Full wwPDB EM Validation Report ⓘ

Mar 3, 2024 – 03:42 PM EST

PDB ID	:	5VY4
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:

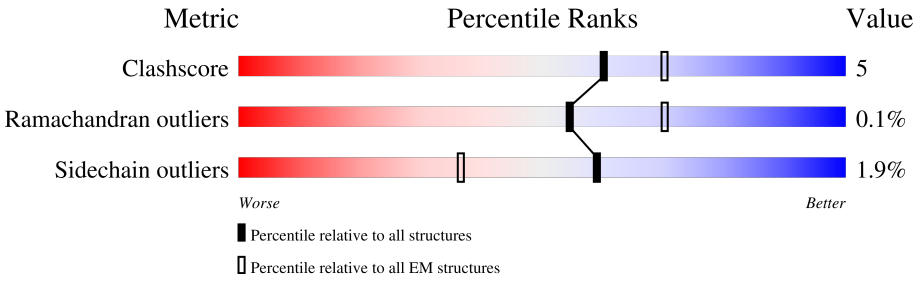
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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 <=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	15% 84% 14% ·
1	1-A	224	15% 86% 12% ·
1	1-C	224	16% 84% 14% ·
1	1-E	224	15% 85% 13% ·
1	1-G	224	15% 86% 12% ·
1	1-I	224	16% 86% 13% ·
1	1-K	224	15% 84% 14% ·
1	1-M	224	15% 84% 14% ·

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Mol	Chain	Length	Quality of chain
1	1-O	224	15% 86% 12%
1	1-Q	224	15% 84% 14%
1	1-S	224	15% 84% 14%
1	1-U	224	16% 86% 13%
1	1-W	224	15% 86% 12%
1	1-Y	224	15% 85% 13%
1	10-0	224	86% 12%
1	10-A	224	84% 13%
1	10-C	224	85% 13%
1	10-E	224	84% 13%
1	10-G	224	83% 14%
1	10-I	224	83% 15%
1	10-K	224	83% 14%
1	10-M	224	83% 14%
1	10-O	224	85% 13%
1	10-Q	224	84% 14%
1	10-S	224	83% 14%
1	10-U	224	83% 15%
1	10-W	224	84% 14%
1	10-Y	224	84% 13%
1	2-0	224	83% 16%
1	2-A	224	83% 15%
1	2-C	224	83% 16%
1	2-E	224	83% 16%
1	2-G	224	83% 16%

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Mol	Chain	Length	Quality of chain
1	2-I	224	83% 16%
1	2-K	224	83% 16%
1	2-M	224	83% 16%
1	2-O	224	82% 17%
1	2-Q	224	82% 17%
1	2-S	224	83% 16%
1	2-U	224	83% 16%
1	2-W	224	83% 15%
1	2-Y	224	83% 16%
1	3-0	224	83% 16%
1	3-A	224	83% 15%
1	3-C	224	83% 15%
1	3-E	224	83% 15%
1	3-G	224	83% 16%
1	3-I	224	82% 16%
1	3-K	224	83% 16%
1	3-M	224	84% 14%
1	3-O	224	83% 16%
1	3-Q	224	83% 15%
1	3-S	224	83% 16%
1	3-U	224	83% 16%
1	3-W	224	83% 16%
1	3-Y	224	83% 16%
1	4-0	224	84% 14%
1	4-A	224	86% 12%

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Mol	Chain	Length	Quality of chain
1	4-C	224	84% 14%
1	4-E	224	85% 13%
1	4-G	224	85% 13%
1	4-I	224	83% 15%
1	4-K	224	84% 13%
1	4-M	224	84% 13%
1	4-O	224	84% 14%
1	4-Q	224	85% 12%
1	4-S	224	85% 13%
1	4-U	224	84% 14%
1	4-W	224	85% 13%
1	4-Y	224	85% 12%
1	5-0	224	83% 15%
1	5-A	224	85% 13%
1	5-C	224	84% 14%
1	5-E	224	84% 14%
1	5-G	224	85% 13%
1	5-I	224	84% 14%
1	5-K	224	83% 15%
1	5-M	224	84% 14%
1	5-O	224	84% 14%
1	5-Q	224	84% 14%
1	5-S	224	83% 15%
1	5-U	224	84% 14%
1	5-W	224	83% 15%

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Mol	Chain	Length	Quality of chain
1	5-Y	224	84% 14%
1	6-0	224	82% 16%
1	6-A	224	82% 17%
1	6-C	224	82% 17%
1	6-E	224	81% 17%
1	6-G	224	81% 17%
1	6-I	224	82% 16%
1	6-K	224	82% 17%
1	6-M	224	81% 17%
1	6-O	224	82% 17%
1	6-Q	224	80% 18%
1	6-S	224	81% 17%
1	6-U	224	81% 17%
1	6-W	224	82% 17%
1	6-Y	224	82% 17%
1	7-0	224	84% 14%
1	7-A	224	84% 14%
1	7-C	224	85% 13%
1	7-E	224	85% 13%
1	7-G	224	85% 13%
1	7-I	224	85% 13%
1	7-K	224	85% 13%
1	7-M	224	84% 14%
1	7-O	224	84% 14%
1	7-Q	224	85% 13%

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Mol	Chain	Length	Quality of chain
1	7-S	224	85% 13%
1	7-U	224	85% 13%
1	7-W	224	85% 13%
1	7-Y	224	85% 13%
1	8-0	224	87% 11%
1	8-A	224	87% 11%
1	8-C	224	87% 11%
1	8-E	224	86% 12%
1	8-G	224	86% 12%
1	8-I	224	84% 13%
1	8-K	224	86% 12%
1	8-M	224	87% 11%
1	8-O	224	87% 11%
1	8-Q	224	87% 11%
1	8-S	224	86% 12%
1	8-U	224	84% 13%
1	8-W	224	86% 12%
1	8-Y	224	86% 12%
1	9-0	224	85% 13%
1	9-A	224	85% 12%
1	9-C	224	86% 12%
1	9-E	224	87% 12%
1	9-G	224	83% 15%
1	9-I	224	83% 16%
1	9-K	224	85% 13%

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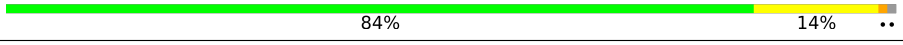
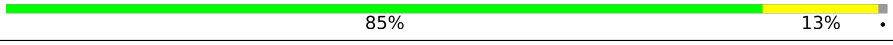
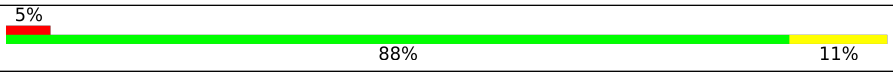
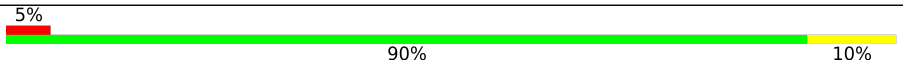
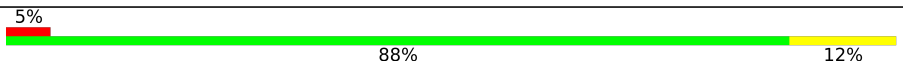
Mol	Chain	Length	Quality of chain
1	9-M	224	
1	9-O	224	
1	9-Q	224	
1	9-S	224	
1	9-U	224	
1	9-W	224	
1	9-Y	224	
2	1-1	203	
2	1-B	203	
2	1-D	203	
2	1-F	203	
2	1-H	203	
2	1-J	203	
2	1-L	203	
2	1-N	203	
2	1-P	203	
2	1-R	203	
2	1-T	203	
2	1-V	203	
2	1-X	203	
2	1-Z	203	
2	10-1	203	
2	10-B	203	
2	10-D	203	
2	10-F	203	

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Mol	Chain	Length	Quality of chain
2	10-H	203	85% 13%
2	10-J	203	87% 10%
2	10-L	203	86% 12%
2	10-N	203	86% 11%
2	10-P	203	85% 13%
2	10-R	203	86% 11%
2	10-T	203	86% 11%
2	10-V	203	84% 14%
2	10-X	203	86% 11%
2	10-Z	203	84% 13%
2	2-1	203	86% 14%
2	2-B	203	85% 15%
2	2-D	203	87% 13%
2	2-F	203	84% 16%
2	2-H	203	84% 16%
2	2-J	203	86% 14%
2	2-L	203	86% 14%
2	2-N	203	86% 14%
2	2-P	203	85% 15%
2	2-R	203	86% 14%
2	2-T	203	87% 13%
2	2-V	203	86% 14%
2	2-X	203	84% 16%
2	2-Z	203	84% 16%
2	3-1	203	88% 12%

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Mol	Chain	Length	Quality of chain
2	3-B	203	88% 12%
2	3-D	203	89% 11%
2	3-F	203	88% 12%
2	3-H	203	88% 12%
2	3-J	203	88% 12%
2	3-L	203	88% 12%
2	3-N	203	88% 12%
2	3-P	203	88% 12%
2	3-R	203	88% 12%
2	3-T	203	88% 12%
2	3-V	203	88% 12%
2	3-X	203	88% 12%
2	3-Z	203	88% 12%
2	4-1	203	88% 11%
2	4-B	203	88% 11%
2	4-D	203	89% 10%
2	4-F	203	89% 10%
2	4-H	203	89% 11%
2	4-J	203	89% 11%
2	4-L	203	88% 11%
2	4-N	203	88% 12%
2	4-P	203	89% 11%
2	4-R	203	88% 11%
2	4-T	203	89% 11%
2	4-V	203	89% 11%

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Mol	Chain	Length	Quality of chain
2	4-X	203	89% 10%
2	4-Z	203	90% 10%
2	5-1	203	84% 15%
2	5-B	203	85% 14%
2	5-D	203	84% 15%
2	5-F	203	84% 15%
2	5-H	203	84% 15%
2	5-J	203	85% 14%
2	5-L	203	85% 14%
2	5-N	203	84% 15%
2	5-P	203	84% 15%
2	5-R	203	84% 15%
2	5-T	203	85% 14%
2	5-V	203	85% 14%
2	5-X	203	84% 15%
2	5-Z	203	84% 15%
2	6-1	203	85% 14%
2	6-B	203	86% 13%
2	6-D	203	84% 15%
2	6-F	203	84% 15%
2	6-H	203	85% 14%
2	6-J	203	86% 13%
2	6-L	203	85% 14%
2	6-N	203	86% 13%
2	6-P	203	86% 13%

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Mol	Chain	Length	Quality of chain
2	6-R	203	86% 13%
2	6-T	203	87% 12%
2	6-V	203	86% 13%
2	6-X	203	86% 13%
2	6-Z	203	85% 14%
2	7-1	203	82% 18%
2	7-B	203	80% 20%
2	7-D	203	81% 19%
2	7-F	203	82% 17%
2	7-H	203	81% 19%
2	7-J	203	81% 19%
2	7-L	203	81% 18%
2	7-N	203	81% 19%
2	7-P	203	81% 19%
2	7-R	203	82% 18%
2	7-T	203	81% 19%
2	7-V	203	81% 19%
2	7-X	203	81% 19%
2	7-Z	203	81% 19%
2	8-1	203	80% 17%
2	8-B	203	80% 18%
2	8-D	203	80% 18%
2	8-F	203	80% 17%
2	8-H	203	80% 17%
2	8-J	203	80% 18%

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Mol	Chain	Length	Quality of chain
2	8-L	203	80% 18%
2	8-N	203	80% 17%
2	8-P	203	79% 18%
2	8-R	203	80% 17%
2	8-T	203	80% 18%
2	8-V	203	80% 17%
2	8-X	203	80% 18%
2	8-Z	203	80% 18%
2	9-1	203	85% 13%
2	9-B	203	85% 13%
2	9-D	203	85% 13%
2	9-F	203	85% 13%
2	9-H	203	85% 13%
2	9-J	203	85% 13%
2	9-L	203	85% 13%
2	9-N	203	85% 13%
2	9-P	203	85% 13%
2	9-R	203	86% 13%
2	9-T	203	85% 13%
2	9-V	203	85% 13%
2	9-X	203	85% 13%
2	9-Z	203	85% 13%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 458920 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	221	Total	C	N	O	S	0	0
			1720	1092	290	335	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	C	N	O	S	0	0
			1720	1092	290	335	3		
1	9-C	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	10-C	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	1-E	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	2-E	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	3-E	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	4-E	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	5-E	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	6-E	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	7-E	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	8-E	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	9-E	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	10-E	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	1-G	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	2-G	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	3-G	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	4-G	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	5-G	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	6-G	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	7-G	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		
1	8-G	221	Total	C	N	O	S	0	0
			1720	1092	290	335	3		

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

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

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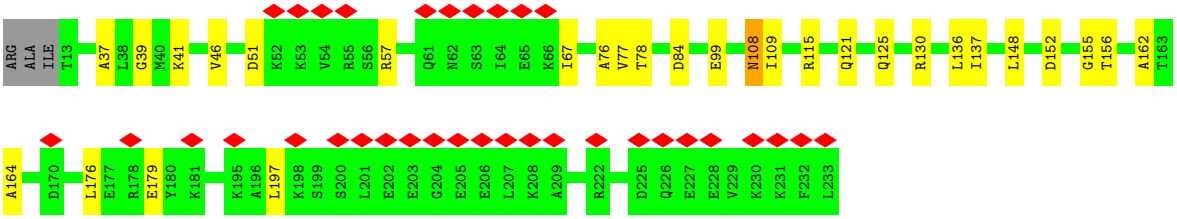
Mol	Chain	Residues	Atoms					AltConf	Trace
2	8-Z	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	9-Z	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	10-Z	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	1-1	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	2-1	203	Total	C	N	O	S	0	0
			1558	985	264	298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

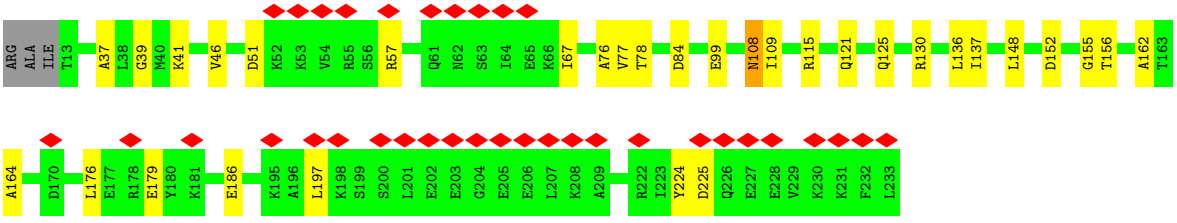
• Molecule 1: Proteasome subunit alpha

Chain 1-A:



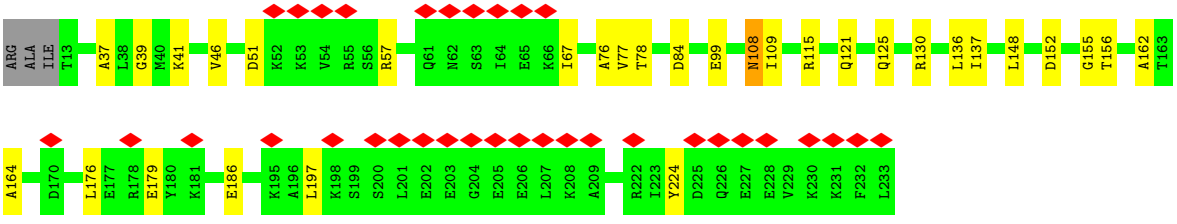
• Molecule 1: Proteasome subunit alpha

Chain 1-C:



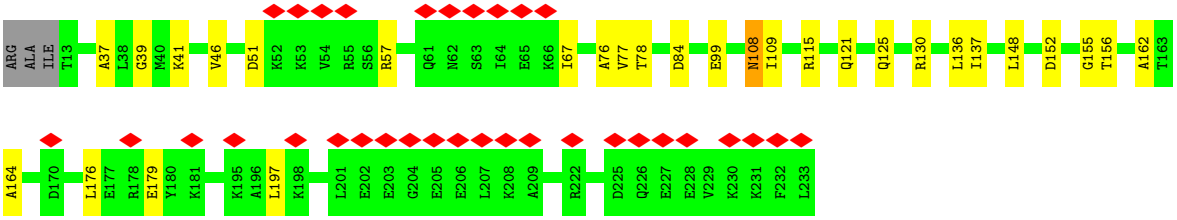
• Molecule 1: Proteasome subunit alpha

Chain 1-E:

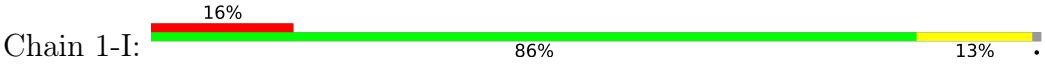


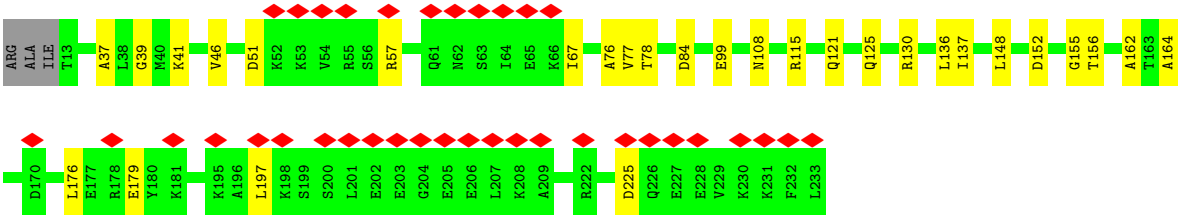
• Molecule 1: Proteasome subunit alpha

Chain 1-G:

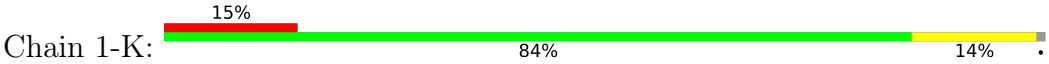


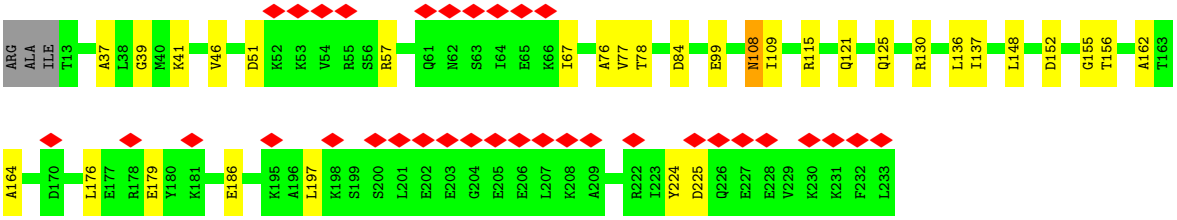
• Molecule 1: Proteasome subunit alpha



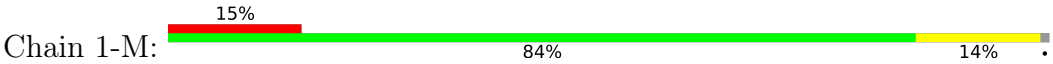


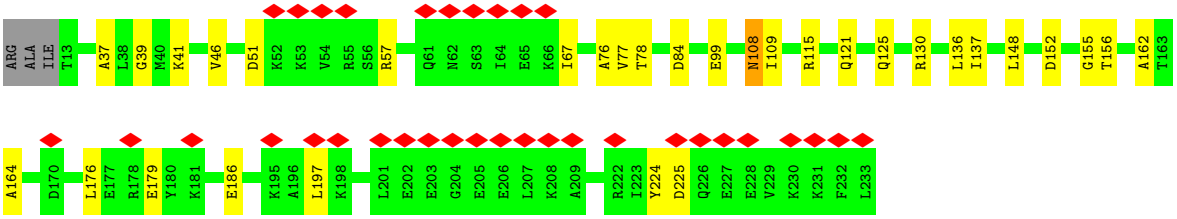
• Molecule 1: Proteasome subunit alpha



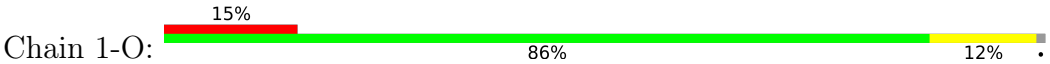


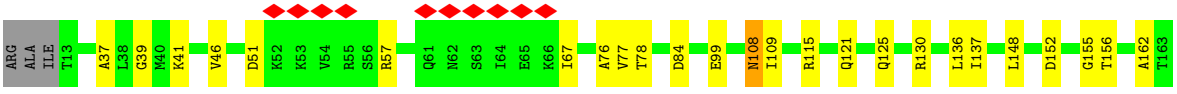
• Molecule 1: Proteasome subunit alpha

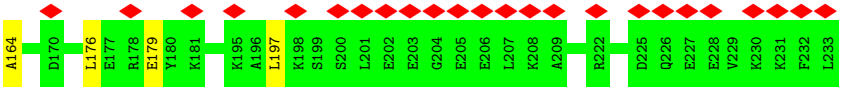




• Molecule 1: Proteasome subunit alpha

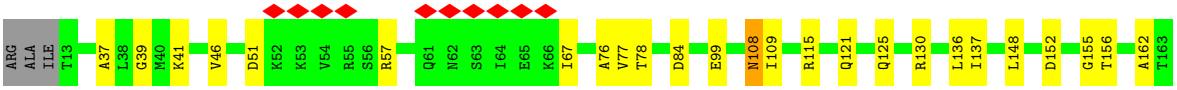


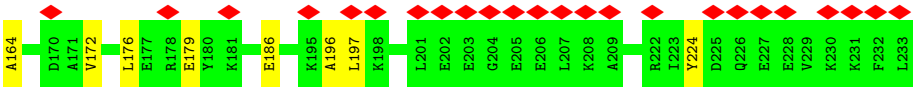




• Molecule 1: Proteasome subunit alpha

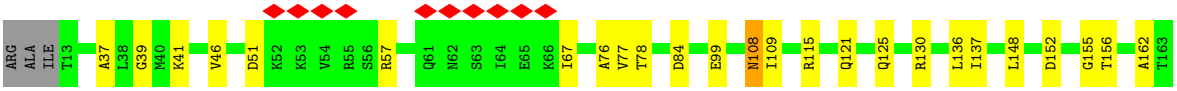
Chain 1-Q:

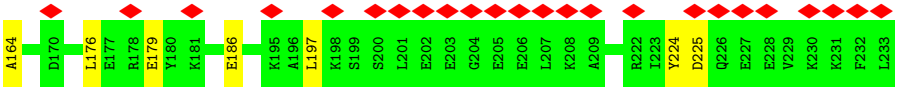




• Molecule 1: Proteasome subunit alpha

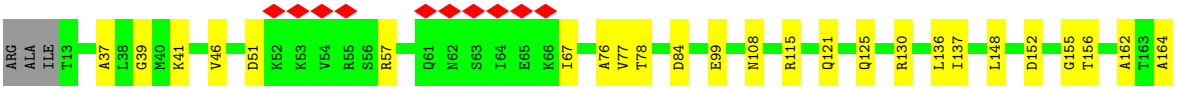
Chain 1-S:

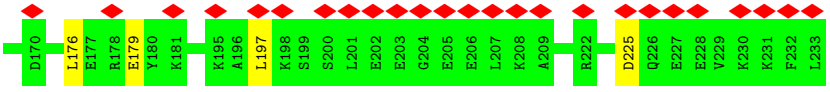




• Molecule 1: Proteasome subunit alpha

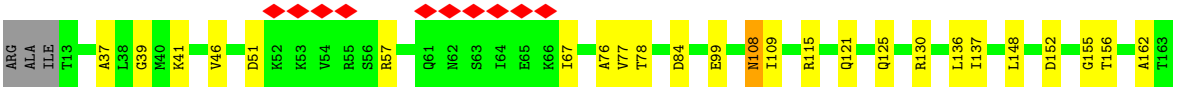
Chain 1-U:





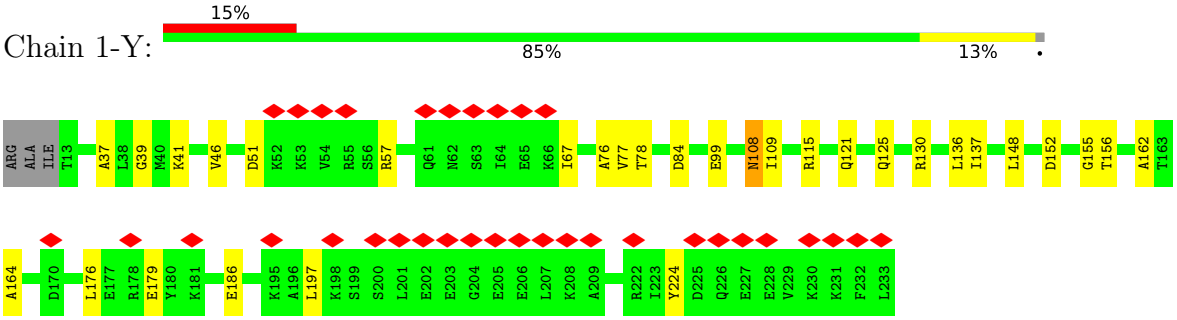
• Molecule 1: Proteasome subunit alpha

Chain 1-W:



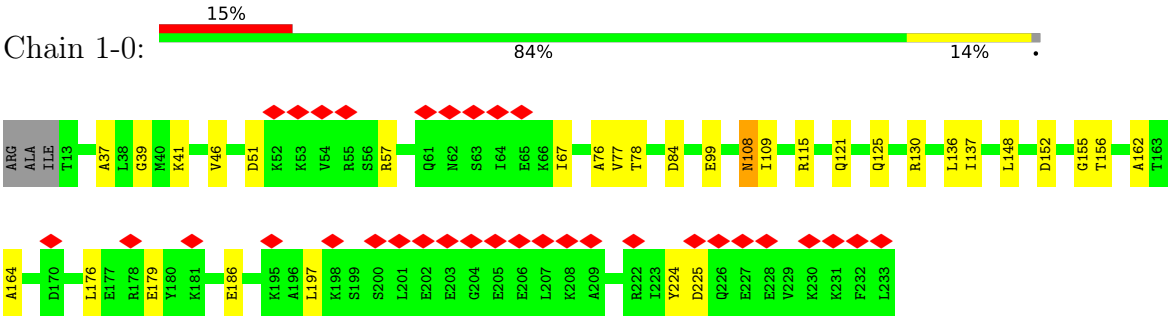
• Molecule 1: Proteasome subunit alpha

Chain 1-Y:



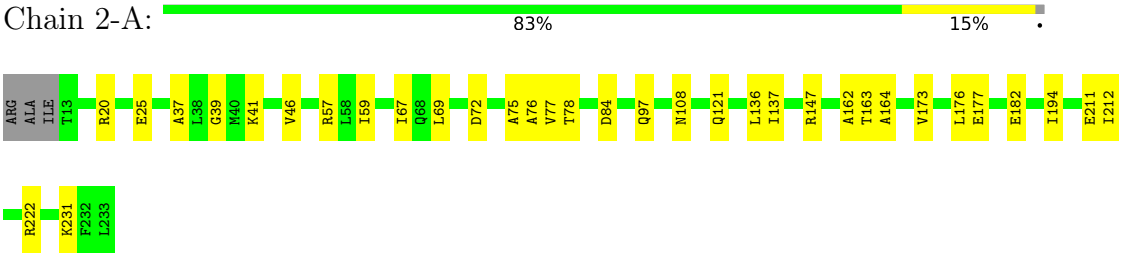
• Molecule 1: Proteasome subunit alpha

Chain 1-0:



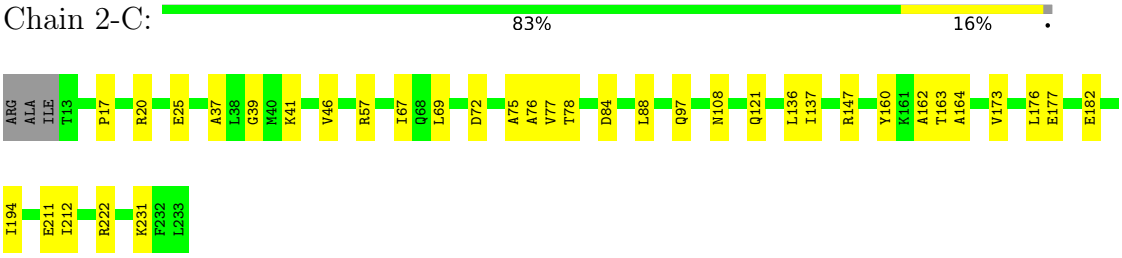
• Molecule 1: Proteasome subunit alpha

Chain 2-A:



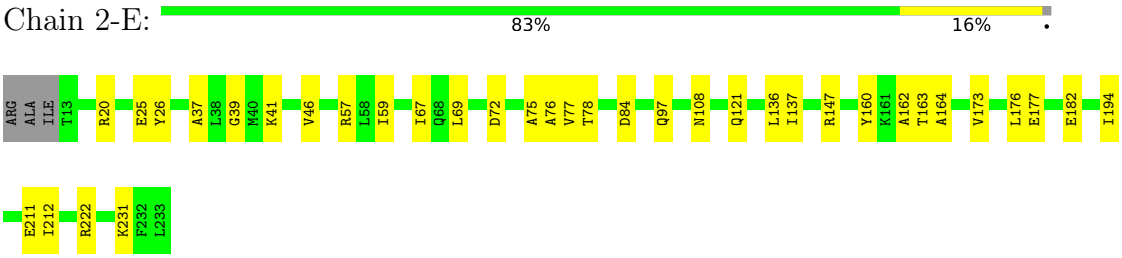
• Molecule 1: Proteasome subunit alpha

Chain 2-C:



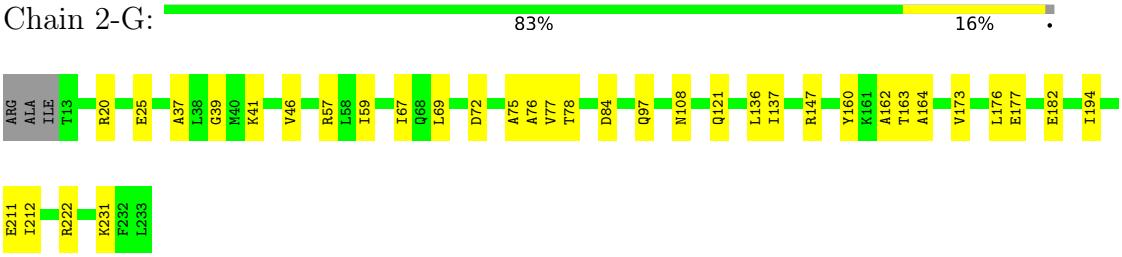
• Molecule 1: Proteasome subunit alpha

Chain 2-E:



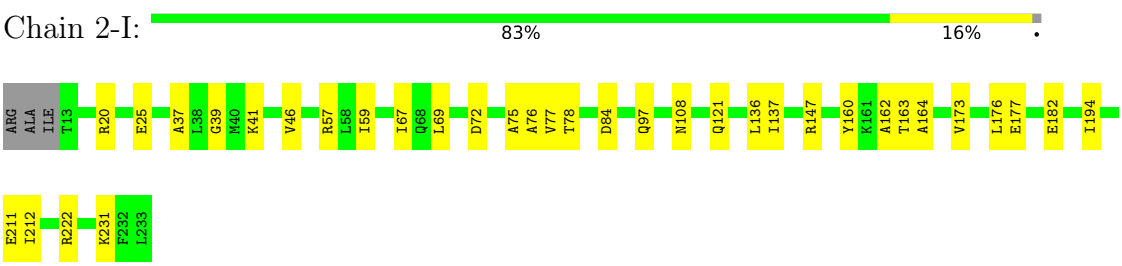
• Molecule 1: Proteasome subunit alpha

Chain 2-G:



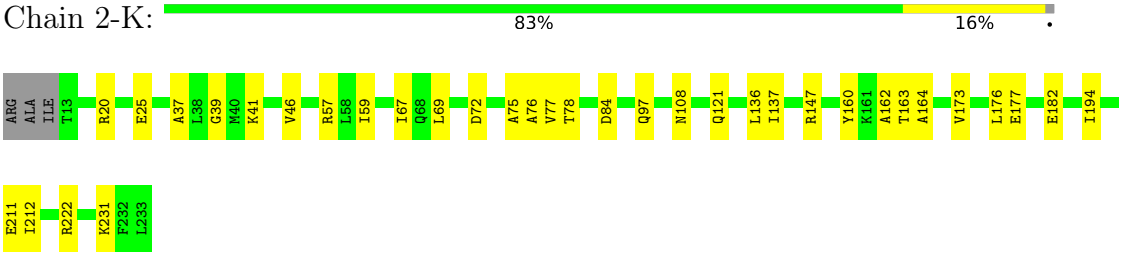
• Molecule 1: Proteasome subunit alpha

Chain 2-I:



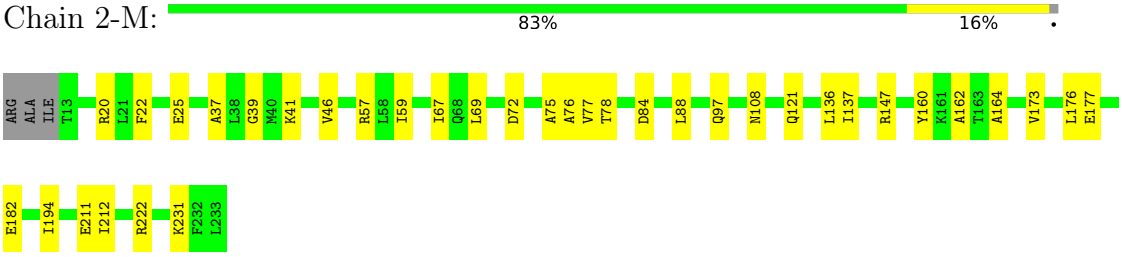
• Molecule 1: Proteasome subunit alpha

Chain 2-K:



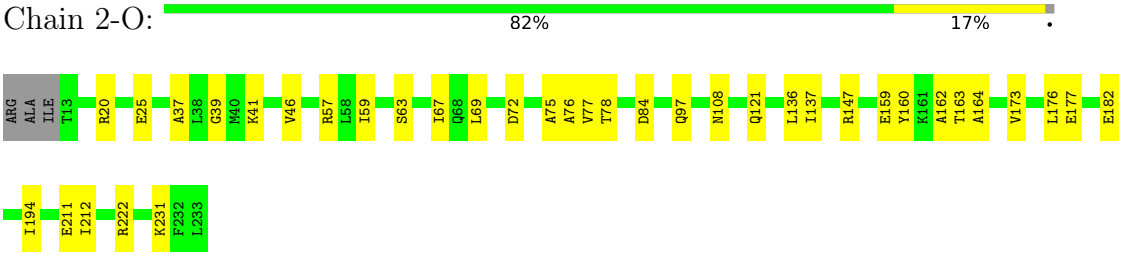
• Molecule 1: Proteasome subunit alpha

Chain 2-M:



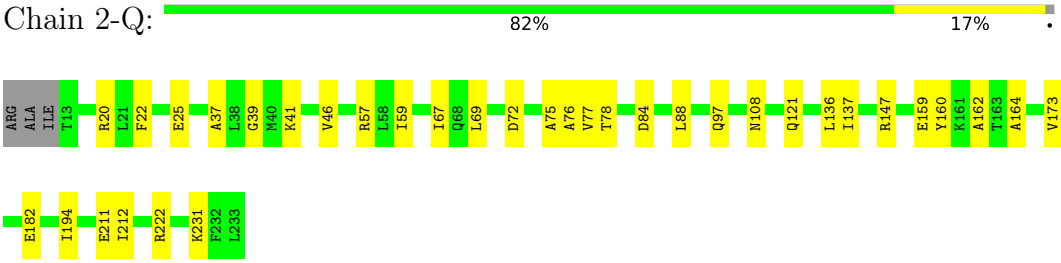
• Molecule 1: Proteasome subunit alpha

Chain 2-O:



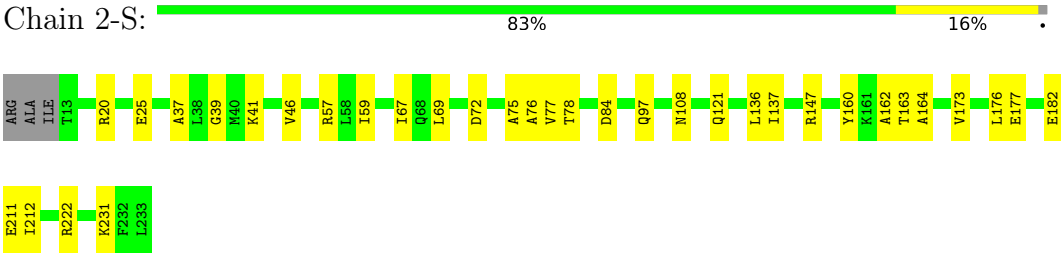
• Molecule 1: Proteasome subunit alpha

Chain 2-Q:



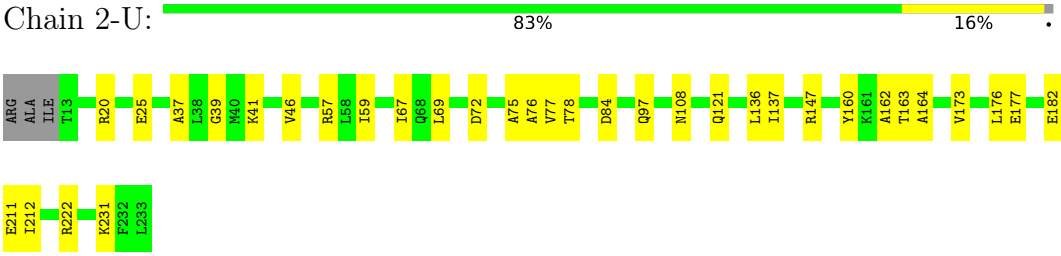
• Molecule 1: Proteasome subunit alpha

Chain 2-S:



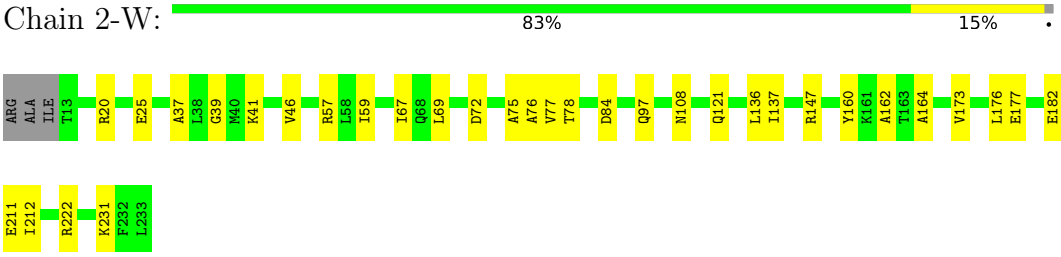
• Molecule 1: Proteasome subunit alpha

Chain 2-U:



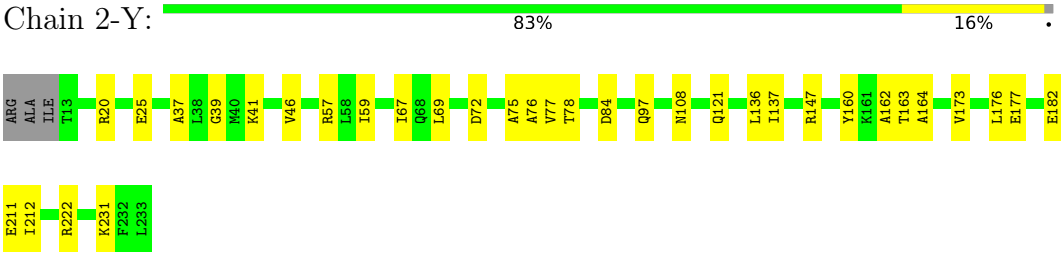
• Molecule 1: Proteasome subunit alpha

Chain 2-W:



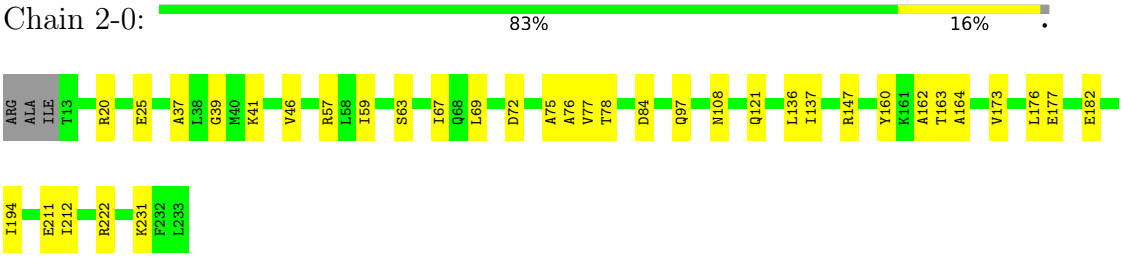
• Molecule 1: Proteasome subunit alpha

Chain 2-Y:



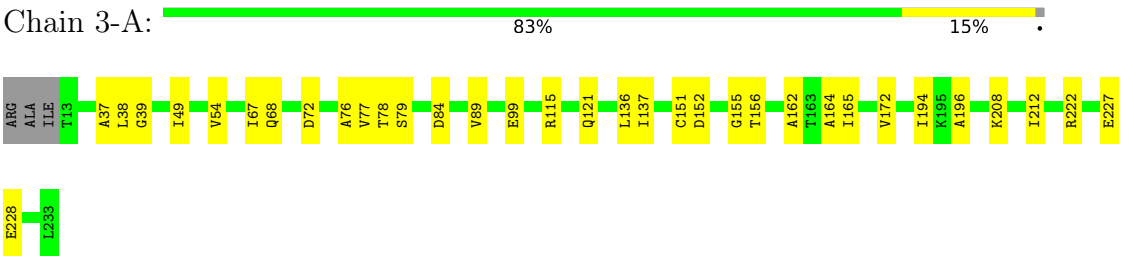
• Molecule 1: Proteasome subunit alpha

Chain 2-0:



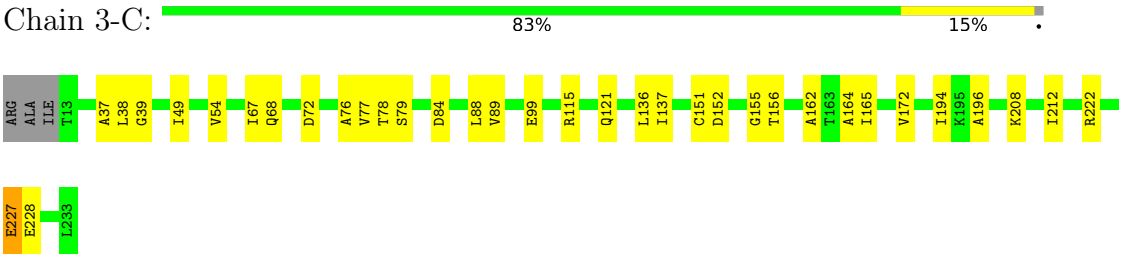
• Molecule 1: Proteasome subunit alpha

Chain 3-A:



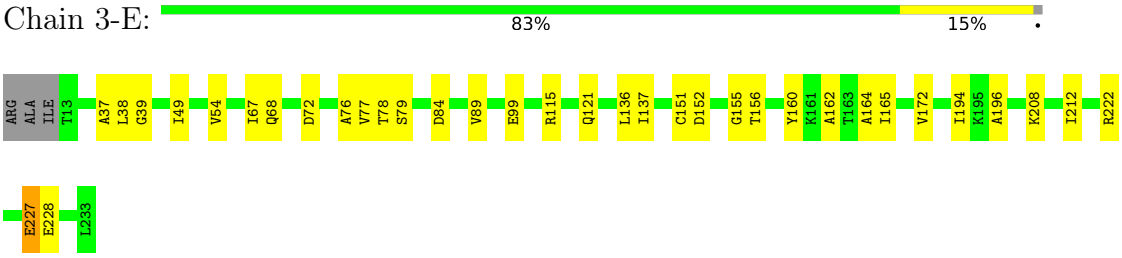
• Molecule 1: Proteasome subunit alpha

Chain 3-C:



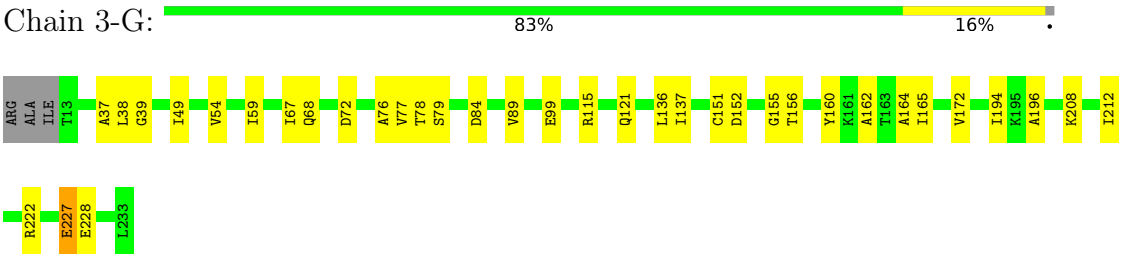
• Molecule 1: Proteasome subunit alpha

Chain 3-E:



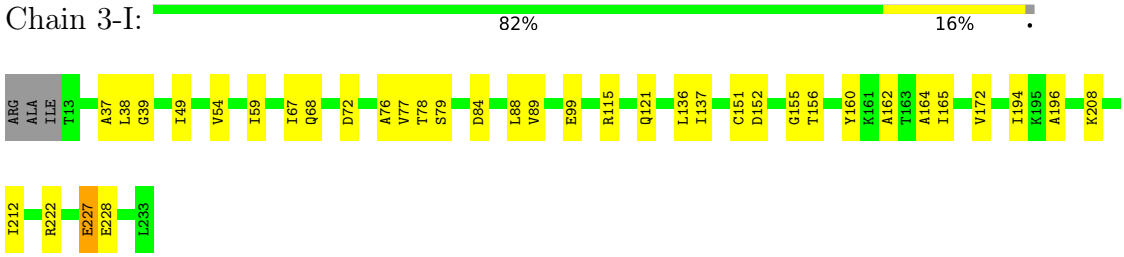
• Molecule 1: Proteasome subunit alpha

Chain 3-G:



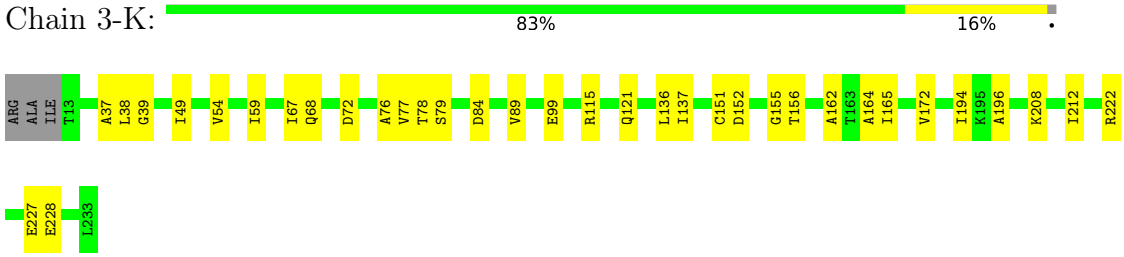
• Molecule 1: Proteasome subunit alpha

Chain 3-I:



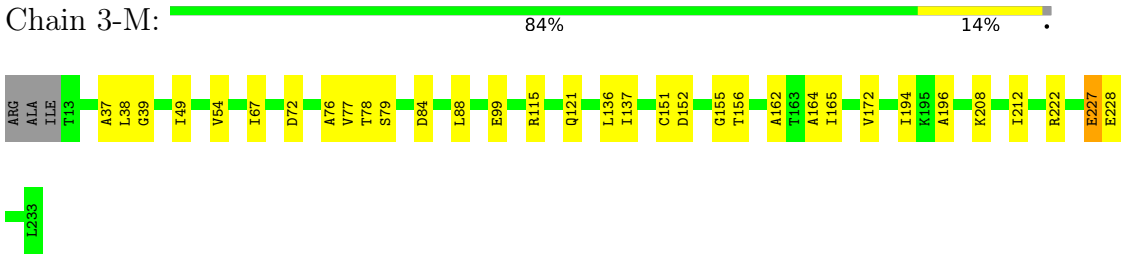
• Molecule 1: Proteasome subunit alpha

Chain 3-K:



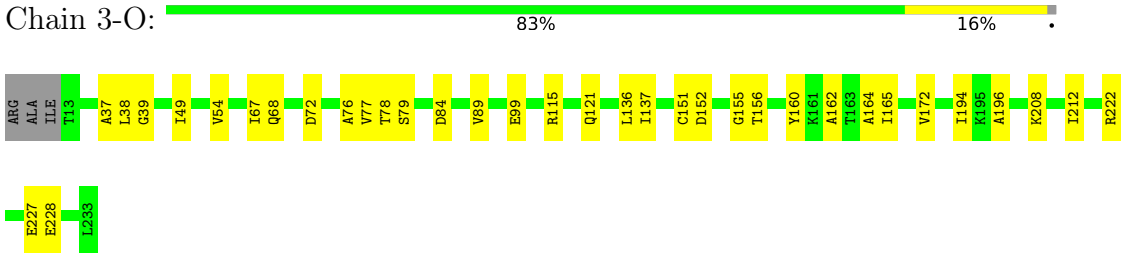
• Molecule 1: Proteasome subunit alpha

Chain 3-M:



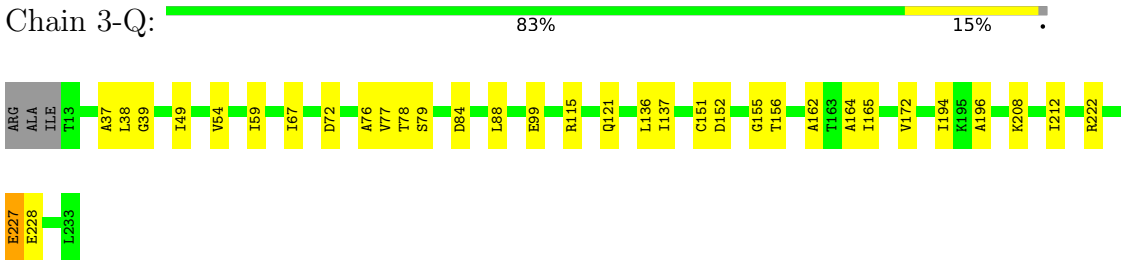
• Molecule 1: Proteasome subunit alpha

Chain 3-O:



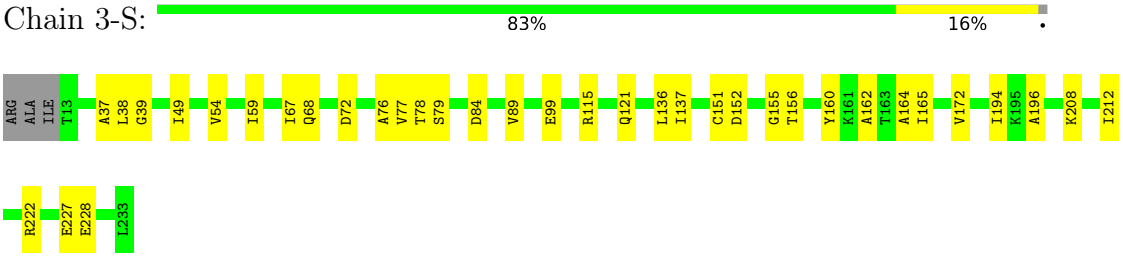
• Molecule 1: Proteasome subunit alpha

Chain 3-Q:



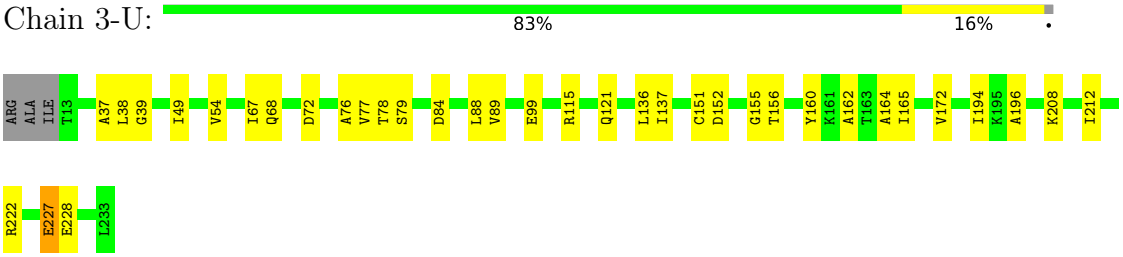
• Molecule 1: Proteasome subunit alpha

Chain 3-S:



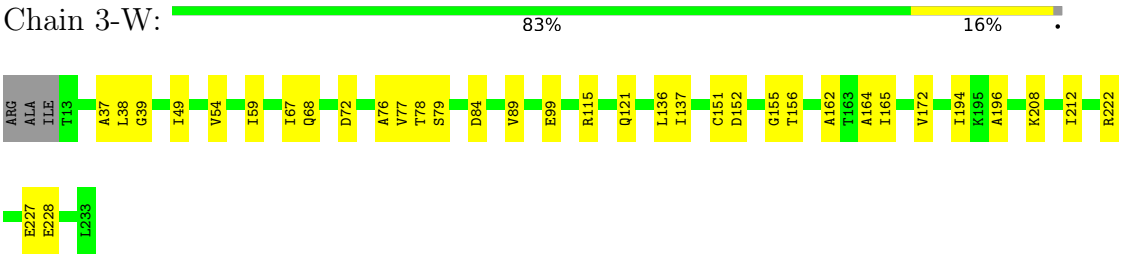
• Molecule 1: Proteasome subunit alpha

Chain 3-U:



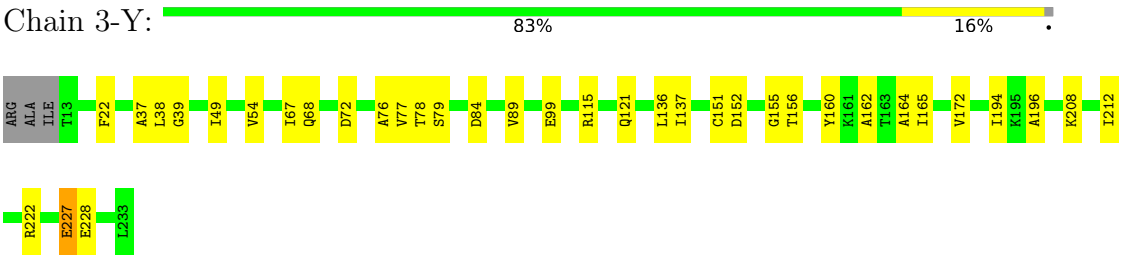
• Molecule 1: Proteasome subunit alpha

Chain 3-W:



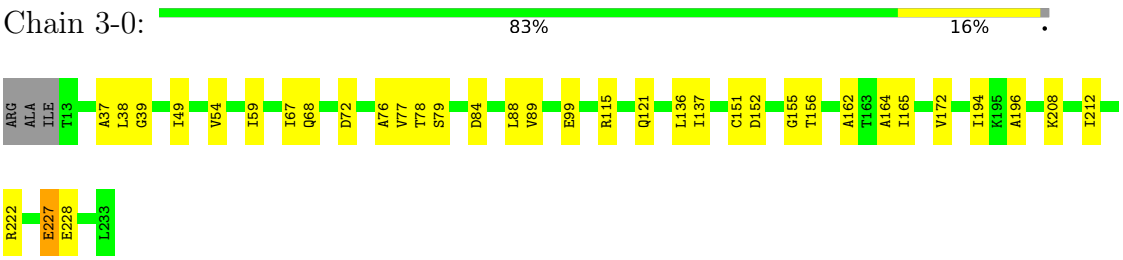
• Molecule 1: Proteasome subunit alpha

Chain 3-Y:



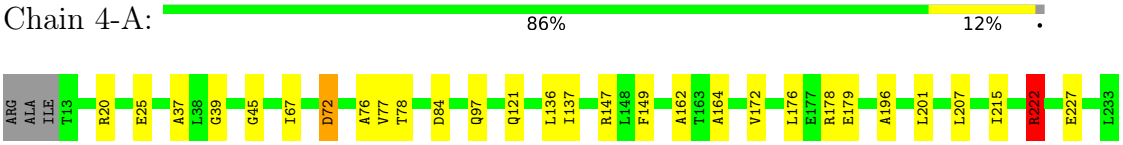
• Molecule 1: Proteasome subunit alpha

Chain 3-0:



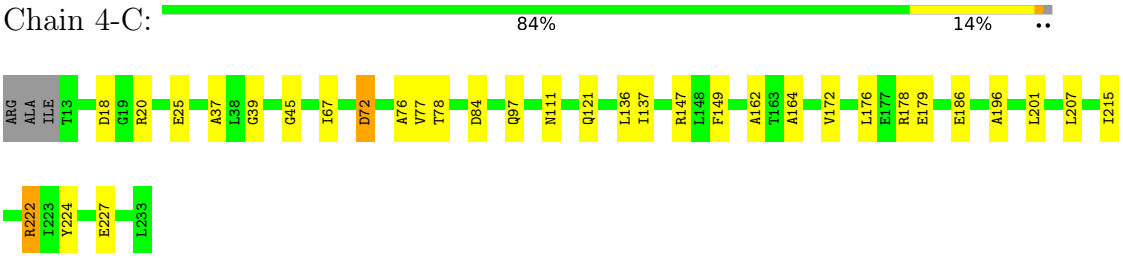
• Molecule 1: Proteasome subunit alpha

Chain 4-A:



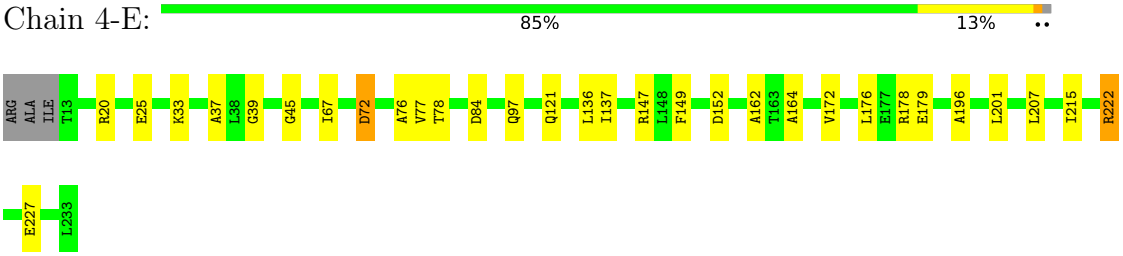
• Molecule 1: Proteasome subunit alpha

Chain 4-C:



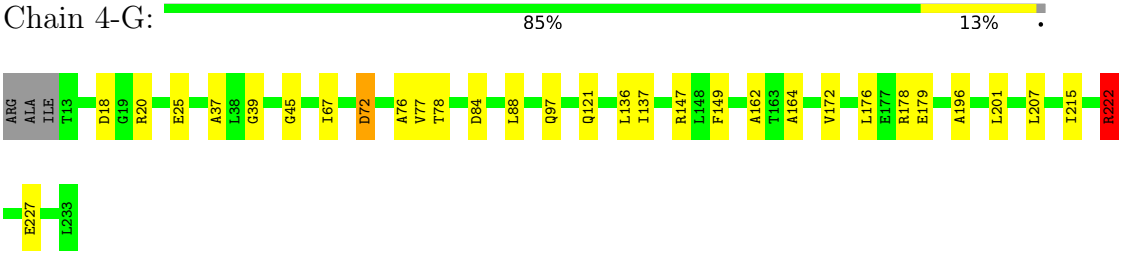
• Molecule 1: Proteasome subunit alpha

Chain 4-E:



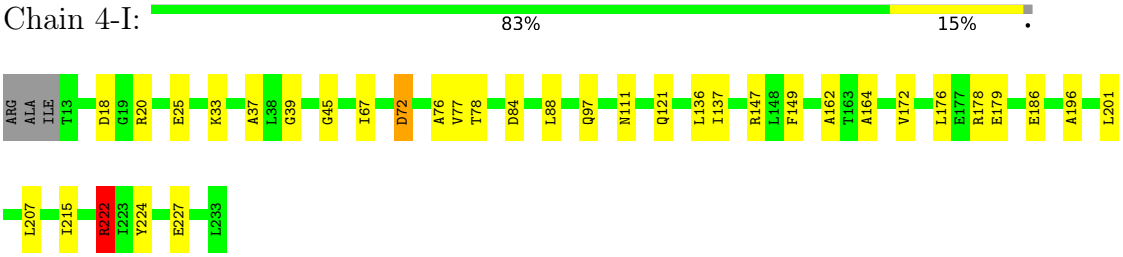
• Molecule 1: Proteasome subunit alpha

Chain 4-G:



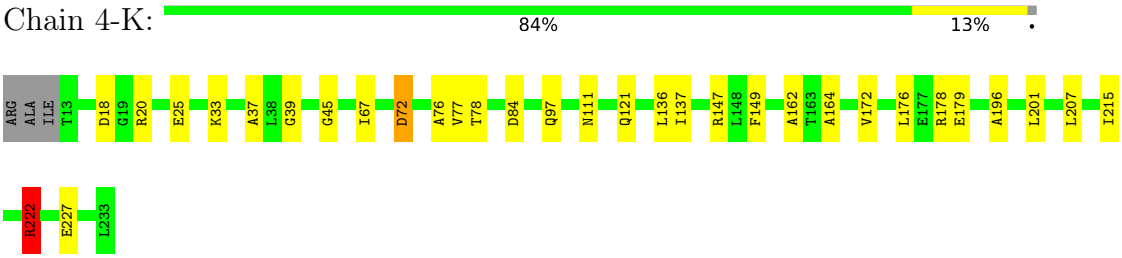
• Molecule 1: Proteasome subunit alpha

Chain 4-I:



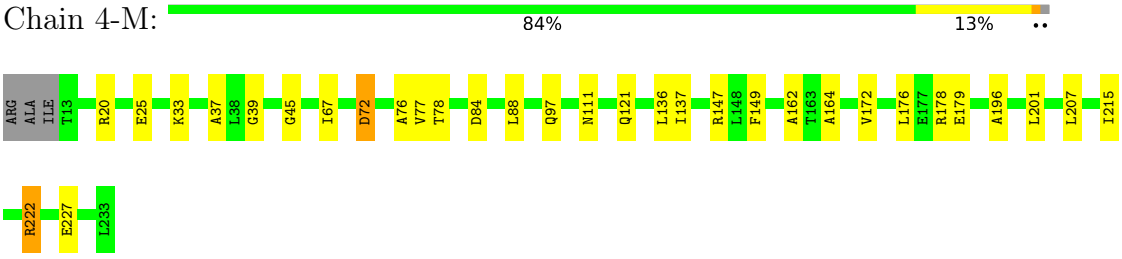
• Molecule 1: Proteasome subunit alpha

Chain 4-K:



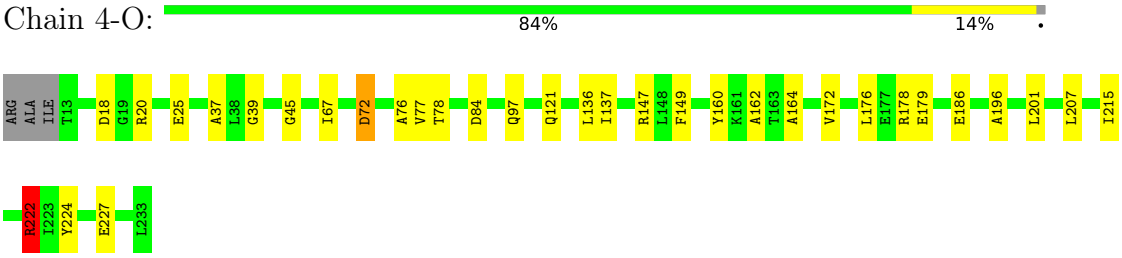
• Molecule 1: Proteasome subunit alpha

Chain 4-M:



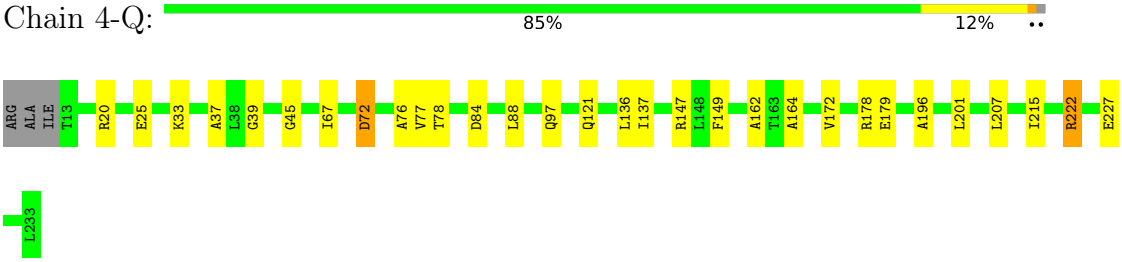
• Molecule 1: Proteasome subunit alpha

Chain 4-O:



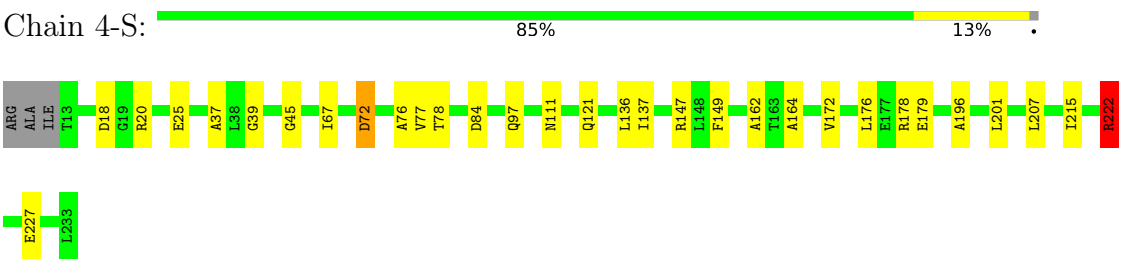
• Molecule 1: Proteasome subunit alpha

Chain 4-Q:



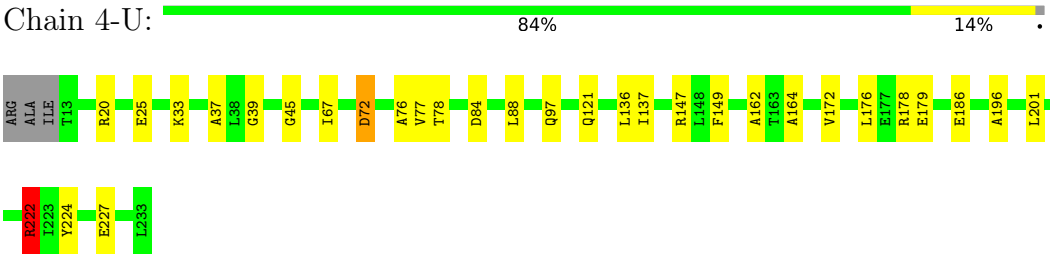
• Molecule 1: Proteasome subunit alpha

Chain 4-S:



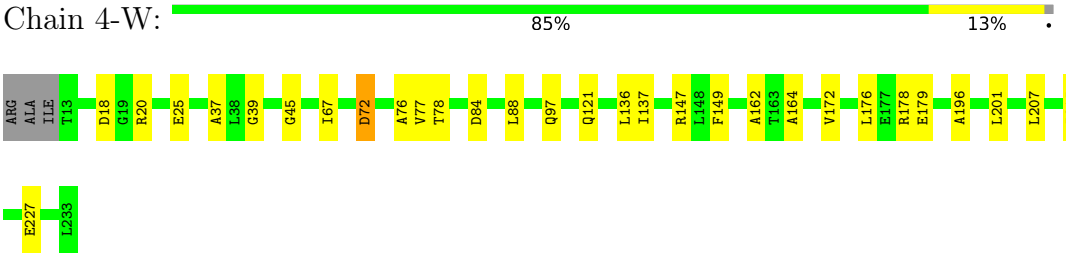
• Molecule 1: Proteasome subunit alpha

Chain 4-U:



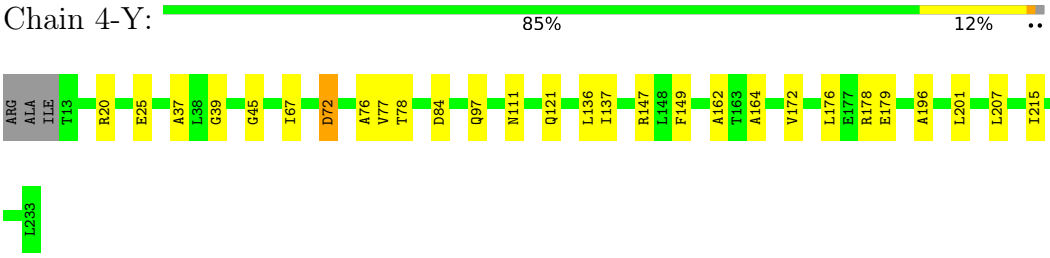
• Molecule 1: Proteasome subunit alpha

Chain 4-W:



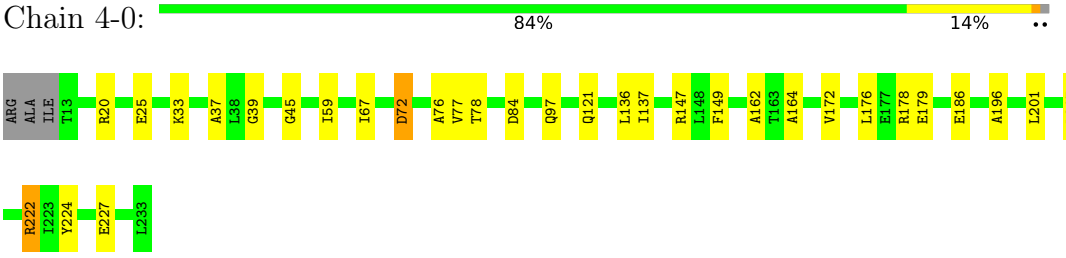
• Molecule 1: Proteasome subunit alpha

Chain 4-Y:



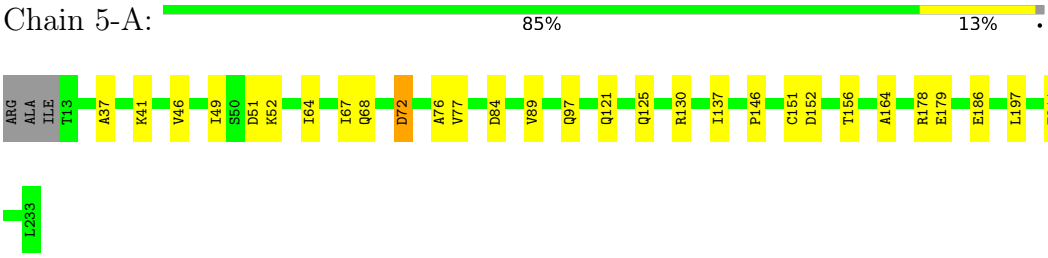
• Molecule 1: Proteasome subunit alpha

Chain 4-0:



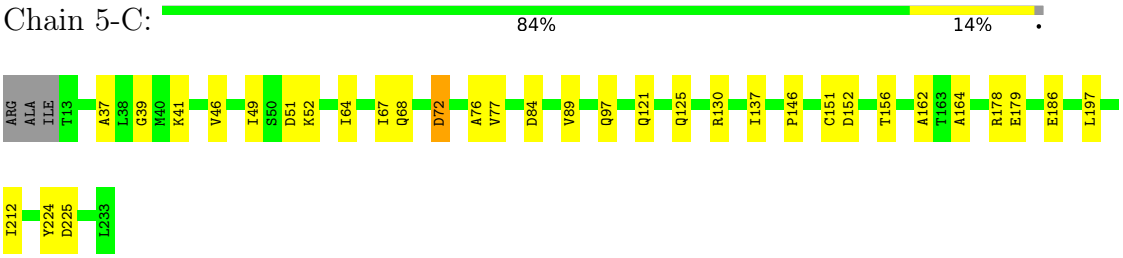
• Molecule 1: Proteasome subunit alpha

Chain 5-A:



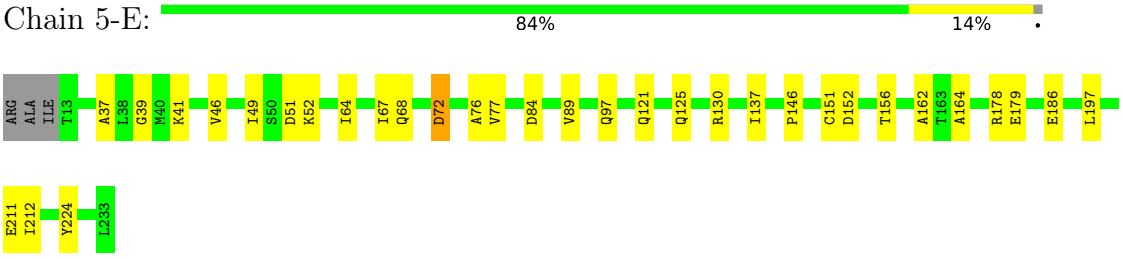
• Molecule 1: Proteasome subunit alpha

Chain 5-C:



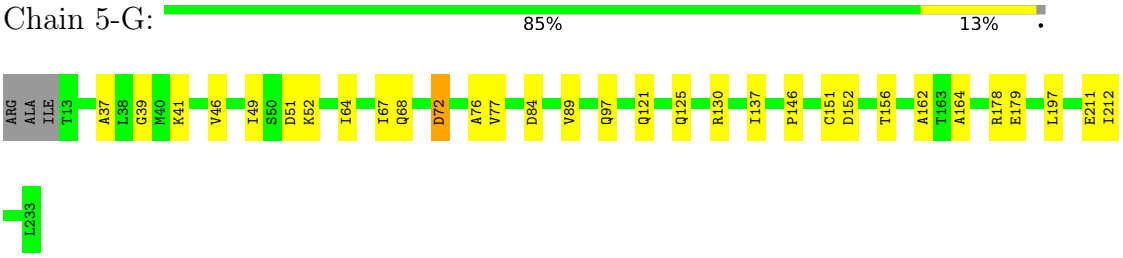
• Molecule 1: Proteasome subunit alpha

Chain 5-E:



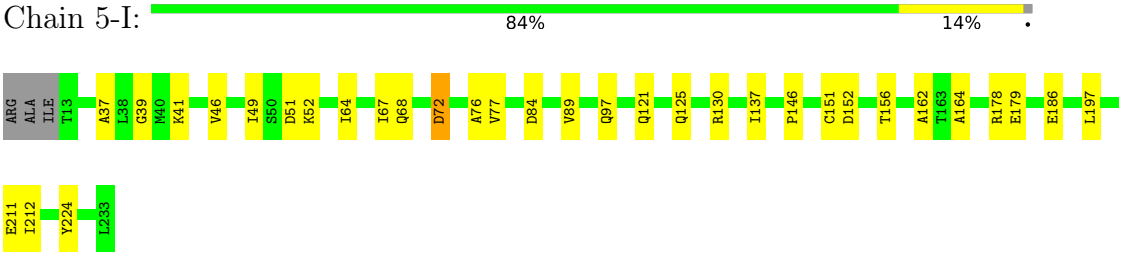
• Molecule 1: Proteasome subunit alpha

Chain 5-G:



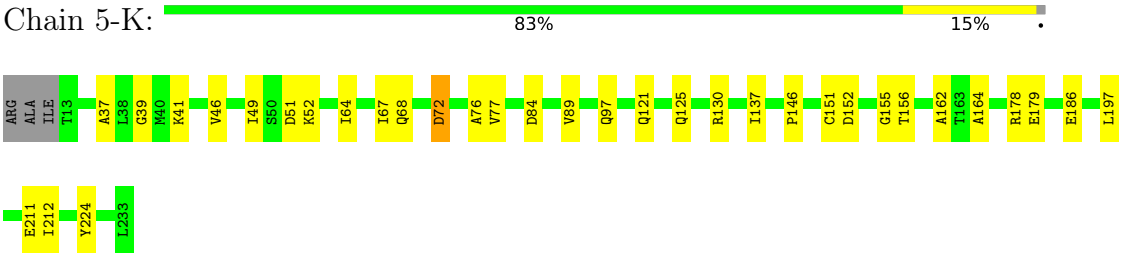
• Molecule 1: Proteasome subunit alpha

Chain 5-I:



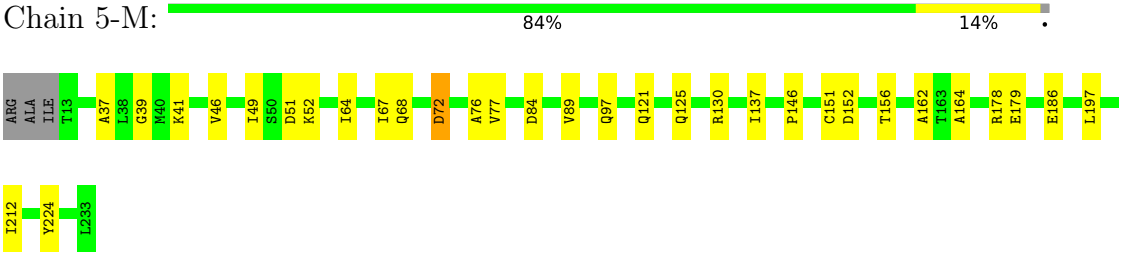
• Molecule 1: Proteasome subunit alpha

Chain 5-K:



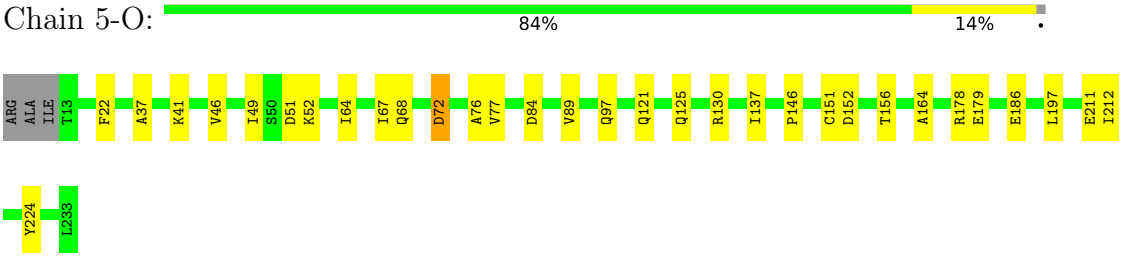
• Molecule 1: Proteasome subunit alpha

Chain 5-M:



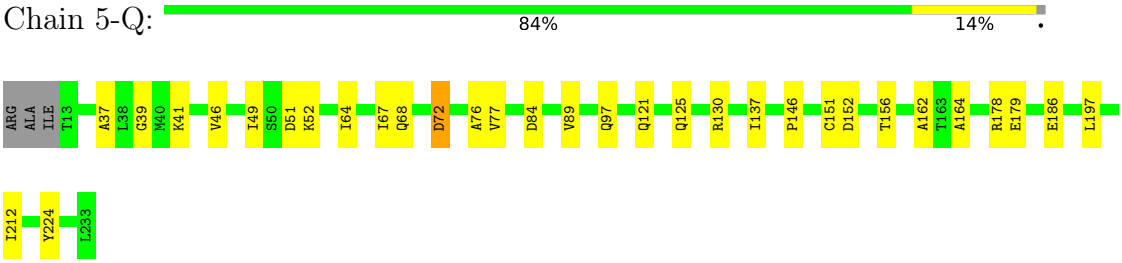
• Molecule 1: Proteasome subunit alpha

Chain 5-O:



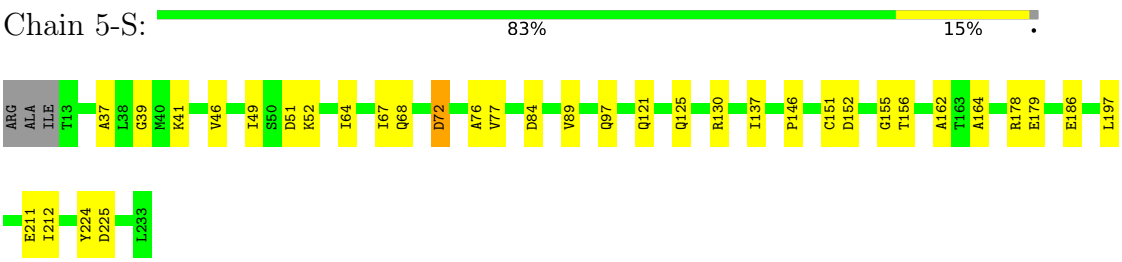
• Molecule 1: Proteasome subunit alpha

Chain 5-Q:



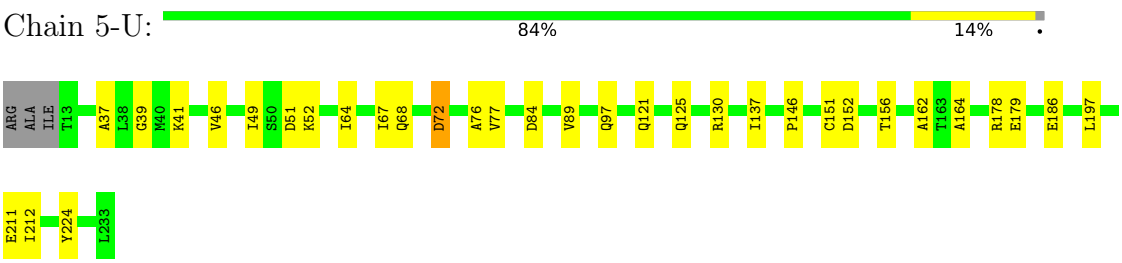
• Molecule 1: Proteasome subunit alpha

Chain 5-S:



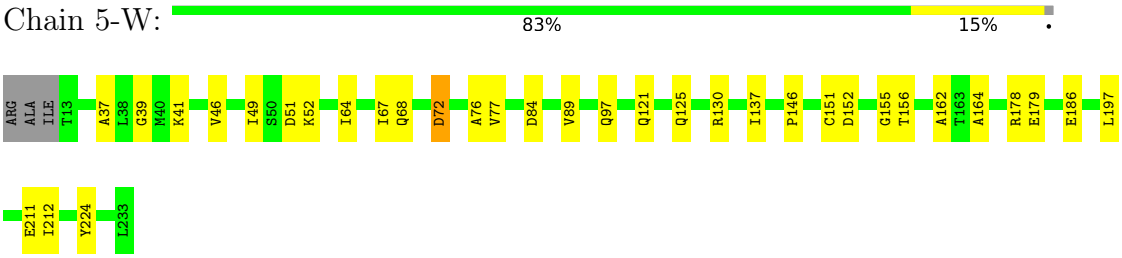
• Molecule 1: Proteasome subunit alpha

Chain 5-U:



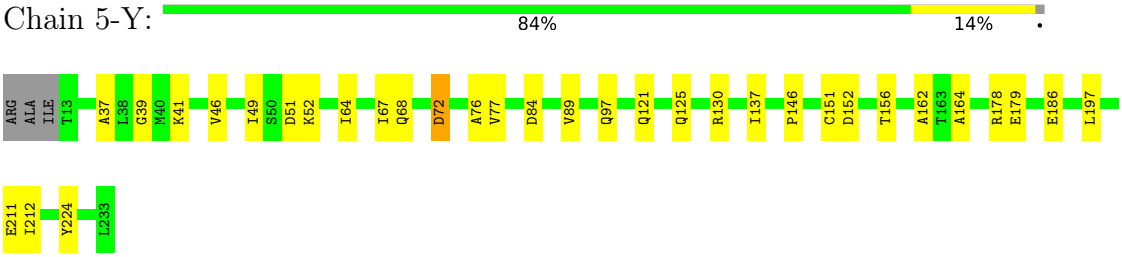
• Molecule 1: Proteasome subunit alpha

Chain 5-W:



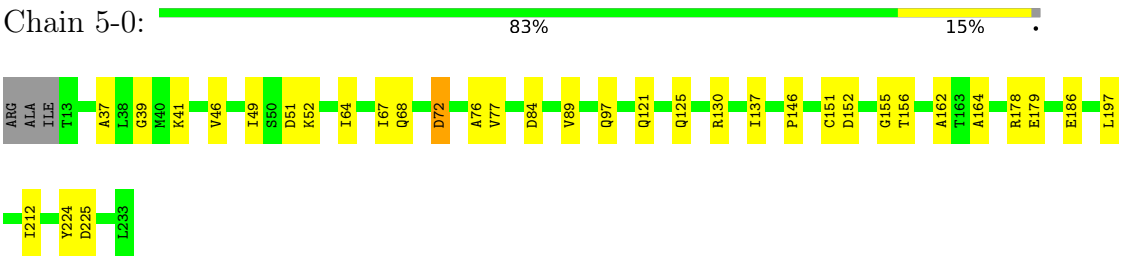
• Molecule 1: Proteasome subunit alpha

Chain 5-Y:



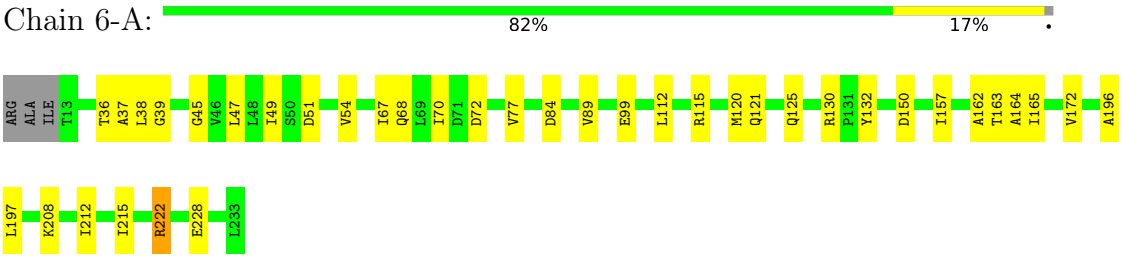
• Molecule 1: Proteasome subunit alpha

Chain 5-0:



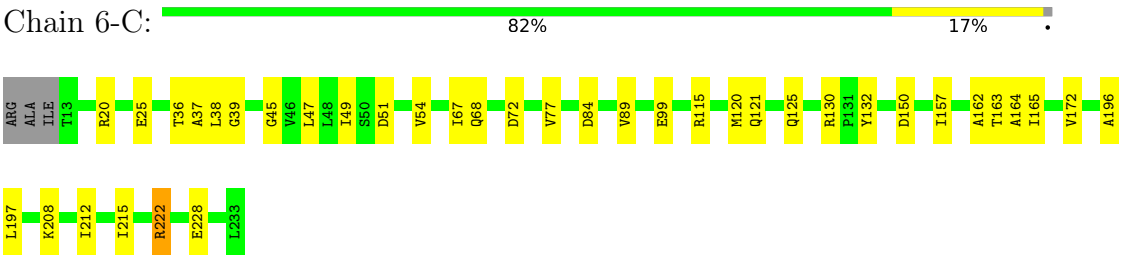
• Molecule 1: Proteasome subunit alpha

Chain 6-A:



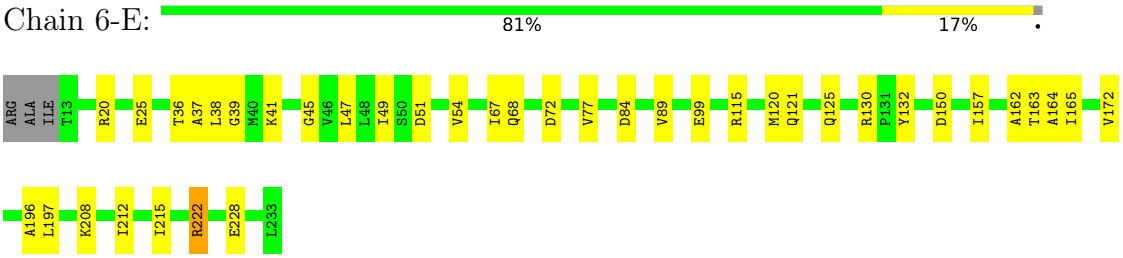
• Molecule 1: Proteasome subunit alpha

Chain 6-C:



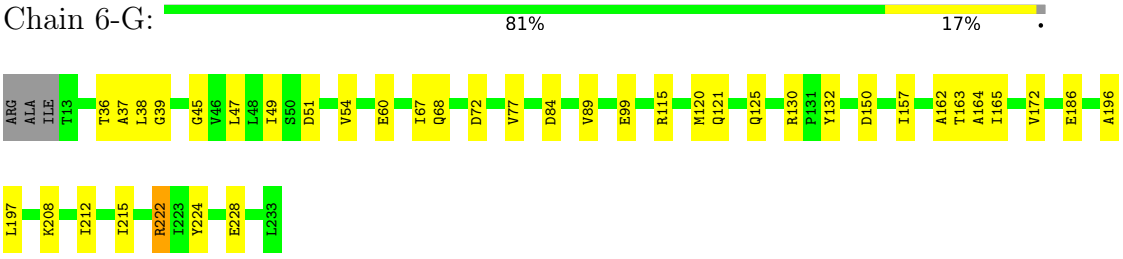
• Molecule 1: Proteasome subunit alpha

Chain 6-E:



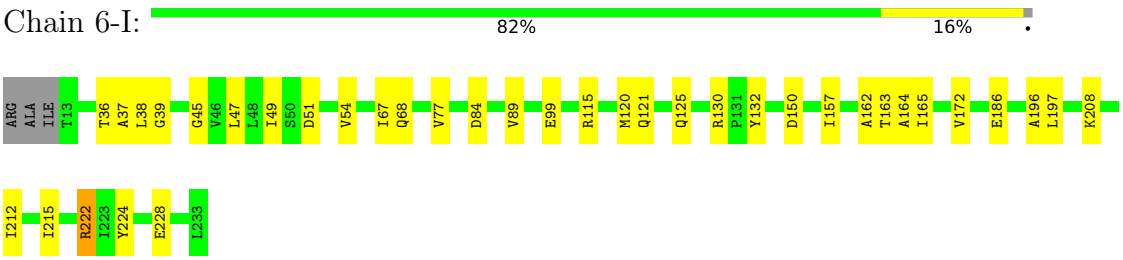
• Molecule 1: Proteasome subunit alpha

Chain 6-G:



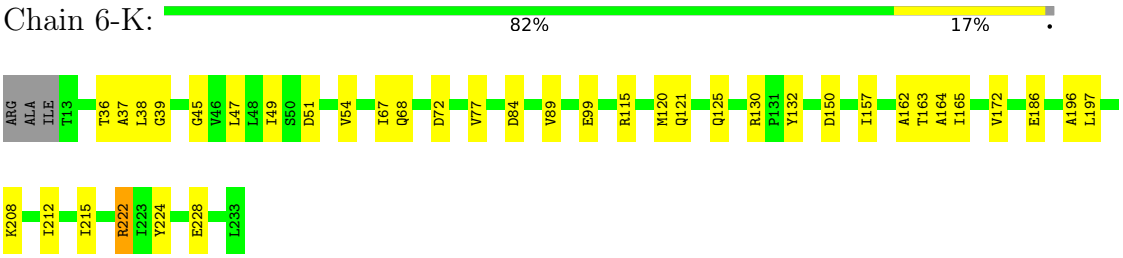
• Molecule 1: Proteasome subunit alpha

Chain 6-I:



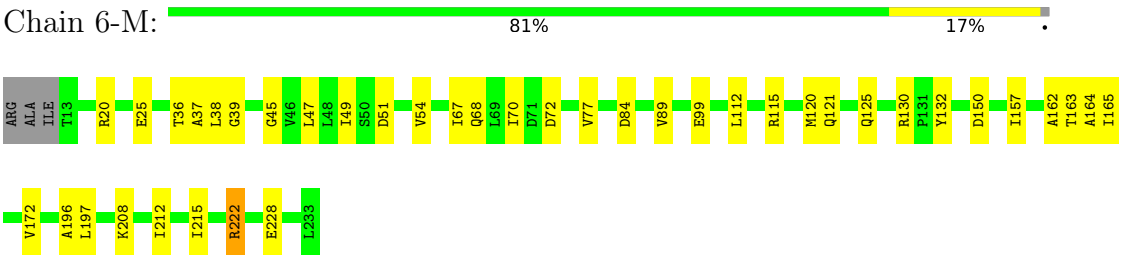
• Molecule 1: Proteasome subunit alpha

Chain 6-K:



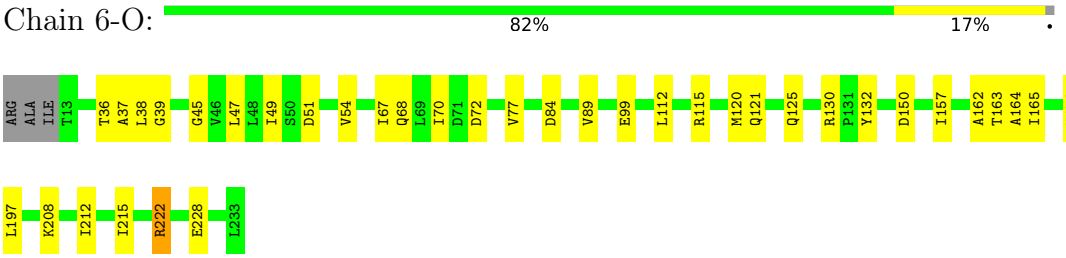
• Molecule 1: Proteasome subunit alpha

Chain 6-M:



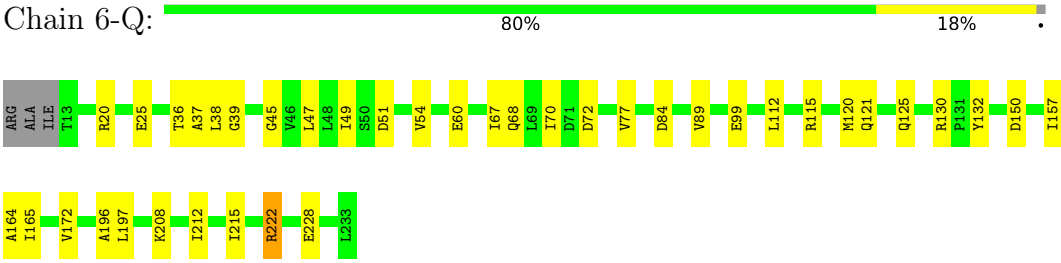
• Molecule 1: Proteasome subunit alpha

Chain 6-O:



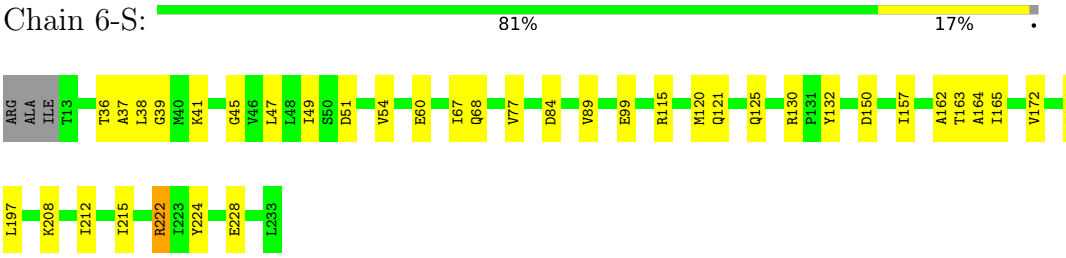
• Molecule 1: Proteasome subunit alpha

Chain 6-Q:



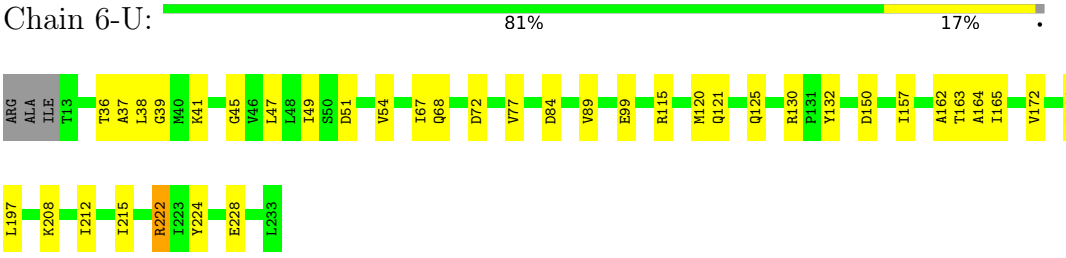
• Molecule 1: Proteasome subunit alpha

Chain 6-S:



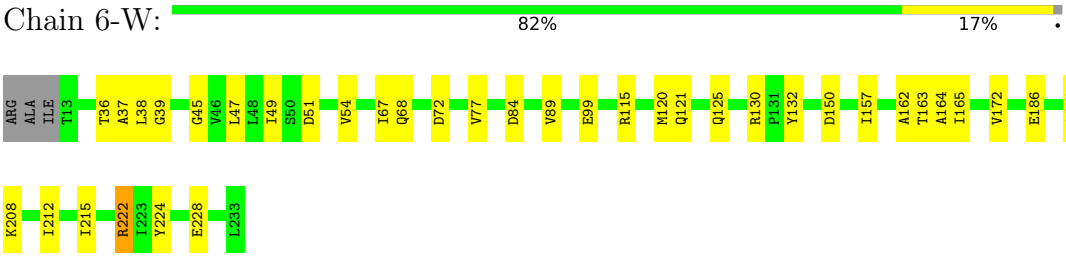
• Molecule 1: Proteasome subunit alpha

Chain 6-U:



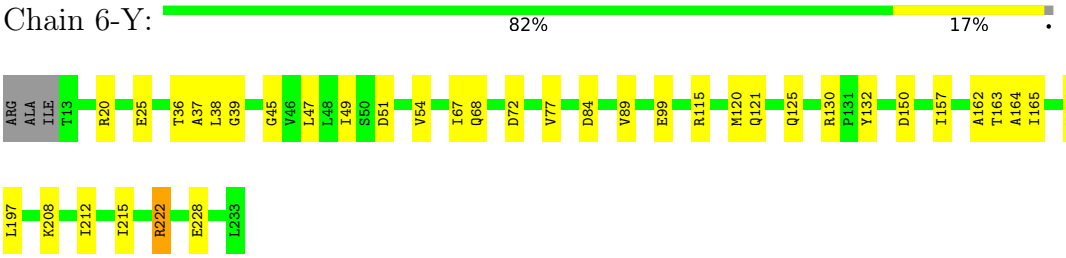
• Molecule 1: Proteasome subunit alpha

Chain 6-W:



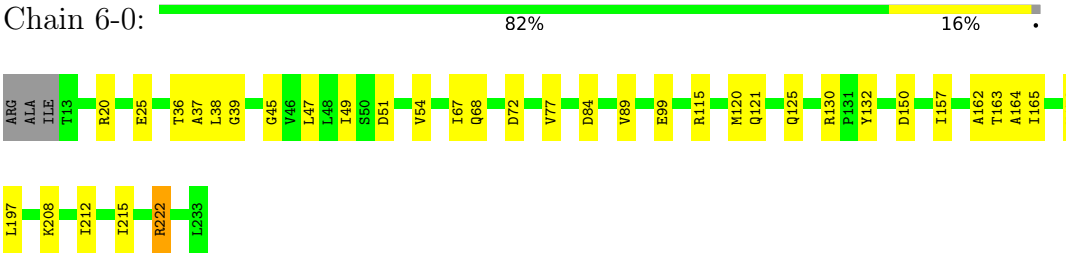
• Molecule 1: Proteasome subunit alpha

Chain 6-Y:



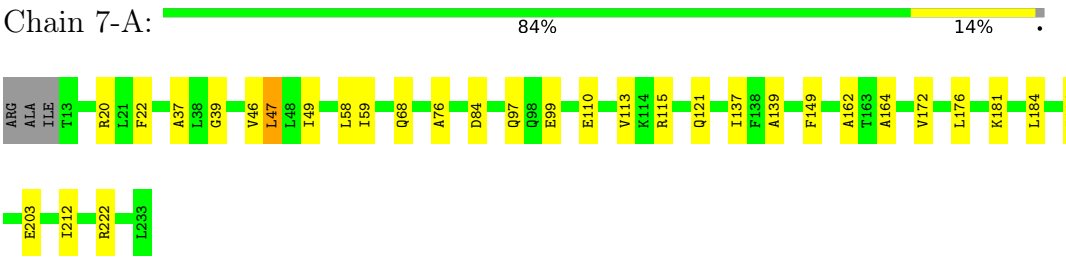
• Molecule 1: Proteasome subunit alpha

Chain 6-0:



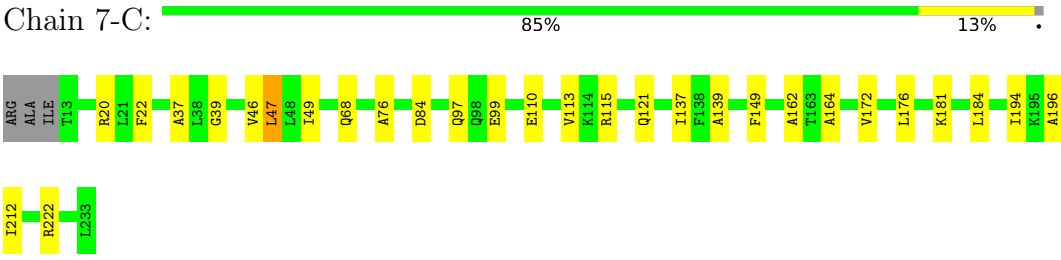
• Molecule 1: Proteasome subunit alpha

Chain 7-A:



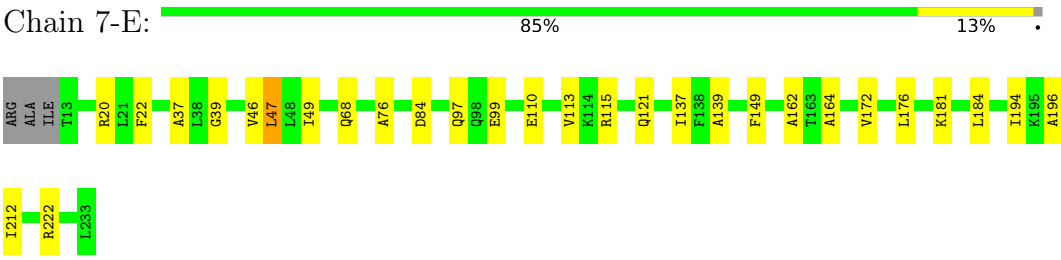
• Molecule 1: Proteasome subunit alpha

Chain 7-C:



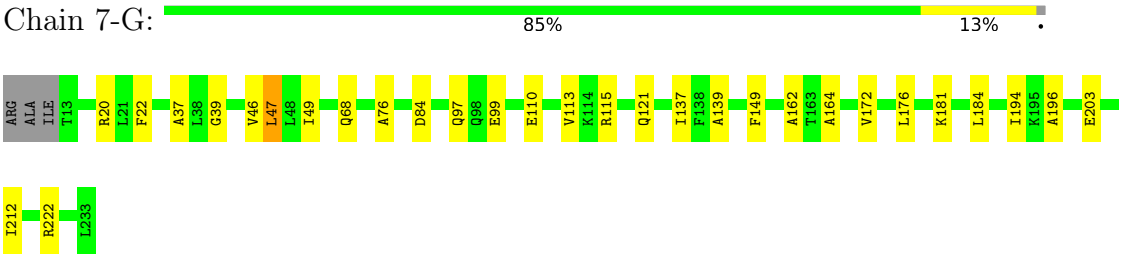
• Molecule 1: Proteasome subunit alpha

Chain 7-E:



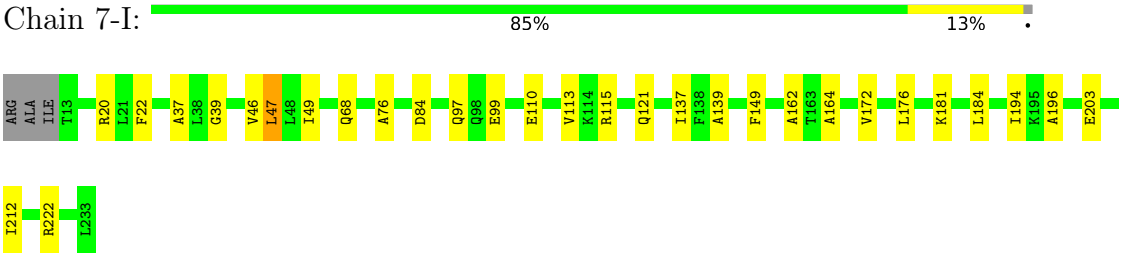
• Molecule 1: Proteasome subunit alpha

Chain 7-G:



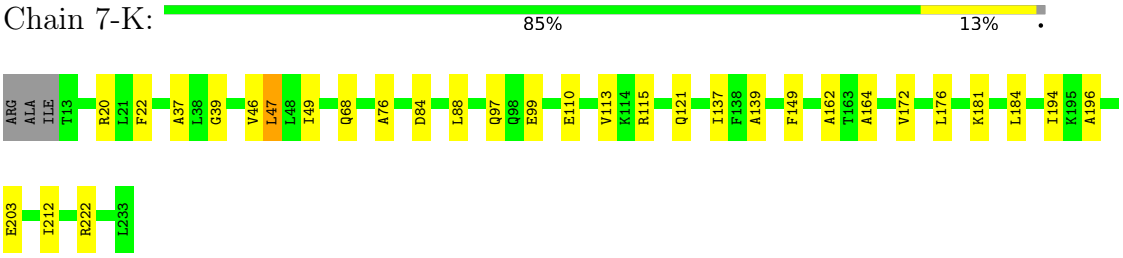
• Molecule 1: Proteasome subunit alpha

Chain 7-I:



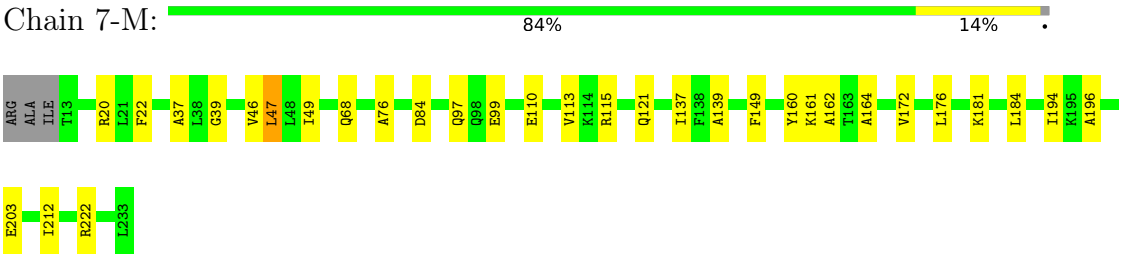
• Molecule 1: Proteasome subunit alpha

Chain 7-K:



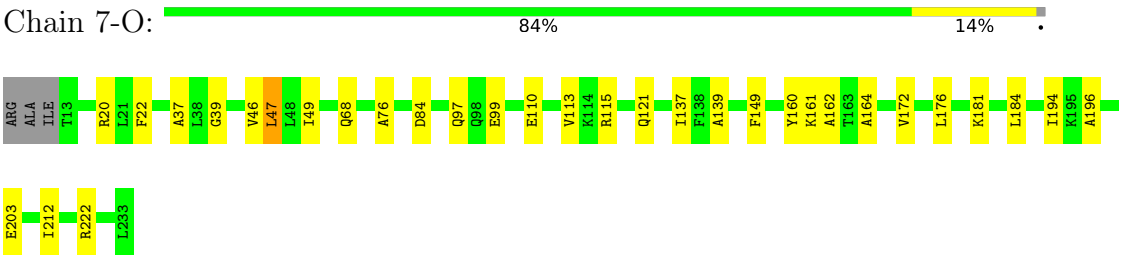
• Molecule 1: Proteasome subunit alpha

Chain 7-M:



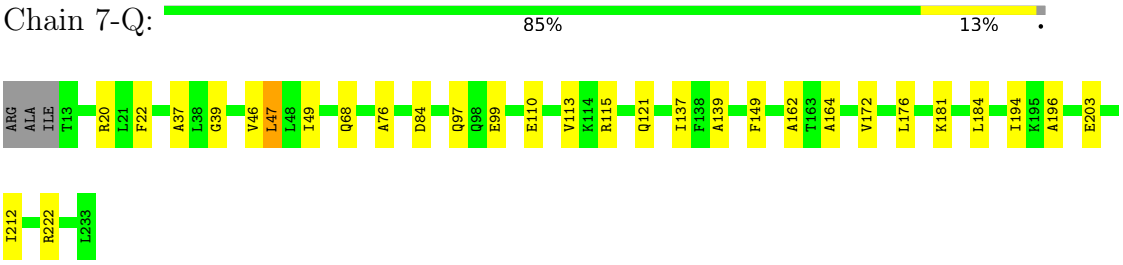
• Molecule 1: Proteasome subunit alpha

Chain 7-O:



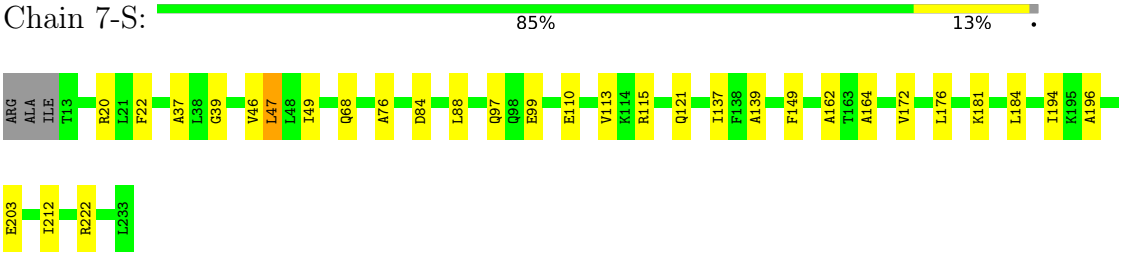
• Molecule 1: Proteasome subunit alpha

Chain 7-Q:



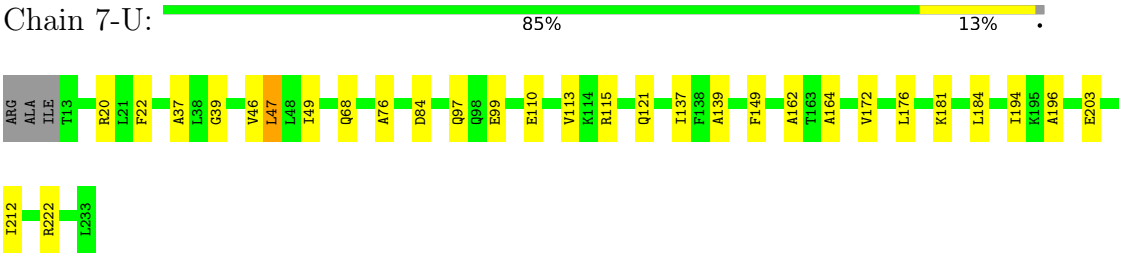
• Molecule 1: Proteasome subunit alpha

Chain 7-S:



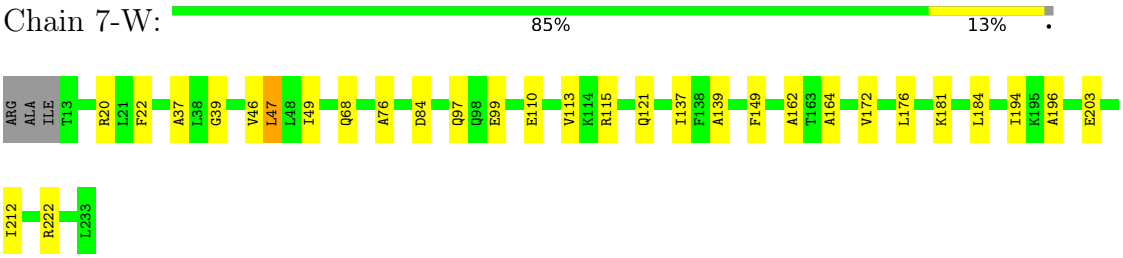
• Molecule 1: Proteasome subunit alpha

Chain 7-U:



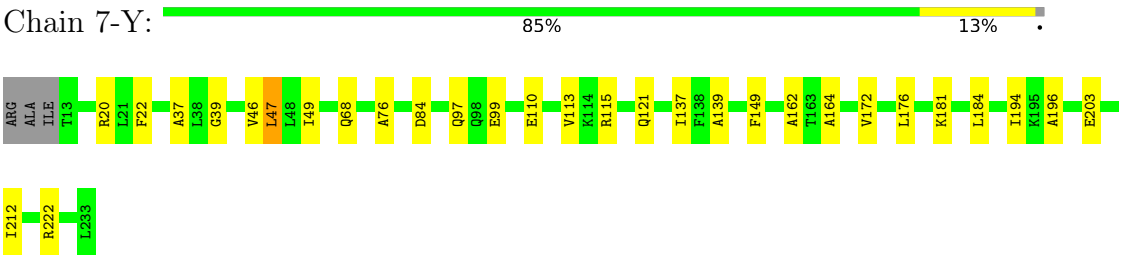
• Molecule 1: Proteasome subunit alpha

Chain 7-W:



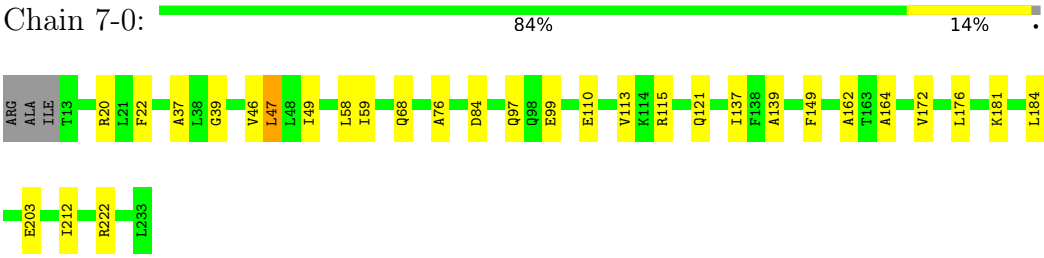
• Molecule 1: Proteasome subunit alpha

Chain 7-Y:



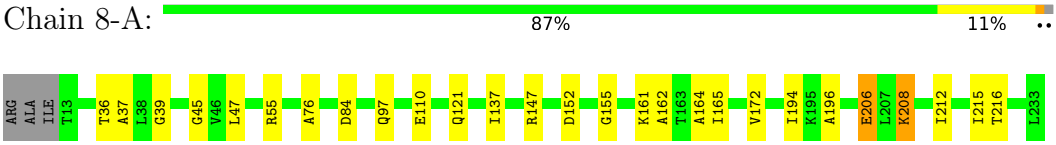
• Molecule 1: Proteasome subunit alpha

Chain 7-0:



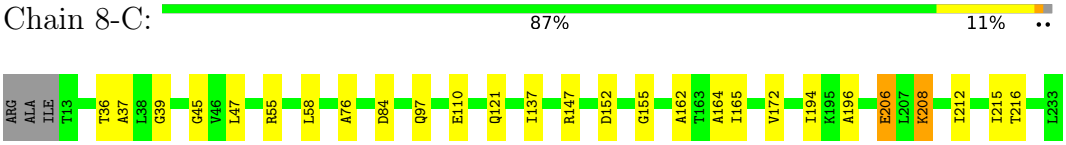
• Molecule 1: Proteasome subunit alpha

Chain 8-A:



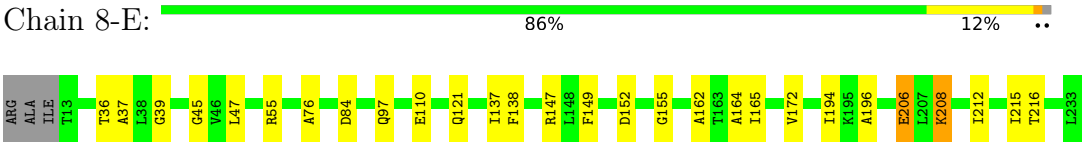
• Molecule 1: Proteasome subunit alpha

Chain 8-C:



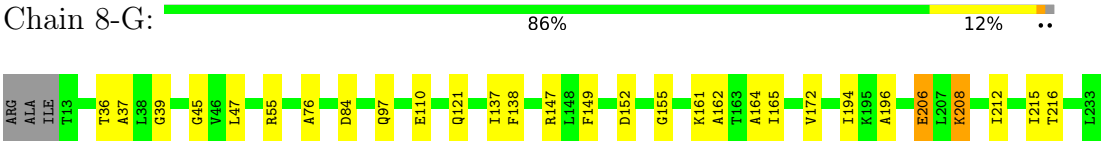
• Molecule 1: Proteasome subunit alpha

Chain 8-E:



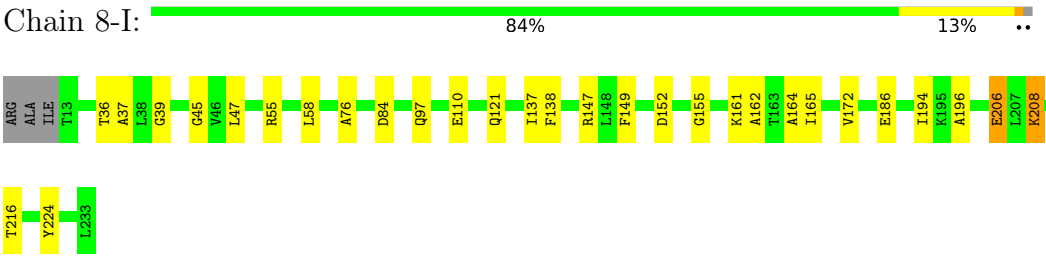
• Molecule 1: Proteasome subunit alpha

Chain 8-G:



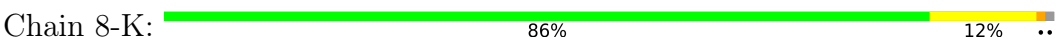
• Molecule 1: Proteasome subunit alpha

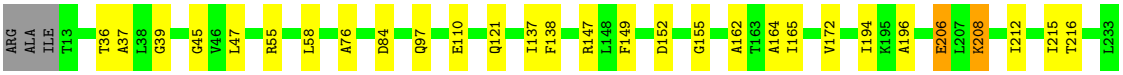
Chain 8-I:



• Molecule 1: Proteasome subunit alpha

Chain 8-K:





• Molecule 1: Proteasome subunit alpha

Chain 8-M:

• Molecule 1: Proteasome subunit alpha

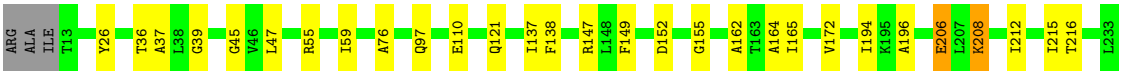
Chain 8-O:

• Molecule 1: Proteasome subunit alpha

Chain 8-Q:

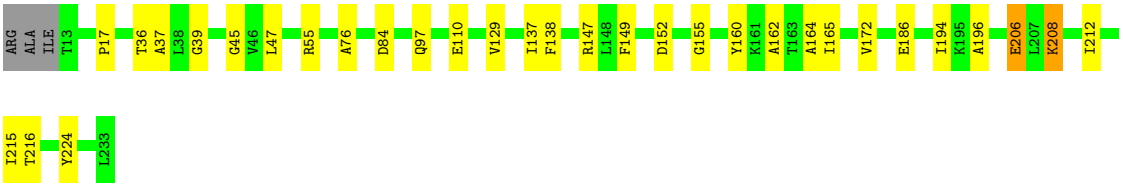
• Molecule 1: Proteasome subunit alpha

Chain 8-S:



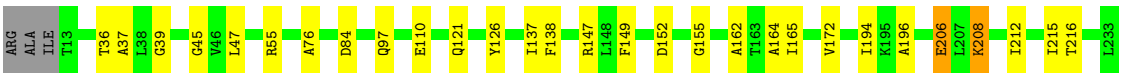
• Molecule 1: Proteasome subunit alpha

Chain 8-U:



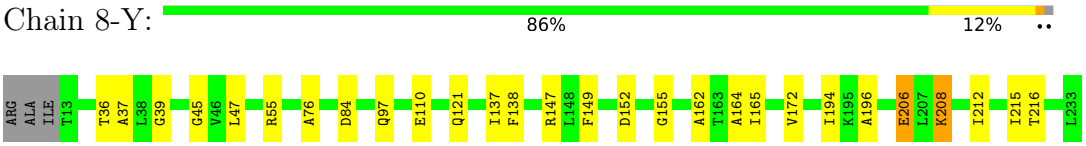
• Molecule 1: Proteasome subunit alpha

Chain 8-W:



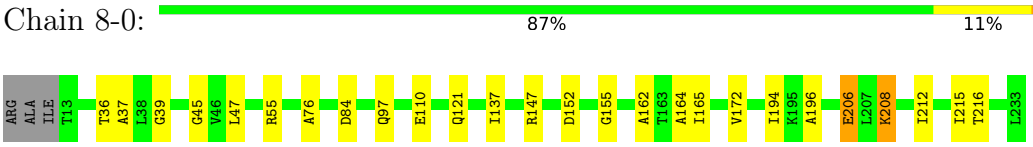
• Molecule 1: Proteasome subunit alpha

Chain 8-Y:



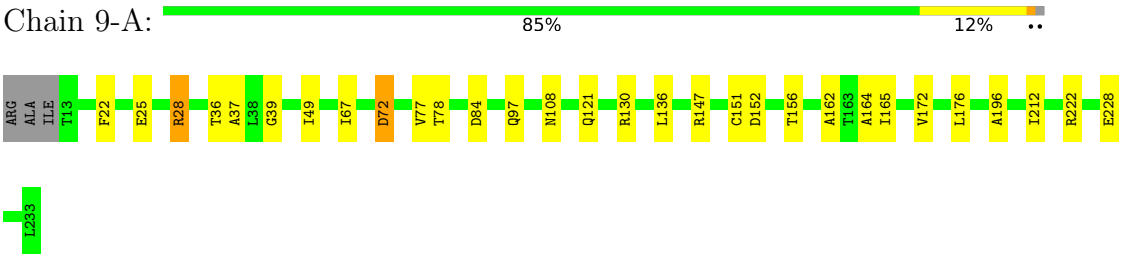
• Molecule 1: Proteasome subunit alpha

Chain 8-0:



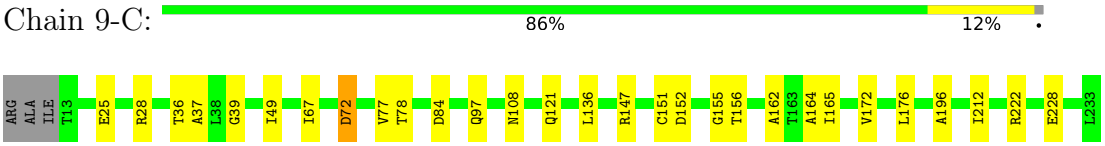
• Molecule 1: Proteasome subunit alpha

Chain 9-A:



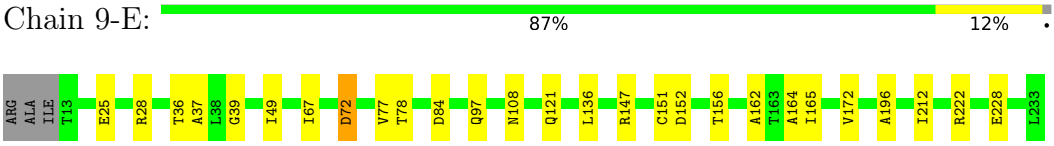
• Molecule 1: Proteasome subunit alpha

Chain 9-C:



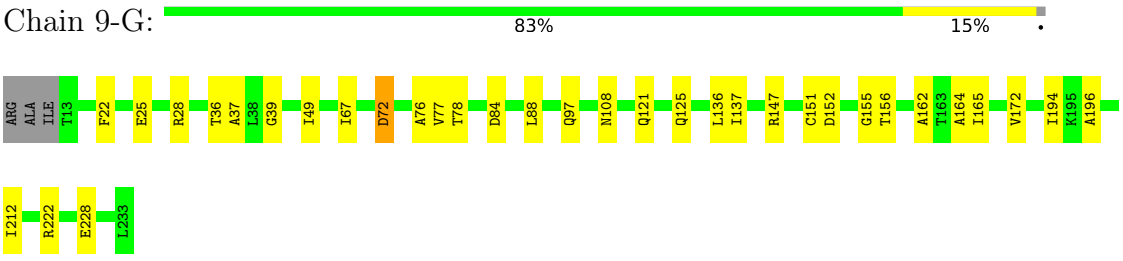
• Molecule 1: Proteasome subunit alpha

Chain 9-E:



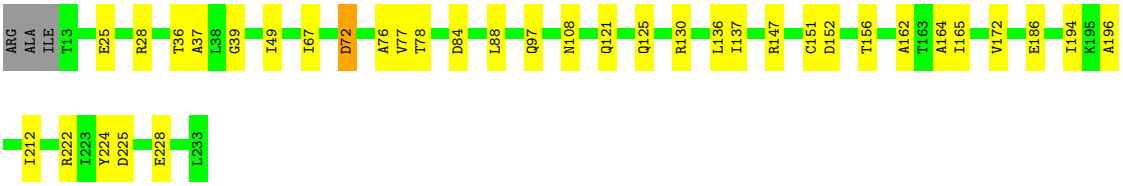
• Molecule 1: Proteasome subunit alpha

Chain 9-G:



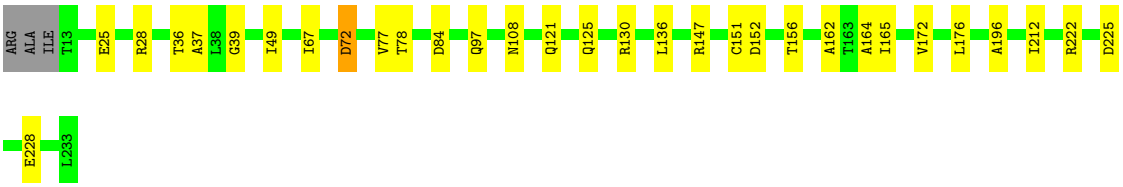
• Molecule 1: Proteasome subunit alpha

Chain 9-I:



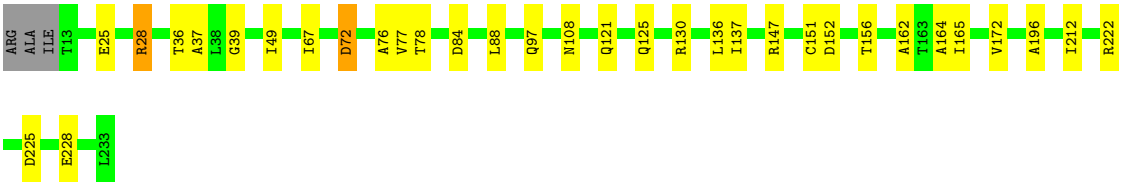
• Molecule 1: Proteasome subunit alpha

Chain 9-K:



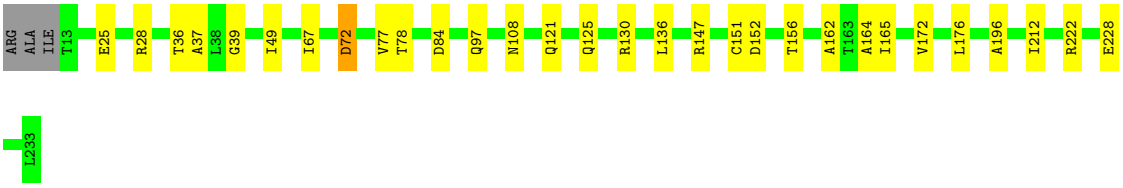
• Molecule 1: Proteasome subunit alpha

Chain 9-M:



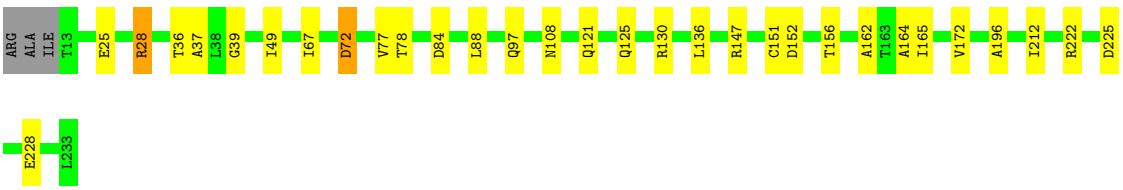
• Molecule 1: Proteasome subunit alpha

Chain 9-O:



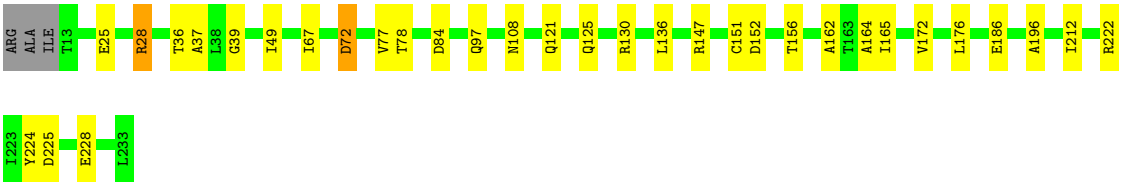
• Molecule 1: Proteasome subunit alpha

Chain 9-Q:



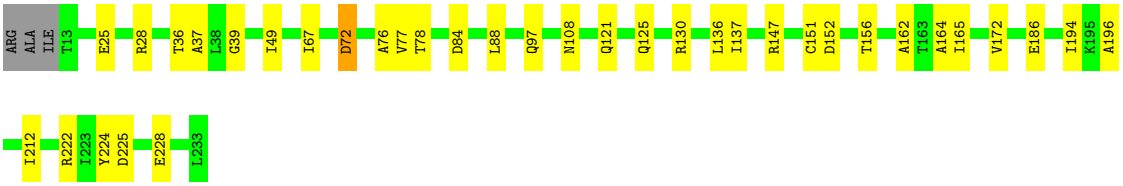
• Molecule 1: Proteasome subunit alpha

Chain 9-S:



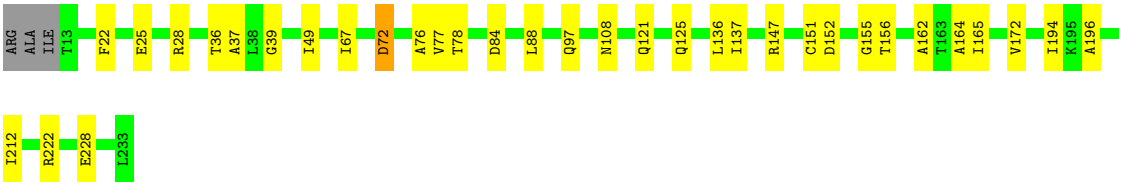
• Molecule 1: Proteasome subunit alpha

Chain 9-U:



• Molecule 1: Proteasome subunit alpha

Chain 9-W:

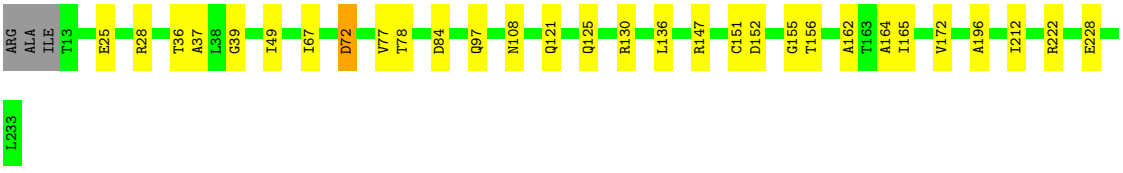


• Molecule 1: Proteasome subunit alpha

Chain 9-Y:

• Molecule 1: Proteasome subunit alpha

Chain 9-0:

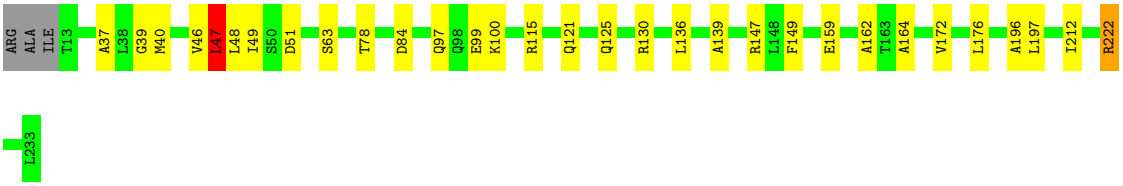


• Molecule 1: Proteasome subunit alpha

Chain 10-A:

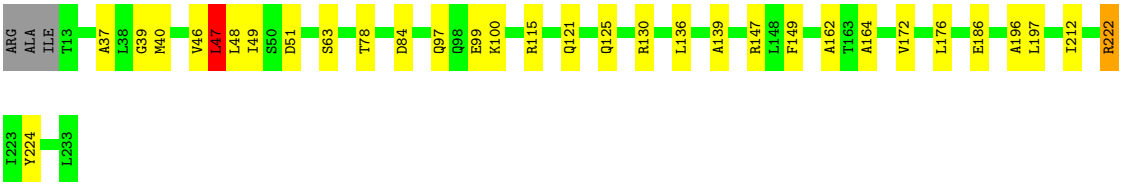
• Molecule 1: Proteasome subunit alpha

Chain 10-C:



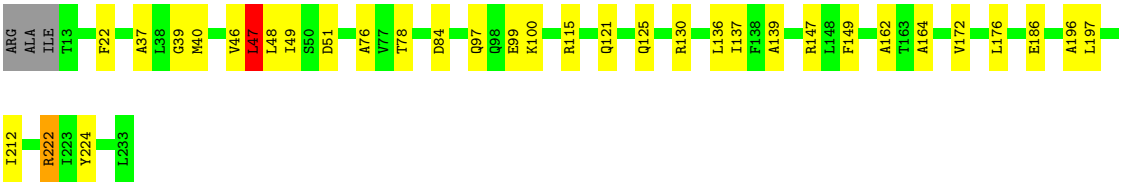
• Molecule 1: Proteasome subunit alpha

Chain 10-E:



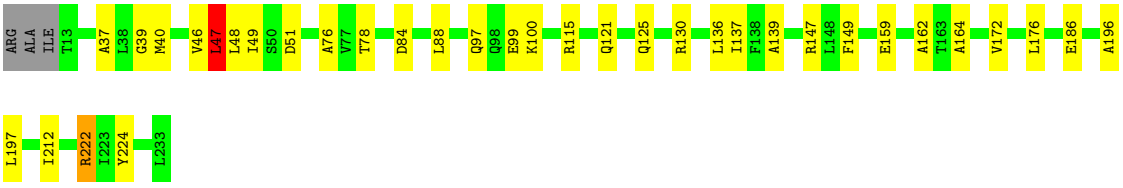
• Molecule 1: Proteasome subunit alpha

Chain 10-G:



• Molecule 1: Proteasome subunit alpha

Chain 10-I:



• Molecule 1: Proteasome subunit alpha

Chain 10-K:

• Molecule 1: Proteasome subunit alpha

Chain 10-M:

• Molecule 1: Proteasome subunit alpha

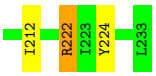
Chain 10-O:

• Molecule 1: Proteasome subunit alpha

Chain 10-Q:

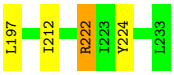
• Molecule 1: Proteasome subunit alpha

Chain 10-S:



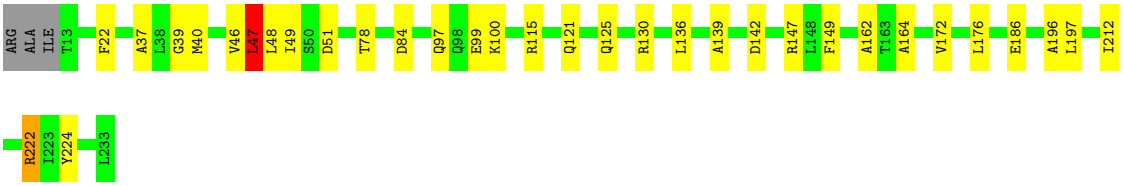
• Molecule 1: Proteasome subunit alpha

Chain 10-U:



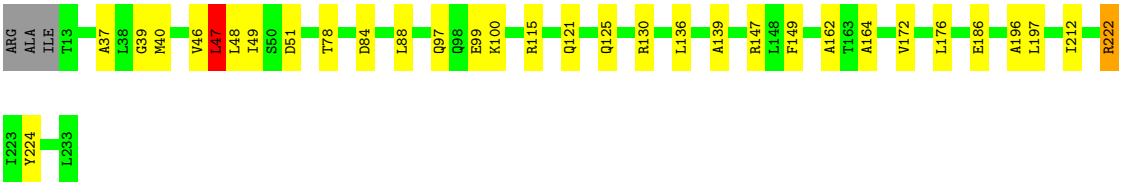
• Molecule 1: Proteasome subunit alpha

Chain 10-W:



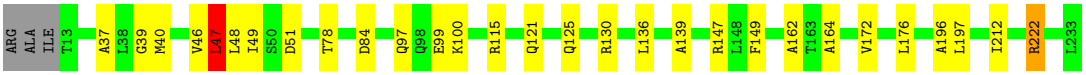
• Molecule 1: Proteasome subunit alpha

Chain 10-Y:



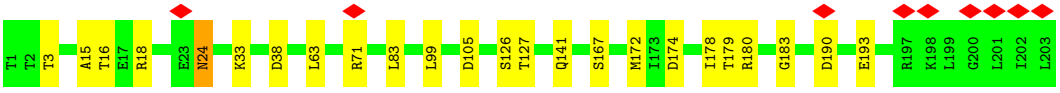
• Molecule 1: Proteasome subunit alpha

Chain 10-0:



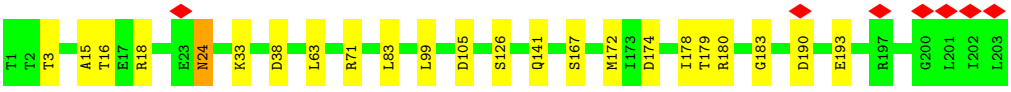
• Molecule 2: Proteasome subunit beta

Chain 1-B:



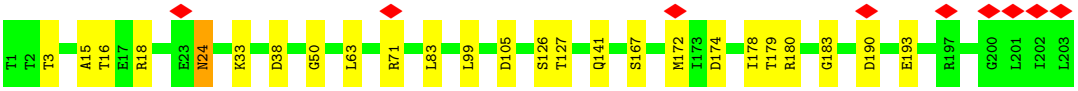
• Molecule 2: Proteasome subunit beta

Chain 1-D:



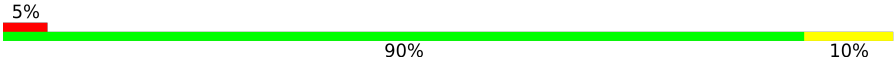
• Molecule 2: Proteasome subunit beta

Chain 1-F:



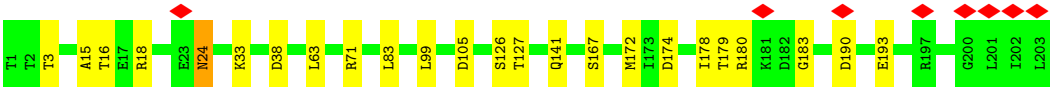
• Molecule 2: Proteasome subunit beta

Chain 1-H:



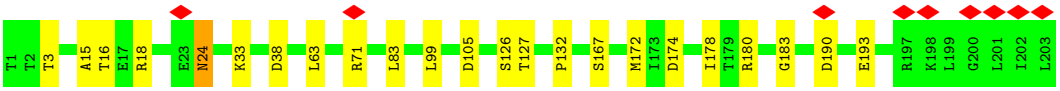
• Molecule 2: Proteasome subunit beta

Chain 1-J:



• Molecule 2: Proteasome subunit beta

Chain 1-L:

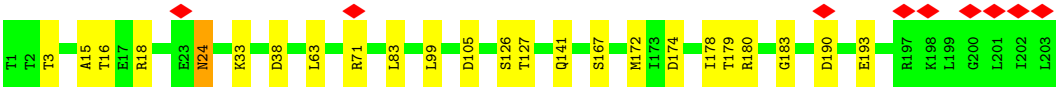


• Molecule 2: Proteasome subunit beta

Chain 1-N:

• Molecule 2: Proteasome subunit beta

Chain 1-P:

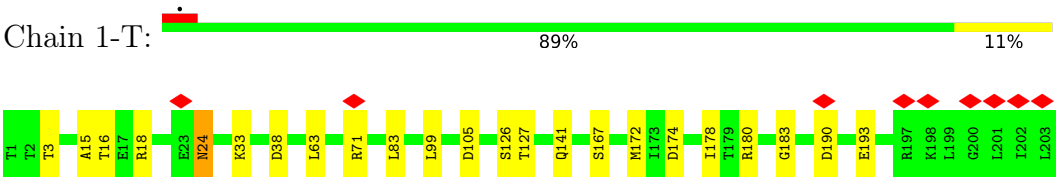


• Molecule 2: Proteasome subunit beta

Chain 1-R:

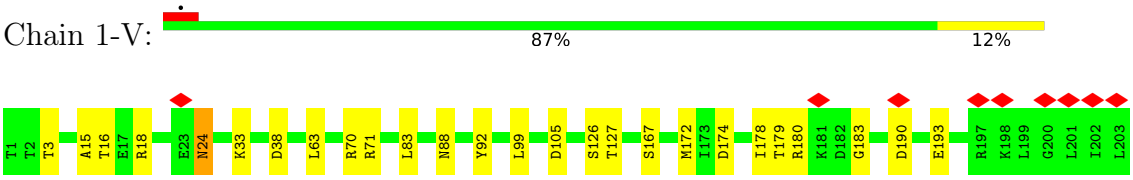
• Molecule 2: Proteasome subunit beta

Chain 1-T:



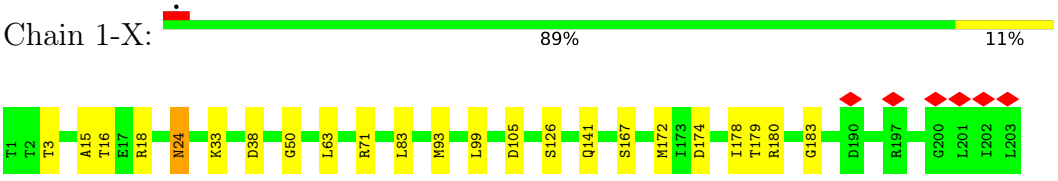
• Molecule 2: Proteasome subunit beta

Chain 1-V:



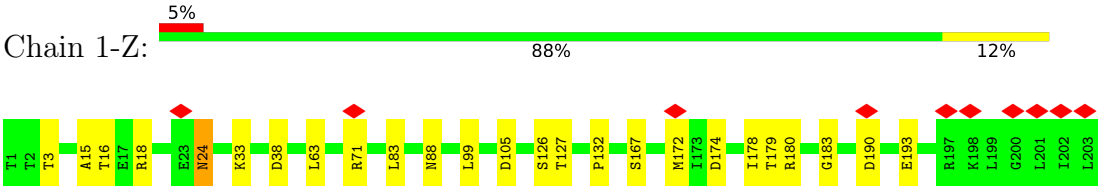
• Molecule 2: Proteasome subunit beta

Chain 1-X:



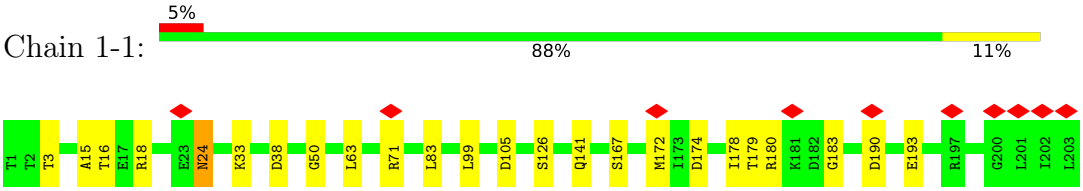
• Molecule 2: Proteasome subunit beta

Chain 1-Z:



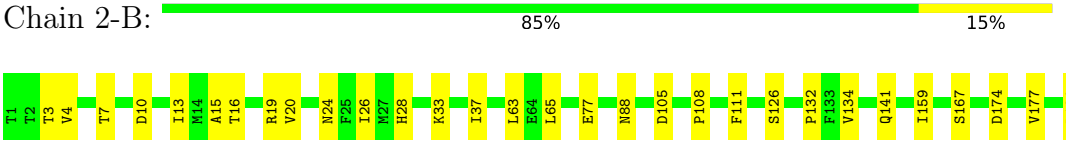
• Molecule 2: Proteasome subunit beta

Chain 1-1:



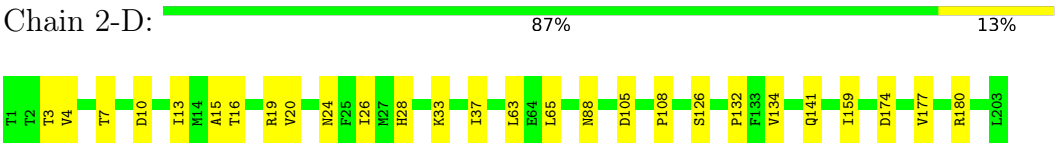
• Molecule 2: Proteasome subunit beta

Chain 2-B:



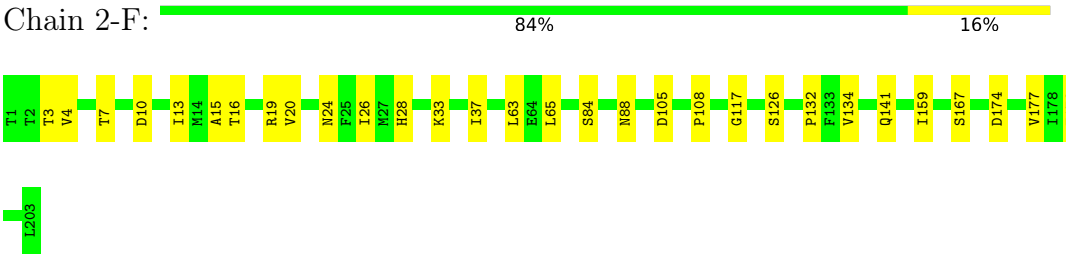
• Molecule 2: Proteasome subunit beta

Chain 2-D:



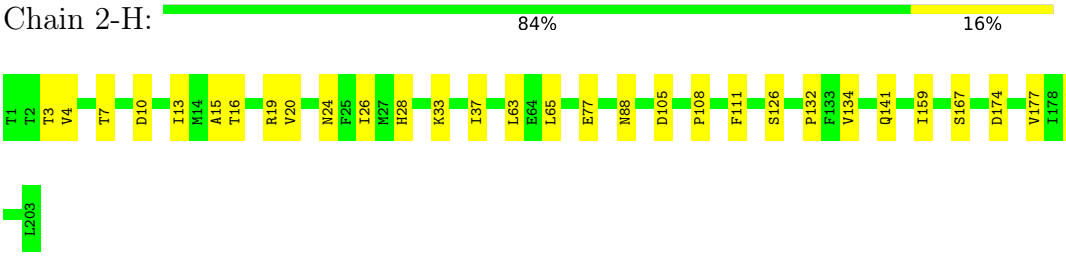
• Molecule 2: Proteasome subunit beta

Chain 2-F:



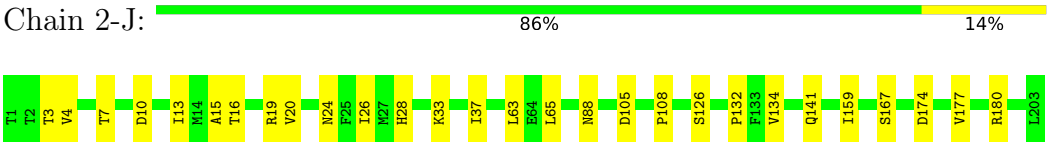
• Molecule 2: Proteasome subunit beta

Chain 2-H:



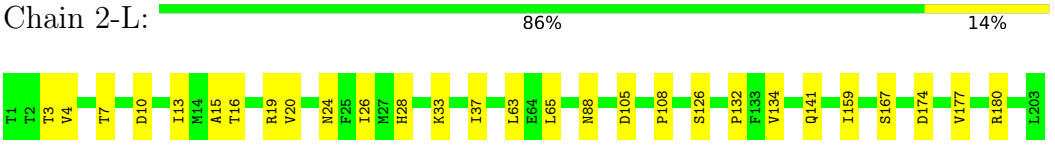
• Molecule 2: Proteasome subunit beta

Chain 2-J:



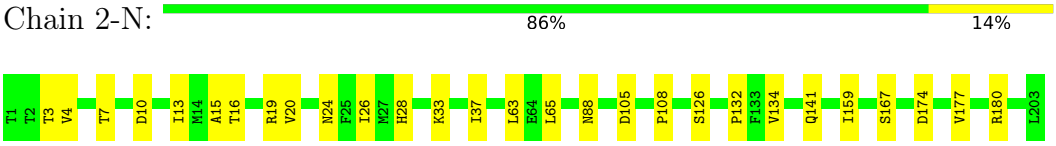
• Molecule 2: Proteasome subunit beta

Chain 2-L:



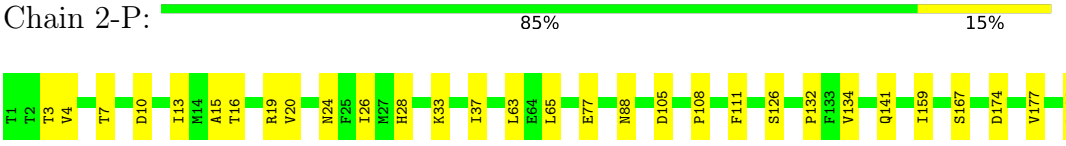
• Molecule 2: Proteasome subunit beta

Chain 2-N:



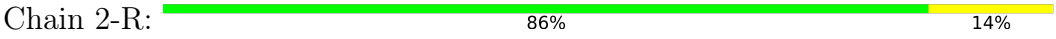
• Molecule 2: Proteasome subunit beta

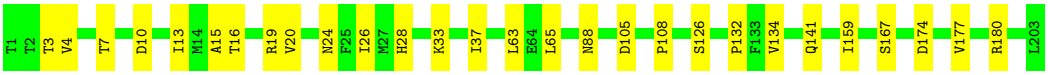
Chain 2-P:



• Molecule 2: Proteasome subunit beta

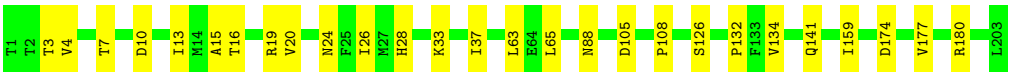
Chain 2-R:





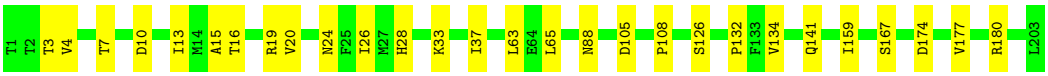
• Molecule 2: Proteasome subunit beta

Chain 2-T:



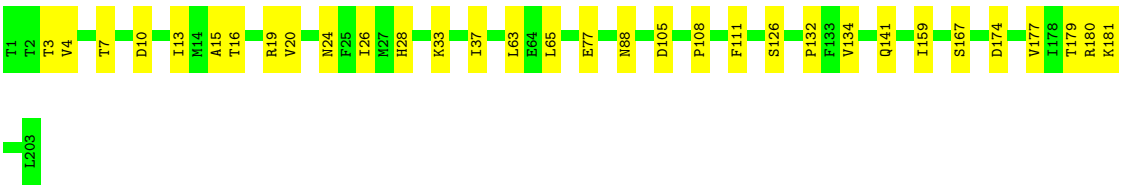
• Molecule 2: Proteasome subunit beta

Chain 2-V:



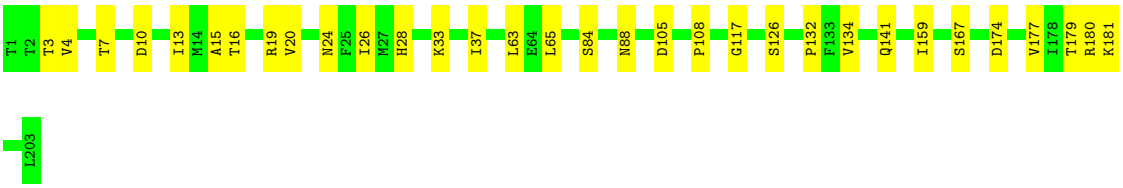
• Molecule 2: Proteasome subunit beta

Chain 2-X:



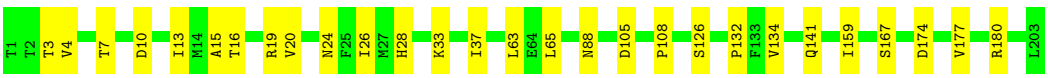
• Molecule 2: Proteasome subunit beta

Chain 2-Z:



• Molecule 2: Proteasome subunit beta

Chain 2-1:

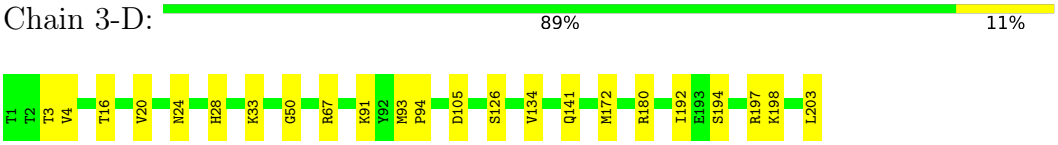


• Molecule 2: Proteasome subunit beta

Chain 3-B:

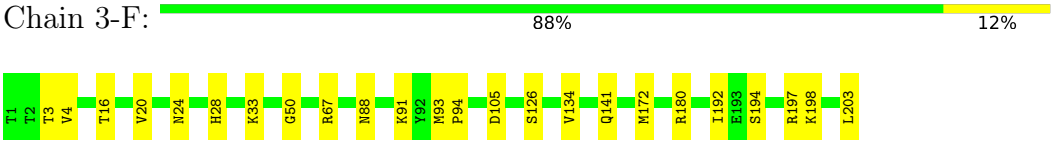
• Molecule 2: Proteasome subunit beta

Chain 3-D:



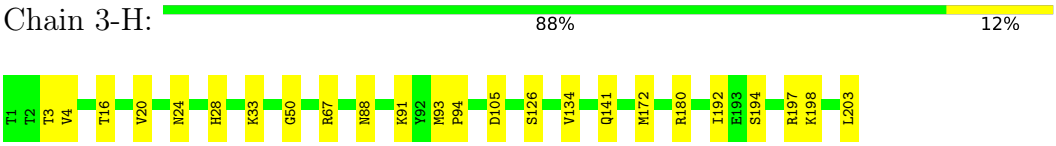
• Molecule 2: Proteasome subunit beta

Chain 3-F:



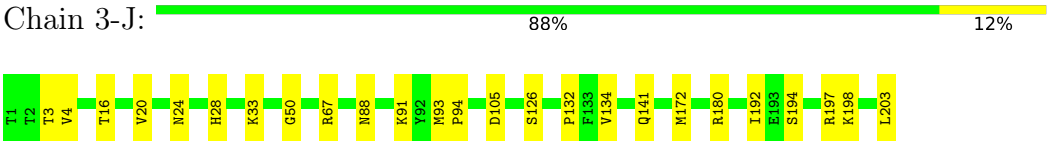
• Molecule 2: Proteasome subunit beta

Chain 3-H:



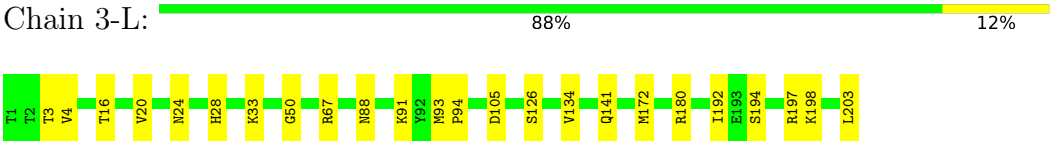
• Molecule 2: Proteasome subunit beta

Chain 3-J:



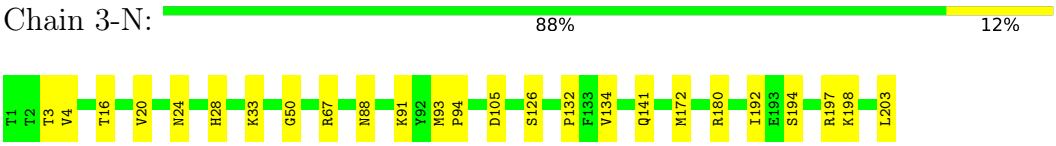
• Molecule 2: Proteasome subunit beta

Chain 3-L:



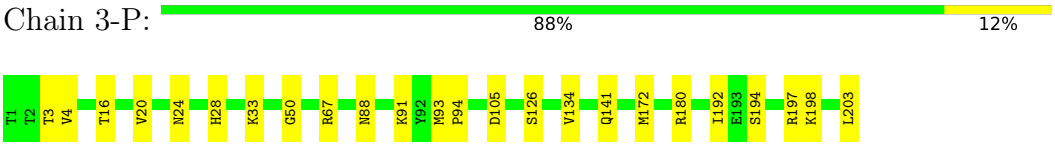
• Molecule 2: Proteasome subunit beta

Chain 3-N:



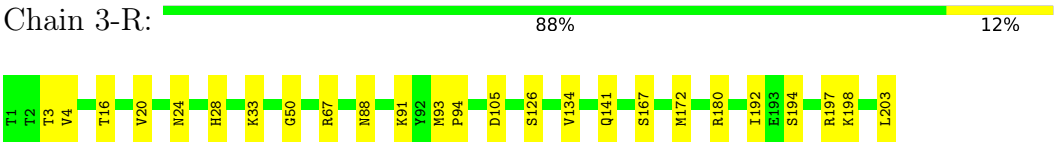
• Molecule 2: Proteasome subunit beta

Chain 3-P:



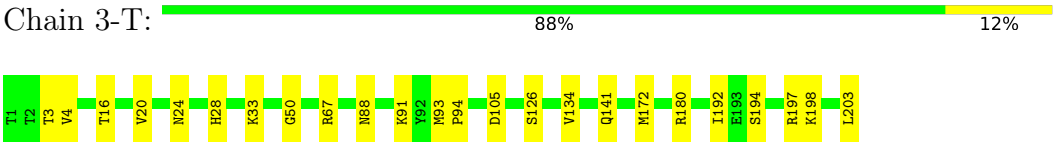
• Molecule 2: Proteasome subunit beta

Chain 3-R:



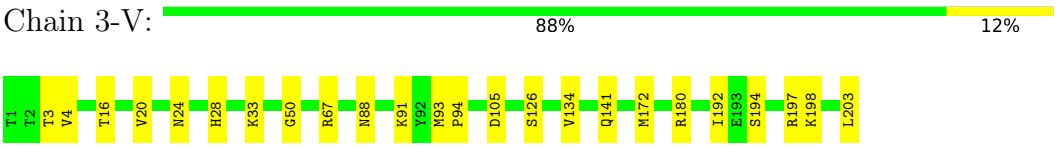
• Molecule 2: Proteasome subunit beta

Chain 3-T:



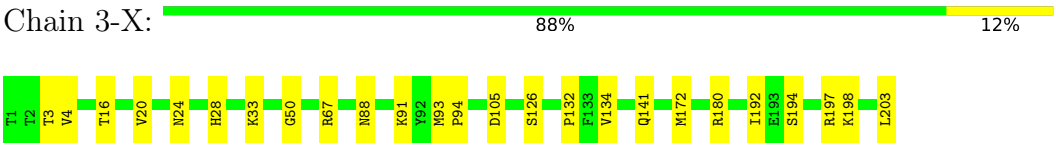
• Molecule 2: Proteasome subunit beta

Chain 3-V:



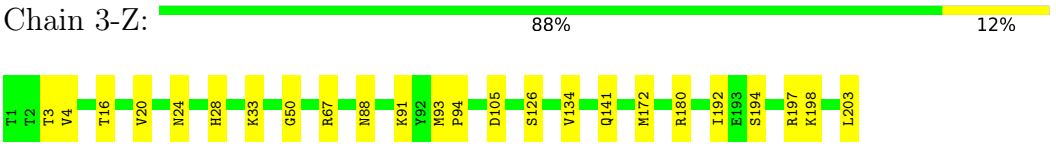
• Molecule 2: Proteasome subunit beta

Chain 3-X:



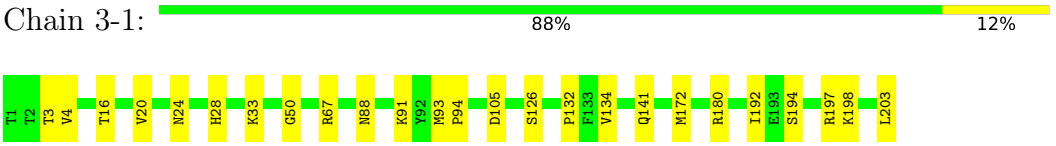
• Molecule 2: Proteasome subunit beta

Chain 3-Z:



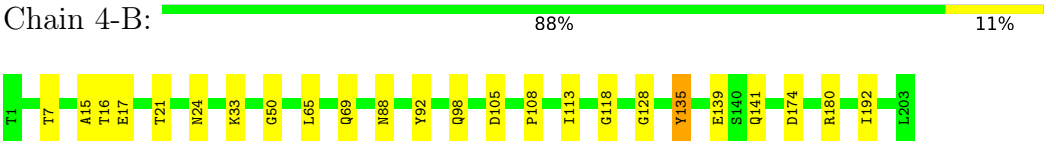
• Molecule 2: Proteasome subunit beta

Chain 3-1:



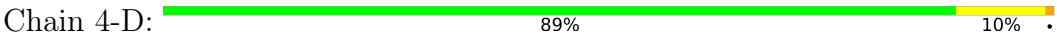
• Molecule 2: Proteasome subunit beta

Chain 4-B:



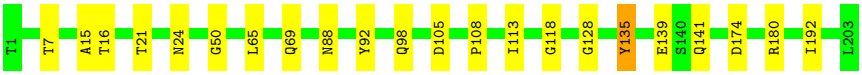
• Molecule 2: Proteasome subunit beta

Chain 4-D:



• Molecule 2: Proteasome subunit beta

Chain 4-F:



• Molecule 2: Proteasome subunit beta

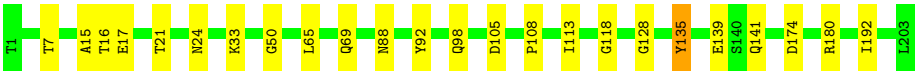
Chain 4-H:

• Molecule 2: Proteasome subunit beta

Chain 4-J:

• Molecule 2: Proteasome subunit beta

Chain 4-L:



• Molecule 2: Proteasome subunit beta

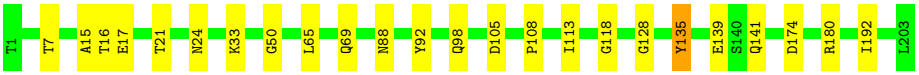
Chain 4-N:

• Molecule 2: Proteasome subunit beta

Chain 4-P:

• Molecule 2: Proteasome subunit beta

Chain 4-R:



• Molecule 2: Proteasome subunit beta

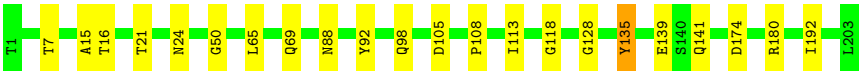
Chain 4-T:

• Molecule 2: Proteasome subunit beta

Chain 4-V:

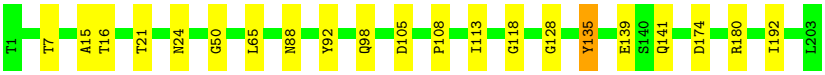
• Molecule 2: Proteasome subunit beta

Chain 4-X:



• Molecule 2: Proteasome subunit beta

Chain 4-Z:

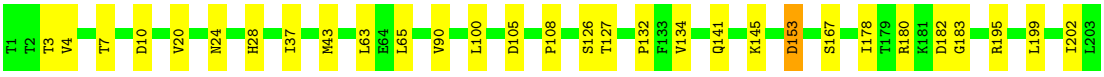


• Molecule 2: Proteasome subunit beta

Chain 4-1:

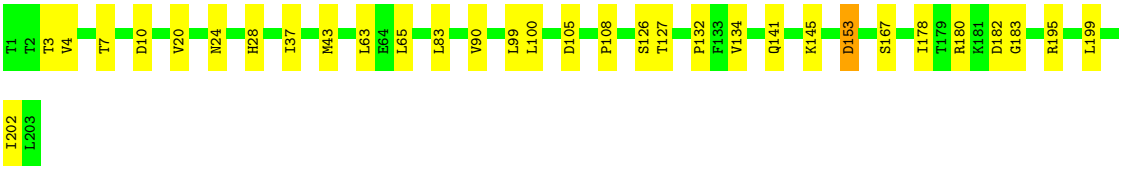
• Molecule 2: Proteasome subunit beta

Chain 5-B:



• Molecule 2: Proteasome subunit beta

Chain 5-D:

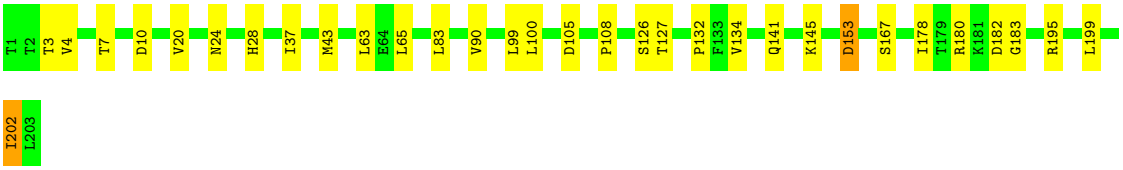


• Molecule 2: Proteasome subunit beta

Chain 5-F:

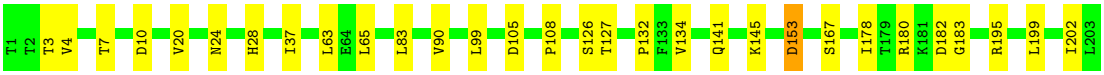
• Molecule 2: Proteasome subunit beta

Chain 5-H:



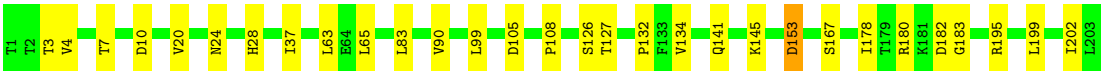
• Molecule 2: Proteasome subunit beta

Chain 5-J:



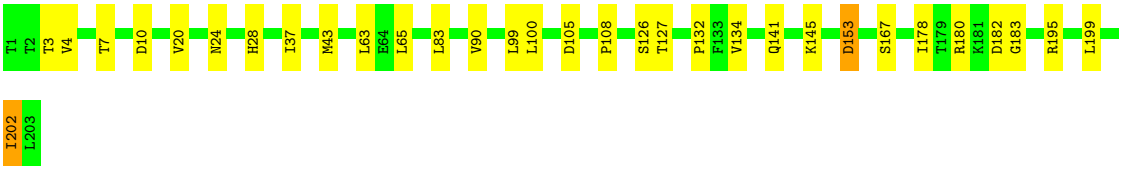
• Molecule 2: Proteasome subunit beta

Chain 5-L:



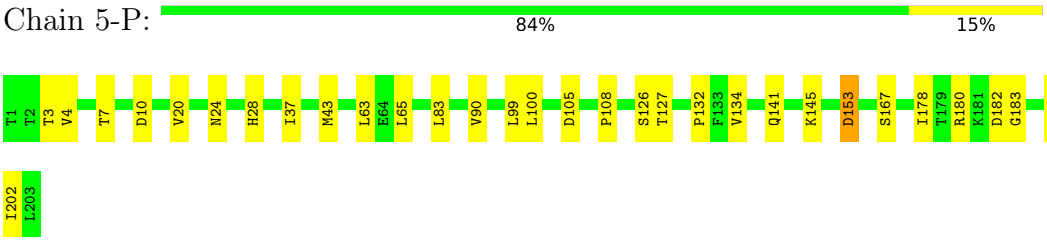
• Molecule 2: Proteasome subunit beta

Chain 5-N:



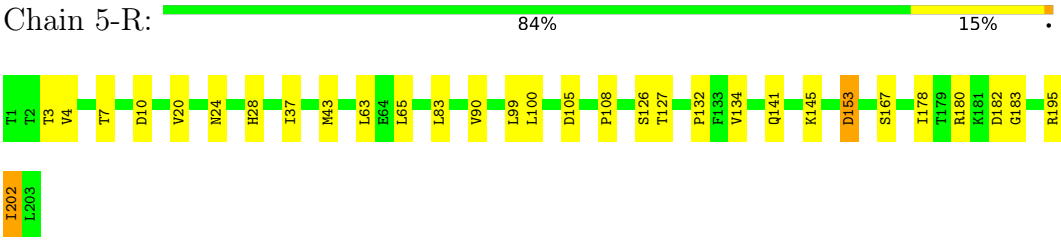
• Molecule 2: Proteasome subunit beta

Chain 5-P:



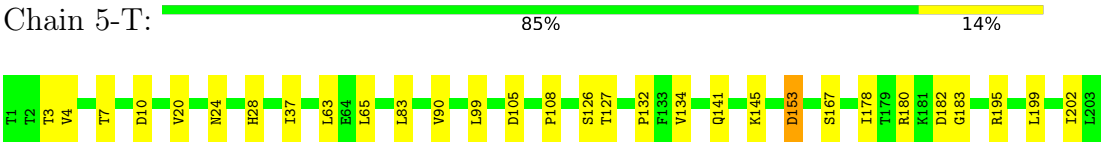
• Molecule 2: Proteasome subunit beta

Chain 5-R:



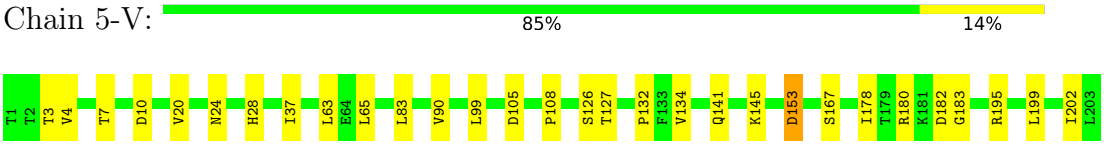
• Molecule 2: Proteasome subunit beta

Chain 5-T:



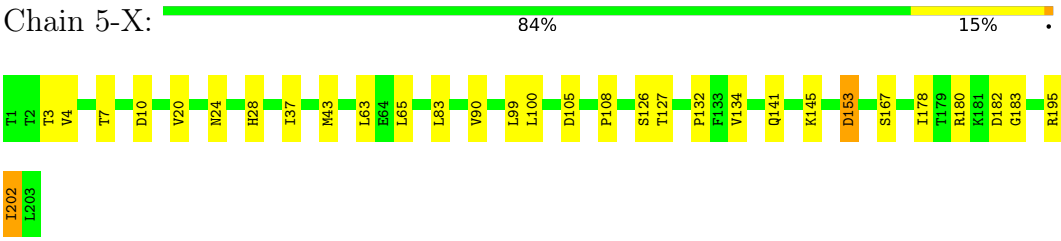
• Molecule 2: Proteasome subunit beta

Chain 5-V:



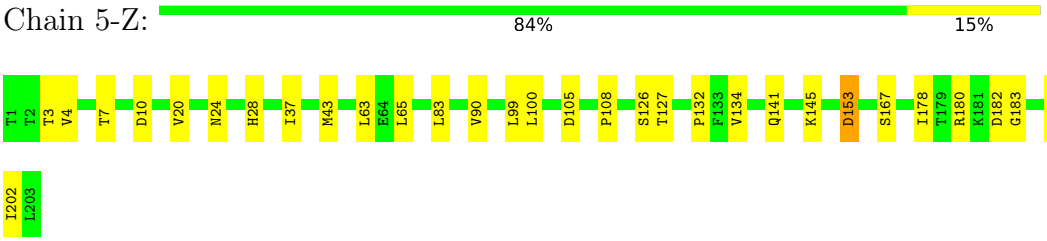
• Molecule 2: Proteasome subunit beta

Chain 5-X:



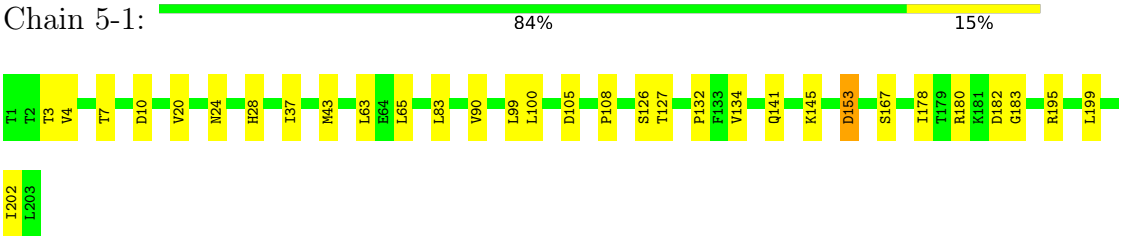
• Molecule 2: Proteasome subunit beta

Chain 5-Z:



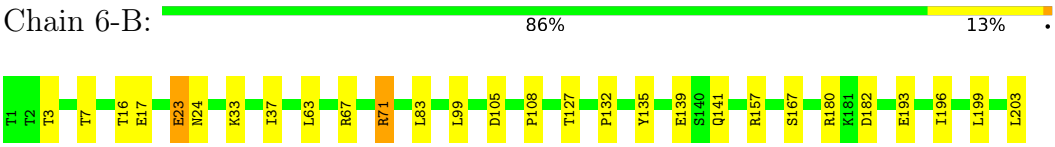
• Molecule 2: Proteasome subunit beta

Chain 5-1:



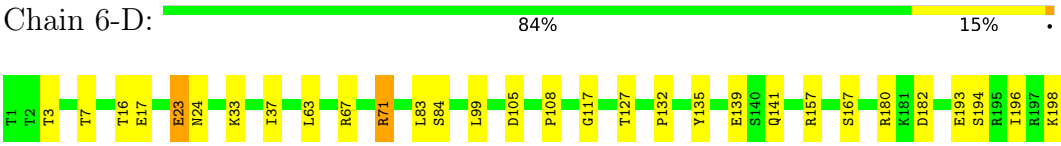
• Molecule 2: Proteasome subunit beta

Chain 6-B:



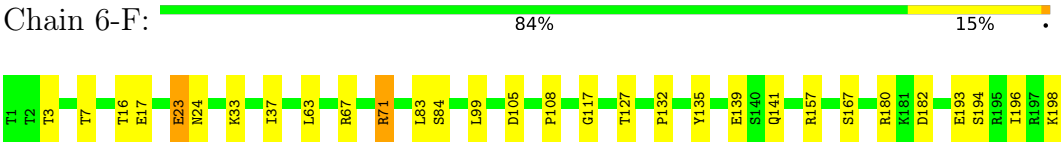
• Molecule 2: Proteasome subunit beta

Chain 6-D:



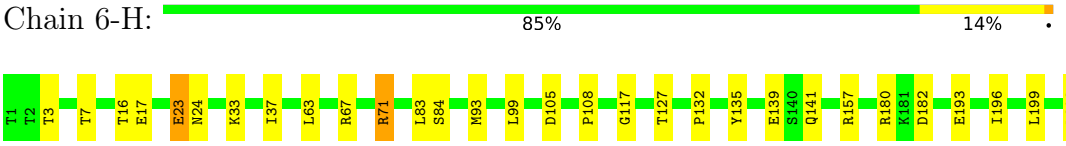
• Molecule 2: Proteasome subunit beta

Chain 6-F:



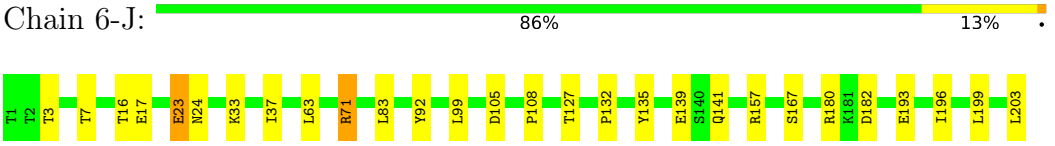
• Molecule 2: Proteasome subunit beta

Chain 6-H:



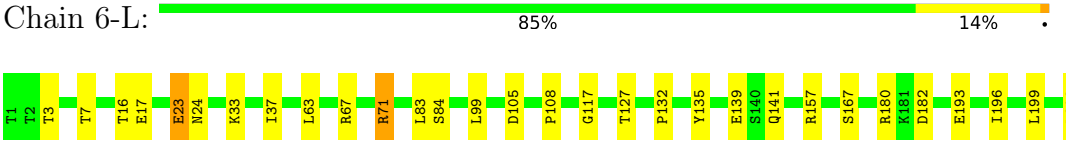
• Molecule 2: Proteasome subunit beta

Chain 6-J:



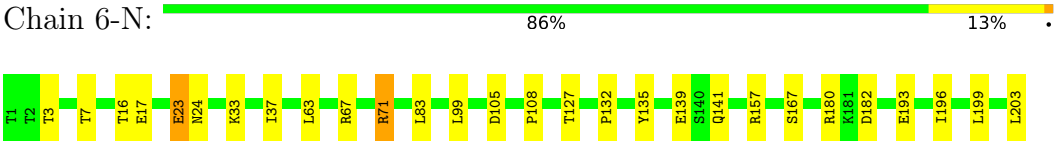
• Molecule 2: Proteasome subunit beta

Chain 6-L:



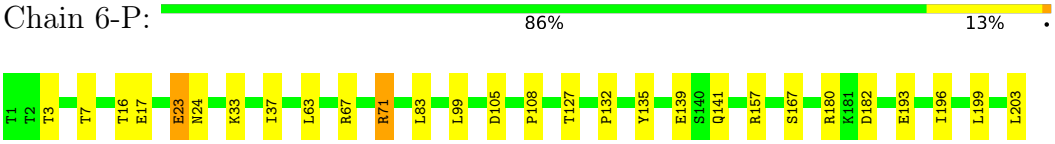
• Molecule 2: Proteasome subunit beta

Chain 6-N:



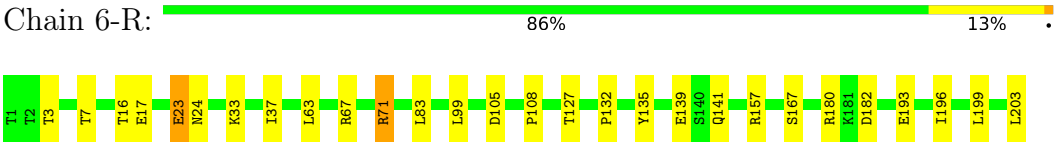
• Molecule 2: Proteasome subunit beta

Chain 6-P:



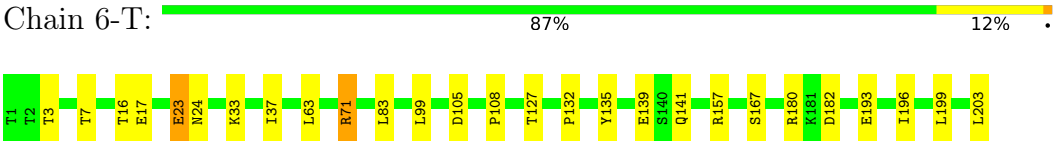
• Molecule 2: Proteasome subunit beta

Chain 6-R:



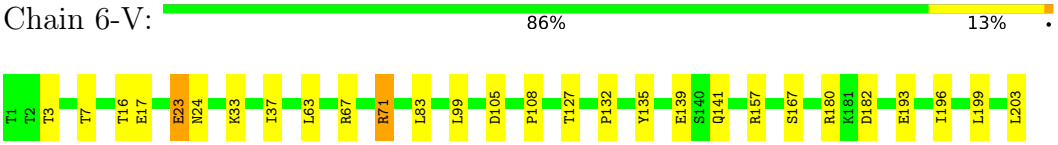
• Molecule 2: Proteasome subunit beta

Chain 6-T:



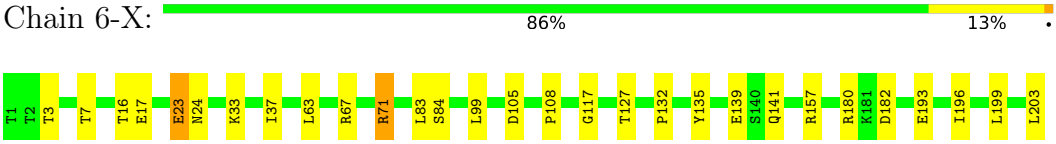
• Molecule 2: Proteasome subunit beta

Chain 6-V:



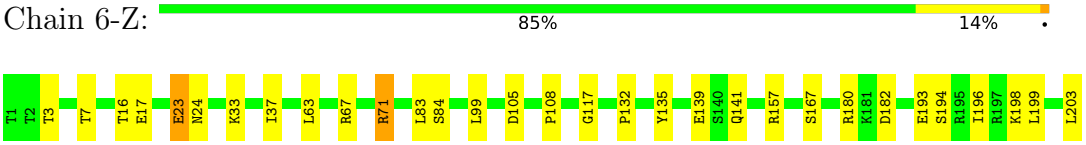
• Molecule 2: Proteasome subunit beta

Chain 6-X:



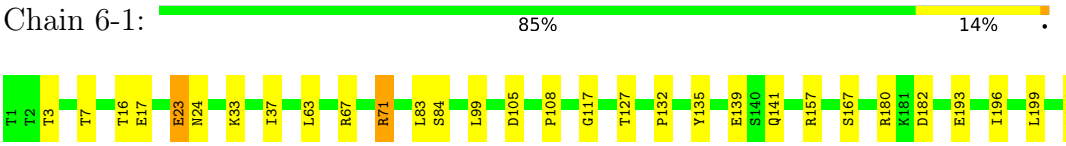
• Molecule 2: Proteasome subunit beta

Chain 6-Z:



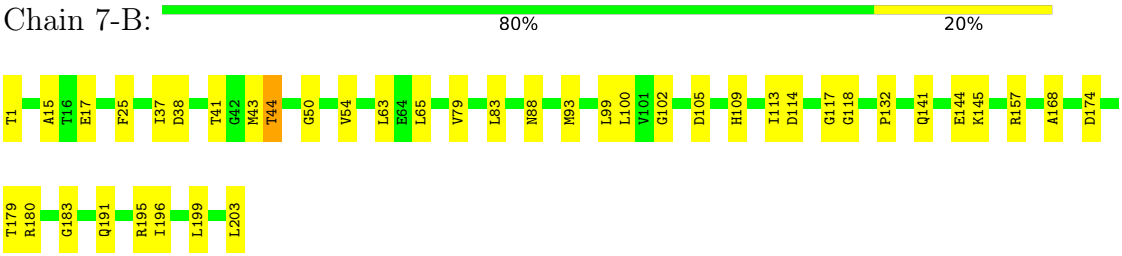
• Molecule 2: Proteasome subunit beta

Chain 6-1:



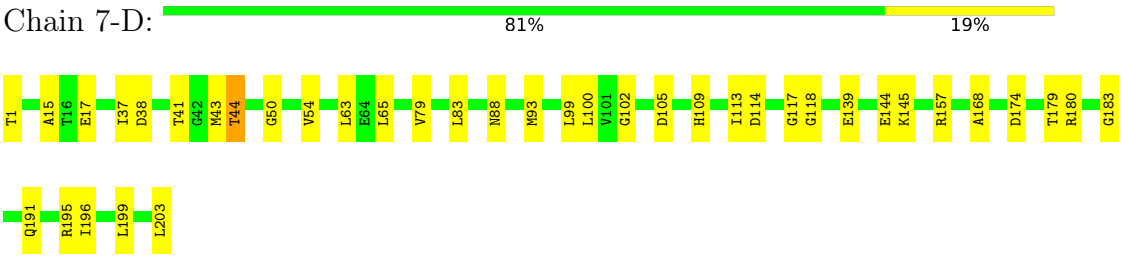
• Molecule 2: Proteasome subunit beta

Chain 7-B:



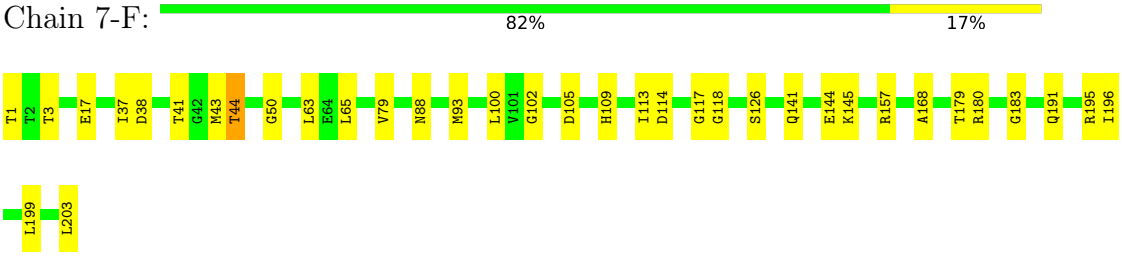
• Molecule 2: Proteasome subunit beta

Chain 7-D:



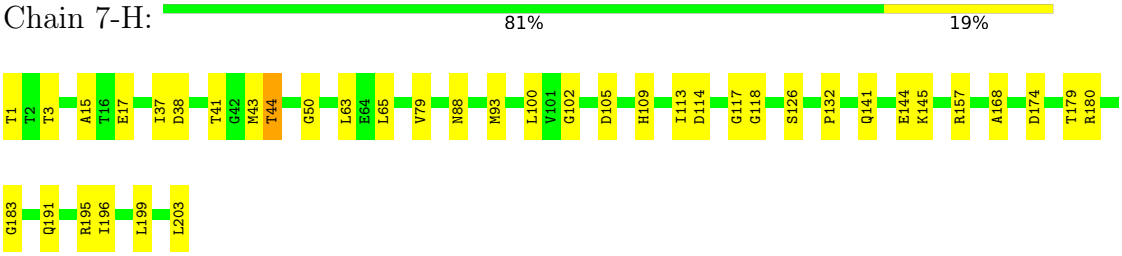
• Molecule 2: Proteasome subunit beta

Chain 7-F:



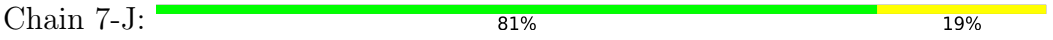
• Molecule 2: Proteasome subunit beta

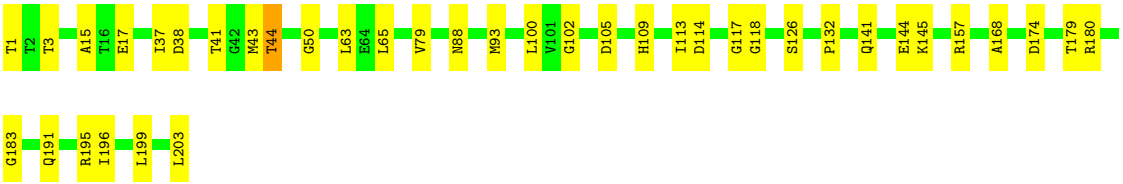
Chain 7-H:



• Molecule 2: Proteasome subunit beta

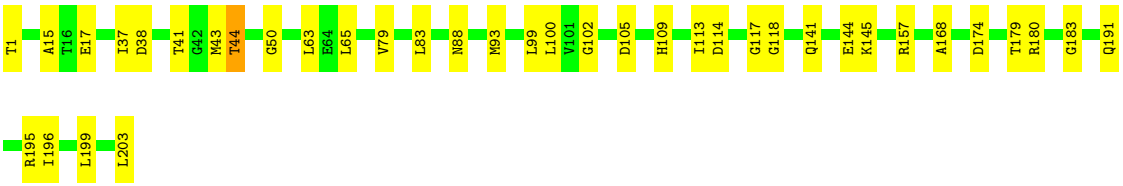
Chain 7-J:





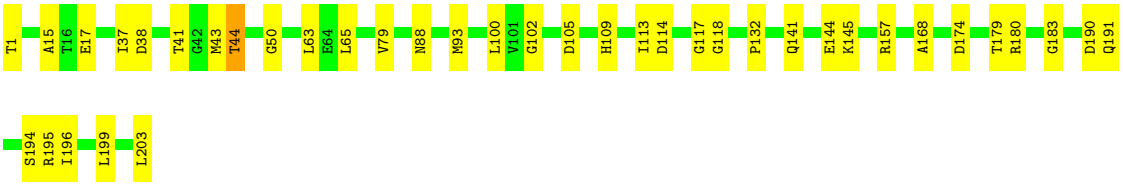
• Molecule 2: Proteasome subunit beta

Chain 7-L:



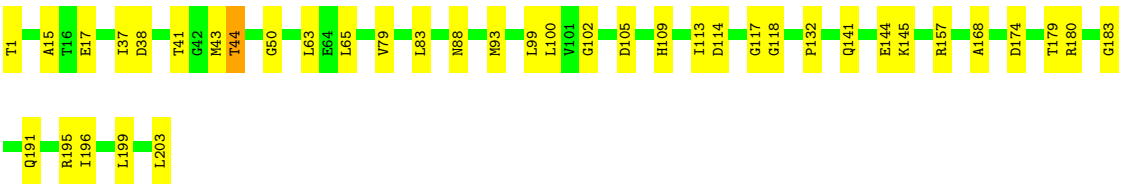
• Molecule 2: Proteasome subunit beta

Chain 7-N:



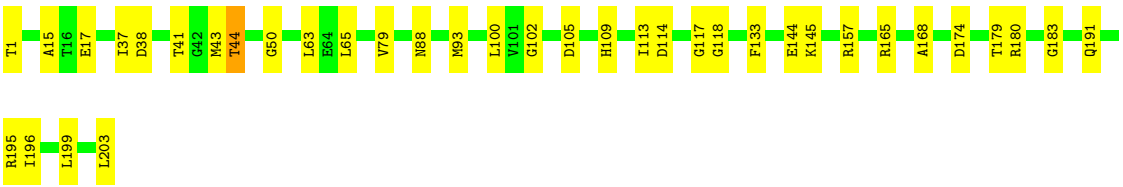
• Molecule 2: Proteasome subunit beta

Chain 7-P:



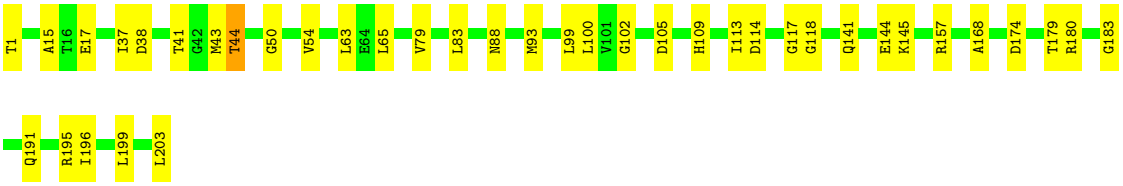
• Molecule 2: Proteasome subunit beta

Chain 7-R:



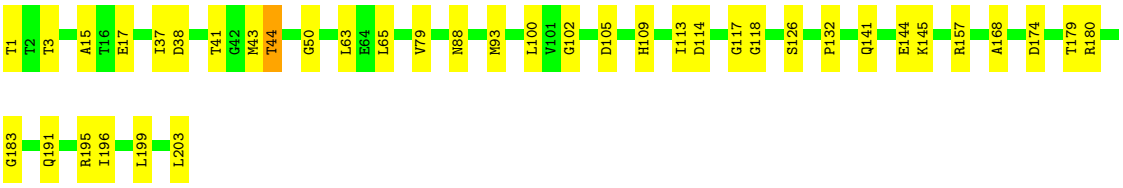
• Molecule 2: Proteasome subunit beta

Chain 7-T:



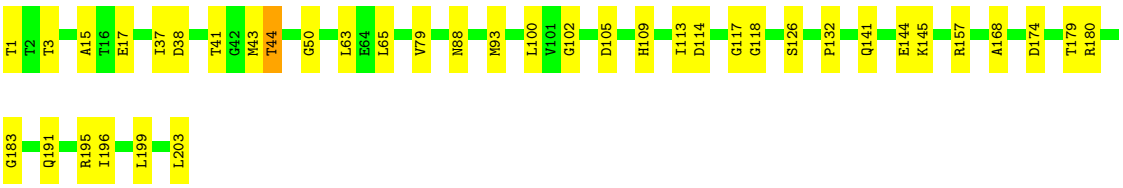
• Molecule 2: Proteasome subunit beta

Chain 7-V:



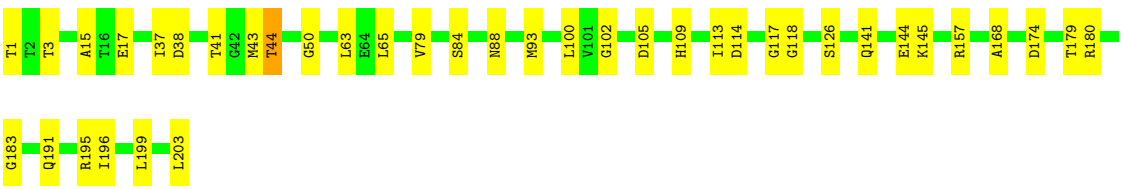
• Molecule 2: Proteasome subunit beta

Chain 7-X:



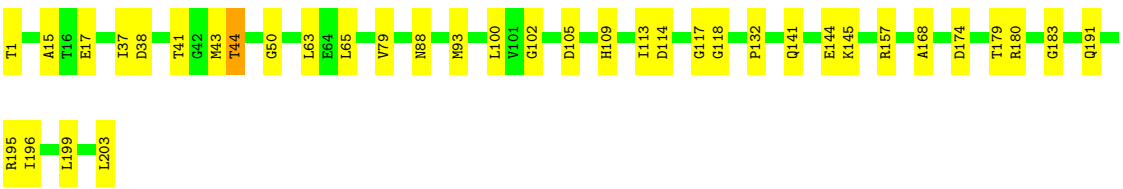
• Molecule 2: Proteasome subunit beta

Chain 7-Z:



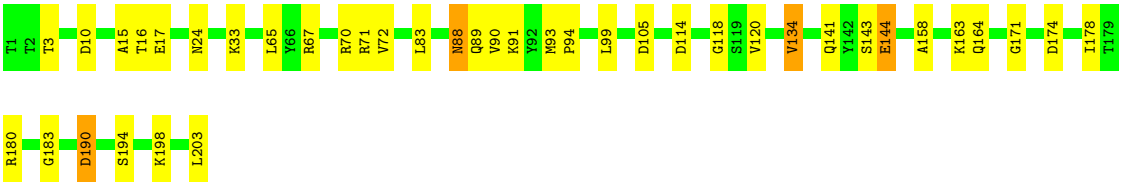
• Molecule 2: Proteasome subunit beta

Chain 7-1:



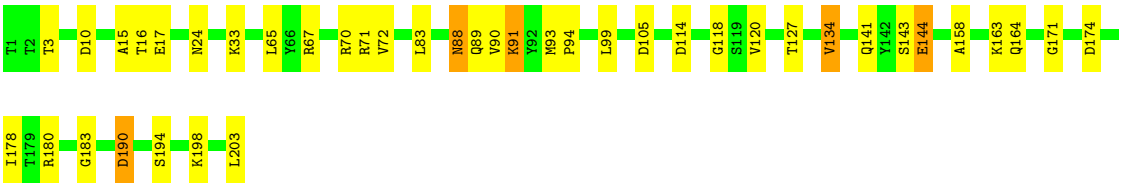
• Molecule 2: Proteasome subunit beta

Chain 8-B:



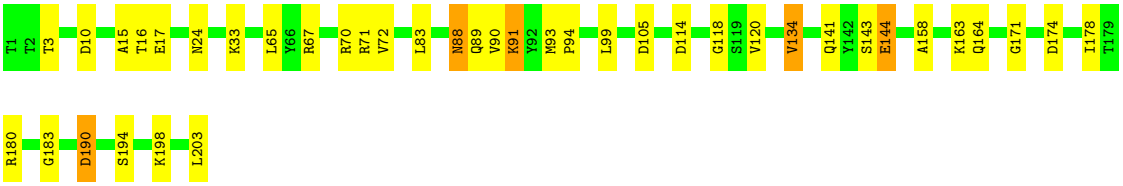
• Molecule 2: Proteasome subunit beta

Chain 8-D:



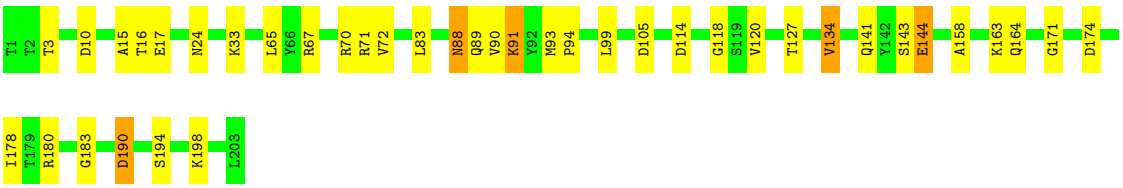
• Molecule 2: Proteasome subunit beta

Chain 8-F:



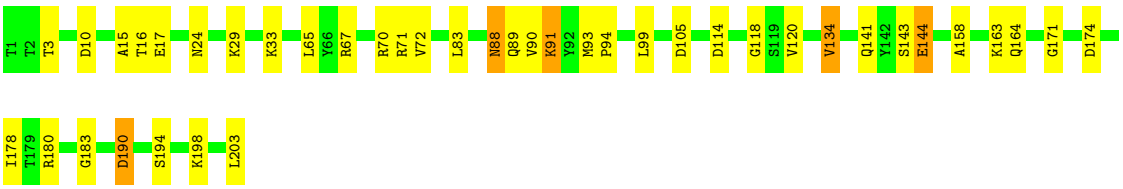
• Molecule 2: Proteasome subunit beta

Chain 8-H:



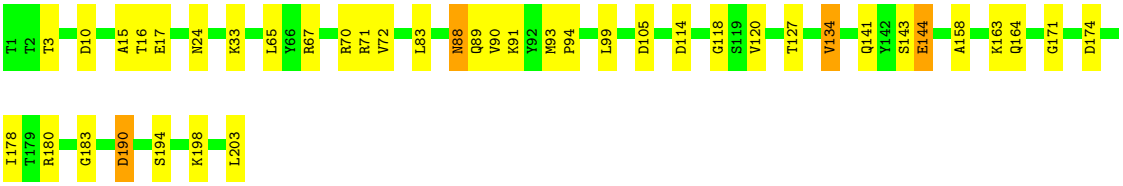
• Molecule 2: Proteasome subunit beta

Chain 8-J:



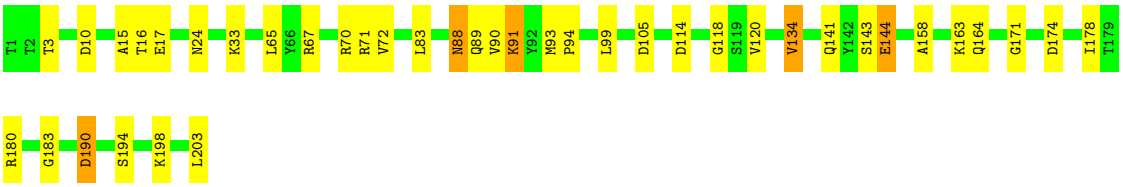
• Molecule 2: Proteasome subunit beta

Chain 8-L:



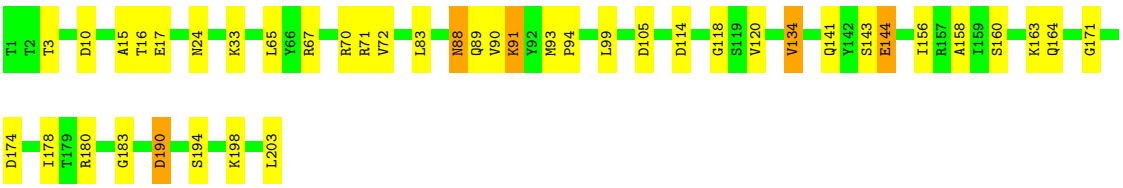
• Molecule 2: Proteasome subunit beta

Chain 8-N:



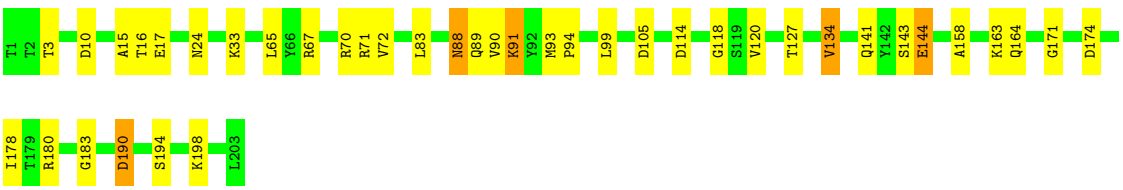
• Molecule 2: Proteasome subunit beta

Chain 8-P:



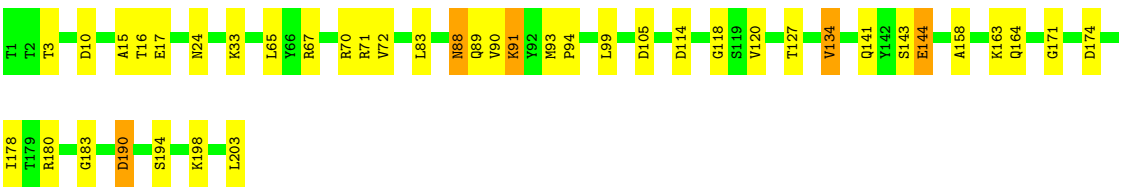
• Molecule 2: Proteasome subunit beta

Chain 8-R:



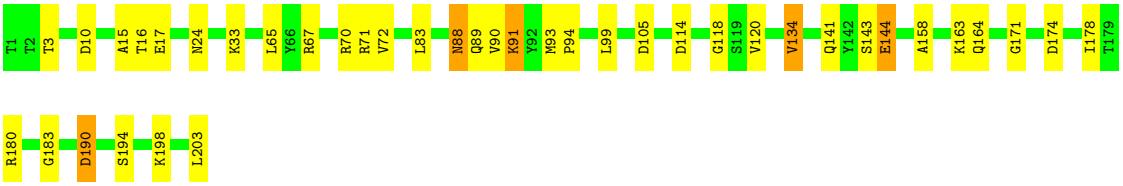
• Molecule 2: Proteasome subunit beta

Chain 8-T:



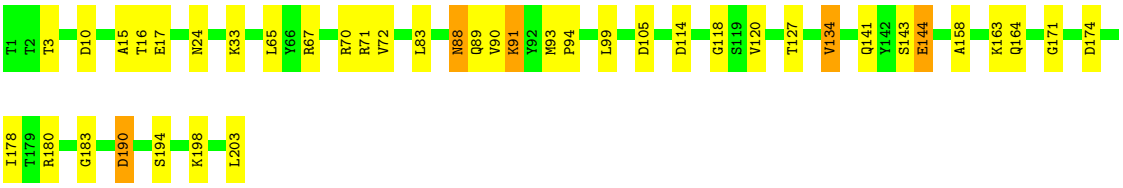
• Molecule 2: Proteasome subunit beta

Chain 8-V:



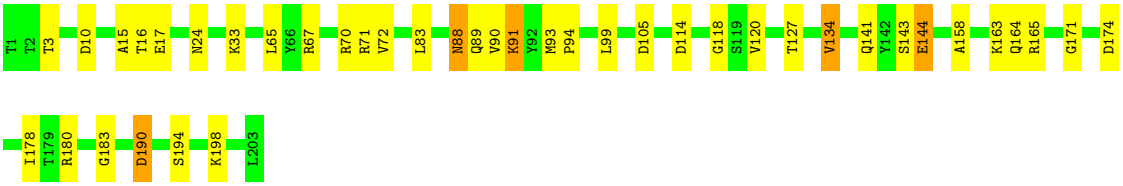
• Molecule 2: Proteasome subunit beta

Chain 8-X:



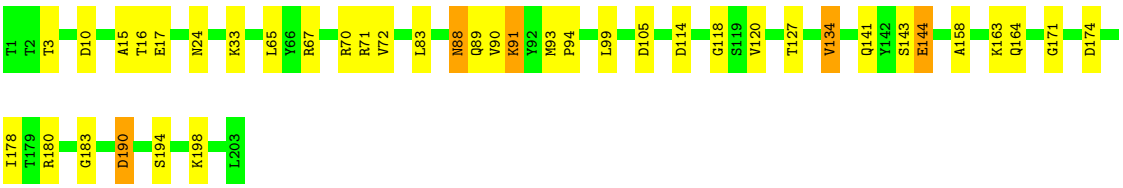
• Molecule 2: Proteasome subunit beta

Chain 8-Z:



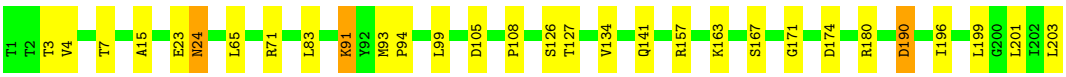
• Molecule 2: Proteasome subunit beta

Chain 8-1:



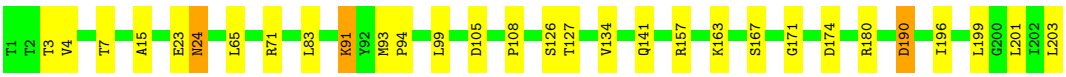
• Molecule 2: Proteasome subunit beta

Chain 9-B:



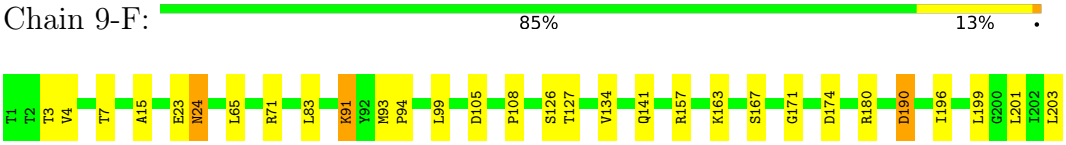
• Molecule 2: Proteasome subunit beta

Chain 9-D:



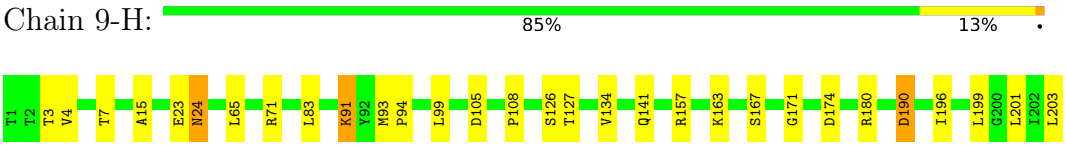
• Molecule 2: Proteasome subunit beta

Chain 9-F:



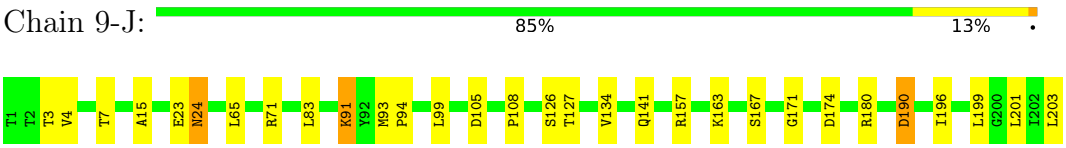
• Molecule 2: Proteasome subunit beta

Chain 9-H:



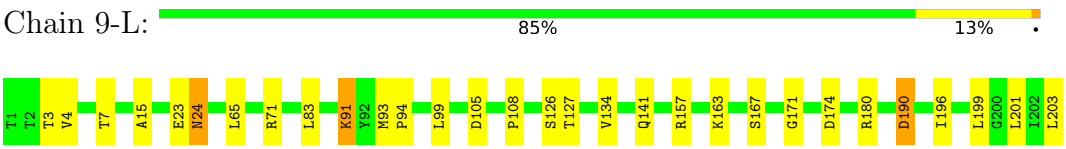
• Molecule 2: Proteasome subunit beta

Chain 9-J:



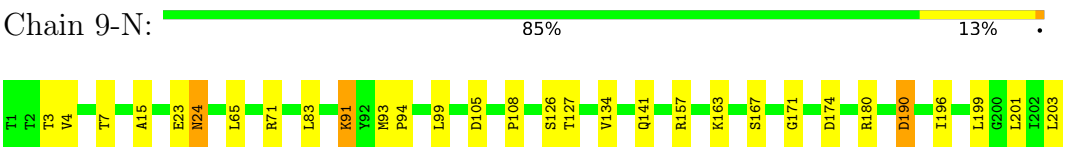
• Molecule 2: Proteasome subunit beta

Chain 9-L:



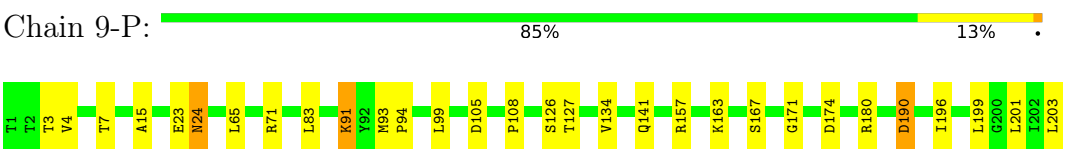
• Molecule 2: Proteasome subunit beta

Chain 9-N:



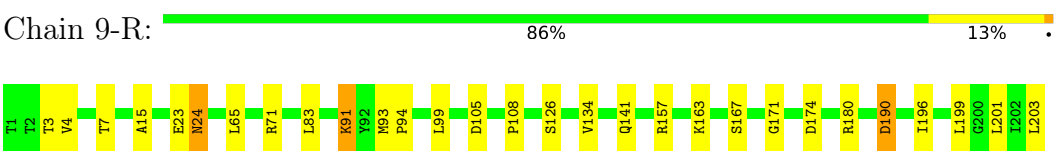
• Molecule 2: Proteasome subunit beta

Chain 9-P:



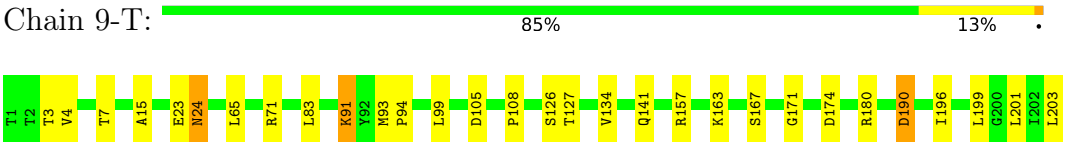
• Molecule 2: Proteasome subunit beta

Chain 9-R:



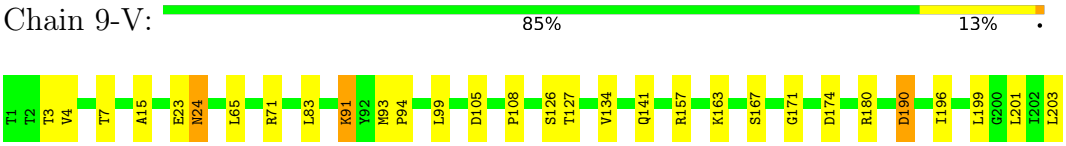
• Molecule 2: Proteasome subunit beta

Chain 9-T:



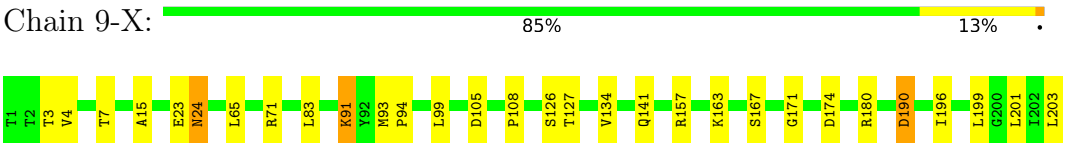
• Molecule 2: Proteasome subunit beta

Chain 9-V:



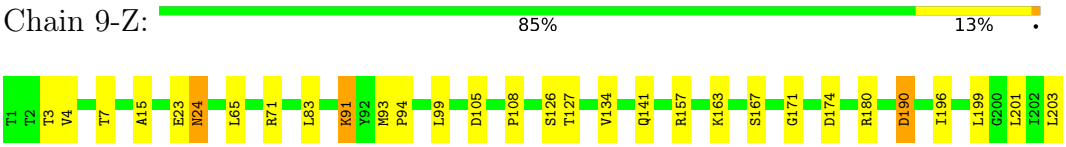
• Molecule 2: Proteasome subunit beta

Chain 9-X:



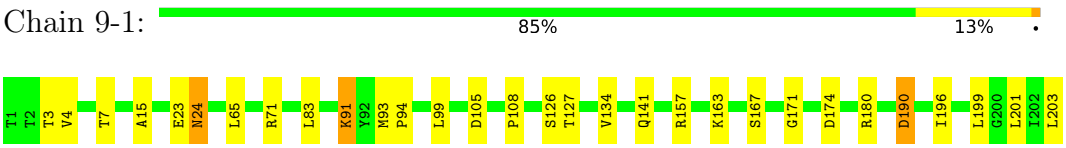
• Molecule 2: Proteasome subunit beta

Chain 9-Z:



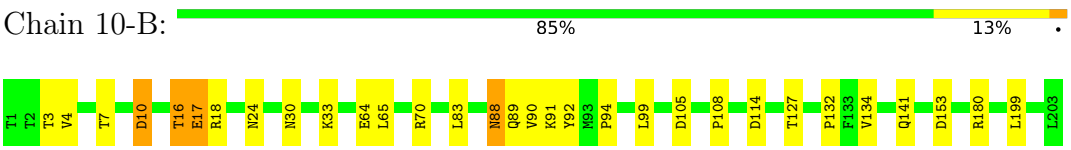
• Molecule 2: Proteasome subunit beta

Chain 9-1:



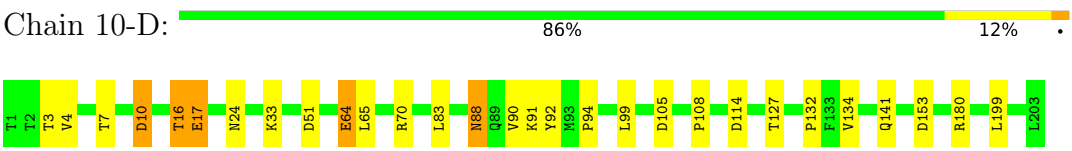
• Molecule 2: Proteasome subunit beta

Chain 10-B:



• Molecule 2: Proteasome subunit beta

Chain 10-D:

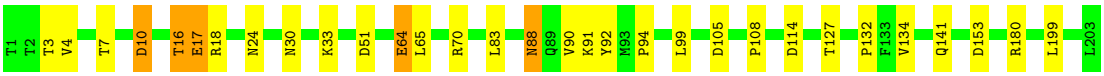


• Molecule 2: Proteasome subunit beta

Chain 10-F:

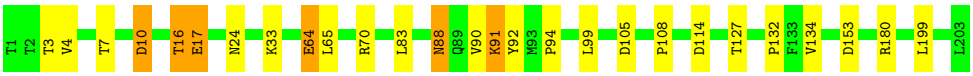
• Molecule 2: Proteasome subunit beta

Chain 10-H:



• Molecule 2: Proteasome subunit beta

Chain 10-J:



• Molecule 2: Proteasome subunit beta

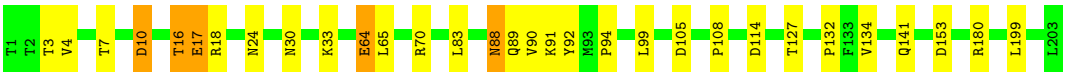
Chain 10-L:

• Molecule 2: Proteasome subunit beta

Chain 10-N:

• Molecule 2: Proteasome subunit beta

Chain 10-P:

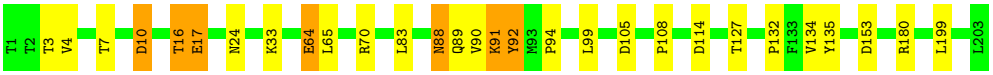


• Molecule 2: Proteasome subunit beta

Chain 10-R:

• Molecule 2: Proteasome subunit beta

Chain 10-T:

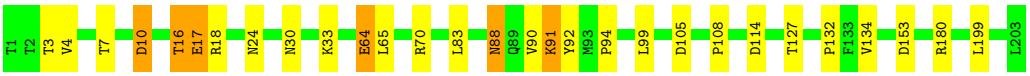


• Molecule 2: Proteasome subunit beta

Chain 10-V:

• Molecule 2: Proteasome subunit beta

Chain 10-X:

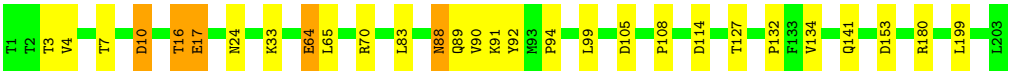


• Molecule 2: Proteasome subunit beta

Chain 10-Z:

• Molecule 2: Proteasome subunit beta

Chain 10-1:



4 Experimental information (i)

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 ($e^-/Å^2$)	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	0.49	0/1743	0.61	1/2348 (0.0%)
1	1-A	0.49	0/1743	0.61	1/2348 (0.0%)
1	1-C	0.49	0/1743	0.61	1/2348 (0.0%)
1	1-E	0.49	0/1743	0.61	1/2348 (0.0%)
1	1-G	0.49	0/1743	0.61	1/2348 (0.0%)
1	1-I	0.49	0/1743	0.61	1/2348 (0.0%)
1	1-K	0.49	0/1743	0.61	1/2348 (0.0%)
1	1-M	0.49	0/1743	0.61	1/2348 (0.0%)
1	1-O	0.49	0/1743	0.61	1/2348 (0.0%)
1	1-Q	0.49	0/1743	0.61	1/2348 (0.0%)
1	1-S	0.49	0/1743	0.61	1/2348 (0.0%)
1	1-U	0.49	0/1743	0.61	1/2348 (0.0%)
1	1-W	0.49	0/1743	0.61	1/2348 (0.0%)
1	1-Y	0.49	0/1743	0.61	1/2348 (0.0%)
1	2-0	0.43	0/1743	0.56	0/2348
1	2-A	0.43	0/1743	0.56	0/2348
1	2-C	0.43	0/1743	0.56	0/2348
1	2-E	0.43	0/1743	0.56	0/2348
1	2-G	0.43	0/1743	0.56	0/2348
1	2-I	0.43	0/1743	0.56	0/2348
1	2-K	0.43	0/1743	0.56	0/2348
1	2-M	0.43	0/1743	0.56	0/2348
1	2-O	0.43	0/1743	0.56	0/2348
1	2-Q	0.43	0/1743	0.56	0/2348
1	2-S	0.43	0/1743	0.56	0/2348
1	2-U	0.43	0/1743	0.56	0/2348
1	2-W	0.43	0/1743	0.56	0/2348
1	2-Y	0.43	0/1743	0.56	0/2348
1	3-0	0.48	0/1743	0.62	1/2348 (0.0%)
1	3-A	0.48	0/1743	0.62	1/2348 (0.0%)
1	3-C	0.48	0/1743	0.62	1/2348 (0.0%)
1	3-E	0.48	0/1743	0.62	1/2348 (0.0%)
1	3-G	0.48	0/1743	0.62	1/2348 (0.0%)
1	3-I	0.48	0/1743	0.62	1/2348 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	3-K	0.48	0/1743	0.62	1/2348 (0.0%)
1	3-M	0.48	0/1743	0.62	1/2348 (0.0%)
1	3-O	0.48	0/1743	0.62	1/2348 (0.0%)
1	3-Q	0.48	0/1743	0.62	1/2348 (0.0%)
1	3-S	0.48	0/1743	0.62	1/2348 (0.0%)
1	3-U	0.48	0/1743	0.62	1/2348 (0.0%)
1	3-W	0.48	0/1743	0.62	1/2348 (0.0%)
1	3-Y	0.48	0/1743	0.62	1/2348 (0.0%)
1	4-0	0.38	0/1743	0.60	2/2348 (0.1%)
1	4-A	0.38	0/1743	0.60	2/2348 (0.1%)
1	4-C	0.38	0/1743	0.60	2/2348 (0.1%)
1	4-E	0.38	0/1743	0.60	2/2348 (0.1%)
1	4-G	0.38	0/1743	0.60	2/2348 (0.1%)
1	4-I	0.38	0/1743	0.60	2/2348 (0.1%)
1	4-K	0.38	0/1743	0.60	2/2348 (0.1%)
1	4-M	0.38	0/1743	0.60	2/2348 (0.1%)
1	4-O	0.38	0/1743	0.60	2/2348 (0.1%)
1	4-Q	0.38	0/1743	0.60	2/2348 (0.1%)
1	4-S	0.38	0/1743	0.60	2/2348 (0.1%)
1	4-U	0.38	0/1743	0.60	2/2348 (0.1%)
1	4-W	0.38	0/1743	0.60	1/2348 (0.0%)
1	4-Y	0.38	0/1743	0.60	2/2348 (0.1%)
1	5-0	0.41	0/1743	0.60	1/2348 (0.0%)
1	5-A	0.41	0/1743	0.60	1/2348 (0.0%)
1	5-C	0.41	0/1743	0.60	1/2348 (0.0%)
1	5-E	0.41	0/1743	0.60	1/2348 (0.0%)
1	5-G	0.41	0/1743	0.60	1/2348 (0.0%)
1	5-I	0.41	0/1743	0.60	1/2348 (0.0%)
1	5-K	0.41	0/1743	0.60	1/2348 (0.0%)
1	5-M	0.41	0/1743	0.60	1/2348 (0.0%)
1	5-O	0.41	0/1743	0.60	1/2348 (0.0%)
1	5-Q	0.41	0/1743	0.60	1/2348 (0.0%)
1	5-S	0.41	0/1743	0.60	1/2348 (0.0%)
1	5-U	0.41	0/1743	0.60	1/2348 (0.0%)
1	5-W	0.41	0/1743	0.60	1/2348 (0.0%)
1	5-Y	0.41	0/1743	0.60	1/2348 (0.0%)
1	6-0	0.40	0/1743	0.61	1/2348 (0.0%)
1	6-A	0.40	0/1743	0.61	1/2348 (0.0%)
1	6-C	0.40	0/1743	0.61	1/2348 (0.0%)
1	6-E	0.40	0/1743	0.61	1/2348 (0.0%)
1	6-G	0.40	0/1743	0.61	1/2348 (0.0%)
1	6-I	0.40	0/1743	0.61	1/2348 (0.0%)
1	6-K	0.40	0/1743	0.61	1/2348 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	6-M	0.40	0/1743	0.61	1/2348 (0.0%)
1	6-O	0.41	0/1743	0.61	1/2348 (0.0%)
1	6-Q	0.41	0/1743	0.61	1/2348 (0.0%)
1	6-S	0.40	0/1743	0.61	1/2348 (0.0%)
1	6-U	0.41	0/1743	0.61	1/2348 (0.0%)
1	6-W	0.40	0/1743	0.61	1/2348 (0.0%)
1	6-Y	0.40	0/1743	0.61	1/2348 (0.0%)
1	7-0	0.43	0/1743	0.60	1/2348 (0.0%)
1	7-A	0.43	0/1743	0.60	1/2348 (0.0%)
1	7-C	0.43	0/1743	0.60	1/2348 (0.0%)
1	7-E	0.43	0/1743	0.60	1/2348 (0.0%)
1	7-G	0.43	0/1743	0.60	1/2348 (0.0%)
1	7-I	0.43	0/1743	0.60	1/2348 (0.0%)
1	7-K	0.43	0/1743	0.60	1/2348 (0.0%)
1	7-M	0.43	0/1743	0.60	1/2348 (0.0%)
1	7-O	0.43	0/1743	0.60	1/2348 (0.0%)
1	7-Q	0.43	0/1743	0.60	1/2348 (0.0%)
1	7-S	0.43	0/1743	0.60	1/2348 (0.0%)
1	7-U	0.43	0/1743	0.60	1/2348 (0.0%)
1	7-W	0.43	0/1743	0.60	1/2348 (0.0%)
1	7-Y	0.43	0/1743	0.60	1/2348 (0.0%)
1	8-0	0.44	0/1743	0.63	1/2348 (0.0%)
1	8-A	0.44	0/1743	0.62	1/2348 (0.0%)
1	8-C	0.44	0/1743	0.62	1/2348 (0.0%)
1	8-E	0.44	0/1743	0.62	1/2348 (0.0%)
1	8-G	0.44	0/1743	0.62	1/2348 (0.0%)
1	8-I	0.44	0/1743	0.62	1/2348 (0.0%)
1	8-K	0.44	0/1743	0.62	1/2348 (0.0%)
1	8-M	0.44	0/1743	0.62	1/2348 (0.0%)
1	8-O	0.44	0/1743	0.62	1/2348 (0.0%)
1	8-Q	0.44	0/1743	0.63	1/2348 (0.0%)
1	8-S	0.44	0/1743	0.63	1/2348 (0.0%)
1	8-U	0.44	0/1743	0.62	1/2348 (0.0%)
1	8-W	0.44	0/1743	0.63	1/2348 (0.0%)
1	8-Y	0.44	0/1743	0.62	1/2348 (0.0%)
1	9-0	0.46	0/1743	0.63	1/2348 (0.0%)
1	9-A	0.46	0/1743	0.63	2/2348 (0.1%)
1	9-C	0.46	0/1743	0.63	1/2348 (0.0%)
1	9-E	0.46	0/1743	0.63	1/2348 (0.0%)
1	9-G	0.46	0/1743	0.63	1/2348 (0.0%)
1	9-I	0.46	0/1743	0.63	1/2348 (0.0%)
1	9-K	0.46	0/1743	0.63	1/2348 (0.0%)
1	9-M	0.46	0/1743	0.63	2/2348 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	9-O	0.46	0/1743	0.63	1/2348 (0.0%)
1	9-Q	0.46	0/1743	0.63	2/2348 (0.1%)
1	9-S	0.46	0/1743	0.63	2/2348 (0.1%)
1	9-U	0.46	0/1743	0.63	1/2348 (0.0%)
1	9-W	0.46	0/1743	0.63	1/2348 (0.0%)
1	9-Y	0.46	0/1743	0.63	1/2348 (0.0%)
1	10-0	0.46	0/1743	0.64	2/2348 (0.1%)
1	10-A	0.46	0/1743	0.64	2/2348 (0.1%)
1	10-C	0.46	0/1743	0.64	2/2348 (0.1%)
1	10-E	0.46	0/1743	0.64	2/2348 (0.1%)
1	10-G	0.46	0/1743	0.64	2/2348 (0.1%)
1	10-I	0.46	0/1743	0.64	2/2348 (0.1%)
1	10-K	0.46	0/1743	0.64	2/2348 (0.1%)
1	10-M	0.46	0/1743	0.64	2/2348 (0.1%)
1	10-O	0.46	0/1743	0.64	2/2348 (0.1%)
1	10-Q	0.46	0/1743	0.64	2/2348 (0.1%)
1	10-S	0.46	0/1743	0.64	2/2348 (0.1%)
1	10-U	0.46	0/1743	0.64	2/2348 (0.1%)
1	10-W	0.46	0/1743	0.64	2/2348 (0.1%)
1	10-Y	0.46	0/1743	0.64	2/2348 (0.1%)
2	1-1	0.60	0/1577	0.65	0/2129
2	1-B	0.60	0/1577	0.65	0/2129
2	1-D	0.60	0/1577	0.65	0/2129
2	1-F	0.60	0/1577	0.65	0/2129
2	1-H	0.60	0/1577	0.65	0/2129
2	1-J	0.60	0/1577	0.65	0/2129
2	1-L	0.60	0/1577	0.65	0/2129
2	1-N	0.60	0/1577	0.65	0/2129
2	1-P	0.60	0/1577	0.65	0/2129
2	1-R	0.60	0/1577	0.65	0/2129
2	1-T	0.60	0/1577	0.65	0/2129
2	1-V	0.60	0/1577	0.65	0/2129
2	1-X	0.60	0/1577	0.65	0/2129
2	1-Z	0.60	0/1577	0.65	0/2129
2	2-1	0.51	0/1577	0.65	1/2129 (0.0%)
2	2-B	0.51	0/1577	0.65	1/2129 (0.0%)
2	2-D	0.51	0/1577	0.65	1/2129 (0.0%)
2	2-F	0.51	0/1577	0.65	1/2129 (0.0%)
2	2-H	0.51	0/1577	0.65	1/2129 (0.0%)
2	2-J	0.52	0/1577	0.65	1/2129 (0.0%)
2	2-L	0.51	0/1577	0.65	1/2129 (0.0%)
2	2-N	0.51	0/1577	0.65	1/2129 (0.0%)
2	2-P	0.51	0/1577	0.65	1/2129 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	2-R	0.51	0/1577	0.65	1/2129 (0.0%)
2	2-T	0.51	0/1577	0.65	1/2129 (0.0%)
2	2-V	0.51	0/1577	0.65	1/2129 (0.0%)
2	2-X	0.51	0/1577	0.65	1/2129 (0.0%)
2	2-Z	0.51	0/1577	0.65	1/2129 (0.0%)
2	3-1	0.56	0/1577	0.68	0/2129
2	3-B	0.56	0/1577	0.68	0/2129
2	3-D	0.56	0/1577	0.68	0/2129
2	3-F	0.56	0/1577	0.68	0/2129
2	3-H	0.56	0/1577	0.68	0/2129
2	3-J	0.56	0/1577	0.68	0/2129
2	3-L	0.56	0/1577	0.68	0/2129
2	3-N	0.56	0/1577	0.68	0/2129
2	3-P	0.56	0/1577	0.68	0/2129
2	3-R	0.56	0/1577	0.68	0/2129
2	3-T	0.56	0/1577	0.68	0/2129
2	3-V	0.56	0/1577	0.68	0/2129
2	3-X	0.56	0/1577	0.68	0/2129
2	3-Z	0.56	0/1577	0.68	0/2129
2	4-1	0.46	0/1577	0.61	0/2129
2	4-B	0.46	0/1577	0.61	0/2129
2	4-D	0.46	0/1577	0.61	0/2129
2	4-F	0.46	0/1577	0.61	0/2129
2	4-H	0.46	0/1577	0.61	0/2129
2	4-J	0.46	0/1577	0.61	0/2129
2	4-L	0.46	0/1577	0.61	0/2129
2	4-N	0.46	0/1577	0.61	0/2129
2	4-P	0.46	0/1577	0.61	0/2129
2	4-R	0.46	0/1577	0.61	0/2129
2	4-T	0.46	0/1577	0.61	0/2129
2	4-V	0.46	0/1577	0.61	0/2129
2	4-X	0.46	0/1577	0.61	0/2129
2	4-Z	0.46	0/1577	0.61	0/2129
2	5-1	0.48	0/1577	0.64	0/2129
2	5-B	0.48	0/1577	0.64	0/2129
2	5-D	0.48	0/1577	0.64	0/2129
2	5-F	0.48	0/1577	0.64	0/2129
2	5-H	0.48	0/1577	0.64	0/2129
2	5-J	0.48	0/1577	0.64	0/2129
2	5-L	0.48	0/1577	0.64	0/2129
2	5-N	0.48	0/1577	0.64	0/2129
2	5-P	0.48	0/1577	0.64	0/2129
2	5-R	0.48	0/1577	0.64	0/2129

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	5-T	0.48	0/1577	0.64	0/2129
2	5-V	0.48	0/1577	0.64	0/2129
2	5-X	0.48	0/1577	0.64	0/2129
2	5-Z	0.48	0/1577	0.64	0/2129
2	6-1	0.47	0/1577	0.69	3/2129 (0.1%)
2	6-B	0.47	0/1577	0.69	3/2129 (0.1%)
2	6-D	0.47	0/1577	0.69	4/2129 (0.2%)
2	6-F	0.47	0/1577	0.69	3/2129 (0.1%)
2	6-H	0.47	0/1577	0.69	3/2129 (0.1%)
2	6-J	0.47	0/1577	0.69	3/2129 (0.1%)
2	6-L	0.47	0/1577	0.69	3/2129 (0.1%)
2	6-N	0.47	0/1577	0.69	3/2129 (0.1%)
2	6-P	0.47	0/1577	0.70	3/2129 (0.1%)
2	6-R	0.47	0/1577	0.69	3/2129 (0.1%)
2	6-T	0.47	0/1577	0.69	3/2129 (0.1%)
2	6-V	0.47	0/1577	0.69	3/2129 (0.1%)
2	6-X	0.47	0/1577	0.69	3/2129 (0.1%)
2	6-Z	0.47	0/1577	0.69	3/2129 (0.1%)
2	7-1	0.50	0/1577	0.67	0/2129
2	7-B	0.50	0/1577	0.68	0/2129
2	7-D	0.50	0/1577	0.68	0/2129
2	7-F	0.50	0/1577	0.67	0/2129
2	7-H	0.50	0/1577	0.67	0/2129
2	7-J	0.50	0/1577	0.67	0/2129
2	7-L	0.50	0/1577	0.68	0/2129
2	7-N	0.50	0/1577	0.68	0/2129
2	7-P	0.50	0/1577	0.68	0/2129
2	7-R	0.50	0/1577	0.67	0/2129
2	7-T	0.50	0/1577	0.68	0/2129
2	7-V	0.50	0/1577	0.67	0/2129
2	7-X	0.50	0/1577	0.68	0/2129
2	7-Z	0.50	0/1577	0.67	0/2129
2	8-1	0.53	0/1577	0.69	1/2129 (0.0%)
2	8-B	0.53	0/1577	0.69	1/2129 (0.0%)
2	8-D	0.53	0/1577	0.69	1/2129 (0.0%)
2	8-F	0.53	0/1577	0.69	1/2129 (0.0%)
2	8-H	0.53	0/1577	0.69	1/2129 (0.0%)
2	8-J	0.53	0/1577	0.69	1/2129 (0.0%)
2	8-L	0.53	0/1577	0.69	1/2129 (0.0%)
2	8-N	0.53	0/1577	0.69	1/2129 (0.0%)
2	8-P	0.53	0/1577	0.69	1/2129 (0.0%)
2	8-R	0.53	0/1577	0.69	1/2129 (0.0%)
2	8-T	0.53	0/1577	0.69	1/2129 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	8-V	0.53	0/1577	0.69	1/2129 (0.0%)
2	8-X	0.53	0/1577	0.69	1/2129 (0.0%)
2	8-Z	0.53	0/1577	0.69	1/2129 (0.0%)
2	9-1	0.57	0/1577	0.66	0/2129
2	9-B	0.57	0/1577	0.66	0/2129
2	9-D	0.57	0/1577	0.66	0/2129
2	9-F	0.57	0/1577	0.66	0/2129
2	9-H	0.57	0/1577	0.66	0/2129
2	9-J	0.57	0/1577	0.66	0/2129
2	9-L	0.57	0/1577	0.66	0/2129
2	9-N	0.57	0/1577	0.66	0/2129
2	9-P	0.57	0/1577	0.66	0/2129
2	9-R	0.57	0/1577	0.66	0/2129
2	9-T	0.57	0/1577	0.66	0/2129
2	9-V	0.57	0/1577	0.66	0/2129
2	9-X	0.57	0/1577	0.66	0/2129
2	9-Z	0.57	0/1577	0.66	0/2129
2	10-1	0.55	0/1577	0.71	4/2129 (0.2%)
2	10-B	0.55	0/1577	0.71	4/2129 (0.2%)
2	10-D	0.55	0/1577	0.71	4/2129 (0.2%)
2	10-F	0.55	0/1577	0.71	4/2129 (0.2%)
2	10-H	0.55	0/1577	0.71	4/2129 (0.2%)
2	10-J	0.55	0/1577	0.71	4/2129 (0.2%)
2	10-L	0.55	0/1577	0.71	4/2129 (0.2%)
2	10-N	0.55	0/1577	0.71	4/2129 (0.2%)
2	10-P	0.55	0/1577	0.71	4/2129 (0.2%)
2	10-R	0.55	0/1577	0.71	4/2129 (0.2%)
2	10-T	0.55	0/1577	0.71	4/2129 (0.2%)
2	10-V	0.55	0/1577	0.71	4/2129 (0.2%)
2	10-X	0.55	0/1577	0.71	4/2129 (0.2%)
2	10-Z	0.55	0/1577	0.71	4/2129 (0.2%)
All	All	0.48	0/464800	0.64	284/626780 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	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.

All (284) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	6-T	71	ARG	NE-CZ-NH1	8.62	124.61	120.30
2	6-P	71	ARG	NE-CZ-NH1	8.61	124.61	120.30
1	5-M	151	CYS	C-N-CA	8.60	143.19	121.70
2	6-X	71	ARG	NE-CZ-NH1	8.59	124.59	120.30
1	5-A	151	CYS	C-N-CA	8.58	143.15	121.70
1	5-E	151	CYS	C-N-CA	8.58	143.15	121.70
1	5-K	151	CYS	C-N-CA	8.58	143.14	121.70
1	5-S	151	CYS	C-N-CA	8.58	143.14	121.70
2	6-1	71	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	5-Y	151	CYS	C-N-CA	8.57	143.13	121.70
1	5-U	151	CYS	C-N-CA	8.57	143.13	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5-G	151	CYS	C-N-CA	8.57	143.12	121.70
1	5-O	151	CYS	C-N-CA	8.57	143.12	121.70
1	5-0	151	CYS	C-N-CA	8.57	143.12	121.70
1	5-Q	151	CYS	C-N-CA	8.56	143.10	121.70
1	5-C	151	CYS	C-N-CA	8.56	143.10	121.70
1	5-I	151	CYS	C-N-CA	8.56	143.09	121.70
1	5-W	151	CYS	C-N-CA	8.55	143.08	121.70
2	6-F	71	ARG	NE-CZ-NH1	8.55	124.58	120.30
2	6-N	71	ARG	NE-CZ-NH1	8.55	124.58	120.30
2	6-V	71	ARG	NE-CZ-NH1	8.55	124.57	120.30
2	6-D	71	ARG	NE-CZ-NH1	8.54	124.57	120.30
2	6-Z	71	ARG	NE-CZ-NH1	8.54	124.57	120.30
2	6-L	71	ARG	NE-CZ-NH1	8.50	124.55	120.30
2	6-B	71	ARG	NE-CZ-NH1	8.49	124.54	120.30
2	6-H	71	ARG	NE-CZ-NH1	8.45	124.53	120.30
2	6-J	71	ARG	NE-CZ-NH1	8.44	124.52	120.30
2	6-R	71	ARG	NE-CZ-NH1	8.44	124.52	120.30
1	4-U	222	ARG	NE-CZ-NH1	8.31	124.45	120.30
1	4-C	222	ARG	NE-CZ-NH1	8.30	124.45	120.30
1	4-M	222	ARG	NE-CZ-NH1	8.27	124.44	120.30
1	4-0	222	ARG	NE-CZ-NH1	8.25	124.42	120.30
1	4-Y	222	ARG	NE-CZ-NH1	8.25	124.42	120.30
1	4-Q	222	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	4-A	222	ARG	NE-CZ-NH1	8.23	124.42	120.30
1	4-G	222	ARG	NE-CZ-NH1	8.23	124.42	120.30
1	4-K	222	ARG	NE-CZ-NH1	8.23	124.42	120.30
1	4-O	222	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	4-I	222	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	4-S	222	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	4-E	222	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	4-W	222	ARG	NE-CZ-NH1	8.11	124.36	120.30
1	6-S	222	ARG	NE-CZ-NH1	7.75	124.18	120.30
1	6-M	222	ARG	NE-CZ-NH1	7.71	124.16	120.30
1	6-O	222	ARG	NE-CZ-NH1	7.71	124.16	120.30
1	6-K	222	ARG	NE-CZ-NH1	7.71	124.15	120.30
1	6-E	222	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	6-Q	222	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	6-U	222	ARG	NE-CZ-NH1	7.69	124.15	120.30
1	6-0	222	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	6-G	222	ARG	NE-CZ-NH1	7.67	124.13	120.30
1	6-W	222	ARG	NE-CZ-NH1	7.67	124.13	120.30
1	6-I	222	ARG	NE-CZ-NH1	7.66	124.13	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6-A	222	ARG	NE-CZ-NH1	7.65	124.12	120.30
1	6-Y	222	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	6-C	222	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	10-U	222	ARG	CG-CD-NE	7.32	127.17	111.80
1	10-K	222	ARG	CG-CD-NE	7.32	127.16	111.80
1	10-C	222	ARG	CG-CD-NE	7.31	127.16	111.80
1	10-G	222	ARG	CG-CD-NE	7.31	127.15	111.80
1	10-M	222	ARG	CG-CD-NE	7.31	127.14	111.80
1	10-Q	222	ARG	CG-CD-NE	7.31	127.14	111.80
1	10-A	222	ARG	CG-CD-NE	7.31	127.14	111.80
1	10-Y	222	ARG	CG-CD-NE	7.31	127.14	111.80
1	10-E	222	ARG	CG-CD-NE	7.30	127.14	111.80
1	10-0	222	ARG	CG-CD-NE	7.30	127.14	111.80
1	10-I	222	ARG	CG-CD-NE	7.30	127.13	111.80
1	10-O	222	ARG	CG-CD-NE	7.30	127.13	111.80
1	10-S	222	ARG	CG-CD-NE	7.29	127.12	111.80
1	10-W	222	ARG	CG-CD-NE	7.27	127.08	111.80
1	7-E	47	LEU	CA-CB-CG	7.00	131.40	115.30
1	7-M	47	LEU	CA-CB-CG	7.00	131.40	115.30
1	7-G	47	LEU	CA-CB-CG	7.00	131.40	115.30
1	7-S	47	LEU	CA-CB-CG	6.99	131.38	115.30
1	7-A	47	LEU	CA-CB-CG	6.99	131.38	115.30
1	7-K	47	LEU	CA-CB-CG	6.99	131.38	115.30
1	7-C	47	LEU	CA-CB-CG	6.99	131.37	115.30
1	7-I	47	LEU	CA-CB-CG	6.99	131.37	115.30
1	7-U	47	LEU	CA-CB-CG	6.99	131.37	115.30
1	7-W	47	LEU	CA-CB-CG	6.99	131.37	115.30
1	7-Q	47	LEU	CA-CB-CG	6.98	131.36	115.30
1	7-0	47	LEU	CA-CB-CG	6.98	131.36	115.30
2	8-X	144	GLU	CA-CB-CG	6.98	128.76	113.40
1	7-Y	47	LEU	CA-CB-CG	6.98	131.34	115.30
1	7-O	47	LEU	CA-CB-CG	6.97	131.34	115.30
2	8-F	144	GLU	CA-CB-CG	6.97	128.74	113.40
2	8-P	144	GLU	CA-CB-CG	6.97	128.74	113.40
2	8-B	144	GLU	CA-CB-CG	6.97	128.74	113.40
2	8-J	144	GLU	CA-CB-CG	6.96	128.71	113.40
2	8-1	144	GLU	CA-CB-CG	6.96	128.71	113.40
2	8-L	144	GLU	CA-CB-CG	6.95	128.69	113.40
2	8-N	144	GLU	CA-CB-CG	6.95	128.69	113.40
2	8-D	144	GLU	CA-CB-CG	6.95	128.69	113.40
2	8-T	144	GLU	CA-CB-CG	6.95	128.69	113.40
2	8-R	144	GLU	CA-CB-CG	6.94	128.67	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	8-Z	144	GLU	CA-CB-CG	6.94	128.67	113.40
2	8-H	144	GLU	CA-CB-CG	6.94	128.66	113.40
2	8-V	144	GLU	CA-CB-CG	6.94	128.66	113.40
2	10-J	17	GLU	CA-CB-CG	6.16	126.95	113.40
2	10-P	17	GLU	CA-CB-CG	6.16	126.94	113.40
2	10-R	17	GLU	CA-CB-CG	6.15	126.93	113.40
2	10-L	17	GLU	CA-CB-CG	6.14	126.92	113.40
2	10-T	17	GLU	CA-CB-CG	6.14	126.92	113.40
2	10-Z	17	GLU	CA-CB-CG	6.14	126.91	113.40
2	10-F	17	GLU	CA-CB-CG	6.14	126.91	113.40
2	10-X	17	GLU	CA-CB-CG	6.14	126.91	113.40
2	10-H	17	GLU	CA-CB-CG	6.14	126.90	113.40
2	10-1	17	GLU	CA-CB-CG	6.14	126.90	113.40
2	10-B	17	GLU	CA-CB-CG	6.12	126.87	113.40
2	10-D	17	GLU	CA-CB-CG	6.12	126.86	113.40
2	10-V	17	GLU	CA-CB-CG	6.12	126.86	113.40
2	10-N	17	GLU	CA-CB-CG	6.12	126.86	113.40
1	3-I	151	CYS	C-N-CA	5.99	136.68	121.70
1	3-0	151	CYS	C-N-CA	5.99	136.68	121.70
1	3-Y	151	CYS	C-N-CA	5.99	136.67	121.70
1	3-A	151	CYS	C-N-CA	5.99	136.66	121.70
1	3-U	151	CYS	C-N-CA	5.99	136.66	121.70
1	3-K	151	CYS	C-N-CA	5.98	136.65	121.70
1	3-E	151	CYS	C-N-CA	5.97	136.64	121.70
1	3-M	151	CYS	C-N-CA	5.97	136.63	121.70
1	3-S	151	CYS	C-N-CA	5.97	136.63	121.70
1	3-C	151	CYS	C-N-CA	5.97	136.62	121.70
1	3-G	151	CYS	C-N-CA	5.97	136.62	121.70
1	3-Q	151	CYS	C-N-CA	5.96	136.61	121.70
1	3-O	151	CYS	C-N-CA	5.96	136.60	121.70
1	3-W	151	CYS	C-N-CA	5.96	136.60	121.70
1	9-U	151	CYS	C-N-CA	5.84	136.31	121.70
1	9-I	151	CYS	C-N-CA	5.84	136.30	121.70
1	9-M	151	CYS	C-N-CA	5.84	136.30	121.70
1	9-K	151	CYS	C-N-CA	5.84	136.29	121.70
1	9-Y	151	CYS	C-N-CA	5.83	136.28	121.70
1	9-0	151	CYS	C-N-CA	5.83	136.28	121.70
1	9-E	151	CYS	C-N-CA	5.83	136.27	121.70
1	9-C	151	CYS	C-N-CA	5.82	136.26	121.70
1	9-S	151	CYS	C-N-CA	5.82	136.26	121.70
1	9-G	151	CYS	C-N-CA	5.82	136.25	121.70
1	9-O	151	CYS	C-N-CA	5.82	136.24	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	9-A	151	CYS	C-N-CA	5.82	136.24	121.70
1	9-W	151	CYS	C-N-CA	5.81	136.24	121.70
1	9-Q	151	CYS	C-N-CA	5.81	136.23	121.70
1	1-E	148	LEU	CA-CB-CG	5.80	128.64	115.30
1	1-W	148	LEU	CA-CB-CG	5.80	128.63	115.30
1	1-O	148	LEU	CA-CB-CG	5.79	128.62	115.30
1	1-I	148	LEU	CA-CB-CG	5.79	128.61	115.30
1	1-S	148	LEU	CA-CB-CG	5.79	128.61	115.30
1	1-A	148	LEU	CA-CB-CG	5.78	128.60	115.30
1	1-C	148	LEU	CA-CB-CG	5.78	128.60	115.30
1	1-0	148	LEU	CA-CB-CG	5.78	128.60	115.30
1	1-G	148	LEU	CA-CB-CG	5.78	128.59	115.30
1	1-K	148	LEU	CA-CB-CG	5.78	128.59	115.30
1	1-Q	148	LEU	CA-CB-CG	5.78	128.60	115.30
1	1-M	148	LEU	CA-CB-CG	5.78	128.59	115.30
1	1-U	148	LEU	CA-CB-CG	5.77	128.57	115.30
1	1-Y	148	LEU	CA-CB-CG	5.77	128.57	115.30
2	6-T	23	GLU	CA-CB-CG	5.59	125.70	113.40
2	6-H	23	GLU	CA-CB-CG	5.59	125.70	113.40
2	6-Z	23	GLU	CA-CB-CG	5.58	125.68	113.40
2	6-D	23	GLU	CA-CB-CG	5.58	125.67	113.40
2	6-N	23	GLU	CA-CB-CG	5.58	125.67	113.40
2	6-V	23	GLU	CA-CB-CG	5.58	125.66	113.40
2	6-B	23	GLU	CA-CB-CG	5.57	125.66	113.40
2	6-L	23	GLU	CA-CB-CG	5.57	125.66	113.40
2	6-F	23	GLU	CA-CB-CG	5.57	125.65	113.40
2	6-X	23	GLU	CA-CB-CG	5.57	125.65	113.40
2	6-P	23	GLU	CA-CB-CG	5.57	125.65	113.40
2	6-1	23	GLU	CA-CB-CG	5.57	125.65	113.40
2	6-R	23	GLU	CA-CB-CG	5.56	125.64	113.40
2	6-J	23	GLU	CA-CB-CG	5.56	125.63	113.40
2	10-R	114	ASP	CB-CG-OD1	5.55	123.29	118.30
2	10-N	114	ASP	CB-CG-OD1	5.52	123.27	118.30
2	10-P	114	ASP	CB-CG-OD1	5.52	123.26	118.30
2	10-J	114	ASP	CB-CG-OD1	5.51	123.26	118.30
2	10-T	114	ASP	CB-CG-OD1	5.50	123.25	118.30
2	10-Z	114	ASP	CB-CG-OD1	5.50	123.25	118.30
1	8-M	47	LEU	CA-CB-CG	5.50	127.94	115.30
2	10-B	114	ASP	CB-CG-OD1	5.50	123.25	118.30
2	10-1	114	ASP	CB-CG-OD1	5.48	123.24	118.30
1	8-A	47	LEU	CA-CB-CG	5.48	127.91	115.30
1	8-O	47	LEU	CA-CB-CG	5.48	127.91	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	10-L	114	ASP	CB-CG-OD1	5.48	123.23	118.30
1	8-C	47	LEU	CA-CB-CG	5.48	127.90	115.30
1	8-I	47	LEU	CA-CB-CG	5.48	127.90	115.30
2	10-F	114	ASP	CB-CG-OD1	5.48	123.23	118.30
1	8-E	47	LEU	CA-CB-CG	5.48	127.90	115.30
1	8-Y	47	LEU	CA-CB-CG	5.48	127.90	115.30
1	8-0	47	LEU	CA-CB-CG	5.48	127.90	115.30
1	8-G	47	LEU	CA-CB-CG	5.48	127.89	115.30
1	8-Q	47	LEU	CA-CB-CG	5.48	127.89	115.30
2	10-X	114	ASP	CB-CG-OD1	5.47	123.23	118.30
1	8-K	47	LEU	CA-CB-CG	5.47	127.89	115.30
1	8-S	47	LEU	CA-CB-CG	5.47	127.87	115.30
1	8-U	47	LEU	CA-CB-CG	5.46	127.87	115.30
1	8-W	47	LEU	CA-CB-CG	5.46	127.87	115.30
2	10-D	114	ASP	CB-CG-OD1	5.46	123.22	118.30
2	10-V	114	ASP	CB-CG-OD1	5.45	123.21	118.30
2	10-H	114	ASP	CB-CG-OD1	5.45	123.20	118.30
1	10-K	47	LEU	C-N-CA	5.44	135.29	121.70
1	10-A	47	LEU	C-N-CA	5.43	135.28	121.70
1	10-0	47	LEU	C-N-CA	5.43	135.28	121.70
1	10-G	47	LEU	C-N-CA	5.43	135.27	121.70
1	10-W	47	LEU	C-N-CA	5.43	135.27	121.70
1	10-Y	47	LEU	C-N-CA	5.42	135.26	121.70
1	10-E	47	LEU	C-N-CA	5.42	135.25	121.70
1	10-U	47	LEU	C-N-CA	5.42	135.26	121.70
1	10-C	47	LEU	C-N-CA	5.42	135.24	121.70
1	10-I	47	LEU	C-N-CA	5.42	135.24	121.70
1	10-S	47	LEU	C-N-CA	5.42	135.24	121.70
1	10-O	47	LEU	C-N-CA	5.42	135.24	121.70
1	10-M	47	LEU	C-N-CA	5.41	135.23	121.70
1	10-Q	47	LEU	C-N-CA	5.41	135.23	121.70
1	4-C	222	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	4-S	222	ARG	NE-CZ-NH2	-5.15	117.73	120.30
2	10-H	92	TYR	CA-CB-CG	5.12	123.12	113.40
2	10-P	92	TYR	CA-CB-CG	5.12	123.12	113.40
2	10-X	92	TYR	CA-CB-CG	5.11	123.11	113.40
1	4-U	222	ARG	NE-CZ-NH2	-5.11	117.75	120.30
2	10-L	92	TYR	CA-CB-CG	5.11	123.11	113.40
2	10-Z	92	TYR	CA-CB-CG	5.11	123.11	113.40
1	4-E	222	ARG	NE-CZ-NH2	-5.11	117.75	120.30
2	10-D	92	TYR	CA-CB-CG	5.11	123.10	113.40
2	6-D	71	ARG	CG-CD-NE	5.10	122.52	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	6-F	71	ARG	CG-CD-NE	5.10	122.51	111.80
2	10-J	90	VAL	CG1-CB-CG2	-5.10	102.74	110.90
2	10-J	92	TYR	CA-CB-CG	5.10	123.09	113.40
2	6-B	71	ARG	CG-CD-NE	5.10	122.51	111.80
2	10-B	92	TYR	CA-CB-CG	5.10	123.09	113.40
2	2-1	10	ASP	CB-CG-OD1	5.10	122.89	118.30
2	6-X	71	ARG	CG-CD-NE	5.10	122.50	111.80
2	10-1	92	TYR	CA-CB-CG	5.10	123.09	113.40
2	2-H	10	ASP	CB-CG-OD1	5.09	122.88	118.30
2	6-P	71	ARG	CG-CD-NE	5.09	122.50	111.80
1	4-O	222	ARG	NE-CZ-NH2	-5.09	117.75	120.30
2	10-N	92	TYR	CA-CB-CG	5.09	123.08	113.40
2	10-R	92	TYR	CA-CB-CG	5.09	123.08	113.40
2	6-R	71	ARG	CG-CD-NE	5.09	122.49	111.80
2	6-T	71	ARG	CG-CD-NE	5.09	122.49	111.80
2	10-V	90	VAL	CG1-CB-CG2	-5.09	102.75	110.90
2	10-F	92	TYR	CA-CB-CG	5.09	123.07	113.40
1	4-I	222	ARG	NE-CZ-NH2	-5.09	117.76	120.30
2	6-H	71	ARG	CG-CD-NE	5.09	122.49	111.80
2	6-V	71	ARG	CG-CD-NE	5.09	122.48	111.80
2	6-N	71	ARG	CG-CD-NE	5.09	122.48	111.80
2	10-T	90	VAL	CG1-CB-CG2	-5.09	102.76	110.90
2	10-T	92	TYR	CA-CB-CG	5.09	123.07	113.40
2	6-1	71	ARG	CG-CD-NE	5.08	122.48	111.80
2	10-V	92	TYR	CA-CB-CG	5.08	123.06	113.40
2	10-X	90	VAL	CG1-CB-CG2	-5.08	102.77	110.90
2	2-R	10	ASP	CB-CG-OD1	5.08	122.87	118.30
2	10-D	90	VAL	CG1-CB-CG2	-5.08	102.77	110.90
2	10-L	90	VAL	CG1-CB-CG2	-5.08	102.77	110.90
2	6-L	71	ARG	CG-CD-NE	5.08	122.47	111.80
2	6-Z	71	ARG	CG-CD-NE	5.08	122.47	111.80
1	4-Y	222	ARG	NE-CZ-NH2	-5.08	117.76	120.30
2	10-F	90	VAL	CG1-CB-CG2	-5.08	102.78	110.90
2	10-H	90	VAL	CG1-CB-CG2	-5.08	102.78	110.90
2	10-R	90	VAL	CG1-CB-CG2	-5.07	102.78	110.90
2	6-J	71	ARG	CG-CD-NE	5.07	122.45	111.80
1	9-S	28	ARG	NE-CZ-NH1	5.07	122.83	120.30
2	10-1	90	VAL	CG1-CB-CG2	-5.07	102.79	110.90
1	4-A	222	ARG	NE-CZ-NH2	-5.07	117.77	120.30
2	10-N	90	VAL	CG1-CB-CG2	-5.07	102.79	110.90
1	4-M	222	ARG	NE-CZ-NH2	-5.06	117.77	120.30
2	10-P	90	VAL	CG1-CB-CG2	-5.06	102.80	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	10-Z	90	VAL	CG1-CB-CG2	-5.06	102.81	110.90
2	2-N	10	ASP	CB-CG-OD1	5.05	122.85	118.30
2	2-T	10	ASP	CB-CG-OD1	5.05	122.85	118.30
2	10-B	90	VAL	CG1-CB-CG2	-5.05	102.82	110.90
1	9-Q	28	ARG	NE-CZ-NH1	5.04	122.82	120.30
2	2-P	10	ASP	CB-CG-OD1	5.04	122.83	118.30
2	2-X	10	ASP	CB-CG-OD1	5.04	122.83	118.30
2	2-D	10	ASP	CB-CG-OD1	5.04	122.83	118.30
1	4-Q	222	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	4-0	222	ARG	NE-CZ-NH2	-5.03	117.78	120.30
2	2-F	10	ASP	CB-CG-OD1	5.03	122.83	118.30
2	6-D	71	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	9-A	28	ARG	NE-CZ-NH1	5.03	122.81	120.30
2	2-B	10	ASP	CB-CG-OD1	5.03	122.83	118.30
2	2-L	10	ASP	CB-CG-OD1	5.03	122.82	118.30
2	2-V	10	ASP	CB-CG-OD1	5.02	122.82	118.30
2	2-J	10	ASP	CB-CG-OD1	5.01	122.81	118.30
1	4-K	222	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	9-M	28	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	4-G	222	ARG	NE-CZ-NH2	-5.01	117.80	120.30
2	2-Z	10	ASP	CB-CG-OD1	5.00	122.80	118.30

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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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	20	0
1	1-I	1720	0	1753	20	0
1	1-K	1720	0	1753	22	0

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	4-M	1720	0	1753	19	0
1	4-O	1720	0	1753	20	0
1	4-Q	1720	0	1753	17	0
1	4-S	1720	0	1753	19	0
1	4-U	1720	0	1753	20	0
1	4-W	1720	0	1753	19	0
1	4-Y	1720	0	1753	17	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	1753	22	0
1	6-A	1720	0	1753	22	0
1	6-C	1720	0	1753	22	0
1	6-E	1720	0	1753	23	0
1	6-G	1720	0	1753	23	0
1	6-I	1720	0	1753	21	0
1	6-K	1720	0	1753	22	0
1	6-M	1720	0	1753	23	0
1	6-O	1720	0	1753	22	0
1	6-Q	1720	0	1753	24	0
1	6-S	1720	0	1753	23	0
1	6-U	1720	0	1753	23	0
1	6-W	1720	0	1753	22	0
1	6-Y	1720	0	1753	22	0
1	7-0	1720	0	1753	19	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	15	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
1	10-A	1720	0	1753	22	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	10-M	1720	0	1753	23	0
1	10-O	1720	0	1753	21	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	21	0
1	10-Y	1720	0	1753	21	0
2	1-1	1558	0	1609	14	0
2	1-B	1558	0	1609	14	0
2	1-D	1558	0	1609	13	0
2	1-F	1558	0	1609	15	0
2	1-H	1558	0	1609	12	0
2	1-J	1558	0	1609	15	0
2	1-L	1558	0	1609	13	0
2	1-N	1558	0	1609	14	0
2	1-P	1558	0	1609	14	0
2	1-R	1558	0	1609	14	0
2	1-T	1558	0	1609	13	0
2	1-V	1558	0	1609	17	0
2	1-X	1558	0	1609	14	0
2	1-Z	1558	0	1609	15	0
2	2-1	1558	0	1609	15	0
2	2-B	1558	0	1609	16	0
2	2-D	1558	0	1609	14	0
2	2-F	1558	0	1609	17	0
2	2-H	1558	0	1609	17	0
2	2-J	1558	0	1609	16	0
2	2-L	1558	0	1609	15	0
2	2-N	1558	0	1609	15	0
2	2-P	1558	0	1609	16	0
2	2-R	1558	0	1609	15	0
2	2-T	1558	0	1609	14	0
2	2-V	1558	0	1609	16	0
2	2-X	1558	0	1609	17	0
2	2-Z	1558	0	1609	17	0
2	3-1	1558	0	1609	14	0
2	3-B	1558	0	1609	13	0
2	3-D	1558	0	1609	12	0
2	3-F	1558	0	1609	13	0
2	3-H	1558	0	1609	13	0
2	3-J	1558	0	1609	14	0
2	3-L	1558	0	1609	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	3-N	1558	0	1609	14	0
2	3-P	1558	0	1609	13	0
2	3-R	1558	0	1609	14	0
2	3-T	1558	0	1609	13	0
2	3-V	1558	0	1609	13	0
2	3-X	1558	0	1609	14	0
2	3-Z	1558	0	1609	13	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	11	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	11	0
2	4-Z	1558	0	1609	11	0
2	5-1	1558	0	1609	17	0
2	5-B	1558	0	1609	15	0
2	5-D	1558	0	1609	16	0
2	5-F	1558	0	1609	17	0
2	5-H	1558	0	1609	18	0
2	5-J	1558	0	1609	16	0
2	5-L	1558	0	1609	16	0
2	5-N	1558	0	1609	17	0
2	5-P	1558	0	1609	17	0
2	5-R	1558	0	1609	18	0
2	5-T	1558	0	1609	16	0
2	5-V	1558	0	1609	16	0
2	5-X	1558	0	1609	18	0
2	5-Z	1558	0	1609	17	0
2	6-1	1558	0	1609	17	0
2	6-B	1558	0	1609	15	0
2	6-D	1558	0	1609	17	0
2	6-F	1558	0	1609	18	0
2	6-H	1558	0	1609	16	0
2	6-J	1558	0	1609	16	0
2	6-L	1558	0	1609	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	6-N	1558	0	1609	16	0
2	6-P	1558	0	1609	15	0
2	6-R	1558	0	1609	16	0
2	6-T	1558	0	1609	15	0
2	6-V	1558	0	1609	16	0
2	6-X	1558	0	1609	15	0
2	6-Z	1558	0	1609	17	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	20	0
2	7-H	1558	0	1609	21	0
2	7-J	1558	0	1609	21	0
2	7-L	1558	0	1609	20	0
2	7-N	1558	0	1609	21	0
2	7-P	1558	0	1609	21	0
2	7-R	1558	0	1609	21	0
2	7-T	1558	0	1609	21	0
2	7-V	1558	0	1609	21	0
2	7-X	1558	0	1609	21	0
2	7-Z	1558	0	1609	21	0
2	8-1	1558	0	1609	18	0
2	8-B	1558	0	1609	17	0
2	8-D	1558	0	1609	19	0
2	8-F	1558	0	1609	18	0
2	8-H	1558	0	1609	19	0
2	8-J	1558	0	1609	20	0
2	8-L	1558	0	1609	19	0
2	8-N	1558	0	1609	19	0
2	8-P	1558	0	1609	19	0
2	8-R	1558	0	1609	18	0
2	8-T	1558	0	1609	19	0
2	8-V	1558	0	1609	19	0
2	8-X	1558	0	1609	19	0
2	8-Z	1558	0	1609	19	0
2	9-1	1558	0	1609	18	0
2	9-B	1558	0	1609	19	0
2	9-D	1558	0	1609	18	0
2	9-F	1558	0	1609	19	0
2	9-H	1558	0	1609	19	0
2	9-J	1558	0	1609	20	0
2	9-L	1558	0	1609	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	9-N	1558	0	1609	19	0
2	9-P	1558	0	1609	19	0
2	9-R	1558	0	1609	18	0
2	9-T	1558	0	1609	18	0
2	9-V	1558	0	1609	20	0
2	9-X	1558	0	1609	20	0
2	9-Z	1558	0	1609	19	0
2	10-1	1558	0	1609	15	0
2	10-B	1558	0	1609	15	0
2	10-D	1558	0	1609	15	0
2	10-F	1558	0	1609	17	0
2	10-H	1558	0	1609	16	0
2	10-J	1558	0	1609	14	0
2	10-L	1558	0	1609	15	0
2	10-N	1558	0	1609	14	0
2	10-P	1558	0	1609	16	0
2	10-R	1558	0	1609	14	0
2	10-T	1558	0	1609	18	0
2	10-V	1558	0	1609	19	0
2	10-X	1558	0	1609	15	0
2	10-Z	1558	0	1609	17	0
All	All	458920	0	470680	4397	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 (4397) 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
1:0:97:GLN:HG3	2:1:65:LEU:HG	1.59	0.83
2:H:141:GLN:HE21	2:V:141:GLN:HE21	1.28	0.80
1:U:97:GLN:HG3	2:V:65:LEU:HG	1.62	0.79
1:M:36:THR:HA	1:M:165:ILE:O	1.84	0.78
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
1:O:36:THR:HA	1:O:165:ILE:O	1.84	0.78
1:Q:36:THR:HA	1:Q:165:ILE:O	1.84	0.78
1:O:37:ALA:O	1:O:164:ALA:HA	1.84	0.78
1:0:37:ALA:O	1:0:164:ALA:HA	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:37:ALA:O	1:M:164:ALA:HA	1.84	0.78
1:Q:37:ALA:O	1:Q:164:ALA:HA	1.84	0.78
1:S:37:ALA:O	1:S:164:ALA:HA	1.84	0.78
1:K:36:THR:HA	1:K:165:ILE:O	1.84	0.78
1:K:37:ALA:O	1:K:164:ALA:HA	1.84	0.78
2:N:141:GLN:HE21	2:1:141:GLN:HE21	1.32	0.78
1:G:37:ALA:O	1:G:164:ALA:HA	1.84	0.78
1:W:37:ALA:O	1:W:164:ALA:HA	1.84	0.78
1:S:36:THR:HA	1:S:165:ILE:O	1.84	0.78
1:E:37:ALA:O	1:E:164:ALA:HA	1.84	0.78
1:Y:37:ALA:O	1:Y:164:ALA:HA	1.84	0.78
1:I:37:ALA:O	1:I:164:ALA:HA	1.84	0.78
1:U:39:GLY:O	1:U:162:ALA:HA	1.84	0.78
1:Y:39:GLY:O	1:Y:162:ALA:HA	1.84	0.78
1:U:37:ALA:O	1:U:164:ALA:HA	1.84	0.78
1:E:39:GLY:O	1:E:162:ALA:HA	1.84	0.78
1:G:39:GLY:O	1:G:162:ALA:HA	1.84	0.78
1:I:39:GLY:O	1:I:162:ALA:HA	1.84	0.78
1:W:39:GLY:O	1:W:162:ALA:HA	1.84	0.78
1:0:36:THR:HA	1:0:165:ILE:O	1.84	0.78
1:K:39:GLY:O	1:K:162:ALA:HA	1.84	0.78
1:C:36:THR:HA	1:C:165:ILE:O	1.84	0.77
1:S:39:GLY:O	1:S:162:ALA:HA	1.84	0.77
1:C:39:GLY:O	1:C:162:ALA:HA	1.84	0.77
1:0:39:GLY:O	1:0:162:ALA:HA	1.84	0.77
1:G:97:GLN:HG3	2:H:65:LEU:HG	1.67	0.77
1:I:36:THR:HA	1:I:165:ILE:O	1.84	0.77
1:M:39:GLY:O	1:M:162:ALA:HA	1.84	0.77
1:Q:39:GLY:O	1:Q:162:ALA:HA	1.84	0.77
1:O:39:GLY:O	1:O:162:ALA:HA	1.84	0.77
1:A:39:GLY:O	1:A:162:ALA:HA	1.84	0.77
1:U:36:THR:HA	1:U:165:ILE:O	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:36:THR:HA	1:W:165:ILE:O	1.84	0.76
1:Y:36:THR:HA	1:Y:165:ILE:O	1.84	0.76
1:G:36:THR:HA	1:G:165:ILE:O	1.84	0.76
1:E:36:THR:HA	1:E:165:ILE:O	1.84	0.76
1:W:37:ALA:O	1:W:164:ALA:HA	1.88	0.74
1:0:37:ALA:O	1:0:164:ALA:HA	1.88	0.74
1:C:37:ALA:O	1:C:164:ALA:HA	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:0:39:GLY:O	1:0:162: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
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
1:0:37:ALA:O	1:0:164: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:0:37:ALA:O	1:0:164: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
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
1:0:37:ALA:O	1:0:164: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:HZ2	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:135:TYR:O	2:D:139:GLU:HB2	1.93	0.69
2:P:135:TYR:O	2:P:139:GLU:HB2	1.93	0.69
2:B:135:TYR:O	2:B:139:GLU:HB2	1.94	0.68
2:1:135:TYR:O	2:1:139:GLU:HB2	1.94	0.68
2:N:135:TYR:O	2:N:139:GLU:HB2	1.93	0.68
2:R:135:TYR:O	2:R:139:GLU:HB2	1.93	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:M:37:ALA:O	1:M:164:ALA:HA	1.94	0.68
1:U:39:GLY:O	1:U:162:ALA:HA	1.94	0.68
1:0:39:GLY:O	1:0:162:ALA:HA	1.94	0.68
1:G:72:ASP:OD1	1:G:72:ASP:N	2.27	0.68
1:Q:37:ALA:O	1:Q:164:ALA:HA	1.94	0.68
2:Z:135:TYR:O	2:Z:139:GLU:HB2	1.93	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
2:F:135:TYR:O	2:F:139:GLU:HB2	1.93	0.68
2:L:135:TYR:O	2:L:139:GLU:HB2	1.94	0.68
2:T:135:TYR:O	2:T:139:GLU:HB2	1.94	0.68
1:A:39:GLY:O	1:A:162:ALA:HA	1.94	0.67
1:S:37:ALA:O	1:S:164: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
2:F:141:GLN:HE21	2:T:141:GLN:HE21	1.41	0.67
1:K:37:ALA:O	1:K:164:ALA:HA	1.94	0.67
2:L:141:GLN:HE21	2:Z:141:GLN:HE21	1.41	0.67
1:O:37:ALA:O	1:O:164:ALA:HA	1.94	0.67
2:N:141:GLN:HE21	2:1:141:GLN:HE21	1.42	0.67
2:B:141:GLN:HE21	2:P:141:GLN:HE21	1.41	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:72:ASP:OD1	1:O:72:ASP:N	2.27	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
1:E:37:ALA:O	1:E:164:ALA:HA	1.94	0.66
2:X:135:TYR:O	2:X:139:GLU:HB2	1.94	0.66
1:Y:37:ALA:O	1:Y:164:ALA:HA	1.94	0.66
2:D:141:GLN:HE21	2:R:141:GLN:HE21	1.40	0.66
2:J:141:GLN:HE21	2:X:141:GLN:HE21	1.43	0.66
2:H:135:TYR:O	2:H:139:GLU:HB2	1.94	0.66
2:J:135:TYR:O	2:J:139:GLU:HB2	1.94	0.66
1:0:37:ALA:O	1:0:164:ALA:HA	1.94	0.66
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:V:135:TYR:O	2:V:139:GLU:HB2	1.94	0.66
1:G:37:ALA:O	1:G:164:ALA:HA	1.94	0.66
2:N:141:GLN:HE21	2:1:141:GLN:HE21	1.41	0.66
1:W:37:ALA:O	1:W:164:ALA:HA	1.94	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
1:0:25:GLU:HA	1:0:28: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:37:ALA:O	1:I:164:ALA:HA	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:U:37:ALA:O	1:U:164:ALA:HA	1.94	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
1:0:39:GLY:O	1:0:162: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
1:0:72:ASP:OD1	1:0:72: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
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
2:H:132:PRO:HB2	2:V:132:PRO:HB2	1.78	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:P:3:THR:HG1	2:P:127:THR:HG1	1.45	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
1:0:72:ASP:OD1	1:0:72: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
2:N:91:LYS:HB3	2:N:93:MET:HG2	1.81	0.63
1:S:72:ASP:N	1:S:72:ASP:OD1	2.27	0.63
1:0:97:GLN:HG3	2:1:65: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
2:1:190:ASP:OD1	2:1:190:ASP:N	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:P:91:LYS:HB3	2:P:93:MET:HG2	1.81	0.63
2:R:91:LYS:HB3	2:R: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
2:J:172:MET:HG3	2:J:203:LEU:HD11	1.81	0.63
2:V:172:MET:HG3	2:V:203:LEU:HD11	1.81	0.63
1:U:72:ASP:N	1:U:72:ASP:OD1	2.30	0.63
2:N:172:MET:HG3	2:N:203:LEU:HD11	1.81	0.63
2:H:190:ASP:N	2:H:190:ASP:OD1	2.30	0.63
1:0:99:GLU:OE1	1:0:115:ARG:NH2	2.32	0.63
2:D:91:LYS:HB3	2:D:93:MET:HG2	1.81	0.63
2:L:172:MET:HG3	2:L:203:LEU:HD11	1.81	0.63
2:R:172:MET:HG3	2:R:203:LEU:HD11	1.81	0.63
2:T:172:MET:HG3	2:T:203:LEU:HD11	1.81	0.63
2:1:91:LYS:HB3	2:1:93: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:L:91:LYS:HB3	2:L:93:MET:HG2	1.81	0.62
2:X:190:ASP:OD1	2:X:190:ASP:N	2.30	0.62
2:T:91:LYS:HB3	2:T:93:MET:HG2	1.81	0.62
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
2:1:172:MET:HG3	2:1:203:LEU:HD11	1.81	0.62
2:T:92:TYR:HB3	2:V:93:MET:SD	2.40	0.62
2:F:172:MET:HG3	2:F:203:LEU:HD11	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:Z:172:MET:HG3	2:Z:203:LEU:HD11	1.81	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
2:D:141:GLN:HE21	2:R:141:GLN:HE21	1.46	0.62
1:O:72:ASP:OD1	1:O:72:ASP:N	2.30	0.62
2:V:91:LYS:HB3	2:V:93:MET:HG2	1.81	0.62
2:X:172:MET:HG3	2:X:203:LEU:HD11	1.81	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
2:J:91:LYS:HB3	2:J:93:MET:HG2	1.81	0.62
1:O:121:GLN:NE2	1:0:84: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
2:H:172:MET:HG3	2:H:203:LEU:HD11	1.81	0.62
2:P:3:THR:HG1	2:P:127:THR:HG1	1.47	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:F:91:LYS:HB3	2:F:93:MET:HG2	1.81	0.61
2:Z:91:LYS:HB3	2:Z:93:MET:HG2	1.81	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
2:P:172:MET:HG3	2:P:203:LEU:HD11	1.81	0.61
2:X:91:LYS:HB3	2:X:93:MET:HG2	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:H:91:LYS:HB3	2:H:93:MET:HG2	1.81	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
1:0:108:ASN:OD1	1:0:147: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
1:0:108:ASN:OD1	1:0:147:ARG:NH1	2.34	0.61
2:B:3:THR:HG1	2:B:127:THR:HG1	1.48	0.61
1:0:99:GLU:OE1	1:0:115: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:X:3:THR:HG1	2:X:127:THR:HG1	1.47	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:3:THR:HG1	2:T:127:THR:HG1	1.48	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
1:Y:99:GLU:OE1	1:Y: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:L:3:THR:HG1	2:L:127:THR:HG1	1.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:3:THR:HG1	2:L:127:THR:HG1	1.48	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
1:M:99:GLU:OE1	1:M:115:ARG:NH2	2.34	0.60
1:Q:99:GLU:OE1	1:Q:115:ARG:NH2	2.34	0.60
2:H:7:THR:HG23	2:H:108:PRO:HB2	1.83	0.60
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
2:J:3:THR:HG1	2:J:127:THR:HG1	1.47	0.60
2:L:7:THR:HG23	2:L:108:PRO:HB2	1.83	0.60
2:T:7:THR:HG23	2:T:108:PRO:HB2	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:B:3:THR:HG1	2:B:127:THR:HG1	1.49	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
2:F:7:THR:HG23	2:F:108:PRO:HB2	1.83	0.60
2:N:7:THR:HG23	2:N:108:PRO:HB2	1.83	0.60
2:R:7:THR:HG23	2:R:108:PRO:HB2	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3:THR:HG1	2:D:127:THR:HG1	1.44	0.60
2:Z:7:THR:HG23	2:Z:108:PRO:HB2	1.83	0.60
2:1:3:THR:HG1	2:1:127:THR:HG1	1.45	0.60
2:T:3:THR:HG1	2:T:127:THR:HG1	1.48	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:I:99:GLU:OE1	1:I: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:O:99:GLU:OE1	1:O:115:ARG:NH2	2.34	0.60
1:U:99:GLU:OE1	1:U:115:ARG:NH2	2.34	0.60
1:Q:97:GLN:HG3	2:R:65:LEU:HG	1.83	0.60
1:W:97:GLN:HG3	2:X:65:LEU:HG	1.83	0.60
2:H:7:THR:HG23	2:H:108:PRO:HB2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:7:THR:HG23	2:D:108:PRO:HB2	1.83	0.60
1:Y:99:GLU:OE1	1:Y:115:ARG:NH2	2.34	0.60
2:H:3:THR:HG1	2:H:127:THR:HG1	1.48	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
1:0:99:GLU:OE1	1:0:115:ARG:NH2	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
2:P:7:THR:HG23	2:P:108:PRO:HB2	1.83	0.60
2:1:7:THR:HG23	2:1:108:PRO:HB2	1.83	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:N	1:S:72:ASP:OD1	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
2:F:3:THR:HG1	2:F:127:THR:HG1	1.50	0.60
2:X:7:THR:HG23	2:X: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
2:1:3:THR:HG1	2:1:127:THR:HG1	1.47	0.60
1:K:99:GLU:OE1	1:K:115:ARG:NH2	2.34	0.59
1:Y:72:ASP:OD1	1:Y:72:ASP:N	2.35	0.59
2:Z:3:THR:HG1	2:Z:127:THR:HG1	1.50	0.59
1:S:99:GLU:OE1	1:S:115:ARG:NH2	2.34	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
2:V:7:THR:HG23	2:V:108:PRO:HB2	1.83	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
1:0:37:ALA:O	1:0:164:ALA:HA	2.03	0.59
1:W:99:GLU:OE1	1:W:115:ARG:NH2	2.34	0.59
1:C:72:ASP:OD1	1:C:72:ASP:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:72:ASP:OD1	1:0:72:ASP:N	2.35	0.59
2:T:105:ASP:O	2:T:180:ARG:NH2	2.36	0.59
1:0:97:GLN:HG3	2:1:65:LEU:HG	1.85	0.59
2:J:7:THR:HG23	2:J:108:PRO:HB2	1.83	0.59
1:C:37:ALA:O	1:C:164:ALA:HA	2.03	0.59
1:G:99:GLU:OE1	1:G:115:ARG:NH2	2.34	0.59
2:N:141:GLN:HE21	2:1:141:GLN:HE21	1.49	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
1:C:99:GLU:OE1	1:C:115:ARG:NH2	2.36	0.59
2:X:3:THR:HG1	2:X:127:THR:HG1	1.49	0.59
1:0:99:GLU:OE1	1:0:115: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:F:3:THR:HG1	2:F:127:THR:HG1	1.49	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
2:1:3:THR:HG22	2:1:16:THR:HG23	1.83	0.59
1:O:37:ALA:O	1:O:164:ALA:HA	2.03	0.59
2:J:141:GLN:HE21	2:X:141:GLN:HE21	1.50	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
2:H:3:THR:HG1	2:H:127:THR:HG1	1.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:S:99:GLU:OE1	1:S:115: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:D:105:ASP:O	2:D:180:ARG:NH2	2.36	0.59
1:K:99:GLU:OE1	1:K:115: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
2:H:3:THR:HG1	2:H:127:THR:HG1	1.50	0.59
1:0:97: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
1:G:99:GLU:OE1	1:G:115:ARG:NH2	2.36	0.58
1:W:99:GLU:OE1	1:W:115:ARG:NH2	2.36	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:97:GLN:HG3	2:X:65:LEU:HG	1.84	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:R:88:ASN:ND2	2:T:50:GLY:O	2.37	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
2:Z:7:THR:HG23	2:Z:108:PRO:HB2	1.84	0.58
1:E:99:GLU:OE1	1:E:115:ARG:NH2	2.36	0.58
1:S:84:ASP:OD1	1:U:121:GLN:NE2	2.34	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	1.84	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
2:1:105:ASP:O	2:1:180:ARG:NH2	2.37	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:L:3:THR:HG1	2:L:127:THR:HG1	1.47	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
1:0:152:ASP:HB3	1:0:156: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
2:H:3:THR:HG1	2:H:127:THR:HG1	1.48	0.58
1:O:99:GLU:OE1	1:O:115:ARG:NH2	2.36	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
2:F:105:ASP:O	2:F:180:ARG:NH2	2.37	0.58
2:P:105:ASP:O	2:P:180:ARG:NH2	2.37	0.58
2:Z:105:ASP:O	2:Z:180:ARG:NH2	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:37:ALA:O	1:W:164:ALA:HA	2.04	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
2:P:193:GLU:HG2	2:P:203:LEU:HD21	1.86	0.58
2:1:193:GLU:HG2	2:1:203:LEU:HD21	1.86	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
1:C:99:GLU:OE1	1:C:115:ARG:NH2	2.36	0.58
2:D:193:GLU:HG2	2:D:203:LEU:HD21	1.86	0.58
2:H:193:GLU:HG2	2:H:203:LEU:HD21	1.86	0.58
1:I:99:GLU:OE1	1:I:115:ARG:NH2	2.36	0.58
1:U:99:GLU:OE1	1:U:115:ARG:NH2	2.36	0.58
2:X:3:THR:HG1	2:X:127:THR:HG1	1.48	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
2:1:7:THR:HG23	2:1:108:PRO:HB2	1.85	0.58
2:R:105:ASP:O	2:R:180:ARG:NH2	2.37	0.58
2:X:93:MET:HG3	2:X:94:PRO:HD3	1.86	0.58
1:O:121:GLN:NE2	1:0:84:ASP:OD1	2.36	0.58
1:M:99:GLU:OE1	1:M:115:ARG:NH2	2.36	0.58
1:Q:99:GLU:OE1	1:Q:115:ARG:NH2	2.36	0.58
2:T:3:THR:HG1	2:T:127:THR:HG1	1.48	0.58
2:X:193:GLU:HG2	2:X:203:LEU:HD21	1.86	0.58
1:0:99:GLU:OE1	1:0:115:ARG:NH2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:93:MET:HG3	2:H:94:PRO:HD3	1.86	0.58
2:N:105:ASP:O	2:N:180:ARG:NH2	2.37	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
2:J:193:GLU:HG2	2:J:203:LEU:HD21	1.86	0.58
2:L:193:GLU:HG2	2:L:203:LEU:HD21	1.86	0.58
2:V:193:GLU:HG2	2:V:203:LEU:HD21	1.86	0.58
2:Z:193:GLU:HG2	2:Z:203:LEU:HD21	1.86	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:F:93:MET:HG3	2:F:94:PRO:HD3	1.86	0.57
2:L:105:ASP:O	2:L:180:ARG:NH2	2.37	0.57
2:T:105:ASP:O	2:T:180:ARG:NH2	2.37	0.57
2:Z:93:MET:HG3	2:Z:94:PRO:HD3	1.86	0.57
1:O:72:ASP:OD1	1:O:72:ASP:N	2.35	0.57
2:P:88:ASN:ND2	2:R:50:GLY:O	2.37	0.57
2:F:193:GLU:HG2	2:F:203:LEU:HD21	1.86	0.57
2:N:193:GLU:HG2	2:N:203:LEU:HD21	1.86	0.57
2:T:193:GLU:HG2	2:T:203:LEU:HD21	1.86	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
2:X:3:THR:HG1	2:X:127:THR:HG1	1.50	0.57
1:0:36:THR:HA	1:0:165: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:I:97:GLN:HG3	2:J:65:LEU:HG	1.86	0.57
2:H:105:ASP:O	2:H:180:ARG:NH2	2.37	0.57
2:N:105:ASP:O	2:N:180:ARG:NH2	2.37	0.57
2:R:193:GLU:HG2	2:R:203:LEU:HD21	1.86	0.57
2:X:105:ASP:O	2:X:180:ARG:NH2	2.37	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
2:H:105:ASP:O	2:H:180:ARG:NH2	2.37	0.57
2:H:141:GLN:HE21	2:V:141:GLN:HE21	1.52	0.57
2:P:93:MET:HG3	2:P:94:PRO:HD3	1.86	0.57
2:1:93:MET:HG3	2:1:94: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
2:R:105:ASP:O	2:R:180:ARG:NH2	2.37	0.57
1:Y:84:ASP:OD1	1:0:121: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
1:0:97: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
2:V:93:MET:HG3	2:V:94:PRO:HD3	1.86	0.57
2:X:105:ASP:O	2:X:180:ARG:NH2	2.37	0.57
2:F:105:ASP:O	2:F:180:ARG:NH2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:105:ASP:O	2:L:180:ARG:NH2	2.38	0.57
1:Q:84:ASP:OD1	1:S:121:GLN:NE2	2.37	0.57
2:T:105:ASP:O	2:T:180:ARG:NH2	2.37	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
1:0:37:ALA:O	1:0:164: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:J:93:MET:HG3	2:J:94:PRO:HD3	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
1:0:41:LYS:HG2	1:0:46:VAL:HG12	1.86	0.57
2:J:105:ASP:O	2:J:180:ARG:NH2	2.37	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: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:P:105:ASP:O	2:P:180:ARG:NH2	2.37	0.57
2:V:105:ASP:O	2:V:180:ARG:NH2	2.38	0.57
2:Z:105:ASP:O	2:Z:180:ARG:NH2	2.37	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
1:0:39:GLY:O	1:0:162:ALA:HA	2.05	0.57
2:F:141:GLN:HE21	2:T:141:GLN:HE21	1.52	0.57
2:L:93:MET:HG3	2:L:94:PRO:HD3	1.86	0.57
2:N:93:MET:HG3	2:N:94:PRO:HD3	1.86	0.57
2:R:93:MET:HG3	2:R:94:PRO:HD3	1.86	0.57
2:T:93:MET:HG3	2:T:94:PRO:HD3	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:3:THR:HG1	2:X:127:THR:HG1	1.52	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
2:1:7:THR:HG23	2:1:108:PRO:HB2	1.87	0.57
1:Y:57:ARG:NH2	1:0:179:GLU:O	2.35	0.57
2:J:105:ASP:O	2:J:180:ARG:NH2	2.37	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: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:D:3:THR:HG1	2:D:127:THR:HG1	1.50	0.57
2:F:10:ASP:N	2:F:10:ASP:OD1	2.37	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
1:0:97:GLN:HG3	2:1:65:LEU:HG	1.87	0.57
2:V:105:ASP:O	2:V:180:ARG:NH2	2.37	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
2:1:105:ASP:O	2:1:180:ARG:NH2	2.37	0.57
2:L:7:THR:HG23	2:L:108:PRO:HB2	1.87	0.57
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
1:0:178:ARG:HG3	1:0:179:GLU:HG2	1.86	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:L:3:THR:HG1	2:L:127:THR:HG1	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:1:7:THR:HG23	2:1:108: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
2:1:3:THR:O	2:1:126:SER:HA	2.05	0.56
2:H:194:SER:O	2:H:198:LYS:HB2	2.05	0.56
2:X:194:SER:O	2:X:198:LYS:HB2	2.05	0.56
2:Z:194:SER:O	2:Z:198:LYS:HB2	2.05	0.56
2:1:194:SER:O	2:1:198:LYS:HB2	2.05	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
2:V:194:SER:O	2:V: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
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
2:F:194:SER:O	2:F:198:LYS:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:39:GLY:O	1:G:162:ALA:HA	2.06	0.56
2:J:194:SER:O	2:J:198:LYS:HB2	2.05	0.56
2:P:194:SER:O	2:P:198:LYS:HB2	2.05	0.56
1:W:39:GLY:O	1:W:162:ALA:HA	2.06	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:D:105:ASP:O	2:D:180:ARG:NH2	2.38	0.56
1:Y:84:ASP:OD1	1:0:121:GLN:NE2	2.38	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	1:0:84: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
2:J:3:THR:HG1	2:J:127:THR:HG1	1.51	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
2:L:194:SER:O	2:L:198:LYS:HB2	2.05	0.56
2:T:194:SER:O	2:T:198:LYS:HB2	2.05	0.56
1:Y:39:GLY:O	1:Y:162:ALA:HA	2.06	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
1:O:121:GLN:NE2	1:0:84:ASP:OD1	2.39	0.56
2:P:179:THR:O	2:P:183:GLY:HA2	2.05	0.56
2:H:163:LYS:NZ	2:H:171:GLY:O	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:121:GLN:NE2	1:E:84:ASP:OD1	2.38	0.56
2:1:105:ASP:O	2:1:180:ARG:NH2	2.38	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
1:I:121:GLN:NE2	1:K:84:ASP:OD1	2.38	0.56
2:R:163:LYS:NZ	2:R:171:GLY:O	2.36	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
1:I:39:GLY:O	1:I:162:ALA:HA	2.05	0.56
2:L:141:GLN:HE21	2:Z:141:GLN:HE21	1.53	0.56
1:U:39:GLY:O	1:U:162:ALA:HA	2.06	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
1:M:97:GLN:HG3	2:N:65:LEU:HG	1.86	0.56
1:Q:39:GLY:O	1:Q:162:ALA:HA	2.05	0.56
1:0:39:GLY:O	1:0:162: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:10:ASP:OD1	2:D:10:ASP:N	2.37	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	1:0:121: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
2:1:10:ASP:OD1	2:1:10:ASP:N	2.37	0.56
1:E:39:GLY:O	1:E:162:ALA:HA	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	1:0:84: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
1:K:121:GLN:NE2	1:M:84:ASP:OD1	2.38	0.56
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:B:141:GLN:HE21	2:P:141:GLN:HE21	1.52	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:O:182:GLU:OE2	1:0:57:ARG:NH1	2.40	0.55
1:U:57:ARG:NH1	1:W:182:GLU:OE2	2.40	0.55
2:N:194:SER:O	2:N:198:LYS:HB2	2.05	0.55
2:R:194:SER:O	2:R:198:LYS:HB2	2.05	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
1:0:39:GLY:O	1:0:162: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:P:88:ASN:ND2	2:R:50:GLY:O	2.40	0.55
1:0:39:GLY:O	1:0:162:ALA:HA	2.05	0.55
2:F:105:ASP:O	2:F:180:ARG:NH2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:Y:57:ARG:NH1	1:0:182: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:F:163:LYS:NZ	2:F:171:GLY:O	2.36	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
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
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
1:M:39:GLY:O	1:M:162:ALA:HA	2.05	0.55
1:S:39:GLY:O	1:S:162:ALA:HA	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:10:ASP:OD1	2:B:10:ASP:N	2.37	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
1:A:84:ASP:OD1	1:M:121:GLN:NE2	2.39	0.55
1:G:172:VAL:HG13	1:G:196:ALA:HB1	1.89	0.55
1:O:172:VAL:HG13	1:O:196:ALA:HB1	1.89	0.55
1:W:172:VAL:HG13	1:W:196:ALA:HB1	1.89	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: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:K:39:GLY:O	1:K:162:ALA:HA	2.06	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
1:I:121:GLN:NE2	1:K:84:ASP:OD1	2.38	0.55
1:K:121:GLN:NE2	1:M:84:ASP:OD1	2.39	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
1:C:41:LYS:HG2	1:C:46:VAL:HG12	1.88	0.55
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
1:Q:39:GLY:O	1:Q:162:ALA:HA	2.06	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:Z:70:ARG:NH2	1:0:99:GLU:OE2	2.40	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:O:39:GLY:O	1:O:162:ALA:HA	2.06	0.55
1:E:172:VAL:HG13	1:E:196:ALA:HB1	1.89	0.55
1:M:172:VAL:HG13	1:M:196:ALA:HB1	1.89	0.55
1:O:84:ASP:OD1	1:Q:121:GLN:NE2	2.39	0.55
1:Q:172:VAL:HG13	1:Q:196:ALA:HB1	1.89	0.55
1:Y:172:VAL:HG13	1:Y:196:ALA:HB1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:P:10:ASP:N	2:P:10:ASP:OD1	2.37	0.55
1:E:179:GLU:O	1:G:57:ARG:NH2	2.39	0.54
2:J:105:ASP:O	2:J:180:ARG:NH2	2.39	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
2:Z:105:ASP:O	2:Z:180:ARG:NH2	2.40	0.54
1:A:39:GLY:O	1:A:162:ALA:HA	2.06	0.54
2:1:105:ASP:O	2:1:180:ARG:NH2	2.39	0.54
1:E:121:GLN:NE2	1:G:84:ASP:OD1	2.39	0.54
1:U:172:VAL:HG13	1:U:196:ALA:HB1	1.89	0.54
1:0:172:VAL:HG13	1:0:196:ALA:HB1	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
1:0:41:LYS:HG2	1:0:46:VAL:HG12	1.88	0.54
2:1:105:ASP:O	2:1:180: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
1:I:172:VAL:HG13	1:I:196:ALA:HB1	1.89	0.54
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
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	1:0:121:GLN:NE2	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:J:141:GLN:HE21	2:X:141:GLN:HE21	1.55	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
1:0:173:VAL:O	1:0:177: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:K:172:VAL:HG13	1:K:196:ALA:HB1	1.89	0.54
1:S:172:VAL:HG13	1:S:196:ALA:HB1	1.89	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
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
2:J:3:THR:OG1	2:J:127:THR:OG1	2.24	0.54
1:O:76:ALA:HA	1:O:137:ILE:O	2.08	0.54
1:W:76:ALA:HA	1:W:137:ILE:O	2.08	0.54
1:Y:84:ASP:OD1	1:0:121:GLN:NE2	2.40	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:E:121:GLN:NE2	1:G:84:ASP:OD1	2.39	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
1:O:121:GLN:NE2	1:0:84:ASP:OD1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:F:3:THR:HG1	2:F:127:THR:HG1	1.48	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
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
2:1:3:THR:OG1	2:1:127:THR:OG1	2.26	0.54
1:G:121:GLN:NE2	1:I:84:ASP:OD1	2.39	0.54
1:U:84:ASP:OD1	1:W:121:GLN:NE2	2.39	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
1:G:121:GLN:NE2	1:I:84:ASP:OD1	2.41	0.54
1:W:84:ASP:OD1	1:Y:121:GLN:NE2	2.39	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
1:0:76:ALA:HA	1:0:137:ILE:O	2.08	0.53
1:G:162:ALA:HB1	1:G:176:LEU:HD13	1.89	0.53
1:0:162:ALA:HB1	1:0:176:LEU:HD13	1.90	0.53
1:I:121:GLN:NE2	1:K:84:ASP:OD1	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:L:50:GLY:O	2:N:88:ASN:ND2	2.41	0.53
1:Y:84:ASP:OD1	1:0:121:GLN:NE2	2.41	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:N:15:ALA:HA	2:N:174:ASP:O	2.08	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
1:G:121:GLN:NE2	1:I:84:ASP:OD1	2.42	0.53
2:P:50:GLY:O	2:1:88:ASN:ND2	2.41	0.53
1:S:84:ASP:OD1	1:U:121:GLN:NE2	2.41	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: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
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
1:U:84:ASP:OD1	1:W:121:GLN:NE2	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:O:99:GLU:HB2	1:O:115:ARG:HH22	1.74	0.53
2:T:88:ASN:ND2	2:V:50:GLY:O	2.41	0.53
1:W:84:ASP:OD1	1:Y:121:GLN:NE2	2.42	0.53
2:D:90:VAL:HG23	2:D:94:PRO:HB3	1.90	0.53
2:D:163:LYS:NZ	2:D:171:GLY:O	2.36	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:V:3:THR:HG1	2:V:127:THR:HG1	1.46	0.53
2:Z:3:THR:HG1	2:Z:127:THR:HG1	1.53	0.53
1:M:99:GLU:HB2	1:M:115:ARG:HH22	1.74	0.53
1:Q:99:GLU:HB2	1:Q:115:ARG:HH22	1.74	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
1:0:97: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: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:E:121:GLN:NE2	1:G:84:ASP:OD1	2.42	0.53
1:0:99:GLU:HB2	1:0:115:ARG:HH22	1.74	0.53
1:O:84:ASP:OD1	1:Q:121:GLN:NE2	2.41	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:15:ALA:HA	2:J:174:ASP:O	2.08	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
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:X:88:ASN:ND2	2:Z:50:GLY:O	2.41	0.53
1:Y:99:GLU:HB2	1:Y:115:ARG:HH22	1.74	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
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
2:B:88:ASN:ND2	2:N:50:GLY:O	2.42	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:J:50:GLY:O	2:L:88:ASN:ND2	2.42	0.53
1:K:99:GLU:HB2	1:K:115:ARG:HH22	1.74	0.53
1:S:99:GLU:HB2	1:S:115:ARG:HH22	1.74	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:3:THR:HG22	2:X:16:THR:HG23	1.90	0.53
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
1:G:99:GLU:HB2	1:G:115:ARG:HH22	1.74	0.52
1:W:99:GLU:HB2	1:W:115:ARG:HH22	1.74	0.52
2:F:178:ILE:HA	2:F:183:GLY:O	2.09	0.52
1:0:37:ALA:O	1:0:164: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
1:K:121:GLN:NE2	1:M:84:ASP:OD1	2.41	0.52
1:U:99:GLU:HB2	1:U:115:ARG:HH22	1.74	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:J:3:THR:HG1	2:J:127:THR:HG1	1.46	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
2:Z:3:THR:HG1	2:Z:127:THR:HG1	1.48	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:I:99:GLU:HB2	1:I:115:ARG:HH22	1.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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	1:0:121:GLN:NE2	2.41	0.52
1:C:37:ALA:O	1:C:164:ALA:HA	2.08	0.52
2:F:50:GLY:O	2:H:88:ASN:ND2	2.42	0.52
1:Q:84:ASP:OD1	1:S:121:GLN:NE2	2.42	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:O:84:ASP:OD1	1:Q:121:GLN:NE2	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	1:0:84: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
1:0:37:ALA:O	1:0:164:ALA:HA	2.08	0.52
2:1:18:ARG:HD3	2:1:172:MET:HB3	1.91	0.52
2:H:50:GLY:O	2:J:88:ASN:ND2	2.42	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:B:132:PRO:HB2	2:P:132:PRO:HB2	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:84:ASP:OD1	1:M:121:GLN:NE2	2.42	0.52
2:R:178:ILE:HA	2:R:183:GLY:O	2.09	0.52
2:F:132:PRO:HB2	2:T:132:PRO:HB2	1.90	0.52
1:I:51:ASP:HB2	1:I:197:LEU:HD11	1.92	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
1:A:121:GLN:NE2	1:C:84:ASP:OD1	2.42	0.52
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
1:0:99:GLU:HB2	1:0:115:ARG:HH22	1.75	0.52
2:Z:88:ASN:ND2	2:1:50:GLY:O	2.42	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
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
1:O:121:GLN:NE2	1:0:84:ASP:OD1	2.42	0.52
1:U:51:ASP:HB2	1:U:197:LEU:HD11	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
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
1:G:51:ASP:HB2	1:G:197:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:51:ASP:HB2	1:W:197:LEU:HD11	1.92	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: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
1:K:51:ASP:HB2	1:K:197:LEU:HD11	1.92	0.51
2:J:141:GLN:HE21	2:X:141:GLN:HE21	1.57	0.51
1:0:181:LYS:HE2	1:0:184: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: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
2:N:132:PRO:HB2	2:1:132:PRO:HB2	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
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
2:D:132:PRO:HB2	2:R:132:PRO:HB2	1.92	0.51
1:0:51:ASP:HB2	1:0:197:LEU:HD11	1.92	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
1:W:99:GLU:HB2	1:W:115:ARG:HH22	1.75	0.51
2:V:88:ASN:ND2	2:X:50:GLY:O	2.43	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
1:E:121:GLN:NE2	1:G:84:ASP:OD1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:3:THR:HG1	2:N:127:THR:HG1	1.56	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
1:S:51:ASP:HB2	1:S:197:LEU:HD11	1.92	0.51
2:L:141:GLN:HE21	2:Z:141:GLN:HE21	1.58	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	1:0:84:ASP:OD1	2.42	0.51
2:H:178:ILE:HA	2:H:183:GLY:O	2.09	0.51
1:A:51:ASP:HB2	1:A:197:LEU:HD11	1.92	0.51
1:0:152:ASP:O	1:0:155: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:H:3:THR:OG1	2:H:127:THR:OG1	2.26	0.51
2:L:153:ASP:OD1	2:L:195:ARG:NH1	2.44	0.51
1:O:51:ASP:HB2	1:O:197:LEU:HD11	1.92	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	1:0:84: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
1:Y:51:ASP:HB2	1:Y:197:LEU:HD11	1.92	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	1:0:121:GLN:NE2	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:99:GLU:HB2	1:U:115:ARG:HH22	1.75	0.50
1:E:51:ASP:HB2	1:E:197:LEU:HD11	1.92	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
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
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:M:51:ASP:HB2	1:M:197:LEU:HD11	1.92	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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:Z:153:ASP:HB3	2:Z:199:LEU:HD11	1.93	0.50
1:Q:51:ASP:HB2	1:Q:197:LEU:HD11	1.92	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
1:Y:84:ASP:OD1	1:0:121:GLN:NE2	2.44	0.50
1:0:41:LYS:HG2	1:0:46: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:L:132:PRO:HB2	2:Z:132:PRO:HB2	1.92	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
1:0:45:GLY:HA3	1:0:215: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
2:1:16:THR:HG21	2:1:33:LYS:HB2	1.94	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: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
1:0:172:VAL:HG13	1:0:196: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:GLY:HA3	1:A:215:ILE:O	2.11	0.49
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: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:3:THR:O	2:J:126:SER:HA	2.12	0.49
2:X:3:THR:O	2:X:126:SER:HA	2.12	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
1:S:152:ASP:O	1:S:155:GLY:N	2.42	0.49
1:Q:152:ASP:O	1:Q:155:GLY:N	2.44	0.49
2:V:3:THR:O	2:V:126:SER:HA	2.13	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
1:0:99:GLU:HB2	1:0:115: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
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:G:54:VAL:HB	1:G:208:LYS:HE2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:3:THR:O	2:H:126:SER:HA	2.13	0.49
1:O:54:VAL:HB	1:O:208:LYS:HE2	1.95	0.49
1:W:54:VAL:HB	1:W:208:LYS:HE2	1.95	0.49
1:Y:67:ILE:HG12	1:Y:77:VAL:HG22	1.94	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
2:V:153:ASP:HB3	2:V:199:LEU:HD11	1.93	0.49
1:0:54:VAL:HB	1:0:208:LYS:HD3	1.94	0.49
1:Q:45:GLY:HA3	1:Q:215:ILE:O	2.11	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:E:54:VAL:HB	1:E:208:LYS:HD3	1.94	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
1:0:152:ASP:O	1:0:155: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
1:0:76:ALA:HA	1:0:137:ILE:O	2.12	0.49
2:F:3:THR:O	2:F:126:SER:HA	2.13	0.49
1:M:78:THR:HG22	1:M:136:LEU:HG	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:152:ASP:O	1:M:155:GLY:N	2.44	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:K:150:ASP:O	1:K:157:ILE:HA	2.13	0.49
1:Y:54:VAL:HB	1:Y:208:LYS:HD3	1.95	0.49
1:G:181:LYS:HE2	1:G:184:LEU:HD21	1.93	0.49
1:0:194:ILE:HD11	1:0:212: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
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:M:54:VAL:HB	1:M:208:LYS:HE2	1.95	0.49
1:O:78:THR:HG22	1:O:136:LEU:HG	1.94	0.49
1:Q:78:THR:HG22	1:Q:136:LEU:HG	1.94	0.49
1:Y:54:VAL:HB	1:Y:208:LYS:HE2	1.95	0.49
2:Z:3:THR:O	2:Z:126:SER:HA	2.13	0.49
1:0:54:VAL:HB	1:0:208:LYS:HE2	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
1:G:121:GLN:NE2	1:I:84:ASP:OD1	2.45	0.49
1:0:49:ILE:HG12	1:0:212:ILE:HG12	1.95	0.49
1:A:54:VAL:HB	1:A:208:LYS:HD3	1.95	0.49
1:S:150:ASP:O	1:S:157:ILE:HA	2.13	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:Q:54:VAL:HB	1:Q: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:O:67:ILE:HG12	1:O:77:VAL:HG22	1.94	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:I:150:ASP:O	1:I:157:ILE:HA	2.13	0.49
1:O:54:VAL:HB	1:O:208:LYS:HD3	1.94	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
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:K:78:THR:HG22	1:K:136:LEU:HG	1.94	0.49
1:U:54:VAL:HB	1:U:208:LYS:HE2	1.95	0.49
1:W:67:ILE:HG12	1:W:77:VAL:HG22	1.95	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
1:A:67:ILE:HG12	1:A:77:VAL:HG22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:150:ASP:O	1:G:157:ILE:HA	2.13	0.49
2:J:132:PRO:HB2	2:X:132:PRO:HB2	1.95	0.49
2:J:167:SER:HB2	2:Z:167:SER:HB2	1.95	0.49
1:K:67:ILE:HG12	1:K:77:VAL:HG22	1.95	0.49
1:O:67:ILE:HG12	1:O:77:VAL:HG22	1.95	0.49
1:S:67:ILE:HG12	1:S:77:VAL:HG22	1.95	0.49
1:U:150:ASP:O	1:U:157:ILE:HA	2.13	0.49
1:W:150:ASP:O	1:W:157:ILE:HA	2.13	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:I:54:VAL:HB	1:I:208:LYS:HE2	1.95	0.49
2:T:3:THR:O	2:T:126:SER:HA	2.13	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
1:E:150:ASP:O	1:E:157:ILE:HA	2.13	0.49
1:0:150:ASP:O	1:0:157:ILE:HA	2.13	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
1:0:162:ALA:HB1	1:0:176:LEU:HD13	1.94	0.49
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
1:0:78:THR:HG22	1:0:136: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:67:ILE:HG12	1:G:77:VAL:HG22	1.95	0.48
1:S:78:THR:HG22	1:S:136:LEU:HG	1.94	0.48
1:0:67:ILE:HG12	1:0:77:VAL:HG22	1.95	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
1:0:20:ARG:NH1	1:0:25:GLU:OE1	2.46	0.48
1:A:49:ILE:HG12	1:A:212:ILE:HG12	1.95	0.48
1:C:150:ASP:O	1:C:157:ILE:HA	2.13	0.48
1:Y:150:ASP:O	1:Y: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
2:L:3:THR:O	2:L:126:SER:HA	2.13	0.48
1:Q:67:ILE:HG12	1:Q:77:VAL:HG22	1.95	0.48
1:G:67:ILE:HG12	1:G:77:VAL:HG22	1.94	0.48
1:W:67:ILE:HG12	1:W:77:VAL:HG22	1.94	0.48
1:0:78:THR:HG22	1:0:136:LEU:HG	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:O:150:ASP:O	1:O: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
1:0:110:GLU:HA	1:0:149: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
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
1:E:99:GLU:OE2	2:H:70:ARG:NH2	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:99:GLU:HB2	1:Q:115:ARG:HH22	1.77	0.48
1:0:172:VAL:HG13	1:0:196: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
2:1:3:THR:HG22	2:1:16:THR:HG23	1.94	0.48
1:G:78:THR:HG22	1:G:136:LEU:HG	1.94	0.48
1:K:54:VAL:HB	1:K:208:LYS:HE2	1.95	0.48
1:0:78:THR:HG22	1:0:136:LEU:HG	1.94	0.48
1:C:20:ARG:NH1	1:C:25:GLU:OE1	2.46	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:I:67:ILE:HG12	1:I:77:VAL:HG22	1.95	0.48
1:M:67:ILE:HG12	1:M:77:VAL:HG22	1.95	0.48
1:M:150:ASP:O	1:M:157:ILE:HA	2.13	0.48
1:Q:67:ILE:HG12	1:Q:77:VAL:HG22	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: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:I:67:ILE:HG12	1:I:77:VAL:HG22	1.95	0.48
1:M:67:ILE:HG12	1:M:77:VAL:HG22	1.95	0.48
1:W:78:THR:HG22	1:W:136:LEU:HG	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
1:G:54:VAL:HB	1:G:208:LYS:HD3	1.95	0.48
2:L:3:THR:HG22	2:L:16:THR:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:39:GLY:HA2	1:M:47:LEU:O	2.14	0.48
1:Q:150:ASP:O	1:Q:157:ILE:HA	2.13	0.48
1:U:67:ILE:HG12	1:U:77:VAL:HG22	1.95	0.48
1:W:54:VAL:HB	1:W:208:LYS:HD3	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
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
1:E:78:THR:HG22	1:E:136:LEU:HG	1.94	0.48
1:K:67:ILE:HG12	1:K:77:VAL:HG22	1.95	0.48
1:S:54:VAL:HB	1:S:208:LYS:HE2	1.95	0.48
1:U:67:ILE:HG12	1:U:77:VAL:HG22	1.95	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
2:J:3:THR:HG22	2:J:16:THR:HG23	1.95	0.48
1:Q:39:GLY:HA2	1:Q:47:LEU:O	2.14	0.48
1:S:39:GLY:HA2	1:S:47:LEU:O	2.14	0.48
2:T:3:THR:HG22	2:T:16:THR:HG23	1.95	0.48
1:0:67:ILE:HG12	1:0:77:VAL:HG22	1.95	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:S:67:ILE:HG12	1:S:77:VAL:HG22	1.95	0.48
1:Y:78:THR:HG22	1:Y:136:LEU:HG	1.94	0.48
2:1:3:THR:O	2:1:126:SER:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:39:GLY:HA2	1:E:47:LEU:O	2.14	0.48
1:K:39:GLY:HA2	1:K:47:LEU:O	2.14	0.48
1:M:54:VAL:HB	1:M:208:LYS:HD3	1.95	0.48
2:V:3:THR:HG22	2:V:16:THR:HG23	1.95	0.48
1:Y:39:GLY:HA2	1:Y:47:LEU:O	2.14	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:I:78:THR:HG22	1:I:136:LEU:HG	1.94	0.48
1:Y:152:ASP:O	1:Y:155:GLY:N	2.44	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
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: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:I:39:GLY:HA2	1:I:47:LEU:O	2.13	0.48
1:O:39:GLY:HA2	1:O:47:LEU:O	2.14	0.48
1:Q:54:VAL:HB	1:Q:208:LYS:HD3	1.95	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
1:0:39:GLY:O	1:0:162: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:0:67:ILE:HG12	1:0:77: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:D:3:THR:HG22	2:D:16:THR:HG23	1.95	0.48
2:N:3:THR:HG22	2:N:16:THR:HG23	1.94	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
1:0:99:GLU:HB2	1:0:115: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
1:0:194:ILE:HD11	1:0:212:ILE:HD11	1.95	0.48
1:E:152:ASP:O	1:E:155:GLY:N	2.44	0.48
1:U:78:THR:HG22	1:U:136:LEU:HG	1.94	0.48
1:S:20:ARG:NH1	1:S:25:GLU:OE1	2.46	0.48
2:H:3:THR:HG22	2:H:16:THR:HG23	1.94	0.48
1:U:39:GLY:HA2	1:U:47:LEU:O	2.14	0.48
2:1:3:THR:HG22	2:1:16:THR:HG23	1.95	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:F:3:THR:OG1	2:F:127:THR:OG1	2.26	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:W:39:GLY:HA2	1:W:47:LEU:O	2.14	0.48
2:X:3:THR:HG22	2:X:16:THR:HG23	1.94	0.48
1:0:39:GLY:HA2	1:0:47: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:16:THR:HG21	2:P:33:LYS:HB2	1.96	0.47
2:1:16:THR:HG21	2:1:33: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
1:G:39:GLY:HA2	1:G:47:LEU:O	2.14	0.47
2:P:3:THR:HG22	2:P:16:THR:HG23	1.94	0.47
2:R:3:THR:HG22	2:R:16:THR:HG23	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
1:O:67:ILE:HG12	1:O:77:VAL:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:3:THR:O	2:P:126:SER:HA	2.13	0.47
2:V:16:THR:HG21	2:V:33:LYS:HB2	1.96	0.47
1:0:152:ASP:HB3	1:0:156:THR:HB	1.96	0.47
1:G:67:ILE:HG12	1:G:77:VAL:HG22	1.95	0.47
1:G:72:ASP:OD2	2:H:67:ARG:NH2	2.48	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:J:16:THR:HG21	2:J:33:LYS:HB2	1.96	0.47
2:N:16:THR:HG21	2:N:33:LYS:HB2	1.96	0.47
2:R:16:THR:HG21	2:R:33:LYS:HB2	1.96	0.47
2:T:16:THR:HG21	2:T: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
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
1:W:67:ILE:HG12	1:W:77:VAL:HG22	1.95	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
2:L:16:THR:HG21	2:L:33:LYS:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:3:THR:O	2:R:126:SER:HA	2.13	0.47
1:0:172:VAL:HG13	1:0:196:ALA:HB1	1.97	0.47
1:A:152:ASP:HB3	1:A:156:THR:HB	1.96	0.47
1:G:178:ARG:HG3	1:G:179:GLU:HG2	1.97	0.47
1:S:54:VAL:HB	1:S:208:LYS:HD3	1.95	0.47
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
1:0:55:ARG:HH22	1:0:208:LYS:NZ	2.13	0.47
1:0:46:VAL:HG11	1:0:139: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
2:N:3:THR:O	2:N:126:SER:HA	2.13	0.47
1:Y:172:VAL:HG13	1:Y:196:ALA:HB1	1.97	0.47
2:Z:16:THR:HG21	2:Z:33:LYS:HB2	1.96	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
1:E:67:ILE:HG12	1:E:77:VAL:HG22	1.95	0.47
1:K:54:VAL:HB	1:K:208:LYS:HD3	1.95	0.47
1:Y:67:ILE:HG12	1:Y:77:VAL:HG22	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
2:H:16:THR:HG21	2:H:33:LYS:HB2	1.96	0.47
2:X:16:THR:HG21	2:X:33:LYS:HB2	1.96	0.47
1:O:78:THR:HG22	1:O:136:LEU:HG	1.95	0.47
1:E:52:LYS:HD2	1:E:64:ILE:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:F:3:THR:HG22	2:F:16:THR:HG23	1.94	0.47
1:I:54:VAL:HB	1:I:208:LYS:HD3	1.95	0.47
2:Z:3:THR:HG22	2:Z:16:THR:HG23	1.95	0.47
1:O:160:TYR:CE1	1:0:59: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
1:G:172:VAL:HG13	1:G:196:ALA:HB1	1.97	0.47
1:I:194:ILE:HD11	1:I:212:ILE:HD11	1.96	0.47
1:O:172:VAL:HG13	1:O:196:ALA:HB1	1.97	0.47
1:U:194:ILE:HD11	1:U:212:ILE:HD11	1.97	0.47
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
1:Y:186:GLU:OE2	1:Y:224:TYR:OH	2.31	0.47
2:H:93:MET:HB2	2:J:92:TYR:CE2	2.49	0.47
1:U:54:VAL:HB	1:U:208:LYS:HD3	1.95	0.47
1:U:72:ASP:OD2	2:V:67:ARG:NH2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:W:172:VAL:HG13	1:W: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
1:I:45:GLY:HA3	1:I:215: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
1:G:76:ALA:HA	1:G:137:ILE:O	2.15	0.47
2:L:163:LYS:NZ	2:L:203:LEU:O	2.41	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: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
1:0:52:LYS:HD2	1:0:64:ILE:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:45:GLY:HA3	1:U:215:ILE:O	2.15	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: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:172:VAL:HG13	1:I:196:ALA:HB1	1.97	0.47
1:U:172:VAL:HG13	1:U:196:ALA:HB1	1.97	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	1:0:130:ARG:O	2.48	0.47
1:C:125:GLN:NE2	1:E:130:ARG:O	2.48	0.47
1:Y:130:ARG:O	1:0:125:GLN:NE2	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
1:O:179:GLU:O	1:0:57:ARG:NH2	2.44	0.46
1:0:77:VAL:HG22	1:0:137:ILE:HB	1.97	0.46
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
1:S:152:ASP:O	1:S:155:GLY:N	2.44	0.46
1:Y:194:ILE:HD11	1:Y:212:ILE:HD11	1.96	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
1:0:51:ASP:HB2	1:0:197:LEU:HD11	1.97	0.46
1:E:125:GLN:NE2	1:G:130:ARG:O	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:1:15:ALA:HA	2:1:174:ASP:O	2.15	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:Z:15:ALA:HA	2:Z:174:ASP:O	2.14	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:Q:130:ARG:O	1:S:125:GLN:NE2	2.49	0.46
1:S:60:GLU:OE2	1:U:41:LYS:NZ	2.40	0.46
1:0:45:GLY:HA3	1:0:215: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
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:W:100:LYS:NZ	2:X:64:GLU:OE2	2.44	0.46
1:0:49:ILE:HG12	1:0:212: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
1:K:152:ASP:O	1:K:155:GLY:N	2.44	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
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
1:O:49:ILE:HG12	1:O:212:ILE:HG12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	1:0:125:GLN:NE2	2.48	0.46
1:0:76:ALA:HA	1:0:137:ILE:O	2.15	0.46
1:0:178:ARG:HG3	1:0:179:GLU:HG2	1.97	0.46
1:E:45:GLY:HA3	1:E:215:ILE:O	2.15	0.46
1:K:45:GLY:HA3	1:K:215:ILE:O	2.15	0.46
1:W:45:GLY:HA3	1:W:215:ILE:O	2.15	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
1:S:20:ARG:NH2	1:S:25:GLU:OE1	2.48	0.46
1:M:194:ILE:HD11	1:M:212:ILE:HD11	1.96	0.46
1:O:194:ILE:HD11	1:O:212:ILE:HD11	1.96	0.46
1:0:152:ASP:O	1:0:155:GLY:N	2.44	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
1:K:125:GLN:NE2	1:M:130:ARG:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:45:GLY:HA3	1:S:215:ILE:O	2.15	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
1:0:76:ALA:HA	1:0:137: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: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
2:1:4:VAL:HG22	2:1:134:VAL:HG11	1.98	0.46
1:M:172:VAL:HG13	1:M:196:ALA:HB1	1.97	0.46
1:S:172:VAL:HG13	1:S:196:ALA:HB1	1.97	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
1:0:186:GLU:OE2	1:0:224:TYR:OH	2.31	0.46
1:A:45:GLY:HA3	1:A:215:ILE:O	2.15	0.46
1:E:68:GLN:HE21	1:E:89:VAL:HG21	1.80	0.46
1:K:68:GLN:HE21	1:K:89:VAL:HG21	1.80	0.46
1:O:45:GLY:HA3	1:O:215:ILE:O	2.15	0.46
1:Y:45:GLY:HA3	1:Y:215:ILE:O	2.15	0.46
2:D:1:THR:N	2:D: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
2:H:15:ALA:HA	2:H:174:ASP:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:172:VAL:HG13	1:0:196: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
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
1:0:78:THR:HG22	1:0:136:LEU:HG	1.97	0.46
2:D:50:GLY:O	2:F:88:ASN:ND2	2.49	0.46
1:K:172:VAL:HG13	1:K:196:ALA:HB1	1.97	0.46
1:Q:172:VAL:HG13	1:Q:196:ALA:HB1	1.97	0.46
1:Q:194:ILE:HD11	1:Q:212:ILE:HD11	1.96	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
1:G:45:GLY:HA3	1:G:215:ILE:O	2.15	0.46
1:O:68:GLN:HE21	1:O:89:VAL:HG21	1.80	0.46
1:S:68:GLN:HE21	1:S:89:VAL:HG21	1.80	0.46
2:T:16:THR:HG21	2:T:33:LYS:HB2	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:4:VAL:HG22	2:R:134:VAL:HG11	1.98	0.46
1:G:194:ILE:HD11	1:G:212:ILE:HD11	1.96	0.46
1:G:227:GLU:H	1:G:227:GLU:HG3	1.60	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
1:0:67:ILE:HG12	1:0:77:VAL:HG22	1.98	0.46
1:G:68:GLN:HE21	1:G:89:VAL:HG21	1.80	0.46
1:Y:68:GLN:HE21	1:Y:89:VAL:HG21	1.80	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
2:F:163:LYS:NZ	2:F:203:LEU:O	2.41	0.46
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
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
1:0:20:ARG:NH2	1:0:25:GLU:OE1	2.48	0.46
1:C:152:ASP:O	1:C:155:GLY:N	2.44	0.46
1:W:194:ILE:HD11	1:W:212:ILE:HD11	1.96	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:I:125:GLN:NE2	1:K:130:ARG:O	2.49	0.46
2:L:16:THR:HG21	2:L:33:LYS:HB2	1.98	0.46
1:W:68:GLN:HE21	1:W:89:VAL:HG21	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:Q:45:GLY:HA3	1:Q:215:ILE:O	2.15	0.45
1:E:51:ASP:HB2	1:E:197:LEU:HD11	1.98	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
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:L:167:SER:HB2	2:1:167:SER:HB2	1.98	0.45
1:M:45:GLY:HA3	1:M:215:ILE:O	2.15	0.45
1:Q:68:GLN:HE21	1:Q:89:VAL:HG21	1.80	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
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
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
1:K:194:ILE:HD11	1:K:212:ILE:HD11	1.97	0.45
1:S:194:ILE:HD11	1:S: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
1:I:68:GLN:HE21	1:I:89:VAL:HG21	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:68:GLN:HE21	1:M:89:VAL:HG21	1.80	0.45
2:R:16:THR:HG21	2:R:33:LYS:HB2	1.98	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
1:0:194:ILE:HD11	1:0:212: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
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
2:1:20:VAL:HB	2:1:28:HIS:HB2	1.98	0.45
1:Y:227:GLU:H	1:Y:227:GLU:HG3	1.60	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
2:D:16:THR:HG21	2:D:33:LYS:HB2	1.98	0.45
2:J:16:THR:HG21	2:J:33:LYS:HB2	1.98	0.45
2:N:16:THR:HG21	2:N:33:LYS:HB2	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:D:167:SER:HB2	2:T:167:SER:HB2	1.98	0.45
1:O:125:GLN:NE2	1:0:130:ARG:O	2.50	0.45
1:U:68:GLN:HE21	1:U:89:VAL:HG21	1.80	0.45
2:V:16:THR:HG21	2:V:33:LYS:HB2	1.98	0.45
2:1:16:THR:HG21	2:1:33:LYS:HB2	1.98	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
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
1:0:51:ASP:HB2	1:0:197: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:78:THR:HG22	1:O:136:LEU:HG	1.97	0.45
2:Z:15:ALA:HA	2:Z:174:ASP:O	2.15	0.45
1:0:194:ILE:HD11	1:0:212:ILE:HD11	1.97	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
1:W:130:ARG:O	1:Y:125:GLN:NE2	2.49	0.45
2:V:44:THR:HG23	2:V:100:LEU:HB2	1.99	0.45
1:0:46:VAL:HG11	1:0:139: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
1:0:28:ARG:NH1	1:0:152: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
1:0:78:THR:HG22	1:0:136: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:S:152:ASP:HB3	1:S:156:THR:HB	1.99	0.45
1:0:152:ASP:HB3	1:0:156: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
1:A:130:ARG:O	1:M:125:GLN:NE2	2.49	0.45
2:N:167:SER:HB2	2:P:167:SER:HB2	1.98	0.45
2:H:44:THR:HG23	2:H:100:LEU:HB2	1.99	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O:152:ASP:HB3	1:O: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:B:167:SER:HB2	2:R:167:SER:HB2	1.98	0.45
1:G:125:GLN:NE2	1:I:130:ARG:O	2.49	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
1:0:113:VAL:HG21	1:0:149: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
1:0:67:ILE:HG12	1:0:77: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
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
1:O:72:ASP:OD2	2:P:67:ARG:NH2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:152:ASP:HB3	1:Q:156:THR:HB	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
2:F:16:THR:HG21	2:F:33:LYS:HB2	1.98	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: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
2:1:19:ARG:HD3	2:1:26:ILE:HG12	1.99	0.45
1:E:72:ASP:OD2	2:F:67:ARG:NH2	2.50	0.45
1:E:227:GLU:H	1:E:227:GLU:HG3	1.60	0.45
1:I:152:ASP:HB3	1:I:156:THR:HB	1.99	0.45
1:K:152:ASP:HB3	1:K:156:THR:HB	1.99	0.45
1:M:152:ASP:HB3	1:M:156:THR:HB	1.99	0.45
1:U:72:ASP:OD2	2:V:67:ARG:NH2	2.50	0.45
1:U:152:ASP:HB3	1:U:156:THR:HB	1.99	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
2:H:17:GLU:OE2	2:H:33:LYS:NZ	2.44	0.45
1:Y:84:ASP:OD1	1:0:121:GLN:NE2	2.49	0.45
1:0:45:GLY:HA3	1:0:215:ILE:O	2.17	0.45
2:N:4:VAL:HG22	2:N:134:VAL:HG11	1.98	0.45
2:Z:16:THR:HG21	2:Z:33:LYS:HB2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
1:U:130:ARG:O	1:W:125:GLN:NE2	2.49	0.44
2:X:16:THR:HG21	2:X:33:LYS:HB2	1.98	0.44
2:F:114:ASP:O	2:F:117:GLY:N	2.47	0.44
2:L:1:THR:N	2:L:168:ALA:O	2.49	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
2:D:163:LYS:NZ	2:D:203:LEU:O	2.41	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:X:163:LYS:NZ	2:X:203:LEU:O	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:4:VAL:HG22	2:V:134:VAL:HG11	1.98	0.44
1:Y:152:ASP:HB3	1:Y:156:THR:HB	1.99	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:H:16:THR:HG21	2:H:33:LYS:HB2	1.98	0.44
2:P:16:THR:HG21	2:P:33:LYS:HB2	1.98	0.44
1:0:68:GLN:HE21	1:0:89:VAL:HG21	1.80	0.44
2:D:114:ASP:O	2:D:117:GLY:N	2.47	0.44
2:T:1:THR:N	2:T:168:ALA:O	2.49	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
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:72:ASP:OD2	2:J:67:ARG:NH2	2.50	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
2:D:84:SER:OG	2:D:117:GLY:O	2.31	0.44
2:J:37:ILE:HG21	2:J:43:MET:HE3	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:P:3:THR:O	2:P:126:SER:HA	2.17	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:G:152:ASP:HB3	1:G:156:THR:HB	1.99	0.44
1:W:152:ASP:O	1:W:155:GLY:N	2.44	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:E:38:LEU:HA	1:E:163:THR:O	2.18	0.44
2:F:167:SER:HB2	2:V:167:SER:HB2	1.99	0.44
1:G:38:LEU:HA	1:G:163:THR:O	2.18	0.44
1:K:120:MET:HG2	1:K:132:TYR:HD2	1.83	0.44
1:M:72:ASP:OD2	2:N:67:ARG:NH2	2.50	0.44
1:W:38:LEU:HA	1:W:163:THR:O	2.18	0.44
1:Y:38:LEU:HA	1:Y:163:THR:O	2.18	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:1:13:ILE:HG12	2:1:177:VAL:HG22	2.00	0.44
1:A:72:ASP:OD2	2:B:67:ARG:NH2	2.51	0.44
1:W:152:ASP:HB3	1:W:156:THR:HB	1.99	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
2:F:84:SER:OG	2:F:117:GLY:O	2.31	0.44
1:I:120:MET:HG2	1:I:132:TYR:HD2	1.83	0.44
1:O:130:ARG:O	1:Q:125:GLN:NE2	2.50	0.44
1:S:120:MET:HG2	1:S:132:TYR:HD2	1.83	0.44
1:U:120:MET:HG2	1:U:132:TYR:HD2	1.83	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:V:37:ILE:HG21	2:V:43:MET:HE3	1.99	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:V:3:THR:O	2:V:126:SER:HA	2.17	0.44
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:G:152:ASP:O	1:G:155:GLY:N	2.44	0.44
1:Y:72:ASP:OD2	2:Z:67:ARG:NH2	2.51	0.44
1:0:72:ASP:OD2	2:1:67:ARG:NH2	2.50	0.44
1:0:76:ALA:HA	1:0:137:ILE:O	2.18	0.44
2:B:3:THR:HG1	2:B:127:THR:HG1	1.53	0.44
1:M:186:GLU:OE2	1:M:224:TYR:OH	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:L:37:ILE:HG21	2:L:43:MET:HE3	1.99	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: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
1:0:110:GLU:HB2	1:0:147: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
1:0:100: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:K:72:ASP:OD2	2:L:67:ARG:NH2	2.51	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
1:O:76:ALA:HA	1:O:137:ILE:O	2.18	0.44
2:D:167:SER:HB2	2:T:167:SER:HB2	1.98	0.44
1:C:72:ASP:OD2	2:D:67:ARG:NH2	2.50	0.44
1:O:72:ASP:OD2	2:P:67:ARG:NH2	2.51	0.44
2:1:84:SER:OG	2:1:117:GLY:O	2.31	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:T:37:ILE:HG21	2:T:43:MET:HE3	2.00	0.44
1:U:49:ILE:HG12	1:U:212:ILE:HG12	2.00	0.44
2:X:37:ILE:HG21	2:X:43:MET:HE3	1.99	0.44
1:Y:76:ALA:HA	1:Y:137:ILE:O	2.18	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:Z:89:GLN:H	2:Z:89:GLN:HG3	1.60	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
1:0:67:ILE:HG12	1:0:77:VAL:HG22	1.99	0.44
1:G:72:ASP:OD2	2:H:67:ARG:NH2	2.51	0.44
1:W:72:ASP:OD2	2:X:67:ARG:NH2	2.51	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
1:E:72:ASP:OD2	2:F:67:ARG:NH2	2.50	0.44
1:G:120:MET:HG2	1:G:132:TYR:HD2	1.83	0.44
1:I:38:LEU:HA	1:I:163:THR:O	2.18	0.44
1:S:130:ARG:O	1:U:125:GLN:NE2	2.50	0.44
1:W:120:MET:HG2	1:W:132:TYR:HD2	1.83	0.44
2:1:83:LEU:HD21	2:1:99:LEU:HD13	2.00	0.44
2:H:37:ILE:HG21	2:H:43:MET:HE3	1.99	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
2:R:1:THR:N	2:R:168:ALA:O	2.49	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
1:0:49:ILE:HG12	1:0:212: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	1:0:125:GLN:NE2	2.51	0.44
1:O:125:GLN:NE2	1:0:130:ARG:O	2.51	0.44
2:P:13:ILE:HG12	2:P:177:VAL:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:20:ARG:NH2	1:Q:25:GLU:OE1	2.48	0.44
1:G:79:SER:HB3	1:G:165:ILE:HG22	2.00	0.44
2:D:135:TYR:O	2:D:139:GLU:HB2	2.18	0.44
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:D:83:LEU:HD21	2:D:99:LEU:HD13	2.00	0.44
1:M:120:MET:HG2	1:M:132:TYR:HD2	1.83	0.44
1:Q:120:MET:HG2	1:Q:132:TYR:HD2	1.83	0.44
2:F:44:THR:HG23	2:F:100:LEU:HB2	1.99	0.44
2:H:1:THR:N	2:H:168:ALA:O	2.49	0.44
2:N:1:THR:N	2:N:168:ALA:O	2.49	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:X:1:THR:N	2:X:168:ALA:O	2.49	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:H:132:PRO:HB2	2:V:132:PRO:HB2	2.00	0.43
1:U:227:GLU:H	1:U:227:GLU:HG3	1.60	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
2:F:83:LEU:HD21	2:F:99:LEU:HD13	2.00	0.43
1:K:38:LEU:HA	1:K:163:THR:O	2.18	0.43
1:U:38:LEU:HA	1:U:163:THR:O	2.18	0.43
2:Z:83:LEU:HD21	2:Z:99:LEU:HD13	2.00	0.43
2:Z:84:SER:OG	2:Z:117:GLY:O	2.31	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: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
1:K:194:ILE:HD11	1:K:212:ILE:HD11	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:Z:13:ILE:HG12	2:Z:177:VAL:HG22	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
1:0:147:ARG:HH21	1:0:149:PHE:HZ	1.65	0.43
2:J:83:LEU:HD21	2:J:99:LEU:HD13	2.00	0.43
2:L:83:LEU:HD21	2:L:99:LEU:HD13	2.00	0.43
2:N:83:LEU:HD21	2:N:99:LEU:HD13	2.00	0.43
2:R:83:LEU:HD21	2:R:99:LEU:HD13	2.00	0.43
2:T:83:LEU:HD21	2:T:99:LEU:HD13	2.00	0.43
1:E:49:ILE:HG12	1:E:212:ILE:HG12	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	1:0:130:ARG:O	2.52	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:79:SER:HB3	1:I:165:ILE:HG22	2.00	0.43
1:W:79:SER:HB3	1:W:165:ILE:HG22	2.00	0.43
1:I:201:LEU:HD11	1:I:207:LEU:HG	2.01	0.43
1:C:38:LEU:HA	1:C:163:THR:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:186:GLU:OE2	1:G:224:TYR:OH	2.33	0.43
1:S:38:LEU:HA	1:S:163:THR:O	2.18	0.43
2:V:83:LEU:HD21	2:V:99:LEU:HD13	2.00	0.43
1:0:38:LEU:HA	1:0:163:THR:O	2.18	0.43
2:B:50:GLY:O	2:D:88:ASN:ND2	2.50	0.43
2:X:38:ASP:HB3	2:X:41:THR:HB	1.99	0.43
1:0:76:ALA:HA	1:0:137: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
1:Q:130:ARG:O	1:S:125:GLN:NE2	2.51	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
1:U:152:ASP:O	1:U:155:GLY:N	2.44	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
1:E:120:MET:HG2	1:E:132:TYR:HD2	1.83	0.43
1:M:38:LEU:HA	1:M:163:THR:O	2.18	0.43
2:P:83:LEU:HD21	2:P:99:LEU:HD13	2.00	0.43
1:W:186:GLU:OE2	1:W:224:TYR:OH	2.33	0.43
2:1:135:TYR:O	2:1:139:GLU:CB	2.66	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
1:0:20:ARG:HH21	1:0:22: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:Y:79:SER:HB3	1:Y:165:ILE:HG22	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:P:17:GLU:OE2	2:P:33:LYS:NZ	2.44	0.43
2:T:135:TYR:O	2:T:139:GLU:HB2	2.18	0.43
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:H:83:LEU:HD21	2:H:99:LEU:HD13	2.00	0.43
2:J:135:TYR:O	2:J:139:GLU:CB	2.66	0.43
1:O:38:LEU:HA	1:O:163:THR:O	2.18	0.43
1:Q:38:LEU:HA	1:Q:163:THR:O	2.18	0.43
2:X:83:LEU:HD21	2:X:99:LEU:HD13	2.00	0.43
1:Y:120:MET:HG2	1:Y:132:TYR:HD2	1.83	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:Y:59:ILE:HG12	1:0:160:TYR:CE1	2.54	0.43
1:C:72:ASP:OD2	2:D:67:ARG:NH2	2.51	0.43
1:M:72:ASP:OD2	2:N:67:ARG:NH2	2.51	0.43
1:U:79:SER:HB3	1:U:165:ILE:HG22	2.00	0.43
2:D:192:ILE:H	2:D:192:ILE:HG13	1.63	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:V:135:TYR:O	2:V:139:GLU:CB	2.66	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:O:159:GLU:OE1	1:0:63:SER:OG	2.29	0.43
1:W:59:ILE:HG12	1:Y:160:TYR:CE1	2.54	0.43
1:I:152:ASP:O	1:I:155:GLY:N	2.44	0.43
1:I:227:GLU:H	1:I:227:GLU:HG3	1.60	0.43
2:V:4:VAL:HG22	2:V:134:VAL:HG11	2.01	0.43
2:B:17:GLU:OE2	2:B:33:LYS:NZ	2.44	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
2:L:135:TYR:O	2:L:139:GLU:CB	2.66	0.43
1:Q:72:ASP:OD2	2:R:67:ARG:NH2	2.51	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:4:VAL:HG22	2:H:134:VAL:HG11	2.01	0.43
1:K:79:SER:HB3	1:K:165:ILE:HG22	2.00	0.43
1:O:152:ASP:O	1:O:155:GLY:N	2.44	0.43
1:Q:88:LEU:HD23	1:Q:88:LEU:HA	1.91	0.43
2:X:4:VAL:HG22	2:X:134:VAL:HG11	2.01	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
1:0:201:LEU:HD11	1:0:207:LEU:HG	2.01	0.43
2:D:3:THR:O	2:D:126:SER:HA	2.19	0.43
2:T:135:TYR:O	2:T:139:GLU:CB	2.66	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	1:0:125:GLN:NE2	2.52	0.43
1:K:160:TYR:CE1	1:M:59:ILE:HG12	2.54	0.43
1:O:59:ILE:HG12	1:Q:160:TYR:CE1	2.54	0.43
2:J:4:VAL:HG22	2:J:134:VAL:HG11	2.01	0.43
2:H:135:TYR:O	2:H:139:GLU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:V:3:THR:HG1	2:V:127:THR:HG1	1.47	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:O:160:TYR:CE1	1:0:59:ILE:HG12	2.54	0.43
1:A:79:SER:HB3	1:A:165:ILE:HG22	2.00	0.43
2:T:4:VAL:HG22	2:T:134:VAL:HG11	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:120:MET:HG2	1:O:132:TYR:HD2	1.83	0.43
1:0:99:GLU:HB2	1:0:115:ARG:HH22	1.84	0.43
2:D:37:ILE:HG21	2:D:43:MET:HE3	2.00	0.43
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:B:167:SER:HB2	2:R:167:SER:HB2	2.01	0.42
2:F:4:VAL:HG22	2:F:134:VAL:HG11	2.01	0.42
2:L:4:VAL:HG22	2:L:134:VAL:HG11	2.01	0.42
1:O:79:SER:HB3	1:O:165:ILE:HG22	2.00	0.42
1:Q:72:ASP:OD2	2:R:67:ARG:NH2	2.52	0.42
1:S:72:ASP:OD2	2:T:67:ARG:NH2	2.52	0.42
1:S:79:SER:HB3	1:S:165:ILE:HG22	2.00	0.42
2:Z:4:VAL:HG22	2:Z:134:VAL:HG11	2.01	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
1:0:120:MET:HG2	1:0:132:TYR:HD2	1.83	0.42
2:J:114:ASP:O	2:J:117:GLY:N	2.47	0.42
1:O:161:LYS:N	1:0:58:LEU:O	2.52	0.42
1:0:36:THR:HA	1:0:165: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
1:0:152:ASP:HB3	1:0:156: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:M:88:LEU:HD23	1:M:88:LEU:HA	1.91	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: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
2:J:157:ARG:HH21	2:J:199:LEU:HD22	1.84	0.42
1:Y:72:ASP:OD2	2:Z:67:ARG:NH2	2.51	0.42
2:N:37:ILE:HG21	2:N:43:MET:HE3	2.01	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
1:0:40:MET:H	1:0:47:LEU:HB3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:K:99:GLU:HB2	1:K:115:ARG:HH22	1.84	0.42
2:N:3:THR:HG1	2:N:127:THR:HG1	1.50	0.42
1:O:99:GLU:HB2	1:O:115:ARG:HH22	1.84	0.42
2:R:3:THR:HG1	2:R:127:THR:HG1	1.50	0.42
2:V:157:ARG:HH21	2:V:199:LEU:HD22	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
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:A:40:MET:HB3	1:A:40:MET:HE2	1.95	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
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:J:167:SER:HB2	2:Z:167:SER:HB2	2.01	0.42
2:N:132:PRO:HB2	2:1:132:PRO:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:0:79:SER:HB3	1:0:165:ILE:HG22	2.00	0.42
1:C:18:ASP:O	1:E:33:LYS:NZ	2.46	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
1:E:99:GLU:HB2	1:E:115:ARG:HH22	1.84	0.42
2:H:157:ARG:HH21	2:H:199:LEU:HD22	1.84	0.42
1:S:99:GLU:HB2	1:S:115:ARG:HH22	1.84	0.42
2:X:157:ARG:HH21	2:X:199:LEU:HD22	1.84	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:37:ILE:HG21	2:R:43:MET:HE3	2.01	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
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:N:84:SER:OG	2:N:117:GLY:O	2.34	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
1:0:162:ALA:HB1	1:0:176: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:Y:99:GLU:HB2	1:Y:115:ARG:HH22	1.84	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
1:O:40:MET:HB3	1:O:40:MET:HE2	1.95	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:M:79:SER:HB3	1:M:165:ILE:HG22	2.00	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
1:0:68:GLN:HE21	1:0:89:VAL:HG21	1.85	0.42
1:0:72:ASP:OD2	2:1:67:ARG:NH2	2.52	0.42
2:B:37:ILE:HG21	2:B:43:MET:HE3	2.00	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:37:ILE:HG21	2:1:43:MET:HE3	2.00	0.42
2:1:157:ARG:HH21	2:1:199:LEU:HD22	1.84	0.42
2:H:91:LYS:HA	2:H:91:LYS:HD2	1.80	0.42
2:H:190:ASP:N	2:H:190:ASP:OD1	2.51	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
1:0:49:ILE:HG12	1:0:212: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
1:0:227:GLU:H	1:0:227:GLU:HG3	1.60	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
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:P:3:THR:HG1	2:P:127:THR:HG1	1.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:3:THR:O	2:X:126:SER:HA	2.19	0.42
1:U:99:GLU:HB2	1:U:115:ARG:HH22	1.84	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:37:ILE:HG21	2:P:43:MET:HE3	2.00	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: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
1:0:78:THR:HG22	1:0:136: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
1:E:186:GLU:OE2	1:E:224:TYR:OH	2.33	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
1:0:67:ILE:HG13	1:0:77: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
1:Q:79:SER:HB3	1:Q:165:ILE:HG22	2.00	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
2:R:98:GLN:NE2	2:R:128:GLY:H	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:41:LYS:NZ	1:G:60:GLU:OE2	2.46	0.42
2:N:135:TYR:O	2:N:139:GLU:CB	2.66	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: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
1:0:162:ALA:HB1	1:0:176: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
2:R:84:SER:OG	2:R:117:GLY:O	2.34	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
1:I:99:GLU:HB2	1:I:115:ARG:HH22	1.84	0.42
2:L:157:ARG:HH21	2:L:199:LEU:HD22	1.84	0.42
2:R:157:ARG:HH21	2:R:199:LEU:HD22	1.84	0.42
2:T:157:ARG:HH21	2:T:199:LEU:HD22	1.84	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: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
2:X:190:ASP:OD1	2:X:190:ASP:N	2.51	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
1:0:147:ARG:HH21	1:0:149: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
1:Y:186:GLU:OE2	1:Y:224:TYR:OH	2.33	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:O:160:TYR:HE1	1:0:59:ILE:HG12	1.85	0.42
1:S:69:LEU:HD23	1:S:75:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:37:ILE:HG22	2:1:63:LEU:HD22	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
2:P:20:VAL:HB	2:P:28:HIS:HB2	2.02	0.42
2:1:4:VAL:HG22	2:1:134: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
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
2:N:157:ARG:HH21	2:N:199:LEU:HD22	1.84	0.42
2:R:135:TYR:O	2:R:139:GLU:CB	2.66	0.42
2:R:196:ILE:HD13	2:R:203:LEU:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:N:4:VAL:HG22	2:N:134:VAL:HG11	2.01	0.41
2:R:4:VAL:HG22	2:R:134:VAL:HG11	2.01	0.41
2:1:20:VAL:HB	2:1:28:HIS:HB2	2.02	0.41
1:K:18:ASP:O	1:M:33:LYS:NZ	2.47	0.41
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:99:GLU:HB2	1:G:115:ARG:HH22	1.84	0.41
2:N:196:ILE:HD13	2:N:203:LEU:HA	2.02	0.41
2:P:196:ILE:HD13	2:P:203:LEU:HA	2.02	0.41
1:Q:99:GLU:HB2	1:Q:115:ARG:HH22	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:Y:22:PHE:HD1	1:Y:22:PHE:HA	1.78	0.41
1:C:162:ALA:HB1	1:C:176:LEU:HD13	2.02	0.41
1:Q:33:LYS:NZ	1:S:18:ASP:O	2.47	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
1:0:162:ALA:HB1	1:0:176: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
1:O:46:VAL:HG13	1:O:146:PRO:HB3	2.02	0.41
1:W:39:GLY:O	1:W:162:ALA:HA	2.20	0.41
2:F:135:TYR:O	2:F:139:GLU:CB	2.66	0.41
2:H:84:SER:OG	2:H:117:GLY:O	2.31	0.41
1:I:186:GLU:OE2	1:I:224:TYR:OH	2.33	0.41
1:M:99:GLU:HB2	1:M:115:ARG:HH22	1.84	0.41
1:W:99:GLU:HB2	1:W:115:ARG:HH22	1.84	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:Y:59:ILE:HG12	1:0:160:TYR:HE1	1.85	0.41
2:N:132:PRO:HB2	2:1:132:PRO:HB2	2.01	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:F:157:ARG:HH21	2:F:199:LEU:HD22	1.84	0.41
1:K:186:GLU:OE2	1:K:224:TYR:OH	2.33	0.41
2:L:196:ILE:HD13	2:L:203:LEU:HA	2.02	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
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
1:0:152:ASP:O	1:0:155: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
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: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
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: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
1:0:46:VAL:HG13	1:0:146:PRO:HB3	2.02	0.41
1:S:186:GLU:OE2	1:S:224:TYR:OH	2.33	0.41
2:T:196:ILE:HD13	2:T:203:LEU:HA	2.02	0.41
2:Z:135:TYR:O	2:Z:139:GLU:CB	2.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:157:ARG:HH21	2:Z:199:LEU:HD22	1.84	0.41
2:1:157:ARG:HH21	2:1:199:LEU:HD22	1.84	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
1:U:138:PHE:HB2	1:U:149:PHE:HB2	2.03	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:V:37:ILE:HG22	2:V:63:LEU:HD22	2.01	0.41
1:0:69:LEU:HD23	1:0:75:ALA:HB2	2.01	0.41
1:E:38:LEU:HB2	1:E:49:ILE:HB	2.02	0.41
2:N:20:VAL:HB	2:N:28:HIS:HB2	2.02	0.41
2:P:4:VAL:HG22	2:P:134:VAL:HG11	2.01	0.41
2:R:20:VAL:HB	2:R:28:HIS:HB2	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
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:D:157:ARG:HH21	2:D:199:LEU:HD22	1.84	0.41
2:L:84:SER:OG	2:L:117:GLY:O	2.31	0.41
1:U:186:GLU:OE2	1:U:224:TYR:OH	2.33	0.41
2:1:196:ILE:HD13	2:1:203:LEU:HA	2.02	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:L:167:SER:HB2	2:1:167:SER:HB2	2.01	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:Q:227:GLU:H	1:Q:227:GLU:HG3	1.60	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:B:157:ARG:HH21	2:B:199:LEU:HD22	1.84	0.41
1:K:72:ASP:OD2	2:L:67:ARG:NH2	2.53	0.41
1:Q:60:GLU:OE2	1:S:41:LYS:NZ	2.45	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:186:GLU:OE2	1:0:224:TYR:OH	2.33	0.41
2:F:37:ILE:HG22	2:F:63:LEU:HD22	2.01	0.41
1:E:68:GLN:HE21	1:E:89:VAL:HG21	1.86	0.41
1:G:68:GLN:HE21	1:G:89:VAL:HG21	1.86	0.41
1:I:68:GLN:HE21	1:I:89:VAL:HG21	1.86	0.41
1:I:76:ALA:HA	1:I:137:ILE:O	2.21	0.41
1:U:68:GLN:HE21	1:U:89:VAL:HG21	1.86	0.41
1:W:68:GLN:HE21	1:W:89:VAL:HG21	1.86	0.41
1:Y:38:LEU:HB2	1:Y:49:ILE:HB	2.02	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
2:L:37:ILE:HG22	2:L:63:LEU:HD22	2.03	0.41
2:P:157:ARG:HH21	2:P:199:LEU:HD22	1.84	0.41
2:X:84:SER:OG	2:X:117:GLY:O	2.31	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
1:0:172:VAL:HG13	1:0:196: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:0:51:ASP:HB2	1:0:197: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:K:38:LEU:HB2	1:K:49:ILE:HB	2.02	0.41
1:M:38:LEU:HB2	1:M:49:ILE:HB	2.02	0.41
1:S:38:LEU:HB2	1:S:49:ILE:HB	2.02	0.41
1:S:76:ALA:HA	1:S:137:ILE:O	2.21	0.41
1:Y:68:GLN:HE21	1:Y:89:VAL:HG21	1.86	0.41
1:0:38:LEU:HB2	1:0:49:ILE:HB	2.02	0.41
1:Y:172:VAL:HG13	1:Y:196:ALA:HB1	2.01	0.41
1:0:172:VAL:HG13	1:0:196: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
1:0:225:ASP:OD1	1:0:225:ASP:N	2.54	0.41
2:D:196:ILE:HD13	2:D:203:LEU:HA	2.02	0.41
2:J:37:ILE:HG22	2:J:63:LEU:HD22	2.03	0.41
2:T:37:ILE:HG22	2:T:63:LEU:HD22	2.03	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: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	1:0:125: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
1:E:160:TYR:CE1	1:G:59:ILE:HG12	2.56	0.41
2:F:20:VAL:HB	2:F:28:HIS:HB2	2.02	0.41
1:K:76:ALA:HA	1:K:137:ILE:O	2.21	0.41
1:O:38:LEU:HB2	1:O:49:ILE:HB	2.02	0.41
1:Q:38:LEU:HB2	1:Q:49:ILE:HB	2.02	0.41
1:U:76:ALA:HA	1:U:137:ILE:O	2.21	0.41
1:W:38:LEU:HB2	1:W:49:ILE:HB	2.01	0.41
2:Z:20:VAL:HB	2:Z:28:HIS:HB2	2.02	0.41
1:0:68:GLN:HE21	1:0:89:VAL:HG21	1.86	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	1:0:33: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:U:49:ILE:HA	1:U:211:GLU:O	2.21	0.41
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
2:D:37:ILE:HG22	2:D:63:LEU:HD22	2.03	0.41
2:F:37:ILE:HG22	2:F:63:LEU:HD22	2.03	0.41
2:F:194:SER:O	2:F:198:LYS:HB2	2.21	0.41
2:J:196:ILE:HD13	2:J:203:LEU:HA	2.02	0.41
2:N:37:ILE:HG22	2:N:63:LEU:HD22	2.03	0.41
2:R:37:ILE:HG22	2:R:63:LEU:HD22	2.03	0.41
2:V:196:ILE:HD13	2:V:203:LEU:HA	2.02	0.41
1:W:72:ASP:OD2	2:X:67:ARG:NH2	2.53	0.41
2:Z:194:SER:O	2:Z:198:LYS:HB2	2.21	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:Z:37:ILE:HG21	2:Z:43:MET:HE3	2.02	0.41
2:B:88:ASN:HD22	2:B:90:VAL:HG12	1.85	0.41
2:D:88:ASN:HD22	2:D:90:VAL:HG12	1.85	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:G:38:LEU:HB2	1:G:49:ILE:HB	2.02	0.41
2:J:132:PRO:HB2	2:X:132:PRO:HB2	2.03	0.41
1:U:88:LEU:HD23	1:U:88:LEU:HA	1.91	0.41
2:X:20:VAL:HB	2:X:28:HIS:HB2	2.02	0.41
1:0:76:ALA:HA	1:0:137:ILE:O	2.21	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: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:V:37:ILE:HG22	2:V:63:LEU:HD22	2.03	0.41
2:Z:37:ILE:HG22	2:Z:63:LEU:HD22	2.03	0.41
2:1:37:ILE:HG22	2:1:63:LEU:HD22	2.03	0.41
2:B:25:PHE:CD1	2:R:133:PHE:HZ	2.39	0.41
2:F:37:ILE:HG21	2:F:43:MET:HE3	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	1:0:130: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
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
2:H:20:VAL:HB	2:H:28:HIS:HB2	2.02	0.40
2:J:20:VAL:HB	2:J:28:HIS:HB2	2.02	0.40
1:M:76:ALA:HA	1:M:137:ILE:O	2.21	0.40
1:O:76:ALA:HA	1:O:137:ILE:O	2.21	0.40
1:O:160:TYR:CE1	1:0:59:ILE:HG12	2.56	0.40
1:Q:76:ALA:HA	1:Q:137:ILE:O	2.21	0.40
1:S:68:GLN:HE21	1:S:89:VAL:HG21	1.86	0.40
1:U:38:LEU:HB2	1:U:49:ILE:HB	2.01	0.40
2:V:20:VAL:HB	2:V:28:HIS:HB2	2.02	0.40
1:W:59:ILE:HG12	1:Y:160:TYR:CE1	2.57	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
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
1:0:39:GLY:O	1:0:162:ALA:HA	2.20	0.40
1:A:49:ILE:HG12	1:A:212:ILE:HG12	2.03	0.40
1:I:49:ILE:HG12	1:I:212:ILE:HG12	2.03	0.40
1:K:49:ILE:HG12	1:K:212:ILE:HG12	2.03	0.40
2:P:37:ILE:HG22	2:P:63:LEU:HD22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:49:ILE:HG12	1:U:212:ILE:HG12	2.03	0.40
2:X:37:ILE:HG22	2:X:63:LEU:HD22	2.03	0.40
1:0:49:ILE:HG12	1:0:212: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
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
1:0:225:ASP:OD1	1:0:225: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:I:88:LEU:HD23	1:I:88:LEU:HA	1.91	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:46:VAL:HG13	1:S:146:PRO:HB3	2.02	0.40
2:V:3:THR:OG1	2:V:127:THR:OG1	2.26	0.40
1:C:20:ARG:NH2	1:C:25:GLU:OE1	2.54	0.40
1:E:20:ARG:NH2	1:E:25:GLU:OE1	2.54	0.40
2:H:196:ILE:HD13	2:H:203:LEU:HA	2.02	0.40
1:O:49:ILE:HG12	1:O:212:ILE:HG12	2.04	0.40
2:X:196:ILE:HD13	2:X:203:LEU:HA	2.02	0.40
2:Z:196:ILE:HD13	2:Z:203:LEU:HA	2.02	0.40
1:0:20:ARG:NH2	1:0:25:GLU:OE1	2.55	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
1:0:108:ASN:HD22	1:0:109:ILE:N	2.20	0.40
2:J:105:ASP:OD1	2:J:105:ASP:N	2.54	0.40
2:Z:179:THR:HG22	2:Z:181:LYS:H	1.86	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:G:76:ALA:HA	1:G:137:ILE:O	2.21	0.40
1:K:68:GLN:HE21	1:K:89:VAL:HG21	1.86	0.40
1:M:227:GLU:H	1:M:227:GLU:HG3	1.60	0.40
1:0:88:LEU:HD23	1:0:88: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:I:18:ASP:O	1:K:33:LYS:NZ	2.46	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
2:F:153:ASP:OD1	2:F:153:ASP:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:153:ASP:OD1	2:Z:153:ASP:N	2.54	0.40
1:A:70:ILE:HG21	1:A:112:LEU:HD21	2.04	0.40
2:F:196:ILE:HD13	2:F:203:LEU:HA	2.02	0.40
1:G:49:ILE:HG12	1:G:212:ILE:HG12	2.03	0.40
2:H:37:ILE:HG22	2:H:63:LEU:HD22	2.03	0.40
1:M:20:ARG:NH2	1:M:25:GLU:OE1	2.55	0.40
1:M:49:ILE:HG12	1:M:212:ILE:HG12	2.03	0.40
1:M:70:ILE:HG21	1:M:112:LEU:HD21	2.03	0.40
1:S:49:ILE:HG12	1:S:212:ILE:HG12	2.04	0.40
1:W:49:ILE:HG12	1:W:212:ILE:HG12	2.03	0.40
1:Y:20:ARG:NH2	1:Y:25:GLU:OE1	2.55	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
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: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:G:160:TYR:CE1	1:I:59:ILE:HG12	2.57	0.40
2:L:20:VAL:HB	2:L:28:HIS:HB2	2.02	0.40
1:O:68:GLN:HE21	1:O:89:VAL:HG21	1.86	0.40
1:Q:59:ILE:HG12	1:S:160:TYR:CE1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:59:ILE:HG12	1:U:160:TYR:CE1	2.57	0.40
2:T:20:VAL:HB	2:T:28:HIS:HB2	2.02	0.40
1:W:76:ALA:HA	1:W:137:ILE:O	2.21	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: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:D:194:SER:O	2:D:198:LYS:HB2	2.21	0.40
1:E:49:ILE:HG12	1:E:212:ILE:HG12	2.03	0.40
1:O:70:ILE:HG21	1:O:112:LEU:HD21	2.04	0.40
1:Q:20:ARG:NH2	1:Q:25:GLU:OE1	2.55	0.40
1:Q:49:ILE:HG12	1:Q:212:ILE:HG12	2.03	0.40
1:Q:70:ILE:HG21	1:Q:112:LEU:HD21	2.04	0.40
1:Y:49:ILE:HG12	1:Y:212:ILE:HG12	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:38:LEU:HB2	1:I:49:ILE:HB	2.02	0.40
1:I:160:TYR:CE1	1:K:59:ILE:HG12	2.57	0.40
1:Y:76:ALA:HA	1:Y: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	1:0:59:ILE:HG12	2.57	0.40
1:W:88:LEU:HD23	1:W:88:LEU:HA	1.92	0.40
1:0:186:GLU:OE2	1:0:224: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: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
1:0:152:ASP:O	1:0:155: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: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
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:W:142:ASP:N	1:W:142:ASP:OD1	2.54	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
1	1-Y	219/224 (98%)	212 (97%)	7 (3%)	0	100	100
1	2-0	219/224 (98%)	208 (95%)	11 (5%)	0	100	100
1	2-A	219/224 (98%)	208 (95%)	11 (5%)	0	100	100
1	2-C	219/224 (98%)	208 (95%)	11 (5%)	0	100	100
1	2-E	219/224 (98%)	208 (95%)	11 (5%)	0	100	100
1	2-G	219/224 (98%)	208 (95%)	11 (5%)	0	100	100
1	2-I	219/224 (98%)	208 (95%)	11 (5%)	0	100	100
1	2-K	219/224 (98%)	208 (95%)	11 (5%)	0	100	100
1	2-M	219/224 (98%)	208 (95%)	11 (5%)	0	100	100
1	2-O	219/224 (98%)	208 (95%)	11 (5%)	0	100	100
1	2-Q	219/224 (98%)	208 (95%)	11 (5%)	0	100	100
1	2-S	219/224 (98%)	208 (95%)	11 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2-U	219/224 (98%)	208 (95%)	11 (5%)	0	100	100
1	2-W	219/224 (98%)	208 (95%)	11 (5%)	0	100	100
1	2-Y	219/224 (98%)	208 (95%)	11 (5%)	0	100	100
1	3-0	219/224 (98%)	209 (95%)	10 (5%)	0	100	100
1	3-A	219/224 (98%)	209 (95%)	10 (5%)	0	100	100
1	3-C	219/224 (98%)	209 (95%)	10 (5%)	0	100	100
1	3-E	219/224 (98%)	209 (95%)	10 (5%)	0	100	100
1	3-G	219/224 (98%)	209 (95%)	10 (5%)	0	100	100
1	3-I	219/224 (98%)	209 (95%)	10 (5%)	0	100	100
1	3-K	219/224 (98%)	209 (95%)	10 (5%)	0	100	100
1	3-M	219/224 (98%)	209 (95%)	10 (5%)	0	100	100
1	3-O	219/224 (98%)	209 (95%)	10 (5%)	0	100	100
1	3-Q	219/224 (98%)	209 (95%)	10 (5%)	0	100	100
1	3-S	219/224 (98%)	209 (95%)	10 (5%)	0	100	100
1	3-U	219/224 (98%)	209 (95%)	10 (5%)	0	100	100
1	3-W	219/224 (98%)	209 (95%)	10 (5%)	0	100	100
1	3-Y	219/224 (98%)	209 (95%)	10 (5%)	0	100	100
1	4-0	219/224 (98%)	212 (97%)	7 (3%)	0	100	100
1	4-A	219/224 (98%)	212 (97%)	7 (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	219/224 (98%)	212 (97%)	7 (3%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	5-0	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	6-0	219/224 (98%)	208 (95%)	11 (5%)	0	100	100
1	6-A	219/224 (98%)	208 (95%)	11 (5%)	0	100	100
1	6-C	219/224 (98%)	208 (95%)	11 (5%)	0	100	100
1	6-E	219/224 (98%)	208 (95%)	11 (5%)	0	100	100
1	6-G	219/224 (98%)	208 (95%)	11 (5%)	0	100	100
1	6-I	219/224 (98%)	208 (95%)	11 (5%)	0	100	100
1	6-K	219/224 (98%)	208 (95%)	11 (5%)	0	100	100
1	6-M	219/224 (98%)	208 (95%)	11 (5%)	0	100	100
1	6-O	219/224 (98%)	208 (95%)	11 (5%)	0	100	100
1	6-Q	219/224 (98%)	208 (95%)	11 (5%)	0	100	100
1	6-S	219/224 (98%)	208 (95%)	11 (5%)	0	100	100
1	6-U	219/224 (98%)	208 (95%)	11 (5%)	0	100	100
1	6-W	219/224 (98%)	208 (95%)	11 (5%)	0	100	100
1	6-Y	219/224 (98%)	208 (95%)	11 (5%)	0	100	100
1	7-0	219/224 (98%)	211 (96%)	8 (4%)	0	100	100
1	7-A	219/224 (98%)	211 (96%)	8 (4%)	0	100	100
1	7-C	219/224 (98%)	211 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
1	9-I	219/224 (98%)	213 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	17	48
1	10-A	219/224 (98%)	208 (95%)	9 (4%)	2 (1%)	17	48
1	10-C	219/224 (98%)	208 (95%)	9 (4%)	2 (1%)	17	48
1	10-E	219/224 (98%)	209 (95%)	8 (4%)	2 (1%)	17	48
1	10-G	219/224 (98%)	209 (95%)	8 (4%)	2 (1%)	17	48
1	10-I	219/224 (98%)	208 (95%)	9 (4%)	2 (1%)	17	48
1	10-K	219/224 (98%)	208 (95%)	9 (4%)	2 (1%)	17	48
1	10-M	219/224 (98%)	208 (95%)	9 (4%)	2 (1%)	17	48
1	10-O	219/224 (98%)	208 (95%)	9 (4%)	2 (1%)	17	48
1	10-Q	219/224 (98%)	209 (95%)	8 (4%)	2 (1%)	17	48
1	10-S	219/224 (98%)	208 (95%)	9 (4%)	2 (1%)	17	48
1	10-U	219/224 (98%)	208 (95%)	9 (4%)	2 (1%)	17	48
1	10-W	219/224 (98%)	208 (95%)	9 (4%)	2 (1%)	17	48
1	10-Y	219/224 (98%)	208 (95%)	9 (4%)	2 (1%)	17	48
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
2	1-P	201/203 (99%)	191 (95%)	10 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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	2-1	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	2-B	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	2-D	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	2-F	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	2-H	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	2-J	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	2-L	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	2-N	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	2-P	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	2-R	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	2-T	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	2-V	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	2-X	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	2-Z	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
2	3-1	201/203 (99%)	189 (94%)	12 (6%)	0	100	100
2	3-B	201/203 (99%)	189 (94%)	12 (6%)	0	100	100
2	3-D	201/203 (99%)	189 (94%)	12 (6%)	0	100	100
2	3-F	201/203 (99%)	189 (94%)	12 (6%)	0	100	100
2	3-H	201/203 (99%)	189 (94%)	12 (6%)	0	100	100
2	3-J	201/203 (99%)	189 (94%)	12 (6%)	0	100	100
2	3-L	201/203 (99%)	189 (94%)	12 (6%)	0	100	100
2	3-N	201/203 (99%)	189 (94%)	12 (6%)	0	100	100
2	3-P	201/203 (99%)	189 (94%)	12 (6%)	0	100	100
2	3-R	201/203 (99%)	189 (94%)	12 (6%)	0	100	100
2	3-T	201/203 (99%)	189 (94%)	12 (6%)	0	100	100
2	3-V	201/203 (99%)	189 (94%)	12 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	3-X	201/203 (99%)	189 (94%)	12 (6%)	0	100	100
2	3-Z	201/203 (99%)	189 (94%)	12 (6%)	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
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	6-1	201/203 (99%)	194 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	6-B	201/203 (99%)	194 (96%)	7 (4%)	0	100	100
2	6-D	201/203 (99%)	194 (96%)	7 (4%)	0	100	100
2	6-F	201/203 (99%)	194 (96%)	7 (4%)	0	100	100
2	6-H	201/203 (99%)	194 (96%)	7 (4%)	0	100	100
2	6-J	201/203 (99%)	194 (96%)	7 (4%)	0	100	100
2	6-L	201/203 (99%)	194 (96%)	7 (4%)	0	100	100
2	6-N	201/203 (99%)	194 (96%)	7 (4%)	0	100	100
2	6-P	201/203 (99%)	194 (96%)	7 (4%)	0	100	100
2	6-R	201/203 (99%)	194 (96%)	7 (4%)	0	100	100
2	6-T	201/203 (99%)	194 (96%)	7 (4%)	0	100	100
2	6-V	201/203 (99%)	194 (96%)	7 (4%)	0	100	100
2	6-X	201/203 (99%)	194 (96%)	7 (4%)	0	100	100
2	6-Z	201/203 (99%)	194 (96%)	7 (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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
2	9-1	201/203 (99%)	191 (95%)	9 (4%)	1 (0%)	29	61
2	9-B	201/203 (99%)	191 (95%)	9 (4%)	1 (0%)	29	61
2	9-D	201/203 (99%)	191 (95%)	9 (4%)	1 (0%)	29	61
2	9-F	201/203 (99%)	191 (95%)	9 (4%)	1 (0%)	29	61
2	9-H	201/203 (99%)	191 (95%)	9 (4%)	1 (0%)	29	61
2	9-J	201/203 (99%)	191 (95%)	9 (4%)	1 (0%)	29	61
2	9-L	201/203 (99%)	191 (95%)	9 (4%)	1 (0%)	29	61
2	9-N	201/203 (99%)	191 (95%)	9 (4%)	1 (0%)	29	61
2	9-P	201/203 (99%)	191 (95%)	9 (4%)	1 (0%)	29	61
2	9-R	201/203 (99%)	191 (95%)	9 (4%)	1 (0%)	29	61
2	9-T	201/203 (99%)	191 (95%)	9 (4%)	1 (0%)	29	61
2	9-V	201/203 (99%)	191 (95%)	9 (4%)	1 (0%)	29	61
2	9-X	201/203 (99%)	191 (95%)	9 (4%)	1 (0%)	29	61
2	9-Z	201/203 (99%)	191 (95%)	9 (4%)	1 (0%)	29	61
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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	58800/59780 (98%)	56189 (96%)	2569 (4%)	42 (0%)	54	81

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

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Mol	Chain	Res	Type
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-0	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	1-A	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	1-C	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	1-E	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	1-G	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	1-I	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	1-K	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	1-M	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	1-O	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	1-Q	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	1-S	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	1-U	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	1-W	184/186 (99%)	183 (100%)	1 (0%)	88	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1-Y	184/186 (99%)	183 (100%)	1 (0%)	88 93
1	2-0	184/186 (99%)	179 (97%)	5 (3%)	44 71
1	2-A	184/186 (99%)	179 (97%)	5 (3%)	44 71
1	2-C	184/186 (99%)	179 (97%)	5 (3%)	44 71
1	2-E	184/186 (99%)	179 (97%)	5 (3%)	44 71
1	2-G	184/186 (99%)	179 (97%)	5 (3%)	44 71
1	2-I	184/186 (99%)	179 (97%)	5 (3%)	44 71
1	2-K	184/186 (99%)	179 (97%)	5 (3%)	44 71
1	2-M	184/186 (99%)	180 (98%)	4 (2%)	52 74
1	2-O	184/186 (99%)	179 (97%)	5 (3%)	44 71
1	2-Q	184/186 (99%)	180 (98%)	4 (2%)	52 74
1	2-S	184/186 (99%)	179 (97%)	5 (3%)	44 71
1	2-U	184/186 (99%)	179 (97%)	5 (3%)	44 71
1	2-W	184/186 (99%)	180 (98%)	4 (2%)	52 74
1	2-Y	184/186 (99%)	179 (97%)	5 (3%)	44 71
1	3-0	184/186 (99%)	181 (98%)	3 (2%)	62 79
1	3-A	184/186 (99%)	181 (98%)	3 (2%)	62 79
1	3-C	184/186 (99%)	181 (98%)	3 (2%)	62 79
1	3-E	184/186 (99%)	181 (98%)	3 (2%)	62 79
1	3-G	184/186 (99%)	181 (98%)	3 (2%)	62 79
1	3-I	184/186 (99%)	181 (98%)	3 (2%)	62 79
1	3-K	184/186 (99%)	181 (98%)	3 (2%)	62 79
1	3-M	184/186 (99%)	181 (98%)	3 (2%)	62 79
1	3-O	184/186 (99%)	181 (98%)	3 (2%)	62 79
1	3-Q	184/186 (99%)	181 (98%)	3 (2%)	62 79
1	3-S	184/186 (99%)	181 (98%)	3 (2%)	62 79
1	3-U	184/186 (99%)	181 (98%)	3 (2%)	62 79
1	3-W	184/186 (99%)	181 (98%)	3 (2%)	62 79
1	3-Y	184/186 (99%)	181 (98%)	3 (2%)	62 79
1	4-0	184/186 (99%)	181 (98%)	3 (2%)	62 79
1	4-A	184/186 (99%)	181 (98%)	3 (2%)	62 79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	4-C	184/186 (99%)	181 (98%)	3 (2%)	62	79
1	4-E	184/186 (99%)	181 (98%)	3 (2%)	62	79
1	4-G	184/186 (99%)	181 (98%)	3 (2%)	62	79
1	4-I	184/186 (99%)	181 (98%)	3 (2%)	62	79
1	4-K	184/186 (99%)	181 (98%)	3 (2%)	62	79
1	4-M	184/186 (99%)	181 (98%)	3 (2%)	62	79
1	4-O	184/186 (99%)	181 (98%)	3 (2%)	62	79
1	4-Q	184/186 (99%)	181 (98%)	3 (2%)	62	79
1	4-S	184/186 (99%)	181 (98%)	3 (2%)	62	79
1	4-U	184/186 (99%)	181 (98%)	3 (2%)	62	79
1	4-W	184/186 (99%)	181 (98%)	3 (2%)	62	79
1	4-Y	184/186 (99%)	181 (98%)	3 (2%)	62	79
1	5-0	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	5-A	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	5-C	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	5-E	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	5-G	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	5-I	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	5-K	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	5-M	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	5-O	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	5-Q	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	5-S	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	5-U	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	5-W	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	5-Y	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	6-0	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	6-A	184/186 (99%)	182 (99%)	2 (1%)	73	85
1	6-C	184/186 (99%)	182 (99%)	2 (1%)	73	85
1	6-E	184/186 (99%)	182 (99%)	2 (1%)	73	85
1	6-G	184/186 (99%)	182 (99%)	2 (1%)	73	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	6-I	184/186 (99%)	182 (99%)	2 (1%)	73	85
1	6-K	184/186 (99%)	182 (99%)	2 (1%)	73	85
1	6-M	184/186 (99%)	182 (99%)	2 (1%)	73	85
1	6-O	184/186 (99%)	182 (99%)	2 (1%)	73	85
1	6-Q	184/186 (99%)	182 (99%)	2 (1%)	73	85
1	6-S	184/186 (99%)	182 (99%)	2 (1%)	73	85
1	6-U	184/186 (99%)	182 (99%)	2 (1%)	73	85
1	6-W	184/186 (99%)	182 (99%)	2 (1%)	73	85
1	6-Y	184/186 (99%)	182 (99%)	2 (1%)	73	85
1	7-0	184/186 (99%)	180 (98%)	4 (2%)	52	74
1	7-A	184/186 (99%)	180 (98%)	4 (2%)	52	74
1	7-C	184/186 (99%)	180 (98%)	4 (2%)	52	74
1	7-E	184/186 (99%)	180 (98%)	4 (2%)	52	74
1	7-G	184/186 (99%)	180 (98%)	4 (2%)	52	74
1	7-I	184/186 (99%)	180 (98%)	4 (2%)	52	74
1	7-K	184/186 (99%)	180 (98%)	4 (2%)	52	74
1	7-M	184/186 (99%)	180 (98%)	4 (2%)	52	74
1	7-O	184/186 (99%)	180 (98%)	4 (2%)	52	74
1	7-Q	184/186 (99%)	180 (98%)	4 (2%)	52	74
1	7-S	184/186 (99%)	180 (98%)	4 (2%)	52	74
1	7-U	184/186 (99%)	180 (98%)	4 (2%)	52	74
1	7-W	184/186 (99%)	180 (98%)	4 (2%)	52	74
1	7-Y	184/186 (99%)	180 (98%)	4 (2%)	52	74
1	8-0	184/186 (99%)	181 (98%)	3 (2%)	62	79
1	8-A	184/186 (99%)	181 (98%)	3 (2%)	62	79
1	8-C	184/186 (99%)	181 (98%)	3 (2%)	62	79
1	8-E	184/186 (99%)	181 (98%)	3 (2%)	62	79
1	8-G	184/186 (99%)	181 (98%)	3 (2%)	62	79
1	8-I	184/186 (99%)	181 (98%)	3 (2%)	62	79
1	8-K	184/186 (99%)	181 (98%)	3 (2%)	62	79
1	8-M	184/186 (99%)	181 (98%)	3 (2%)	62	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	8-O	184/186 (99%)	181 (98%)	3 (2%)	62	79
1	8-Q	184/186 (99%)	181 (98%)	3 (2%)	62	79
1	8-S	184/186 (99%)	181 (98%)	3 (2%)	62	79
1	8-U	184/186 (99%)	181 (98%)	3 (2%)	62	79
1	8-W	184/186 (99%)	181 (98%)	3 (2%)	62	79
1	8-Y	184/186 (99%)	181 (98%)	3 (2%)	62	79
1	9-0	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	9-A	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	9-C	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	9-E	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	9-G	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	9-I	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	9-K	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	9-M	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	9-O	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	9-Q	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	9-S	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	9-U	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	9-W	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	9-Y	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	10-0	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	10-A	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	10-C	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	10-E	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	10-G	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	10-I	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	10-K	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	10-M	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	10-O	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	10-Q	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	10-S	184/186 (99%)	183 (100%)	1 (0%)	88	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	10-U	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	10-W	184/186 (99%)	183 (100%)	1 (0%)	88	93
1	10-Y	184/186 (99%)	183 (100%)	1 (0%)	88	93
2	1-1	170/170 (100%)	168 (99%)	2 (1%)	71	83
2	1-B	170/170 (100%)	168 (99%)	2 (1%)	71	83
2	1-D	170/170 (100%)	168 (99%)	2 (1%)	71	83
2	1-F	170/170 (100%)	168 (99%)	2 (1%)	71	83
2	1-H	170/170 (100%)	168 (99%)	2 (1%)	71	83
2	1-J	170/170 (100%)	168 (99%)	2 (1%)	71	83
2	1-L	170/170 (100%)	168 (99%)	2 (1%)	71	83
2	1-N	170/170 (100%)	168 (99%)	2 (1%)	71	83
2	1-P	170/170 (100%)	168 (99%)	2 (1%)	71	83
2	1-R	170/170 (100%)	168 (99%)	2 (1%)	71	83
2	1-T	170/170 (100%)	168 (99%)	2 (1%)	71	83
2	1-V	170/170 (100%)	168 (99%)	2 (1%)	71	83
2	1-X	170/170 (100%)	168 (99%)	2 (1%)	71	83
2	1-Z	170/170 (100%)	168 (99%)	2 (1%)	71	83
2	2-1	170/170 (100%)	169 (99%)	1 (1%)	86	91
2	2-B	170/170 (100%)	169 (99%)	1 (1%)	86	91
2	2-D	170/170 (100%)	169 (99%)	1 (1%)	86	91
2	2-F	170/170 (100%)	169 (99%)	1 (1%)	86	91
2	2-H	170/170 (100%)	169 (99%)	1 (1%)	86	91
2	2-J	170/170 (100%)	169 (99%)	1 (1%)	86	91
2	2-L	170/170 (100%)	169 (99%)	1 (1%)	86	91
2	2-N	170/170 (100%)	169 (99%)	1 (1%)	86	91
2	2-P	170/170 (100%)	169 (99%)	1 (1%)	86	91
2	2-R	170/170 (100%)	169 (99%)	1 (1%)	86	91
2	2-T	170/170 (100%)	169 (99%)	1 (1%)	86	91
2	2-V	170/170 (100%)	169 (99%)	1 (1%)	86	91
2	2-X	170/170 (100%)	169 (99%)	1 (1%)	86	91
2	2-Z	170/170 (100%)	169 (99%)	1 (1%)	86	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	3-1	170/170 (100%)	168 (99%)	2 (1%)	71	83
2	3-B	170/170 (100%)	168 (99%)	2 (1%)	71	83
2	3-D	170/170 (100%)	168 (99%)	2 (1%)	71	83
2	3-F	170/170 (100%)	168 (99%)	2 (1%)	71	83
2	3-H	170/170 (100%)	168 (99%)	2 (1%)	71	83
2	3-J	170/170 (100%)	168 (99%)	2 (1%)	71	83
2	3-L	170/170 (100%)	168 (99%)	2 (1%)	71	83
2	3-N	170/170 (100%)	168 (99%)	2 (1%)	71	83
2	3-P	170/170 (100%)	168 (99%)	2 (1%)	71	83
2	3-R	170/170 (100%)	168 (99%)	2 (1%)	71	83
2	3-T	170/170 (100%)	168 (99%)	2 (1%)	71	83
2	3-V	170/170 (100%)	168 (99%)	2 (1%)	71	83
2	3-X	170/170 (100%)	168 (99%)	2 (1%)	71	83
2	3-Z	170/170 (100%)	168 (99%)	2 (1%)	71	83
2	4-1	170/170 (100%)	166 (98%)	4 (2%)	49	73
2	4-B	170/170 (100%)	166 (98%)	4 (2%)	49	73
2	4-D	170/170 (100%)	166 (98%)	4 (2%)	49	73
2	4-F	170/170 (100%)	166 (98%)	4 (2%)	49	73
2	4-H	170/170 (100%)	166 (98%)	4 (2%)	49	73
2	4-J	170/170 (100%)	166 (98%)	4 (2%)	49	73
2	4-L	170/170 (100%)	166 (98%)	4 (2%)	49	73
2	4-N	170/170 (100%)	166 (98%)	4 (2%)	49	73
2	4-P	170/170 (100%)	166 (98%)	4 (2%)	49	73
2	4-R	170/170 (100%)	166 (98%)	4 (2%)	49	73
2	4-T	170/170 (100%)	166 (98%)	4 (2%)	49	73
2	4-V	170/170 (100%)	166 (98%)	4 (2%)	49	73
2	4-X	170/170 (100%)	166 (98%)	4 (2%)	49	73
2	4-Z	170/170 (100%)	166 (98%)	4 (2%)	49	73
2	5-1	170/170 (100%)	164 (96%)	6 (4%)	36	64
2	5-B	170/170 (100%)	164 (96%)	6 (4%)	36	64
2	5-D	170/170 (100%)	164 (96%)	6 (4%)	36	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	5-F	170/170 (100%)	164 (96%)	6 (4%)	36	64
2	5-H	170/170 (100%)	164 (96%)	6 (4%)	36	64
2	5-J	170/170 (100%)	164 (96%)	6 (4%)	36	64
2	5-L	170/170 (100%)	164 (96%)	6 (4%)	36	64
2	5-N	170/170 (100%)	164 (96%)	6 (4%)	36	64
2	5-P	170/170 (100%)	164 (96%)	6 (4%)	36	64
2	5-R	170/170 (100%)	164 (96%)	6 (4%)	36	64
2	5-T	170/170 (100%)	164 (96%)	6 (4%)	36	64
2	5-V	170/170 (100%)	164 (96%)	6 (4%)	36	64
2	5-X	170/170 (100%)	164 (96%)	6 (4%)	36	64
2	5-Z	170/170 (100%)	164 (96%)	6 (4%)	36	64
2	6-1	170/170 (100%)	165 (97%)	5 (3%)	42	69
2	6-B	170/170 (100%)	165 (97%)	5 (3%)	42	69
2	6-D	170/170 (100%)	165 (97%)	5 (3%)	42	69
2	6-F	170/170 (100%)	165 (97%)	5 (3%)	42	69
2	6-H	170/170 (100%)	165 (97%)	5 (3%)	42	69
2	6-J	170/170 (100%)	165 (97%)	5 (3%)	42	69
2	6-L	170/170 (100%)	165 (97%)	5 (3%)	42	69
2	6-N	170/170 (100%)	165 (97%)	5 (3%)	42	69
2	6-P	170/170 (100%)	165 (97%)	5 (3%)	42	69
2	6-R	170/170 (100%)	165 (97%)	5 (3%)	42	69
2	6-T	170/170 (100%)	165 (97%)	5 (3%)	42	69
2	6-V	170/170 (100%)	165 (97%)	5 (3%)	42	69
2	6-X	170/170 (100%)	165 (97%)	5 (3%)	42	69
2	6-Z	170/170 (100%)	165 (97%)	5 (3%)	42	69
2	7-1	170/170 (100%)	168 (99%)	2 (1%)	71	83
2	7-B	170/170 (100%)	168 (99%)	2 (1%)	71	83
2	7-D	170/170 (100%)	168 (99%)	2 (1%)	71	83
2	7-F	170/170 (100%)	168 (99%)	2 (1%)	71	83
2	7-H	170/170 (100%)	168 (99%)	2 (1%)	71	83
2	7-J	170/170 (100%)	168 (99%)	2 (1%)	71	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	7-L	170/170 (100%)	168 (99%)	2 (1%)	71	83
2	7-N	170/170 (100%)	168 (99%)	2 (1%)	71	83
2	7-P	170/170 (100%)	168 (99%)	2 (1%)	71	83
2	7-R	170/170 (100%)	168 (99%)	2 (1%)	71	83
2	7-T	170/170 (100%)	168 (99%)	2 (1%)	71	83
2	7-V	170/170 (100%)	168 (99%)	2 (1%)	71	83
2	7-X	170/170 (100%)	168 (99%)	2 (1%)	71	83
2	7-Z	170/170 (100%)	168 (99%)	2 (1%)	71	83
2	8-1	170/170 (100%)	156 (92%)	14 (8%)	11	36
2	8-B	170/170 (100%)	156 (92%)	14 (8%)	11	36
2	8-D	170/170 (100%)	156 (92%)	14 (8%)	11	36
2	8-F	170/170 (100%)	156 (92%)	14 (8%)	11	36
2	8-H	170/170 (100%)	156 (92%)	14 (8%)	11	36
2	8-J	170/170 (100%)	156 (92%)	14 (8%)	11	36
2	8-L	170/170 (100%)	156 (92%)	14 (8%)	11	36
2	8-N	170/170 (100%)	156 (92%)	14 (8%)	11	36
2	8-P	170/170 (100%)	156 (92%)	14 (8%)	11	36
2	8-R	170/170 (100%)	156 (92%)	14 (8%)	11	36
2	8-T	170/170 (100%)	156 (92%)	14 (8%)	11	36
2	8-V	170/170 (100%)	156 (92%)	14 (8%)	11	36
2	8-X	170/170 (100%)	156 (92%)	14 (8%)	11	36
2	8-Z	170/170 (100%)	156 (92%)	14 (8%)	11	36
2	9-1	170/170 (100%)	167 (98%)	3 (2%)	59	78
2	9-B	170/170 (100%)	167 (98%)	3 (2%)	59	78
2	9-D	170/170 (100%)	167 (98%)	3 (2%)	59	78
2	9-F	170/170 (100%)	167 (98%)	3 (2%)	59	78
2	9-H	170/170 (100%)	167 (98%)	3 (2%)	59	78
2	9-J	170/170 (100%)	167 (98%)	3 (2%)	59	78
2	9-L	170/170 (100%)	167 (98%)	3 (2%)	59	78
2	9-N	170/170 (100%)	167 (98%)	3 (2%)	59	78
2	9-P	170/170 (100%)	167 (98%)	3 (2%)	59	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	9-R	170/170 (100%)	167 (98%)	3 (2%)	59	78
2	9-T	170/170 (100%)	167 (98%)	3 (2%)	59	78
2	9-V	170/170 (100%)	167 (98%)	3 (2%)	59	78
2	9-X	170/170 (100%)	167 (98%)	3 (2%)	59	78
2	9-Z	170/170 (100%)	167 (98%)	3 (2%)	59	78
2	10-1	170/170 (100%)	164 (96%)	6 (4%)	36	64
2	10-B	170/170 (100%)	164 (96%)	6 (4%)	36	64
2	10-D	170/170 (100%)	164 (96%)	6 (4%)	36	64
2	10-F	170/170 (100%)	164 (96%)	6 (4%)	36	64
2	10-H	170/170 (100%)	164 (96%)	6 (4%)	36	64
2	10-J	170/170 (100%)	164 (96%)	6 (4%)	36	64
2	10-L	170/170 (100%)	164 (96%)	6 (4%)	36	64
2	10-N	170/170 (100%)	164 (96%)	6 (4%)	36	64
2	10-P	170/170 (100%)	164 (96%)	6 (4%)	36	64
2	10-R	170/170 (100%)	164 (96%)	6 (4%)	36	64
2	10-T	170/170 (100%)	164 (96%)	6 (4%)	36	64
2	10-V	170/170 (100%)	164 (96%)	6 (4%)	36	64
2	10-X	170/170 (100%)	164 (96%)	6 (4%)	36	64
2	10-Z	170/170 (100%)	164 (96%)	6 (4%)	36	64
All	All	49560/49840 (99%)	48598 (98%)	962 (2%)	59	77

All (962) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	108	ASN
2	1-B	24	ASN
2	1-B	71	ARG
1	1-C	108	ASN
2	1-D	24	ASN
2	1-D	71	ARG
1	1-E	108	ASN
2	1-F	24	ASN
2	1-F	71	ARG
1	1-G	108	ASN
2	1-H	24	ASN

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Mol	Chain	Res	Type
2	1-H	71	ARG
1	1-I	108	ASN
2	1-J	24	ASN
2	1-J	71	ARG
1	1-K	108	ASN
2	1-L	24	ASN
2	1-L	71	ARG
1	1-M	108	ASN
2	1-N	24	ASN
2	1-N	71	ARG
1	1-O	108	ASN
2	1-P	24	ASN
2	1-P	71	ARG
1	1-Q	108	ASN
2	1-R	24	ASN
2	1-R	71	ARG
1	1-S	108	ASN
2	1-T	24	ASN
2	1-T	71	ARG
1	1-U	108	ASN
2	1-V	24	ASN
2	1-V	71	ARG
1	1-W	108	ASN
2	1-X	24	ASN
2	1-X	71	ARG
1	1-Y	108	ASN
2	1-Z	24	ASN
2	1-Z	71	ARG
1	1-0	108	ASN
2	1-1	24	ASN
2	1-1	71	ARG
1	2-A	72	ASP
1	2-A	163	THR
1	2-A	211	GLU
1	2-A	222	ARG
1	2-A	231	LYS
2	2-B	88	ASN
1	2-C	72	ASP
1	2-C	163	THR
1	2-C	211	GLU
1	2-C	222	ARG
1	2-C	231	LYS

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Mol	Chain	Res	Type
2	2-D	88	ASN
1	2-E	72	ASP
1	2-E	163	THR
1	2-E	211	GLU
1	2-E	222	ARG
1	2-E	231	LYS
2	2-F	88	ASN
1	2-G	72	ASP
1	2-G	163	THR
1	2-G	211	GLU
1	2-G	222	ARG
1	2-G	231	LYS
2	2-H	88	ASN
1	2-I	72	ASP
1	2-I	163	THR
1	2-I	211	GLU
1	2-I	222	ARG
1	2-I	231	LYS
2	2-J	88	ASN
1	2-K	72	ASP
1	2-K	163	THR
1	2-K	211	GLU
1	2-K	222	ARG
1	2-K	231	LYS
2	2-L	88	ASN
1	2-M	72	ASP
1	2-M	211	GLU
1	2-M	222	ARG
1	2-M	231	LYS
2	2-N	88	ASN
1	2-O	72	ASP
1	2-O	163	THR
1	2-O	211	GLU
1	2-O	222	ARG
1	2-O	231	LYS
2	2-P	88	ASN
1	2-Q	72	ASP
1	2-Q	211	GLU
1	2-Q	222	ARG
1	2-Q	231	LYS
2	2-R	88	ASN
1	2-S	72	ASP

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Mol	Chain	Res	Type
1	2-S	163	THR
1	2-S	211	GLU
1	2-S	222	ARG
1	2-S	231	LYS
2	2-T	88	ASN
1	2-U	72	ASP
1	2-U	163	THR
1	2-U	211	GLU
1	2-U	222	ARG
1	2-U	231	LYS
2	2-V	88	ASN
1	2-W	72	ASP
1	2-W	211	GLU
1	2-W	222	ARG
1	2-W	231	LYS
2	2-X	88	ASN
1	2-Y	72	ASP
1	2-Y	163	THR
1	2-Y	211	GLU
1	2-Y	222	ARG
1	2-Y	231	LYS
2	2-Z	88	ASN
1	2-0	72	ASP
1	2-0	163	THR
1	2-0	211	GLU
1	2-0	222	ARG
1	2-0	231	LYS
2	2-1	88	ASN
1	3-A	222	ARG
1	3-A	227	GLU
1	3-A	228	GLU
2	3-B	192	ILE
2	3-B	197	ARG
1	3-C	222	ARG
1	3-C	227	GLU
1	3-C	228	GLU
2	3-D	192	ILE
2	3-D	197	ARG
1	3-E	222	ARG
1	3-E	227	GLU
1	3-E	228	GLU
2	3-F	192	ILE

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Mol	Chain	Res	Type
2	3-F	197	ARG
1	3-G	222	ARG
1	3-G	227	GLU
1	3-G	228	GLU
2	3-H	192	ILE
2	3-H	197	ARG
1	3-I	222	ARG
1	3-I	227	GLU
1	3-I	228	GLU
2	3-J	192	ILE
2	3-J	197	ARG
1	3-K	222	ARG
1	3-K	227	GLU
1	3-K	228	GLU
2	3-L	192	ILE
2	3-L	197	ARG
1	3-M	222	ARG
1	3-M	227	GLU
1	3-M	228	GLU
2	3-N	192	ILE
2	3-N	197	ARG
1	3-O	222	ARG
1	3-O	227	GLU
1	3-O	228	GLU
2	3-P	192	ILE
2	3-P	197	ARG
1	3-Q	222	ARG
1	3-Q	227	GLU
1	3-Q	228	GLU
2	3-R	192	ILE
2	3-R	197	ARG
1	3-S	222	ARG
1	3-S	227	GLU
1	3-S	228	GLU
2	3-T	192	ILE
2	3-T	197	ARG
1	3-U	222	ARG
1	3-U	227	GLU
1	3-U	228	GLU
2	3-V	192	ILE
2	3-V	197	ARG
1	3-W	222	ARG

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Mol	Chain	Res	Type
1	3-W	227	GLU
1	3-W	228	GLU
2	3-X	192	ILE
2	3-X	197	ARG
1	3-Y	222	ARG
1	3-Y	227	GLU
1	3-Y	228	GLU
2	3-Z	192	ILE
2	3-Z	197	ARG
1	3-0	222	ARG
1	3-0	227	GLU
1	3-0	228	GLU
2	3-1	192	ILE
2	3-1	197	ARG
1	4-A	72	ASP
1	4-A	222	ARG
1	4-A	227	GLU
2	4-B	16	THR
2	4-B	21	THR
2	4-B	135	TYR
2	4-B	192	ILE
1	4-C	72	ASP
1	4-C	222	ARG
1	4-C	227	GLU
2	4-D	16	THR
2	4-D	21	THR
2	4-D	135	TYR
2	4-D	192	ILE
1	4-E	72	ASP
1	4-E	222	ARG
1	4-E	227	GLU
2	4-F	16	THR
2	4-F	21	THR
2	4-F	135	TYR
2	4-F	192	ILE
1	4-G	72	ASP
1	4-G	222	ARG
1	4-G	227	GLU
2	4-H	16	THR
2	4-H	21	THR
2	4-H	135	TYR
2	4-H	192	ILE

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Mol	Chain	Res	Type
1	4-I	72	ASP
1	4-I	222	ARG
1	4-I	227	GLU
2	4-J	16	THR
2	4-J	21	THR
2	4-J	135	TYR
2	4-J	192	ILE
1	4-K	72	ASP
1	4-K	222	ARG
1	4-K	227	GLU
2	4-L	16	THR
2	4-L	21	THR
2	4-L	135	TYR
2	4-L	192	ILE
1	4-M	72	ASP
1	4-M	222	ARG
1	4-M	227	GLU
2	4-N	16	THR
2	4-N	21	THR
2	4-N	135	TYR
2	4-N	192	ILE
1	4-O	72	ASP
1	4-O	222	ARG
1	4-O	227	GLU
2	4-P	16	THR
2	4-P	21	THR
2	4-P	135	TYR
2	4-P	192	ILE
1	4-Q	72	ASP
1	4-Q	222	ARG
1	4-Q	227	GLU
2	4-R	16	THR
2	4-R	21	THR
2	4-R	135	TYR
2	4-R	192	ILE
1	4-S	72	ASP
1	4-S	222	ARG
1	4-S	227	GLU
2	4-T	16	THR
2	4-T	21	THR
2	4-T	135	TYR
2	4-T	192	ILE

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Mol	Chain	Res	Type
1	4-U	72	ASP
1	4-U	222	ARG
1	4-U	227	GLU
2	4-V	16	THR
2	4-V	21	THR
2	4-V	135	TYR
2	4-V	192	ILE
1	4-W	72	ASP
1	4-W	222	ARG
1	4-W	227	GLU
2	4-X	16	THR
2	4-X	21	THR
2	4-X	135	TYR
2	4-X	192	ILE
1	4-Y	72	ASP
1	4-Y	222	ARG
1	4-Y	227	GLU
2	4-Z	16	THR
2	4-Z	21	THR
2	4-Z	135	TYR
2	4-Z	192	ILE
1	4-0	72	ASP
1	4-0	222	ARG
1	4-0	227	GLU
2	4-1	16	THR
2	4-1	21	THR
2	4-1	135	TYR
2	4-1	192	ILE
1	5-A	72	ASP
2	5-B	10	ASP
2	5-B	90	VAL
2	5-B	145	LYS
2	5-B	153	ASP
2	5-B	182	ASP
2	5-B	202	ILE
1	5-C	72	ASP
2	5-D	10	ASP
2	5-D	90	VAL
2	5-D	145	LYS
2	5-D	153	ASP
2	5-D	182	ASP
2	5-D	202	ILE

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Mol	Chain	Res	Type
1	5-E	72	ASP
2	5-F	10	ASP
2	5-F	90	VAL
2	5-F	145	LYS
2	5-F	153	ASP
2	5-F	182	ASP
2	5-F	202	ILE
1	5-G	72	ASP
2	5-H	10	ASP
2	5-H	90	VAL
2	5-H	145	LYS
2	5-H	153	ASP
2	5-H	182	ASP
2	5-H	202	ILE
1	5-I	72	ASP
2	5-J	10	ASP
2	5-J	90	VAL
2	5-J	145	LYS
2	5-J	153	ASP
2	5-J	182	ASP
2	5-J	202	ILE
1	5-K	72	ASP
2	5-L	10	ASP
2	5-L	90	VAL
2	5-L	145	LYS
2	5-L	153	ASP
2	5-L	182	ASP
2	5-L	202	ILE
1	5-M	72	ASP
2	5-N	10	ASP
2	5-N	90	VAL
2	5-N	145	LYS
2	5-N	153	ASP
2	5-N	182	ASP
2	5-N	202	ILE
1	5-O	72	ASP
2	5-P	10	ASP
2	5-P	90	VAL
2	5-P	145	LYS
2	5-P	153	ASP
2	5-P	182	ASP
2	5-P	202	ILE

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Mol	Chain	Res	Type
1	5-Q	72	ASP
2	5-R	10	ASP
2	5-R	90	VAL
2	5-R	145	LYS
2	5-R	153	ASP
2	5-R	182	ASP
2	5-R	202	ILE
1	5-S	72	ASP
2	5-T	10	ASP
2	5-T	90	VAL
2	5-T	145	LYS
2	5-T	153	ASP
2	5-T	182	ASP
2	5-T	202	ILE
1	5-U	72	ASP
2	5-V	10	ASP
2	5-V	90	VAL
2	5-V	145	LYS
2	5-V	153	ASP
2	5-V	182	ASP
2	5-V	202	ILE
1	5-W	72	ASP
2	5-X	10	ASP
2	5-X	90	VAL
2	5-X	145	LYS
2	5-X	153	ASP
2	5-X	182	ASP
2	5-X	202	ILE
1	5-Y	72	ASP
2	5-Z	10	ASP
2	5-Z	90	VAL
2	5-Z	145	LYS
2	5-Z	153	ASP
2	5-Z	182	ASP
2	5-Z	202	ILE
1	5-0	72	ASP
2	5-1	10	ASP
2	5-1	90	VAL
2	5-1	145	LYS
2	5-1	153	ASP
2	5-1	182	ASP
2	5-1	202	ILE

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Mol	Chain	Res	Type
1	6-A	222	ARG
1	6-A	228	GLU
2	6-B	17	GLU
2	6-B	23	GLU
2	6-B	24	ASN
2	6-B	71	ARG
2	6-B	182	ASP
1	6-C	222	ARG
1	6-C	228	GLU
2	6-D	17	GLU
2	6-D	23	GLU
2	6-D	24	ASN
2	6-D	71	ARG
2	6-D	182	ASP
1	6-E	222	ARG
1	6-E	228	GLU
2	6-F	17	GLU
2	6-F	23	GLU
2	6-F	24	ASN
2	6-F	71	ARG
2	6-F	182	ASP
1	6-G	222	ARG
1	6-G	228	GLU
2	6-H	17	GLU
2	6-H	23	GLU
2	6-H	24	ASN
2	6-H	71	ARG
2	6-H	182	ASP
1	6-I	222	ARG
1	6-I	228	GLU
2	6-J	17	GLU
2	6-J	23	GLU
2	6-J	24	ASN
2	6-J	71	ARG
2	6-J	182	ASP
1	6-K	222	ARG
1	6-K	228	GLU
2	6-L	17	GLU
2	6-L	23	GLU
2	6-L	24	ASN
2	6-L	71	ARG
2	6-L	182	ASP

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Mol	Chain	Res	Type
1	6-M	222	ARG
1	6-M	228	GLU
2	6-N	17	GLU
2	6-N	23	GLU
2	6-N	24	ASN
2	6-N	71	ARG
2	6-N	182	ASP
1	6-O	222	ARG
1	6-O	228	GLU
2	6-P	17	GLU
2	6-P	23	GLU
2	6-P	24	ASN
2	6-P	71	ARG
2	6-P	182	ASP
1	6-Q	222	ARG
1	6-Q	228	GLU
2	6-R	17	GLU
2	6-R	23	GLU
2	6-R	24	ASN
2	6-R	71	ARG
2	6-R	182	ASP
1	6-S	222	ARG
1	6-S	228	GLU
2	6-T	17	GLU
2	6-T	23	GLU
2	6-T	24	ASN
2	6-T	71	ARG
2	6-T	182	ASP
1	6-U	222	ARG
1	6-U	228	GLU
2	6-V	17	GLU
2	6-V	23	GLU
2	6-V	24	ASN
2	6-V	71	ARG
2	6-V	182	ASP
1	6-W	222	ARG
1	6-W	228	GLU
2	6-X	17	GLU
2	6-X	23	GLU
2	6-X	24	ASN
2	6-X	71	ARG
2	6-X	182	ASP

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Mol	Chain	Res	Type
1	6-Y	222	ARG
1	6-Y	228	GLU
2	6-Z	17	GLU
2	6-Z	23	GLU
2	6-Z	24	ASN
2	6-Z	71	ARG
2	6-Z	182	ASP
1	6-0	222	ARG
2	6-1	17	GLU
2	6-1	23	GLU
2	6-1	24	ASN
2	6-1	71	ARG
2	6-1	182	ASP
1	7-A	47	LEU
1	7-A	68	GLN
1	7-A	203	GLU
1	7-A	222	ARG
2	7-B	17	GLU
2	7-B	44	THR
1	7-C	47	LEU
1	7-C	68	GLN
1	7-C	203	GLU
1	7-C	222	ARG
2	7-D	17	GLU
2	7-D	44	THR
1	7-E	47	LEU
1	7-E	68	GLN
1	7-E	203	GLU
1	7-E	222	ARG
2	7-F	17	GLU
2	7-F	44	THR
1	7-G	47	LEU
1	7-G	68	GLN
1	7-G	203	GLU
1	7-G	222	ARG
2	7-H	17	GLU
2	7-H	44	THR
1	7-I	47	LEU
1	7-I	68	GLN
1	7-I	203	GLU
1	7-I	222	ARG
2	7-J	17	GLU

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Mol	Chain	Res	Type
2	7-J	44	THR
1	7-K	47	LEU
1	7-K	68	GLN
1	7-K	203	GLU
1	7-K	222	ARG
2	7-L	17	GLU
2	7-L	44	THR
1	7-M	47	LEU
1	7-M	68	GLN
1	7-M	203	GLU
1	7-M	222	ARG
2	7-N	17	GLU
2	7-N	44	THR
1	7-O	47	LEU
1	7-O	68	GLN
1	7-O	203	GLU
1	7-O	222	ARG
2	7-P	17	GLU
2	7-P	44	THR
1	7-Q	47	LEU
1	7-Q	68	GLN
1	7-Q	203	GLU
1	7-Q	222	ARG
2	7-R	17	GLU
2	7-R	44	THR
1	7-S	47	LEU
1	7-S	68	GLN
1	7-S	203	GLU
1	7-S	222	ARG
2	7-T	17	GLU
2	7-T	44	THR
1	7-U	47	LEU
1	7-U	68	GLN
1	7-U	203	GLU
1	7-U	222	ARG
2	7-V	17	GLU
2	7-V	44	THR
1	7-W	47	LEU
1	7-W	68	GLN
1	7-W	203	GLU
1	7-W	222	ARG
2	7-X	17	GLU

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Mol	Chain	Res	Type
2	7-X	44	THR
1	7-Y	47	LEU
1	7-Y	68	GLN
1	7-Y	203	GLU
1	7-Y	222	ARG
2	7-Z	17	GLU
2	7-Z	44	THR
1	7-0	47	LEU
1	7-0	68	GLN
1	7-0	203	GLU
1	7-0	222	ARG
2	7-1	17	GLU
2	7-1	44	THR
1	8-A	206	GLU
1	8-A	208	LYS
1	8-A	216	THR
2	8-B	10	ASP
2	8-B	17	GLU
2	8-B	67	ARG
2	8-B	71	ARG
2	8-B	88	ASN
2	8-B	89	GLN
2	8-B	91	LYS
2	8-B	93	MET
2	8-B	120	VAL
2	8-B	134	VAL
2	8-B	143	SER
2	8-B	144	GLU
2	8-B	164	GLN
2	8-B	190	ASP
1	8-C	206	GLU
1	8-C	208	LYS
1	8-C	216	THR
2	8-D	10	ASP
2	8-D	17	GLU
2	8-D	67	ARG
2	8-D	71	ARG
2	8-D	88	ASN
2	8-D	89	GLN
2	8-D	91	LYS
2	8-D	93	MET
2	8-D	120	VAL

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Mol	Chain	Res	Type
2	8-D	134	VAL
2	8-D	143	SER
2	8-D	144	GLU
2	8-D	164	GLN
2	8-D	190	ASP
1	8-E	206	GLU
1	8-E	208	LYS
1	8-E	216	THR
2	8-F	10	ASP
2	8-F	17	GLU
2	8-F	67	ARG
2	8-F	71	ARG
2	8-F	88	ASN
2	8-F	89	GLN
2	8-F	91	LYS
2	8-F	93	MET
2	8-F	120	VAL
2	8-F	134	VAL
2	8-F	143	SER
2	8-F	144	GLU
2	8-F	164	GLN
2	8-F	190	ASP
1	8-G	206	GLU
1	8-G	208	LYS
1	8-G	216	THR
2	8-H	10	ASP
2	8-H	17	GLU
2	8-H	67	ARG
2	8-H	71	ARG
2	8-H	88	ASN
2	8-H	89	GLN
2	8-H	91	LYS
2	8-H	93	MET
2	8-H	120	VAL
2	8-H	134	VAL
2	8-H	143	SER
2	8-H	144	GLU
2	8-H	164	GLN
2	8-H	190	ASP
1	8-I	206	GLU
1	8-I	208	LYS
1	8-I	216	THR

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Mol	Chain	Res	Type
2	8-J	10	ASP
2	8-J	17	GLU
2	8-J	67	ARG
2	8-J	71	ARG
2	8-J	88	ASN
2	8-J	89	GLN
2	8-J	91	LYS
2	8-J	93	MET
2	8-J	120	VAL
2	8-J	134	VAL
2	8-J	143	SER
2	8-J	144	GLU
2	8-J	164	GLN
2	8-J	190	ASP
1	8-K	206	GLU
1	8-K	208	LYS
1	8-K	216	THR
2	8-L	10	ASP
2	8-L	17	GLU
2	8-L	67	ARG
2	8-L	71	ARG
2	8-L	88	ASN
2	8-L	89	GLN
2	8-L	91	LYS
2	8-L	93	MET
2	8-L	120	VAL
2	8-L	134	VAL
2	8-L	143	SER
2	8-L	144	GLU
2	8-L	164	GLN
2	8-L	190	ASP
1	8-M	206	GLU
1	8-M	208	LYS
1	8-M	216	THR
2	8-N	10	ASP
2	8-N	17	GLU
2	8-N	67	ARG
2	8-N	71	ARG
2	8-N	88	ASN
2	8-N	89	GLN
2	8-N	91	LYS
2	8-N	93	MET

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Mol	Chain	Res	Type
2	8-N	120	VAL
2	8-N	134	VAL
2	8-N	143	SER
2	8-N	144	GLU
2	8-N	164	GLN
2	8-N	190	ASP
1	8-O	206	GLU
1	8-O	208	LYS
1	8-O	216	THR
2	8-P	10	ASP
2	8-P	17	GLU
2	8-P	67	ARG
2	8-P	71	ARG
2	8-P	88	ASN
2	8-P	89	GLN
2	8-P	91	LYS
2	8-P	93	MET
2	8-P	120	VAL
2	8-P	134	VAL
2	8-P	143	SER
2	8-P	144	GLU
2	8-P	164	GLN
2	8-P	190	ASP
1	8-Q	206	GLU
1	8-Q	208	LYS
1	8-Q	216	THR
2	8-R	10	ASP
2	8-R	17	GLU
2	8-R	67	ARG
2	8-R	71	ARG
2	8-R	88	ASN
2	8-R	89	GLN
2	8-R	91	LYS
2	8-R	93	MET
2	8-R	120	VAL
2	8-R	134	VAL
2	8-R	143	SER
2	8-R	144	GLU
2	8-R	164	GLN
2	8-R	190	ASP
1	8-S	206	GLU
1	8-S	208	LYS

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Mol	Chain	Res	Type
1	8-S	216	THR
2	8-T	10	ASP
2	8-T	17	GLU
2	8-T	67	ARG
2	8-T	71	ARG
2	8-T	88	ASN
2	8-T	89	GLN
2	8-T	91	LYS
2	8-T	93	MET
2	8-T	120	VAL
2	8-T	134	VAL
2	8-T	143	SER
2	8-T	144	GLU
2	8-T	164	GLN
2	8-T	190	ASP
1	8-U	206	GLU
1	8-U	208	LYS
1	8-U	216	THR
2	8-V	10	ASP
2	8-V	17	GLU
2	8-V	67	ARG
2	8-V	71	ARG
2	8-V	88	ASN
2	8-V	89	GLN
2	8-V	91	LYS
2	8-V	93	MET
2	8-V	120	VAL
2	8-V	134	VAL
2	8-V	143	SER
2	8-V	144	GLU
2	8-V	164	GLN
2	8-V	190	ASP
1	8-W	206	GLU
1	8-W	208	LYS
1	8-W	216	THR
2	8-X	10	ASP
2	8-X	17	GLU
2	8-X	67	ARG
2	8-X	71	ARG
2	8-X	88	ASN
2	8-X	89	GLN
2	8-X	91	LYS

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Mol	Chain	Res	Type
2	8-X	93	MET
2	8-X	120	VAL
2	8-X	134	VAL
2	8-X	143	SER
2	8-X	144	GLU
2	8-X	164	GLN
2	8-X	190	ASP
1	8-Y	206	GLU
1	8-Y	208	LYS
1	8-Y	216	THR
2	8-Z	10	ASP
2	8-Z	17	GLU
2	8-Z	67	ARG
2	8-Z	71	ARG
2	8-Z	88	ASN
2	8-Z	89	GLN
2	8-Z	91	LYS
2	8-Z	93	MET
2	8-Z	120	VAL
2	8-Z	134	VAL
2	8-Z	143	SER
2	8-Z	144	GLU
2	8-Z	164	GLN
2	8-Z	190	ASP
1	8-0	206	GLU
1	8-0	208	LYS
1	8-0	216	THR
2	8-1	10	ASP
2	8-1	17	GLU
2	8-1	67	ARG
2	8-1	71	ARG
2	8-1	88	ASN
2	8-1	89	GLN
2	8-1	91	LYS
2	8-1	93	MET
2	8-1	120	VAL
2	8-1	134	VAL
2	8-1	143	SER
2	8-1	144	GLU
2	8-1	164	GLN
2	8-1	190	ASP
1	9-A	72	ASP

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Mol	Chain	Res	Type
2	9-B	24	ASN
2	9-B	71	ARG
2	9-B	190	ASP
1	9-C	72	ASP
2	9-D	24	ASN
2	9-D	71	ARG
2	9-D	190	ASP
1	9-E	72	ASP
2	9-F	24	ASN
2	9-F	71	ARG
2	9-F	190	ASP
1	9-G	72	ASP
2	9-H	24	ASN
2	9-H	71	ARG
2	9-H	190	ASP
1	9-I	72	ASP
2	9-J	24	ASN
2	9-J	71	ARG
2	9-J	190	ASP
1	9-K	72	ASP
2	9-L	24	ASN
2	9-L	71	ARG
2	9-L	190	ASP
1	9-M	72	ASP
2	9-N	24	ASN
2	9-N	71	ARG
2	9-N	190	ASP
1	9-O	72	ASP
2	9-P	24	ASN
2	9-P	71	ARG
2	9-P	190	ASP
1	9-Q	72	ASP
2	9-R	24	ASN
2	9-R	71	ARG
2	9-R	190	ASP
1	9-S	72	ASP
2	9-T	24	ASN
2	9-T	71	ARG
2	9-T	190	ASP
1	9-U	72	ASP
2	9-V	24	ASN
2	9-V	71	ARG

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Mol	Chain	Res	Type
2	9-V	190	ASP
1	9-W	72	ASP
2	9-X	24	ASN
2	9-X	71	ARG
2	9-X	190	ASP
1	9-Y	72	ASP
2	9-Z	24	ASN
2	9-Z	71	ARG
2	9-Z	190	ASP
1	9-0	72	ASP
2	9-1	24	ASN
2	9-1	71	ARG
2	9-1	190	ASP
1	10-A	222	ARG
2	10-B	10	ASP
2	10-B	16	THR
2	10-B	17	GLU
2	10-B	64	GLU
2	10-B	88	ASN
2	10-B	91	LYS
1	10-C	222	ARG
2	10-D	10	ASP
2	10-D	16	THR
2	10-D	17	GLU
2	10-D	64	GLU
2	10-D	88	ASN
2	10-D	91	LYS
1	10-E	222	ARG
2	10-F	10	ASP
2	10-F	16	THR
2	10-F	17	GLU
2	10-F	64	GLU
2	10-F	88	ASN
2	10-F	91	LYS
1	10-G	222	ARG
2	10-H	10	ASP
2	10-H	16	THR
2	10-H	17	GLU
2	10-H	64	GLU
2	10-H	88	ASN
2	10-H	91	LYS
1	10-I	222	ARG

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Mol	Chain	Res	Type
2	10-J	10	ASP
2	10-J	16	THR
2	10-J	17	GLU
2	10-J	64	GLU
2	10-J	88	ASN
2	10-J	91	LYS
1	10-K	222	ARG
2	10-L	10	ASP
2	10-L	16	THR
2	10-L	17	GLU
2	10-L	64	GLU
2	10-L	88	ASN
2	10-L	91	LYS
1	10-M	222	ARG
2	10-N	10	ASP
2	10-N	16	THR
2	10-N	17	GLU
2	10-N	64	GLU
2	10-N	88	ASN
2	10-N	91	LYS
1	10-O	222	ARG
2	10-P	10	ASP
2	10-P	16	THR
2	10-P	17	GLU
2	10-P	64	GLU
2	10-P	88	ASN
2	10-P	91	LYS
1	10-Q	222	ARG
2	10-R	10	ASP
2	10-R	16	THR
2	10-R	17	GLU
2	10-R	64	GLU
2	10-R	88	ASN
2	10-R	91	LYS
1	10-S	222	ARG
2	10-T	10	ASP
2	10-T	16	THR
2	10-T	17	GLU
2	10-T	64	GLU
2	10-T	88	ASN
2	10-T	91	LYS
1	10-U	222	ARG

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Mol	Chain	Res	Type
2	10-V	10	ASP
2	10-V	16	THR
2	10-V	17	GLU
2	10-V	64	GLU
2	10-V	88	ASN
2	10-V	91	LYS
1	10-W	222	ARG
2	10-X	10	ASP
2	10-X	16	THR
2	10-X	17	GLU
2	10-X	64	GLU
2	10-X	88	ASN
2	10-X	91	LYS
1	10-Y	222	ARG
2	10-Z	10	ASP
2	10-Z	16	THR
2	10-Z	17	GLU
2	10-Z	64	GLU
2	10-Z	88	ASN
2	10-Z	91	LYS
1	10-0	222	ARG
2	10-1	10	ASP
2	10-1	16	THR
2	10-1	17	GLU
2	10-1	64	GLU
2	10-1	88	ASN
2	10-1	91	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (149) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	108	ASN
1	1-C	108	ASN
1	1-E	108	ASN
1	1-G	108	ASN
1	1-I	108	ASN
2	1-J	141	GLN
1	1-K	108	ASN
1	1-M	108	ASN
1	1-O	108	ASN
1	1-Q	108	ASN
1	1-S	108	ASN

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Mol	Chain	Res	Type
1	1-U	108	ASN
1	1-W	108	ASN
1	1-Y	108	ASN
1	1-0	108	ASN
2	2-D	88	ASN
2	2-D	141	GLN
2	2-J	141	GLN
2	2-L	141	GLN
2	2-P	141	GLN
2	2-T	141	GLN
2	2-V	141	GLN
2	2-1	141	GLN
2	3-B	141	GLN
2	3-D	141	GLN
2	3-H	88	ASN
2	3-H	141	GLN
2	3-L	141	GLN
2	3-R	88	ASN
2	3-T	141	GLN
2	3-X	88	ASN
2	3-X	141	GLN
2	3-1	141	GLN
1	4-A	111	ASN
2	4-B	30	ASN
2	4-B	98	GLN
2	4-B	141	GLN
1	4-C	111	ASN
2	4-D	30	ASN
2	4-D	98	GLN
2	4-D	141	GLN
1	4-E	111	ASN
2	4-F	30	ASN
2	4-F	98	GLN
1	4-G	111	ASN
2	4-H	30	ASN
2	4-H	98	GLN
1	4-I	111	ASN
2	4-J	30	ASN
2	4-J	98	GLN
2	4-J	141	GLN
1	4-K	111	ASN
2	4-L	30	ASN

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Mol	Chain	Res	Type
2	4-L	98	GLN
2	4-L	141	GLN
1	4-M	111	ASN
2	4-N	30	ASN
2	4-N	98	GLN
2	4-N	141	GLN
2	4-P	30	ASN
2	4-P	98	GLN
1	4-Q	111	ASN
2	4-R	30	ASN
2	4-R	98	GLN
1	4-S	111	ASN
2	4-T	30	ASN
2	4-T	98	GLN
2	4-T	141	GLN
1	4-U	111	ASN
2	4-V	30	ASN
2	4-V	98	GLN
2	4-V	141	GLN
1	4-W	111	ASN
2	4-X	30	ASN
2	4-X	98	GLN
1	4-Y	111	ASN
2	4-Z	30	ASN
2	4-Z	98	GLN
1	4-0	111	ASN
2	4-1	30	ASN
2	4-1	98	GLN
2	5-B	141	GLN
2	5-D	141	GLN
2	5-J	141	GLN
2	5-L	141	GLN
2	5-T	141	GLN
1	5-U	68	GLN
2	5-V	141	GLN
2	5-1	141	GLN
2	6-B	141	GLN
2	6-H	141	GLN
2	6-L	141	GLN
2	6-R	141	GLN
2	6-T	141	GLN
2	6-X	141	GLN

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Mol	Chain	Res	Type
2	6-1	141	GLN
2	7-D	88	ASN
2	7-L	141	GLN
2	7-N	141	GLN
2	7-P	141	GLN
2	7-R	88	ASN
2	7-T	141	GLN
2	7-V	141	GLN
2	7-X	141	GLN
2	8-B	88	ASN
2	8-D	88	ASN
2	8-D	141	GLN
2	8-F	88	ASN
2	8-H	88	ASN
2	8-J	88	ASN
2	8-L	88	ASN
2	8-L	141	GLN
2	8-N	88	ASN
2	8-N	141	GLN
2	8-P	88	ASN
2	8-P	141	GLN
2	8-R	88	ASN
2	8-T	88	ASN
2	8-T	141	GLN
1	8-U	111	ASN
2	8-V	88	ASN
2	8-V	141	GLN
2	8-X	88	ASN
2	8-X	141	GLN
2	8-Z	88	ASN
2	8-1	88	ASN
2	9-B	141	GLN
2	9-D	141	GLN
2	9-F	141	GLN
2	9-V	141	GLN
2	9-X	141	GLN
2	9-Z	141	GLN
2	9-1	141	GLN
2	10-B	88	ASN
2	10-D	88	ASN
2	10-F	88	ASN
2	10-H	88	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	10-J	88	ASN
2	10-L	88	ASN
2	10-N	88	ASN
2	10-P	88	ASN
2	10-R	88	ASN
2	10-T	88	ASN
2	10-V	88	ASN
2	10-V	141	GLN
2	10-X	88	ASN
2	10-Z	28	HIS
2	10-Z	88	ASN
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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

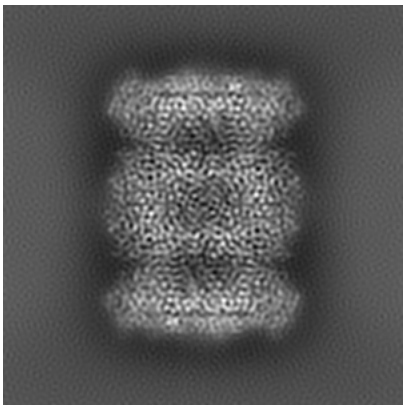
6 Map visualisation

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.

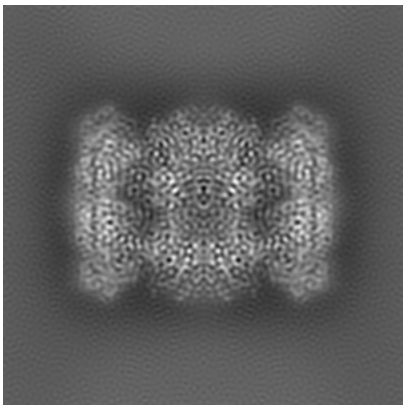
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

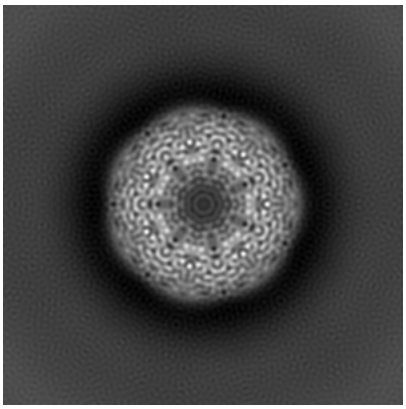
6.1.1 Primary map



X

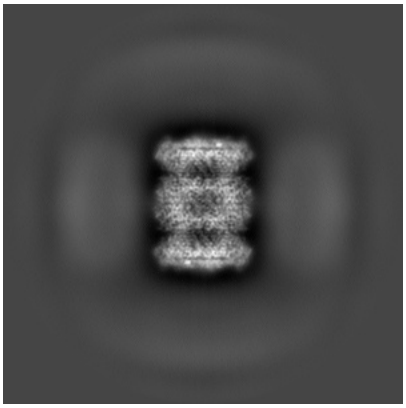


Y

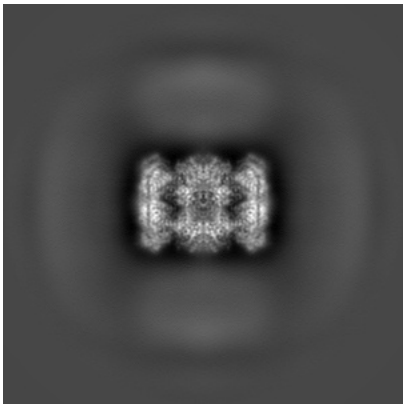


Z

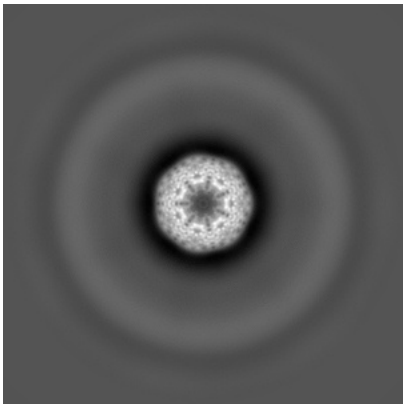
6.1.2 Raw map



X



Y

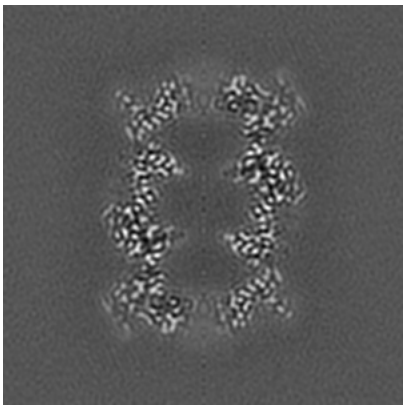


Z

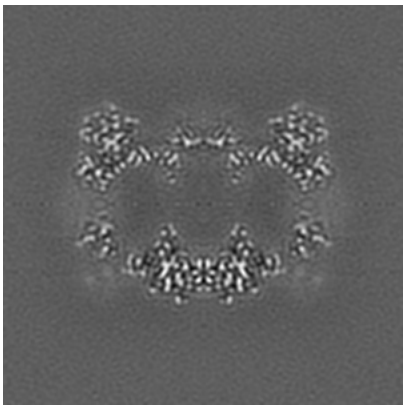
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

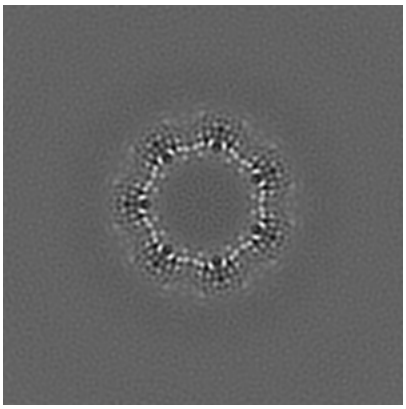
6.2.1 Primary map



X Index: 128

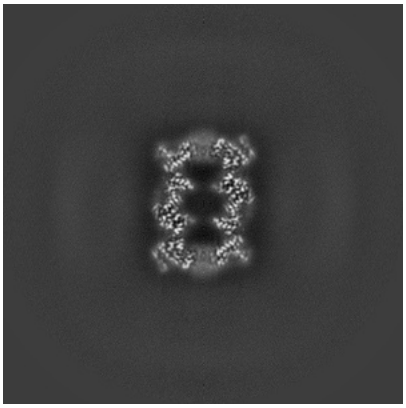


Y Index: 128

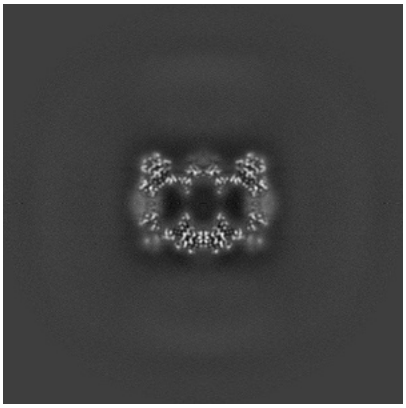


Z Index: 128

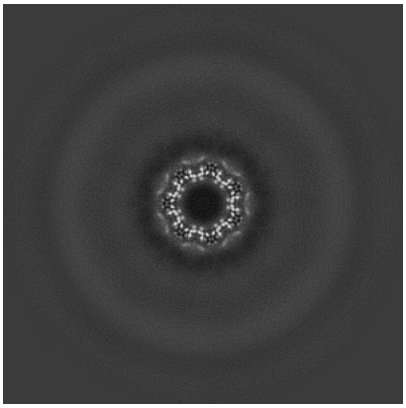
6.2.2 Raw map



X Index: 256



Y Index: 256

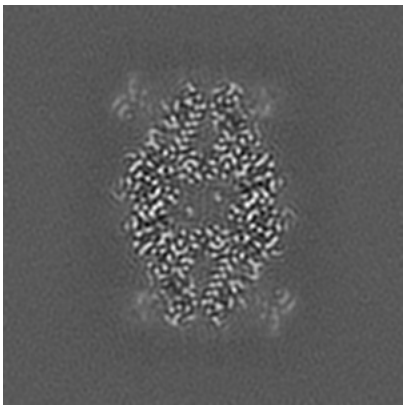


Z Index: 256

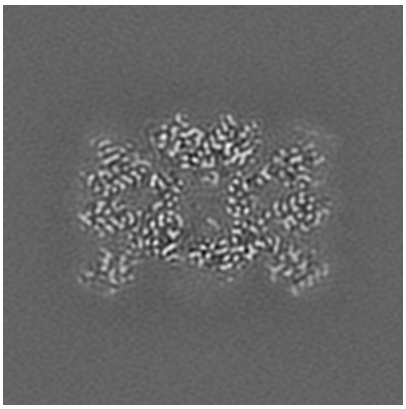
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

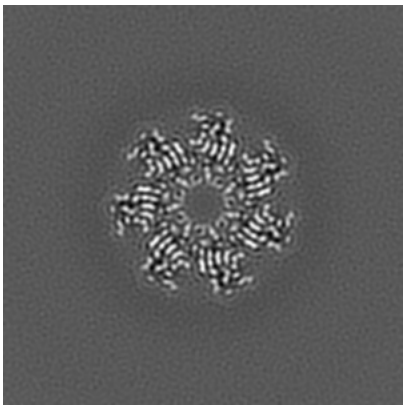
6.3.1 Primary map



X Index: 100

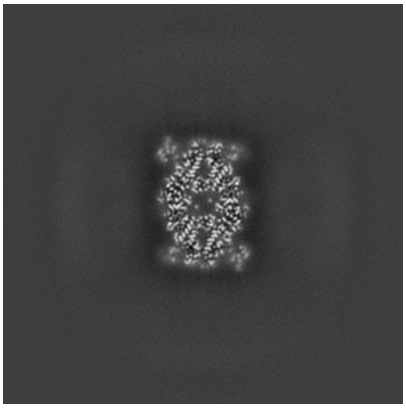


Y Index: 155

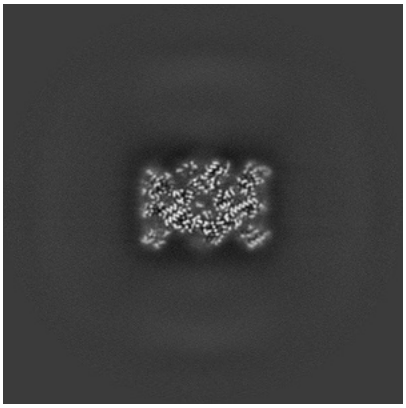


Z Index: 148

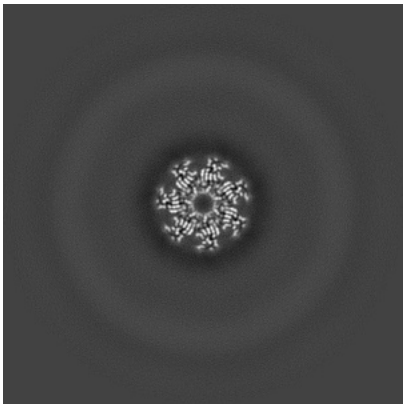
6.3.2 Raw map



X Index: 229



Y Index: 286

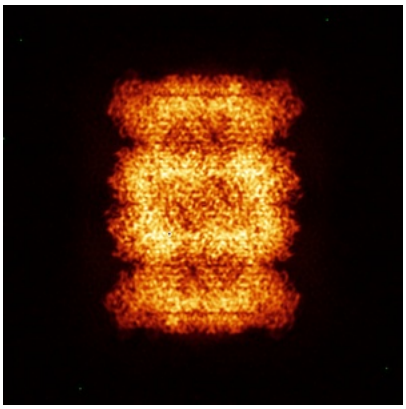


Z Index: 236

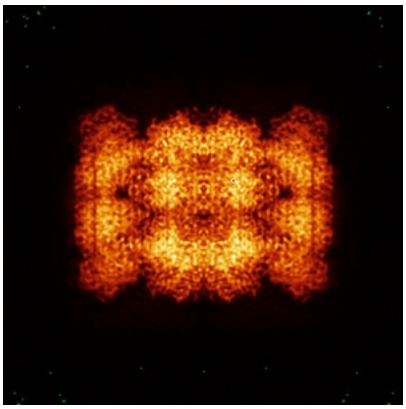
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

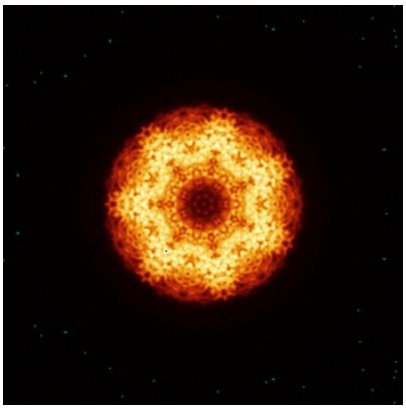
6.4.1 Primary map



X

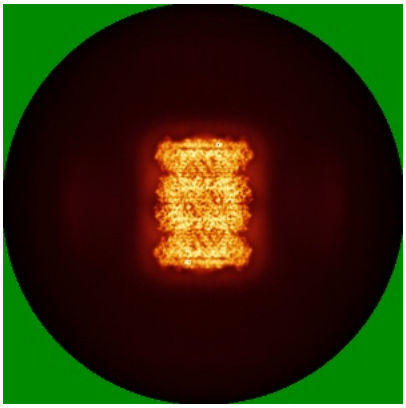


Y

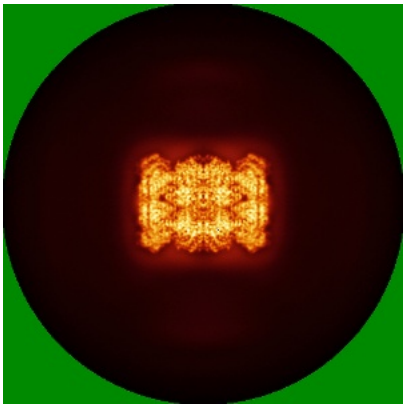


Z

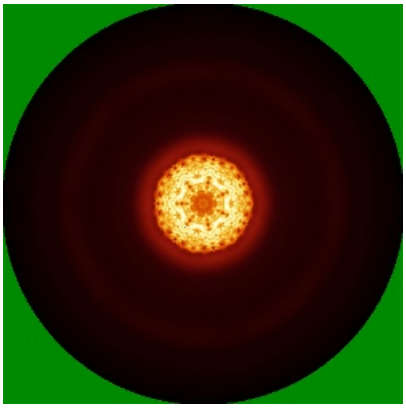
6.4.2 Raw map



X



Y

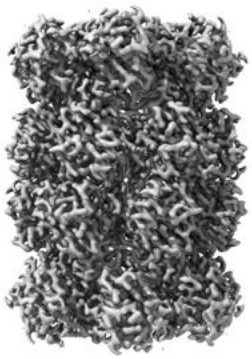


Z

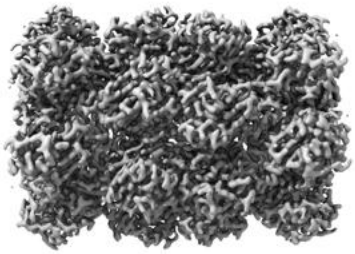
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

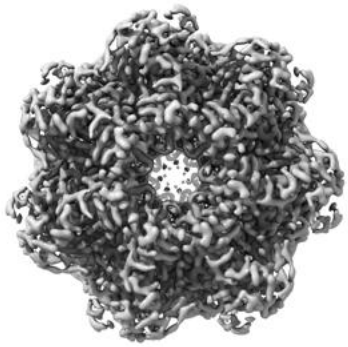
6.5.1 Primary map



X



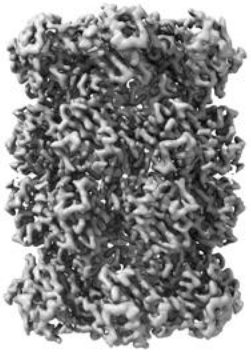
Y



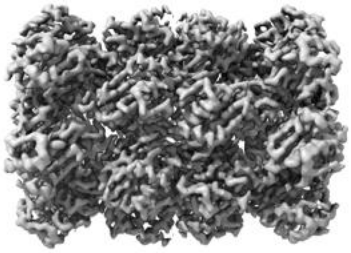
Z

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.

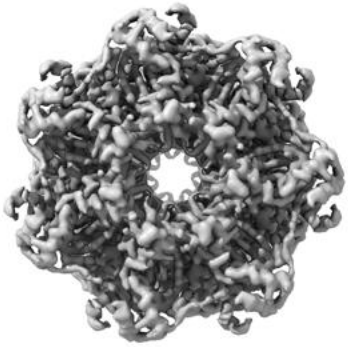
6.5.2 Raw map



X



Y



Z

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

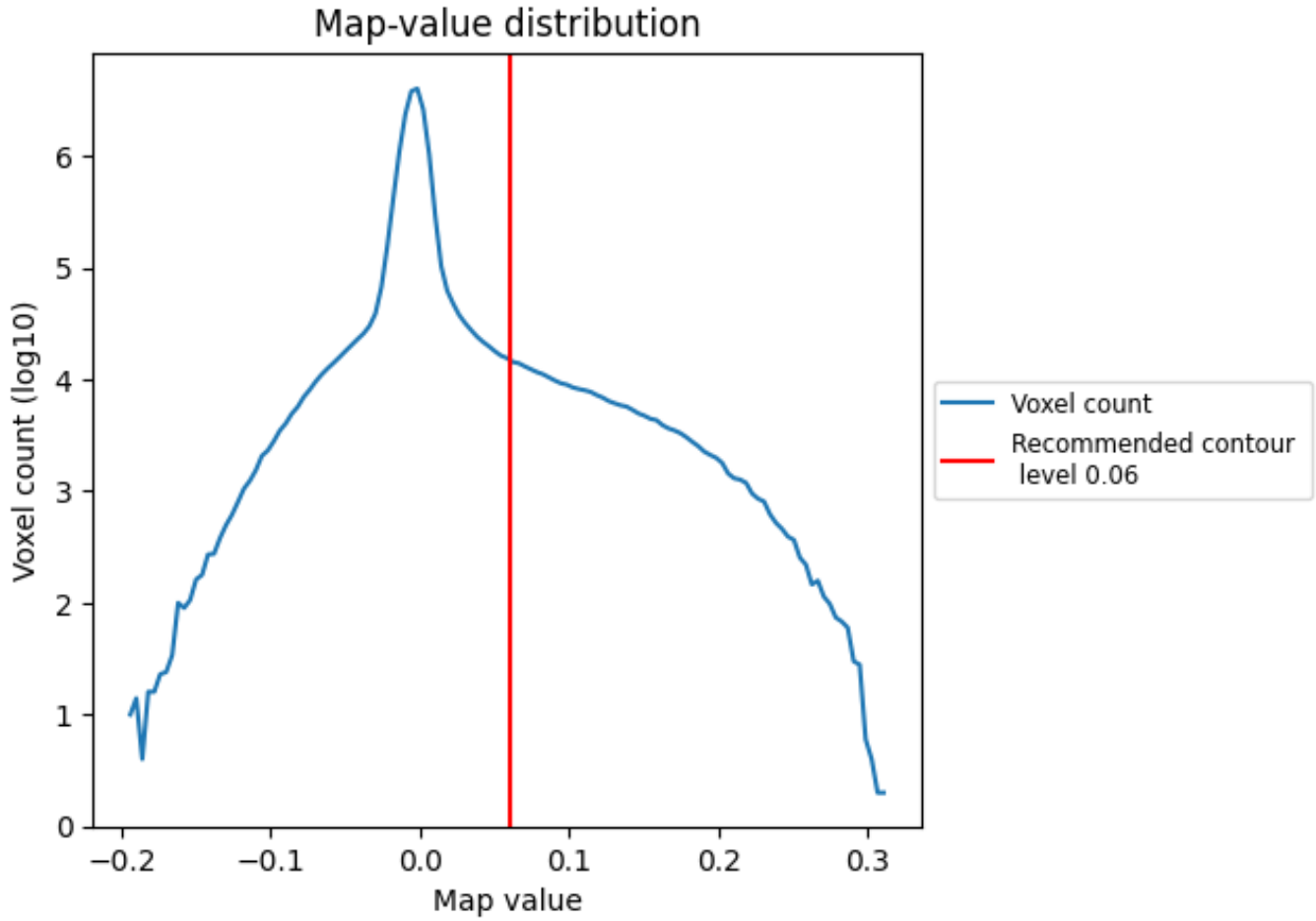
6.6 Mask visualisation (i)

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

7 Map analysis

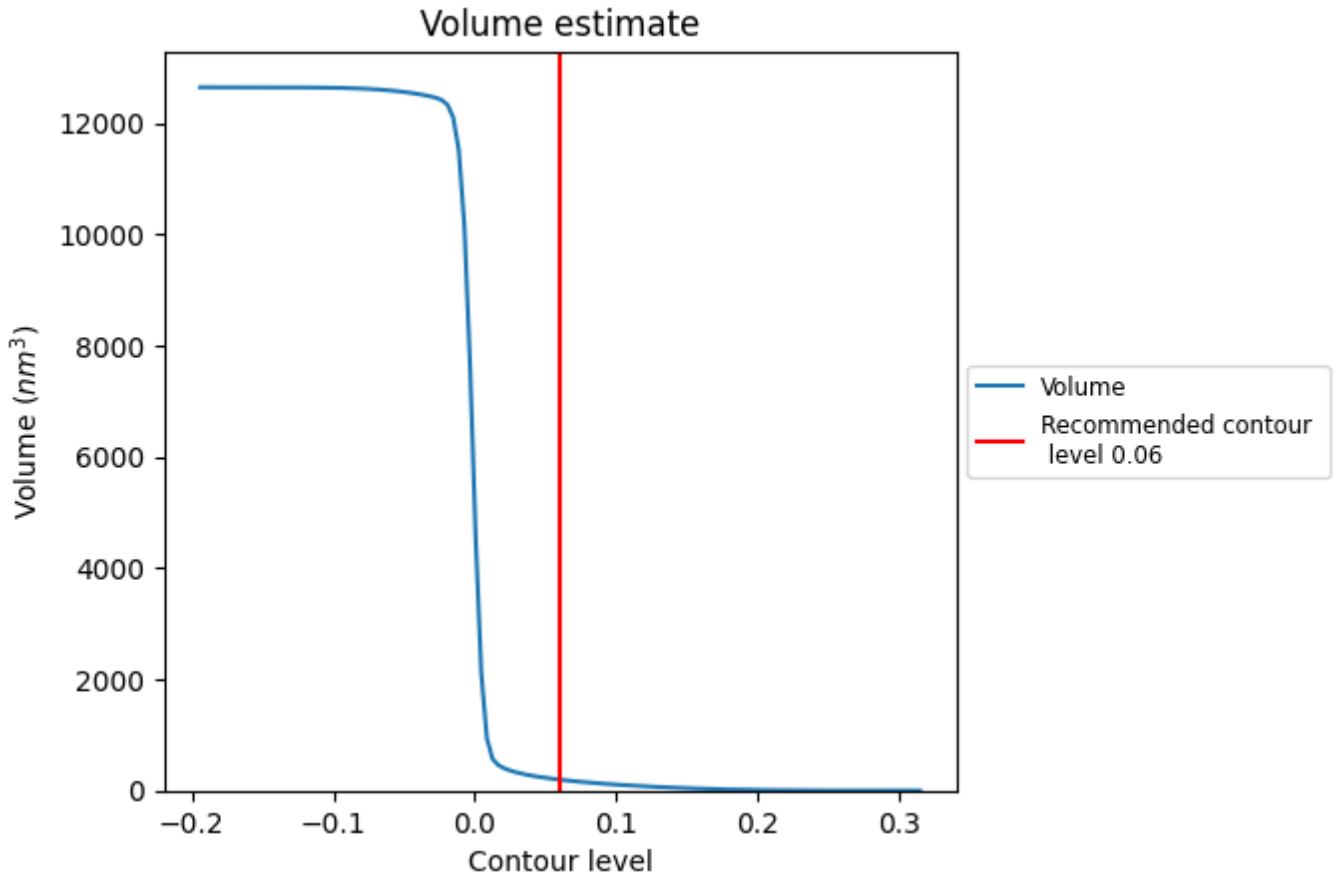
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

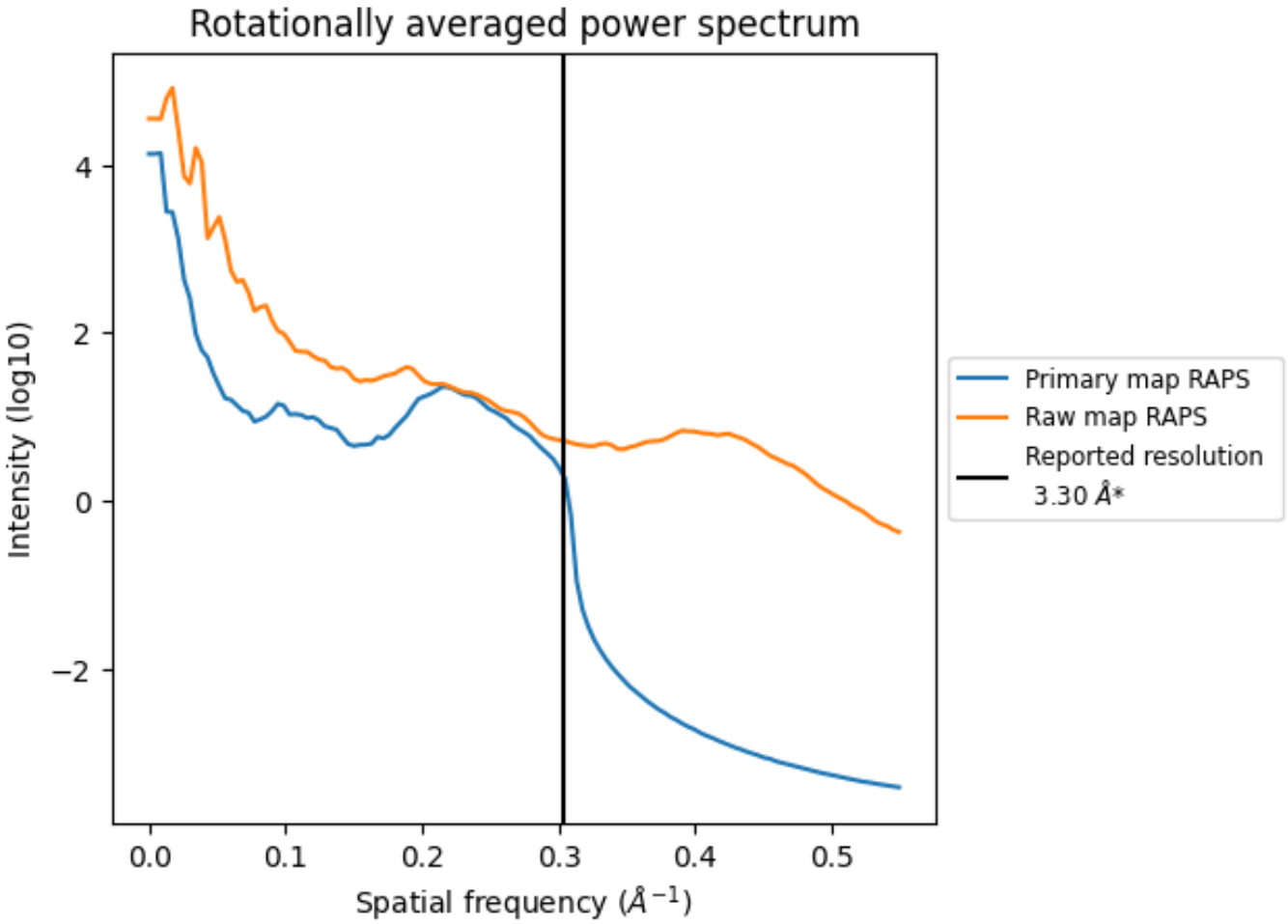
7.2 Volume estimate



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 (i)

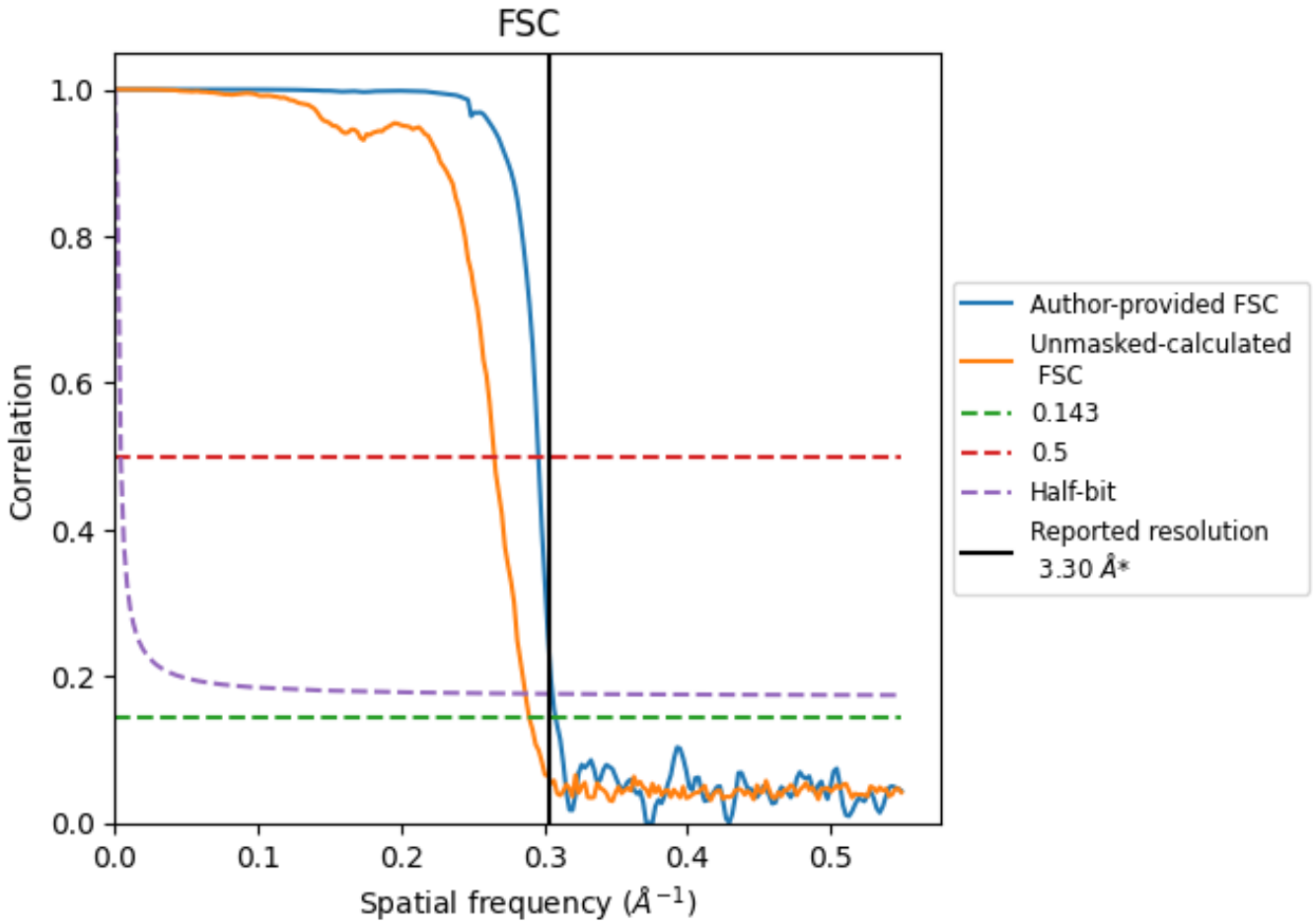


*Reported resolution corresponds to spatial frequency of 0.303 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8.2 Resolution estimates (i)

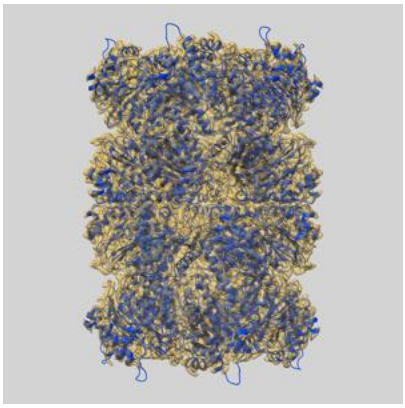
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.25	3.38	3.27
Unmasked-calculated*	3.45	3.77	3.49

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

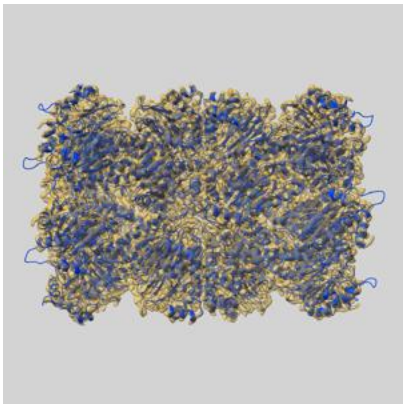
9 Map-model fit

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 28.

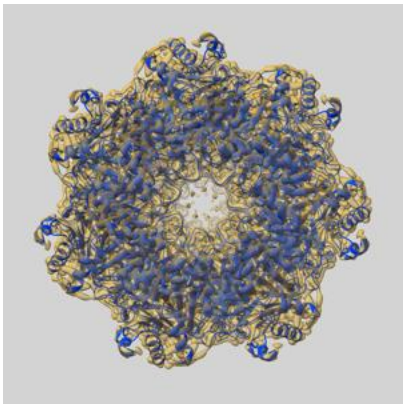
9.1 Map-model overlay



X



Y



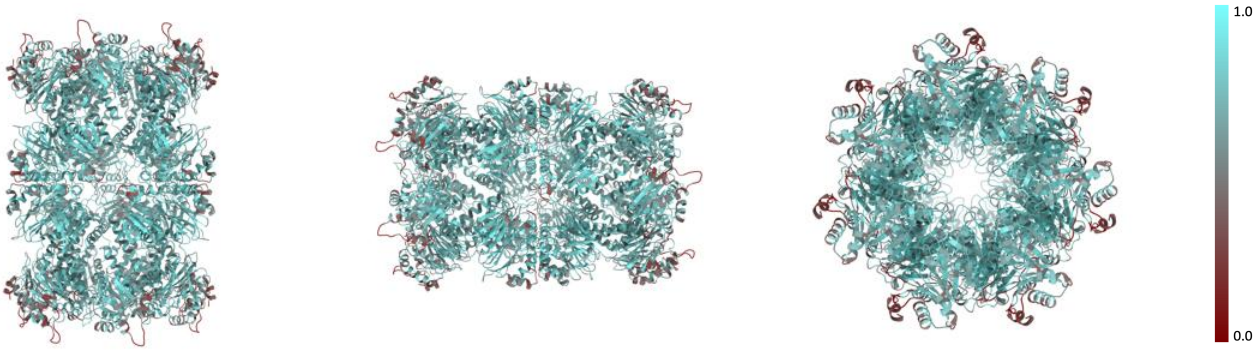
Z

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

This section was not generated.

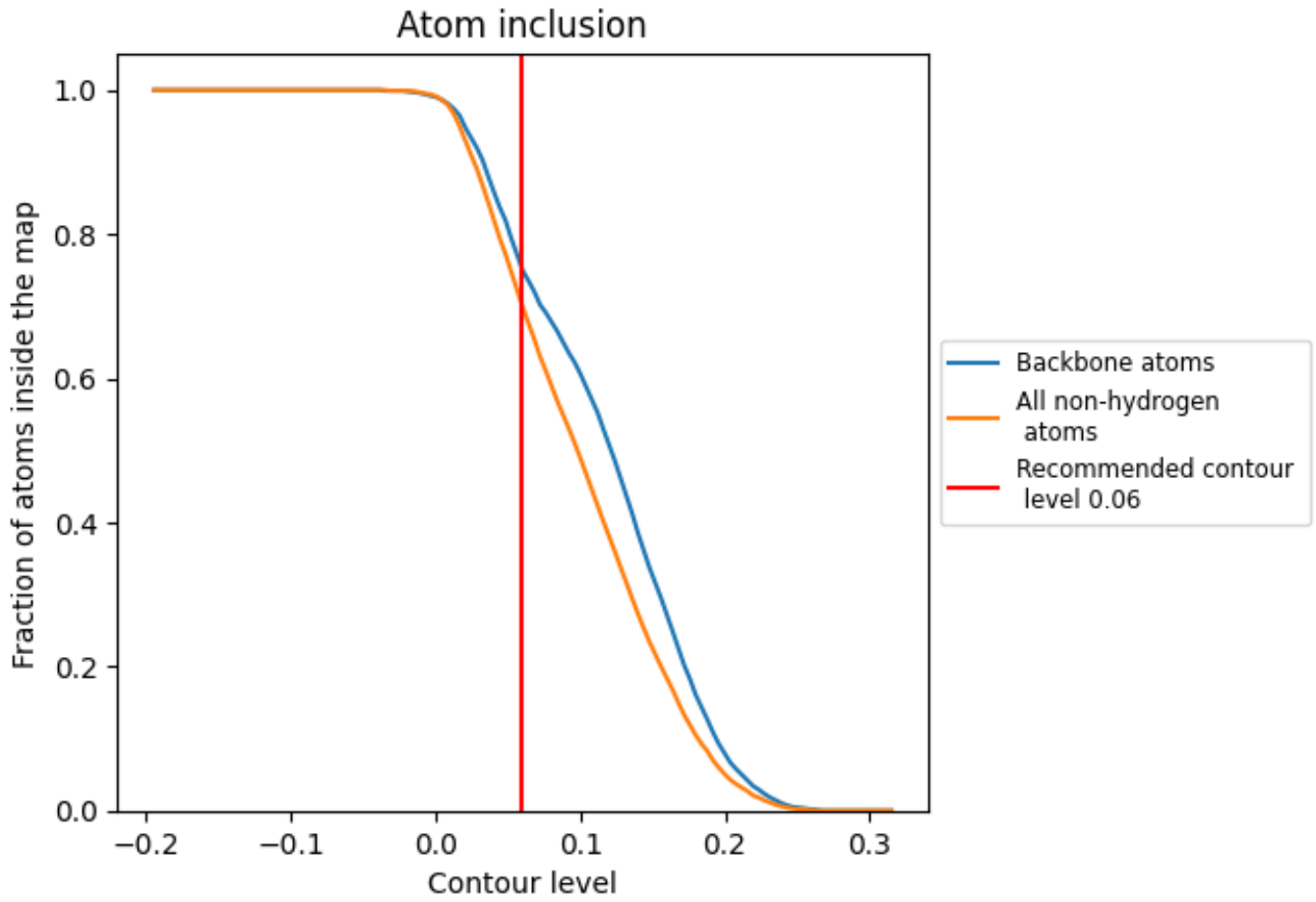
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (i)



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
All	0.7000
0	0.6470
1	0.7620
A	0.6440
B	0.7590
C	0.6470
D	0.7580
E	0.6460
F	0.7580
G	0.6510
H	0.7560
I	0.6430
J	0.7630
K	0.6430
L	0.7640
M	0.6460
N	0.7630
O	0.6460
P	0.7580
Q	0.6460
R	0.7620
S	0.6440
T	0.7600
U	0.6440
V	0.7600
W	0.6510
X	0.7600
Y	0.6460
Z	0.7510