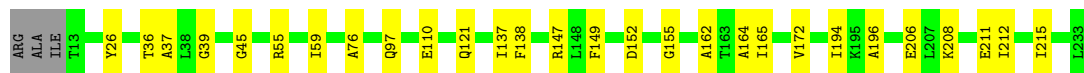
- Molecule 1: Proteasome subunit alpha

Chain 8-Q:  88% 11% .



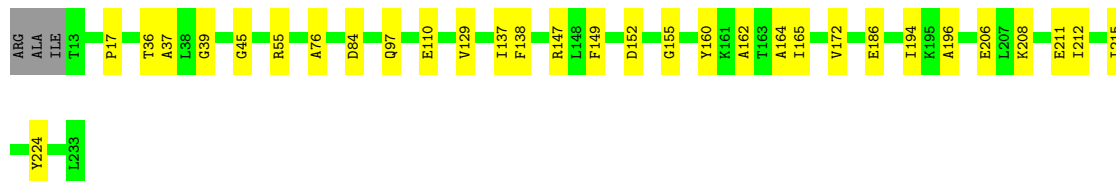
- Molecule 1: Proteasome subunit alpha

Chain 8-S:  86% 12% .



- Molecule 1: Proteasome subunit alpha

Chain 8-U:  85% 14% .



- Molecule 1: Proteasome subunit alpha

Chain 8-W:  86% 12% .



- Molecule 1: Proteasome subunit alpha

Chain 8-Y:  86% 13% .

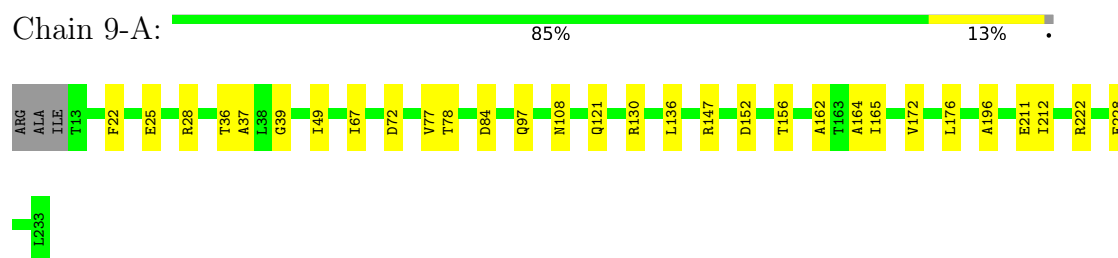


- Molecule 1: Proteasome subunit alpha

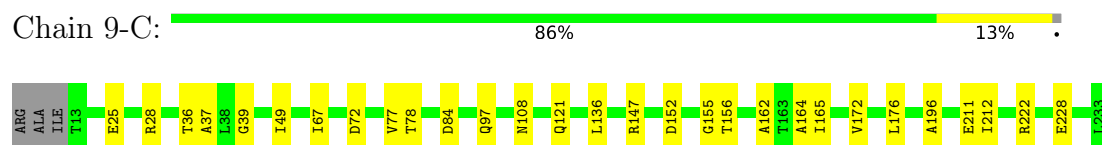
Chain 8-0:  88% 11% .



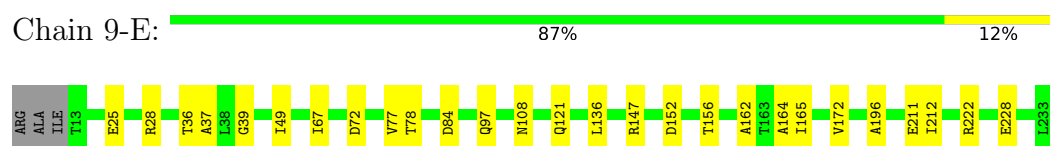
• Molecule 1: Proteasome subunit alpha



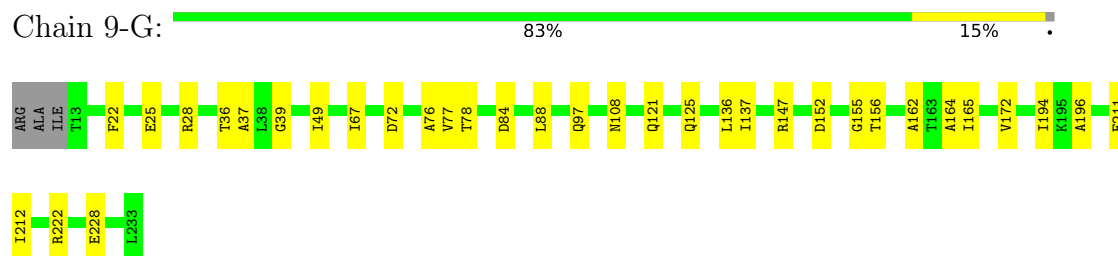
• Molecule 1: Proteasome subunit alpha



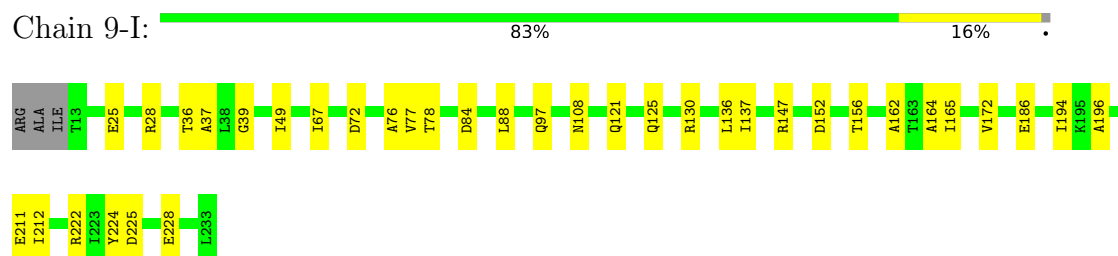
• Molecule 1: Proteasome subunit alpha



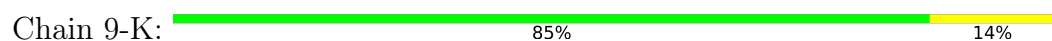
• Molecule 1: Proteasome subunit alpha

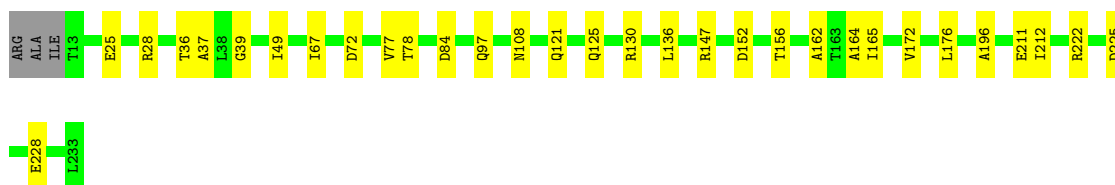


• Molecule 1: Proteasome subunit alpha



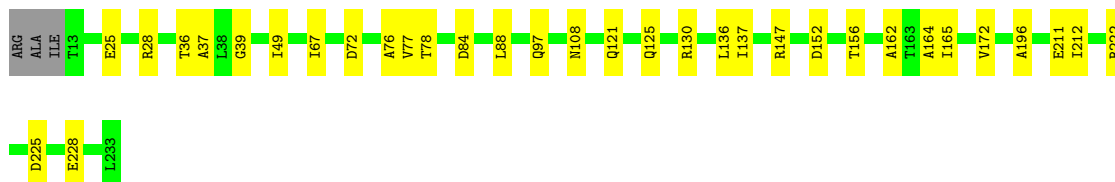
• Molecule 1: Proteasome subunit alpha





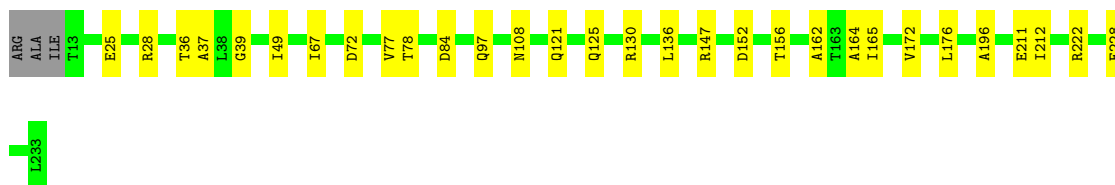
- Molecule 1: Proteasome subunit alpha

Chain 9-M: 84% 15%



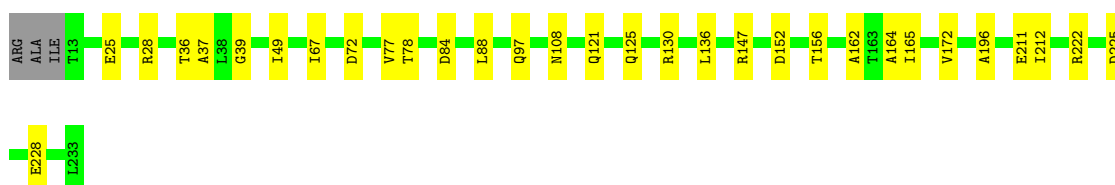
- Molecule 1: Proteasome subunit alpha

Chain 9-O: 85% 13%



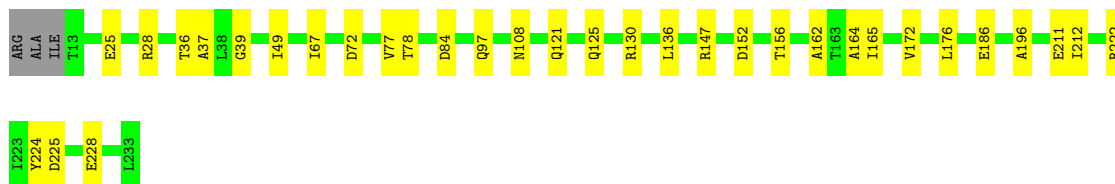
- Molecule 1: Proteasome subunit alpha

Chain 9-Q: 85% 14%



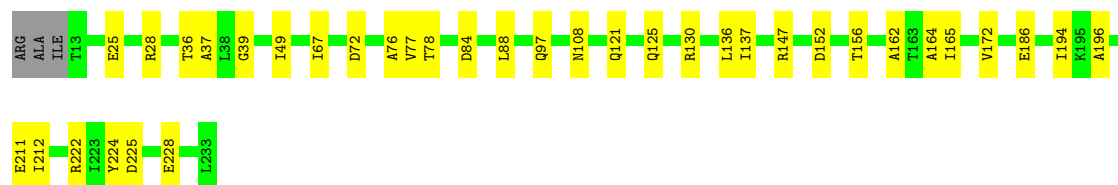
- Molecule 1: Proteasome subunit alpha

Chain 9-S: 84% 15%



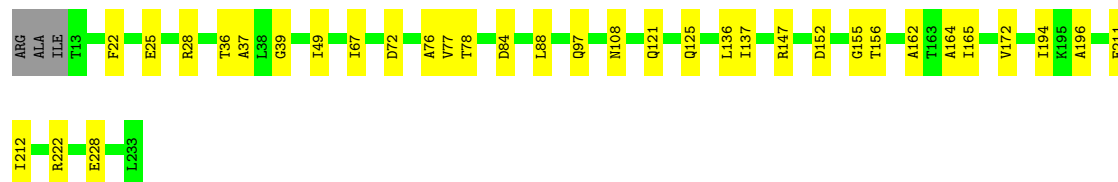
- Molecule 1: Proteasome subunit alpha

Chain 9-U: 83% 16%



- Molecule 1: Proteasome subunit alpha

Chain 9-W: 83% 15%



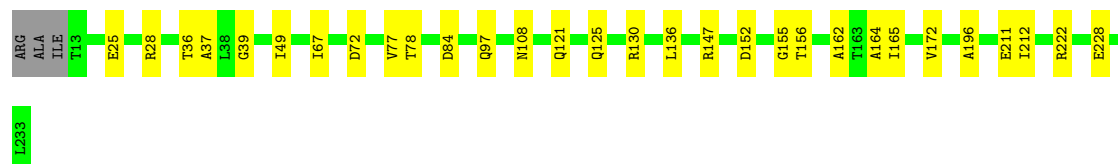
- Molecule 1: Proteasome subunit alpha

Chain 9-Y: 86% 12%



- Molecule 1: Proteasome subunit alpha

Chain 9-0: 85% 13%



- Molecule 1: Proteasome subunit alpha

Chain 10-A: 84% 14%



- Molecule 1: Proteasome subunit alpha

Chain 10-C: 85% 13%



L233

- Molecule 1: Proteasome subunit alpha

Chain 10-E:  84% 14%Y224
L233

- Molecule 1: Proteasome subunit alpha

Chain 10-G:  83% 15%E211
I212
Y224
L233

- Molecule 1: Proteasome subunit alpha

Chain 10-I:  83% 15%L197
E211
I212
Y224
L233

- Molecule 1: Proteasome subunit alpha

Chain 10-K:  83% 15%E211
I212
Y224
L233

- Molecule 1: Proteasome subunit alpha

Chain 10-M:  83% 15%



- Molecule 1: Proteasome subunit alpha

Chain 10-O:  85% 13%



- Molecule 1: Proteasome subunit alpha

Chain 10-Q:  84% 14%



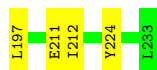
- Molecule 1: Proteasome subunit alpha

Chain 10-S:  83% 15%



- Molecule 1: Proteasome subunit alpha

Chain 10-U:  83% 15%



- Molecule 1: Proteasome subunit alpha

Chain 10-W:  84% 14%





- Molecule 1: Proteasome subunit alpha

Chain 10-Y: 84% 14%



- Molecule 1: Proteasome subunit alpha

Chain 10-0: 86% 12%



- Molecule 2: Proteasome subunit beta

Chain 1-B: 86% 13%



- Molecule 2: Proteasome subunit beta

Chain 1-D: 87% 13%



- Molecule 2: Proteasome subunit beta

Chain 1-F: 87% 13%

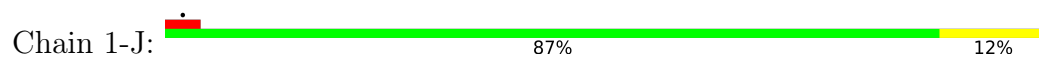


- Molecule 2: Proteasome subunit beta

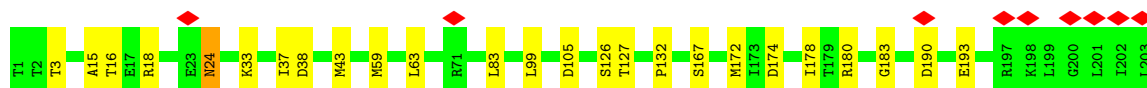
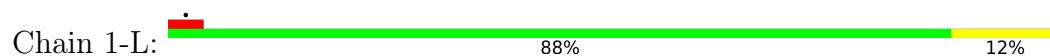
Chain 1-H: 5% 88% 12%



- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta

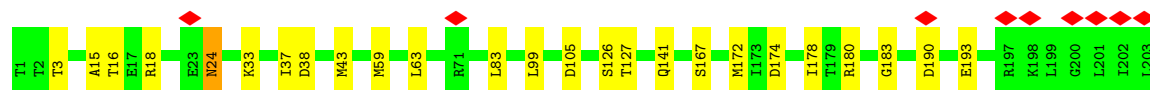


- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta

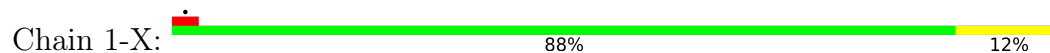




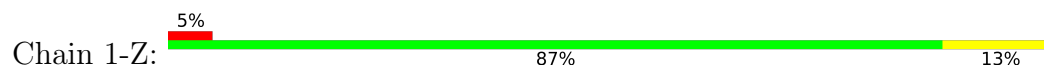
- Molecule 2: Proteasome subunit beta



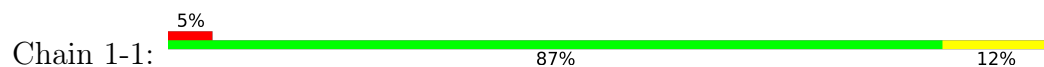
- Molecule 2: Proteasome subunit beta



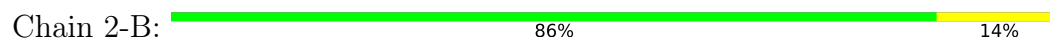
- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta





- Molecule 2: Proteasome subunit beta

Chain 2-F: 85% 15%



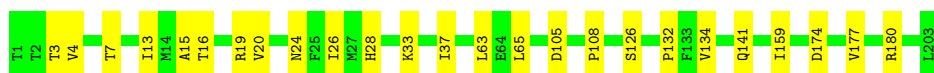
- Molecule 2: Proteasome subunit beta

Chain 2-H: 84% 16%



- Molecule 2: Proteasome subunit beta

Chain 2-J: 88% 12%



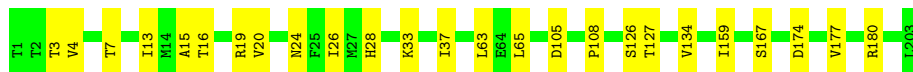
- Molecule 2: Proteasome subunit beta

Chain 2-L: 87% 13%



- Molecule 2: Proteasome subunit beta

Chain 2-N: 88% 12%



- Molecule 2: Proteasome subunit beta

Chain 2-P: 86% 14%



- Molecule 2: Proteasome subunit beta

Chain 2-R:  87% 13%



- Molecule 2: Proteasome subunit beta

Chain 2-T:  87% 13%



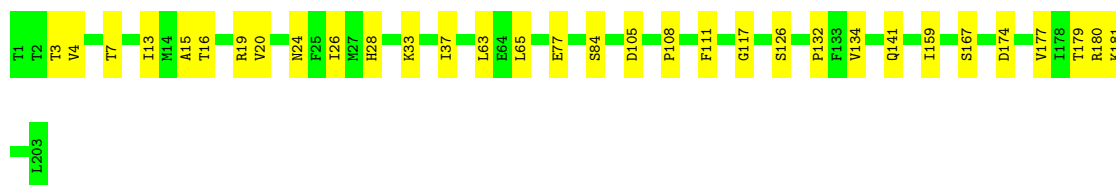
- Molecule 2: Proteasome subunit beta

Chain 2-V:  87% 13%



- Molecule 2: Proteasome subunit beta

Chain 2-X:  84% 16%



- Molecule 2: Proteasome subunit beta

Chain 2-Z:  90% 10%



- Molecule 2: Proteasome subunit beta

Chain 2-1:  99% 1%



- Molecule 2: Proteasome subunit beta

Chain 3-B:  86% 11% 3%

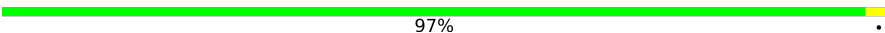


- Molecule 2: Proteasome subunit beta

Chain 3-D:  89% 11%



- Molecule 2: Proteasome subunit beta

Chain 3-F:  97% .

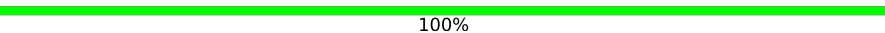


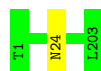
- Molecule 2: Proteasome subunit beta

Chain 3-H:  100%

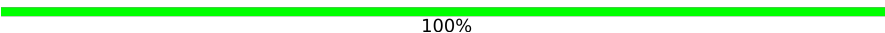


- Molecule 2: Proteasome subunit beta

Chain 3-J:  100%

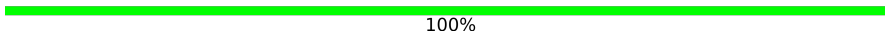


- Molecule 2: Proteasome subunit beta

Chain 3-L:  100%

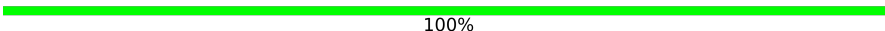


- Molecule 2: Proteasome subunit beta

Chain 3-N:  100%



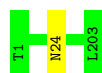
- Molecule 2: Proteasome subunit beta

Chain 3-P:  100%



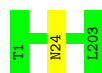
- Molecule 2: Proteasome subunit beta

Chain 3-R:  100%



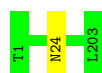
- Molecule 2: Proteasome subunit beta

Chain 3-T:  100%



- Molecule 2: Proteasome subunit beta

Chain 3-V:  100%



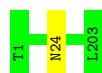
- Molecule 2: Proteasome subunit beta

Chain 3-X:  100%



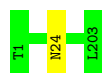
- Molecule 2: Proteasome subunit beta

Chain 3-Z:  100%



- Molecule 2: Proteasome subunit beta

Chain 3-1:  100%



- Molecule 2: Proteasome subunit beta

Chain 4-B:  90% 10%



- Molecule 2: Proteasome subunit beta

Chain 4-D:  90% 10%



- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta





- Molecule 2: Proteasome subunit beta



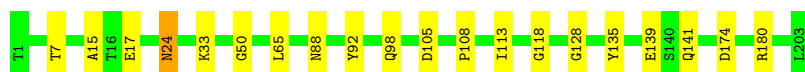
- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta



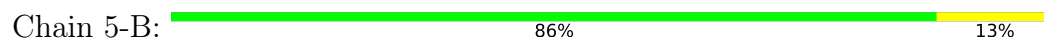
- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta

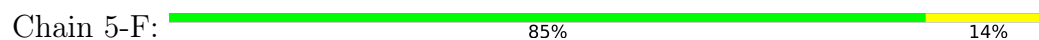


- Molecule 2: Proteasome subunit beta

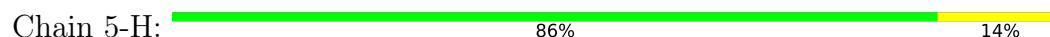




- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta



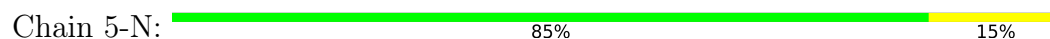
- Molecule 2: Proteasome subunit beta



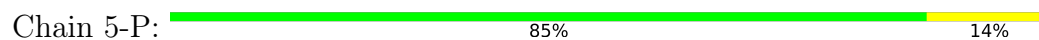
- Molecule 2: Proteasome subunit beta



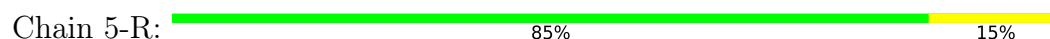
- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta

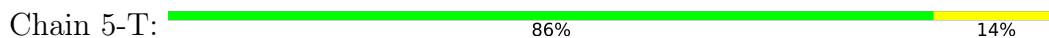


- Molecule 2: Proteasome subunit beta

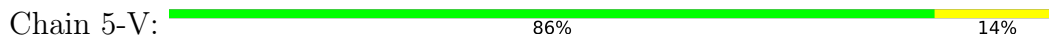




- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta



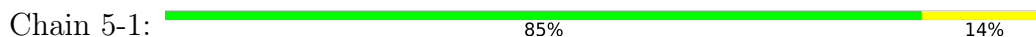
- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta



There are no outlier residues recorded for this chain.

- Molecule 2: Proteasome subunit beta

Chain 6-F:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: Proteasome subunit beta

Chain 6-H:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: Proteasome subunit beta

Chain 6-J:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: Proteasome subunit beta

Chain 6-L:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: Proteasome subunit beta

Chain 6-N:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: Proteasome subunit beta

Chain 6-P:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: Proteasome subunit beta

Chain 6-R:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: Proteasome subunit beta

Chain 6-T:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: Proteasome subunit beta

Chain 6-V:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: Proteasome subunit beta

Chain 6-X:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: Proteasome subunit beta

Chain 6-Z:  100%

There are no outlier residues recorded for this chain.

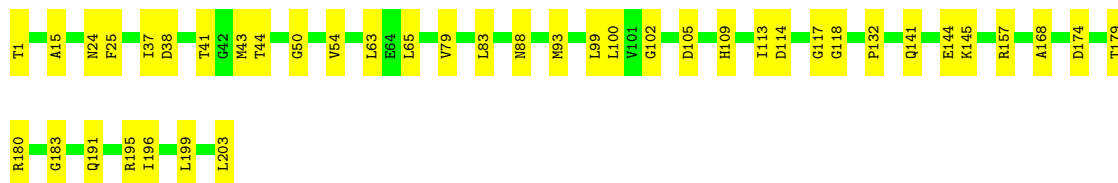
- Molecule 2: Proteasome subunit beta

Chain 6-1:  100%

There are no outlier residues recorded for this chain.

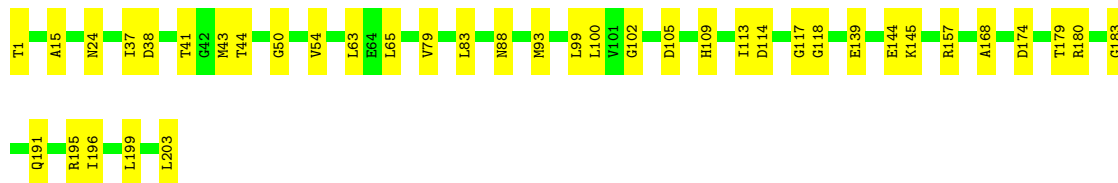
- Molecule 2: Proteasome subunit beta

Chain 7-B:  80% 20%



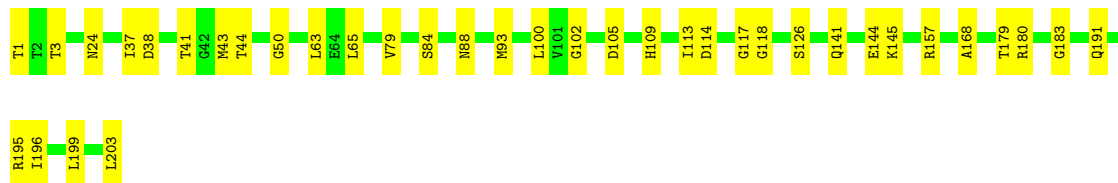
- Molecule 2: Proteasome subunit beta

Chain 7-D:  81% 19%



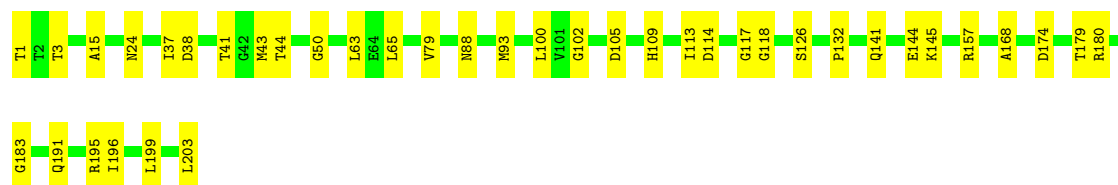
- Molecule 2: Proteasome subunit beta

Chain 7-F:  82% 18%



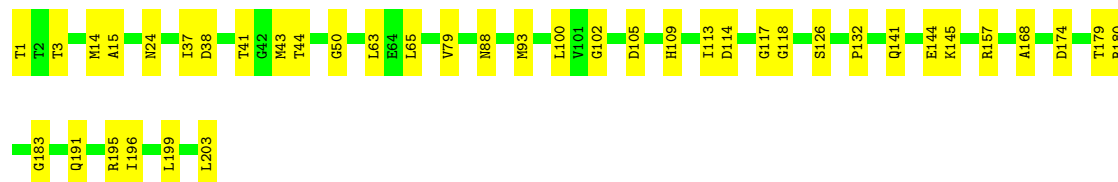
- Molecule 2: Proteasome subunit beta

Chain 7-H:  81% 19%



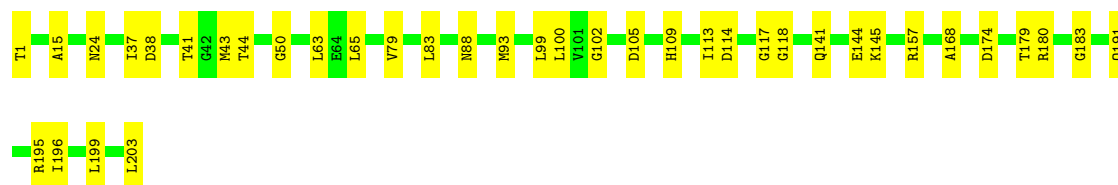
- Molecule 2: Proteasome subunit beta

Chain 7-J: 80% 20%



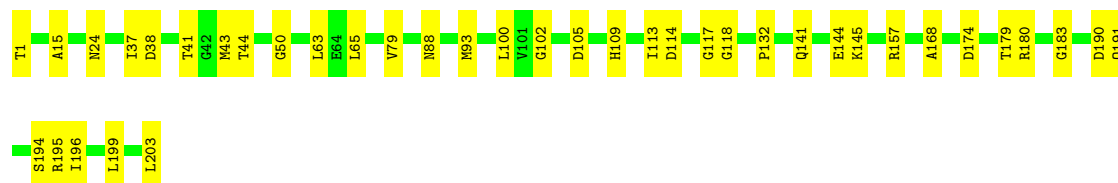
- Molecule 2: Proteasome subunit beta

Chain 7-L: 81% 19%



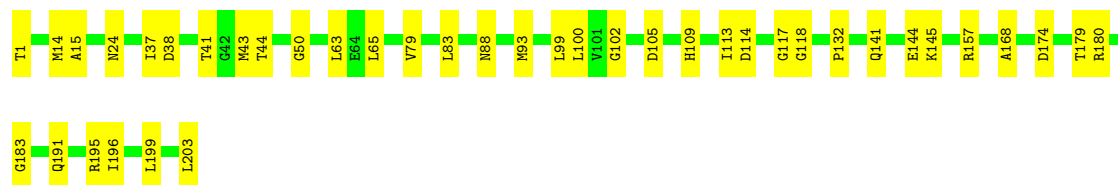
- Molecule 2: Proteasome subunit beta

Chain 7-N: 81% 19%



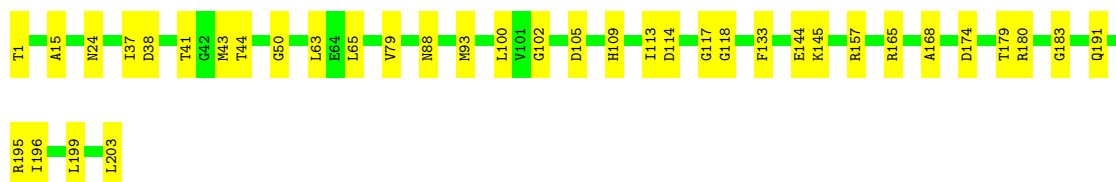
- Molecule 2: Proteasome subunit beta

Chain 7-P: 80% 20%

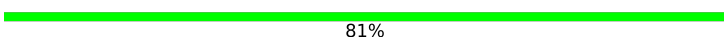
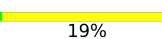


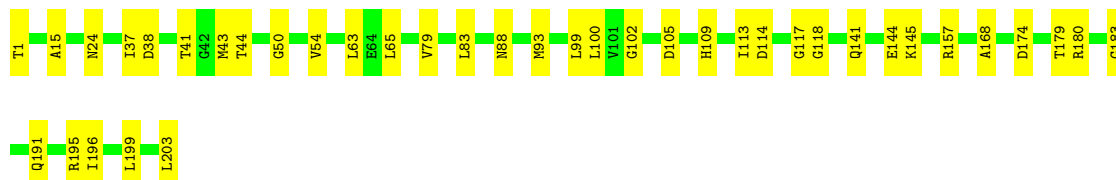
- Molecule 2: Proteasome subunit beta

Chain 7-R: 82% 18%

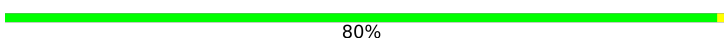
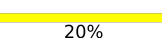


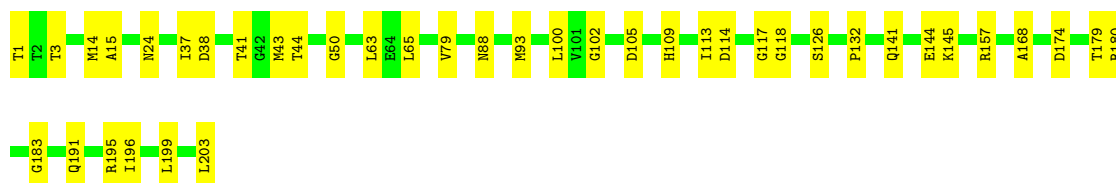
- Molecule 2: Proteasome subunit beta

Chain 7-T:  81%  19%

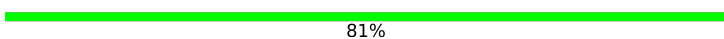
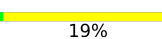


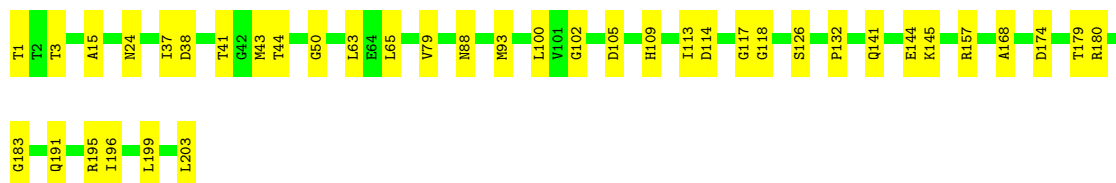
- Molecule 2: Proteasome subunit beta

Chain 7-V:  80%  20%

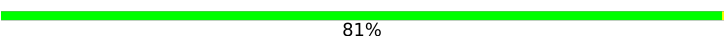
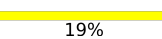


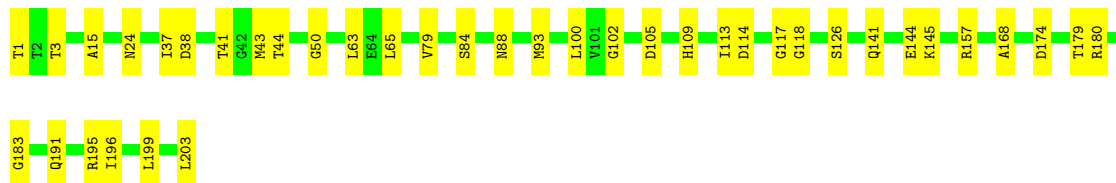
- Molecule 2: Proteasome subunit beta

Chain 7-X:  81%  19%

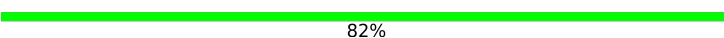
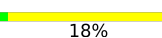


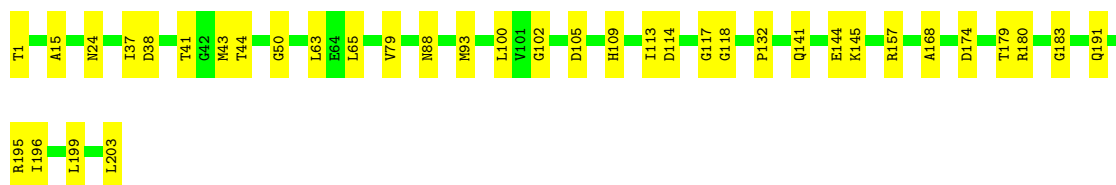
- Molecule 2: Proteasome subunit beta

Chain 7-Z:  81%  19%



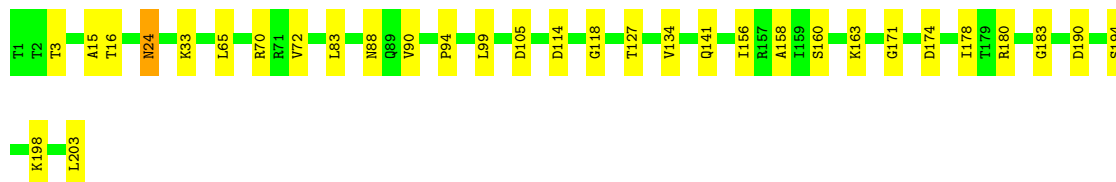
- Molecule 2: Proteasome subunit beta

Chain 7-1:  82%  18%



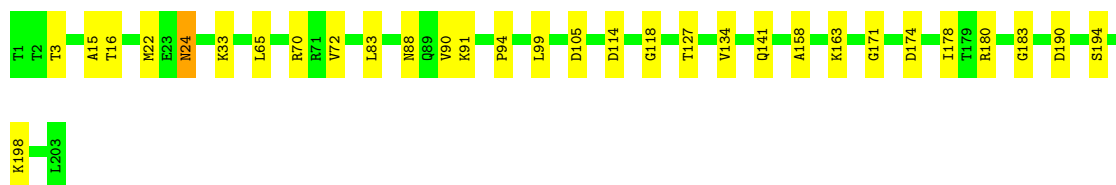
- Molecule 2: Proteasome subunit beta

Chain 8-B: 84% 15%



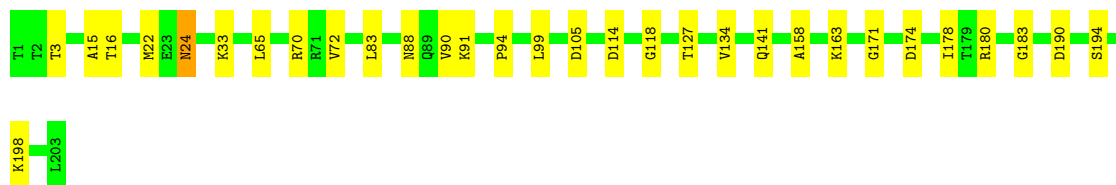
- Molecule 2: Proteasome subunit beta

Chain 8-D: 85% 15%



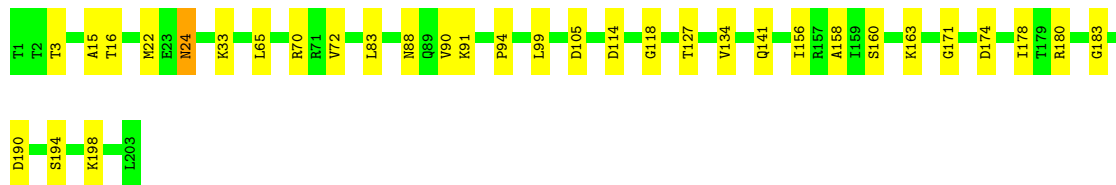
- Molecule 2: Proteasome subunit beta

Chain 8-F: 85% 15%



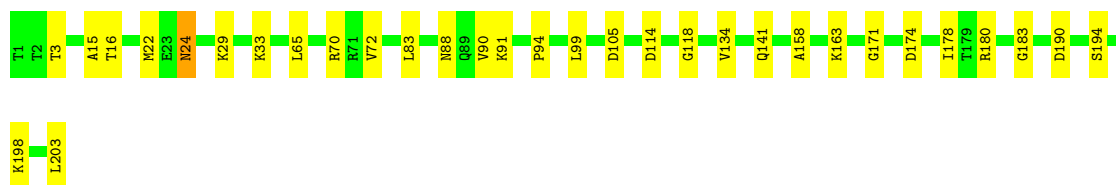
- Molecule 2: Proteasome subunit beta

Chain 8-H: 84% 16%



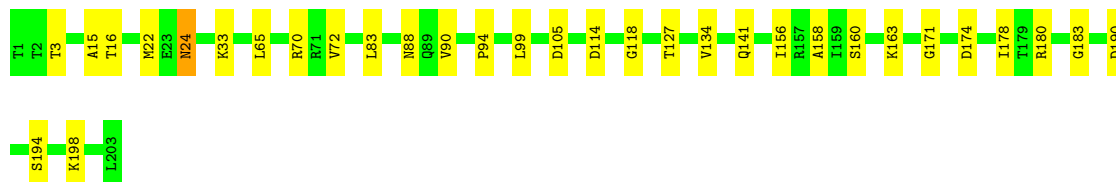
- Molecule 2: Proteasome subunit beta

Chain 8-J: 84% 15%



- Molecule 2: Proteasome subunit beta

Chain 8-L: 84% 15%



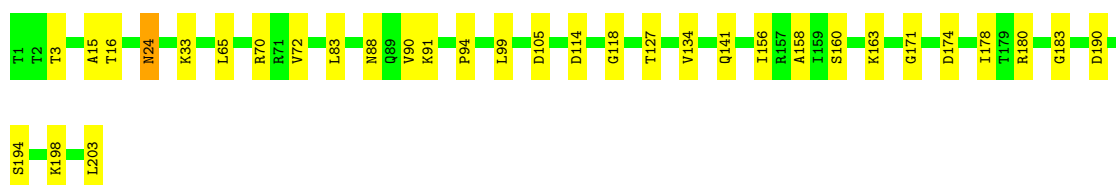
- Molecule 2: Proteasome subunit beta

Chain 8-N: 85% 15%



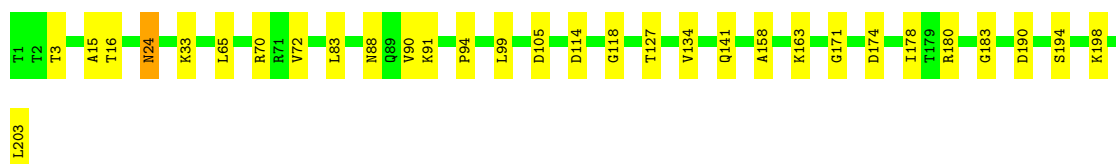
- Molecule 2: Proteasome subunit beta

Chain 8-P: 84% 16%



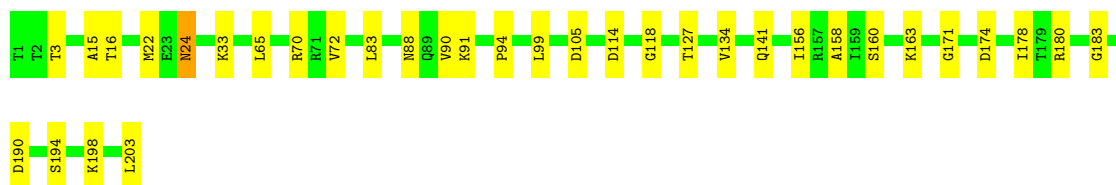
- Molecule 2: Proteasome subunit beta

Chain 8-R: 85% 15%



- Molecule 2: Proteasome subunit beta

Chain 8-T: 83% 16%



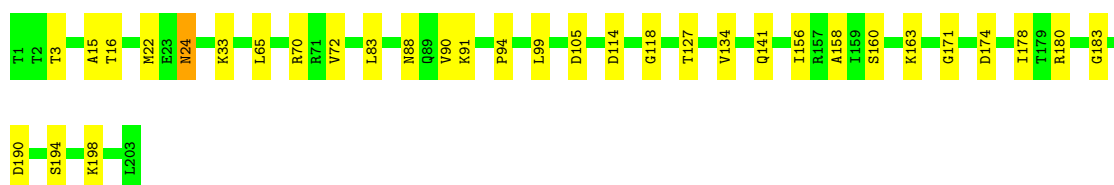
- Molecule 2: Proteasome subunit beta

Chain 8-V: 85% 14%



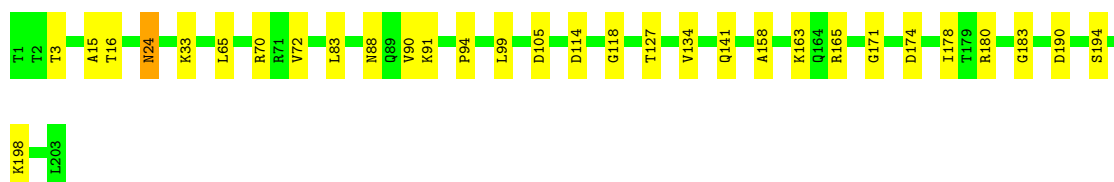
- Molecule 2: Proteasome subunit beta

Chain 8-X: 84% 16%



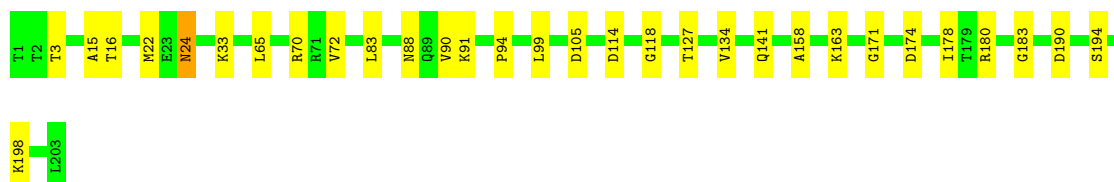
- Molecule 2: Proteasome subunit beta

Chain 8-Z: 85% 15%



- Molecule 2: Proteasome subunit beta

Chain 8-1: 85% 15%



- Molecule 2: Proteasome subunit beta

Chain 9-B: 85% 14%



● Molecule 2: Proteasome subunit beta

Chain 9-D:  85% 14%

● Molecule 2: Proteasome subunit beta

Chain 9-F:  85% 14%

● Molecule 2: Proteasome subunit beta

Chain 9-H:  85% 14%

● Molecule 2: Proteasome subunit beta

Chain 9-J:  85% 14%

● Molecule 2: Proteasome subunit beta

Chain 9-L:  85% 14%

● Molecule 2: Proteasome subunit beta

Chain 9-N:  85% 14%

● Molecule 2: Proteasome subunit beta

Chain 9-P:  85% 14%

● Molecule 2: Proteasome subunit beta

Chain 9-R:  85% 14% .



- Molecule 2: Proteasome subunit beta

Chain 9-T:  85% 14% .



- Molecule 2: Proteasome subunit beta

Chain 9-V:  85% 14% .



- Molecule 2: Proteasome subunit beta

Chain 9-X:  85% 14% .



- Molecule 2: Proteasome subunit beta

Chain 9-Z:  85% 14% .



- Molecule 2: Proteasome subunit beta

Chain 9-1:  85% 14% .



- Molecule 2: Proteasome subunit beta

Chain 10-B:  86% 14%



- Molecule 2: Proteasome subunit beta

Chain 10-D:  86% 13%



- Molecule 2: Proteasome subunit beta

Chain 10-F: 86% 14%



- Molecule 2: Proteasome subunit beta

Chain 10-H: 86% 14%



- Molecule 2: Proteasome subunit beta

Chain 10-J: 88% 12%



- Molecule 2: Proteasome subunit beta

Chain 10-L: 87% 13%



- Molecule 2: Proteasome subunit beta

Chain 10-N: 87% 13%



- Molecule 2: Proteasome subunit beta

Chain 10-P: 85% 14%



- Molecule 2: Proteasome subunit beta

Chain 10-R: 87% 13%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D7	Depositor
Number of particles used	96254	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	65	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	45000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.315	Depositor
Minimum map value	-0.194	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	232.96, 232.96, 232.96	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.91, 0.91, 0.91	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1-0	0.18	0/1743	0.23	0/2348
1	1-A	0.18	0/1743	0.23	0/2348
1	1-C	0.18	0/1743	0.23	0/2348
1	1-E	0.18	0/1743	0.23	0/2348
1	1-G	0.18	0/1743	0.23	0/2348
1	1-I	0.18	0/1743	0.23	0/2348
1	1-K	0.18	0/1743	0.24	0/2348
1	1-M	0.18	0/1743	0.23	0/2348
1	1-O	0.18	0/1743	0.23	0/2348
1	1-Q	0.18	0/1743	0.24	0/2348
1	1-S	0.18	0/1743	0.23	0/2348
1	1-U	0.18	0/1743	0.24	0/2348
1	1-W	0.18	0/1743	0.23	0/2348
1	1-Y	0.18	0/1743	0.23	0/2348
1	2-0	0.18	0/1743	0.23	0/2348
1	2-A	0.18	0/1743	0.23	0/2348
1	2-C	0.18	0/1743	0.23	0/2348
1	2-E	0.18	0/1743	0.23	0/2348
1	2-G	0.18	0/1696	0.24	0/2285
1	2-I	0.18	0/1743	0.23	0/2348
1	2-K	0.18	0/1743	0.24	0/2348
1	2-M	0.18	0/1743	0.23	0/2348
1	2-O	0.18	0/1743	0.23	0/2348
1	2-Q	0.18	0/1743	0.24	0/2348
1	2-S	0.18	0/1743	0.23	0/2348
1	2-U	0.18	0/1743	0.24	0/2348
1	2-W	0.18	0/1743	0.23	0/2348
1	2-Y	0.18	0/1743	0.23	0/2348
1	3-0	0.18	0/1743	0.23	0/2348
1	3-A	0.18	0/1743	0.23	0/2348
1	3-C	0.18	0/1743	0.23	0/2348
1	3-E	0.18	0/1743	0.23	0/2348
1	3-G	0.18	0/1639	0.23	0/2209
1	3-I	0.18	0/1729	0.23	0/2330

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	3-K	0.18	0/1743	0.24	0/2348
1	3-M	0.18	0/1743	0.23	0/2348
1	3-O	0.18	0/1743	0.23	0/2348
1	3-Q	0.18	0/1743	0.24	0/2348
1	3-S	0.18	0/1743	0.23	0/2348
1	3-U	0.18	0/1743	0.24	0/2348
1	3-W	0.18	0/1743	0.23	0/2348
1	3-Y	0.18	0/1743	0.23	0/2348
1	4-0	0.18	0/1743	0.23	0/2348
1	4-A	0.18	0/1665	0.24	0/2241
1	4-C	0.18	0/1743	0.23	0/2348
1	4-E	0.18	0/1743	0.23	0/2348
1	4-G	0.18	0/1743	0.23	0/2348
1	4-I	0.18	0/1743	0.23	0/2348
1	4-K	0.18	0/1743	0.24	0/2348
1	4-M	0.18	0/1743	0.23	0/2348
1	4-O	0.18	0/1571	0.23	0/2113
1	4-Q	0.18	0/1743	0.24	0/2348
1	4-S	0.18	0/1743	0.23	0/2348
1	4-U	0.18	0/1743	0.24	0/2348
1	4-W	0.18	0/1743	0.23	0/2348
1	4-Y	0.18	0/1743	0.23	0/2348
1	5-0	0.18	0/1743	0.23	0/2348
1	5-A	0.18	0/1743	0.23	0/2348
1	5-C	0.18	0/1743	0.23	0/2348
1	5-E	0.18	0/1743	0.23	0/2348
1	5-G	0.18	0/1743	0.23	0/2348
1	5-I	0.18	0/1743	0.23	0/2348
1	5-K	0.18	0/1743	0.24	0/2348
1	5-M	0.18	0/1743	0.23	0/2348
1	5-O	0.18	0/1743	0.23	0/2348
1	5-Q	0.18	0/1743	0.24	0/2348
1	5-S	0.18	0/1743	0.23	0/2348
1	5-U	0.18	0/1743	0.24	0/2348
1	5-W	0.18	0/1743	0.23	0/2348
1	5-Y	0.18	0/1743	0.23	0/2348
1	6-0	0.18	0/1743	0.23	0/2348
1	6-A	0.18	0/1743	0.23	0/2348
1	6-C	0.18	0/1743	0.23	0/2348
1	6-E	0.18	0/1743	0.23	0/2348
1	6-G	0.18	0/1743	0.23	0/2348
1	6-I	0.18	0/1743	0.23	0/2348
1	6-K	0.18	0/1743	0.24	0/2348

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	6-M	0.18	0/1743	0.23	0/2348
1	6-O	0.18	0/1743	0.23	0/2348
1	6-Q	0.18	0/1743	0.24	0/2348
1	6-S	0.18	0/1743	0.23	0/2348
1	6-U	0.18	0/1743	0.24	0/2348
1	6-W	0.18	0/1743	0.23	0/2348
1	6-Y	0.18	0/1743	0.23	0/2348
1	7-0	0.18	0/1743	0.23	0/2348
1	7-A	0.18	0/1743	0.23	0/2348
1	7-C	0.18	0/1743	0.23	0/2348
1	7-E	0.18	0/1743	0.23	0/2348
1	7-G	0.18	0/1743	0.23	0/2348
1	7-I	0.18	0/1743	0.23	0/2348
1	7-K	0.18	0/1743	0.24	0/2348
1	7-M	0.18	0/1743	0.23	0/2348
1	7-O	0.18	0/1743	0.23	0/2348
1	7-Q	0.18	0/1743	0.24	0/2348
1	7-S	0.18	0/1743	0.23	0/2348
1	7-U	0.18	0/1743	0.24	0/2348
1	7-W	0.18	0/1743	0.23	0/2348
1	7-Y	0.18	0/1743	0.23	0/2348
1	8-0	0.18	0/1743	0.23	0/2348
1	8-A	0.18	0/1743	0.23	0/2348
1	8-C	0.18	0/1743	0.23	0/2348
1	8-E	0.18	0/1743	0.23	0/2348
1	8-G	0.18	0/1743	0.23	0/2348
1	8-I	0.18	0/1743	0.23	0/2348
1	8-K	0.18	0/1743	0.24	0/2348
1	8-M	0.18	0/1743	0.23	0/2348
1	8-O	0.18	0/1743	0.23	0/2348
1	8-Q	0.18	0/1743	0.24	0/2348
1	8-S	0.18	0/1743	0.23	0/2348
1	8-U	0.18	0/1743	0.24	0/2348
1	8-W	0.18	0/1743	0.23	0/2348
1	8-Y	0.18	0/1743	0.23	0/2348
1	9-0	0.18	0/1743	0.23	0/2348
1	9-A	0.18	0/1743	0.23	0/2348
1	9-C	0.18	0/1743	0.23	0/2348
1	9-E	0.18	0/1743	0.23	0/2348
1	9-G	0.18	0/1743	0.23	0/2348
1	9-I	0.18	0/1743	0.23	0/2348
1	9-K	0.18	0/1743	0.24	0/2348
1	9-M	0.18	0/1743	0.23	0/2348

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	9-O	0.18	0/1743	0.23	0/2348
1	9-Q	0.18	0/1743	0.24	0/2348
1	9-S	0.18	0/1743	0.23	0/2348
1	9-U	0.18	0/1743	0.24	0/2348
1	9-W	0.18	0/1743	0.23	0/2348
1	9-Y	0.18	0/1743	0.23	0/2348
1	10-0	0.18	0/1743	0.23	0/2348
1	10-A	0.18	0/1743	0.23	0/2348
1	10-C	0.18	0/1743	0.23	0/2348
1	10-E	0.18	0/1743	0.23	0/2348
1	10-G	0.18	0/1743	0.23	0/2348
1	10-I	0.18	0/1743	0.23	0/2348
1	10-K	0.18	0/1743	0.24	0/2348
1	10-M	0.18	0/1743	0.23	0/2348
1	10-O	0.18	0/1743	0.23	0/2348
1	10-Q	0.18	0/1743	0.24	0/2348
1	10-S	0.18	0/1743	0.23	0/2348
1	10-U	0.18	0/1743	0.24	0/2348
1	10-W	0.18	0/1743	0.23	0/2348
1	10-Y	0.18	0/1743	0.23	0/2348
2	1-1	0.27	0/1577	0.32	0/2129
2	1-B	0.27	0/1577	0.32	0/2129
2	1-D	0.27	0/1577	0.32	0/2129
2	1-F	0.27	0/1577	0.32	0/2129
2	1-H	0.27	0/1577	0.32	0/2129
2	1-J	0.27	0/1577	0.32	0/2129
2	1-L	0.27	0/1577	0.32	0/2129
2	1-N	0.27	0/1577	0.32	0/2129
2	1-P	0.27	0/1577	0.32	0/2129
2	1-R	0.27	0/1577	0.32	0/2129
2	1-T	0.27	0/1577	0.32	0/2129
2	1-V	0.27	0/1577	0.32	0/2129
2	1-X	0.27	0/1577	0.32	0/2129
2	1-Z	0.27	0/1577	0.32	0/2129
2	2-1	0.27	0/1577	0.32	0/2129
2	2-B	0.27	0/1577	0.32	0/2129
2	2-D	0.27	0/1577	0.32	0/2129
2	2-F	0.27	0/1577	0.32	0/2129
2	2-H	0.27	0/1577	0.32	0/2129
2	2-J	0.27	0/1577	0.32	0/2129
2	2-L	0.27	0/1577	0.32	0/2129
2	2-N	0.27	0/1577	0.32	0/2129
2	2-P	0.27	0/1577	0.32	0/2129

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	2-R	0.27	0/1577	0.32	0/2129
2	2-T	0.27	0/1577	0.32	0/2129
2	2-V	0.27	0/1577	0.32	0/2129
2	2-X	0.27	0/1577	0.32	0/2129
2	2-Z	0.27	0/1524	0.32	0/2054
2	3-1	0.27	0/1577	0.32	0/2129
2	3-B	0.27	0/1533	0.32	0/2069
2	3-D	0.27	0/1577	0.32	0/2129
2	3-F	0.28	0/1369	0.32	0/1845
2	3-H	0.27	0/1523	0.32	0/2053
2	3-J	0.27	0/1486	0.32	0/2000
2	3-L	0.27	0/1577	0.32	0/2129
2	3-N	0.27	0/1577	0.32	0/2129
2	3-P	0.27	0/1577	0.32	0/2129
2	3-R	0.27	0/1577	0.32	0/2129
2	3-T	0.27	0/1577	0.32	0/2129
2	3-V	0.27	0/1577	0.32	0/2129
2	3-X	0.27	0/1577	0.32	0/2129
2	3-Z	0.27	0/1577	0.32	0/2129
2	4-1	0.27	0/1577	0.32	0/2129
2	4-B	0.27	0/1577	0.32	0/2129
2	4-D	0.27	0/1577	0.32	0/2129
2	4-F	0.27	0/1577	0.32	0/2129
2	4-H	0.27	0/1577	0.32	0/2129
2	4-J	0.27	0/1577	0.32	0/2129
2	4-L	0.27	0/1577	0.32	0/2129
2	4-N	0.27	0/1577	0.32	0/2129
2	4-P	0.27	0/1577	0.32	0/2129
2	4-R	0.27	0/1577	0.32	0/2129
2	4-T	0.27	0/1577	0.32	0/2129
2	4-V	0.27	0/1577	0.32	0/2129
2	4-X	0.27	0/1577	0.32	0/2129
2	4-Z	0.27	0/1577	0.32	0/2129
2	5-1	0.27	0/1577	0.32	0/2129
2	5-B	0.27	0/1577	0.32	0/2129
2	5-D	0.27	0/1577	0.32	0/2129
2	5-F	0.27	0/1577	0.32	0/2129
2	5-H	0.27	0/1577	0.32	0/2129
2	5-J	0.27	0/1577	0.32	0/2129
2	5-L	0.27	0/1577	0.32	0/2129
2	5-N	0.27	0/1577	0.32	0/2129
2	5-P	0.27	0/1577	0.32	0/2129
2	5-R	0.27	0/1577	0.32	0/2129

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	5-T	0.27	0/1577	0.32	0/2129
2	5-V	0.27	0/1577	0.32	0/2129
2	5-X	0.27	0/1577	0.32	0/2129
2	5-Z	0.27	0/1577	0.32	0/2129
2	6-1	0.27	0/1577	0.32	0/2129
2	6-B	0.27	0/1577	0.32	0/2129
2	6-D	0.27	0/944	0.29	0/1261
2	6-F	0.27	0/1577	0.32	0/2129
2	6-H	0.27	0/1577	0.32	0/2129
2	6-J	0.27	0/1577	0.32	0/2129
2	6-L	0.27	0/1577	0.32	0/2129
2	6-N	0.27	0/1577	0.32	0/2129
2	6-P	0.27	0/1577	0.32	0/2129
2	6-R	0.27	0/1577	0.32	0/2129
2	6-T	0.27	0/1577	0.32	0/2129
2	6-V	0.27	0/1577	0.32	0/2129
2	6-X	0.27	0/1577	0.32	0/2129
2	6-Z	0.27	0/1577	0.32	0/2129
2	7-1	0.27	0/1577	0.32	0/2129
2	7-B	0.27	0/1577	0.32	0/2129
2	7-D	0.27	0/1577	0.32	0/2129
2	7-F	0.27	0/1577	0.32	0/2129
2	7-H	0.27	0/1577	0.32	0/2129
2	7-J	0.27	0/1577	0.32	0/2129
2	7-L	0.27	0/1577	0.32	0/2129
2	7-N	0.27	0/1577	0.32	0/2129
2	7-P	0.27	0/1577	0.32	0/2129
2	7-R	0.27	0/1577	0.32	0/2129
2	7-T	0.27	0/1577	0.32	0/2129
2	7-V	0.27	0/1577	0.32	0/2129
2	7-X	0.27	0/1577	0.32	0/2129
2	7-Z	0.27	0/1577	0.32	0/2129
2	8-1	0.27	0/1577	0.32	0/2129
2	8-B	0.27	0/1577	0.32	0/2129
2	8-D	0.27	0/1577	0.32	0/2129
2	8-F	0.27	0/1577	0.32	0/2129
2	8-H	0.27	0/1577	0.32	0/2129
2	8-J	0.27	0/1577	0.32	0/2129
2	8-L	0.27	0/1577	0.32	0/2129
2	8-N	0.27	0/1577	0.32	0/2129
2	8-P	0.27	0/1577	0.32	0/2129
2	8-R	0.27	0/1577	0.32	0/2129
2	8-T	0.27	0/1577	0.32	0/2129

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	8-V	0.27	0/1577	0.32	0/2129
2	8-X	0.27	0/1577	0.32	0/2129
2	8-Z	0.27	0/1577	0.32	0/2129
2	9-1	0.27	0/1577	0.32	0/2129
2	9-B	0.27	0/1577	0.32	0/2129
2	9-D	0.27	0/1577	0.32	0/2129
2	9-F	0.27	0/1577	0.32	0/2129
2	9-H	0.27	0/1577	0.32	0/2129
2	9-J	0.27	0/1577	0.32	0/2129
2	9-L	0.27	0/1577	0.32	0/2129
2	9-N	0.27	0/1577	0.32	0/2129
2	9-P	0.27	0/1577	0.32	0/2129
2	9-R	0.27	0/1577	0.32	0/2129
2	9-T	0.27	0/1577	0.32	0/2129
2	9-V	0.27	0/1577	0.32	0/2129
2	9-X	0.27	0/1577	0.32	0/2129
2	9-Z	0.27	0/1577	0.32	0/2129
2	10-1	0.27	0/1577	0.32	0/2129
2	10-B	0.27	0/1577	0.32	0/2129
2	10-D	0.27	0/1577	0.32	0/2129
2	10-F	0.27	0/1577	0.32	0/2129
2	10-H	0.27	0/1577	0.32	0/2129
2	10-J	0.27	0/1577	0.32	0/2129
2	10-L	0.27	0/1577	0.32	0/2129
2	10-N	0.27	0/1577	0.32	0/2129
2	10-P	0.27	0/1577	0.32	0/2129
2	10-R	0.27	0/1577	0.32	0/2129
2	10-T	0.27	0/1577	0.32	0/2129
2	10-V	0.27	0/1577	0.32	0/2129
2	10-X	0.27	0/1577	0.32	0/2129
2	10-Z	0.27	0/1577	0.32	0/2129
All	All	0.23	0/463302	0.28	0/624726

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	8-0	0	1
1	8-A	0	1
1	8-C	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	8-E	0	1
1	8-G	0	1
1	8-I	0	1
1	8-K	0	1
1	8-M	0	1
1	8-O	0	1
1	8-Q	0	1
1	8-S	0	1
1	8-U	0	1
1	8-W	0	1
1	8-Y	0	1
1	10-0	0	1
1	10-A	0	1
1	10-C	0	1
1	10-E	0	1
1	10-G	0	1
1	10-I	0	1
1	10-K	0	1
1	10-M	0	1
1	10-O	0	1
1	10-Q	0	1
1	10-S	0	1
1	10-U	0	1
1	10-W	0	1
1	10-Y	0	1
2	1-1	0	1
2	1-B	0	1
2	1-D	0	1
2	1-F	0	1
2	1-H	0	1
2	1-J	0	1
2	1-L	0	1
2	1-N	0	1
2	1-P	0	1
2	1-R	0	1
2	1-T	0	1
2	1-V	0	1
2	1-X	0	1
2	1-Z	0	1
2	2-1	0	2
2	2-B	0	2
2	2-D	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	2-F	0	2
2	2-H	0	2
2	2-J	0	2
2	2-L	0	2
2	2-N	0	2
2	2-P	0	2
2	2-R	0	2
2	2-T	0	2
2	2-V	0	2
2	2-X	0	2
2	2-Z	0	2
2	3-1	0	1
2	3-B	0	1
2	3-D	0	1
2	3-F	0	1
2	3-H	0	1
2	3-J	0	1
2	3-L	0	1
2	3-N	0	1
2	3-P	0	1
2	3-R	0	1
2	3-T	0	1
2	3-V	0	1
2	3-X	0	1
2	3-Z	0	1
2	4-1	0	2
2	4-B	0	2
2	4-D	0	2
2	4-F	0	2
2	4-H	0	2
2	4-J	0	2
2	4-L	0	2
2	4-N	0	2
2	4-P	0	2
2	4-R	0	2
2	4-T	0	2
2	4-V	0	2
2	4-X	0	2
2	4-Z	0	2
2	5-1	0	1
2	5-B	0	1
2	5-D	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	5-F	0	1
2	5-H	0	1
2	5-J	0	1
2	5-L	0	1
2	5-N	0	1
2	5-P	0	1
2	5-R	0	1
2	5-T	0	1
2	5-V	0	1
2	5-X	0	1
2	5-Z	0	1
2	7-1	0	1
2	7-B	0	1
2	7-D	0	1
2	7-F	0	1
2	7-H	0	1
2	7-J	0	1
2	7-L	0	1
2	7-N	0	1
2	7-P	0	1
2	7-R	0	1
2	7-T	0	1
2	7-V	0	1
2	7-X	0	1
2	7-Z	0	1
2	8-1	0	1
2	8-B	0	1
2	8-D	0	1
2	8-F	0	1
2	8-H	0	1
2	8-J	0	1
2	8-L	0	1
2	8-N	0	1
2	8-P	0	1
2	8-R	0	1
2	8-T	0	1
2	8-V	0	1
2	8-X	0	1
2	8-Z	0	1
2	9-1	0	1
2	9-B	0	1
2	9-D	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	9-F	0	1
2	9-H	0	1
2	9-J	0	1
2	9-L	0	1
2	9-N	0	1
2	9-P	0	1
2	9-R	0	1
2	9-T	0	1
2	9-V	0	1
2	9-X	0	1
2	9-Z	0	1
2	10-1	0	3
2	10-B	0	3
2	10-D	0	3
2	10-F	0	3
2	10-H	0	3
2	10-J	0	3
2	10-L	0	3
2	10-N	0	3
2	10-P	0	3
2	10-R	0	3
2	10-T	0	3
2	10-V	0	3
2	10-X	0	3
2	10-Z	0	3
All	All	0	210

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (210) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1-1	24	ASN	Peptide
2	1-B	24	ASN	Peptide
2	1-D	24	ASN	Peptide
2	1-F	24	ASN	Peptide
2	1-H	24	ASN	Peptide
2	1-J	24	ASN	Peptide
2	1-L	24	ASN	Peptide
2	1-N	24	ASN	Peptide

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Mol	Chain	Res	Type	Group
2	1-P	24	ASN	Peptide
2	1-R	24	ASN	Peptide
2	1-T	24	ASN	Peptide
2	1-V	24	ASN	Peptide
2	1-X	24	ASN	Peptide
2	1-Z	24	ASN	Peptide
1	10-0	47	LEU	Peptide
2	10-1	24	ASN	Peptide
2	10-1	88	ASN	Peptide
2	10-1	94	PRO	Peptide
1	10-A	47	LEU	Peptide
2	10-B	24	ASN	Peptide
2	10-B	88	ASN	Peptide
2	10-B	94	PRO	Peptide
1	10-C	47	LEU	Peptide
2	10-D	24	ASN	Peptide
2	10-D	88	ASN	Peptide
2	10-D	94	PRO	Peptide
1	10-E	47	LEU	Peptide
2	10-F	24	ASN	Peptide
2	10-F	88	ASN	Peptide
2	10-F	94	PRO	Peptide
1	10-G	47	LEU	Peptide
2	10-H	24	ASN	Peptide
2	10-H	88	ASN	Peptide
2	10-H	94	PRO	Peptide
1	10-I	47	LEU	Peptide
2	10-J	24	ASN	Peptide
2	10-J	88	ASN	Peptide
2	10-J	94	PRO	Peptide
1	10-K	47	LEU	Peptide
2	10-L	24	ASN	Peptide
2	10-L	88	ASN	Peptide
2	10-L	94	PRO	Peptide
1	10-M	47	LEU	Peptide
2	10-N	24	ASN	Peptide
2	10-N	88	ASN	Peptide
2	10-N	94	PRO	Peptide
1	10-O	47	LEU	Peptide
2	10-P	24	ASN	Peptide
2	10-P	88	ASN	Peptide
2	10-P	94	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	10-Q	47	LEU	Peptide
2	10-R	24	ASN	Peptide
2	10-R	88	ASN	Peptide
2	10-R	94	PRO	Peptide
1	10-S	47	LEU	Peptide
2	10-T	24	ASN	Peptide
2	10-T	88	ASN	Peptide
2	10-T	94	PRO	Peptide
1	10-U	47	LEU	Peptide
2	10-V	24	ASN	Peptide
2	10-V	88	ASN	Peptide
2	10-V	94	PRO	Peptide
1	10-W	47	LEU	Peptide
2	10-X	24	ASN	Peptide
2	10-X	88	ASN	Peptide
2	10-X	94	PRO	Peptide
1	10-Y	47	LEU	Peptide
2	10-Z	24	ASN	Peptide
2	10-Z	88	ASN	Peptide
2	10-Z	94	PRO	Peptide
2	2-1	159	ILE	Peptide
2	2-1	24	ASN	Peptide
2	2-B	159	ILE	Peptide
2	2-B	24	ASN	Peptide
2	2-D	159	ILE	Peptide
2	2-D	24	ASN	Peptide
2	2-F	159	ILE	Peptide
2	2-F	24	ASN	Peptide
2	2-H	159	ILE	Peptide
2	2-H	24	ASN	Peptide
2	2-J	159	ILE	Peptide
2	2-J	24	ASN	Peptide
2	2-L	159	ILE	Peptide
2	2-L	24	ASN	Peptide
2	2-N	159	ILE	Peptide
2	2-N	24	ASN	Peptide
2	2-P	159	ILE	Peptide
2	2-P	24	ASN	Peptide
2	2-R	159	ILE	Peptide
2	2-R	24	ASN	Peptide
2	2-T	159	ILE	Peptide
2	2-T	24	ASN	Peptide

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Mol	Chain	Res	Type	Group
2	2-V	159	ILE	Peptide
2	2-V	24	ASN	Peptide
2	2-X	159	ILE	Peptide
2	2-X	24	ASN	Peptide
2	2-Z	159	ILE	Peptide
2	2-Z	24	ASN	Peptide
2	3-1	24	ASN	Peptide
2	3-B	24	ASN	Peptide
2	3-D	24	ASN	Peptide
2	3-F	24	ASN	Peptide
2	3-H	24	ASN	Peptide
2	3-J	24	ASN	Peptide
2	3-L	24	ASN	Peptide
2	3-N	24	ASN	Peptide
2	3-P	24	ASN	Peptide
2	3-R	24	ASN	Peptide
2	3-T	24	ASN	Peptide
2	3-V	24	ASN	Peptide
2	3-X	24	ASN	Peptide
2	3-Z	24	ASN	Peptide
2	4-1	24	ASN	Peptide
2	4-1	92	TYR	Peptide
2	4-B	24	ASN	Peptide
2	4-B	92	TYR	Peptide
2	4-D	24	ASN	Peptide
2	4-D	92	TYR	Peptide
2	4-F	24	ASN	Peptide
2	4-F	92	TYR	Peptide
2	4-H	24	ASN	Peptide
2	4-H	92	TYR	Peptide
2	4-J	24	ASN	Peptide
2	4-J	92	TYR	Peptide
2	4-L	24	ASN	Peptide
2	4-L	92	TYR	Peptide
2	4-N	24	ASN	Peptide
2	4-N	92	TYR	Peptide
2	4-P	24	ASN	Peptide
2	4-P	92	TYR	Peptide
2	4-R	24	ASN	Peptide
2	4-R	92	TYR	Peptide
2	4-T	24	ASN	Peptide
2	4-T	92	TYR	Peptide

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Mol	Chain	Res	Type	Group
2	4-V	24	ASN	Peptide
2	4-V	92	TYR	Peptide
2	4-X	24	ASN	Peptide
2	4-X	92	TYR	Peptide
2	4-Z	24	ASN	Peptide
2	4-Z	92	TYR	Peptide
2	5-1	24	ASN	Peptide
2	5-B	24	ASN	Peptide
2	5-D	24	ASN	Peptide
2	5-F	24	ASN	Peptide
2	5-H	24	ASN	Peptide
2	5-J	24	ASN	Peptide
2	5-L	24	ASN	Peptide
2	5-N	24	ASN	Peptide
2	5-P	24	ASN	Peptide
2	5-R	24	ASN	Peptide
2	5-T	24	ASN	Peptide
2	5-V	24	ASN	Peptide
2	5-X	24	ASN	Peptide
2	5-Z	24	ASN	Peptide
2	7-1	93	MET	Peptide
2	7-B	93	MET	Peptide
2	7-D	93	MET	Peptide
2	7-F	93	MET	Peptide
2	7-H	93	MET	Peptide
2	7-J	93	MET	Peptide
2	7-L	93	MET	Peptide
2	7-N	93	MET	Peptide
2	7-P	93	MET	Peptide
2	7-R	93	MET	Peptide
2	7-T	93	MET	Peptide
2	7-V	93	MET	Peptide
2	7-X	93	MET	Peptide
2	7-Z	93	MET	Peptide
1	8-0	206	GLU	Peptide
2	8-1	24	ASN	Peptide
1	8-A	206	GLU	Peptide
2	8-B	24	ASN	Peptide
1	8-C	206	GLU	Peptide
2	8-D	24	ASN	Peptide
1	8-E	206	GLU	Peptide
2	8-F	24	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	8-G	206	GLU	Peptide
2	8-H	24	ASN	Peptide
1	8-I	206	GLU	Peptide
2	8-J	24	ASN	Peptide
1	8-K	206	GLU	Peptide
2	8-L	24	ASN	Peptide
1	8-M	206	GLU	Peptide
2	8-N	24	ASN	Peptide
1	8-O	206	GLU	Peptide
2	8-P	24	ASN	Peptide
1	8-Q	206	GLU	Peptide
2	8-R	24	ASN	Peptide
1	8-S	206	GLU	Peptide
2	8-T	24	ASN	Peptide
1	8-U	206	GLU	Peptide
2	8-V	24	ASN	Peptide
1	8-W	206	GLU	Peptide
2	8-X	24	ASN	Peptide
1	8-Y	206	GLU	Peptide
2	8-Z	24	ASN	Peptide
2	9-1	23	GLU	Peptide
2	9-B	23	GLU	Peptide
2	9-D	23	GLU	Peptide
2	9-F	23	GLU	Peptide
2	9-H	23	GLU	Peptide
2	9-J	23	GLU	Peptide
2	9-L	23	GLU	Peptide
2	9-N	23	GLU	Peptide
2	9-P	23	GLU	Peptide
2	9-R	23	GLU	Peptide
2	9-T	23	GLU	Peptide
2	9-V	23	GLU	Peptide
2	9-X	23	GLU	Peptide
2	9-Z	23	GLU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-0	1720	0	1753	22	0
1	1-A	1720	0	1753	20	0
1	1-C	1720	0	1753	22	0
1	1-E	1720	0	1753	21	0
1	1-G	1720	0	1753	21	0
1	1-I	1720	0	1753	20	0
1	1-K	1720	0	1753	22	0
1	1-M	1720	0	1753	22	0
1	1-O	1720	0	1753	20	0
1	1-Q	1720	0	1753	22	0
1	1-S	1720	0	1753	22	0
1	1-U	1720	0	1753	20	0
1	1-W	1720	0	1753	22	0
1	1-Y	1720	0	1753	21	0
1	2-0	1720	0	0	0	0
1	2-A	1720	0	1753	19	0
1	2-C	1720	0	1753	21	0
1	2-E	1720	0	1753	22	0
1	2-G	1675	0	1707	21	0
1	2-I	1720	0	1753	22	0
1	2-K	1720	0	1753	22	0
1	2-M	1720	0	1753	23	0
1	2-O	1720	0	1753	18	0
1	2-Q	1720	0	1753	24	0
1	2-S	1720	0	1753	22	0
1	2-U	1720	0	1753	21	0
1	2-W	1720	0	1753	20	0
1	2-Y	1720	0	1753	17	0
1	3-0	1720	0	0	0	0
1	3-A	1720	0	1753	17	0
1	3-C	1720	0	1753	20	0
1	3-E	1720	0	1753	17	0
1	3-G	1720	0	0	0	0
1	3-I	1720	0	0	0	0
1	3-K	1720	0	0	0	0
1	3-M	1720	0	0	0	0
1	3-O	1720	0	0	0	0
1	3-Q	1720	0	0	0	0
1	3-S	1720	0	0	0	0
1	3-U	1720	0	0	0	0
1	3-W	1720	0	0	0	0
1	3-Y	1720	0	0	0	0
1	4-0	1720	0	1753	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	4-A	1630	0	1680	19	0
1	4-C	1720	0	1753	20	0
1	4-E	1720	0	1753	19	0
1	4-G	1720	0	1753	20	0
1	4-I	1720	0	1753	22	0
1	4-K	1720	0	1753	20	0
1	4-M	1720	0	1753	20	0
1	4-O	1540	0	1578	18	0
1	4-Q	1720	0	1753	17	0
1	4-S	1720	0	1753	20	0
1	4-U	1720	0	1753	21	0
1	4-W	1720	0	1753	20	0
1	4-Y	1720	0	1753	18	0
1	5-0	1720	0	1753	21	0
1	5-A	1720	0	1753	19	0
1	5-C	1720	0	1753	20	0
1	5-E	1720	0	1753	20	0
1	5-G	1720	0	1753	19	0
1	5-I	1720	0	1753	20	0
1	5-K	1720	0	1753	21	0
1	5-M	1720	0	1753	19	0
1	5-O	1720	0	1753	20	0
1	5-Q	1720	0	1753	19	0
1	5-S	1720	0	1753	22	0
1	5-U	1720	0	1753	20	0
1	5-W	1720	0	1753	21	0
1	5-Y	1720	0	1753	20	0
1	6-0	1720	0	0	0	0
1	6-A	1720	0	1753	20	0
1	6-C	1720	0	1753	19	0
1	6-E	1720	0	0	0	0
1	6-G	1720	0	0	0	0
1	6-I	1720	0	0	0	0
1	6-K	1720	0	0	0	0
1	6-M	1720	0	0	0	0
1	6-O	1720	0	0	0	0
1	6-Q	1720	0	0	0	0
1	6-S	1720	0	0	0	0
1	6-U	1720	0	0	0	0
1	6-W	1720	0	0	0	0
1	6-Y	1720	0	0	0	0
1	7-0	1720	0	1753	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	7-A	1720	0	1753	19	0
1	7-C	1720	0	1753	17	0
1	7-E	1720	0	1753	17	0
1	7-G	1720	0	1753	17	0
1	7-I	1720	0	1753	17	0
1	7-K	1720	0	1753	18	0
1	7-M	1720	0	1753	19	0
1	7-O	1720	0	1753	19	0
1	7-Q	1720	0	1753	17	0
1	7-S	1720	0	1753	18	0
1	7-U	1720	0	1753	17	0
1	7-W	1720	0	1753	17	0
1	7-Y	1720	0	1753	17	0
1	8-0	1720	0	1753	13	0
1	8-A	1720	0	1753	15	0
1	8-C	1720	0	1753	14	0
1	8-E	1720	0	1753	15	0
1	8-G	1720	0	1753	16	0
1	8-I	1720	0	1753	18	0
1	8-K	1720	0	1753	16	0
1	8-M	1720	0	1753	14	0
1	8-O	1720	0	1753	14	0
1	8-Q	1720	0	1753	14	0
1	8-S	1720	0	1753	16	0
1	8-U	1720	0	1753	19	0
1	8-W	1720	0	1753	17	0
1	8-Y	1720	0	1753	16	0
1	9-0	1720	0	1753	19	0
1	9-A	1720	0	1753	19	0
1	9-C	1720	0	1753	18	0
1	9-E	1720	0	1753	16	0
1	9-G	1720	0	1753	22	0
1	9-I	1720	0	1753	23	0
1	9-K	1720	0	1753	20	0
1	9-M	1720	0	1753	21	0
1	9-O	1720	0	1753	19	0
1	9-Q	1720	0	1753	20	0
1	9-S	1720	0	1753	21	0
1	9-U	1720	0	1753	23	0
1	9-W	1720	0	1753	22	0
1	9-Y	1720	0	1753	17	0
1	10-0	1720	0	1753	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	10-A	1720	0	1753	21	0
1	10-C	1720	0	1753	21	0
1	10-E	1720	0	1753	21	0
1	10-G	1720	0	1753	22	0
1	10-I	1720	0	1753	23	0
1	10-K	1720	0	1753	23	0
1	10-M	1720	0	1753	23	0
1	10-O	1720	0	1753	20	0
1	10-Q	1720	0	1753	22	0
1	10-S	1720	0	1753	23	0
1	10-U	1720	0	1753	23	0
1	10-W	1720	0	1753	20	0
1	10-Y	1720	0	1753	21	0
2	1-1	1558	0	1609	16	0
2	1-B	1558	0	1609	18	0
2	1-D	1558	0	1609	16	0
2	1-F	1558	0	1609	17	0
2	1-H	1558	0	1609	15	0
2	1-J	1558	0	1609	17	0
2	1-L	1558	0	1609	15	0
2	1-N	1558	0	1609	16	0
2	1-P	1558	0	1609	17	0
2	1-R	1558	0	1609	16	0
2	1-T	1558	0	1609	15	0
2	1-V	1558	0	1609	19	0
2	1-X	1558	0	1609	16	0
2	1-Z	1558	0	1609	17	0
2	2-1	1558	0	0	0	0
2	2-B	1558	0	1609	18	0
2	2-D	1558	0	1609	14	0
2	2-F	1558	0	1609	17	0
2	2-H	1558	0	1609	18	0
2	2-J	1558	0	1609	15	0
2	2-L	1558	0	1609	15	0
2	2-N	1558	0	1609	15	0
2	2-P	1558	0	1609	18	0
2	2-R	1558	0	1609	17	0
2	2-T	1558	0	1609	15	0
2	2-V	1558	0	1609	16	0
2	2-X	1558	0	1609	18	0
2	2-Z	1558	0	1175	12	0
2	3-1	1558	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	3-B	1513	0	1572	12	0
2	3-D	1558	0	1609	12	0
2	3-F	1558	0	506	3	0
2	3-H	1558	0	0	0	0
2	3-J	1558	0	0	0	0
2	3-L	1558	0	0	0	0
2	3-N	1558	0	0	0	0
2	3-P	1558	0	0	0	0
2	3-R	1558	0	0	0	0
2	3-T	1558	0	0	0	0
2	3-V	1558	0	0	0	0
2	3-X	1558	0	0	0	0
2	3-Z	1558	0	0	0	0
2	4-1	1558	0	1609	14	0
2	4-B	1558	0	1609	12	0
2	4-D	1558	0	1609	12	0
2	4-F	1558	0	1609	12	0
2	4-H	1558	0	1609	11	0
2	4-J	1558	0	1609	11	0
2	4-L	1558	0	1609	12	0
2	4-N	1558	0	1609	13	0
2	4-P	1558	0	1609	11	0
2	4-R	1558	0	1609	12	0
2	4-T	1558	0	1609	11	0
2	4-V	1558	0	1609	11	0
2	4-X	1558	0	1609	12	0
2	4-Z	1558	0	1609	12	0
2	5-1	1558	0	1609	19	0
2	5-B	1558	0	1609	17	0
2	5-D	1558	0	1609	18	0
2	5-F	1558	0	1609	18	0
2	5-H	1558	0	1609	19	0
2	5-J	1558	0	1609	18	0
2	5-L	1558	0	1609	18	0
2	5-N	1558	0	1609	19	0
2	5-P	1558	0	1609	19	0
2	5-R	1558	0	1609	20	0
2	5-T	1558	0	1609	18	0
2	5-V	1558	0	1609	18	0
2	5-X	1558	0	1609	19	0
2	5-Z	1558	0	1609	18	0
2	6-1	1558	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	6-B	1558	0	1609	14	0
2	6-D	1558	0	78	0	0
2	6-F	1558	0	0	0	0
2	6-H	1558	0	0	0	0
2	6-J	1558	0	0	0	0
2	6-L	1558	0	0	0	0
2	6-N	1558	0	0	0	0
2	6-P	1558	0	0	0	0
2	6-R	1558	0	0	0	0
2	6-T	1558	0	0	0	0
2	6-V	1558	0	0	0	0
2	6-X	1558	0	0	0	0
2	6-Z	1558	0	0	0	0
2	7-1	1558	0	1609	20	0
2	7-B	1558	0	1609	24	0
2	7-D	1558	0	1609	23	0
2	7-F	1558	0	1609	21	0
2	7-H	1558	0	1609	21	0
2	7-J	1558	0	1609	22	0
2	7-L	1558	0	1609	20	0
2	7-N	1558	0	1609	21	0
2	7-P	1558	0	1609	22	0
2	7-R	1558	0	1609	21	0
2	7-T	1558	0	1609	21	0
2	7-V	1558	0	1609	22	0
2	7-X	1558	0	1609	21	0
2	7-Z	1558	0	1609	21	0
2	8-1	1558	0	1609	19	0
2	8-B	1558	0	1609	19	0
2	8-D	1558	0	1609	19	0
2	8-F	1558	0	1609	20	0
2	8-H	1558	0	1609	22	0
2	8-J	1558	0	1609	21	0
2	8-L	1558	0	1609	20	0
2	8-N	1558	0	1609	20	0
2	8-P	1558	0	1609	20	0
2	8-R	1558	0	1609	19	0
2	8-T	1558	0	1609	21	0
2	8-V	1558	0	1609	19	0
2	8-X	1558	0	1609	20	0
2	8-Z	1558	0	1609	19	0
2	9-1	1558	0	1609	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	9-B	1558	0	1609	21	0
2	9-D	1558	0	1609	20	0
2	9-F	1558	0	1609	21	0
2	9-H	1558	0	1609	21	0
2	9-J	1558	0	1609	22	0
2	9-L	1558	0	1609	20	0
2	9-N	1558	0	1609	21	0
2	9-P	1558	0	1609	21	0
2	9-R	1558	0	1609	20	0
2	9-T	1558	0	1609	20	0
2	9-V	1558	0	1609	22	0
2	9-X	1558	0	1609	22	0
2	9-Z	1558	0	1609	21	0
2	10-1	1558	0	1609	17	0
2	10-B	1558	0	1609	18	0
2	10-D	1558	0	1609	18	0
2	10-F	1558	0	1609	19	0
2	10-H	1558	0	1609	18	0
2	10-J	1558	0	1609	16	0
2	10-L	1558	0	1609	17	0
2	10-N	1558	0	1609	17	0
2	10-P	1558	0	1609	19	0
2	10-R	1558	0	1609	17	0
2	10-T	1558	0	1609	22	0
2	10-V	1558	0	1609	23	0
2	10-X	1558	0	1609	18	0
2	10-Z	1558	0	1609	20	0
All	All	458560	0	386593	3747	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (3747) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:GLN:HG3	2:D:65:LEU:HG	1.60	0.84
1:O:97:GLN:HG3	2:1:65:LEU:HG	1.59	0.83
1:U:97:GLN:HG3	2:V:65:LEU:HG	1.62	0.79
1:A:37:ALA:O	1:A:164:ALA:HA	1.84	0.78
1:C:37:ALA:O	1:C:164:ALA:HA	1.84	0.78
1:A:36:THR:HA	1:A:165:ILE:O	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:141:GLN:HE21	2:1:141:GLN:HE21	1.32	0.78
1:E:37:ALA:O	1:E:164:ALA:HA	1.84	0.78
1:C:36:THR:HA	1:C:165:ILE:O	1.84	0.77
1:C:39:GLY:O	1:C:162:ALA:HA	1.84	0.77
1:G:97:GLN:HG3	2:H:65:LEU:HG	1.67	0.77
1:A:39:GLY:O	1:A:162:ALA:HA	1.84	0.77
2:D:141:GLN:HE21	2:R:141:GLN:HE21	1.33	0.77
1:A:97:GLN:HG3	2:B:65:LEU:HG	1.67	0.76
1:W:37:ALA:O	1:W:164:ALA:HA	1.88	0.74
1:O:37:ALA:O	1:O:164:ALA:HA	1.88	0.74
1:C:37:ALA:O	1:C:164:ALA:HA	1.88	0.74
1:G:37:ALA:O	1:G:164:ALA:HA	1.88	0.74
1:A:37:ALA:O	1:A:164:ALA:HA	1.88	0.74
1:O:37:ALA:O	1:O:164:ALA:HA	1.88	0.74
1:K:37:ALA:O	1:K:164:ALA:HA	1.88	0.73
1:M:37:ALA:O	1:M:164:ALA:HA	1.88	0.73
1:E:37:ALA:O	1:E:164:ALA:HA	1.88	0.73
1:Q:37:ALA:O	1:Q:164:ALA:HA	1.88	0.73
1:Y:37:ALA:O	1:Y:164:ALA:HA	1.88	0.73
1:S:37:ALA:O	1:S:164:ALA:HA	1.88	0.73
1:E:37:ALA:O	1:E:164:ALA:HA	1.88	0.73
1:I:37:ALA:O	1:I:164:ALA:HA	1.88	0.73
1:U:37:ALA:O	1:U:164:ALA:HA	1.88	0.73
1:A:37:ALA:O	1:A:164:ALA:HA	1.88	0.73
1:Y:37:ALA:O	1:Y:164:ALA:HA	1.88	0.73
1:O:37:ALA:O	1:O:164:ALA:HA	1.88	0.73
1:G:37:ALA:O	1:G:164:ALA:HA	1.88	0.73
1:U:37:ALA:O	1:U:164:ALA:HA	1.88	0.73
1:C:39:GLY:O	1:C:162:ALA:HA	1.89	0.73
1:O:39:GLY:O	1:O:162:ALA:HA	1.89	0.73
2:B:141:GLN:HE21	2:P:141:GLN:HE21	1.36	0.73
1:W:37:ALA:O	1:W:164:ALA:HA	1.88	0.73
1:U:39:GLY:O	1:U:162:ALA:HA	1.89	0.73
1:I:39:GLY:O	1:I:162:ALA:HA	1.89	0.72
1:M:39:GLY:O	1:M:162:ALA:HA	1.89	0.72
1:O:39:GLY:O	1:O:162:ALA:HA	1.89	0.72
1:Q:39:GLY:O	1:Q:162:ALA:HA	1.89	0.72
1:I:37:ALA:O	1:I:164:ALA:HA	1.88	0.72
1:S:39:GLY:O	1:S:162:ALA:HA	1.89	0.72
1:S:37:ALA:O	1:S:164:ALA:HA	1.88	0.72
1:A:39:GLY:O	1:A:162:ALA:HA	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:39:GLY:O	1:K:162:ALA:HA	1.89	0.72
1:K:37:ALA:O	1:K:164:ALA:HA	1.88	0.72
1:C:37:ALA:O	1:C:164:ALA:HA	1.88	0.72
1:O:37:ALA:O	1:O:164:ALA:HA	1.88	0.72
1:E:39:GLY:O	1:E:162:ALA:HA	1.89	0.72
1:Y:39:GLY:O	1:Y:162:ALA:HA	1.89	0.72
2:D:91:LYS:HB2	2:D:93:MET:HG2	1.72	0.72
1:Q:37:ALA:O	1:Q:164:ALA:HA	1.88	0.72
2:1:91:LYS:HB2	2:1:93:MET:HG2	1.72	0.72
2:T:91:LYS:HB2	2:T:93:MET:HG2	1.72	0.72
1:Q:37:ALA:O	1:Q:164:ALA:HA	1.90	0.71
1:M:37:ALA:O	1:M:164:ALA:HA	1.88	0.71
2:J:91:LYS:HB2	2:J:93:MET:HG2	1.72	0.71
2:V:91:LYS:HB2	2:V:93:MET:HG2	1.72	0.71
1:W:39:GLY:O	1:W:162:ALA:HA	1.89	0.71
1:M:37:ALA:O	1:M:164:ALA:HA	1.90	0.71
2:B:91:LYS:HB2	2:B:93:MET:HG2	1.72	0.71
2:L:91:LYS:HB2	2:L:93:MET:HG2	1.72	0.71
1:G:39:GLY:O	1:G:162:ALA:HA	1.89	0.71
2:P:91:LYS:HB2	2:P:93:MET:HG2	1.72	0.71
2:Z:91:LYS:HB2	2:Z:93:MET:HG2	1.72	0.71
1:A:37:ALA:O	1:A:164:ALA:HA	1.90	0.71
1:C:37:ALA:O	1:C:164:ALA:HA	1.90	0.71
1:O:37:ALA:O	1:O:164:ALA:HA	1.90	0.71
2:F:91:LYS:HB2	2:F:93:MET:HG2	1.72	0.71
1:Y:37:ALA:O	1:Y:164:ALA:HA	1.91	0.71
1:S:37:ALA:O	1:S:164:ALA:HA	1.90	0.71
1:O:37:ALA:O	1:O:164:ALA:HA	1.90	0.71
2:R:91:LYS:HB2	2:R:93:MET:HG2	1.72	0.71
1:E:37:ALA:O	1:E:164:ALA:HA	1.91	0.71
2:H:91:LYS:HB2	2:H:93:MET:HG2	1.72	0.71
2:N:91:LYS:HB2	2:N:93:MET:HG2	1.72	0.71
1:G:37:ALA:O	1:G:164:ALA:HA	1.90	0.71
1:W:37:ALA:O	1:W:164:ALA:HA	1.90	0.71
1:Y:37:ALA:O	1:Y:164:ALA:HA	1.90	0.71
2:X:91:LYS:HB2	2:X:93:MET:HG2	1.72	0.71
1:G:37:ALA:O	1:G:164:ALA:HA	1.91	0.71
1:E:37:ALA:O	1:E:164:ALA:HA	1.90	0.71
1:K:37:ALA:O	1:K:164:ALA:HA	1.90	0.71
1:W:37:ALA:O	1:W:164:ALA:HA	1.91	0.71
1:S:37:ALA:O	1:S:164:ALA:HA	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:37:ALA:O	1:K:164:ALA:HA	1.91	0.70
1:C:37:ALA:O	1:C:164:ALA:HA	1.91	0.70
2:T:91:LYS:HB2	2:V:93:MET:HE3	1.71	0.70
1:O:37:ALA:O	1:O:164:ALA:HA	1.91	0.70
1:I:37:ALA:O	1:I:164:ALA:HA	1.90	0.70
1:A:37:ALA:O	1:A:164:ALA:HA	1.91	0.70
2:T:91:LYS:HZ1	2:V:95:TYR:HE1	1.40	0.70
1:U:37:ALA:O	1:U:164:ALA:HA	1.90	0.70
1:M:37:ALA:O	1:M:164:ALA:HA	1.91	0.70
1:O:37:ALA:O	1:O:164:ALA:HA	1.91	0.70
2:T:92:TYR:HD1	2:V:93:MET:HE1	1.55	0.70
1:U:97:GLN:HG3	2:V:65:LEU:HG	1.72	0.70
1:I:37:ALA:O	1:I:164:ALA:HA	1.91	0.70
1:U:37:ALA:O	1:U:164:ALA:HA	1.91	0.70
1:Q:37:ALA:O	1:Q:164:ALA:HA	1.91	0.70
2:J:132:PRO:HB2	2:X:132:PRO:HB2	1.74	0.69
2:B:135:TYR:O	2:B:139:GLU:HB2	1.94	0.68
1:W:39:GLY:O	1:W:162:ALA:HA	1.94	0.68
1:K:39:GLY:O	1:K:162:ALA:HA	1.94	0.68
1:C:39:GLY:O	1:C:162:ALA:HA	1.94	0.68
1:E:39:GLY:O	1:E:162:ALA:HA	1.94	0.68
1:G:39:GLY:O	1:G:162:ALA:HA	1.94	0.68
1:I:39:GLY:O	1:I:162:ALA:HA	1.94	0.68
1:S:39:GLY:O	1:S:162:ALA:HA	1.94	0.68
1:Y:39:GLY:O	1:Y:162:ALA:HA	1.94	0.68
1:W:72:ASP:OD1	1:W:72:ASP:N	2.27	0.68
1:U:39:GLY:O	1:U:162:ALA:HA	1.94	0.68
1:O:39:GLY:O	1:O:162:ALA:HA	1.94	0.68
1:G:72:ASP:OD1	1:G:72:ASP:N	2.27	0.68
1:M:39:GLY:O	1:M:162:ALA:HA	1.94	0.68
1:O:39:GLY:O	1:O:162:ALA:HA	1.94	0.68
1:Q:39:GLY:O	1:Q:162:ALA:HA	1.94	0.68
1:C:72:ASP:OD1	1:C:72:ASP:N	2.27	0.68
1:A:39:GLY:O	1:A:162:ALA:HA	1.94	0.67
2:L:141:GLN:HE21	2:Z:141:GLN:HE21	1.42	0.67
1:A:37:ALA:O	1:A:164:ALA:HA	1.94	0.67
1:O:72:ASP:OD1	1:O:72:ASP:N	2.27	0.67
2:F:93:MET:HE3	2:H:91:LYS:HB2	1.76	0.67
1:A:72:ASP:OD1	1:A:72:ASP:N	2.27	0.66
1:C:37:ALA:O	1:C:164:ALA:HA	1.94	0.66
2:J:141:GLN:HE21	2:X:141:GLN:HE21	1.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:141:GLN:HE21	2:V:141:GLN:HE21	1.43	0.66
2:L:141:GLN:HE21	2:Z:141:GLN:HE21	1.43	0.66
1:C:97:GLN:HG3	2:D:65:LEU:HG	1.77	0.66
2:F:141:GLN:HE21	2:T:141:GLN:HE21	1.43	0.66
1:C:25:GLU:HA	1:C:28:ARG:HD2	1.78	0.66
1:O:25:GLU:HA	1:O:28:ARG:HD2	1.78	0.66
1:U:84:ASP:OD1	1:W:121:GLN:NE2	2.29	0.66
1:A:25:GLU:HA	1:A:28:ARG:HD2	1.78	0.66
1:O:25:GLU:HA	1:O:28:ARG:HD2	1.78	0.66
1:E:25:GLU:HA	1:E:28:ARG:HD2	1.78	0.65
1:Y:25:GLU:HA	1:Y:28:ARG:HD2	1.78	0.65
2:B:141:GLN:HE21	2:P:141:GLN:HE21	1.44	0.65
2:B:141:GLN:HE21	2:P:141:GLN:HE21	1.44	0.65
2:H:141:GLN:HE21	2:V:141:GLN:HE21	1.43	0.65
1:E:39:GLY:O	1:E:162:ALA:HA	1.97	0.65
2:J:141:GLN:HE21	2:X:141:GLN:HE21	1.44	0.65
1:G:39:GLY:O	1:G:162:ALA:HA	1.97	0.65
1:W:39:GLY:O	1:W:162:ALA:HA	1.97	0.65
1:Y:39:GLY:O	1:Y:162:ALA:HA	1.97	0.65
1:O:97:GLN:HG3	2:P:65:LEU:HG	1.78	0.65
1:U:39:GLY:O	1:U:162:ALA:HA	1.97	0.65
1:M:72:ASP:OD1	1:M:72:ASP:N	2.30	0.65
1:I:39:GLY:O	1:I:162:ALA:HA	1.97	0.65
1:M:25:GLU:HA	1:M:28:ARG:HD2	1.78	0.65
1:Q:25:GLU:HA	1:Q:28:ARG:HD2	1.78	0.65
1:Q:72:ASP:N	1:Q:72:ASP:OD1	2.30	0.65
2:D:141:GLN:HE21	2:R:141:GLN:HE21	1.45	0.65
1:K:39:GLY:O	1:K:162:ALA:HA	1.97	0.64
2:H:141:GLN:HE21	2:V:141:GLN:HE21	1.45	0.64
1:A:39:GLY:O	1:A:162:ALA:HA	1.97	0.64
1:C:39:GLY:O	1:C:162:ALA:HA	1.97	0.64
1:O:39:GLY:O	1:O:162:ALA:HA	1.97	0.64
1:W:25:GLU:HA	1:W:28:ARG:HD2	1.78	0.64
1:O:39:GLY:O	1:O:162:ALA:HA	1.97	0.64
1:S:39:GLY:O	1:S:162:ALA:HA	1.97	0.64
1:M:72:ASP:OD1	1:M:72:ASP:N	2.27	0.64
1:C:72:ASP:OD1	1:C:72:ASP:N	2.30	0.64
1:G:25:GLU:HA	1:G:28:ARG:HD2	1.78	0.64
1:O:72:ASP:OD1	1:O:72:ASP:N	2.30	0.64
1:Q:72:ASP:N	1:Q:72:ASP:OD1	2.27	0.64
2:R:88:ASN:ND2	2:T:50:GLY:O	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:72:ASP:OD1	1:E:72:ASP:N	2.30	0.64
2:J:190:ASP:OD1	2:J:190:ASP:N	2.30	0.64
2:V:190:ASP:OD1	2:V:190:ASP:N	2.30	0.64
1:Y:72:ASP:OD1	1:Y:72:ASP:N	2.30	0.64
1:M:39:GLY:O	1:M:162:ALA:HA	1.97	0.64
1:Q:39:GLY:O	1:Q:162:ALA:HA	1.97	0.64
1:K:25:GLU:HA	1:K:28:ARG:HD2	1.78	0.64
1:S:25:GLU:HA	1:S:28:ARG:HD2	1.78	0.64
2:H:3:THR:HG1	2:H:127:THR:HG1	1.46	0.64
1:G:72:ASP:N	1:G:72:ASP:OD1	2.30	0.64
1:W:72:ASP:OD1	1:W:72:ASP:N	2.30	0.64
1:O:72:ASP:OD1	1:O:72:ASP:N	2.27	0.63
2:B:54:VAL:HG21	2:D:88:ASN:HD22	1.63	0.63
1:K:72:ASP:OD1	1:K:72:ASP:N	2.27	0.63
1:S:72:ASP:OD1	1:S:72:ASP:N	2.27	0.63
1:O:97:GLN:HG3	2:I:65:LEU:HG	1.81	0.63
2:D:190:ASP:OD1	2:D:190:ASP:N	2.30	0.63
2:F:190:ASP:N	2:F:190:ASP:OD1	2.30	0.63
1:K:72:ASP:OD1	1:K:72:ASP:N	2.30	0.63
2:N:190:ASP:OD1	2:N:190:ASP:N	2.30	0.63
2:R:190:ASP:N	2:R:190:ASP:OD1	2.30	0.63
2:I:190:ASP:OD1	2:I:190:ASP:N	2.30	0.63
2:F:132:PRO:HB2	2:T:132:PRO:HB2	1.80	0.63
2:B:91:LYS:HB3	2:B:93:MET:HG2	1.81	0.63
1:M:97:GLN:HG3	2:N:65:LEU:HG	1.80	0.63
1:K:97:GLN:HG3	2:L:65:LEU:HG	1.80	0.63
2:L:190:ASP:OD1	2:L:190:ASP:N	2.30	0.63
1:U:25:GLU:HA	1:U:28:ARG:HD2	1.78	0.63
2:Z:190:ASP:OD1	2:Z:190:ASP:N	2.30	0.63
2:J:141:GLN:HE21	2:X:141:GLN:HE21	1.47	0.63
1:I:25:GLU:HA	1:I:28:ARG:HD2	1.78	0.63
1:S:72:ASP:N	1:S:72:ASP:OD1	2.30	0.63
2:T:190:ASP:N	2:T:190:ASP:OD1	2.30	0.63
1:I:72:ASP:N	1:I:72:ASP:OD1	2.30	0.63
1:U:72:ASP:N	1:U:72:ASP:OD1	2.30	0.63
2:H:190:ASP:N	2:H:190:ASP:OD1	2.30	0.63
1:O:99:GLU:OE1	1:O:115:ARG:NH2	2.32	0.63
2:D:91:LYS:HB3	2:D:93:MET:HG2	1.81	0.63
2:H:141:GLN:HE21	2:V:141:GLN:HE21	1.47	0.63
1:C:99:GLU:OE1	1:C:115:ARG:NH2	2.33	0.62
2:X:190:ASP:OD1	2:X:190:ASP:N	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:97:GLN:HG3	2:X:65:LEU:HG	1.80	0.62
1:G:108:ASN:OD1	1:G:147:ARG:NH1	2.33	0.62
2:J:141:GLN:HE21	2:X:141:GLN:HE21	1.47	0.62
2:D:172:MET:HG3	2:D:203:LEU:HD11	1.81	0.62
2:T:92:TYR:HB3	2:V:93:MET:SD	2.40	0.62
1:E:72:ASP:OD1	1:E:72:ASP:N	2.27	0.62
1:Y:72:ASP:OD1	1:Y:72:ASP:N	2.27	0.62
1:A:72:ASP:OD1	1:A:72:ASP:N	2.30	0.62
2:B:141:GLN:HE21	2:P:141:GLN:HE21	1.46	0.62
1:W:108:ASN:OD1	1:W:147:ARG:NH1	2.33	0.62
1:Q:99:GLU:OE1	1:Q:115:ARG:NH2	2.32	0.62
1:Y:99:GLU:OE1	1:Y:115:ARG:NH2	2.32	0.62
1:A:97:GLN:HG3	2:B:65:LEU:HG	1.82	0.62
1:A:99:GLU:OE1	1:A:115:ARG:NH2	2.32	0.62
1:E:99:GLU:OE1	1:E:115:ARG:NH2	2.32	0.62
1:I:99:GLU:OE1	1:I:115:ARG:NH2	2.32	0.62
1:M:99:GLU:OE1	1:M:115:ARG:NH2	2.32	0.62
1:O:99:GLU:OE1	1:O:115:ARG:NH2	2.32	0.62
1:U:99:GLU:OE1	1:U:115:ARG:NH2	2.32	0.62
2:F:141:GLN:HE21	2:T:141:GLN:HE21	1.48	0.62
1:O:72:ASP:OD1	1:O:72:ASP:N	2.30	0.62
2:B:141:GLN:HE21	2:P:141:GLN:HE21	1.48	0.62
2:F:141:GLN:HE21	2:T:141:GLN:HE21	1.47	0.62
2:L:141:GLN:HE21	2:Z:141:GLN:HE21	1.47	0.62
1:Q:108:ASN:OD1	1:Q:147:ARG:NH1	2.33	0.62
2:H:132:PRO:HB2	2:V:132:PRO:HB2	1.82	0.62
1:O:121:GLN:NE2	1:O:84:ASP:OD1	2.33	0.62
1:O:97:GLN:HG3	2:P:65:LEU:HG	1.82	0.62
1:E:108:ASN:OD1	1:E:147:ARG:NH1	2.33	0.62
1:I:108:ASN:OD1	1:I:147:ARG:NH1	2.33	0.62
1:M:108:ASN:OD1	1:M:147:ARG:NH1	2.33	0.62
1:Y:108:ASN:OD1	1:Y:147:ARG:NH1	2.33	0.62
1:G:99:GLU:OE1	1:G:115:ARG:NH2	2.32	0.62
1:U:108:ASN:OD1	1:U:147:ARG:NH1	2.33	0.62
1:K:99:GLU:OE1	1:K:115:ARG:NH2	2.32	0.61
1:S:99:GLU:OE1	1:S:115:ARG:NH2	2.32	0.61
1:W:99:GLU:OE1	1:W:115:ARG:NH2	2.32	0.61
2:B:132:PRO:HB2	2:P:132:PRO:HB2	1.81	0.61
1:C:97:GLN:HG3	2:D:65:LEU:HG	1.82	0.61
2:D:141:GLN:HE21	2:R:141:GLN:HE21	1.48	0.61
2:N:141:GLN:HE21	2:1:141:GLN:HE21	1.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:172:MET:HG3	2:B:203:LEU:HD11	1.81	0.61
1:K:97:GLN:HG3	2:L:65:LEU:HG	1.83	0.61
1:A:108:ASN:OD1	1:A:147:ARG:NH1	2.33	0.61
1:O:108:ASN:OD1	1:O:147:ARG:NH1	2.33	0.61
1:S:108:ASN:OD1	1:S:147:ARG:NH1	2.33	0.61
2:L:7:THR:HG23	2:L:108:PRO:HB2	1.83	0.61
1:O:97:GLN:HG3	2:P:65:LEU:HG	1.82	0.61
1:O:108:ASN:OD1	1:O:147:ARG:NH1	2.33	0.61
2:T:7:THR:HG23	2:T:108:PRO:HB2	1.83	0.61
1:C:108:ASN:OD1	1:C:147:ARG:NH1	2.33	0.61
1:K:108:ASN:OD1	1:K:147:ARG:NH1	2.33	0.61
1:C:97:GLN:HG3	2:D:65:LEU:HG	1.83	0.61
1:I:72:ASP:OD1	1:I:72:ASP:N	2.27	0.61
1:Y:97:GLN:HG3	2:Z:65:LEU:HG	1.83	0.61
1:K:108:ASN:OD1	1:K:147:ARG:NH1	2.34	0.61
1:S:108:ASN:OD1	1:S:147:ARG:NH1	2.34	0.61
1:O:99:GLU:OE1	1:O:115:ARG:NH2	2.34	0.61
2:N:141:GLN:HE21	2:1:141:GLN:HE21	1.47	0.61
1:C:108:ASN:OD1	1:C:147:ARG:NH1	2.34	0.61
1:M:108:ASN:OD1	1:M:147:ARG:NH1	2.34	0.61
1:U:72:ASP:OD1	1:U:72:ASP:N	2.27	0.61
1:C:99:GLU:OE1	1:C:115:ARG:NH2	2.34	0.61
2:D:141:GLN:HE21	2:R:141:GLN:HE21	1.47	0.61
2:P:190:ASP:OD1	2:P:190:ASP:N	2.30	0.61
2:L:153:ASP:HB2	2:L:199:LEU:HD11	1.83	0.61
2:N:153:ASP:HB2	2:N:199:LEU:HD11	1.83	0.61
2:R:153:ASP:HB2	2:R:199:LEU:HD11	1.83	0.61
2:T:153:ASP:HB2	2:T:199:LEU:HD11	1.83	0.61
1:E:99:GLU:OE1	1:E:115:ARG:NH2	2.34	0.61
2:N:7:THR:HG23	2:N:108:PRO:HB2	1.83	0.61
1:G:99:GLU:OE1	1:G:115:ARG:NH2	2.34	0.61
2:F:141:GLN:HE21	2:T:141:GLN:HE21	1.47	0.61
2:B:153:ASP:HB2	2:B:199:LEU:HD11	1.83	0.61
2:D:153:ASP:HB2	2:D:199:LEU:HD11	1.83	0.61
2:N:132:PRO:HB2	2:1:132:PRO:HB2	1.82	0.61
2:P:153:ASP:HB2	2:P:199:LEU:HD11	1.83	0.61
2:1:153:ASP:HB2	2:1:199:LEU:HD11	1.83	0.61
2:J:3:THR:HG22	2:J:16:THR:HG23	1.83	0.60
2:V:3:THR:HG22	2:V:16:THR:HG23	1.83	0.60
1:Q:108:ASN:OD1	1:Q:147:ARG:NH1	2.34	0.60
2:H:7:THR:HG23	2:H:108:PRO:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:97:GLN:HG3	2:R:65:LEU:HG	1.83	0.60
1:U:97:GLN:HG3	2:V:65:LEU:HG	1.83	0.60
1:K:99:GLU:OE1	1:K:115:ARG:NH2	2.34	0.60
1:S:99:GLU:OE1	1:S:115:ARG:NH2	2.34	0.60
1:W:99:GLU:OE1	1:W:115:ARG:NH2	2.34	0.60
2:D:132:PRO:HB2	2:R:132:PRO:HB2	1.82	0.60
1:U:108:ASN:OD1	1:U:147:ARG:NH1	2.34	0.60
1:E:97:GLN:HG3	2:F:65:LEU:HG	1.83	0.60
2:F:7:THR:HG23	2:F:108:PRO:HB2	1.83	0.60
2:R:7:THR:HG23	2:R:108:PRO:HB2	1.83	0.60
1:S:97:GLN:HG3	2:T:65:LEU:HG	1.84	0.60
1:U:97:GLN:HG3	2:V:65:LEU:HG	1.83	0.60
2:X:7:THR:HG23	2:X:108:PRO:HB2	1.83	0.60
2:Z:7:THR:HG23	2:Z:108:PRO:HB2	1.83	0.60
1:C:97:GLN:HG3	2:D:65:LEU:HG	1.84	0.60
1:A:99:GLU:OE1	1:A:115:ARG:NH2	2.34	0.60
1:O:99:GLU:OE1	1:O:115:ARG:NH2	2.34	0.60
2:B:190:ASP:OD1	2:B:190:ASP:N	2.30	0.60
2:X:3:THR:HG22	2:X:16:THR:HG23	1.83	0.60
1:I:108:ASN:OD1	1:I:147:ARG:NH1	2.34	0.60
2:J:50:GLY:O	2:L:88:ASN:ND2	2.35	0.60
1:S:97:GLN:HG3	2:T:65:LEU:HG	1.84	0.60
2:H:3:THR:HG22	2:H:16:THR:HG23	1.83	0.60
2:J:7:THR:HG23	2:J:108:PRO:HB2	1.83	0.60
2:V:7:THR:HG23	2:V:108:PRO:HB2	1.83	0.60
1:M:97:GLN:HG3	2:N:65:LEU:HG	1.84	0.60
2:L:3:THR:HG22	2:L:16:THR:HG23	1.83	0.60
1:A:99:GLU:OE1	1:A:115:ARG:NH2	2.34	0.60
1:A:97:GLN:HG3	2:B:65:LEU:HG	1.83	0.60
1:G:72:ASP:N	1:G:72:ASP:OD1	2.35	0.60
1:M:97:GLN:HG3	2:N:65:LEU:HG	1.84	0.60
1:W:72:ASP:OD1	1:W:72:ASP:N	2.35	0.60
1:E:99:GLU:OE1	1:E:115:ARG:NH2	2.34	0.60
2:J:141:GLN:HE21	2:X:141:GLN:HE21	1.49	0.60
2:T:3:THR:HG22	2:T:16:THR:HG23	1.83	0.60
1:A:108:ASN:OD1	1:A:147:ARG:NH1	2.34	0.60
1:E:108:ASN:OD1	1:E:147:ARG:NH1	2.34	0.60
1:G:108:ASN:OD1	1:G:147:ARG:NH1	2.34	0.60
1:W:108:ASN:OD1	1:W:147:ARG:NH1	2.34	0.60
1:Y:108:ASN:OD1	1:Y:147:ARG:NH1	2.34	0.60
1:Q:97:GLN:HG3	2:R:65:LEU:HG	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:97:GLN:HG3	2:X:65:LEU:HG	1.83	0.60
1:I:99:GLU:OE1	1:I:115:ARG:NH2	2.34	0.60
1:Q:99:GLU:OE1	1:Q:115:ARG:NH2	2.34	0.60
1:U:99:GLU:OE1	1:U:115:ARG:NH2	2.34	0.60
2:B:132:PRO:HB2	2:P:132:PRO:HB2	1.82	0.60
2:L:132:PRO:HB2	2:Z:132:PRO:HB2	1.83	0.60
2:N:3:THR:HG22	2:N:16:THR:HG23	1.83	0.60
2:R:3:THR:HG22	2:R:16:THR:HG23	1.83	0.60
1:C:99:GLU:OE1	1:C:115:ARG:NH2	2.34	0.60
1:I:97:GLN:HG3	2:J:65:LEU:HG	1.84	0.60
1:W:97:GLN:HG3	2:X:65:LEU:HG	1.83	0.60
1:Y:97:GLN:HG3	2:Z:65:LEU:HG	1.84	0.60
1:A:97:GLN:HG3	2:B:65:LEU:HG	1.84	0.60
2:B:7:THR:HG23	2:B:108:PRO:HB2	1.83	0.60
1:Y:99:GLU:OE1	1:Y:115:ARG:NH2	2.34	0.60
1:Q:97:GLN:HG3	2:R:65:LEU:HG	1.84	0.60
2:J:153:ASP:HB2	2:J:199:LEU:HD11	1.83	0.60
1:O:108:ASN:OD1	1:O:147:ARG:NH1	2.34	0.60
1:G:97:GLN:HG3	2:H:65:LEU:HG	1.83	0.60
1:O:97:GLN:HG3	2:P:65:LEU:HG	1.84	0.60
1:M:99:GLU:OE1	1:M:115:ARG:NH2	2.34	0.60
2:F:153:ASP:HB2	2:F:199:LEU:HD11	1.83	0.60
1:W:97:GLN:HG3	2:X:65:LEU:HG	1.83	0.60
1:E:72:ASP:OD1	1:E:72:ASP:N	2.35	0.60
1:K:72:ASP:OD1	1:K:72:ASP:N	2.35	0.60
1:S:72:ASP:OD1	1:S:72:ASP:N	2.35	0.60
2:Z:153:ASP:HB2	2:Z:199:LEU:HD11	1.83	0.60
2:1:7:THR:HG23	2:1:108:PRO:HB2	1.83	0.60
1:E:97:GLN:HG3	2:F:65:LEU:HG	1.83	0.60
2:V:153:ASP:HB2	2:V:199:LEU:HD11	1.83	0.60
2:Z:91:LYS:HB2	2:1:93:MET:HE3	1.83	0.60
1:Y:72:ASP:OD1	1:Y:72:ASP:N	2.35	0.59
2:B:7:THR:HG23	2:B:108:PRO:HB2	1.83	0.59
2:D:7:THR:HG23	2:D:108:PRO:HB2	1.83	0.59
2:P:7:THR:HG23	2:P:108:PRO:HB2	1.83	0.59
2:L:7:THR:HG23	2:L:108:PRO:HB2	1.84	0.59
2:L:105:ASP:O	2:L:180:ARG:NH2	2.36	0.59
2:T:7:THR:HG23	2:T:108:PRO:HB2	1.84	0.59
1:G:97:GLN:HG3	2:H:65:LEU:HG	1.83	0.59
2:F:3:THR:HG22	2:F:16:THR:HG23	1.83	0.59
2:Z:3:THR:HG22	2:Z:16:THR:HG23	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:ASP:OD1	1:C:72:ASP:N	2.35	0.59
1:O:72:ASP:OD1	1:O:72:ASP:N	2.35	0.59
2:T:105:ASP:O	2:T:180:ARG:NH2	2.36	0.59
1:O:97:GLN:HG3	2:I:65:LEU:HG	1.85	0.59
1:C:37:ALA:O	1:C:164:ALA:HA	2.03	0.59
2:D:3:THR:HG22	2:D:16:THR:HG23	1.83	0.59
1:S:37:ALA:O	1:S:164:ALA:HA	2.03	0.59
1:E:97:GLN:HG3	2:F:65:LEU:HG	1.85	0.59
1:I:121:GLN:NE2	1:K:84:ASP:OD1	2.35	0.59
2:H:163:LYS:NZ	2:H:171:GLY:O	2.36	0.59
1:C:99:GLU:OE1	1:C:115:ARG:NH2	2.36	0.59
1:O:99:GLU:OE1	1:O:115:ARG:NH2	2.36	0.59
1:K:37:ALA:O	1:K:164:ALA:HA	2.03	0.59
1:I:72:ASP:N	1:I:72:ASP:OD1	2.35	0.59
2:F:105:ASP:O	2:F:180:ARG:NH2	2.36	0.59
2:H:105:ASP:O	2:H:180:ARG:NH2	2.36	0.59
2:N:105:ASP:O	2:N:180:ARG:NH2	2.36	0.59
2:Z:105:ASP:O	2:Z:180:ARG:NH2	2.36	0.59
2:P:3:THR:HG22	2:P:16:THR:HG23	1.85	0.59
2:P:163:LYS:NZ	2:P:171:GLY:O	2.36	0.59
1:A:99:GLU:OE1	1:A:115:ARG:NH2	2.36	0.59
2:I:3:THR:HG22	2:I:16:THR:HG23	1.83	0.59
1:O:37:ALA:O	1:O:164:ALA:HA	2.03	0.59
1:U:72:ASP:N	1:U:72:ASP:OD1	2.35	0.59
2:R:105:ASP:O	2:R:180:ARG:NH2	2.36	0.59
2:V:7:THR:HG23	2:V:108:PRO:HB2	1.84	0.59
1:Q:97:GLN:HG3	2:R:65:LEU:HG	1.85	0.59
1:I:99:GLU:OE1	1:I:115:ARG:NH2	2.36	0.59
2:B:3:THR:HG22	2:B:16:THR:HG23	1.83	0.59
1:O:152:ASP:HB3	1:O:156:THR:HB	1.85	0.59
2:P:3:THR:HG22	2:P:16:THR:HG23	1.83	0.59
1:A:37:ALA:O	1:A:164:ALA:HA	2.03	0.59
1:E:37:ALA:O	1:E:164:ALA:HA	2.03	0.59
1:I:37:ALA:O	1:I:164:ALA:HA	2.03	0.59
1:U:37:ALA:O	1:U:164:ALA:HA	2.03	0.59
2:J:7:THR:HG23	2:J:108:PRO:HB2	1.84	0.59
2:J:105:ASP:O	2:J:180:ARG:NH2	2.36	0.59
2:V:105:ASP:O	2:V:180:ARG:NH2	2.36	0.59
2:X:105:ASP:O	2:X:180:ARG:NH2	2.36	0.59
2:B:3:THR:HG22	2:B:16:THR:HG23	1.85	0.59
1:M:97:GLN:HG3	2:N:65:LEU:HG	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:99:GLU:OE1	1:O:115:ARG:NH2	2.36	0.59
1:U:99:GLU:OE1	1:U:115:ARG:NH2	2.36	0.59
1:K:152:ASP:HB3	1:K:156:THR:HB	1.85	0.59
1:M:152:ASP:HB3	1:M:156:THR:HB	1.85	0.59
1:Q:152:ASP:HB3	1:Q:156:THR:HB	1.85	0.59
2:T:3:THR:HG1	2:T:127:THR:HG1	1.50	0.59
1:Y:37:ALA:O	1:Y:164:ALA:HA	2.03	0.59
2:B:105:ASP:O	2:B:180:ARG:NH2	2.36	0.59
2:P:105:ASP:O	2:P:180:ARG:NH2	2.36	0.59
2:1:105:ASP:O	2:1:180:ARG:NH2	2.36	0.59
1:M:97:GLN:HG3	2:N:65:LEU:HG	1.85	0.59
2:Z:3:THR:HG22	2:Z:16:THR:HG23	1.85	0.59
1:S:152:ASP:HB3	1:S:156:THR:HB	1.85	0.59
1:G:37:ALA:O	1:G:164:ALA:HA	2.03	0.59
2:L:3:THR:HG1	2:L:127:THR:HG1	1.49	0.59
2:D:105:ASP:O	2:D:180:ARG:NH2	2.36	0.59
2:F:3:THR:HG22	2:F:16:THR:HG23	1.85	0.59
2:N:3:THR:HG22	2:N:16:THR:HG23	1.85	0.59
1:O:97:GLN:HG3	2:1:65:LEU:HG	1.84	0.59
1:A:152:ASP:HB3	1:A:156:THR:HB	1.85	0.58
1:Q:37:ALA:O	1:Q:164:ALA:HA	2.03	0.58
2:L:141:GLN:HE21	2:Z:141:GLN:HE21	1.51	0.58
2:N:7:THR:HG23	2:N:108:PRO:HB2	1.84	0.58
2:D:3:THR:HG22	2:D:16:THR:HG23	1.85	0.58
2:R:3:THR:HG22	2:R:16:THR:HG23	1.85	0.58
2:1:3:THR:HG22	2:1:16:THR:HG23	1.85	0.58
1:A:97:GLN:HG3	2:B:65:LEU:HG	1.85	0.58
1:G:97:GLN:HG3	2:H:65:LEU:HG	1.84	0.58
2:X:3:THR:HG1	2:X:127:THR:HG1	1.50	0.58
1:G:99:GLU:OE1	1:G:115:ARG:NH2	2.36	0.58
2:H:141:GLN:HE21	2:V:141:GLN:HE21	1.50	0.58
1:W:99:GLU:OE1	1:W:115:ARG:NH2	2.36	0.58
2:X:92:TYR:HD1	2:Z:93:MET:HE1	1.68	0.58
1:M:37:ALA:O	1:M:164:ALA:HA	2.03	0.58
1:W:37:ALA:O	1:W:164:ALA:HA	2.03	0.58
2:D:163:LYS:NZ	2:D:171:GLY:O	2.36	0.58
1:W:97:GLN:HG3	2:X:65:LEU:HG	1.84	0.58
2:H:153:ASP:HB2	2:H:199:LEU:HD11	1.83	0.58
1:C:152:ASP:HB3	1:C:156:THR:HB	1.85	0.58
2:H:7:THR:HG23	2:H:108:PRO:HB2	1.84	0.58
2:R:7:THR:HG23	2:R:108:PRO:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:7:THR:HG23	2:Z:108:PRO:HB2	1.84	0.58
1:K:97:GLN:HG3	2:L:65:LEU:HG	1.84	0.58
1:U:97:GLN:HG3	2:V:65:LEU:HG	1.84	0.58
1:K:99:GLU:OE1	1:K:115:ARG:NH2	2.36	0.58
2:F:7:THR:HG23	2:F:108:PRO:HB2	1.84	0.58
2:X:7:THR:HG23	2:X:108:PRO:HB2	1.84	0.58
2:1:163:LYS:NZ	2:1:171:GLY:O	2.36	0.58
1:I:97:GLN:HG3	2:J:65:LEU:HG	1.84	0.58
1:S:97:GLN:HG3	2:T:65:LEU:HG	1.84	0.58
1:Q:99:GLU:OE1	1:Q:115:ARG:NH2	2.36	0.58
1:S:99:GLU:OE1	1:S:115:ARG:NH2	2.36	0.58
1:O:152:ASP:HB3	1:O:156:THR:HB	1.85	0.58
2:B:105:ASP:O	2:B:180:ARG:NH2	2.37	0.58
2:D:105:ASP:O	2:D:180:ARG:NH2	2.37	0.58
1:M:72:ASP:OD1	1:M:72:ASP:N	2.35	0.58
1:I:97:GLN:HG3	2:J:65:LEU:HG	1.85	0.58
1:K:97:GLN:HG3	2:L:65:LEU:HG	1.84	0.58
1:M:99:GLU:OE1	1:M:115:ARG:NH2	2.36	0.58
2:X:153:ASP:HB2	2:X:199:LEU:HD11	1.83	0.58
1:K:121:GLN:NE2	1:M:84:ASP:OD1	2.36	0.58
1:W:84:ASP:OD1	1:Y:121:GLN:NE2	2.37	0.58
1:A:99:GLU:OE1	1:A:115:ARG:NH2	2.36	0.58
2:H:3:THR:HG22	2:H:16:THR:HG23	1.85	0.58
2:X:3:THR:HG22	2:X:16:THR:HG23	1.85	0.58
1:G:37:ALA:O	1:G:164:ALA:HA	2.04	0.58
1:W:37:ALA:O	1:W:164:ALA:HA	2.04	0.58
2:J:93:MET:HE3	2:L:91:LYS:HB2	1.85	0.58
2:R:91:LYS:HB2	2:T:93:MET:HE3	1.84	0.58
1:Y:99:GLU:OE1	1:Y:115:ARG:NH2	2.36	0.58
1:K:97:GLN:HG3	2:L:65:LEU:HG	1.86	0.58
1:Q:72:ASP:N	1:Q:72:ASP:OD1	2.35	0.58
1:S:84:ASP:OD1	1:U:121:GLN:NE2	2.36	0.58
1:E:99:GLU:OE1	1:E:115:ARG:NH2	2.36	0.58
2:X:70:ARG:NH2	1:Y:99:GLU:OE2	2.36	0.58
1:E:152:ASP:HB3	1:E:156:THR:HB	1.85	0.58
1:Y:152:ASP:HB3	1:Y:156:THR:HB	1.85	0.58
2:T:7:THR:HG23	2:T:108:PRO:HB2	1.85	0.58
2:D:7:THR:HG23	2:D:108:PRO:HB2	1.84	0.58
1:Q:84:ASP:OD1	1:S:121:GLN:NE2	2.37	0.58
2:1:7:THR:HG23	2:1:108:PRO:HB2	1.84	0.58
2:B:193:GLU:HG2	2:B:203:LEU:HD21	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:GLU:OE1	1:C:115:ARG:NH2	2.36	0.58
1:E:36:THR:HA	1:E:165:ILE:O	2.04	0.58
1:G:36:THR:HA	1:G:165:ILE:O	2.04	0.58
1:I:36:THR:HA	1:I:165:ILE:O	2.04	0.58
2:J:105:ASP:O	2:J:180:ARG:NH2	2.37	0.58
1:U:36:THR:HA	1:U:165:ILE:O	2.04	0.58
2:V:105:ASP:O	2:V:180:ARG:NH2	2.37	0.58
1:W:36:THR:HA	1:W:165:ILE:O	2.04	0.58
1:O:121:GLN:NE2	1:O:84:ASP:OD1	2.36	0.58
2:L:105:ASP:O	2:L:180:ARG:NH2	2.37	0.58
1:Y:37:ALA:O	1:Y:164:ALA:HA	2.04	0.58
1:Y:97:GLN:HG3	2:Z:65:LEU:HG	1.84	0.58
1:I:152:ASP:HB3	1:I:156:THR:HB	1.85	0.58
2:D:7:THR:HG23	2:D:108:PRO:HB2	1.85	0.58
2:L:7:THR:HG23	2:L:108:PRO:HB2	1.86	0.58
1:A:72:ASP:OD1	1:A:72:ASP:N	2.35	0.58
1:U:84:ASP:OD1	1:W:121:GLN:NE2	2.37	0.58
1:O:97:GLN:HG3	2:P:65:LEU:HG	1.86	0.58
1:C:36:THR:HA	1:C:165:ILE:O	2.04	0.58
1:E:37:ALA:O	1:E:164:ALA:HA	2.04	0.58
2:H:105:ASP:O	2:H:180:ARG:NH2	2.37	0.58
1:I:37:ALA:O	1:I:164:ALA:HA	2.04	0.58
2:T:105:ASP:O	2:T:180:ARG:NH2	2.37	0.58
2:X:105:ASP:O	2:X:180:ARG:NH2	2.37	0.58
1:Y:36:THR:HA	1:Y:165:ILE:O	2.04	0.58
1:G:97:GLN:HG3	2:H:65:LEU:HG	1.85	0.58
1:E:39:GLY:O	1:E:162:ALA:HA	2.04	0.57
2:P:88:ASN:ND2	2:R:50:GLY:O	2.37	0.57
2:T:3:THR:HG22	2:T:16:THR:HG23	1.85	0.57
1:C:37:ALA:O	1:C:164:ALA:HA	2.04	0.57
1:M:36:THR:HA	1:M:165:ILE:O	2.04	0.57
1:Q:36:THR:HA	1:Q:165:ILE:O	2.04	0.57
1:U:37:ALA:O	1:U:164:ALA:HA	2.04	0.57
1:O:36:THR:HA	1:O:165:ILE:O	2.04	0.57
1:U:152:ASP:HB3	1:U:156:THR:HB	1.85	0.57
1:W:152:ASP:HB3	1:W:156:THR:HB	1.85	0.57
2:H:7:THR:HG23	2:H:108:PRO:HB2	1.85	0.57
1:K:97:GLN:HG3	2:L:65:LEU:HG	1.86	0.57
2:P:7:THR:HG23	2:P:108:PRO:HB2	1.85	0.57
1:O:178:ARG:HG3	1:O:179:GLU:HG2	1.86	0.57
1:A:121:GLN:NE2	1:C:84:ASP:OD1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:97:GLN:HG3	2:J:65:LEU:HG	1.86	0.57
1:S:97:GLN:HG3	2:T:65:LEU:HG	1.87	0.57
2:L:3:THR:HG22	2:L:16:THR:HG23	1.85	0.57
2:V:3:THR:HG22	2:V:16:THR:HG23	1.85	0.57
1:E:97:GLN:HG3	2:F:65:LEU:HG	1.85	0.57
1:S:36:THR:HA	1:S:165:ILE:O	2.04	0.57
1:E:97:GLN:HG3	2:F:65:LEU:HG	1.86	0.57
2:B:7:THR:HG23	2:B:108:PRO:HB2	1.86	0.57
1:G:39:GLY:O	1:G:162:ALA:HA	2.05	0.57
1:I:39:GLY:O	1:I:162:ALA:HA	2.05	0.57
1:M:97:GLN:HG3	2:N:65:LEU:HG	1.86	0.57
1:W:39:GLY:O	1:W:162:ALA:HA	2.05	0.57
2:X:7:THR:HG23	2:X:108:PRO:HB2	1.86	0.57
1:Y:39:GLY:O	1:Y:162:ALA:HA	2.05	0.57
2:D:93:MET:HG3	2:D:94:PRO:HD3	1.86	0.57
1:A:178:ARG:HG3	1:A:179:GLU:HG2	1.86	0.57
2:B:7:THR:HG23	2:B:108:PRO:HB2	1.84	0.57
2:P:7:THR:HG23	2:P:108:PRO:HB2	1.84	0.57
1:Y:84:ASP:OD1	1:O:121:GLN:NE2	2.37	0.57
1:G:121:GLN:NE2	1:I:84:ASP:OD1	2.37	0.57
2:T:3:THR:HG1	2:T:127:THR:HG1	1.51	0.57
2:J:10:ASP:OD1	2:J:10:ASP:N	2.37	0.57
1:O:97:GLN:HG3	2:1:65:LEU:HG	1.85	0.57
1:G:152:ASP:HB3	1:G:156:THR:HB	1.85	0.57
1:C:39:GLY:O	1:C:162:ALA:HA	2.04	0.57
2:B:93:MET:HG3	2:B:94:PRO:HD3	1.86	0.57
1:A:36:THR:HA	1:A:165:ILE:O	2.04	0.57
1:K:36:THR:HA	1:K:165:ILE:O	2.04	0.57
1:O:36:THR:HA	1:O:165:ILE:O	2.04	0.57
1:O:37:ALA:O	1:O:164:ALA:HA	2.04	0.57
1:A:99:GLU:OE2	2:D:70:ARG:NH2	2.37	0.57
1:C:97:GLN:HG3	2:D:65:LEU:HG	1.85	0.57
2:R:10:ASP:N	2:R:10:ASP:OD1	2.37	0.57
1:S:97:GLN:HG3	2:T:65:LEU:HG	1.85	0.57
2:V:10:ASP:OD1	2:V:10:ASP:N	2.37	0.57
1:G:97:GLN:HG3	2:H:65:LEU:HG	1.85	0.57
1:S:39:GLY:O	1:S:162:ALA:HA	2.04	0.57
1:U:39:GLY:O	1:U:162:ALA:HA	2.05	0.57
2:V:7:THR:HG23	2:V:108:PRO:HB2	1.86	0.57
2:B:88:ASN:ND2	2:N:50:GLY:O	2.38	0.57
1:C:41:LYS:HG2	1:C:46:VAL:HG12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:41:LYS:HG2	1:O:46:VAL:HG12	1.86	0.57
2:J:3:THR:HG22	2:J:16:THR:HG23	1.85	0.57
1:Q:37:ALA:O	1:Q:164:ALA:HA	2.04	0.57
2:L:93:MET:HE3	2:N:91:LYS:HB2	1.86	0.57
2:N:10:ASP:OD1	2:N:10:ASP:N	2.37	0.57
2:P:3:THR:HG1	2:P:127:THR:HG1	1.52	0.57
2:J:7:THR:HG23	2:J:108:PRO:HB2	1.85	0.57
1:A:41:LYS:HG2	1:A:46:VAL:HG12	1.86	0.57
2:L:3:THR:HG1	2:L:127:THR:HG1	1.52	0.57
1:M:37:ALA:O	1:M:164:ALA:HA	2.04	0.57
1:K:39:GLY:O	1:K:162:ALA:HA	2.05	0.57
1:E:178:ARG:HG3	1:E:179:GLU:HG2	1.86	0.57
1:Y:178:ARG:HG3	1:Y:179:GLU:HG2	1.86	0.57
1:O:41:LYS:HG2	1:O:46:VAL:HG12	1.86	0.57
2:B:105:ASP:O	2:B:180:ARG:NH2	2.38	0.57
2:L:50:GLY:O	2:N:88:ASN:ND2	2.38	0.57
2:B:7:THR:HG23	2:B:108:PRO:HB2	1.87	0.57
2:D:7:THR:HG23	2:D:108:PRO:HB2	1.87	0.57
2:N:105:ASP:O	2:N:180:ARG:NH2	2.37	0.57
2:P:7:THR:HG23	2:P:108:PRO:HB2	1.87	0.57
2:I:7:THR:HG23	2:I:108:PRO:HB2	1.87	0.57
1:Y:57:ARG:NH2	1:O:179:GLU:O	2.35	0.57
1:G:178:ARG:HG3	1:G:179:GLU:HG2	1.86	0.57
2:L:50:GLY:O	2:N:88:ASN:ND2	2.38	0.57
1:M:178:ARG:HG3	1:M:179:GLU:HG2	1.86	0.57
1:W:178:ARG:HG3	1:W:179:GLU:HG2	1.86	0.57
2:X:3:THR:HG1	2:X:127:THR:HG1	1.52	0.57
2:R:105:ASP:O	2:R:180:ARG:NH2	2.37	0.57
2:Z:105:ASP:O	2:Z:180:ARG:NH2	2.37	0.57
2:F:10:ASP:N	2:F:10:ASP:OD1	2.37	0.57
2:J:3:THR:HG1	2:J:127:THR:HG1	1.49	0.57
2:F:3:THR:O	2:F:126:SER:HA	2.05	0.57
2:R:7:THR:HG23	2:R:108:PRO:HB2	1.85	0.57
2:Z:3:THR:O	2:Z:126:SER:HA	2.05	0.57
1:S:178:ARG:HG3	1:S:179:GLU:HG2	1.86	0.57
2:H:179:THR:O	2:H:183:GLY:HA2	2.05	0.57
1:K:97:GLN:HG3	2:L:65:LEU:HG	1.87	0.57
2:D:105:ASP:O	2:D:180:ARG:NH2	2.37	0.57
2:F:105:ASP:O	2:F:180:ARG:NH2	2.37	0.57
2:I:105:ASP:O	2:I:180:ARG:NH2	2.37	0.57
2:L:7:THR:HG23	2:L:108:PRO:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:7:THR:HG23	2:T:108:PRO:HB2	1.87	0.57
2:X:7:THR:HG23	2:X:108:PRO:HB2	1.86	0.57
2:F:7:THR:HG23	2:F:108:PRO:HB2	1.86	0.57
2:N:7:THR:HG23	2:N:108:PRO:HB2	1.86	0.57
2:Z:7:THR:HG23	2:Z:108:PRO:HB2	1.85	0.57
1:C:178:ARG:HG3	1:C:179:GLU:HG2	1.86	0.57
1:Q:178:ARG:HG3	1:Q:179:GLU:HG2	1.86	0.57
1:O:178:ARG:HG3	1:O:179:GLU:HG2	1.86	0.57
2:T:3:THR:HG1	2:T:127:THR:HG1	1.53	0.57
1:W:84:ASP:OD1	1:Y:121:GLN:NE2	2.38	0.57
2:B:105:ASP:O	2:B:180:ARG:NH2	2.37	0.57
2:B:7:THR:HG23	2:B:108:PRO:HB2	1.86	0.57
2:D:7:THR:HG23	2:D:108:PRO:HB2	1.87	0.57
2:H:7:THR:HG23	2:H:108:PRO:HB2	1.86	0.57
1:S:84:ASP:OD1	1:U:121:GLN:NE2	2.38	0.57
2:Z:10:ASP:OD1	2:Z:10:ASP:N	2.37	0.57
2:I:7:THR:HG23	2:I:108:PRO:HB2	1.86	0.57
1:I:97:GLN:HG3	2:J:65:LEU:HG	1.86	0.56
1:M:39:GLY:O	1:M:162:ALA:HA	2.05	0.56
1:Q:39:GLY:O	1:Q:162:ALA:HA	2.04	0.56
1:K:178:ARG:HG3	1:K:179:GLU:HG2	1.86	0.56
1:A:84:ASP:OD1	1:M:121:GLN:NE2	2.36	0.56
1:G:41:LYS:HG2	1:G:46:VAL:HG12	1.86	0.56
2:X:179:THR:O	2:X:183:GLY:HA2	2.05	0.56
1:A:37:ALA:O	1:A:164:ALA:HA	2.04	0.56
1:O:37:ALA:O	1:O:164:ALA:HA	2.04	0.56
2:L:10:ASP:OD1	2:L:10:ASP:N	2.37	0.56
1:O:97:GLN:HG3	2:P:65:LEU:HG	1.85	0.56
2:P:7:THR:HG23	2:P:108:PRO:HB2	1.87	0.56
2:T:10:ASP:OD1	2:T:10:ASP:N	2.37	0.56
1:A:39:GLY:O	1:A:162:ALA:HA	2.05	0.56
2:D:3:THR:O	2:D:126:SER:HA	2.05	0.56
1:O:97:GLN:HG3	2:P:65:LEU:HG	1.87	0.56
2:D:194:SER:O	2:D:198:LYS:HB2	2.05	0.56
1:U:178:ARG:HG3	1:U:179:GLU:HG2	1.86	0.56
1:A:121:GLN:NE2	1:C:84:ASP:OD1	2.38	0.56
2:P:105:ASP:O	2:P:180:ARG:NH2	2.37	0.56
1:A:39:GLY:O	1:A:162:ALA:HA	2.05	0.56
1:O:39:GLY:O	1:O:162:ALA:HA	2.05	0.56
2:V:3:THR:HG1	2:V:127:THR:HG1	1.51	0.56
2:H:3:THR:O	2:H:126:SER:HA	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:39:GLY:O	1:O:162:ALA:HA	2.05	0.56
2:X:3:THR:O	2:X:126:SER:HA	2.05	0.56
2:B:194:SER:O	2:B:198:LYS:HB2	2.05	0.56
1:E:39:GLY:O	1:E:162:ALA:HA	2.05	0.56
1:I:178:ARG:HG3	1:I:179:GLU:HG2	1.86	0.56
2:T:88:ASN:ND2	2:V:50:GLY:O	2.39	0.56
2:T:105:ASP:O	2:T:180:ARG:NH2	2.39	0.56
1:S:41:LYS:HG2	1:S:46:VAL:HG12	1.86	0.56
2:F:179:THR:O	2:F:183:GLY:HA2	2.05	0.56
1:Y:97:GLN:HG3	2:Z:65:LEU:HG	1.87	0.56
2:Z:179:THR:O	2:Z:183:GLY:HA2	2.05	0.56
1:O:121:GLN:NE2	1:O:84:ASP:OD1	2.38	0.56
1:Q:84:ASP:OD1	1:S:121:GLN:NE2	2.36	0.56
2:X:163:LYS:NZ	2:X:171:GLY:O	2.36	0.56
1:K:37:ALA:O	1:K:164:ALA:HA	2.04	0.56
1:S:37:ALA:O	1:S:164:ALA:HA	2.04	0.56
1:Y:97:GLN:HG3	2:Z:65:LEU:HG	1.87	0.56
1:C:39:GLY:O	1:C:162:ALA:HA	2.05	0.56
1:W:39:GLY:O	1:W:162:ALA:HA	2.05	0.56
2:V:3:THR:O	2:V:126:SER:HA	2.05	0.56
1:W:97:GLN:HG3	2:X:65:LEU:HG	1.86	0.56
1:K:41:LYS:HG2	1:K:46:VAL:HG12	1.86	0.56
1:A:121:GLN:NE2	1:C:84:ASP:OD1	2.39	0.56
2:P:179:THR:O	2:P:183:GLY:HA2	2.05	0.56
2:N:7:THR:HG23	2:N:108:PRO:HB2	1.87	0.56
1:C:99:GLU:OE2	2:F:70:ARG:NH2	2.36	0.56
1:G:39:GLY:O	1:G:162:ALA:HA	2.05	0.56
2:J:3:THR:O	2:J:126:SER:HA	2.05	0.56
2:L:3:THR:O	2:L:126:SER:HA	2.05	0.56
1:Q:97:GLN:HG3	2:R:65:LEU:HG	1.88	0.56
2:T:3:THR:O	2:T:126:SER:HA	2.05	0.56
1:U:41:LYS:HG2	1:U:46:VAL:HG12	1.87	0.56
1:W:41:LYS:HG2	1:W:46:VAL:HG12	1.88	0.56
2:F:50:GLY:O	2:H:88:ASN:ND2	2.39	0.56
2:L:105:ASP:O	2:L:180:ARG:NH2	2.39	0.56
1:C:121:GLN:NE2	1:E:84:ASP:OD1	2.36	0.56
1:E:41:LYS:HG2	1:E:46:VAL:HG12	1.86	0.56
1:O:84:ASP:OD1	1:Q:121:GLN:NE2	2.37	0.56
1:Y:41:LYS:HG2	1:Y:46:VAL:HG12	1.86	0.56
1:A:84:ASP:OD1	1:M:121:GLN:NE2	2.39	0.56
2:Z:88:ASN:ND2	2:1:50:GLY:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:121:GLN:NE2	1:K:84:ASP:OD1	2.38	0.56
1:S:97:GLN:HG3	2:T:65:LEU:HG	1.88	0.56
2:F:7:THR:HG23	2:F:108:PRO:HB2	1.87	0.56
2:R:7:THR:HG23	2:R:108:PRO:HB2	1.87	0.56
2:V:7:THR:HG23	2:V:108:PRO:HB2	1.87	0.56
1:I:39:GLY:O	1:I:162:ALA:HA	2.05	0.56
1:U:39:GLY:O	1:U:162:ALA:HA	2.05	0.56
1:G:41:LYS:HG2	1:G:46:VAL:HG12	1.87	0.56
1:I:41:LYS:HG2	1:I:46:VAL:HG12	1.88	0.56
2:P:3:THR:O	2:P:126:SER:HA	2.05	0.56
2:J:105:ASP:O	2:J:180:ARG:NH2	2.39	0.56
2:V:105:ASP:O	2:V:180:ARG:NH2	2.39	0.56
1:W:41:LYS:HG2	1:W:46:VAL:HG12	1.86	0.56
2:B:179:THR:O	2:B:183:GLY:HA2	2.05	0.56
2:F:50:GLY:O	2:H:88:ASN:ND2	2.39	0.56
2:P:50:GLY:O	2:1:88:ASN:ND2	2.39	0.56
2:Z:163:LYS:NZ	2:Z:171:GLY:O	2.36	0.56
2:H:7:THR:HG23	2:H:108:PRO:HB2	1.87	0.56
2:L:7:THR:HG23	2:L:108:PRO:HB2	1.87	0.56
2:T:7:THR:HG23	2:T:108:PRO:HB2	1.87	0.56
2:X:7:THR:HG23	2:X:108:PRO:HB2	1.87	0.56
2:Z:7:THR:HG23	2:Z:108:PRO:HB2	1.87	0.56
2:B:93:MET:HE3	2:D:91:LYS:HB2	1.87	0.56
1:M:97:GLN:HG3	2:N:65:LEU:HG	1.86	0.56
2:P:93:MET:HE3	2:1:91:LYS:HB2	1.87	0.56
1:Q:39:GLY:O	1:Q:162:ALA:HA	2.05	0.56
1:O:39:GLY:O	1:O:162:ALA:HA	2.05	0.56
2:1:105:ASP:O	2:1:180:ARG:NH2	2.39	0.56
2:D:50:GLY:O	2:F:88:ASN:ND2	2.39	0.56
2:V:88:ASN:ND2	2:X:50:GLY:O	2.39	0.56
2:X:105:ASP:O	2:X:180:ARG:NH2	2.39	0.56
1:Q:41:LYS:HG2	1:Q:46:VAL:HG12	1.86	0.56
1:I:97:GLN:HG3	2:J:65:LEU:HG	1.88	0.56
1:O:84:ASP:OD1	1:Q:121:GLN:NE2	2.38	0.56
2:P:88:ASN:ND2	2:R:50:GLY:O	2.39	0.56
2:J:7:THR:HG23	2:J:108:PRO:HB2	1.86	0.56
2:N:7:THR:HG23	2:N:108:PRO:HB2	1.86	0.56
2:B:105:ASP:O	2:B:180:ARG:NH2	2.39	0.56
2:D:105:ASP:O	2:D:180:ARG:NH2	2.39	0.56
2:F:105:ASP:O	2:F:180:ARG:NH2	2.39	0.56
1:M:39:GLY:O	1:M:162:ALA:HA	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:105:ASP:O	2:P:180:ARG:NH2	2.39	0.56
2:Z:105:ASP:O	2:Z:180:ARG:NH2	2.39	0.56
2:B:3:THR:O	2:B:126:SER:HA	2.05	0.56
1:Y:97:GLN:HG3	2:Z:65:LEU:HG	1.87	0.56
2:H:105:ASP:O	2:H:180:ARG:NH2	2.39	0.56
2:N:105:ASP:O	2:N:180:ARG:NH2	2.39	0.56
2:R:105:ASP:O	2:R:180:ARG:NH2	2.39	0.56
2:X:88:ASN:ND2	2:Z:50:GLY:O	2.39	0.56
1:A:121:GLN:NE2	1:C:84:ASP:OD1	2.38	0.56
2:D:179:THR:O	2:D:183:GLY:HA2	2.05	0.56
1:E:97:GLN:HG3	2:F:65:LEU:HG	1.88	0.56
1:U:97:GLN:HG3	2:V:65:LEU:HG	1.88	0.56
1:I:97:GLN:HG3	2:J:65:LEU:HG	1.86	0.56
2:B:91:LYS:HB2	2:N:93:MET:HE3	1.87	0.56
1:Q:97:GLN:HG3	2:R:65:LEU:HG	1.86	0.56
2:R:7:THR:HG23	2:R:108:PRO:HB2	1.86	0.56
2:Z:7:THR:HG23	2:Z:108:PRO:HB2	1.86	0.56
1:U:41:LYS:HG2	1:U:46:VAL:HG12	1.86	0.56
1:Y:84:ASP:OD1	1:O:121:GLN:NE2	2.37	0.56
1:G:97:GLN:HG3	2:H:65:LEU:HG	1.87	0.56
2:V:179:THR:O	2:V:183:GLY:HA2	2.05	0.56
2:X:88:ASN:ND2	2:Z:50:GLY:O	2.39	0.56
1:O:84:ASP:OD1	1:Q:121:GLN:NE2	2.38	0.56
1:W:152:ASP:O	1:W:155:GLY:N	2.36	0.56
1:M:39:GLY:O	1:M:162:ALA:HA	2.06	0.56
1:A:84:ASP:OD1	1:M:121:GLN:NE2	2.38	0.56
2:F:7:THR:HG23	2:F:108:PRO:HB2	1.87	0.56
1:E:39:GLY:O	1:E:162:ALA:HA	2.05	0.56
1:A:41:LYS:HG2	1:A:46:VAL:HG12	1.88	0.56
2:N:3:THR:O	2:N:126:SER:HA	2.05	0.56
2:R:3:THR:O	2:R:126:SER:HA	2.05	0.56
1:Y:41:LYS:HG2	1:Y:46:VAL:HG12	1.88	0.56
2:H:50:GLY:O	2:J:88:ASN:ND2	2.39	0.56
1:I:41:LYS:HG2	1:I:46:VAL:HG12	1.86	0.56
1:M:41:LYS:HG2	1:M:46:VAL:HG12	1.86	0.56
1:O:121:GLN:NE2	1:O:84:ASP:OD1	2.39	0.56
1:W:97:GLN:HG3	2:X:65:LEU:HG	1.87	0.56
2:1:179:THR:O	2:1:183:GLY:HA2	2.05	0.56
1:E:121:GLN:NE2	1:G:84:ASP:OD1	2.39	0.56
2:F:163:LYS:NZ	2:F:171:GLY:O	2.36	0.56
1:K:121:GLN:NE2	1:M:84:ASP:OD1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:39:GLY:O	1:O:162:ALA:HA	2.06	0.56
2:N:105:ASP:O	2:N:180:ARG:NH2	2.39	0.55
2:R:105:ASP:O	2:R:180:ARG:NH2	2.39	0.55
1:E:41:LYS:HG2	1:E:46:VAL:HG12	1.87	0.55
1:O:41:LYS:HG2	1:O:46:VAL:HG12	1.88	0.55
2:J:179:THR:O	2:J:183:GLY:HA2	2.05	0.55
1:A:84:ASP:OD1	1:M:121:GLN:NE2	2.39	0.55
1:G:152:ASP:O	1:G:155:GLY:N	2.36	0.55
1:Q:152:ASP:O	1:Q:155:GLY:N	2.36	0.55
1:A:39:GLY:O	1:A:162:ALA:HA	2.06	0.55
1:Q:39:GLY:O	1:Q:162:ALA:HA	2.07	0.55
2:L:105:ASP:O	2:L:180:ARG:NH2	2.39	0.55
1:O:57:ARG:NH2	1:Q:179:GLU:O	2.38	0.55
1:Y:39:GLY:O	1:Y:162:ALA:HA	2.05	0.55
1:U:57:ARG:NH1	1:W:182:GLU:OE2	2.40	0.55
2:T:179:THR:O	2:T:183:GLY:HA2	2.05	0.55
1:C:39:GLY:O	1:C:162:ALA:HA	2.07	0.55
1:O:39:GLY:O	1:O:162:ALA:HA	2.06	0.55
1:E:121:GLN:NE2	1:G:84:ASP:OD1	2.38	0.55
2:R:70:ARG:NH2	1:S:99:GLU:OE2	2.39	0.55
2:T:105:ASP:O	2:T:180:ARG:NH2	2.39	0.55
1:A:173:VAL:O	1:A:177:GLU:HB2	2.06	0.55
2:F:105:ASP:O	2:F:180:ARG:NH2	2.39	0.55
1:W:84:ASP:OD1	1:Y:121:GLN:NE2	2.39	0.55
2:J:50:GLY:O	2:L:88:ASN:ND2	2.39	0.55
2:L:179:THR:O	2:L:183:GLY:HA2	2.05	0.55
1:M:152:ASP:O	1:M:155:GLY:N	2.36	0.55
1:Y:152:ASP:O	1:Y:155:GLY:N	2.36	0.55
2:J:7:THR:HG23	2:J:108:PRO:HB2	1.87	0.55
1:K:39:GLY:O	1:K:162:ALA:HA	2.06	0.55
1:S:39:GLY:O	1:S:162:ALA:HA	2.06	0.55
1:M:173:VAL:O	1:M:177:GLU:HB2	2.06	0.55
1:Q:57:ARG:NH1	1:S:182:GLU:OE2	2.40	0.55
1:C:39:GLY:O	1:C:162:ALA:HA	2.06	0.55
2:B:50:GLY:O	2:D:88:ASN:ND2	2.39	0.55
2:R:88:ASN:ND2	2:T:50:GLY:O	2.39	0.55
2:Z:105:ASP:O	2:Z:180:ARG:NH2	2.39	0.55
2:V:7:THR:HG23	2:V:108:PRO:HB2	1.87	0.55
2:H:105:ASP:O	2:H:180:ARG:NH2	2.39	0.55
1:K:39:GLY:O	1:K:162:ALA:HA	2.05	0.55
1:S:39:GLY:O	1:S:162:ALA:HA	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:57:ARG:NH2	1:Y:179:GLU:O	2.38	0.55
1:K:41:LYS:HG2	1:K:46:VAL:HG12	1.88	0.55
1:O:57:ARG:NH1	1:Q:182:GLU:OE2	2.40	0.55
1:Q:173:VAL:O	1:Q:177:GLU:HB2	2.06	0.55
1:S:41:LYS:HG2	1:S:46:VAL:HG12	1.88	0.55
1:E:152:ASP:O	1:E:155:GLY:N	2.36	0.55
2:X:10:ASP:OD1	2:X:10:ASP:N	2.37	0.55
1:A:57:ARG:NH2	1:M:179:GLU:O	2.39	0.55
1:G:173:VAL:O	1:G:177:GLU:HB2	2.06	0.55
1:I:173:VAL:O	1:I:177:GLU:HB2	2.06	0.55
1:M:41:LYS:HG2	1:M:46:VAL:HG12	1.88	0.55
2:N:3:THR:HG1	2:N:127:THR:HG1	1.49	0.55
1:O:173:VAL:O	1:O:177:GLU:HB2	2.06	0.55
1:Q:41:LYS:HG2	1:Q:46:VAL:HG12	1.88	0.55
2:R:3:THR:HG1	2:R:127:THR:HG1	1.49	0.55
2:B:105:ASP:O	2:B:180:ARG:NH2	2.39	0.55
2:P:105:ASP:O	2:P:180:ARG:NH2	2.39	0.55
1:K:121:GLN:NE2	1:M:84:ASP:OD1	2.40	0.55
2:N:179:THR:O	2:N:183:GLY:HA2	2.05	0.55
1:I:39:GLY:O	1:I:162:ALA:HA	2.07	0.55
1:U:39:GLY:O	1:U:162:ALA:HA	2.07	0.55
2:B:3:THR:HG1	2:B:127:THR:HG1	1.54	0.55
2:X:105:ASP:O	2:X:180:ARG:NH2	2.39	0.55
1:U:173:VAL:O	1:U:177:GLU:HB2	2.06	0.55
1:W:173:VAL:O	1:W:177:GLU:HB2	2.06	0.55
2:R:179:THR:O	2:R:183:GLY:HA2	2.05	0.55
2:H:10:ASP:N	2:H:10:ASP:OD1	2.37	0.55
2:J:43:MET:HE1	2:J:59:MET:HG3	1.89	0.55
2:V:43:MET:HE1	2:V:59:MET:HG3	1.89	0.55
2:R:105:ASP:O	2:R:180:ARG:NH2	2.40	0.55
1:S:57:ARG:NH1	1:U:182:GLU:OE2	2.39	0.55
1:S:84:ASP:OD1	1:U:121:GLN:NE2	2.40	0.55
1:W:57:ARG:NH1	1:Y:182:GLU:OE2	2.40	0.55
1:I:121:GLN:NE2	1:K:84:ASP:OD1	2.40	0.55
1:A:172:VAL:HG13	1:A:196:ALA:HB1	1.89	0.55
2:H:50:GLY:O	2:J:88:ASN:ND2	2.39	0.55
2:V:163:LYS:NZ	2:V:171:GLY:O	2.36	0.55
1:E:39:GLY:O	1:E:162:ALA:HA	2.06	0.55
2:L:43:MET:HE1	2:L:59:MET:HG3	1.89	0.55
2:T:43:MET:HE1	2:T:59:MET:HG3	1.89	0.55
1:C:41:LYS:HG2	1:C:46:VAL:HG12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:105:ASP:O	2:N:180:ARG:NH2	2.40	0.55
1:U:97:GLN:HG3	2:V:65:LEU:HG	1.88	0.55
2:D:105:ASP:O	2:D:180:ARG:NH2	2.39	0.55
1:S:84:ASP:OD1	1:U:121:GLN:NE2	2.40	0.55
2:J:163:LYS:NZ	2:J:171:GLY:O	2.36	0.55
1:G:39:GLY:O	1:G:162:ALA:HA	2.06	0.55
2:J:43:MET:HE1	2:J:59:MET:HG3	1.89	0.55
2:V:43:MET:HE1	2:V:59:MET:HG3	1.89	0.55
2:Z:70:ARG:NH2	1:O:99:GLU:OE2	2.40	0.55
2:N:43:MET:HE1	2:N:59:MET:HG3	1.89	0.55
2:R:43:MET:HE1	2:R:59:MET:HG3	1.89	0.55
2:V:105:ASP:O	2:V:180:ARG:NH2	2.39	0.55
1:A:97:GLN:HG3	2:B:65:LEU:HG	1.89	0.55
1:I:121:GLN:NE2	1:K:84:ASP:OD1	2.40	0.55
2:V:88:ASN:ND2	2:X:50:GLY:O	2.39	0.55
1:C:121:GLN:NE2	1:E:84:ASP:OD1	2.38	0.55
1:W:39:GLY:O	1:W:162:ALA:HA	2.07	0.55
1:Y:39:GLY:O	1:Y:162:ALA:HA	2.07	0.55
1:E:179:GLU:O	1:G:57:ARG:NH2	2.39	0.54
2:H:43:MET:HE1	2:H:59:MET:HG3	1.89	0.54
2:J:105:ASP:O	2:J:180:ARG:NH2	2.39	0.54
2:X:43:MET:HE1	2:X:59:MET:HG3	1.89	0.54
2:B:105:ASP:O	2:B:180:ARG:NH2	2.40	0.54
1:E:121:GLN:NE2	1:G:84:ASP:OD1	2.39	0.54
2:F:105:ASP:O	2:F:180:ARG:NH2	2.40	0.54
1:K:121:GLN:NE2	1:M:84:ASP:OD1	2.40	0.54
1:K:182:GLU:OE2	1:M:57:ARG:NH1	2.40	0.54
1:Q:84:ASP:OD1	1:S:121:GLN:NE2	2.40	0.54
1:S:97:GLN:HG3	2:T:65:LEU:HG	1.89	0.54
1:A:39:GLY:O	1:A:162:ALA:HA	2.06	0.54
2:I:105:ASP:O	2:I:180:ARG:NH2	2.39	0.54
1:E:121:GLN:NE2	1:G:84:ASP:OD1	2.39	0.54
2:N:43:MET:HE1	2:N:59:MET:HG3	1.89	0.54
2:T:43:MET:HE1	2:T:59:MET:HG3	1.89	0.54
2:D:105:ASP:O	2:D:180:ARG:NH2	2.40	0.54
2:P:105:ASP:O	2:P:180:ARG:NH2	2.40	0.54
1:K:121:GLN:NE2	1:M:84:ASP:OD1	2.40	0.54
1:Q:84:ASP:OD1	1:S:121:GLN:NE2	2.40	0.54
1:U:84:ASP:OD1	1:W:121:GLN:NE2	2.40	0.54
1:C:172:VAL:HG13	1:C:196:ALA:HB1	1.89	0.54
2:L:43:MET:HE1	2:L:59:MET:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:121:GLN:NE2	1:I:84:ASP:OD1	2.40	0.54
1:A:162:ALA:HB1	1:A:176:LEU:HD13	1.89	0.54
1:M:162:ALA:HB1	1:M:176:LEU:HD13	1.89	0.54
1:Q:162:ALA:HB1	1:Q:176:LEU:HD13	1.89	0.54
1:G:121:GLN:NE2	1:I:84:ASP:OD1	2.40	0.54
2:R:43:MET:HE1	2:R:59:MET:HG3	1.89	0.54
1:U:84:ASP:OD1	1:W:121:GLN:NE2	2.40	0.54
2:H:105:ASP:O	2:H:180:ARG:NH2	2.40	0.54
1:U:84:ASP:OD1	1:W:121:GLN:NE2	2.40	0.54
2:X:105:ASP:O	2:X:180:ARG:NH2	2.40	0.54
1:Y:84:ASP:OD1	1:O:121:GLN:NE2	2.39	0.54
2:B:43:MET:HE1	2:B:59:MET:HG3	1.89	0.54
2:P:43:MET:HE1	2:P:59:MET:HG3	1.89	0.54
1:Q:57:ARG:NH2	1:S:179:GLU:O	2.39	0.54
1:W:84:ASP:OD1	1:Y:121:GLN:NE2	2.41	0.54
1:I:121:GLN:NE2	1:K:84:ASP:OD1	2.41	0.54
1:O:162:ALA:HB1	1:O:176:LEU:HD13	1.90	0.54
1:A:84:ASP:OD1	1:M:121:GLN:NE2	2.40	0.54
1:S:84:ASP:OD1	1:U:121:GLN:NE2	2.41	0.54
2:B:15:ALA:HA	2:B:174:ASP:O	2.08	0.54
2:D:15:ALA:HA	2:D:174:ASP:O	2.08	0.54
2:P:15:ALA:HA	2:P:174:ASP:O	2.08	0.54
2:1:15:ALA:HA	2:1:174:ASP:O	2.08	0.54
1:E:76:ALA:HA	1:E:137:ILE:O	2.08	0.54
1:K:179:GLU:O	1:M:57:ARG:NH2	2.39	0.54
1:C:173:VAL:O	1:C:177:GLU:HB2	2.06	0.54
1:E:173:VAL:O	1:E:177:GLU:HB2	2.06	0.54
1:E:182:GLU:OE2	1:G:57:ARG:NH1	2.41	0.54
1:K:173:VAL:O	1:K:177:GLU:HB2	2.06	0.54
1:S:173:VAL:O	1:S:177:GLU:HB2	2.06	0.54
1:A:121:GLN:NE2	1:C:84:ASP:OD1	2.40	0.54
1:C:121:GLN:NE2	1:E:84:ASP:OD1	2.40	0.54
1:Q:84:ASP:OD1	1:S:121:GLN:NE2	2.41	0.54
2:T:88:ASN:ND2	2:V:50:GLY:O	2.40	0.54
1:U:84:ASP:OD1	1:W:121:GLN:NE2	2.40	0.54
2:X:43:MET:HE1	2:X:59:MET:HG3	1.89	0.54
1:I:121:GLN:NE2	1:K:84:ASP:OD1	2.41	0.54
2:P:16:THR:HG21	2:P:33:LYS:HB2	1.90	0.54
1:A:76:ALA:HA	1:A:137:ILE:O	2.08	0.54
1:G:76:ALA:HA	1:G:137:ILE:O	2.08	0.54
1:O:76:ALA:HA	1:O:137:ILE:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:76:ALA:HA	1:W:137:ILE:O	2.08	0.54
1:Y:173:VAL:O	1:Y:177:GLU:HB2	2.06	0.54
1:E:121:GLN:NE2	1:G:84:ASP:OD1	2.40	0.54
1:I:76:ALA:HA	1:I:137:ILE:O	2.08	0.54
1:Y:76:ALA:HA	1:Y:137:ILE:O	2.08	0.54
1:O:84:ASP:OD1	1:Q:121:GLN:NE2	2.40	0.54
2:T:105:ASP:O	2:T:180:ARG:NH2	2.40	0.54
1:W:84:ASP:OD1	1:Y:121:GLN:NE2	2.40	0.54
2:D:3:THR:OG1	2:D:127:THR:OG1	2.26	0.54
2:D:50:GLY:O	2:F:88:ASN:ND2	2.41	0.54
1:W:84:ASP:OD1	1:Y:121:GLN:NE2	2.40	0.54
2:H:43:MET:HE1	2:H:59:MET:HG3	1.89	0.54
1:I:222:ARG:NH2	1:I:228:GLU:OE2	2.41	0.54
1:U:222:ARG:NH2	1:U:228:GLU:OE2	2.41	0.54
2:B:16:THR:HG21	2:B:33:LYS:HB2	1.90	0.54
1:U:76:ALA:HA	1:U:137:ILE:O	2.08	0.54
2:V:3:THR:OG1	2:V:127:THR:OG1	2.24	0.54
2:Z:43:MET:HE1	2:Z:59:MET:HG3	1.89	0.54
1:A:84:ASP:OD1	1:M:121:GLN:NE2	2.41	0.54
1:K:162:ALA:HB1	1:K:176:LEU:HD13	1.89	0.54
2:L:105:ASP:O	2:L:180:ARG:NH2	2.40	0.54
1:S:162:ALA:HB1	1:S:176:LEU:HD13	1.90	0.54
2:Z:3:THR:OG1	2:Z:127:THR:OG1	2.26	0.54
2:1:3:THR:OG1	2:1:127:THR:OG1	2.26	0.54
2:P:43:MET:HE1	2:P:59:MET:HG3	1.89	0.54
1:K:99:GLU:OE2	2:N:70:ARG:NH2	2.41	0.54
2:F:3:THR:HG1	2:F:127:THR:HG1	1.51	0.54
2:F:43:MET:HE1	2:F:59:MET:HG3	1.89	0.54
1:G:121:GLN:NE2	1:I:84:ASP:OD1	2.41	0.54
1:C:121:GLN:NE2	1:E:84:ASP:OD1	2.41	0.54
1:G:121:GLN:NE2	1:I:84:ASP:OD1	2.41	0.54
2:B:105:ASP:O	2:B:180:ARG:NH2	2.41	0.54
1:G:222:ARG:NH2	1:G:228:GLU:OE2	2.41	0.54
1:K:222:ARG:NH2	1:K:228:GLU:OE2	2.41	0.54
2:R:15:ALA:HA	2:R:174:ASP:O	2.08	0.54
1:S:222:ARG:NH2	1:S:228:GLU:OE2	2.41	0.54
1:W:222:ARG:NH2	1:W:228:GLU:OE2	2.41	0.54
2:L:3:THR:HG22	2:L:16:THR:HG23	1.90	0.54
2:N:16:THR:HG21	2:N:33:LYS:HB2	1.90	0.54
2:T:3:THR:HG22	2:T:16:THR:HG23	1.90	0.54
1:C:76:ALA:HA	1:C:137:ILE:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:76:ALA:HA	1:0:137:ILE:O	2.08	0.53
2:1:43:MET:HE1	2:1:59:MET:HG3	1.89	0.53
1:G:162:ALA:HB1	1:G:176:LEU:HD13	1.89	0.53
1:E:121:GLN:NE2	1:G:84:ASP:OD1	2.41	0.53
2:F:90:VAL:HG23	2:F:94:PRO:HB3	1.90	0.53
2:P:105:ASP:O	2:P:180:ARG:NH2	2.41	0.53
1:E:222:ARG:NH2	1:E:228:GLU:OE2	2.41	0.53
2:J:3:THR:OG1	2:J:127:THR:OG1	2.26	0.53
2:V:3:THR:OG1	2:V:127:THR:OG1	2.26	0.53
1:Y:222:ARG:NH2	1:Y:228:GLU:OE2	2.41	0.53
1:I:99:GLU:OE2	2:L:70:ARG:NH2	2.41	0.53
1:A:37:ALA:O	1:A:164:ALA:HA	2.08	0.53
2:D:43:MET:HE1	2:D:59:MET:HG3	1.89	0.53
2:V:105:ASP:O	2:V:180:ARG:NH2	2.40	0.53
1:W:162:ALA:HB1	1:W:176:LEU:HD13	1.89	0.53
2:P:3:THR:OG1	2:P:127:THR:OG1	2.26	0.53
2:F:105:ASP:O	2:F:180:ARG:NH2	2.41	0.53
2:Z:105:ASP:O	2:Z:180:ARG:NH2	2.41	0.53
2:B:43:MET:HE1	2:B:59:MET:HG3	1.89	0.53
2:F:43:MET:HE1	2:F:59:MET:HG3	1.89	0.53
2:N:15:ALA:HA	2:N:174:ASP:O	2.08	0.53
2:1:43:MET:HE1	2:1:59:MET:HG3	1.89	0.53
1:Q:84:ASP:OD1	1:S:121:GLN:NE2	2.41	0.53
2:R:16:THR:HG21	2:R:33:LYS:HB2	1.90	0.53
1:G:121:GLN:NE2	1:I:84:ASP:OD1	2.42	0.53
1:M:76:ALA:HA	1:M:137:ILE:O	2.08	0.53
1:O:37:ALA:O	1:O:164:ALA:HA	2.08	0.53
1:A:121:GLN:NE2	1:C:84:ASP:OD1	2.41	0.53
1:G:182:GLU:OE2	1:I:57:ARG:NH1	2.42	0.53
2:J:105:ASP:O	2:J:180:ARG:NH2	2.40	0.53
2:D:105:ASP:O	2:D:180:ARG:NH2	2.41	0.53
2:N:105:ASP:O	2:N:180:ARG:NH2	2.41	0.53
2:R:105:ASP:O	2:R:180:ARG:NH2	2.41	0.53
2:V:90:VAL:HG23	2:V:94:PRO:HB3	1.90	0.53
2:X:90:VAL:HG23	2:X:94:PRO:HB3	1.90	0.53
2:Z:90:VAL:HG23	2:Z:94:PRO:HB3	1.90	0.53
1:C:222:ARG:NH2	1:C:228:GLU:OE2	2.41	0.53
2:D:43:MET:HE1	2:D:59:MET:HG3	1.89	0.53
2:F:15:ALA:HA	2:F:174:ASP:O	2.08	0.53
1:0:222:ARG:NH2	1:0:228:GLU:OE2	2.41	0.53
2:J:3:THR:HG22	2:J:16:THR:HG23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:121:GLN:NE2	1:M:84:ASP:OD1	2.41	0.53
2:1:16:THR:HG21	2:1:33:LYS:HB2	1.90	0.53
1:I:121:GLN:NE2	1:K:84:ASP:OD1	2.42	0.53
1:C:162:ALA:HB1	1:C:176:LEU:HD13	1.89	0.53
2:H:3:THR:OG1	2:H:127:THR:OG1	2.26	0.53
1:I:37:ALA:O	1:I:164:ALA:HA	2.09	0.53
2:H:90:VAL:HG23	2:H:94:PRO:HB3	1.90	0.53
2:1:105:ASP:O	2:1:180:ARG:NH2	2.41	0.53
1:M:222:ARG:NH2	1:M:228:GLU:OE2	2.41	0.53
1:Q:222:ARG:NH2	1:Q:228:GLU:OE2	2.41	0.53
2:T:15:ALA:HA	2:T:174:ASP:O	2.08	0.53
2:Z:15:ALA:HA	2:Z:174:ASP:O	2.08	0.53
2:Z:43:MET:HE1	2:Z:59:MET:HG3	1.89	0.53
1:O:99:GLU:OE2	2:1:70:ARG:NH2	2.41	0.53
2:V:3:THR:HG22	2:V:16:THR:HG23	1.90	0.53
1:E:121:GLN:NE2	1:G:84:ASP:OD1	2.42	0.53
1:K:76:ALA:HA	1:K:137:ILE:O	2.08	0.53
1:Q:76:ALA:HA	1:Q:137:ILE:O	2.08	0.53
1:S:76:ALA:HA	1:S:137:ILE:O	2.08	0.53
1:U:84:ASP:OD1	1:W:121:GLN:NE2	2.42	0.53
1:A:99:GLU:HB2	1:A:115:ARG:HH22	1.74	0.53
2:D:90:VAL:HG23	2:D:94:PRO:HB3	1.90	0.53
2:L:15:ALA:HA	2:L:174:ASP:O	2.08	0.53
2:D:16:THR:HG21	2:D:33:LYS:HB2	1.90	0.53
2:Z:3:THR:HG1	2:Z:127:THR:HG1	1.53	0.53
1:K:37:ALA:O	1:K:164:ALA:HA	2.09	0.53
1:S:37:ALA:O	1:S:164:ALA:HA	2.09	0.53
1:O:97:GLN:HG3	2:1:65:LEU:HG	1.91	0.53
2:J:90:VAL:HG23	2:J:94:PRO:HB3	1.90	0.53
2:T:90:VAL:HG23	2:T:94:PRO:HB3	1.90	0.53
1:U:152:ASP:O	1:U:155:GLY:N	2.36	0.53
2:1:90:VAL:HG23	2:1:94:PRO:HB3	1.90	0.53
2:B:10:ASP:OD1	2:B:10:ASP:N	2.37	0.53
2:F:167:SER:HB2	2:V:167:SER:HB2	1.91	0.53
2:L:18:ARG:HD3	2:L:172:MET:HB3	1.91	0.53
1:M:37:ALA:O	1:M:164:ALA:HA	2.08	0.53
1:Q:37:ALA:O	1:Q:164:ALA:HA	2.08	0.53
1:S:84:ASP:OD1	1:U:121:GLN:NE2	2.42	0.53
1:I:162:ALA:HB1	1:I:176:LEU:HD13	1.89	0.53
1:C:99:GLU:HB2	1:C:115:ARG:HH22	1.74	0.53
1:O:84:ASP:OD1	1:Q:121:GLN:NE2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:141:GLN:HE21	2:1:141:GLN:HE21	1.55	0.53
1:U:37:ALA:O	1:U:164:ALA:HA	2.09	0.53
2:J:15:ALA:HA	2:J:174:ASP:O	2.08	0.53
2:V:15:ALA:HA	2:V:174:ASP:O	2.08	0.53
2:H:3:THR:HG22	2:H:16:THR:HG23	1.90	0.53
2:R:3:THR:HG22	2:R:16:THR:HG23	1.90	0.53
2:1:10:ASP:OD1	2:1:10:ASP:N	2.37	0.53
1:I:37:ALA:O	1:I:164:ALA:HA	2.08	0.53
2:T:18:ARG:HD3	2:T:172:MET:HB3	1.91	0.53
2:N:141:GLN:HE21	2:1:141:GLN:HE21	1.56	0.53
2:L:90:VAL:HG23	2:L:94:PRO:HB3	1.90	0.53
1:O:222:ARG:NH2	1:O:228:GLU:OE2	2.41	0.53
2:D:10:ASP:OD1	2:D:10:ASP:N	2.37	0.53
1:U:162:ALA:HB1	1:U:176:LEU:HD13	1.89	0.53
1:Y:162:ALA:HB1	1:Y:176:LEU:HD13	1.89	0.53
1:C:121:GLN:NE2	1:E:84:ASP:OD1	2.41	0.53
1:E:99:GLU:HB2	1:E:115:ARG:HH22	1.74	0.53
2:P:178:ILE:HA	2:P:183:GLY:O	2.09	0.53
1:Q:37:ALA:O	1:Q:164:ALA:HA	2.09	0.53
2:B:105:ASP:O	2:B:180:ARG:NH2	2.42	0.53
1:C:97:GLN:HG3	2:D:65:LEU:HG	1.91	0.53
2:P:105:ASP:O	2:P:180:ARG:NH2	2.42	0.53
2:H:105:ASP:O	2:H:180:ARG:NH2	2.41	0.53
2:X:105:ASP:O	2:X:180:ARG:NH2	2.41	0.53
1:A:97:GLN:HG3	2:B:65:LEU:HG	1.90	0.53
2:D:3:THR:HG22	2:D:16:THR:HG23	1.90	0.53
2:N:3:THR:HG22	2:N:16:THR:HG23	1.90	0.53
2:V:16:THR:HG21	2:V:33:LYS:HB2	1.90	0.53
1:E:162:ALA:HB1	1:E:176:LEU:HD13	1.89	0.53
2:B:178:ILE:HA	2:B:183:GLY:O	2.09	0.53
1:C:37:ALA:O	1:C:164:ALA:HA	2.09	0.53
1:G:37:ALA:O	1:G:164:ALA:HA	2.09	0.53
1:M:37:ALA:O	1:M:164:ALA:HA	2.09	0.53
1:W:37:ALA:O	1:W:164:ALA:HA	2.09	0.53
2:Z:178:ILE:HA	2:Z:183:GLY:O	2.09	0.53
1:I:152:ASP:O	1:I:155:GLY:N	2.36	0.53
1:A:222:ARG:NH2	1:A:228:GLU:OE2	2.41	0.53
2:P:10:ASP:N	2:P:10:ASP:OD1	2.37	0.53
2:P:70:ARG:NH2	1:Q:99:GLU:OE2	2.41	0.53
2:T:16:THR:HG21	2:T:33:LYS:HB2	1.90	0.53
2:X:3:THR:HG22	2:X:16:THR:HG23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:GLU:O	1:C:57:ARG:NH2	2.40	0.52
2:N:18:ARG:HD3	2:N:172:MET:HB3	1.91	0.52
2:R:18:ARG:HD3	2:R:172:MET:HB3	1.91	0.52
1:U:37:ALA:O	1:U:164:ALA:HA	2.08	0.52
1:I:182:GLU:OE2	1:K:57:ARG:NH1	2.42	0.52
2:F:178:ILE:HA	2:F:183:GLY:O	2.09	0.52
1:O:37:ALA:O	1:O:164:ALA:HA	2.09	0.52
2:L:105:ASP:O	2:L:180:ARG:NH2	2.41	0.52
1:O:152:ASP:O	1:O:155:GLY:N	2.36	0.52
2:P:90:VAL:HG23	2:P:94:PRO:HB3	1.90	0.52
2:V:105:ASP:O	2:V:180:ARG:NH2	2.41	0.52
2:H:15:ALA:HA	2:H:174:ASP:O	2.08	0.52
2:X:15:ALA:HA	2:X:174:ASP:O	2.08	0.52
2:1:3:THR:HG22	2:1:16:THR:HG23	1.90	0.52
1:W:37:ALA:O	1:W:164:ALA:HA	2.08	0.52
2:1:105:ASP:O	2:1:180:ARG:NH2	2.42	0.52
1:A:152:ASP:O	1:A:155:GLY:N	2.36	0.52
2:B:90:VAL:HG23	2:B:94:PRO:HB3	1.90	0.52
2:N:90:VAL:HG23	2:N:94:PRO:HB3	1.90	0.52
2:R:90:VAL:HG23	2:R:94:PRO:HB3	1.90	0.52
2:T:105:ASP:O	2:T:180:ARG:NH2	2.41	0.52
2:L:16:THR:HG21	2:L:33:LYS:HB2	1.90	0.52
1:W:84:ASP:OD1	1:Y:121:GLN:NE2	2.42	0.52
1:G:37:ALA:O	1:G:164:ALA:HA	2.08	0.52
1:K:37:ALA:O	1:K:164:ALA:HA	2.08	0.52
1:K:121:GLN:NE2	1:M:84:ASP:OD1	2.42	0.52
1:O:84:ASP:OD1	1:Q:121:GLN:NE2	2.41	0.52
1:Q:84:ASP:OD1	1:S:121:GLN:NE2	2.41	0.52
1:S:37:ALA:O	1:S:164:ALA:HA	2.08	0.52
1:E:37:ALA:O	1:E:164:ALA:HA	2.09	0.52
2:D:105:ASP:O	2:D:180:ARG:NH2	2.42	0.52
2:J:105:ASP:O	2:J:180:ARG:NH2	2.41	0.52
1:O:84:ASP:OD1	1:Q:121:GLN:NE2	2.41	0.52
2:Z:16:THR:HG21	2:Z:33:LYS:HB2	1.90	0.52
1:O:37:ALA:O	1:O:164:ALA:HA	2.09	0.52
2:Z:105:ASP:O	2:Z:180:ARG:NH2	2.42	0.52
2:L:134:VAL:HG12	2:L:158:ALA:HB1	1.92	0.52
2:L:163:LYS:NZ	2:L:171:GLY:O	2.36	0.52
2:N:134:VAL:HG12	2:N:158:ALA:HB1	1.92	0.52
2:P:134:VAL:HG12	2:P:158:ALA:HB1	1.92	0.52
2:T:134:VAL:HG12	2:T:158:ALA:HB1	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:3:THR:HG22	2:F:16:THR:HG23	1.90	0.52
1:G:99:GLU:OE2	2:J:70:ARG:NH2	2.40	0.52
1:Y:84:ASP:OD1	1:O:121:GLN:NE2	2.41	0.52
1:C:37:ALA:O	1:C:164:ALA:HA	2.08	0.52
1:A:37:ALA:O	1:A:164:ALA:HA	2.09	0.52
2:L:178:ILE:HA	2:L:183:GLY:O	2.09	0.52
1:Y:37:ALA:O	1:Y:164:ALA:HA	2.09	0.52
2:F:105:ASP:O	2:F:180:ARG:NH2	2.42	0.52
2:B:134:VAL:HG12	2:B:158:ALA:HB1	1.92	0.52
2:J:134:VAL:HG12	2:J:158:ALA:HB1	1.92	0.52
2:R:134:VAL:HG12	2:R:158:ALA:HB1	1.92	0.52
2:T:163:LYS:NZ	2:T:171:GLY:O	2.36	0.52
2:V:134:VAL:HG12	2:V:158:ALA:HB1	1.92	0.52
2:B:70:ARG:NH2	1:M:99:GLU:OE2	2.42	0.52
2:Z:3:THR:HG22	2:Z:16:THR:HG23	1.90	0.52
1:C:121:GLN:NE2	1:E:84:ASP:OD1	2.42	0.52
1:S:152:ASP:O	1:S:155:GLY:N	2.36	0.52
2:F:16:THR:HG21	2:F:33:LYS:HB2	1.90	0.52
1:O:121:GLN:NE2	1:O:84:ASP:OD1	2.41	0.52
2:D:18:ARG:HD3	2:D:172:MET:HB3	1.91	0.52
2:J:18:ARG:HD3	2:J:172:MET:HB3	1.91	0.52
1:O:37:ALA:O	1:O:164:ALA:HA	2.08	0.52
2:1:18:ARG:HD3	2:1:172:MET:HB3	1.91	0.52
2:N:178:ILE:HA	2:N:183:GLY:O	2.09	0.52
2:T:178:ILE:HA	2:T:183:GLY:O	2.09	0.52
2:J:105:ASP:O	2:J:180:ARG:NH2	2.42	0.52
2:V:105:ASP:O	2:V:180:ARG:NH2	2.42	0.52
2:H:16:THR:HG21	2:H:33:LYS:HB2	1.90	0.52
2:J:16:THR:HG21	2:J:33:LYS:HB2	1.90	0.52
1:A:84:ASP:OD1	1:M:121:GLN:NE2	2.42	0.52
1:I:179:GLU:O	1:K:57:ARG:NH2	2.39	0.52
1:S:57:ARG:NH2	1:U:179:GLU:O	2.39	0.52
1:Y:37:ALA:O	1:Y:164:ALA:HA	2.08	0.52
2:R:178:ILE:HA	2:R:183:GLY:O	2.09	0.52
2:F:93:MET:HE2	2:F:94:PRO:HG3	1.91	0.52
2:L:3:THR:OG1	2:L:127:THR:OG1	2.26	0.52
2:N:93:MET:HE2	2:N:94:PRO:HG3	1.91	0.52
2:B:3:THR:HG22	2:B:16:THR:HG23	1.90	0.52
2:P:3:THR:HG22	2:P:16:THR:HG23	1.90	0.52
2:P:91:LYS:HB2	2:R:93:MET:HE3	1.91	0.52
1:A:121:GLN:NE2	1:C:84:ASP:OD1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:37:ALA:O	1:E:164:ALA:HA	2.08	0.52
2:V:18:ARG:HD3	2:V:172:MET:HB3	1.91	0.52
2:X:18:ARG:HD3	2:X:172:MET:HB3	1.91	0.52
1:O:99:GLU:HB2	1:O:115:ARG:HH22	1.75	0.52
2:J:178:ILE:HA	2:J:183:GLY:O	2.09	0.52
2:N:105:ASP:O	2:N:180:ARG:NH2	2.42	0.52
2:R:105:ASP:O	2:R:180:ARG:NH2	2.42	0.52
2:Z:93:MET:HE2	2:Z:94:PRO:HG3	1.91	0.52
1:C:99:GLU:HB2	1:C:115:ARG:HH22	1.75	0.52
1:C:179:GLU:O	1:E:57:ARG:NH2	2.39	0.52
1:E:99:GLU:HB2	1:E:115:ARG:HH22	1.75	0.52
1:Y:99:GLU:HB2	1:Y:115:ARG:HH22	1.75	0.52
1:A:121:GLN:NE2	1:C:84:ASP:OD1	2.42	0.52
2:R:93:MET:HE2	2:R:94:PRO:HG3	1.92	0.52
2:Z:18:ARG:HD3	2:Z:172:MET:HB3	1.91	0.51
2:Z:153:ASP:OD1	2:Z:195:ARG:NH1	2.43	0.51
2:X:105:ASP:O	2:X:180:ARG:NH2	2.42	0.51
2:H:134:VAL:HG12	2:H:158:ALA:HB1	1.92	0.51
2:X:134:VAL:HG12	2:X:158:ALA:HB1	1.92	0.51
2:1:134:VAL:HG12	2:1:158:ALA:HB1	1.92	0.51
2:L:93:MET:HE2	2:L:94:PRO:HG3	1.91	0.51
2:T:93:MET:HE2	2:T:94:PRO:HG3	1.91	0.51
2:1:93:MET:HE2	2:1:94:PRO:HG3	1.91	0.51
1:A:121:GLN:NE2	1:C:84:ASP:OD1	2.42	0.51
2:B:18:ARG:HD3	2:B:172:MET:HB3	1.91	0.51
2:F:18:ARG:HD3	2:F:172:MET:HB3	1.91	0.51
2:P:18:ARG:HD3	2:P:172:MET:HB3	1.91	0.51
2:F:153:ASP:OD1	2:F:195:ARG:NH1	2.43	0.51
2:N:153:ASP:OD1	2:N:195:ARG:NH1	2.43	0.51
2:R:153:ASP:OD1	2:R:195:ARG:NH1	2.44	0.51
2:H:105:ASP:O	2:H:180:ARG:NH2	2.42	0.51
2:L:105:ASP:O	2:L:180:ARG:NH2	2.42	0.51
2:T:105:ASP:O	2:T:180:ARG:NH2	2.42	0.51
2:D:134:VAL:HG12	2:D:158:ALA:HB1	1.92	0.51
1:K:152:ASP:O	1:K:155:GLY:N	2.36	0.51
2:H:93:MET:HE2	2:H:94:PRO:HG3	1.92	0.51
2:X:93:MET:HE2	2:X:94:PRO:HG3	1.91	0.51
2:X:16:THR:HG21	2:X:33:LYS:HB2	1.90	0.51
1:A:57:ARG:NH1	1:M:182:GLU:OE2	2.44	0.51
2:D:153:ASP:OD1	2:D:195:ARG:NH1	2.43	0.51
2:V:178:ILE:HA	2:V:183:GLY:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:141:GLN:HE21	2:X:141:GLN:HE21	1.57	0.51
1:O:181:LYS:HE2	1:O:184:LEU:HD21	1.93	0.51
2:B:163:LYS:NZ	2:B:171:GLY:O	2.36	0.51
2:Z:134:VAL:HG12	2:Z:158:ALA:HB1	1.92	0.51
2:D:93:MET:HE2	2:D:94:PRO:HG3	1.92	0.51
2:H:167:SER:HB2	2:X:167:SER:HB2	1.92	0.51
2:1:153:ASP:OD1	2:1:195:ARG:NH1	2.43	0.51
1:C:51:ASP:HB2	1:C:197:LEU:HD11	1.92	0.51
1:C:181:LYS:HE2	1:C:184:LEU:HD21	1.93	0.51
2:F:134:VAL:HG12	2:F:158:ALA:HB1	1.92	0.51
2:J:93:MET:HE2	2:J:94:PRO:HG3	1.91	0.51
2:V:93:MET:HE2	2:V:94:PRO:HG3	1.92	0.51
1:C:121:GLN:NE2	1:E:84:ASP:OD1	2.42	0.51
2:H:18:ARG:HD3	2:H:172:MET:HB3	1.91	0.51
2:D:178:ILE:HA	2:D:183:GLY:O	2.09	0.51
2:P:153:ASP:OD1	2:P:195:ARG:NH1	2.43	0.51
2:X:178:ILE:HA	2:X:183:GLY:O	2.09	0.51
2:1:178:ILE:HA	2:1:183:GLY:O	2.09	0.51
1:E:181:LYS:HE2	1:E:184:LEU:HD21	1.93	0.51
1:O:181:LYS:HE2	1:O:184:LEU:HD21	1.93	0.51
2:V:91:LYS:HB2	2:X:93:MET:HE3	1.93	0.51
1:W:99:GLU:HB2	1:W:115:ARG:HH22	1.75	0.51
2:B:153:ASP:OD1	2:B:195:ARG:NH1	2.43	0.51
1:A:181:LYS:HE2	1:A:184:LEU:HD21	1.93	0.51
2:H:141:GLN:HE21	2:V:141:GLN:HE21	1.57	0.51
1:Y:181:LYS:HE2	1:Y:184:LEU:HD21	1.93	0.51
1:I:45:GLY:HA3	1:I:215:ILE:O	2.11	0.51
1:S:26:TYR:CD1	1:U:17:PRO:HA	2.46	0.51
1:U:45:GLY:HA3	1:U:215:ILE:O	2.11	0.51
2:B:93:MET:HE2	2:B:94:PRO:HG3	1.92	0.51
1:E:121:GLN:NE2	1:G:84:ASP:OD1	2.44	0.51
2:P:93:MET:HE2	2:P:94:PRO:HG3	1.91	0.51
1:O:99:GLU:HB2	1:O:115:ARG:HH22	1.75	0.51
1:W:41:LYS:HG2	1:W:46:VAL:HG12	1.93	0.51
2:B:43:MET:HE1	2:B:59:MET:HG3	1.92	0.51
2:L:141:GLN:HE21	2:Z:141:GLN:HE21	1.58	0.51
2:P:3:THR:OG1	2:P:127:THR:OG1	2.25	0.51
1:G:41:LYS:HG2	1:G:46:VAL:HG12	1.93	0.51
1:G:99:GLU:HB2	1:G:115:ARG:HH22	1.75	0.51
1:O:121:GLN:NE2	1:O:84:ASP:OD1	2.42	0.51
2:H:178:ILE:HA	2:H:183:GLY:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:ASP:HB2	1:A:197:LEU:HD11	1.92	0.51
1:O:152:ASP:O	1:O:155:GLY:N	2.36	0.51
1:A:99:GLU:HB2	1:A:115:ARG:HH22	1.75	0.51
1:U:41:LYS:HG2	1:U:46:VAL:HG12	1.93	0.51
2:L:153:ASP:OD1	2:L:195:ARG:NH1	2.44	0.51
2:B:3:THR:OG1	2:B:127:THR:OG1	2.25	0.51
2:J:29:LYS:HE2	2:Z:165:ARG:NH2	2.26	0.51
1:W:84:ASP:OD1	1:Y:121:GLN:NE2	2.44	0.51
1:E:41:LYS:HG2	1:E:46:VAL:HG12	1.93	0.51
1:I:41:LYS:HG2	1:I:46:VAL:HG12	1.93	0.51
1:I:99:GLU:HB2	1:I:115:ARG:HH22	1.75	0.51
1:M:99:GLU:HB2	1:M:115:ARG:HH22	1.75	0.51
1:Y:41:LYS:HG2	1:Y:46:VAL:HG12	1.93	0.51
1:E:97:GLN:HG3	2:F:65:LEU:HG	1.93	0.51
2:T:153:ASP:OD1	2:T:195:ARG:NH1	2.44	0.51
1:U:181:LYS:HE2	1:U:184:LEU:HD21	1.93	0.51
1:O:121:GLN:NE2	1:O:84:ASP:OD1	2.44	0.51
1:Q:99:GLU:HB2	1:Q:115:ARG:HH22	1.75	0.50
2:B:153:ASP:HB3	2:B:199:LEU:HD11	1.93	0.50
2:P:153:ASP:HB3	2:P:199:LEU:HD11	1.93	0.50
2:R:153:ASP:HB3	2:R:199:LEU:HD11	1.93	0.50
2:F:141:GLN:HE21	2:T:141:GLN:HE21	1.58	0.50
1:I:181:LYS:HE2	1:I:184:LEU:HD21	1.93	0.50
1:Q:181:LYS:HE2	1:Q:184:LEU:HD21	1.93	0.50
1:K:45:GLY:HA3	1:K:215:ILE:O	2.11	0.50
1:A:84:ASP:OD1	1:M:121:GLN:NE2	2.44	0.50
1:U:84:ASP:OD1	1:W:121:GLN:NE2	2.44	0.50
1:Y:84:ASP:OD1	1:O:121:GLN:NE2	2.44	0.50
2:H:93:MET:HE3	2:J:91:LYS:HB2	1.93	0.50
2:T:92:TYR:CD1	2:V:93:MET:HE1	2.42	0.50
2:X:91:LYS:HD3	2:Z:51:ASP:OD1	2.11	0.50
2:B:3:THR:OG1	2:B:127:THR:OG1	2.24	0.50
1:U:99:GLU:HB2	1:U:115:ARG:HH22	1.75	0.50
1:E:110:GLU:HA	1:E:149:PHE:HE2	1.77	0.50
1:C:152:ASP:O	1:C:155:GLY:N	2.36	0.50
2:N:163:LYS:NZ	2:N:171:GLY:O	2.36	0.50
1:G:121:GLN:NE2	1:I:84:ASP:OD1	2.44	0.50
2:N:3:THR:HG1	2:N:127:THR:HG1	1.57	0.50
1:O:84:ASP:OD1	1:Q:121:GLN:NE2	2.44	0.50
1:S:84:ASP:OD1	1:U:121:GLN:NE2	2.44	0.50
1:K:41:LYS:HG2	1:K:46:VAL:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:41:LYS:HG2	1:S:46:VAL:HG12	1.93	0.50
2:N:153:ASP:HB3	2:N:199:LEU:HD11	1.93	0.50
1:I:110:GLU:HA	1:I:149:PHE:HE2	1.77	0.50
1:K:110:GLU:HA	1:K:149:PHE:HE2	1.77	0.50
1:M:181:LYS:HE2	1:M:184:LEU:HD21	1.93	0.50
1:S:110:GLU:HA	1:S:149:PHE:HE2	1.77	0.50
1:U:110:GLU:HA	1:U:149:PHE:HE2	1.77	0.50
1:Y:110:GLU:HA	1:Y:149:PHE:HE2	1.77	0.50
1:E:45:GLY:HA3	1:E:215:ILE:O	2.11	0.50
1:Y:45:GLY:HA3	1:Y:215:ILE:O	2.11	0.50
1:I:121:GLN:NE2	1:K:84:ASP:OD1	2.44	0.50
1:A:110:GLU:HA	1:A:149:PHE:HE2	1.77	0.50
1:K:181:LYS:HE2	1:K:184:LEU:HD21	1.93	0.50
1:Q:110:GLU:HA	1:Q:149:PHE:HE2	1.77	0.50
1:W:110:GLU:HA	1:W:149:PHE:HE2	1.77	0.50
1:G:45:GLY:HA3	1:G:215:ILE:O	2.11	0.50
2:R:163:LYS:NZ	2:R:171:GLY:O	2.36	0.50
1:S:45:GLY:HA3	1:S:215:ILE:O	2.11	0.50
1:Q:84:ASP:OD1	1:S:121:GLN:NE2	2.44	0.50
2:N:37:ILE:HD13	2:N:43:MET:HE3	1.94	0.50
2:P:37:ILE:HD13	2:P:43:MET:HE3	1.94	0.50
2:T:37:ILE:HD13	2:T:43:MET:HE3	1.94	0.50
2:V:37:ILE:HD13	2:V:43:MET:HE3	1.94	0.50
2:H:16:THR:HG21	2:H:33:LYS:HB2	1.94	0.50
2:X:16:THR:HG21	2:X:33:LYS:HB2	1.94	0.50
2:F:153:ASP:HB3	2:F:199:LEU:HD11	1.93	0.50
2:H:153:ASP:OD1	2:H:195:ARG:NH1	2.43	0.50
2:J:153:ASP:OD1	2:J:195:ARG:NH1	2.44	0.50
2:X:153:ASP:OD1	2:X:195:ARG:NH1	2.44	0.50
1:G:110:GLU:HA	1:G:149:PHE:HE2	1.77	0.50
1:M:110:GLU:HA	1:M:149:PHE:HE2	1.77	0.50
1:S:181:LYS:HE2	1:S:184:LEU:HD21	1.93	0.50
1:K:121:GLN:NE2	1:M:84:ASP:OD1	2.44	0.50
1:C:41:LYS:HG2	1:C:46:VAL:HG12	1.93	0.50
2:J:37:ILE:HD13	2:J:43:MET:HE3	1.94	0.50
2:L:37:ILE:HD13	2:L:43:MET:HE3	1.94	0.50
2:R:37:ILE:HD13	2:R:43:MET:HE3	1.94	0.50
1:A:76:ALA:HA	1:A:137:ILE:O	2.12	0.50
2:V:16:THR:HG21	2:V:33:LYS:HB2	1.94	0.50
2:Z:16:THR:HG21	2:Z:33:LYS:HB2	1.94	0.50
2:V:153:ASP:OD1	2:V:195:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:153:ASP:HB3	2:Z:199:LEU:HD11	1.93	0.50
1:O:110:GLU:HA	1:O:149:PHE:HE2	1.77	0.50
1:C:45:GLY:HA3	1:C:215:ILE:O	2.11	0.50
1:W:45:GLY:HA3	1:W:215:ILE:O	2.11	0.50
1:A:121:GLN:NE2	1:C:84:ASP:OD1	2.44	0.50
2:B:37:ILE:HD13	2:B:43:MET:HE3	1.94	0.50
2:H:37:ILE:HD13	2:H:43:MET:HE3	1.94	0.50
2:X:37:ILE:HD13	2:X:43:MET:HE3	1.94	0.50
1:Y:84:ASP:OD1	1:O:121:GLN:NE2	2.44	0.50
1:O:41:LYS:HG2	1:O:46:VAL:HG12	1.93	0.50
2:F:16:THR:HG21	2:F:33:LYS:HB2	1.94	0.50
1:G:76:ALA:HA	1:G:137:ILE:O	2.12	0.50
2:J:16:THR:HG21	2:J:33:LYS:HB2	1.94	0.50
2:D:16:THR:HG21	2:D:33:LYS:HB2	1.94	0.50
1:W:76:ALA:HA	1:W:137:ILE:O	2.12	0.50
1:O:45:GLY:HA3	1:O:215:ILE:O	2.11	0.50
1:E:172:VAL:HG13	1:E:196:ALA:HB1	1.94	0.50
1:S:99:GLU:HB2	1:S:115:ARG:HH22	1.75	0.50
1:E:76:ALA:HA	1:E:137:ILE:O	2.12	0.50
1:O:76:ALA:HA	1:O:137:ILE:O	2.12	0.50
1:U:76:ALA:HA	1:U:137:ILE:O	2.12	0.50
1:Y:76:ALA:HA	1:Y:137:ILE:O	2.12	0.50
2:D:153:ASP:HB3	2:D:199:LEU:HD11	1.93	0.50
2:T:153:ASP:HB3	2:T:199:LEU:HD11	1.93	0.50
2:1:153:ASP:HB3	2:1:199:LEU:HD11	1.93	0.50
2:N:3:THR:OG1	2:N:127:THR:OG1	2.25	0.50
2:R:3:THR:OG1	2:R:127:THR:OG1	2.25	0.50
1:C:172:VAL:HG13	1:C:196:ALA:HB1	1.94	0.50
1:Y:172:VAL:HG13	1:Y:196:ALA:HB1	1.94	0.50
1:O:172:VAL:HG13	1:O:196:ALA:HB1	1.94	0.50
2:T:70:ARG:NH2	1:U:99:GLU:OE2	2.45	0.50
2:B:15:ALA:HA	2:B:174:ASP:O	2.12	0.49
1:K:99:GLU:HB2	1:K:115:ARG:HH22	1.75	0.49
2:P:15:ALA:HA	2:P:174:ASP:O	2.12	0.49
1:I:76:ALA:HA	1:I:137:ILE:O	2.12	0.49
1:K:76:ALA:HA	1:K:137:ILE:O	2.12	0.49
1:S:76:ALA:HA	1:S:137:ILE:O	2.12	0.49
1:M:67:ILE:HG12	1:M:77:VAL:HG22	1.94	0.49
1:Q:67:ILE:HG12	1:Q:77:VAL:HG22	1.94	0.49
2:L:153:ASP:HB3	2:L:199:LEU:HD11	1.93	0.49
1:A:45:GLY:HA3	1:A:215:ILE:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:45:GLY:HA3	1:M:215:ILE:O	2.11	0.49
1:Y:97:GLN:HG3	2:Z:65:LEU:HG	1.93	0.49
2:T:196:ILE:HD13	2:T:203:LEU:HG	1.94	0.49
2:F:37:ILE:HD13	2:F:43:MET:HE3	1.94	0.49
2:L:3:THR:HG22	2:L:16:THR:HG23	1.94	0.49
2:L:16:THR:HG21	2:L:33:LYS:HB2	1.94	0.49
2:T:3:THR:HG22	2:T:16:THR:HG23	1.94	0.49
2:T:16:THR:HG21	2:T:33:LYS:HB2	1.94	0.49
2:J:153:ASP:HB3	2:J:199:LEU:HD11	1.93	0.49
2:X:153:ASP:HB3	2:X:199:LEU:HD11	1.93	0.49
1:O:162:ALA:HB1	1:O:176:LEU:HD13	1.94	0.49
1:Q:162:ALA:HB1	1:Q:176:LEU:HD13	1.94	0.49
1:O:172:VAL:HG13	1:O:196:ALA:HB1	1.94	0.49
2:R:196:ILE:HD13	2:R:203:LEU:HG	1.94	0.49
1:W:172:VAL:HG13	1:W:196:ALA:HB1	1.94	0.49
1:C:99:GLU:HB2	1:C:115:ARG:HH22	1.77	0.49
1:E:99:GLU:HB2	1:E:115:ARG:HH22	1.77	0.49
2:D:37:ILE:HD13	2:D:43:MET:HE3	1.94	0.49
1:S:152:ASP:O	1:S:155:GLY:N	2.42	0.49
2:1:37:ILE:HD13	2:1:43:MET:HE3	1.94	0.49
1:A:162:ALA:HB1	1:A:176:LEU:HD13	1.95	0.49
1:M:162:ALA:HB1	1:M:176:LEU:HD13	1.95	0.49
2:F:70:ARG:HB3	2:F:72:VAL:HG12	1.94	0.49
1:O:45:GLY:HA3	1:O:215:ILE:O	2.11	0.49
1:A:172:VAL:HG13	1:A:196:ALA:HB1	1.94	0.49
1:G:172:VAL:HG13	1:G:196:ALA:HB1	1.94	0.49
2:L:196:ILE:HD13	2:L:203:LEU:HG	1.94	0.49
2:N:196:ILE:HD13	2:N:203:LEU:HG	1.94	0.49
1:Y:99:GLU:HB2	1:Y:115:ARG:HH22	1.78	0.49
1:O:99:GLU:HB2	1:O:115:ARG:HH22	1.78	0.49
1:G:179:GLU:O	1:I:57:ARG:NH2	2.40	0.49
2:J:16:THR:HG21	2:J:33:LYS:HB2	1.94	0.49
1:Q:41:LYS:HG2	1:Q:46:VAL:HG12	1.93	0.49
2:R:15:ALA:HA	2:R:174:ASP:O	2.12	0.49
1:U:57:ARG:NH2	1:W:179:GLU:O	2.40	0.49
2:V:16:THR:HG21	2:V:33:LYS:HB2	1.94	0.49
2:Z:37:ILE:HD13	2:Z:43:MET:HE3	1.94	0.49
1:C:76:ALA:HA	1:C:137:ILE:O	2.12	0.49
1:O:63:SER:OG	1:Q:159:GLU:OE1	2.29	0.49
1:Y:78:THR:HG22	1:Y:136:LEU:HG	1.95	0.49
2:H:153:ASP:HB3	2:H:199:LEU:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:153:ASP:HB3	2:V:199:LEU:HD11	1.93	0.49
1:Q:45:GLY:HA3	1:Q:215:ILE:O	2.11	0.49
1:W:100:LYS:NZ	2:X:64:GLU:OE2	2.44	0.49
1:M:41:LYS:HG2	1:M:46:VAL:HG12	1.93	0.49
2:N:15:ALA:HA	2:N:174:ASP:O	2.12	0.49
2:T:16:THR:HG21	2:T:33:LYS:HB2	1.95	0.49
2:X:16:THR:HG21	2:X:33:LYS:HB2	1.94	0.49
1:Y:152:ASP:O	1:Y:155:GLY:N	2.42	0.49
2:J:3:THR:HG22	2:J:16:THR:HG23	1.94	0.49
1:A:54:VAL:HB	1:A:208:LYS:HE2	1.95	0.49
1:A:78:THR:HG22	1:A:136:LEU:HG	1.94	0.49
1:E:54:VAL:HB	1:E:208:LYS:HE2	1.95	0.49
1:E:20:ARG:NH1	1:E:25:GLU:OE1	2.46	0.49
1:E:78:THR:HG22	1:E:136:LEU:HG	1.95	0.49
1:K:67:ILE:HG12	1:K:77:VAL:HG22	1.94	0.49
1:M:20:ARG:NH1	1:M:25:GLU:OE1	2.46	0.49
1:Q:20:ARG:NH1	1:Q:25:GLU:OE1	2.46	0.49
1:C:54:VAL:HB	1:C:208:LYS:HD3	1.95	0.49
1:K:162:ALA:HB1	1:K:176:LEU:HD13	1.94	0.49
2:D:70:ARG:HB3	2:D:72:VAL:HG12	1.94	0.49
2:H:94:PRO:O	2:J:91:LYS:NZ	2.29	0.49
2:P:196:ILE:HD13	2:P:203:LEU:HG	1.94	0.49
2:V:196:ILE:HD13	2:V:203:LEU:HG	1.94	0.49
1:A:41:LYS:HG2	1:A:46:VAL:HG12	1.93	0.49
1:K:152:ASP:O	1:K:155:GLY:N	2.42	0.49
2:L:16:THR:HG21	2:L:33:LYS:HB2	1.95	0.49
1:W:152:ASP:O	1:W:155:GLY:N	2.42	0.49
1:O:152:ASP:O	1:O:155:GLY:N	2.42	0.49
2:P:16:THR:HG21	2:P:33:LYS:HB2	1.94	0.49
2:V:3:THR:HG22	2:V:16:THR:HG23	1.94	0.49
2:X:3:THR:HG22	2:X:16:THR:HG23	1.94	0.49
1:S:67:ILE:HG12	1:S:77:VAL:HG22	1.94	0.49
1:Y:20:ARG:NH1	1:Y:25:GLU:OE1	2.46	0.49
1:G:181:LYS:HE2	1:G:184:LEU:HD21	1.93	0.49
1:O:194:ILE:HD11	1:O:212:ILE:HD11	1.95	0.49
2:N:70:ARG:HB3	2:N:72:VAL:HG12	1.94	0.49
2:B:196:ILE:HD13	2:B:203:LEU:HG	1.94	0.49
2:J:196:ILE:HD13	2:J:203:LEU:HG	1.94	0.49
1:A:99:GLU:HB2	1:A:115:ARG:HH22	1.77	0.49
1:O:99:GLU:HB2	1:O:115:ARG:HH22	1.77	0.49
1:S:100:LYS:NZ	2:T:64:GLU:OE2	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:99:GLU:HB2	1:W:115:ARG:HH22	1.77	0.49
2:D:15:ALA:HA	2:D:174:ASP:O	2.12	0.49
1:O:41:LYS:HG2	1:O:46:VAL:HG12	1.93	0.49
2:1:15:ALA:HA	2:1:174:ASP:O	2.12	0.49
2:D:132:PRO:HB2	2:R:132:PRO:HB2	1.94	0.49
2:H:3:THR:HG22	2:H:16:THR:HG23	1.94	0.49
1:E:67:ILE:HG12	1:E:77:VAL:HG22	1.95	0.49
1:A:67:ILE:HG12	1:A:77:VAL:HG22	1.94	0.49
1:W:78:THR:HG22	1:W:136:LEU:HG	1.95	0.49
1:C:49:ILE:HG12	1:C:212:ILE:HG12	1.95	0.49
2:F:3:THR:OG1	2:F:127:THR:OG1	2.26	0.49
1:G:121:GLN:NE2	1:I:84:ASP:OD1	2.45	0.49
2:L:43:MET:HE1	2:L:59:MET:HG3	1.95	0.49
1:O:49:ILE:HG12	1:O:212:ILE:HG12	1.95	0.49
1:A:54:VAL:HB	1:A:208:LYS:HD3	1.95	0.49
1:O:194:ILE:HD11	1:O:212:ILE:HD11	1.95	0.49
1:Q:194:ILE:HD11	1:Q:212:ILE:HD11	1.95	0.49
1:S:162:ALA:HB1	1:S:176:LEU:HD13	1.95	0.49
1:W:181:LYS:HE2	1:W:184:LEU:HD21	1.93	0.49
2:N:163:LYS:NZ	2:N:203:LEU:O	2.41	0.49
2:R:70:ARG:HB3	2:R:72:VAL:HG12	1.94	0.49
2:R:163:LYS:NZ	2:R:203:LEU:O	2.41	0.49
2:Z:70:ARG:HB3	2:Z:72:VAL:HG12	1.94	0.49
1:G:99:GLU:HB2	1:G:115:ARG:HH22	1.78	0.49
1:E:152:ASP:O	1:E:155:GLY:N	2.42	0.49
2:R:16:THR:HG21	2:R:33:LYS:HB2	1.94	0.49
2:1:16:THR:HG21	2:1:33:LYS:HB2	1.95	0.49
2:B:3:THR:HG1	2:B:127:THR:HG1	1.56	0.49
2:B:16:THR:HG21	2:B:33:LYS:HB2	1.94	0.49
2:R:3:THR:HG22	2:R:16:THR:HG23	1.94	0.49
1:C:54:VAL:HB	1:C:208:LYS:HE2	1.95	0.49
1:G:20:ARG:NH1	1:G:25:GLU:OE1	2.46	0.49
1:G:78:THR:HG22	1:G:136:LEU:HG	1.95	0.49
1:W:20:ARG:NH1	1:W:25:GLU:OE1	2.46	0.49
1:I:49:ILE:HG12	1:I:212:ILE:HG12	1.95	0.49
1:S:49:ILE:HG12	1:S:212:ILE:HG12	1.95	0.49
1:U:49:ILE:HG12	1:U:212:ILE:HG12	1.95	0.49
1:Y:49:ILE:HG12	1:Y:212:ILE:HG12	1.95	0.49
1:A:194:ILE:HD11	1:A:212:ILE:HD11	1.95	0.49
1:C:110:GLU:HA	1:C:149:PHE:HE2	1.76	0.49
1:K:194:ILE:HD11	1:K:212:ILE:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:194:ILE:HD11	1:M:212:ILE:HD11	1.95	0.49
1:S:194:ILE:HD11	1:S:212:ILE:HD11	1.95	0.49
2:H:70:ARG:HB3	2:H:72:VAL:HG12	1.94	0.49
2:1:70:ARG:HB3	2:1:72:VAL:HG12	1.94	0.49
1:I:172:VAL:HG13	1:I:196:ALA:HB1	1.94	0.49
1:M:172:VAL:HG13	1:M:196:ALA:HB1	1.94	0.49
1:Q:172:VAL:HG13	1:Q:196:ALA:HB1	1.94	0.49
1:U:172:VAL:HG13	1:U:196:ALA:HB1	1.94	0.49
1:C:78:THR:HG22	1:C:136:LEU:HG	1.95	0.49
1:C:152:ASP:O	1:C:155:GLY:N	2.42	0.49
1:G:152:ASP:O	1:G:155:GLY:N	2.42	0.49
2:H:16:THR:HG21	2:H:33:LYS:HB2	1.95	0.49
2:P:16:THR:HG21	2:P:33:LYS:HB2	1.94	0.49
1:Y:78:THR:HG22	1:Y:136:LEU:HG	1.95	0.49
2:N:3:THR:HG22	2:N:16:THR:HG23	1.94	0.49
1:E:49:ILE:HG12	1:E:212:ILE:HG12	1.95	0.49
1:K:49:ILE:HG12	1:K:212:ILE:HG12	1.95	0.49
2:T:43:MET:HE1	2:T:59:MET:HG3	1.95	0.49
1:A:67:ILE:HG12	1:A:77:VAL:HG22	1.95	0.49
1:C:194:ILE:HD11	1:C:212:ILE:HD11	1.95	0.49
1:K:99:GLU:HB2	1:K:115:ARG:HH22	1.77	0.49
2:L:70:ARG:HB3	2:L:72:VAL:HG12	1.94	0.49
2:X:70:ARG:HB3	2:X:72:VAL:HG12	1.94	0.49
1:E:172:VAL:HG13	1:E:196:ALA:HB1	1.95	0.49
1:Y:172:VAL:HG13	1:Y:196:ALA:HB1	1.95	0.49
2:D:16:THR:HG21	2:D:33:LYS:HB2	1.95	0.49
1:E:78:THR:HG22	1:E:136:LEU:HG	1.95	0.49
1:K:78:THR:HG22	1:K:136:LEU:HG	1.95	0.49
2:N:16:THR:HG21	2:N:33:LYS:HB2	1.95	0.49
1:S:78:THR:HG22	1:S:136:LEU:HG	1.95	0.49
2:Z:16:THR:HG21	2:Z:33:LYS:HB2	1.94	0.49
1:M:76:ALA:HA	1:M:137:ILE:O	2.12	0.49
1:C:67:ILE:HG12	1:C:77:VAL:HG22	1.95	0.49
1:E:67:ILE:HG12	1:E:77:VAL:HG22	1.94	0.49
1:I:78:THR:HG22	1:I:136:LEU:HG	1.95	0.49
2:J:43:MET:HE1	2:J:59:MET:HG3	1.95	0.49
1:A:99:GLU:HB2	1:A:115:ARG:HH22	1.78	0.49
1:C:162:ALA:HB1	1:C:176:LEU:HD13	1.94	0.49
1:W:99:GLU:HB2	1:W:115:ARG:HH22	1.78	0.49
1:Y:99:GLU:HB2	1:Y:115:ARG:HH22	1.78	0.49
1:O:162:ALA:HB1	1:O:176:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:172:VAL:HG13	1:K:196:ALA:HB1	1.94	0.49
2:B:16:THR:HG21	2:B:33:LYS:HB2	1.95	0.48
2:F:16:THR:HG21	2:F:33:LYS:HB2	1.95	0.48
1:M:78:THR:HG22	1:M:136:LEU:HG	1.95	0.48
1:O:78:THR:HG22	1:O:136:LEU:HG	1.95	0.48
2:N:16:THR:HG21	2:N:33:LYS:HB2	1.94	0.48
2:R:16:THR:HG21	2:R:33:LYS:HB2	1.94	0.48
1:C:78:THR:HG22	1:C:136:LEU:HG	1.94	0.48
1:C:78:THR:HG22	1:C:136:LEU:HG	1.95	0.48
1:U:78:THR:HG22	1:U:136:LEU:HG	1.95	0.48
1:Y:67:ILE:HG12	1:Y:77:VAL:HG22	1.94	0.48
1:O:20:ARG:NH1	1:O:25:GLU:OE1	2.46	0.48
1:A:49:ILE:HG12	1:A:212:ILE:HG12	1.95	0.48
2:R:43:MET:HE1	2:R:59:MET:HG3	1.95	0.48
2:V:43:MET:HE1	2:V:59:MET:HG3	1.95	0.48
1:C:150:ASP:O	1:C:157:ILE:HA	2.13	0.48
1:E:99:GLU:HB2	1:E:115:ARG:HH22	1.78	0.48
1:G:99:GLU:HB2	1:G:115:ARG:HH22	1.78	0.48
1:S:99:GLU:HB2	1:S:115:ARG:HH22	1.78	0.48
2:T:70:ARG:HB3	2:T:72:VAL:HG12	1.94	0.48
1:C:172:VAL:HG13	1:C:196:ALA:HB1	1.95	0.48
1:I:99:GLU:HB2	1:I:115:ARG:HH22	1.77	0.48
1:M:99:GLU:HB2	1:M:115:ARG:HH22	1.77	0.48
1:U:99:GLU:HB2	1:U:115:ARG:HH22	1.77	0.48
1:O:78:THR:HG22	1:O:136:LEU:HG	1.95	0.48
1:Q:78:THR:HG22	1:Q:136:LEU:HG	1.95	0.48
1:Q:76:ALA:HA	1:Q:137:ILE:O	2.12	0.48
1:G:67:ILE:HG12	1:G:77:VAL:HG22	1.94	0.48
2:H:17:GLU:OE2	2:H:33:LYS:NZ	2.44	0.48
1:W:67:ILE:HG12	1:W:77:VAL:HG22	1.94	0.48
1:O:78:THR:HG22	1:O:136:LEU:HG	1.95	0.48
2:N:43:MET:HE1	2:N:59:MET:HG3	1.95	0.48
1:O:49:ILE:HG12	1:O:212:ILE:HG12	1.95	0.48
1:Q:49:ILE:HG12	1:Q:212:ILE:HG12	1.95	0.48
1:W:49:ILE:HG12	1:W:212:ILE:HG12	1.95	0.48
1:A:150:ASP:O	1:A:157:ILE:HA	2.13	0.48
1:I:162:ALA:HB1	1:I:176:LEU:HD13	1.95	0.48
1:O:99:GLU:HB2	1:O:115:ARG:HH22	1.78	0.48
1:O:110:GLU:HA	1:O:149:PHE:HE2	1.77	0.48
2:F:163:LYS:NZ	2:F:171:GLY:O	2.46	0.48
2:J:163:LYS:NZ	2:J:171:GLY:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:172:VAL:HG13	1:S:196:ALA:HB1	1.94	0.48
2:V:163:LYS:NZ	2:V:171:GLY:O	2.46	0.48
2:X:196:ILE:HD13	2:X:203:LEU:HG	1.94	0.48
2:1:163:LYS:NZ	2:1:171:GLY:O	2.46	0.48
2:D:93:MET:HE3	2:F:91:LYS:HB2	1.95	0.48
1:E:99:GLU:OE2	2:H:70:ARG:NH2	2.45	0.48
1:Q:99:GLU:HB2	1:Q:115:ARG:HH22	1.77	0.48
1:O:172:VAL:HG13	1:O:196:ALA:HB1	1.95	0.48
1:G:78:THR:HG22	1:G:136:LEU:HG	1.95	0.48
2:J:15:ALA:HA	2:J:174:ASP:O	2.12	0.48
2:L:15:ALA:HA	2:L:174:ASP:O	2.12	0.48
2:V:15:ALA:HA	2:V:174:ASP:O	2.12	0.48
1:W:78:THR:HG22	1:W:136:LEU:HG	1.95	0.48
1:C:121:GLN:NE2	1:E:84:ASP:OD1	2.45	0.48
1:C:20:ARG:NH1	1:C:25:GLU:OE1	2.46	0.48
2:X:17:GLU:OE2	2:X:33:LYS:NZ	2.44	0.48
1:G:49:ILE:HG12	1:G:212:ILE:HG12	1.95	0.48
1:M:49:ILE:HG12	1:M:212:ILE:HG12	1.95	0.48
1:E:194:ILE:HD11	1:E:212:ILE:HD11	1.95	0.48
1:U:162:ALA:HB1	1:U:176:LEU:HD13	1.95	0.48
1:Y:194:ILE:HD11	1:Y:212:ILE:HD11	1.95	0.48
2:R:16:THR:HG21	2:R:33:LYS:HB2	1.96	0.48
2:D:163:LYS:NZ	2:D:171:GLY:O	2.46	0.48
2:F:3:THR:OG1	2:F:127:THR:OG1	2.26	0.48
2:H:196:ILE:HD13	2:H:203:LEU:HG	1.94	0.48
2:P:163:LYS:NZ	2:P:171:GLY:O	2.46	0.48
2:Z:163:LYS:NZ	2:Z:171:GLY:O	2.46	0.48
1:W:172:VAL:HG13	1:W:196:ALA:HB1	1.95	0.48
1:A:78:THR:HG22	1:A:136:LEU:HG	1.95	0.48
1:I:78:THR:HG22	1:I:136:LEU:HG	1.95	0.48
2:T:15:ALA:HA	2:T:174:ASP:O	2.12	0.48
1:C:160:TYR:CE1	1:E:59:ILE:HG12	2.48	0.48
2:D:3:THR:HG22	2:D:16:THR:HG23	1.94	0.48
1:O:20:ARG:NH1	1:O:25:GLU:OE1	2.46	0.48
1:E:152:ASP:HB3	1:E:156:THR:HB	1.96	0.48
2:H:167:SER:HB2	2:X:167:SER:HB2	1.95	0.48
2:B:16:THR:HG21	2:B:33:LYS:HB2	1.96	0.48
2:N:16:THR:HG21	2:N:33:LYS:HB2	1.96	0.48
2:P:16:THR:HG21	2:P:33:LYS:HB2	1.96	0.48
2:P:70:ARG:HB3	2:P:72:VAL:HG12	1.94	0.48
2:R:163:LYS:NZ	2:R:171:GLY:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:163:LYS:NZ	2:X:171:GLY:O	2.46	0.48
1:A:130:ARG:O	1:M:125:GLN:NE2	2.46	0.48
1:G:172:VAL:HG13	1:G:196:ALA:HB1	1.95	0.48
1:K:99:GLU:HB2	1:K:115:ARG:HH22	1.77	0.48
1:S:99:GLU:HB2	1:S:115:ARG:HH22	1.77	0.48
1:U:78:THR:HG22	1:U:136:LEU:HG	1.95	0.48
2:D:43:MET:HE1	2:D:59:MET:HG3	1.94	0.48
1:E:78:THR:HG22	1:E:136:LEU:HG	1.94	0.48
1:U:67:ILE:HG12	1:U:77:VAL:HG22	1.94	0.48
2:1:17:GLU:OE2	2:1:33:LYS:NZ	2.44	0.48
1:W:152:ASP:HB3	1:W:156:THR:HB	1.96	0.48
1:Y:152:ASP:HB3	1:Y:156:THR:HB	1.96	0.48
1:A:39:GLY:O	1:A:162:ALA:HA	2.14	0.48
2:B:70:ARG:HB3	2:B:72:VAL:HG12	1.94	0.48
2:B:163:LYS:NZ	2:B:171:GLY:O	2.46	0.48
2:F:196:ILE:HD13	2:F:203:LEU:HG	1.94	0.48
2:H:163:LYS:NZ	2:H:171:GLY:O	2.46	0.48
2:Z:196:ILE:HD13	2:Z:203:LEU:HG	1.94	0.48
1:U:100:LYS:NZ	2:V:64:GLU:OE2	2.46	0.48
2:F:3:THR:HG22	2:F:16:THR:HG23	1.94	0.48
2:Z:3:THR:HG22	2:Z:16:THR:HG23	1.94	0.48
2:D:3:THR:O	2:D:126:SER:HA	2.13	0.48
1:A:20:ARG:NH1	1:A:25:GLU:OE1	2.46	0.48
1:I:20:ARG:NH1	1:I:25:GLU:OE1	2.46	0.48
1:I:67:ILE:HG12	1:I:77:VAL:HG22	1.94	0.48
2:F:141:GLN:HE21	2:T:141:GLN:HE21	1.62	0.48
1:C:67:ILE:HG12	1:C:77:VAL:HG22	1.95	0.48
1:O:39:GLY:O	1:O:162:ALA:HA	2.14	0.48
1:Q:39:GLY:O	1:Q:162:ALA:HA	2.14	0.48
2:L:163:LYS:NZ	2:L:171:GLY:O	2.46	0.48
2:N:163:LYS:NZ	2:N:171:GLY:O	2.46	0.48
2:T:163:LYS:NZ	2:T:171:GLY:O	2.46	0.48
2:1:3:THR:OG1	2:1:127:THR:OG1	2.26	0.48
1:O:172:VAL:HG13	1:O:196:ALA:HB1	1.95	0.48
1:I:194:ILE:HD11	1:I:212:ILE:HD11	1.95	0.48
1:K:194:ILE:HD11	1:K:212:ILE:HD11	1.96	0.48
2:P:3:THR:HG22	2:P:16:THR:HG23	1.94	0.48
1:U:194:ILE:HD11	1:U:212:ILE:HD11	1.95	0.48
1:C:67:ILE:HG12	1:C:77:VAL:HG22	1.94	0.48
2:D:17:GLU:OE2	2:D:33:LYS:NZ	2.44	0.48
1:U:20:ARG:NH1	1:U:25:GLU:OE1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:125:GLN:NE2	1:I:130:ARG:O	2.47	0.48
1:G:152:ASP:HB3	1:G:156:THR:HB	1.96	0.48
2:H:43:MET:HE1	2:H:59:MET:HG3	1.95	0.48
2:J:141:GLN:HE21	2:X:141:GLN:HE21	1.62	0.48
1:K:152:ASP:HB3	1:K:156:THR:HB	1.96	0.48
1:A:39:GLY:HA2	1:A:47:LEU:O	2.13	0.48
1:E:162:ALA:HB1	1:E:176:LEU:HD13	1.94	0.48
1:M:39:GLY:O	1:M:162:ALA:HA	2.14	0.48
1:O:39:GLY:O	1:O:162:ALA:HA	2.14	0.48
2:V:70:ARG:HB3	2:V:72:VAL:HG12	1.94	0.48
1:A:172:VAL:HG13	1:A:196:ALA:HB1	1.95	0.48
2:H:15:ALA:HA	2:H:174:ASP:O	2.12	0.48
2:B:3:THR:HG22	2:B:16:THR:HG23	1.94	0.48
1:S:194:ILE:HD11	1:S:212:ILE:HD11	1.96	0.48
1:K:20:ARG:NH1	1:K:25:GLU:OE1	2.46	0.48
1:K:78:THR:HG22	1:K:136:LEU:HG	1.95	0.48
1:O:67:ILE:HG12	1:O:77:VAL:HG22	1.94	0.48
1:I:152:ASP:HB3	1:I:156:THR:HB	1.96	0.48
2:L:141:GLN:HE21	2:Z:141:GLN:HE21	1.62	0.48
1:S:152:ASP:HB3	1:S:156:THR:HB	1.96	0.48
1:U:152:ASP:HB3	1:U:156:THR:HB	1.96	0.48
2:X:43:MET:HE1	2:X:59:MET:HG3	1.95	0.48
1:C:39:GLY:O	1:C:162:ALA:HA	2.14	0.48
1:Q:97:GLN:HG3	2:R:65:LEU:HG	1.96	0.48
1:Y:162:ALA:HB1	1:Y:176:LEU:HD13	1.94	0.48
1:O:99:GLU:HB2	1:O:115:ARG:HH22	1.78	0.48
2:B:15:ALA:HA	2:B:174:ASP:O	2.14	0.48
2:J:70:ARG:HB3	2:J:72:VAL:HG12	1.94	0.48
2:N:15:ALA:HA	2:N:174:ASP:O	2.14	0.48
2:P:15:ALA:HA	2:P:174:ASP:O	2.14	0.48
2:R:15:ALA:HA	2:R:174:ASP:O	2.14	0.48
2:D:3:THR:OG1	2:D:127:THR:OG1	2.26	0.48
2:Z:3:THR:OG1	2:Z:127:THR:OG1	2.26	0.48
2:F:15:ALA:HA	2:F:174:ASP:O	2.12	0.48
1:C:160:TYR:HE1	1:E:59:ILE:HG12	1.78	0.48
1:E:152:ASP:O	1:E:155:GLY:N	2.44	0.48
1:S:20:ARG:NH1	1:S:25:GLU:OE1	2.46	0.48
1:C:99:GLU:HB2	1:C:115:ARG:HH22	1.78	0.48
2:T:16:THR:HG21	2:T:33:LYS:HB2	1.96	0.48
2:1:196:ILE:HD13	2:1:203:LEU:HG	1.94	0.48
1:I:172:VAL:HG13	1:I:196:ALA:HB1	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:172:VAL:HG13	1:M:196:ALA:HB1	1.95	0.48
1:Q:172:VAL:HG13	1:Q:196:ALA:HB1	1.95	0.48
2:Z:15:ALA:HA	2:Z:174:ASP:O	2.12	0.48
1:A:67:ILE:HG12	1:A:77:VAL:HG22	1.94	0.48
2:B:43:MET:HE1	2:B:59:MET:HG3	1.95	0.48
1:S:78:THR:HG22	1:S:136:LEU:HG	1.95	0.48
1:C:152:ASP:HB3	1:C:156:THR:HB	1.96	0.48
2:D:43:MET:HE1	2:D:59:MET:HG3	1.95	0.48
1:Q:152:ASP:HB3	1:Q:156:THR:HB	1.96	0.48
2:B:3:THR:HG22	2:B:16:THR:HG23	1.94	0.48
1:C:39:GLY:HA2	1:C:47:LEU:O	2.14	0.48
1:G:162:ALA:HB1	1:G:176:LEU:HD13	1.95	0.48
1:I:99:GLU:HB2	1:I:115:ARG:HH22	1.78	0.48
1:K:39:GLY:O	1:K:162:ALA:HA	2.14	0.48
1:U:99:GLU:HB2	1:U:115:ARG:HH22	1.78	0.48
1:W:162:ALA:HB1	1:W:176:LEU:HD13	1.94	0.48
2:D:15:ALA:HA	2:D:174:ASP:O	2.14	0.48
2:L:16:THR:HG21	2:L:33:LYS:HB2	1.96	0.48
1:U:172:VAL:HG13	1:U:196:ALA:HB1	1.95	0.48
1:C:194:ILE:HD11	1:C:212:ILE:HD11	1.95	0.47
2:B:3:THR:O	2:B:126:SER:HA	2.12	0.47
2:B:16:THR:HG21	2:B:33:LYS:HB2	1.96	0.47
2:D:16:THR:HG21	2:D:33:LYS:HB2	1.96	0.47
2:P:15:ALA:HA	2:P:174:ASP:O	2.14	0.47
1:I:52:LYS:HD2	1:I:64:ILE:HG23	1.96	0.47
1:K:52:LYS:HD2	1:K:64:ILE:HG23	1.96	0.47
1:M:152:ASP:HB3	1:M:156:THR:HB	1.96	0.47
1:O:152:ASP:HB3	1:O:156:THR:HB	1.96	0.47
1:S:52:LYS:HD2	1:S:64:ILE:HG23	1.96	0.47
1:U:52:LYS:HD2	1:U:64:ILE:HG23	1.96	0.47
1:W:52:LYS:HD2	1:W:64:ILE:HG23	1.96	0.47
2:1:43:MET:HE1	2:1:59:MET:HG3	1.95	0.47
1:M:99:GLU:HB2	1:M:115:ARG:HH22	1.78	0.47
1:S:39:GLY:O	1:S:162:ALA:HA	2.14	0.47
1:C:121:GLN:NE2	1:E:84:ASP:OD1	2.47	0.47
1:S:172:VAL:HG13	1:S:196:ALA:HB1	1.95	0.47
2:B:167:SER:HB2	2:R:167:SER:HB2	1.96	0.47
2:N:141:GLN:HE21	2:1:141:GLN:HE21	1.62	0.47
2:X:15:ALA:HA	2:X:174:ASP:O	2.13	0.47
1:A:182:GLU:OE2	1:C:57:ARG:NH1	2.47	0.47
1:M:194:ILE:HD11	1:M:212:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:43:MET:HE1	2:F:59:MET:HG3	1.94	0.47
1:O:152:ASP:HB3	1:O:156:THR:HB	1.96	0.47
1:E:39:GLY:O	1:E:162:ALA:HA	2.14	0.47
1:G:39:GLY:O	1:G:162:ALA:HA	2.14	0.47
2:P:191:GLN:HE21	2:P:195:ARG:HH21	1.63	0.47
1:U:194:ILE:HD11	1:U:212:ILE:HD11	1.95	0.47
2:1:15:ALA:HA	2:1:174:ASP:O	2.14	0.47
2:1:16:THR:HG21	2:1:33:LYS:HB2	1.96	0.47
2:D:196:ILE:HD13	2:D:203:LEU:HG	1.94	0.47
1:K:172:VAL:HG13	1:K:196:ALA:HB1	1.95	0.47
1:O:46:VAL:HG11	1:O:139:ALA:HB1	1.96	0.47
1:G:77:VAL:HG22	1:G:137:ILE:HB	1.96	0.47
1:W:77:VAL:HG22	1:W:137:ILE:HB	1.96	0.47
2:F:16:THR:HG21	2:F:33:LYS:HB2	1.96	0.47
2:B:15:ALA:HA	2:B:174:ASP:O	2.14	0.47
2:P:50:GLY:O	2:1:88:ASN:ND2	2.47	0.47
2:R:15:ALA:HA	2:R:174:ASP:O	2.14	0.47
2:Z:17:GLU:OE2	2:Z:33:LYS:NZ	2.44	0.47
2:B:43:MET:HE1	2:B:59:MET:HG3	1.95	0.47
1:G:52:LYS:HD2	1:G:64:ILE:HG23	1.96	0.47
1:W:186:GLU:OE2	1:W:224:TYR:OH	2.31	0.47
2:B:113:ILE:HA	2:B:118:GLY:O	2.14	0.47
2:D:113:ILE:HA	2:D:118:GLY:O	2.14	0.47
2:N:191:GLN:HE21	2:N:195:ARG:HH21	1.63	0.47
2:P:113:ILE:HA	2:P:118:GLY:O	2.14	0.47
1:Q:99:GLU:HB2	1:Q:115:ARG:HH22	1.78	0.47
2:R:191:GLN:HE21	2:R:195:ARG:HH21	1.63	0.47
1:W:39:GLY:O	1:W:162:ALA:HA	2.14	0.47
1:Y:39:GLY:O	1:Y:162:ALA:HA	2.14	0.47
1:A:46:VAL:HG11	1:A:139:ALA:HB1	1.96	0.47
1:A:194:ILE:HD11	1:A:212:ILE:HD11	1.95	0.47
1:G:194:ILE:HD11	1:G:212:ILE:HD11	1.95	0.47
1:Q:194:ILE:HD11	1:Q:212:ILE:HD11	1.96	0.47
1:C:172:VAL:HG13	1:C:196:ALA:HB1	1.97	0.47
1:C:18:ASP:O	1:E:33:LYS:NZ	2.46	0.47
2:F:17:GLU:OE2	2:F:33:LYS:NZ	2.44	0.47
1:A:152:ASP:HB3	1:A:156:THR:HB	1.96	0.47
2:F:43:MET:HE1	2:F:59:MET:HG3	1.95	0.47
1:G:178:ARG:HG3	1:G:179:GLU:HG2	1.97	0.47
2:P:43:MET:HE1	2:P:59:MET:HG3	1.95	0.47
2:Z:43:MET:HE1	2:Z:59:MET:HG3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:191:GLN:HE21	2:B:195:ARG:HH21	1.63	0.47
1:G:194:ILE:HD11	1:G:212:ILE:HD11	1.95	0.47
1:I:39:GLY:O	1:I:162:ALA:HA	2.14	0.47
1:I:194:ILE:HD11	1:I:212:ILE:HD11	1.95	0.47
2:L:15:ALA:HA	2:L:174:ASP:O	2.14	0.47
1:O:55:ARG:HH22	1:O:208:LYS:NZ	2.13	0.47
1:O:46:VAL:HG11	1:O:139:ALA:HB1	1.96	0.47
2:N:167:SER:HB2	2:P:167:SER:HB2	1.96	0.47
1:O:194:ILE:HD11	1:O:212:ILE:HD11	1.96	0.47
1:W:194:ILE:HD11	1:W:212:ILE:HD11	1.95	0.47
1:E:172:VAL:HG13	1:E:196:ALA:HB1	1.97	0.47
1:A:78:THR:HG22	1:A:136:LEU:HG	1.95	0.47
2:N:15:ALA:HA	2:N:174:ASP:O	2.14	0.47
1:Q:78:THR:HG22	1:Q:136:LEU:HG	1.95	0.47
2:D:139:GLU:OE2	2:R:165:ARG:NH2	2.34	0.47
2:1:113:ILE:HA	2:1:118:GLY:O	2.14	0.47
1:C:55:ARG:HH22	1:C:208:LYS:NZ	2.13	0.47
2:D:16:THR:HG21	2:D:33:LYS:HB2	1.96	0.47
1:I:76:ALA:HA	1:I:137:ILE:O	2.15	0.47
2:T:15:ALA:HA	2:T:174:ASP:O	2.14	0.47
1:I:49:ILE:HG12	1:I:212:ILE:HG12	1.96	0.47
1:Q:46:VAL:HG11	1:Q:139:ALA:HB1	1.96	0.47
1:E:77:VAL:HG22	1:E:137:ILE:HB	1.96	0.47
1:U:77:VAL:HG22	1:U:137:ILE:HB	1.97	0.47
1:E:194:ILE:HD11	1:E:212:ILE:HD11	1.95	0.47
1:Y:194:ILE:HD11	1:Y:212:ILE:HD11	1.96	0.47
1:E:52:LYS:HD2	1:E:64:ILE:HG23	1.96	0.47
1:W:178:ARG:HG3	1:W:179:GLU:HG2	1.97	0.47
1:Y:52:LYS:HD2	1:Y:64:ILE:HG23	1.96	0.47
1:O:160:TYR:CE1	1:O:59:ILE:HG12	2.49	0.47
2:V:113:ILE:HA	2:V:118:GLY:O	2.14	0.47
1:W:194:ILE:HD11	1:W:212:ILE:HD11	1.95	0.47
2:1:191:GLN:HE21	2:1:195:ARG:HH21	1.63	0.47
2:J:16:THR:HG21	2:J:33:LYS:HB2	1.96	0.47
1:C:46:VAL:HG11	1:C:139:ALA:HB1	1.96	0.47
1:M:46:VAL:HG11	1:M:139:ALA:HB1	1.96	0.47
1:U:49:ILE:HG12	1:U:212:ILE:HG12	1.96	0.47
1:I:77:VAL:HG22	1:I:137:ILE:HB	1.97	0.47
1:Y:77:VAL:HG22	1:Y:137:ILE:HB	1.96	0.47
2:B:15:ALA:HA	2:B:174:ASP:O	2.15	0.47
2:P:15:ALA:HA	2:P:174:ASP:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:15:ALA:HA	2:J:174:ASP:O	2.14	0.47
1:M:78:THR:HG22	1:M:136:LEU:HG	1.95	0.47
2:V:15:ALA:HA	2:V:174:ASP:O	2.14	0.47
2:X:113:ILE:HA	2:X:118:GLY:O	2.15	0.47
2:1:15:ALA:HA	2:1:174:ASP:O	2.14	0.47
1:E:178:ARG:HG3	1:E:179:GLU:HG2	1.97	0.47
1:G:76:ALA:HA	1:G:137:ILE:O	2.15	0.47
1:I:76:ALA:HA	1:I:137:ILE:O	2.15	0.47
1:I:125:GLN:NE2	1:K:130:ARG:O	2.48	0.47
1:M:52:LYS:HD2	1:M:64:ILE:HG23	1.97	0.47
1:O:76:ALA:HA	1:O:137:ILE:O	2.15	0.47
1:Q:52:LYS:HD2	1:Q:64:ILE:HG23	1.96	0.47
1:S:130:ARG:O	1:U:125:GLN:NE2	2.48	0.47
1:U:76:ALA:HA	1:U:137:ILE:O	2.15	0.47
1:U:130:ARG:O	1:W:125:GLN:NE2	2.48	0.47
1:Y:178:ARG:HG3	1:Y:179:GLU:HG2	1.97	0.47
2:D:191:GLN:HE21	2:D:195:ARG:HH21	1.63	0.47
2:J:113:ILE:HA	2:J:118:GLY:O	2.14	0.47
1:U:39:GLY:O	1:U:162:ALA:HA	2.14	0.47
2:H:3:THR:OG1	2:H:127:THR:OG1	2.25	0.47
1:U:76:ALA:HA	1:U:137:ILE:O	2.15	0.47
2:V:16:THR:HG21	2:V:33:LYS:HB2	1.96	0.47
2:Z:16:THR:HG21	2:Z:33:LYS:HB2	1.96	0.47
1:G:49:ILE:HG12	1:G:212:ILE:HG12	1.97	0.47
1:W:49:ILE:HG12	1:W:212:ILE:HG12	1.97	0.47
1:Y:46:VAL:HG11	1:Y:139:ALA:HB1	1.96	0.47
1:Y:49:ILE:HG12	1:Y:212:ILE:HG12	1.96	0.47
1:G:20:ARG:NH2	1:G:25:GLU:OE1	2.48	0.47
1:I:20:ARG:NH2	1:I:25:GLU:OE1	2.48	0.47
1:U:20:ARG:NH2	1:U:25:GLU:OE1	2.48	0.47
1:A:172:VAL:HG13	1:A:196:ALA:HB1	1.97	0.47
2:D:15:ALA:HA	2:D:174:ASP:O	2.14	0.47
2:J:113:ILE:HA	2:J:118:GLY:O	2.15	0.47
2:V:113:ILE:HA	2:V:118:GLY:O	2.15	0.47
1:A:76:ALA:HA	1:A:137:ILE:O	2.15	0.47
1:A:125:GLN:NE2	1:C:130:ARG:O	2.48	0.47
2:L:167:SER:HB2	2:1:167:SER:HB2	1.96	0.47
1:U:178:ARG:HG3	1:U:179:GLU:HG2	1.97	0.47
1:W:76:ALA:HA	1:W:137:ILE:O	2.15	0.47
2:L:191:GLN:HE21	2:L:195:ARG:HH21	1.63	0.47
1:A:55:ARG:HH22	1:A:208:LYS:NZ	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:76:ALA:HA	1:G:137:ILE:O	2.15	0.47
1:M:76:ALA:HA	1:M:137:ILE:O	2.15	0.47
1:O:55:ARG:HH22	1:O:208:LYS:NZ	2.13	0.47
1:O:76:ALA:HA	1:O:137:ILE:O	2.15	0.47
1:Q:76:ALA:HA	1:Q:137:ILE:O	2.15	0.47
1:W:76:ALA:HA	1:W:137:ILE:O	2.15	0.47
1:E:46:VAL:HG11	1:E:139:ALA:HB1	1.96	0.47
1:E:49:ILE:HG12	1:E:212:ILE:HG12	1.96	0.47
1:W:20:ARG:NH2	1:W:25:GLU:OE1	2.48	0.47
2:H:113:ILE:HA	2:H:118:GLY:O	2.15	0.47
1:I:18:ASP:O	1:K:33:LYS:NZ	2.46	0.47
1:C:52:LYS:HD2	1:C:64:ILE:HG23	1.96	0.47
1:E:76:ALA:HA	1:E:137:ILE:O	2.15	0.47
1:Y:76:ALA:HA	1:Y:137:ILE:O	2.15	0.47
1:O:52:LYS:HD2	1:O:64:ILE:HG23	1.96	0.47
2:T:191:GLN:HE21	2:T:195:ARG:HH21	1.63	0.47
2:X:113:ILE:HA	2:X:118:GLY:O	2.14	0.47
1:A:76:ALA:HA	1:A:137:ILE:O	2.15	0.47
1:K:76:ALA:HA	1:K:137:ILE:O	2.15	0.47
2:X:16:THR:HG21	2:X:33:LYS:HB2	1.96	0.47
2:Z:3:THR:OG1	2:Z:127:THR:OG1	2.25	0.47
2:J:43:MET:HE1	2:J:59:MET:HG3	1.97	0.47
2:T:43:MET:HE1	2:T:59:MET:HG3	1.97	0.47
2:V:43:MET:HE1	2:V:59:MET:HG3	1.97	0.47
2:D:141:GLN:HE21	2:R:141:GLN:HE21	1.63	0.47
1:E:194:ILE:HD11	1:E:212:ILE:HD11	1.96	0.47
1:I:178:ARG:HG3	1:I:179:GLU:HG2	1.97	0.47
1:K:125:GLN:NE2	1:M:130:ARG:O	2.48	0.47
1:M:76:ALA:HA	1:M:137:ILE:O	2.15	0.47
1:O:125:GLN:NE2	1:O:130:ARG:O	2.48	0.47
2:H:113:ILE:HA	2:H:118:GLY:O	2.14	0.47
2:T:113:ILE:HA	2:T:118:GLY:O	2.14	0.47
2:H:16:THR:HG21	2:H:33:LYS:HB2	1.96	0.47
1:I:55:ARG:HH22	1:I:208:LYS:NZ	2.13	0.47
1:K:55:ARG:HH22	1:K:208:LYS:NZ	2.13	0.47
1:S:76:ALA:HA	1:S:137:ILE:O	2.15	0.47
2:T:163:LYS:NZ	2:T:203:LEU:O	2.41	0.47
1:A:186:GLU:OE2	1:A:224:TYR:OH	2.30	0.47
2:L:43:MET:HE1	2:L:59:MET:HG3	1.97	0.47
1:O:179:GLU:O	1:O:57:ARG:NH2	2.44	0.46
1:O:77:VAL:HG22	1:O:137:ILE:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:78:THR:HG22	1:E:136:LEU:HG	1.97	0.46
1:G:78:THR:HG22	1:G:136:LEU:HG	1.97	0.46
2:J:15:ALA:HA	2:J:174:ASP:O	2.15	0.46
2:B:17:GLU:OE2	2:B:33:LYS:NZ	2.44	0.46
2:P:17:GLU:OE2	2:P:33:LYS:NZ	2.44	0.46
1:S:33:LYS:NZ	1:U:18:ASP:O	2.46	0.46
1:W:33:LYS:NZ	1:Y:18:ASP:O	2.45	0.46
1:A:51:ASP:HB2	1:A:197:LEU:HD11	1.97	0.46
1:A:130:ARG:O	1:M:125:GLN:NE2	2.48	0.46
1:O:51:ASP:HB2	1:O:197:LEU:HD11	1.97	0.46
1:O:130:ARG:O	1:Q:125:GLN:NE2	2.48	0.46
1:S:76:ALA:HA	1:S:137:ILE:O	2.15	0.46
1:O:51:ASP:HB2	1:O:197:LEU:HD11	1.97	0.46
2:L:113:ILE:HA	2:L:118:GLY:O	2.14	0.46
1:E:55:ARG:HH22	1:E:208:LYS:NZ	2.13	0.46
1:E:76:ALA:HA	1:E:137:ILE:O	2.15	0.46
2:F:15:ALA:HA	2:F:174:ASP:O	2.14	0.46
2:F:16:THR:HG21	2:F:33:LYS:HB2	1.96	0.46
1:S:55:ARG:HH22	1:S:208:LYS:NZ	2.13	0.46
1:U:55:ARG:HH22	1:U:208:LYS:NZ	2.13	0.46
1:Y:55:ARG:HH22	1:Y:208:LYS:NZ	2.13	0.46
1:I:100:LYS:NZ	2:J:64:GLU:OE2	2.48	0.46
1:O:186:GLU:OE2	1:O:224:TYR:OH	2.30	0.46
1:S:46:VAL:HG11	1:S:139:ALA:HB1	1.96	0.46
1:W:78:THR:HG22	1:W:136:LEU:HG	1.97	0.46
1:Y:78:THR:HG22	1:Y:136:LEU:HG	1.97	0.46
2:T:113:ILE:HA	2:T:118:GLY:O	2.15	0.46
2:V:17:GLU:OE2	2:V:33:LYS:NZ	2.44	0.46
2:X:15:ALA:HA	2:X:174:ASP:O	2.14	0.46
1:C:51:ASP:HB2	1:C:197:LEU:HD11	1.97	0.46
1:K:76:ALA:HA	1:K:137:ILE:O	2.15	0.46
1:O:52:LYS:HD2	1:O:64:ILE:HG23	1.96	0.46
1:Q:76:ALA:HA	1:Q:137:ILE:O	2.15	0.46
1:I:46:VAL:HG11	1:I:139:ALA:HB1	1.98	0.46
2:R:113:ILE:HA	2:R:118:GLY:O	2.14	0.46
1:S:46:VAL:HG11	1:S:139:ALA:HB1	1.98	0.46
1:U:46:VAL:HG11	1:U:139:ALA:HB1	1.98	0.46
2:Z:191:GLN:HE21	2:Z:195:ARG:HH21	1.62	0.46
2:F:3:THR:OG1	2:F:127:THR:OG1	2.25	0.46
2:F:94:PRO:O	2:H:91:LYS:NZ	2.36	0.46
2:Z:15:ALA:HA	2:Z:174:ASP:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:46:VAL:HG11	1:I:139:ALA:HB1	1.96	0.46
2:L:141:GLN:HE21	2:Z:141:GLN:HE21	1.63	0.46
1:O:100:LYS:NZ	2:P:64:GLU:OE2	2.49	0.46
1:Q:49:ILE:HG12	1:Q:212:ILE:HG12	1.96	0.46
1:U:46:VAL:HG11	1:U:139:ALA:HB1	1.96	0.46
2:D:15:ALA:HA	2:D:174:ASP:O	2.15	0.46
2:N:15:ALA:HA	2:N:174:ASP:O	2.15	0.46
2:R:15:ALA:HA	2:R:174:ASP:O	2.15	0.46
2:V:15:ALA:HA	2:V:174:ASP:O	2.15	0.46
2:J:17:GLU:OE2	2:J:33:LYS:NZ	2.44	0.46
2:L:15:ALA:HA	2:L:174:ASP:O	2.14	0.46
2:T:15:ALA:HA	2:T:174:ASP:O	2.14	0.46
1:A:52:LYS:HD2	1:A:64:ILE:HG23	1.97	0.46
2:B:141:GLN:HE21	2:P:141:GLN:HE21	1.63	0.46
1:C:178:ARG:HG3	1:C:179:GLU:HG2	1.96	0.46
1:I:51:ASP:HB2	1:I:197:LEU:HD11	1.97	0.46
1:U:51:ASP:HB2	1:U:197:LEU:HD11	1.97	0.46
2:V:37:ILE:HG22	2:V:63:LEU:HD22	1.97	0.46
1:C:45:GLY:HA3	1:C:215:ILE:O	2.15	0.46
1:K:46:VAL:HG11	1:K:139:ALA:HB1	1.98	0.46
2:N:113:ILE:HA	2:N:118:GLY:O	2.14	0.46
2:J:15:ALA:HA	2:J:174:ASP:O	2.14	0.46
1:Y:76:ALA:HA	1:Y:137:ILE:O	2.15	0.46
1:A:49:ILE:HG12	1:A:212:ILE:HG12	1.97	0.46
1:C:49:ILE:HG12	1:C:212:ILE:HG12	1.96	0.46
2:H:43:MET:HE1	2:H:59:MET:HG3	1.97	0.46
1:K:46:VAL:HG11	1:K:139:ALA:HB1	1.96	0.46
1:K:49:ILE:HG12	1:K:212:ILE:HG12	1.96	0.46
1:M:49:ILE:HG12	1:M:212:ILE:HG12	1.96	0.46
1:S:49:ILE:HG12	1:S:212:ILE:HG12	1.96	0.46
1:W:46:VAL:HG11	1:W:139:ALA:HB1	1.96	0.46
1:O:49:ILE:HG12	1:O:212:ILE:HG12	1.96	0.46
1:C:77:VAL:HG22	1:C:137:ILE:HB	1.97	0.46
1:W:130:ARG:O	1:Y:125:GLN:NE2	2.48	0.46
2:F:113:ILE:HA	2:F:118:GLY:O	2.15	0.46
2:H:15:ALA:HA	2:H:174:ASP:O	2.14	0.46
1:A:178:ARG:HG3	1:A:179:GLU:HG2	1.96	0.46
2:J:37:ILE:HG22	2:J:63:LEU:HD22	1.97	0.46
2:X:37:ILE:HG22	2:X:63:LEU:HD22	1.97	0.46
2:F:191:GLN:HE21	2:F:195:ARG:HH21	1.63	0.46
1:G:46:VAL:HG11	1:G:139:ALA:HB1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:172:VAL:HG13	1:G:196:ALA:HB1	1.98	0.46
2:V:15:ALA:HA	2:V:174:ASP:O	2.14	0.46
2:B:167:SER:HB2	2:R:167:SER:HB2	1.97	0.46
1:E:28:ARG:NH1	1:E:152:ASP:OD1	2.49	0.46
1:U:28:ARG:NH1	1:U:152:ASP:OD1	2.49	0.46
1:Y:28:ARG:NH1	1:Y:152:ASP:OD1	2.49	0.46
1:K:100:LYS:NZ	2:L:64:GLU:OE2	2.48	0.46
2:N:43:MET:HE1	2:N:59:MET:HG3	1.97	0.46
1:O:49:ILE:HG12	1:O:212:ILE:HG12	1.97	0.46
2:R:43:MET:HE1	2:R:59:MET:HG3	1.97	0.46
1:M:77:VAL:HG22	1:M:137:ILE:HB	1.96	0.46
1:Q:77:VAL:HG22	1:Q:137:ILE:HB	1.97	0.46
1:C:78:THR:HG22	1:C:136:LEU:HG	1.97	0.46
1:K:20:ARG:NH2	1:K:25:GLU:OE1	2.48	0.46
2:V:20:VAL:HB	2:V:28:HIS:HB2	1.98	0.46
1:A:194:ILE:HD11	1:A:212:ILE:HD11	1.97	0.46
2:L:113:ILE:HA	2:L:118:GLY:O	2.15	0.46
2:Z:113:ILE:HA	2:Z:118:GLY:O	2.15	0.46
2:H:37:ILE:HG22	2:H:63:LEU:HD22	1.97	0.46
1:Y:130:ARG:O	1:O:125:GLN:NE2	2.48	0.46
1:O:76:ALA:HA	1:O:137:ILE:O	2.15	0.46
1:O:178:ARG:HG3	1:O:179:GLU:HG2	1.97	0.46
2:F:113:ILE:HA	2:F:118:GLY:O	2.14	0.46
1:Q:46:VAL:HG11	1:Q:139:ALA:HB1	1.98	0.46
1:W:46:VAL:HG11	1:W:139:ALA:HB1	1.98	0.46
2:Z:113:ILE:HA	2:Z:118:GLY:O	2.14	0.46
1:A:172:VAL:HG13	1:A:196:ALA:HB1	1.98	0.46
1:E:172:VAL:HG13	1:E:196:ALA:HB1	1.98	0.46
1:O:172:VAL:HG13	1:O:196:ALA:HB1	1.98	0.46
1:W:172:VAL:HG13	1:W:196:ALA:HB1	1.98	0.46
2:F:167:SER:HB2	2:V:167:SER:HB2	1.97	0.46
1:I:28:ARG:NH1	1:I:152:ASP:OD1	2.49	0.46
1:G:46:VAL:HG11	1:G:139:ALA:HB1	1.96	0.46
1:G:78:THR:HG22	1:G:136:LEU:HG	1.97	0.46
1:A:77:VAL:HG22	1:A:137:ILE:HB	1.97	0.46
1:O:77:VAL:HG22	1:O:137:ILE:HB	1.97	0.46
2:B:4:VAL:HG22	2:B:134:VAL:HG11	1.98	0.46
1:C:20:ARG:NH2	1:C:25:GLU:OE1	2.48	0.46
2:H:15:ALA:HA	2:H:174:ASP:O	2.15	0.46
1:I:78:THR:HG22	1:I:136:LEU:HG	1.97	0.46
2:J:20:VAL:HB	2:J:28:HIS:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:20:ARG:NH2	1:S:25:GLU:OE1	2.48	0.46
1:C:76:ALA:HA	1:C:137:ILE:O	2.15	0.46
2:D:141:GLN:HE21	2:R:141:GLN:HE21	1.63	0.46
1:G:51:ASP:HB2	1:G:197:LEU:HD11	1.97	0.46
1:K:51:ASP:HB2	1:K:197:LEU:HD11	1.97	0.46
2:Z:37:ILE:HG22	2:Z:63:LEU:HD22	1.97	0.46
1:A:68:GLN:HE21	1:A:89:VAL:HG21	1.80	0.46
2:J:191:GLN:HE21	2:J:195:ARG:HH21	1.63	0.46
1:M:46:VAL:HG11	1:M:139:ALA:HB1	1.98	0.46
2:V:191:GLN:HE21	2:V:195:ARG:HH21	1.63	0.46
1:Y:172:VAL:HG13	1:Y:196:ALA:HB1	1.98	0.46
1:O:76:ALA:HA	1:O:137:ILE:O	2.15	0.46
2:P:3:THR:OG1	2:P:127:THR:OG1	2.26	0.46
1:M:186:GLU:OE2	1:M:224:TYR:OH	2.30	0.46
2:X:43:MET:HE1	2:X:59:MET:HG3	1.97	0.46
2:D:167:SER:HB2	2:T:167:SER:HB2	1.96	0.46
1:K:77:VAL:HG22	1:K:137:ILE:HB	1.97	0.46
1:O:152:ASP:O	1:O:155:GLY:N	2.42	0.46
1:S:77:VAL:HG22	1:S:137:ILE:HB	1.97	0.46
2:D:4:VAL:HG22	2:D:134:VAL:HG11	1.98	0.46
2:H:20:VAL:HB	2:H:28:HIS:HB2	1.98	0.46
1:O:20:ARG:NH2	1:O:25:GLU:OE1	2.48	0.46
2:P:4:VAL:HG22	2:P:134:VAL:HG11	1.98	0.46
2:T:15:ALA:HA	2:T:174:ASP:O	2.15	0.46
1:U:78:THR:HG22	1:U:136:LEU:HG	1.97	0.46
2:X:15:ALA:HA	2:X:174:ASP:O	2.15	0.46
2:B:113:ILE:HA	2:B:118:GLY:O	2.15	0.46
1:C:186:GLU:OE2	1:C:224:TYR:OH	2.31	0.46
2:F:37:ILE:HG22	2:F:63:LEU:HD22	1.97	0.46
2:H:141:GLN:HE21	2:V:141:GLN:HE21	1.64	0.46
1:M:51:ASP:HB2	1:M:197:LEU:HD11	1.97	0.46
1:O:178:ARG:HG3	1:O:179:GLU:HG2	1.97	0.46
1:Q:130:ARG:O	1:S:125:GLN:NE2	2.48	0.46
1:S:51:ASP:HB2	1:S:197:LEU:HD11	1.97	0.46
1:W:130:ARG:O	1:Y:125:GLN:NE2	2.48	0.46
1:O:186:GLU:OE2	1:O:224:TYR:OH	2.31	0.46
1:A:45:GLY:HA3	1:A:215:ILE:O	2.15	0.46
2:D:1:THR:N	2:D:168:ALA:O	2.49	0.46
2:X:1:THR:N	2:X:168:ALA:O	2.49	0.46
2:X:191:GLN:HE21	2:X:195:ARG:HH21	1.62	0.46
1:G:55:ARG:HH22	1:G:208:LYS:NZ	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:15:ALA:HA	2:H:174:ASP:O	2.14	0.46
1:O:172:VAL:HG13	1:O:196:ALA:HB1	1.98	0.46
2:H:167:SER:HB2	2:X:167:SER:HB2	1.97	0.46
1:E:78:THR:HG22	1:E:136:LEU:HG	1.97	0.46
1:U:51:ASP:HB2	1:U:197:LEU:HD11	1.98	0.46
1:W:78:THR:HG22	1:W:136:LEU:HG	1.97	0.46
2:1:43:MET:HE1	2:1:59:MET:HG3	1.97	0.46
1:A:125:GLN:NE2	1:C:130:ARG:O	2.49	0.46
1:I:125:GLN:NE2	1:K:130:ARG:O	2.49	0.46
1:S:130:ARG:O	1:U:125:GLN:NE2	2.49	0.46
1:U:152:ASP:O	1:U:155:GLY:N	2.42	0.46
2:L:15:ALA:HA	2:L:174:ASP:O	2.15	0.46
2:X:20:VAL:HB	2:X:28:HIS:HB2	1.98	0.46
2:P:113:ILE:HA	2:P:118:GLY:O	2.15	0.46
1:E:51:ASP:HB2	1:E:197:LEU:HD11	1.97	0.46
1:G:67:ILE:HG12	1:G:77:VAL:HG22	1.98	0.46
1:K:178:ARG:HG3	1:K:179:GLU:HG2	1.96	0.46
2:L:37:ILE:HG22	2:L:63:LEU:HD22	1.97	0.46
1:S:178:ARG:HG3	1:S:179:GLU:HG2	1.97	0.46
2:T:37:ILE:HG22	2:T:63:LEU:HD22	1.97	0.46
1:W:67:ILE:HG12	1:W:77:VAL:HG22	1.98	0.46
1:Y:51:ASP:HB2	1:Y:197:LEU:HD11	1.97	0.46
2:H:1:THR:N	2:H:168:ALA:O	2.49	0.46
1:Y:46:VAL:HG11	1:Y:139:ALA:HB1	1.98	0.46
2:1:1:THR:N	2:1:168:ALA:O	2.49	0.46
1:C:76:ALA:HA	1:C:137:ILE:O	2.15	0.46
1:C:172:VAL:HG13	1:C:196:ALA:HB1	1.98	0.46
2:J:167:SER:HB2	2:Z:167:SER:HB2	1.97	0.46
1:S:28:ARG:NH1	1:S:152:ASP:OD1	2.49	0.46
1:Q:186:GLU:OE2	1:Q:224:TYR:OH	2.30	0.46
1:S:51:ASP:HB2	1:S:197:LEU:HD11	1.98	0.46
1:Y:78:THR:HG22	1:Y:136:LEU:HG	1.97	0.46
2:L:167:SER:HB2	2:1:167:SER:HB2	1.96	0.46
1:Q:130:ARG:O	1:S:125:GLN:NE2	2.49	0.46
2:N:4:VAL:HG22	2:N:134:VAL:HG11	1.98	0.46
2:R:4:VAL:HG22	2:R:134:VAL:HG11	1.98	0.46
2:Z:15:ALA:HA	2:Z:174:ASP:O	2.14	0.46
1:Q:51:ASP:HB2	1:Q:197:LEU:HD11	1.97	0.46
1:O:67:ILE:HG12	1:O:77:VAL:HG22	1.98	0.46
2:H:191:GLN:HE21	2:H:195:ARG:HH21	1.63	0.46
2:1:114:ASP:O	2:1:117:GLY:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:172:VAL:HG13	1:I:196:ALA:HB1	1.98	0.46
1:M:172:VAL:HG13	1:M:196:ALA:HB1	1.98	0.46
1:U:129:VAL:HG12	1:W:126:TYR:CD1	2.51	0.46
1:U:172:VAL:HG13	1:U:196:ALA:HB1	1.98	0.46
1:W:55:ARG:HH22	1:W:208:LYS:NZ	2.13	0.46
2:X:15:ALA:HA	2:X:174:ASP:O	2.14	0.46
1:K:28:ARG:NH1	1:K:152:ASP:OD1	2.49	0.46
1:A:78:THR:HG22	1:A:136:LEU:HG	1.97	0.46
2:D:43:MET:HE1	2:D:59:MET:HG3	1.97	0.46
1:K:51:ASP:HB2	1:K:197:LEU:HD11	1.98	0.46
1:M:100:LYS:NZ	2:N:64:GLU:OE2	2.49	0.46
1:A:152:ASP:O	1:A:155:GLY:N	2.42	0.46
1:Q:67:ILE:HG12	1:Q:77:VAL:HG22	1.98	0.46
1:C:152:ASP:O	1:C:155:GLY:N	2.44	0.46
2:Z:88:ASN:ND2	2:1:50:GLY:O	2.49	0.46
2:B:37:ILE:HG22	2:B:63:LEU:HD22	1.97	0.46
1:C:67:ILE:HG12	1:C:77:VAL:HG22	1.98	0.46
1:U:67:ILE:HG12	1:U:77:VAL:HG22	1.98	0.46
1:Y:67:ILE:HG12	1:Y:77:VAL:HG22	1.98	0.46
1:E:46:VAL:HG11	1:E:139:ALA:HB1	1.98	0.46
1:Q:172:VAL:HG13	1:Q:196:ALA:HB1	1.98	0.46
1:G:51:ASP:HB2	1:G:197:LEU:HD11	1.98	0.46
1:I:51:ASP:HB2	1:I:197:LEU:HD11	1.98	0.46
1:M:78:THR:HG22	1:M:136:LEU:HG	1.97	0.46
1:I:152:ASP:O	1:I:155:GLY:N	2.42	0.45
1:Q:78:THR:HG22	1:Q:136:LEU:HG	1.97	0.45
2:F:15:ALA:HA	2:F:174:ASP:O	2.14	0.45
1:C:125:GLN:NE2	1:E:130:ARG:O	2.49	0.45
1:E:67:ILE:HG12	1:E:77:VAL:HG22	1.98	0.45
1:I:67:ILE:HG12	1:I:77:VAL:HG22	1.98	0.45
2:P:37:ILE:HG22	2:P:63:LEU:HD22	1.97	0.45
1:W:51:ASP:HB2	1:W:197:LEU:HD11	1.97	0.45
1:E:51:ASP:HB2	1:E:197:LEU:HD11	1.98	0.45
2:F:43:MET:HE1	2:F:59:MET:HG3	1.97	0.45
2:P:43:MET:HE1	2:P:59:MET:HG3	1.97	0.45
1:Q:100:LYS:NZ	2:R:64:GLU:OE2	2.49	0.45
1:W:51:ASP:HB2	1:W:197:LEU:HD11	1.98	0.45
1:Y:51:ASP:HB2	1:Y:197:LEU:HD11	1.98	0.45
1:K:125:GLN:NE2	1:M:130:ARG:O	2.49	0.45
1:A:59:ILE:HG12	1:M:160:TYR:CE1	2.51	0.45
1:K:67:ILE:HG12	1:K:77:VAL:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:67:ILE:HG12	1:M:77:VAL:HG22	1.99	0.45
2:D:113:ILE:HA	2:D:118:GLY:O	2.15	0.45
2:R:37:ILE:HG22	2:R:63:LEU:HD22	1.97	0.45
2:B:1:THR:N	2:B:168:ALA:O	2.49	0.45
2:N:63:LEU:HD21	2:N:79:VAL:HG22	1.99	0.45
2:P:1:THR:N	2:P:168:ALA:O	2.49	0.45
1:Q:113:VAL:HG21	1:Q:149:PHE:HD2	1.81	0.45
2:D:167:SER:HB2	2:T:167:SER:HB2	1.97	0.45
2:B:43:MET:HE1	2:B:59:MET:HG3	1.97	0.45
1:G:125:GLN:NE2	1:I:130:ARG:O	2.49	0.45
1:U:78:THR:HG22	1:U:136:LEU:HG	1.97	0.45
2:Z:43:MET:HE1	2:Z:59:MET:HG3	1.97	0.45
1:C:125:GLN:NE2	1:E:130:ARG:O	2.49	0.45
1:O:130:ARG:O	1:Q:125:GLN:NE2	2.50	0.45
1:U:130:ARG:O	1:W:125:GLN:NE2	2.50	0.45
2:B:20:VAL:HB	2:B:28:HIS:HB2	1.98	0.45
2:F:4:VAL:HG22	2:F:134:VAL:HG11	1.98	0.45
2:L:20:VAL:HB	2:L:28:HIS:HB2	1.98	0.45
1:M:78:THR:HG22	1:M:136:LEU:HG	1.97	0.45
2:Z:4:VAL:HG22	2:Z:134:VAL:HG11	1.98	0.45
1:C:194:ILE:HD11	1:C:212:ILE:HD11	1.96	0.45
2:N:37:ILE:HG22	2:N:63:LEU:HD22	1.97	0.45
1:S:186:GLU:OE2	1:S:224:TYR:OH	2.31	0.45
2:B:63:LEU:HD21	2:B:79:VAL:HG22	1.99	0.45
1:M:113:VAL:HG21	1:M:149:PHE:HD2	1.82	0.45
1:O:46:VAL:HG11	1:O:139:ALA:HB1	1.98	0.45
2:R:63:LEU:HD21	2:R:79:VAL:HG22	1.99	0.45
1:A:194:ILE:HD11	1:A:212:ILE:HD11	1.98	0.45
1:C:194:ILE:HD11	1:C:212:ILE:HD11	1.98	0.45
1:O:194:ILE:HD11	1:O:212:ILE:HD11	1.98	0.45
1:A:28:ARG:NH1	1:A:152:ASP:OD1	2.49	0.45
1:O:28:ARG:NH1	1:O:152:ASP:OD1	2.49	0.45
1:I:78:THR:HG22	1:I:136:LEU:HG	1.97	0.45
1:K:186:GLU:OE2	1:K:224:TYR:OH	2.30	0.45
1:O:78:THR:HG22	1:O:136:LEU:HG	1.97	0.45
1:Q:78:THR:HG22	1:Q:136:LEU:HG	1.97	0.45
2:R:105:ASP:O	2:R:180:ARG:NH2	2.50	0.45
2:T:105:ASP:O	2:T:180:ARG:NH2	2.50	0.45
2:T:135:TYR:CD2	2:V:25:PHE:HZ	2.34	0.45
2:X:105:ASP:O	2:X:180:ARG:NH2	2.50	0.45
2:1:105:ASP:O	2:1:180:ARG:NH2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:78:THR:HG22	1:S:136:LEU:HG	1.97	0.45
2:T:20:VAL:HB	2:T:28:HIS:HB2	1.98	0.45
2:1:113:ILE:HA	2:1:118:GLY:O	2.15	0.45
1:K:186:GLU:OE2	1:K:224:TYR:OH	2.31	0.45
1:A:46:VAL:HG11	1:A:139:ALA:HB1	1.98	0.45
2:L:63:LEU:HD21	2:L:79:VAL:HG22	1.99	0.45
2:P:63:LEU:HD21	2:P:79:VAL:HG22	1.99	0.45
1:K:110:GLU:HB2	1:K:147:ARG:HH21	1.81	0.45
1:K:172:VAL:HG13	1:K:196:ALA:HB1	1.98	0.45
1:O:194:ILE:HD11	1:O:212:ILE:HD11	1.99	0.45
1:S:110:GLU:HB2	1:S:147:ARG:HH21	1.81	0.45
2:L:24:ASN:N	2:L:24:ASN:OD1	2.50	0.45
2:T:24:ASN:N	2:T:24:ASN:OD1	2.50	0.45
2:D:105:ASP:O	2:D:180:ARG:NH2	2.50	0.45
2:D:141:GLN:HE21	2:R:141:GLN:HE21	1.63	0.45
2:F:105:ASP:O	2:F:180:ARG:NH2	2.50	0.45
1:G:100:LYS:NZ	2:H:64:GLU:OE2	2.48	0.45
2:N:105:ASP:O	2:N:180:ARG:NH2	2.50	0.45
1:Q:51:ASP:HB2	1:Q:197:LEU:HD11	1.98	0.45
1:E:125:GLN:NE2	1:G:130:ARG:O	2.49	0.45
1:G:125:GLN:NE2	1:I:130:ARG:O	2.50	0.45
1:A:78:THR:HG22	1:A:136:LEU:HG	1.97	0.45
1:K:78:THR:HG22	1:K:136:LEU:HG	1.97	0.45
2:L:4:VAL:HG22	2:L:134:VAL:HG11	1.98	0.45
1:O:67:ILE:HG12	1:O:77:VAL:HG22	1.98	0.45
2:P:20:VAL:HB	2:P:28:HIS:HB2	1.98	0.45
1:S:67:ILE:HG12	1:S:77:VAL:HG22	1.99	0.45
2:T:4:VAL:HG22	2:T:134:VAL:HG11	1.98	0.45
1:E:18:ASP:O	1:G:33:LYS:NZ	2.46	0.45
2:R:113:ILE:HA	2:R:118:GLY:O	2.15	0.45
1:A:67:ILE:HG12	1:A:77:VAL:HG22	1.98	0.45
2:D:37:ILE:HG22	2:D:63:LEU:HD22	1.97	0.45
1:M:178:ARG:HG3	1:M:179:GLU:HG2	1.97	0.45
2:1:37:ILE:HG22	2:1:63:LEU:HD22	1.97	0.45
1:C:46:VAL:HG11	1:C:139:ALA:HB1	1.98	0.45
2:D:63:LEU:HD21	2:D:79:VAL:HG22	1.99	0.45
2:T:63:LEU:HD21	2:T:79:VAL:HG22	1.99	0.45
2:1:63:LEU:HD21	2:1:79:VAL:HG22	1.99	0.45
1:S:172:VAL:HG13	1:S:196:ALA:HB1	1.98	0.45
1:G:28:ARG:NH1	1:G:152:ASP:OD1	2.49	0.45
1:M:28:ARG:NH1	1:M:152:ASP:OD1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:67:ILE:HG12	1:O:77:VAL:HG22	1.99	0.45
1:Q:28:ARG:NH1	1:Q:152:ASP:OD1	2.49	0.45
2:Z:157:ARG:HH21	2:Z:199:LEU:HD22	1.82	0.45
2:H:105:ASP:O	2:H:180:ARG:NH2	2.50	0.45
2:L:105:ASP:O	2:L:180:ARG:NH2	2.50	0.45
1:M:51:ASP:HB2	1:M:197:LEU:HD11	1.98	0.45
2:Z:105:ASP:O	2:Z:180:ARG:NH2	2.50	0.45
1:O:51:ASP:HB2	1:O:197:LEU:HD11	1.98	0.45
1:A:130:ARG:O	1:M:125:GLN:NE2	2.50	0.45
2:V:88:ASN:ND2	2:X:50:GLY:O	2.50	0.45
1:A:67:ILE:HG12	1:A:77:VAL:HG22	1.98	0.45
2:D:20:VAL:HB	2:D:28:HIS:HB2	1.98	0.45
1:O:78:THR:HG22	1:O:136:LEU:HG	1.97	0.45
2:P:3:THR:OG1	2:P:127:THR:OG1	2.25	0.45
2:N:113:ILE:HA	2:N:118:GLY:O	2.15	0.45
2:B:4:VAL:HG22	2:B:134:VAL:HG11	1.98	0.45
1:O:67:ILE:HG12	1:O:77:VAL:HG22	1.98	0.45
2:V:44:THR:HG23	2:V:100:LEU:HB2	1.99	0.45
1:O:46:VAL:HG11	1:O:139:ALA:HB1	1.98	0.45
1:A:208:LYS:HE2	1:A:208:LYS:HB2	1.73	0.45
1:A:67:ILE:HG12	1:A:77:VAL:HG22	1.99	0.45
1:I:67:ILE:HG12	1:I:77:VAL:HG22	1.99	0.45
2:L:157:ARG:HH21	2:L:199:LEU:HD22	1.82	0.45
1:U:67:ILE:HG12	1:U:77:VAL:HG22	1.99	0.45
1:O:28:ARG:NH1	1:O:152:ASP:OD1	2.49	0.45
1:A:125:GLN:NE2	1:C:130:ARG:O	2.50	0.45
1:C:78:THR:HG22	1:C:136:LEU:HG	1.97	0.45
2:J:105:ASP:O	2:J:180:ARG:NH2	2.50	0.45
1:K:78:THR:HG22	1:K:136:LEU:HG	1.97	0.45
1:S:186:GLU:OE2	1:S:224:TYR:OH	2.30	0.45
1:O:78:THR:HG22	1:O:136:LEU:HG	1.97	0.45
1:Q:152:ASP:O	1:Q:155:GLY:N	2.42	0.45
1:A:59:ILE:HG12	1:M:160:TYR:HE1	1.82	0.45
2:F:15:ALA:HA	2:F:174:ASP:O	2.15	0.45
2:F:20:VAL:HB	2:F:28:HIS:HB2	1.98	0.45
1:C:152:ASP:HB3	1:C:156:THR:HB	1.99	0.45
1:E:45:GLY:HA3	1:E:215:ILE:O	2.17	0.45
1:K:45:GLY:HA3	1:K:215:ILE:O	2.17	0.45
2:L:17:GLU:OE2	2:L:33:LYS:NZ	2.44	0.45
2:P:4:VAL:HG22	2:P:134:VAL:HG11	1.99	0.45
2:H:44:THR:HG23	2:H:100:LEU:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:44:THR:HG23	2:J:100:LEU:HB2	1.99	0.45
2:P:44:THR:HG23	2:P:100:LEU:HB2	1.99	0.45
1:W:113:VAL:HG21	1:W:149:PHE:HD2	1.81	0.45
2:X:44:THR:HG23	2:X:100:LEU:HB2	1.98	0.45
1:C:28:ARG:NH1	1:C:152:ASP:OD1	2.49	0.45
2:F:157:ARG:HH21	2:F:199:LEU:HD22	1.82	0.45
2:N:24:ASN:OD1	2:N:24:ASN:N	2.50	0.45
1:Q:67:ILE:HG12	1:Q:77:VAL:HG22	1.99	0.45
2:R:24:ASN:OD1	2:R:24:ASN:N	2.50	0.45
1:W:28:ARG:NH1	1:W:152:ASP:OD1	2.49	0.45
1:C:51:ASP:HB2	1:C:197:LEU:HD11	1.98	0.45
2:P:105:ASP:O	2:P:180:ARG:NH2	2.50	0.45
1:S:78:THR:HG22	1:S:136:LEU:HG	1.97	0.45
2:T:91:LYS:HD3	2:V:51:ASP:OD1	2.17	0.45
2:V:105:ASP:O	2:V:180:ARG:NH2	2.50	0.45
1:U:67:ILE:HG12	1:U:77:VAL:HG22	1.98	0.45
2:Z:20:VAL:HB	2:Z:28:HIS:HB2	1.98	0.45
1:A:152:ASP:HB3	1:A:156:THR:HB	1.99	0.45
1:S:45:GLY:HA3	1:S:215:ILE:O	2.17	0.45
1:W:147:ARG:HH21	1:W:149:PHE:HZ	1.65	0.45
1:Y:45:GLY:HA3	1:Y:215:ILE:O	2.17	0.45
2:D:4:VAL:HG22	2:D:134:VAL:HG11	1.98	0.45
1:K:67:ILE:HG12	1:K:77:VAL:HG22	1.98	0.45
1:Q:178:ARG:HG3	1:Q:179:GLU:HG2	1.97	0.45
1:S:67:ILE:HG12	1:S:77:VAL:HG22	1.98	0.45
2:1:4:VAL:HG22	2:1:134:VAL:HG11	1.98	0.45
2:F:1:THR:N	2:F:168:ALA:O	2.49	0.45
2:F:63:LEU:HD21	2:F:79:VAL:HG22	1.99	0.45
1:G:113:VAL:HG21	1:G:149:PHE:HD2	1.81	0.45
2:Z:1:THR:N	2:Z:168:ALA:O	2.49	0.45
1:O:113:VAL:HG21	1:O:149:PHE:HD2	1.81	0.45
2:H:114:ASP:HB3	2:H:118:GLY:H	1.82	0.45
1:U:194:ILE:HD11	1:U:212:ILE:HD11	1.98	0.45
1:M:67:ILE:HG12	1:M:77:VAL:HG22	1.99	0.45
1:S:67:ILE:HG12	1:S:77:VAL:HG22	1.99	0.45
2:T:157:ARG:HH21	2:T:199:LEU:HD22	1.82	0.45
1:O:67:ILE:HG12	1:O:77:VAL:HG22	1.99	0.45
2:B:105:ASP:O	2:B:180:ARG:NH2	2.50	0.45
2:1:3:THR:O	2:1:126:SER:HA	2.17	0.45
2:D:19:ARG:HD3	2:D:26:ILE:HG12	1.99	0.45
1:I:67:ILE:HG12	1:I:77:VAL:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:19:ARG:HD3	2:J:26:ILE:HG12	1.99	0.45
2:Z:19:ARG:HD3	2:Z:26:ILE:HG12	1.99	0.45
2:R:17:GLU:OE2	2:R:33:LYS:NZ	2.44	0.45
2:T:17:GLU:OE2	2:T:33:LYS:NZ	2.44	0.45
2:B:16:THR:HG21	2:B:33:LYS:HB2	1.98	0.45
1:C:68:GLN:HE21	1:C:89:VAL:HG21	1.80	0.45
1:A:113:VAL:HG21	1:A:149:PHE:HD2	1.81	0.45
2:B:44:THR:HG23	2:B:100:LEU:HB2	1.99	0.45
1:E:113:VAL:HG21	1:E:149:PHE:HD2	1.81	0.45
1:K:113:VAL:HG21	1:K:149:PHE:HD2	1.81	0.45
2:J:114:ASP:HB3	2:J:118:GLY:H	1.82	0.45
1:M:55:ARG:HH22	1:M:208:LYS:NZ	2.13	0.45
1:Q:194:ILE:HD11	1:Q:212:ILE:HD11	1.98	0.45
2:X:114:ASP:HB3	2:X:118:GLY:H	1.82	0.45
1:G:67:ILE:HG12	1:G:77:VAL:HG22	1.99	0.45
2:H:24:ASN:OD1	2:H:24:ASN:N	2.50	0.45
2:J:157:ARG:HH21	2:J:199:LEU:HD22	1.82	0.45
2:V:157:ARG:HH21	2:V:199:LEU:HD22	1.82	0.45
2:X:24:ASN:OD1	2:X:24:ASN:N	2.50	0.45
2:D:3:THR:OG1	2:D:127:THR:OG1	2.26	0.45
2:D:3:THR:O	2:D:126:SER:HA	2.17	0.45
1:M:152:ASP:O	1:M:155:GLY:N	2.42	0.45
2:F:19:ARG:HD3	2:F:26:ILE:HG12	1.99	0.45
2:V:19:ARG:HD3	2:V:26:ILE:HG12	1.99	0.45
1:E:227:GLU:H	1:E:227:GLU:HG3	1.60	0.45
1:C:45:GLY:HA3	1:C:215:ILE:O	2.17	0.45
1:G:147:ARG:HH21	1:G:149:PHE:HZ	1.65	0.45
1:Y:84:ASP:OD1	1:O:121:GLN:NE2	2.49	0.45
1:O:45:GLY:HA3	1:O:215:ILE:O	2.17	0.45
2:N:4:VAL:HG22	2:N:134:VAL:HG11	1.98	0.45
1:C:113:VAL:HG21	1:C:149:PHE:HD2	1.81	0.45
2:D:44:THR:HG23	2:D:100:LEU:HB2	1.99	0.45
2:H:63:LEU:HD21	2:H:79:VAL:HG22	1.99	0.45
2:J:63:LEU:HD21	2:J:79:VAL:HG22	1.99	0.45
1:S:113:VAL:HG21	1:S:149:PHE:HD2	1.81	0.45
2:X:63:LEU:HD21	2:X:79:VAL:HG22	1.99	0.45
1:Y:113:VAL:HG21	1:Y:149:PHE:HD2	1.81	0.45
2:Z:63:LEU:HD21	2:Z:79:VAL:HG22	1.99	0.45
1:E:194:ILE:HD11	1:E:212:ILE:HD11	1.98	0.45
1:G:110:GLU:HB2	1:G:147:ARG:HH21	1.81	0.45
1:I:194:ILE:HD11	1:I:212:ILE:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:194:ILE:HD11	1:M:212:ILE:HD11	1.98	0.45
1:Q:55:ARG:HH22	1:Q:208:LYS:NZ	2.13	0.45
1:Y:194:ILE:HD11	1:Y:212:ILE:HD11	1.98	0.45
1:C:67:ILE:HG12	1:C:77:VAL:HG22	1.99	0.45
1:K:67:ILE:HG12	1:K:77:VAL:HG22	1.99	0.45
2:L:167:SER:HB2	2:1:167:SER:HB2	1.97	0.45
1:A:51:ASP:HB2	1:A:197:LEU:HD11	1.98	0.45
2:Z:88:ASN:ND2	2:1:50:GLY:O	2.50	0.44
2:N:20:VAL:HB	2:N:28:HIS:HB2	1.98	0.44
2:T:19:ARG:HD3	2:T:26:ILE:HG12	1.99	0.44
1:A:33:LYS:NZ	1:M:18:ASP:O	2.46	0.44
1:A:45:GLY:HA3	1:A:215:ILE:O	2.17	0.44
1:E:147:ARG:HH21	1:E:149:PHE:HZ	1.65	0.44
1:U:147:ARG:HH21	1:U:149:PHE:HZ	1.65	0.44
1:E:186:GLU:OE2	1:E:224:TYR:OH	2.31	0.44
2:R:4:VAL:HG22	2:R:134:VAL:HG11	1.98	0.44
2:F:114:ASP:O	2:F:117:GLY:N	2.47	0.44
1:O:113:VAL:HG21	1:O:149:PHE:HD2	1.81	0.44
2:1:44:THR:HG23	2:1:100:LEU:HB2	1.99	0.44
1:K:208:LYS:HE2	1:K:208:LYS:HB2	1.73	0.44
1:S:208:LYS:HE2	1:S:208:LYS:HB2	1.73	0.44
2:V:114:ASP:HB3	2:V:118:GLY:H	1.82	0.44
1:W:110:GLU:HB2	1:W:147:ARG:HH21	1.81	0.44
2:1:3:THR:OG1	2:1:127:THR:OG1	2.25	0.44
1:W:67:ILE:HG12	1:W:77:VAL:HG22	1.99	0.44
1:O:51:ASP:HB2	1:O:197:LEU:HD11	1.98	0.44
1:S:130:ARG:O	1:U:125:GLN:NE2	2.50	0.44
2:L:19:ARG:HD3	2:L:26:ILE:HG12	1.99	0.44
2:R:20:VAL:HB	2:R:28:HIS:HB2	1.98	0.44
2:V:4:VAL:HG22	2:V:134:VAL:HG11	1.98	0.44
1:I:45:GLY:HA3	1:I:215:ILE:O	2.17	0.44
1:O:45:GLY:HA3	1:O:215:ILE:O	2.17	0.44
1:S:76:ALA:HA	1:S:137:ILE:O	2.18	0.44
1:U:45:GLY:HA3	1:U:215:ILE:O	2.17	0.44
1:Y:147:ARG:HH21	1:Y:149:PHE:HZ	1.65	0.44
1:Q:67:ILE:HG12	1:Q:77:VAL:HG22	1.98	0.44
1:A:125:GLN:NE2	1:C:130:ARG:O	2.50	0.44
2:D:114:ASP:O	2:D:117:GLY:N	2.47	0.44
2:V:63:LEU:HD21	2:V:79:VAL:HG22	1.99	0.44
1:M:208:LYS:HB2	1:M:208:LYS:HE2	1.73	0.44
1:Q:208:LYS:HB2	1:Q:208:LYS:HE2	1.73	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:208:LYS:HE2	1:U:208:LYS:HB2	1.73	0.44
2:B:157:ARG:HH21	2:B:199:LEU:HD22	1.82	0.44
2:B:3:THR:O	2:B:126:SER:HA	2.17	0.44
2:J:4:VAL:HG22	2:J:134:VAL:HG11	1.98	0.44
1:E:152:ASP:HB3	1:E:156:THR:HB	1.99	0.44
1:I:147:ARG:HH21	1:I:149:PHE:HZ	1.65	0.44
1:K:76:ALA:HA	1:K:137:ILE:O	2.18	0.44
1:M:45:GLY:HA3	1:M:215:ILE:O	2.17	0.44
2:N:17:GLU:OE2	2:N:33:LYS:NZ	2.44	0.44
2:1:192:ILE:H	2:1:192:ILE:HG13	1.63	0.44
1:A:186:GLU:OE2	1:A:224:TYR:OH	2.31	0.44
2:B:167:SER:HB2	2:R:167:SER:HB2	1.99	0.44
2:J:4:VAL:HG22	2:J:134:VAL:HG11	1.99	0.44
1:M:67:ILE:HG12	1:M:77:VAL:HG22	1.98	0.44
1:O:186:GLU:OE2	1:O:224:TYR:OH	2.31	0.44
2:V:4:VAL:HG22	2:V:134:VAL:HG11	1.98	0.44
1:Y:186:GLU:OE2	1:Y:224:TYR:OH	2.31	0.44
2:R:44:THR:HG23	2:R:100:LEU:HB2	1.98	0.44
2:V:1:THR:N	2:V:168:ALA:O	2.49	0.44
2:D:3:THR:OG1	2:D:127:THR:OG1	2.25	0.44
1:I:208:LYS:HE2	1:I:208:LYS:HB2	1.73	0.44
1:O:208:LYS:HE2	1:O:208:LYS:HB2	1.73	0.44
1:U:110:GLU:HB2	1:U:147:ARG:HH21	1.81	0.44
1:G:152:ASP:HB3	1:G:156:THR:HB	1.99	0.44
2:P:157:ARG:HH21	2:P:199:LEU:HD22	1.82	0.44
1:Q:225:ASP:OD1	1:Q:225:ASP:N	2.50	0.44
2:V:24:ASN:OD1	2:V:24:ASN:N	2.49	0.44
1:E:186:GLU:OE2	1:E:224:TYR:OH	2.30	0.44
2:D:84:SER:OG	2:D:117:GLY:O	2.34	0.44
2:P:3:THR:O	2:P:126:SER:HA	2.17	0.44
2:B:3:THR:OG1	2:B:127:THR:OG1	2.25	0.44
1:E:20:ARG:NH2	1:E:25:GLU:OE1	2.48	0.44
2:H:4:VAL:HG22	2:H:134:VAL:HG11	1.98	0.44
1:I:76:ALA:HA	1:I:137:ILE:O	2.18	0.44
1:Q:45:GLY:HA3	1:Q:215:ILE:O	2.17	0.44
2:F:167:SER:HB2	2:V:167:SER:HB2	1.99	0.44
2:H:4:VAL:HG22	2:H:134:VAL:HG11	1.99	0.44
1:A:49:ILE:HG12	1:A:212:ILE:HG12	2.00	0.44
2:N:44:THR:HG23	2:N:100:LEU:HB2	1.99	0.44
1:O:49:ILE:HG12	1:O:212:ILE:HG12	2.00	0.44
1:O:76:ALA:HA	1:O:137:ILE:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:44:THR:HG23	2:T:100:LEU:HB2	1.99	0.44
2:Z:114:ASP:O	2:Z:117:GLY:N	2.47	0.44
2:D:91:LYS:HA	2:D:91:LYS:HD2	1.80	0.44
2:F:114:ASP:HB3	2:F:118:GLY:H	1.82	0.44
1:I:110:GLU:HB2	1:I:147:ARG:HH21	1.81	0.44
2:Z:114:ASP:HB3	2:Z:118:GLY:H	1.82	0.44
2:H:157:ARG:HH21	2:H:199:LEU:HD22	1.82	0.44
2:N:157:ARG:HH21	2:N:199:LEU:HD22	1.82	0.44
2:R:157:ARG:HH21	2:R:199:LEU:HD22	1.82	0.44
1:W:152:ASP:HB3	1:W:156:THR:HB	2.00	0.44
2:X:157:ARG:HH21	2:X:199:LEU:HD22	1.82	0.44
1:E:125:GLN:NE2	1:G:130:ARG:O	2.50	0.44
1:U:130:ARG:O	1:W:125:GLN:NE2	2.51	0.44
1:W:130:ARG:O	1:Y:125:GLN:NE2	2.50	0.44
2:X:3:THR:O	2:X:126:SER:HA	2.17	0.44
2:Z:3:THR:O	2:Z:126:SER:HA	2.17	0.44
1:A:20:ARG:NH2	1:A:25:GLU:OE1	2.48	0.44
2:B:19:ARG:HD3	2:B:26:ILE:HG12	1.99	0.44
1:E:67:ILE:HG12	1:E:77:VAL:HG22	1.98	0.44
2:H:19:ARG:HD3	2:H:26:ILE:HG12	1.99	0.44
2:P:3:THR:HG1	2:P:127:THR:HG1	1.62	0.44
2:P:19:ARG:HD3	2:P:26:ILE:HG12	1.99	0.44
2:R:19:ARG:HD3	2:R:26:ILE:HG12	1.99	0.44
2:X:19:ARG:HD3	2:X:26:ILE:HG12	1.99	0.44
1:Y:20:ARG:NH2	1:Y:25:GLU:OE1	2.48	0.44
1:Y:67:ILE:HG12	1:Y:77:VAL:HG22	1.98	0.44
1:A:72:ASP:OD2	2:B:67:ARG:NH2	2.51	0.44
1:K:18:ASP:O	1:M:33:LYS:NZ	2.47	0.44
1:U:76:ALA:HA	1:U:137:ILE:O	2.18	0.44
2:X:4:VAL:HG22	2:X:134:VAL:HG11	1.98	0.44
1:G:76:ALA:HA	1:G:137:ILE:O	2.18	0.44
2:J:1:THR:N	2:J:168:ALA:O	2.49	0.44
2:L:44:THR:HG23	2:L:100:LEU:HB2	1.99	0.44
2:N:1:THR:N	2:N:168:ALA:O	2.49	0.44
2:Z:190:ASP:OD1	2:Z:190:ASP:N	2.51	0.44
1:E:67:ILE:HG12	1:E:77:VAL:HG22	1.99	0.44
2:J:24:ASN:OD1	2:J:24:ASN:N	2.50	0.44
1:Y:186:GLU:OE2	1:Y:224:TYR:OH	2.30	0.44
2:F:3:THR:O	2:F:126:SER:HA	2.17	0.44
2:J:3:THR:OG1	2:J:127:THR:OG1	2.24	0.44
2:V:3:THR:O	2:V:126:SER:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:13:ILE:HG12	2:D:177:VAL:HG22	2.00	0.44
1:G:67:ILE:HG12	1:G:77:VAL:HG22	1.98	0.44
2:R:13:ILE:HG12	2:R:177:VAL:HG22	2.00	0.44
1:W:67:ILE:HG12	1:W:77:VAL:HG22	1.98	0.44
2:X:4:VAL:HG22	2:X:134:VAL:HG11	1.98	0.44
1:Q:33:LYS:NZ	1:S:18:ASP:O	2.47	0.44
1:O:76:ALA:HA	1:O:137:ILE:O	2.18	0.44
1:M:186:GLU:OE2	1:M:224:TYR:OH	2.31	0.44
1:Q:186:GLU:OE2	1:Q:224:TYR:OH	2.31	0.44
1:A:76:ALA:HA	1:A:137:ILE:O	2.18	0.44
1:E:76:ALA:HA	1:E:137:ILE:O	2.18	0.44
1:M:49:ILE:HG12	1:M:212:ILE:HG12	2.00	0.44
1:U:76:ALA:HA	1:U:137:ILE:O	2.18	0.44
1:W:76:ALA:HA	1:W:137:ILE:O	2.18	0.44
1:A:110:GLU:HB2	1:A:147:ARG:HH21	1.81	0.44
2:B:114:ASP:HB3	2:B:118:GLY:H	1.82	0.44
2:B:156:ILE:O	2:B:160:SER:OG	2.32	0.44
2:F:190:ASP:N	2:F:190:ASP:OD1	2.51	0.44
1:O:110:GLU:HB2	1:O:147:ARG:HH21	1.81	0.44
1:O:110:GLU:HB2	1:O:147:ARG:HH21	1.81	0.44
2:D:24:ASN:OD1	2:D:24:ASN:N	2.50	0.44
1:E:152:ASP:HB3	1:E:156:THR:HB	1.99	0.44
2:P:24:ASN:OD1	2:P:24:ASN:N	2.50	0.44
1:Y:67:ILE:HG12	1:Y:77:VAL:HG22	1.99	0.44
2:1:24:ASN:OD1	2:1:24:ASN:N	2.50	0.44
1:O:100:LYS:NZ	2:1:64:GLU:OE2	2.48	0.44
2:H:3:THR:O	2:H:126:SER:HA	2.17	0.44
2:J:3:THR:O	2:J:126:SER:HA	2.17	0.44
1:M:20:ARG:NH2	1:M:25:GLU:OE1	2.48	0.44
2:N:19:ARG:HD3	2:N:26:ILE:HG12	2.00	0.44
1:A:76:ALA:HA	1:A:137:ILE:O	2.18	0.44
1:G:45:GLY:HA3	1:G:215:ILE:O	2.17	0.44
2:D:167:SER:HB2	2:T:167:SER:HB2	1.98	0.44
1:I:49:ILE:HG12	1:I:212:ILE:HG12	2.00	0.44
1:I:76:ALA:HA	1:I:137:ILE:O	2.18	0.44
1:I:113:VAL:HG21	1:I:149:PHE:HD2	1.82	0.44
1:Q:49:ILE:HG12	1:Q:212:ILE:HG12	2.00	0.44
2:R:1:THR:N	2:R:168:ALA:O	2.49	0.44
1:U:49:ILE:HG12	1:U:212:ILE:HG12	2.00	0.44
1:Y:76:ALA:HA	1:Y:137:ILE:O	2.18	0.44
2:1:37:ILE:HD13	2:1:43:MET:HE2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:114:ASP:HB3	2:P:118:GLY:H	1.82	0.44
2:1:91:LYS:HA	2:1:91:LYS:HD2	1.80	0.44
2:1:190:ASP:OD1	2:1:190:ASP:N	2.51	0.44
2:B:24:ASN:OD1	2:B:24:ASN:N	2.50	0.44
1:U:152:ASP:HB3	1:U:156:THR:HB	1.99	0.44
1:Y:152:ASP:HB3	1:Y:156:THR:HB	1.99	0.44
2:P:3:THR:OG1	2:P:127:THR:OG1	2.26	0.44
2:Z:89:GLN:H	2:Z:89:GLN:HG3	1.60	0.44
1:W:186:GLU:OE2	1:W:224:TYR:OH	2.33	0.44
2:B:13:ILE:HG12	2:B:177:VAL:HG22	2.00	0.44
1:C:67:ILE:HG12	1:C:77:VAL:HG22	1.98	0.44
2:N:13:ILE:HG12	2:N:177:VAL:HG22	2.00	0.44
1:C:76:ALA:HA	1:C:137:ILE:O	2.18	0.44
1:G:76:ALA:HA	1:G:137:ILE:O	2.18	0.44
1:M:76:ALA:HA	1:M:137:ILE:O	2.18	0.44
2:L:4:VAL:HG22	2:L:134:VAL:HG11	1.99	0.44
2:T:4:VAL:HG22	2:T:134:VAL:HG11	1.98	0.44
2:B:37:ILE:HD13	2:B:43:MET:HE2	2.00	0.44
2:D:37:ILE:HD13	2:D:43:MET:HE2	2.00	0.44
1:K:49:ILE:HG12	1:K:212:ILE:HG12	2.00	0.44
1:K:76:ALA:HA	1:K:137:ILE:O	2.18	0.44
1:S:49:ILE:HG12	1:S:212:ILE:HG12	2.00	0.44
1:S:76:ALA:HA	1:S:137:ILE:O	2.18	0.44
2:Z:37:ILE:HD13	2:Z:43:MET:HE2	2.00	0.44
1:O:49:ILE:HG12	1:O:212:ILE:HG12	2.00	0.44
1:C:110:GLU:HB2	1:C:147:ARG:HH21	1.81	0.44
2:D:190:ASP:OD1	2:D:190:ASP:N	2.51	0.44
2:L:114:ASP:HB3	2:L:118:GLY:H	1.82	0.44
1:M:36:THR:HA	1:M:165:ILE:O	2.18	0.44
2:P:156:ILE:O	2:P:160:SER:OG	2.32	0.44
1:A:152:ASP:HB3	1:A:156:THR:HB	1.99	0.44
1:I:152:ASP:HB3	1:I:156:THR:HB	1.99	0.44
1:M:152:ASP:HB3	1:M:156:THR:HB	1.99	0.44
1:Q:152:ASP:HB3	1:Q:156:THR:HB	1.99	0.44
2:V:4:VAL:HG22	2:V:134:VAL:HG11	2.00	0.44
1:Y:130:ARG:O	1:O:125:GLN:NE2	2.51	0.44
1:G:186:GLU:OE2	1:G:224:TYR:OH	2.33	0.44
1:O:125:GLN:NE2	1:O:130:ARG:O	2.51	0.44
2:P:13:ILE:HG12	2:P:177:VAL:HG22	2.00	0.44
1:Q:20:ARG:NH2	1:Q:25:GLU:OE1	2.48	0.44
2:D:135:TYR:O	2:D:139:GLU:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:147:ARG:HH21	1:S:149:PHE:HZ	1.65	0.44
1:W:45:GLY:HA3	1:W:215:ILE:O	2.17	0.44
2:1:135:TYR:O	2:1:139:GLU:HB2	2.18	0.44
2:F:4:VAL:HG22	2:F:134:VAL:HG11	1.98	0.44
2:J:167:SER:HB2	2:Z:167:SER:HB2	1.99	0.44
2:Z:4:VAL:HG22	2:Z:134:VAL:HG11	1.98	0.44
1:A:72:ASP:OD2	2:B:67:ARG:NH2	2.51	0.44
2:F:37:ILE:HD13	2:F:43:MET:HE2	2.00	0.44
2:F:44:THR:HG23	2:F:100:LEU:HB2	1.99	0.44
2:J:37:ILE:HD13	2:J:43:MET:HE2	2.00	0.44
2:P:37:ILE:HD13	2:P:43:MET:HE2	2.00	0.44
2:R:88:ASN:HD22	2:T:54:VAL:HG21	1.83	0.44
1:U:113:VAL:HG21	1:U:149:PHE:HD2	1.82	0.44
2:Z:44:THR:HG23	2:Z:100:LEU:HB2	1.99	0.44
1:E:110:GLU:HB2	1:E:147:ARG:HH21	1.81	0.44
1:Q:36:THR:HA	1:Q:165:ILE:O	2.18	0.44
1:Y:110:GLU:HB2	1:Y:147:ARG:HH21	1.81	0.44
1:O:152:ASP:HB3	1:O:156:THR:HB	2.00	0.44
2:B:3:THR:OG1	2:B:127:THR:OG1	2.26	0.44
2:P:84:SER:OG	2:P:117:GLY:O	2.34	0.43
2:H:132:PRO:HB2	2:V:132:PRO:HB2	2.00	0.43
1:I:111:ASN:HD21	2:L:69:GLN:HB3	1.83	0.43
1:K:147:ARG:HH21	1:K:149:PHE:HZ	1.65	0.43
1:Q:76:ALA:HA	1:Q:137:ILE:O	2.18	0.43
1:W:76:ALA:HA	1:W:137:ILE:O	2.18	0.43
2:Z:135:TYR:O	2:Z:139:GLU:HB2	2.18	0.43
1:C:49:ILE:HG12	1:C:212:ILE:HG12	2.00	0.43
1:C:76:ALA:HA	1:C:137:ILE:O	2.18	0.43
2:N:37:ILE:HD13	2:N:43:MET:HE2	2.00	0.43
2:R:37:ILE:HD13	2:R:43:MET:HE2	2.00	0.43
2:V:37:ILE:HD13	2:V:43:MET:HE2	2.00	0.43
2:V:38:ASP:HB3	2:V:41:THR:HB	1.99	0.43
1:W:49:ILE:HG12	1:W:212:ILE:HG12	2.00	0.43
2:X:37:ILE:HD13	2:X:43:MET:HE2	2.00	0.43
1:K:194:ILE:HD11	1:K:212:ILE:HD11	1.98	0.43
1:S:36:THR:HA	1:S:165:ILE:O	2.18	0.43
2:T:114:ASP:HB3	2:T:118:GLY:H	1.82	0.43
2:B:4:VAL:HG22	2:B:134:VAL:HG11	2.00	0.43
2:D:4:VAL:HG22	2:D:134:VAL:HG11	2.00	0.43
2:P:4:VAL:HG22	2:P:134:VAL:HG11	2.00	0.43
2:1:4:VAL:HG22	2:1:134:VAL:HG11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:125:GLN:NE2	1:K:130:ARG:O	2.51	0.43
2:J:132:PRO:HB2	2:X:132:PRO:HB2	2.00	0.43
2:D:43:MET:HE2	2:D:83:LEU:HD11	2.00	0.43
1:C:147:ARG:HH21	1:C:149:PHE:HZ	1.65	0.43
1:E:76:ALA:HA	1:E:137:ILE:O	2.18	0.43
2:F:135:TYR:O	2:F:139:GLU:HB2	2.18	0.43
1:U:201:LEU:HD11	1:U:207:LEU:HG	2.01	0.43
1:Y:76:ALA:HA	1:Y:137:ILE:O	2.18	0.43
1:O:147:ARG:HH21	1:O:149:PHE:HZ	1.65	0.43
1:E:49:ILE:HG12	1:E:212:ILE:HG12	2.00	0.43
2:H:37:ILE:HD13	2:H:43:MET:HE2	2.00	0.43
2:J:38:ASP:HB3	2:J:41:THR:HB	2.00	0.43
1:Y:49:ILE:HG12	1:Y:212:ILE:HG12	2.00	0.43
2:J:91:LYS:HA	2:J:91:LYS:HD2	1.80	0.43
1:K:36:THR:HA	1:K:165:ILE:O	2.18	0.43
1:M:110:GLU:HB2	1:M:147:ARG:HH21	1.81	0.43
2:R:114:ASP:HB3	2:R:118:GLY:H	1.82	0.43
2:Z:24:ASN:OD1	2:Z:24:ASN:N	2.50	0.43
2:H:4:VAL:HG22	2:H:134:VAL:HG11	2.00	0.43
2:J:4:VAL:HG22	2:J:134:VAL:HG11	2.00	0.43
1:O:125:GLN:NE2	1:O:130:ARG:O	2.52	0.43
2:H:84:SER:OG	2:H:117:GLY:O	2.34	0.43
2:L:3:THR:OG1	2:L:127:THR:OG1	2.24	0.43
2:T:3:THR:O	2:T:126:SER:HA	2.17	0.43
2:F:13:ILE:HG12	2:F:177:VAL:HG22	2.00	0.43
2:F:167:SER:HB2	2:V:167:SER:HB2	2.00	0.43
1:Q:59:ILE:HG12	1:S:160:TYR:CE1	2.53	0.43
1:E:79:SER:HB3	1:E:165:ILE:HG22	2.00	0.43
1:I:201:LEU:HD11	1:I:207:LEU:HG	2.01	0.43
2:X:3:THR:OG1	2:X:127:THR:OG1	2.26	0.43
1:C:38:LEU:HA	1:C:163:THR:O	2.18	0.43
2:B:50:GLY:O	2:D:88:ASN:ND2	2.50	0.43
2:L:37:ILE:HD13	2:L:43:MET:HE2	2.00	0.43
2:X:38:ASP:HB3	2:X:41:THR:HB	1.99	0.43
1:O:76:ALA:HA	1:O:137:ILE:O	2.18	0.43
2:B:163:LYS:NZ	2:B:203:LEU:O	2.41	0.43
1:G:194:ILE:HD11	1:G:212:ILE:HD11	1.98	0.43
2:N:114:ASP:HB3	2:N:118:GLY:H	1.82	0.43
2:F:24:ASN:OD1	2:F:24:ASN:N	2.50	0.43
2:R:4:VAL:HG22	2:R:134:VAL:HG11	2.00	0.43
1:E:100:LYS:NZ	2:F:64:GLU:OE2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:130:ARG:O	1:S:125:GLN:NE2	2.51	0.43
2:B:84:SER:OG	2:B:117:GLY:O	2.34	0.43
2:L:3:THR:O	2:L:126:SER:HA	2.17	0.43
2:R:3:THR:O	2:R:126:SER:HA	2.17	0.43
2:T:3:THR:OG1	2:T:127:THR:OG1	2.24	0.43
1:C:182:GLU:OE2	1:E:57:ARG:NH1	2.51	0.43
2:F:84:SER:OG	2:F:117:GLY:O	2.32	0.43
2:B:135:TYR:O	2:B:139:GLU:HB2	2.18	0.43
1:O:147:ARG:HH21	1:O:149:PHE:HZ	1.65	0.43
2:P:135:TYR:O	2:P:139:GLU:HB2	2.18	0.43
1:S:201:LEU:HD11	1:S:207:LEU:HG	2.01	0.43
2:B:83:LEU:HD21	2:B:99:LEU:HD13	2.00	0.43
2:B:54:VAL:CG2	2:D:88:ASN:HD22	2.28	0.43
1:C:20:ARG:HH21	1:C:22:PHE:HE1	1.67	0.43
1:G:49:ILE:HG12	1:G:212:ILE:HG12	2.00	0.43
2:H:38:ASP:HB3	2:H:41:THR:HB	1.99	0.43
2:H:114:ASP:O	2:H:117:GLY:N	2.47	0.43
2:R:114:ASP:O	2:R:117:GLY:N	2.47	0.43
2:T:37:ILE:HD13	2:T:43:MET:HE2	2.00	0.43
1:O:20:ARG:HH21	1:O:22:PHE:HE1	1.67	0.43
2:B:190:ASP:OD1	2:B:190:ASP:N	2.51	0.43
2:P:190:ASP:OD1	2:P:190:ASP:N	2.51	0.43
1:Q:110:GLU:HB2	1:Q:147:ARG:HH21	1.81	0.43
1:S:194:ILE:HD11	1:S:212:ILE:HD11	1.99	0.43
1:W:194:ILE:HD11	1:W:212:ILE:HD11	1.99	0.43
2:N:4:VAL:HG22	2:N:134:VAL:HG11	2.00	0.43
1:K:125:GLN:NE2	1:M:130:ARG:O	2.51	0.43
2:F:178:ILE:HA	2:F:183:GLY:O	2.19	0.43
2:N:3:THR:O	2:N:126:SER:HA	2.17	0.43
2:N:83:LEU:HD21	2:N:99:LEU:HD13	2.01	0.43
2:R:83:LEU:HD21	2:R:99:LEU:HD13	2.01	0.43
1:G:160:TYR:CE1	1:I:59:ILE:HG12	2.54	0.43
1:I:160:TYR:CE1	1:K:59:ILE:HG12	2.54	0.43
2:L:13:ILE:HG12	2:L:177:VAL:HG22	2.00	0.43
1:S:59:ILE:HG12	1:U:160:TYR:CE1	2.54	0.43
2:T:13:ILE:HG12	2:T:177:VAL:HG22	2.00	0.43
1:U:59:ILE:HG12	1:W:160:TYR:CE1	2.54	0.43
2:B:43:MET:HE2	2:B:83:LEU:HD11	2.00	0.43
1:A:147:ARG:HH21	1:A:149:PHE:HZ	1.65	0.43
1:K:201:LEU:HD11	1:K:207:LEU:HG	2.01	0.43
2:T:135:TYR:O	2:T:139:GLU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:20:VAL:HB	2:V:28:HIS:HB2	2.00	0.43
1:A:38:LEU:HA	1:A:163:THR:O	2.18	0.43
2:B:88:ASN:ND2	2:N:50:GLY:O	2.51	0.43
1:G:36:THR:HA	1:G:165:ILE:O	2.18	0.43
1:W:36:THR:HA	1:W:165:ILE:O	2.18	0.43
1:M:225:ASP:OD1	1:M:225:ASP:N	2.50	0.43
1:O:130:ARG:O	1:Q:125:GLN:NE2	2.52	0.43
2:P:4:VAL:HG22	2:P:134:VAL:HG11	2.00	0.43
2:X:4:VAL:HG22	2:X:134:VAL:HG11	2.00	0.43
2:F:141:GLN:HE21	2:T:141:GLN:HE21	1.67	0.43
2:N:178:ILE:HA	2:N:183:GLY:O	2.19	0.43
2:R:178:ILE:HA	2:R:183:GLY:O	2.19	0.43
1:U:196:ALA:O	1:U:199:SER:OG	2.34	0.43
1:C:72:ASP:OD2	2:D:67:ARG:NH2	2.51	0.43
2:D:192:ILE:H	2:D:192:ILE:HG13	1.63	0.43
2:X:135:TYR:O	2:X:139:GLU:HB2	2.18	0.43
2:J:20:VAL:HB	2:J:28:HIS:HB2	2.00	0.43
2:X:20:VAL:HB	2:X:28:HIS:HB2	2.00	0.43
1:M:76:ALA:HA	1:M:137:ILE:O	2.18	0.43
2:P:91:LYS:HD2	2:P:91:LYS:HA	1.80	0.43
2:J:93:MET:HG3	2:J:94:PRO:HD3	2.01	0.43
1:S:225:ASP:OD1	1:S:225:ASP:N	2.50	0.43
2:B:4:VAL:HG22	2:B:134:VAL:HG11	2.00	0.43
2:1:4:VAL:HG22	2:1:134:VAL:HG11	2.00	0.43
2:B:83:LEU:HD21	2:B:99:LEU:HD13	2.01	0.43
2:J:167:SER:HB2	2:Z:167:SER:HB2	2.00	0.43
1:M:162:ALA:HB1	1:M:176:LEU:HD13	2.00	0.43
1:Q:162:ALA:HB1	1:Q:176:LEU:HD13	2.00	0.43
2:Z:178:ILE:HA	2:Z:183:GLY:O	2.19	0.43
2:1:83:LEU:HD21	2:1:99:LEU:HD13	2.01	0.43
1:I:196:ALA:O	1:I:199:SER:OG	2.34	0.43
1:W:59:ILE:HG12	1:Y:160:TYR:CE1	2.54	0.43
1:A:18:ASP:O	1:C:33:LYS:NZ	2.46	0.43
1:M:201:LEU:HD11	1:M:207:LEU:HG	2.01	0.43
2:H:20:VAL:HB	2:H:28:HIS:HB2	2.00	0.43
2:H:132:PRO:HB2	2:V:132:PRO:HB2	2.01	0.43
1:Y:20:ARG:HH21	1:Y:22:PHE:HE1	1.67	0.43
2:P:163:LYS:NZ	2:P:203:LEU:O	2.41	0.43
2:R:190:ASP:N	2:R:190:ASP:OD1	2.51	0.43
2:T:91:LYS:NZ	2:V:94:PRO:O	2.36	0.43
2:V:91:LYS:HA	2:V:91:LYS:HD2	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:4:VAL:HG22	2:F:134:VAL:HG11	2.00	0.43
1:K:225:ASP:OD1	1:K:225:ASP:N	2.50	0.43
2:T:93:MET:HG3	2:T:94:PRO:HD3	2.01	0.43
2:V:93:MET:HG3	2:V:94:PRO:HD3	2.01	0.43
2:X:203:LEU:HD13	2:X:203:LEU:HA	1.87	0.43
2:1:157:ARG:HH21	2:1:199:LEU:HD22	1.82	0.43
1:C:100:LYS:NZ	2:D:64:GLU:OE2	2.49	0.43
2:D:4:VAL:HG22	2:D:134:VAL:HG11	2.00	0.43
2:F:89:GLN:H	2:F:89:GLN:HG3	1.60	0.43
2:L:4:VAL:HG22	2:L:134:VAL:HG11	2.00	0.43
2:T:4:VAL:HG22	2:T:134:VAL:HG11	2.00	0.43
2:Z:4:VAL:HG22	2:Z:134:VAL:HG11	2.00	0.43
2:D:83:LEU:HD21	2:D:99:LEU:HD13	2.01	0.43
2:L:83:LEU:HD21	2:L:99:LEU:HD13	2.01	0.43
2:Z:84:SER:OG	2:Z:117:GLY:O	2.32	0.43
2:L:135:TYR:O	2:L:139:GLU:HB2	2.18	0.43
2:N:135:TYR:O	2:N:139:GLU:HB2	2.18	0.43
1:O:186:GLU:OE2	1:O:224:TYR:OH	2.34	0.43
1:Q:147:ARG:HH21	1:Q:149:PHE:HZ	1.65	0.43
1:Q:201:LEU:HD11	1:Q:207:LEU:HG	2.01	0.43
2:R:135:TYR:O	2:R:139:GLU:HB2	2.18	0.43
1:O:201:LEU:HD11	1:O:207:LEU:HG	2.01	0.43
2:D:3:THR:O	2:D:126:SER:HA	2.19	0.43
1:A:20:ARG:HH21	1:A:22:PHE:HE1	1.67	0.43
1:E:20:ARG:HH21	1:E:22:PHE:HE1	1.67	0.43
2:N:114:ASP:O	2:N:117:GLY:N	2.47	0.43
2:X:114:ASP:O	2:X:117:GLY:N	2.47	0.43
1:I:36:THR:HA	1:I:165:ILE:O	2.18	0.43
1:I:161:LYS:N	1:K:58:LEU:O	2.48	0.43
2:N:190:ASP:OD1	2:N:190:ASP:N	2.51	0.43
1:K:152:ASP:HB3	1:K:156:THR:HB	1.99	0.43
1:S:152:ASP:HB3	1:S:156:THR:HB	1.99	0.43
2:Z:4:VAL:HG22	2:Z:134:VAL:HG11	2.00	0.43
2:R:89:GLN:H	2:R:89:GLN:HG3	1.60	0.43
2:F:167:SER:HB2	2:V:167:SER:HB2	2.00	0.43
2:J:83:LEU:HD21	2:J:99:LEU:HD13	2.01	0.43
1:O:162:ALA:HB1	1:O:176:LEU:HD13	2.00	0.43
2:P:83:LEU:HD21	2:P:99:LEU:HD13	2.01	0.43
2:X:178:ILE:HA	2:X:183:GLY:O	2.19	0.43
1:Y:130:ARG:O	1:O:125:GLN:NE2	2.52	0.43
1:K:160:TYR:CE1	1:M:59:ILE:HG12	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:59:ILE:HG12	1:Q:160:TYR:CE1	2.54	0.43
2:H:135:TYR:O	2:H:139:GLU:HB2	2.18	0.43
1:W:201:LEU:HD11	1:W:207:LEU:HG	2.01	0.43
1:I:186:GLU:OE2	1:I:224:TYR:OH	2.31	0.43
2:Z:3:THR:O	2:Z:126:SER:HA	2.19	0.43
2:1:3:THR:O	2:1:126:SER:HA	2.19	0.43
2:F:38:ASP:HB3	2:F:41:THR:HB	1.99	0.43
1:O:20:ARG:HH21	1:O:22:PHE:HE1	1.67	0.43
1:Q:76:ALA:HA	1:Q:137:ILE:O	2.18	0.43
1:A:36:THR:HA	1:A:165:ILE:O	2.18	0.43
1:O:36:THR:HA	1:O:165:ILE:O	2.18	0.43
2:B:3:THR:OG1	2:B:127:THR:OG1	2.26	0.43
1:C:152:ASP:HB3	1:C:156:THR:HB	1.99	0.43
2:D:157:ARG:HH21	2:D:199:LEU:HD22	1.82	0.43
2:L:93:MET:HG3	2:L:94:PRO:HD3	2.01	0.43
1:A:40:MET:H	1:A:47:LEU:HB3	1.83	0.43
2:F:4:VAL:HG22	2:F:134:VAL:HG11	2.00	0.43
1:I:162:ALA:HB1	1:I:176:LEU:HD13	2.01	0.43
1:K:40:MET:H	1:K:47:LEU:HB3	1.83	0.43
1:M:40:MET:H	1:M:47:LEU:HB3	1.83	0.43
1:S:40:MET:H	1:S:47:LEU:HB3	1.83	0.43
1:U:88:LEU:HD23	1:U:88:LEU:HA	1.90	0.43
1:U:162:ALA:HB1	1:U:176:LEU:HD13	2.01	0.43
1:W:40:MET:H	1:W:47:LEU:HB3	1.83	0.43
2:X:18:ARG:NE	2:X:30:ASN:OD1	2.48	0.43
2:B:178:ILE:HA	2:B:183:GLY:O	2.19	0.43
2:P:178:ILE:HA	2:P:183:GLY:O	2.19	0.43
2:T:83:LEU:HD21	2:T:99:LEU:HD13	2.01	0.43
1:A:79:SER:HB3	1:A:165:ILE:HG22	2.00	0.43
1:C:201:LEU:HD11	1:C:207:LEU:HG	2.01	0.43
1:G:201:LEU:HD11	1:G:207:LEU:HG	2.01	0.43
1:M:147:ARG:HH21	1:M:149:PHE:HZ	1.65	0.43
2:V:135:TYR:O	2:V:139:GLU:HB2	2.18	0.43
2:B:20:VAL:HB	2:B:28:HIS:HB2	2.00	0.43
2:D:20:VAL:HB	2:D:28:HIS:HB2	2.00	0.43
2:F:3:THR:O	2:F:126:SER:HA	2.19	0.43
2:J:132:PRO:HB2	2:X:132:PRO:HB2	2.01	0.43
2:P:20:VAL:HB	2:P:28:HIS:HB2	2.00	0.43
1:A:120:MET:HG2	1:A:132:TYR:HD2	1.83	0.43
1:C:120:MET:HG2	1:C:132:TYR:HD2	1.83	0.43
2:F:84:SER:OG	2:F:117:GLY:O	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:157:ARG:HH21	2:J:199:LEU:HD22	1.84	0.43
2:V:157:ARG:HH21	2:V:199:LEU:HD22	1.84	0.43
2:Z:38:ASP:HB3	2:Z:41:THR:HB	1.99	0.43
2:D:114:ASP:HB3	2:D:118:GLY:H	1.82	0.43
1:U:36:THR:HA	1:U:165:ILE:O	2.18	0.43
2:L:4:VAL:HG22	2:L:134:VAL:HG11	2.00	0.43
2:T:4:VAL:HG22	2:T:134:VAL:HG11	2.00	0.43
1:G:147:ARG:HH21	1:G:149:PHE:HZ	1.67	0.43
1:K:162:ALA:HB1	1:K:176:LEU:HD13	2.01	0.43
2:V:83:LEU:HD21	2:V:99:LEU:HD13	2.01	0.43
1:W:147:ARG:HH21	1:W:149:PHE:HZ	1.67	0.43
1:A:162:ALA:HB1	1:A:176:LEU:HD13	2.01	0.42
1:E:162:ALA:HB1	1:E:176:LEU:HD13	2.00	0.42
1:K:162:ALA:HB1	1:K:176:LEU:HD13	2.00	0.42
1:E:160:TYR:CE1	1:G:59:ILE:HG12	2.54	0.42
2:X:13:ILE:HG12	2:X:177:VAL:HG22	2.00	0.42
2:1:20:VAL:HB	2:1:28:HIS:HB2	2.00	0.42
1:C:99:GLU:HB2	1:C:115:ARG:HH22	1.84	0.42
2:J:114:ASP:O	2:J:117:GLY:N	2.47	0.42
1:O:161:LYS:N	1:O:58:LEU:O	2.52	0.42
1:O:36:THR:HA	1:O:165:ILE:O	2.18	0.42
1:A:78:THR:HG22	1:A:136:LEU:HG	2.00	0.42
2:B:93:MET:HG3	2:B:94:PRO:HD3	2.01	0.42
2:N:93:MET:HG3	2:N:94:PRO:HD3	2.01	0.42
2:P:93:MET:HG3	2:P:94:PRO:HD3	2.01	0.42
1:O:152:ASP:HB3	1:O:156:THR:HB	1.99	0.42
1:G:40:MET:H	1:G:47:LEU:HB3	1.83	0.42
2:H:18:ARG:NE	2:H:30:ASN:OD1	2.48	0.42
1:I:88:LEU:HD23	1:I:88:LEU:HA	1.90	0.42
2:N:4:VAL:HG22	2:N:134:VAL:HG11	2.00	0.42
1:O:40:MET:H	1:O:47:LEU:HB3	1.83	0.42
1:Q:40:MET:H	1:Q:47:LEU:HB3	1.83	0.42
2:F:83:LEU:HD21	2:F:99:LEU:HD13	2.01	0.42
2:J:178:ILE:HA	2:J:183:GLY:O	2.19	0.42
1:S:162:ALA:HB1	1:S:176:LEU:HD13	2.01	0.42
2:Z:83:LEU:HD21	2:Z:99:LEU:HD13	2.01	0.42
1:G:69:LEU:HD23	1:G:75:ALA:HB2	2.01	0.42
2:H:13:ILE:HG12	2:H:177:VAL:HG22	2.00	0.42
2:J:13:ILE:HG12	2:J:177:VAL:HG22	2.00	0.42
2:L:132:PRO:HB2	2:Z:132:PRO:HB2	2.00	0.42
2:N:167:SER:HB2	2:P:167:SER:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:13:ILE:HG12	2:V:177:VAL:HG22	2.00	0.42
1:W:69:LEU:HD23	1:W:75:ALA:HB2	2.01	0.42
1:A:152:ASP:O	1:A:155:GLY:N	2.44	0.42
1:I:186:GLU:OE2	1:I:224:TYR:OH	2.34	0.42
2:J:135:TYR:O	2:J:139:GLU:HB2	2.18	0.42
2:B:3:THR:O	2:B:126:SER:HA	2.19	0.42
2:B:3:THR:HG1	2:B:127:THR:HG1	1.53	0.42
2:P:3:THR:O	2:P:126:SER:HA	2.19	0.42
2:T:20:VAL:HB	2:T:28:HIS:HB2	2.00	0.42
1:U:186:GLU:OE2	1:U:224:TYR:OH	2.31	0.42
1:C:36:THR:HA	1:C:165:ILE:O	2.18	0.42
2:R:83:LEU:HD21	2:R:99:LEU:HD13	2.01	0.42
2:D:3:THR:O	2:D:126:SER:HA	2.19	0.42
2:R:93:MET:HG3	2:R:94:PRO:HD3	2.01	0.42
1:U:49:ILE:HG12	1:U:212:ILE:HG12	2.01	0.42
2:1:3:THR:O	2:1:126:SER:HA	2.19	0.42
1:C:40:MET:H	1:C:47:LEU:HB3	1.83	0.42
1:E:147:ARG:HH21	1:E:149:PHE:HZ	1.67	0.42
1:I:186:GLU:OE2	1:I:224:TYR:OH	2.30	0.42
2:J:83:LEU:HD21	2:J:99:LEU:HD13	2.01	0.42
2:L:83:LEU:HD21	2:L:99:LEU:HD13	2.01	0.42
2:P:89:GLN:H	2:P:89:GLN:HG3	1.60	0.42
2:R:4:VAL:HG22	2:R:134:VAL:HG11	2.00	0.42
1:S:162:ALA:HB1	1:S:176:LEU:HD13	2.01	0.42
1:U:147:ARG:HH21	1:U:149:PHE:HZ	1.67	0.42
1:O:40:MET:H	1:O:47:LEU:HB3	1.83	0.42
2:H:178:ILE:HA	2:H:183:GLY:O	2.19	0.42
2:V:83:LEU:HD21	2:V:99:LEU:HD13	2.01	0.42
2:B:37:ILE:HG22	2:B:63:LEU:HD22	2.01	0.42
1:I:160:TYR:HE1	1:K:59:ILE:HG12	1.85	0.42
2:N:37:ILE:HG22	2:N:63:LEU:HD22	2.01	0.42
2:R:37:ILE:HG22	2:R:63:LEU:HD22	2.01	0.42
2:D:98:GLN:NE2	2:D:128:GLY:H	2.18	0.42
2:1:98:GLN:NE2	2:1:128:GLY:H	2.18	0.42
2:N:3:THR:OG1	2:N:127:THR:OG1	2.26	0.42
2:R:3:THR:OG1	2:R:127:THR:OG1	2.26	0.42
1:A:99:GLU:HB2	1:A:115:ARG:HH22	1.84	0.42
2:B:38:ASP:HB3	2:B:41:THR:HB	1.99	0.42
2:L:114:ASP:O	2:L:117:GLY:N	2.47	0.42
2:T:38:ASP:HB3	2:T:41:THR:HB	1.99	0.42
2:B:83:LEU:HD21	2:B:99:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:178:ILE:HA	2:B:183:GLY:O	2.20	0.42
2:N:83:LEU:HD21	2:N:99:LEU:HD13	2.01	0.42
2:P:83:LEU:HD21	2:P:99:LEU:HD13	2.01	0.42
2:1:114:ASP:HB3	2:1:118:GLY:H	1.82	0.42
1:A:49:ILE:HG12	1:A:212:ILE:HG12	2.01	0.42
1:M:49:ILE:HG12	1:M:212:ILE:HG12	2.01	0.42
1:M:78:THR:HG22	1:M:136:LEU:HG	2.00	0.42
1:O:49:ILE:HG12	1:O:212:ILE:HG12	2.01	0.42
1:Q:49:ILE:HG12	1:Q:212:ILE:HG12	2.02	0.42
1:G:162:ALA:HB1	1:G:176:LEU:HD13	2.01	0.42
1:O:162:ALA:HB1	1:O:176:LEU:HD13	2.01	0.42
2:T:83:LEU:HD21	2:T:99:LEU:HD13	2.01	0.42
1:W:162:ALA:HB1	1:W:176:LEU:HD13	2.01	0.42
2:X:91:LYS:HB2	2:Z:93:MET:HE3	2.01	0.42
1:Y:147:ARG:HH21	1:Y:149:PHE:HZ	1.67	0.42
2:V:178:ILE:HA	2:V:183:GLY:O	2.19	0.42
1:Y:162:ALA:HB1	1:Y:176:LEU:HD13	2.00	0.42
1:E:160:TYR:HE1	1:G:59:ILE:HG12	1.85	0.42
1:I:69:LEU:HD23	1:I:75:ALA:HB2	2.01	0.42
2:P:37:ILE:HG22	2:P:63:LEU:HD22	2.01	0.42
1:C:79:SER:HB3	1:C:165:ILE:HG22	2.00	0.42
1:U:186:GLU:OE2	1:U:224:TYR:OH	2.34	0.42
1:A:68:GLN:HE21	1:A:89:VAL:HG21	1.85	0.42
2:L:20:VAL:HB	2:L:28:HIS:HB2	2.01	0.42
2:L:132:PRO:HB2	2:Z:132:PRO:HB2	2.01	0.42
2:B:3:THR:OG1	2:B:127:THR:OG1	2.26	0.42
2:D:157:ARG:HH21	2:D:199:LEU:HD22	1.84	0.42
2:L:38:ASP:HB3	2:L:41:THR:HB	1.99	0.42
2:R:38:ASP:HB3	2:R:41:THR:HB	1.99	0.42
2:Z:84:SER:OG	2:Z:117:GLY:O	2.34	0.42
2:F:178:ILE:HA	2:F:183:GLY:O	2.20	0.42
2:H:178:ILE:HA	2:H:183:GLY:O	2.20	0.42
2:N:91:LYS:HD2	2:N:91:LYS:HA	1.80	0.42
2:X:178:ILE:HA	2:X:183:GLY:O	2.20	0.42
2:B:3:THR:O	2:B:126:SER:HA	2.19	0.42
1:E:49:ILE:HG12	1:E:212:ILE:HG12	2.01	0.42
2:F:203:LEU:HA	2:F:203:LEU:HD13	1.87	0.42
1:G:49:ILE:HG12	1:G:212:ILE:HG12	2.01	0.42
2:H:93:MET:HG3	2:H:94:PRO:HD3	2.01	0.42
1:K:49:ILE:HG12	1:K:212:ILE:HG12	2.02	0.42
2:N:167:SER:HB2	2:P:167:SER:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:78:THR:HG22	1:O:136:LEU:HG	2.00	0.42
2:Z:203:LEU:HA	2:Z:203:LEU:HD13	1.87	0.42
1:A:162:ALA:HB1	1:A:176:LEU:HD13	2.01	0.42
1:C:125:GLN:NE2	1:E:130:ARG:O	2.53	0.42
2:D:51:ASP:OD1	2:F:91:LYS:HD3	2.20	0.42
2:D:190:ASP:HA	2:D:193:GLU:HG2	2.02	0.42
2:L:178:ILE:HA	2:L:183:GLY:O	2.19	0.42
2:T:178:ILE:HA	2:T:183:GLY:O	2.19	0.42
2:X:83:LEU:HD21	2:X:99:LEU:HD13	2.01	0.42
1:O:162:ALA:HB1	1:O:176:LEU:HD13	2.00	0.42
1:E:69:LEU:HD23	1:E:75:ALA:HB2	2.01	0.42
1:U:69:LEU:HD23	1:U:75:ALA:HB2	2.01	0.42
1:Y:69:LEU:HD23	1:Y:75:ALA:HB2	2.01	0.42
1:O:68:GLN:HE21	1:O:89:VAL:HG21	1.85	0.42
1:K:20:ARG:HH21	1:K:22:PHE:HE1	1.67	0.42
2:N:38:ASP:HB3	2:N:41:THR:HB	1.99	0.42
2:P:38:ASP:HB3	2:P:41:THR:HB	1.99	0.42
2:V:114:ASP:O	2:V:117:GLY:N	2.47	0.42
2:P:178:ILE:HA	2:P:183:GLY:O	2.20	0.42
2:T:190:ASP:OD1	2:T:190:ASP:N	2.51	0.42
1:C:49:ILE:HG12	1:C:212:ILE:HG12	2.01	0.42
1:I:49:ILE:HG12	1:I:212:ILE:HG12	2.02	0.42
2:P:3:THR:O	2:P:126:SER:HA	2.19	0.42
1:Q:78:THR:HG22	1:Q:136:LEU:HG	2.00	0.42
1:S:49:ILE:HG12	1:S:212:ILE:HG12	2.02	0.42
1:W:49:ILE:HG12	1:W:212:ILE:HG12	2.01	0.42
1:Y:49:ILE:HG12	1:Y:212:ILE:HG12	2.01	0.42
2:D:83:LEU:HD21	2:D:99:LEU:HD13	2.01	0.42
1:G:186:GLU:OE2	1:G:224:TYR:OH	2.30	0.42
1:I:147:ARG:HH21	1:I:149:PHE:HZ	1.67	0.42
2:P:83:LEU:HD21	2:P:99:LEU:HD13	2.01	0.42
1:W:186:GLU:OE2	1:W:224:TYR:OH	2.30	0.42
2:X:83:LEU:HD21	2:X:99:LEU:HD13	2.01	0.42
2:1:83:LEU:HD21	2:1:99:LEU:HD13	2.01	0.42
2:1:190:ASP:HA	2:1:193:GLU:HG2	2.02	0.42
1:O:59:ILE:HG12	1:Q:160:TYR:HE1	1.85	0.42
1:S:172:VAL:HG13	1:S:196:ALA:HB1	2.01	0.42
1:C:68:GLN:HE21	1:C:89:VAL:HG21	1.85	0.42
2:H:3:THR:O	2:H:126:SER:HA	2.19	0.42
1:K:68:GLN:HE21	1:K:89:VAL:HG21	1.85	0.42
1:O:68:GLN:HE21	1:O:89:VAL:HG21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:157:ARG:HH21	2:B:199:LEU:HD22	1.84	0.42
1:M:172:VAL:HG13	1:M:196:ALA:HB1	2.02	0.42
2:P:157:ARG:HH21	2:P:199:LEU:HD22	1.84	0.42
2:P:196:ILE:HD13	2:P:203:LEU:HA	2.02	0.42
2:R:196:ILE:HD13	2:R:203:LEU:HA	2.02	0.42
1:S:20:ARG:HH21	1:S:22:PHE:HE1	1.67	0.42
2:V:144:GLU:HG2	2:V:145:LYS:HD2	2.02	0.42
2:1:157:ARG:HH21	2:1:199:LEU:HD22	1.84	0.42
2:F:22:MET:HE2	2:F:22:MET:HB3	1.93	0.42
2:H:91:LYS:HA	2:H:91:LYS:HD2	1.80	0.42
2:L:94:PRO:O	2:N:91:LYS:NZ	2.34	0.42
2:Z:178:ILE:HA	2:Z:183:GLY:O	2.20	0.42
2:D:93:MET:HG3	2:D:94:PRO:HD3	2.01	0.42
2:J:203:LEU:HD13	2:J:203:LEU:HA	1.87	0.42
2:V:4:VAL:HG22	2:V:134:VAL:HG11	2.00	0.42
1:W:152:ASP:O	1:W:155:GLY:N	2.36	0.42
2:X:93:MET:HG3	2:X:94:PRO:HD3	2.01	0.42
1:O:49:ILE:HG12	1:O:212:ILE:HG12	2.01	0.42
2:1:93:MET:HG3	2:1:94:PRO:HD3	2.01	0.42
2:B:83:LEU:HD21	2:B:99:LEU:HD13	2.01	0.42
1:E:40:MET:H	1:E:47:LEU:HB3	1.83	0.42
2:N:89:GLN:H	2:N:89:GLN:HG3	1.60	0.42
1:Y:40:MET:H	1:Y:47:LEU:HB3	1.83	0.42
1:C:162:ALA:HB1	1:C:176:LEU:HD13	2.00	0.42
2:D:178:ILE:HA	2:D:183:GLY:O	2.19	0.42
1:G:67:ILE:HG13	1:G:77:VAL:HG12	2.02	0.42
1:G:162:ALA:HB1	1:G:176:LEU:HD13	2.00	0.42
2:L:38:ASP:HB2	2:L:63:LEU:HD13	2.02	0.42
2:P:190:ASP:HA	2:P:193:GLU:HG2	2.02	0.42
2:T:38:ASP:HB2	2:T:63:LEU:HD13	2.02	0.42
2:B:132:PRO:HB2	2:P:132:PRO:HB2	2.00	0.42
1:W:59:ILE:HG12	1:Y:160:TYR:HE1	1.85	0.42
1:E:201:LEU:HD11	1:E:207:LEU:HG	2.01	0.42
1:G:18:ASP:O	1:I:33:LYS:NZ	2.46	0.42
2:H:98:GLN:NE2	2:H:128:GLY:H	2.18	0.42
1:K:172:VAL:HG13	1:K:196:ALA:HB1	2.01	0.42
2:N:98:GLN:NE2	2:N:128:GLY:H	2.18	0.42
2:V:98:GLN:NE2	2:V:128:GLY:H	2.18	0.42
2:X:98:GLN:NE2	2:X:128:GLY:H	2.18	0.42
1:Y:201:LEU:HD11	1:Y:207:LEU:HG	2.01	0.42
2:B:132:PRO:HB2	2:P:132:PRO:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:20:VAL:HB	2:F:28:HIS:HB2	2.00	0.42
2:L:3:THR:O	2:L:126:SER:HA	2.19	0.42
1:M:68:GLN:HE21	1:M:89:VAL:HG21	1.85	0.42
2:N:20:VAL:HB	2:N:28:HIS:HB2	2.00	0.42
2:X:3:THR:O	2:X:126:SER:HA	2.19	0.42
2:B:196:ILE:HD13	2:B:203:LEU:HA	2.02	0.42
2:H:144:GLU:HG2	2:H:145:LYS:HD2	2.02	0.42
2:J:144:GLU:HG2	2:J:145:LYS:HD2	2.02	0.42
1:K:172:VAL:HG13	1:K:196:ALA:HB1	2.02	0.42
2:N:196:ILE:HD13	2:N:203:LEU:HA	2.02	0.42
2:P:15:ALA:HA	2:P:174:ASP:O	2.20	0.42
2:P:144:GLU:HG2	2:P:145:LYS:HD2	2.02	0.42
1:Q:172:VAL:HG13	1:Q:196:ALA:HB1	2.02	0.42
1:S:172:VAL:HG13	1:S:196:ALA:HB1	2.02	0.42
2:T:114:ASP:O	2:T:117:GLY:N	2.47	0.42
2:T:196:ILE:HD13	2:T:203:LEU:HA	2.02	0.42
1:U:20:ARG:HH21	1:U:22:PHE:HE1	1.67	0.42
1:E:36:THR:HA	1:E:165:ILE:O	2.18	0.42
2:L:190:ASP:OD1	2:L:190:ASP:N	2.51	0.42
2:R:91:LYS:HD2	2:R:91:LYS:HA	1.80	0.42
2:X:91:LYS:HA	2:X:91:LYS:HD2	1.80	0.42
2:X:156:ILE:O	2:X:160:SER:OG	2.32	0.42
2:Z:91:LYS:HA	2:Z:91:LYS:HD2	1.80	0.42
2:J:4:VAL:HG22	2:J:134:VAL:HG11	2.00	0.42
1:K:78:THR:HG22	1:K:136:LEU:HG	2.00	0.42
2:V:196:ILE:HG23	2:V:201:LEU:HB2	2.02	0.42
1:O:78:THR:HG22	1:O:136:LEU:HG	2.00	0.42
1:C:162:ALA:HB1	1:C:176:LEU:HD13	2.01	0.42
2:N:141:GLN:HE21	2:1:141:GLN:HE21	1.66	0.42
1:Y:162:ALA:HB1	1:Y:176:LEU:HD13	2.01	0.42
2:F:190:ASP:HA	2:F:193:GLU:HG2	2.02	0.42
2:H:83:LEU:HD21	2:H:99:LEU:HD13	2.01	0.42
2:R:38:ASP:HB2	2:R:63:LEU:HD13	2.02	0.42
1:W:67:ILE:HG13	1:W:77:VAL:HG12	2.02	0.42
1:O:67:ILE:HG13	1:O:77:VAL:HG12	2.02	0.42
2:1:178:ILE:HA	2:1:183:GLY:O	2.19	0.42
2:L:37:ILE:HG22	2:L:63:LEU:HD22	2.01	0.42
1:Q:59:ILE:HG12	1:S:160:TYR:HE1	1.85	0.42
2:X:37:ILE:HG22	2:X:63:LEU:HD22	2.01	0.42
2:J:98:GLN:NE2	2:J:128:GLY:H	2.18	0.42
1:O:201:LEU:HD11	1:O:207:LEU:HG	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:98:GLN:NE2	2:R:128:GLY:H	2.18	0.42
1:U:172:VAL:HG13	1:U:196:ALA:HB1	2.01	0.42
1:E:68:GLN:HE21	1:E:89:VAL:HG21	1.85	0.42
2:F:132:PRO:HB2	2:T:132:PRO:HB2	2.01	0.42
1:Q:68:GLN:HE21	1:Q:89:VAL:HG21	1.85	0.42
2:R:20:VAL:HB	2:R:28:HIS:HB2	2.01	0.42
1:S:68:GLN:HE21	1:S:89:VAL:HG21	1.85	0.42
2:T:3:THR:O	2:T:126:SER:HA	2.19	0.42
1:Y:68:GLN:HE21	1:Y:89:VAL:HG21	1.85	0.42
2:Z:20:VAL:HB	2:Z:28:HIS:HB2	2.00	0.42
2:B:14:MET:HE2	2:B:44:THR:HG23	2.02	0.42
1:A:58:LEU:O	1:M:161:LYS:N	2.53	0.42
2:B:144:GLU:HG2	2:B:145:LYS:HD2	2.02	0.42
2:L:196:ILE:HD13	2:L:203:LEU:HA	2.02	0.42
2:X:144:GLU:HG2	2:X:145:LYS:HD2	2.02	0.42
2:X:157:ARG:HH21	2:X:199:LEU:HD22	1.84	0.42
2:H:156:ILE:O	2:H:160:SER:OG	2.32	0.42
2:L:83:LEU:HD21	2:L:99:LEU:HD13	2.01	0.42
2:N:178:ILE:HA	2:N:183:GLY:O	2.20	0.42
2:F:196:ILE:HG23	2:F:201:LEU:HB2	2.02	0.42
2:H:3:THR:O	2:H:126:SER:HA	2.19	0.42
1:Q:88:LEU:HD23	1:Q:88:LEU:HA	1.92	0.42
2:X:3:THR:O	2:X:126:SER:HA	2.19	0.42
2:Z:3:THR:O	2:Z:126:SER:HA	2.19	0.42
2:Z:196:ILE:HG23	2:Z:201:LEU:HB2	2.02	0.42
1:E:162:ALA:HB1	1:E:176:LEU:HD13	2.01	0.42
1:U:186:GLU:OE2	1:U:224:TYR:OH	2.30	0.42
1:O:162:ALA:HB1	1:O:176:LEU:HD13	2.01	0.42
2:B:190:ASP:HA	2:B:193:GLU:HG2	2.02	0.42
1:E:67:ILE:HG13	1:E:77:VAL:HG12	2.02	0.42
1:K:186:GLU:OE2	1:K:224:TYR:OH	2.33	0.42
1:M:225:ASP:OD1	1:M:225:ASP:N	2.53	0.42
2:N:38:ASP:HB2	2:N:63:LEU:HD13	2.02	0.42
1:Y:67:ILE:HG13	1:Y:77:VAL:HG12	2.02	0.42
2:H:37:ILE:HG22	2:H:63:LEU:HD22	2.01	0.42
2:T:37:ILE:HG22	2:T:63:LEU:HD22	2.01	0.42
1:A:201:LEU:HD11	1:A:207:LEU:HG	2.01	0.42
1:I:172:VAL:HG13	1:I:196:ALA:HB1	2.01	0.42
1:M:172:VAL:HG13	1:M:196:ALA:HB1	2.01	0.42
1:G:46:VAL:HG13	1:G:146:PRO:HB3	2.02	0.42
1:I:68:GLN:HE21	1:I:89:VAL:HG21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:68:GLN:HE21	1:U:89:VAL:HG21	1.85	0.42
2:B:15:ALA:HA	2:B:174:ASP:O	2.20	0.42
2:D:38:ASP:HB3	2:D:41:THR:HB	2.00	0.42
2:D:196:ILE:HD13	2:D:203:LEU:HA	2.02	0.42
2:H:157:ARG:HH21	2:H:199:LEU:HD22	1.84	0.42
1:I:20:ARG:HH21	1:I:22:PHE:HE1	1.67	0.42
1:I:172:VAL:HG13	1:I:196:ALA:HB1	2.02	0.42
2:L:144:GLU:HG2	2:L:145:LYS:HD2	2.02	0.42
2:N:15:ALA:HA	2:N:174:ASP:O	2.20	0.42
2:T:1:THR:N	2:T:168:ALA:O	2.49	0.42
2:V:196:ILE:HD13	2:V:203:LEU:HA	2.02	0.42
2:1:196:ILE:HD13	2:1:203:LEU:HA	2.02	0.42
2:F:88:ASN:HD22	2:F:90:VAL:HG12	1.85	0.42
2:R:178:ILE:HA	2:R:183:GLY:O	2.20	0.42
1:Y:36:THR:HA	1:Y:165:ILE:O	2.18	0.42
1:C:78:THR:HG22	1:C:136:LEU:HG	2.01	0.42
2:F:3:THR:O	2:F:126:SER:HA	2.19	0.42
2:H:4:VAL:HG22	2:H:134:VAL:HG11	2.00	0.42
2:H:196:ILE:HG23	2:H:201:LEU:HB2	2.02	0.42
2:J:3:THR:O	2:J:126:SER:HA	2.19	0.42
2:J:196:ILE:HG23	2:J:201:LEU:HB2	2.02	0.42
2:V:3:THR:O	2:V:126:SER:HA	2.19	0.42
2:X:4:VAL:HG22	2:X:134:VAL:HG11	2.00	0.42
2:H:83:LEU:HD21	2:H:99:LEU:HD13	2.01	0.42
1:K:147:ARG:HH21	1:K:149:PHE:HZ	1.67	0.42
1:S:147:ARG:HH21	1:S:149:PHE:HZ	1.67	0.42
1:O:147:ARG:HH21	1:O:149:PHE:HZ	1.67	0.42
1:C:67:ILE:HG13	1:C:77:VAL:HG12	2.02	0.42
1:I:67:ILE:HG13	1:I:77:VAL:HG12	2.02	0.42
1:W:162:ALA:HB1	1:W:176:LEU:HD13	2.01	0.42
2:Z:190:ASP:HA	2:Z:193:GLU:HG2	2.02	0.42
2:D:37:ILE:HG22	2:D:63:LEU:HD22	2.01	0.42
1:K:69:LEU:HD23	1:K:75:ALA:HB2	2.01	0.42
1:K:160:TYR:HE1	1:M:59:ILE:HG12	1.85	0.42
1:S:69:LEU:HD23	1:S:75:ALA:HB2	2.01	0.42
2:B:20:VAL:HB	2:B:28:HIS:HB2	2.02	0.42
2:D:4:VAL:HG22	2:D:134:VAL:HG11	2.01	0.42
1:Q:172:VAL:HG13	1:Q:196:ALA:HB1	2.01	0.42
2:Z:88:ASN:HD22	2:1:54:VAL:HG21	1.84	0.42
1:G:39:GLY:O	1:G:162:ALA:HA	2.20	0.42
2:J:3:THR:O	2:J:126:SER:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:39:GLY:O	1:U:162:ALA:HA	2.20	0.42
2:V:3:THR:O	2:V:126:SER:HA	2.19	0.42
1:W:46:VAL:HG13	1:W:146:PRO:HB3	2.02	0.42
1:A:172:VAL:HG13	1:A:196:ALA:HB1	2.02	0.42
2:D:102:GLY:HA2	2:D:109:HIS:O	2.20	0.42
2:D:144:GLU:HG2	2:D:145:LYS:HD2	2.02	0.42
2:F:144:GLU:HG2	2:F:145:LYS:HD2	2.02	0.42
2:F:157:ARG:HH21	2:F:199:LEU:HD22	1.84	0.42
2:J:196:ILE:HD13	2:J:203:LEU:HA	2.02	0.42
2:L:102:GLY:HA2	2:L:109:HIS:O	2.20	0.42
1:O:172:VAL:HG13	1:O:196:ALA:HB1	2.02	0.42
2:R:15:ALA:HA	2:R:174:ASP:O	2.20	0.42
2:R:144:GLU:HG2	2:R:145:LYS:HD2	2.02	0.42
2:R:157:ARG:HH21	2:R:199:LEU:HD22	1.84	0.42
2:T:102:GLY:HA2	2:T:109:HIS:O	2.20	0.42
2:T:144:GLU:HG2	2:T:145:LYS:HD2	2.02	0.42
1:U:172:VAL:HG13	1:U:196:ALA:HB1	2.02	0.42
2:Z:144:GLU:HG2	2:Z:145:LYS:HD2	2.02	0.42
2:1:38:ASP:HB3	2:1:41:THR:HB	1.99	0.42
2:1:102:GLY:HA2	2:1:109:HIS:O	2.20	0.42
2:1:144:GLU:HG2	2:1:145:LYS:HD2	2.02	0.42
2:T:83:LEU:HD21	2:T:99:LEU:HD13	2.01	0.42
2:Z:88:ASN:HD22	2:Z:90:VAL:HG12	1.85	0.42
1:G:78:THR:HG22	1:G:136:LEU:HG	2.00	0.42
1:G:152:ASP:O	1:G:155:GLY:N	2.36	0.42
2:N:3:THR:O	2:N:126:SER:HA	2.19	0.42
1:S:78:THR:HG22	1:S:136:LEU:HG	2.01	0.42
2:X:196:ILE:HG23	2:X:201:LEU:HB2	2.02	0.42
2:Z:93:MET:HG3	2:Z:94:PRO:HD3	2.01	0.42
1:C:147:ARG:HH21	1:C:149:PHE:HZ	1.67	0.42
1:I:40:MET:H	1:I:47:LEU:HB3	1.83	0.42
2:B:141:GLN:HE21	2:P:141:GLN:HE21	1.67	0.41
2:J:38:ASP:HB2	2:J:63:LEU:HD13	2.02	0.41
2:L:132:PRO:HB2	2:Z:132:PRO:HB2	2.01	0.41
1:S:186:GLU:OE2	1:S:224:TYR:OH	2.33	0.41
1:S:225:ASP:OD1	1:S:225:ASP:N	2.53	0.41
1:U:67:ILE:HG13	1:U:77:VAL:HG12	2.02	0.41
2:V:38:ASP:HB2	2:V:63:LEU:HD13	2.02	0.41
2:X:38:ASP:HB2	2:X:63:LEU:HD13	2.02	0.41
1:C:69:LEU:HD23	1:C:75:ALA:HB2	2.01	0.41
1:O:69:LEU:HD23	1:O:75:ALA:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:88:LEU:HD23	1:Q:88:LEU:HA	1.92	0.41
1:I:39:GLY:O	1:I:162:ALA:HA	2.20	0.41
2:N:3:THR:O	2:N:126:SER:HA	2.19	0.41
2:N:202:ILE:H	2:N:202:ILE:HG13	1.72	0.41
2:R:3:THR:O	2:R:126:SER:HA	2.19	0.41
2:B:196:ILE:HD13	2:B:203:LEU:HA	2.02	0.41
1:G:20:ARG:HH21	1:G:22:PHE:HE1	1.67	0.41
2:J:102:GLY:HA2	2:J:109:HIS:O	2.20	0.41
2:N:157:ARG:HH21	2:N:199:LEU:HD22	1.84	0.41
2:V:102:GLY:HA2	2:V:109:HIS:O	2.20	0.41
1:W:172:VAL:HG13	1:W:196:ALA:HB1	2.02	0.41
2:H:88:ASN:HD22	2:H:90:VAL:HG12	1.85	0.41
2:V:178:ILE:HA	2:V:183:GLY:O	2.20	0.41
1:Y:208:LYS:HB2	1:Y:208:LYS:HE2	1.73	0.41
2:D:83:LEU:HD21	2:D:99:LEU:HD13	2.02	0.41
2:F:93:MET:HG3	2:F:94:PRO:HD3	2.01	0.41
1:I:186:GLU:OE2	1:I:224:TYR:OH	2.33	0.41
2:P:203:LEU:HA	2:P:203:LEU:HD13	1.87	0.41
1:W:78:THR:HG22	1:W:136:LEU:HG	2.01	0.41
2:B:89:GLN:H	2:B:89:GLN:HG3	1.60	0.41
1:U:40:MET:H	1:U:47:LEU:HB3	1.83	0.41
1:K:225:ASP:OD1	1:K:225:ASP:N	2.53	0.41
1:A:69:LEU:HD23	1:A:75:ALA:HB2	2.01	0.41
1:S:59:ILE:HG12	1:U:160:TYR:HE1	1.85	0.41
2:D:20:VAL:HB	2:D:28:HIS:HB2	2.02	0.41
1:C:162:ALA:HB1	1:C:176:LEU:HD13	2.02	0.41
2:T:98:GLN:NE2	2:T:128:GLY:H	2.18	0.41
1:U:33:LYS:NZ	1:W:18:ASP:O	2.46	0.41
1:O:162:ALA:HB1	1:O:176:LEU:HD13	2.02	0.41
1:A:46:VAL:HG13	1:A:146:PRO:HB3	2.02	0.41
1:E:125:GLN:NE2	1:G:130:ARG:O	2.52	0.41
2:N:14:MET:HE2	2:N:44:THR:HG23	2.03	0.41
1:O:46:VAL:HG13	1:O:146:PRO:HB3	2.02	0.41
2:R:14:MET:HE2	2:R:44:THR:HG23	2.03	0.41
1:W:39:GLY:O	1:W:162:ALA:HA	2.20	0.41
2:B:102:GLY:HA2	2:B:109:HIS:O	2.20	0.41
2:F:102:GLY:HA2	2:F:109:HIS:O	2.20	0.41
2:L:1:THR:N	2:L:168:ALA:O	2.49	0.41
2:N:144:GLU:HG2	2:N:145:LYS:HD2	2.02	0.41
2:Z:102:GLY:HA2	2:Z:109:HIS:O	2.20	0.41
2:Z:157:ARG:HH21	2:Z:199:LEU:HD22	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:15:ALA:HA	2:1:174:ASP:O	2.20	0.41
2:J:178:ILE:HA	2:J:183:GLY:O	2.20	0.41
2:X:88:ASN:HD22	2:X:90:VAL:HG12	1.85	0.41
2:1:83:LEU:HD21	2:1:99:LEU:HD13	2.01	0.41
2:1:178:ILE:HA	2:1:183:GLY:O	2.20	0.41
1:E:78:THR:HG22	1:E:136:LEU:HG	2.00	0.41
2:L:196:ILE:HG23	2:L:201:LEU:HB2	2.02	0.41
1:M:88:LEU:HD23	1:M:88:LEU:HA	1.92	0.41
2:R:3:THR:O	2:R:126:SER:HA	2.19	0.41
2:R:83:LEU:HD21	2:R:99:LEU:HD13	2.02	0.41
2:T:83:LEU:HD21	2:T:99:LEU:HD13	2.02	0.41
2:T:196:ILE:HG23	2:T:201:LEU:HB2	2.02	0.41
1:U:186:GLU:OE2	1:U:224:TYR:OH	2.33	0.41
2:V:203:LEU:HD13	2:V:203:LEU:HA	1.87	0.41
2:1:83:LEU:HD21	2:1:99:LEU:HD13	2.02	0.41
1:Y:100:LYS:NZ	2:Z:64:GLU:OE2	2.50	0.41
2:F:50:GLY:O	2:H:88:ASN:ND2	2.53	0.41
1:O:67:ILE:HG13	1:O:77:VAL:HG12	2.02	0.41
1:U:162:ALA:HB1	1:U:176:LEU:HD13	2.00	0.41
2:L:98:GLN:NE2	2:L:128:GLY:H	2.18	0.41
1:K:39:GLY:O	1:K:162:ALA:HA	2.20	0.41
1:S:39:GLY:O	1:S:162:ALA:HA	2.20	0.41
2:N:102:GLY:HA2	2:N:109:HIS:O	2.20	0.41
1:W:20:ARG:HH21	1:W:22:PHE:HE1	1.67	0.41
2:D:83:LEU:HD21	2:D:99:LEU:HD13	2.01	0.41
2:J:83:LEU:HD21	2:J:99:LEU:HD13	2.01	0.41
2:T:22:MET:HE2	2:T:22:MET:HB3	1.93	0.41
1:W:208:LYS:HB2	1:W:208:LYS:HE2	1.73	0.41
2:B:83:LEU:HD21	2:B:99:LEU:HD13	2.02	0.41
2:B:203:LEU:HA	2:B:203:LEU:HD13	1.87	0.41
1:G:88:LEU:HD23	1:G:88:LEU:HA	1.92	0.41
1:I:78:THR:HG22	1:I:136:LEU:HG	2.00	0.41
2:L:3:THR:O	2:L:126:SER:HA	2.19	0.41
2:N:83:LEU:HD21	2:N:99:LEU:HD13	2.02	0.41
2:V:83:LEU:HD21	2:V:99:LEU:HD13	2.02	0.41
1:Y:78:THR:HG22	1:Y:136:LEU:HG	2.00	0.41
2:Z:83:LEU:HD21	2:Z:99:LEU:HD13	2.02	0.41
1:O:152:ASP:O	1:O:155:GLY:N	2.36	0.41
1:A:58:LEU:O	1:M:161:LYS:N	2.50	0.41
1:Q:63:SER:OG	1:S:159:GLU:OE1	2.37	0.41
1:A:67:ILE:HG13	1:A:77:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:38:ASP:HB2	2:H:63:LEU:HD13	2.02	0.41
1:I:162:ALA:HB1	1:I:176:LEU:HD13	2.00	0.41
2:F:132:PRO:HB2	2:T:132:PRO:HB2	2.02	0.41
2:N:3:THR:OG1	2:N:127:THR:OG1	2.25	0.41
2:X:84:SER:OG	2:X:117:GLY:O	2.32	0.41
2:B:4:VAL:HG22	2:B:134:VAL:HG11	2.01	0.41
1:C:227:GLU:H	1:C:227:GLU:HG3	1.60	0.41
2:B:14:MET:HE2	2:B:44:THR:HG23	2.03	0.41
1:C:46:VAL:HG13	1:C:146:PRO:HB3	2.02	0.41
1:E:39:GLY:O	1:E:162:ALA:HA	2.20	0.41
2:L:14:MET:HE2	2:L:44:THR:HG23	2.03	0.41
2:P:14:MET:HE2	2:P:44:THR:HG23	2.03	0.41
2:V:153:ASP:OD1	2:V:153:ASP:N	2.54	0.41
1:Y:39:GLY:O	1:Y:162:ALA:HA	2.20	0.41
1:O:46:VAL:HG13	1:O:146:PRO:HB3	2.02	0.41
1:G:172:VAL:HG13	1:G:196:ALA:HB1	2.02	0.41
2:J:15:ALA:HA	2:J:174:ASP:O	2.20	0.41
2:P:102:GLY:HA2	2:P:109:HIS:O	2.20	0.41
2:R:102:GLY:HA2	2:R:109:HIS:O	2.20	0.41
2:T:157:ARG:HH21	2:T:199:LEU:HD22	1.84	0.41
2:V:15:ALA:HA	2:V:174:ASP:O	2.20	0.41
2:D:178:ILE:HA	2:D:183:GLY:O	2.20	0.41
2:H:190:ASP:OD1	2:H:190:ASP:N	2.51	0.41
1:U:138:PHE:HB2	1:U:149:PHE:HB2	2.03	0.41
2:X:190:ASP:OD1	2:X:190:ASP:N	2.51	0.41
2:F:83:LEU:HD21	2:F:99:LEU:HD13	2.02	0.41
2:L:83:LEU:HD21	2:L:99:LEU:HD13	2.02	0.41
2:T:3:THR:O	2:T:126:SER:HA	2.19	0.41
2:F:83:LEU:HD21	2:F:99:LEU:HD13	2.01	0.41
2:Z:83:LEU:HD21	2:Z:99:LEU:HD13	2.01	0.41
2:P:38:ASP:HB2	2:P:63:LEU:HD13	2.02	0.41
2:R:3:THR:OG1	2:R:127:THR:OG1	2.25	0.41
2:V:37:ILE:HG22	2:V:63:LEU:HD22	2.01	0.41
1:E:38:LEU:HB2	1:E:49:ILE:HB	2.02	0.41
2:B:98:GLN:NE2	2:B:128:GLY:H	2.18	0.41
2:F:98:GLN:NE2	2:F:128:GLY:H	2.18	0.41
1:M:88:LEU:HD23	1:M:88:LEU:HA	1.92	0.41
2:P:98:GLN:NE2	2:P:128:GLY:H	2.18	0.41
1:S:162:ALA:HB1	1:S:176:LEU:HD13	2.02	0.41
2:Z:98:GLN:NE2	2:Z:128:GLY:H	2.18	0.41
1:G:68:GLN:HE21	1:G:89:VAL:HG21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:153:ASP:OD1	2:J:153:ASP:N	2.54	0.41
2:R:202:ILE:H	2:R:202:ILE:HG13	1.73	0.41
2:V:3:THR:OG1	2:V:127:THR:OG1	2.26	0.41
2:D:15:ALA:HA	2:D:174:ASP:O	2.20	0.41
2:H:196:ILE:HD13	2:H:203:LEU:HA	2.02	0.41
2:J:14:MET:HE3	2:J:14:MET:HB2	1.92	0.41
2:P:114:ASP:O	2:P:117:GLY:N	2.47	0.41
1:E:208:LYS:HB2	1:E:208:LYS:HE2	1.73	0.41
2:L:22:MET:HE2	2:L:22:MET:HB3	1.93	0.41
2:L:156:ILE:O	2:L:160:SER:OG	2.32	0.41
1:U:186:GLU:OE2	1:U:224:TYR:OH	2.38	0.41
2:V:83:LEU:HD21	2:V:99:LEU:HD13	2.01	0.41
2:1:22:MET:HE2	2:1:22:MET:HB3	1.93	0.41
2:D:196:ILE:HG23	2:D:201:LEU:HB2	2.02	0.41
2:J:83:LEU:HD21	2:J:99:LEU:HD13	2.02	0.41
1:U:88:LEU:HD23	1:U:88:LEU:HA	1.92	0.41
1:W:88:LEU:HD23	1:W:88:LEU:HA	1.92	0.41
2:1:196:ILE:HG23	2:1:201:LEU:HB2	2.02	0.41
1:K:159:GLU:OE1	1:M:63:SER:OG	2.37	0.41
2:B:38:ASP:HB2	2:B:63:LEU:HD13	2.02	0.41
2:V:92:TYR:CE2	2:X:93:MET:HB3	2.56	0.41
2:J:37:ILE:HG22	2:J:63:LEU:HD22	2.01	0.41
1:S:196:ALA:O	1:S:199:SER:OG	2.34	0.41
2:Z:37:ILE:HG22	2:Z:63:LEU:HD22	2.01	0.41
1:C:38:LEU:HB2	1:C:49:ILE:HB	2.02	0.41
1:A:172:VAL:HG13	1:A:196:ALA:HB1	2.01	0.41
1:E:162:ALA:HB1	1:E:176:LEU:HD13	2.02	0.41
1:K:162:ALA:HB1	1:K:176:LEU:HD13	2.02	0.41
1:O:172:VAL:HG13	1:O:196:ALA:HB1	2.01	0.41
2:L:153:ASP:OD1	2:L:153:ASP:N	2.54	0.41
2:T:14:MET:HE2	2:T:44:THR:HG23	2.03	0.41
2:B:157:ARG:HH21	2:B:199:LEU:HD22	1.84	0.41
2:H:102:GLY:HA2	2:H:109:HIS:O	2.20	0.41
1:Q:20:ARG:HH21	1:Q:22:PHE:HE1	1.67	0.41
2:X:102:GLY:HA2	2:X:109:HIS:O	2.20	0.41
2:X:196:ILE:HD13	2:X:203:LEU:HA	2.02	0.41
1:Y:172:VAL:HG13	1:Y:196:ALA:HB1	2.02	0.41
2:F:91:LYS:HA	2:F:91:LYS:HD2	1.80	0.41
1:I:138:PHE:HB2	1:I:149:PHE:HB2	2.03	0.41
2:J:163:LYS:NZ	2:J:203:LEU:O	2.41	0.41
2:J:190:ASP:OD1	2:J:190:ASP:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:178:ILE:HA	2:L:183:GLY:O	2.20	0.41
2:N:88:ASN:HD22	2:N:90:VAL:HG12	1.85	0.41
2:X:194:SER:O	2:X:198:LYS:HB2	2.21	0.41
2:P:83:LEU:HD21	2:P:99:LEU:HD13	2.03	0.41
1:U:78:THR:HG22	1:U:136:LEU:HG	2.00	0.41
2:F:179:THR:O	2:F:183:GLY:HA2	2.21	0.41
2:H:179:THR:O	2:H:183:GLY:HA2	2.21	0.41
1:M:51:ASP:HB2	1:M:197:LEU:HD11	2.03	0.41
1:Q:51:ASP:HB2	1:Q:197:LEU:HD11	2.03	0.41
1:S:67:ILE:HG13	1:S:77:VAL:HG12	2.02	0.41
2:Z:179:THR:O	2:Z:183:GLY:HA2	2.21	0.41
1:O:186:GLU:OE2	1:O:224:TYR:OH	2.33	0.41
2:F:37:ILE:HG22	2:F:63:LEU:HD22	2.01	0.41
2:H:84:SER:OG	2:H:117:GLY:O	2.32	0.41
1:K:196:ALA:O	1:K:199:SER:OG	2.34	0.41
1:E:68:GLN:HE21	1:E:89:VAL:HG21	1.86	0.41
1:E:152:ASP:OD1	1:E:152:ASP:N	2.54	0.41
1:Y:162:ALA:HB1	1:Y:176:LEU:HD13	2.03	0.41
1:C:225:ASP:OD1	1:C:225:ASP:N	2.54	0.41
1:M:46:VAL:HG13	1:M:146:PRO:HB3	2.02	0.41
1:Q:46:VAL:HG13	1:Q:146:PRO:HB3	2.02	0.41
1:S:152:ASP:O	1:S:155:GLY:N	2.39	0.41
2:T:153:ASP:OD1	2:T:153:ASP:N	2.54	0.41
1:W:68:GLN:HE21	1:W:89:VAL:HG21	1.85	0.41
1:Y:46:VAL:HG13	1:Y:146:PRO:HB3	2.02	0.41
1:C:172:VAL:HG13	1:C:196:ALA:HB1	2.02	0.41
2:D:54:VAL:HG21	2:F:88:ASN:HD22	1.85	0.41
1:E:172:VAL:HG13	1:E:196:ALA:HB1	2.02	0.41
2:F:196:ILE:HD13	2:F:203:LEU:HA	2.02	0.41
2:L:157:ARG:HH21	2:L:199:LEU:HD22	1.84	0.41
1:O:172:VAL:HG13	1:O:196:ALA:HB1	2.02	0.41
2:H:194:SER:O	2:H:198:LYS:HB2	2.21	0.41
1:I:186:GLU:OE2	1:I:224:TYR:OH	2.38	0.41
2:J:88:ASN:HD22	2:J:90:VAL:HG12	1.85	0.41
2:P:88:ASN:HD22	2:P:90:VAL:HG12	1.85	0.41
2:R:88:ASN:HD22	2:R:90:VAL:HG12	1.85	0.41
1:S:59:ILE:HG12	1:U:160:TYR:HE1	1.85	0.41
1:W:138:PHE:HB2	1:W:149:PHE:HB2	2.03	0.41
1:Y:186:GLU:OE2	1:Y:224:TYR:OH	2.38	0.41
2:Z:83:LEU:HD21	2:Z:99:LEU:HD13	2.01	0.41
1:C:152:ASP:O	1:C:155:GLY:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:83:LEU:HD21	2:H:99:LEU:HD13	2.02	0.41
1:U:225:ASP:OD1	1:U:225:ASP:N	2.50	0.41
2:X:83:LEU:HD21	2:X:99:LEU:HD13	2.02	0.41
2:P:18:ARG:NE	2:P:30:ASN:OD1	2.48	0.41
1:Q:147:ARG:HH21	1:Q:149:PHE:HZ	1.67	0.41
1:A:51:ASP:HB2	1:A:197:LEU:HD11	2.03	0.41
1:C:51:ASP:HB2	1:C:197:LEU:HD11	2.03	0.41
1:K:67:ILE:HG13	1:K:77:VAL:HG12	2.02	0.41
2:N:179:THR:O	2:N:183:GLY:HA2	2.21	0.41
1:O:51:ASP:HB2	1:O:197:LEU:HD11	2.03	0.41
1:Q:67:ILE:HG13	1:Q:77:VAL:HG12	2.02	0.41
2:R:179:THR:O	2:R:183:GLY:HA2	2.21	0.41
1:O:51:ASP:HB2	1:O:197:LEU:HD11	2.03	0.41
1:C:17:PRO:HA	1:E:26:TYR:CD1	2.55	0.41
1:G:160:TYR:HE1	1:I:59:ILE:HG12	1.85	0.41
2:H:167:SER:HB2	2:X:167:SER:HB2	2.02	0.41
1:M:69:LEU:HD23	1:M:75:ALA:HB2	2.01	0.41
1:Y:172:VAL:HG13	1:Y:196:ALA:HB1	2.01	0.41
1:O:172:VAL:HG13	1:O:196:ALA:HB1	2.01	0.41
1:E:46:VAL:HG13	1:E:146:PRO:HB3	2.02	0.41
2:H:43:MET:HA	2:H:100:LEU:O	2.21	0.41
1:U:46:VAL:HG13	1:U:146:PRO:HB3	2.02	0.41
1:O:225:ASP:OD1	1:O:225:ASP:N	2.54	0.41
2:B:114:ASP:O	2:B:117:GLY:N	2.47	0.41
1:M:20:ARG:HH21	1:M:22:PHE:HE1	1.67	0.41
2:V:14:MET:HE3	2:V:14:MET:HB2	1.92	0.41
2:Z:196:ILE:HD13	2:Z:203:LEU:HA	2.02	0.41
2:D:194:SER:O	2:D:198:LYS:HB2	2.21	0.41
1:G:138:PHE:HB2	1:G:149:PHE:HB2	2.03	0.41
1:G:208:LYS:HB2	1:G:208:LYS:HE2	1.73	0.41
2:V:190:ASP:OD1	2:V:190:ASP:N	2.51	0.41
2:1:88:ASN:HD22	2:1:90:VAL:HG12	1.85	0.41
2:1:194:SER:O	2:1:198:LYS:HB2	2.21	0.41
1:G:22:PHE:HD1	1:G:22:PHE:HA	1.78	0.41
1:Y:130:ARG:O	1:O:125:GLN:NE2	2.54	0.41
1:A:159:GLU:OE1	1:C:63:SER:OG	2.38	0.41
2:B:18:ARG:NE	2:B:30:ASN:OD1	2.48	0.41
1:I:159:GLU:OE1	1:K:63:SER:OG	2.37	0.41
1:M:147:ARG:HH21	1:M:149:PHE:HZ	1.67	0.41
1:O:147:ARG:HH21	1:O:149:PHE:HZ	1.67	0.41
1:Q:162:ALA:HB1	1:Q:176:LEU:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:89:GLN:H	2:V:89:GLN:HG3	1.60	0.41
1:C:186:GLU:OE2	1:C:224:TYR:OH	2.33	0.41
2:D:179:THR:O	2:D:183:GLY:HA2	2.21	0.41
1:E:51:ASP:HB2	1:E:197:LEU:HD11	2.03	0.41
2:F:38:ASP:HB2	2:F:63:LEU:HD13	2.02	0.41
2:J:190:ASP:HA	2:J:193:GLU:HG2	2.02	0.41
2:L:190:ASP:HA	2:L:193:GLU:HG2	2.02	0.41
1:M:67:ILE:HG13	1:M:77:VAL:HG12	2.02	0.41
2:R:84:SER:OG	2:R:117:GLY:O	2.34	0.41
2:T:190:ASP:HA	2:T:193:GLU:HG2	2.02	0.41
1:U:225:ASP:OD1	1:U:225:ASP:N	2.53	0.41
2:V:190:ASP:HA	2:V:193:GLU:HG2	2.02	0.41
1:Y:51:ASP:HB2	1:Y:197:LEU:HD11	2.03	0.41
2:Z:38:ASP:HB2	2:Z:63:LEU:HD13	2.02	0.41
2:B:167:SER:HB2	2:R:167:SER:HB2	2.02	0.41
1:Q:69:LEU:HD23	1:Q:75:ALA:HB2	2.01	0.41
1:Q:88:LEU:HD23	1:Q:88:LEU:HA	1.94	0.41
1:A:38:LEU:HB2	1:A:49:ILE:HB	2.02	0.41
1:C:68:GLN:HE21	1:C:89:VAL:HG21	1.86	0.41
2:F:20:VAL:HB	2:F:28:HIS:HB2	2.02	0.41
2:B:69:GLN:HB3	1:M:111:ASN:HD21	1.86	0.41
1:C:172:VAL:HG13	1:C:196:ALA:HB1	2.01	0.41
1:E:172:VAL:HG13	1:E:196:ALA:HB1	2.01	0.41
1:G:172:VAL:HG13	1:G:196:ALA:HB1	2.01	0.41
1:G:222:ARG:HG2	1:G:222:ARG:HH11	1.86	0.41
1:I:222:ARG:HG2	1:I:222:ARG:HH11	1.86	0.41
2:N:132:PRO:HB2	2:1:132:PRO:HB2	2.02	0.41
1:O:18:ASP:O	1:O:33:LYS:NZ	2.46	0.41
1:U:222:ARG:HG2	1:U:222:ARG:HH11	1.86	0.41
1:W:172:VAL:HG13	1:W:196:ALA:HB1	2.01	0.41
1:W:222:ARG:HG2	1:W:222:ARG:HH11	1.86	0.41
2:D:43:MET:HA	2:D:100:LEU:O	2.21	0.41
2:F:43:MET:HA	2:F:100:LEU:O	2.21	0.41
2:F:83:LEU:HD21	2:F:99:LEU:HD13	2.03	0.41
1:G:49:ILE:HA	1:G:211:GLU:O	2.21	0.41
2:H:153:ASP:OD1	2:H:153:ASP:N	2.54	0.41
2:H:202:ILE:H	2:H:202:ILE:HG13	1.73	0.41
1:I:49:ILE:HA	1:I:211:GLU:O	2.21	0.41
2:J:83:LEU:HD21	2:J:99:LEU:HD13	2.03	0.41
2:P:3:THR:HG1	2:P:127:THR:HG1	1.54	0.41
1:U:49:ILE:HA	1:U:211:GLU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:83:LEU:HD21	2:V:99:LEU:HD13	2.03	0.41
2:X:43:MET:HA	2:X:100:LEU:O	2.21	0.41
2:X:83:LEU:HD21	2:X:99:LEU:HD13	2.03	0.41
2:X:153:ASP:OD1	2:X:153:ASP:N	2.54	0.41
2:Z:83:LEU:HD21	2:Z:99:LEU:HD13	2.03	0.41
2:1:43:MET:HA	2:1:100:LEU:O	2.21	0.41
2:1:83:LEU:HD21	2:1:99:LEU:HD13	2.03	0.41
1:A:59:ILE:HG12	1:M:160:TYR:CE1	2.55	0.41
2:H:15:ALA:HA	2:H:174:ASP:O	2.20	0.41
2:L:15:ALA:HA	2:L:174:ASP:O	2.20	0.41
2:N:132:PRO:HB2	2:1:132:PRO:HB2	2.02	0.41
2:T:15:ALA:HA	2:T:174:ASP:O	2.20	0.41
2:X:15:ALA:HA	2:X:174:ASP:O	2.20	0.41
2:B:88:ASN:HD22	2:B:90:VAL:HG12	1.85	0.41
2:D:22:MET:HE2	2:D:22:MET:HB3	1.93	0.41
2:D:88:ASN:HD22	2:D:90:VAL:HG12	1.85	0.41
2:J:22:MET:HE2	2:J:22:MET:HB3	1.93	0.41
2:N:194:SER:O	2:N:198:LYS:HB2	2.21	0.41
2:R:194:SER:O	2:R:198:LYS:HB2	2.21	0.41
2:T:156:ILE:O	2:T:160:SER:OG	2.32	0.41
2:T:178:ILE:HA	2:T:183:GLY:O	2.20	0.41
2:V:88:ASN:HD22	2:V:90:VAL:HG12	1.85	0.41
1:I:88:LEU:HD23	1:I:88:LEU:HA	1.92	0.41
1:I:225:ASP:OD1	1:I:225:ASP:N	2.50	0.41
1:K:125:GLN:NE2	1:M:130:ARG:O	2.54	0.41
2:N:196:ILE:HG23	2:N:201:LEU:HB2	2.02	0.41
1:O:130:ARG:O	1:Q:125:GLN:NE2	2.54	0.41
2:P:196:ILE:HG23	2:P:201:LEU:HB2	2.02	0.41
1:Q:130:ARG:O	1:S:125:GLN:NE2	2.54	0.41
1:S:186:GLU:OE2	1:S:224:TYR:OH	2.33	0.41
1:A:147:ARG:HH21	1:A:149:PHE:HZ	1.67	0.41
1:G:22:PHE:HD1	1:G:22:PHE:HA	1.76	0.41
1:M:22:PHE:HD1	1:M:22:PHE:HA	1.76	0.41
1:M:162:ALA:HB1	1:M:176:LEU:HD13	2.01	0.41
1:S:88:LEU:HD23	1:S:88:LEU:HA	1.90	0.41
1:I:225:ASP:OD1	1:I:225:ASP:N	2.53	0.41
2:J:179:THR:O	2:J:183:GLY:HA2	2.21	0.41
1:K:51:ASP:HB2	1:K:197:LEU:HD11	2.03	0.41
1:Q:186:GLU:OE2	1:Q:224:TYR:OH	2.33	0.41
1:S:51:ASP:HB2	1:S:197:LEU:HD11	2.03	0.41
2:V:179:THR:O	2:V:183:GLY:HA2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:179:THR:O	2:X:183:GLY:HA2	2.21	0.41
1:M:22:PHE:HD1	1:M:22:PHE:HA	1.79	0.41
2:R:69:GLN:HB3	1:S:111:ASN:HD21	1.86	0.41
1:U:162:ALA:HB1	1:U:176:LEU:HD13	2.02	0.41
2:B:43:MET:HA	2:B:100:LEU:O	2.21	0.41
2:D:83:LEU:HD21	2:D:99:LEU:HD13	2.03	0.41
1:I:46:VAL:HG13	1:I:146:PRO:HB3	2.02	0.41
2:N:43:MET:HA	2:N:100:LEU:O	2.21	0.41
1:W:49:ILE:HA	1:W:211:GLU:O	2.21	0.41
2:Z:43:MET:HA	2:Z:100:LEU:O	2.21	0.41
2:1:14:MET:HE2	2:1:44:THR:HG23	2.03	0.41
2:B:37:ILE:HG22	2:B:63:LEU:HD22	2.03	0.41
1:C:49:ILE:HG12	1:C:212:ILE:HG12	2.03	0.41
2:B:25:PHE:CD1	2:R:133:PHE:HZ	2.39	0.41
2:H:3:THR:O	2:H:126:SER:HA	2.21	0.41
1:K:88:LEU:HD23	1:K:88:LEU:HA	1.93	0.41
1:K:138:PHE:HB2	1:K:149:PHE:HB2	2.03	0.41
2:L:194:SER:O	2:L:198:LYS:HB2	2.21	0.41
1:S:138:PHE:HB2	1:S:149:PHE:HB2	2.03	0.41
2:T:194:SER:O	2:T:198:LYS:HB2	2.21	0.41
2:X:83:LEU:HD21	2:X:99:LEU:HD13	2.01	0.41
1:O:125:GLN:NE2	1:O:130:ARG:O	2.54	0.41
2:R:196:ILE:HG23	2:R:201:LEU:HB2	2.02	0.41
2:L:89:GLN:H	2:L:89:GLN:HG3	1.60	0.41
1:C:108:ASN:HD22	1:C:109:ILE:N	2.19	0.40
2:D:38:ASP:HB2	2:D:63:LEU:HD13	2.02	0.40
1:M:186:GLU:OE2	1:M:224:TYR:OH	2.33	0.40
2:N:84:SER:OG	2:N:117:GLY:O	2.34	0.40
1:S:108:ASN:HD22	1:S:109:ILE:N	2.19	0.40
1:W:51:ASP:HB2	1:W:197:LEU:HD11	2.03	0.40
2:H:179:THR:HG22	2:H:181:LYS:H	1.86	0.40
1:A:76:ALA:HA	1:A:137:ILE:O	2.21	0.40
1:G:162:ALA:HB1	1:G:176:LEU:HD13	2.03	0.40
1:O:162:ALA:HB1	1:O:176:LEU:HD13	2.02	0.40
1:W:162:ALA:HB1	1:W:176:LEU:HD13	2.02	0.40
1:C:39:GLY:O	1:C:162:ALA:HA	2.20	0.40
2:J:3:THR:OG1	2:J:127:THR:OG1	2.26	0.40
1:K:46:VAL:HG13	1:K:146:PRO:HB3	2.02	0.40
2:L:83:LEU:HD21	2:L:99:LEU:HD13	2.03	0.40
1:M:39:GLY:O	1:M:162:ALA:HA	2.20	0.40
2:R:43:MET:HA	2:R:100:LEU:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:83:LEU:HD21	2:T:99:LEU:HD13	2.03	0.40
1:W:152:ASP:O	1:W:155:GLY:N	2.39	0.40
2:X:202:ILE:H	2:X:202:ILE:HG13	1.72	0.40
1:O:39:GLY:O	1:O:162:ALA:HA	2.20	0.40
1:A:49:ILE:HG12	1:A:212:ILE:HG12	2.03	0.40
2:J:3:THR:O	2:J:126:SER:HA	2.21	0.40
1:S:88:LEU:HD23	1:S:88:LEU:HA	1.93	0.40
2:V:3:THR:O	2:V:126:SER:HA	2.21	0.40
2:X:3:THR:O	2:X:126:SER:HA	2.21	0.40
1:E:138:PHE:HB2	1:E:149:PHE:HB2	2.03	0.40
2:F:83:LEU:HD21	2:F:99:LEU:HD13	2.01	0.40
2:F:194:SER:O	2:F:198:LYS:HB2	2.21	0.40
2:H:83:LEU:HD21	2:H:99:LEU:HD13	2.01	0.40
2:T:88:ASN:HD22	2:T:90:VAL:HG12	1.85	0.40
2:X:22:MET:HE2	2:X:22:MET:HB3	1.93	0.40
1:Y:138:PHE:HB2	1:Y:149:PHE:HB2	2.03	0.40
2:B:196:ILE:HG23	2:B:201:LEU:HB2	2.02	0.40
1:I:125:GLN:NE2	1:K:130:ARG:O	2.54	0.40
1:K:162:ALA:HB1	1:K:176:LEU:HD13	2.04	0.40
1:O:162:ALA:HB1	1:O:176:LEU:HD13	2.04	0.40
1:S:130:ARG:O	1:U:125:GLN:NE2	2.54	0.40
1:S:162:ALA:HB1	1:S:176:LEU:HD13	2.04	0.40
1:U:130:ARG:O	1:W:125:GLN:NE2	2.54	0.40
2:H:51:ASP:OD1	2:J:91:LYS:HD3	2.21	0.40
1:G:51:ASP:HB2	1:G:197:LEU:HD11	2.03	0.40
1:K:108:ASN:HD22	1:K:109:ILE:N	2.20	0.40
1:O:108:ASN:HD22	1:O:109:ILE:N	2.19	0.40
1:Y:186:GLU:OE2	1:Y:224:TYR:OH	2.33	0.40
1:O:225:ASP:OD1	1:O:225:ASP:N	2.53	0.40
2:1:38:ASP:HB2	2:1:63:LEU:HD13	2.02	0.40
2:1:179:THR:O	2:1:183:GLY:HA2	2.21	0.40
1:M:88:LEU:HD23	1:M:88:LEU:HA	1.94	0.40
2:V:105:ASP:OD1	2:V:105:ASP:N	2.54	0.40
2:X:179:THR:HG22	2:X:181:LYS:H	1.86	0.40
1:C:76:ALA:HA	1:C:137:ILE:O	2.21	0.40
1:A:162:ALA:HB1	1:A:176:LEU:HD13	2.02	0.40
1:I:162:ALA:HB1	1:I:176:LEU:HD13	2.02	0.40
1:U:88:LEU:HD23	1:U:88:LEU:HA	1.92	0.40
2:D:14:MET:HE2	2:D:44:THR:HG23	2.03	0.40
2:H:83:LEU:HD21	2:H:99:LEU:HD13	2.04	0.40
1:K:152:ASP:O	1:K:155:GLY:N	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:3:THR:OG1	2:L:127:THR:OG1	2.26	0.40
1:O:22:PHE:HD1	1:O:22:PHE:HA	1.80	0.40
2:P:43:MET:HA	2:P:100:LEU:O	2.21	0.40
1:Q:39:GLY:O	1:Q:162:ALA:HA	2.21	0.40
1:S:46:VAL:HG13	1:S:146:PRO:HB3	2.02	0.40
1:C:20:ARG:NH2	1:C:25:GLU:OE1	2.54	0.40
1:G:161:LYS:N	1:I:58:LEU:O	2.49	0.40
2:J:194:SER:O	2:J:198:LYS:HB2	2.21	0.40
1:U:129:VAL:HG12	1:W:126:TYR:HD1	1.86	0.40
1:A:22:PHE:HD1	1:A:22:PHE:HA	1.78	0.40
1:G:125:GLN:NE2	1:I:130:ARG:O	2.54	0.40
2:N:163:LYS:NZ	2:N:203:LEU:HD11	2.37	0.40
2:R:163:LYS:NZ	2:R:203:LEU:HD11	2.37	0.40
2:B:141:GLN:HE21	2:P:141:GLN:HE21	1.67	0.40
2:N:83:LEU:HD21	2:N:99:LEU:HD13	2.01	0.40
2:R:83:LEU:HD21	2:R:99:LEU:HD13	2.01	0.40
1:S:63:SER:OG	1:U:159:GLU:OE1	2.36	0.40
2:T:89:GLN:H	2:T:89:GLN:HG3	1.60	0.40
1:U:51:ASP:HB2	1:U:197:LEU:HD11	2.03	0.40
1:W:108:ASN:HD22	1:W:109:ILE:N	2.19	0.40
1:O:108:ASN:HD22	1:O:109:ILE:N	2.20	0.40
2:J:105:ASP:OD1	2:J:105:ASP:N	2.54	0.40
1:A:68:GLN:HE21	1:A:89:VAL:HG21	1.86	0.40
1:C:88:LEU:HD23	1:C:88:LEU:HA	1.91	0.40
1:C:111:ASN:HD21	2:F:69:GLN:HB3	1.87	0.40
1:C:186:GLU:OE2	1:C:224:TYR:OH	2.34	0.40
1:K:111:ASN:HD21	2:N:69:GLN:HB3	1.86	0.40
1:O:222:ARG:HG2	1:O:222:ARG:HH11	1.86	0.40
1:S:222:ARG:HG2	1:S:222:ARG:HH11	1.86	0.40
2:X:69:GLN:HB3	1:Y:111:ASN:HD21	1.86	0.40
1:A:49:ILE:HA	1:A:211:GLU:O	2.21	0.40
1:K:49:ILE:HA	1:K:211:GLU:O	2.21	0.40
1:O:49:ILE:HA	1:O:211:GLU:O	2.21	0.40
2:T:3:THR:OG1	2:T:127:THR:OG1	2.26	0.40
2:Z:14:MET:HE2	2:Z:44:THR:HG23	2.02	0.40
1:A:70:ILE:HG21	1:A:112:LEU:HD21	2.04	0.40
2:P:14:MET:HE3	2:P:14:MET:HB2	1.92	0.40
2:B:194:SER:O	2:B:198:LYS:HB2	2.21	0.40
2:V:163:LYS:NZ	2:V:203:LEU:O	2.41	0.40
2:Z:194:SER:O	2:Z:198:LYS:HB2	2.21	0.40
1:A:162:ALA:HB1	1:A:176:LEU:HD13	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:194:ILE:HD11	1:G:212:ILE:HD11	2.04	0.40
1:W:22:PHE:HD1	1:W:22:PHE:HA	1.78	0.40
1:W:194:ILE:HD11	1:W:212:ILE:HD11	2.04	0.40
1:C:159:GLU:OE1	1:E:63:SER:OG	2.37	0.40
1:U:76:ALA:HA	1:U:137:ILE:O	2.22	0.40
1:W:22:PHE:HD1	1:W:22:PHE:HA	1.76	0.40
2:Z:18:ARG:NE	2:Z:30:ASN:OD1	2.48	0.40
2:1:89:GLN:H	2:1:89:GLN:HG3	1.60	0.40
1:A:108:ASN:HD22	1:A:109:ILE:N	2.20	0.40
1:C:225:ASP:OD1	1:C:225:ASP:N	2.53	0.40
1:E:108:ASN:HD22	1:E:109:ILE:N	2.20	0.40
1:E:186:GLU:OE2	1:E:224:TYR:OH	2.33	0.40
1:G:108:ASN:HD22	1:G:109:ILE:N	2.19	0.40
1:I:51:ASP:HB2	1:I:197:LEU:HD11	2.03	0.40
1:M:108:ASN:HD22	1:M:109:ILE:N	2.19	0.40
2:B:77:GLU:HG2	2:B:111:PHE:HZ	1.87	0.40
1:C:88:LEU:HD23	1:C:88:LEU:HA	1.94	0.40
2:F:179:THR:HG22	2:F:181:LYS:H	1.86	0.40
2:H:77:GLU:HG2	2:H:111:PHE:HZ	1.87	0.40
1:Q:22:PHE:HD1	1:Q:22:PHE:HA	1.79	0.40
1:A:222:ARG:HG2	1:A:222:ARG:HH11	1.86	0.40
1:G:88:LEU:HD23	1:G:88:LEU:HA	1.92	0.40
2:J:14:MET:HE2	2:J:44:THR:HG23	2.03	0.40
2:N:83:LEU:HD21	2:N:99:LEU:HD13	2.03	0.40
2:N:167:SER:HB2	2:P:167:SER:HB2	2.03	0.40
1:S:49:ILE:HA	1:S:211:GLU:O	2.21	0.40
2:V:14:MET:HE2	2:V:44:THR:HG23	2.03	0.40
2:F:3:THR:O	2:F:126:SER:HA	2.21	0.40
2:H:132:PRO:HB2	2:V:132:PRO:HB2	2.04	0.40
2:J:132:PRO:HB2	2:X:132:PRO:HB2	2.04	0.40
2:N:190:ASP:O	2:N:194:SER:HB3	2.22	0.40
2:P:83:LEU:HD21	2:P:99:LEU:HD13	2.04	0.40
2:L:88:ASN:HD22	2:L:90:VAL:HG12	1.85	0.40
2:P:194:SER:O	2:P:198:LYS:HB2	2.21	0.40
2:H:163:LYS:NZ	2:H:203:LEU:HD11	2.37	0.40
1:I:76:ALA:HA	1:I:137:ILE:O	2.22	0.40
1:I:194:ILE:HD11	1:I:212:ILE:HD11	2.04	0.40
2:J:163:LYS:NZ	2:J:203:LEU:HD11	2.37	0.40
1:U:76:ALA:HA	1:U:137:ILE:O	2.22	0.40
1:W:76:ALA:HA	1:W:137:ILE:O	2.22	0.40
2:X:163:LYS:NZ	2:X:203:LEU:HD11	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:88:LEU:HD23	1:K:88:LEU:HA	1.90	0.40
2:B:179:THR:O	2:B:183:GLY:HA2	2.21	0.40
2:N:190:ASP:HA	2:N:193:GLU:HG2	2.02	0.40
2:P:179:THR:O	2:P:183:GLY:HA2	2.21	0.40
1:Q:108:ASN:HD22	1:Q:109:ILE:N	2.20	0.40
1:Q:172:VAL:HG13	1:Q:196:ALA:HB1	2.04	0.40
2:R:190:ASP:HA	2:R:193:GLU:HG2	2.02	0.40
2:V:70:ARG:NH2	1:W:99:GLU:OE2	2.55	0.40
1:Y:108:ASN:HD22	1:Y:109:ILE:N	2.20	0.40
2:P:77:GLU:HG2	2:P:111:PHE:HZ	1.87	0.40
2:X:77:GLU:HG2	2:X:111:PHE:HZ	1.87	0.40
1:E:76:ALA:HA	1:E:137:ILE:O	2.21	0.40
1:I:88:LEU:HD23	1:I:88:LEU:HA	1.92	0.40
1:K:222:ARG:HG2	1:K:222:ARG:HH11	1.86	0.40
1:M:162:ALA:HB1	1:M:176:LEU:HD13	2.02	0.40
1:O:160:TYR:CE1	1:O:59:ILE:HG12	2.57	0.40
1:W:88:LEU:HD23	1:W:88:LEU:HA	1.92	0.40
1:O:186:GLU:OE2	1:O:224:TYR:OH	2.34	0.40
2:D:132:PRO:HB2	2:R:132:PRO:HB2	2.03	0.40
1:E:49:ILE:HA	1:E:211:GLU:O	2.21	0.40
2:F:14:MET:HE2	2:F:44:THR:HG23	2.03	0.40
2:N:132:PRO:HB2	2:1:132:PRO:HB2	2.02	0.40
2:P:83:LEU:HD21	2:P:99:LEU:HD13	2.03	0.40
2:R:83:LEU:HD21	2:R:99:LEU:HD13	2.03	0.40
2:R:153:ASP:OD1	2:R:153:ASP:N	2.54	0.40
1:S:225:ASP:OD1	1:S:225:ASP:N	2.54	0.40
1:Y:49:ILE:HA	1:Y:211:GLU:O	2.21	0.40
1:O:152:ASP:O	1:O:155:GLY:N	2.39	0.40
2:1:153:ASP:OD1	2:1:153:ASP:N	2.54	0.40
2:B:83:LEU:HD21	2:B:99:LEU:HD13	2.04	0.40
2:D:83:LEU:HD21	2:D:99:LEU:HD13	2.04	0.40
2:L:83:LEU:HD21	2:L:99:LEU:HD13	2.04	0.40
2:T:83:LEU:HD21	2:T:99:LEU:HD13	2.04	0.40
2:Z:3:THR:O	2:Z:126:SER:HA	2.21	0.40
2:Z:15:ALA:HA	2:Z:174:ASP:O	2.20	0.40
1:A:161:LYS:N	1:C:58:LEU:O	2.47	0.40
2:H:22:MET:HE2	2:H:22:MET:HB3	1.93	0.40
2:V:194:SER:O	2:V:198:LYS:HB2	2.21	0.40
1:A:130:ARG:O	1:M:125:GLN:NE2	2.55	0.40
1:C:162:ALA:HB1	1:C:176:LEU:HD13	2.04	0.40
1:G:76:ALA:HA	1:G:137:ILE:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:76:ALA:HA	1:M:137:ILE:O	2.22	0.40
1:U:194:ILE:HD11	1:U:212:ILE:HD11	2.04	0.40
2:V:163:LYS:NZ	2:V:203:LEU:HD11	2.37	0.40
2:F:18:ARG:NE	2:F:30:ASN:OD1	2.48	0.40
1:G:76:ALA:HA	1:G:137:ILE:O	2.22	0.40
1:I:76:ALA:HA	1:I:137:ILE:O	2.22	0.40
1:Q:22:PHE:HD1	1:Q:22:PHE:HA	1.76	0.40
1:Y:88:LEU:HD23	1:Y:88:LEU:HA	1.90	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	1-0	219/224 (98%)	212 (97%)	7 (3%)	0	100	100
1	1-A	219/224 (98%)	212 (97%)	7 (3%)	0	100	100
1	1-C	219/224 (98%)	212 (97%)	7 (3%)	0	100	100
1	1-E	219/224 (98%)	212 (97%)	7 (3%)	0	100	100
1	1-G	219/224 (98%)	212 (97%)	7 (3%)	0	100	100
1	1-I	219/224 (98%)	212 (97%)	7 (3%)	0	100	100
1	1-K	219/224 (98%)	212 (97%)	7 (3%)	0	100	100
1	1-M	219/224 (98%)	212 (97%)	7 (3%)	0	100	100
1	1-O	219/224 (98%)	212 (97%)	7 (3%)	0	100	100
1	1-Q	219/224 (98%)	212 (97%)	7 (3%)	0	100	100
1	1-S	219/224 (98%)	212 (97%)	7 (3%)	0	100	100
1	1-U	219/224 (98%)	212 (97%)	7 (3%)	0	100	100
1	1-W	219/224 (98%)	212 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-Y	219/224 (98%)	212 (97%)	7 (3%)	0	100	100
1	4-O	219/224 (98%)	212 (97%)	7 (3%)	0	100	100
1	4-A	208/224 (93%)	202 (97%)	6 (3%)	0	100	100
1	4-C	219/224 (98%)	212 (97%)	7 (3%)	0	100	100
1	4-E	219/224 (98%)	212 (97%)	7 (3%)	0	100	100
1	4-G	219/224 (98%)	212 (97%)	7 (3%)	0	100	100
1	4-I	219/224 (98%)	212 (97%)	7 (3%)	0	100	100
1	4-K	219/224 (98%)	212 (97%)	7 (3%)	0	100	100
1	4-M	219/224 (98%)	212 (97%)	7 (3%)	0	100	100
1	4-O	196/224 (88%)	189 (96%)	7 (4%)	0	100	100
1	4-Q	219/224 (98%)	212 (97%)	7 (3%)	0	100	100
1	4-S	219/224 (98%)	212 (97%)	7 (3%)	0	100	100
1	4-U	219/224 (98%)	212 (97%)	7 (3%)	0	100	100
1	4-W	219/224 (98%)	212 (97%)	7 (3%)	0	100	100
1	4-Y	219/224 (98%)	212 (97%)	7 (3%)	0	100	100
1	5-O	219/224 (98%)	211 (96%)	8 (4%)	0	100	100
1	5-A	219/224 (98%)	211 (96%)	8 (4%)	0	100	100
1	5-C	219/224 (98%)	211 (96%)	8 (4%)	0	100	100
1	5-E	219/224 (98%)	211 (96%)	8 (4%)	0	100	100
1	5-G	219/224 (98%)	211 (96%)	8 (4%)	0	100	100
1	5-I	219/224 (98%)	211 (96%)	8 (4%)	0	100	100
1	5-K	219/224 (98%)	211 (96%)	8 (4%)	0	100	100
1	5-M	219/224 (98%)	211 (96%)	8 (4%)	0	100	100
1	5-O	219/224 (98%)	211 (96%)	8 (4%)	0	100	100
1	5-Q	219/224 (98%)	211 (96%)	8 (4%)	0	100	100
1	5-S	219/224 (98%)	211 (96%)	8 (4%)	0	100	100
1	5-U	219/224 (98%)	211 (96%)	8 (4%)	0	100	100
1	5-W	219/224 (98%)	211 (96%)	8 (4%)	0	100	100
1	5-Y	219/224 (98%)	211 (96%)	8 (4%)	0	100	100
1	7-O	219/224 (98%)	211 (96%)	8 (4%)	0	100	100
1	7-A	219/224 (98%)	211 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	7-C	219/224 (98%)	211 (96%)	8 (4%)	0	100	100
1	7-E	219/224 (98%)	211 (96%)	8 (4%)	0	100	100
1	7-G	219/224 (98%)	211 (96%)	8 (4%)	0	100	100
1	7-I	219/224 (98%)	211 (96%)	8 (4%)	0	100	100
1	7-K	219/224 (98%)	211 (96%)	8 (4%)	0	100	100
1	7-M	219/224 (98%)	211 (96%)	8 (4%)	0	100	100
1	7-O	219/224 (98%)	211 (96%)	8 (4%)	0	100	100
1	7-Q	219/224 (98%)	211 (96%)	8 (4%)	0	100	100
1	7-S	219/224 (98%)	211 (96%)	8 (4%)	0	100	100
1	7-U	219/224 (98%)	211 (96%)	8 (4%)	0	100	100
1	7-W	219/224 (98%)	211 (96%)	8 (4%)	0	100	100
1	7-Y	219/224 (98%)	211 (96%)	8 (4%)	0	100	100
1	8-0	219/224 (98%)	215 (98%)	4 (2%)	0	100	100
1	8-A	219/224 (98%)	215 (98%)	4 (2%)	0	100	100
1	8-C	219/224 (98%)	215 (98%)	4 (2%)	0	100	100
1	8-E	219/224 (98%)	215 (98%)	4 (2%)	0	100	100
1	8-G	219/224 (98%)	215 (98%)	4 (2%)	0	100	100
1	8-I	219/224 (98%)	215 (98%)	4 (2%)	0	100	100
1	8-K	219/224 (98%)	215 (98%)	4 (2%)	0	100	100
1	8-M	219/224 (98%)	215 (98%)	4 (2%)	0	100	100
1	8-O	219/224 (98%)	215 (98%)	4 (2%)	0	100	100
1	8-Q	219/224 (98%)	215 (98%)	4 (2%)	0	100	100
1	8-S	219/224 (98%)	215 (98%)	4 (2%)	0	100	100
1	8-U	219/224 (98%)	215 (98%)	4 (2%)	0	100	100
1	8-W	219/224 (98%)	215 (98%)	4 (2%)	0	100	100
1	8-Y	219/224 (98%)	215 (98%)	4 (2%)	0	100	100
1	9-0	219/224 (98%)	213 (97%)	6 (3%)	0	100	100
1	9-A	219/224 (98%)	213 (97%)	6 (3%)	0	100	100
1	9-C	219/224 (98%)	213 (97%)	6 (3%)	0	100	100
1	9-E	219/224 (98%)	213 (97%)	6 (3%)	0	100	100
1	9-G	219/224 (98%)	213 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	9-I	219/224 (98%)	213 (97%)	6 (3%)	0	100	100
1	9-K	219/224 (98%)	213 (97%)	6 (3%)	0	100	100
1	9-M	219/224 (98%)	213 (97%)	6 (3%)	0	100	100
1	9-O	219/224 (98%)	213 (97%)	6 (3%)	0	100	100
1	9-Q	219/224 (98%)	213 (97%)	6 (3%)	0	100	100
1	9-S	219/224 (98%)	213 (97%)	6 (3%)	0	100	100
1	9-U	219/224 (98%)	213 (97%)	6 (3%)	0	100	100
1	9-W	219/224 (98%)	213 (97%)	6 (3%)	0	100	100
1	9-Y	219/224 (98%)	213 (97%)	6 (3%)	0	100	100
1	10-0	219/224 (98%)	208 (95%)	9 (4%)	2 (1%)	14	43
1	10-A	219/224 (98%)	208 (95%)	9 (4%)	2 (1%)	14	43
1	10-C	219/224 (98%)	208 (95%)	9 (4%)	2 (1%)	14	43
1	10-E	219/224 (98%)	209 (95%)	8 (4%)	2 (1%)	14	43
1	10-G	219/224 (98%)	209 (95%)	8 (4%)	2 (1%)	14	43
1	10-I	219/224 (98%)	208 (95%)	9 (4%)	2 (1%)	14	43
1	10-K	219/224 (98%)	208 (95%)	9 (4%)	2 (1%)	14	43
1	10-M	219/224 (98%)	208 (95%)	9 (4%)	2 (1%)	14	43
1	10-O	219/224 (98%)	208 (95%)	9 (4%)	2 (1%)	14	43
1	10-Q	219/224 (98%)	209 (95%)	8 (4%)	2 (1%)	14	43
1	10-S	219/224 (98%)	208 (95%)	9 (4%)	2 (1%)	14	43
1	10-U	219/224 (98%)	208 (95%)	9 (4%)	2 (1%)	14	43
1	10-W	219/224 (98%)	208 (95%)	9 (4%)	2 (1%)	14	43
1	10-Y	219/224 (98%)	208 (95%)	9 (4%)	2 (1%)	14	43
2	1-1	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	1-B	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	1-D	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	1-F	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	1-H	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	1-J	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	1-L	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	1-N	201/203 (99%)	191 (95%)	10 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1-P	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	1-R	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	1-T	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	1-V	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	1-X	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	1-Z	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	4-1	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	4-B	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	4-D	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	4-F	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	4-H	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	4-J	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	4-L	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	4-N	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	4-P	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	4-R	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	4-T	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	4-V	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	4-X	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	4-Z	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	5-1	201/203 (99%)	193 (96%)	8 (4%)	0	100	100
2	5-B	201/203 (99%)	193 (96%)	8 (4%)	0	100	100
2	5-D	201/203 (99%)	193 (96%)	8 (4%)	0	100	100
2	5-F	201/203 (99%)	193 (96%)	8 (4%)	0	100	100
2	5-H	201/203 (99%)	193 (96%)	8 (4%)	0	100	100
2	5-J	201/203 (99%)	193 (96%)	8 (4%)	0	100	100
2	5-L	201/203 (99%)	193 (96%)	8 (4%)	0	100	100
2	5-N	201/203 (99%)	193 (96%)	8 (4%)	0	100	100
2	5-P	201/203 (99%)	193 (96%)	8 (4%)	0	100	100
2	5-R	201/203 (99%)	193 (96%)	8 (4%)	0	100	100
2	5-T	201/203 (99%)	193 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	5-V	201/203 (99%)	193 (96%)	8 (4%)	0	100	100
2	5-X	201/203 (99%)	193 (96%)	8 (4%)	0	100	100
2	5-Z	201/203 (99%)	193 (96%)	8 (4%)	0	100	100
2	7-1	201/203 (99%)	183 (91%)	18 (9%)	0	100	100
2	7-B	201/203 (99%)	183 (91%)	18 (9%)	0	100	100
2	7-D	201/203 (99%)	183 (91%)	18 (9%)	0	100	100
2	7-F	201/203 (99%)	183 (91%)	18 (9%)	0	100	100
2	7-H	201/203 (99%)	183 (91%)	18 (9%)	0	100	100
2	7-J	201/203 (99%)	183 (91%)	18 (9%)	0	100	100
2	7-L	201/203 (99%)	183 (91%)	18 (9%)	0	100	100
2	7-N	201/203 (99%)	183 (91%)	18 (9%)	0	100	100
2	7-P	201/203 (99%)	183 (91%)	18 (9%)	0	100	100
2	7-R	201/203 (99%)	183 (91%)	18 (9%)	0	100	100
2	7-T	201/203 (99%)	183 (91%)	18 (9%)	0	100	100
2	7-V	201/203 (99%)	183 (91%)	18 (9%)	0	100	100
2	7-X	201/203 (99%)	183 (91%)	18 (9%)	0	100	100
2	7-Z	201/203 (99%)	183 (91%)	18 (9%)	0	100	100
2	8-1	201/203 (99%)	193 (96%)	8 (4%)	0	100	100
2	8-B	201/203 (99%)	192 (96%)	9 (4%)	0	100	100
2	8-D	201/203 (99%)	192 (96%)	9 (4%)	0	100	100
2	8-F	201/203 (99%)	192 (96%)	9 (4%)	0	100	100
2	8-H	201/203 (99%)	192 (96%)	9 (4%)	0	100	100
2	8-J	201/203 (99%)	192 (96%)	9 (4%)	0	100	100
2	8-L	201/203 (99%)	192 (96%)	9 (4%)	0	100	100
2	8-N	201/203 (99%)	192 (96%)	9 (4%)	0	100	100
2	8-P	201/203 (99%)	193 (96%)	8 (4%)	0	100	100
2	8-R	201/203 (99%)	193 (96%)	8 (4%)	0	100	100
2	8-T	201/203 (99%)	192 (96%)	9 (4%)	0	100	100
2	8-V	201/203 (99%)	193 (96%)	8 (4%)	0	100	100
2	8-X	201/203 (99%)	192 (96%)	9 (4%)	0	100	100
2	8-Z	201/203 (99%)	192 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	9-1	201/203 (99%)	191 (95%)	9 (4%)	1 (0%)	24	55
2	9-B	201/203 (99%)	191 (95%)	9 (4%)	1 (0%)	24	55
2	9-D	201/203 (99%)	191 (95%)	9 (4%)	1 (0%)	24	55
2	9-F	201/203 (99%)	191 (95%)	9 (4%)	1 (0%)	24	55
2	9-H	201/203 (99%)	191 (95%)	9 (4%)	1 (0%)	24	55
2	9-J	201/203 (99%)	191 (95%)	9 (4%)	1 (0%)	24	55
2	9-L	201/203 (99%)	191 (95%)	9 (4%)	1 (0%)	24	55
2	9-N	201/203 (99%)	191 (95%)	9 (4%)	1 (0%)	24	55
2	9-P	201/203 (99%)	191 (95%)	9 (4%)	1 (0%)	24	55
2	9-R	201/203 (99%)	191 (95%)	9 (4%)	1 (0%)	24	55
2	9-T	201/203 (99%)	191 (95%)	9 (4%)	1 (0%)	24	55
2	9-V	201/203 (99%)	191 (95%)	9 (4%)	1 (0%)	24	55
2	9-X	201/203 (99%)	191 (95%)	9 (4%)	1 (0%)	24	55
2	9-Z	201/203 (99%)	191 (95%)	9 (4%)	1 (0%)	24	55
2	10-1	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	10-B	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	10-D	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	10-F	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	10-H	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	10-J	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	10-L	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	10-N	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	10-P	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	10-R	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	10-T	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	10-V	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	10-X	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	10-Z	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
All	All	41126/41846 (98%)	39370 (96%)	1714 (4%)	42 (0%)	49	75

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	10-A	47	LEU
1	10-A	48	LEU
1	10-C	47	LEU
1	10-C	48	LEU
1	10-E	47	LEU
1	10-E	48	LEU
1	10-G	47	LEU
1	10-G	48	LEU
1	10-I	47	LEU
1	10-I	48	LEU
1	10-K	47	LEU
1	10-K	48	LEU
1	10-M	47	LEU
1	10-M	48	LEU
1	10-O	47	LEU
1	10-O	48	LEU
1	10-Q	47	LEU
1	10-Q	48	LEU
1	10-S	47	LEU
1	10-S	48	LEU
1	10-U	47	LEU
1	10-U	48	LEU
1	10-W	47	LEU
1	10-W	48	LEU
1	10-Y	47	LEU
1	10-Y	48	LEU
1	10-0	47	LEU
1	10-0	48	LEU
2	9-B	91	LYS
2	9-D	91	LYS
2	9-F	91	LYS
2	9-H	91	LYS
2	9-J	91	LYS
2	9-L	91	LYS
2	9-N	91	LYS
2	9-P	91	LYS
2	9-R	91	LYS
2	9-T	91	LYS
2	9-V	91	LYS
2	9-X	91	LYS
2	9-Z	91	LYS
2	9-1	91	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-0	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	1-A	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	1-C	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	1-E	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	1-G	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	1-I	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	1-K	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	1-M	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	1-O	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	1-Q	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	1-S	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	1-U	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	1-W	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	1-Y	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	4-0	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	4-A	176/186 (95%)	175 (99%)	1 (1%)	78	81
1	4-C	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	4-E	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	4-G	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	4-I	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	4-K	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	4-M	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	4-O	165/186 (89%)	164 (99%)	1 (1%)	78	81
1	4-Q	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	4-S	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	4-U	184/186 (99%)	183 (100%)	1 (0%)	81	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	4-W	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	4-Y	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	5-0	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	5-A	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	5-C	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	5-E	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	5-G	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	5-I	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	5-K	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	5-M	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	5-O	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	5-Q	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	5-S	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	5-U	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	5-W	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	5-Y	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	7-0	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	7-A	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	7-C	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	7-E	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	7-G	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	7-I	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	7-K	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	7-M	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	7-O	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	7-Q	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	7-S	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	7-U	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	7-W	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	7-Y	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	8-0	184/186 (99%)	183 (100%)	1 (0%)	81	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	8-A	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	8-C	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	8-E	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	8-G	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	8-I	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	8-K	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	8-M	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	8-O	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	8-Q	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	8-S	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	8-U	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	8-W	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	8-Y	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	9-0	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	9-A	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	9-C	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	9-E	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	9-G	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	9-I	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	9-K	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	9-M	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	9-O	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	9-Q	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	9-S	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	9-U	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	9-W	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	9-Y	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	10-0	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	10-A	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	10-C	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	10-E	184/186 (99%)	183 (100%)	1 (0%)	81	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	10-G	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	10-I	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	10-K	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	10-M	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	10-O	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	10-Q	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	10-S	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	10-U	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	10-W	184/186 (99%)	183 (100%)	1 (0%)	81	83
1	10-Y	184/186 (99%)	183 (100%)	1 (0%)	81	83
2	1-1	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	1-B	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	1-D	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	1-F	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	1-H	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	1-J	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	1-L	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	1-N	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	1-P	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	1-R	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	1-T	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	1-V	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	1-X	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	1-Z	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	4-1	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	4-B	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	4-D	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	4-F	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	4-H	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	4-J	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	4-L	170/170 (100%)	169 (99%)	1 (1%)	78	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	4-N	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	4-P	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	4-R	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	4-T	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	4-V	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	4-X	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	4-Z	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	5-1	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	5-B	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	5-D	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	5-F	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	5-H	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	5-J	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	5-L	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	5-N	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	5-P	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	5-R	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	5-T	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	5-V	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	5-X	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	5-Z	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	7-1	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	7-B	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	7-D	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	7-F	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	7-H	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	7-J	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	7-L	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	7-N	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	7-P	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	7-R	170/170 (100%)	169 (99%)	1 (1%)	78	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	7-T	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	7-V	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	7-X	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	7-Z	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	8-1	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	8-B	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	8-D	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	8-F	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	8-H	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	8-J	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	8-L	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	8-N	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	8-P	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	8-R	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	8-T	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	8-V	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	8-X	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	8-Z	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	9-1	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	9-B	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	9-D	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	9-F	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	9-H	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	9-J	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	9-L	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	9-N	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	9-P	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	9-R	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	9-T	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	9-V	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	9-X	170/170 (100%)	169 (99%)	1 (1%)	78	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	9-Z	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	10-1	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	10-B	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	10-D	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	10-F	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	10-H	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	10-J	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	10-L	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	10-N	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	10-P	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	10-R	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	10-T	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	10-V	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	10-X	170/170 (100%)	169 (99%)	1 (1%)	78	81
2	10-Z	170/170 (100%)	169 (99%)	1 (1%)	78	81
All	All	34665/34888 (99%)	34469 (99%)	196 (1%)	76	81

All (196) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	211	GLU
2	1-B	24	ASN
1	1-C	211	GLU
2	1-D	24	ASN
1	1-E	211	GLU
2	1-F	24	ASN
1	1-G	211	GLU
2	1-H	24	ASN
1	1-I	211	GLU
2	1-J	24	ASN
1	1-K	211	GLU
2	1-L	24	ASN
1	1-M	211	GLU
2	1-N	24	ASN
1	1-O	211	GLU
2	1-P	24	ASN
1	1-Q	211	GLU

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Mol	Chain	Res	Type
2	1-R	24	ASN
1	1-S	211	GLU
2	1-T	24	ASN
1	1-U	211	GLU
2	1-V	24	ASN
1	1-W	211	GLU
2	1-X	24	ASN
1	1-Y	211	GLU
2	1-Z	24	ASN
1	1-0	211	GLU
2	1-1	24	ASN
1	4-A	211	GLU
2	4-B	24	ASN
1	4-C	211	GLU
2	4-D	24	ASN
1	4-E	211	GLU
2	4-F	24	ASN
1	4-G	211	GLU
2	4-H	24	ASN
1	4-I	211	GLU
2	4-J	24	ASN
1	4-K	211	GLU
2	4-L	24	ASN
1	4-M	211	GLU
2	4-N	24	ASN
1	4-O	211	GLU
2	4-P	24	ASN
1	4-Q	211	GLU
2	4-R	24	ASN
1	4-S	211	GLU
2	4-T	24	ASN
1	4-U	211	GLU
2	4-V	24	ASN
1	4-W	211	GLU
2	4-X	24	ASN
1	4-Y	211	GLU
2	4-Z	24	ASN
1	4-0	211	GLU
2	4-1	24	ASN
1	5-A	211	GLU
2	5-B	24	ASN
1	5-C	211	GLU

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Mol	Chain	Res	Type
2	5-D	24	ASN
1	5-E	211	GLU
2	5-F	24	ASN
1	5-G	211	GLU
2	5-H	24	ASN
1	5-I	211	GLU
2	5-J	24	ASN
1	5-K	211	GLU
2	5-L	24	ASN
1	5-M	211	GLU
2	5-N	24	ASN
1	5-O	211	GLU
2	5-P	24	ASN
1	5-Q	211	GLU
2	5-R	24	ASN
1	5-S	211	GLU
2	5-T	24	ASN
1	5-U	211	GLU
2	5-V	24	ASN
1	5-W	211	GLU
2	5-X	24	ASN
1	5-Y	211	GLU
2	5-Z	24	ASN
1	5-0	211	GLU
2	5-1	24	ASN
1	7-A	211	GLU
2	7-B	24	ASN
1	7-C	211	GLU
2	7-D	24	ASN
1	7-E	211	GLU
2	7-F	24	ASN
1	7-G	211	GLU
2	7-H	24	ASN
1	7-I	211	GLU
2	7-J	24	ASN
1	7-K	211	GLU
2	7-L	24	ASN
1	7-M	211	GLU
2	7-N	24	ASN
1	7-O	211	GLU
2	7-P	24	ASN
1	7-Q	211	GLU

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Mol	Chain	Res	Type
2	7-R	24	ASN
1	7-S	211	GLU
2	7-T	24	ASN
1	7-U	211	GLU
2	7-V	24	ASN
1	7-W	211	GLU
2	7-X	24	ASN
1	7-Y	211	GLU
2	7-Z	24	ASN
1	7-0	211	GLU
2	7-1	24	ASN
1	8-A	211	GLU
2	8-B	24	ASN
1	8-C	211	GLU
2	8-D	24	ASN
1	8-E	211	GLU
2	8-F	24	ASN
1	8-G	211	GLU
2	8-H	24	ASN
1	8-I	211	GLU
2	8-J	24	ASN
1	8-K	211	GLU
2	8-L	24	ASN
1	8-M	211	GLU
2	8-N	24	ASN
1	8-O	211	GLU
2	8-P	24	ASN
1	8-Q	211	GLU
2	8-R	24	ASN
1	8-S	211	GLU
2	8-T	24	ASN
1	8-U	211	GLU
2	8-V	24	ASN
1	8-W	211	GLU
2	8-X	24	ASN
1	8-Y	211	GLU
2	8-Z	24	ASN
1	8-0	211	GLU
2	8-1	24	ASN
1	9-A	211	GLU
2	9-B	24	ASN
1	9-C	211	GLU

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Mol	Chain	Res	Type
2	9-D	24	ASN
1	9-E	211	GLU
2	9-F	24	ASN
1	9-G	211	GLU
2	9-H	24	ASN
1	9-I	211	GLU
2	9-J	24	ASN
1	9-K	211	GLU
2	9-L	24	ASN
1	9-M	211	GLU
2	9-N	24	ASN
1	9-O	211	GLU
2	9-P	24	ASN
1	9-Q	211	GLU
2	9-R	24	ASN
1	9-S	211	GLU
2	9-T	24	ASN
1	9-U	211	GLU
2	9-V	24	ASN
1	9-W	211	GLU
2	9-X	24	ASN
1	9-Y	211	GLU
2	9-Z	24	ASN
1	9-0	211	GLU
2	9-1	24	ASN
1	10-A	211	GLU
2	10-B	24	ASN
1	10-C	211	GLU
2	10-D	24	ASN
1	10-E	211	GLU
2	10-F	24	ASN
1	10-G	211	GLU
2	10-H	24	ASN
1	10-I	211	GLU
2	10-J	24	ASN
1	10-K	211	GLU
2	10-L	24	ASN
1	10-M	211	GLU
2	10-N	24	ASN
1	10-O	211	GLU
2	10-P	24	ASN
1	10-Q	211	GLU

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Mol	Chain	Res	Type
2	10-R	24	ASN
1	10-S	211	GLU
2	10-T	24	ASN
1	10-U	211	GLU
2	10-V	24	ASN
1	10-W	211	GLU
2	10-X	24	ASN
1	10-Y	211	GLU
2	10-Z	24	ASN
1	10-0	211	GLU
2	10-1	24	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (305) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	97	GLN
1	1-A	108	ASN
2	1-B	24	ASN
2	1-B	28	HIS
1	1-C	97	GLN
1	1-C	108	ASN
2	1-D	24	ASN
1	1-E	97	GLN
1	1-E	108	ASN
1	1-E	111	ASN
1	1-E	119	GLN
2	1-F	24	ASN
2	1-F	28	HIS
1	1-G	97	GLN
1	1-G	108	ASN
2	1-H	24	ASN
1	1-I	97	GLN
1	1-I	108	ASN
2	1-J	24	ASN
2	1-J	28	HIS
2	1-J	141	GLN
1	1-K	97	GLN
1	1-K	108	ASN
2	1-L	24	ASN
2	1-L	28	HIS
1	1-M	97	GLN
1	1-M	108	ASN

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Mol	Chain	Res	Type
2	1-N	24	ASN
2	1-N	28	HIS
2	1-N	141	GLN
1	1-O	97	GLN
1	1-O	108	ASN
1	1-O	119	GLN
2	1-P	24	ASN
2	1-P	28	HIS
2	1-P	141	GLN
1	1-Q	97	GLN
1	1-Q	108	ASN
1	1-Q	119	GLN
2	1-R	24	ASN
2	1-R	28	HIS
2	1-R	141	GLN
1	1-S	97	GLN
1	1-S	108	ASN
2	1-T	24	ASN
2	1-T	28	HIS
2	1-T	141	GLN
1	1-U	97	GLN
1	1-U	108	ASN
2	1-V	28	HIS
1	1-W	97	GLN
1	1-W	108	ASN
1	1-W	111	ASN
2	1-X	24	ASN
1	1-Y	97	GLN
1	1-Y	108	ASN
2	1-Z	24	ASN
1	1-0	97	GLN
1	1-0	108	ASN
1	1-0	111	ASN
1	1-0	119	GLN
2	1-1	24	ASN
1	4-A	97	GLN
1	4-A	111	ASN
2	4-B	73	ASN
2	4-B	98	GLN
2	4-B	141	GLN
1	4-C	97	GLN
1	4-C	111	ASN

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Mol	Chain	Res	Type
2	4-D	73	ASN
2	4-D	98	GLN
2	4-D	141	GLN
1	4-E	97	GLN
1	4-E	111	ASN
2	4-F	73	ASN
2	4-F	98	GLN
1	4-G	97	GLN
1	4-G	111	ASN
2	4-H	98	GLN
1	4-I	97	GLN
1	4-I	111	ASN
2	4-J	28	HIS
2	4-J	73	ASN
2	4-J	98	GLN
1	4-K	97	GLN
1	4-K	111	ASN
2	4-L	98	GLN
2	4-L	141	GLN
1	4-M	97	GLN
1	4-M	111	ASN
2	4-N	28	HIS
2	4-N	73	ASN
2	4-N	98	GLN
1	4-O	97	GLN
1	4-O	111	ASN
2	4-P	73	ASN
2	4-P	98	GLN
1	4-Q	97	GLN
1	4-Q	111	ASN
2	4-R	28	HIS
2	4-R	73	ASN
2	4-R	98	GLN
1	4-S	97	GLN
1	4-S	111	ASN
2	4-T	28	HIS
2	4-T	73	ASN
2	4-T	98	GLN
2	4-T	141	GLN
1	4-U	97	GLN
1	4-U	111	ASN
2	4-V	28	HIS

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Mol	Chain	Res	Type
2	4-V	73	ASN
2	4-V	98	GLN
2	4-V	141	GLN
1	4-W	97	GLN
1	4-W	111	ASN
2	4-X	73	ASN
2	4-X	98	GLN
2	4-X	141	GLN
1	4-Y	97	GLN
1	4-Y	111	ASN
2	4-Z	73	ASN
2	4-Z	88	ASN
2	4-Z	98	GLN
1	4-0	97	GLN
1	4-0	111	ASN
2	4-1	28	HIS
2	4-1	73	ASN
2	4-1	98	GLN
2	4-1	141	GLN
1	5-A	68	GLN
1	5-A	97	GLN
2	5-B	28	HIS
2	5-B	141	GLN
1	5-C	68	GLN
1	5-C	97	GLN
2	5-D	28	HIS
1	5-E	68	GLN
1	5-E	97	GLN
1	5-E	111	ASN
2	5-F	28	HIS
2	5-F	141	GLN
1	5-G	68	GLN
2	5-H	141	GLN
1	5-I	68	GLN
1	5-I	111	ASN
2	5-J	28	HIS
2	5-J	141	GLN
1	5-K	68	GLN
2	5-L	28	HIS
1	5-M	68	GLN
1	5-M	97	GLN
1	5-M	111	ASN

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Mol	Chain	Res	Type
2	5-N	141	GLN
1	5-O	68	GLN
1	5-O	97	GLN
2	5-P	28	HIS
1	5-Q	68	GLN
1	5-Q	97	GLN
1	5-Q	111	ASN
2	5-R	28	HIS
2	5-R	141	GLN
1	5-S	68	GLN
2	5-T	28	HIS
1	5-U	68	GLN
2	5-V	28	HIS
1	5-W	68	GLN
1	5-W	97	GLN
1	5-W	111	ASN
2	5-X	28	HIS
1	5-Y	68	GLN
1	5-Y	111	ASN
2	5-Z	28	HIS
2	5-Z	141	GLN
1	5-0	68	GLN
1	5-0	97	GLN
1	5-0	111	ASN
2	5-1	28	HIS
2	7-B	28	HIS
2	7-B	191	GLN
1	7-C	111	ASN
2	7-D	88	ASN
2	7-D	191	GLN
1	7-E	111	ASN
2	7-F	191	GLN
1	7-G	111	ASN
2	7-H	141	GLN
2	7-H	191	GLN
1	7-I	111	ASN
2	7-J	28	HIS
2	7-J	191	GLN
1	7-K	111	ASN
2	7-L	191	GLN
1	7-M	111	ASN
2	7-N	141	GLN

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Mol	Chain	Res	Type
2	7-N	191	GLN
1	7-O	111	ASN
2	7-P	141	GLN
2	7-P	191	GLN
1	7-Q	111	ASN
2	7-R	88	ASN
2	7-R	191	GLN
2	7-T	28	HIS
2	7-T	141	GLN
2	7-T	191	GLN
1	7-U	111	ASN
2	7-V	28	HIS
2	7-V	191	GLN
1	7-W	111	ASN
2	7-X	141	GLN
2	7-X	191	GLN
1	7-Y	111	ASN
2	7-Z	141	GLN
2	7-Z	191	GLN
1	7-0	111	ASN
2	7-1	191	GLN
2	8-B	85	ASN
2	8-B	88	ASN
2	8-D	85	ASN
2	8-D	88	ASN
2	8-D	141	GLN
2	8-F	85	ASN
2	8-F	88	ASN
2	8-F	141	GLN
2	8-H	85	ASN
2	8-H	88	ASN
2	8-H	141	GLN
2	8-J	85	ASN
2	8-J	88	ASN
2	8-L	85	ASN
2	8-L	88	ASN
2	8-L	141	GLN
2	8-N	85	ASN
2	8-N	88	ASN
2	8-P	85	ASN
2	8-P	88	ASN
2	8-P	141	GLN

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Mol	Chain	Res	Type
2	8-R	85	ASN
2	8-R	88	ASN
2	8-T	85	ASN
2	8-T	88	ASN
1	8-U	111	ASN
2	8-V	85	ASN
2	8-V	88	ASN
2	8-X	85	ASN
2	8-X	88	ASN
2	8-X	141	GLN
2	8-Z	85	ASN
2	8-Z	88	ASN
2	8-1	85	ASN
2	8-1	88	ASN
2	8-1	141	GLN
1	9-A	111	ASN
1	9-C	111	ASN
2	9-D	141	GLN
1	9-E	111	ASN
2	9-F	141	GLN
1	9-G	111	ASN
1	9-I	111	ASN
2	9-J	141	GLN
1	9-K	111	ASN
1	9-M	111	ASN
1	9-O	111	ASN
2	9-P	141	GLN
1	9-S	111	ASN
1	9-U	111	ASN
2	9-V	141	GLN
1	9-W	97	GLN
1	9-W	111	ASN
1	9-Y	111	ASN
2	9-Z	141	GLN
1	9-0	111	ASN
2	9-1	141	GLN
2	10-B	28	HIS
2	10-B	88	ASN
2	10-D	28	HIS
2	10-D	88	ASN
2	10-F	28	HIS
2	10-F	73	ASN

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Mol	Chain	Res	Type
2	10-F	88	ASN
2	10-H	28	HIS
2	10-H	88	ASN
2	10-H	141	GLN
2	10-J	28	HIS
2	10-J	88	ASN
2	10-L	28	HIS
2	10-L	88	ASN
2	10-N	28	HIS
2	10-N	88	ASN
2	10-P	28	HIS
2	10-P	88	ASN
2	10-R	28	HIS
2	10-R	88	ASN
2	10-R	141	GLN
2	10-T	28	HIS
2	10-T	88	ASN
2	10-V	88	ASN
1	10-W	97	GLN
2	10-X	28	HIS
2	10-X	88	ASN
2	10-Z	28	HIS
2	10-Z	73	ASN
2	10-Z	88	ASN
2	10-1	28	HIS
2	10-1	88	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

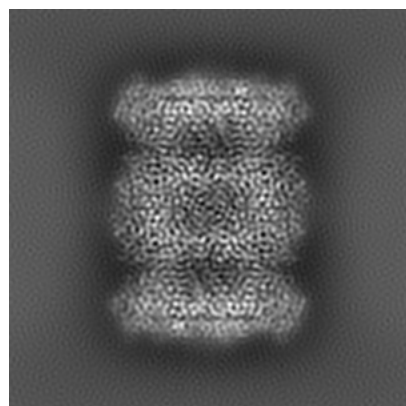
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8742. These allow visual inspection of the internal detail of the map and identification of artifacts.

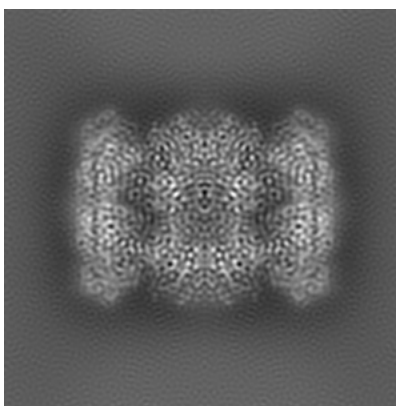
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

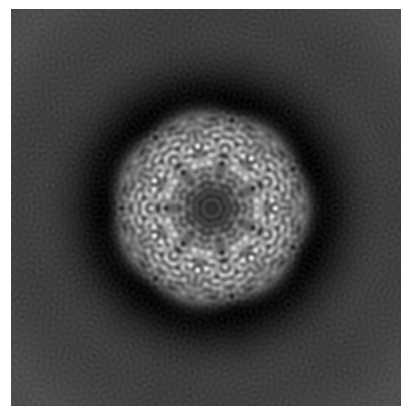
6.1.1 Primary map



X

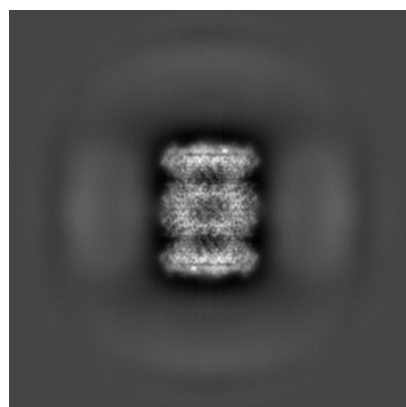


Y

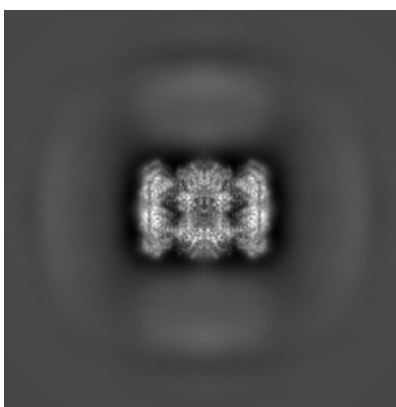


Z

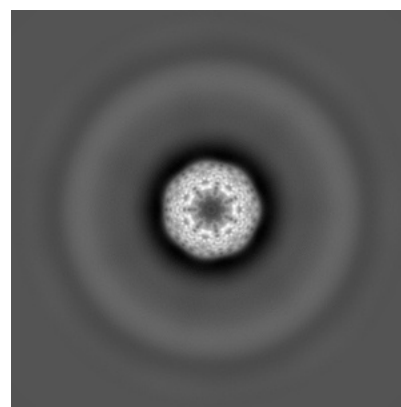
6.1.2 Raw map



X



Y

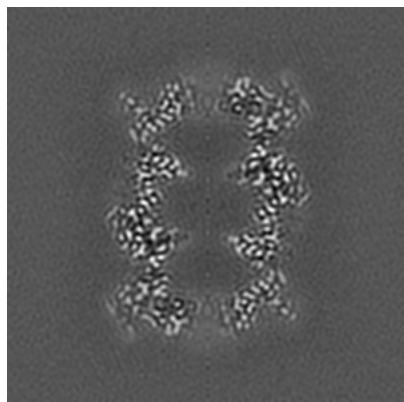


Z

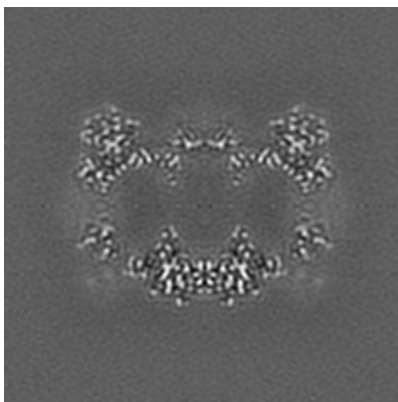
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

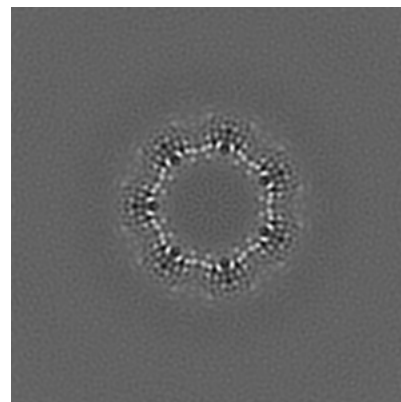
6.2.1 Primary map



X Index: 128

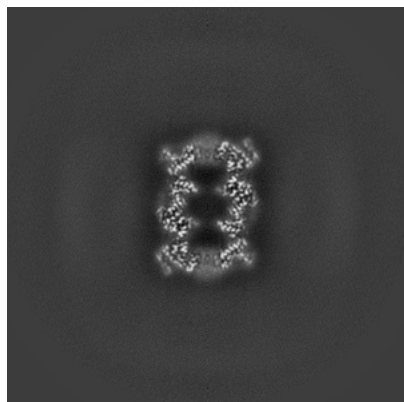


Y Index: 128

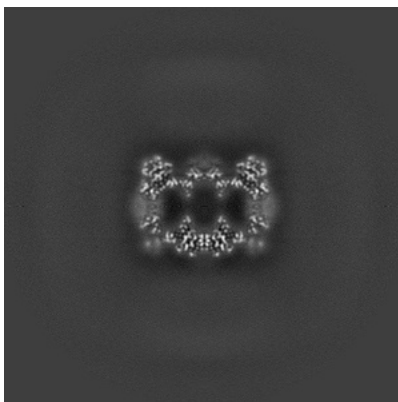


Z Index: 128

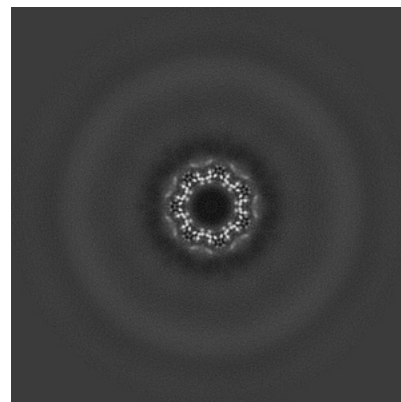
6.2.2 Raw map



X Index: 256



Y Index: 256

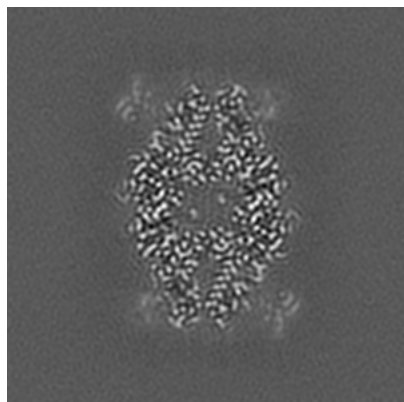


Z Index: 256

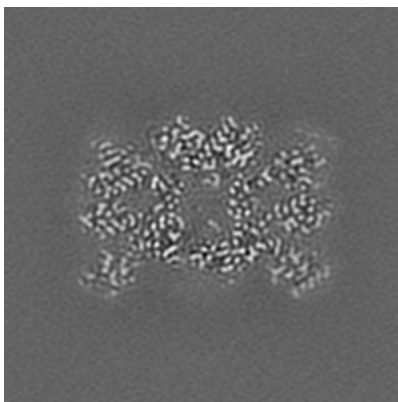
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

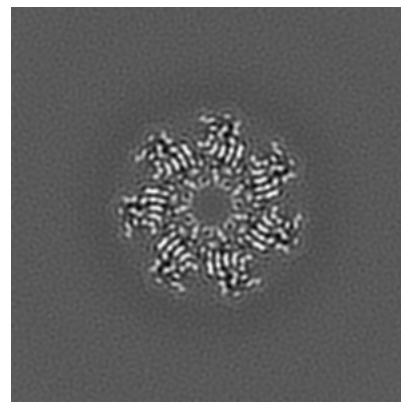
6.3.1 Primary map



X Index: 100

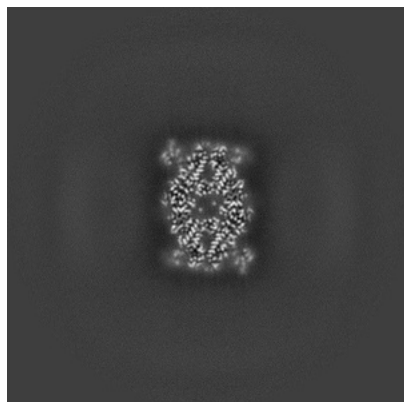


Y Index: 155

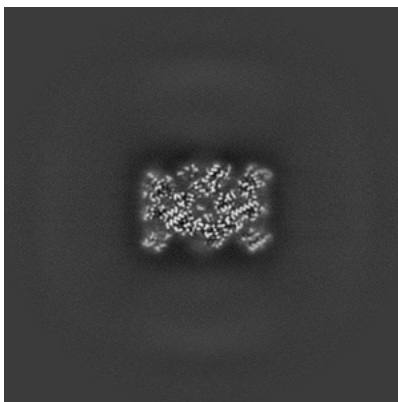


Z Index: 148

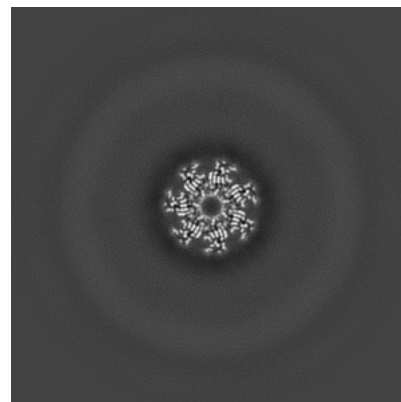
6.3.2 Raw map



X Index: 229



Y Index: 286

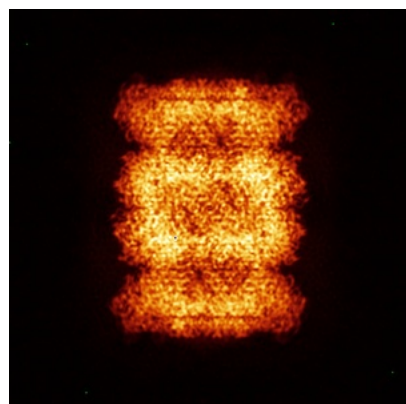


Z Index: 236

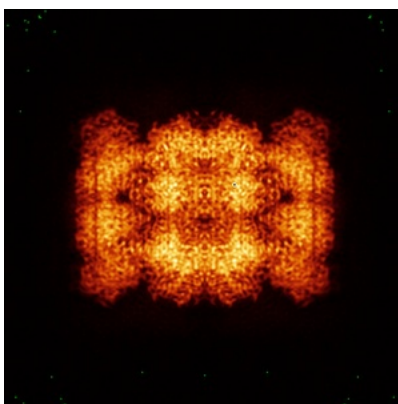
The images above show the largest variance slices of the map in three orthogonal directions.

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

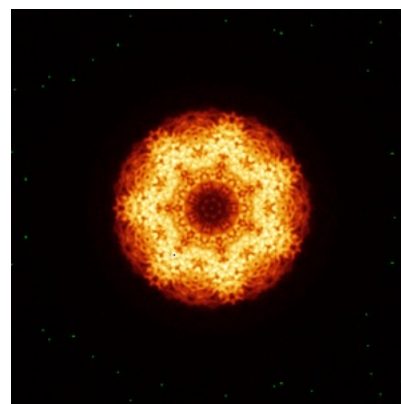
6.4.1 Primary map



X

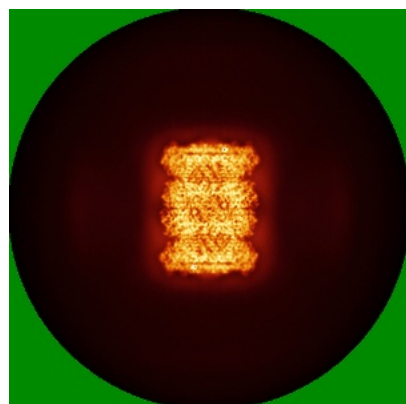


Y

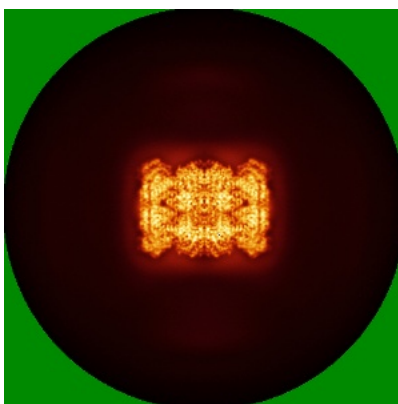


Z

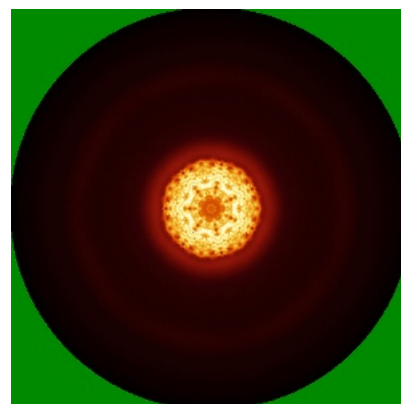
6.4.2 Raw map



X



Y

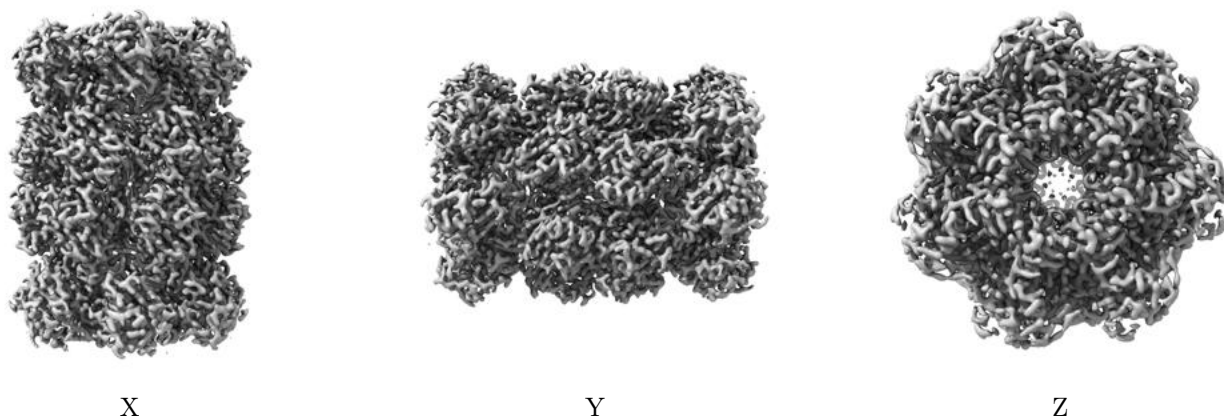


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

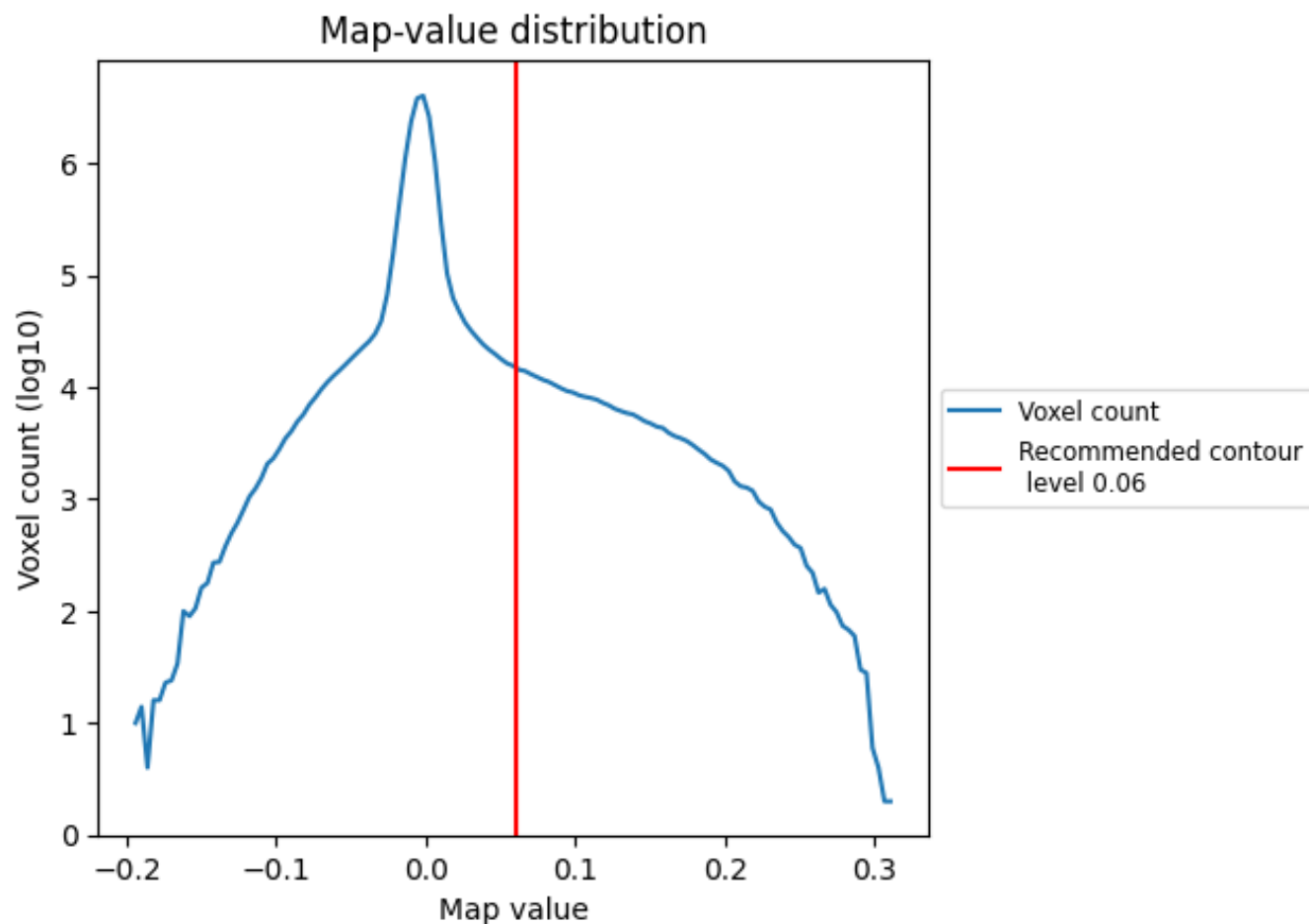
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

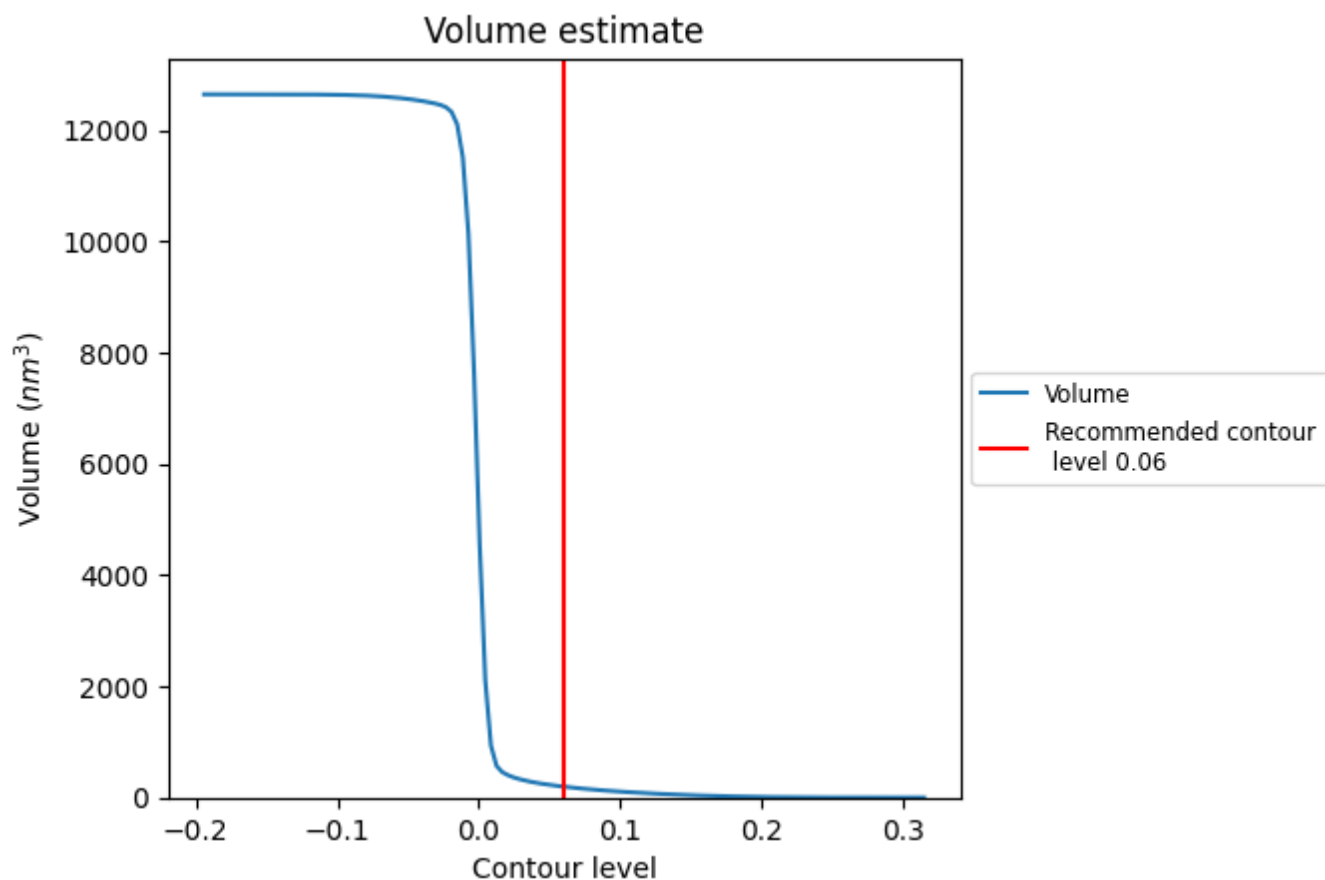
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

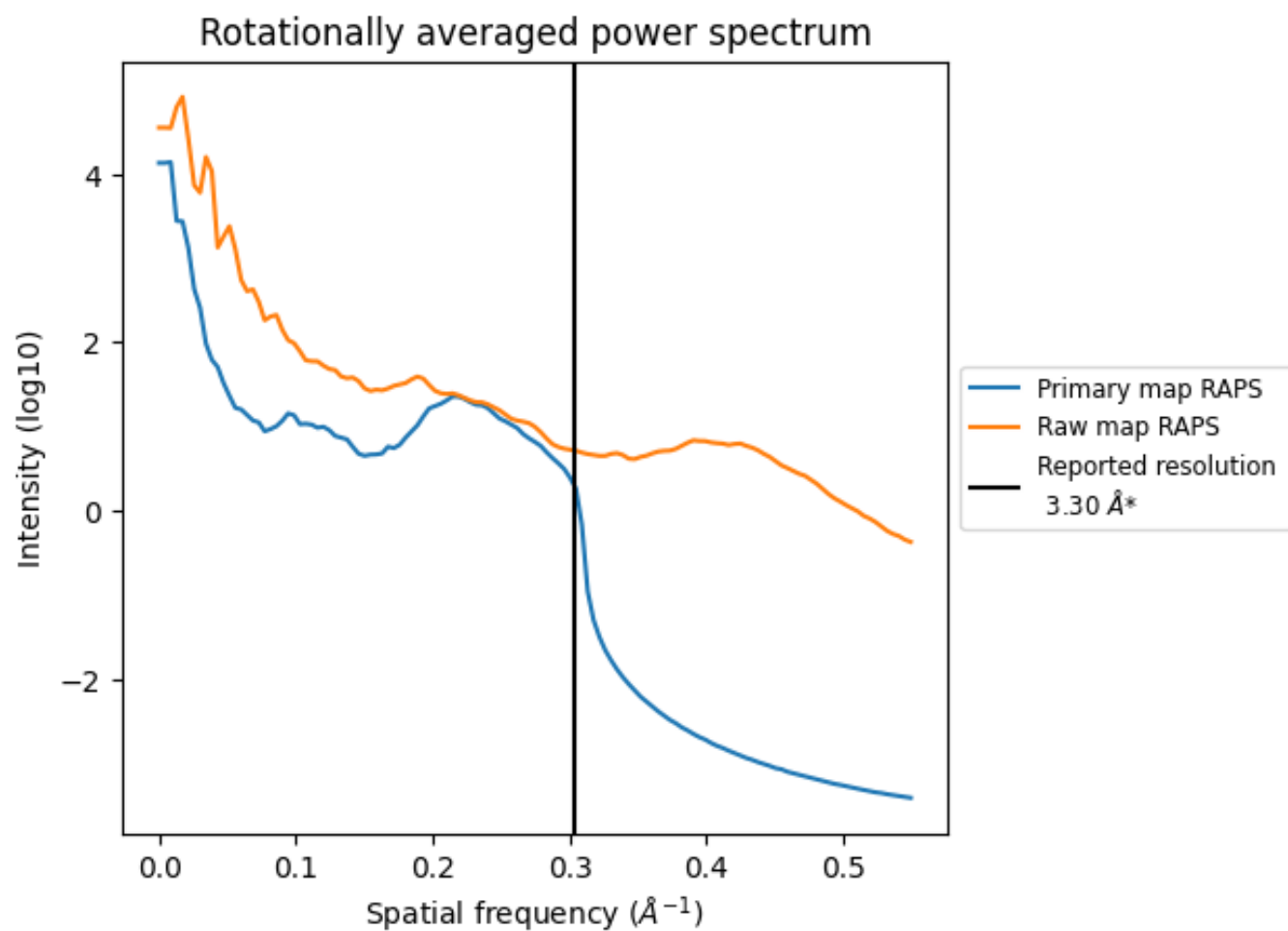
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 197 nm^3 ; this corresponds to an approximate mass of 178 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

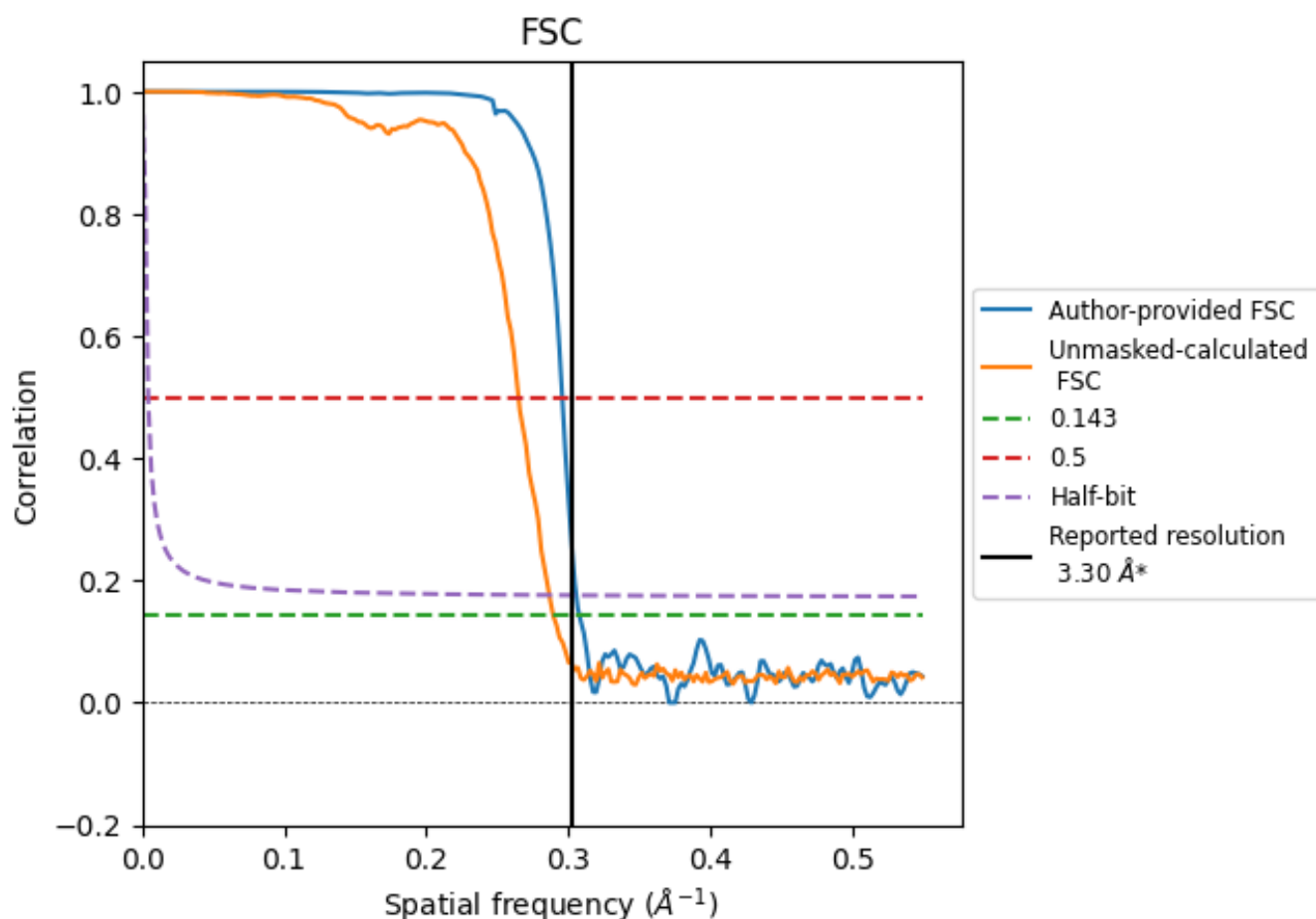


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

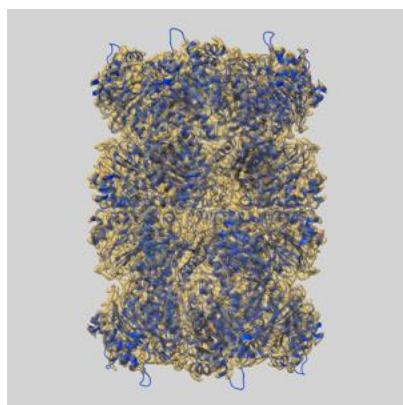
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.25	3.38	3.27
Unmasked-calculated*	3.45	3.77	3.49

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

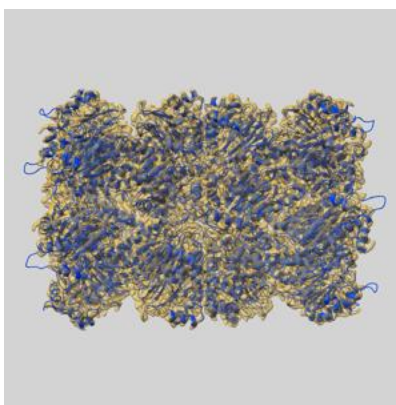
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8742 and PDB model 5VY4. Per-residue inclusion information can be found in section [3](#) on page [29](#).

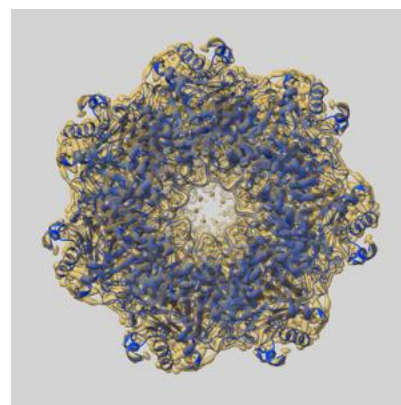
9.1 Map-model overlay [i](#)



X



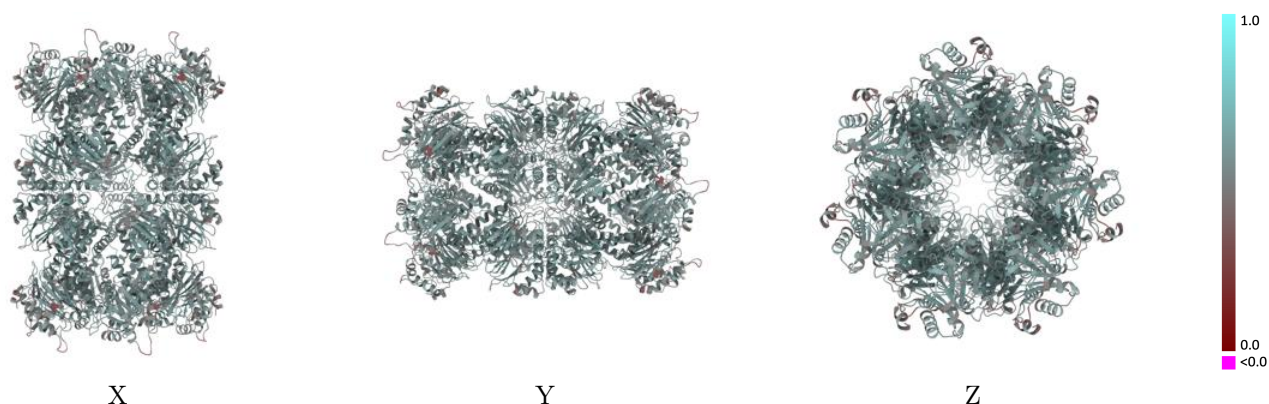
Y



Z

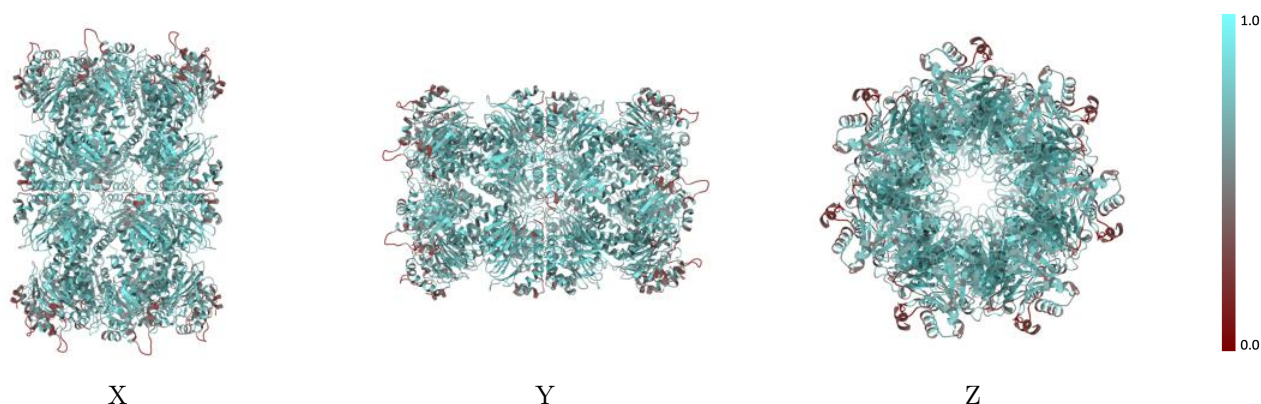
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



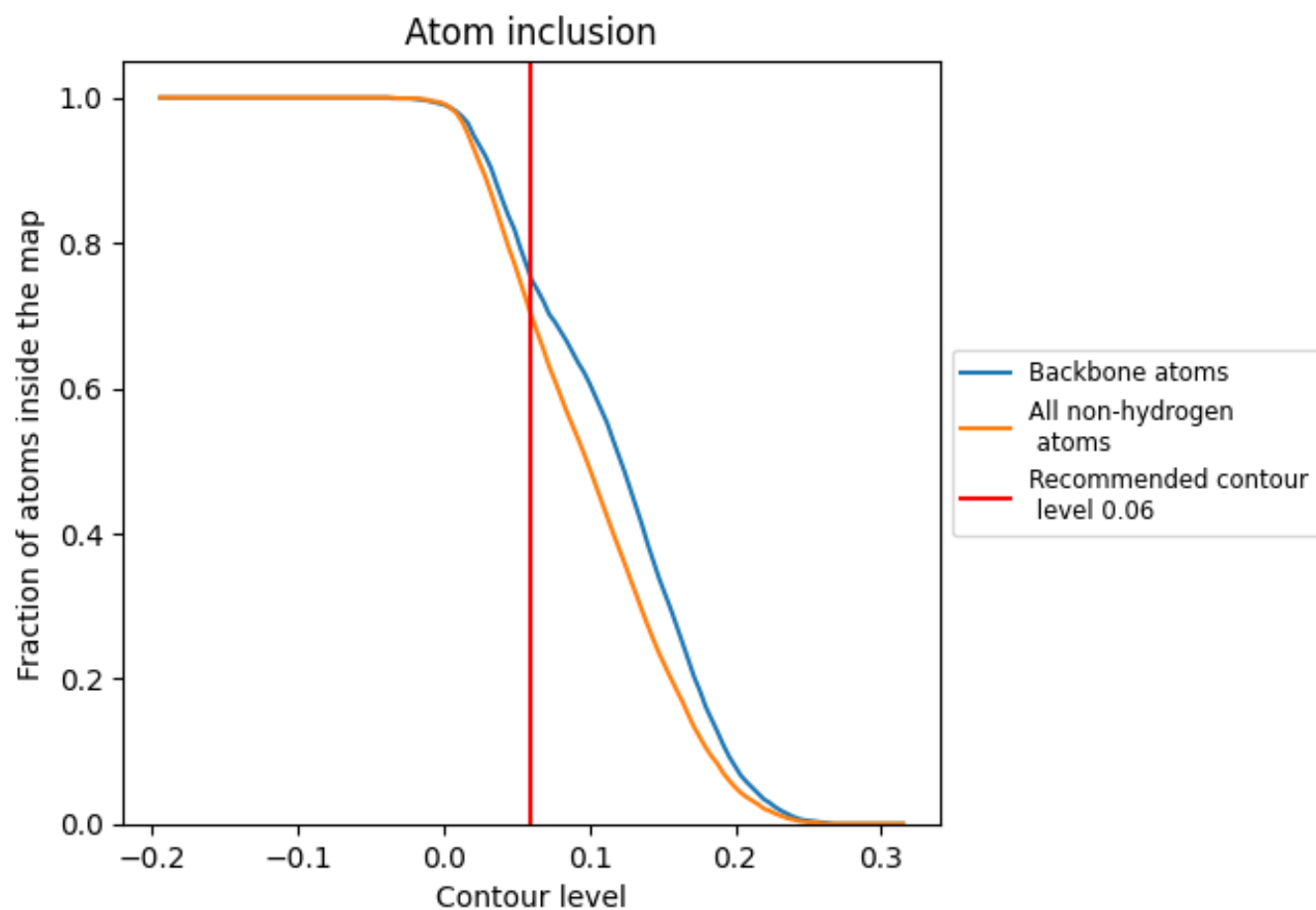
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

9.4 Atom inclusion ⓘ



At the recommended contour level, 75% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7000	 0.5510
0	 0.6470	 0.5410
1	 0.7620	 0.5680
A	 0.6440	 0.5390
B	 0.7590	 0.5670
C	 0.6470	 0.5400
D	 0.7580	 0.5650
E	 0.6460	 0.5380
F	 0.7580	 0.5640
G	 0.6510	 0.5360
H	 0.7560	 0.5640
I	 0.6430	 0.5390
J	 0.7630	 0.5660
K	 0.6430	 0.5380
L	 0.7640	 0.5680
M	 0.6460	 0.5400
N	 0.7630	 0.5650
O	 0.6460	 0.5380
P	 0.7580	 0.5660
Q	 0.6460	 0.5400
R	 0.7620	 0.5660
S	 0.6440	 0.5370
T	 0.7600	 0.5670
U	 0.6440	 0.5370
V	 0.7600	 0.5620
W	 0.6510	 0.5370
X	 0.7600	 0.5660
Y	 0.6460	 0.5400
Z	 0.7510	 0.5640

