



Full wwPDB EM Validation Report ⓘ

Nov 27, 2022 – 12:59 PM EST

PDB ID : 6V21
EMDB ID : EMD-21024
Title : Mouse heavy chain apoferritin determined using single-particle cryo-EM at 200 keV
Authors : Wu, M.; Lander, G.C.; Herzik, M.A.
Deposited on : 2019-11-21
Resolution : 1.75 Å(reported)
Based on initial model : 3WNW

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

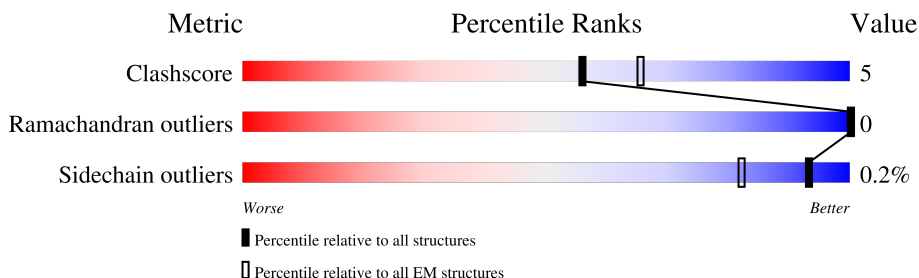
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 1.75 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.









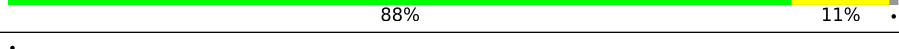
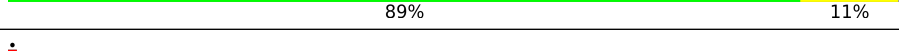
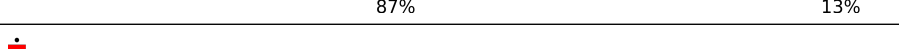
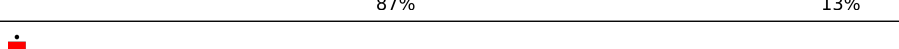
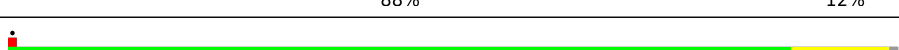

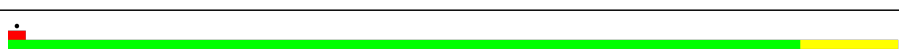

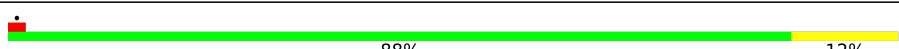





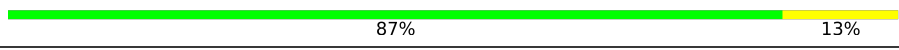
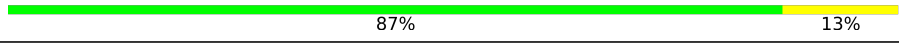



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1-A	174	
1	1-B	174	
1	1-C	174	
1	1-D	174	
1	1-E	174	
1	1-F	174	
1	1-G	174	
1	1-H	174	











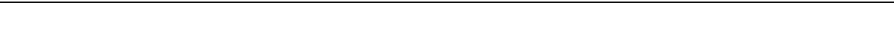

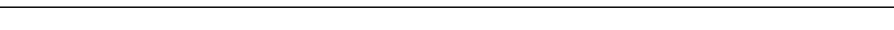
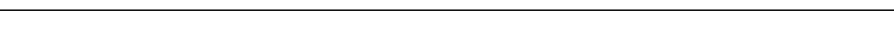











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Mol	Chain	Length	Quality of chain
1	1-I	174	 88% 11%
1	1-J	174	 88% 12%
1	1-K	174	 87% 12%
1	1-L	174	 88% 12%
1	1-M	174	 87% 13%
1	1-N	174	 88% 11%
1	1-O	174	 88% 11%
1	1-P	174	 89% 11%
1	1-Q	174	 87% 13%
1	1-R	174	 87% 13%
1	1-S	174	 88% 12%
1	1-T	174	 88% 11%
1	1-U	174	 89% 11%
1	1-V	174	 89% 11%
1	1-W	174	 86% 14%
1	1-X	174	 88% 12%
1	10-A	174	 86% 13%
1	10-B	174	 87% 13%
1	10-C	174	 86% 14%
1	10-D	174	 87% 13%
1	10-E	174	 85% 14%
1	10-F	174	 87% 13%
1	10-G	174	 87% 13%
1	10-H	174	 87% 13%
1	10-I	174	 85% 14%














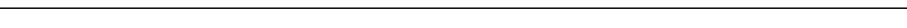











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Mol	Chain	Length	Quality of chain
1	10-J	174	 86% 14%
1	10-K	174	 85% 14% .
1	10-L	174	 87% 13%
1	10-M	174	 86% 13% .
1	10-N	174	 84% 15% .
1	10-O	174	 85% 14% .
1	10-P	174	 86% 14% .
1	10-Q	174	 83% 17% .
1	10-R	174	 86% 14%
1	10-S	174	 84% 16%
1	10-T	174	 84% 15% .
1	10-U	174	 83% 16% .
1	10-V	174	 86% 14%
1	10-W	174	 84% 15% .
1	10-X	174	 86% 14%
1	2-A	174	 87% 12% ..
1	2-B	174	 87% 12% ..
1	2-C	174	 85% 14% ..
1	2-D	174	 87% 11% ..
1	2-E	174	 86% 13% ..
1	2-F	174	 87% 13% .
1	2-G	174	 86% 14% .
1	2-H	174	 87% 12% ..
1	2-I	174	 86% 13% ..
1	2-J	174	 86% 13% .













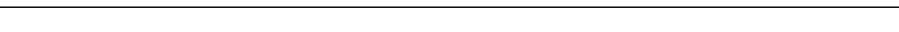

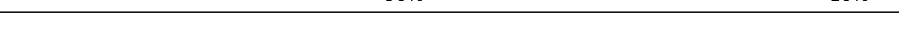

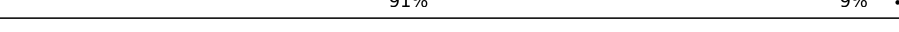








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Mol	Chain	Length	Quality of chain
1	2-K	174	 85% 14% ..
1	2-L	174	 87% 13% .
1	2-M	174	 87% 12% ..
1	2-N	174	 87% 12% ..
1	2-O	174	 85% 14% ..
1	2-P	174	 86% 13% ..
1	2-Q	174	 84% 15% ..
1	2-R	174	 85% 14% .
1	2-S	174	 87% 12% .
1	2-T	174	 87% 12% ..
1	2-U	174	 84% 15% ..
1	2-V	174	 86% 13% .
1	2-W	174	 84% 15% ..
1	2-X	174	 86% 13% .
1	3-A	174	 86% 14% .
1	3-B	174	 88% 11% .
1	3-C	174	 86% 13% .
1	3-D	174	 87% 12% .
1	3-E	174	 87% 12% .
1	3-F	174	 86% 14%
1	3-G	174	 87% 13%
1	3-H	174	 88% 11% .
1	3-I	174	 87% 12% .
1	3-J	174	 89% 11%
1	3-K	174	 87% 12% .


























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Mol	Chain	Length	Quality of chain
1	3-L	174	 87% 13%
1	3-M	174	 87% 13%
1	3-N	174	 86% 13%
1	3-O	174	 87% 13%
1	3-P	174	 88% 11%
1	3-Q	174	 87% 12%
1	3-R	174	 87% 13%
1	3-S	174	 86% 14%
1	3-T	174	 86% 13%
1	3-U	174	 86% 13%
1	3-V	174	 89% 11%
1	3-W	174	 87% 12%
1	3-X	174	 87% 13%
1	4-A	174	 90% 10%
1	4-B	174	 91% 8%
1	4-C	174	 91% 9%
1	4-D	174	 91% 9%
1	4-E	174	 91% 8%
1	4-F	174	 92% 8%
1	4-G	174	 91% 9%
1	4-H	174	 91% 8%
1	4-I	174	 91% 8%
1	4-J	174	 91% 9%
1	4-K	174	 90% 9%
1	4-L	174	 91% 9%












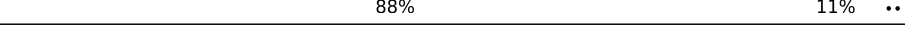







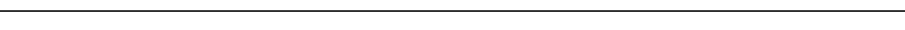

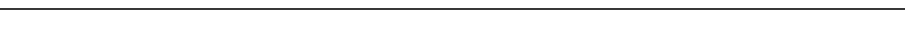
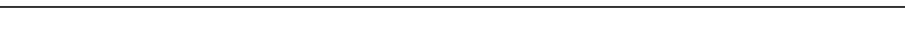


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Mol	Chain	Length	Quality of chain
1	4-M	174	 91% 8% .
1	4-N	174	 93% 7% .
1	4-O	174	 91% 9% .
1	4-P	174	 90% 9% .
1	4-Q	174	 90% 10% .
1	4-R	174	 91% 9%
1	4-S	174	 93% 7%
1	4-T	174	 92% 7% .
1	4-U	174	 91% 9% .
1	4-V	174	 92% 8%
1	4-W	174	 91% 9% .
1	4-X	174	 91% 9%
1	5-A	174	 91% 8% ..
1	5-B	174	 90% 9% ..
1	5-C	174	 91% 7% ..
1	5-D	174	 89% 10% ..
1	5-E	174	 91% 7% ..
1	5-F	174	 90% 10% .
1	5-G	174	 91% 9% .
1	5-H	174	 90% 9% ..
1	5-I	174	 91% 8% ..
1	5-J	174	 91% 9% .
1	5-K	174	 91% 7% ..
1	5-L	174	 90% 9% .
1	5-M	174	 91% 8% ..














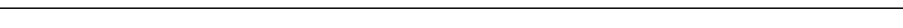











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Mol	Chain	Length	Quality of chain
1	5-N	174	 89% 10% ..
1	5-O	174	 92% 7% .
1	5-P	174	 90% 9% ..
1	5-Q	174	 89% 10% ..
1	5-R	174	 90% 9% .
1	5-S	174	 92% 7% .
1	5-T	174	 89% 10% ..
1	5-U	174	 91% 9% .
1	5-V	174	 91% 8% .
1	5-W	174	 89% 10% ..
1	5-X	174	 90% 9% .
1	6-A	174	 88% 11% ..
1	6-B	174	 88% 11% ..
1	6-C	174	 87% 12% ..
1	6-D	174	 88% 11% ..
1	6-E	174	 87% 12% ..
1	6-F	174	 89% 11% .
1	6-G	174	 89% 11% .
1	6-H	174	 88% 11% ..
1	6-I	174	 87% 12% ..
1	6-J	174	 89% 11% .
1	6-K	174	 87% 11% ..
1	6-L	174	 89% 11% .
1	6-M	174	 88% 11% ..
1	6-N	174	 87% 11% ..














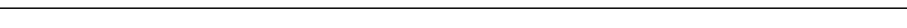











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Mol	Chain	Length	Quality of chain
1	6-O	174	 87% 11% ..
1	6-P	174	 88% 11% ..
1	6-Q	174	 87% 12% ..
1	6-R	174	 88% 11% .
1	6-S	174	 89% 11% .
1	6-T	174	 87% 11% ..
1	6-U	174	 88% 11% ..
1	6-V	174	 89% 11% .
1	6-W	174	 87% 12% ..
1	6-X	174	 89% 11% .
1	7-A	174	 89% 11% .
1	7-B	174	 89% 10% .
1	7-C	174	 88% 11% .
1	7-D	174	 89% 11% .
1	7-E	174	 87% 13% .
1	7-F	174	 90% 10%
1	7-G	174	 89% 11%
1	7-H	174	 89% 10% .
1	7-I	174	 88% 11% .
1	7-J	174	 89% 11%
1	7-K	174	 87% 13% .
1	7-L	174	 90% 10%
1	7-M	174	 87% 12% .
1	7-N	174	 89% 11% .
1	7-O	174	 87% 12% .











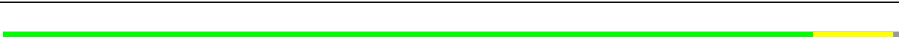


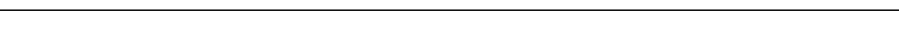
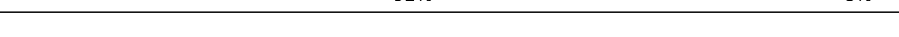
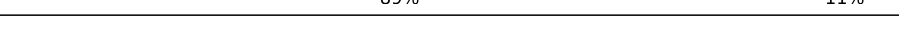


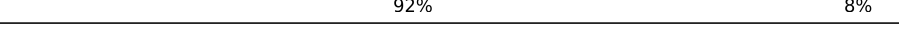
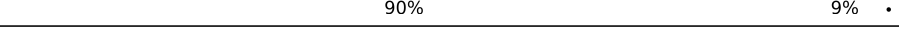





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Mol	Chain	Length	Quality of chain
1	7-P	174	 90% 10% .
1	7-Q	174	 86% 14% .
1	7-R	174	 89% 11%
1	7-S	174	 87% 13%
1	7-T	174	 89% 11% .
1	7-U	174	 87% 13% .
1	7-V	174	 91% 9%
1	7-W	174	 86% 13% .
1	7-X	174	 87% 13%
1	8-A	174	 87% 13% .
1	8-B	174	 86% 13% .
1	8-C	174	 88% 11% .
1	8-D	174	 88% 11% .
1	8-E	174	 88% 11% .
1	8-F	174	 87% 13%
1	8-G	174	 87% 13%
1	8-H	174	 86% 13% .
1	8-I	174	 88% 11% .
1	8-J	174	 89% 11%
1	8-K	174	 87% 12% .
1	8-L	174	 87% 13%
1	8-M	174	 89% 10% .
1	8-N	174	 87% 13% .
1	8-O	174	 87% 13% .
1	8-P	174	 90% 9% .



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Mol	Chain	Length	Quality of chain
1	8-Q	174	 86% 13%
1	8-R	174	 87% 13%
1	8-S	174	 90% 10%
1	8-T	174	 87% 13%
1	8-U	174	 89% 10%
1	8-V	174	 90% 10%
1	8-W	174	 86% 13%
1	8-X	174	 86% 14%
1	9-A	174	 91% 8%
1	9-B	174	 91% 8%
1	9-C	174	 91% 9%
1	9-D	174	 91% 8%
1	9-E	174	 90% 9%
1	9-F	174	 92% 8%
1	9-G	174	 89% 11%
1	9-H	174	 91% 8%
1	9-I	174	 91% 9%
1	9-J	174	 92% 8%
1	9-K	174	 90% 9%
1	9-L	174	 90% 10%
1	9-M	174	 91% 8%
1	9-N	174	 89% 10%
1	9-O	174	 90% 9%
1	9-P	174	 91% 8%
1	9-Q	174	 91% 8%

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Mol	Chain	Length	Quality of chain
1	9-R	174	 90%10%
1	9-S	174	 91%9%
1	9-T	174	 90%9%.
1	9-U	174	 90%9%.
1	9-V	174	 92%8%
1	9-W	174	 90%9%.
1	9-X	174	 91%9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 358232 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 Ferritin heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1-A	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	2-A	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	3-A	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	4-A	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	5-A	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	6-A	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	7-A	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	8-A	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	9-A	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	10-A	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	1-B	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	2-B	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	3-B	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	4-B	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	5-B	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	6-B	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	7-B	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	8-B	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	9-B	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	10-B	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	1-C	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	2-C	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	3-C	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	4-C	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	5-C	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	6-C	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	7-C	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	8-C	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	9-C	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	10-C	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	1-D	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	2-D	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	3-D	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	4-D	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	5-D	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	6-D	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	7-D	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	8-D	173	Total 1415	C 887	N 248	O 272	S 8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	9-D	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	10-D	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	1-E	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	2-E	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	3-E	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	4-E	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	5-E	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	6-E	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	7-E	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	8-E	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	9-E	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	10-E	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	1-F	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	2-F	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	3-F	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	4-F	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	5-F	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	6-F	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	7-F	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	8-F	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	9-F	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	10-F	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	1-G	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	2-G	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	3-G	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	4-G	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	5-G	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	6-G	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	7-G	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	8-G	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	9-G	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	10-G	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	1-H	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	2-H	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	3-H	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	4-H	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	5-H	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	6-H	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	7-H	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	8-H	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	9-H	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	10-H	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	1-I	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	2-I	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	3-I	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	4-I	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	5-I	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	6-I	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	7-I	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	8-I	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	9-I	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	10-I	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	1-J	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	2-J	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	3-J	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	4-J	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	5-J	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	6-J	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	7-J	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	8-J	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	9-J	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	10-J	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	1-K	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	2-K	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	3-K	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	4-K	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	5-K	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	6-K	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	7-K	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	8-K	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	9-K	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	10-K	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	1-L	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	2-L	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	3-L	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	4-L	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	5-L	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	6-L	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	7-L	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	8-L	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	9-L	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	10-L	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	1-M	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	2-M	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	3-M	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	4-M	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	5-M	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	6-M	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	7-M	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	8-M	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	9-M	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	10-M	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	1-N	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	2-N	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	3-N	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	4-N	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	5-N	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	6-N	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	7-N	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	8-N	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	9-N	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	10-N	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	1-O	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	2-O	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	3-O	173	Total 1415	C 887	N 248	O 272	S 8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	4-O	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	5-O	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	6-O	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	7-O	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	8-O	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	9-O	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	10-O	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	1-P	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	2-P	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	3-P	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	4-P	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	5-P	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	6-P	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	7-P	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	8-P	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	9-P	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	10-P	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	1-Q	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	2-Q	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	3-Q	173	Total 1415	C 887	N 248	O 272	S 8	0	0
1	4-Q	173	Total 1415	C 887	N 248	O 272	S 8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	5-Q	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	6-Q	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	7-Q	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	8-Q	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	9-Q	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	10-Q	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	1-R	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	2-R	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	3-R	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	4-R	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	5-R	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	6-R	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	7-R	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	8-R	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	9-R	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	10-R	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	1-S	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	2-S	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	3-S	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	4-S	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	5-S	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	6-S	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	7-S	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	8-S	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	9-S	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	10-S	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	1-T	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	2-T	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	3-T	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	4-T	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	5-T	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	6-T	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	7-T	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	8-T	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	9-T	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	10-T	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	1-U	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	2-U	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	3-U	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	4-U	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	5-U	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	6-U	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	7-U	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	8-U	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	9-U	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	10-U	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	1-V	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	2-V	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	3-V	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	4-V	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	5-V	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	6-V	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	7-V	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	8-V	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	9-V	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	10-V	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	1-W	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	2-W	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	3-W	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	4-W	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	5-W	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	6-W	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	7-W	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	8-W	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	9-W	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	10-W	173	Total	C	N	O	S	0	0
			1415	887	248	272	8		
1	1-X	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	2-X	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	3-X	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	4-X	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	5-X	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	6-X	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	7-X	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	8-X	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	9-X	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		
1	10-X	174	Total	C	N	O	S	0	0
			1425	893	251	273	8		

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		AltConf
2	1-A	75	Total	O	0
			75	75	
2	2-A	75	Total	O	0
			75	75	
2	3-A	75	Total	O	0
			75	75	
2	4-A	75	Total	O	0
			75	75	
2	5-A	75	Total	O	0
			75	75	
2	6-A	75	Total	O	0
			75	75	

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Mol	Chain	Residues	Atoms		AltConf
2	7-A	75	Total 75	O 75	0
2	8-A	75	Total 75	O 75	0
2	9-A	75	Total 75	O 75	0
2	10-A	75	Total 75	O 75	0
2	1-B	74	Total 74	O 74	0
2	2-B	74	Total 74	O 74	0
2	3-B	75	Total 75	O 75	0
2	4-B	74	Total 74	O 74	0
2	5-B	74	Total 74	O 74	0
2	6-B	74	Total 74	O 74	0
2	7-B	74	Total 74	O 74	0
2	8-B	74	Total 74	O 74	0
2	9-B	74	Total 74	O 74	0
2	10-B	75	Total 75	O 75	0
2	1-C	74	Total 74	O 74	0
2	2-C	74	Total 74	O 74	0
2	3-C	74	Total 74	O 74	0
2	4-C	74	Total 74	O 74	0
2	5-C	74	Total 74	O 74	0
2	6-C	74	Total 74	O 74	0
2	7-C	74	Total 74	O 74	0

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Mol	Chain	Residues	Atoms		AltConf
2	8-C	74	Total 74	O 74	0
2	9-C	74	Total 74	O 74	0
2	10-C	74	Total 74	O 74	0
2	1-D	74	Total 74	O 74	0
2	2-D	74	Total 74	O 74	0
2	3-D	74	Total 74	O 74	0
2	4-D	74	Total 74	O 74	0
2	5-D	74	Total 74	O 74	0
2	6-D	74	Total 74	O 74	0
2	7-D	74	Total 74	O 74	0
2	8-D	74	Total 74	O 74	0
2	9-D	74	Total 74	O 74	0
2	10-D	74	Total 74	O 74	0
2	1-E	75	Total 75	O 75	0
2	2-E	75	Total 75	O 75	0
2	3-E	75	Total 75	O 75	0
2	4-E	75	Total 75	O 75	0
2	5-E	75	Total 75	O 75	0
2	6-E	75	Total 75	O 75	0
2	7-E	75	Total 75	O 75	0
2	8-E	75	Total 75	O 75	0

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Mol	Chain	Residues	Atoms		AltConf
2	9-E	75	Total 75	O 75	0
2	10-E	75	Total 75	O 75	0
2	1-F	75	Total 75	O 75	0
2	2-F	75	Total 75	O 75	0
2	3-F	75	Total 75	O 75	0
2	4-F	75	Total 75	O 75	0
2	5-F	75	Total 75	O 75	0
2	6-F	75	Total 75	O 75	0
2	7-F	75	Total 75	O 75	0
2	8-F	75	Total 75	O 75	0
2	9-F	75	Total 75	O 75	0
2	10-F	75	Total 75	O 75	0
2	1-G	75	Total 75	O 75	0
2	2-G	75	Total 75	O 75	0
2	3-G	75	Total 75	O 75	0
2	4-G	75	Total 75	O 75	0
2	5-G	75	Total 75	O 75	0
2	6-G	75	Total 75	O 75	0
2	7-G	75	Total 75	O 75	0
2	8-G	75	Total 75	O 75	0
2	9-G	75	Total 75	O 75	0

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Mol	Chain	Residues	Atoms		AltConf
2	10-G	75	Total 75	O 75	0
2	1-H	75	Total 75	O 75	0
2	2-H	75	Total 75	O 75	0
2	3-H	75	Total 75	O 75	0
2	4-H	75	Total 75	O 75	0
2	5-H	75	Total 75	O 75	0
2	6-H	75	Total 75	O 75	0
2	7-H	75	Total 75	O 75	0
2	8-H	75	Total 75	O 75	0
2	9-H	75	Total 75	O 75	0
2	10-H	75	Total 75	O 75	0
2	1-I	74	Total 74	O 74	0
2	2-I	74	Total 74	O 74	0
2	3-I	74	Total 74	O 74	0
2	4-I	74	Total 74	O 74	0
2	5-I	74	Total 74	O 74	0
2	6-I	74	Total 74	O 74	0
2	7-I	74	Total 74	O 74	0
2	8-I	74	Total 74	O 74	0
2	9-I	74	Total 74	O 74	0
2	10-I	74	Total 74	O 74	0

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Mol	Chain	Residues	Atoms		AltConf
2	1-J	76	Total 76	O 76	0
2	2-J	76	Total 76	O 76	0
2	3-J	76	Total 76	O 76	0
2	4-J	76	Total 76	O 76	0
2	5-J	76	Total 76	O 76	0
2	6-J	76	Total 76	O 76	0
2	7-J	76	Total 76	O 76	0
2	8-J	76	Total 76	O 76	0
2	9-J	76	Total 76	O 76	0
2	10-J	76	Total 76	O 76	0
2	1-K	72	Total 72	O 72	0
2	2-K	72	Total 72	O 72	0
2	3-K	72	Total 72	O 72	0
2	4-K	72	Total 72	O 72	0
2	5-K	72	Total 72	O 72	0
2	6-K	72	Total 72	O 72	0
2	7-K	72	Total 72	O 72	0
2	8-K	72	Total 72	O 72	0
2	9-K	72	Total 72	O 72	0
2	10-K	72	Total 72	O 72	0
2	1-L	74	Total 74	O 74	0

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Mol	Chain	Residues	Atoms		AltConf
2	2-L	74	Total 74	O 74	0
2	3-L	74	Total 74	O 74	0
2	4-L	74	Total 74	O 74	0
2	5-L	74	Total 74	O 74	0
2	6-L	74	Total 74	O 74	0
2	7-L	74	Total 74	O 74	0
2	8-L	74	Total 74	O 74	0
2	9-L	74	Total 74	O 74	0
2	10-L	74	Total 74	O 74	0
2	1-M	73	Total 73	O 73	0
2	2-M	73	Total 73	O 73	0
2	3-M	73	Total 73	O 73	0
2	4-M	73	Total 73	O 73	0
2	5-M	73	Total 73	O 73	0
2	6-M	73	Total 73	O 73	0
2	7-M	73	Total 73	O 73	0
2	8-M	73	Total 73	O 73	0
2	9-M	73	Total 73	O 73	0
2	10-M	73	Total 73	O 73	0
2	1-N	75	Total 75	O 75	0
2	2-N	75	Total 75	O 75	0

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Mol	Chain	Residues	Atoms		AltConf
2	3-N	75	Total 75	O 75	0
2	4-N	75	Total 75	O 75	0
2	5-N	75	Total 75	O 75	0
2	6-N	75	Total 75	O 75	0
2	7-N	75	Total 75	O 75	0
2	8-N	75	Total 75	O 75	0
2	9-N	75	Total 75	O 75	0
2	10-N	75	Total 75	O 75	0
2	1-O	75	Total 75	O 75	0
2	2-O	75	Total 75	O 75	0
2	3-O	75	Total 75	O 75	0
2	4-O	75	Total 75	O 75	0
2	5-O	75	Total 75	O 75	0
2	6-O	75	Total 75	O 75	0
2	7-O	75	Total 75	O 75	0
2	8-O	75	Total 75	O 75	0
2	9-O	75	Total 75	O 75	0
2	10-O	75	Total 75	O 75	0
2	1-P	74	Total 74	O 74	0
2	2-P	74	Total 74	O 74	0
2	3-P	74	Total 74	O 74	0

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Mol	Chain	Residues	Atoms		AltConf
2	4-P	74	Total 74	O 74	0
2	5-P	74	Total 74	O 74	0
2	6-P	74	Total 74	O 74	0
2	7-P	74	Total 74	O 74	0
2	8-P	74	Total 74	O 74	0
2	9-P	74	Total 74	O 74	0
2	10-P	74	Total 74	O 74	0
2	1-Q	74	Total 74	O 74	0
2	2-Q	74	Total 74	O 74	0
2	3-Q	74	Total 74	O 74	0
2	4-Q	74	Total 74	O 74	0
2	5-Q	74	Total 74	O 74	0
2	6-Q	74	Total 74	O 74	0
2	7-Q	74	Total 74	O 74	0
2	8-Q	74	Total 74	O 74	0
2	9-Q	74	Total 74	O 74	0
2	10-Q	74	Total 74	O 74	0
2	1-R	74	Total 74	O 74	0
2	2-R	74	Total 74	O 74	0
2	3-R	74	Total 74	O 74	0
2	4-R	74	Total 74	O 74	0

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Mol	Chain	Residues	Atoms		AltConf
2	5-R	74	Total 74	O 74	0
2	6-R	74	Total 74	O 74	0
2	7-R	74	Total 74	O 74	0
2	8-R	74	Total 74	O 74	0
2	9-R	74	Total 74	O 74	0
2	10-R	74	Total 74	O 74	0
2	1-S	75	Total 75	O 75	0
2	2-S	75	Total 75	O 75	0
2	3-S	75	Total 75	O 75	0
2	4-S	75	Total 75	O 75	0
2	5-S	75	Total 75	O 75	0
2	6-S	75	Total 75	O 75	0
2	7-S	75	Total 75	O 75	0
2	8-S	75	Total 75	O 75	0
2	9-S	75	Total 75	O 75	0
2	10-S	75	Total 75	O 75	0
2	1-T	75	Total 75	O 75	0
2	2-T	75	Total 75	O 75	0
2	3-T	75	Total 75	O 75	0
2	4-T	75	Total 75	O 75	0
2	5-T	75	Total 75	O 75	0

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Mol	Chain	Residues	Atoms		AltConf
2	6-T	75	Total 75	O 75	0
2	7-T	75	Total 75	O 75	0
2	8-T	75	Total 75	O 75	0
2	9-T	75	Total 75	O 75	0
2	10-T	75	Total 75	O 75	0
2	1-U	74	Total 74	O 74	0
2	2-U	74	Total 74	O 74	0
2	3-U	74	Total 74	O 74	0
2	4-U	74	Total 74	O 74	0
2	5-U	74	Total 74	O 74	0
2	6-U	74	Total 74	O 74	0
2	7-U	74	Total 74	O 74	0
2	8-U	74	Total 74	O 74	0
2	9-U	74	Total 74	O 74	0
2	10-U	74	Total 74	O 74	0
2	1-V	75	Total 75	O 75	0
2	2-V	75	Total 75	O 75	0
2	3-V	75	Total 75	O 75	0
2	4-V	75	Total 75	O 75	0
2	5-V	75	Total 75	O 75	0
2	6-V	75	Total 75	O 75	0

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Mol	Chain	Residues	Atoms		AltConf
2	7-V	75	Total 75	O 75	0
2	8-V	75	Total 75	O 75	0
2	9-V	75	Total 75	O 75	0
2	10-V	75	Total 75	O 75	0
2	1-W	73	Total 73	O 73	0
2	2-W	73	Total 73	O 73	0
2	3-W	73	Total 73	O 73	0
2	4-W	73	Total 73	O 73	0
2	5-W	73	Total 73	O 73	0
2	6-W	73	Total 73	O 73	0
2	7-W	73	Total 73	O 73	0
2	8-W	73	Total 73	O 73	0
2	9-W	73	Total 73	O 73	0
2	10-W	73	Total 73	O 73	0
2	1-X	73	Total 73	O 73	0
2	2-X	73	Total 73	O 73	0
2	3-X	73	Total 73	O 73	0
2	4-X	73	Total 73	O 73	0
2	5-X	73	Total 73	O 73	0
2	6-X	73	Total 73	O 73	0
2	7-X	73	Total 73	O 73	0

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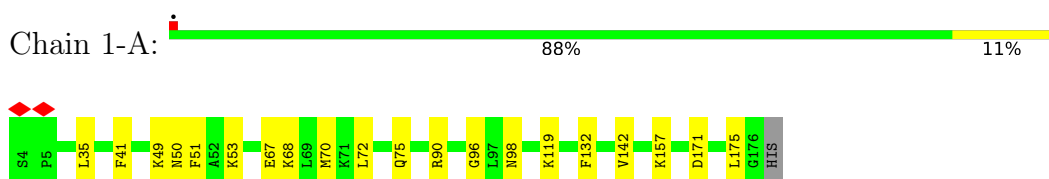
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Mol	Chain	Residues	Atoms		AltConf
2	8-X	73	Total 73	O 73	0
2	9-X	73	Total 73	O 73	0
2	10-X	73	Total 73	O 73	0

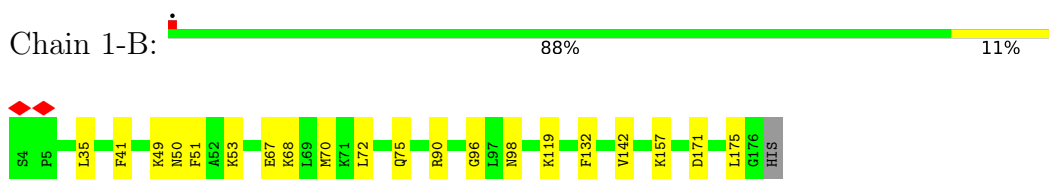
3 Residue-property plots [i](#)

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

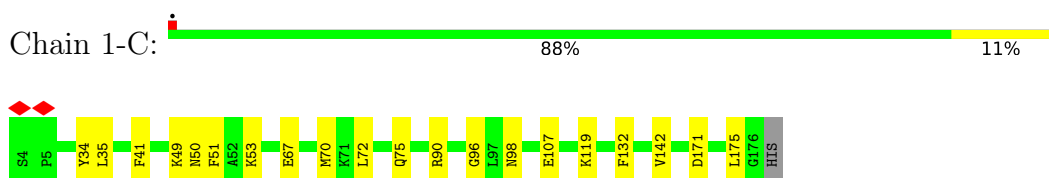
- Molecule 1: Ferritin heavy chain



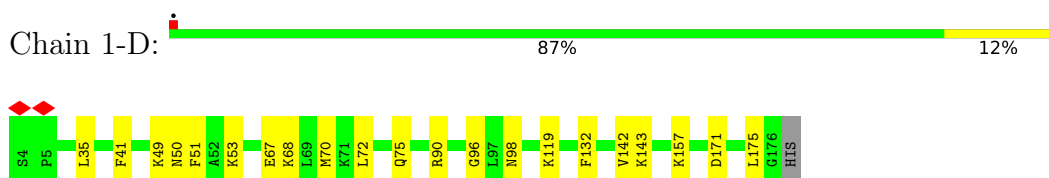
- Molecule 1: Ferritin heavy chain



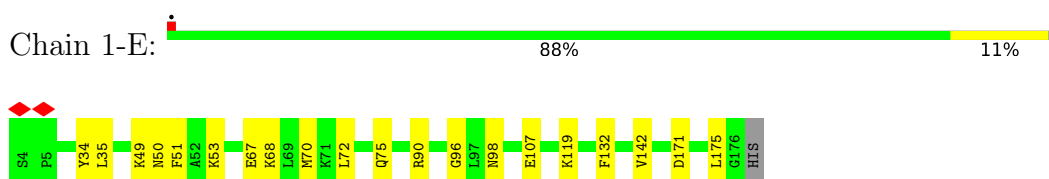
- Molecule 1: Ferritin heavy chain




- Molecule 1: Ferritin heavy chain



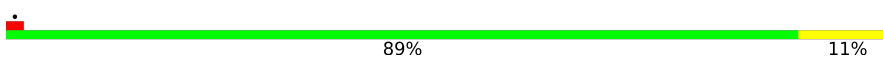
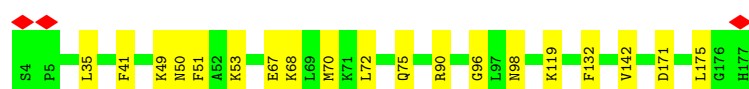
- Molecule 1: Ferritin heavy chain




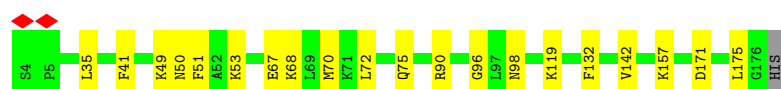
● Molecule 1: Ferritin heavy chain

Chain 1-F:  89% 11%


● Molecule 1: Ferritin heavy chain

Chain 1-G:  89% 11%


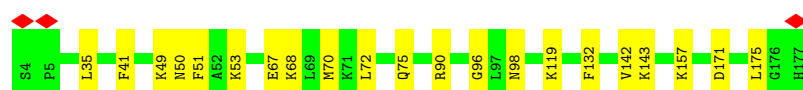
● Molecule 1: Ferritin heavy chain

Chain 1-H:  88% 11%


● Molecule 1: Ferritin heavy chain

Chain 1-I:  88% 11%


● Molecule 1: Ferritin heavy chain

Chain 1-J:  88% 12%

● Molecule 1: Ferritin heavy chain

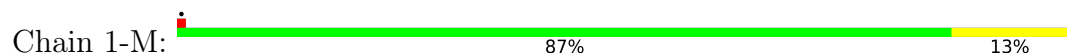
Chain 1-K:  87% 12%

● Molecule 1: Ferritin heavy chain

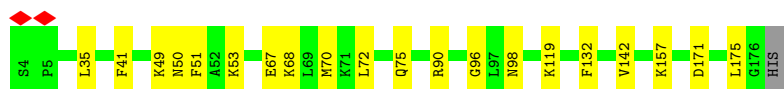
Chain 1-L:  88% 12%



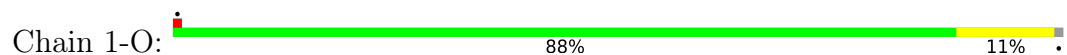
- Molecule 1: Ferritin heavy chain



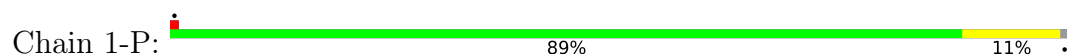
- Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain



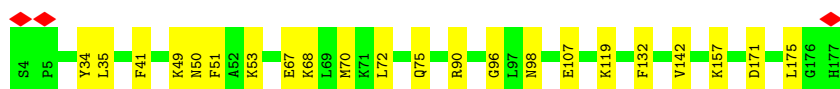
- Molecule 1: Ferritin heavy chain



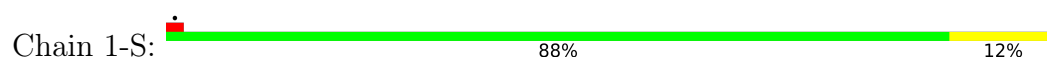
- Molecule 1: Ferritin heavy chain



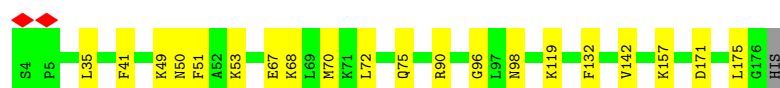
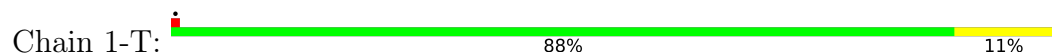
- Molecule 1: Ferritin heavy chain



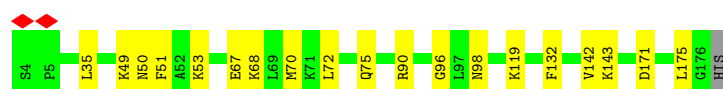
- Molecule 1: Ferritin heavy chain



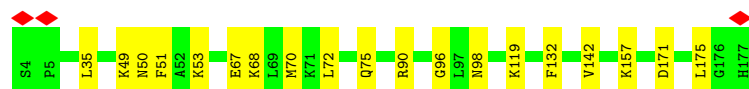
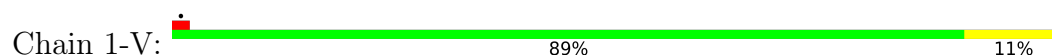
- Molecule 1: Ferritin heavy chain



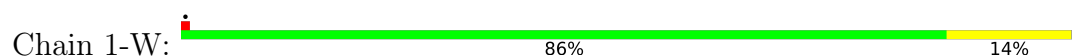
- Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain

Chain 2-B:  87% 12% ..




- Molecule 1: Ferritin heavy chain

Chain 2-C:  85% 14% ..



- Molecule 1: Ferritin heavy chain

Chain 2-D:  87% 11% ..




- Molecule 1: Ferritin heavy chain

Chain 2-E:  86% 13% ..




- Molecule 1: Ferritin heavy chain

Chain 2-F:  87% 13% .



- Molecule 1: Ferritin heavy chain

Chain 2-G:  86% 14% .




- Molecule 1: Ferritin heavy chain

Chain 2-H:  87% 12% ..



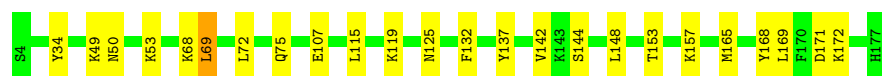
- Molecule 1: Ferritin heavy chain

Chain 2-I:  86% 13% ..




• Molecule 1: Ferritin heavy chain

Chain 2-J:  86% 13% .




• Molecule 1: Ferritin heavy chain

Chain 2-K:  85% 14% ..




• Molecule 1: Ferritin heavy chain

Chain 2-L:  87% 13% .




• Molecule 1: Ferritin heavy chain

Chain 2-M:  87% 12% ..




• Molecule 1: Ferritin heavy chain

Chain 2-N:  87% 12% ..




• Molecule 1: Ferritin heavy chain

Chain 2-O:  85% 14% ..




• Molecule 1: Ferritin heavy chain

Chain 2-P:  86% 13% ..




• Molecule 1: Ferritin heavy chain

Chain 2-Q:  84% 15% ..




• Molecule 1: Ferritin heavy chain

Chain 2-R:  85% 14% .




• Molecule 1: Ferritin heavy chain

Chain 2-S:  87% 12% .




• Molecule 1: Ferritin heavy chain

Chain 2-T:  87% 12% ..




• Molecule 1: Ferritin heavy chain

Chain 2-U:  84% 15% ..




• Molecule 1: Ferritin heavy chain

Chain 2-V:  86% 13% .




• Molecule 1: Ferritin heavy chain

Chain 2-W:  84% 15% ..




- Molecule 1: Ferritin heavy chain

Chain 2-X:  86% 13% .



- Molecule 1: Ferritin heavy chain

Chain 3-A:  86% 14% .




- Molecule 1: Ferritin heavy chain

Chain 3-B:  88% 11% .




- Molecule 1: Ferritin heavy chain

Chain 3-C:  86% 13% .




- Molecule 1: Ferritin heavy chain

Chain 3-D:  87% 12% .




- Molecule 1: Ferritin heavy chain

Chain 3-E:  87% 12% .



- Molecule 1: Ferritin heavy chain

Chain 3-F:  86% 14%



- Molecule 1: Ferritin heavy chain

Chain 3-G:  87% 13%




- Molecule 1: Ferritin heavy chain

Chain 3-H:  88% 11%




- Molecule 1: Ferritin heavy chain

Chain 3-I:  87% 12%



- Molecule 1: Ferritin heavy chain

Chain 3-J:  89% 11%




- Molecule 1: Ferritin heavy chain

Chain 3-K:  87% 12%




- Molecule 1: Ferritin heavy chain

Chain 3-L:  87% 13%




- Molecule 1: Ferritin heavy chain

Chain 3-M:  87% 13%




- Molecule 1: Ferritin heavy chain

Chain 3-N:  86% 13%




- Molecule 1: Ferritin heavy chain

Chain 3-O:  87% 13%




- Molecule 1: Ferritin heavy chain

Chain 3-P:  88% 11%




- Molecule 1: Ferritin heavy chain

Chain 3-Q:  87% 12%




- Molecule 1: Ferritin heavy chain

Chain 3-R:  87% 13%




- Molecule 1: Ferritin heavy chain

Chain 3-S:  86% 14%




- Molecule 1: Ferritin heavy chain

Chain 3-T:  86% 13%



- Molecule 1: Ferritin heavy chain

Chain 3-U:  86% 13%



- Molecule 1: Ferritin heavy chain

Chain 3-V:  89% 11%



- Molecule 1: Ferritin heavy chain

Chain 3-W:  87% 12%



- Molecule 1: Ferritin heavy chain

Chain 3-X:  87% 13%



- Molecule 1: Ferritin heavy chain

Chain 4-A:  90% 10%



- Molecule 1: Ferritin heavy chain

Chain 4-B:  91% 8%



- Molecule 1: Ferritin heavy chain

Chain 4-C:  91% 9% .



- Molecule 1: Ferritin heavy chain

Chain 4-D:  91% 9% .



- Molecule 1: Ferritin heavy chain

Chain 4-E:  91% 8% .



- Molecule 1: Ferritin heavy chain

Chain 4-F:  92% 8% .



- Molecule 1: Ferritin heavy chain

Chain 4-G:  91% 9% .




- Molecule 1: Ferritin heavy chain

Chain 4-H:  91% 8% .




- Molecule 1: Ferritin heavy chain

Chain 4-I:  91% 8% .



- Molecule 1: Ferritin heavy chain

Chain 4-J:  91% 9%



- Molecule 1: Ferritin heavy chain

Chain 4-K:  90% 9%



- Molecule 1: Ferritin heavy chain

Chain 4-L:  91% 9%



- Molecule 1: Ferritin heavy chain

Chain 4-M:  91% 8%



- Molecule 1: Ferritin heavy chain

Chain 4-N:  93% 7%



- Molecule 1: Ferritin heavy chain

Chain 4-O:  91% 9%



- Molecule 1: Ferritin heavy chain

Chain 4-P:  90% 9%



- Molecule 1: Ferritin heavy chain

Chain 4-Q:  90% 10%



- Molecule 1: Ferritin heavy chain

Chain 4-R:  91% 9%



- Molecule 1: Ferritin heavy chain

Chain 4-S:  93% 7%



- Molecule 1: Ferritin heavy chain

Chain 4-T:  92% 7%



- Molecule 1: Ferritin heavy chain

Chain 4-U:  91% 9%



- Molecule 1: Ferritin heavy chain

Chain 4-V:  92% 8%



- Molecule 1: Ferritin heavy chain

Chain 4-W:  91% 9%



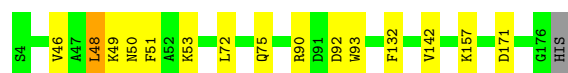
- Molecule 1: Ferritin heavy chain

Chain 4-X:  91% 9%



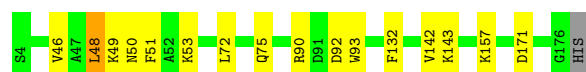
- Molecule 1: Ferritin heavy chain

Chain 5-A:  91% 8% ..



- Molecule 1: Ferritin heavy chain

Chain 5-B:  90% 9% ..



- Molecule 1: Ferritin heavy chain

Chain 5-C:  91% 7% ..



- Molecule 1: Ferritin heavy chain

Chain 5-D:  89% 10% ..



- Molecule 1: Ferritin heavy chain

Chain 5-E:  91% 7% ..



- Molecule 1: Ferritin heavy chain

Chain 5-F:  90% 10% ..



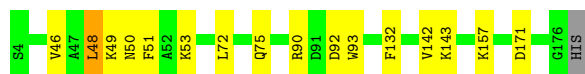
- Molecule 1: Ferritin heavy chain

Chain 5-G:  91% 9% .




• Molecule 1: Ferritin heavy chain

Chain 5-H:  90% 9% ..



• Molecule 1: Ferritin heavy chain

Chain 5-I:  91% 8% ..



• Molecule 1: Ferritin heavy chain

Chain 5-J:  91% 9% .



• Molecule 1: Ferritin heavy chain

Chain 5-K:  91% 7% ..



• Molecule 1: Ferritin heavy chain

Chain 5-L:  90% 9% .




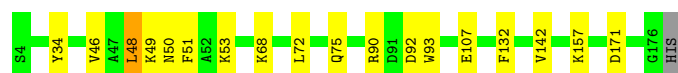
• Molecule 1: Ferritin heavy chain

Chain 5-M:  91% 8% ..



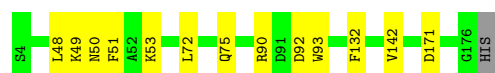
• Molecule 1: Ferritin heavy chain

Chain 5-N:  89% 10% ..



- Molecule 1: Ferritin heavy chain

Chain 5-O:  92% 7% .




- Molecule 1: Ferritin heavy chain

Chain 5-P:  90% 9% ..



- Molecule 1: Ferritin heavy chain

Chain 5-Q:  89% 10% ..



- Molecule 1: Ferritin heavy chain

Chain 5-R:  90% 9% .



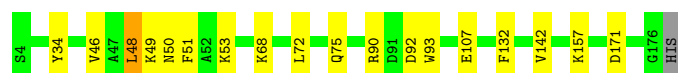
- Molecule 1: Ferritin heavy chain

Chain 5-S:  92% 7% .



- Molecule 1: Ferritin heavy chain

Chain 5-T:  89% 10% ..



- Molecule 1: Ferritin heavy chain

Chain 5-U:  91% 9% .



• Molecule 1: Ferritin heavy chain

Chain 5-V:  91% 8% .



• Molecule 1: Ferritin heavy chain

Chain 5-W:  89% 10% ..



• Molecule 1: Ferritin heavy chain

Chain 5-X:  90% 9% .




• Molecule 1: Ferritin heavy chain

Chain 6-A:  88% 11% ..




• Molecule 1: Ferritin heavy chain

Chain 6-B:  88% 11% ..




• Molecule 1: Ferritin heavy chain

Chain 6-C:  87% 12% ..




• Molecule 1: Ferritin heavy chain

Chain 6-D:  88% 11% ..




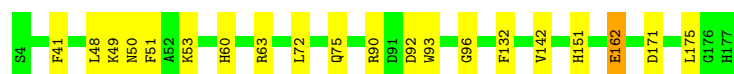
- Molecule 1: Ferritin heavy chain

Chain 6-E:  87% 12% ..




- Molecule 1: Ferritin heavy chain

Chain 6-F:  89% 11% .




- Molecule 1: Ferritin heavy chain

Chain 6-G:  89% 11% .




- Molecule 1: Ferritin heavy chain

Chain 6-H:  88% 11% ..




- Molecule 1: Ferritin heavy chain

Chain 6-I:  87% 12% ..




- Molecule 1: Ferritin heavy chain

Chain 6-J:  89% 11% .




- Molecule 1: Ferritin heavy chain

Chain 6-K:  87% 11% ..




- Molecule 1: Ferritin heavy chain

Chain 6-L:  89% 11% .



- Molecule 1: Ferritin heavy chain

Chain 6-M:  88% 11% ..




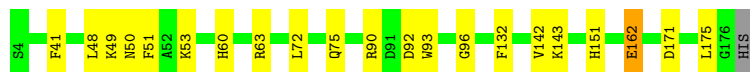
- Molecule 1: Ferritin heavy chain

Chain 6-N:  87% 11% ..




- Molecule 1: Ferritin heavy chain

Chain 6-O:  87% 11% ..




- Molecule 1: Ferritin heavy chain

Chain 6-P:  88% 11% ..




- Molecule 1: Ferritin heavy chain

Chain 6-Q:  87% 12% ..



- Molecule 1: Ferritin heavy chain

Chain 6-R:  88% 11% .




- Molecule 1: Ferritin heavy chain

Chain 6-S:  89% 11% .



- Molecule 1: Ferritin heavy chain

Chain 6-T:  87% 11% ..



- Molecule 1: Ferritin heavy chain

Chain 6-U:  88% 11% ..



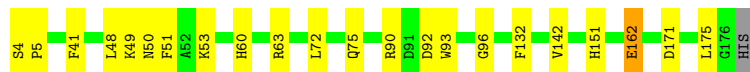
- Molecule 1: Ferritin heavy chain

Chain 6-V:  89% 11% .



- Molecule 1: Ferritin heavy chain

Chain 6-W:  87% 12% ..




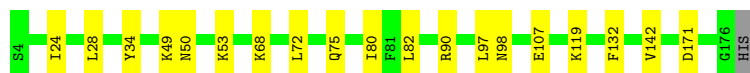
- Molecule 1: Ferritin heavy chain

Chain 6-X:  89% 11% .




- Molecule 1: Ferritin heavy chain

Chain 7-A:  89% 11%




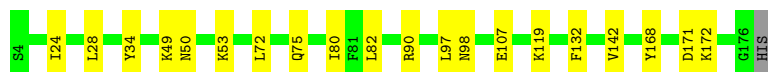
• Molecule 1: Ferritin heavy chain

Chain 7-B:  89% 10%



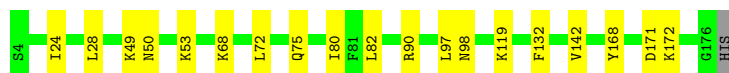
• Molecule 1: Ferritin heavy chain

Chain 7-C:  88% 11%




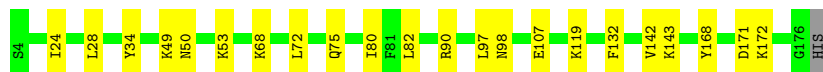
• Molecule 1: Ferritin heavy chain

Chain 7-D:  89% 11%



• Molecule 1: Ferritin heavy chain

Chain 7-E:  87% 13%



• Molecule 1: Ferritin heavy chain

Chain 7-F:  90% 10%



• Molecule 1: Ferritin heavy chain

Chain 7-G:  89% 11%




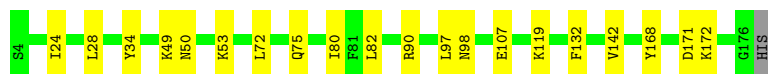
• Molecule 1: Ferritin heavy chain

Chain 7-H:  89% 10%



- Molecule 1: Ferritin heavy chain

Chain 7-I:  88% 11%




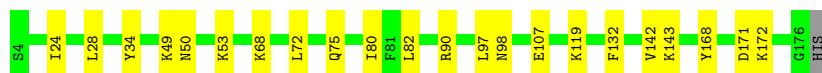
- Molecule 1: Ferritin heavy chain

Chain 7-J:  89% 11%



- Molecule 1: Ferritin heavy chain

Chain 7-K:  87% 13%




- Molecule 1: Ferritin heavy chain

Chain 7-L:  90% 10%



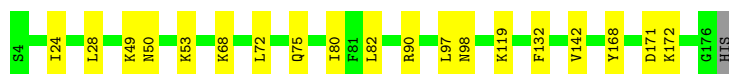
- Molecule 1: Ferritin heavy chain

Chain 7-M:  87% 12%




- Molecule 1: Ferritin heavy chain

Chain 7-N:  89% 11%



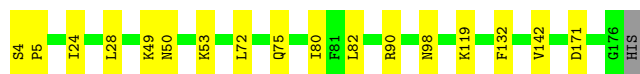
- Molecule 1: Ferritin heavy chain

Chain 7-O:  87% 12% .




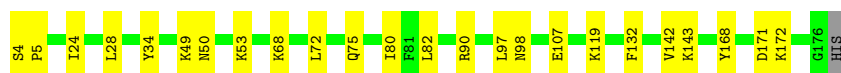
- Molecule 1: Ferritin heavy chain

Chain 7-P:  90% 10% .



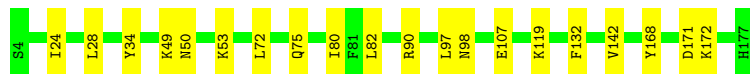
- Molecule 1: Ferritin heavy chain

Chain 7-Q:  86% 14% .




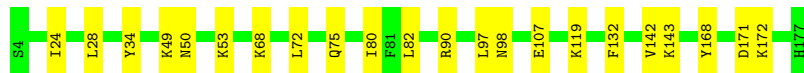
- Molecule 1: Ferritin heavy chain

Chain 7-R:  89% 11% .



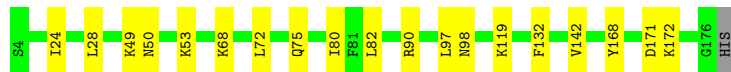
- Molecule 1: Ferritin heavy chain

Chain 7-S:  87% 13% .



- Molecule 1: Ferritin heavy chain

Chain 7-T:  89% 11% .



- Molecule 1: Ferritin heavy chain

Chain 7-U:  87% 13% .



- Molecule 1: Ferritin heavy chain

Chain 7-V:  91% 9%




- Molecule 1: Ferritin heavy chain

Chain 7-W:  86% 13%



- Molecule 1: Ferritin heavy chain

Chain 7-X:  87% 13%




- Molecule 1: Ferritin heavy chain

Chain 8-A:  87% 13%




- Molecule 1: Ferritin heavy chain

Chain 8-B:  86% 13%



- Molecule 1: Ferritin heavy chain

Chain 8-C:  88% 11%




- Molecule 1: Ferritin heavy chain

Chain 8-D:  88% 11%




- Molecule 1: Ferritin heavy chain

Chain 8-E:  88% 11%



- Molecule 1: Ferritin heavy chain

Chain 8-F:  87% 13%




- Molecule 1: Ferritin heavy chain

Chain 8-G:  87% 13%



- Molecule 1: Ferritin heavy chain

Chain 8-H:  86% 13%



- Molecule 1: Ferritin heavy chain

Chain 8-I:  88% 11%



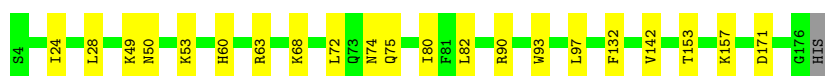
- Molecule 1: Ferritin heavy chain

Chain 8-J:  89% 11%




- Molecule 1: Ferritin heavy chain

Chain 8-K:  87% 12%



- Molecule 1: Ferritin heavy chain

Chain 8-L:  87% 13%



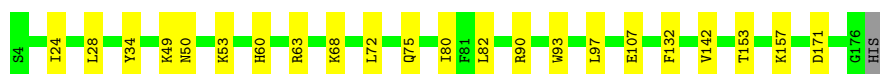
- Molecule 1: Ferritin heavy chain

Chain 8-M:  89% 10%




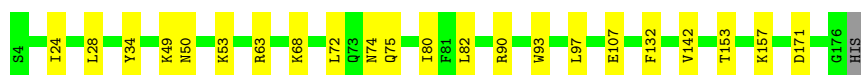
- Molecule 1: Ferritin heavy chain

Chain 8-N:  87% 13%



- Molecule 1: Ferritin heavy chain

Chain 8-O:  87% 13%




- Molecule 1: Ferritin heavy chain

Chain 8-P:  90% 9%



- Molecule 1: Ferritin heavy chain

Chain 8-Q:  86% 13%




- Molecule 1: Ferritin heavy chain

Chain 8-R:  87% 13%




- Molecule 1: Ferritin heavy chain

Chain 8-S:  90% 10%



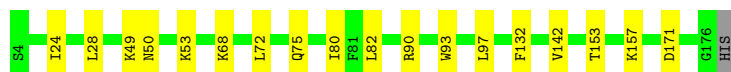
- Molecule 1: Ferritin heavy chain

Chain 8-T:  87% 13%



- Molecule 1: Ferritin heavy chain

Chain 8-U:  89% 10%




- Molecule 1: Ferritin heavy chain

Chain 8-V:  90% 10%



- Molecule 1: Ferritin heavy chain

Chain 8-W:  86% 13%



- Molecule 1: Ferritin heavy chain

Chain 8-X:  86% 14%



- Molecule 1: Ferritin heavy chain

Chain 9-A:  91% 8%



- Molecule 1: Ferritin heavy chain

Chain 9-B:  91% 8%



● Molecule 1: Ferritin heavy chain

Chain 9-C:  91% 9%



● Molecule 1: Ferritin heavy chain

Chain 9-D:  91% 8%



● Molecule 1: Ferritin heavy chain

Chain 9-E:  90% 9%



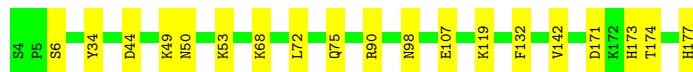
● Molecule 1: Ferritin heavy chain

Chain 9-F:  92% 8%



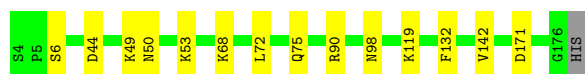
● Molecule 1: Ferritin heavy chain

Chain 9-G:  89% 11%



● Molecule 1: Ferritin heavy chain

Chain 9-H:  91% 8%



● Molecule 1: Ferritin heavy chain

Chain 9-I:  91% 9%



- Molecule 1: Ferritin heavy chain

Chain 9-J:  92% 8%



- Molecule 1: Ferritin heavy chain

Chain 9-K:  90% 9%



- Molecule 1: Ferritin heavy chain

Chain 9-L:  90% 10%



- Molecule 1: Ferritin heavy chain

Chain 9-M:  91% 8%



- Molecule 1: Ferritin heavy chain

Chain 9-N:  89% 10%



- Molecule 1: Ferritin heavy chain

Chain 9-O:  90% 9%



- Molecule 1: Ferritin heavy chain

Chain 9-P:  91% 8%



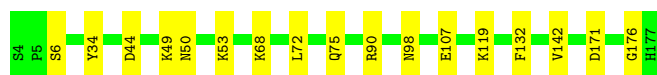
• Molecule 1: Ferritin heavy chain

Chain 9-Q:  91% 8%



• Molecule 1: Ferritin heavy chain

Chain 9-R:  90% 10%



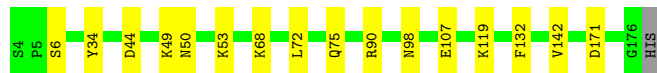
• Molecule 1: Ferritin heavy chain

Chain 9-S:  91% 9%



• Molecule 1: Ferritin heavy chain

Chain 9-T:  90% 9%



• Molecule 1: Ferritin heavy chain

Chain 9-U:  90% 9%



• Molecule 1: Ferritin heavy chain

Chain 9-V:  92% 8%



• Molecule 1: Ferritin heavy chain

Chain 9-W:  90% 9%



- Molecule 1: Ferritin heavy chain

Chain 9-X:  91% 9%




- Molecule 1: Ferritin heavy chain

Chain 10-A:  86% 13%



- Molecule 1: Ferritin heavy chain

Chain 10-B:  87% 13%



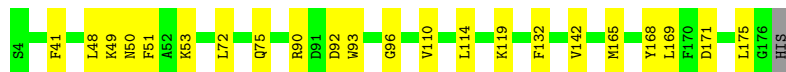
- Molecule 1: Ferritin heavy chain

Chain 10-C:  86% 14%



- Molecule 1: Ferritin heavy chain

Chain 10-D:  87% 13%



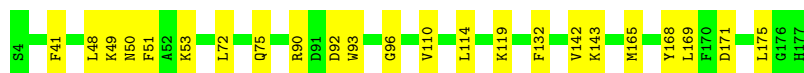
- Molecule 1: Ferritin heavy chain

Chain 10-E:  85% 14%



- Molecule 1: Ferritin heavy chain

Chain 10-F:  87% 13%



- Molecule 1: Ferritin heavy chain

Chain 10-G:  87% 13%




- Molecule 1: Ferritin heavy chain

Chain 10-H:  87% 13%




- Molecule 1: Ferritin heavy chain

Chain 10-I:  85% 14%




- Molecule 1: Ferritin heavy chain

Chain 10-J:  86% 14%



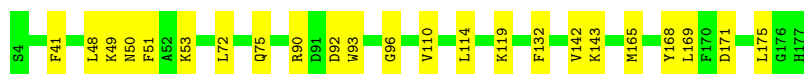
- Molecule 1: Ferritin heavy chain

Chain 10-K:  85% 14%




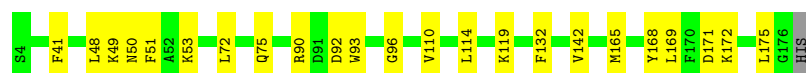
- Molecule 1: Ferritin heavy chain

Chain 10-L:  87% 13%




- Molecule 1: Ferritin heavy chain

Chain 10-M:  86% 13%




• Molecule 1: Ferritin heavy chain

Chain 10-N:  84% 15%




• Molecule 1: Ferritin heavy chain

Chain 10-O:  85% 14%




• Molecule 1: Ferritin heavy chain

Chain 10-P:  86% 14%



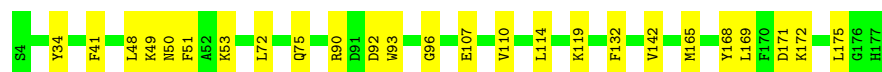
• Molecule 1: Ferritin heavy chain

Chain 10-Q:  83% 17%




• Molecule 1: Ferritin heavy chain

Chain 10-R:  86% 14%




• Molecule 1: Ferritin heavy chain

Chain 10-S:  84% 16%




• Molecule 1: Ferritin heavy chain

Chain 10-T:  84% 15%




- Molecule 1: Ferritin heavy chain

Chain 10-U:  83% 16%




- Molecule 1: Ferritin heavy chain

Chain 10-V:  86% 14%




- Molecule 1: Ferritin heavy chain

Chain 10-W:  84% 15%



- Molecule 1: Ferritin heavy chain

Chain 10-X:  86% 14%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, O	Depositor
Number of particles used	241878	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	73000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.251	Depositor
Minimum map value	-0.140	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.039	Depositor
Map size (Å)	215.80798, 215.80798, 215.80798	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.562, 0.562, 0.562	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-A	0.37	0/1444	0.56	0/1943
1	1-B	0.37	0/1444	0.55	0/1943
1	1-C	0.37	0/1444	0.56	0/1943
1	1-D	0.37	0/1444	0.56	0/1943
1	1-E	0.37	0/1444	0.56	0/1943
1	1-F	0.37	0/1455	0.55	0/1958
1	1-G	0.37	0/1455	0.56	0/1958
1	1-H	0.37	0/1444	0.55	0/1943
1	1-I	0.37	0/1444	0.56	0/1943
1	1-J	0.37	0/1455	0.56	0/1958
1	1-K	0.37	0/1444	0.56	0/1943
1	1-L	0.37	0/1455	0.56	0/1958
1	1-M	0.37	0/1444	0.56	0/1943
1	1-N	0.37	0/1444	0.56	0/1943
1	1-O	0.37	0/1444	0.55	0/1943
1	1-P	0.37	0/1444	0.56	0/1943
1	1-Q	0.37	0/1444	0.55	0/1943
1	1-R	0.37	0/1455	0.55	0/1958
1	1-S	0.37	0/1455	0.55	0/1958
1	1-T	0.37	0/1444	0.55	0/1943
1	1-U	0.37	0/1444	0.56	0/1943
1	1-V	0.37	0/1455	0.55	0/1958
1	1-W	0.37	0/1444	0.56	0/1943
1	1-X	0.37	0/1455	0.55	0/1958
1	2-A	0.36	0/1444	0.54	0/1943
1	2-B	0.36	0/1444	0.54	0/1943
1	2-C	0.36	0/1444	0.54	0/1943
1	2-D	0.36	0/1444	0.54	0/1943
1	2-E	0.35	0/1444	0.53	0/1943
1	2-F	0.36	0/1455	0.53	0/1958
1	2-G	0.36	0/1455	0.54	0/1958
1	2-H	0.36	0/1444	0.54	0/1943
1	2-I	0.36	0/1444	0.54	0/1943
1	2-J	0.36	0/1455	0.54	0/1958

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	2-K	0.36	0/1444	0.54	0/1943
1	2-L	0.36	0/1455	0.53	0/1958
1	2-M	0.36	0/1444	0.53	0/1943
1	2-N	0.36	0/1444	0.54	0/1943
1	2-O	0.36	0/1444	0.54	0/1943
1	2-P	0.36	0/1444	0.53	0/1943
1	2-Q	0.36	0/1444	0.54	0/1943
1	2-R	0.36	0/1455	0.53	0/1958
1	2-S	0.36	0/1455	0.53	0/1958
1	2-T	0.36	0/1444	0.54	0/1943
1	2-U	0.36	0/1444	0.54	0/1943
1	2-V	0.36	0/1455	0.54	0/1958
1	2-W	0.36	0/1444	0.54	0/1943
1	2-X	0.36	0/1455	0.54	0/1958
1	3-A	0.42	0/1444	0.60	0/1943
1	3-B	0.41	0/1444	0.60	0/1943
1	3-C	0.41	0/1444	0.60	0/1943
1	3-D	0.41	0/1444	0.60	0/1943
1	3-E	0.41	0/1444	0.60	0/1943
1	3-F	0.41	0/1455	0.60	0/1958
1	3-G	0.41	0/1455	0.60	0/1958
1	3-H	0.41	0/1444	0.60	0/1943
1	3-I	0.41	0/1444	0.60	0/1943
1	3-J	0.42	0/1455	0.60	0/1958
1	3-K	0.41	0/1444	0.60	0/1943
1	3-L	0.41	0/1455	0.60	0/1958
1	3-M	0.42	0/1444	0.60	0/1943
1	3-N	0.41	0/1444	0.60	0/1943
1	3-O	0.41	0/1444	0.60	0/1943
1	3-P	0.41	0/1444	0.60	0/1943
1	3-Q	0.42	0/1444	0.60	0/1943
1	3-R	0.41	0/1455	0.60	0/1958
1	3-S	0.41	0/1455	0.60	0/1958
1	3-T	0.41	0/1444	0.60	0/1943
1	3-U	0.41	0/1444	0.60	0/1943
1	3-V	0.42	0/1455	0.60	0/1958
1	3-W	0.41	0/1444	0.60	0/1943
1	3-X	0.41	0/1455	0.60	0/1958
1	4-A	0.34	0/1444	0.54	0/1943
1	4-B	0.34	0/1444	0.54	0/1943
1	4-C	0.34	0/1444	0.55	0/1943
1	4-D	0.34	0/1444	0.55	0/1943
1	4-E	0.34	0/1444	0.55	0/1943

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	4-F	0.34	0/1455	0.54	0/1958
1	4-G	0.34	0/1455	0.54	0/1958
1	4-H	0.34	0/1444	0.54	0/1943
1	4-I	0.34	0/1444	0.54	0/1943
1	4-J	0.34	0/1455	0.55	0/1958
1	4-K	0.34	0/1444	0.54	0/1943
1	4-L	0.34	0/1455	0.55	0/1958
1	4-M	0.34	0/1444	0.54	0/1943
1	4-N	0.34	0/1444	0.54	0/1943
1	4-O	0.34	0/1444	0.54	0/1943
1	4-P	0.34	0/1444	0.55	0/1943
1	4-Q	0.34	0/1444	0.54	0/1943
1	4-R	0.34	0/1455	0.54	0/1958
1	4-S	0.34	0/1455	0.54	0/1958
1	4-T	0.34	0/1444	0.55	0/1943
1	4-U	0.34	0/1444	0.55	0/1943
1	4-V	0.34	0/1455	0.55	0/1958
1	4-W	0.34	0/1444	0.55	0/1943
1	4-X	0.34	0/1455	0.55	0/1958
1	5-A	0.40	0/1444	0.60	1/1943 (0.1%)
1	5-B	0.40	0/1444	0.59	1/1943 (0.1%)
1	5-C	0.40	0/1444	0.59	1/1943 (0.1%)
1	5-D	0.40	0/1444	0.59	1/1943 (0.1%)
1	5-E	0.40	0/1444	0.59	1/1943 (0.1%)
1	5-F	0.40	0/1455	0.59	1/1958 (0.1%)
1	5-G	0.40	0/1455	0.59	1/1958 (0.1%)
1	5-H	0.40	0/1444	0.59	1/1943 (0.1%)
1	5-I	0.40	0/1444	0.60	1/1943 (0.1%)
1	5-J	0.40	0/1455	0.59	1/1958 (0.1%)
1	5-K	0.40	0/1444	0.59	1/1943 (0.1%)
1	5-L	0.40	0/1455	0.60	1/1958 (0.1%)
1	5-M	0.40	0/1444	0.59	1/1943 (0.1%)
1	5-N	0.40	0/1444	0.59	1/1943 (0.1%)
1	5-O	0.40	0/1444	0.59	1/1943 (0.1%)
1	5-P	0.40	0/1444	0.59	1/1943 (0.1%)
1	5-Q	0.40	0/1444	0.59	1/1943 (0.1%)
1	5-R	0.40	0/1455	0.59	1/1958 (0.1%)
1	5-S	0.40	0/1455	0.59	1/1958 (0.1%)
1	5-T	0.40	0/1444	0.59	1/1943 (0.1%)
1	5-U	0.40	0/1444	0.59	1/1943 (0.1%)
1	5-V	0.40	0/1455	0.59	1/1958 (0.1%)
1	5-W	0.40	0/1444	0.59	1/1943 (0.1%)
1	5-X	0.40	0/1455	0.59	1/1958 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	6-A	0.38	0/1444	0.57	0/1943
1	6-B	0.38	0/1444	0.57	0/1943
1	6-C	0.38	0/1444	0.57	0/1943
1	6-D	0.38	0/1444	0.57	0/1943
1	6-E	0.38	0/1444	0.57	0/1943
1	6-F	0.38	0/1455	0.57	0/1958
1	6-G	0.38	0/1455	0.57	0/1958
1	6-H	0.38	0/1444	0.57	0/1943
1	6-I	0.38	0/1444	0.57	0/1943
1	6-J	0.38	0/1455	0.57	0/1958
1	6-K	0.38	0/1444	0.57	0/1943
1	6-L	0.38	0/1455	0.57	0/1958
1	6-M	0.38	0/1444	0.57	0/1943
1	6-N	0.38	0/1444	0.57	0/1943
1	6-O	0.38	0/1444	0.57	0/1943
1	6-P	0.38	0/1444	0.57	0/1943
1	6-Q	0.38	0/1444	0.57	0/1943
1	6-R	0.38	0/1455	0.57	0/1958
1	6-S	0.38	0/1455	0.57	0/1958
1	6-T	0.38	0/1444	0.57	0/1943
1	6-U	0.38	0/1444	0.57	0/1943
1	6-V	0.38	0/1455	0.57	0/1958
1	6-W	0.38	0/1444	0.57	0/1943
1	6-X	0.38	0/1455	0.57	0/1958
1	7-A	0.36	0/1444	0.55	0/1943
1	7-B	0.36	0/1444	0.55	0/1943
1	7-C	0.36	0/1444	0.55	0/1943
1	7-D	0.36	0/1444	0.55	0/1943
1	7-E	0.36	0/1444	0.55	0/1943
1	7-F	0.36	0/1455	0.55	0/1958
1	7-G	0.36	0/1455	0.55	0/1958
1	7-H	0.36	0/1444	0.55	0/1943
1	7-I	0.36	0/1444	0.55	0/1943
1	7-J	0.36	0/1455	0.55	0/1958
1	7-K	0.36	0/1444	0.55	0/1943
1	7-L	0.36	0/1455	0.55	0/1958
1	7-M	0.36	0/1444	0.55	0/1943
1	7-N	0.36	0/1444	0.55	0/1943
1	7-O	0.36	0/1444	0.55	0/1943
1	7-P	0.36	0/1444	0.55	0/1943
1	7-Q	0.36	0/1444	0.55	0/1943
1	7-R	0.36	0/1455	0.55	0/1958
1	7-S	0.36	0/1455	0.55	0/1958

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	7-T	0.36	0/1444	0.55	0/1943
1	7-U	0.36	0/1444	0.55	0/1943
1	7-V	0.36	0/1455	0.55	0/1958
1	7-W	0.36	0/1444	0.55	0/1943
1	7-X	0.36	0/1455	0.56	0/1958
1	8-A	0.41	0/1444	0.58	0/1943
1	8-B	0.41	0/1444	0.58	0/1943
1	8-C	0.41	0/1444	0.58	0/1943
1	8-D	0.41	0/1444	0.58	0/1943
1	8-E	0.41	0/1444	0.58	0/1943
1	8-F	0.41	0/1455	0.58	0/1958
1	8-G	0.41	0/1455	0.58	0/1958
1	8-H	0.41	0/1444	0.58	0/1943
1	8-I	0.41	0/1444	0.58	0/1943
1	8-J	0.41	0/1455	0.58	0/1958
1	8-K	0.41	0/1444	0.58	0/1943
1	8-L	0.41	0/1455	0.58	0/1958
1	8-M	0.41	0/1444	0.58	0/1943
1	8-N	0.41	0/1444	0.58	0/1943
1	8-O	0.41	0/1444	0.58	0/1943
1	8-P	0.41	0/1444	0.58	0/1943
1	8-Q	0.41	0/1444	0.58	0/1943
1	8-R	0.41	0/1455	0.58	0/1958
1	8-S	0.41	0/1455	0.58	0/1958
1	8-T	0.41	0/1444	0.58	0/1943
1	8-U	0.41	0/1444	0.58	0/1943
1	8-V	0.41	0/1455	0.58	0/1958
1	8-W	0.41	0/1444	0.58	0/1943
1	8-X	0.41	0/1455	0.59	0/1958
1	9-A	0.32	0/1444	0.51	0/1943
1	9-B	0.32	0/1444	0.51	0/1943
1	9-C	0.33	0/1444	0.51	0/1943
1	9-D	0.32	0/1444	0.51	0/1943
1	9-E	0.33	0/1444	0.51	0/1943
1	9-F	0.32	0/1455	0.51	0/1958
1	9-G	0.33	0/1455	0.52	0/1958
1	9-H	0.33	0/1444	0.51	0/1943
1	9-I	0.33	0/1444	0.51	0/1943
1	9-J	0.32	0/1455	0.51	0/1958
1	9-K	0.32	0/1444	0.51	0/1943
1	9-L	0.33	0/1455	0.52	0/1958
1	9-M	0.32	0/1444	0.51	0/1943
1	9-N	0.32	0/1444	0.51	0/1943

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	9-O	0.32	0/1444	0.51	0/1943
1	9-P	0.32	0/1444	0.51	0/1943
1	9-Q	0.32	0/1444	0.51	0/1943
1	9-R	0.33	0/1455	0.52	0/1958
1	9-S	0.33	0/1455	0.52	0/1958
1	9-T	0.32	0/1444	0.51	0/1943
1	9-U	0.32	0/1444	0.51	0/1943
1	9-V	0.33	0/1455	0.51	0/1958
1	9-W	0.32	0/1444	0.51	0/1943
1	9-X	0.33	0/1455	0.51	0/1958
1	10-A	0.36	0/1444	0.56	0/1943
1	10-B	0.36	0/1444	0.56	0/1943
1	10-C	0.36	0/1444	0.56	0/1943
1	10-D	0.36	0/1444	0.56	0/1943
1	10-E	0.36	0/1444	0.56	0/1943
1	10-F	0.36	0/1455	0.56	0/1958
1	10-G	0.36	0/1455	0.56	0/1958
1	10-H	0.36	0/1444	0.56	0/1943
1	10-I	0.36	0/1444	0.56	0/1943
1	10-J	0.36	0/1455	0.56	0/1958
1	10-K	0.36	0/1444	0.56	0/1943
1	10-L	0.36	0/1455	0.56	0/1958
1	10-M	0.36	0/1444	0.56	0/1943
1	10-N	0.36	0/1444	0.56	0/1943
1	10-O	0.36	0/1444	0.56	0/1943
1	10-P	0.36	0/1444	0.56	0/1943
1	10-Q	0.36	0/1444	0.56	0/1943
1	10-R	0.36	0/1455	0.56	0/1958
1	10-S	0.36	0/1455	0.56	0/1958
1	10-T	0.36	0/1444	0.56	0/1943
1	10-U	0.36	0/1444	0.56	0/1943
1	10-V	0.36	0/1455	0.56	0/1958
1	10-W	0.36	0/1444	0.56	0/1943
1	10-X	0.36	0/1455	0.56	0/1958
All	All	0.37	0/347440	0.56	24/467520 (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	1-X	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	9-R	0	1
All	All	0	2

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5-B	51	PHE	CB-CG-CD2	-5.29	117.09	120.80
1	5-W	51	PHE	CB-CG-CD2	-5.27	117.11	120.80
1	5-A	51	PHE	CB-CG-CD2	-5.27	117.11	120.80
1	5-J	51	PHE	CB-CG-CD2	-5.27	117.11	120.80
1	5-N	51	PHE	CB-CG-CD2	-5.27	117.11	120.80
1	5-P	51	PHE	CB-CG-CD2	-5.27	117.11	120.80
1	5-E	51	PHE	CB-CG-CD2	-5.26	117.11	120.80
1	5-H	51	PHE	CB-CG-CD2	-5.24	117.14	120.80
1	5-D	51	PHE	CB-CG-CD2	-5.22	117.14	120.80
1	5-I	51	PHE	CB-CG-CD2	-5.22	117.14	120.80
1	5-C	51	PHE	CB-CG-CD2	-5.21	117.16	120.80
1	5-O	51	PHE	CB-CG-CD2	-5.20	117.16	120.80
1	5-Q	51	PHE	CB-CG-CD2	-5.20	117.16	120.80
1	5-R	51	PHE	CB-CG-CD2	-5.20	117.16	120.80
1	5-U	51	PHE	CB-CG-CD2	-5.20	117.16	120.80
1	5-K	51	PHE	CB-CG-CD2	-5.17	117.18	120.80
1	5-T	51	PHE	CB-CG-CD2	-5.16	117.19	120.80
1	5-F	51	PHE	CB-CG-CD2	-5.15	117.19	120.80
1	5-L	51	PHE	CB-CG-CD2	-5.15	117.19	120.80
1	5-X	51	PHE	CB-CG-CD2	-5.15	117.19	120.80
1	5-G	51	PHE	CB-CG-CD2	-5.14	117.20	120.80
1	5-M	51	PHE	CB-CG-CD2	-5.14	117.20	120.80
1	5-S	51	PHE	CB-CG-CD2	-5.14	117.20	120.80
1	5-V	51	PHE	CB-CG-CD2	-5.14	117.20	120.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-X	176	GLY	Peptide
1	9-R	176	GLY	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	1415	0	1364	19	0
1	1-B	1415	0	1364	18	0
1	1-C	1415	0	1364	17	0
1	1-D	1415	0	1364	19	0
1	1-E	1415	0	1364	17	0
1	1-F	1425	0	1371	18	0
1	1-G	1425	0	1371	17	0
1	1-H	1415	0	1364	18	0
1	1-I	1415	0	1364	17	0
1	1-J	1425	0	1371	19	0
1	1-K	1415	0	1364	18	0
1	1-L	1425	0	1371	18	0
1	1-M	1415	0	1364	19	0
1	1-N	1415	0	1364	18	0
1	1-O	1415	0	1364	21	0
1	1-P	1415	0	1364	18	0
1	1-Q	1415	0	1364	19	0
1	1-R	1425	0	1371	20	0
1	1-S	1425	0	1371	18	0
1	1-T	1415	0	1364	18	0
1	1-U	1415	0	1364	18	0
1	1-V	1425	0	1371	20	0
1	1-W	1415	0	1364	20	0
1	1-X	1425	0	1371	18	0
1	2-A	1415	0	1364	19	0
1	2-B	1415	0	1364	21	0
1	2-C	1415	0	1364	22	0
1	2-D	1415	0	1364	19	0
1	2-E	1415	0	1364	19	0
1	2-F	1425	0	1371	22	0
1	2-G	1425	0	1371	23	0
1	2-H	1415	0	1364	19	0
1	2-I	1415	0	1364	22	0
1	2-J	1425	0	1371	21	0
1	2-K	1415	0	1364	22	0
1	2-L	1425	0	1371	22	0
1	2-M	1415	0	1364	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2-N	1415	0	1364	20	0
1	2-O	1415	0	1364	23	0
1	2-P	1415	0	1364	21	0
1	2-Q	1415	0	1364	23	0
1	2-R	1425	0	1371	24	0
1	2-S	1425	0	1371	21	0
1	2-T	1415	0	1364	20	0
1	2-U	1415	0	1364	23	0
1	2-V	1425	0	1371	21	0
1	2-W	1415	0	1364	23	0
1	2-X	1425	0	1371	22	0
1	3-A	1415	0	1364	20	0
1	3-B	1415	0	1364	18	0
1	3-C	1415	0	1364	19	0
1	3-D	1415	0	1364	19	0
1	3-E	1415	0	1364	19	0
1	3-F	1425	0	1371	21	0
1	3-G	1425	0	1371	19	0
1	3-H	1415	0	1364	18	0
1	3-I	1415	0	1364	19	0
1	3-J	1425	0	1371	18	0
1	3-K	1415	0	1364	19	0
1	3-L	1425	0	1371	20	0
1	3-M	1415	0	1364	20	0
1	3-N	1415	0	1364	20	0
1	3-O	1415	0	1364	19	0
1	3-P	1415	0	1364	18	0
1	3-Q	1415	0	1364	19	0
1	3-R	1425	0	1371	19	0
1	3-S	1425	0	1371	23	0
1	3-T	1415	0	1364	20	0
1	3-U	1415	0	1364	20	0
1	3-V	1425	0	1371	18	0
1	3-W	1415	0	1364	19	0
1	3-X	1425	0	1371	20	0
1	4-A	1415	0	1364	13	0
1	4-B	1415	0	1364	10	0
1	4-C	1415	0	1364	10	0
1	4-D	1415	0	1364	11	0
1	4-E	1415	0	1364	10	0
1	4-F	1425	0	1371	10	0
1	4-G	1425	0	1371	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	4-H	1415	0	1364	11	0
1	4-I	1415	0	1364	10	0
1	4-J	1425	0	1371	12	0
1	4-K	1415	0	1364	11	0
1	4-L	1425	0	1371	11	0
1	4-M	1415	0	1364	10	0
1	4-N	1415	0	1364	9	0
1	4-O	1415	0	1364	10	0
1	4-P	1415	0	1364	11	0
1	4-Q	1415	0	1364	11	0
1	4-R	1425	0	1371	11	0
1	4-S	1425	0	1371	9	0
1	4-T	1415	0	1364	9	0
1	4-U	1415	0	1364	10	0
1	4-V	1425	0	1371	10	0
1	4-W	1415	0	1364	10	0
1	4-X	1425	0	1371	11	0
1	5-A	1415	0	1364	10	0
1	5-B	1415	0	1364	10	0
1	5-C	1415	0	1364	8	0
1	5-D	1415	0	1364	13	0
1	5-E	1415	0	1364	8	0
1	5-F	1425	0	1371	11	0
1	5-G	1425	0	1371	9	0
1	5-H	1415	0	1364	11	0
1	5-I	1415	0	1364	11	0
1	5-J	1425	0	1371	10	0
1	5-K	1415	0	1364	8	0
1	5-L	1425	0	1371	10	0
1	5-M	1415	0	1364	9	0
1	5-N	1415	0	1364	11	0
1	5-O	1415	0	1364	7	0
1	5-P	1415	0	1364	10	0
1	5-Q	1415	0	1364	11	0
1	5-R	1425	0	1371	10	0
1	5-S	1425	0	1371	8	0
1	5-T	1415	0	1364	11	0
1	5-U	1415	0	1364	8	0
1	5-V	1425	0	1371	9	0
1	5-W	1415	0	1364	11	0
1	5-X	1425	0	1371	10	0
1	6-A	1415	0	1364	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	6-B	1415	0	1364	16	0
1	6-C	1415	0	1364	17	0
1	6-D	1415	0	1364	17	0
1	6-E	1415	0	1364	18	0
1	6-F	1425	0	1371	18	0
1	6-G	1425	0	1371	16	0
1	6-H	1415	0	1364	16	0
1	6-I	1415	0	1364	17	0
1	6-J	1425	0	1371	17	0
1	6-K	1415	0	1364	18	0
1	6-L	1425	0	1371	18	0
1	6-M	1415	0	1364	16	0
1	6-N	1415	0	1364	17	0
1	6-O	1415	0	1364	17	0
1	6-P	1415	0	1364	16	0
1	6-Q	1415	0	1364	17	0
1	6-R	1425	0	1371	17	0
1	6-S	1425	0	1371	16	0
1	6-T	1415	0	1364	17	0
1	6-U	1415	0	1364	16	0
1	6-V	1425	0	1371	16	0
1	6-W	1415	0	1364	17	0
1	6-X	1425	0	1371	16	0
1	7-A	1415	0	1364	13	0
1	7-B	1415	0	1364	12	0
1	7-C	1415	0	1364	13	0
1	7-D	1415	0	1364	13	0
1	7-E	1415	0	1364	15	0
1	7-F	1425	0	1371	13	0
1	7-G	1425	0	1371	13	0
1	7-H	1415	0	1364	12	0
1	7-I	1415	0	1364	13	0
1	7-J	1425	0	1371	14	0
1	7-K	1415	0	1364	15	0
1	7-L	1425	0	1371	13	0
1	7-M	1415	0	1364	14	0
1	7-N	1415	0	1364	13	0
1	7-O	1415	0	1364	14	0
1	7-P	1415	0	1364	11	0
1	7-Q	1415	0	1364	16	0
1	7-R	1425	0	1371	13	0
1	7-S	1425	0	1371	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	7-T	1415	0	1364	13	0
1	7-U	1415	0	1364	15	0
1	7-V	1425	0	1371	11	0
1	7-W	1415	0	1364	15	0
1	7-X	1425	0	1371	15	0
1	8-A	1415	0	1364	17	0
1	8-B	1415	0	1364	19	0
1	8-C	1415	0	1364	17	0
1	8-D	1415	0	1364	17	0
1	8-E	1415	0	1364	17	0
1	8-F	1425	0	1371	18	0
1	8-G	1425	0	1371	17	0
1	8-H	1415	0	1364	19	0
1	8-I	1415	0	1364	17	0
1	8-J	1425	0	1371	17	0
1	8-K	1415	0	1364	18	0
1	8-L	1425	0	1371	19	0
1	8-M	1415	0	1364	16	0
1	8-N	1415	0	1364	18	0
1	8-O	1415	0	1364	18	0
1	8-P	1415	0	1364	14	0
1	8-Q	1415	0	1364	18	0
1	8-R	1425	0	1371	18	0
1	8-S	1425	0	1371	15	0
1	8-T	1415	0	1364	18	0
1	8-U	1415	0	1364	15	0
1	8-V	1425	0	1371	15	0
1	8-W	1415	0	1364	18	0
1	8-X	1425	0	1371	20	0
1	9-A	1415	0	1364	11	0
1	9-B	1415	0	1364	11	0
1	9-C	1415	0	1364	11	0
1	9-D	1415	0	1364	11	0
1	9-E	1415	0	1364	12	0
1	9-F	1425	0	1371	11	0
1	9-G	1425	0	1371	15	0
1	9-H	1415	0	1364	11	0
1	9-I	1415	0	1364	11	0
1	9-J	1425	0	1371	11	0
1	9-K	1415	0	1364	12	0
1	9-L	1425	0	1371	15	0
1	9-M	1415	0	1364	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	9-N	1415	0	1364	13	0
1	9-O	1415	0	1364	12	0
1	9-P	1415	0	1364	11	0
1	9-Q	1415	0	1364	11	0
1	9-R	1425	0	1371	12	0
1	9-S	1425	0	1371	14	0
1	9-T	1415	0	1364	12	0
1	9-U	1415	0	1364	12	0
1	9-V	1425	0	1371	11	0
1	9-W	1415	0	1364	12	0
1	9-X	1425	0	1371	12	0
1	10-A	1415	0	1364	20	0
1	10-B	1415	0	1364	20	0
1	10-C	1415	0	1364	20	0
1	10-D	1415	0	1364	19	0
1	10-E	1415	0	1364	21	0
1	10-F	1425	0	1371	20	0
1	10-G	1425	0	1371	19	0
1	10-H	1415	0	1364	19	0
1	10-I	1415	0	1364	21	0
1	10-J	1425	0	1371	21	0
1	10-K	1415	0	1364	21	0
1	10-L	1425	0	1371	20	0
1	10-M	1415	0	1364	21	0
1	10-N	1415	0	1364	22	0
1	10-O	1415	0	1364	21	0
1	10-P	1415	0	1364	20	0
1	10-Q	1415	0	1364	24	0
1	10-R	1425	0	1371	21	0
1	10-S	1425	0	1371	25	0
1	10-T	1415	0	1364	22	0
1	10-U	1415	0	1364	23	0
1	10-V	1425	0	1371	20	0
1	10-W	1415	0	1364	22	0
1	10-X	1425	0	1371	20	0
2	1-A	75	0	0	2	0
2	1-B	74	0	0	2	0
2	1-C	74	0	0	1	0
2	1-D	74	0	0	2	0
2	1-E	75	0	0	1	0
2	1-F	75	0	0	2	0
2	1-G	75	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	1-H	75	0	0	2	0
2	1-I	74	0	0	1	0
2	1-J	76	0	0	2	0
2	1-K	72	0	0	1	0
2	1-L	74	0	0	1	0
2	1-M	73	0	0	2	0
2	1-N	75	0	0	2	0
2	1-O	75	0	0	1	0
2	1-P	74	0	0	2	0
2	1-Q	74	0	0	1	0
2	1-R	74	0	0	2	0
2	1-S	75	0	0	1	0
2	1-T	75	0	0	2	0
2	1-U	74	0	0	1	0
2	1-V	75	0	0	2	0
2	1-W	73	0	0	1	0
2	1-X	73	0	0	1	0
2	2-A	75	0	0	2	0
2	2-B	74	0	0	2	0
2	2-C	74	0	0	2	0
2	2-D	74	0	0	2	0
2	2-E	75	0	0	1	0
2	2-F	75	0	0	2	0
2	2-G	75	0	0	2	0
2	2-H	75	0	0	2	0
2	2-I	74	0	0	2	0
2	2-J	76	0	0	2	0
2	2-K	72	0	0	2	0
2	2-L	74	0	0	2	0
2	2-M	73	0	0	2	0
2	2-N	75	0	0	2	0
2	2-O	75	0	0	2	0
2	2-P	74	0	0	2	0
2	2-Q	74	0	0	2	0
2	2-R	74	0	0	2	0
2	2-S	75	0	0	2	0
2	2-T	75	0	0	2	0
2	2-U	74	0	0	2	0
2	2-V	75	0	0	2	0
2	2-W	73	0	0	2	0
2	2-X	73	0	0	2	0
2	3-A	75	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	3-B	75	0	0	1	0
2	3-C	74	0	0	0	0
2	3-D	74	0	0	0	0
2	3-E	75	0	0	0	0
2	3-F	75	0	0	0	0
2	3-G	75	0	0	0	0
2	3-H	75	0	0	0	0
2	3-I	74	0	0	0	0
2	3-J	76	0	0	0	0
2	3-K	72	0	0	0	0
2	3-L	74	0	0	0	0
2	3-M	73	0	0	0	0
2	3-N	75	0	0	0	0
2	3-O	75	0	0	0	0
2	3-P	74	0	0	0	0
2	3-Q	74	0	0	0	0
2	3-R	74	0	0	0	0
2	3-S	75	0	0	0	0
2	3-T	75	0	0	0	0
2	3-U	74	0	0	0	0
2	3-V	75	0	0	0	0
2	3-W	73	0	0	0	0
2	3-X	73	0	0	0	0
2	4-A	75	0	0	4	0
2	4-B	74	0	0	2	0
2	4-C	74	0	0	1	0
2	4-D	74	0	0	3	0
2	4-E	75	0	0	1	0
2	4-F	75	0	0	2	0
2	4-G	75	0	0	1	0
2	4-H	75	0	0	2	0
2	4-I	74	0	0	1	0
2	4-J	76	0	0	2	0
2	4-K	72	0	0	1	0
2	4-L	74	0	0	1	0
2	4-M	73	0	0	2	0
2	4-N	75	0	0	1	0
2	4-O	75	0	0	1	0
2	4-P	74	0	0	1	0
2	4-Q	74	0	0	1	0
2	4-R	74	0	0	2	0
2	4-S	75	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	4-T	75	0	0	1	0
2	4-U	74	0	0	1	0
2	4-V	75	0	0	1	0
2	4-W	73	0	0	1	0
2	4-X	73	0	0	1	0
2	5-A	75	0	0	2	0
2	5-B	74	0	0	1	0
2	5-C	74	0	0	0	0
2	5-D	74	0	0	1	0
2	5-E	75	0	0	0	0
2	5-F	75	0	0	1	0
2	5-G	75	0	0	0	0
2	5-H	75	0	0	1	0
2	5-I	74	0	0	0	0
2	5-J	76	0	0	1	0
2	5-K	72	0	0	0	0
2	5-L	74	0	0	0	0
2	5-M	73	0	0	0	0
2	5-N	75	0	0	1	0
2	5-O	75	0	0	0	0
2	5-P	74	0	0	1	0
2	5-Q	74	0	0	0	0
2	5-R	74	0	0	1	0
2	5-S	75	0	0	0	0
2	5-T	75	0	0	1	0
2	5-U	74	0	0	0	0
2	5-V	75	0	0	1	0
2	5-W	73	0	0	0	0
2	5-X	73	0	0	0	0
2	6-A	75	0	0	1	0
2	6-B	74	0	0	1	0
2	6-C	74	0	0	1	0
2	6-D	74	0	0	1	0
2	6-E	75	0	0	1	0
2	6-F	75	0	0	1	0
2	6-G	75	0	0	1	0
2	6-H	75	0	0	1	0
2	6-I	74	0	0	1	0
2	6-J	76	0	0	1	0
2	6-K	72	0	0	1	0
2	6-L	74	0	0	1	0
2	6-M	73	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	6-N	75	0	0	1	0
2	6-O	75	0	0	1	0
2	6-P	74	0	0	1	0
2	6-Q	74	0	0	1	0
2	6-R	74	0	0	2	0
2	6-S	75	0	0	1	0
2	6-T	75	0	0	1	0
2	6-U	74	0	0	1	0
2	6-V	75	0	0	1	0
2	6-W	73	0	0	1	0
2	6-X	73	0	0	1	0
2	7-A	75	0	0	1	0
2	7-B	74	0	0	1	0
2	7-C	74	0	0	1	0
2	7-D	74	0	0	1	0
2	7-E	75	0	0	1	0
2	7-F	75	0	0	1	0
2	7-G	75	0	0	1	0
2	7-H	75	0	0	1	0
2	7-I	74	0	0	1	0
2	7-J	76	0	0	1	0
2	7-K	72	0	0	1	0
2	7-L	74	0	0	1	0
2	7-M	73	0	0	1	0
2	7-N	75	0	0	1	0
2	7-O	75	0	0	1	0
2	7-P	74	0	0	1	0
2	7-Q	74	0	0	1	0
2	7-R	74	0	0	1	0
2	7-S	75	0	0	1	0
2	7-T	75	0	0	1	0
2	7-U	74	0	0	1	0
2	7-V	75	0	0	1	0
2	7-W	73	0	0	1	0
2	7-X	73	0	0	1	0
2	8-A	75	0	0	0	0
2	8-B	74	0	0	0	0
2	8-C	74	0	0	0	0
2	8-D	74	0	0	0	0
2	8-E	75	0	0	0	0
2	8-F	75	0	0	0	0
2	8-G	75	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	8-H	75	0	0	0	0
2	8-I	74	0	0	0	0
2	8-J	76	0	0	0	0
2	8-K	72	0	0	0	0
2	8-L	74	0	0	0	0
2	8-M	73	0	0	0	0
2	8-N	75	0	0	0	0
2	8-O	75	0	0	0	0
2	8-P	74	0	0	0	0
2	8-Q	74	0	0	0	0
2	8-R	74	0	0	0	0
2	8-S	75	0	0	0	0
2	8-T	75	0	0	0	0
2	8-U	74	0	0	0	0
2	8-V	75	0	0	0	0
2	8-W	73	0	0	0	0
2	8-X	73	0	0	0	0
2	9-A	75	0	0	1	0
2	9-B	74	0	0	1	0
2	9-C	74	0	0	1	0
2	9-D	74	0	0	1	0
2	9-E	75	0	0	1	0
2	9-F	75	0	0	1	0
2	9-G	75	0	0	1	0
2	9-H	75	0	0	1	0
2	9-I	74	0	0	1	0
2	9-J	76	0	0	1	0
2	9-K	72	0	0	1	0
2	9-L	74	0	0	1	0
2	9-M	73	0	0	1	0
2	9-N	75	0	0	1	0
2	9-O	75	0	0	1	0
2	9-P	74	0	0	1	0
2	9-Q	74	0	0	1	0
2	9-R	74	0	0	1	0
2	9-S	75	0	0	1	0
2	9-T	75	0	0	1	0
2	9-U	74	0	0	1	0
2	9-V	75	0	0	1	0
2	9-W	73	0	0	1	0
2	9-X	73	0	0	1	0
2	10-A	75	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	10-B	75	0	0	3	0
2	10-C	74	0	0	1	0
2	10-D	74	0	0	1	0
2	10-E	75	0	0	1	0
2	10-F	75	0	0	1	0
2	10-G	75	0	0	1	0
2	10-H	75	0	0	1	0
2	10-I	74	0	0	1	0
2	10-J	76	0	0	1	0
2	10-K	72	0	0	1	0
2	10-L	74	0	0	1	0
2	10-M	73	0	0	1	0
2	10-N	75	0	0	1	0
2	10-O	75	0	0	1	0
2	10-P	74	0	0	1	0
2	10-Q	74	0	0	1	0
2	10-R	74	0	0	1	0
2	10-S	75	0	0	1	0
2	10-T	75	0	0	1	0
2	10-U	74	0	0	1	0
2	10-V	75	0	0	1	0
2	10-W	73	0	0	1	0
2	10-X	73	0	0	1	0
All	All	358232	0	327920	3486	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 (3486) 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:X:176:GLY:O	1:X:177:HIS:ND1	1.91	1.02
1:X:162:GLU:N	1:X:162:GLU:OE1	2.10	0.85
1:I:162:GLU:OE1	1:I:162:GLU:N	2.10	0.85
1:R:162:GLU:OE1	1:R:162:GLU:N	2.10	0.85
1:C:162:GLU:N	1:C:162:GLU:OE1	2.10	0.85
1:K:162:GLU:OE1	1:K:162:GLU:N	2.10	0.85
1:E:162:GLU:N	1:E:162:GLU:OE1	2.10	0.85
1:N:162:GLU:N	1:N:162:GLU:OE1	2.10	0.85
1:T:162:GLU:N	1:T:162:GLU:OE1	2.10	0.85
1:U:162:GLU:OE1	1:U:162:GLU:N	2.10	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:GLU:OE1	1:A:162:GLU:N	2.10	0.84
1:D:162:GLU:OE1	1:D:162:GLU:N	2.10	0.84
1:O:162:GLU:N	1:O:162:GLU:OE1	2.10	0.84
1:M:162:GLU:N	1:M:162:GLU:OE1	2.10	0.84
1:S:162:GLU:N	1:S:162:GLU:OE1	2.10	0.84
1:G:162:GLU:N	1:G:162:GLU:OE1	2.10	0.84
1:P:162:GLU:OE1	1:P:162:GLU:N	2.10	0.84
1:F:162:GLU:OE1	1:F:162:GLU:N	2.10	0.84
1:V:162:GLU:N	1:V:162:GLU:OE1	2.10	0.84
1:L:162:GLU:N	1:L:162:GLU:OE1	2.10	0.84
1:B:162:GLU:N	1:B:162:GLU:OE1	2.10	0.83
1:J:162:GLU:N	1:J:162:GLU:OE1	2.10	0.83
1:H:162:GLU:N	1:H:162:GLU:OE1	2.10	0.83
1:Q:162:GLU:N	1:Q:162:GLU:OE1	2.10	0.83
1:W:162:GLU:OE1	1:W:162:GLU:N	2.10	0.83
1:X:176:GLY:O	1:X:177:HIS:ND1	2.12	0.82
1:A:75:GLN:OE1	2:A:201:HOH:O	1.98	0.81
1:S:173:HIS:HA	1:S:177:HIS:CE1	2.16	0.80
1:E:51:PHE:HE2	1:E:96:GLY:HA3	1.51	0.76
1:J:51:PHE:HE2	1:J:96:GLY:HA3	1.51	0.76
1:K:51:PHE:HE2	1:K:96:GLY:HA3	1.51	0.76
1:N:51:PHE:HE2	1:N:96:GLY:HA3	1.51	0.76
1:D:51:PHE:HE2	1:D:96:GLY:HA3	1.51	0.76
1:T:51:PHE:HE2	1:T:96:GLY:HA3	1.51	0.75
1:H:51:PHE:HE2	1:H:96:GLY:HA3	1.51	0.75
1:B:51:PHE:HE2	1:B:96:GLY:HA3	1.51	0.75
1:V:51:PHE:HE2	1:V:96:GLY:HA3	1.51	0.75
1:W:51:PHE:HE2	1:W:96:GLY:HA3	1.51	0.75
1:P:51:PHE:HE2	1:P:96:GLY:HA3	1.51	0.75
1:Q:51:PHE:HE2	1:Q:96:GLY:HA3	1.51	0.75
1:O:51:PHE:HE2	1:O:96:GLY:HA3	1.51	0.74
1:A:51:PHE:HE2	1:A:96:GLY:HA3	1.51	0.74
1:X:51:PHE:HE2	1:X:96:GLY:HA3	1.51	0.74
1:U:51:PHE:HE2	1:U:96:GLY:HA3	1.51	0.74
1:C:51:PHE:HE2	1:C:96:GLY:HA3	1.51	0.74
1:G:51:PHE:HE2	1:G:96:GLY:HA3	1.51	0.74
1:M:51:PHE:HE2	1:M:96:GLY:HA3	1.51	0.74
1:R:51:PHE:HE2	1:R:96:GLY:HA3	1.51	0.74
1:S:51:PHE:HE2	1:S:96:GLY:HA3	1.51	0.74
1:F:51:PHE:HE2	1:F:96:GLY:HA3	1.51	0.74
1:I:51:PHE:HE2	1:I:96:GLY:HA3	1.51	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:51:PHE:HE2	1:L:96:GLY:HA3	1.51	0.74
1:S:173:HIS:O	1:S:177:HIS:HD2	1.70	0.73
1:X:176:GLY:O	1:X:177:HIS:CG	2.42	0.72
1:L:173:HIS:O	1:L:177:HIS:CD2	2.42	0.72
1:S:173:HIS:O	1:S:177:HIS:ND1	2.22	0.72
1:C:165:MET:HG3	1:C:169:LEU:HD23	1.73	0.71
1:B:70:MET:HE1	1:E:35:LEU:HD11	1.73	0.71
1:F:165:MET:HG3	1:F:169:LEU:HD23	1.73	0.71
1:I:165:MET:HG3	1:I:169:LEU:HD23	1.73	0.71
1:L:165:MET:HG3	1:L:169:LEU:HD23	1.73	0.71
1:N:165:MET:HG3	1:N:169:LEU:HD23	1.73	0.71
1:Q:165:MET:HG3	1:Q:169:LEU:HD23	1.73	0.71
1:T:165:MET:HG3	1:T:169:LEU:HD23	1.73	0.71
1:U:165:MET:HG3	1:U:169:LEU:HD23	1.72	0.71
1:O:165:MET:HG3	1:O:169:LEU:HD23	1.73	0.71
1:W:165:MET:HG3	1:W:169:LEU:HD23	1.73	0.71
1:R:165:MET:HG3	1:R:169:LEU:HD23	1.73	0.71
1:X:165:MET:HG3	1:X:169:LEU:HD23	1.73	0.71
1:Q:125:ASN:HB3	1:R:119:LYS:HE3	1.72	0.71
1:C:165:MET:HG3	1:C:169:LEU:HD23	1.73	0.71
1:A:165:MET:HG3	1:A:169:LEU:HD23	1.72	0.71
1:G:165:MET:HG3	1:G:169:LEU:HD23	1.72	0.71
1:I:165:MET:HG3	1:I:169:LEU:HD23	1.73	0.71
1:S:165:MET:HG3	1:S:169:LEU:HD23	1.73	0.70
1:F:165:MET:HG3	1:F:169:LEU:HD23	1.73	0.70
1:M:165:MET:HG3	1:M:169:LEU:HD23	1.73	0.70
1:L:165:MET:HG3	1:L:169:LEU:HD23	1.73	0.70
1:K:165:MET:HG3	1:K:169:LEU:HD23	1.72	0.70
1:N:165:MET:HG3	1:N:169:LEU:HD23	1.73	0.70
1:S:165:MET:HG3	1:S:169:LEU:HD23	1.73	0.70
1:E:165:MET:HG3	1:E:169:LEU:HD23	1.73	0.70
1:M:165:MET:HG3	1:M:169:LEU:HD23	1.73	0.70
1:O:165:MET:HG3	1:O:169:LEU:HD23	1.73	0.70
1:U:165:MET:HG3	1:U:169:LEU:HD23	1.73	0.70
1:T:165:MET:HG3	1:T:169:LEU:HD23	1.73	0.70
1:X:165:MET:HG3	1:X:169:LEU:HD23	1.73	0.70
1:H:70:MET:HE1	1:K:35:LEU:HD11	1.74	0.70
1:Q:165:MET:HG3	1:Q:169:LEU:HD23	1.73	0.70
1:R:165:MET:HG3	1:R:169:LEU:HD23	1.73	0.70
1:W:165:MET:HG3	1:W:169:LEU:HD23	1.73	0.70
1:B:165:MET:HG3	1:B:169:LEU:HD23	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:165:MET:HG3	1:H:169:LEU:HD23	1.73	0.70
1:J:165:MET:HG3	1:J:169:LEU:HD23	1.72	0.70
1:G:165:MET:HG3	1:G:169:LEU:HD23	1.73	0.70
1:D:165:MET:HG3	1:D:169:LEU:HD23	1.73	0.69
1:E:125:ASN:HB3	1:F:119:LYS:HE3	1.74	0.69
1:A:165:MET:HG3	1:A:169:LEU:HD23	1.73	0.69
1:V:165:MET:HG3	1:V:169:LEU:HD23	1.72	0.69
1:P:165:MET:HG3	1:P:169:LEU:HD23	1.73	0.69
1:B:119:LYS:NZ	2:B:201:HOH:O	2.26	0.69
1:J:165:MET:HG3	1:J:169:LEU:HD23	1.73	0.69
1:H:119:LYS:NZ	2:H:201:HOH:O	2.00	0.69
1:D:165:MET:HG3	1:D:169:LEU:HD23	1.73	0.69
1:S:173:HIS:O	1:S:177:HIS:HD2	1.73	0.69
1:X:176:GLY:O	1:X:177:HIS:CG	2.46	0.69
1:H:165:MET:HG3	1:H:169:LEU:HD23	1.73	0.69
1:B:165:MET:HG3	1:B:169:LEU:HD23	1.73	0.69
1:E:165:MET:HG3	1:E:169:LEU:HD23	1.73	0.69
1:W:119:LYS:NZ	2:W:201:HOH:O	2.00	0.68
1:K:165:MET:HG3	1:K:169:LEU:HD23	1.73	0.68
1:C:70:MET:HE1	1:J:35:LEU:HD11	1.75	0.68
1:P:165:MET:HG3	1:P:169:LEU:HD23	1.73	0.68
1:V:165:MET:HG3	1:V:169:LEU:HD23	1.73	0.68
1:H:35:LEU:HD11	1:K:70:MET:HE1	1.75	0.68
1:Q:119:LYS:NZ	2:Q:201:HOH:O	2.00	0.68
1:B:35:LEU:HD11	1:E:70:MET:HE1	1.75	0.68
1:D:35:LEU:HD11	1:I:70:MET:HE1	1.75	0.68
1:N:35:LEU:HD11	1:Q:70:MET:HE1	1.76	0.68
1:S:173:HIS:HA	1:S:177:HIS:HE1	1.58	0.68
1:R:119:LYS:NZ	2:R:201:HOH:O	1.99	0.67
1:B:119:LYS:NZ	2:B:201:HOH:O	2.00	0.67
1:T:35:LEU:HD11	1:W:70:MET:HE1	1.77	0.67
1:S:119:LYS:HE3	1:U:125:ASN:HB3	1.77	0.67
1:I:119:LYS:NZ	2:I:201:HOH:O	2.00	0.66
1:M:90:ARG:NH1	1:M:98:ASN:HD21	1.93	0.66
1:N:90:ARG:NH1	1:N:98:ASN:HD21	1.93	0.66
1:T:90:ARG:NH1	1:T:98:ASN:HD21	1.93	0.66
1:I:168:TYR:HD2	1:I:169:LEU:HD22	1.60	0.66
1:C:119:LYS:NZ	2:C:201:HOH:O	2.00	0.66
1:A:90:ARG:NH1	1:A:98:ASN:HD21	1.93	0.66
1:D:90:ARG:NH1	1:D:98:ASN:HD21	1.93	0.66
1:J:90:ARG:NH1	1:J:98:ASN:HD21	1.93	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:90:ARG:NH1	1:S:98:ASN:HD21	1.93	0.66
1:C:168:TYR:HD2	1:C:169:LEU:HD22	1.61	0.66
1:Q:168:TYR:HD2	1:Q:169:LEU:HD22	1.60	0.66
1:W:168:TYR:HD2	1:W:169:LEU:HD22	1.61	0.66
1:L:90:ARG:NH1	1:L:98:ASN:HD21	1.93	0.66
1:G:168:TYR:HD2	1:G:169:LEU:HD22	1.61	0.66
1:F:90:ARG:NH1	1:F:98:ASN:HD21	1.93	0.66
1:G:90:ARG:NH1	1:G:98:ASN:HD21	1.93	0.66
1:R:168:TYR:HD2	1:R:169:LEU:HD22	1.61	0.66
1:X:168:TYR:HD2	1:X:169:LEU:HD22	1.61	0.66
1:K:125:ASN:HB3	1:L:119:LYS:HE3	1.78	0.66
1:V:90:ARG:NH1	1:V:98:ASN:HD21	1.93	0.66
1:A:168:TYR:HD2	1:A:169:LEU:HD22	1.61	0.66
1:B:90:ARG:NH1	1:B:98:ASN:HD21	1.93	0.66
1:E:90:ARG:NH1	1:E:98:ASN:HD21	1.93	0.66
1:H:90:ARG:NH1	1:H:98:ASN:HD21	1.93	0.66
1:O:90:ARG:NH1	1:O:98:ASN:HD21	1.93	0.66
1:U:90:ARG:NH1	1:U:98:ASN:HD21	1.93	0.66
1:N:168:TYR:HD2	1:N:169:LEU:HD22	1.61	0.66
1:T:168:TYR:HD2	1:T:169:LEU:HD22	1.61	0.66
1:K:90:ARG:NH1	1:K:98:ASN:HD21	1.93	0.66
1:P:90:ARG:NH1	1:P:98:ASN:HD21	1.93	0.66
1:D:168:TYR:HD2	1:D:169:LEU:HD22	1.61	0.66
1:V:168:TYR:HD2	1:V:169:LEU:HD22	1.61	0.66
1:J:168:TYR:HD2	1:J:169:LEU:HD22	1.61	0.66
1:P:119:LYS:HE3	1:R:125:ASN:HB3	1.78	0.66
1:Q:90:ARG:NH1	1:Q:98:ASN:HD21	1.93	0.66
1:M:168:TYR:HD2	1:M:169:LEU:HD22	1.61	0.66
1:P:168:TYR:HD2	1:P:169:LEU:HD22	1.61	0.66
1:W:90:ARG:NH1	1:W:98:ASN:HD21	1.93	0.65
1:Q:51:PHE:HE2	1:Q:96:GLY:HA3	1.62	0.65
1:R:51:PHE:HE2	1:R:96:GLY:HA3	1.62	0.65
1:S:168:TYR:HD2	1:S:169:LEU:HD22	1.61	0.65
1:B:168:TYR:HD2	1:B:169:LEU:HD22	1.61	0.65
1:F:168:TYR:HD2	1:F:169:LEU:HD22	1.61	0.65
1:H:168:TYR:HD2	1:H:169:LEU:HD22	1.61	0.65
1:F:51:PHE:HE2	1:F:96:GLY:HA3	1.62	0.65
1:L:51:PHE:HE2	1:L:96:GLY:HA3	1.62	0.65
1:W:51:PHE:HE2	1:W:96:GLY:HA3	1.62	0.65
1:X:51:PHE:HE2	1:X:96:GLY:HA3	1.62	0.65
1:L:168:TYR:HD2	1:L:169:LEU:HD22	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:ARG:NH1	1:C:98:ASN:HD21	1.93	0.65
1:R:90:ARG:NH1	1:R:98:ASN:HD21	1.93	0.65
1:X:119:LYS:NZ	2:X:201:HOH:O	2.00	0.65
1:G:51:PHE:HE2	1:G:96:GLY:HA3	1.62	0.65
1:I:90:ARG:NH1	1:I:98:ASN:HD21	1.93	0.65
1:C:51:PHE:HE2	1:C:96:GLY:HA3	1.62	0.65
1:I:51:PHE:HE2	1:I:96:GLY:HA3	1.62	0.65
1:J:51:PHE:HE2	1:J:96:GLY:HA3	1.62	0.65
1:T:70:MET:HE1	1:W:35:LEU:HD11	1.77	0.65
1:U:51:PHE:HE2	1:U:96:GLY:HA3	1.62	0.65
1:C:168:TYR:HD2	1:C:169:LEU:HD22	1.62	0.65
1:X:168:TYR:HD2	1:X:169:LEU:HD22	1.62	0.65
1:X:90:ARG:NH1	1:X:98:ASN:HD21	1.93	0.65
1:A:51:PHE:HE2	1:A:96:GLY:HA3	1.62	0.65
1:O:51:PHE:HE2	1:O:96:GLY:HA3	1.62	0.65
1:I:168:TYR:HD2	1:I:169:LEU:HD22	1.62	0.65
1:Q:168:TYR:HD2	1:Q:169:LEU:HD22	1.62	0.65
1:K:168:TYR:HD2	1:K:169:LEU:HD22	1.61	0.65
1:N:51:PHE:HE2	1:N:96:GLY:HA3	1.62	0.64
1:S:119:LYS:NZ	2:S:201:HOH:O	1.99	0.64
1:R:168:TYR:HD2	1:R:169:LEU:HD22	1.62	0.64
1:R:153:THR:HG22	1:R:157:LYS:NZ	2.12	0.64
1:D:51:PHE:HE2	1:D:96:GLY:HA3	1.62	0.64
1:S:51:PHE:HE2	1:S:96:GLY:HA3	1.62	0.64
1:G:119:LYS:HE3	1:I:125:ASN:HB3	1.78	0.64
1:W:168:TYR:HD2	1:W:169:LEU:HD22	1.62	0.64
1:X:153:THR:HG22	1:X:157:LYS:NZ	2.12	0.64
1:E:168:TYR:HD2	1:E:169:LEU:HD22	1.61	0.64
1:T:51:PHE:HE2	1:T:96:GLY:HA3	1.62	0.64
1:V:51:PHE:HE2	1:V:96:GLY:HA3	1.62	0.64
1:W:125:ASN:HB3	1:X:119:LYS:HE3	1.79	0.64
1:C:153:THR:HG22	1:C:157:LYS:NZ	2.13	0.64
1:I:153:THR:HG22	1:I:157:LYS:NZ	2.13	0.64
1:K:153:THR:HG22	1:K:157:LYS:NZ	2.12	0.64
1:P:51:PHE:HE2	1:P:96:GLY:HA3	1.62	0.64
1:A:168:TYR:HD2	1:A:169:LEU:HD22	1.62	0.64
1:G:168:TYR:HD2	1:G:169:LEU:HD22	1.63	0.64
1:A:153:THR:HG22	1:A:157:LYS:NZ	2.12	0.64
1:E:153:THR:HG22	1:E:157:LYS:NZ	2.12	0.64
1:G:153:THR:HG22	1:G:157:LYS:NZ	2.12	0.64
1:M:51:PHE:HE2	1:M:96:GLY:HA3	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:168:TYR:HD2	1:D:169:LEU:HD22	1.62	0.64
1:J:51:PHE:CE2	1:J:96:GLY:HA3	2.33	0.64
1:M:51:PHE:CE2	1:M:96:GLY:HA3	2.33	0.64
1:S:51:PHE:CE2	1:S:96:GLY:HA3	2.33	0.64
1:T:168:TYR:HD2	1:T:169:LEU:HD22	1.62	0.64
1:X:51:PHE:CE2	1:X:96:GLY:HA3	2.33	0.64
1:Q:153:THR:HG22	1:Q:157:LYS:NZ	2.13	0.64
1:W:153:THR:HG22	1:W:157:LYS:NZ	2.12	0.64
1:O:168:TYR:HD2	1:O:169:LEU:HD22	1.61	0.64
1:N:119:LYS:NZ	2:N:201:HOH:O	2.00	0.64
1:D:51:PHE:CE2	1:D:96:GLY:HA3	2.33	0.64
1:R:51:PHE:CE2	1:R:96:GLY:HA3	2.33	0.64
1:H:153:THR:HG22	1:H:157:LYS:NZ	2.12	0.64
1:P:153:THR:HG22	1:P:157:LYS:NZ	2.12	0.64
1:V:153:THR:HG22	1:V:157:LYS:NZ	2.12	0.64
1:U:168:TYR:HD2	1:U:169:LEU:HD22	1.61	0.64
1:E:51:PHE:HE2	1:E:96:GLY:HA3	1.62	0.64
1:D:110:VAL:O	1:D:114:LEU:HD13	1.98	0.64
1:F:168:TYR:HD2	1:F:169:LEU:HD22	1.62	0.64
1:J:110:VAL:O	1:J:114:LEU:HD13	1.98	0.64
1:L:168:TYR:HD2	1:L:169:LEU:HD22	1.62	0.64
1:K:51:PHE:HE2	1:K:96:GLY:HA3	1.62	0.64
1:N:70:MET:HE1	1:Q:35:LEU:HD11	1.78	0.64
1:N:168:TYR:HD2	1:N:169:LEU:HD22	1.63	0.64
1:R:110:VAL:O	1:R:114:LEU:HD13	1.98	0.64
1:V:168:TYR:HD2	1:V:169:LEU:HD22	1.62	0.64
1:X:110:VAL:O	1:X:114:LEU:HD13	1.98	0.64
1:B:153:THR:HG22	1:B:157:LYS:NZ	2.12	0.64
1:T:119:LYS:NZ	2:T:201:HOH:O	2.00	0.64
1:Q:51:PHE:CE2	1:Q:96:GLY:HA3	2.33	0.64
1:W:51:PHE:CE2	1:W:96:GLY:HA3	2.33	0.64
1:M:153:THR:HG22	1:M:157:LYS:NZ	2.13	0.64
1:N:153:THR:HG22	1:N:157:LYS:NZ	2.12	0.64
1:O:153:THR:HG22	1:O:157:LYS:NZ	2.12	0.64
1:S:153:THR:HG22	1:S:157:LYS:NZ	2.12	0.64
1:B:168:TYR:HD2	1:B:169:LEU:HD22	1.62	0.63
1:H:168:TYR:HD2	1:H:169:LEU:HD22	1.62	0.63
1:J:168:TYR:HD2	1:J:169:LEU:HD22	1.63	0.63
1:U:153:THR:HG22	1:U:157:LYS:NZ	2.12	0.63
1:M:168:TYR:HD2	1:M:169:LEU:HD22	1.62	0.63
1:P:168:TYR:HD2	1:P:169:LEU:HD22	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:153:THR:HG22	1:T:157:LYS:NZ	2.13	0.63
1:M:125:ASN:HB3	1:N:119:LYS:HE3	1.79	0.63
1:B:51:PHE:CE2	1:B:96:GLY:HA3	2.33	0.63
1:S:168:TYR:HD2	1:S:169:LEU:HD22	1.62	0.63
1:Q:51:PHE:HE2	1:Q:96:GLY:HA3	1.64	0.63
1:U:51:PHE:HE2	1:U:96:GLY:HA3	1.64	0.63
1:C:110:VAL:O	1:C:114:LEU:HD13	1.98	0.63
1:H:51:PHE:CE2	1:H:96:GLY:HA3	2.33	0.63
1:I:110:VAL:O	1:I:114:LEU:HD13	1.98	0.63
1:Q:110:VAL:O	1:Q:114:LEU:HD13	1.98	0.63
1:W:110:VAL:O	1:W:114:LEU:HD13	1.98	0.63
1:W:51:PHE:HE2	1:W:96:GLY:HA3	1.64	0.63
1:D:153:THR:HG22	1:D:157:LYS:NZ	2.12	0.63
1:F:153:THR:HG22	1:F:157:LYS:NZ	2.12	0.63
1:G:110:VAL:O	1:G:114:LEU:HD13	1.98	0.63
1:O:51:PHE:HE2	1:O:96:GLY:HA3	1.64	0.63
1:L:153:THR:HG22	1:L:157:LYS:NZ	2.12	0.63
1:P:67:GLU:HA	1:P:70:MET:HE2	1.81	0.63
1:A:110:VAL:O	1:A:114:LEU:HD13	1.98	0.63
1:T:51:PHE:CE2	1:T:96:GLY:HA3	2.33	0.63
1:F:51:PHE:HE2	1:F:96:GLY:HA3	1.64	0.63
1:J:119:LYS:HE3	1:L:125:ASN:HB3	1.80	0.63
1:K:119:LYS:NZ	2:K:201:HOH:O	2.00	0.63
1:C:153:THR:HG22	1:C:157:LYS:NZ	2.14	0.63
1:F:110:VAL:O	1:F:114:LEU:HD13	1.98	0.63
1:I:153:THR:HG22	1:I:157:LYS:NZ	2.14	0.63
1:K:51:PHE:CE2	1:K:96:GLY:HA3	2.33	0.63
1:K:110:VAL:O	1:K:114:LEU:HD13	1.98	0.63
1:M:110:VAL:O	1:M:114:LEU:HD13	1.98	0.63
1:N:51:PHE:CE2	1:N:96:GLY:HA3	2.33	0.63
1:O:51:PHE:CE2	1:O:96:GLY:HA3	2.33	0.63
1:R:153:THR:HG22	1:R:157:LYS:NZ	2.14	0.63
1:L:51:PHE:HE2	1:L:96:GLY:HA3	1.64	0.63
1:N:51:PHE:HE2	1:N:96:GLY:HA3	1.64	0.63
1:T:51:PHE:HE2	1:T:96:GLY:HA3	1.64	0.63
1:J:153:THR:HG22	1:J:157:LYS:NZ	2.13	0.63
1:B:51:PHE:HE2	1:B:96:GLY:HA3	1.62	0.63
1:V:67:GLU:HA	1:V:70:MET:HE2	1.81	0.63
1:H:125:ASN:HB3	1:I:119:LYS:HE3	1.79	0.63
1:M:119:LYS:NZ	2:M:201:HOH:O	2.00	0.63
1:U:119:LYS:NZ	2:U:201:HOH:O	2.00	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:110:VAL:O	1:E:114:LEU:HD13	1.98	0.63
1:K:153:THR:HG22	1:K:157:LYS:NZ	2.14	0.63
1:L:110:VAL:O	1:L:114:LEU:HD13	1.98	0.63
1:P:110:VAL:O	1:P:114:LEU:HD13	1.98	0.63
1:U:51:PHE:CE2	1:U:96:GLY:HA3	2.33	0.63
1:X:153:THR:HG22	1:X:157:LYS:NZ	2.14	0.63
1:V:51:PHE:HE2	1:V:96:GLY:HA3	1.64	0.63
1:A:153:THR:HG22	1:A:157:LYS:NZ	2.14	0.63
1:E:51:PHE:CE2	1:E:96:GLY:HA3	2.33	0.63
1:E:153:THR:HG22	1:E:157:LYS:NZ	2.14	0.63
1:G:153:THR:HG22	1:G:157:LYS:NZ	2.14	0.63
1:O:110:VAL:O	1:O:114:LEU:HD13	1.98	0.63
1:O:168:TYR:HD2	1:O:169:LEU:HD22	1.62	0.63
1:Q:153:THR:HG22	1:Q:157:LYS:NZ	2.14	0.63
1:S:110:VAL:O	1:S:114:LEU:HD13	1.98	0.63
1:E:51:PHE:HE2	1:E:96:GLY:HA3	1.64	0.63
1:H:51:PHE:HE2	1:H:96:GLY:HA3	1.62	0.62
1:N:110:VAL:O	1:N:114:LEU:HD13	1.98	0.62
1:U:110:VAL:O	1:U:114:LEU:HD13	1.98	0.62
1:U:168:TYR:HD2	1:U:169:LEU:HD22	1.62	0.62
1:K:51:PHE:HE2	1:K:96:GLY:HA3	1.64	0.62
1:P:51:PHE:HE2	1:P:96:GLY:HA3	1.64	0.62
1:A:70:MET:HE1	1:R:35:LEU:HD11	1.79	0.62
1:B:110:VAL:O	1:B:114:LEU:HD13	1.98	0.62
1:H:110:VAL:O	1:H:114:LEU:HD13	1.98	0.62
1:H:153:THR:HG22	1:H:157:LYS:NZ	2.14	0.62
1:K:168:TYR:HD2	1:K:169:LEU:HD22	1.62	0.62
1:T:110:VAL:O	1:T:114:LEU:HD13	1.98	0.62
1:V:110:VAL:O	1:V:114:LEU:HD13	1.98	0.62
1:V:153:THR:HG22	1:V:157:LYS:NZ	2.14	0.62
1:W:153:THR:HG22	1:W:157:LYS:NZ	2.14	0.62
1:A:51:PHE:HE2	1:A:96:GLY:HA3	1.64	0.62
1:R:51:PHE:HE2	1:R:96:GLY:HA3	1.65	0.62
1:A:119:LYS:HE3	1:C:125:ASN:HB3	1.80	0.62
1:P:153:THR:HG22	1:P:157:LYS:NZ	2.14	0.62
1:G:51:PHE:HE2	1:G:96:GLY:HA3	1.64	0.62
1:F:51:PHE:HE2	1:F:96:GLY:HA3	1.64	0.62
1:X:51:PHE:HE2	1:X:96:GLY:HA3	1.65	0.62
1:G:70:MET:HE1	1:X:35:LEU:HD11	1.79	0.62
1:B:153:THR:HG22	1:B:157:LYS:NZ	2.14	0.62
1:R:51:PHE:HE2	1:R:96:GLY:HA3	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:51:PHE:HE2	1:X:96:GLY:HA3	1.64	0.62
1:L:51:PHE:HE2	1:L:96:GLY:HA3	1.65	0.62
1:N:51:PHE:HE2	1:N:96:GLY:HA3	1.65	0.62
1:U:51:PHE:HE2	1:U:96:GLY:HA3	1.65	0.62
1:C:35:LEU:HD11	1:J:70:MET:HE1	1.81	0.62
1:D:119:LYS:HE3	1:F:125:ASN:HB3	1.80	0.62
1:G:119:LYS:NZ	2:G:201:HOH:O	1.99	0.62
1:M:153:THR:HG22	1:M:157:LYS:NZ	2.14	0.62
1:O:51:PHE:HE2	1:O:96:GLY:HA3	1.65	0.62
1:T:51:PHE:HE2	1:T:96:GLY:HA3	1.65	0.62
1:A:119:LYS:NZ	2:A:202:HOH:O	2.00	0.62
1:O:153:THR:HG22	1:O:157:LYS:NZ	2.14	0.62
1:U:153:THR:HG22	1:U:157:LYS:NZ	2.14	0.62
1:Q:51:PHE:HE2	1:Q:96:GLY:HA3	1.65	0.62
1:R:67:GLU:HA	1:R:70:MET:HE2	1.81	0.62
1:F:49:LYS:O	1:F:53:LYS:HG2	2.00	0.62
1:E:168:TYR:HD2	1:E:169:LEU:HD22	1.63	0.62
1:N:153:THR:HG22	1:N:157:LYS:NZ	2.14	0.62
1:S:153:THR:HG22	1:S:157:LYS:NZ	2.14	0.62
1:M:51:PHE:HE2	1:M:96:GLY:HA3	1.64	0.62
1:L:49:LYS:O	1:L:53:LYS:HG2	2.00	0.62
1:F:51:PHE:CE2	1:F:96:GLY:HA3	2.33	0.62
1:T:153:THR:HG22	1:T:157:LYS:NZ	2.14	0.62
1:E:51:PHE:HE2	1:E:96:GLY:HA3	1.65	0.62
1:W:51:PHE:HE2	1:W:96:GLY:HA3	1.65	0.62
1:D:70:MET:HE1	1:I:35:LEU:HD11	1.81	0.62
1:S:51:PHE:HE2	1:S:96:GLY:HA3	1.64	0.62
1:A:51:PHE:HE2	1:A:96:GLY:HA3	1.65	0.62
1:C:110:VAL:O	1:C:114:LEU:HD13	2.00	0.62
1:I:110:VAL:O	1:I:114:LEU:HD13	2.00	0.62
1:X:110:VAL:O	1:X:114:LEU:HD13	2.00	0.62
1:L:70:MET:HE1	1:S:35:LEU:HD11	1.82	0.62
1:N:49:LYS:O	1:N:53:LYS:HG2	2.00	0.62
1:O:119:LYS:NZ	2:O:201:HOH:O	2.00	0.62
1:T:49:LYS:O	1:T:53:LYS:HG2	2.00	0.62
1:A:51:PHE:CE2	1:A:96:GLY:HA3	2.33	0.62
1:D:153:THR:HG22	1:D:157:LYS:NZ	2.14	0.62
1:G:51:PHE:CE2	1:G:96:GLY:HA3	2.33	0.62
1:L:51:PHE:CE2	1:L:96:GLY:HA3	2.33	0.62
1:L:153:THR:HG22	1:L:157:LYS:NZ	2.14	0.62
1:G:51:PHE:HE2	1:G:96:GLY:HA3	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:51:PHE:HE2	1:J:96:GLY:HA3	1.65	0.62
1:J:119:LYS:NZ	2:J:201:HOH:O	1.99	0.61
1:Q:49:LYS:O	1:Q:53:LYS:HG2	2.00	0.61
1:W:49:LYS:O	1:W:53:LYS:HG2	2.00	0.61
1:F:153:THR:HG22	1:F:157:LYS:NZ	2.14	0.61
1:L:173:HIS:O	1:L:177:HIS:NE2	2.33	0.61
1:K:51:PHE:HE2	1:K:96:GLY:HA3	1.65	0.61
1:R:110:VAL:O	1:R:114:LEU:HD13	2.00	0.61
1:V:49:LYS:O	1:V:53:LYS:HG2	2.00	0.61
1:J:153:THR:HG22	1:J:157:LYS:NZ	2.14	0.61
1:D:51:PHE:HE2	1:D:96:GLY:HA3	1.65	0.61
1:D:110:VAL:O	1:D:114:LEU:HD13	2.00	0.61
1:U:110:VAL:O	1:U:114:LEU:HD13	2.00	0.61
1:X:67:GLU:HA	1:X:70:MET:HE2	1.82	0.61
1:H:49:LYS:O	1:H:53:LYS:HG2	2.00	0.61
1:P:49:LYS:O	1:P:53:LYS:HG2	2.00	0.61
1:R:49:LYS:O	1:R:53:LYS:HG2	2.00	0.61
1:T:125:ASN:HB3	1:U:119:LYS:HE3	1.81	0.61
1:X:49:LYS:O	1:X:53:LYS:HG2	2.00	0.61
1:B:51:PHE:HE2	1:B:96:GLY:HA3	1.64	0.61
1:I:51:PHE:HE2	1:I:96:GLY:HA3	1.65	0.61
1:J:110:VAL:O	1:J:114:LEU:HD13	2.00	0.61
1:B:49:LYS:O	1:B:53:LYS:HG2	2.00	0.61
1:P:119:LYS:NZ	2:P:201:HOH:O	2.00	0.61
1:P:51:PHE:CE2	1:P:96:GLY:HA3	2.33	0.61
1:V:51:PHE:CE2	1:V:96:GLY:HA3	2.33	0.61
1:D:51:PHE:HE2	1:D:96:GLY:HA3	1.64	0.61
1:H:51:PHE:HE2	1:H:96:GLY:HA3	1.64	0.61
1:J:51:PHE:HE2	1:J:96:GLY:HA3	1.64	0.61
1:B:110:VAL:O	1:B:114:LEU:HD13	2.00	0.61
1:H:110:VAL:O	1:H:114:LEU:HD13	2.00	0.61
1:O:110:VAL:O	1:O:114:LEU:HD13	2.00	0.61
1:U:67:GLU:HA	1:U:70:MET:HE2	1.82	0.61
1:I:51:PHE:HE2	1:I:96:GLY:HA3	1.64	0.61
1:C:51:PHE:HE2	1:C:96:GLY:HA3	1.65	0.61
1:P:110:VAL:O	1:P:114:LEU:HD13	2.00	0.61
1:V:51:PHE:HE2	1:V:96:GLY:HA3	1.65	0.61
1:D:49:LYS:O	1:D:53:LYS:HG2	2.00	0.61
1:I:51:PHE:CE2	1:I:96:GLY:HA3	2.33	0.61
1:N:110:VAL:O	1:N:114:LEU:HD13	2.00	0.61
1:S:51:PHE:HE2	1:S:96:GLY:HA3	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:110:VAL:O	1:V:114:LEU:HD13	2.00	0.61
1:J:49:LYS:O	1:J:53:LYS:HG2	2.00	0.61
1:C:51:PHE:HE2	1:C:96:GLY:HA3	1.64	0.61
1:O:67:GLU:HA	1:O:70:MET:HE2	1.82	0.61
1:A:49:LYS:O	1:A:53:LYS:HG2	2.00	0.61
1:E:49:LYS:O	1:E:53:LYS:HG2	2.00	0.61
1:K:49:LYS:O	1:K:53:LYS:HG2	2.00	0.61
1:A:51:PHE:CE2	1:A:96:GLY:HA3	2.36	0.61
1:G:51:PHE:CE2	1:G:96:GLY:HA3	2.36	0.61
1:A:11:ASN:ND2	2:B:201:HOH:O	2.33	0.61
1:G:110:VAL:O	1:G:114:LEU:HD13	2.00	0.61
1:M:51:PHE:HE2	1:M:96:GLY:HA3	1.65	0.61
1:P:51:PHE:HE2	1:P:96:GLY:HA3	1.65	0.61
1:T:110:VAL:O	1:T:114:LEU:HD13	2.00	0.61
1:C:51:PHE:CE2	1:C:96:GLY:HA3	2.33	0.61
1:I:51:PHE:CE2	1:I:96:GLY:HA3	2.36	0.61
1:R:51:PHE:CE2	1:R:96:GLY:HA3	2.36	0.61
1:X:51:PHE:CE2	1:X:96:GLY:HA3	2.36	0.61
1:C:49:LYS:O	1:C:53:LYS:HG2	2.00	0.60
1:G:49:LYS:O	1:G:53:LYS:HG2	2.00	0.60
1:I:49:LYS:O	1:I:53:LYS:HG2	2.00	0.60
1:C:51:PHE:CE2	1:C:96:GLY:HA3	2.36	0.60
1:U:51:PHE:CE2	1:U:96:GLY:HA3	2.36	0.60
1:A:110:VAL:O	1:A:114:LEU:HD13	2.00	0.60
1:Q:110:VAL:O	1:Q:114:LEU:HD13	2.00	0.60
1:W:110:VAL:O	1:W:114:LEU:HD13	2.00	0.60
1:F:70:MET:HE1	1:M:35:LEU:HD11	1.83	0.60
1:F:35:LEU:HD11	1:M:70:MET:HE1	1.83	0.60
1:L:35:LEU:HD11	1:S:70:MET:HE1	1.83	0.60
1:S:49:LYS:O	1:S:53:LYS:HG2	2.00	0.60
1:F:51:PHE:CE2	1:F:96:GLY:HA3	2.36	0.60
1:L:51:PHE:CE2	1:L:96:GLY:HA3	2.36	0.60
1:O:51:PHE:CE2	1:O:96:GLY:HA3	2.36	0.60
1:T:24:ILE:O	1:T:28:LEU:HD13	2.02	0.60
1:L:110:VAL:O	1:L:114:LEU:HD13	2.00	0.60
1:M:110:VAL:O	1:M:114:LEU:HD13	2.00	0.60
1:S:110:VAL:O	1:S:114:LEU:HD13	2.00	0.60
1:U:49:LYS:O	1:U:53:LYS:HG2	2.00	0.60
1:V:119:LYS:HE3	1:X:125:ASN:HB3	1.83	0.60
1:V:119:LYS:NZ	2:V:201:HOH:O	2.00	0.60
1:E:24:ILE:O	1:E:28:LEU:HD13	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:49:LYS:O	1:M:53:LYS:HG2	2.00	0.60
1:O:49:LYS:O	1:O:53:LYS:HG2	2.00	0.60
1:K:24:ILE:O	1:K:28:LEU:HD13	2.02	0.60
1:N:24:ILE:O	1:N:28:LEU:HD13	2.02	0.60
1:F:110:VAL:O	1:F:114:LEU:HD13	2.00	0.60
1:H:51:PHE:HE2	1:H:96:GLY:HA3	1.65	0.60
1:L:119:LYS:NZ	2:L:201:HOH:O	2.00	0.60
1:V:51:PHE:CE2	1:V:96:GLY:HA3	2.36	0.60
1:B:51:PHE:HE2	1:B:96:GLY:HA3	1.65	0.60
1:G:173:HIS:O	1:G:177:HIS:CE1	2.54	0.60
1:L:90:ARG:NH1	1:L:98:ASN:HD21	2.00	0.60
1:O:24:ILE:O	1:O:28:LEU:HD13	2.02	0.60
1:W:24:ILE:O	1:W:28:LEU:HD13	2.02	0.60
1:M:67:GLU:HA	1:M:70:MET:HE2	1.84	0.60
1:S:67:GLU:HA	1:S:70:MET:HE2	1.84	0.60
1:P:51:PHE:CE2	1:P:96:GLY:HA3	2.36	0.60
1:F:90:ARG:NH1	1:F:98:ASN:HD21	2.00	0.60
1:Q:24:ILE:O	1:Q:28:LEU:HD13	2.02	0.60
1:U:24:ILE:O	1:U:28:LEU:HD13	2.02	0.60
1:E:110:VAL:O	1:E:114:LEU:HD13	2.00	0.60
1:K:110:VAL:O	1:K:114:LEU:HD13	2.00	0.60
1:F:67:GLU:HA	1:F:70:MET:HE2	1.84	0.60
1:D:119:LYS:NZ	2:D:201:HOH:O	2.00	0.60
1:T:51:PHE:CE2	1:T:96:GLY:HA3	2.36	0.60
1:C:90:ARG:NH1	1:C:98:ASN:HD21	2.00	0.60
1:I:90:ARG:NH1	1:I:98:ASN:HD21	2.00	0.60
1:N:90:ARG:NH1	1:N:98:ASN:HD21	2.00	0.60
1:T:90:ARG:NH1	1:T:98:ASN:HD21	2.00	0.60
1:W:90:ARG:NH1	1:W:98:ASN:HD21	2.00	0.60
1:A:24:ILE:O	1:A:28:LEU:HD13	2.02	0.60
1:G:24:ILE:O	1:G:28:LEU:HD13	2.02	0.60
1:V:24:ILE:O	1:V:28:LEU:HD13	2.02	0.60
1:C:51:PHE:CE2	1:C:96:GLY:HA3	2.37	0.60
1:G:51:PHE:CE2	1:G:96:GLY:HA3	2.37	0.60
1:I:51:PHE:CE2	1:I:96:GLY:HA3	2.37	0.60
1:Q:90:ARG:NH1	1:Q:98:ASN:HD21	2.00	0.60
1:J:24:ILE:O	1:J:28:LEU:HD13	2.02	0.60
1:P:24:ILE:O	1:P:28:LEU:HD13	2.02	0.60
1:A:51:PHE:CE2	1:A:96:GLY:HA3	2.37	0.59
1:J:51:PHE:CE2	1:J:96:GLY:HA3	2.36	0.59
1:N:51:PHE:CE2	1:N:96:GLY:HA3	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:51:PHE:CE2	1:S:96:GLY:HA3	2.36	0.59
1:B:90:ARG:NH1	1:B:98:ASN:HD21	2.00	0.59
1:D:24:ILE:O	1:D:28:LEU:HD13	2.02	0.59
1:E:51:PHE:CE2	1:E:96:GLY:HA3	2.36	0.59
1:M:51:PHE:CE2	1:M:96:GLY:HA3	2.36	0.59
1:A:90:ARG:NH1	1:A:98:ASN:HD21	2.00	0.59
1:G:90:ARG:NH1	1:G:98:ASN:HD21	2.00	0.59
1:H:90:ARG:NH1	1:H:98:ASN:HD21	2.00	0.59
1:A:34:TYR:OH	1:A:107:GLU:OE2	2.17	0.59
1:C:24:ILE:O	1:C:28:LEU:HD13	2.02	0.59
1:D:51:PHE:CE2	1:D:96:GLY:HA3	2.36	0.59
1:F:24:ILE:O	1:F:28:LEU:HD13	2.02	0.59
1:I:24:ILE:O	1:I:28:LEU:HD13	2.02	0.59
1:O:51:PHE:CE2	1:O:96:GLY:HA3	2.37	0.59
1:K:51:PHE:CE2	1:K:96:GLY:HA3	2.36	0.59
1:L:24:ILE:O	1:L:28:LEU:HD13	2.02	0.59
1:R:24:ILE:O	1:R:28:LEU:HD13	2.02	0.59
1:X:24:ILE:O	1:X:28:LEU:HD13	2.02	0.59
1:F:51:PHE:CE2	1:F:96:GLY:HA3	2.37	0.59
1:J:51:PHE:CE2	1:J:96:GLY:HA3	2.37	0.59
1:L:51:PHE:CE2	1:L:96:GLY:HA3	2.37	0.59
1:F:119:LYS:NZ	2:F:201:HOH:O	1.99	0.59
1:Q:51:PHE:CE2	1:Q:96:GLY:HA3	2.36	0.59
1:W:51:PHE:CE2	1:W:96:GLY:HA3	2.36	0.59
1:D:51:PHE:CE2	1:D:96:GLY:HA3	2.38	0.59
1:S:51:PHE:CE2	1:S:96:GLY:HA3	2.37	0.59
1:U:51:PHE:CE2	1:U:96:GLY:HA3	2.37	0.59
1:N:125:ASN:HB3	1:O:119:LYS:HE3	1.83	0.59
1:B:24:ILE:O	1:B:28:LEU:HD13	2.02	0.59
1:H:24:ILE:O	1:H:28:LEU:HD13	2.02	0.59
1:M:24:ILE:O	1:M:28:LEU:HD13	2.02	0.59
1:E:90:ARG:NH1	1:E:98:ASN:HD21	2.00	0.59
1:K:90:ARG:NH1	1:K:98:ASN:HD21	2.00	0.59
1:U:90:ARG:NH1	1:U:98:ASN:HD21	2.00	0.59
1:S:24:ILE:O	1:S:28:LEU:HD13	2.02	0.59
1:M:51:PHE:CE2	1:M:96:GLY:HA3	2.37	0.59
1:X:51:PHE:CE2	1:X:96:GLY:HA3	2.37	0.59
1:J:125:ASN:HB3	1:K:119:LYS:HE3	1.84	0.59
1:V:125:ASN:HB3	1:W:119:LYS:HE3	1.84	0.59
1:O:90:ARG:NH1	1:O:98:ASN:HD21	2.00	0.59
1:S:90:ARG:NH1	1:S:98:ASN:HD21	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:67:GLU:HA	1:L:70:MET:HE2	1.85	0.59
1:P:35:LEU:HD11	1:U:70:MET:HE1	1.85	0.59
1:R:51:PHE:CE2	1:R:96:GLY:HA3	2.37	0.59
1:T:51:PHE:CE2	1:T:96:GLY:HA3	2.37	0.59
1:P:125:ASN:HB3	1:Q:119:LYS:HE3	1.84	0.59
1:M:90:ARG:NH1	1:M:98:ASN:HD21	2.00	0.59
1:R:90:ARG:NH1	1:R:98:ASN:HD21	2.00	0.59
1:X:90:ARG:NH1	1:X:98:ASN:HD21	2.00	0.59
1:N:51:PHE:CE2	1:N:96:GLY:HA3	2.37	0.58
1:H:51:PHE:CE2	1:H:96:GLY:HA3	2.36	0.58
1:O:70:MET:HE1	1:V:35:LEU:HD11	1.85	0.58
1:Q:51:PHE:CE2	1:Q:96:GLY:HA3	2.37	0.58
1:C:51:PHE:CE2	1:C:96:GLY:HA3	2.39	0.58
1:I:51:PHE:CE2	1:I:96:GLY:HA3	2.39	0.58
1:E:51:PHE:CE2	1:E:96:GLY:HA3	2.37	0.58
1:B:51:PHE:CE2	1:B:96:GLY:HA3	2.36	0.58
1:A:51:PHE:CE2	1:A:96:GLY:HA3	2.39	0.58
1:G:51:PHE:CE2	1:G:96:GLY:HA3	2.39	0.58
1:K:51:PHE:CE2	1:K:96:GLY:HA3	2.37	0.58
1:P:51:PHE:CE2	1:P:96:GLY:HA3	2.37	0.58
1:W:51:PHE:CE2	1:W:96:GLY:HA3	2.37	0.58
1:A:125:ASN:HB3	1:B:119:LYS:HE3	1.84	0.58
1:U:51:PHE:CE2	1:U:96:GLY:HA3	2.39	0.58
1:H:51:PHE:CE2	1:H:96:GLY:HA3	2.37	0.58
1:V:51:PHE:CE2	1:V:96:GLY:HA3	2.37	0.58
1:P:90:ARG:NH1	1:P:98:ASN:HD21	2.00	0.58
1:V:90:ARG:NH1	1:V:98:ASN:HD21	2.00	0.58
1:D:90:ARG:NH1	1:D:98:ASN:HD21	2.00	0.58
1:J:90:ARG:NH1	1:J:98:ASN:HD21	2.00	0.58
1:F:51:PHE:CE2	1:F:96:GLY:HA3	2.39	0.58
1:L:51:PHE:CE2	1:L:96:GLY:HA3	2.39	0.58
1:O:51:PHE:CE2	1:O:96:GLY:HA3	2.39	0.58
1:B:51:PHE:CE2	1:B:96:GLY:HA3	2.37	0.58
1:B:125:ASN:HB3	1:C:119:LYS:HE3	1.84	0.58
1:G:34:TYR:OH	1:G:107:GLU:OE2	2.18	0.58
1:G:35:LEU:HD11	1:X:70:MET:HE1	1.86	0.58
1:R:51:PHE:CE2	1:R:96:GLY:HA3	2.39	0.58
1:C:153:THR:HG22	1:C:157:LYS:NZ	2.19	0.58
1:M:119:LYS:HE3	1:O:125:ASN:HB3	1.85	0.58
1:J:51:PHE:CE2	1:J:96:GLY:HA3	2.39	0.58
1:G:125:ASN:HB3	1:H:119:LYS:HE3	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:TYR:OH	1:A:107:GLU:OE2	2.19	0.57
1:D:51:PHE:CE2	1:D:96:GLY:HA3	2.39	0.57
1:X:51:PHE:CE2	1:X:96:GLY:HA3	2.39	0.57
1:I:153:THR:HG22	1:I:157:LYS:NZ	2.19	0.57
1:N:24:ILE:O	1:N:28:LEU:HD13	2.05	0.57
1:T:24:ILE:O	1:T:28:LEU:HD13	2.05	0.57
1:H:153:THR:HG22	1:H:157:LYS:NZ	2.19	0.57
1:O:24:ILE:O	1:O:28:LEU:HD13	2.05	0.57
1:S:51:PHE:CE2	1:S:96:GLY:HA3	2.39	0.57
1:T:51:PHE:CE2	1:T:96:GLY:HA3	2.39	0.57
1:O:35:LEU:HD11	1:V:70:MET:HE1	1.87	0.57
1:B:153:THR:HG22	1:B:157:LYS:NZ	2.19	0.57
1:G:153:THR:HG22	1:G:157:LYS:NZ	2.19	0.57
1:O:153:THR:HG22	1:O:157:LYS:NZ	2.19	0.57
1:N:90:ARG:NH1	1:N:98:ASN:HD21	2.03	0.57
1:T:90:ARG:NH1	1:T:98:ASN:HD21	2.03	0.57
1:E:24:ILE:O	1:E:28:LEU:HD13	2.05	0.57
1:K:24:ILE:O	1:K:28:LEU:HD13	2.05	0.57
1:U:24:ILE:O	1:U:28:LEU:HD13	2.05	0.57
1:A:153:THR:HG22	1:A:157:LYS:HZ2	1.67	0.57
1:E:51:PHE:CE2	1:E:96:GLY:HA3	2.39	0.57
1:M:51:PHE:CE2	1:M:96:GLY:HA3	2.39	0.57
1:N:51:PHE:CE2	1:N:96:GLY:HA3	2.39	0.57
1:V:51:PHE:CE2	1:V:96:GLY:HA3	2.39	0.57
1:A:153:THR:HG22	1:A:157:LYS:NZ	2.19	0.57
1:R:153:THR:HG22	1:R:157:LYS:NZ	2.19	0.57
1:S:125:ASN:HB3	1:T:119:LYS:HE3	1.85	0.57
1:U:153:THR:HG22	1:U:157:LYS:NZ	2.19	0.57
1:X:153:THR:HG22	1:X:157:LYS:NZ	2.19	0.57
1:C:153:THR:HG22	1:C:157:LYS:HZ3	1.69	0.57
1:H:34:TYR:OH	1:H:107:GLU:OE2	2.17	0.57
1:E:153:THR:HG22	1:E:157:LYS:NZ	2.19	0.57
1:E:90:ARG:NH1	1:E:98:ASN:HD21	2.03	0.57
1:G:90:ARG:NH1	1:G:98:ASN:HD21	2.03	0.57
1:Q:90:ARG:NH1	1:Q:98:ASN:HD21	2.03	0.57
1:W:90:ARG:NH1	1:W:98:ASN:HD21	2.03	0.57
1:P:24:ILE:O	1:P:28:LEU:HD13	2.05	0.57
1:V:24:ILE:O	1:V:28:LEU:HD13	2.05	0.57
1:G:153:THR:HG22	1:G:157:LYS:HZ2	1.67	0.57
1:H:51:PHE:CE2	1:H:96:GLY:HA3	2.39	0.57
1:K:51:PHE:CE2	1:K:96:GLY:HA3	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:51:PHE:CE2	1:P:96:GLY:HA3	2.39	0.57
1:Q:51:PHE:CE2	1:Q:96:GLY:HA3	2.39	0.57
1:K:153:THR:HG22	1:K:157:LYS:NZ	2.19	0.57
1:A:90:ARG:NH1	1:A:98:ASN:HD21	2.03	0.57
1:K:90:ARG:NH1	1:K:98:ASN:HD21	2.03	0.57
1:L:24:ILE:O	1:L:28:LEU:HD13	2.05	0.57
1:Q:24:ILE:O	1:Q:28:LEU:HD13	2.05	0.57
1:W:24:ILE:O	1:W:28:LEU:HD13	2.05	0.57
1:C:144:SER:O	1:C:148:LEU:HD13	2.05	0.57
1:I:144:SER:O	1:I:148:LEU:HD13	2.05	0.57
1:Q:153:THR:HG22	1:Q:157:LYS:NZ	2.19	0.57
1:F:24:ILE:O	1:F:28:LEU:HD13	2.05	0.57
1:B:51:PHE:CE2	1:B:96:GLY:HA3	2.39	0.57
1:F:153:THR:HG22	1:F:157:LYS:NZ	2.19	0.57
1:V:153:THR:HG22	1:V:157:LYS:NZ	2.19	0.57
1:W:153:THR:HG22	1:W:157:LYS:NZ	2.19	0.57
1:B:24:ILE:O	1:B:28:LEU:HD13	2.05	0.57
1:S:173:HIS:O	1:S:177:HIS:CD2	2.57	0.57
1:W:51:PHE:CE2	1:W:96:GLY:HA3	2.39	0.57
1:J:144:SER:O	1:J:148:LEU:HD13	2.05	0.57
1:L:153:THR:HG22	1:L:157:LYS:NZ	2.19	0.57
1:P:153:THR:HG22	1:P:157:LYS:NZ	2.19	0.57
1:X:24:ILE:O	1:X:28:LEU:HD13	2.05	0.57
1:G:34:TYR:OH	1:G:107:GLU:OE2	2.17	0.57
1:N:153:THR:HG22	1:N:157:LYS:NZ	2.19	0.56
1:T:153:THR:HG22	1:T:157:LYS:NZ	2.19	0.56
1:D:90:ARG:NH1	1:D:98:ASN:HD21	2.03	0.56
1:X:177:HIS:O	1:X:177:HIS:ND1	2.38	0.56
1:H:24:ILE:O	1:H:28:LEU:HD13	2.05	0.56
1:M:24:ILE:O	1:M:28:LEU:HD13	2.05	0.56
1:R:24:ILE:O	1:R:28:LEU:HD13	2.05	0.56
1:P:70:MET:HE1	1:U:35:LEU:HD11	1.87	0.56
1:D:144:SER:O	1:D:148:LEU:HD13	2.05	0.56
1:H:144:SER:O	1:H:148:LEU:HD13	2.05	0.56
1:M:153:THR:HG22	1:M:157:LYS:NZ	2.19	0.56
1:S:153:THR:HG22	1:S:157:LYS:NZ	2.19	0.56
1:J:75:GLN:HG2	1:K:142:VAL:HG12	1.87	0.56
1:J:90:ARG:NH1	1:J:98:ASN:HD21	2.03	0.56
1:S:24:ILE:O	1:S:28:LEU:HD13	2.05	0.56
1:A:35:LEU:HD11	1:R:70:MET:HE1	1.87	0.56
1:O:119:LYS:HD2	2:O:201:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:SER:O	1:B:148:LEU:HD13	2.05	0.56
1:R:144:SER:O	1:R:148:LEU:HD13	2.05	0.56
1:S:144:SER:O	1:S:148:LEU:HD13	2.05	0.56
1:G:153:THR:HG22	1:G:157:LYS:HZ2	1.68	0.56
1:B:90:ARG:NH1	1:B:98:ASN:HD21	2.03	0.56
1:X:90:ARG:NH1	1:X:98:ASN:HD21	2.03	0.56
1:A:144:SER:O	1:A:148:LEU:HD13	2.05	0.56
1:G:144:SER:O	1:G:148:LEU:HD13	2.05	0.56
1:M:144:SER:O	1:M:148:LEU:HD13	2.05	0.56
1:P:144:SER:O	1:P:148:LEU:HD13	2.05	0.56
1:V:144:SER:O	1:V:148:LEU:HD13	2.05	0.56
1:X:144:SER:O	1:X:148:LEU:HD13	2.05	0.56
1:I:90:ARG:NH1	1:I:98:ASN:HD21	2.03	0.56
1:P:34:TYR:OH	1:P:107:GLU:OE2	2.18	0.56
1:G:173:HIS:O	1:G:177:HIS:CE1	2.58	0.56
1:H:90:ARG:NH1	1:H:98:ASN:HD21	2.03	0.56
1:D:24:ILE:O	1:D:28:LEU:HD13	2.05	0.56
1:G:24:ILE:O	1:G:28:LEU:HD13	2.05	0.56
1:D:67:GLU:HA	1:D:70:MET:HE2	1.86	0.56
1:J:67:GLU:HA	1:J:70:MET:HE2	1.86	0.56
1:E:144:SER:O	1:E:148:LEU:HD13	2.05	0.56
1:N:144:SER:O	1:N:148:LEU:HD13	2.05	0.56
1:C:90:ARG:NH1	1:C:98:ASN:HD21	2.03	0.56
1:M:90:ARG:NH1	1:M:98:ASN:HD21	2.03	0.56
1:R:90:ARG:NH1	1:R:98:ASN:HD21	2.03	0.56
1:V:90:ARG:NH1	1:V:98:ASN:HD21	2.03	0.56
1:A:24:ILE:O	1:A:28:LEU:HD13	2.05	0.56
1:J:24:ILE:O	1:J:28:LEU:HD13	2.05	0.56
1:J:153:THR:HG22	1:J:157:LYS:NZ	2.19	0.56
1:K:144:SER:O	1:K:148:LEU:HD13	2.05	0.56
1:T:144:SER:O	1:T:148:LEU:HD13	2.05	0.56
1:S:90:ARG:NH1	1:S:98:ASN:HD21	2.03	0.56
1:Q:90:ARG:NH1	1:Q:98:ASN:HD21	2.04	0.56
1:W:90:ARG:NH1	1:W:98:ASN:HD21	2.04	0.56
1:D:153:THR:HG22	1:D:157:LYS:NZ	2.19	0.56
1:T:90:ARG:NH1	1:T:98:ASN:HD21	2.04	0.56
1:L:90:ARG:NH1	1:L:98:ASN:HD21	2.03	0.56
1:U:90:ARG:NH1	1:U:98:ASN:HD21	2.03	0.56
1:A:119:LYS:HD2	2:A:202:HOH:O	2.07	0.56
1:N:90:ARG:NH1	1:N:98:ASN:HD21	2.04	0.56
1:P:90:ARG:NH1	1:P:98:ASN:HD21	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:ARG:NH1	1:C:98:ASN:HD21	2.04	0.55
1:G:119:LYS:HD2	2:G:201:HOH:O	2.07	0.55
1:P:90:ARG:NH1	1:P:98:ASN:HD21	2.04	0.55
1:F:90:ARG:NH1	1:F:98:ASN:HD21	2.03	0.55
1:O:90:ARG:NH1	1:O:98:ASN:HD21	2.03	0.55
1:I:90:ARG:NH1	1:I:98:ASN:HD21	2.04	0.55
1:V:90:ARG:NH1	1:V:98:ASN:HD21	2.04	0.55
1:Q:144:SER:O	1:Q:148:LEU:HD13	2.05	0.55
1:U:144:SER:O	1:U:148:LEU:HD13	2.05	0.55
1:W:144:SER:O	1:W:148:LEU:HD13	2.05	0.55
1:H:75:GLN:HG2	1:I:142:VAL:HG12	1.88	0.55
1:J:75:GLN:HG2	1:K:142:VAL:HG12	1.88	0.55
1:U:119:LYS:HD2	2:U:201:HOH:O	2.07	0.55
1:F:144:SER:O	1:F:148:LEU:HD13	2.05	0.55
1:O:144:SER:O	1:O:148:LEU:HD13	2.05	0.55
1:D:75:GLN:HG2	1:E:142:VAL:HG12	1.88	0.55
1:S:142:VAL:HG12	1:U:75:GLN:HG2	1.89	0.55
1:F:119:LYS:HD2	2:F:201:HOH:O	2.07	0.55
1:I:119:LYS:HD2	2:I:201:HOH:O	2.06	0.55
1:L:119:LYS:HD2	2:L:201:HOH:O	2.06	0.55
1:B:90:ARG:NH1	1:B:98:ASN:HD21	2.04	0.55
1:D:90:ARG:NH1	1:D:98:ASN:HD21	2.04	0.55
1:J:90:ARG:NH1	1:J:98:ASN:HD21	2.04	0.55
1:N:67:GLU:HA	1:N:70:MET:HE2	1.88	0.55
1:R:119:LYS:HD2	2:R:201:HOH:O	2.07	0.55
1:X:119:LYS:HD2	2:X:201:HOH:O	2.06	0.55
1:A:153:THR:HG22	1:A:157:LYS:HZ2	1.70	0.55
1:C:24:ILE:O	1:C:28:LEU:HD13	2.05	0.55
1:I:24:ILE:O	1:I:28:LEU:HD13	2.05	0.55
1:S:142:VAL:HG12	1:U:75:GLN:HG2	1.89	0.55
1:K:153:THR:HG22	1:K:157:LYS:HZ3	1.71	0.55
1:T:153:THR:HG22	1:T:157:LYS:HZ2	1.71	0.55
1:C:119:LYS:HD2	2:C:201:HOH:O	2.07	0.55
1:E:90:ARG:NH1	1:E:98:ASN:HD21	2.04	0.55
1:H:90:ARG:NH1	1:H:98:ASN:HD21	2.04	0.55
1:P:119:LYS:HD2	2:P:201:HOH:O	2.06	0.55
1:X:90:ARG:NH1	1:X:98:ASN:HD21	2.04	0.55
1:L:144:SER:O	1:L:148:LEU:HD13	2.05	0.55
1:M:115:LEU:O	1:M:119:LYS:HG2	2.07	0.55
1:F:90:ARG:NH1	1:F:98:ASN:HD21	2.04	0.55
1:V:119:LYS:HD2	2:V:201:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:GLN:HG2	1:E:142:VAL:HG12	1.89	0.55
1:D:75:GLN:HG2	1:E:142:VAL:HG12	1.89	0.55
1:S:142:VAL:HG12	1:U:75:GLN:HG2	1.89	0.55
1:E:119:LYS:HD2	2:E:228:HOH:O	2.07	0.55
1:K:90:ARG:NH1	1:K:98:ASN:HD21	2.04	0.55
1:S:142:VAL:HG12	1:U:75:GLN:HG2	1.89	0.55
1:L:165:MET:O	1:L:169:LEU:HD23	2.07	0.55
1:V:142:VAL:HG12	1:X:75:GLN:HG2	1.89	0.55
1:G:90:ARG:NH1	1:G:98:ASN:HD21	2.04	0.55
1:K:119:LYS:HD2	2:K:201:HOH:O	2.07	0.55
1:L:90:ARG:NH1	1:L:98:ASN:HD21	2.04	0.55
1:R:90:ARG:NH1	1:R:98:ASN:HD21	2.04	0.55
1:T:115:LEU:O	1:T:119:LYS:HG2	2.07	0.55
1:F:165:MET:O	1:F:169:LEU:HD23	2.07	0.55
1:K:165:MET:O	1:K:169:LEU:HD23	2.07	0.55
1:V:165:MET:O	1:V:169:LEU:HD23	2.07	0.55
1:H:75:GLN:HG2	1:I:142:VAL:HG12	1.88	0.55
1:W:75:GLN:HG2	1:X:142:VAL:HG12	1.89	0.55
1:P:142:VAL:HG12	1:R:75:GLN:HG2	1.89	0.55
1:S:142:VAL:HG12	1:U:75:GLN:HG2	1.89	0.55
1:V:142:VAL:HG12	1:X:75:GLN:HG2	1.89	0.55
1:A:67:GLU:HA	1:A:70:MET:HE2	1.87	0.55
1:A:90:ARG:NH1	1:A:98:ASN:HD21	2.04	0.55
1:S:90:ARG:NH1	1:S:98:ASN:HD21	2.04	0.55
1:C:115:LEU:O	1:C:119:LYS:HG2	2.07	0.55
1:D:75:GLN:HG2	1:E:142:VAL:HG12	1.89	0.55
1:E:165:MET:O	1:E:169:LEU:HD23	2.07	0.55
1:J:165:MET:O	1:J:169:LEU:HD23	2.07	0.55
1:M:165:MET:O	1:M:169:LEU:HD23	2.07	0.55
1:M:142:VAL:HG12	1:O:75:GLN:HG2	1.89	0.55
1:M:142:VAL:HG12	1:O:75:GLN:HG2	1.89	0.55
1:M:90:ARG:NH1	1:M:98:ASN:HD21	2.04	0.54
1:G:75:GLN:HG2	1:H:142:VAL:HG12	1.89	0.54
1:J:75:GLN:HG2	1:K:142:VAL:HG12	1.89	0.54
1:A:165:MET:O	1:A:169:LEU:HD23	2.07	0.54
1:H:165:MET:O	1:H:169:LEU:HD23	2.07	0.54
1:P:165:MET:O	1:P:169:LEU:HD23	2.07	0.54
1:S:165:MET:O	1:S:169:LEU:HD23	2.07	0.54
1:B:75:GLN:HG2	1:C:142:VAL:HG12	1.88	0.54
1:M:142:VAL:HG12	1:O:75:GLN:HG2	1.90	0.54
1:W:34:TYR:OH	1:W:107:GLU:OE2	2.18	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:90:ARG:HH12	1:K:98:ASN:HD21	1.55	0.54
1:G:67:GLU:HA	1:G:70:MET:HE2	1.87	0.54
1:N:119:LYS:HD2	2:N:201:HOH:O	2.06	0.54
1:V:142:VAL:HG12	1:X:75:GLN:HG2	1.89	0.54
1:W:75:GLN:HG2	1:X:142:VAL:HG12	1.89	0.54
1:B:165:MET:O	1:B:169:LEU:HD23	2.07	0.54
1:D:165:MET:O	1:D:169:LEU:HD23	2.07	0.54
1:G:165:MET:O	1:G:169:LEU:HD23	2.07	0.54
1:N:165:MET:O	1:N:169:LEU:HD23	2.07	0.54
1:T:165:MET:O	1:T:169:LEU:HD23	2.07	0.54
1:P:75:GLN:HG2	1:Q:142:VAL:HG12	1.88	0.54
1:W:75:GLN:HG2	1:X:142:VAL:HG12	1.89	0.54
1:Q:75:GLN:HG2	1:R:142:VAL:HG12	1.89	0.54
1:E:90:ARG:HH12	1:E:98:ASN:HD21	1.56	0.54
1:H:75:GLN:HG2	1:I:142:VAL:HG12	1.88	0.54
1:J:142:VAL:HG12	1:L:75:GLN:HG2	1.89	0.54
1:Q:75:GLN:HG2	1:R:142:VAL:HG12	1.89	0.54
1:W:75:GLN:HG2	1:X:142:VAL:HG12	1.89	0.54
1:D:119:LYS:HD2	2:D:201:HOH:O	2.06	0.54
1:J:119:LYS:HD2	2:J:201:HOH:O	2.06	0.54
1:T:119:LYS:HD2	2:T:201:HOH:O	2.06	0.54
1:P:142:VAL:HG12	1:R:75:GLN:HG2	1.89	0.54
1:O:165:MET:O	1:O:169:LEU:HD23	2.07	0.54
1:U:165:MET:O	1:U:169:LEU:HD23	2.07	0.54
1:W:165:MET:O	1:W:169:LEU:HD23	2.07	0.54
1:Q:75:GLN:HG2	1:R:142:VAL:HG12	1.89	0.54
1:P:142:VAL:HG12	1:R:75:GLN:HG2	1.90	0.54
1:C:34:TYR:OH	1:C:107:GLU:OE2	2.21	0.54
1:D:153:THR:HG22	1:D:157:LYS:HZ3	1.72	0.54
1:J:153:THR:HG22	1:J:157:LYS:HZ3	1.72	0.54
1:D:75:GLN:HG2	1:E:142:VAL:HG12	1.89	0.54
1:D:142:VAL:HG12	1:F:75:GLN:HG2	1.89	0.54
1:V:90:ARG:HH12	1:V:98:ASN:HD21	1.56	0.54
1:W:75:GLN:HG2	1:X:142:VAL:HG12	1.89	0.54
1:J:75:GLN:HG2	1:K:142:VAL:HG12	1.89	0.54
1:P:142:VAL:HG12	1:R:75:GLN:HG2	1.90	0.54
1:P:142:VAL:HG12	1:R:75:GLN:HG2	1.90	0.54
1:Q:75:GLN:HG2	1:R:142:VAL:HG12	1.89	0.54
1:V:142:VAL:HG12	1:X:75:GLN:HG2	1.90	0.54
1:Q:75:GLN:HG2	1:R:142:VAL:HG12	1.89	0.54
1:Q:119:LYS:HD2	2:Q:201:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:67:GLU:HA	1:T:70:MET:HE2	1.90	0.54
1:W:119:LYS:HD2	2:W:201:HOH:O	2.07	0.54
1:V:115:LEU:O	1:V:119:LYS:HG2	2.07	0.54
1:J:75:GLN:HG2	1:K:142:VAL:HG12	1.90	0.54
1:Q:165:MET:O	1:Q:169:LEU:HD23	2.07	0.54
1:V:75:GLN:HG2	1:W:142:VAL:HG12	1.89	0.54
1:B:75:GLN:HG2	1:C:142:VAL:HG12	1.89	0.54
1:I:34:TYR:OH	1:I:107:GLU:OE2	2.21	0.54
1:G:75:GLN:HG2	1:H:142:VAL:HG12	1.89	0.54
1:P:90:ARG:HH12	1:P:98:ASN:HD21	1.56	0.54
1:J:142:VAL:HG12	1:L:75:GLN:HG2	1.89	0.54
1:S:142:VAL:HG12	1:U:75:GLN:HG2	1.90	0.54
1:U:90:ARG:NH1	1:U:98:ASN:HD21	2.04	0.54
1:N:75:GLN:HG2	1:O:142:VAL:HG12	1.88	0.54
1:G:34:TYR:OH	1:G:107:GLU:OE2	2.19	0.54
1:J:153:THR:HG22	1:J:157:LYS:HZ3	1.72	0.54
1:C:34:TYR:OH	1:C:107:GLU:OE2	2.21	0.54
1:N:75:GLN:HG2	1:O:142:VAL:HG12	1.88	0.54
1:J:75:GLN:HG2	1:K:142:VAL:HG12	1.90	0.54
1:P:142:VAL:HG12	1:R:75:GLN:HG2	1.90	0.54
1:A:90:ARG:HH12	1:A:98:ASN:HD21	1.56	0.54
1:D:142:VAL:HG12	1:F:75:GLN:HG2	1.89	0.54
1:A:75:GLN:HG2	1:B:142:VAL:HG12	1.90	0.54
1:B:119:LYS:HD2	2:B:201:HOH:O	2.06	0.54
1:H:119:LYS:HD2	2:H:201:HOH:O	2.06	0.54
1:W:67:GLU:HA	1:W:70:MET:HE2	1.90	0.54
1:B:115:LEU:O	1:B:119:LYS:HG2	2.07	0.54
1:C:153:THR:HG22	1:C:157:LYS:HZ3	1.72	0.54
1:D:142:VAL:HG12	1:F:75:GLN:HG2	1.89	0.54
1:H:115:LEU:O	1:H:119:LYS:HG2	2.07	0.54
1:J:142:VAL:HG12	1:L:75:GLN:HG2	1.89	0.54
1:K:115:LEU:O	1:K:119:LYS:HG2	2.07	0.54
1:S:142:VAL:HG12	1:U:75:GLN:HG2	1.90	0.54
1:V:142:VAL:HG12	1:X:75:GLN:HG2	1.90	0.54
1:W:75:GLN:HG2	1:X:142:VAL:HG12	1.90	0.54
1:G:75:GLN:HG2	1:H:142:VAL:HG12	1.89	0.54
1:H:90:ARG:HH12	1:H:98:ASN:HD21	1.56	0.54
1:T:90:ARG:HH12	1:T:98:ASN:HD21	1.56	0.54
1:A:75:GLN:HG2	1:B:142:VAL:HG12	1.89	0.54
1:D:75:GLN:HG2	1:E:142:VAL:HG12	1.90	0.54
1:G:75:GLN:HG2	1:H:142:VAL:HG12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:90:ARG:NH1	1:O:98:ASN:HD21	2.04	0.54
1:V:142:VAL:HG12	1:X:75:GLN:HG2	1.90	0.54
1:A:75:GLN:HG2	1:B:142:VAL:HG12	1.89	0.54
1:M:142:VAL:HG12	1:O:75:GLN:HG2	1.90	0.54
1:A:34:TYR:OH	1:A:107:GLU:OE2	2.21	0.54
1:I:90:ARG:HH12	1:I:98:ASN:HD21	1.56	0.54
1:A:75:GLN:HG2	1:B:142:VAL:HG12	1.90	0.54
1:V:75:GLN:HG2	1:W:142:VAL:HG12	1.89	0.54
1:J:75:GLN:HG2	1:K:142:VAL:HG12	1.90	0.54
1:V:142:VAL:HG12	1:X:75:GLN:HG2	1.90	0.54
1:B:75:GLN:HG2	1:C:142:VAL:HG12	1.89	0.54
1:V:75:GLN:HG2	1:W:142:VAL:HG12	1.89	0.54
1:P:142:VAL:HG12	1:R:75:GLN:HG2	1.90	0.54
1:W:75:GLN:HG2	1:X:142:VAL:HG12	1.90	0.54
1:A:75:GLN:HG2	1:B:142:VAL:HG12	1.90	0.54
1:C:90:ARG:HH12	1:C:98:ASN:HD21	1.56	0.54
1:H:75:GLN:HG2	1:I:142:VAL:HG12	1.89	0.54
1:V:142:VAL:HG12	1:X:75:GLN:HG2	1.90	0.54
1:A:75:GLN:HG2	1:B:142:VAL:HG12	1.90	0.54
1:G:75:GLN:HG2	1:H:142:VAL:HG12	1.90	0.54
1:D:142:VAL:HG12	1:F:75:GLN:HG2	1.90	0.54
1:P:75:GLN:HG2	1:Q:142:VAL:HG12	1.89	0.54
1:N:80:ILE:HG22	1:N:82:LEU:HD12	1.90	0.54
1:P:142:VAL:HG12	1:R:75:GLN:HG2	1.90	0.54
1:T:80:ILE:HG22	1:T:82:LEU:HD12	1.90	0.54
1:B:90:ARG:HH12	1:B:98:ASN:HD21	1.56	0.54
1:G:90:ARG:HH12	1:G:98:ASN:HD21	1.56	0.54
1:N:90:ARG:HH12	1:N:98:ASN:HD21	1.56	0.54
1:P:75:GLN:HG2	1:Q:142:VAL:HG12	1.89	0.54
1:D:51:PHE:CD1	1:D:175:LEU:HD12	2.43	0.54
1:G:75:GLN:HG2	1:H:142:VAL:HG12	1.89	0.54
1:N:75:GLN:HG2	1:O:142:VAL:HG12	1.89	0.54
1:T:51:PHE:CD1	1:T:175:LEU:HD12	2.43	0.54
1:D:142:VAL:HG12	1:F:75:GLN:HG2	1.90	0.54
1:I:165:MET:O	1:I:169:LEU:HD23	2.07	0.54
1:P:142:VAL:HG12	1:R:75:GLN:HG2	1.90	0.54
1:X:90:ARG:HH12	1:X:98:ASN:HD21	1.56	0.54
1:F:49:LYS:O	1:F:53:LYS:HG2	2.08	0.54
1:J:142:VAL:HG12	1:L:75:GLN:HG2	1.90	0.54
1:Q:75:GLN:HG2	1:R:142:VAL:HG12	1.90	0.54
1:A:142:VAL:HG12	1:C:75:GLN:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:80:ILE:HG22	1:E:82:LEU:HD12	1.90	0.54
1:K:80:ILE:HG22	1:K:82:LEU:HD12	1.90	0.54
1:W:75:GLN:HG2	1:X:142:VAL:HG12	1.90	0.54
1:A:75:GLN:HG2	1:B:142:VAL:HG12	1.89	0.54
1:J:75:GLN:HG2	1:K:142:VAL:HG12	1.90	0.54
1:A:51:PHE:CD1	1:A:175:LEU:HD12	2.43	0.54
1:B:51:PHE:CD1	1:B:175:LEU:HD12	2.43	0.54
1:G:142:VAL:HG12	1:I:75:GLN:HG2	1.89	0.54
1:I:51:PHE:CD1	1:I:175:LEU:HD12	2.43	0.54
1:J:51:PHE:CD1	1:J:175:LEU:HD12	2.43	0.54
1:N:51:PHE:CD1	1:N:175:LEU:HD12	2.43	0.54
1:N:75:GLN:HG2	1:O:142:VAL:HG12	1.89	0.53
1:W:75:GLN:HG2	1:X:142:VAL:HG12	1.90	0.53
1:P:75:GLN:HG2	1:Q:142:VAL:HG12	1.89	0.53
1:E:153:THR:HG22	1:E:157:LYS:HZ3	1.72	0.53
1:H:75:GLN:HG2	1:I:142:VAL:HG12	1.89	0.53
1:R:90:ARG:HH12	1:R:98:ASN:HD21	1.56	0.53
1:M:142:VAL:HG12	1:O:75:GLN:HG2	1.91	0.53
1:S:142:VAL:HG12	1:U:75:GLN:HG2	1.90	0.53
1:G:75:GLN:HG2	1:H:142:VAL:HG12	1.90	0.53
1:L:49:LYS:O	1:L:53:LYS:HG2	2.08	0.53
1:M:142:VAL:HG12	1:O:75:GLN:HG2	1.90	0.53
1:N:75:GLN:HG2	1:O:142:VAL:HG12	1.89	0.53
1:A:75:GLN:HG2	1:B:142:VAL:HG12	1.90	0.53
1:J:142:VAL:HG12	1:L:75:GLN:HG2	1.89	0.53
1:Q:75:GLN:HG2	1:R:142:VAL:HG12	1.90	0.53
1:S:142:VAL:HG12	1:U:75:GLN:HG2	1.90	0.53
1:U:80:ILE:HG22	1:U:82:LEU:HD12	1.90	0.53
1:V:75:GLN:HG2	1:W:142:VAL:HG12	1.90	0.53
1:A:142:VAL:HG12	1:C:75:GLN:HG2	1.89	0.53
1:C:51:PHE:CD1	1:C:175:LEU:HD12	2.43	0.53
1:H:51:PHE:CD1	1:H:175:LEU:HD12	2.43	0.53
1:M:51:PHE:CD1	1:M:175:LEU:HD12	2.43	0.53
1:S:51:PHE:CD1	1:S:175:LEU:HD12	2.43	0.53
1:W:51:PHE:CD1	1:W:175:LEU:HD12	2.43	0.53
1:Q:75:GLN:HG2	1:R:142:VAL:HG12	1.90	0.53
1:T:51:PHE:CD1	1:T:175:LEU:HD12	2.44	0.53
1:O:115:LEU:O	1:O:119:LYS:HG2	2.08	0.53
1:U:168:TYR:HD2	1:U:169:LEU:HD12	1.74	0.53
1:C:165:MET:O	1:C:169:LEU:HD23	2.07	0.53
1:Q:75:GLN:HG2	1:R:142:VAL:HG12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:GLN:HG2	1:E:142:VAL:HG12	1.90	0.53
1:A:49:LYS:O	1:A:53:LYS:HG2	2.08	0.53
1:G:49:LYS:O	1:G:53:LYS:HG2	2.08	0.53
1:D:75:GLN:HG2	1:E:142:VAL:HG12	1.90	0.53
1:O:80:ILE:HG22	1:O:82:LEU:HD12	1.90	0.53
1:R:153:THR:HG22	1:R:157:LYS:HZ3	1.73	0.53
1:R:90:ARG:HH12	1:R:98:ASN:HD21	1.55	0.53
1:G:51:PHE:CD1	1:G:175:LEU:HD12	2.43	0.53
1:X:51:PHE:CD1	1:X:175:LEU:HD12	2.43	0.53
1:D:51:PHE:CD1	1:D:175:LEU:HD12	2.44	0.53
1:E:67:GLU:HA	1:E:70:MET:HE2	1.91	0.53
1:H:75:GLN:HG2	1:I:142:VAL:HG12	1.90	0.53
1:Q:115:LEU:O	1:Q:119:LYS:HG2	2.07	0.53
1:B:75:GLN:HG2	1:C:142:VAL:HG12	1.90	0.53
1:V:142:VAL:HG12	1:X:75:GLN:HG2	1.90	0.53
1:A:142:VAL:HG12	1:C:75:GLN:HG2	1.89	0.53
1:G:90:ARG:HH12	1:G:98:ASN:HD21	1.56	0.53
1:J:142:VAL:HG12	1:L:75:GLN:HG2	1.90	0.53
1:E:49:LYS:O	1:E:53:LYS:HG2	2.08	0.53
1:H:49:LYS:O	1:H:53:LYS:HG2	2.08	0.53
1:K:49:LYS:O	1:K:53:LYS:HG2	2.08	0.53
1:P:80:ILE:HG22	1:P:82:LEU:HD12	1.90	0.53
1:V:80:ILE:HG22	1:V:82:LEU:HD12	1.90	0.53
1:F:51:PHE:CD1	1:F:175:LEU:HD12	2.43	0.53
1:Q:51:PHE:CD1	1:Q:175:LEU:HD12	2.43	0.53
1:R:51:PHE:CD1	1:R:175:LEU:HD12	2.43	0.53
1:B:51:PHE:CD1	1:B:175:LEU:HD12	2.44	0.53
1:J:51:PHE:CD1	1:J:175:LEU:HD12	2.44	0.53
1:J:75:GLN:HG2	1:K:142:VAL:HG12	1.91	0.53
1:J:142:VAL:HG12	1:L:75:GLN:HG2	1.90	0.53
1:M:51:PHE:CD1	1:M:175:LEU:HD12	2.44	0.53
1:N:51:PHE:CD1	1:N:175:LEU:HD12	2.44	0.53
1:S:51:PHE:CD1	1:S:175:LEU:HD12	2.44	0.53
1:S:119:LYS:HD2	2:S:201:HOH:O	2.07	0.53
1:O:168:TYR:HD2	1:O:169:LEU:HD12	1.74	0.53
1:U:115:LEU:O	1:U:119:LYS:HG2	2.08	0.53
1:W:115:LEU:O	1:W:119:LYS:HG2	2.07	0.53
1:K:153:THR:HG22	1:K:157:LYS:HZ3	1.72	0.53
1:X:165:MET:O	1:X:169:LEU:HD23	2.07	0.53
1:O:90:ARG:HH12	1:O:98:ASN:HD21	1.56	0.53
1:B:75:GLN:HG2	1:C:142:VAL:HG12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:LYS:O	1:B:53:LYS:HG2	2.08	0.53
1:G:142:VAL:HG12	1:I:75:GLN:HG2	1.90	0.53
1:S:142:VAL:HG12	1:U:75:GLN:HG2	1.90	0.53
1:U:49:LYS:O	1:U:53:LYS:HG2	2.08	0.53
1:Q:80:ILE:HG22	1:Q:82:LEU:HD12	1.90	0.53
1:A:142:VAL:HG12	1:C:75:GLN:HG2	1.89	0.53
1:D:75:GLN:HG2	1:E:142:VAL:HG12	1.90	0.53
1:L:51:PHE:CD1	1:L:175:LEU:HD12	2.43	0.53
1:P:51:PHE:CD1	1:P:175:LEU:HD12	2.43	0.53
1:V:51:PHE:CD1	1:V:175:LEU:HD12	2.43	0.53
1:V:75:GLN:HG2	1:W:142:VAL:HG12	1.89	0.53
1:A:51:PHE:CD1	1:A:175:LEU:HD12	2.44	0.53
1:G:51:PHE:CD1	1:G:175:LEU:HD12	2.44	0.53
1:H:51:PHE:CD1	1:H:175:LEU:HD12	2.44	0.53
1:I:51:PHE:CD1	1:I:175:LEU:HD12	2.44	0.53
1:W:51:PHE:CD1	1:W:175:LEU:HD12	2.44	0.53
1:A:142:VAL:HG12	1:C:75:GLN:HG2	1.89	0.53
1:A:168:TYR:HD2	1:A:169:LEU:HD12	1.74	0.53
1:D:115:LEU:O	1:D:119:LYS:HG2	2.09	0.53
1:G:142:VAL:HG12	1:I:75:GLN:HG2	1.89	0.53
1:G:168:TYR:HD2	1:G:169:LEU:HD12	1.74	0.53
1:N:115:LEU:O	1:N:119:LYS:HG2	2.08	0.53
1:S:75:GLN:HG2	1:T:142:VAL:HG12	1.89	0.53
1:A:75:GLN:HG2	1:B:142:VAL:HG12	1.90	0.53
1:A:90:ARG:HH12	1:A:98:ASN:HD21	1.56	0.53
1:B:90:ARG:HH12	1:B:98:ASN:HD21	1.56	0.53
1:D:142:VAL:HG12	1:F:75:GLN:HG2	1.90	0.53
1:G:142:VAL:HG12	1:I:75:GLN:HG2	1.89	0.53
1:H:90:ARG:HH12	1:H:98:ASN:HD21	1.56	0.53
1:J:142:VAL:HG12	1:L:75:GLN:HG2	1.90	0.53
1:U:90:ARG:HH12	1:U:98:ASN:HD21	1.56	0.53
1:D:142:VAL:HG12	1:F:75:GLN:HG2	1.90	0.53
1:S:75:GLN:HG2	1:T:142:VAL:HG12	1.90	0.53
1:A:142:VAL:HG12	1:C:75:GLN:HG2	1.90	0.53
1:O:49:LYS:O	1:O:53:LYS:HG2	2.08	0.53
1:S:49:LYS:O	1:S:53:LYS:HG2	2.08	0.53
1:E:80:ILE:HG22	1:E:82:LEU:HD12	1.91	0.53
1:K:80:ILE:HG22	1:K:82:LEU:HD12	1.91	0.53
1:N:80:ILE:HG22	1:N:82:LEU:HD12	1.91	0.53
1:T:75:GLN:HG2	1:U:142:VAL:HG12	1.89	0.53
1:T:80:ILE:HG22	1:T:82:LEU:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:80:ILE:HG22	1:V:82:LEU:HD12	1.91	0.53
1:D:142:VAL:HG12	1:F:75:GLN:HG2	1.90	0.53
1:N:153:THR:HG22	1:N:157:LYS:HZ3	1.73	0.53
1:R:80:ILE:HG22	1:R:82:LEU:HD12	1.90	0.53
1:W:80:ILE:HG22	1:W:82:LEU:HD12	1.90	0.53
1:X:90:ARG:HH12	1:X:98:ASN:HD21	1.56	0.53
1:C:51:PHE:CD1	1:C:175:LEU:HD12	2.44	0.53
1:K:67:GLU:HA	1:K:70:MET:HE2	1.91	0.53
1:M:119:LYS:HD2	2:M:201:HOH:O	2.07	0.53
1:R:51:PHE:CD1	1:R:175:LEU:HD12	2.44	0.53
1:M:75:GLN:HG2	1:N:142:VAL:HG12	1.89	0.53
1:V:168:TYR:HD2	1:V:169:LEU:HD12	1.74	0.53
1:D:142:VAL:HG12	1:F:75:GLN:HG2	1.90	0.53
1:G:75:GLN:HG2	1:H:142:VAL:HG12	1.90	0.53
1:N:75:GLN:HG2	1:O:142:VAL:HG12	1.90	0.53
1:R:165:MET:O	1:R:169:LEU:HD23	2.07	0.53
1:G:75:GLN:HG2	1:H:142:VAL:HG12	1.90	0.53
1:T:75:GLN:HG2	1:U:142:VAL:HG12	1.89	0.53
1:M:49:LYS:O	1:M:53:LYS:HG2	2.08	0.53
1:S:75:GLN:HG2	1:T:142:VAL:HG12	1.90	0.53
1:X:80:ILE:HG22	1:X:82:LEU:HD12	1.90	0.53
1:O:51:PHE:CD1	1:O:175:LEU:HD12	2.43	0.53
1:U:51:PHE:CD1	1:U:175:LEU:HD12	2.43	0.53
1:F:51:PHE:CD1	1:F:175:LEU:HD12	2.44	0.53
1:Q:51:PHE:CD1	1:Q:175:LEU:HD12	2.44	0.53
1:S:75:GLN:HG2	1:T:142:VAL:HG12	1.90	0.53
1:V:51:PHE:CD1	1:V:175:LEU:HD12	2.44	0.53
1:H:75:GLN:HG2	1:I:142:VAL:HG12	1.90	0.53
1:J:115:LEU:O	1:J:119:LYS:HG2	2.09	0.53
1:P:168:TYR:HD2	1:P:169:LEU:HD12	1.74	0.53
1:T:75:GLN:HG2	1:U:142:VAL:HG12	1.89	0.53
1:Q:165:MET:HG3	1:Q:169:LEU:CD2	2.39	0.53
1:W:165:MET:HG3	1:W:169:LEU:CD2	2.39	0.53
1:W:75:GLN:HG2	1:X:142:VAL:HG12	1.90	0.53
1:J:75:GLN:HG2	1:K:142:VAL:HG12	1.91	0.53
1:N:49:LYS:O	1:N:53:LYS:HG2	2.08	0.53
1:P:80:ILE:HG22	1:P:82:LEU:HD12	1.91	0.53
1:P:142:VAL:HG12	1:R:75:GLN:HG2	1.91	0.53
1:R:119:LYS:HD2	2:R:201:HOH:O	2.09	0.53
1:V:142:VAL:HG12	1:X:75:GLN:HG2	1.91	0.53
1:A:142:VAL:HG12	1:C:75:GLN:HG2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:GLN:HG2	1:C:142:VAL:HG12	1.89	0.53
1:S:75:GLN:HG2	1:T:142:VAL:HG12	1.89	0.53
1:L:51:PHE:CD1	1:L:175:LEU:HD12	2.44	0.53
1:M:75:GLN:HG2	1:N:142:VAL:HG12	1.90	0.53
1:P:51:PHE:CD1	1:P:175:LEU:HD12	2.44	0.53
1:X:51:PHE:CD1	1:X:175:LEU:HD12	2.44	0.53
1:A:115:LEU:O	1:A:119:LYS:HG2	2.08	0.53
1:M:165:MET:HG3	1:M:169:LEU:CD2	2.39	0.53
1:L:90:ARG:HH12	1:L:98:ASN:HD21	1.56	0.53
1:M:75:GLN:HG2	1:N:142:VAL:HG12	1.90	0.53
1:D:75:GLN:HG2	1:E:142:VAL:HG12	1.90	0.53
1:N:75:GLN:HG2	1:O:142:VAL:HG12	1.90	0.53
1:T:49:LYS:O	1:T:53:LYS:HG2	2.08	0.53
1:A:119:LYS:HD2	2:A:202:HOH:O	2.09	0.53
1:E:75:GLN:HG2	1:F:142:VAL:HG12	1.89	0.53
1:G:142:VAL:HG12	1:I:75:GLN:HG2	1.90	0.53
1:H:153:THR:HG22	1:H:157:LYS:HZ2	1.73	0.53
1:N:75:GLN:HG2	1:O:142:VAL:HG12	1.90	0.53
1:S:75:GLN:HG2	1:T:142:VAL:HG12	1.89	0.53
1:M:75:GLN:HG2	1:N:142:VAL:HG12	1.89	0.53
1:B:75:GLN:HG2	1:C:142:VAL:HG12	1.90	0.53
1:Q:67:GLU:HA	1:Q:70:MET:HE2	1.91	0.53
1:F:168:TYR:HD2	1:F:169:LEU:HD12	1.74	0.53
1:I:115:LEU:O	1:I:119:LYS:HG2	2.09	0.53
1:Q:168:TYR:HD2	1:Q:169:LEU:HD12	1.74	0.53
1:S:115:LEU:O	1:S:119:LYS:HG2	2.09	0.53
1:W:168:TYR:HD2	1:W:169:LEU:HD12	1.74	0.53
1:P:75:GLN:HG2	1:Q:142:VAL:HG12	1.90	0.53
1:T:153:THR:HG22	1:T:157:LYS:HZ3	1.73	0.53
1:V:75:GLN:HG2	1:W:142:VAL:HG12	1.90	0.53
1:M:75:GLN:HG2	1:N:142:VAL:HG12	1.90	0.53
1:W:90:ARG:HH12	1:W:98:ASN:HD21	1.56	0.53
1:N:75:GLN:HG2	1:O:142:VAL:HG12	1.90	0.53
1:P:75:GLN:HG2	1:Q:142:VAL:HG12	1.90	0.53
1:Q:75:GLN:HG2	1:R:142:VAL:HG12	1.91	0.53
1:V:75:GLN:HG2	1:W:142:VAL:HG12	1.90	0.53
1:C:49:LYS:O	1:C:53:LYS:HG2	2.08	0.53
1:E:75:GLN:HG2	1:F:142:VAL:HG12	1.90	0.53
1:I:49:LYS:O	1:I:53:LYS:HG2	2.08	0.53
1:G:119:LYS:HD2	2:G:201:HOH:O	2.09	0.53
1:V:119:LYS:HD2	2:V:201:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:119:LYS:HD2	2:X:201:HOH:O	2.09	0.53
1:B:75:GLN:HG2	1:C:142:VAL:HG12	1.90	0.53
1:V:75:GLN:HG2	1:W:142:VAL:HG12	1.90	0.53
1:D:90:ARG:HH12	1:D:98:ASN:HD21	1.56	0.53
1:K:75:GLN:HG2	1:L:142:VAL:HG12	1.89	0.53
1:M:90:ARG:HH12	1:M:98:ASN:HD21	1.56	0.53
1:T:75:GLN:HG2	1:U:142:VAL:HG12	1.90	0.53
1:B:75:GLN:HG2	1:C:142:VAL:HG12	1.90	0.53
1:O:51:PHE:CD1	1:O:175:LEU:HD12	2.44	0.53
1:W:34:TYR:OH	1:W:107:GLU:OE2	2.22	0.53
1:P:115:LEU:O	1:P:119:LYS:HG2	2.09	0.53
1:D:153:THR:HG22	1:D:157:LYS:HZ3	1.73	0.53
1:J:142:VAL:HG12	1:L:75:GLN:HG2	1.91	0.53
1:N:165:MET:HG3	1:N:169:LEU:CD2	2.39	0.53
1:S:75:GLN:HG2	1:T:142:VAL:HG12	1.90	0.53
1:K:75:GLN:HG2	1:L:142:VAL:HG12	1.90	0.53
1:D:142:VAL:HG12	1:F:75:GLN:HG2	1.91	0.53
1:M:75:GLN:HG2	1:N:142:VAL:HG12	1.90	0.53
1:S:80:ILE:HG22	1:S:82:LEU:HD12	1.90	0.53
1:I:119:LYS:HD2	2:I:201:HOH:O	2.09	0.53
1:J:90:ARG:HH12	1:J:98:ASN:HD21	1.56	0.53
1:M:75:GLN:HG2	1:N:142:VAL:HG12	1.89	0.53
1:O:119:LYS:HD2	2:O:201:HOH:O	2.09	0.53
1:A:142:VAL:HG12	1:C:75:GLN:HG2	1.90	0.52
1:U:51:PHE:CD1	1:U:175:LEU:HD12	2.44	0.52
1:G:115:LEU:O	1:G:119:LYS:HG2	2.09	0.52
1:K:75:GLN:HG2	1:L:142:VAL:HG12	1.89	0.52
1:K:168:TYR:HD2	1:K:169:LEU:HD12	1.74	0.52
1:T:165:MET:HG3	1:T:169:LEU:CD2	2.39	0.52
1:D:71:LYS:NZ	2:D:202:HOH:O	2.31	0.52
1:F:90:ARG:HH12	1:F:98:ASN:HD21	1.56	0.52
1:A:75:GLN:HG2	1:B:142:VAL:HG12	1.91	0.52
1:I:119:LYS:HD2	2:I:201:HOH:O	2.09	0.52
1:J:142:VAL:HG12	1:L:75:GLN:HG2	1.91	0.52
1:M:80:ILE:HG22	1:M:82:LEU:HD12	1.91	0.52
1:P:119:LYS:HD2	2:P:201:HOH:O	2.09	0.52
1:B:80:ILE:HG22	1:B:82:LEU:HD12	1.90	0.52
1:B:153:THR:HG22	1:B:157:LYS:HZ2	1.73	0.52
1:H:75:GLN:HG2	1:I:142:VAL:HG12	1.90	0.52
1:I:80:ILE:HG22	1:I:82:LEU:HD12	1.90	0.52
1:P:75:GLN:HG2	1:Q:142:VAL:HG12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:153:THR:HG22	1:P:157:LYS:HZ2	1.73	0.52
1:S:90:ARG:HH12	1:S:98:ASN:HD21	1.56	0.52
1:E:75:GLN:HG2	1:F:142:VAL:HG12	1.89	0.52
1:B:168:TYR:HD2	1:B:169:LEU:HD12	1.74	0.52
1:E:168:TYR:HD2	1:E:169:LEU:HD12	1.74	0.52
1:L:168:TYR:HD2	1:L:169:LEU:HD12	1.74	0.52
1:A:142:VAL:HG12	1:C:75:GLN:HG2	1.90	0.52
1:E:75:GLN:HG2	1:F:142:VAL:HG12	1.89	0.52
1:Q:90:ARG:HH12	1:Q:98:ASN:HD21	1.56	0.52
1:Q:49:LYS:O	1:Q:53:LYS:HG2	2.08	0.52
1:W:49:LYS:O	1:W:53:LYS:HG2	2.08	0.52
1:A:80:ILE:HG22	1:A:82:LEU:HD12	1.91	0.52
1:G:75:GLN:HG2	1:H:142:VAL:HG12	1.91	0.52
1:G:80:ILE:HG22	1:G:82:LEU:HD12	1.91	0.52
1:H:80:ILE:HG22	1:H:82:LEU:HD12	1.91	0.52
1:Q:80:ILE:HG22	1:Q:82:LEU:HD12	1.91	0.52
1:U:80:ILE:HG22	1:U:82:LEU:HD12	1.91	0.52
1:W:80:ILE:HG22	1:W:82:LEU:HD12	1.91	0.52
1:C:80:ILE:HG22	1:C:82:LEU:HD12	1.90	0.52
1:F:80:ILE:HG22	1:F:82:LEU:HD12	1.90	0.52
1:L:80:ILE:HG22	1:L:82:LEU:HD12	1.90	0.52
1:M:80:ILE:HG22	1:M:82:LEU:HD12	1.90	0.52
1:P:75:GLN:HG2	1:Q:142:VAL:HG12	1.90	0.52
1:X:115:LEU:O	1:X:119:LYS:HG2	2.08	0.52
1:M:75:GLN:HG2	1:N:142:VAL:HG12	1.90	0.52
1:S:75:GLN:HG2	1:T:142:VAL:HG12	1.90	0.52
1:B:75:GLN:HG2	1:C:142:VAL:HG12	1.90	0.52
1:X:49:LYS:O	1:X:53:LYS:HG2	2.08	0.52
1:S:80:ILE:HG22	1:S:82:LEU:HD12	1.91	0.52
1:H:80:ILE:HG22	1:H:82:LEU:HD12	1.90	0.52
1:V:153:THR:HG22	1:V:157:LYS:HZ2	1.73	0.52
1:E:51:PHE:CD1	1:E:175:LEU:HD12	2.43	0.52
1:E:75:GLN:HG2	1:F:142:VAL:HG12	1.90	0.52
1:P:75:GLN:HG2	1:Q:142:VAL:HG12	1.90	0.52
1:D:168:TYR:HD2	1:D:169:LEU:HD12	1.74	0.52
1:H:168:TYR:HD2	1:H:169:LEU:HD12	1.74	0.52
1:J:168:TYR:HD2	1:J:169:LEU:HD12	1.74	0.52
1:L:115:LEU:O	1:L:119:LYS:HG2	2.09	0.52
1:R:168:TYR:HD2	1:R:169:LEU:HD12	1.74	0.52
1:S:168:TYR:HD2	1:S:169:LEU:HD12	1.74	0.52
1:A:165:MET:HG3	1:A:169:LEU:CD2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:165:MET:HG3	1:G:169:LEU:CD2	2.39	0.52
1:S:51:PHE:CD1	1:S:175:LEU:HD12	2.45	0.52
1:V:49:LYS:O	1:V:53:LYS:HG2	2.08	0.52
1:B:80:ILE:HG22	1:B:82:LEU:HD12	1.91	0.52
1:G:142:VAL:HG12	1:I:75:GLN:HG2	1.90	0.52
1:O:80:ILE:HG22	1:O:82:LEU:HD12	1.91	0.52
1:A:80:ILE:HG22	1:A:82:LEU:HD12	1.90	0.52
1:G:80:ILE:HG22	1:G:82:LEU:HD12	1.90	0.52
1:N:75:GLN:HG2	1:O:142:VAL:HG12	1.90	0.52
1:O:153:THR:HG22	1:O:157:LYS:HZ2	1.73	0.52
1:F:90:ARG:HH12	1:F:98:ASN:HD21	1.55	0.52
1:Q:90:ARG:HH12	1:Q:98:ASN:HD21	1.56	0.52
1:H:75:GLN:HG2	1:I:142:VAL:HG12	1.90	0.52
1:T:75:GLN:HG2	1:U:142:VAL:HG12	1.90	0.52
1:M:142:VAL:HG12	1:O:75:GLN:HG2	1.92	0.52
1:X:168:TYR:HD2	1:X:169:LEU:HD12	1.74	0.52
1:H:75:GLN:HG2	1:I:142:VAL:HG12	1.90	0.52
1:J:51:PHE:CD1	1:J:175:LEU:HD12	2.45	0.52
1:M:51:PHE:CD1	1:M:175:LEU:HD12	2.45	0.52
1:W:119:LYS:HD2	2:W:201:HOH:O	2.09	0.52
1:K:75:GLN:HG2	1:L:142:VAL:HG12	1.89	0.52
1:E:75:GLN:HG2	1:F:142:VAL:HG12	1.89	0.52
1:G:119:LYS:HD2	2:G:201:HOH:O	2.10	0.52
1:K:51:PHE:CD1	1:K:175:LEU:HD12	2.43	0.52
1:V:119:LYS:HD2	2:V:201:HOH:O	2.10	0.52
1:K:75:GLN:HG2	1:L:142:VAL:HG12	1.90	0.52
1:K:75:GLN:HG2	1:L:142:VAL:HG12	1.90	0.52
1:I:90:ARG:HD3	1:I:92:ASP:O	2.10	0.52
1:M:90:ARG:HD3	1:M:92:ASP:O	2.10	0.52
1:S:90:ARG:HD3	1:S:92:ASP:O	2.10	0.52
1:B:51:PHE:CD1	1:B:175:LEU:HD12	2.45	0.52
1:D:49:LYS:O	1:D:53:LYS:HG2	2.08	0.52
1:D:51:PHE:CD1	1:D:175:LEU:HD12	2.45	0.52
1:H:51:PHE:CD1	1:H:175:LEU:HD12	2.45	0.52
1:N:51:PHE:CD1	1:N:175:LEU:HD12	2.45	0.52
1:P:49:LYS:O	1:P:53:LYS:HG2	2.08	0.52
1:R:49:LYS:O	1:R:53:LYS:HG2	2.08	0.52
1:T:51:PHE:CD1	1:T:175:LEU:HD12	2.45	0.52
1:Q:119:LYS:HD2	2:Q:201:HOH:O	2.09	0.52
1:R:80:ILE:HG22	1:R:82:LEU:HD12	1.91	0.52
1:W:34:TYR:OH	1:W:107:GLU:OE2	2.21	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:75:GLN:HG2	1:F:142:VAL:HG12	1.90	0.52
1:A:119:LYS:HD2	2:A:202:HOH:O	2.10	0.52
1:P:119:LYS:HD2	2:P:201:HOH:O	2.10	0.52
1:T:75:GLN:HG2	1:U:142:VAL:HG12	1.90	0.52
1:G:142:VAL:HG12	1:I:75:GLN:HG2	1.90	0.52
1:E:75:GLN:HG2	1:F:142:VAL:HG12	1.90	0.52
1:M:168:TYR:HD2	1:M:169:LEU:HD12	1.74	0.52
1:N:168:TYR:HD2	1:N:169:LEU:HD12	1.74	0.52
1:G:142:VAL:HG12	1:I:75:GLN:HG2	1.91	0.52
1:J:90:ARG:HH12	1:J:98:ASN:HD21	1.56	0.52
1:M:90:ARG:HH12	1:M:98:ASN:HD21	1.56	0.52
1:S:90:ARG:HH12	1:S:98:ASN:HD21	1.56	0.52
1:A:142:VAL:HG12	1:C:75:GLN:HG2	1.90	0.52
1:C:90:ARG:HD3	1:C:92:ASP:O	2.10	0.52
1:X:90:ARG:HD3	1:X:92:ASP:O	2.10	0.52
1:J:49:LYS:O	1:J:53:LYS:HG2	2.08	0.52
1:W:51:PHE:CD1	1:W:175:LEU:HD12	2.45	0.52
1:F:119:LYS:HD2	2:F:201:HOH:O	2.09	0.52
1:K:119:LYS:HD2	2:K:201:HOH:O	2.08	0.52
1:L:119:LYS:HD2	2:L:201:HOH:O	2.09	0.52
1:M:119:LYS:HD2	2:M:201:HOH:O	2.09	0.52
1:T:75:GLN:HG2	1:U:142:VAL:HG12	1.90	0.52
1:U:153:THR:HG22	1:U:157:LYS:HZ2	1.73	0.52
1:L:90:ARG:HH12	1:L:98:ASN:HD21	1.56	0.52
1:W:90:ARG:HH12	1:W:98:ASN:HD21	1.56	0.52
1:E:51:PHE:CD1	1:E:175:LEU:HD12	2.44	0.52
1:L:165:MET:HG3	1:L:169:LEU:CD2	2.39	0.52
1:T:75:GLN:HG2	1:U:142:VAL:HG12	1.90	0.52
1:T:90:ARG:HH12	1:T:98:ASN:HD21	1.56	0.52
1:E:90:ARG:HD3	1:E:92:ASP:O	2.10	0.52
1:K:90:ARG:HD3	1:K:92:ASP:O	2.10	0.52
1:R:90:ARG:HD3	1:R:92:ASP:O	2.10	0.52
1:T:75:GLN:HG2	1:U:142:VAL:HG12	1.90	0.52
1:P:51:PHE:CD1	1:P:175:LEU:HD12	2.45	0.52
1:Q:51:PHE:CD1	1:Q:175:LEU:HD12	2.45	0.52
1:V:51:PHE:CD1	1:V:175:LEU:HD12	2.45	0.52
1:C:119:LYS:HD2	2:C:201:HOH:O	2.09	0.52
1:S:119:LYS:HD2	2:S:201:HOH:O	2.09	0.52
1:X:80:ILE:HG22	1:X:82:LEU:HD12	1.91	0.52
1:K:75:GLN:HG2	1:L:142:VAL:HG12	1.90	0.52
1:K:51:PHE:CD1	1:K:175:LEU:HD12	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:75:GLN:HG2	1:W:142:VAL:HG12	1.91	0.52
1:F:115:LEU:O	1:F:119:LYS:HG2	2.10	0.52
1:J:165:MET:HG3	1:J:169:LEU:CD2	2.39	0.52
1:R:153:THR:HG22	1:R:157:LYS:HZ3	1.75	0.52
1:X:165:MET:HG3	1:X:169:LEU:CD2	2.39	0.52
1:D:90:ARG:HH12	1:D:98:ASN:HD21	1.56	0.52
1:N:90:ARG:HH12	1:N:98:ASN:HD21	1.56	0.52
1:A:51:PHE:CD1	1:A:175:LEU:HD12	2.45	0.52
1:C:51:PHE:CD1	1:C:175:LEU:HD12	2.45	0.52
1:I:51:PHE:CD1	1:I:175:LEU:HD12	2.45	0.52
1:U:51:PHE:CD1	1:U:175:LEU:HD12	2.45	0.52
1:D:80:ILE:HG22	1:D:82:LEU:HD12	1.91	0.52
1:O:119:LYS:HD2	2:O:201:HOH:O	2.09	0.52
1:Q:34:TYR:OH	1:Q:107:GLU:OE2	2.21	0.52
1:U:119:LYS:HD2	2:U:201:HOH:O	2.09	0.52
1:G:174:THR:HA	1:G:177:HIS:NE2	2.25	0.52
1:P:119:LYS:HD2	2:P:201:HOH:O	2.10	0.52
1:R:119:LYS:HD2	2:R:201:HOH:O	2.10	0.52
1:V:119:LYS:HD2	2:V:201:HOH:O	2.10	0.52
1:R:119:LYS:HD2	2:R:201:HOH:O	2.10	0.52
1:T:168:TYR:HD2	1:T:169:LEU:HD12	1.74	0.52
1:F:165:MET:HG3	1:F:169:LEU:CD2	2.39	0.52
1:P:153:THR:HG22	1:P:157:LYS:HZ2	1.74	0.52
1:R:165:MET:HG3	1:R:169:LEU:CD2	2.39	0.52
1:V:153:THR:HG22	1:V:157:LYS:HZ2	1.74	0.52
1:D:90:ARG:HD3	1:D:92:ASP:O	2.10	0.52
1:J:90:ARG:HD3	1:J:92:ASP:O	2.10	0.52
1:P:90:ARG:HD3	1:P:92:ASP:O	2.10	0.52
1:G:51:PHE:CD1	1:G:175:LEU:HD12	2.45	0.52
1:O:51:PHE:CD1	1:O:175:LEU:HD12	2.45	0.52
1:P:75:GLN:HG2	1:Q:142:VAL:HG12	1.90	0.52
1:V:75:GLN:HG2	1:W:142:VAL:HG12	1.90	0.52
1:S:75:GLN:HG2	1:T:142:VAL:HG12	1.91	0.52
1:L:153:THR:HG22	1:L:157:LYS:HZ3	1.75	0.52
1:M:142:VAL:HG12	1:O:75:GLN:HG2	1.92	0.52
1:A:119:LYS:HD2	2:A:202:HOH:O	2.10	0.52
1:C:119:LYS:HD2	2:C:201:HOH:O	2.10	0.52
1:I:119:LYS:HD2	2:I:201:HOH:O	2.10	0.52
1:C:168:TYR:HD2	1:C:169:LEU:HD12	1.74	0.51
1:C:165:MET:HG3	1:C:169:LEU:CD2	2.39	0.51
1:D:51:PHE:CD1	1:D:175:LEU:HD12	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:165:MET:HG3	1:E:169:LEU:CD2	2.39	0.51
1:F:90:ARG:HD3	1:F:92:ASP:O	2.10	0.51
1:V:90:ARG:HD3	1:V:92:ASP:O	2.10	0.51
1:F:51:PHE:CD1	1:F:175:LEU:HD12	2.45	0.51
1:L:51:PHE:CD1	1:L:175:LEU:HD12	2.45	0.51
1:X:51:PHE:CD1	1:X:175:LEU:HD12	2.45	0.51
1:J:80:ILE:HG22	1:J:82:LEU:HD12	1.91	0.51
1:X:119:LYS:HD2	2:X:201:HOH:O	2.10	0.51
1:F:119:LYS:HD2	2:F:201:HOH:O	2.10	0.51
1:U:119:LYS:HD2	2:U:201:HOH:O	2.10	0.51
1:X:119:LYS:HD2	2:X:201:HOH:O	2.10	0.51
1:I:67:GLU:HA	1:I:70:MET:HE2	1.91	0.51
1:R:176:GLY:O	1:R:177:HIS:ND1	2.44	0.51
1:W:153:THR:HG22	1:W:157:LYS:HZ3	1.73	0.51
1:B:51:PHE:CD1	1:B:175:LEU:HD12	2.46	0.51
1:D:165:MET:HG3	1:D:169:LEU:CD2	2.39	0.51
1:I:165:MET:HG3	1:I:169:LEU:CD2	2.39	0.51
1:J:51:PHE:CD1	1:J:175:LEU:HD12	2.46	0.51
1:K:165:MET:HG3	1:K:169:LEU:CD2	2.39	0.51
1:B:90:ARG:HD3	1:B:92:ASP:O	2.10	0.51
1:L:90:ARG:HD3	1:L:92:ASP:O	2.10	0.51
1:X:34:TYR:OH	1:X:107:GLU:OE2	2.18	0.51
1:M:75:GLN:HG2	1:N:142:VAL:HG12	1.91	0.51
1:R:51:PHE:CD1	1:R:175:LEU:HD12	2.45	0.51
1:I:80:ILE:HG22	1:I:82:LEU:HD12	1.91	0.51
1:M:75:GLN:HG2	1:N:142:VAL:HG12	1.91	0.51
1:D:80:ILE:HG22	1:D:82:LEU:HD12	1.90	0.51
1:F:153:THR:HG22	1:F:157:LYS:HZ3	1.75	0.51
1:G:119:LYS:HD2	2:G:201:HOH:O	2.10	0.51
1:L:119:LYS:HD2	2:L:201:HOH:O	2.10	0.51
1:I:168:TYR:HD2	1:I:169:LEU:HD12	1.74	0.51
1:A:51:PHE:CD1	1:A:175:LEU:HD12	2.46	0.51
1:H:51:PHE:CD1	1:H:175:LEU:HD12	2.46	0.51
1:M:51:PHE:CD1	1:M:175:LEU:HD12	2.46	0.51
1:N:51:PHE:CD1	1:N:175:LEU:HD12	2.46	0.51
1:S:51:PHE:CD1	1:S:175:LEU:HD12	2.46	0.51
1:T:51:PHE:CD1	1:T:175:LEU:HD12	2.46	0.51
1:E:90:ARG:HH12	1:E:98:ASN:HD21	1.56	0.51
1:H:90:ARG:HD3	1:H:92:ASP:O	2.10	0.51
1:K:75:GLN:HG2	1:L:142:VAL:HG12	1.91	0.51
1:N:90:ARG:HD3	1:N:92:ASP:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:90:ARG:HD3	1:T:92:ASP:O	2.10	0.51
1:U:90:ARG:HD3	1:U:92:ASP:O	2.10	0.51
1:N:60:HIS:CD2	1:N:63:ARG:HH12	2.29	0.51
1:C:80:ILE:HG22	1:C:82:LEU:HD12	1.91	0.51
1:I:153:THR:HG22	1:I:157:LYS:HZ2	1.76	0.51
1:X:153:THR:HG22	1:X:157:LYS:HZ2	1.74	0.51
1:O:90:ARG:HH12	1:O:98:ASN:HD21	1.55	0.51
1:W:34:TYR:OH	1:W:107:GLU:OE2	2.22	0.51
1:Q:153:THR:HG22	1:Q:157:LYS:HZ3	1.73	0.51
1:G:51:PHE:CD1	1:G:175:LEU:HD12	2.46	0.51
1:I:51:PHE:CD1	1:I:175:LEU:HD12	2.46	0.51
1:W:34:TYR:OH	1:W:107:GLU:OE2	2.21	0.51
1:A:90:ARG:HD3	1:A:92:ASP:O	2.10	0.51
1:G:90:ARG:HD3	1:G:92:ASP:O	2.10	0.51
1:O:90:ARG:HD3	1:O:92:ASP:O	2.10	0.51
1:A:60:HIS:CD2	1:A:63:ARG:HH12	2.29	0.51
1:G:60:HIS:CD2	1:G:63:ARG:HH12	2.29	0.51
1:O:60:HIS:CD2	1:O:63:ARG:HH12	2.29	0.51
1:Q:60:HIS:CD2	1:Q:63:ARG:HH12	2.29	0.51
1:T:60:HIS:CD2	1:T:63:ARG:HH12	2.29	0.51
1:W:60:HIS:CD2	1:W:63:ARG:HH12	2.29	0.51
1:B:119:LYS:HD2	2:B:201:HOH:O	2.09	0.51
1:C:153:THR:HG22	1:C:157:LYS:HZ2	1.76	0.51
1:J:80:ILE:HG22	1:J:82:LEU:HD12	1.90	0.51
1:Q:153:THR:HG22	1:Q:157:LYS:HZ3	1.73	0.51
1:Q:119:LYS:HD2	2:Q:201:HOH:O	2.10	0.51
1:W:119:LYS:HD2	2:W:201:HOH:O	2.10	0.51
1:K:119:LYS:HD2	2:K:201:HOH:O	2.10	0.51
1:C:51:PHE:CD1	1:C:175:LEU:HD12	2.46	0.51
1:W:51:PHE:CD1	1:W:175:LEU:HD12	2.46	0.51
1:K:90:ARG:HH12	1:K:98:ASN:HD21	1.56	0.51
1:K:119:LYS:HD2	2:K:201:HOH:O	2.10	0.51
1:E:75:GLN:HG2	1:F:142:VAL:HG12	1.91	0.51
1:S:60:HIS:CD2	1:S:63:ARG:HH12	2.29	0.51
1:U:60:HIS:CD2	1:U:63:ARG:HH12	2.29	0.51
1:L:80:ILE:HG22	1:L:82:LEU:HD12	1.91	0.51
1:B:49:LYS:O	1:B:53:LYS:HG2	2.11	0.51
1:L:119:LYS:HD2	2:L:201:HOH:O	2.10	0.51
1:O:119:LYS:HD2	2:O:201:HOH:O	2.10	0.51
1:U:90:ARG:HH12	1:U:98:ASN:HD21	1.56	0.51
1:U:119:LYS:HD2	2:U:201:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:51:PHE:CD1	1:F:175:LEU:HD12	2.46	0.51
1:P:51:PHE:CD1	1:P:175:LEU:HD12	2.46	0.51
1:Q:51:PHE:CD1	1:Q:175:LEU:HD12	2.46	0.51
1:R:51:PHE:CD1	1:R:175:LEU:HD12	2.46	0.51
1:V:51:PHE:CD1	1:V:175:LEU:HD12	2.46	0.51
1:X:51:PHE:CD1	1:X:175:LEU:HD12	2.46	0.51
1:X:34:TYR:OH	1:X:107:GLU:OE2	2.21	0.51
1:U:34:TYR:OH	1:U:107:GLU:OE2	2.18	0.51
1:B:60:HIS:CD2	1:B:63:ARG:HH12	2.29	0.51
1:H:60:HIS:CD2	1:H:63:ARG:HH12	2.29	0.51
1:M:60:HIS:CD2	1:M:63:ARG:HH12	2.29	0.51
1:F:80:ILE:HG22	1:F:82:LEU:HD12	1.91	0.51
1:J:119:LYS:HD2	2:J:201:HOH:O	2.09	0.51
1:H:49:LYS:O	1:H:53:LYS:HG2	2.11	0.51
1:W:153:THR:HG22	1:W:157:LYS:HZ3	1.73	0.51
1:F:119:LYS:HD2	2:F:201:HOH:O	2.10	0.51
1:J:119:LYS:HD2	2:J:201:HOH:O	2.10	0.51
1:W:90:ARG:HD3	1:W:92:ASP:O	2.10	0.51
1:D:119:LYS:HD2	2:D:201:HOH:O	2.09	0.51
1:E:119:LYS:HD2	2:E:228:HOH:O	2.09	0.51
1:H:119:LYS:HD2	2:H:201:HOH:O	2.09	0.51
1:D:119:LYS:HD2	2:D:201:HOH:O	2.10	0.51
1:E:119:LYS:HD2	2:E:228:HOH:O	2.10	0.51
1:Q:34:TYR:OH	1:Q:107:GLU:OE2	2.22	0.51
1:Q:119:LYS:HD2	2:Q:201:HOH:O	2.10	0.51
1:W:119:LYS:HD2	2:W:201:HOH:O	2.10	0.51
1:X:90:ARG:HH12	1:X:98:ASN:HD21	1.59	0.51
1:F:153:THR:HG22	1:F:157:LYS:HZ3	1.76	0.51
1:L:51:PHE:CD1	1:L:175:LEU:HD12	2.46	0.51
1:O:119:LYS:HD2	2:O:201:HOH:O	2.11	0.51
1:R:34:TYR:OH	1:R:107:GLU:OE2	2.21	0.51
1:R:119:LYS:HD2	2:R:201:HOH:O	2.11	0.51
1:Q:90:ARG:HD3	1:Q:92:ASP:O	2.10	0.51
1:S:75:GLN:HG2	1:T:142:VAL:HG12	1.92	0.51
1:C:119:LYS:HD2	2:C:201:HOH:O	2.10	0.51
1:A:90:ARG:HH12	1:A:98:ASN:HD21	1.59	0.51
1:E:75:GLN:HG2	1:F:142:VAL:HG12	1.91	0.51
1:H:153:THR:HG22	1:H:157:LYS:HZ2	1.75	0.51
1:O:51:PHE:CD1	1:O:175:LEU:HD12	2.46	0.51
1:Q:153:THR:HG22	1:Q:157:LYS:HZ3	1.73	0.51
1:U:51:PHE:CD1	1:U:175:LEU:HD12	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:34:TYR:OH	1:Q:107:GLU:OE2	2.21	0.51
1:X:119:LYS:HD2	2:X:201:HOH:O	2.11	0.51
1:E:51:PHE:CD1	1:E:175:LEU:HD12	2.45	0.51
1:E:49:LYS:O	1:E:53:LYS:HG2	2.11	0.51
1:K:49:LYS:O	1:K:53:LYS:HG2	2.11	0.51
1:R:34:TYR:OH	1:R:107:GLU:OE2	2.17	0.51
1:E:34:TYR:OH	1:E:107:GLU:OE2	2.23	0.51
1:M:142:VAL:HG12	1:O:75:GLN:HG2	1.93	0.51
1:G:90:ARG:HH12	1:G:98:ASN:HD21	1.59	0.51
1:H:67:GLU:HA	1:H:70:MET:HE2	1.93	0.51
1:R:90:ARG:HH12	1:R:98:ASN:HD21	1.59	0.51
1:W:34:TYR:OH	1:W:107:GLU:OE2	2.22	0.51
1:B:165:MET:HG3	1:B:169:LEU:CD2	2.39	0.51
1:N:153:THR:HG22	1:N:157:LYS:HZ2	1.75	0.51
1:P:165:MET:HG3	1:P:169:LEU:CD2	2.39	0.51
1:V:119:LYS:HD2	2:V:201:HOH:O	2.11	0.51
1:F:60:HIS:CD2	1:F:63:ARG:HH12	2.29	0.51
1:K:51:PHE:CD1	1:K:175:LEU:HD12	2.45	0.51
1:L:60:HIS:CD2	1:L:63:ARG:HH12	2.29	0.51
1:X:34:TYR:OH	1:X:107:GLU:OE2	2.17	0.51
1:X:177:HIS:O	1:X:177:HIS:ND1	2.44	0.50
1:V:165:MET:HG3	1:V:169:LEU:CD2	2.39	0.50
1:A:119:LYS:HD2	2:A:202:HOH:O	2.11	0.50
1:P:119:LYS:HD2	2:P:201:HOH:O	2.11	0.50
1:V:90:ARG:HH12	1:V:98:ASN:HD21	1.56	0.50
1:C:60:HIS:CD2	1:C:63:ARG:HH12	2.29	0.50
1:G:49:LYS:O	1:G:53:LYS:HG2	2.11	0.50
1:E:119:LYS:HD2	2:E:228:HOH:O	2.10	0.50
1:N:119:LYS:HD2	2:N:201:HOH:O	2.10	0.50
1:J:153:THR:HG22	1:J:157:LYS:HZ3	1.76	0.50
1:H:165:MET:HG3	1:H:169:LEU:CD2	2.39	0.50
1:R:34:TYR:OH	1:R:107:GLU:OE2	2.19	0.50
1:U:119:LYS:HD2	2:U:201:HOH:O	2.11	0.50
1:V:60:HIS:CD2	1:V:63:ARG:HH12	2.29	0.50
1:A:49:LYS:O	1:A:53:LYS:HG2	2.11	0.50
1:S:49:LYS:O	1:S:53:LYS:HG2	2.11	0.50
1:V:49:LYS:O	1:V:53:LYS:HG2	2.11	0.50
1:R:90:ARG:HD3	1:R:92:ASP:O	2.12	0.50
1:S:90:ARG:HD3	1:S:92:ASP:O	2.12	0.50
1:X:90:ARG:HD3	1:X:92:ASP:O	2.12	0.50
1:D:90:ARG:HH12	1:D:98:ASN:HD21	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:34:TYR:OH	1:I:107:GLU:OE2	2.22	0.50
1:M:142:VAL:HG12	1:O:75:GLN:HG2	1.94	0.50
1:U:90:ARG:HH12	1:U:98:ASN:HD21	1.59	0.50
1:D:153:THR:HG22	1:D:157:LYS:HZ3	1.76	0.50
1:V:34:TYR:OH	1:V:107:GLU:OE2	2.22	0.50
1:U:165:MET:HG3	1:U:169:LEU:CD2	2.39	0.50
1:G:119:LYS:HD2	2:G:201:HOH:O	2.11	0.50
1:P:90:ARG:HH12	1:P:98:ASN:HD21	1.56	0.50
1:Q:119:LYS:HD2	2:Q:201:HOH:O	2.11	0.50
1:W:119:LYS:HD2	2:W:201:HOH:O	2.11	0.50
1:G:142:VAL:HG12	1:I:75:GLN:HG2	1.92	0.50
1:H:49:LYS:O	1:H:53:LYS:HG2	2.12	0.50
1:E:60:HIS:CD2	1:E:63:ARG:HH12	2.29	0.50
1:I:60:HIS:CD2	1:I:63:ARG:HH12	2.29	0.50
1:P:60:HIS:CD2	1:P:63:ARG:HH12	2.29	0.50
1:T:75:GLN:HG2	1:U:142:VAL:HG12	1.93	0.50
1:X:60:HIS:CD2	1:X:63:ARG:HH12	2.29	0.50
1:B:49:LYS:O	1:B:53:LYS:HG2	2.12	0.50
1:H:49:LYS:O	1:H:53:LYS:HG2	2.12	0.50
1:T:119:LYS:HD2	2:T:201:HOH:O	2.09	0.50
1:M:49:LYS:O	1:M:53:LYS:HG2	2.11	0.50
1:Q:49:LYS:O	1:Q:53:LYS:HG2	2.11	0.50
1:W:49:LYS:O	1:W:53:LYS:HG2	2.11	0.50
1:K:34:TYR:OH	1:K:107:GLU:OE2	2.23	0.50
1:K:119:LYS:HD2	2:K:201:HOH:O	2.10	0.50
1:D:90:ARG:HD3	1:D:92:ASP:O	2.12	0.50
1:F:90:ARG:HD3	1:F:92:ASP:O	2.12	0.50
1:J:90:ARG:HD3	1:J:92:ASP:O	2.12	0.50
1:M:90:ARG:HD3	1:M:92:ASP:O	2.12	0.50
1:T:90:ARG:HD3	1:T:92:ASP:O	2.12	0.50
1:T:119:LYS:HD2	2:T:201:HOH:O	2.10	0.50
1:B:49:LYS:O	1:B:53:LYS:HG2	2.12	0.50
1:C:34:TYR:OH	1:C:107:GLU:OE2	2.22	0.50
1:H:49:LYS:O	1:H:53:LYS:HG2	2.12	0.50
1:J:90:ARG:HH12	1:J:98:ASN:HD21	1.59	0.50
1:O:90:ARG:HH12	1:O:98:ASN:HD21	1.59	0.50
1:Q:34:TYR:OH	1:Q:107:GLU:OE2	2.22	0.50
1:B:49:LYS:O	1:B:53:LYS:HG2	2.12	0.50
1:K:49:LYS:O	1:K:53:LYS:HG2	2.12	0.50
1:N:119:LYS:HD2	2:N:201:HOH:O	2.09	0.50
1:H:90:ARG:HD3	1:H:92:ASP:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:LYS:O	1:B:53:LYS:HG2	2.12	0.50
1:H:49:LYS:O	1:H:53:LYS:HG2	2.12	0.50
1:K:49:LYS:O	1:K:53:LYS:HG2	2.12	0.50
1:O:153:THR:HG22	1:O:157:LYS:HZ2	1.75	0.50
1:O:165:MET:HG3	1:O:169:LEU:CD2	2.39	0.50
1:X:153:THR:HG22	1:X:157:LYS:HZ2	1.76	0.50
1:F:119:LYS:HD2	2:F:201:HOH:O	2.11	0.50
1:L:119:LYS:HD2	2:L:201:HOH:O	2.11	0.50
1:E:49:LYS:O	1:E:53:LYS:HG2	2.12	0.50
1:K:60:HIS:CD2	1:K:63:ARG:HH12	2.29	0.50
1:R:60:HIS:CD2	1:R:63:ARG:HH12	2.29	0.50
1:K:49:LYS:O	1:K:53:LYS:HG2	2.12	0.50
1:E:153:THR:HG22	1:E:157:LYS:HZ3	1.75	0.50
1:O:49:LYS:O	1:O:53:LYS:HG2	2.11	0.50
1:P:49:LYS:O	1:P:53:LYS:HG2	2.11	0.50
1:R:49:LYS:O	1:R:53:LYS:HG2	2.11	0.50
1:U:49:LYS:O	1:U:53:LYS:HG2	2.11	0.50
1:D:44:ASP:OD2	1:I:6:SER:OG	2.29	0.50
1:B:90:ARG:HD3	1:B:92:ASP:O	2.12	0.50
1:B:119:LYS:HD2	2:B:236:HOH:O	2.10	0.50
1:L:90:ARG:HD3	1:L:92:ASP:O	2.12	0.50
1:N:90:ARG:HD3	1:N:92:ASP:O	2.12	0.50
1:N:165:MET:HG3	1:N:169:LEU:CD2	2.42	0.50
1:C:67:GLU:HA	1:C:70:MET:HE2	1.92	0.50
1:E:49:LYS:O	1:E:53:LYS:HG2	2.12	0.50
1:E:90:ARG:HH12	1:E:98:ASN:HD21	1.59	0.50
1:K:90:ARG:HH12	1:K:98:ASN:HD21	1.59	0.50
1:N:90:ARG:HH12	1:N:98:ASN:HD21	1.59	0.50
1:R:115:LEU:O	1:R:119:LYS:HG2	2.10	0.50
1:E:49:LYS:O	1:E:53:LYS:HG2	2.12	0.50
1:E:119:LYS:HD2	2:E:228:HOH:O	2.11	0.50
1:I:119:LYS:HD2	2:I:201:HOH:O	2.11	0.50
1:C:90:ARG:HD3	1:C:92:ASP:O	2.12	0.50
1:H:119:LYS:HD2	2:H:201:HOH:O	2.10	0.50
1:I:90:ARG:HD3	1:I:92:ASP:O	2.12	0.50
1:T:165:MET:HG3	1:T:169:LEU:CD2	2.42	0.50
1:C:90:ARG:HH12	1:C:98:ASN:HD21	1.59	0.50
1:K:49:LYS:O	1:K:53:LYS:HG2	2.12	0.50
1:T:90:ARG:HH12	1:T:98:ASN:HD21	1.59	0.50
1:I:69:LEU:HD13	1:I:137:TYR:OH	2.12	0.50
1:U:153:THR:HG22	1:U:157:LYS:HZ2	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:LYS:O	1:A:53:LYS:HG2	2.12	0.50
1:F:34:TYR:OH	1:F:107:GLU:OE2	2.18	0.50
1:M:49:LYS:O	1:M:53:LYS:HG2	2.12	0.50
1:A:49:LYS:O	1:A:53:LYS:HG2	2.12	0.50
1:E:49:LYS:O	1:E:53:LYS:HG2	2.12	0.50
1:G:49:LYS:O	1:G:53:LYS:HG2	2.12	0.50
1:V:49:LYS:O	1:V:53:LYS:HG2	2.12	0.50
1:X:49:LYS:O	1:X:53:LYS:HG2	2.11	0.50
1:H:119:LYS:HD2	2:H:201:HOH:O	2.10	0.50
1:K:90:ARG:HD3	1:K:92:ASP:O	2.12	0.50
1:A:49:LYS:O	1:A:53:LYS:HG2	2.12	0.50
1:G:49:LYS:O	1:G:53:LYS:HG2	2.12	0.50
1:C:69:LEU:HD13	1:C:137:TYR:OH	2.12	0.50
1:T:153:THR:HG22	1:T:157:LYS:HZ3	1.77	0.50
1:D:90:ARG:HD3	1:D:92:ASP:O	2.12	0.50
1:E:51:PHE:CD1	1:E:175:LEU:HD12	2.46	0.50
1:L:90:ARG:HD3	1:L:92:ASP:O	2.12	0.50
1:L:153:THR:HG22	1:L:157:LYS:HZ3	1.77	0.50
1:G:49:LYS:O	1:G:53:LYS:HG2	2.12	0.50
1:S:49:LYS:O	1:S:53:LYS:HG2	2.12	0.50
1:B:119:LYS:HD2	2:B:201:HOH:O	2.10	0.50
1:J:119:LYS:HD2	2:J:201:HOH:O	2.10	0.50
1:M:119:LYS:HD2	2:M:201:HOH:O	2.10	0.50
1:N:119:LYS:HD2	2:N:201:HOH:O	2.10	0.50
1:E:90:ARG:HD3	1:E:92:ASP:O	2.12	0.50
1:S:49:LYS:O	1:S:53:LYS:HG2	2.12	0.50
1:N:153:THR:HG22	1:N:157:LYS:HZ3	1.77	0.50
1:F:90:ARG:HD3	1:F:92:ASP:O	2.12	0.50
1:K:51:PHE:CD1	1:K:175:LEU:HD12	2.46	0.50
1:S:49:LYS:O	1:S:53:LYS:HG2	2.12	0.50
1:T:90:ARG:HD3	1:T:92:ASP:O	2.12	0.50
1:U:34:TYR:OH	1:U:107:GLU:OE2	2.19	0.50
1:B:49:LYS:O	1:B:53:LYS:HG2	2.12	0.50
1:C:119:LYS:HD2	2:C:201:HOH:O	2.11	0.50
1:H:49:LYS:O	1:H:53:LYS:HG2	2.12	0.50
1:Q:49:LYS:O	1:Q:53:LYS:HG2	2.12	0.50
1:R:34:TYR:OH	1:R:107:GLU:OE2	2.18	0.50
1:S:49:LYS:O	1:S:53:LYS:HG2	2.12	0.50
1:S:119:LYS:HD2	2:S:201:HOH:O	2.10	0.50
1:G:165:MET:HG3	1:G:169:LEU:CD2	2.42	0.50
1:M:119:LYS:HD2	2:M:201:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:119:LYS:HD2	2:S:201:HOH:O	2.10	0.50
1:I:90:ARG:HH12	1:I:98:ASN:HD21	1.59	0.49
1:U:49:LYS:O	1:U:53:LYS:HG2	2.12	0.49
1:V:49:LYS:O	1:V:53:LYS:HG2	2.12	0.49
1:K:69:LEU:HD13	1:K:137:TYR:OH	2.12	0.49
1:Q:69:LEU:HD13	1:Q:137:TYR:OH	2.12	0.49
1:A:49:LYS:O	1:A:53:LYS:HG2	2.12	0.49
1:G:49:LYS:O	1:G:53:LYS:HG2	2.12	0.49
1:M:49:LYS:O	1:M:53:LYS:HG2	2.12	0.49
1:N:90:ARG:HD3	1:N:92:ASP:O	2.12	0.49
1:R:90:ARG:HD3	1:R:92:ASP:O	2.12	0.49
1:S:90:ARG:HD3	1:S:92:ASP:O	2.12	0.49
1:R:49:LYS:O	1:R:53:LYS:HG2	2.12	0.49
1:V:49:LYS:O	1:V:53:LYS:HG2	2.12	0.49
1:W:49:LYS:O	1:W:53:LYS:HG2	2.12	0.49
1:M:49:LYS:O	1:M:53:LYS:HG2	2.12	0.49
1:P:49:LYS:O	1:P:53:LYS:HG2	2.12	0.49
1:R:49:LYS:O	1:R:53:LYS:HG2	2.12	0.49
1:D:49:LYS:O	1:D:53:LYS:HG2	2.11	0.49
1:D:119:LYS:HD2	2:D:201:HOH:O	2.10	0.49
1:T:119:LYS:HD2	2:T:201:HOH:O	2.10	0.49
1:A:165:MET:HG3	1:A:169:LEU:CD2	2.42	0.49
1:F:165:MET:O	1:F:169:LEU:HD23	2.12	0.49
1:K:165:MET:O	1:K:169:LEU:HD23	2.12	0.49
1:L:165:MET:O	1:L:169:LEU:HD23	2.12	0.49
1:W:90:ARG:HD3	1:W:92:ASP:O	2.12	0.49
1:M:49:LYS:O	1:M:53:LYS:HG2	2.12	0.49
1:P:49:LYS:O	1:P:53:LYS:HG2	2.12	0.49
1:Q:49:LYS:O	1:Q:53:LYS:HG2	2.12	0.49
1:R:49:LYS:O	1:R:53:LYS:HG2	2.12	0.49
1:W:49:LYS:O	1:W:53:LYS:HG2	2.12	0.49
1:E:69:LEU:HD13	1:E:137:TYR:OH	2.12	0.49
1:F:69:LEU:HD13	1:F:137:TYR:OH	2.12	0.49
1:W:69:LEU:HD13	1:W:137:TYR:OH	2.12	0.49
1:E:90:ARG:HD3	1:E:92:ASP:O	2.12	0.49
1:J:90:ARG:HD3	1:J:92:ASP:O	2.12	0.49
1:K:90:ARG:HD3	1:K:92:ASP:O	2.12	0.49
1:M:90:ARG:HD3	1:M:92:ASP:O	2.12	0.49
1:W:49:LYS:O	1:W:53:LYS:HG2	2.12	0.49
1:W:153:THR:HG22	1:W:157:LYS:HZ3	1.75	0.49
1:X:90:ARG:HD3	1:X:92:ASP:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:119:LYS:HD2	2:S:201:HOH:O	2.11	0.49
1:L:34:TYR:OH	1:L:107:GLU:OE2	2.18	0.49
1:P:49:LYS:O	1:P:53:LYS:HG2	2.12	0.49
1:U:49:LYS:O	1:U:53:LYS:HG2	2.12	0.49
1:D:60:HIS:CD2	1:D:63:ARG:HH12	2.29	0.49
1:J:60:HIS:CD2	1:J:63:ARG:HH12	2.29	0.49
1:Q:49:LYS:O	1:Q:53:LYS:HG2	2.12	0.49
1:U:49:LYS:O	1:U:53:LYS:HG2	2.12	0.49
1:W:49:LYS:O	1:W:53:LYS:HG2	2.12	0.49
1:X:49:LYS:O	1:X:53:LYS:HG2	2.12	0.49
1:X:34:TYR:OH	1:X:107:GLU:OE2	2.23	0.49
1:Q:90:ARG:HD3	1:Q:92:ASP:O	2.12	0.49
1:B:67:GLU:HA	1:B:70:MET:HE2	1.94	0.49
1:P:90:ARG:HH12	1:P:98:ASN:HD21	1.59	0.49
1:A:69:LEU:HD13	1:A:137:TYR:OH	2.12	0.49
1:G:69:LEU:HD13	1:G:137:TYR:OH	2.12	0.49
1:H:69:LEU:HD13	1:H:137:TYR:OH	2.12	0.49
1:K:153:THR:HG22	1:K:157:LYS:HZ3	1.76	0.49
1:L:69:LEU:HD13	1:L:137:TYR:OH	2.12	0.49
1:X:69:LEU:HD13	1:X:137:TYR:OH	2.12	0.49
1:P:49:LYS:O	1:P:53:LYS:HG2	2.12	0.49
1:Q:49:LYS:O	1:Q:53:LYS:HG2	2.12	0.49
1:V:49:LYS:O	1:V:53:LYS:HG2	2.12	0.49
1:A:49:LYS:O	1:A:53:LYS:HG2	2.12	0.49
1:O:49:LYS:O	1:O:53:LYS:HG2	2.12	0.49
1:O:49:LYS:O	1:O:53:LYS:HG2	2.12	0.49
1:A:165:MET:O	1:A:169:LEU:HD23	2.12	0.49
1:E:165:MET:O	1:E:169:LEU:HD23	2.13	0.49
1:H:165:MET:O	1:H:169:LEU:HD23	2.12	0.49
1:J:165:MET:O	1:J:169:LEU:HD23	2.12	0.49
1:M:165:MET:O	1:M:169:LEU:HD23	2.12	0.49
1:P:90:ARG:HD3	1:P:92:ASP:O	2.12	0.49
1:P:165:MET:O	1:P:169:LEU:HD23	2.12	0.49
1:V:165:MET:O	1:V:169:LEU:HD23	2.12	0.49
1:O:49:LYS:O	1:O:53:LYS:HG2	2.12	0.49
1:X:49:LYS:O	1:X:53:LYS:HG2	2.12	0.49
1:C:90:ARG:HD3	1:C:92:ASP:O	2.12	0.49
1:H:90:ARG:HD3	1:H:92:ASP:O	2.12	0.49
1:R:49:LYS:O	1:R:53:LYS:HG2	2.12	0.49
1:U:49:LYS:O	1:U:53:LYS:HG2	2.12	0.49
1:X:49:LYS:O	1:X:53:LYS:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:49:LYS:O	1:E:53:LYS:HG2	2.12	0.49
1:G:49:LYS:O	1:G:53:LYS:HG2	2.12	0.49
1:K:49:LYS:O	1:K:53:LYS:HG2	2.12	0.49
1:N:119:LYS:HD2	2:N:201:HOH:O	2.11	0.49
1:X:49:LYS:O	1:X:53:LYS:HG2	2.12	0.49
1:I:49:LYS:O	1:I:53:LYS:HG2	2.11	0.49
1:J:49:LYS:O	1:J:53:LYS:HG2	2.11	0.49
1:N:49:LYS:O	1:N:53:LYS:HG2	2.11	0.49
1:S:153:THR:HG22	1:S:157:LYS:HZ2	1.77	0.49
1:I:90:ARG:HH12	1:I:98:ASN:HD21	1.56	0.49
1:B:165:MET:O	1:B:169:LEU:HD23	2.12	0.49
1:D:165:MET:O	1:D:169:LEU:HD23	2.12	0.49
1:G:165:MET:O	1:G:169:LEU:HD23	2.12	0.49
1:V:90:ARG:HD3	1:V:92:ASP:O	2.12	0.49
1:X:165:MET:HG3	1:X:169:LEU:CD2	2.42	0.49
1:V:90:ARG:HH12	1:V:98:ASN:HD21	1.59	0.49
1:B:69:LEU:HD13	1:B:137:TYR:OH	2.12	0.49
1:R:69:LEU:HD13	1:R:137:TYR:OH	2.12	0.49
1:B:90:ARG:HD3	1:B:92:ASP:O	2.12	0.49
1:I:153:THR:HG22	1:I:157:LYS:HZ2	1.78	0.49
1:O:49:LYS:O	1:O:53:LYS:HG2	2.12	0.49
1:P:49:LYS:O	1:P:53:LYS:HG2	2.12	0.49
1:T:119:LYS:HD2	2:T:201:HOH:O	2.11	0.49
1:V:49:LYS:O	1:V:53:LYS:HG2	2.12	0.49
1:A:75:GLN:OE1	2:A:201:HOH:O	2.19	0.49
1:K:75:GLN:HG2	1:L:142:VAL:HG12	1.92	0.49
1:C:49:LYS:O	1:C:53:LYS:HG2	2.11	0.49
1:F:49:LYS:O	1:F:53:LYS:HG2	2.11	0.49
1:L:49:LYS:O	1:L:53:LYS:HG2	2.11	0.49
1:T:49:LYS:O	1:T:53:LYS:HG2	2.11	0.49
1:R:34:TYR:OH	1:R:107:GLU:OE2	2.23	0.49
1:Q:165:MET:O	1:Q:169:LEU:HD23	2.12	0.49
1:S:165:MET:O	1:S:169:LEU:HD23	2.12	0.49
1:U:165:MET:O	1:U:169:LEU:HD23	2.12	0.49
1:W:165:MET:O	1:W:169:LEU:HD23	2.12	0.49
1:B:153:THR:HG22	1:B:157:LYS:HZ2	1.77	0.49
1:I:90:ARG:HD3	1:I:92:ASP:O	2.12	0.49
1:M:119:LYS:HD2	2:M:201:HOH:O	2.11	0.49
1:S:49:LYS:O	1:S:53:LYS:HG2	2.12	0.49
1:W:49:LYS:O	1:W:53:LYS:HG2	2.12	0.49
1:M:153:THR:HG22	1:M:157:LYS:HZ2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:ARG:HH12	1:C:98:ASN:HD21	1.56	0.49
1:C:165:MET:HG3	1:C:169:LEU:CD2	2.42	0.49
1:H:49:LYS:O	1:H:53:LYS:HG2	2.13	0.49
1:J:165:MET:HG3	1:J:169:LEU:CD2	2.42	0.49
1:T:165:MET:O	1:T:169:LEU:HD23	2.12	0.49
1:D:49:LYS:O	1:D:53:LYS:HG2	2.12	0.49
1:F:90:ARG:HH12	1:F:98:ASN:HD21	1.59	0.49
1:S:90:ARG:HH12	1:S:98:ASN:HD21	1.59	0.49
1:O:49:LYS:O	1:O:53:LYS:HG2	2.12	0.49
1:R:49:LYS:O	1:R:53:LYS:HG2	2.12	0.49
1:U:49:LYS:O	1:U:53:LYS:HG2	2.12	0.49
1:X:49:LYS:O	1:X:53:LYS:HG2	2.12	0.49
1:G:34:TYR:OH	1:G:107:GLU:OE2	2.21	0.49
1:B:49:LYS:O	1:B:53:LYS:HG2	2.13	0.49
1:E:165:MET:HG3	1:E:169:LEU:CD2	2.42	0.49
1:I:165:MET:HG3	1:I:169:LEU:CD2	2.42	0.49
1:N:165:MET:O	1:N:169:LEU:HD23	2.12	0.49
1:R:165:MET:HG3	1:R:169:LEU:CD2	2.42	0.49
1:N:69:LEU:HD13	1:N:137:TYR:OH	2.12	0.49
1:O:69:LEU:HD13	1:O:137:TYR:OH	2.12	0.49
1:S:165:MET:HG3	1:S:169:LEU:CD2	2.39	0.49
1:K:75:GLN:HG2	1:L:142:VAL:HG12	1.93	0.49
1:M:49:LYS:O	1:M:53:LYS:HG2	2.12	0.49
1:Q:49:LYS:O	1:Q:53:LYS:HG2	2.12	0.49
1:D:49:LYS:O	1:D:53:LYS:HG2	2.12	0.49
1:X:34:TYR:OH	1:X:107:GLU:OE2	2.21	0.49
1:D:165:MET:HG3	1:D:169:LEU:CD2	2.42	0.49
1:O:165:MET:O	1:O:169:LEU:HD23	2.12	0.49
1:M:90:ARG:HH12	1:M:98:ASN:HD21	1.59	0.49
1:T:69:LEU:HD13	1:T:137:TYR:OH	2.12	0.49
1:U:69:LEU:HD13	1:U:137:TYR:OH	2.12	0.49
1:Q:90:ARG:HD3	1:Q:92:ASP:O	2.12	0.49
1:D:49:LYS:O	1:D:53:LYS:HG2	2.12	0.49
1:J:49:LYS:O	1:J:53:LYS:HG2	2.12	0.49
1:I:49:LYS:O	1:I:53:LYS:HG2	2.12	0.49
1:J:49:LYS:O	1:J:53:LYS:HG2	2.12	0.49
1:A:49:LYS:O	1:A:53:LYS:HG2	2.13	0.49
1:C:34:TYR:OH	1:C:107:GLU:OE2	2.22	0.49
1:K:49:LYS:O	1:K:53:LYS:HG2	2.13	0.49
1:K:165:MET:HG3	1:K:169:LEU:CD2	2.42	0.49
1:B:90:ARG:HH12	1:B:98:ASN:HD21	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:90:ARG:HH12	1:H:98:ASN:HD21	1.59	0.49
1:J:49:LYS:O	1:J:53:LYS:HG2	2.12	0.49
1:L:90:ARG:HH12	1:L:98:ASN:HD21	1.59	0.49
1:M:69:LEU:HD13	1:M:137:TYR:OH	2.12	0.49
1:X:34:TYR:OH	1:X:107:GLU:OE2	2.19	0.49
1:H:119:LYS:HD2	2:H:201:HOH:O	2.11	0.49
1:I:34:TYR:OH	1:I:107:GLU:OE2	2.21	0.49
1:J:119:LYS:HD2	2:J:201:HOH:O	2.11	0.49
1:R:34:TYR:OH	1:R:107:GLU:OE2	2.21	0.49
1:E:49:LYS:O	1:E:53:LYS:HG2	2.13	0.49
1:G:49:LYS:O	1:G:53:LYS:HG2	2.13	0.49
1:I:34:TYR:OH	1:I:107:GLU:OE2	2.22	0.49
1:I:165:MET:O	1:I:169:LEU:HD23	2.12	0.49
1:X:34:TYR:OH	1:X:107:GLU:OE2	2.22	0.49
1:I:49:LYS:O	1:I:53:LYS:HG2	2.12	0.48
1:A:153:THR:HG22	1:A:157:LYS:HZ3	1.77	0.48
1:C:34:TYR:OH	1:C:107:GLU:OE2	2.19	0.48
1:D:49:LYS:O	1:D:53:LYS:HG2	2.12	0.48
1:J:49:LYS:O	1:J:53:LYS:HG2	2.12	0.48
1:W:90:ARG:HD3	1:W:92:ASP:O	2.12	0.48
1:T:49:LYS:O	1:T:53:LYS:HG2	2.12	0.48
1:A:34:TYR:OH	1:A:107:GLU:OE2	2.21	0.48
1:F:49:LYS:O	1:F:53:LYS:HG2	2.12	0.48
1:C:49:LYS:O	1:C:53:LYS:HG2	2.12	0.48
1:F:49:LYS:O	1:F:53:LYS:HG2	2.12	0.48
1:L:49:LYS:O	1:L:53:LYS:HG2	2.12	0.48
1:N:49:LYS:O	1:N:53:LYS:HG2	2.12	0.48
1:Q:90:ARG:HH12	1:Q:98:ASN:HD21	1.59	0.48
1:S:69:LEU:HD13	1:S:137:TYR:OH	2.12	0.48
1:X:34:TYR:OH	1:X:107:GLU:OE2	2.22	0.48
1:B:119:LYS:HD2	2:B:201:HOH:O	2.11	0.48
1:F:49:LYS:O	1:F:53:LYS:HG2	2.12	0.48
1:I:49:LYS:O	1:I:53:LYS:HG2	2.12	0.48
1:C:49:LYS:O	1:C:53:LYS:HG2	2.12	0.48
1:L:49:LYS:O	1:L:53:LYS:HG2	2.12	0.48
1:N:49:LYS:O	1:N:53:LYS:HG2	2.12	0.48
1:F:153:THR:HG22	1:F:157:LYS:HZ2	1.78	0.48
1:L:174:THR:HA	1:L:177:HIS:CE1	2.48	0.48
1:C:165:MET:O	1:C:169:LEU:HD23	2.12	0.48
1:R:34:TYR:OH	1:R:107:GLU:OE2	2.22	0.48
1:R:49:LYS:O	1:R:53:LYS:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:49:LYS:O	1:S:53:LYS:HG2	2.13	0.48
1:U:49:LYS:O	1:U:53:LYS:HG2	2.13	0.48
1:U:90:ARG:HD3	1:U:92:ASP:O	2.12	0.48
1:V:49:LYS:O	1:V:53:LYS:HG2	2.13	0.48
1:T:49:LYS:O	1:T:53:LYS:HG2	2.12	0.48
1:W:90:ARG:HH12	1:W:98:ASN:HD21	1.59	0.48
1:F:49:LYS:O	1:F:53:LYS:HG2	2.12	0.48
1:M:153:THR:HG22	1:M:157:LYS:HZ2	1.78	0.48
1:O:90:ARG:HD3	1:O:92:ASP:O	2.12	0.48
1:S:153:THR:HG22	1:S:157:LYS:HZ2	1.78	0.48
1:D:49:LYS:O	1:D:53:LYS:HG2	2.12	0.48
1:D:119:LYS:HD2	2:D:201:HOH:O	2.11	0.48
1:C:49:LYS:O	1:C:53:LYS:HG2	2.12	0.48
1:L:49:LYS:O	1:L:53:LYS:HG2	2.12	0.48
1:N:49:LYS:O	1:N:53:LYS:HG2	2.12	0.48
1:T:49:LYS:O	1:T:53:LYS:HG2	2.12	0.48
1:H:165:MET:HG3	1:H:169:LEU:CD2	2.42	0.48
1:M:49:LYS:O	1:M:53:LYS:HG2	2.13	0.48
1:P:49:LYS:O	1:P:53:LYS:HG2	2.13	0.48
1:P:165:MET:HG3	1:P:169:LEU:CD2	2.42	0.48
1:Q:49:LYS:O	1:Q:53:LYS:HG2	2.13	0.48
1:W:49:LYS:O	1:W:53:LYS:HG2	2.13	0.48
1:X:49:LYS:O	1:X:53:LYS:HG2	2.13	0.48
1:C:49:LYS:O	1:C:53:LYS:HG2	2.12	0.48
1:I:49:LYS:O	1:I:53:LYS:HG2	2.12	0.48
1:N:49:LYS:O	1:N:53:LYS:HG2	2.12	0.48
1:T:49:LYS:O	1:T:53:LYS:HG2	2.12	0.48
1:U:90:ARG:HD3	1:U:92:ASP:O	2.12	0.48
1:B:165:MET:HG3	1:B:169:LEU:CD2	2.42	0.48
1:G:90:ARG:HD3	1:G:92:ASP:O	2.12	0.48
1:O:49:LYS:O	1:O:53:LYS:HG2	2.13	0.48
1:O:90:ARG:HD3	1:O:92:ASP:O	2.12	0.48
1:C:34:TYR:OH	1:C:107:GLU:OE2	2.22	0.48
1:P:69:LEU:HD13	1:P:137:TYR:OH	2.12	0.48
1:R:34:TYR:OH	1:R:107:GLU:OE2	2.22	0.48
1:V:69:LEU:HD13	1:V:137:TYR:OH	2.12	0.48
1:L:49:LYS:O	1:L:53:LYS:HG2	2.12	0.48
1:F:49:LYS:O	1:F:53:LYS:HG2	2.12	0.48
1:I:49:LYS:O	1:I:53:LYS:HG2	2.12	0.48
1:J:49:LYS:O	1:J:53:LYS:HG2	2.12	0.48
1:L:34:TYR:OH	1:L:107:GLU:OE2	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:153:THR:HG22	1:L:157:LYS:HZ2	1.78	0.48
1:V:165:MET:HG3	1:V:169:LEU:CD2	2.42	0.48
1:X:165:MET:O	1:X:169:LEU:HD23	2.12	0.48
1:I:34:TYR:OH	1:I:107:GLU:OE2	2.22	0.48
1:J:69:LEU:HD13	1:J:137:TYR:OH	2.12	0.48
1:H:49:LYS:O	1:H:53:LYS:HG2	2.14	0.48
1:A:90:ARG:HD3	1:A:92:ASP:O	2.12	0.48
1:D:69:LEU:HD13	1:D:137:TYR:OH	2.12	0.48
1:V:153:THR:HG22	1:V:157:LYS:HZ3	1.76	0.48
1:V:90:ARG:HD3	1:V:92:ASP:O	2.12	0.48
1:C:49:LYS:O	1:C:53:LYS:HG2	2.12	0.48
1:L:49:LYS:O	1:L:53:LYS:HG2	2.12	0.48
1:T:49:LYS:O	1:T:53:LYS:HG2	2.12	0.48
1:O:151:HIS:HD2	2:O:242:HOH:O	1.97	0.48
1:A:49:LYS:O	1:A:53:LYS:HG2	2.14	0.48
1:B:49:LYS:O	1:B:53:LYS:HG2	2.14	0.48
1:O:165:MET:HG3	1:O:169:LEU:CD2	2.42	0.48
1:U:165:MET:HG3	1:U:169:LEU:CD2	2.42	0.48
1:P:153:THR:HG22	1:P:157:LYS:HZ3	1.76	0.48
1:P:90:ARG:HD3	1:P:92:ASP:O	2.12	0.48
1:N:49:LYS:O	1:N:53:LYS:HG2	2.12	0.48
1:X:153:THR:HG22	1:X:157:LYS:HZ3	1.79	0.48
1:G:49:LYS:O	1:G:53:LYS:HG2	2.14	0.48
1:S:173:HIS:O	1:S:177:HIS:CD2	2.60	0.48
1:S:173:HIS:HA	1:S:177:HIS:CD2	2.49	0.48
1:W:151:HIS:HD2	2:W:244:HOH:O	1.97	0.48
1:M:153:THR:HG22	1:M:157:LYS:HZ3	1.77	0.48
1:K:49:LYS:O	1:K:53:LYS:HG2	2.14	0.48
1:R:49:LYS:O	1:R:53:LYS:HG2	2.14	0.48
1:V:49:LYS:O	1:V:53:LYS:HG2	2.14	0.48
1:R:165:MET:O	1:R:169:LEU:HD23	2.13	0.48
1:S:173:HIS:HA	1:S:177:HIS:CD2	2.48	0.48
1:Q:151:HIS:HD2	2:Q:245:HOH:O	1.97	0.48
1:U:151:HIS:HD2	2:U:244:HOH:O	1.97	0.48
1:F:82:LEU:HD12	1:F:82:LEU:N	2.29	0.48
1:L:82:LEU:HD12	1:L:82:LEU:N	2.29	0.48
1:Q:82:LEU:HD12	1:Q:82:LEU:N	2.29	0.48
1:S:153:THR:HG22	1:S:157:LYS:HZ3	1.77	0.48
1:E:49:LYS:O	1:E:53:LYS:HG2	2.14	0.48
1:O:49:LYS:O	1:O:53:LYS:HG2	2.14	0.48
1:P:49:LYS:O	1:P:53:LYS:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:49:LYS:O	1:U:53:LYS:HG2	2.14	0.48
1:W:34:TYR:OH	1:W:107:GLU:OE2	2.23	0.48
1:X:49:LYS:O	1:X:53:LYS:HG2	2.14	0.48
1:D:49:LYS:O	1:D:53:LYS:HG2	2.13	0.48
1:L:165:MET:HG3	1:L:169:LEU:CD2	2.42	0.48
1:O:82:LEU:HD12	1:O:82:LEU:N	2.29	0.47
1:U:82:LEU:HD12	1:U:82:LEU:N	2.29	0.47
1:W:82:LEU:HD12	1:W:82:LEU:N	2.29	0.47
1:Q:49:LYS:O	1:Q:53:LYS:HG2	2.14	0.47
1:W:49:LYS:O	1:W:53:LYS:HG2	2.14	0.47
1:F:165:MET:HG3	1:F:169:LEU:CD2	2.42	0.47
1:J:49:LYS:O	1:J:53:LYS:HG2	2.13	0.47
1:F:153:THR:HG22	1:F:157:LYS:HZ3	1.79	0.47
1:L:153:THR:HG22	1:L:157:LYS:HZ2	1.79	0.47
1:I:151:HIS:HD2	2:I:241:HOH:O	1.97	0.47
1:N:151:HIS:HD2	2:N:243:HOH:O	1.97	0.47
1:A:82:LEU:HD12	1:A:82:LEU:N	2.29	0.47
1:C:82:LEU:HD12	1:C:82:LEU:N	2.29	0.47
1:I:49:LYS:O	1:I:53:LYS:HG2	2.13	0.47
1:C:151:HIS:HD2	2:C:244:HOH:O	1.97	0.47
1:E:82:LEU:HD12	1:E:82:LEU:N	2.29	0.47
1:G:82:LEU:HD12	1:G:82:LEU:N	2.29	0.47
1:I:82:LEU:HD12	1:I:82:LEU:N	2.29	0.47
1:K:82:LEU:HD12	1:K:82:LEU:N	2.29	0.47
1:N:82:LEU:HD12	1:N:82:LEU:N	2.29	0.47
1:T:82:LEU:HD12	1:T:82:LEU:N	2.29	0.47
1:F:49:LYS:O	1:F:53:LYS:HG2	2.13	0.47
1:X:177:HIS:O	1:X:177:HIS:ND1	2.48	0.47
1:R:151:HIS:HD2	2:R:243:HOH:O	1.98	0.47
1:S:49:LYS:O	1:S:53:LYS:HG2	2.14	0.47
1:C:49:LYS:O	1:C:53:LYS:HG2	2.13	0.47
1:L:49:LYS:O	1:L:53:LYS:HG2	2.13	0.47
1:X:151:HIS:HD2	2:X:243:HOH:O	1.98	0.47
1:L:34:TYR:OH	1:L:107:GLU:OE2	2.17	0.47
1:M:49:LYS:O	1:M:53:LYS:HG2	2.14	0.47
1:N:49:LYS:O	1:N:53:LYS:HG2	2.13	0.47
1:N:53:LYS:HD3	2:N:267:HOH:O	2.15	0.47
1:A:90:ARG:HD3	1:A:92:ASP:O	2.12	0.47
1:T:49:LYS:O	1:T:53:LYS:HG2	2.13	0.47
1:T:53:LYS:HD3	2:T:267:HOH:O	2.15	0.47
1:G:90:ARG:HD3	1:G:92:ASP:O	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:HIS:HD2	2:B:244:HOH:O	1.97	0.47
1:F:151:HIS:HD2	2:F:245:HOH:O	1.98	0.47
1:H:151:HIS:HD2	2:H:245:HOH:O	1.97	0.47
1:L:151:HIS:HD2	2:L:243:HOH:O	1.98	0.47
1:B:82:LEU:HD12	1:B:82:LEU:N	2.29	0.47
1:M:82:LEU:HD12	1:M:82:LEU:N	2.29	0.47
1:R:82:LEU:HD12	1:R:82:LEU:N	2.29	0.47
1:V:82:LEU:HD12	1:V:82:LEU:N	2.29	0.47
1:X:82:LEU:HD12	1:X:82:LEU:N	2.29	0.47
1:D:49:LYS:O	1:D:53:LYS:HG2	2.14	0.47
1:F:49:LYS:O	1:F:53:LYS:HG2	2.14	0.47
1:L:49:LYS:O	1:L:53:LYS:HG2	2.14	0.47
1:S:34:TYR:OH	1:S:107:GLU:OE2	2.21	0.47
1:C:153:THR:HG22	1:C:157:LYS:HZ3	1.78	0.47
1:H:82:LEU:HD12	1:H:82:LEU:N	2.29	0.47
1:P:82:LEU:HD12	1:P:82:LEU:N	2.29	0.47
1:S:82:LEU:HD12	1:S:82:LEU:N	2.29	0.47
1:G:142:VAL:HG12	1:I:75:GLN:HG2	1.96	0.47
1:O:53:LYS:HD3	2:O:268:HOH:O	2.15	0.47
1:S:53:LYS:HD3	2:S:268:HOH:O	2.15	0.47
1:F:34:TYR:OH	1:F:107:GLU:OE2	2.17	0.47
1:I:49:LYS:O	1:I:53:LYS:HG2	2.14	0.47
1:S:165:MET:HG3	1:S:169:LEU:CD2	2.42	0.47
1:G:153:THR:HG22	1:G:157:LYS:HZ3	1.79	0.47
1:D:151:HIS:HD2	2:D:243:HOH:O	1.97	0.47
1:M:34:TYR:OH	1:M:107:GLU:OE2	2.21	0.47
1:B:34:TYR:OH	1:B:107:GLU:OE2	2.17	0.47
1:D:82:LEU:HD12	1:D:82:LEU:N	2.29	0.47
1:I:153:THR:HG22	1:I:157:LYS:HZ3	1.78	0.47
1:W:34:TYR:OH	1:W:107:GLU:OE2	2.17	0.47
1:C:49:LYS:O	1:C:53:LYS:HG2	2.14	0.47
1:J:49:LYS:O	1:J:53:LYS:HG2	2.14	0.47
1:S:34:TYR:OH	1:S:107:GLU:OE2	2.22	0.47
1:R:34:TYR:OH	1:R:107:GLU:OE2	2.22	0.46
1:V:53:LYS:HD3	2:V:267:HOH:O	2.15	0.46
1:E:153:THR:HG22	1:E:157:LYS:HZ2	1.78	0.46
1:M:53:LYS:HD3	2:M:265:HOH:O	2.15	0.46
1:U:53:LYS:HD3	2:U:266:HOH:O	2.15	0.46
1:P:169:LEU:HD22	1:P:169:LEU:N	2.31	0.46
1:U:169:LEU:HD22	1:U:169:LEU:N	2.31	0.46
1:E:90:ARG:HD2	1:E:93:TRP:CE3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:90:ARG:HD2	1:K:93:TRP:CE3	2.51	0.46
1:J:82:LEU:HD12	1:J:82:LEU:N	2.29	0.46
1:M:165:MET:HG3	1:M:169:LEU:CD2	2.42	0.46
1:R:67:GLU:HA	1:R:70:MET:CE	2.46	0.46
1:X:67:GLU:HA	1:X:70:MET:CE	2.46	0.46
1:B:53:LYS:HD3	2:B:266:HOH:O	2.15	0.46
1:P:53:LYS:HD3	2:P:266:HOH:O	2.15	0.46
1:W:169:LEU:HD22	1:W:169:LEU:N	2.31	0.46
1:E:151:HIS:HD2	2:E:243:HOH:O	1.97	0.46
1:K:151:HIS:HD2	2:K:240:HOH:O	1.97	0.46
1:Q:90:ARG:HD2	1:Q:93:TRP:CE3	2.51	0.46
1:W:90:ARG:HD2	1:W:93:TRP:CE3	2.51	0.46
1:X:90:ARG:HD2	1:X:93:TRP:CE3	2.51	0.46
1:Q:165:MET:HG3	1:Q:169:LEU:CD2	2.42	0.46
1:W:165:MET:HG3	1:W:169:LEU:CD2	2.42	0.46
1:H:53:LYS:HD3	2:H:267:HOH:O	2.14	0.46
1:F:153:THR:HG22	1:F:157:LYS:HZ2	1.80	0.46
1:G:169:LEU:HD22	1:G:169:LEU:N	2.31	0.46
1:Q:169:LEU:HD22	1:Q:169:LEU:N	2.31	0.46
1:V:169:LEU:HD22	1:V:169:LEU:N	2.31	0.46
1:C:90:ARG:HD2	1:C:93:TRP:CE3	2.51	0.46
1:I:90:ARG:HD2	1:I:93:TRP:CE3	2.51	0.46
1:J:151:HIS:HD2	2:J:247:HOH:O	1.97	0.46
1:M:151:HIS:HD2	2:M:242:HOH:O	1.97	0.46
1:P:151:HIS:HD2	2:P:243:HOH:O	1.97	0.46
1:R:90:ARG:HD2	1:R:93:TRP:CE3	2.51	0.46
1:Q:34:TYR:OH	1:Q:107:GLU:OE2	2.17	0.46
1:N:49:LYS:O	1:N:53:LYS:HG2	2.14	0.46
1:D:53:LYS:HD3	2:D:266:HOH:O	2.15	0.46
1:J:53:LYS:HD3	2:J:268:HOH:O	2.15	0.46
1:R:53:LYS:HD3	2:R:266:HOH:O	2.15	0.46
1:X:53:LYS:HD3	2:X:265:HOH:O	2.15	0.46
1:A:169:LEU:HD22	1:A:169:LEU:N	2.31	0.46
1:D:169:LEU:HD22	1:D:169:LEU:N	2.31	0.46
1:M:153:THR:HG22	1:M:157:LYS:HZ3	1.78	0.46
1:X:153:THR:HG22	1:X:157:LYS:HZ3	1.81	0.46
1:A:71:LYS:NZ	2:A:201:HOH:O	2.10	0.46
1:D:50:ASN:HB2	1:D:171:ASP:OD1	2.16	0.46
1:J:50:ASN:HB2	1:J:171:ASP:OD1	2.16	0.46
1:A:90:ARG:HD2	1:A:93:TRP:CE3	2.51	0.46
1:B:90:ARG:HD2	1:B:93:TRP:CE3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:90:ARG:HD2	1:H:93:TRP:CE3	2.51	0.46
1:O:90:ARG:HD2	1:O:93:TRP:CE3	2.51	0.46
1:U:90:ARG:HD2	1:U:93:TRP:CE3	2.51	0.46
1:T:49:LYS:O	1:T:53:LYS:HG2	2.14	0.46
1:A:67:GLU:HA	1:A:70:MET:CE	2.46	0.46
1:E:153:THR:HG22	1:E:157:LYS:HZ3	1.79	0.46
1:L:153:THR:HG22	1:L:157:LYS:HZ3	1.80	0.46
1:J:169:LEU:HD22	1:J:169:LEU:N	2.31	0.46
1:M:50:ASN:HB2	1:M:171:ASP:OD1	2.16	0.46
1:S:50:ASN:HB2	1:S:171:ASP:OD1	2.16	0.46
1:A:151:HIS:HD2	2:A:245:HOH:O	1.98	0.46
1:F:90:ARG:HD2	1:F:93:TRP:CE3	2.51	0.46
1:G:90:ARG:HD2	1:G:93:TRP:CE3	2.51	0.46
1:T:90:ARG:HD2	1:T:93:TRP:CE3	2.50	0.46
1:V:151:HIS:HD2	2:V:246:HOH:O	1.97	0.46
1:G:67:GLU:HA	1:G:70:MET:CE	2.46	0.46
1:I:153:THR:HG22	1:I:157:LYS:HZ3	1.78	0.46
1:B:50:ASN:HB2	1:B:171:ASP:OD1	2.16	0.46
1:H:50:ASN:HB2	1:H:171:ASP:OD1	2.16	0.46
1:L:90:ARG:HD2	1:L:93:TRP:CE3	2.51	0.46
1:N:90:ARG:HD2	1:N:93:TRP:CE3	2.51	0.46
1:C:169:LEU:HD22	1:C:169:LEU:N	2.31	0.46
1:I:169:LEU:HD22	1:I:169:LEU:N	2.31	0.46
1:M:169:LEU:HD22	1:M:169:LEU:N	2.31	0.46
1:S:169:LEU:HD22	1:S:169:LEU:N	2.31	0.46
1:F:50:ASN:HB2	1:F:171:ASP:OD1	2.16	0.46
1:L:50:ASN:HB2	1:L:171:ASP:OD1	2.16	0.46
1:Q:50:ASN:HB2	1:Q:171:ASP:OD1	2.16	0.46
1:W:50:ASN:HB2	1:W:171:ASP:OD1	2.16	0.46
1:S:151:HIS:HD2	2:S:245:HOH:O	1.98	0.46
1:O:34:TYR:OH	1:O:107:GLU:OE2	2.17	0.46
1:Q:153:THR:HG22	1:Q:157:LYS:HZ2	1.81	0.46
1:J:67:GLU:HA	1:J:70:MET:CE	2.46	0.46
1:L:67:GLU:HA	1:L:70:MET:CE	2.46	0.46
1:B:169:LEU:HD22	1:B:169:LEU:N	2.31	0.46
1:E:169:LEU:HD22	1:E:169:LEU:N	2.31	0.46
1:S:153:THR:HG22	1:S:157:LYS:HZ3	1.78	0.46
1:J:50:ASN:HB2	1:J:171:ASP:OD1	2.16	0.46
1:V:50:ASN:HB2	1:V:171:ASP:OD1	2.16	0.46
1:G:151:HIS:HD2	2:G:246:HOH:O	1.98	0.46
1:R:153:THR:HG22	1:R:157:LYS:HZ2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:153:THR:HG22	1:W:157:LYS:HZ2	1.80	0.46
1:D:67:GLU:HA	1:D:70:MET:CE	2.46	0.46
1:F:53:LYS:HD3	2:F:266:HOH:O	2.15	0.46
1:Q:53:LYS:HD3	2:Q:266:HOH:O	2.15	0.46
1:W:53:LYS:HD3	2:W:265:HOH:O	2.15	0.46
1:H:169:LEU:HD22	1:H:169:LEU:N	2.31	0.46
1:K:169:LEU:HD22	1:K:169:LEU:N	2.31	0.46
1:D:50:ASN:HB2	1:D:171:ASP:OD1	2.16	0.46
1:F:50:ASN:HB2	1:F:171:ASP:OD1	2.16	0.46
1:H:50:ASN:HB2	1:H:171:ASP:OD1	2.16	0.46
1:M:50:ASN:HB2	1:M:171:ASP:OD1	2.16	0.46
1:P:50:ASN:HB2	1:P:171:ASP:OD1	2.16	0.46
1:D:90:ARG:HD2	1:D:93:TRP:CE3	2.51	0.46
1:C:67:GLU:HA	1:C:70:MET:CE	2.46	0.45
1:E:34:TYR:OH	1:E:107:GLU:OE2	2.22	0.45
1:F:67:GLU:HA	1:F:70:MET:CE	2.46	0.45
1:H:67:GLU:HA	1:H:70:MET:CE	2.46	0.45
1:I:67:GLU:HA	1:I:70:MET:CE	2.46	0.45
1:E:53:LYS:HD3	2:E:267:HOH:O	2.15	0.45
1:M:50:ASN:HB2	1:M:171:ASP:OD1	2.17	0.45
1:R:169:LEU:HD22	1:R:169:LEU:N	2.31	0.45
1:B:50:ASN:HB2	1:B:171:ASP:OD1	2.16	0.45
1:L:50:ASN:HB2	1:L:171:ASP:OD1	2.16	0.45
1:S:50:ASN:HB2	1:S:171:ASP:OD1	2.17	0.45
1:G:50:ASN:HB2	1:G:171:ASP:OD1	2.16	0.45
1:J:90:ARG:HD2	1:J:93:TRP:CE3	2.51	0.45
1:N:90:ARG:HD3	1:N:92:ASP:O	2.17	0.45
1:V:153:THR:HG22	1:V:157:LYS:HZ3	1.80	0.45
1:J:50:ASN:HB2	1:J:171:ASP:OD1	2.17	0.45
1:M:50:ASN:HB2	1:M:171:ASP:OD1	2.17	0.45
1:O:67:GLU:HA	1:O:70:MET:CE	2.46	0.45
1:Q:67:GLU:HA	1:Q:70:MET:CE	2.46	0.45
1:U:67:GLU:HA	1:U:70:MET:CE	2.46	0.45
1:W:67:GLU:HA	1:W:70:MET:CE	2.46	0.45
1:C:53:LYS:HD3	2:C:266:HOH:O	2.15	0.45
1:G:174:THR:O	1:G:177:HIS:CD2	2.70	0.45
1:K:53:LYS:HD3	2:K:263:HOH:O	2.15	0.45
1:F:50:ASN:HB2	1:F:171:ASP:OD1	2.17	0.45
1:L:50:ASN:HB2	1:L:171:ASP:OD1	2.17	0.45
1:S:50:ASN:HB2	1:S:171:ASP:OD1	2.17	0.45
1:X:169:LEU:HD22	1:X:169:LEU:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:50:ASN:HB2	1:Q:171:ASP:OD1	2.16	0.45
1:W:50:ASN:HB2	1:W:171:ASP:OD1	2.16	0.45
1:A:50:ASN:HB2	1:A:171:ASP:OD1	2.16	0.45
1:T:50:ASN:HB2	1:T:171:ASP:OD1	2.16	0.45
1:E:90:ARG:HD3	1:E:92:ASP:O	2.17	0.45
1:K:90:ARG:HD3	1:K:92:ASP:O	2.17	0.45
1:T:90:ARG:HD3	1:T:92:ASP:O	2.17	0.45
1:D:50:ASN:HB2	1:D:171:ASP:OD1	2.17	0.45
1:N:34:TYR:OH	1:N:107:GLU:OE2	2.17	0.45
1:I:34:TYR:OH	1:I:107:GLU:OE2	2.23	0.45
1:D:50:ASN:HB2	1:D:171:ASP:OD1	2.17	0.45
1:S:50:ASN:HB2	1:S:171:ASP:OD1	2.17	0.45
1:B:67:GLU:HA	1:B:70:MET:CE	2.46	0.45
1:I:53:LYS:HD3	2:I:266:HOH:O	2.15	0.45
1:L:53:LYS:HD3	2:L:266:HOH:O	2.15	0.45
1:B:50:ASN:HB2	1:B:171:ASP:OD1	2.17	0.45
1:D:50:ASN:HB2	1:D:171:ASP:OD1	2.17	0.45
1:H:50:ASN:HB2	1:H:171:ASP:OD1	2.17	0.45
1:J:50:ASN:HB2	1:J:171:ASP:OD1	2.17	0.45
1:I:50:ASN:HB2	1:I:171:ASP:OD1	2.16	0.45
1:N:50:ASN:HB2	1:N:171:ASP:OD1	2.16	0.45
1:A:41:PHE:CE1	1:A:51:PHE:HD2	2.35	0.45
1:J:90:ARG:HD3	1:J:92:ASP:O	2.17	0.45
1:A:97:LEU:HD13	1:A:97:LEU:C	2.37	0.45
1:D:97:LEU:HD13	1:D:97:LEU:C	2.37	0.45
1:F:97:LEU:HD13	1:F:97:LEU:C	2.37	0.45
1:J:50:ASN:HB2	1:J:171:ASP:OD1	2.17	0.45
1:L:50:ASN:HB2	1:L:171:ASP:OD1	2.17	0.45
1:L:97:LEU:HD13	1:L:97:LEU:C	2.37	0.45
1:M:50:ASN:HB2	1:M:171:ASP:OD1	2.17	0.45
1:P:153:THR:HG22	1:P:157:LYS:HZ3	1.80	0.45
1:C:34:TYR:OH	1:C:107:GLU:OE2	2.23	0.45
1:L:44:ASP:OD2	1:S:6:SER:OG	2.33	0.45
1:B:50:ASN:HB2	1:B:171:ASP:OD1	2.17	0.45
1:H:50:ASN:HB2	1:H:171:ASP:OD1	2.17	0.45
1:L:50:ASN:HB2	1:L:171:ASP:OD1	2.17	0.45
1:K:34:TYR:OH	1:K:107:GLU:OE2	2.22	0.45
1:D:50:ASN:HB2	1:D:171:ASP:OD1	2.17	0.45
1:G:53:LYS:HD3	2:G:267:HOH:O	2.15	0.45
1:J:50:ASN:HB2	1:J:171:ASP:OD1	2.17	0.45
1:L:50:ASN:HB2	1:L:171:ASP:OD1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:50:ASN:HB2	1:M:171:ASP:OD1	2.17	0.45
1:W:50:ASN:HB2	1:W:171:ASP:OD1	2.17	0.45
1:P:50:ASN:HB2	1:P:171:ASP:OD1	2.16	0.45
1:V:50:ASN:HB2	1:V:171:ASP:OD1	2.16	0.45
1:C:50:ASN:HB2	1:C:171:ASP:OD1	2.16	0.45
1:K:50:ASN:HB2	1:K:171:ASP:OD1	2.16	0.45
1:R:50:ASN:HB2	1:R:171:ASP:OD1	2.16	0.45
1:C:90:ARG:HD3	1:C:92:ASP:O	2.17	0.45
1:G:41:PHE:CE1	1:G:51:PHE:HD2	2.35	0.45
1:L:41:PHE:CE1	1:L:51:PHE:HD2	2.35	0.45
1:M:90:ARG:HD3	1:M:92:ASP:O	2.17	0.45
1:S:90:ARG:HD3	1:S:92:ASP:O	2.17	0.45
1:F:50:ASN:HB2	1:F:171:ASP:OD1	2.17	0.45
1:G:97:LEU:HD13	1:G:97:LEU:C	2.37	0.45
1:H:50:ASN:HB2	1:H:171:ASP:OD1	2.17	0.45
1:J:97:LEU:C	1:J:97:LEU:HD13	2.37	0.45
1:S:50:ASN:HB2	1:S:171:ASP:OD1	2.17	0.45
1:J:50:ASN:HB2	1:J:171:ASP:OD1	2.17	0.45
1:F:50:ASN:HB2	1:F:171:ASP:OD1	2.17	0.45
1:M:50:ASN:HB2	1:M:171:ASP:OD1	2.17	0.45
1:S:50:ASN:HB2	1:S:171:ASP:OD1	2.17	0.45
1:F:50:ASN:HB2	1:F:171:ASP:OD1	2.17	0.45
1:G:173:HIS:O	1:G:177:HIS:ND1	2.50	0.45
1:S:50:ASN:HB2	1:S:171:ASP:OD1	2.17	0.45
1:G:50:ASN:HB2	1:G:171:ASP:OD1	2.16	0.45
1:E:50:ASN:HB2	1:E:171:ASP:OD1	2.16	0.45
1:D:90:ARG:HD3	1:D:92:ASP:O	2.17	0.45
1:F:41:PHE:CE1	1:F:51:PHE:HD2	2.35	0.45
1:I:90:ARG:HD3	1:I:92:ASP:O	2.17	0.45
1:R:41:PHE:CE1	1:R:51:PHE:HD2	2.35	0.45
1:B:50:ASN:HB2	1:B:171:ASP:OD1	2.17	0.45
1:S:97:LEU:HD13	1:S:97:LEU:C	2.37	0.45
1:U:97:LEU:HD13	1:U:97:LEU:C	2.37	0.45
1:D:50:ASN:HB2	1:D:171:ASP:OD1	2.17	0.45
1:F:50:ASN:HB2	1:F:171:ASP:OD1	2.17	0.45
1:L:50:ASN:HB2	1:L:171:ASP:OD1	2.17	0.45
1:M:50:ASN:HB2	1:M:171:ASP:OD1	2.17	0.45
1:Q:50:ASN:HB2	1:Q:171:ASP:OD1	2.17	0.45
1:W:50:ASN:HB2	1:W:171:ASP:OD1	2.17	0.45
1:D:50:ASN:HB2	1:D:171:ASP:OD1	2.17	0.45
1:F:50:ASN:HB2	1:F:171:ASP:OD1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:50:ASN:HB2	1:J:171:ASP:OD1	2.17	0.45
1:L:50:ASN:HB2	1:L:171:ASP:OD1	2.17	0.45
1:B:50:ASN:HB2	1:B:171:ASP:OD1	2.17	0.45
1:H:50:ASN:HB2	1:H:171:ASP:OD1	2.17	0.45
1:F:34:TYR:OH	1:F:107:GLU:OE2	2.19	0.45
1:F:169:LEU:HD22	1:F:169:LEU:N	2.31	0.45
1:O:169:LEU:HD22	1:O:169:LEU:N	2.31	0.45
1:Q:50:ASN:HB2	1:Q:171:ASP:OD1	2.17	0.45
1:A:50:ASN:HB2	1:A:171:ASP:OD1	2.16	0.45
1:I:50:ASN:HB2	1:I:171:ASP:OD1	2.16	0.45
1:T:50:ASN:HB2	1:T:171:ASP:OD1	2.16	0.45
1:X:50:ASN:HB2	1:X:171:ASP:OD1	2.16	0.45
1:C:41:PHE:CE1	1:C:51:PHE:HD2	2.35	0.45
1:I:41:PHE:CE1	1:I:51:PHE:HD2	2.35	0.45
1:S:90:ARG:HD2	1:S:93:TRP:CE3	2.51	0.45
1:T:151:HIS:HD2	2:T:244:HOH:O	1.99	0.45
1:X:41:PHE:CE1	1:X:51:PHE:HD2	2.35	0.45
1:F:82:LEU:HD12	1:F:82:LEU:N	2.32	0.45
1:O:82:LEU:HD12	1:O:82:LEU:N	2.32	0.45
1:Q:82:LEU:HD12	1:Q:82:LEU:N	2.32	0.45
1:U:82:LEU:HD12	1:U:82:LEU:N	2.32	0.45
1:W:82:LEU:HD12	1:W:82:LEU:N	2.32	0.45
1:O:97:LEU:C	1:O:97:LEU:HD13	2.37	0.45
1:T:34:TYR:OH	1:T:107:GLU:OE2	2.17	0.45
1:H:50:ASN:HB2	1:H:171:ASP:OD1	2.17	0.45
1:S:50:ASN:HB2	1:S:171:ASP:OD1	2.17	0.45
1:V:50:ASN:HB2	1:V:171:ASP:OD1	2.17	0.45
1:H:50:ASN:HB2	1:H:171:ASP:OD1	2.17	0.45
1:K:67:GLU:HA	1:K:70:MET:CE	2.46	0.45
1:A:53:LYS:HD3	2:A:267:HOH:O	2.15	0.45
1:Q:50:ASN:HB2	1:Q:171:ASP:OD1	2.17	0.45
1:W:50:ASN:HB2	1:W:171:ASP:OD1	2.17	0.45
1:G:50:ASN:HB2	1:G:171:ASP:OD1	2.17	0.45
1:L:169:LEU:HD22	1:L:169:LEU:N	2.31	0.45
1:N:50:ASN:HB2	1:N:171:ASP:OD1	2.17	0.45
1:T:50:ASN:HB2	1:T:171:ASP:OD1	2.17	0.45
1:V:50:ASN:HB2	1:V:171:ASP:OD1	2.17	0.45
1:C:50:ASN:HB2	1:C:171:ASP:OD1	2.16	0.45
1:E:50:ASN:HB2	1:E:171:ASP:OD1	2.16	0.45
1:K:50:ASN:HB2	1:K:171:ASP:OD1	2.16	0.45
1:N:50:ASN:HB2	1:N:171:ASP:OD1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:90:ARG:HD3	1:H:92:ASP:O	2.17	0.45
1:M:90:ARG:HD2	1:M:93:TRP:CE3	2.51	0.45
1:N:41:PHE:CE1	1:N:51:PHE:HD2	2.35	0.45
1:P:90:ARG:HD2	1:P:93:TRP:CE3	2.51	0.45
1:T:41:PHE:CE1	1:T:51:PHE:HD2	2.35	0.45
1:W:90:ARG:HD3	1:W:92:ASP:O	2.16	0.45
1:A:82:LEU:HD12	1:A:82:LEU:N	2.32	0.45
1:G:82:LEU:HD12	1:G:82:LEU:N	2.32	0.45
1:L:82:LEU:HD12	1:L:82:LEU:N	2.32	0.45
1:M:97:LEU:C	1:M:97:LEU:HD13	2.37	0.45
1:B:50:ASN:HB2	1:B:171:ASP:OD1	2.17	0.45
1:B:50:ASN:HB2	1:B:171:ASP:OD1	2.17	0.45
1:E:67:GLU:HA	1:E:70:MET:CE	2.46	0.45
1:S:34:TYR:OH	1:S:107:GLU:OE2	2.22	0.45
1:C:50:ASN:HB2	1:C:171:ASP:OD1	2.17	0.45
1:I:50:ASN:HB2	1:I:171:ASP:OD1	2.17	0.45
1:P:50:ASN:HB2	1:P:171:ASP:OD1	2.17	0.45
1:J:34:TYR:OH	1:J:107:GLU:OE2	2.21	0.45
1:O:50:ASN:HB2	1:O:171:ASP:OD1	2.16	0.45
1:B:90:ARG:HD3	1:B:92:ASP:O	2.17	0.45
1:R:90:ARG:HD3	1:R:92:ASP:O	2.17	0.45
1:V:90:ARG:HD2	1:V:93:TRP:CE3	2.51	0.45
1:X:90:ARG:HD3	1:X:92:ASP:O	2.17	0.45
1:D:50:ASN:HB2	1:D:171:ASP:OD1	2.17	0.45
1:S:50:ASN:HB2	1:S:171:ASP:OD1	2.17	0.45
1:N:50:ASN:HB2	1:N:171:ASP:OD1	2.17	0.45
1:Q:50:ASN:HB2	1:Q:171:ASP:OD1	2.17	0.45
1:R:97:LEU:C	1:R:97:LEU:HD13	2.37	0.45
1:T:50:ASN:HB2	1:T:171:ASP:OD1	2.17	0.45
1:W:50:ASN:HB2	1:W:171:ASP:OD1	2.17	0.45
1:L:6:SER:OG	1:S:44:ASP:OD2	2.34	0.45
1:W:50:ASN:HB2	1:W:171:ASP:OD1	2.17	0.45
1:G:50:ASN:HB2	1:G:171:ASP:OD1	2.17	0.45
1:I:50:ASN:HB2	1:I:171:ASP:OD1	2.17	0.45
1:N:50:ASN:HB2	1:N:171:ASP:OD1	2.17	0.45
1:P:50:ASN:HB2	1:P:171:ASP:OD1	2.17	0.45
1:W:50:ASN:HB2	1:W:171:ASP:OD1	2.17	0.45
1:I:50:ASN:HB2	1:I:171:ASP:OD1	2.17	0.45
1:T:50:ASN:HB2	1:T:171:ASP:OD1	2.17	0.45
1:V:50:ASN:HB2	1:V:171:ASP:OD1	2.17	0.45
1:A:50:ASN:HB2	1:A:171:ASP:OD1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:50:ASN:HB2	1:X:171:ASP:OD1	2.16	0.45
1:U:50:ASN:HB2	1:U:171:ASP:OD1	2.16	0.45
1:Q:41:PHE:CE1	1:Q:51:PHE:HD2	2.35	0.45
1:Q:90:ARG:HD3	1:Q:92:ASP:O	2.17	0.45
1:W:41:PHE:CE1	1:W:51:PHE:HD2	2.35	0.45
1:C:82:LEU:HD12	1:C:82:LEU:N	2.32	0.45
1:I:82:LEU:HD12	1:I:82:LEU:N	2.32	0.45
1:J:50:ASN:HB2	1:J:171:ASP:OD1	2.17	0.45
1:L:50:ASN:HB2	1:L:171:ASP:OD1	2.17	0.45
1:M:50:ASN:HB2	1:M:171:ASP:OD1	2.17	0.45
1:R:82:LEU:HD12	1:R:82:LEU:N	2.32	0.45
1:T:82:LEU:HD12	1:T:82:LEU:N	2.32	0.45
1:C:50:ASN:HB2	1:C:171:ASP:OD1	2.17	0.45
1:I:50:ASN:HB2	1:I:171:ASP:OD1	2.17	0.45
1:U:153:THR:HG22	1:U:157:LYS:HZ3	1.80	0.45
1:X:97:LEU:HD13	1:X:97:LEU:C	2.37	0.45
1:Q:50:ASN:HB2	1:Q:171:ASP:OD1	2.17	0.45
1:V:50:ASN:HB2	1:V:171:ASP:OD1	2.17	0.45
1:A:50:ASN:HB2	1:A:171:ASP:OD1	2.17	0.45
1:C:50:ASN:HB2	1:C:171:ASP:OD1	2.17	0.45
1:E:50:ASN:HB2	1:E:171:ASP:OD1	2.17	0.45
1:Q:50:ASN:HB2	1:Q:171:ASP:OD1	2.17	0.45
1:T:67:GLU:HA	1:T:70:MET:CE	2.46	0.45
1:V:50:ASN:HB2	1:V:171:ASP:OD1	2.17	0.45
1:C:50:ASN:HB2	1:C:171:ASP:OD1	2.17	0.45
1:N:50:ASN:HB2	1:N:171:ASP:OD1	2.17	0.45
1:P:50:ASN:HB2	1:P:171:ASP:OD1	2.17	0.45
1:R:153:THR:HG22	1:R:157:LYS:HZ2	1.82	0.45
1:T:169:LEU:HD22	1:T:169:LEU:N	2.31	0.45
1:R:50:ASN:HB2	1:R:171:ASP:OD1	2.17	0.45
1:M:41:PHE:CE1	1:M:51:PHE:HD2	2.35	0.45
1:B:50:ASN:HB2	1:B:171:ASP:OD1	2.17	0.45
1:E:34:TYR:OH	1:E:107:GLU:OE2	2.21	0.45
1:E:82:LEU:HD12	1:E:82:LEU:N	2.32	0.45
1:F:50:ASN:HB2	1:F:171:ASP:OD1	2.17	0.45
1:H:50:ASN:HB2	1:H:171:ASP:OD1	2.17	0.45
1:K:82:LEU:HD12	1:K:82:LEU:N	2.32	0.45
1:N:82:LEU:HD12	1:N:82:LEU:N	2.32	0.45
1:E:97:LEU:C	1:E:97:LEU:HD13	2.37	0.45
1:G:50:ASN:HB2	1:G:171:ASP:OD1	2.17	0.45
1:P:50:ASN:HB2	1:P:171:ASP:OD1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:50:ASN:HB2	1:V:171:ASP:OD1	2.17	0.45
1:N:44:ASP:OD2	1:Q:6:SER:OG	2.35	0.45
1:T:44:ASP:OD2	1:W:6:SER:OG	2.35	0.45
1:T:50:ASN:HB2	1:T:171:ASP:OD1	2.17	0.45
1:I:50:ASN:HB2	1:I:171:ASP:OD1	2.17	0.44
1:N:50:ASN:HB2	1:N:171:ASP:OD1	2.17	0.44
1:N:67:GLU:HA	1:N:70:MET:CE	2.46	0.44
1:P:50:ASN:HB2	1:P:171:ASP:OD1	2.17	0.44
1:T:50:ASN:HB2	1:T:171:ASP:OD1	2.17	0.44
1:G:50:ASN:HB2	1:G:171:ASP:OD1	2.17	0.44
1:E:50:ASN:HB2	1:E:171:ASP:OD1	2.17	0.44
1:K:50:ASN:HB2	1:K:171:ASP:OD1	2.17	0.44
1:N:169:LEU:HD22	1:N:169:LEU:N	2.31	0.44
1:W:153:THR:HG22	1:W:157:LYS:HZ2	1.82	0.44
1:D:50:ASN:HB2	1:D:171:ASP:OD1	2.18	0.44
1:L:50:ASN:HB2	1:L:171:ASP:OD1	2.18	0.44
1:M:50:ASN:HB2	1:M:171:ASP:OD1	2.18	0.44
1:O:90:ARG:HD3	1:O:92:ASP:O	2.17	0.44
1:S:41:PHE:CE1	1:S:51:PHE:HD2	2.35	0.44
1:U:90:ARG:HD3	1:U:92:ASP:O	2.16	0.44
1:M:82:LEU:HD12	1:M:82:LEU:N	2.32	0.44
1:Q:50:ASN:HB2	1:Q:171:ASP:OD1	2.17	0.44
1:W:50:ASN:HB2	1:W:171:ASP:OD1	2.17	0.44
1:X:82:LEU:HD12	1:X:82:LEU:N	2.32	0.44
1:A:50:ASN:HB2	1:A:171:ASP:OD1	2.17	0.44
1:C:97:LEU:C	1:C:97:LEU:HD13	2.37	0.44
1:I:97:LEU:HD13	1:I:97:LEU:C	2.37	0.44
1:K:97:LEU:HD13	1:K:97:LEU:C	2.37	0.44
1:Q:97:LEU:C	1:Q:97:LEU:HD13	2.37	0.44
1:T:97:LEU:C	1:T:97:LEU:HD13	2.37	0.44
1:B:44:ASP:OD2	1:E:6:SER:OG	2.35	0.44
1:C:6:SER:OG	1:J:44:ASP:OD2	2.35	0.44
1:C:50:ASN:HB2	1:C:171:ASP:OD1	2.17	0.44
1:P:50:ASN:HB2	1:P:171:ASP:OD1	2.17	0.44
1:T:50:ASN:HB2	1:T:171:ASP:OD1	2.17	0.44
1:C:50:ASN:HB2	1:C:171:ASP:OD1	2.17	0.44
1:G:50:ASN:HB2	1:G:171:ASP:OD1	2.17	0.44
1:M:34:TYR:OH	1:M:107:GLU:OE2	2.22	0.44
1:U:50:ASN:HB2	1:U:171:ASP:OD1	2.16	0.44
1:F:50:ASN:HB2	1:F:171:ASP:OD1	2.18	0.44
1:H:50:ASN:HB2	1:H:171:ASP:OD1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:50:ASN:HB2	1:J:171:ASP:OD1	2.18	0.44
1:S:50:ASN:HB2	1:S:171:ASP:OD1	2.18	0.44
1:B:82:LEU:HD12	1:B:82:LEU:N	2.32	0.44
1:N:97:LEU:HD13	1:N:97:LEU:C	2.37	0.44
1:O:153:THR:HG22	1:O:157:LYS:HZ3	1.80	0.44
1:V:97:LEU:C	1:V:97:LEU:HD13	2.37	0.44
1:G:34:TYR:OH	1:G:107:GLU:OE2	2.23	0.44
1:G:50:ASN:HB2	1:G:171:ASP:OD1	2.17	0.44
1:I:50:ASN:HB2	1:I:171:ASP:OD1	2.17	0.44
1:N:50:ASN:HB2	1:N:171:ASP:OD1	2.17	0.44
1:K:50:ASN:HB2	1:K:171:ASP:OD1	2.17	0.44
1:R:50:ASN:HB2	1:R:171:ASP:OD1	2.17	0.44
1:A:50:ASN:HB2	1:A:171:ASP:OD1	2.17	0.44
1:A:50:ASN:HB2	1:A:171:ASP:OD1	2.17	0.44
1:K:50:ASN:HB2	1:K:171:ASP:OD1	2.17	0.44
1:R:50:ASN:HB2	1:R:171:ASP:OD1	2.17	0.44
1:O:50:ASN:HB2	1:O:171:ASP:OD1	2.16	0.44
1:B:41:PHE:CE1	1:B:51:PHE:HD2	2.35	0.44
1:B:50:ASN:HB2	1:B:171:ASP:OD1	2.18	0.44
1:H:41:PHE:CE1	1:H:51:PHE:HD2	2.35	0.44
1:L:90:ARG:HD3	1:L:92:ASP:O	2.17	0.44
1:V:41:PHE:CE1	1:V:51:PHE:HD2	2.35	0.44
1:H:82:LEU:HD12	1:H:82:LEU:N	2.32	0.44
1:S:82:LEU:HD12	1:S:82:LEU:N	2.32	0.44
1:B:97:LEU:HD13	1:B:97:LEU:C	2.37	0.44
1:E:50:ASN:HB2	1:E:171:ASP:OD1	2.17	0.44
1:H:97:LEU:C	1:H:97:LEU:HD13	2.37	0.44
1:K:50:ASN:HB2	1:K:171:ASP:OD1	2.17	0.44
1:E:50:ASN:HB2	1:E:171:ASP:OD1	2.17	0.44
1:H:44:ASP:OD2	1:K:6:SER:OG	2.35	0.44
1:X:50:ASN:HB2	1:X:171:ASP:OD1	2.17	0.44
1:V:67:GLU:HA	1:V:70:MET:CE	2.46	0.44
1:E:50:ASN:HB2	1:E:171:ASP:OD1	2.17	0.44
1:O:50:ASN:HB2	1:O:171:ASP:OD1	2.16	0.44
1:U:153:THR:HG22	1:U:157:LYS:HZ3	1.81	0.44
1:X:50:ASN:HB2	1:X:171:ASP:OD1	2.17	0.44
1:F:90:ARG:HD3	1:F:92:ASP:O	2.17	0.44
1:P:41:PHE:CE1	1:P:51:PHE:HD2	2.35	0.44
1:C:50:ASN:HB2	1:C:171:ASP:OD1	2.17	0.44
1:I:50:ASN:HB2	1:I:171:ASP:OD1	2.17	0.44
1:K:34:TYR:OH	1:K:107:GLU:OE2	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:50:ASN:HB2	1:N:171:ASP:OD1	2.17	0.44
1:T:50:ASN:HB2	1:T:171:ASP:OD1	2.17	0.44
1:V:50:ASN:HB2	1:V:171:ASP:OD1	2.17	0.44
1:P:97:LEU:HD13	1:P:97:LEU:C	2.37	0.44
1:R:50:ASN:HB2	1:R:171:ASP:OD1	2.17	0.44
1:W:97:LEU:C	1:W:97:LEU:HD13	2.37	0.44
1:A:50:ASN:HB2	1:A:171:ASP:OD1	2.17	0.44
1:E:50:ASN:HB2	1:E:171:ASP:OD1	2.17	0.44
1:K:50:ASN:HB2	1:K:171:ASP:OD1	2.17	0.44
1:R:50:ASN:HB2	1:R:171:ASP:OD1	2.17	0.44
1:G:174:THR:HA	1:G:177:HIS:NE2	2.33	0.44
1:U:50:ASN:HB2	1:U:171:ASP:OD1	2.17	0.44
1:A:90:ARG:HD3	1:A:92:ASP:O	2.17	0.44
1:G:90:ARG:HD3	1:G:92:ASP:O	2.17	0.44
1:P:50:ASN:HB2	1:P:171:ASP:OD1	2.17	0.44
1:V:82:LEU:HD12	1:V:82:LEU:N	2.32	0.44
1:G:44:ASP:OD2	1:X:6:SER:OG	2.36	0.44
1:K:50:ASN:HB2	1:K:171:ASP:OD1	2.17	0.44
1:O:50:ASN:HB2	1:O:171:ASP:OD1	2.17	0.44
1:U:50:ASN:HB2	1:U:171:ASP:OD1	2.17	0.44
1:P:67:GLU:HA	1:P:70:MET:CE	2.46	0.44
1:S:67:GLU:HA	1:S:70:MET:CE	2.46	0.44
1:O:153:THR:HG22	1:O:157:LYS:HZ2	1.81	0.44
1:R:50:ASN:HB2	1:R:171:ASP:OD1	2.17	0.44
1:U:50:ASN:HB2	1:U:171:ASP:OD1	2.17	0.44
1:X:50:ASN:HB2	1:X:171:ASP:OD1	2.17	0.44
1:V:153:THR:HG22	1:V:157:LYS:HZ3	1.82	0.44
1:D:41:PHE:CE1	1:D:51:PHE:HD2	2.35	0.44
1:J:41:PHE:CE1	1:J:51:PHE:HD2	2.35	0.44
1:N:50:ASN:HB2	1:N:171:ASP:OD1	2.18	0.44
1:Q:50:ASN:HB2	1:Q:171:ASP:OD1	2.18	0.44
1:T:50:ASN:HB2	1:T:171:ASP:OD1	2.18	0.44
1:W:50:ASN:HB2	1:W:171:ASP:OD1	2.18	0.44
1:G:50:ASN:HB2	1:G:171:ASP:OD1	2.17	0.44
1:P:82:LEU:HD12	1:P:82:LEU:N	2.32	0.44
1:R:50:ASN:HB2	1:R:171:ASP:OD1	2.17	0.44
1:E:34:TYR:OH	1:E:107:GLU:OE2	2.22	0.44
1:J:34:TYR:OH	1:J:107:GLU:OE2	2.22	0.44
1:T:34:TYR:OH	1:T:107:GLU:OE2	2.22	0.44
1:M:67:GLU:HA	1:M:70:MET:CE	2.46	0.44
1:X:50:ASN:HB2	1:X:171:ASP:OD1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:153:THR:HG22	1:U:157:LYS:HZ2	1.81	0.44
1:A:11:ASN:ND2	2:B:201:HOH:O	2.51	0.44
1:P:72:LEU:HD22	1:P:132:PHE:CD2	2.53	0.44
1:A:72:LEU:HD22	1:A:132:PHE:CD2	2.53	0.44
1:C:50:ASN:HB2	1:C:171:ASP:OD1	2.18	0.44
1:D:72:LEU:HD22	1:D:132:PHE:CD2	2.53	0.44
1:I:50:ASN:HB2	1:I:171:ASP:OD1	2.18	0.44
1:J:72:LEU:HD22	1:J:132:PHE:CD2	2.53	0.44
1:K:41:PHE:CE1	1:K:51:PHE:HD2	2.35	0.44
1:O:41:PHE:CE1	1:O:51:PHE:HD2	2.35	0.44
1:P:50:ASN:HB2	1:P:171:ASP:OD1	2.18	0.44
1:U:41:PHE:CE1	1:U:51:PHE:HD2	2.35	0.44
1:V:50:ASN:HB2	1:V:171:ASP:OD1	2.18	0.44
1:A:50:ASN:HB2	1:A:171:ASP:OD1	2.17	0.44
1:E:50:ASN:HB2	1:E:171:ASP:OD1	2.17	0.44
1:J:82:LEU:HD12	1:J:82:LEU:N	2.32	0.44
1:O:50:ASN:HB2	1:O:171:ASP:OD1	2.17	0.44
1:U:50:ASN:HB2	1:U:171:ASP:OD1	2.17	0.44
1:X:50:ASN:HB2	1:X:171:ASP:OD1	2.17	0.44
1:N:6:SER:OG	1:Q:44:ASP:OD2	2.36	0.44
1:U:50:ASN:HB2	1:U:171:ASP:OD1	2.17	0.44
1:X:50:ASN:HB2	1:X:171:ASP:OD1	2.17	0.44
1:J:72:LEU:HD22	1:J:132:PHE:CD2	2.53	0.44
1:H:153:THR:HG22	1:H:157:LYS:HZ2	1.83	0.44
1:O:50:ASN:HB2	1:O:171:ASP:OD1	2.17	0.44
1:O:153:THR:HG22	1:O:157:LYS:HZ3	1.81	0.44
1:P:153:THR:HG22	1:P:157:LYS:HZ3	1.82	0.44
1:N:72:LEU:HD22	1:N:132:PHE:CD2	2.53	0.44
1:O:72:LEU:HD22	1:O:132:PHE:CD2	2.53	0.44
1:Q:72:LEU:HD22	1:Q:132:PHE:CD2	2.53	0.44
1:T:72:LEU:HD22	1:T:132:PHE:CD2	2.53	0.44
1:V:72:LEU:HD22	1:V:132:PHE:CD2	2.53	0.44
1:W:72:LEU:HD22	1:W:132:PHE:CD2	2.53	0.44
1:G:72:LEU:HD22	1:G:132:PHE:CD2	2.53	0.44
1:R:72:LEU:HD22	1:R:132:PHE:CD2	2.53	0.44
1:X:72:LEU:HD22	1:X:132:PHE:CD2	2.53	0.44
1:D:82:LEU:HD12	1:D:82:LEU:N	2.32	0.44
1:K:50:ASN:HB2	1:K:171:ASP:OD1	2.17	0.44
1:D:72:LEU:HD22	1:D:132:PHE:CD2	2.53	0.44
1:G:6:SER:OG	1:X:44:ASP:OD2	2.36	0.44
1:P:72:LEU:HD22	1:P:132:PHE:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:72:LEU:HD22	1:V:132:PHE:CD2	2.53	0.44
1:D:72:LEU:HD22	1:D:132:PHE:CD2	2.53	0.44
1:O:169:LEU:HD22	1:O:169:LEU:N	2.33	0.44
1:U:169:LEU:HD22	1:U:169:LEU:N	2.33	0.44
1:X:72:LEU:HD22	1:X:132:PHE:CD2	2.53	0.44
1:X:169:LEU:HD22	1:X:169:LEU:N	2.33	0.44
1:U:50:ASN:HB2	1:U:171:ASP:OD1	2.17	0.44
1:F:72:LEU:HD22	1:F:132:PHE:CD2	2.53	0.44
1:J:72:LEU:HD22	1:J:132:PHE:CD2	2.53	0.44
1:L:72:LEU:HD22	1:L:132:PHE:CD2	2.53	0.44
1:U:72:LEU:HD22	1:U:132:PHE:CD2	2.53	0.44
1:X:72:LEU:HD22	1:X:132:PHE:CD2	2.53	0.44
1:E:41:PHE:CE1	1:E:51:PHE:HD2	2.35	0.44
1:G:50:ASN:HB2	1:G:171:ASP:OD1	2.18	0.44
1:R:50:ASN:HB2	1:R:171:ASP:OD1	2.17	0.44
1:J:72:LEU:HD22	1:J:132:PHE:CD2	2.53	0.44
1:O:50:ASN:HB2	1:O:171:ASP:OD1	2.17	0.44
1:Q:72:LEU:HD22	1:Q:132:PHE:CD2	2.53	0.44
1:T:6:SER:OG	1:W:44:ASP:OD2	2.36	0.44
1:U:72:LEU:HD22	1:U:132:PHE:CD2	2.53	0.44
1:W:72:LEU:HD22	1:W:132:PHE:CD2	2.53	0.44
1:X:72:LEU:HD22	1:X:132:PHE:CD2	2.53	0.44
1:D:169:LEU:HD22	1:D:169:LEU:N	2.33	0.44
1:J:169:LEU:HD22	1:J:169:LEU:N	2.33	0.44
1:O:72:LEU:HD22	1:O:132:PHE:CD2	2.53	0.44
1:P:169:LEU:HD22	1:P:169:LEU:N	2.33	0.44
1:Q:169:LEU:HD22	1:Q:169:LEU:N	2.33	0.44
1:R:72:LEU:HD22	1:R:132:PHE:CD2	2.53	0.44
1:R:169:LEU:HD22	1:R:169:LEU:N	2.33	0.44
1:W:169:LEU:HD22	1:W:169:LEU:N	2.33	0.44
1:O:50:ASN:HB2	1:O:171:ASP:OD1	2.17	0.43
1:B:153:THR:HG22	1:B:157:LYS:HZ2	1.83	0.43
1:D:72:LEU:HD22	1:D:132:PHE:CD2	2.53	0.43
1:J:72:LEU:HD22	1:J:132:PHE:CD2	2.53	0.43
1:R:72:LEU:HD22	1:R:132:PHE:CD2	2.53	0.43
1:V:72:LEU:HD22	1:V:132:PHE:CD2	2.53	0.43
1:X:72:LEU:HD22	1:X:132:PHE:CD2	2.53	0.43
1:Q:153:THR:HG22	1:Q:157:LYS:HZ2	1.83	0.43
1:D:72:LEU:HD22	1:D:132:PHE:CD2	2.53	0.43
1:E:34:TYR:OH	1:E:107:GLU:OE2	2.21	0.43
1:R:72:LEU:HD22	1:R:132:PHE:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ASN:HB2	1:A:171:ASP:OD1	2.18	0.43
1:O:72:LEU:HD22	1:O:132:PHE:CD2	2.53	0.43
1:U:72:LEU:HD22	1:U:132:PHE:CD2	2.53	0.43
1:V:72:LEU:HD22	1:V:132:PHE:CD2	2.53	0.43
1:X:50:ASN:HB2	1:X:171:ASP:OD1	2.17	0.43
1:A:44:ASP:OD2	1:R:6:SER:OG	2.36	0.43
1:D:6:SER:OG	1:I:44:ASP:OD2	2.35	0.43
1:H:6:SER:OG	1:K:44:ASP:OD2	2.36	0.43
1:N:72:LEU:HD22	1:N:132:PHE:CD2	2.53	0.43
1:O:72:LEU:HD22	1:O:132:PHE:CD2	2.53	0.43
1:R:72:LEU:HD22	1:R:132:PHE:CD2	2.53	0.43
1:T:72:LEU:HD22	1:T:132:PHE:CD2	2.53	0.43
1:A:72:LEU:HD22	1:A:132:PHE:CD2	2.53	0.43
1:A:169:LEU:HD22	1:A:169:LEU:N	2.33	0.43
1:G:72:LEU:HD22	1:G:132:PHE:CD2	2.53	0.43
1:K:34:TYR:OH	1:K:107:GLU:OE2	2.22	0.43
1:P:72:LEU:HD22	1:P:132:PHE:CD2	2.53	0.43
1:V:72:LEU:HD22	1:V:132:PHE:CD2	2.53	0.43
1:V:169:LEU:HD22	1:V:169:LEU:N	2.33	0.43
1:O:72:LEU:HD22	1:O:132:PHE:CD2	2.53	0.43
1:P:72:LEU:HD22	1:P:132:PHE:CD2	2.53	0.43
1:U:72:LEU:HD22	1:U:132:PHE:CD2	2.53	0.43
1:N:153:THR:HG22	1:N:157:LYS:HZ3	1.81	0.43
1:E:72:LEU:HD22	1:E:132:PHE:CD2	2.53	0.43
1:K:72:LEU:HD22	1:K:132:PHE:CD2	2.53	0.43
1:E:50:ASN:HB2	1:E:171:ASP:OD1	2.18	0.43
1:P:72:LEU:HD22	1:P:132:PHE:CD2	2.53	0.43
1:U:50:ASN:HB2	1:U:171:ASP:OD1	2.17	0.43
1:A:6:SER:OG	1:R:44:ASP:OD2	2.36	0.43
1:B:6:SER:OG	1:E:44:ASP:OD2	2.36	0.43
1:L:72:LEU:HD22	1:L:132:PHE:CD2	2.53	0.43
1:L:72:LEU:HD22	1:L:132:PHE:CD2	2.53	0.43
1:U:72:LEU:HD22	1:U:132:PHE:CD2	2.53	0.43
1:E:34:TYR:OH	1:E:107:GLU:OE2	2.22	0.43
1:Q:72:LEU:HD22	1:Q:132:PHE:CD2	2.53	0.43
1:A:72:LEU:HD22	1:A:132:PHE:CD2	2.53	0.43
1:B:72:LEU:HD22	1:B:132:PHE:CD2	2.53	0.43
1:G:72:LEU:HD22	1:G:132:PHE:CD2	2.53	0.43
1:H:72:LEU:HD22	1:H:132:PHE:CD2	2.53	0.43
1:S:72:LEU:HD22	1:S:132:PHE:CD2	2.53	0.43
1:K:50:ASN:HB2	1:K:171:ASP:OD1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:90:ARG:HD3	1:V:92:ASP:O	2.17	0.43
1:J:72:LEU:HD22	1:J:132:PHE:CD2	2.54	0.43
1:A:72:LEU:HD22	1:A:132:PHE:CD2	2.53	0.43
1:B:72:LEU:HD22	1:B:132:PHE:CD2	2.53	0.43
1:E:72:LEU:HD22	1:E:132:PHE:CD2	2.53	0.43
1:F:72:LEU:HD22	1:F:132:PHE:CD2	2.53	0.43
1:G:72:LEU:HD22	1:G:132:PHE:CD2	2.53	0.43
1:K:72:LEU:HD22	1:K:132:PHE:CD2	2.53	0.43
1:O:6:SER:OG	1:V:44:ASP:OD2	2.35	0.43
1:B:169:LEU:HD22	1:B:169:LEU:N	2.33	0.43
1:F:90:ARG:HD2	1:F:93:TRP:CE3	2.54	0.43
1:G:90:ARG:HD2	1:G:93:TRP:CE3	2.54	0.43
1:G:169:LEU:HD22	1:G:169:LEU:N	2.33	0.43
1:M:169:LEU:HD22	1:M:169:LEU:N	2.33	0.43
1:N:34:TYR:OH	1:N:107:GLU:OE2	2.22	0.43
1:F:157:LYS:HG3	2:F:220:HOH:O	2.18	0.43
1:A:72:LEU:HD22	1:A:132:PHE:CD2	2.53	0.43
1:G:72:LEU:HD22	1:G:132:PHE:CD2	2.53	0.43
1:J:34:TYR:OH	1:J:107:GLU:OE2	2.22	0.43
1:L:72:LEU:HD22	1:L:132:PHE:CD2	2.53	0.43
1:S:153:THR:HG22	1:S:157:LYS:HZ3	1.82	0.43
1:W:72:LEU:HD22	1:W:132:PHE:CD2	2.53	0.43
1:K:34:TYR:OH	1:K:107:GLU:OE2	2.21	0.43
1:M:72:LEU:HD22	1:M:132:PHE:CD2	2.53	0.43
1:P:90:ARG:HD3	1:P:92:ASP:O	2.16	0.43
1:R:50:ASN:HB2	1:R:171:ASP:OD1	2.18	0.43
1:D:72:LEU:HD22	1:D:132:PHE:CD2	2.54	0.43
1:O:50:ASN:HB2	1:O:171:ASP:OD1	2.17	0.43
1:V:72:LEU:HD22	1:V:132:PHE:CD2	2.54	0.43
1:H:72:LEU:HD22	1:H:132:PHE:CD2	2.53	0.43
1:A:90:ARG:HD2	1:A:93:TRP:CE3	2.54	0.43
1:B:72:LEU:HD22	1:B:132:PHE:CD2	2.53	0.43
1:C:169:LEU:HD22	1:C:169:LEU:N	2.33	0.43
1:H:169:LEU:HD22	1:H:169:LEU:N	2.33	0.43
1:L:90:ARG:HD2	1:L:93:TRP:CE3	2.54	0.43
1:P:90:ARG:HD2	1:P:93:TRP:CE3	2.54	0.43
1:Q:72:LEU:HD22	1:Q:132:PHE:CD2	2.53	0.43
1:S:169:LEU:HD22	1:S:169:LEU:N	2.33	0.43
1:T:72:LEU:HD22	1:T:132:PHE:CD2	2.53	0.43
1:W:72:LEU:HD22	1:W:132:PHE:CD2	2.53	0.43
1:R:157:LYS:HG3	2:R:218:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:LEU:HD22	1:B:132:PHE:CD2	2.53	0.43
1:F:72:LEU:HD22	1:F:132:PHE:CD2	2.53	0.43
1:K:72:LEU:HD22	1:K:132:PHE:CD2	2.53	0.43
1:N:72:LEU:HD22	1:N:132:PHE:CD2	2.53	0.43
1:T:72:LEU:HD22	1:T:132:PHE:CD2	2.53	0.43
1:B:72:LEU:HD22	1:B:132:PHE:CD2	2.53	0.43
1:E:72:LEU:HD22	1:E:132:PHE:CD2	2.53	0.43
1:O:48:LEU:HD13	1:O:51:PHE:CE2	2.54	0.43
1:U:50:ASN:HB2	1:U:171:ASP:OD1	2.18	0.43
1:X:50:ASN:HB2	1:X:171:ASP:OD1	2.18	0.43
1:Q:72:LEU:HD22	1:Q:132:PHE:CD2	2.54	0.43
1:U:72:LEU:HD22	1:U:132:PHE:CD2	2.54	0.43
1:X:72:LEU:HD22	1:X:132:PHE:CD2	2.54	0.43
1:O:44:ASP:OD2	1:V:6:SER:OG	2.36	0.43
1:P:44:ASP:OD2	1:U:6:SER:OG	2.35	0.43
1:D:90:ARG:HD2	1:D:93:TRP:CE3	2.54	0.43
1:E:72:LEU:HD22	1:E:132:PHE:CD2	2.53	0.43
1:F:72:LEU:HD22	1:F:132:PHE:CD2	2.53	0.43
1:H:72:LEU:HD22	1:H:132:PHE:CD2	2.53	0.43
1:I:90:ARG:HD2	1:I:93:TRP:CE3	2.54	0.43
1:I:169:LEU:HD22	1:I:169:LEU:N	2.33	0.43
1:K:72:LEU:HD22	1:K:132:PHE:CD2	2.53	0.43
1:M:90:ARG:HD2	1:M:93:TRP:CE3	2.54	0.43
1:N:72:LEU:HD22	1:N:132:PHE:CD2	2.53	0.43
1:V:90:ARG:HD2	1:V:93:TRP:CE3	2.54	0.43
1:E:72:LEU:HD22	1:E:132:PHE:CD2	2.53	0.43
1:H:72:LEU:HD22	1:H:132:PHE:CD2	2.53	0.43
1:B:153:THR:HG22	1:B:157:LYS:HZ3	1.79	0.43
1:P:34:TYR:OH	1:P:107:GLU:OE2	2.21	0.43
1:A:48:LEU:HD13	1:A:51:PHE:CE2	2.54	0.43
1:H:72:LEU:HD22	1:H:132:PHE:CD2	2.53	0.43
1:K:72:LEU:HD22	1:K:132:PHE:CD2	2.53	0.43
1:U:48:LEU:HD13	1:U:51:PHE:CE2	2.54	0.43
1:W:48:LEU:HD13	1:W:51:PHE:CE2	2.54	0.43
1:O:72:LEU:HD22	1:O:132:PHE:CD2	2.54	0.43
1:P:72:LEU:HD22	1:P:132:PHE:CD2	2.54	0.43
1:R:72:LEU:HD22	1:R:132:PHE:CD2	2.54	0.43
1:W:72:LEU:HD22	1:W:132:PHE:CD2	2.54	0.43
1:A:68:LYS:HG2	1:A:132:PHE:HZ	1.84	0.43
1:G:68:LYS:HG2	1:G:132:PHE:HZ	1.84	0.43
1:H:143:LYS:HE2	1:H:143:LYS:HB2	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:153:THR:HG22	1:H:157:LYS:HZ3	1.80	0.43
1:C:44:ASP:OD2	1:J:6:SER:OG	2.36	0.43
1:C:90:ARG:HD2	1:C:93:TRP:CE3	2.54	0.43
1:S:90:ARG:HD2	1:S:93:TRP:CE3	2.54	0.43
1:M:153:THR:HG22	1:M:157:LYS:HZ3	1.82	0.43
1:O:34:TYR:OH	1:O:107:GLU:OE2	2.19	0.43
1:S:34:TYR:OH	1:S:107:GLU:OE2	2.19	0.43
1:N:34:TYR:OH	1:N:107:GLU:OE2	2.18	0.43
1:B:48:LEU:HD13	1:B:51:PHE:CE2	2.54	0.43
1:H:48:LEU:HD13	1:H:51:PHE:CE2	2.54	0.43
1:I:72:LEU:HD22	1:I:132:PHE:CD2	2.53	0.43
1:L:72:LEU:HD22	1:L:132:PHE:CD2	2.53	0.43
1:M:48:LEU:HD13	1:M:51:PHE:CE2	2.54	0.43
1:O:50:ASN:HB2	1:O:171:ASP:OD1	2.18	0.43
1:Q:48:LEU:HD13	1:Q:51:PHE:CE2	2.54	0.43
1:S:48:LEU:HD13	1:S:51:PHE:CE2	2.54	0.43
1:A:72:LEU:HD22	1:A:132:PHE:CD2	2.54	0.43
1:G:72:LEU:HD22	1:G:132:PHE:CD2	2.54	0.43
1:L:72:LEU:HD22	1:L:132:PHE:CD2	2.54	0.43
1:N:153:THR:HG22	1:N:157:LYS:HZ2	1.80	0.43
1:M:72:LEU:HD22	1:M:132:PHE:CD2	2.53	0.43
1:P:6:SER:OG	1:U:44:ASP:OD2	2.36	0.43
1:E:169:LEU:HD22	1:E:169:LEU:N	2.33	0.43
1:J:90:ARG:HD2	1:J:93:TRP:CE3	2.54	0.43
1:K:169:LEU:HD22	1:K:169:LEU:N	2.33	0.43
1:Q:90:ARG:HD2	1:Q:93:TRP:CE3	2.54	0.43
1:A:157:LYS:HG3	2:A:220:HOH:O	2.18	0.43
1:J:72:LEU:HD22	1:J:132:PHE:CD2	2.54	0.43
1:V:72:LEU:HD22	1:V:132:PHE:CD2	2.54	0.43
1:X:72:LEU:HD22	1:X:132:PHE:CD2	2.54	0.43
1:K:34:TYR:OH	1:K:107:GLU:OE2	2.22	0.43
1:C:72:LEU:HD22	1:C:132:PHE:CD2	2.53	0.43
1:D:48:LEU:HD13	1:D:51:PHE:CE2	2.54	0.43
1:E:34:TYR:OH	1:E:107:GLU:OE2	2.27	0.43
1:F:72:LEU:HD22	1:F:132:PHE:CD2	2.53	0.43
1:G:48:LEU:HD13	1:G:51:PHE:CE2	2.54	0.43
1:Q:72:LEU:HD22	1:Q:132:PHE:CD2	2.53	0.43
1:S:72:LEU:HD22	1:S:132:PHE:CD2	2.53	0.43
1:B:72:LEU:HD22	1:B:132:PHE:CD2	2.54	0.43
1:K:72:LEU:HD22	1:K:132:PHE:CD2	2.54	0.43
1:N:72:LEU:HD22	1:N:132:PHE:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:72:LEU:HD22	1:T:132:PHE:CD2	2.54	0.43
1:B:143:LYS:HE2	1:B:143:LYS:HB2	1.89	0.43
1:D:153:THR:HG22	1:D:157:LYS:HZ2	1.82	0.43
1:J:68:LYS:HG2	1:J:132:PHE:HZ	1.84	0.43
1:F:6:SER:OG	1:M:44:ASP:OD2	2.36	0.43
1:S:72:LEU:HD22	1:S:132:PHE:CD2	2.53	0.43
1:N:41:PHE:CE1	1:N:51:PHE:HD2	2.37	0.43
1:R:41:PHE:CE1	1:R:51:PHE:HD2	2.37	0.43
1:W:90:ARG:HD2	1:W:93:TRP:CE3	2.54	0.43
1:X:41:PHE:CE1	1:X:51:PHE:HD2	2.37	0.43
1:D:72:LEU:HD22	1:D:132:PHE:CD2	2.54	0.43
1:P:72:LEU:HD22	1:P:132:PHE:CD2	2.54	0.43
1:Q:72:LEU:HD22	1:Q:132:PHE:CD2	2.54	0.43
1:R:72:LEU:HD22	1:R:132:PHE:CD2	2.54	0.43
1:M:72:LEU:HD22	1:M:132:PHE:CD2	2.53	0.43
1:X:153:THR:HG22	1:X:157:LYS:HZ3	1.84	0.43
1:C:72:LEU:HD22	1:C:132:PHE:CD2	2.53	0.43
1:D:72:LEU:HD22	1:D:132:PHE:CD2	2.54	0.43
1:H:143:LYS:HE2	1:H:143:LYS:HB2	1.90	0.43
1:J:72:LEU:HD22	1:J:132:PHE:CD2	2.54	0.43
1:X:72:LEU:HD22	1:X:132:PHE:CD2	2.54	0.43
1:J:48:LEU:HD13	1:J:51:PHE:CE2	2.54	0.43
1:M:72:LEU:HD22	1:M:132:PHE:CD2	2.53	0.43
1:N:72:LEU:HD22	1:N:132:PHE:CD2	2.53	0.43
1:T:72:LEU:HD22	1:T:132:PHE:CD2	2.53	0.43
1:E:72:LEU:HD22	1:E:132:PHE:CD2	2.54	0.43
1:F:72:LEU:HD22	1:F:132:PHE:CD2	2.54	0.43
1:H:72:LEU:HD22	1:H:132:PHE:CD2	2.54	0.43
1:B:153:THR:HG22	1:B:157:LYS:HZ3	1.80	0.43
1:F:44:ASP:OD2	1:M:6:SER:OG	2.36	0.43
1:G:41:PHE:CE1	1:G:51:PHE:HD2	2.37	0.43
1:S:72:LEU:HD22	1:S:132:PHE:CD2	2.53	0.43
1:T:41:PHE:CE1	1:T:51:PHE:HD2	2.37	0.43
1:L:72:LEU:HD22	1:L:132:PHE:CD2	2.54	0.43
1:O:72:LEU:HD22	1:O:132:PHE:CD2	2.54	0.43
1:U:72:LEU:HD22	1:U:132:PHE:CD2	2.54	0.43
1:W:72:LEU:HD22	1:W:132:PHE:CD2	2.54	0.43
1:R:153:THR:HG22	1:R:157:LYS:HZ3	1.84	0.43
1:J:72:LEU:HD22	1:J:132:PHE:CD2	2.54	0.43
1:N:34:TYR:OH	1:N:107:GLU:OE2	2.19	0.43
1:I:72:LEU:HD22	1:I:132:PHE:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:LYS:HE2	1:B:143:LYS:HB2	1.90	0.43
1:G:90:ARG:HD2	1:G:93:TRP:CE3	2.54	0.43
1:O:72:LEU:HD22	1:O:132:PHE:CD2	2.54	0.43
1:P:72:LEU:HD22	1:P:132:PHE:CD2	2.54	0.43
1:R:72:LEU:HD22	1:R:132:PHE:CD2	2.54	0.43
1:V:72:LEU:HD22	1:V:132:PHE:CD2	2.54	0.43
1:R:72:LEU:HD22	1:R:132:PHE:CE2	2.54	0.43
1:D:68:LYS:HG2	1:D:132:PHE:HZ	1.84	0.43
1:J:153:THR:HG22	1:J:157:LYS:HZ2	1.82	0.43
1:T:68:LYS:HG2	1:T:132:PHE:HZ	1.84	0.43
1:A:41:PHE:CE1	1:A:51:PHE:HD2	2.37	0.43
1:B:90:ARG:HD2	1:B:93:TRP:CE3	2.54	0.43
1:N:90:ARG:HD2	1:N:93:TRP:CE3	2.54	0.43
1:T:90:ARG:HD2	1:T:93:TRP:CE3	2.54	0.43
1:A:72:LEU:HD22	1:A:132:PHE:CD2	2.54	0.42
1:G:72:LEU:HD22	1:G:132:PHE:CD2	2.54	0.42
1:K:72:LEU:HD22	1:K:132:PHE:CD2	2.54	0.42
1:T:72:LEU:HD22	1:T:132:PHE:CD2	2.54	0.42
1:B:165:MET:HG3	1:B:169:LEU:HD22	2.02	0.42
1:H:165:MET:HG3	1:H:169:LEU:HD22	2.02	0.42
1:I:153:THR:HG22	1:I:157:LYS:HZ2	1.84	0.42
1:Q:165:MET:HG3	1:Q:169:LEU:HD22	2.01	0.42
1:S:72:LEU:HD22	1:S:132:PHE:CD2	2.53	0.42
1:W:165:MET:HG3	1:W:169:LEU:HD22	2.01	0.42
1:R:72:LEU:HD22	1:R:132:PHE:CD2	2.54	0.42
1:V:72:LEU:HD22	1:V:132:PHE:CD2	2.54	0.42
1:X:72:LEU:HD22	1:X:132:PHE:CD2	2.54	0.42
1:A:90:ARG:HD2	1:A:93:TRP:CE3	2.54	0.42
1:I:90:ARG:HD2	1:I:93:TRP:CE3	2.54	0.42
1:L:72:LEU:HD22	1:L:132:PHE:CD2	2.54	0.42
1:Q:72:LEU:HD22	1:Q:132:PHE:CD2	2.54	0.42
1:T:34:TYR:OH	1:T:107:GLU:OE2	2.18	0.42
1:U:72:LEU:HD22	1:U:132:PHE:CD2	2.54	0.42
1:C:48:LEU:HD13	1:C:51:PHE:CE2	2.54	0.42
1:E:72:LEU:HD22	1:E:132:PHE:CE2	2.54	0.42
1:K:72:LEU:HD22	1:K:132:PHE:CE2	2.54	0.42
1:M:72:LEU:HD22	1:M:132:PHE:CE2	2.54	0.42
1:S:72:LEU:HD22	1:S:132:PHE:CE2	2.54	0.42
1:V:72:LEU:HD22	1:V:132:PHE:CE2	2.54	0.42
1:W:72:LEU:HD22	1:W:132:PHE:CD2	2.53	0.42
1:X:72:LEU:HD22	1:X:132:PHE:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:LEU:HD22	1:C:132:PHE:CD2	2.53	0.42
1:C:41:PHE:CE1	1:C:51:PHE:HD2	2.37	0.42
1:I:41:PHE:CE1	1:I:51:PHE:HD2	2.37	0.42
1:M:72:LEU:HD22	1:M:132:PHE:CD2	2.53	0.42
1:O:90:ARG:HD2	1:O:93:TRP:CE3	2.54	0.42
1:T:169:LEU:HD22	1:T:169:LEU:N	2.33	0.42
1:U:90:ARG:HD2	1:U:93:TRP:CE3	2.54	0.42
1:B:72:LEU:HD22	1:B:132:PHE:CD2	2.54	0.42
1:B:157:LYS:HG3	2:B:219:HOH:O	2.19	0.42
1:F:72:LEU:HD22	1:F:132:PHE:CD2	2.54	0.42
1:J:157:LYS:HG3	2:J:221:HOH:O	2.18	0.42
1:N:72:LEU:HD22	1:N:132:PHE:CD2	2.54	0.42
1:A:165:MET:HG3	1:A:169:LEU:HD22	2.01	0.42
1:B:153:THR:HG22	1:B:157:LYS:HZ3	1.84	0.42
1:D:165:MET:HG3	1:D:169:LEU:HD22	2.01	0.42
1:J:165:MET:HG3	1:J:169:LEU:HD22	2.01	0.42
1:M:165:MET:HG3	1:M:169:LEU:HD22	2.01	0.42
1:D:72:LEU:HD22	1:D:132:PHE:CD2	2.54	0.42
1:P:72:LEU:HD22	1:P:132:PHE:CD2	2.54	0.42
1:D:68:LYS:HG2	1:D:132:PHE:HZ	1.85	0.42
1:J:68:LYS:HG2	1:J:132:PHE:HZ	1.85	0.42
1:C:90:ARG:HD2	1:C:93:TRP:CE3	2.55	0.42
1:G:72:LEU:HD22	1:G:132:PHE:CD2	2.54	0.42
1:L:90:ARG:HD2	1:L:93:TRP:CE3	2.54	0.42
1:T:72:LEU:HD22	1:T:132:PHE:CD2	2.54	0.42
1:W:72:LEU:HD22	1:W:132:PHE:CD2	2.54	0.42
1:X:90:ARG:HD2	1:X:93:TRP:CE3	2.54	0.42
1:C:72:LEU:HD22	1:C:132:PHE:CE2	2.54	0.42
1:I:48:LEU:HD13	1:I:51:PHE:CE2	2.54	0.42
1:I:72:LEU:HD22	1:I:132:PHE:CE2	2.54	0.42
1:P:48:LEU:HD13	1:P:51:PHE:CE2	2.54	0.42
1:P:72:LEU:HD22	1:P:132:PHE:CE2	2.54	0.42
1:R:48:LEU:HD13	1:R:51:PHE:CE2	2.54	0.42
1:M:72:LEU:HD22	1:M:132:PHE:CD2	2.54	0.42
1:Q:72:LEU:HD22	1:Q:132:PHE:CD2	2.54	0.42
1:V:72:LEU:HD22	1:V:132:PHE:CD2	2.54	0.42
1:W:72:LEU:HD22	1:W:132:PHE:CD2	2.54	0.42
1:F:41:PHE:CE1	1:F:51:PHE:HD2	2.37	0.42
1:L:41:PHE:CE1	1:L:51:PHE:HD2	2.37	0.42
1:E:72:LEU:HD22	1:E:132:PHE:CD2	2.54	0.42
1:H:72:LEU:HD22	1:H:132:PHE:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:157:LYS:HG3	2:H:219:HOH:O	2.19	0.42
1:G:165:MET:HG3	1:G:169:LEU:HD22	2.01	0.42
1:R:153:THR:HG22	1:R:157:LYS:HZ2	1.83	0.42
1:S:165:MET:HG3	1:S:169:LEU:HD22	2.01	0.42
1:H:153:THR:HG22	1:H:157:LYS:HZ3	1.81	0.42
1:L:72:LEU:HD22	1:L:132:PHE:CD2	2.54	0.42
1:O:72:LEU:HD22	1:O:132:PHE:CD2	2.54	0.42
1:Q:72:LEU:HD22	1:Q:132:PHE:CD2	2.54	0.42
1:T:34:TYR:OH	1:T:107:GLU:OE2	2.19	0.42
1:U:72:LEU:HD22	1:U:132:PHE:CD2	2.54	0.42
1:W:72:LEU:HD22	1:W:132:PHE:CD2	2.54	0.42
1:T:68:LYS:HG2	1:T:132:PHE:HZ	1.84	0.42
1:A:72:LEU:HD22	1:A:132:PHE:CD2	2.54	0.42
1:D:90:ARG:HD2	1:D:93:TRP:CE3	2.54	0.42
1:F:72:LEU:HD22	1:F:132:PHE:CD2	2.54	0.42
1:F:90:ARG:HD2	1:F:93:TRP:CE3	2.54	0.42
1:K:72:LEU:HD22	1:K:132:PHE:CD2	2.54	0.42
1:N:72:LEU:HD22	1:N:132:PHE:CD2	2.54	0.42
1:D:72:LEU:HD22	1:D:132:PHE:CE2	2.54	0.42
1:K:72:LEU:HD22	1:K:132:PHE:CD2	2.54	0.42
1:N:68:LYS:HG2	1:N:132:PHE:HZ	1.84	0.42
1:N:72:LEU:HD22	1:N:132:PHE:CD2	2.54	0.42
1:O:72:LEU:HD22	1:O:132:PHE:CD2	2.54	0.42
1:G:174:THR:O	1:G:177:HIS:CD2	2.72	0.42
1:I:72:LEU:HD22	1:I:132:PHE:CD2	2.53	0.42
1:F:169:LEU:HD22	1:F:169:LEU:N	2.33	0.42
1:H:90:ARG:HD2	1:H:93:TRP:CE3	2.54	0.42
1:L:169:LEU:HD22	1:L:169:LEU:N	2.33	0.42
1:M:41:PHE:CE1	1:M:51:PHE:HD2	2.37	0.42
1:N:169:LEU:HD22	1:N:169:LEU:N	2.33	0.42
1:X:90:ARG:HD2	1:X:93:TRP:CE3	2.54	0.42
1:M:157:LYS:HG3	2:M:217:HOH:O	2.18	0.42
1:N:68:LYS:HG2	1:N:132:PHE:HZ	1.85	0.42
1:P:165:MET:HG3	1:P:169:LEU:HD22	2.01	0.42
1:Q:68:LYS:HG2	1:Q:132:PHE:HZ	1.85	0.42
1:T:68:LYS:HG2	1:T:132:PHE:HZ	1.85	0.42
1:V:165:MET:HG3	1:V:169:LEU:HD22	2.01	0.42
1:A:72:LEU:HD22	1:A:132:PHE:CD2	2.54	0.42
1:B:72:LEU:HD22	1:B:132:PHE:CD2	2.54	0.42
1:G:72:LEU:HD22	1:G:132:PHE:CD2	2.54	0.42
1:N:72:LEU:HD22	1:N:132:PHE:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:72:LEU:HD22	1:T:132:PHE:CD2	2.54	0.42
1:N:68:LYS:HG2	1:N:132:PHE:HZ	1.85	0.42
1:B:72:LEU:HD22	1:B:132:PHE:CD2	2.54	0.42
1:E:72:LEU:HD22	1:E:132:PHE:CD2	2.54	0.42
1:H:72:LEU:HD22	1:H:132:PHE:CD2	2.54	0.42
1:R:90:ARG:HD2	1:R:93:TRP:CE3	2.54	0.42
1:E:48:LEU:HD13	1:E:51:PHE:CE2	2.54	0.42
1:J:72:LEU:HD22	1:J:132:PHE:CE2	2.54	0.42
1:K:143:LYS:HE2	1:K:143:LYS:HB2	1.91	0.42
1:V:48:LEU:HD13	1:V:51:PHE:CE2	2.54	0.42
1:S:72:LEU:HD22	1:S:132:PHE:CD2	2.54	0.42
1:F:72:LEU:HD22	1:F:132:PHE:CD2	2.54	0.42
1:L:72:LEU:HD22	1:L:132:PHE:CD2	2.54	0.42
1:P:72:LEU:HD22	1:P:132:PHE:CD2	2.54	0.42
1:T:72:LEU:HD22	1:T:132:PHE:CD2	2.54	0.42
1:V:68:LYS:HG2	1:V:132:PHE:HZ	1.84	0.42
1:E:90:ARG:HD2	1:E:93:TRP:CE3	2.54	0.42
1:J:41:PHE:CE1	1:J:51:PHE:HD2	2.37	0.42
1:R:90:ARG:HD2	1:R:93:TRP:CE3	2.54	0.42
1:S:41:PHE:CE1	1:S:51:PHE:HD2	2.37	0.42
1:W:41:PHE:CE1	1:W:51:PHE:HD2	2.37	0.42
1:C:72:LEU:HD22	1:C:132:PHE:CD2	2.53	0.42
1:S:153:THR:HG22	1:S:157:LYS:HZ2	1.85	0.42
1:W:68:LYS:HG2	1:W:132:PHE:HZ	1.85	0.42
1:X:153:THR:HG22	1:X:157:LYS:HZ2	1.83	0.42
1:F:72:LEU:HD22	1:F:132:PHE:CD2	2.54	0.42
1:H:72:LEU:HD22	1:H:132:PHE:CD2	2.54	0.42
1:K:72:LEU:HD22	1:K:132:PHE:CD2	2.54	0.42
1:G:68:LYS:HG2	1:G:132:PHE:HZ	1.84	0.42
1:M:90:ARG:HD2	1:M:93:TRP:CE3	2.54	0.42
1:S:90:ARG:HD2	1:S:93:TRP:CE3	2.54	0.42
1:C:34:TYR:OH	1:C:107:GLU:OE2	2.27	0.42
1:K:48:LEU:HD13	1:K:51:PHE:CE2	2.54	0.42
1:X:48:LEU:HD13	1:X:51:PHE:CE2	2.54	0.42
1:E:72:LEU:HD22	1:E:132:PHE:CD2	2.54	0.42
1:M:68:LYS:HG2	1:M:132:PHE:HZ	1.84	0.42
1:M:72:LEU:HD22	1:M:132:PHE:CD2	2.54	0.42
1:P:68:LYS:HG2	1:P:132:PHE:HZ	1.84	0.42
1:Q:68:LYS:HG2	1:Q:132:PHE:HZ	1.84	0.42
1:S:68:LYS:HG2	1:S:132:PHE:HZ	1.84	0.42
1:U:72:LEU:HD22	1:U:132:PHE:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:48:LEU:HD13	1:O:51:PHE:CE2	2.55	0.42
1:Q:41:PHE:CE1	1:Q:51:PHE:HD2	2.37	0.42
1:U:48:LEU:HD13	1:U:51:PHE:CE2	2.55	0.42
1:M:72:LEU:HD22	1:M:132:PHE:CD2	2.54	0.42
1:O:70:MET:HE1	1:V:35:LEU:HD21	2.00	0.42
1:E:165:MET:HG3	1:E:169:LEU:HD22	2.01	0.42
1:G:69:LEU:HD13	1:G:137:TYR:CZ	2.55	0.42
1:J:68:LYS:HG2	1:J:132:PHE:HZ	1.85	0.42
1:K:165:MET:HG3	1:K:169:LEU:HD22	2.01	0.42
1:X:168:TYR:O	1:X:172:LYS:HG2	2.20	0.42
1:E:72:LEU:HD22	1:E:132:PHE:CD2	2.54	0.42
1:Q:68:LYS:HG2	1:Q:132:PHE:HZ	1.85	0.42
1:W:68:LYS:HG2	1:W:132:PHE:HZ	1.84	0.42
1:D:63:ARG:CZ	1:I:63:ARG:CZ	2.97	0.42
1:J:90:ARG:HD2	1:J:93:TRP:CE3	2.55	0.42
1:O:90:ARG:HD2	1:O:93:TRP:CE3	2.54	0.42
1:P:90:ARG:HD2	1:P:93:TRP:CE3	2.54	0.42
1:V:90:ARG:HD2	1:V:93:TRP:CE3	2.54	0.42
1:F:72:LEU:HD22	1:F:132:PHE:CE2	2.54	0.42
1:N:72:LEU:HD22	1:N:132:PHE:CE2	2.54	0.42
1:T:72:LEU:HD22	1:T:132:PHE:CE2	2.54	0.42
1:B:72:LEU:HD22	1:B:132:PHE:CD2	2.54	0.42
1:D:72:LEU:HD22	1:D:132:PHE:CD2	2.54	0.42
1:H:72:LEU:HD22	1:H:132:PHE:CD2	2.54	0.42
1:J:72:LEU:HD22	1:J:132:PHE:CD2	2.54	0.42
1:S:72:LEU:HD22	1:S:132:PHE:CD2	2.54	0.42
1:X:72:LEU:HD22	1:X:132:PHE:CD2	2.54	0.42
1:D:41:PHE:CE1	1:D:51:PHE:HD2	2.37	0.42
1:G:48:LEU:HD13	1:G:51:PHE:CE2	2.55	0.42
1:I:72:LEU:HD22	1:I:132:PHE:CD2	2.53	0.42
1:K:90:ARG:HD2	1:K:93:TRP:CE3	2.54	0.42
1:S:48:LEU:HD13	1:S:51:PHE:CE2	2.55	0.42
1:A:69:LEU:HD13	1:A:137:TYR:CZ	2.55	0.42
1:D:68:LYS:HG2	1:D:132:PHE:HZ	1.85	0.42
1:H:69:LEU:HD13	1:H:137:TYR:CZ	2.55	0.42
1:I:72:LEU:HD22	1:I:132:PHE:CD2	2.53	0.42
1:K:168:TYR:O	1:K:172:LYS:HG2	2.20	0.42
1:R:176:GLY:O	1:R:177:HIS:CG	2.72	0.42
1:T:168:TYR:O	1:T:172:LYS:HG2	2.20	0.42
1:A:68:LYS:HG2	1:A:132:PHE:HZ	1.84	0.42
1:S:68:LYS:HG2	1:S:132:PHE:HZ	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:90:ARG:HD2	1:N:93:TRP:CE3	2.54	0.42
1:T:90:ARG:HD2	1:T:93:TRP:CE3	2.54	0.42
1:U:90:ARG:HD2	1:U:93:TRP:CE3	2.54	0.42
1:A:72:LEU:HD22	1:A:132:PHE:CE2	2.54	0.42
1:O:143:LYS:HE2	1:O:143:LYS:HB2	1.91	0.42
1:C:72:LEU:HD22	1:C:132:PHE:CD2	2.54	0.42
1:R:72:LEU:HD22	1:R:132:PHE:CD2	2.54	0.42
1:W:68:LYS:HG2	1:W:132:PHE:HZ	1.84	0.42
1:A:48:LEU:HD13	1:A:51:PHE:CE2	2.55	0.42
1:B:48:LEU:HD13	1:B:51:PHE:CE2	2.55	0.42
1:C:72:LEU:HD22	1:C:132:PHE:CD2	2.53	0.42
1:H:48:LEU:HD13	1:H:51:PHE:CE2	2.55	0.42
1:J:48:LEU:HD13	1:J:51:PHE:CE2	2.55	0.42
1:M:48:LEU:HD13	1:M:51:PHE:CE2	2.55	0.42
1:O:41:PHE:CE1	1:O:51:PHE:HD2	2.37	0.42
1:D:157:LYS:HG3	2:D:218:HOH:O	2.19	0.42
1:S:72:LEU:HD22	1:S:132:PHE:CD2	2.54	0.42
1:T:68:LYS:HG2	1:T:132:PHE:HZ	1.85	0.42
1:E:168:TYR:O	1:E:172:LYS:HG2	2.20	0.42
1:M:153:THR:HG22	1:M:157:LYS:HZ2	1.85	0.42
1:N:168:TYR:O	1:N:172:LYS:HG2	2.20	0.42
1:O:68:LYS:HG2	1:O:132:PHE:HZ	1.85	0.42
1:O:69:LEU:HD13	1:O:137:TYR:CZ	2.55	0.42
1:Q:168:TYR:O	1:Q:172:LYS:HG2	2.20	0.42
1:R:168:TYR:O	1:R:172:LYS:HG2	2.20	0.42
1:S:168:TYR:O	1:S:172:LYS:HG2	2.20	0.42
1:U:68:LYS:HG2	1:U:132:PHE:HZ	1.85	0.42
1:U:168:TYR:HD2	1:U:169:LEU:CD1	2.33	0.42
1:W:168:TYR:O	1:W:172:LYS:HG2	2.20	0.42
1:X:69:LEU:HD13	1:X:137:TYR:CZ	2.55	0.42
1:M:68:LYS:HG2	1:M:132:PHE:HZ	1.85	0.42
1:M:72:LEU:HD22	1:M:132:PHE:CD2	2.54	0.42
1:F:48:LEU:HD13	1:F:51:PHE:CE2	2.54	0.42
1:I:34:TYR:OH	1:I:107:GLU:OE2	2.27	0.42
1:L:48:LEU:HD13	1:L:51:PHE:CE2	2.54	0.42
1:L:72:LEU:HD22	1:L:132:PHE:CE2	2.54	0.42
1:F:80:ILE:HG22	1:F:82:LEU:CD1	2.50	0.42
1:L:80:ILE:HG22	1:L:82:LEU:CD1	2.50	0.42
1:O:63:ARG:CZ	1:V:63:ARG:CZ	2.97	0.42
1:B:41:PHE:CE1	1:B:51:PHE:HD2	2.37	0.42
1:D:48:LEU:HD13	1:D:51:PHE:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:41:PHE:CE1	1:H:51:PHE:HD2	2.37	0.42
1:Q:48:LEU:HD13	1:Q:51:PHE:CE2	2.55	0.42
1:U:41:PHE:CE1	1:U:51:PHE:HD2	2.37	0.42
1:V:41:PHE:CE1	1:V:51:PHE:HD2	2.37	0.42
1:W:48:LEU:HD13	1:W:51:PHE:CE2	2.55	0.42
1:D:68:LYS:HG2	1:D:132:PHE:HZ	1.85	0.42
1:N:68:LYS:HG2	1:N:132:PHE:HZ	1.85	0.42
1:V:157:LYS:HG3	2:V:221:HOH:O	2.18	0.42
1:B:69:LEU:HD13	1:B:137:TYR:CZ	2.55	0.42
1:I:168:TYR:O	1:I:172:LYS:HG2	2.20	0.42
1:J:168:TYR:O	1:J:172:LYS:HG2	2.20	0.42
1:K:68:LYS:HG2	1:K:132:PHE:HZ	1.85	0.42
1:M:168:TYR:O	1:M:172:LYS:HG2	2.20	0.42
1:N:69:LEU:HD13	1:N:137:TYR:CZ	2.55	0.42
1:N:165:MET:HG3	1:N:169:LEU:HD22	2.01	0.42
1:T:69:LEU:HD13	1:T:137:TYR:CZ	2.55	0.42
1:U:69:LEU:HD13	1:U:137:TYR:CZ	2.55	0.42
1:V:69:LEU:HD13	1:V:137:TYR:CZ	2.55	0.42
1:D:153:THR:HG22	1:D:157:LYS:HZ2	1.83	0.42
1:S:72:LEU:HD22	1:S:132:PHE:CD2	2.54	0.42
1:G:72:LEU:HD22	1:G:132:PHE:CE2	2.54	0.42
1:H:72:LEU:HD22	1:H:132:PHE:CE2	2.54	0.42
1:N:48:LEU:HD13	1:N:51:PHE:CE2	2.54	0.42
1:Q:72:LEU:HD22	1:Q:132:PHE:CE2	2.54	0.42
1:T:48:LEU:HD13	1:T:51:PHE:CE2	2.54	0.42
1:A:72:LEU:HD22	1:A:132:PHE:CD2	2.54	0.42
1:G:72:LEU:HD22	1:G:132:PHE:CD2	2.54	0.42
1:T:153:THR:HG22	1:T:157:LYS:HZ3	1.83	0.42
1:K:41:PHE:CE1	1:K:51:PHE:HD2	2.37	0.42
1:P:41:PHE:CE1	1:P:51:PHE:HD2	2.37	0.42
1:J:68:LYS:HG2	1:J:132:PHE:HZ	1.85	0.42
1:Q:68:LYS:HG2	1:Q:132:PHE:HZ	1.85	0.42
1:W:68:LYS:HG2	1:W:132:PHE:HZ	1.85	0.42
1:C:168:TYR:O	1:C:172:LYS:HG2	2.20	0.42
1:D:69:LEU:HD13	1:D:137:TYR:CZ	2.55	0.42
1:D:168:TYR:O	1:D:172:LYS:HG2	2.20	0.42
1:F:68:LYS:HG2	1:F:132:PHE:HZ	1.85	0.42
1:F:168:TYR:HD2	1:F:169:LEU:CD1	2.33	0.42
1:L:68:LYS:HG2	1:L:132:PHE:HZ	1.85	0.42
1:L:143:LYS:HE2	1:L:143:LYS:HB2	1.90	0.42
1:L:168:TYR:HD2	1:L:169:LEU:CD1	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:168:TYR:HD2	1:O:169:LEU:CD1	2.33	0.42
1:P:69:LEU:HD13	1:P:137:TYR:CZ	2.55	0.42
1:R:69:LEU:HD13	1:R:137:TYR:CZ	2.55	0.42
1:R:165:MET:HG3	1:R:169:LEU:HD22	2.01	0.42
1:T:165:MET:HG3	1:T:169:LEU:HD22	2.02	0.42
1:X:165:MET:HG3	1:X:169:LEU:HD22	2.02	0.42
1:M:72:LEU:HD22	1:M:132:PHE:CD2	2.54	0.42
1:F:68:LYS:HG2	1:F:132:PHE:HZ	1.84	0.42
1:R:157:LYS:HG3	2:R:218:HOH:O	2.20	0.42
1:B:72:LEU:HD22	1:B:132:PHE:CE2	2.54	0.42
1:W:72:LEU:HD22	1:W:132:PHE:CE2	2.54	0.42
1:I:72:LEU:HD22	1:I:132:PHE:CD2	2.54	0.42
1:A:80:ILE:HG22	1:A:82:LEU:CD1	2.50	0.42
1:C:72:LEU:HD22	1:C:132:PHE:CD2	2.54	0.42
1:F:68:LYS:HG2	1:F:132:PHE:HZ	1.84	0.42
1:H:68:LYS:HG2	1:H:132:PHE:HZ	1.84	0.42
1:D:68:LYS:HG2	1:D:132:PHE:HZ	1.85	0.42
1:C:72:LEU:HD22	1:C:132:PHE:CD2	2.54	0.41
1:O:70:MET:CE	1:V:35:LEU:HD11	2.50	0.41
1:B:68:LYS:HG2	1:B:132:PHE:HZ	1.85	0.41
1:B:168:TYR:O	1:B:172:LYS:HG2	2.20	0.41
1:E:68:LYS:HG2	1:E:132:PHE:HZ	1.85	0.41
1:H:168:TYR:O	1:H:172:LYS:HG2	2.20	0.41
1:J:69:LEU:HD13	1:J:137:TYR:CZ	2.55	0.41
1:O:168:TYR:O	1:O:172:LYS:HG2	2.20	0.41
1:S:72:LEU:HD22	1:S:132:PHE:CD2	2.54	0.41
1:O:68:LYS:HG2	1:O:132:PHE:HZ	1.84	0.41
1:C:46:VAL:O	1:C:48:LEU:HD13	2.20	0.41
1:E:90:ARG:HD2	1:E:93:TRP:CE3	2.54	0.41
1:Q:90:ARG:HD2	1:Q:93:TRP:CE3	2.55	0.41
1:B:68:LYS:HG2	1:B:132:PHE:HZ	1.84	0.41
1:G:80:ILE:HG22	1:G:82:LEU:CD1	2.50	0.41
1:I:72:LEU:HD22	1:I:132:PHE:CD2	2.54	0.41
1:K:68:LYS:HG2	1:K:132:PHE:HZ	1.84	0.41
1:L:68:LYS:HG2	1:L:132:PHE:HZ	1.84	0.41
1:U:80:ILE:HG22	1:U:82:LEU:CD1	2.50	0.41
1:J:68:LYS:HG2	1:J:132:PHE:HZ	1.85	0.41
1:N:68:LYS:HG2	1:N:132:PHE:HZ	1.85	0.41
1:Q:68:LYS:HG2	1:Q:132:PHE:HZ	1.85	0.41
1:T:34:TYR:OH	1:T:107:GLU:OE2	2.23	0.41
1:T:68:LYS:HG2	1:T:132:PHE:HZ	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:157:LYS:HG3	2:T:218:HOH:O	2.19	0.41
1:H:68:LYS:HG2	1:H:132:PHE:HZ	1.85	0.41
1:I:153:THR:HG22	1:I:157:LYS:HZ3	1.83	0.41
1:U:168:TYR:O	1:U:172:LYS:HG2	2.20	0.41
1:V:168:TYR:O	1:V:172:LYS:HG2	2.20	0.41
1:F:157:LYS:HG3	2:F:220:HOH:O	2.20	0.41
1:K:68:LYS:HG2	1:K:132:PHE:HZ	1.85	0.41
1:L:68:LYS:HG2	1:L:132:PHE:HZ	1.85	0.41
1:B:90:ARG:HD2	1:B:93:TRP:CE3	2.54	0.41
1:H:90:ARG:HD2	1:H:93:TRP:CE3	2.55	0.41
1:I:46:VAL:O	1:I:48:LEU:HD13	2.21	0.41
1:K:90:ARG:HD2	1:K:93:TRP:CE3	2.54	0.41
1:Q:46:VAL:O	1:Q:48:LEU:HD13	2.21	0.41
1:I:80:ILE:HG22	1:I:82:LEU:CD1	2.50	0.41
1:R:68:LYS:HG2	1:R:132:PHE:HZ	1.84	0.41
1:E:41:PHE:CE1	1:E:51:PHE:HD2	2.37	0.41
1:I:72:LEU:HD22	1:I:132:PHE:CD2	2.54	0.41
1:L:143:LYS:HE2	1:L:143:LYS:HB2	1.91	0.41
1:N:157:LYS:HG3	2:N:218:HOH:O	2.19	0.41
1:O:68:LYS:HG2	1:O:132:PHE:HZ	1.85	0.41
1:F:69:LEU:HD13	1:F:137:TYR:CZ	2.55	0.41
1:K:69:LEU:HD13	1:K:137:TYR:CZ	2.55	0.41
1:L:69:LEU:HD13	1:L:137:TYR:CZ	2.55	0.41
1:O:165:MET:HG3	1:O:169:LEU:HD22	2.01	0.41
1:Q:168:TYR:HD2	1:Q:169:LEU:CD1	2.33	0.41
1:S:68:LYS:HG2	1:S:132:PHE:HZ	1.85	0.41
1:U:4:SER:HA	1:U:5:PRO:HD3	1.93	0.41
1:W:168:TYR:HD2	1:W:169:LEU:CD1	2.33	0.41
1:E:68:LYS:HG2	1:E:132:PHE:HZ	1.84	0.41
1:U:68:LYS:HG2	1:U:132:PHE:HZ	1.84	0.41
1:C:72:LEU:HD22	1:C:132:PHE:CD2	2.54	0.41
1:H:46:VAL:O	1:H:48:LEU:HD13	2.21	0.41
1:L:46:VAL:O	1:L:48:LEU:HD13	2.20	0.41
1:R:157:LYS:HG3	2:R:218:HOH:O	2.20	0.41
1:W:46:VAL:O	1:W:48:LEU:HD13	2.21	0.41
1:W:90:ARG:HD2	1:W:93:TRP:CE3	2.54	0.41
1:A:60:HIS:CD2	1:R:63:ARG:CZ	3.04	0.41
1:C:80:ILE:HG22	1:C:82:LEU:CD1	2.50	0.41
1:O:68:LYS:HG2	1:O:132:PHE:HZ	1.84	0.41
1:O:80:ILE:HG22	1:O:82:LEU:CD1	2.50	0.41
1:W:68:LYS:HG2	1:W:132:PHE:HZ	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:LEU:HD13	1:C:51:PHE:CE2	2.55	0.41
1:F:68:LYS:HG2	1:F:132:PHE:HZ	1.85	0.41
1:U:68:LYS:HG2	1:U:132:PHE:HZ	1.85	0.41
1:C:69:LEU:HD13	1:C:137:TYR:CZ	2.55	0.41
1:E:69:LEU:HD13	1:E:137:TYR:CZ	2.55	0.41
1:I:69:LEU:HD13	1:I:137:TYR:CZ	2.55	0.41
1:M:68:LYS:HG2	1:M:132:PHE:HZ	1.85	0.41
1:P:68:LYS:HG2	1:P:132:PHE:HZ	1.85	0.41
1:L:143:LYS:HE2	1:L:143:LYS:HB2	1.90	0.41
1:A:157:LYS:HG3	2:A:220:HOH:O	2.21	0.41
1:B:46:VAL:O	1:B:48:LEU:HD13	2.21	0.41
1:F:46:VAL:O	1:F:48:LEU:HD13	2.20	0.41
1:I:72:LEU:HD22	1:I:132:PHE:CD2	2.54	0.41
1:U:72:LEU:HD22	1:U:132:PHE:CE2	2.54	0.41
1:C:63:ARG:CZ	1:J:60:HIS:CD2	3.04	0.41
1:C:68:LYS:HG2	1:C:132:PHE:HZ	1.84	0.41
1:E:68:LYS:HG2	1:E:132:PHE:HZ	1.84	0.41
1:K:153:THR:HG22	1:K:157:LYS:HZ2	1.83	0.41
1:Q:90:ARG:HD2	1:Q:93:TRP:CE3	2.56	0.41
1:U:68:LYS:HG2	1:U:132:PHE:HZ	1.84	0.41
1:W:90:ARG:HD2	1:W:93:TRP:CE3	2.56	0.41
1:X:68:LYS:HG2	1:X:132:PHE:HZ	1.84	0.41
1:X:80:ILE:HG22	1:X:82:LEU:CD1	2.50	0.41
1:N:34:TYR:OH	1:N:107:GLU:OE2	2.23	0.41
1:I:48:LEU:HD13	1:I:51:PHE:CE2	2.55	0.41
1:P:48:LEU:HD13	1:P:51:PHE:CE2	2.55	0.41
1:R:48:LEU:HD13	1:R:51:PHE:CE2	2.55	0.41
1:V:48:LEU:HD13	1:V:51:PHE:CE2	2.55	0.41
1:X:48:LEU:HD13	1:X:51:PHE:CE2	2.55	0.41
1:K:68:LYS:HG2	1:K:132:PHE:HZ	1.85	0.41
1:P:157:LYS:HG3	2:P:218:HOH:O	2.19	0.41
1:S:68:LYS:HG2	1:S:132:PHE:HZ	1.85	0.41
1:F:143:LYS:HE2	1:F:143:LYS:HB2	1.90	0.41
1:N:168:TYR:HD2	1:N:169:LEU:CD1	2.33	0.41
1:P:168:TYR:O	1:P:172:LYS:HG2	2.20	0.41
1:T:168:TYR:HD2	1:T:169:LEU:CD1	2.33	0.41
1:U:143:LYS:HE2	1:U:143:LYS:HB2	1.90	0.41
1:U:165:MET:HG3	1:U:169:LEU:HD22	2.01	0.41
1:W:143:LYS:HE2	1:W:143:LYS:HB2	1.90	0.41
1:C:72:LEU:HD22	1:C:132:PHE:CD2	2.54	0.41
1:G:46:VAL:O	1:G:48:LEU:HD13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:157:LYS:HG3	2:H:219:HOH:O	2.20	0.41
1:A:97:LEU:HD13	1:A:97:LEU:C	2.41	0.41
1:D:68:LYS:HG2	1:D:132:PHE:HZ	1.86	0.41
1:J:97:LEU:C	1:J:97:LEU:HD13	2.41	0.41
1:L:97:LEU:HD13	1:L:97:LEU:C	2.41	0.41
1:N:68:LYS:HG2	1:N:132:PHE:HZ	1.86	0.41
1:T:68:LYS:HG2	1:T:132:PHE:HZ	1.86	0.41
1:F:90:ARG:HD2	1:F:93:TRP:CE3	2.56	0.41
1:G:60:HIS:CD2	1:X:63:ARG:CZ	3.04	0.41
1:H:90:ARG:HD2	1:H:93:TRP:CE3	2.56	0.41
1:I:68:LYS:HG2	1:I:132:PHE:HZ	1.84	0.41
1:J:80:ILE:HG22	1:J:82:LEU:CD1	2.50	0.41
1:L:60:HIS:CD2	1:S:63:ARG:CZ	3.04	0.41
1:N:80:ILE:HG22	1:N:82:LEU:CD1	2.50	0.41
1:Q:143:LYS:HE2	1:Q:143:LYS:HB2	1.89	0.41
1:R:80:ILE:HG22	1:R:82:LEU:CD1	2.50	0.41
1:R:90:ARG:HD2	1:R:93:TRP:CE3	2.56	0.41
1:S:80:ILE:HG22	1:S:82:LEU:CD1	2.50	0.41
1:X:90:ARG:HD2	1:X:93:TRP:CE3	2.56	0.41
1:F:68:LYS:HG2	1:F:132:PHE:HZ	1.85	0.41
1:O:68:LYS:HG2	1:O:132:PHE:HZ	1.85	0.41
1:S:68:LYS:HG2	1:S:132:PHE:HZ	1.85	0.41
1:L:68:LYS:HG2	1:L:132:PHE:HZ	1.85	0.41
1:M:68:LYS:HG2	1:M:132:PHE:HZ	1.85	0.41
1:K:143:LYS:HE2	1:K:143:LYS:HB2	1.90	0.41
1:M:69:LEU:HD13	1:M:137:TYR:CZ	2.55	0.41
1:O:4:SER:HA	1:O:5:PRO:HD3	1.93	0.41
1:S:69:LEU:HD13	1:S:137:TYR:CZ	2.55	0.41
1:V:68:LYS:HG2	1:V:132:PHE:HZ	1.85	0.41
1:X:68:LYS:HG2	1:X:132:PHE:HZ	1.85	0.41
1:A:157:LYS:HG3	2:A:220:HOH:O	2.20	0.41
1:H:157:LYS:HG3	2:H:219:HOH:O	2.20	0.41
1:R:68:LYS:HG2	1:R:132:PHE:HZ	1.85	0.41
1:X:68:LYS:HG2	1:X:132:PHE:HZ	1.84	0.41
1:D:97:LEU:HD13	1:D:97:LEU:C	2.41	0.41
1:F:97:LEU:HD13	1:F:97:LEU:C	2.41	0.41
1:G:97:LEU:HD13	1:G:97:LEU:C	2.41	0.41
1:J:68:LYS:HG2	1:J:132:PHE:HZ	1.86	0.41
1:L:143:LYS:HE2	1:L:143:LYS:HB2	1.91	0.41
1:A:90:ARG:HD2	1:A:93:TRP:CE3	2.56	0.41
1:B:90:ARG:HD2	1:B:93:TRP:CE3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:ARG:HD2	1:C:93:TRP:CE3	2.56	0.41
1:D:80:ILE:HG22	1:D:82:LEU:CD1	2.50	0.41
1:F:60:HIS:CD2	1:M:63:ARG:CZ	3.04	0.41
1:L:90:ARG:HD2	1:L:93:TRP:CE3	2.56	0.41
1:P:80:ILE:HG22	1:P:82:LEU:CD1	2.50	0.41
1:T:60:HIS:CD2	1:W:63:ARG:CZ	3.04	0.41
1:T:80:ILE:HG22	1:T:82:LEU:CD1	2.50	0.41
1:M:68:LYS:HG2	1:M:132:PHE:HZ	1.85	0.41
1:U:68:LYS:HG2	1:U:132:PHE:HZ	1.85	0.41
1:E:48:LEU:HD13	1:E:51:PHE:CE2	2.55	0.41
1:K:48:LEU:HD13	1:K:51:PHE:CE2	2.55	0.41
1:B:68:LYS:HG2	1:B:132:PHE:HZ	1.85	0.41
1:E:68:LYS:HG2	1:E:132:PHE:HZ	1.85	0.41
1:O:35:LEU:HD21	1:V:70:MET:HE1	2.01	0.41
1:E:143:LYS:HE2	1:E:143:LYS:HB2	1.90	0.41
1:G:68:LYS:HG2	1:G:132:PHE:HZ	1.85	0.41
1:Q:69:LEU:HD13	1:Q:137:TYR:CZ	2.55	0.41
1:R:68:LYS:HG2	1:R:132:PHE:HZ	1.85	0.41
1:W:69:LEU:HD13	1:W:137:TYR:CZ	2.55	0.41
1:I:72:LEU:HD22	1:I:132:PHE:CD2	2.54	0.41
1:A:46:VAL:O	1:A:48:LEU:HD13	2.21	0.41
1:B:157:LYS:HG3	2:B:219:HOH:O	2.21	0.41
1:D:157:LYS:HG3	2:D:218:HOH:O	2.20	0.41
1:H:75:GLN:HG2	1:I:142:VAL:CG1	2.51	0.41
1:M:46:VAL:O	1:M:48:LEU:HD13	2.21	0.41
1:S:46:VAL:O	1:S:48:LEU:HD13	2.20	0.41
1:O:72:LEU:HD22	1:O:132:PHE:CE2	2.54	0.41
1:Q:68:LYS:HG2	1:Q:132:PHE:HZ	1.86	0.41
1:W:68:LYS:HG2	1:W:132:PHE:HZ	1.86	0.41
1:E:90:ARG:HD2	1:E:93:TRP:CE3	2.56	0.41
1:G:90:ARG:HD2	1:G:93:TRP:CE3	2.56	0.41
1:I:90:ARG:HD2	1:I:93:TRP:CE3	2.56	0.41
1:K:90:ARG:HD2	1:K:93:TRP:CE3	2.56	0.41
1:O:90:ARG:HD2	1:O:93:TRP:CE3	2.56	0.41
1:V:80:ILE:HG22	1:V:82:LEU:CD1	2.50	0.41
1:W:143:LYS:HE2	1:W:143:LYS:HB2	1.89	0.41
1:L:68:LYS:HG2	1:L:132:PHE:HZ	1.85	0.41
1:F:48:LEU:HD13	1:F:51:PHE:CE2	2.55	0.41
1:L:143:LYS:HE2	1:L:143:LYS:HB2	1.91	0.41
1:U:4:SER:HA	1:U:5:PRO:HD3	1.94	0.41
1:F:143:LYS:HE2	1:F:143:LYS:HB2	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:68:LYS:HG2	1:H:132:PHE:HZ	1.85	0.41
1:J:143:LYS:HB2	1:J:143:LYS:HE2	1.90	0.41
1:R:41:PHE:CE1	1:R:51:PHE:HD2	2.39	0.41
1:I:68:LYS:HG2	1:I:132:PHE:HZ	1.85	0.41
1:B:157:LYS:HG3	2:B:219:HOH:O	2.20	0.41
1:H:68:LYS:HG2	1:H:132:PHE:HZ	1.85	0.41
1:U:4:SER:HA	1:U:5:PRO:HD3	1.93	0.41
1:D:46:VAL:O	1:D:48:LEU:HD13	2.21	0.41
1:F:157:LYS:HG3	2:F:220:HOH:O	2.20	0.41
1:J:46:VAL:O	1:J:48:LEU:HD13	2.21	0.41
1:L:143:LYS:HE2	1:L:143:LYS:HB2	1.90	0.41
1:O:4:SER:HA	1:O:5:PRO:HD3	1.93	0.41
1:S:97:LEU:HD13	1:S:97:LEU:C	2.41	0.41
1:U:97:LEU:HD13	1:U:97:LEU:C	2.41	0.41
1:B:80:ILE:HG22	1:B:82:LEU:CD1	2.50	0.41
1:C:60:HIS:CD2	1:J:63:ARG:CZ	3.04	0.41
1:D:60:HIS:CD2	1:I:63:ARG:CZ	3.04	0.41
1:M:80:ILE:HG22	1:M:82:LEU:CD1	2.50	0.41
1:U:90:ARG:HD2	1:U:93:TRP:CE3	2.56	0.41
1:K:68:LYS:HG2	1:K:132:PHE:HZ	1.85	0.41
1:L:48:LEU:HD13	1:L:51:PHE:CE2	2.55	0.41
1:N:48:LEU:HD13	1:N:51:PHE:CE2	2.55	0.41
1:T:48:LEU:HD13	1:T:51:PHE:CE2	2.55	0.41
1:G:68:LYS:HG2	1:G:132:PHE:HZ	1.85	0.41
1:J:41:PHE:CE1	1:J:51:PHE:HD2	2.39	0.41
1:Q:4:SER:HA	1:Q:5:PRO:HD3	1.94	0.41
1:U:143:LYS:HE2	1:U:143:LYS:HB2	1.90	0.41
1:X:41:PHE:CE1	1:X:51:PHE:HD2	2.39	0.41
1:A:68:LYS:HG2	1:A:132:PHE:HZ	1.85	0.41
1:C:68:LYS:HG2	1:C:132:PHE:HZ	1.85	0.41
1:C:165:MET:HG3	1:C:169:LEU:HD22	2.01	0.41
1:C:168:TYR:HD2	1:C:169:LEU:CD1	2.33	0.41
1:F:165:MET:HG3	1:F:169:LEU:HD22	2.01	0.41
1:I:165:MET:HG3	1:I:169:LEU:HD22	2.01	0.41
1:I:168:TYR:HD2	1:I:169:LEU:CD1	2.33	0.41
1:L:153:THR:HG22	1:L:157:LYS:HZ2	1.86	0.41
1:O:143:LYS:HE2	1:O:143:LYS:HB2	1.90	0.41
1:O:153:THR:HG22	1:O:157:LYS:HZ3	1.85	0.41
1:Q:143:LYS:HE2	1:Q:143:LYS:HB2	1.90	0.41
1:D:143:LYS:HB2	1:D:143:LYS:HE2	1.90	0.41
1:F:143:LYS:HE2	1:F:143:LYS:HB2	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:153:THR:HG22	1:J:157:LYS:HZ2	1.84	0.41
1:T:153:THR:HG22	1:T:157:LYS:HZ2	1.83	0.41
1:B:68:LYS:HG2	1:B:132:PHE:HZ	1.85	0.41
1:G:34:TYR:OH	1:G:107:GLU:OE2	2.21	0.41
1:H:63:ARG:CZ	1:K:63:ARG:CZ	2.99	0.41
1:V:68:LYS:HG2	1:V:132:PHE:HZ	1.85	0.41
1:D:143:LYS:HB2	1:D:143:LYS:HE2	1.90	0.41
1:N:46:VAL:O	1:N:48:LEU:HD13	2.21	0.41
1:Q:34:TYR:OH	1:Q:107:GLU:OE2	2.18	0.41
1:X:46:VAL:O	1:X:48:LEU:HD13	2.20	0.41
1:Q:4:SER:HA	1:Q:5:PRO:HD3	1.94	0.41
1:C:97:LEU:C	1:C:97:LEU:HD13	2.41	0.41
1:F:68:LYS:HG2	1:F:132:PHE:HZ	1.86	0.41
1:F:143:LYS:HE2	1:F:143:LYS:HB2	1.91	0.41
1:I:97:LEU:HD13	1:I:97:LEU:C	2.41	0.41
1:L:68:LYS:HG2	1:L:132:PHE:HZ	1.86	0.41
1:M:97:LEU:C	1:M:97:LEU:HD13	2.41	0.41
1:O:68:LYS:HG2	1:O:132:PHE:HZ	1.86	0.41
1:O:97:LEU:C	1:O:97:LEU:HD13	2.41	0.41
1:S:68:LYS:HG2	1:S:132:PHE:HZ	1.86	0.41
1:U:68:LYS:HG2	1:U:132:PHE:HZ	1.86	0.41
1:G:63:ARG:CZ	1:X:60:HIS:CD2	3.04	0.41
1:H:63:ARG:CZ	1:K:60:HIS:CD2	3.04	0.41
1:K:80:ILE:HG22	1:K:82:LEU:CD1	2.50	0.41
1:L:143:LYS:HE2	1:L:143:LYS:HB2	1.89	0.41
1:N:60:HIS:CD2	1:Q:63:ARG:CZ	3.04	0.41
1:B:68:LYS:HG2	1:B:132:PHE:HZ	1.85	0.41
1:E:68:LYS:HG2	1:E:132:PHE:HZ	1.85	0.41
1:G:68:LYS:HG2	1:G:132:PHE:HZ	1.85	0.41
1:U:4:SER:HA	1:U:5:PRO:HD3	1.93	0.41
1:O:4:SER:HA	1:O:5:PRO:HD3	1.94	0.41
1:W:143:LYS:HE2	1:W:143:LYS:HB2	1.91	0.41
1:A:68:LYS:HG2	1:A:132:PHE:HZ	1.85	0.41
1:D:41:PHE:CE1	1:D:51:PHE:HD2	2.39	0.41
1:N:41:PHE:CE1	1:N:51:PHE:HD2	2.39	0.41
1:P:68:LYS:HG2	1:P:132:PHE:HZ	1.85	0.41
1:T:41:PHE:CE1	1:T:51:PHE:HD2	2.39	0.41
1:V:68:LYS:HG2	1:V:132:PHE:HZ	1.85	0.41
1:W:143:LYS:HE2	1:W:143:LYS:HB2	1.91	0.41
1:D:168:TYR:HD2	1:D:169:LEU:CD1	2.33	0.41
1:P:4:SER:HA	1:P:5:PRO:HD3	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:68:LYS:HG2	1:P:132:PHE:HZ	1.84	0.41
1:T:46:VAL:O	1:T:48:LEU:HD13	2.21	0.41
1:V:157:LYS:HG3	2:V:221:HOH:O	2.20	0.41
1:N:143:LYS:HE2	1:N:143:LYS:HB2	1.91	0.41
1:T:143:LYS:HE2	1:T:143:LYS:HB2	1.91	0.41
1:K:68:LYS:HG2	1:K:132:PHE:HZ	1.86	0.41
1:P:4:SER:HA	1:P:5:PRO:HD3	1.93	0.41
1:T:97:LEU:HD13	1:T:97:LEU:C	2.41	0.41
1:U:34:TYR:OH	1:U:107:GLU:OE2	2.21	0.41
1:B:63:ARG:CZ	1:E:60:HIS:CD2	3.04	0.41
1:D:63:ARG:CZ	1:I:60:HIS:CD2	3.04	0.41
1:E:80:ILE:HG22	1:E:82:LEU:CD1	2.50	0.41
1:H:60:HIS:CD2	1:K:63:ARG:CZ	3.04	0.41
1:H:80:ILE:HG22	1:H:82:LEU:CD1	2.50	0.41
1:J:90:ARG:HD2	1:J:93:TRP:CE3	2.56	0.41
1:E:143:LYS:HE2	1:E:143:LYS:HB2	1.91	0.41
1:B:41:PHE:CE1	1:B:51:PHE:HD2	2.39	0.40
1:H:41:PHE:CE1	1:H:51:PHE:HD2	2.39	0.40
1:Q:143:LYS:HE2	1:Q:143:LYS:HB2	1.90	0.40
1:R:68:LYS:HG2	1:R:132:PHE:HZ	1.85	0.40
1:W:4:SER:HA	1:W:5:PRO:HD3	1.94	0.40
1:X:68:LYS:HG2	1:X:132:PHE:HZ	1.85	0.40
1:C:143:LYS:HB2	1:C:143:LYS:HE2	1.90	0.40
1:E:168:TYR:HD2	1:E:169:LEU:CD1	2.33	0.40
1:L:165:MET:HG3	1:L:169:LEU:HD22	2.01	0.40
1:P:168:TYR:HD2	1:P:169:LEU:CD1	2.33	0.40
1:E:153:THR:HG22	1:E:157:LYS:HZ2	1.84	0.40
1:C:68:LYS:HG2	1:C:132:PHE:HZ	1.84	0.40
1:O:4:SER:HA	1:O:5:PRO:HD3	1.93	0.40
1:N:157:LYS:HG3	2:N:218:HOH:O	2.20	0.40
1:R:46:VAL:O	1:R:48:LEU:HD13	2.21	0.40
1:T:157:LYS:HG3	2:T:218:HOH:O	2.21	0.40
1:E:97:LEU:C	1:E:97:LEU:HD13	2.41	0.40
1:K:97:LEU:HD13	1:K:97:LEU:C	2.41	0.40
1:K:168:TYR:O	1:K:172:LYS:HG2	2.22	0.40
1:M:68:LYS:HG2	1:M:132:PHE:HZ	1.86	0.40
1:M:168:TYR:O	1:M:172:LYS:HG2	2.21	0.40
1:N:97:LEU:HD13	1:N:97:LEU:C	2.41	0.40
1:N:168:TYR:O	1:N:172:LYS:HG2	2.21	0.40
1:Q:4:SER:HA	1:Q:5:PRO:HD3	1.93	0.40
1:R:168:TYR:O	1:R:172:LYS:HG2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:143:LYS:HB2	1:S:143:LYS:HE2	1.91	0.40
1:U:143:LYS:HE2	1:U:143:LYS:HB2	1.91	0.40
1:W:143:LYS:HE2	1:W:143:LYS:HB2	1.91	0.40
1:X:168:TYR:O	1:X:172:LYS:HG2	2.22	0.40
1:A:63:ARG:CZ	1:R:60:HIS:CD2	3.04	0.40
1:D:90:ARG:HD2	1:D:93:TRP:CE3	2.56	0.40
1:F:143:LYS:HE2	1:F:143:LYS:HB2	1.89	0.40
1:T:63:ARG:CZ	1:W:60:HIS:CD2	3.04	0.40
1:T:90:ARG:HD2	1:T:93:TRP:CE3	2.56	0.40
1:F:143:LYS:HE2	1:F:143:LYS:HB2	1.91	0.40
1:U:143:LYS:HE2	1:U:143:LYS:HB2	1.91	0.40
1:D:143:LYS:HB2	1:D:143:LYS:HE2	1.90	0.40
1:L:34:TYR:OH	1:L:107:GLU:OE2	2.22	0.40
1:A:168:TYR:O	1:A:172:LYS:HG2	2.20	0.40
1:J:168:TYR:HD2	1:J:169:LEU:CD1	2.33	0.40
1:K:168:TYR:HD2	1:K:169:LEU:CD1	2.33	0.40
1:X:168:TYR:HD2	1:X:169:LEU:CD1	2.33	0.40
1:A:90:ARG:HD2	1:A:93:TRP:CE3	2.57	0.40
1:K:153:THR:HG22	1:K:157:LYS:HZ2	1.84	0.40
1:W:143:LYS:HE2	1:W:143:LYS:HB2	1.90	0.40
1:D:157:LYS:HG3	2:D:218:HOH:O	2.20	0.40
1:I:68:LYS:HG2	1:I:132:PHE:HZ	1.85	0.40
1:J:157:LYS:HG3	2:J:221:HOH:O	2.20	0.40
1:F:143:LYS:HE2	1:F:143:LYS:HB2	1.90	0.40
1:P:157:LYS:HG3	2:P:218:HOH:O	2.20	0.40
1:Q:143:LYS:HE2	1:Q:143:LYS:HB2	1.90	0.40
1:W:4:SER:HA	1:W:5:PRO:HD3	1.94	0.40
1:E:68:LYS:HG2	1:E:132:PHE:HZ	1.86	0.40
1:E:168:TYR:O	1:E:172:LYS:HG2	2.22	0.40
1:I:168:TYR:O	1:I:172:LYS:HG2	2.22	0.40
1:J:168:TYR:O	1:J:172:LYS:HG2	2.21	0.40
1:Q:168:TYR:O	1:Q:172:LYS:HG2	2.22	0.40
1:R:97:LEU:C	1:R:97:LEU:HD13	2.41	0.40
1:T:168:TYR:O	1:T:172:LYS:HG2	2.22	0.40
1:W:168:TYR:O	1:W:172:LYS:HG2	2.22	0.40
1:N:90:ARG:HD2	1:N:93:TRP:CE3	2.56	0.40
1:A:68:LYS:HG2	1:A:132:PHE:HZ	1.86	0.40
1:H:68:LYS:HG2	1:H:132:PHE:HZ	1.85	0.40
1:O:4:SER:HA	1:O:5:PRO:HD3	1.93	0.40
1:R:68:LYS:HG2	1:R:132:PHE:HZ	1.85	0.40
1:U:34:TYR:OH	1:U:107:GLU:OE2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:4:SER:HA	1:V:5:PRO:HD3	1.94	0.40
1:O:143:LYS:HE2	1:O:143:LYS:HB2	1.90	0.40
1:G:168:TYR:O	1:G:172:LYS:HG2	2.20	0.40
1:Q:4:SER:HA	1:Q:5:PRO:HD3	1.94	0.40
1:R:168:TYR:HD2	1:R:169:LEU:CD1	2.33	0.40
1:S:168:TYR:HD2	1:S:169:LEU:CD1	2.33	0.40
1:V:168:TYR:HD2	1:V:169:LEU:CD1	2.33	0.40
1:F:90:ARG:HD2	1:F:93:TRP:CE3	2.57	0.40
1:G:90:ARG:HD2	1:G:93:TRP:CE3	2.57	0.40
1:L:90:ARG:HD2	1:L:93:TRP:CE3	2.57	0.40
1:J:157:LYS:HG3	2:J:221:HOH:O	2.21	0.40
1:M:143:LYS:HB2	1:M:143:LYS:HE2	1.90	0.40
1:V:46:VAL:O	1:V:48:LEU:HD13	2.21	0.40
1:E:75:GLN:HG2	1:F:142:VAL:CG1	2.52	0.40
1:J:142:VAL:CG1	1:L:75:GLN:HG2	2.52	0.40
1:B:68:LYS:HG2	1:B:132:PHE:HZ	1.86	0.40
1:C:168:TYR:O	1:C:172:LYS:HG2	2.22	0.40
1:D:168:TYR:O	1:D:172:LYS:HG2	2.22	0.40
1:J:143:LYS:HB2	1:J:143:LYS:HE2	1.91	0.40
1:Q:97:LEU:C	1:Q:97:LEU:HD13	2.41	0.40
1:S:168:TYR:O	1:S:172:LYS:HG2	2.22	0.40
1:B:60:HIS:CD2	1:E:63:ARG:CZ	3.04	0.40
1:K:74:ASN:C	1:L:146:LYS:HZ2	2.25	0.40
1:M:146:LYS:HZ2	1:O:74:ASN:C	2.25	0.40
1:K:143:LYS:HE2	1:K:143:LYS:HB2	1.91	0.40
1:O:143:LYS:HE2	1:O:143:LYS:HB2	1.91	0.40
1:Q:143:LYS:HE2	1:Q:143:LYS:HB2	1.91	0.40
1:G:41:PHE:CE1	1:G:51:PHE:HD2	2.39	0.40
1:I:68:LYS:HG2	1:I:132:PHE:HZ	1.85	0.40
1:M:143:LYS:HB2	1:M:143:LYS:HE2	1.90	0.40
1:O:41:PHE:CE1	1:O:51:PHE:HD2	2.39	0.40
1:Q:41:PHE:CE1	1:Q:51:PHE:HD2	2.39	0.40
1:W:41:PHE:CE1	1:W:51:PHE:HD2	2.39	0.40
1:F:168:TYR:O	1:F:172:LYS:HG2	2.20	0.40
1:L:168:TYR:O	1:L:172:LYS:HG2	2.20	0.40
1:M:168:TYR:HD2	1:M:169:LEU:CD1	2.33	0.40
1:U:34:TYR:OH	1:U:107:GLU:OE2	2.22	0.40
1:W:4:SER:HA	1:W:5:PRO:HD3	1.93	0.40
1:I:90:ARG:HD2	1:I:93:TRP:CE3	2.57	0.40
1:M:90:ARG:HD2	1:M:93:TRP:CE3	2.57	0.40
1:M:143:LYS:HB2	1:M:143:LYS:HE2	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:143:LYS:HE2	1:Q:143:LYS:HB2	1.90	0.40
1:M:157:LYS:HG3	2:M:217:HOH:O	2.21	0.40
1:V:4:SER:HA	1:V:5:PRO:HD3	1.93	0.40
1:E:46:VAL:O	1:E:48:LEU:HD13	2.21	0.40
1:N:68:LYS:HG2	1:N:132:PHE:HZ	1.87	0.40
1:P:46:VAL:O	1:P:48:LEU:HD13	2.21	0.40
1:Q:68:LYS:HG2	1:Q:132:PHE:HZ	1.87	0.40
1:T:68:LYS:HG2	1:T:132:PHE:HZ	1.87	0.40
1:W:68:LYS:HG2	1:W:132:PHE:HZ	1.87	0.40
1:K:75:GLN:HG2	1:L:142:VAL:CG1	2.52	0.40
1:E:143:LYS:HE2	1:E:143:LYS:HB2	1.91	0.40
1:K:143:LYS:HE2	1:K:143:LYS:HB2	1.91	0.40
1:Q:143:LYS:HE2	1:Q:143:LYS:HB2	1.91	0.40
1:U:168:TYR:O	1:U:172:LYS:HG2	2.22	0.40
1:W:4:SER:HA	1:W:5:PRO:HD3	1.93	0.40
1:N:63:ARG:CZ	1:Q:60:HIS:CD2	3.04	0.40
1:V:68:LYS:HG2	1:V:132:PHE:HZ	1.85	0.40
1:M:72:LEU:HD22	1:M:132:PHE:CE2	2.57	0.40
1:M:168:TYR:O	1:M:172:LYS:HG2	2.22	0.40
1:N:68:LYS:HG2	1:N:132:PHE:HZ	1.87	0.40
1:S:72:LEU:HD22	1:S:132:PHE:CE2	2.57	0.40
1:W:68:LYS:HG2	1:W:132:PHE:HZ	1.87	0.40
1:A:35:LEU:HD21	1:R:70:MET:HE1	2.03	0.40
1:A:41:PHE:CE1	1:A:51:PHE:HD2	2.39	0.40
1:C:41:PHE:CE1	1:C:51:PHE:HD2	2.39	0.40
1:K:41:PHE:CE1	1:K:51:PHE:HD2	2.39	0.40
1:P:70:MET:HE1	1:U:35:LEU:HD21	2.03	0.40
1:S:41:PHE:CE1	1:S:51:PHE:HD2	2.39	0.40
1:B:168:TYR:HD2	1:B:169:LEU:CD1	2.33	0.40
1:F:168:TYR:CD2	1:F:169:LEU:HD12	2.56	0.40
1:C:90:ARG:HD2	1:C:93:TRP:CE3	2.57	0.40
1:E:168:TYR:O	1:E:172:LYS:HG2	2.22	0.40
1:K:168:TYR:O	1:K:172:LYS:HG2	2.22	0.40
1:N:168:TYR:O	1:N:172:LYS:HG2	2.22	0.40
1:S:90:ARG:HD2	1:S:93:TRP:CE3	2.57	0.40
1:T:168:TYR:O	1:T:172:LYS:HG2	2.22	0.40
1:U:143:LYS:HE2	1:U:143:LYS:HB2	1.90	0.40
1:X:168:TYR:O	1:X:172:LYS:HG2	2.22	0.40
1:J:143:LYS:HB2	1:J:143:LYS:HE2	1.92	0.40
1:L:143:LYS:HE2	1:L:143:LYS:HB2	1.92	0.40
1:P:4:SER:HA	1:P:5:PRO:HD3	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:4:SER:HA	1:Q:5:PRO:HD3	1.93	0.40
1:D:63:ARG:NH2	1:I:63:ARG:CZ	2.85	0.40
1:D:68:LYS:HG2	1:D:132:PHE:HZ	1.87	0.40
1:J:68:LYS:HG2	1:J:132:PHE:HZ	1.87	0.40
1:K:46:VAL:O	1:K:48:LEU:HD13	2.21	0.40
1:W:143:LYS:HE2	1:W:143:LYS:HB2	1.90	0.40
1:D:142:VAL:CG1	1:F:75:GLN:HG2	2.52	0.40
1:R:157:LYS:HG3	2:R:218:HOH:O	2.22	0.40
1:A:68:LYS:HG2	1:A:132:PHE:HZ	1.86	0.40
1:B:168:TYR:O	1:B:172:LYS:HG2	2.22	0.40
1:G:68:LYS:HG2	1:G:132:PHE:HZ	1.86	0.40
1:H:68:LYS:HG2	1:H:132:PHE:HZ	1.86	0.40
1:H:168:TYR:O	1:H:172:LYS:HG2	2.22	0.40
1:O:168:TYR:O	1:O:172:LYS:HG2	2.22	0.40
1:V:97:LEU:HD13	1:V:97:LEU:C	2.41	0.40
1:X:97:LEU:C	1:X:97:LEU:HD13	2.41	0.40
1:L:143:LYS:HE2	1:L:143:LYS:HB2	1.93	0.40
1:N:168:TYR:O	1:N:172:LYS:HG2	2.22	0.40
1:P:68:LYS:HG2	1:P:132:PHE:HZ	1.85	0.40
1:X:68:LYS:HG2	1:X:132:PHE:HZ	1.85	0.40
1:I:168:TYR:O	1:I:172:LYS:HG2	2.22	0.40
1:J:168:TYR:O	1:J:172:LYS:HG2	2.22	0.40
1:N:168:TYR:O	1:N:172:LYS:HG2	2.22	0.40
1:P:4:SER:HA	1:P:5:PRO:HD3	1.94	0.40
1:Q:4:SER:HA	1:Q:5:PRO:HD3	1.94	0.40
1:Q:68:LYS:HG2	1:Q:132:PHE:HZ	1.87	0.40
1:Q:168:TYR:O	1:Q:172:LYS:HG2	2.22	0.40
1:R:168:TYR:O	1:R:172:LYS:HG2	2.22	0.40
1:S:168:TYR:O	1:S:172:LYS:HG2	2.22	0.40
1:T:68:LYS:HG2	1:T:132:PHE:HZ	1.87	0.40
1:T:168:TYR:O	1:T:172:LYS:HG2	2.22	0.40
1:U:168:TYR:O	1:U:172:LYS:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-A	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	1-B	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	1-C	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	1-D	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	1-E	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	1-F	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	1-G	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	1-H	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	1-I	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	1-J	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	1-K	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	1-L	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	1-M	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	1-N	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	1-O	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	1-P	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	1-Q	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	1-R	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	1-S	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	1-T	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	1-U	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	1-V	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	1-W	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	1-X	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	2-A	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	2-B	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	2-C	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	2-D	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	2-E	171/174 (98%)	167 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2-F	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	2-G	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	2-H	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	2-I	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	2-J	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	2-K	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	2-L	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	2-M	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	2-N	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	2-O	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	2-P	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	2-Q	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	2-R	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	2-S	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	2-T	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	2-U	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	2-V	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	2-W	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	2-X	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	3-A	171/174 (98%)	165 (96%)	6 (4%)	0	100	100
1	3-B	171/174 (98%)	165 (96%)	6 (4%)	0	100	100
1	3-C	171/174 (98%)	165 (96%)	6 (4%)	0	100	100
1	3-D	171/174 (98%)	165 (96%)	6 (4%)	0	100	100
1	3-E	171/174 (98%)	165 (96%)	6 (4%)	0	100	100
1	3-F	172/174 (99%)	166 (96%)	6 (4%)	0	100	100
1	3-G	172/174 (99%)	166 (96%)	6 (4%)	0	100	100
1	3-H	171/174 (98%)	165 (96%)	6 (4%)	0	100	100
1	3-I	171/174 (98%)	165 (96%)	6 (4%)	0	100	100
1	3-J	172/174 (99%)	166 (96%)	6 (4%)	0	100	100
1	3-K	171/174 (98%)	165 (96%)	6 (4%)	0	100	100
1	3-L	172/174 (99%)	166 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3-M	171/174 (98%)	165 (96%)	6 (4%)	0	100	100
1	3-N	171/174 (98%)	165 (96%)	6 (4%)	0	100	100
1	3-O	171/174 (98%)	165 (96%)	6 (4%)	0	100	100
1	3-P	171/174 (98%)	165 (96%)	6 (4%)	0	100	100
1	3-Q	171/174 (98%)	165 (96%)	6 (4%)	0	100	100
1	3-R	172/174 (99%)	166 (96%)	6 (4%)	0	100	100
1	3-S	172/174 (99%)	166 (96%)	6 (4%)	0	100	100
1	3-T	171/174 (98%)	165 (96%)	6 (4%)	0	100	100
1	3-U	171/174 (98%)	165 (96%)	6 (4%)	0	100	100
1	3-V	172/174 (99%)	166 (96%)	6 (4%)	0	100	100
1	3-W	171/174 (98%)	165 (96%)	6 (4%)	0	100	100
1	3-X	172/174 (99%)	166 (96%)	6 (4%)	0	100	100
1	4-A	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	4-B	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	4-C	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	4-D	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	4-E	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	4-F	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	4-G	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	4-H	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	4-I	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	4-J	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	4-K	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	4-L	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	4-M	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	4-N	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	4-O	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	4-P	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	4-Q	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	4-R	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	4-S	172/174 (99%)	168 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	4-T	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	4-U	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	4-V	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	4-W	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	4-X	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	5-A	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	5-B	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	5-C	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	5-D	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	5-E	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	5-F	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	5-G	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	5-H	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	5-I	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	5-J	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	5-K	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	5-L	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	5-M	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	5-N	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	5-O	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	5-P	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	5-Q	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	5-R	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	5-S	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	5-T	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	5-U	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	5-V	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	5-W	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	5-X	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	6-A	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	6-B	171/174 (98%)	167 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	6-C	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	6-D	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	6-E	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	6-F	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	6-G	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	6-H	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	6-I	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	6-J	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	6-K	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	6-L	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	6-M	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	6-N	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	6-O	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	6-P	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	6-Q	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	6-R	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	6-S	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	6-T	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	6-U	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	6-V	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	6-W	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	6-X	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	7-A	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	7-B	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	7-C	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	7-D	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	7-E	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	7-F	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	7-G	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	7-H	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	7-I	171/174 (98%)	167 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	7-J	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	7-K	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	7-L	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	7-M	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	7-N	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	7-O	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	7-P	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	7-Q	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	7-R	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	7-S	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	7-T	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	7-U	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	7-V	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	7-W	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	7-X	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	8-A	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	8-B	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	8-C	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	8-D	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	8-E	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	8-F	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	8-G	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	8-H	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	8-I	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	8-J	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	8-K	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	8-L	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	8-M	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	8-N	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	8-O	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	8-P	171/174 (98%)	167 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	8-Q	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	8-R	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	8-S	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	8-T	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	8-U	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	8-V	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	8-W	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	8-X	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	9-A	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	9-B	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	9-C	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	9-D	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	9-E	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	9-F	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	9-G	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	9-H	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	9-I	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	9-J	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	9-K	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	9-L	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	9-M	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	9-N	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	9-O	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	9-P	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	9-Q	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	9-R	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	9-S	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	9-T	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	9-U	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
1	9-V	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	9-W	171/174 (98%)	167 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	9-X	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
1	10-A	171/174 (98%)	165 (96%)	6 (4%)	0	100	100
1	10-B	171/174 (98%)	165 (96%)	6 (4%)	0	100	100
1	10-C	171/174 (98%)	165 (96%)	6 (4%)	0	100	100
1	10-D	171/174 (98%)	165 (96%)	6 (4%)	0	100	100
1	10-E	171/174 (98%)	165 (96%)	6 (4%)	0	100	100
1	10-F	172/174 (99%)	166 (96%)	6 (4%)	0	100	100
1	10-G	172/174 (99%)	166 (96%)	6 (4%)	0	100	100
1	10-H	171/174 (98%)	165 (96%)	6 (4%)	0	100	100
1	10-I	171/174 (98%)	165 (96%)	6 (4%)	0	100	100
1	10-J	172/174 (99%)	166 (96%)	6 (4%)	0	100	100
1	10-K	171/174 (98%)	165 (96%)	6 (4%)	0	100	100
1	10-L	172/174 (99%)	166 (96%)	6 (4%)	0	100	100
1	10-M	171/174 (98%)	165 (96%)	6 (4%)	0	100	100
1	10-N	171/174 (98%)	165 (96%)	6 (4%)	0	100	100
1	10-O	171/174 (98%)	165 (96%)	6 (4%)	0	100	100
1	10-P	171/174 (98%)	165 (96%)	6 (4%)	0	100	100
1	10-Q	171/174 (98%)	165 (96%)	6 (4%)	0	100	100
1	10-R	172/174 (99%)	166 (96%)	6 (4%)	0	100	100
1	10-S	172/174 (99%)	166 (96%)	6 (4%)	0	100	100
1	10-T	171/174 (98%)	165 (96%)	6 (4%)	0	100	100
1	10-U	171/174 (98%)	165 (96%)	6 (4%)	0	100	100
1	10-V	172/174 (99%)	166 (96%)	6 (4%)	0	100	100
1	10-W	171/174 (98%)	165 (96%)	6 (4%)	0	100	100
1	10-X	172/174 (99%)	166 (96%)	6 (4%)	0	100	100
All	All	41120/41760 (98%)	40064 (97%)	1056 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-A	153/154 (99%)	153 (100%)	0	100	100
1	1-B	153/154 (99%)	153 (100%)	0	100	100
1	1-C	153/154 (99%)	153 (100%)	0	100	100
1	1-D	153/154 (99%)	153 (100%)	0	100	100
1	1-E	153/154 (99%)	153 (100%)	0	100	100
1	1-F	154/154 (100%)	154 (100%)	0	100	100
1	1-G	154/154 (100%)	154 (100%)	0	100	100
1	1-H	153/154 (99%)	153 (100%)	0	100	100
1	1-I	153/154 (99%)	153 (100%)	0	100	100
1	1-J	154/154 (100%)	154 (100%)	0	100	100
1	1-K	153/154 (99%)	153 (100%)	0	100	100
1	1-L	154/154 (100%)	154 (100%)	0	100	100
1	1-M	153/154 (99%)	153 (100%)	0	100	100
1	1-N	153/154 (99%)	153 (100%)	0	100	100
1	1-O	153/154 (99%)	153 (100%)	0	100	100
1	1-P	153/154 (99%)	153 (100%)	0	100	100
1	1-Q	153/154 (99%)	153 (100%)	0	100	100
1	1-R	154/154 (100%)	154 (100%)	0	100	100
1	1-S	154/154 (100%)	154 (100%)	0	100	100
1	1-T	153/154 (99%)	153 (100%)	0	100	100
1	1-U	153/154 (99%)	153 (100%)	0	100	100
1	1-V	154/154 (100%)	154 (100%)	0	100	100
1	1-W	153/154 (99%)	153 (100%)	0	100	100
1	1-X	154/154 (100%)	154 (100%)	0	100	100
1	2-A	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	2-B	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	2-C	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	2-D	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	2-E	153/154 (99%)	152 (99%)	1 (1%)	84	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2-F	154/154 (100%)	153 (99%)	1 (1%)	86	79
1	2-G	154/154 (100%)	153 (99%)	1 (1%)	86	79
1	2-H	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	2-I	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	2-J	154/154 (100%)	153 (99%)	1 (1%)	86	79
1	2-K	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	2-L	154/154 (100%)	153 (99%)	1 (1%)	86	79
1	2-M	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	2-N	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	2-O	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	2-P	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	2-Q	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	2-R	154/154 (100%)	153 (99%)	1 (1%)	86	79
1	2-S	154/154 (100%)	153 (99%)	1 (1%)	86	79
1	2-T	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	2-U	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	2-V	154/154 (100%)	153 (99%)	1 (1%)	86	79
1	2-W	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	2-X	154/154 (100%)	153 (99%)	1 (1%)	86	79
1	3-A	153/154 (99%)	153 (100%)	0	100	100
1	3-B	153/154 (99%)	153 (100%)	0	100	100
1	3-C	153/154 (99%)	153 (100%)	0	100	100
1	3-D	153/154 (99%)	153 (100%)	0	100	100
1	3-E	153/154 (99%)	153 (100%)	0	100	100
1	3-F	154/154 (100%)	154 (100%)	0	100	100
1	3-G	154/154 (100%)	154 (100%)	0	100	100
1	3-H	153/154 (99%)	153 (100%)	0	100	100
1	3-I	153/154 (99%)	153 (100%)	0	100	100
1	3-J	154/154 (100%)	154 (100%)	0	100	100
1	3-K	153/154 (99%)	153 (100%)	0	100	100
1	3-L	154/154 (100%)	154 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	3-M	153/154 (99%)	153 (100%)	0	100	100
1	3-N	153/154 (99%)	153 (100%)	0	100	100
1	3-O	153/154 (99%)	153 (100%)	0	100	100
1	3-P	153/154 (99%)	153 (100%)	0	100	100
1	3-Q	153/154 (99%)	153 (100%)	0	100	100
1	3-R	154/154 (100%)	154 (100%)	0	100	100
1	3-S	154/154 (100%)	154 (100%)	0	100	100
1	3-T	153/154 (99%)	153 (100%)	0	100	100
1	3-U	153/154 (99%)	153 (100%)	0	100	100
1	3-V	154/154 (100%)	154 (100%)	0	100	100
1	3-W	153/154 (99%)	153 (100%)	0	100	100
1	3-X	154/154 (100%)	154 (100%)	0	100	100
1	4-A	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	4-B	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	4-C	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	4-D	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	4-E	153/154 (99%)	153 (100%)	0	100	100
1	4-F	154/154 (100%)	153 (99%)	1 (1%)	86	79
1	4-G	154/154 (100%)	153 (99%)	1 (1%)	86	79
1	4-H	153/154 (99%)	153 (100%)	0	100	100
1	4-I	153/154 (99%)	153 (100%)	0	100	100
1	4-J	154/154 (100%)	154 (100%)	0	100	100
1	4-K	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	4-L	154/154 (100%)	153 (99%)	1 (1%)	86	79
1	4-M	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	4-N	153/154 (99%)	153 (100%)	0	100	100
1	4-O	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	4-P	153/154 (99%)	153 (100%)	0	100	100
1	4-Q	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	4-R	154/154 (100%)	153 (99%)	1 (1%)	86	79
1	4-S	154/154 (100%)	153 (99%)	1 (1%)	86	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	4-T	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	4-U	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	4-V	154/154 (100%)	154 (100%)	0	100	100
1	4-W	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	4-X	154/154 (100%)	153 (99%)	1 (1%)	86	79
1	5-A	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	5-B	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	5-C	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	5-D	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	5-E	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	5-F	154/154 (100%)	153 (99%)	1 (1%)	86	79
1	5-G	154/154 (100%)	153 (99%)	1 (1%)	86	79
1	5-H	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	5-I	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	5-J	154/154 (100%)	153 (99%)	1 (1%)	86	79
1	5-K	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	5-L	154/154 (100%)	153 (99%)	1 (1%)	86	79
1	5-M	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	5-N	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	5-O	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	5-P	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	5-Q	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	5-R	154/154 (100%)	153 (99%)	1 (1%)	86	79
1	5-S	154/154 (100%)	153 (99%)	1 (1%)	86	79
1	5-T	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	5-U	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	5-V	154/154 (100%)	153 (99%)	1 (1%)	86	79
1	5-W	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	5-X	154/154 (100%)	153 (99%)	1 (1%)	86	79
1	6-A	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	6-B	153/154 (99%)	152 (99%)	1 (1%)	84	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	6-C	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	6-D	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	6-E	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	6-F	154/154 (100%)	153 (99%)	1 (1%)	86	79
1	6-G	154/154 (100%)	153 (99%)	1 (1%)	86	79
1	6-H	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	6-I	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	6-J	154/154 (100%)	153 (99%)	1 (1%)	86	79
1	6-K	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	6-L	154/154 (100%)	153 (99%)	1 (1%)	86	79
1	6-M	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	6-N	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	6-O	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	6-P	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	6-Q	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	6-R	154/154 (100%)	153 (99%)	1 (1%)	86	79
1	6-S	154/154 (100%)	153 (99%)	1 (1%)	86	79
1	6-T	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	6-U	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	6-V	154/154 (100%)	153 (99%)	1 (1%)	86	79
1	6-W	153/154 (99%)	152 (99%)	1 (1%)	84	75
1	6-X	154/154 (100%)	153 (99%)	1 (1%)	86	79
1	7-A	153/154 (99%)	153 (100%)	0	100	100
1	7-B	153/154 (99%)	153 (100%)	0	100	100
1	7-C	153/154 (99%)	153 (100%)	0	100	100
1	7-D	153/154 (99%)	153 (100%)	0	100	100
1	7-E	153/154 (99%)	153 (100%)	0	100	100
1	7-F	154/154 (100%)	154 (100%)	0	100	100
1	7-G	154/154 (100%)	154 (100%)	0	100	100
1	7-H	153/154 (99%)	153 (100%)	0	100	100
1	7-I	153/154 (99%)	153 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	7-J	154/154 (100%)	154 (100%)	0	100	100
1	7-K	153/154 (99%)	153 (100%)	0	100	100
1	7-L	154/154 (100%)	154 (100%)	0	100	100
1	7-M	153/154 (99%)	153 (100%)	0	100	100
1	7-N	153/154 (99%)	153 (100%)	0	100	100
1	7-O	153/154 (99%)	153 (100%)	0	100	100
1	7-P	153/154 (99%)	153 (100%)	0	100	100
1	7-Q	153/154 (99%)	153 (100%)	0	100	100
1	7-R	154/154 (100%)	154 (100%)	0	100	100
1	7-S	154/154 (100%)	154 (100%)	0	100	100
1	7-T	153/154 (99%)	153 (100%)	0	100	100
1	7-U	153/154 (99%)	153 (100%)	0	100	100
1	7-V	154/154 (100%)	154 (100%)	0	100	100
1	7-W	153/154 (99%)	153 (100%)	0	100	100
1	7-X	154/154 (100%)	154 (100%)	0	100	100
1	8-A	153/154 (99%)	153 (100%)	0	100	100
1	8-B	153/154 (99%)	153 (100%)	0	100	100
1	8-C	153/154 (99%)	153 (100%)	0	100	100
1	8-D	153/154 (99%)	153 (100%)	0	100	100
1	8-E	153/154 (99%)	153 (100%)	0	100	100
1	8-F	154/154 (100%)	154 (100%)	0	100	100
1	8-G	154/154 (100%)	154 (100%)	0	100	100
1	8-H	153/154 (99%)	153 (100%)	0	100	100
1	8-I	153/154 (99%)	153 (100%)	0	100	100
1	8-J	154/154 (100%)	154 (100%)	0	100	100
1	8-K	153/154 (99%)	153 (100%)	0	100	100
1	8-L	154/154 (100%)	154 (100%)	0	100	100
1	8-M	153/154 (99%)	153 (100%)	0	100	100
1	8-N	153/154 (99%)	153 (100%)	0	100	100
1	8-O	153/154 (99%)	153 (100%)	0	100	100
1	8-P	153/154 (99%)	153 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	8-Q	153/154 (99%)	153 (100%)	0	100	100
1	8-R	154/154 (100%)	154 (100%)	0	100	100
1	8-S	154/154 (100%)	154 (100%)	0	100	100
1	8-T	153/154 (99%)	153 (100%)	0	100	100
1	8-U	153/154 (99%)	153 (100%)	0	100	100
1	8-V	154/154 (100%)	154 (100%)	0	100	100
1	8-W	153/154 (99%)	153 (100%)	0	100	100
1	8-X	154/154 (100%)	154 (100%)	0	100	100
1	9-A	153/154 (99%)	153 (100%)	0	100	100
1	9-B	153/154 (99%)	153 (100%)	0	100	100
1	9-C	153/154 (99%)	153 (100%)	0	100	100
1	9-D	153/154 (99%)	153 (100%)	0	100	100
1	9-E	153/154 (99%)	153 (100%)	0	100	100
1	9-F	154/154 (100%)	154 (100%)	0	100	100
1	9-G	154/154 (100%)	154 (100%)	0	100	100
1	9-H	153/154 (99%)	153 (100%)	0	100	100
1	9-I	153/154 (99%)	153 (100%)	0	100	100
1	9-J	154/154 (100%)	154 (100%)	0	100	100
1	9-K	153/154 (99%)	153 (100%)	0	100	100
1	9-L	154/154 (100%)	154 (100%)	0	100	100
1	9-M	153/154 (99%)	153 (100%)	0	100	100
1	9-N	153/154 (99%)	153 (100%)	0	100	100
1	9-O	153/154 (99%)	153 (100%)	0	100	100
1	9-P	153/154 (99%)	153 (100%)	0	100	100
1	9-Q	153/154 (99%)	153 (100%)	0	100	100
1	9-R	154/154 (100%)	154 (100%)	0	100	100
1	9-S	154/154 (100%)	154 (100%)	0	100	100
1	9-T	153/154 (99%)	153 (100%)	0	100	100
1	9-U	153/154 (99%)	153 (100%)	0	100	100
1	9-V	154/154 (100%)	154 (100%)	0	100	100
1	9-W	153/154 (99%)	153 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	9-X	154/154 (100%)	154 (100%)	0	100	100
1	10-A	153/154 (99%)	153 (100%)	0	100	100
1	10-B	153/154 (99%)	153 (100%)	0	100	100
1	10-C	153/154 (99%)	153 (100%)	0	100	100
1	10-D	153/154 (99%)	153 (100%)	0	100	100
1	10-E	153/154 (99%)	153 (100%)	0	100	100
1	10-F	154/154 (100%)	154 (100%)	0	100	100
1	10-G	154/154 (100%)	154 (100%)	0	100	100
1	10-H	153/154 (99%)	153 (100%)	0	100	100
1	10-I	153/154 (99%)	153 (100%)	0	100	100
1	10-J	154/154 (100%)	154 (100%)	0	100	100
1	10-K	153/154 (99%)	153 (100%)	0	100	100
1	10-L	154/154 (100%)	154 (100%)	0	100	100
1	10-M	153/154 (99%)	153 (100%)	0	100	100
1	10-N	153/154 (99%)	153 (100%)	0	100	100
1	10-O	153/154 (99%)	153 (100%)	0	100	100
1	10-P	153/154 (99%)	153 (100%)	0	100	100
1	10-Q	153/154 (99%)	153 (100%)	0	100	100
1	10-R	154/154 (100%)	154 (100%)	0	100	100
1	10-S	154/154 (100%)	154 (100%)	0	100	100
1	10-T	153/154 (99%)	153 (100%)	0	100	100
1	10-U	153/154 (99%)	153 (100%)	0	100	100
1	10-V	154/154 (100%)	154 (100%)	0	100	100
1	10-W	153/154 (99%)	153 (100%)	0	100	100
1	10-X	154/154 (100%)	154 (100%)	0	100	100
All	All	36800/36960 (100%)	36711 (100%)	89 (0%)	93	91

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2-A	69	LEU
1	2-B	69	LEU
1	2-C	69	LEU

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Mol	Chain	Res	Type
1	2-D	69	LEU
1	2-E	69	LEU
1	2-F	69	LEU
1	2-G	69	LEU
1	2-H	69	LEU
1	2-I	69	LEU
1	2-J	69	LEU
1	2-K	69	LEU
1	2-L	69	LEU
1	2-M	69	LEU
1	2-N	69	LEU
1	2-O	69	LEU
1	2-P	69	LEU
1	2-Q	69	LEU
1	2-R	69	LEU
1	2-S	69	LEU
1	2-T	69	LEU
1	2-U	69	LEU
1	2-V	69	LEU
1	2-W	69	LEU
1	2-X	69	LEU
1	4-A	48	LEU
1	4-B	48	LEU
1	4-C	48	LEU
1	4-D	48	LEU
1	4-F	48	LEU
1	4-G	48	LEU
1	4-K	48	LEU
1	4-L	48	LEU
1	4-M	48	LEU
1	4-O	48	LEU
1	4-Q	48	LEU
1	4-R	48	LEU
1	4-S	48	LEU
1	4-T	48	LEU
1	4-U	48	LEU
1	4-W	48	LEU
1	4-X	48	LEU
1	5-A	48	LEU
1	5-B	48	LEU
1	5-C	48	LEU
1	5-D	48	LEU

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Mol	Chain	Res	Type
1	5-E	48	LEU
1	5-F	48	LEU
1	5-G	48	LEU
1	5-H	48	LEU
1	5-I	48	LEU
1	5-J	48	LEU
1	5-K	48	LEU
1	5-L	48	LEU
1	5-M	48	LEU
1	5-N	48	LEU
1	5-O	48	LEU
1	5-P	48	LEU
1	5-Q	48	LEU
1	5-R	48	LEU
1	5-S	48	LEU
1	5-T	48	LEU
1	5-U	48	LEU
1	5-V	48	LEU
1	5-W	48	LEU
1	5-X	48	LEU
1	6-A	162	GLU
1	6-B	162	GLU
1	6-C	162	GLU
1	6-D	162	GLU
1	6-E	162	GLU
1	6-F	162	GLU
1	6-G	162	GLU
1	6-H	162	GLU
1	6-I	162	GLU
1	6-J	162	GLU
1	6-K	162	GLU
1	6-L	162	GLU
1	6-M	162	GLU
1	6-N	162	GLU
1	6-O	162	GLU
1	6-P	162	GLU
1	6-Q	162	GLU
1	6-R	162	GLU
1	6-S	162	GLU
1	6-T	162	GLU
1	6-U	162	GLU
1	6-V	162	GLU

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Mol	Chain	Res	Type
1	6-W	162	GLU
1	6-X	162	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (383) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	60	HIS
1	1-A	98	ASN
1	1-B	60	HIS
1	1-B	98	ASN
1	1-C	60	HIS
1	1-C	98	ASN
1	1-D	60	HIS
1	1-D	98	ASN
1	1-E	60	HIS
1	1-E	98	ASN
1	1-F	60	HIS
1	1-F	98	ASN
1	1-G	60	HIS
1	1-G	98	ASN
1	1-H	60	HIS
1	1-H	98	ASN
1	1-I	60	HIS
1	1-I	98	ASN
1	1-J	60	HIS
1	1-J	98	ASN
1	1-K	60	HIS
1	1-K	98	ASN
1	1-L	60	HIS
1	1-L	98	ASN
1	1-M	60	HIS
1	1-M	98	ASN
1	1-N	60	HIS
1	1-N	98	ASN
1	1-O	60	HIS
1	1-O	98	ASN
1	1-P	60	HIS
1	1-P	98	ASN
1	1-Q	60	HIS
1	1-Q	98	ASN
1	1-R	60	HIS
1	1-R	98	ASN

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Mol	Chain	Res	Type
1	1-S	60	HIS
1	1-S	98	ASN
1	1-T	60	HIS
1	1-T	98	ASN
1	1-U	60	HIS
1	1-U	98	ASN
1	1-V	60	HIS
1	1-V	98	ASN
1	1-W	60	HIS
1	1-W	98	ASN
1	1-X	60	HIS
1	1-X	98	ASN
1	2-A	60	HIS
1	2-B	60	HIS
1	2-C	60	HIS
1	2-D	60	HIS
1	2-E	60	HIS
1	2-F	60	HIS
1	2-G	60	HIS
1	2-H	60	HIS
1	2-I	60	HIS
1	2-J	60	HIS
1	2-K	60	HIS
1	2-L	60	HIS
1	2-M	60	HIS
1	2-N	60	HIS
1	2-O	60	HIS
1	2-P	60	HIS
1	2-Q	60	HIS
1	2-R	60	HIS
1	2-S	60	HIS
1	2-T	60	HIS
1	2-U	60	HIS
1	2-V	60	HIS
1	2-W	60	HIS
1	2-X	60	HIS
1	3-A	11	ASN
1	3-A	60	HIS
1	3-B	60	HIS
1	3-C	60	HIS
1	3-D	60	HIS
1	3-E	60	HIS

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Mol	Chain	Res	Type
1	3-F	60	HIS
1	3-G	60	HIS
1	3-H	60	HIS
1	3-I	60	HIS
1	3-J	60	HIS
1	3-K	60	HIS
1	3-L	60	HIS
1	3-M	60	HIS
1	3-N	60	HIS
1	3-O	60	HIS
1	3-P	60	HIS
1	3-Q	60	HIS
1	3-R	60	HIS
1	3-S	60	HIS
1	3-S	177	HIS
1	3-T	60	HIS
1	3-U	60	HIS
1	3-V	60	HIS
1	3-W	60	HIS
1	3-X	60	HIS
1	4-A	60	HIS
1	4-A	98	ASN
1	4-B	60	HIS
1	4-B	98	ASN
1	4-C	60	HIS
1	4-C	98	ASN
1	4-D	60	HIS
1	4-D	98	ASN
1	4-E	60	HIS
1	4-E	98	ASN
1	4-F	60	HIS
1	4-F	98	ASN
1	4-G	60	HIS
1	4-G	98	ASN
1	4-H	60	HIS
1	4-H	98	ASN
1	4-I	60	HIS
1	4-I	98	ASN
1	4-J	60	HIS
1	4-J	98	ASN
1	4-K	98	ASN
1	4-L	60	HIS

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Mol	Chain	Res	Type
1	4-L	98	ASN
1	4-M	60	HIS
1	4-M	98	ASN
1	4-N	60	HIS
1	4-N	98	ASN
1	4-O	60	HIS
1	4-O	98	ASN
1	4-P	60	HIS
1	4-P	98	ASN
1	4-Q	60	HIS
1	4-Q	98	ASN
1	4-R	60	HIS
1	4-R	98	ASN
1	4-S	60	HIS
1	4-S	98	ASN
1	4-T	60	HIS
1	4-T	98	ASN
1	4-U	60	HIS
1	4-U	98	ASN
1	4-V	60	HIS
1	4-V	98	ASN
1	4-W	60	HIS
1	4-W	98	ASN
1	4-X	60	HIS
1	4-X	98	ASN
1	5-A	60	HIS
1	5-B	60	HIS
1	5-C	60	HIS
1	5-D	60	HIS
1	5-E	60	HIS
1	5-F	60	HIS
1	5-G	60	HIS
1	5-H	60	HIS
1	5-I	60	HIS
1	5-J	60	HIS
1	5-K	60	HIS
1	5-L	60	HIS
1	5-M	60	HIS
1	5-N	60	HIS
1	5-O	60	HIS
1	5-P	60	HIS
1	5-Q	60	HIS

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Mol	Chain	Res	Type
1	5-R	60	HIS
1	5-S	60	HIS
1	5-T	60	HIS
1	5-U	60	HIS
1	5-V	60	HIS
1	5-W	60	HIS
1	5-X	60	HIS
1	6-A	60	HIS
1	6-A	151	HIS
1	6-B	60	HIS
1	6-B	151	HIS
1	6-C	60	HIS
1	6-C	151	HIS
1	6-D	60	HIS
1	6-D	151	HIS
1	6-E	60	HIS
1	6-E	151	HIS
1	6-F	60	HIS
1	6-F	151	HIS
1	6-G	60	HIS
1	6-G	151	HIS
1	6-H	60	HIS
1	6-H	151	HIS
1	6-I	60	HIS
1	6-I	151	HIS
1	6-J	60	HIS
1	6-J	151	HIS
1	6-K	60	HIS
1	6-K	151	HIS
1	6-L	60	HIS
1	6-L	151	HIS
1	6-M	60	HIS
1	6-M	151	HIS
1	6-N	60	HIS
1	6-N	151	HIS
1	6-O	60	HIS
1	6-O	151	HIS
1	6-P	60	HIS
1	6-P	151	HIS
1	6-Q	60	HIS
1	6-Q	151	HIS
1	6-R	60	HIS

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Mol	Chain	Res	Type
1	6-R	151	HIS
1	6-S	60	HIS
1	6-S	151	HIS
1	6-T	60	HIS
1	6-T	151	HIS
1	6-U	60	HIS
1	6-U	151	HIS
1	6-V	60	HIS
1	6-V	151	HIS
1	6-W	60	HIS
1	6-W	151	HIS
1	6-X	60	HIS
1	6-X	151	HIS
1	7-A	60	HIS
1	7-A	98	ASN
1	7-B	60	HIS
1	7-B	98	ASN
1	7-C	60	HIS
1	7-C	98	ASN
1	7-D	60	HIS
1	7-D	98	ASN
1	7-E	60	HIS
1	7-E	98	ASN
1	7-F	60	HIS
1	7-F	98	ASN
1	7-G	60	HIS
1	7-G	98	ASN
1	7-H	60	HIS
1	7-H	98	ASN
1	7-I	60	HIS
1	7-I	98	ASN
1	7-J	60	HIS
1	7-J	98	ASN
1	7-K	60	HIS
1	7-K	98	ASN
1	7-L	60	HIS
1	7-L	98	ASN
1	7-M	60	HIS
1	7-M	98	ASN
1	7-N	60	HIS
1	7-N	98	ASN
1	7-O	60	HIS

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Mol	Chain	Res	Type
1	7-O	98	ASN
1	7-P	60	HIS
1	7-P	98	ASN
1	7-Q	60	HIS
1	7-Q	98	ASN
1	7-R	60	HIS
1	7-R	98	ASN
1	7-S	60	HIS
1	7-S	98	ASN
1	7-T	60	HIS
1	7-T	98	ASN
1	7-U	60	HIS
1	7-U	98	ASN
1	7-V	60	HIS
1	7-V	98	ASN
1	7-W	60	HIS
1	7-W	98	ASN
1	7-X	60	HIS
1	7-X	98	ASN
1	8-A	60	HIS
1	8-A	98	ASN
1	8-B	60	HIS
1	8-B	98	ASN
1	8-C	60	HIS
1	8-C	98	ASN
1	8-D	60	HIS
1	8-D	98	ASN
1	8-E	60	HIS
1	8-E	98	ASN
1	8-F	60	HIS
1	8-F	98	ASN
1	8-G	60	HIS
1	8-G	98	ASN
1	8-H	60	HIS
1	8-H	98	ASN
1	8-I	60	HIS
1	8-I	98	ASN
1	8-J	60	HIS
1	8-J	98	ASN
1	8-K	60	HIS
1	8-K	98	ASN
1	8-L	60	HIS

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Mol	Chain	Res	Type
1	8-L	98	ASN
1	8-M	60	HIS
1	8-M	98	ASN
1	8-N	60	HIS
1	8-O	60	HIS
1	8-O	98	ASN
1	8-P	60	HIS
1	8-P	98	ASN
1	8-Q	60	HIS
1	8-R	60	HIS
1	8-R	98	ASN
1	8-S	60	HIS
1	8-S	98	ASN
1	8-T	60	HIS
1	8-U	60	HIS
1	8-U	98	ASN
1	8-V	60	HIS
1	8-V	98	ASN
1	8-W	60	HIS
1	8-W	98	ASN
1	8-X	60	HIS
1	8-X	98	ASN
1	9-A	60	HIS
1	9-A	98	ASN
1	9-B	60	HIS
1	9-B	98	ASN
1	9-C	60	HIS
1	9-C	98	ASN
1	9-D	98	ASN
1	9-E	60	HIS
1	9-E	98	ASN
1	9-F	60	HIS
1	9-F	98	ASN
1	9-G	60	HIS
1	9-G	98	ASN
1	9-H	60	HIS
1	9-H	98	ASN
1	9-I	98	ASN
1	9-J	60	HIS
1	9-J	98	ASN
1	9-K	60	HIS
1	9-K	98	ASN

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Mol	Chain	Res	Type
1	9-L	60	HIS
1	9-L	98	ASN
1	9-L	177	HIS
1	9-M	60	HIS
1	9-M	98	ASN
1	9-N	60	HIS
1	9-N	98	ASN
1	9-O	60	HIS
1	9-O	98	ASN
1	9-P	60	HIS
1	9-P	98	ASN
1	9-Q	60	HIS
1	9-Q	98	ASN
1	9-R	60	HIS
1	9-R	98	ASN
1	9-S	60	HIS
1	9-S	98	ASN
1	9-T	60	HIS
1	9-T	98	ASN
1	9-U	60	HIS
1	9-U	98	ASN
1	9-V	60	HIS
1	9-V	98	ASN
1	9-W	60	HIS
1	9-W	98	ASN
1	9-X	60	HIS
1	9-X	98	ASN
1	10-A	11	ASN
1	10-A	60	HIS
1	10-B	60	HIS
1	10-C	60	HIS
1	10-D	60	HIS
1	10-E	60	HIS
1	10-F	60	HIS
1	10-G	60	HIS
1	10-H	60	HIS
1	10-I	60	HIS
1	10-J	60	HIS
1	10-K	60	HIS
1	10-L	60	HIS
1	10-M	60	HIS
1	10-N	60	HIS

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Mol	Chain	Res	Type
1	10-O	60	HIS
1	10-P	60	HIS
1	10-Q	60	HIS
1	10-R	60	HIS
1	10-S	60	HIS
1	10-S	177	HIS
1	10-T	60	HIS
1	10-U	60	HIS
1	10-V	60	HIS
1	10-W	60	HIS
1	10-X	60	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

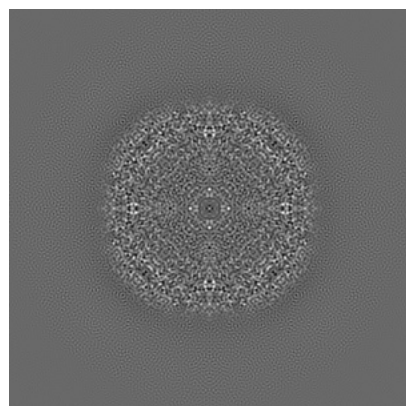
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21024. These allow visual inspection of the internal detail of the map and identification of artifacts.

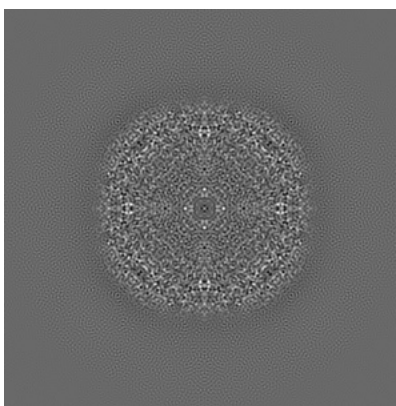
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

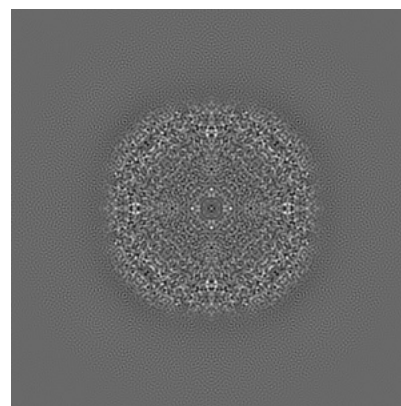
6.1.1 Primary map



X

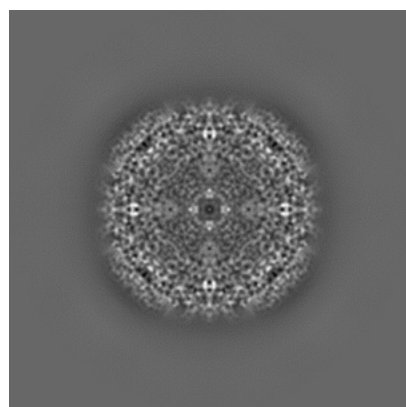


Y

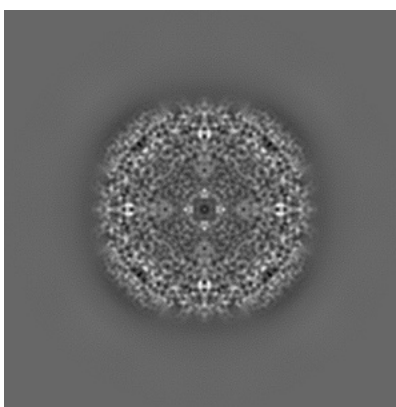


Z

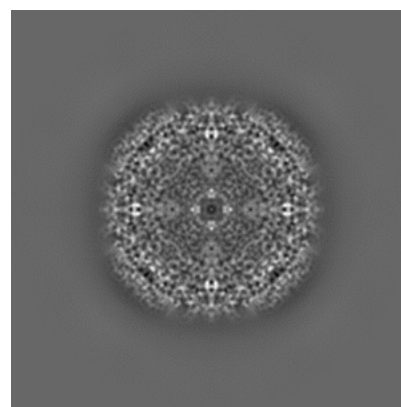
6.1.2 Raw map



X



Y

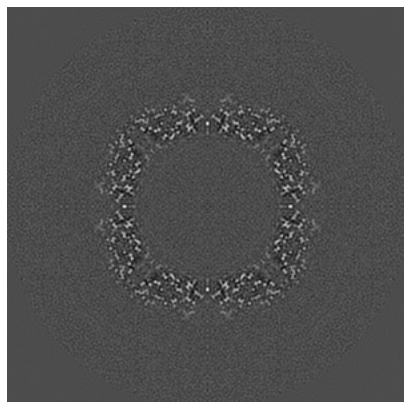


Z

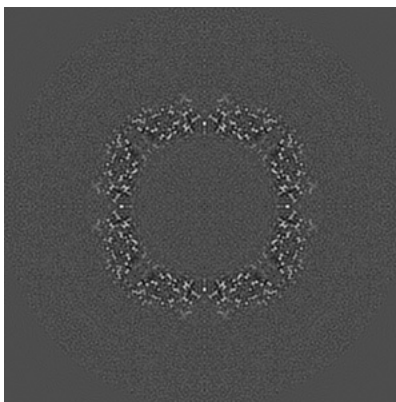
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

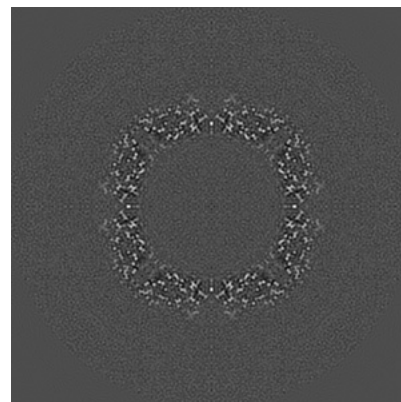
6.2.1 Primary map



X Index: 192

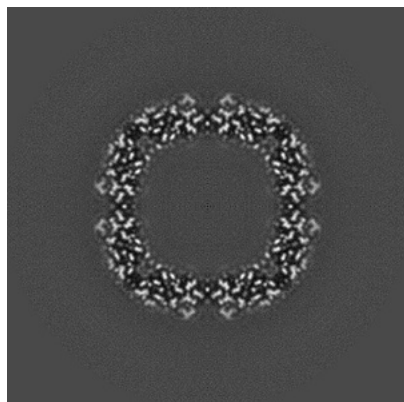


Y Index: 192

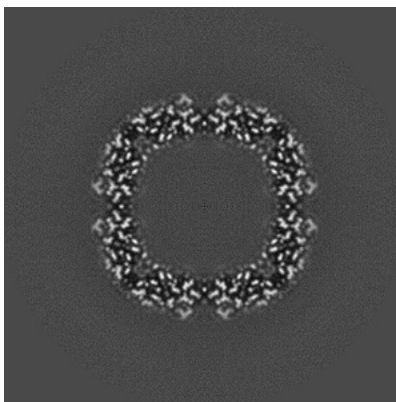


Z Index: 192

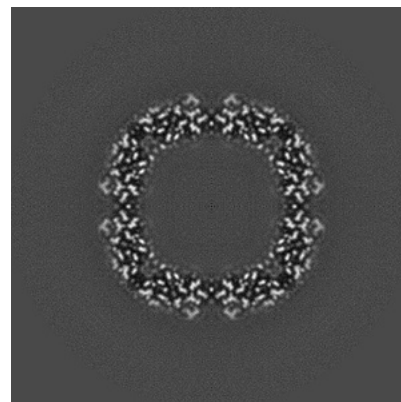
6.2.2 Raw map



X Index: 192



Y Index: 192

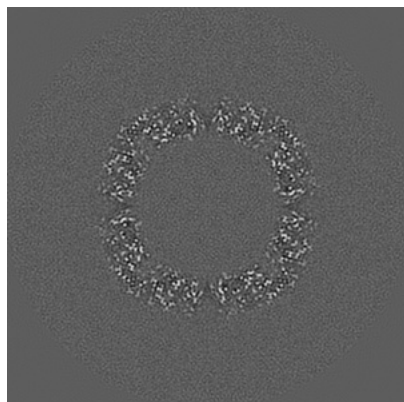


Z Index: 192

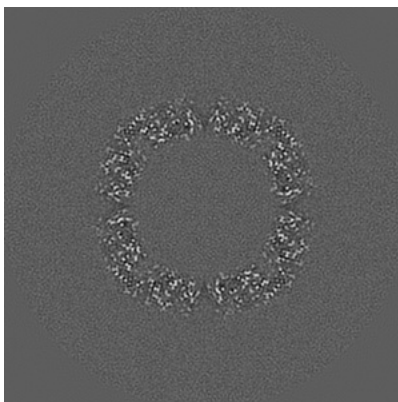
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

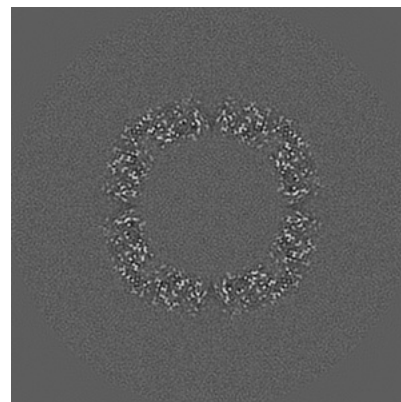
6.3.1 Primary map



X Index: 194

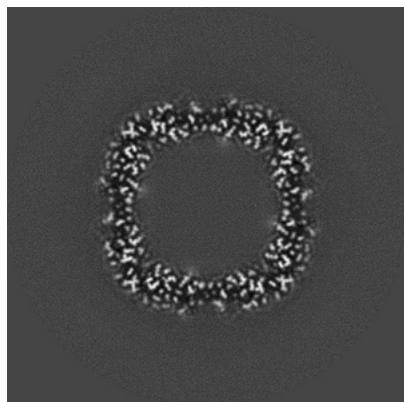


Y Index: 194

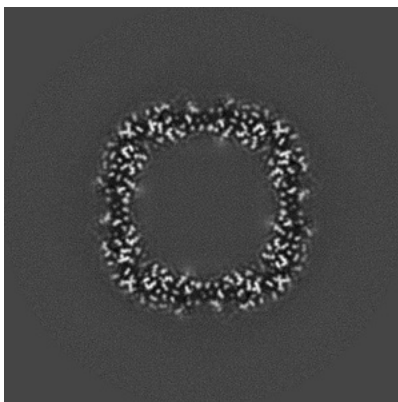


Z Index: 194

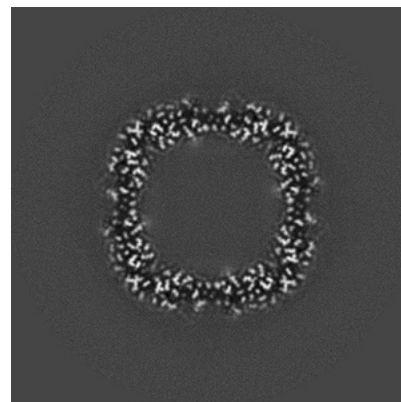
6.3.2 Raw map



X Index: 188



Y Index: 188

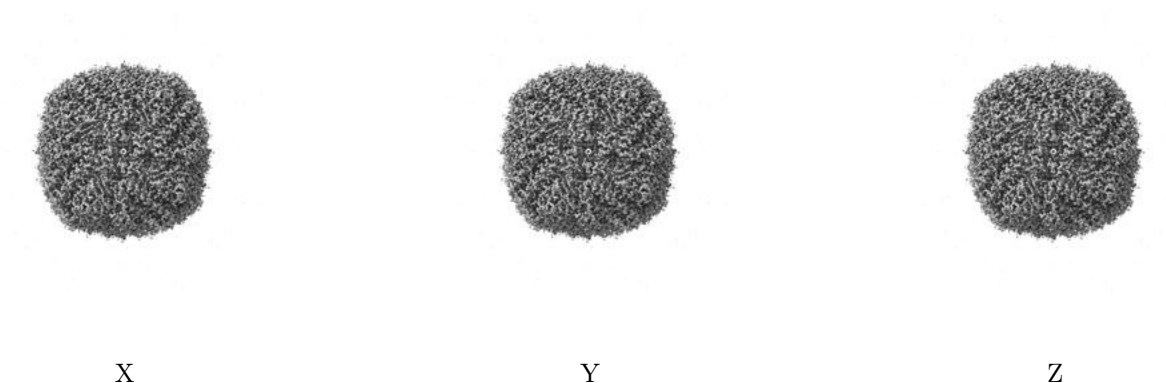


Z Index: 196

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

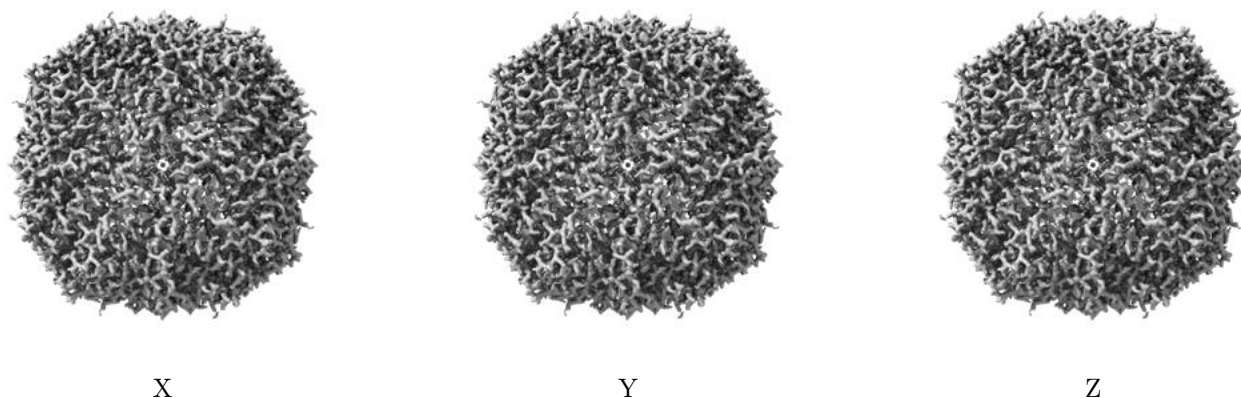
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.039. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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.

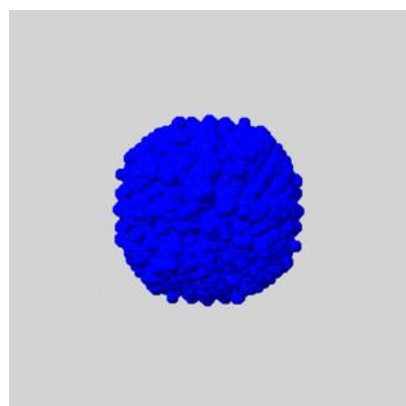
6.5 Mask visualisation [i](#)

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

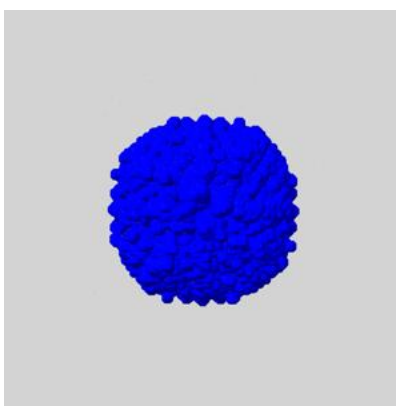
A mask typically either:

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

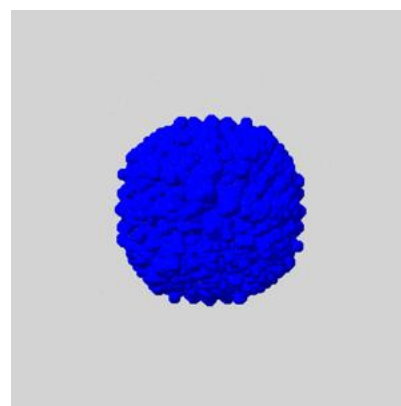
6.5.1 emd_21024_msk_1.map [i](#)



X



Y

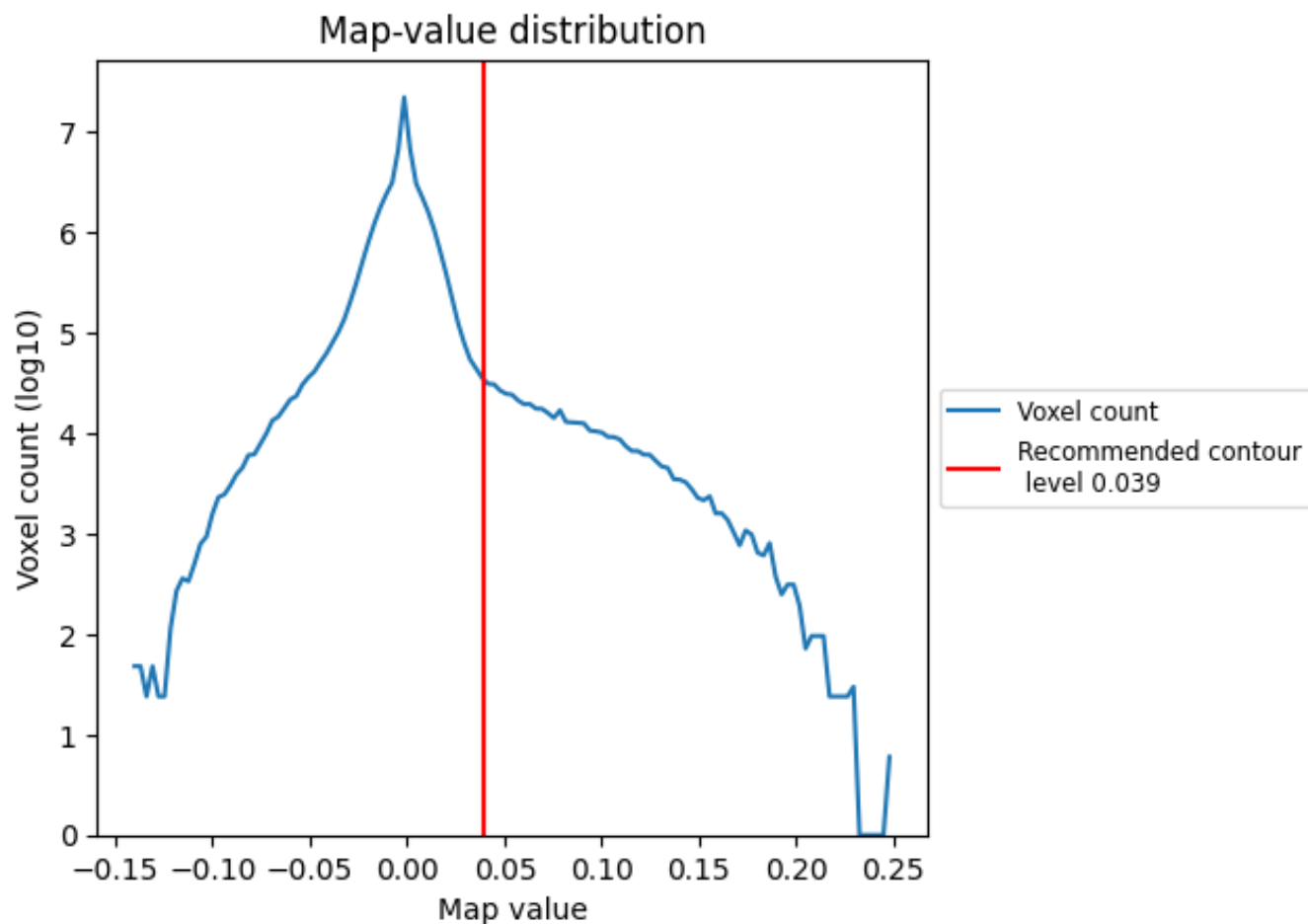


Z

7 Map analysis [i](#)

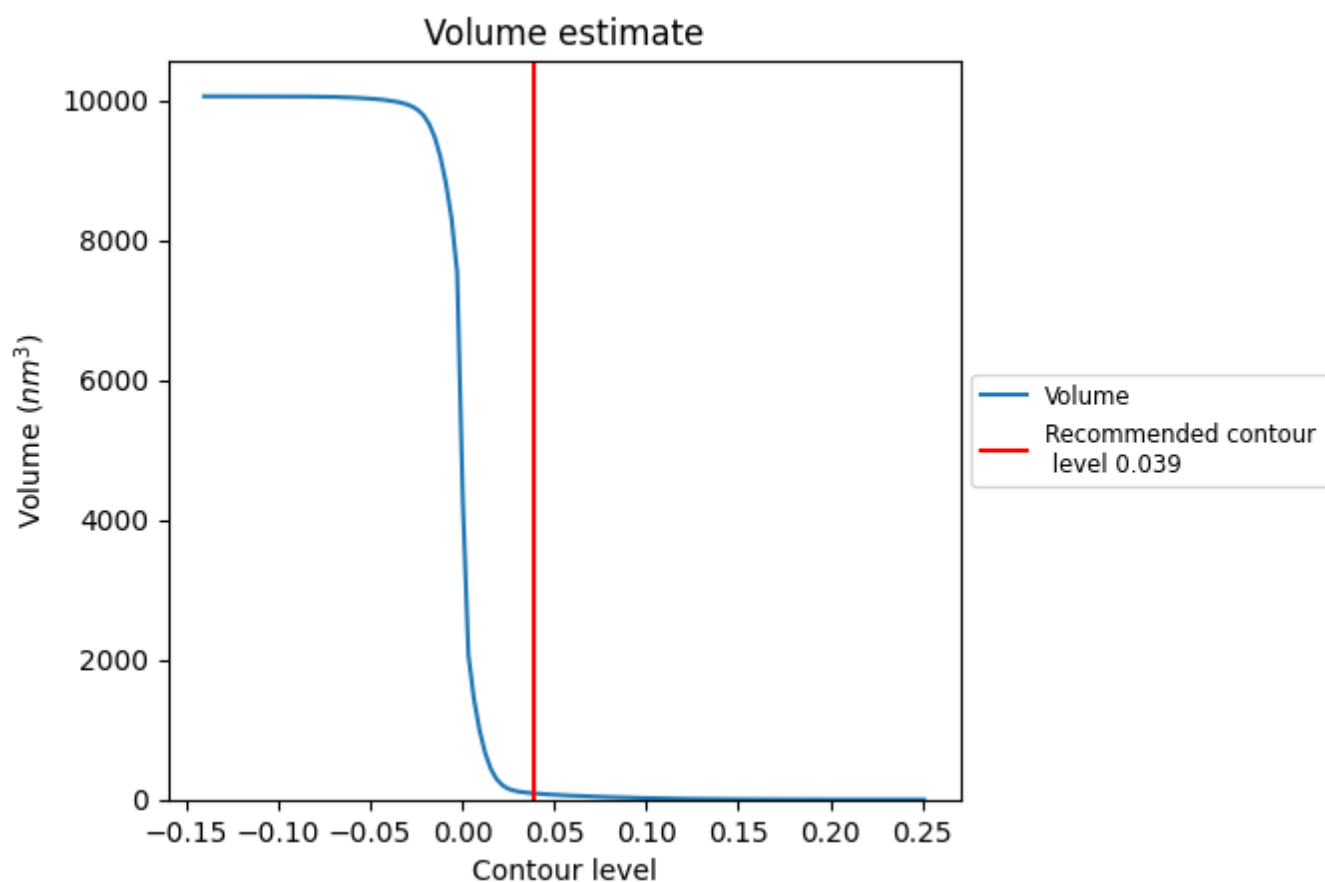
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

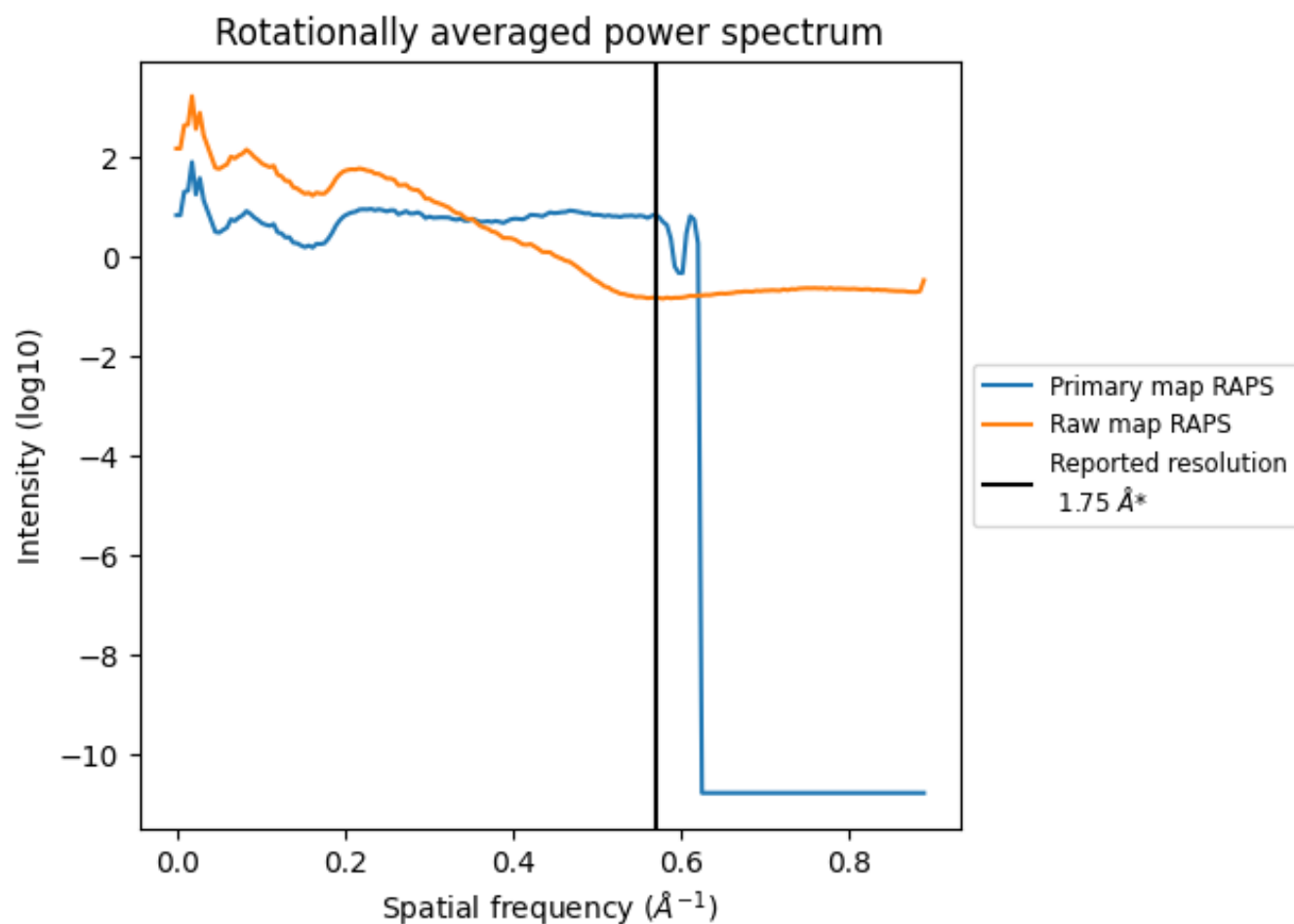
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 89 nm^3 ; this corresponds to an approximate mass of 80 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

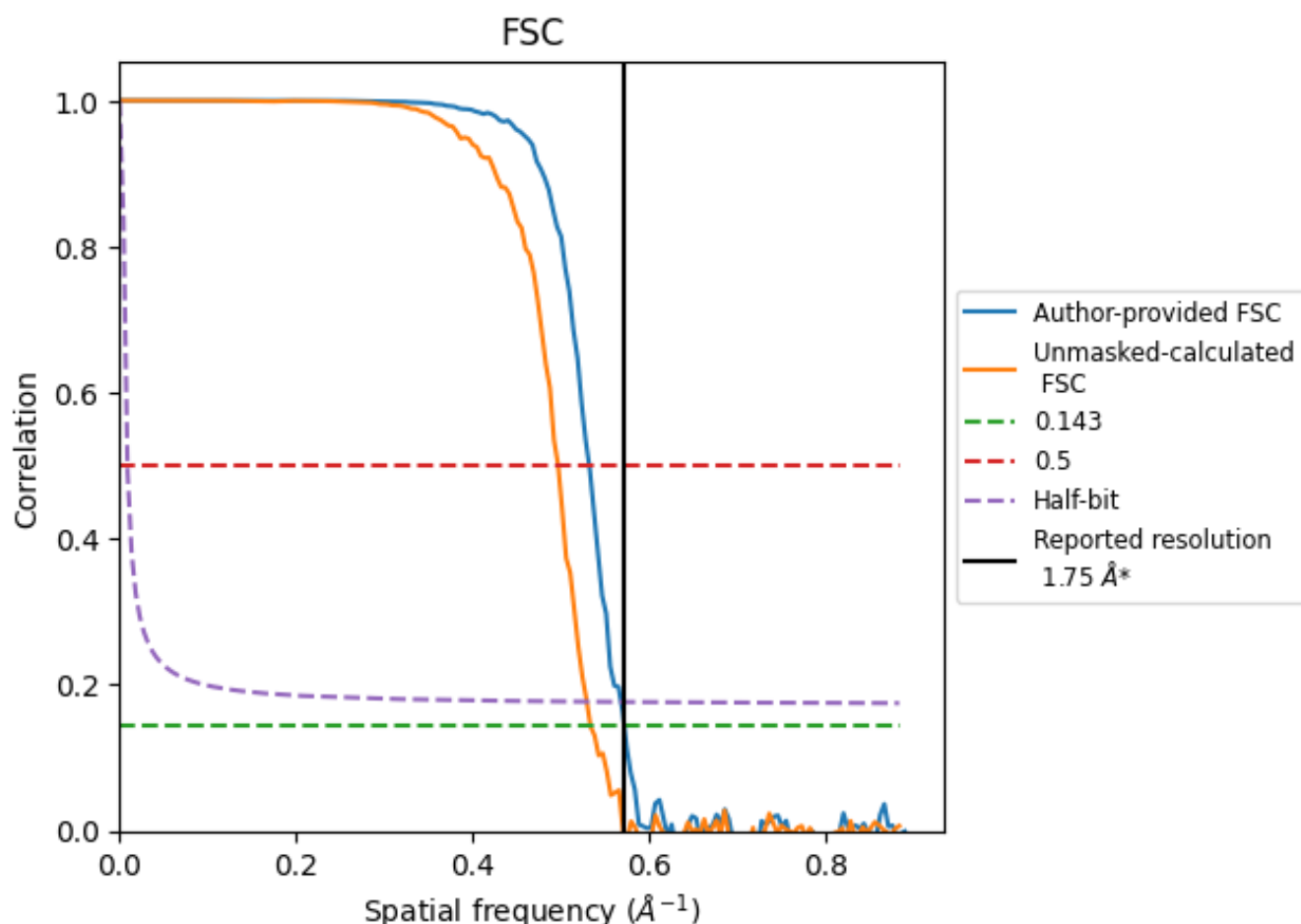


*Reported resolution corresponds to spatial frequency of 0.571 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.571 Å⁻¹

8.2 Resolution estimates [i](#)

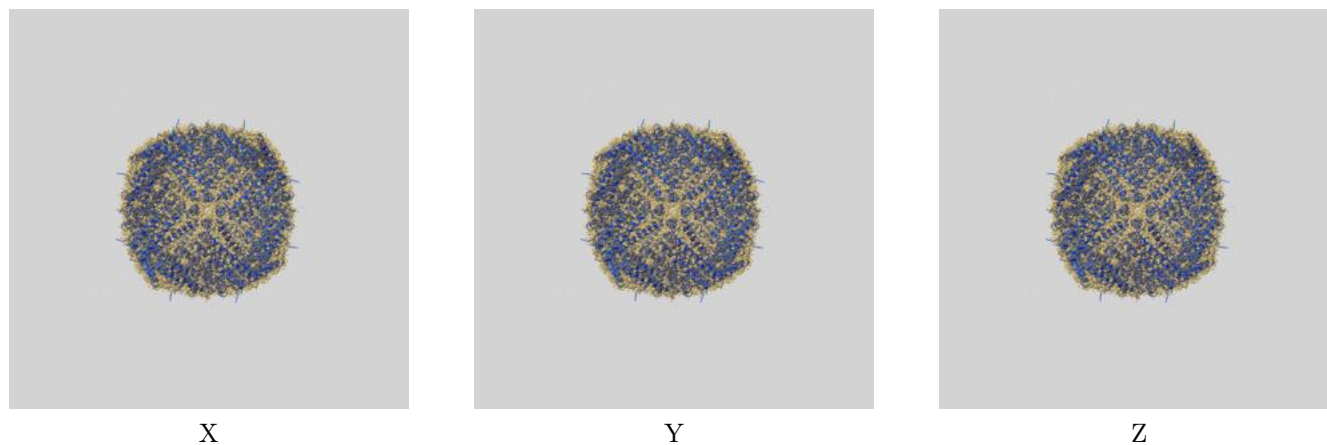
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.75	-	-
Author-provided FSC curve	1.75	1.88	1.76
Unmasked-calculated*	1.87	2.01	1.89

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

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21024 and PDB model 6V21. Per-residue inclusion information can be found in [section 3](#) on [page 37](#).

9.1 Map-model overlay [i](#)

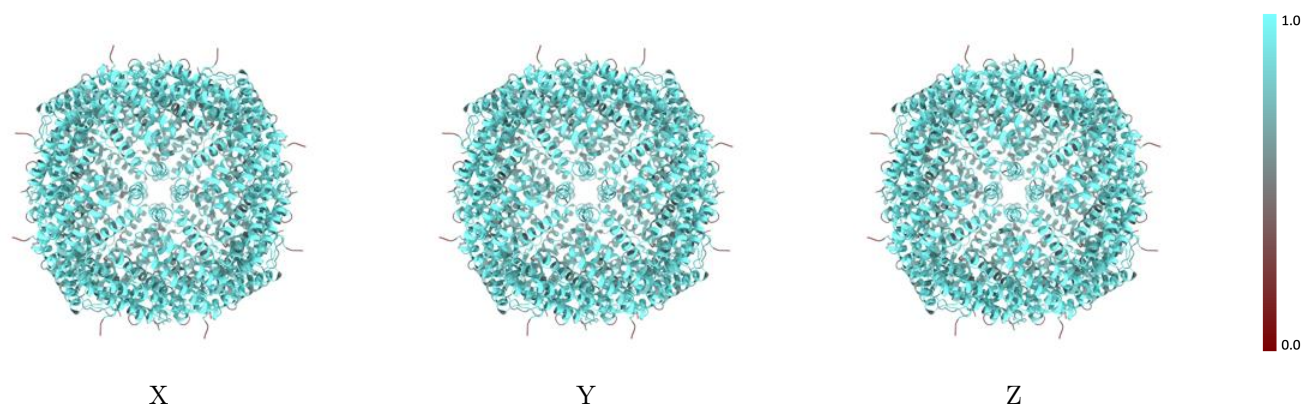


The images above show the 3D surface view of the map at the recommended contour level 0.039 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

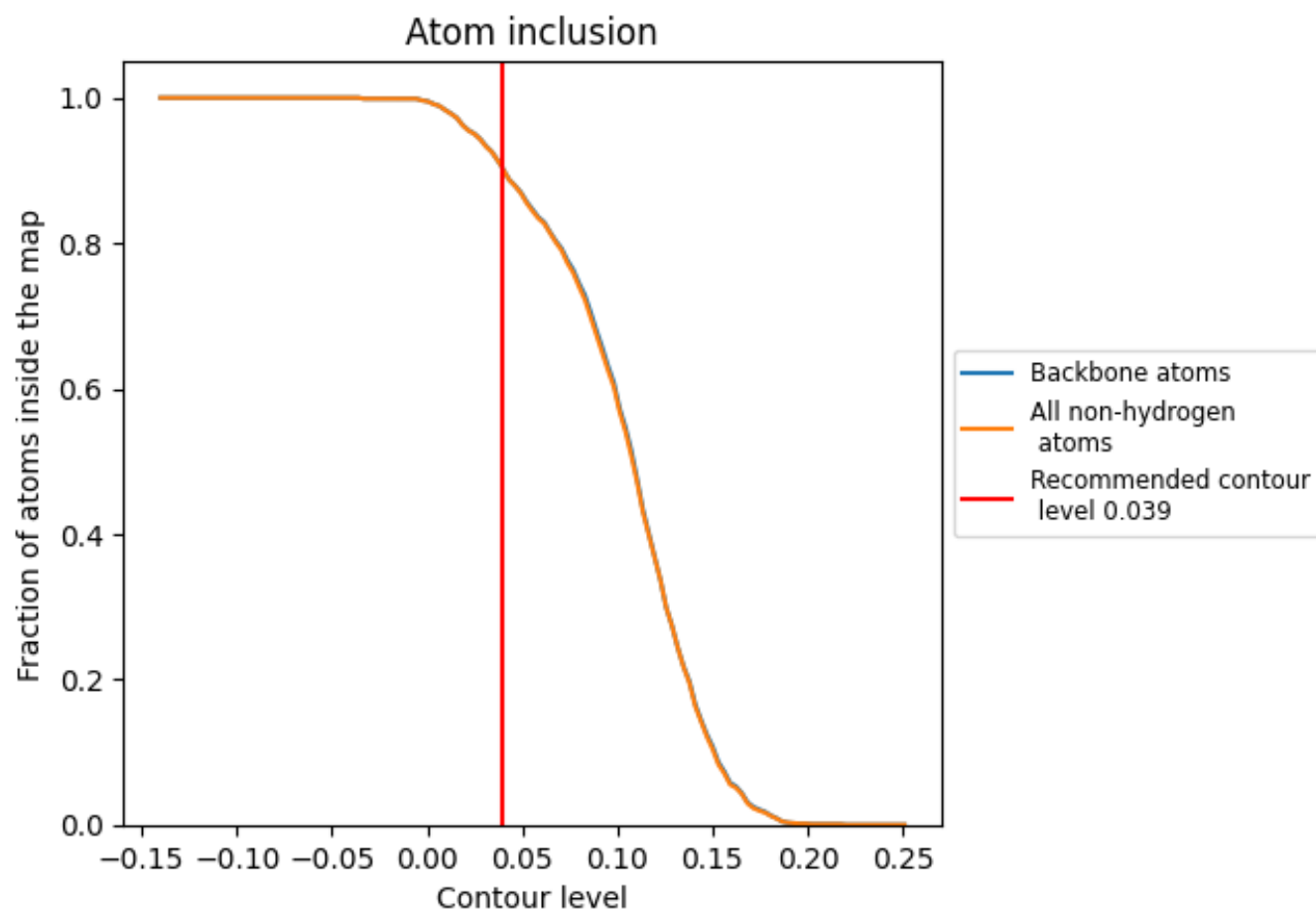
This section was not generated.

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.039).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 91% 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 (0.039) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	<div></div> 0.9064
A	<div></div> 0.9107
B	<div></div> 0.9114
C	<div></div> 0.9107
D	<div></div> 0.9122
E	<div></div> 0.9107
F	<div></div> 0.9049
G	<div></div> 0.9049
H	<div></div> 0.9114
I	<div></div> 0.9107
J	<div></div> 0.9056
K	<div></div> 0.9107
L	<div></div> 0.9049
M	<div></div> 0.9107
N	<div></div> 0.9107
O	<div></div> 0.9114
P	<div></div> 0.9114
Q	<div></div> 0.9107
R	<div></div> 0.9049
S	<div></div> 0.9049
T	<div></div> 0.9114
U	<div></div> 0.9107
V	<div></div> 0.9049
W	<div></div> 0.9107
X	<div></div> 0.9049

