



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:32 PM UTC

PDB ID : 4R7Z / pdb_00004r7z
Title : PfMCM-AAA double-octamer
Authors : Miller, J.M.; Arachea, B.T.; Epling, L.B.; Enemark, E.J.
Deposited on : 2014-08-28
Resolution : 3.80 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

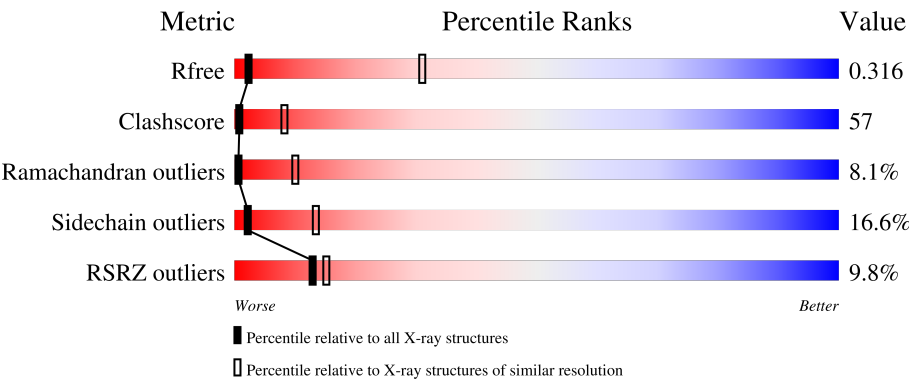
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	338	11% 29% 46% 18% • 7%
1	B	338	4% 30% 46% 17% • 7%
1	C	338	4% 29% 47% 17% • 7%
1	D	338	6% 29% 47% 17% • 7%
1	E	338	8% 28% 46% 18% • 7%

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Mol	Chain	Length	Quality of chain
1	F	338	
1	G	338	
1	H	338	
1	I	338	
1	J	338	
1	K	338	
1	L	338	
1	M	338	
1	N	338	
1	O	338	
1	P	338	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MG	D	1002	-	-	-	X
3	MG	I	1002	-	-	-	X
3	MG	L	1002	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 39296 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Cell division control protein 21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	0	0
			2428	1533	440	448	7			
1	B	316	Total	C	N	O	S	0	0	0
			2428	1533	440	448	7			
1	C	316	Total	C	N	O	S	0	0	0
			2428	1533	440	448	7			
1	D	316	Total	C	N	O	S	0	0	0
			2428	1533	440	448	7			
1	E	316	Total	C	N	O	S	0	0	0
			2428	1533	440	448	7			
1	F	316	Total	C	N	O	S	0	0	0
			2428	1533	440	448	7			
1	G	316	Total	C	N	O	S	0	0	0
			2428	1533	440	448	7			
1	H	316	Total	C	N	O	S	0	0	0
			2428	1533	440	448	7			
1	I	316	Total	C	N	O	S	0	0	0
			2428	1533	440	448	7			
1	J	316	Total	C	N	O	S	0	0	0
			2428	1533	440	448	7			
1	K	316	Total	C	N	O	S	0	0	0
			2428	1533	440	448	7			
1	L	316	Total	C	N	O	S	0	0	0
			2428	1533	440	448	7			
1	M	316	Total	C	N	O	S	0	0	0
			2428	1533	440	448	7			
1	N	316	Total	C	N	O	S	0	0	0
			2428	1533	440	448	7			
1	O	316	Total	C	N	O	S	0	0	0
			2428	1533	440	448	7			
1	P	316	Total	C	N	O	S	0	0	0
			2428	1533	440	448	7			

There are 528 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	353	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	354	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	355	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	356	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	357	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	358	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	359	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	360	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	361	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	729	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	730	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	731	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	732	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	733	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	734	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	735	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	736	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	737	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	738	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	739	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	740	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	741	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	742	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	743	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	744	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	745	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	746	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	747	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	748	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	749	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	750	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	751	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	752	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	353	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	354	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	355	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	356	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	357	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	358	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	359	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	360	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	361	UNK	-	SEE REMARK 999	UNP Q8U3I4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	729	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	730	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	731	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	732	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	733	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	734	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	735	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	736	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	737	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	738	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	739	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	740	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	741	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	742	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	743	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	744	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	745	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	746	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	747	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	748	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	749	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	750	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	751	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	752	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	353	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	354	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	355	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	356	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	357	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	358	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	359	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	360	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	361	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	729	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	730	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	731	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	732	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	733	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	734	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	735	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	736	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	737	UNK	-	SEE REMARK 999	UNP Q8U3I4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	738	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	739	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	740	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	741	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	742	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	743	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	744	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	745	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	746	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	747	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	748	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	749	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	750	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	751	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	752	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	353	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	354	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	355	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	356	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	357	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	358	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	359	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	360	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	361	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	729	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	730	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	731	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	732	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	733	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	734	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	735	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	736	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	737	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	738	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	739	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	740	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	741	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	742	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	743	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	744	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	745	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	746	UNK	-	SEE REMARK 999	UNP Q8U3I4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	747	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	748	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	749	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	750	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	751	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	752	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	353	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	354	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	355	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	356	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	357	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	358	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	359	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	360	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	361	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	729	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	730	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	731	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	732	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	733	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	734	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	735	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	736	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	737	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	738	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	739	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	740	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	741	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	742	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	743	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	744	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	745	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	746	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	747	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	748	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	749	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	750	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	751	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	752	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	353	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	354	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	355	UNK	-	SEE REMARK 999	UNP Q8U3I4

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Chain	Residue	Modelled	Actual	Comment	Reference
F	356	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	357	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	358	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	359	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	360	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	361	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	729	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	730	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	731	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	732	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	733	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	734	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	735	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	736	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	737	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	738	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	739	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	740	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	741	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	742	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	743	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	744	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	745	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	746	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	747	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	748	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	749	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	750	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	751	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	752	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	353	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	354	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	355	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	356	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	357	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	358	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	359	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	360	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	361	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	729	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	730	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	731	UNK	-	SEE REMARK 999	UNP Q8U3I4

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Chain	Residue	Modelled	Actual	Comment	Reference
G	732	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	733	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	734	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	735	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	736	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	737	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	738	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	739	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	740	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	741	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	742	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	743	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	744	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	745	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	746	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	747	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	748	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	749	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	750	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	751	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	752	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	353	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	354	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	355	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	356	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	357	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	358	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	359	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	360	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	361	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	729	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	730	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	731	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	732	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	733	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	734	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	735	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	736	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	737	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	738	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	739	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	740	UNK	-	SEE REMARK 999	UNP Q8U3I4

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Chain	Residue	Modelled	Actual	Comment	Reference
H	741	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	742	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	743	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	744	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	745	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	746	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	747	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	748	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	749	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	750	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	751	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	752	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	353	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	354	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	355	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	356	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	357	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	358	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	359	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	360	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	361	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	729	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	730	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	731	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	732	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	733	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	734	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	735	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	736	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	737	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	738	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	739	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	740	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	741	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	742	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	743	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	744	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	745	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	746	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	747	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	748	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	749	UNK	-	SEE REMARK 999	UNP Q8U3I4

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Chain	Residue	Modelled	Actual	Comment	Reference
I	750	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	751	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	752	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	353	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	354	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	355	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	356	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	357	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	358	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	359	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	360	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	361	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	729	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	730	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	731	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	732	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	733	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	734	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	735	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	736	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	737	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	738	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	739	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	740	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	741	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	742	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	743	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	744	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	745	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	746	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	747	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	748	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	749	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	750	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	751	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	752	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	353	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	354	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	355	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	356	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	357	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	358	UNK	-	SEE REMARK 999	UNP Q8U3I4

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Chain	Residue	Modelled	Actual	Comment	Reference
K	359	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	360	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	361	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	729	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	730	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	731	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	732	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	733	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	734	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	735	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	736	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	737	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	738	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	739	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	740	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	741	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	742	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	743	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	744	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	745	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	746	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	747	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	748	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	749	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	750	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	751	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	752	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	353	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	354	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	355	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	356	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	357	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	358	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	359	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	360	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	361	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	729	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	730	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	731	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	732	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	733	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	734	UNK	-	SEE REMARK 999	UNP Q8U3I4

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Chain	Residue	Modelled	Actual	Comment	Reference
L	735	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	736	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	737	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	738	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	739	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	740	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	741	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	742	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	743	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	744	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	745	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	746	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	747	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	748	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	749	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	750	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	751	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	752	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	353	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	354	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	355	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	356	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	357	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	358	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	359	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	360	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	361	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	729	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	730	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	731	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	732	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	733	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	734	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	735	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	736	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	737	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	738	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	739	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	740	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	741	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	742	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	743	UNK	-	SEE REMARK 999	UNP Q8U3I4

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Chain	Residue	Modelled	Actual	Comment	Reference
M	744	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	745	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	746	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	747	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	748	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	749	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	750	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	751	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	752	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	353	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	354	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	355	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	356	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	357	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	358	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	359	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	360	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	361	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	729	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	730	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	731	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	732	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	733	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	734	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	735	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	736	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	737	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	738	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	739	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	740	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	741	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	742	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	743	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	744	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	745	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	746	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	747	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	748	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	749	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	750	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	751	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	752	UNK	-	SEE REMARK 999	UNP Q8U3I4

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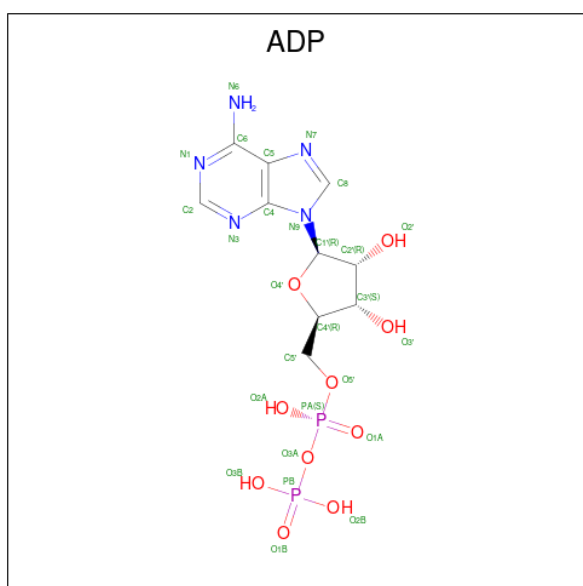
Chain	Residue	Modelled	Actual	Comment	Reference
O	353	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	354	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	355	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	356	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	357	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	358	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	359	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	360	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	361	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	729	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	730	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	731	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	732	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	733	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	734	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	735	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	736	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	737	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	738	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	739	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	740	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	741	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	742	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	743	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	744	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	745	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	746	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	747	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	748	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	749	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	750	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	751	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	752	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	353	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	354	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	355	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	356	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	357	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	358	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	359	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	360	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	361	UNK	-	SEE REMARK 999	UNP Q8U3I4

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Chain	Residue	Modelled	Actual	Comment	Reference
P	729	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	730	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	731	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	732	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	733	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	734	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	735	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	736	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	737	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	738	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	739	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	740	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	741	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	742	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	743	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	744	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	745	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	746	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	747	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	748	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	749	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	750	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	751	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	752	UNK	-	SEE REMARK 999	UNP Q8U3I4

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	M	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	N	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	O	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	P	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

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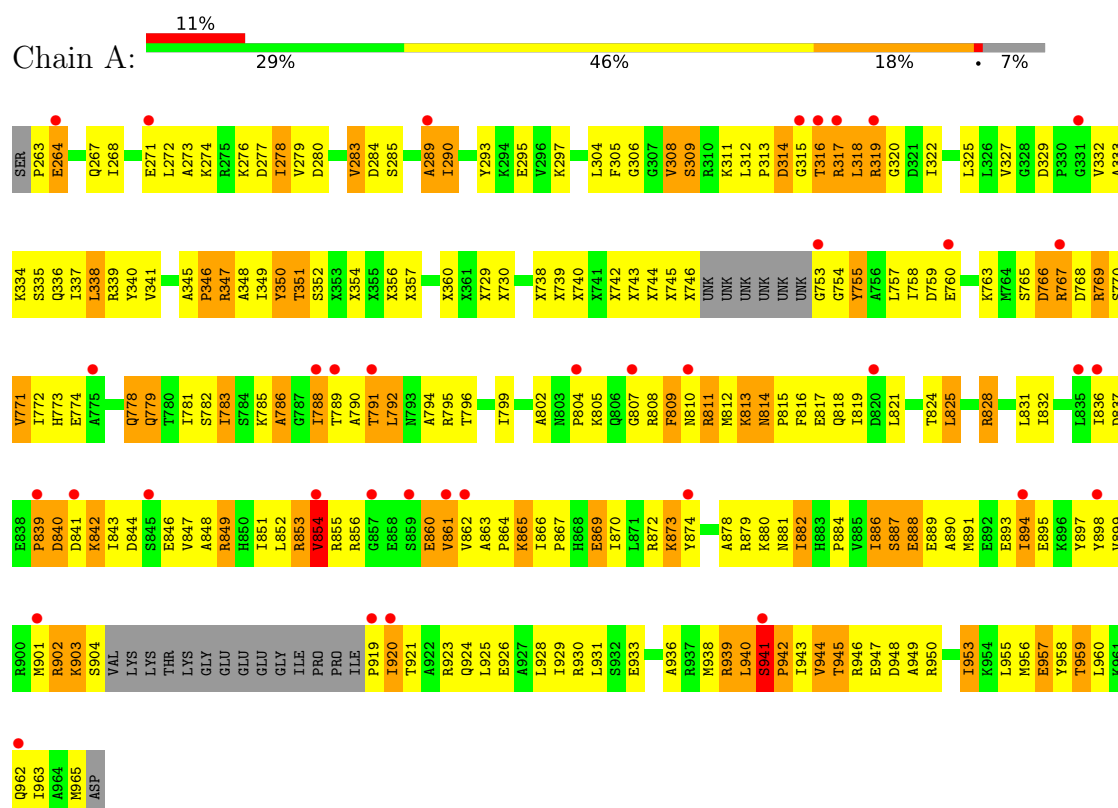
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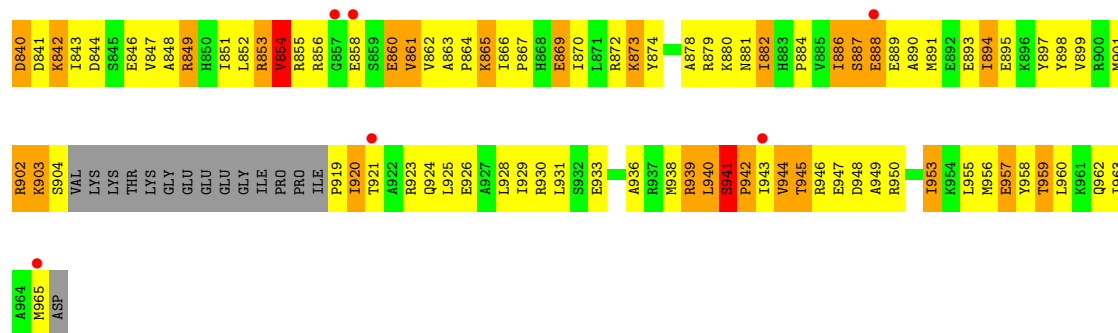
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total 1	Mg 1	0	0
3	F	1	Total 1	Mg 1	0	0
3	G	1	Total 1	Mg 1	0	0
3	H	1	Total 1	Mg 1	0	0
3	I	1	Total 1	Mg 1	0	0
3	J	1	Total 1	Mg 1	0	0
3	K	1	Total 1	Mg 1	0	0
3	L	1	Total 1	Mg 1	0	0
3	M	1	Total 1	Mg 1	0	0
3	N	1	Total 1	Mg 1	0	0
3	O	1	Total 1	Mg 1	0	0
3	P	1	Total 1	Mg 1	0	0

3 Residue-property plots

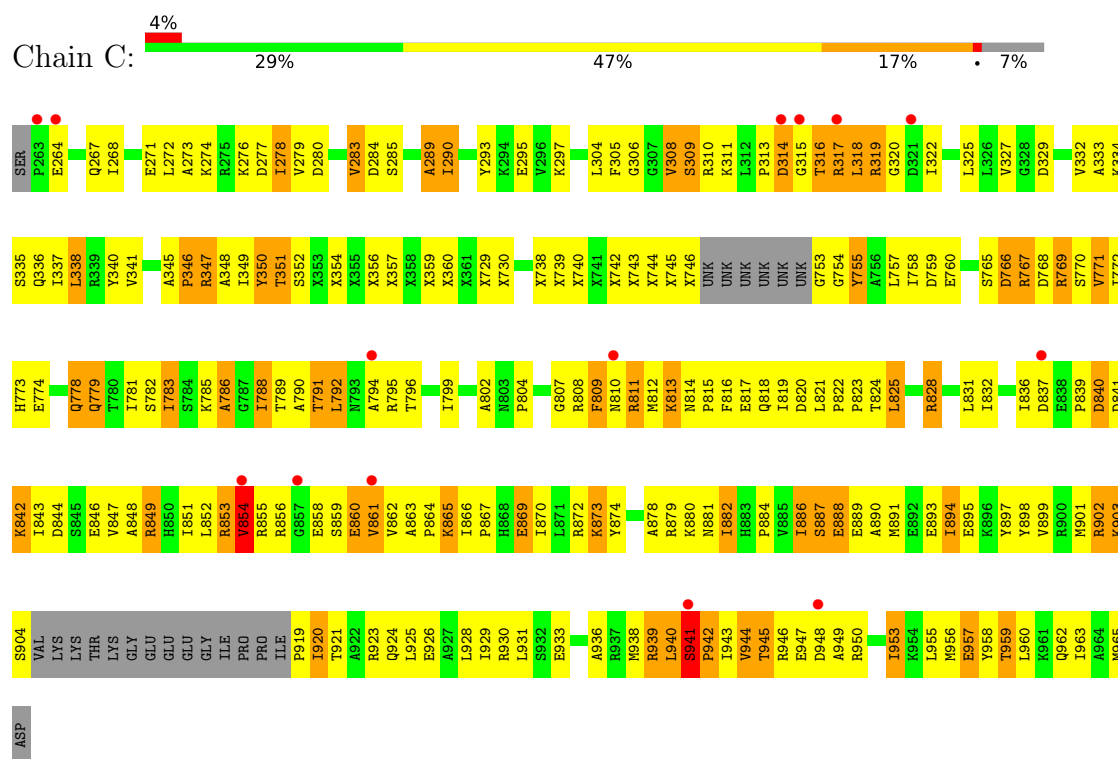
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: Cell division control protein 21

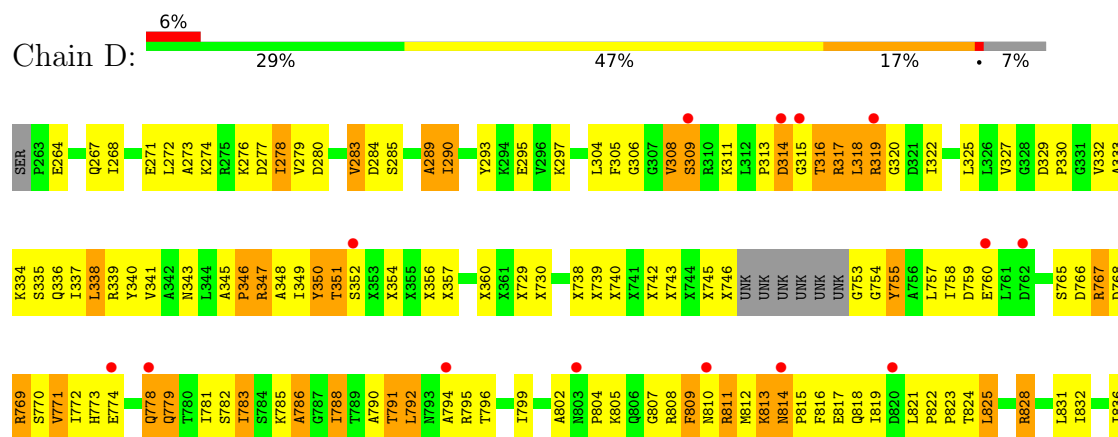


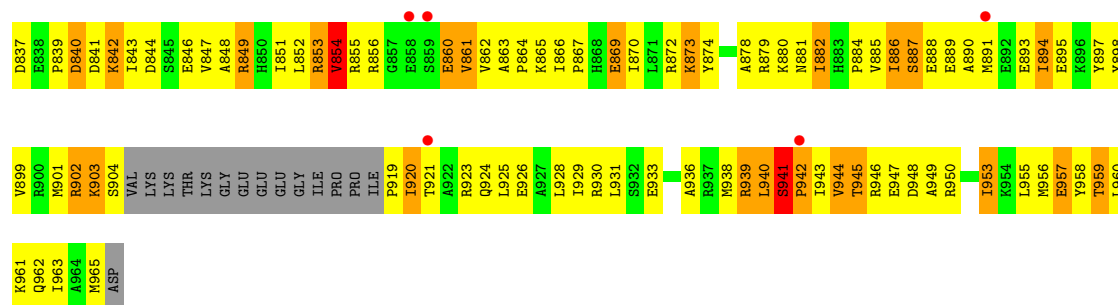


• Molecule 1: Cell division control protein 21

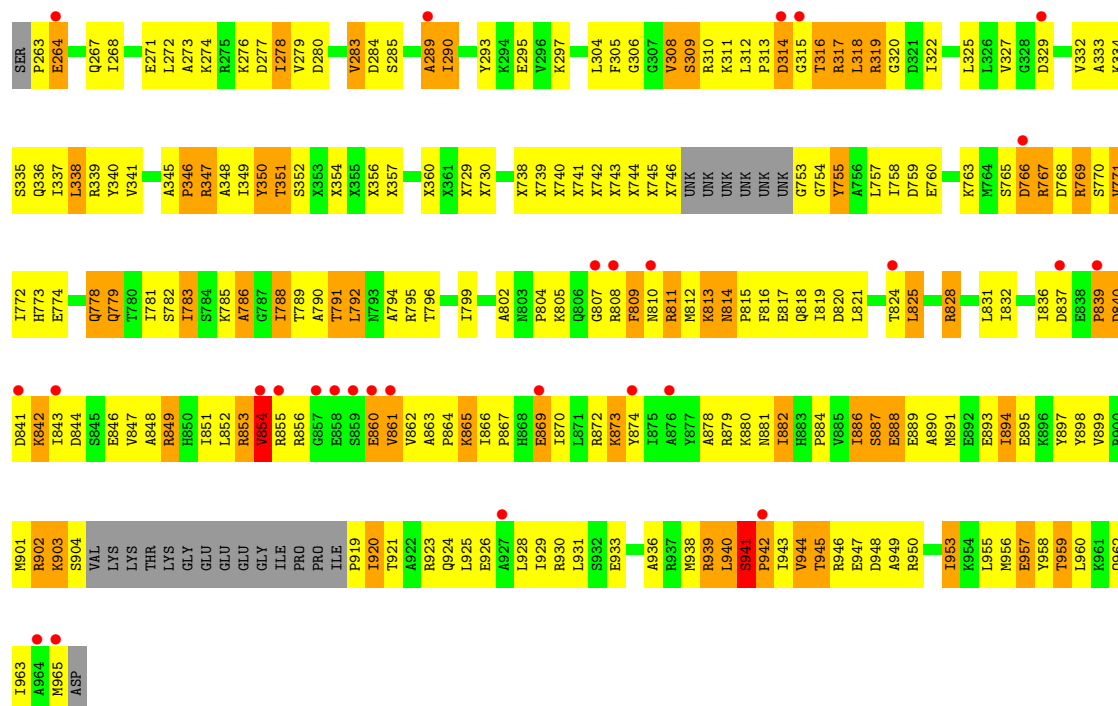


• Molecule 1: Cell division control protein 21

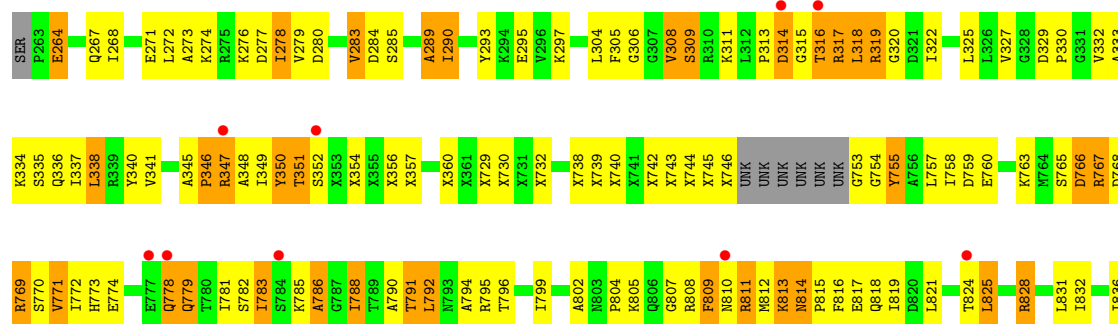


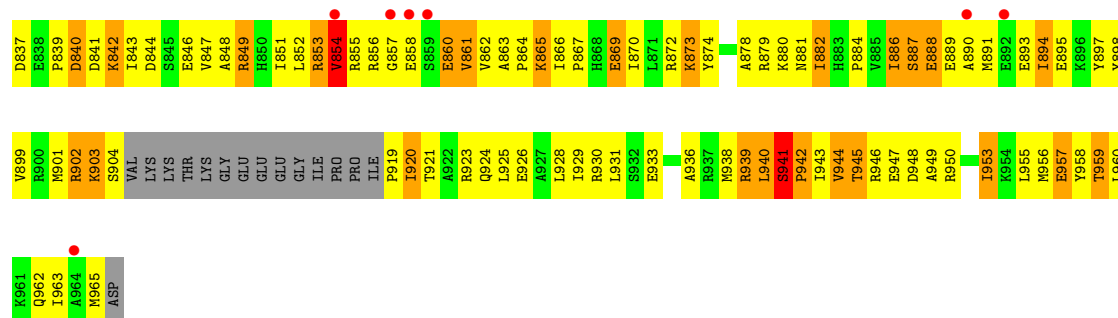


• Molecule 1: Cell division control protein 21

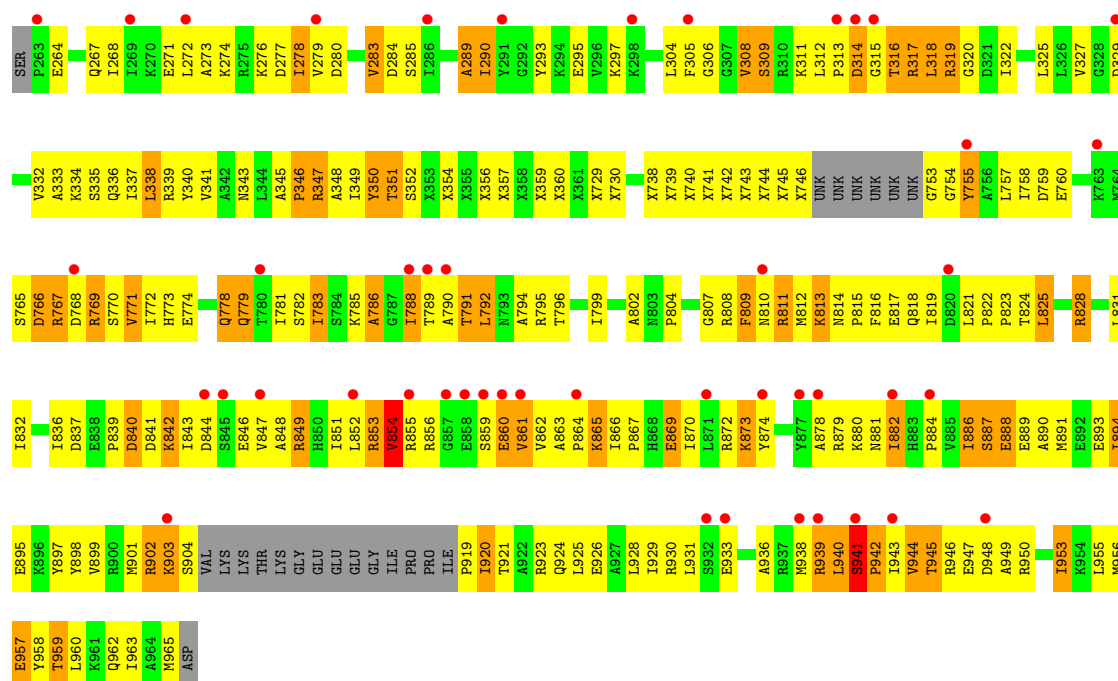


• Molecule 1: Cell division control protein 21

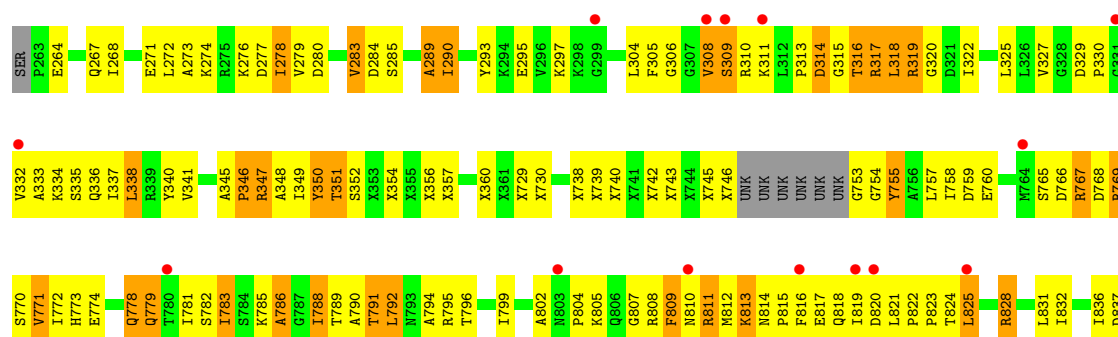


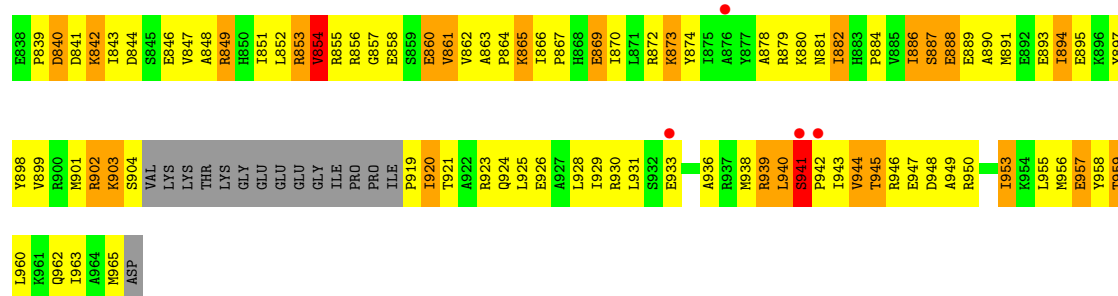


• Molecule 1: Cell division control protein 21

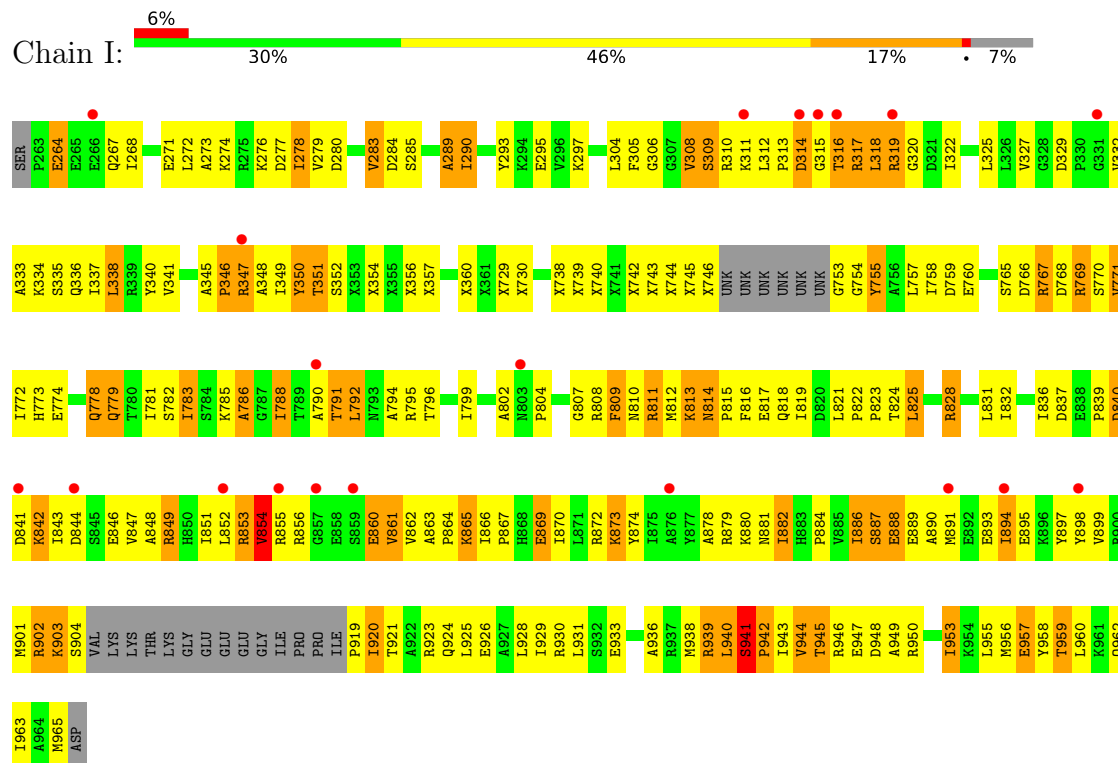


• Molecule 1: Cell division control protein 21

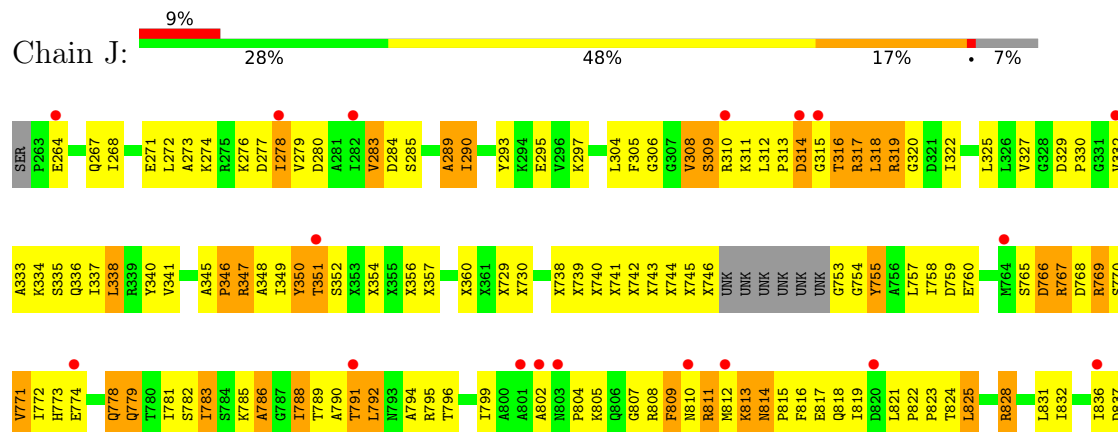


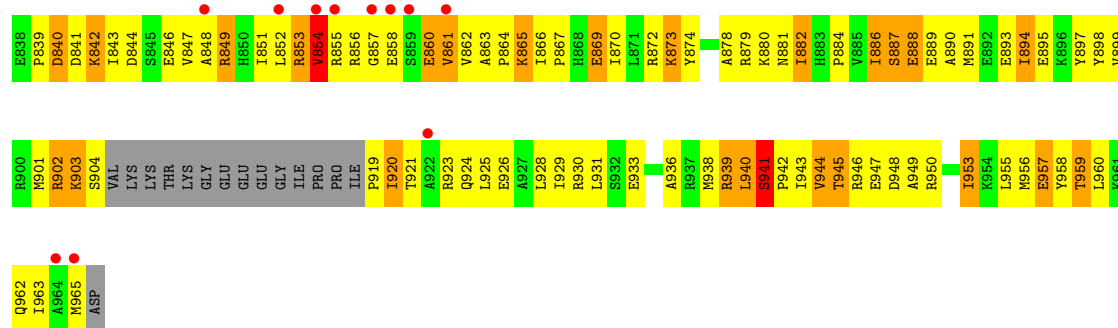


• Molecule 1: Cell division control protein 21

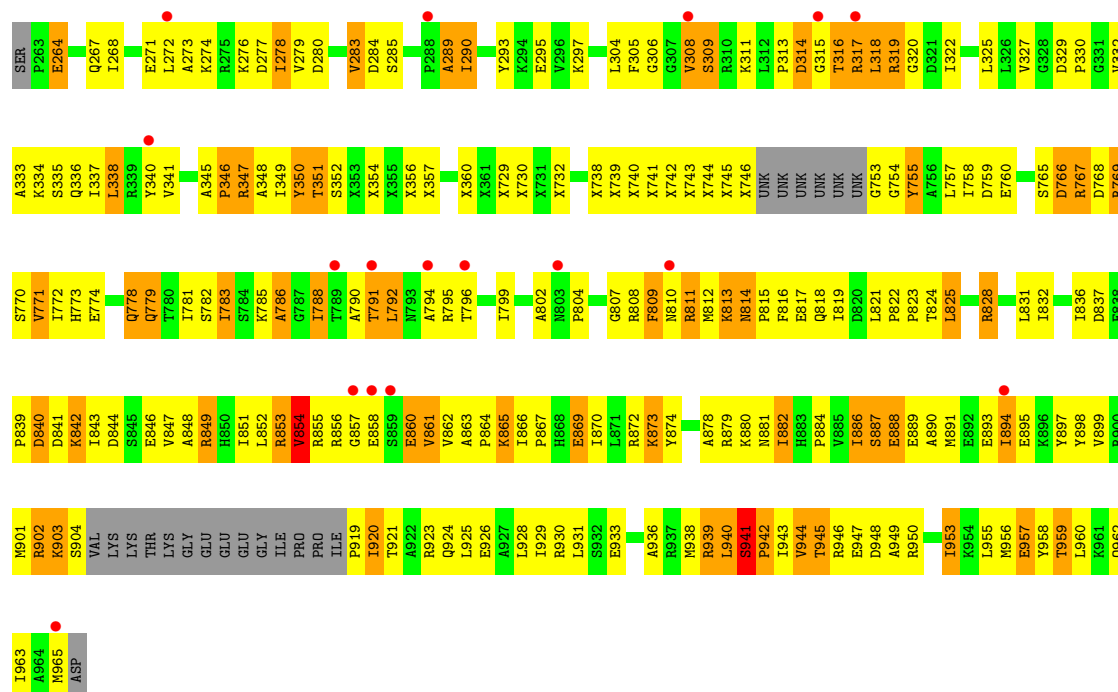


• Molecule 1: Cell division control protein 21

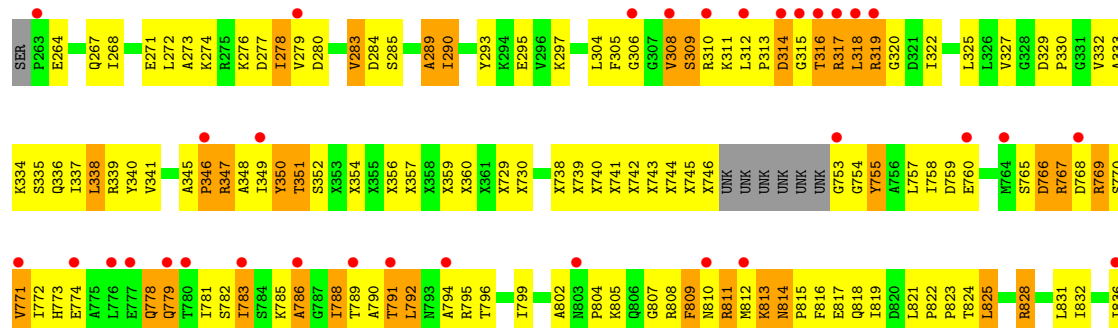


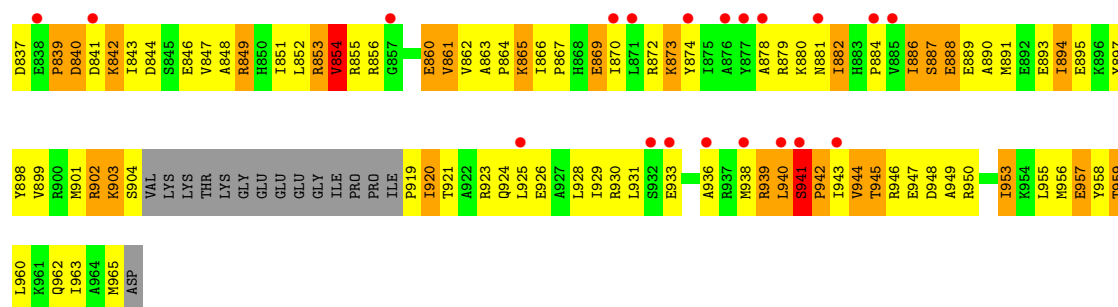


• Molecule 1: Cell division control protein 21

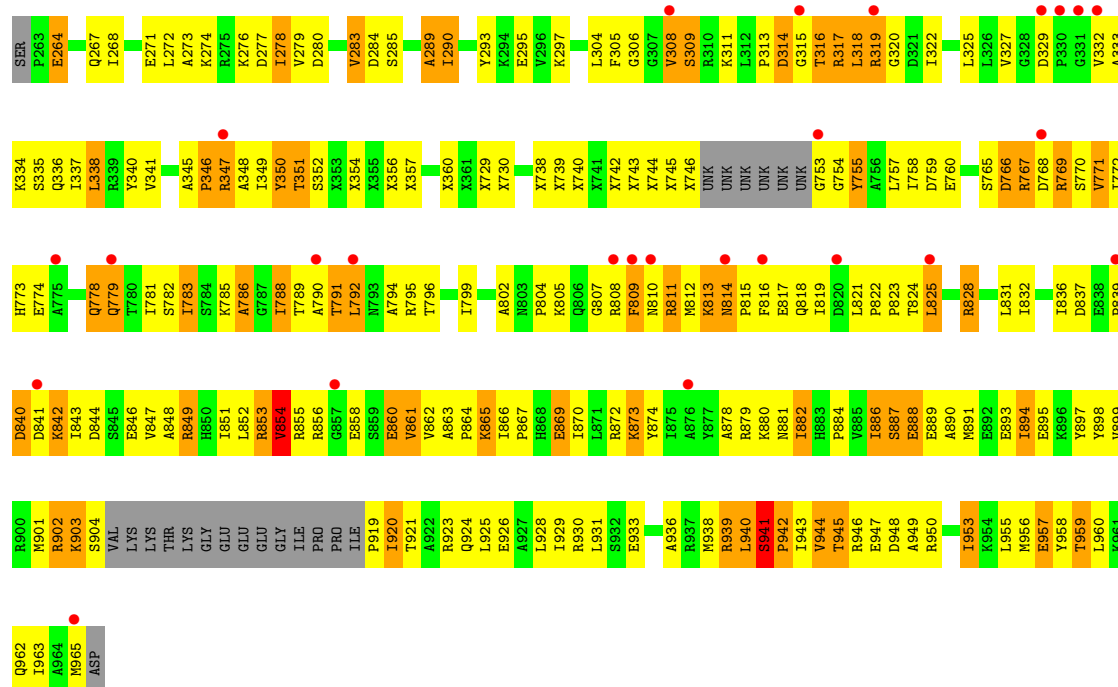


• Molecule 1: Cell division control protein 21

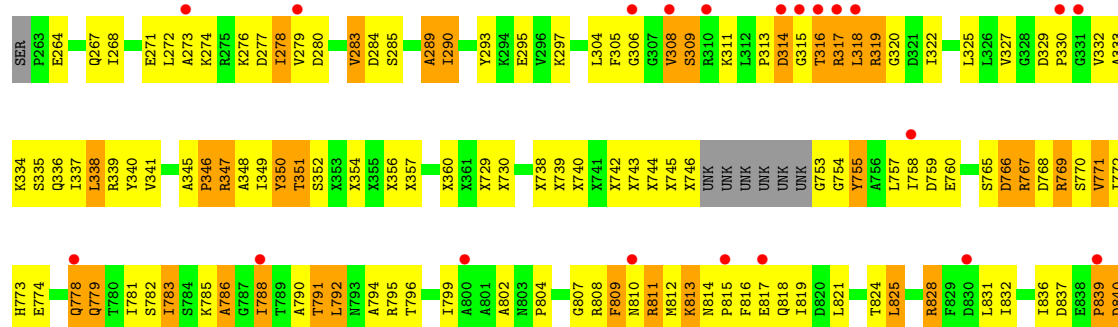


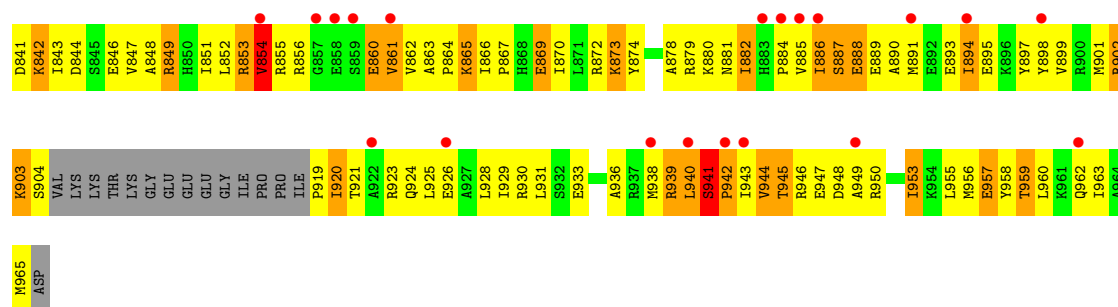


• Molecule 1: Cell division control protein 21

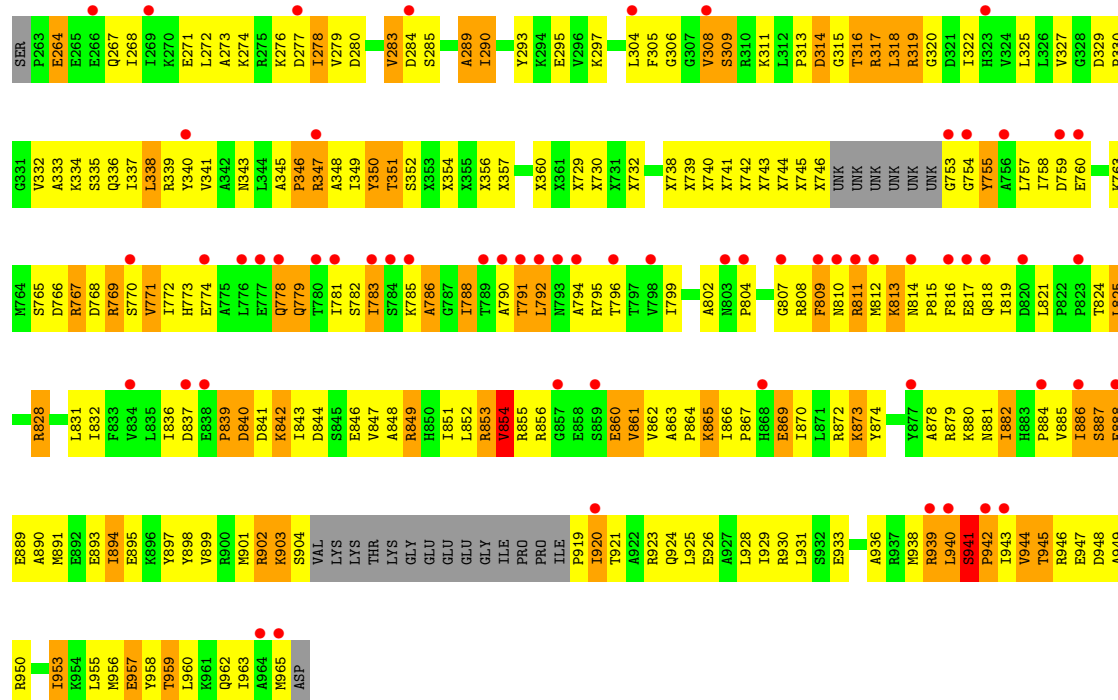


• Molecule 1: Cell division control protein 21

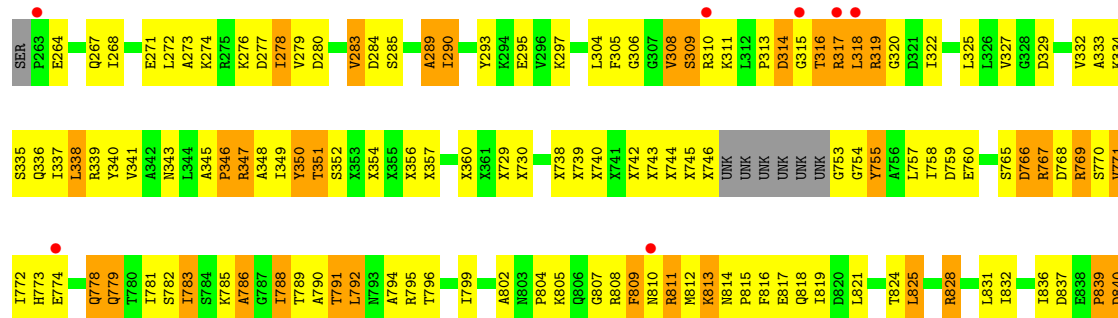


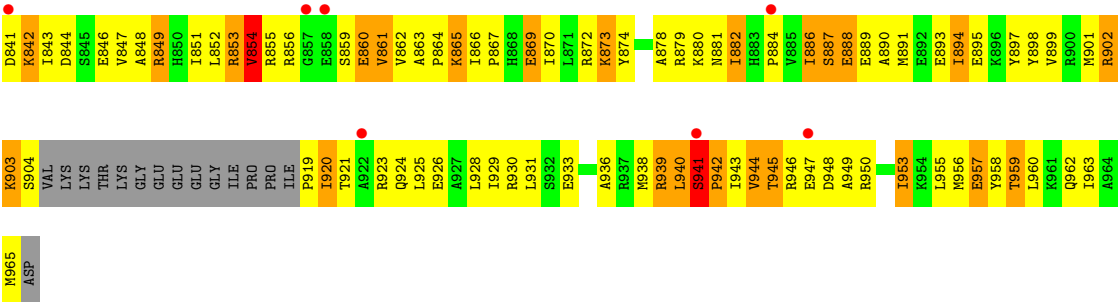


• Molecule 1: Cell division control protein 21



• Molecule 1: Cell division control protein 21





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	124.96Å 127.08Å 128.03Å 71.85° 72.82° 80.39°	Depositor
Resolution (Å)	48.37 – 3.80 48.37 – 3.80	Depositor EDS
% Data completeness (in resolution range)	98.4 (48.37-3.80) 98.4 (48.37-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 3.77Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.301 , 0.314 0.302 , 0.316	Depositor DCC
R_{free} test set	3522 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	82.7	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 94.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.004 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	39296	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.61	0/2326	1.10	14/3133 (0.4%)
1	B	0.61	0/2326	1.10	14/3133 (0.4%)
1	C	0.61	0/2326	1.11	14/3133 (0.4%)
1	D	0.61	0/2326	1.10	14/3133 (0.4%)
1	E	0.61	0/2326	1.10	14/3133 (0.4%)
1	F	0.61	0/2326	1.11	14/3133 (0.4%)
1	G	0.61	0/2326	1.10	14/3133 (0.4%)
1	H	0.61	0/2326	1.11	14/3133 (0.4%)
1	I	0.61	0/2326	1.11	14/3133 (0.4%)
1	J	0.61	0/2326	1.11	14/3133 (0.4%)
1	K	0.61	0/2326	1.10	14/3133 (0.4%)
1	L	0.61	0/2326	1.10	14/3133 (0.4%)
1	M	0.61	0/2326	1.10	14/3133 (0.4%)
1	N	0.61	0/2326	1.10	14/3133 (0.4%)
1	O	0.61	0/2326	1.10	14/3133 (0.4%)
1	P	0.61	0/2326	1.11	14/3133 (0.4%)
All	All	0.61	0/37216	1.11	224/50128 (0.4%)

There are no bond length outliers.

All (224) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	920	ILE	N-CA-C	9.84	123.58	109.51
1	E	920	ILE	N-CA-C	9.83	123.57	109.51
1	J	920	ILE	N-CA-C	9.83	123.56	109.51
1	O	920	ILE	N-CA-C	9.82	123.56	109.51
1	K	920	ILE	N-CA-C	9.82	123.55	109.51
1	I	920	ILE	N-CA-C	9.81	123.54	109.51
1	B	920	ILE	N-CA-C	9.81	123.54	109.51
1	A	920	ILE	N-CA-C	9.81	123.54	109.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	920	ILE	N-CA-C	9.80	123.53	109.51
1	L	920	ILE	N-CA-C	9.80	123.53	109.51
1	G	920	ILE	N-CA-C	9.80	123.52	109.51
1	D	920	ILE	N-CA-C	9.79	123.52	109.51
1	P	920	ILE	N-CA-C	9.80	123.52	109.51
1	H	920	ILE	N-CA-C	9.79	123.51	109.51
1	F	920	ILE	N-CA-C	9.79	123.51	109.51
1	N	920	ILE	N-CA-C	9.79	123.51	109.51
1	L	264	GLU	N-CA-C	-7.19	103.98	112.89
1	H	264	GLU	N-CA-C	-7.18	103.98	112.89
1	M	264	GLU	N-CA-C	-7.18	103.99	112.89
1	C	264	GLU	N-CA-C	-7.18	103.99	112.89
1	B	264	GLU	N-CA-C	-7.17	104.00	112.89
1	E	264	GLU	N-CA-C	-7.17	104.00	112.89
1	N	264	GLU	N-CA-C	-7.17	104.00	112.89
1	F	264	GLU	N-CA-C	-7.17	104.00	112.89
1	P	264	GLU	N-CA-C	-7.17	104.00	112.89
1	J	264	GLU	N-CA-C	-7.17	104.00	112.89
1	A	264	GLU	N-CA-C	-7.16	104.01	112.89
1	O	264	GLU	N-CA-C	-7.16	104.02	112.89
1	G	264	GLU	N-CA-C	-7.15	104.03	112.89
1	I	264	GLU	N-CA-C	-7.14	104.04	112.89
1	D	264	GLU	N-CA-C	-7.13	104.05	112.89
1	K	264	GLU	N-CA-C	-7.12	104.06	112.89
1	K	865	LYS	N-CA-C	-7.04	104.66	113.18
1	B	865	LYS	N-CA-C	-7.03	104.67	113.18
1	G	865	LYS	N-CA-C	-7.03	104.67	113.18
1	L	865	LYS	N-CA-C	-7.03	104.67	113.18
1	C	865	LYS	N-CA-C	-7.03	104.68	113.18
1	D	865	LYS	N-CA-C	-7.02	104.69	113.18
1	E	865	LYS	N-CA-C	-7.02	104.69	113.18
1	H	865	LYS	N-CA-C	-7.02	104.69	113.18
1	I	865	LYS	N-CA-C	-7.01	104.70	113.18
1	A	865	LYS	N-CA-C	-7.01	104.70	113.18
1	J	865	LYS	N-CA-C	-7.00	104.71	113.18
1	P	865	LYS	N-CA-C	-7.00	104.71	113.18
1	F	865	LYS	N-CA-C	-6.99	104.72	113.18
1	O	865	LYS	N-CA-C	-6.99	104.72	113.18
1	N	865	LYS	N-CA-C	-6.98	104.74	113.18
1	M	865	LYS	N-CA-C	-6.96	104.75	113.18
1	G	825	LEU	N-CA-C	-6.55	104.22	112.93
1	M	825	LEU	N-CA-C	-6.55	104.22	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	825	LEU	N-CA-C	-6.54	104.22	112.93
1	H	825	LEU	N-CA-C	-6.54	104.23	112.93
1	K	825	LEU	N-CA-C	-6.54	104.22	112.93
1	C	825	LEU	N-CA-C	-6.54	104.23	112.93
1	I	825	LEU	N-CA-C	-6.54	104.23	112.93
1	J	825	LEU	N-CA-C	-6.54	104.23	112.93
1	A	825	LEU	N-CA-C	-6.54	104.24	112.93
1	B	825	LEU	N-CA-C	-6.53	104.24	112.93
1	N	825	LEU	N-CA-C	-6.53	104.24	112.93
1	L	825	LEU	N-CA-C	-6.53	104.25	112.93
1	O	825	LEU	N-CA-C	-6.53	104.25	112.93
1	P	825	LEU	N-CA-C	-6.52	104.26	112.93
1	E	825	LEU	N-CA-C	-6.52	104.26	112.93
1	D	825	LEU	N-CA-C	-6.52	104.26	112.93
1	E	817	GLU	N-CA-C	-6.50	105.50	113.50
1	I	817	GLU	N-CA-C	-6.50	105.51	113.50
1	C	817	GLU	N-CA-C	-6.49	105.52	113.50
1	G	817	GLU	N-CA-C	-6.49	105.52	113.50
1	J	817	GLU	N-CA-C	-6.49	105.52	113.50
1	K	817	GLU	N-CA-C	-6.48	105.53	113.50
1	N	817	GLU	N-CA-C	-6.48	105.53	113.50
1	M	817	GLU	N-CA-C	-6.48	105.53	113.50
1	L	817	GLU	N-CA-C	-6.48	105.53	113.50
1	A	817	GLU	N-CA-C	-6.48	105.53	113.50
1	B	817	GLU	N-CA-C	-6.47	105.54	113.50
1	P	817	GLU	N-CA-C	-6.47	105.54	113.50
1	O	817	GLU	N-CA-C	-6.47	105.54	113.50
1	F	817	GLU	N-CA-C	-6.47	105.54	113.50
1	H	817	GLU	N-CA-C	-6.44	105.58	113.50
1	D	817	GLU	N-CA-C	-6.43	105.59	113.50
1	N	919	PRO	CA-C-N	6.27	129.14	120.49
1	N	919	PRO	C-N-CA	6.27	129.14	120.49
1	F	919	PRO	CA-C-N	6.27	129.14	120.49
1	F	919	PRO	C-N-CA	6.27	129.14	120.49
1	P	919	PRO	CA-C-N	6.26	129.13	120.49
1	P	919	PRO	C-N-CA	6.26	129.13	120.49
1	D	919	PRO	CA-C-N	6.25	129.12	120.49
1	D	919	PRO	C-N-CA	6.25	129.12	120.49
1	H	919	PRO	CA-C-N	6.25	129.12	120.49
1	H	919	PRO	C-N-CA	6.25	129.12	120.49
1	M	919	PRO	CA-C-N	6.25	129.11	120.49
1	M	919	PRO	C-N-CA	6.25	129.11	120.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	919	PRO	CA-C-N	6.25	129.11	120.49
1	J	919	PRO	C-N-CA	6.25	129.11	120.49
1	I	919	PRO	CA-C-N	6.24	129.11	120.49
1	I	919	PRO	C-N-CA	6.24	129.11	120.49
1	A	919	PRO	CA-C-N	6.24	129.10	120.49
1	A	919	PRO	C-N-CA	6.24	129.10	120.49
1	B	919	PRO	CA-C-N	6.23	129.09	120.49
1	B	919	PRO	C-N-CA	6.23	129.09	120.49
1	L	919	PRO	CA-C-N	6.23	129.09	120.49
1	L	919	PRO	C-N-CA	6.23	129.09	120.49
1	E	919	PRO	CA-C-N	6.22	129.07	120.49
1	E	919	PRO	C-N-CA	6.22	129.07	120.49
1	K	919	PRO	CA-C-N	6.22	129.07	120.49
1	K	919	PRO	C-N-CA	6.22	129.07	120.49
1	C	919	PRO	CA-C-N	6.21	129.06	120.49
1	C	919	PRO	C-N-CA	6.21	129.06	120.49
1	O	919	PRO	CA-C-N	6.21	129.06	120.49
1	O	919	PRO	C-N-CA	6.21	129.06	120.49
1	G	919	PRO	CA-C-N	6.20	129.05	120.49
1	G	919	PRO	C-N-CA	6.20	129.05	120.49
1	G	888	GLU	N-CA-C	-6.12	103.92	111.75
1	L	888	GLU	N-CA-C	-6.11	103.93	111.75
1	I	888	GLU	N-CA-C	-6.10	103.94	111.75
1	N	888	GLU	N-CA-C	-6.10	103.94	111.75
1	O	888	GLU	N-CA-C	-6.10	103.94	111.75
1	B	888	GLU	N-CA-C	-6.09	103.95	111.75
1	F	888	GLU	N-CA-C	-6.09	103.96	111.75
1	A	888	GLU	N-CA-C	-6.09	103.96	111.75
1	D	888	GLU	N-CA-C	-6.08	103.97	111.75
1	C	888	GLU	N-CA-C	-6.08	103.97	111.75
1	M	888	GLU	N-CA-C	-6.07	103.98	111.75
1	P	888	GLU	N-CA-C	-6.07	103.98	111.75
1	J	888	GLU	N-CA-C	-6.07	103.98	111.75
1	K	888	GLU	N-CA-C	-6.07	103.98	111.75
1	E	888	GLU	N-CA-C	-6.06	103.99	111.75
1	H	888	GLU	N-CA-C	-6.04	104.02	111.75
1	E	873	LYS	N-CA-C	-5.89	104.44	111.69
1	C	873	LYS	N-CA-C	-5.89	104.45	111.69
1	K	873	LYS	N-CA-C	-5.88	104.46	111.69
1	O	873	LYS	N-CA-C	-5.87	104.47	111.69
1	M	873	LYS	N-CA-C	-5.87	104.47	111.69
1	I	873	LYS	N-CA-C	-5.87	104.47	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	873	LYS	N-CA-C	-5.86	104.49	111.69
1	K	758	ILE	N-CA-C	5.86	115.75	106.32
1	G	758	ILE	N-CA-C	5.86	115.75	106.32
1	H	873	LYS	N-CA-C	-5.85	104.49	111.69
1	A	873	LYS	N-CA-C	-5.85	104.49	111.69
1	F	873	LYS	N-CA-C	-5.85	104.49	111.69
1	L	873	LYS	N-CA-C	-5.85	104.50	111.69
1	N	758	ILE	N-CA-C	5.85	115.74	106.32
1	M	758	ILE	N-CA-C	5.84	115.73	106.32
1	B	873	LYS	N-CA-C	-5.84	104.50	111.69
1	P	873	LYS	N-CA-C	-5.84	104.50	111.69
1	G	873	LYS	N-CA-C	-5.84	104.51	111.69
1	N	873	LYS	N-CA-C	-5.84	104.51	111.69
1	J	873	LYS	N-CA-C	-5.84	104.51	111.69
1	O	758	ILE	N-CA-C	5.84	115.72	106.32
1	D	758	ILE	N-CA-C	5.84	115.72	106.32
1	J	758	ILE	N-CA-C	5.84	115.72	106.32
1	A	758	ILE	N-CA-C	5.83	115.71	106.32
1	C	758	ILE	N-CA-C	5.83	115.71	106.32
1	E	758	ILE	N-CA-C	5.83	115.71	106.32
1	H	758	ILE	N-CA-C	5.83	115.71	106.32
1	B	758	ILE	N-CA-C	5.83	115.71	106.32
1	I	758	ILE	N-CA-C	5.83	115.71	106.32
1	F	758	ILE	N-CA-C	5.82	115.70	106.32
1	P	758	ILE	N-CA-C	5.82	115.69	106.32
1	L	758	ILE	N-CA-C	5.82	115.68	106.32
1	H	308	VAL	N-CA-C	5.55	116.19	110.36
1	F	308	VAL	N-CA-C	5.54	116.18	110.36
1	B	308	VAL	N-CA-C	5.54	116.18	110.36
1	K	308	VAL	N-CA-C	5.54	116.17	110.36
1	G	308	VAL	N-CA-C	5.53	116.17	110.36
1	J	308	VAL	N-CA-C	5.53	116.17	110.36
1	L	308	VAL	N-CA-C	5.53	116.17	110.36
1	N	308	VAL	N-CA-C	5.52	116.16	110.36
1	A	308	VAL	N-CA-C	5.52	116.15	110.36
1	O	308	VAL	N-CA-C	5.50	116.14	110.36
1	C	308	VAL	N-CA-C	5.50	116.13	110.36
1	E	308	VAL	N-CA-C	5.50	116.13	110.36
1	P	308	VAL	N-CA-C	5.49	116.12	110.36
1	M	308	VAL	N-CA-C	5.49	116.12	110.36
1	I	308	VAL	N-CA-C	5.48	116.11	110.36
1	D	308	VAL	N-CA-C	5.47	116.11	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	879	ARG	N-CA-C	-5.37	107.04	113.21
1	C	879	ARG	N-CA-C	-5.37	107.04	113.21
1	I	879	ARG	N-CA-C	-5.36	107.05	113.21
1	P	879	ARG	N-CA-C	-5.36	107.05	113.21
1	H	879	ARG	N-CA-C	-5.36	107.05	113.21
1	D	879	ARG	N-CA-C	-5.35	107.05	113.21
1	M	879	ARG	N-CA-C	-5.35	107.06	113.21
1	A	879	ARG	N-CA-C	-5.35	107.06	113.21
1	N	879	ARG	N-CA-C	-5.34	107.07	113.21
1	K	879	ARG	N-CA-C	-5.34	107.07	113.21
1	G	879	ARG	N-CA-C	-5.34	107.07	113.21
1	J	879	ARG	N-CA-C	-5.34	107.07	113.21
1	L	879	ARG	N-CA-C	-5.34	107.07	113.21
1	F	879	ARG	N-CA-C	-5.33	107.08	113.21
1	B	879	ARG	N-CA-C	-5.33	107.08	113.21
1	E	879	ARG	N-CA-C	-5.33	107.08	113.21
1	J	814	ASN	N-CA-C	5.33	117.33	109.50
1	I	814	ASN	N-CA-C	5.31	117.30	109.50
1	L	814	ASN	N-CA-C	5.30	117.30	109.50
1	F	814	ASN	N-CA-C	5.30	117.29	109.50
1	A	814	ASN	N-CA-C	5.30	117.29	109.50
1	K	814	ASN	N-CA-C	5.30	117.28	109.50
1	N	814	ASN	N-CA-C	5.29	117.28	109.50
1	H	814	ASN	N-CA-C	5.29	117.28	109.50
1	D	814	ASN	N-CA-C	5.29	117.28	109.50
1	O	814	ASN	N-CA-C	5.29	117.28	109.50
1	P	814	ASN	N-CA-C	5.29	117.27	109.50
1	E	814	ASN	N-CA-C	5.28	117.26	109.50
1	M	814	ASN	N-CA-C	5.28	117.26	109.50
1	G	814	ASN	N-CA-C	5.28	117.26	109.50
1	C	814	ASN	N-CA-C	5.27	117.25	109.50
1	B	814	ASN	N-CA-C	5.27	117.25	109.50
1	B	920	ILE	CB-CA-C	-5.06	103.15	111.51
1	E	920	ILE	CB-CA-C	-5.06	103.16	111.51
1	M	920	ILE	CB-CA-C	-5.05	103.18	111.51
1	J	920	ILE	CB-CA-C	-5.05	103.18	111.51
1	N	920	ILE	CB-CA-C	-5.05	103.18	111.51
1	D	920	ILE	CB-CA-C	-5.05	103.18	111.51
1	A	920	ILE	CB-CA-C	-5.04	103.19	111.51
1	P	920	ILE	CB-CA-C	-5.04	103.19	111.51
1	H	920	ILE	CB-CA-C	-5.04	103.20	111.51
1	L	920	ILE	CB-CA-C	-5.03	103.20	111.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	920	ILE	CB-CA-C	-5.03	103.20	111.51
1	I	920	ILE	CB-CA-C	-5.03	103.21	111.51
1	G	920	ILE	CB-CA-C	-5.03	103.21	111.51
1	C	920	ILE	CB-CA-C	-5.03	103.22	111.51
1	F	920	ILE	CB-CA-C	-5.03	103.22	111.51
1	K	920	ILE	CB-CA-C	-5.02	103.22	111.51

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2428	0	2425	291	6
1	B	2428	0	2425	278	20
1	C	2428	0	2425	299	1
1	D	2428	0	2425	318	0
1	E	2428	0	2425	293	6
1	F	2428	0	2425	290	4
1	G	2428	0	2425	321	1
1	H	2428	0	2425	290	0
1	I	2428	0	2425	337	6
1	J	2428	0	2425	361	0
1	K	2428	0	2425	323	21
1	L	2428	0	2425	311	0
1	M	2428	0	2425	308	6
1	N	2428	0	2425	303	0
1	O	2428	0	2425	308	3
1	P	2428	0	2425	322	2
2	A	27	0	12	3	0
2	B	27	0	12	3	0
2	C	27	0	12	3	0
2	D	27	0	12	3	0
2	E	27	0	12	3	0
2	F	27	0	12	3	0
2	G	27	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	27	0	12	3	0
2	I	27	0	12	3	0
2	J	27	0	12	3	0
2	K	27	0	12	4	0
2	L	27	0	12	3	0
2	M	27	0	12	3	0
2	N	27	0	12	3	0
2	O	27	0	12	3	0
2	P	27	0	12	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
All	All	39296	0	38992	4473	38

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 57.

All (4473) 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:D:785:LYS:HG3	1:M:785:LYS:CG	1.32	1.56
1:G:730:UNK:CB	1:K:729:UNK:C	1.92	1.44
1:D:785:LYS:CG	1:M:785:LYS:HG3	0.98	1.44
1:E:788:ILE:HG22	1:L:741:UNK:CB	1.47	1.42
1:E:740:UNK:CA	1:L:789:THR:O	1.68	1.41
1:D:785:LYS:C	1:M:785:LYS:HG2	1.44	1.39
1:J:891:MET:HE1	1:K:856:ARG:CZ	1.57	1.34
1:G:789:THR:O	1:J:740:UNK:HA	1.20	1.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:891:MET:HE1	1:J:856:ARG:CZ	1.56	1.33
1:A:785:LYS:CG	1:P:785:LYS:CG	2.05	1.33
1:D:785:LYS:CG	1:M:785:LYS:CG	1.93	1.33
1:D:785:LYS:O	1:M:785:LYS:HG2	1.19	1.32
1:G:730:UNK:CB	1:K:729:UNK:O	1.76	1.31
1:O:316:THR:HG21	1:P:339:ARG:CD	1.63	1.27
1:D:785:LYS:CB	1:M:785:LYS:HG3	1.66	1.26
1:I:891:MET:CE	1:J:856:ARG:CZ	2.15	1.24
1:A:785:LYS:HG3	1:P:785:LYS:CG	1.65	1.22
1:A:785:LYS:HG2	1:P:785:LYS:CG	1.69	1.21
1:E:740:UNK:HA	1:L:789:THR:C	1.65	1.21
1:E:741:UNK:CB	1:L:788:ILE:HA	1.70	1.19
1:H:785:LYS:HG3	1:I:785:LYS:CG	1.71	1.19
1:A:785:LYS:CG	1:P:785:LYS:HG2	1.67	1.19
1:E:741:UNK:CB	1:L:788:ILE:CG2	2.21	1.18
1:I:898:TYR:CD2	1:J:848:ALA:HB2	1.78	1.18
1:F:891:MET:HE1	1:G:856:ARG:NE	1.57	1.18
1:K:941:SER:HB3	1:K:943:ILE:H	1.08	1.18
1:N:891:MET:HE2	1:O:852:LEU:HB3	1.23	1.18
1:B:788:ILE:HG22	1:O:741:UNK:N	1.59	1.17
1:O:316:THR:CG2	1:P:339:ARG:HD2	1.73	1.17
1:C:941:SER:HB3	1:C:943:ILE:H	1.08	1.17
1:G:789:THR:O	1:J:740:UNK:CA	1.93	1.17
1:P:941:SER:HB3	1:P:943:ILE:H	1.08	1.17
1:L:941:SER:HB3	1:L:943:ILE:H	1.08	1.17
1:D:730:UNK:CB	1:N:730:UNK:CB	2.22	1.16
1:E:941:SER:HB3	1:E:943:ILE:H	1.08	1.16
1:D:785:LYS:CB	1:M:785:LYS:CG	2.20	1.15
1:G:941:SER:HB3	1:G:943:ILE:H	1.08	1.15
1:I:941:SER:HB3	1:I:943:ILE:H	1.08	1.15
1:F:941:SER:HB3	1:F:943:ILE:H	1.08	1.14
1:D:785:LYS:O	1:M:785:LYS:CG	1.94	1.14
1:G:730:UNK:CB	1:K:730:UNK:CB	2.25	1.14
1:D:785:LYS:HB3	1:M:785:LYS:HB3	1.30	1.14
1:B:941:SER:HB3	1:B:943:ILE:H	1.08	1.13
1:H:941:SER:HB3	1:H:943:ILE:H	1.08	1.13
1:M:941:SER:HB3	1:M:943:ILE:H	1.08	1.12
1:A:789:THR:O	1:P:740:UNK:HA	1.49	1.11
1:F:891:MET:HE1	1:G:856:ARG:CZ	1.78	1.11
1:D:785:LYS:HB3	1:M:785:LYS:CB	1.80	1.11
1:I:856:ARG:HH12	1:P:888:GLU:HG2	1.14	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:941:SER:HB3	1:A:943:ILE:H	1.08	1.10
1:L:312:LEU:HD11	1:M:858:GLU:HA	1.26	1.10
1:C:359:UNK:CB	1:O:732:UNK:HA	1.80	1.10
1:I:894:ILE:HD11	1:J:852:LEU:HD11	1.27	1.10
1:D:941:SER:HB3	1:D:943:ILE:H	1.08	1.10
1:N:891:MET:HG3	1:O:852:LEU:HG	1.11	1.10
1:A:785:LYS:CG	1:P:785:LYS:HG3	1.77	1.09
1:G:312:LEU:HD21	1:H:858:GLU:HG3	1.29	1.09
1:J:941:SER:HB3	1:J:943:ILE:H	1.08	1.09
1:F:894:ILE:HD11	1:G:852:LEU:HD11	1.26	1.09
1:N:941:SER:HB3	1:N:943:ILE:H	1.08	1.09
1:C:891:MET:HE1	1:D:856:ARG:NE	1.67	1.09
1:E:740:UNK:HA	1:L:789:THR:O	0.92	1.09
1:I:891:MET:HE1	1:J:856:ARG:NH2	1.68	1.09
1:O:941:SER:HB3	1:O:943:ILE:H	1.08	1.09
1:I:852:LEU:HD11	1:P:894:ILE:HD11	1.27	1.09
1:F:888:GLU:HG2	1:G:856:ARG:HH12	1.07	1.08
1:O:313:PRO:O	1:P:343:ASN:ND2	1.86	1.08
1:A:785:LYS:HG2	1:P:785:LYS:HG3	1.16	1.08
1:C:888:GLU:HG2	1:D:856:ARG:HH12	0.95	1.08
1:I:898:TYR:HD2	1:J:848:ALA:HB2	1.11	1.08
1:C:894:ILE:HD11	1:D:852:LEU:HD11	1.31	1.08
1:I:310:ARG:NH1	1:J:858:GLU:OE2	1.88	1.07
1:E:741:UNK:CB	1:L:788:ILE:HG22	1.83	1.06
1:N:885:VAL:HG13	1:O:856:ARG:HB2	1.32	1.06
1:I:856:ARG:CZ	1:P:891:MET:HE1	1.86	1.06
1:N:891:MET:HG3	1:O:852:LEU:CG	1.84	1.06
1:H:867:PRO:HB2	1:H:870:ILE:HD13	1.38	1.06
1:J:894:ILE:HD11	1:K:852:LEU:HD11	1.37	1.06
1:K:867:PRO:HB2	1:K:870:ILE:HD13	1.38	1.06
1:N:867:PRO:HB2	1:N:870:ILE:HD13	1.38	1.06
1:C:867:PRO:HB2	1:C:870:ILE:HD13	1.38	1.05
1:A:867:PRO:HB2	1:A:870:ILE:HD13	1.38	1.05
1:M:867:PRO:HB2	1:M:870:ILE:HD13	1.38	1.05
1:B:867:PRO:HB2	1:B:870:ILE:HD13	1.38	1.05
1:G:867:PRO:HB2	1:G:870:ILE:HD13	1.38	1.05
1:I:856:ARG:NE	1:P:891:MET:HE1	1.72	1.05
1:O:867:PRO:HB2	1:O:870:ILE:HD13	1.38	1.05
1:G:730:UNK:CB	1:K:730:UNK:N	2.18	1.04
1:F:867:PRO:HB2	1:F:870:ILE:HD13	1.38	1.04
1:D:867:PRO:HB2	1:D:870:ILE:HD13	1.38	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:310:ARG:NH1	1:K:858:GLU:OE2	1.89	1.04
1:P:867:PRO:HB2	1:P:870:ILE:HD13	1.38	1.03
1:J:867:PRO:HB2	1:J:870:ILE:HD13	1.38	1.03
1:N:316:THR:HG21	1:O:339:ARG:CD	1.89	1.03
1:I:886:ILE:O	1:J:856:ARG:NH1	1.90	1.02
1:D:785:LYS:HG2	1:M:785:LYS:HG3	1.38	1.02
1:E:740:UNK:N	1:L:789:THR:O	1.93	1.02
1:I:867:PRO:HB2	1:I:870:ILE:HD13	1.38	1.02
1:L:867:PRO:HB2	1:L:870:ILE:HD13	1.38	1.02
1:I:856:ARG:HD3	1:P:891:MET:CE	1.90	1.01
1:J:902:ARG:NH1	1:K:844:ASP:OD1	1.92	1.01
1:I:894:ILE:CD1	1:J:852:LEU:HD11	1.89	1.01
1:I:898:TYR:HD2	1:J:848:ALA:CB	1.73	1.00
1:E:788:ILE:CG2	1:L:741:UNK:CB	2.40	1.00
1:E:867:PRO:HB2	1:E:870:ILE:HD13	1.38	1.00
1:H:785:LYS:HG3	1:I:785:LYS:HG3	1.41	1.00
1:H:785:LYS:CG	1:I:785:LYS:HG3	1.92	1.00
1:G:730:UNK:CB	1:K:730:UNK:CA	2.39	0.99
1:E:740:UNK:O	1:L:789:THR:OG1	1.79	0.99
1:C:888:GLU:HG2	1:D:856:ARG:NH1	1.79	0.98
1:C:891:MET:CE	1:D:856:ARG:HD3	1.94	0.98
1:F:891:MET:CE	1:G:856:ARG:HD3	1.93	0.98
1:I:929:ILE:HD11	1:J:852:LEU:HD13	1.45	0.96
1:I:856:ARG:CD	1:P:891:MET:HE1	1.95	0.96
1:J:312:LEU:HD11	1:K:858:GLU:HA	1.47	0.96
1:N:891:MET:HE2	1:O:852:LEU:CB	1.95	0.96
1:I:891:MET:HE1	1:J:856:ARG:NE	1.81	0.96
1:G:789:THR:OG1	1:J:740:UNK:O	1.83	0.95
1:I:886:ILE:HB	1:J:856:ARG:HD3	1.49	0.95
1:D:785:LYS:C	1:M:785:LYS:CG	2.37	0.95
1:A:339:ARG:HD2	1:H:316:THR:HG21	1.49	0.95
1:N:903:LYS:NZ	1:O:839:PRO:HB3	1.81	0.94
1:D:785:LYS:HG3	1:M:785:LYS:CD	1.97	0.94
1:I:894:ILE:HD11	1:J:852:LEU:CD1	1.98	0.94
1:H:785:LYS:HG3	1:I:785:LYS:HG2	1.48	0.93
1:G:312:LEU:HD11	1:H:858:GLU:HA	1.50	0.93
1:N:885:VAL:CG1	1:O:856:ARG:HB2	1.98	0.93
1:F:891:MET:HE1	1:G:856:ARG:CD	1.97	0.93
1:C:891:MET:HE1	1:D:856:ARG:CZ	1.97	0.93
1:I:310:ARG:NH2	1:J:857:GLY:O	2.02	0.92
1:E:741:UNK:CB	1:L:788:ILE:HG23	1.98	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:312:LEU:CD1	1:H:858:GLU:HA	2.00	0.92
1:E:741:UNK:CB	1:L:788:ILE:CA	2.46	0.91
1:G:789:THR:C	1:J:740:UNK:HA	1.95	0.91
1:J:310:ARG:NH2	1:K:857:GLY:O	2.03	0.91
1:H:785:LYS:HG2	1:I:785:LYS:O	1.70	0.91
1:C:891:MET:HE1	1:D:856:ARG:CD	1.99	0.91
1:J:898:TYR:CD2	1:K:848:ALA:HB2	2.05	0.91
1:F:902:ARG:NH1	1:G:844:ASP:OD1	2.03	0.90
1:G:869:GLU:HA	1:G:872:ARG:HH12	1.36	0.90
1:M:869:GLU:HA	1:M:872:ARG:HH12	1.36	0.90
1:H:869:GLU:HA	1:H:872:ARG:HH12	1.36	0.90
1:N:316:THR:HG21	1:O:339:ARG:HD2	1.49	0.90
1:H:785:LYS:CG	1:I:785:LYS:CG	2.48	0.90
1:B:869:GLU:HA	1:B:872:ARG:HH12	1.37	0.90
1:E:869:GLU:HA	1:E:872:ARG:HH12	1.36	0.90
1:F:869:GLU:HA	1:F:872:ARG:HH12	1.36	0.90
1:L:869:GLU:HA	1:L:872:ARG:HH12	1.36	0.90
1:N:869:GLU:HA	1:N:872:ARG:HH12	1.36	0.90
1:J:891:MET:CE	1:K:856:ARG:CZ	2.49	0.90
1:C:869:GLU:HA	1:C:872:ARG:HH12	1.36	0.90
1:I:869:GLU:HA	1:I:872:ARG:HH12	1.36	0.90
1:O:869:GLU:HA	1:O:872:ARG:HH12	1.36	0.90
1:N:769:ARG:CB	1:N:769:ARG:HH11	1.85	0.90
1:B:729:UNK:O	1:P:729:UNK:O	1.89	0.90
1:A:869:GLU:HA	1:A:872:ARG:HH12	1.36	0.90
1:N:903:LYS:NZ	1:O:839:PRO:CB	2.35	0.90
1:M:769:ARG:CB	1:M:769:ARG:HH11	1.85	0.89
1:E:740:UNK:C	1:L:789:THR:H	1.84	0.89
1:E:769:ARG:CB	1:E:769:ARG:HH11	1.85	0.89
1:H:769:ARG:CB	1:H:769:ARG:HH11	1.85	0.89
1:F:769:ARG:HH11	1:F:769:ARG:CB	1.85	0.89
1:J:769:ARG:CB	1:J:769:ARG:HH11	1.85	0.89
1:K:869:GLU:HA	1:K:872:ARG:HH12	1.37	0.89
1:C:785:LYS:HG3	1:N:785:LYS:CG	2.03	0.89
1:L:854:VAL:HG13	1:L:862:VAL:HB	1.55	0.89
1:E:854:VAL:HG13	1:E:862:VAL:HB	1.55	0.89
1:A:854:VAL:HG13	1:A:862:VAL:HB	1.55	0.89
1:B:854:VAL:HG13	1:B:862:VAL:HB	1.55	0.89
1:G:854:VAL:HG13	1:G:862:VAL:HB	1.55	0.89
1:O:769:ARG:CB	1:O:769:ARG:HH11	1.85	0.89
1:B:769:ARG:CB	1:B:769:ARG:HH11	1.85	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:785:LYS:HE3	1:M:785:LYS:HE3	1.55	0.88
1:G:741:UNK:CB	1:J:788:ILE:HG22	2.02	0.88
1:I:769:ARG:CB	1:I:769:ARG:HH11	1.85	0.88
1:J:312:LEU:HD21	1:K:858:GLU:HB3	1.53	0.88
1:P:769:ARG:CB	1:P:769:ARG:HH11	1.85	0.88
1:C:769:ARG:CB	1:C:769:ARG:HH11	1.85	0.88
1:D:854:VAL:HG13	1:D:862:VAL:HB	1.55	0.88
1:H:854:VAL:HG13	1:H:862:VAL:HB	1.55	0.88
1:L:769:ARG:CB	1:L:769:ARG:HH11	1.85	0.88
1:A:769:ARG:CB	1:A:769:ARG:HH11	1.85	0.88
1:C:730:UNK:CB	1:O:729:UNK:C	2.50	0.88
1:K:769:ARG:CB	1:K:769:ARG:HH11	1.85	0.88
1:D:769:ARG:CB	1:D:769:ARG:HH11	1.85	0.88
1:G:769:ARG:CB	1:G:769:ARG:HH11	1.85	0.88
1:D:729:UNK:O	1:N:729:UNK:O	1.91	0.87
1:N:854:VAL:HG13	1:N:862:VAL:HB	1.55	0.87
1:A:941:SER:HB3	1:A:943:ILE:N	1.90	0.87
1:J:869:GLU:HA	1:J:872:ARG:HH12	1.36	0.87
1:L:941:SER:HB3	1:L:943:ILE:N	1.90	0.87
1:M:854:VAL:HG13	1:M:862:VAL:HB	1.55	0.87
1:J:854:VAL:HG13	1:J:862:VAL:HB	1.55	0.87
1:P:869:GLU:HA	1:P:872:ARG:HH12	1.37	0.87
1:D:869:GLU:HA	1:D:872:ARG:HH12	1.36	0.87
1:L:312:LEU:CD1	1:M:858:GLU:HA	2.04	0.87
1:J:891:MET:HE1	1:K:856:ARG:NH1	1.89	0.87
1:K:854:VAL:HG13	1:K:862:VAL:HB	1.55	0.87
1:J:941:SER:HB3	1:J:943:ILE:N	1.90	0.87
1:O:941:SER:HB3	1:O:943:ILE:N	1.90	0.87
1:F:941:SER:HB3	1:F:943:ILE:N	1.90	0.87
1:D:941:SER:HB3	1:D:943:ILE:N	1.90	0.86
1:I:891:MET:HE3	1:J:856:ARG:CZ	2.04	0.86
1:P:941:SER:HB3	1:P:943:ILE:N	1.90	0.86
1:I:854:VAL:HG13	1:I:862:VAL:HB	1.55	0.86
1:O:854:VAL:HG13	1:O:862:VAL:HB	1.55	0.86
1:P:854:VAL:HG13	1:P:862:VAL:HB	1.55	0.86
1:D:769:ARG:HH11	1:D:769:ARG:HB2	1.41	0.86
1:I:941:SER:HB3	1:I:943:ILE:N	1.90	0.86
1:F:769:ARG:HH11	1:F:769:ARG:HB2	1.41	0.86
1:F:888:GLU:HG2	1:G:856:ARG:NH1	1.90	0.86
1:E:941:SER:HB3	1:E:943:ILE:N	1.90	0.86
1:H:941:SER:HB3	1:H:943:ILE:N	1.90	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:769:ARG:HH11	1:A:769:ARG:HB2	1.41	0.86
1:C:854:VAL:HG13	1:C:862:VAL:HB	1.55	0.86
1:G:941:SER:HB3	1:G:943:ILE:N	1.90	0.86
1:O:769:ARG:HH11	1:O:769:ARG:HB2	1.41	0.86
1:A:785:LYS:HG3	1:P:785:LYS:HG2	0.89	0.86
1:B:312:LEU:HD11	1:C:858:GLU:HA	1.58	0.86
1:F:854:VAL:HG13	1:F:862:VAL:HB	1.55	0.86
1:B:941:SER:HB3	1:B:943:ILE:N	1.90	0.85
1:G:769:ARG:HH11	1:G:769:ARG:HB2	1.41	0.85
1:K:769:ARG:HH11	1:K:769:ARG:HB2	1.41	0.85
1:N:769:ARG:HH11	1:N:769:ARG:HB2	1.41	0.85
1:E:754:GLY:O	1:E:796:THR:HB	1.77	0.85
1:D:754:GLY:O	1:D:796:THR:HB	1.77	0.85
1:J:769:ARG:HH11	1:J:769:ARG:HB2	1.41	0.85
1:E:789:THR:O	1:L:740:UNK:HA	1.76	0.85
1:K:902:ARG:HG2	1:L:844:ASP:OD2	1.76	0.85
1:C:769:ARG:HH11	1:C:769:ARG:HB2	1.41	0.85
1:E:769:ARG:HH11	1:E:769:ARG:HB2	1.41	0.85
1:K:941:SER:HB3	1:K:943:ILE:N	1.90	0.85
1:C:290:ILE:HD11	1:C:297:LYS:HE3	1.59	0.85
1:F:754:GLY:O	1:F:796:THR:HB	1.77	0.85
1:J:290:ILE:HD11	1:J:297:LYS:HE3	1.59	0.85
1:C:941:SER:HB3	1:C:943:ILE:N	1.90	0.85
1:G:754:GLY:O	1:G:796:THR:HB	1.77	0.85
1:J:754:GLY:O	1:J:796:THR:HB	1.77	0.85
1:N:941:SER:HB3	1:N:943:ILE:N	1.90	0.85
1:I:290:ILE:HD11	1:I:297:LYS:HE3	1.59	0.85
1:I:754:GLY:O	1:I:796:THR:HB	1.77	0.85
1:C:754:GLY:O	1:C:796:THR:HB	1.77	0.84
1:H:863:ALA:HB1	1:H:864:PRO:HD2	1.59	0.84
1:M:941:SER:HB3	1:M:943:ILE:N	1.90	0.84
1:B:754:GLY:O	1:B:796:THR:HB	1.77	0.84
1:G:290:ILE:HD11	1:G:297:LYS:HE3	1.59	0.84
1:I:863:ALA:HB1	1:I:864:PRO:HD2	1.59	0.84
1:J:863:ALA:HB1	1:J:864:PRO:HD2	1.59	0.84
1:H:769:ARG:HH11	1:H:769:ARG:HB2	1.41	0.84
1:I:891:MET:CE	1:J:856:ARG:NE	2.39	0.84
1:L:754:GLY:O	1:L:796:THR:HB	1.77	0.84
1:M:290:ILE:HD11	1:M:297:LYS:HE3	1.59	0.84
1:A:754:GLY:O	1:A:796:THR:HB	1.77	0.84
1:E:863:ALA:HB1	1:E:864:PRO:HD2	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:316:THR:OG1	1:P:339:ARG:HD3	1.77	0.84
1:P:754:GLY:O	1:P:796:THR:HB	1.77	0.84
1:K:290:ILE:HD11	1:K:297:LYS:HE3	1.59	0.84
1:P:290:ILE:HD11	1:P:297:LYS:HE3	1.59	0.84
1:B:863:ALA:HB1	1:B:864:PRO:HD2	1.59	0.84
1:L:290:ILE:HD11	1:L:297:LYS:HE3	1.59	0.84
1:N:754:GLY:O	1:N:796:THR:HB	1.77	0.84
1:O:316:THR:CG2	1:P:339:ARG:CD	2.44	0.84
1:P:863:ALA:HB1	1:P:864:PRO:HD2	1.59	0.84
1:E:290:ILE:HD11	1:E:297:LYS:HE3	1.59	0.84
1:N:863:ALA:HB1	1:N:864:PRO:HD2	1.59	0.84
1:K:754:GLY:O	1:K:796:THR:HB	1.77	0.84
1:N:313:PRO:O	1:O:343:ASN:ND2	2.11	0.84
1:B:769:ARG:HH11	1:B:769:ARG:HB2	1.41	0.83
1:M:769:ARG:HH11	1:M:769:ARG:HB2	1.41	0.83
1:N:903:LYS:HZ1	1:O:839:PRO:HB3	1.39	0.83
1:A:290:ILE:HD11	1:A:297:LYS:HE3	1.59	0.83
1:C:863:ALA:HB1	1:C:864:PRO:HD2	1.59	0.83
1:I:769:ARG:HH11	1:I:769:ARG:HB2	1.41	0.83
1:G:789:THR:OG1	1:J:740:UNK:C	2.26	0.83
1:J:902:ARG:HH11	1:K:844:ASP:CG	1.86	0.83
1:A:730:UNK:CB	1:I:730:UNK:CB	2.57	0.83
1:F:863:ALA:HB1	1:F:864:PRO:HD2	1.60	0.83
1:J:926:GLU:OE2	2:K:1001:ADP:O3'	1.95	0.83
1:L:769:ARG:HH11	1:L:769:ARG:HB2	1.41	0.83
1:M:754:GLY:O	1:M:796:THR:HB	1.77	0.83
1:N:290:ILE:HD11	1:N:297:LYS:HE3	1.59	0.83
1:D:290:ILE:HD11	1:D:297:LYS:HE3	1.59	0.83
1:F:290:ILE:HD11	1:F:297:LYS:HE3	1.59	0.83
1:H:754:GLY:O	1:H:796:THR:HB	1.77	0.83
1:P:769:ARG:HH11	1:P:769:ARG:HB2	1.41	0.83
1:O:863:ALA:HB1	1:O:864:PRO:HD2	1.59	0.83
1:A:863:ALA:HB1	1:A:864:PRO:HD2	1.59	0.82
1:G:312:LEU:HD21	1:H:858:GLU:CG	2.07	0.82
1:G:863:ALA:HB1	1:G:864:PRO:HD2	1.59	0.82
1:L:863:ALA:HB1	1:L:864:PRO:HD2	1.60	0.82
1:A:740:UNK:HA	1:P:789:THR:O	1.79	0.82
1:G:789:THR:O	1:J:739:UNK:C	2.28	0.82
1:K:863:ALA:HB1	1:K:864:PRO:HD2	1.60	0.82
1:M:863:ALA:HB1	1:M:864:PRO:HD2	1.59	0.82
1:B:290:ILE:HD11	1:B:297:LYS:HE3	1.59	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:785:LYS:HG2	1:N:785:LYS:O	1.80	0.82
1:D:730:UNK:CB	1:N:730:UNK:N	2.43	0.82
1:H:290:ILE:HD11	1:H:297:LYS:HE3	1.59	0.82
1:O:754:GLY:O	1:O:796:THR:HB	1.77	0.82
1:N:316:THR:HG21	1:O:339:ARG:HD3	1.60	0.81
1:D:863:ALA:HB1	1:D:864:PRO:HD2	1.60	0.81
1:J:929:ILE:HD11	1:K:852:LEU:HD13	1.61	0.81
1:M:891:MET:HG3	1:N:852:LEU:HG	1.61	0.81
1:O:290:ILE:HD11	1:O:297:LYS:HE3	1.59	0.81
1:I:895:GLU:OE1	1:J:849:ARG:HG2	1.80	0.81
1:I:844:ASP:OD1	1:P:902:ARG:NH1	2.14	0.80
1:A:730:UNK:CB	1:I:729:UNK:C	2.60	0.80
1:B:730:UNK:CB	1:P:730:UNK:CB	2.60	0.79
1:F:903:LYS:HD2	1:G:841:ASP:OD2	1.83	0.79
1:F:894:ILE:CD1	1:G:852:LEU:HD11	2.10	0.79
1:F:316:THR:HG21	1:G:339:ARG:CD	2.12	0.79
1:G:789:THR:O	1:J:740:UNK:N	2.16	0.79
1:J:898:TYR:CE2	1:K:848:ALA:HB2	2.18	0.79
1:I:902:ARG:NH1	1:J:844:ASP:OD1	2.16	0.78
1:J:902:ARG:NH1	1:K:844:ASP:CG	2.42	0.78
1:C:785:LYS:HG3	1:N:785:LYS:HG3	1.63	0.78
1:C:891:MET:HE1	1:D:856:ARG:HD3	1.62	0.78
1:F:898:TYR:CD2	1:G:848:ALA:HB2	2.19	0.78
1:G:788:ILE:HA	1:J:741:UNK:CB	2.13	0.78
1:I:929:ILE:O	1:I:933:GLU:HG3	1.84	0.78
1:D:785:LYS:O	1:M:785:LYS:CB	2.31	0.78
1:D:785:LYS:HB3	1:M:785:LYS:CG	2.00	0.78
1:E:741:UNK:CA	1:L:788:ILE:HA	2.14	0.78
1:G:886:ILE:N	1:G:886:ILE:HD12	1.99	0.78
1:N:929:ILE:O	1:N:933:GLU:HG3	1.84	0.78
1:O:929:ILE:O	1:O:933:GLU:HG3	1.84	0.78
1:C:929:ILE:O	1:C:933:GLU:HG3	1.84	0.77
1:E:929:ILE:O	1:E:933:GLU:HG3	1.84	0.77
1:H:929:ILE:O	1:H:933:GLU:HG3	1.84	0.77
1:J:886:ILE:N	1:J:886:ILE:HD12	2.00	0.77
1:N:886:ILE:HD12	1:N:886:ILE:N	2.00	0.77
1:C:886:ILE:HD12	1:C:886:ILE:N	2.00	0.77
1:C:888:GLU:CG	1:D:856:ARG:HH12	1.89	0.77
1:G:929:ILE:O	1:G:933:GLU:HG3	1.84	0.77
1:B:929:ILE:O	1:B:933:GLU:HG3	1.84	0.77
1:F:902:ARG:HH11	1:G:844:ASP:CG	1.91	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:929:ILE:O	1:F:933:GLU:HG3	1.84	0.77
1:I:898:TYR:CE2	1:J:848:ALA:HB2	2.20	0.77
1:C:869:GLU:O	1:C:873:LYS:HD3	1.85	0.77
1:D:869:GLU:O	1:D:873:LYS:HD3	1.85	0.77
1:D:929:ILE:O	1:D:933:GLU:HG3	1.84	0.77
1:H:854:VAL:CG1	1:H:862:VAL:HB	2.15	0.77
1:B:869:GLU:O	1:B:873:LYS:HD3	1.85	0.77
1:C:327:VAL:HG12	1:C:802:ALA:HB3	1.67	0.77
1:D:730:UNK:CB	1:N:729:UNK:C	2.63	0.77
1:M:869:GLU:O	1:M:873:LYS:HD3	1.85	0.77
1:N:327:VAL:HG12	1:N:802:ALA:HB3	1.67	0.77
1:O:888:GLU:HG2	1:P:856:ARG:HH12	1.46	0.77
1:A:886:ILE:HD12	1:A:886:ILE:N	2.00	0.77
1:E:854:VAL:CG1	1:E:862:VAL:HB	2.15	0.77
1:F:891:MET:CE	1:G:856:ARG:CD	2.59	0.77
1:I:854:VAL:CG1	1:I:862:VAL:HB	2.15	0.77
1:J:327:VAL:HG12	1:J:802:ALA:HB3	1.67	0.77
1:J:869:GLU:O	1:J:873:LYS:HD3	1.85	0.77
1:K:327:VAL:HG12	1:K:802:ALA:HB3	1.67	0.77
1:L:886:ILE:N	1:L:886:ILE:HD12	2.00	0.77
1:O:327:VAL:HG12	1:O:802:ALA:HB3	1.67	0.77
1:P:929:ILE:O	1:P:933:GLU:HG3	1.84	0.77
1:E:886:ILE:N	1:E:886:ILE:HD12	1.99	0.77
1:K:869:GLU:O	1:K:873:LYS:HD3	1.85	0.77
1:A:929:ILE:O	1:A:933:GLU:HG3	1.84	0.77
1:F:854:VAL:CG1	1:F:862:VAL:HB	2.15	0.77
1:H:886:ILE:HD12	1:H:886:ILE:N	2.00	0.77
1:I:886:ILE:HD12	1:I:886:ILE:N	2.00	0.77
1:O:854:VAL:CG1	1:O:862:VAL:HB	2.15	0.77
1:A:854:VAL:CG1	1:A:862:VAL:HB	2.15	0.76
1:H:869:GLU:O	1:H:873:LYS:HD3	1.85	0.76
1:J:929:ILE:O	1:J:933:GLU:HG3	1.84	0.76
1:N:891:MET:CG	1:O:852:LEU:HG	2.06	0.76
1:O:886:ILE:N	1:O:886:ILE:HD12	1.99	0.76
1:K:854:VAL:CG1	1:K:862:VAL:HB	2.15	0.76
1:K:929:ILE:O	1:K:933:GLU:HG3	1.84	0.76
1:L:869:GLU:O	1:L:873:LYS:HD3	1.85	0.76
1:A:327:VAL:HG12	1:A:802:ALA:HB3	1.67	0.76
1:E:869:GLU:O	1:E:873:LYS:HD3	1.85	0.76
1:G:757:LEU:HD23	1:G:799:ILE:HB	1.68	0.76
1:I:757:LEU:HD23	1:I:799:ILE:HB	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:929:ILE:O	1:L:933:GLU:HG3	1.84	0.76
1:O:869:GLU:O	1:O:873:LYS:HD3	1.85	0.76
1:B:854:VAL:CG1	1:B:862:VAL:HB	2.15	0.76
1:D:886:ILE:N	1:D:886:ILE:HD12	1.99	0.76
1:G:869:GLU:O	1:G:873:LYS:HD3	1.85	0.76
1:I:869:GLU:O	1:I:873:LYS:HD3	1.85	0.76
1:L:312:LEU:HD21	1:M:858:GLU:HG3	1.65	0.76
1:M:929:ILE:O	1:M:933:GLU:HG3	1.84	0.76
1:B:757:LEU:HD23	1:B:799:ILE:HB	1.68	0.76
1:B:886:ILE:N	1:B:886:ILE:HD12	2.00	0.76
1:G:327:VAL:HG12	1:G:802:ALA:HB3	1.67	0.76
1:J:891:MET:CE	1:K:856:ARG:NH1	2.49	0.76
1:M:327:VAL:HG12	1:M:802:ALA:HB3	1.67	0.76
1:P:869:GLU:O	1:P:873:LYS:HD3	1.85	0.76
1:A:869:GLU:O	1:A:873:LYS:HD3	1.85	0.76
1:E:327:VAL:HG12	1:E:802:ALA:HB3	1.67	0.76
1:E:757:LEU:HD23	1:E:799:ILE:HB	1.68	0.76
1:I:327:VAL:HG12	1:I:802:ALA:HB3	1.67	0.76
1:K:886:ILE:HD12	1:K:886:ILE:N	2.00	0.76
1:M:886:ILE:N	1:M:886:ILE:HD12	2.00	0.76
1:F:316:THR:HG21	1:G:339:ARG:HD2	1.67	0.76
1:L:854:VAL:CG1	1:L:862:VAL:HB	2.15	0.76
1:M:854:VAL:CG1	1:M:862:VAL:HB	2.15	0.76
1:P:327:VAL:HG12	1:P:802:ALA:HB3	1.67	0.76
1:P:854:VAL:CG1	1:P:862:VAL:HB	2.15	0.76
1:B:788:ILE:HG22	1:O:740:UNK:C	2.16	0.76
1:F:886:ILE:HD12	1:F:886:ILE:N	1.99	0.76
1:G:854:VAL:CG1	1:G:862:VAL:HB	2.15	0.76
1:H:815:PRO:HD3	1:H:965:MET:HE2	1.68	0.76
1:I:929:ILE:CD1	1:J:852:LEU:HD13	2.16	0.76
1:B:815:PRO:HD3	1:B:965:MET:HE2	1.68	0.76
1:E:815:PRO:HD3	1:E:965:MET:HE2	1.68	0.76
1:F:327:VAL:HG12	1:F:802:ALA:HB3	1.67	0.76
1:F:869:GLU:O	1:F:873:LYS:HD3	1.85	0.76
1:J:854:VAL:CG1	1:J:862:VAL:HB	2.15	0.76
1:L:312:LEU:HD21	1:M:858:GLU:CG	2.16	0.76
1:O:757:LEU:HD23	1:O:799:ILE:HB	1.68	0.76
1:A:815:PRO:HD3	1:A:965:MET:HE2	1.68	0.75
1:D:757:LEU:HD23	1:D:799:ILE:HB	1.68	0.75
1:J:815:PRO:HD3	1:J:965:MET:HE2	1.68	0.75
1:B:327:VAL:HG12	1:B:802:ALA:HB3	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:349:ILE:HG21	1:J:743:UNK:O	1.87	0.75
1:K:781:ILE:HG22	1:K:782:SER:H	1.52	0.75
1:L:815:PRO:HD3	1:L:965:MET:HE2	1.68	0.75
1:O:781:ILE:HG22	1:O:782:SER:H	1.52	0.75
1:C:854:VAL:CG1	1:C:862:VAL:HB	2.15	0.75
1:H:349:ILE:HG21	1:H:743:UNK:O	1.87	0.75
1:I:349:ILE:HG21	1:I:743:UNK:O	1.87	0.75
1:M:781:ILE:HG22	1:M:782:SER:H	1.52	0.75
1:N:349:ILE:HG21	1:N:743:UNK:O	1.87	0.75
1:A:757:LEU:HD23	1:A:799:ILE:HB	1.68	0.75
1:C:757:LEU:HD23	1:C:799:ILE:HB	1.68	0.75
1:D:854:VAL:CG1	1:D:862:VAL:HB	2.15	0.75
1:E:920:ILE:HD12	1:E:924:GLN:HG3	1.69	0.75
1:F:349:ILE:HG21	1:F:743:UNK:O	1.87	0.75
1:G:781:ILE:HG22	1:G:782:SER:H	1.52	0.75
1:H:920:ILE:HD12	1:H:924:GLN:HG3	1.69	0.75
1:L:920:ILE:HD12	1:L:924:GLN:HG3	1.69	0.75
1:N:815:PRO:HD3	1:N:965:MET:HE2	1.68	0.75
1:N:869:GLU:O	1:N:873:LYS:HD3	1.85	0.75
1:P:886:ILE:HD12	1:P:886:ILE:N	2.00	0.75
1:A:920:ILE:HD12	1:A:924:GLN:HG3	1.69	0.75
1:B:349:ILE:HG21	1:B:743:UNK:O	1.87	0.75
1:F:815:PRO:HD3	1:F:965:MET:HE2	1.68	0.75
1:M:349:ILE:HG21	1:M:743:UNK:O	1.87	0.75
1:M:757:LEU:HD23	1:M:799:ILE:HB	1.68	0.75
1:N:757:LEU:HD23	1:N:799:ILE:HB	1.68	0.75
1:O:815:PRO:HD3	1:O:965:MET:HE2	1.68	0.75
1:P:815:PRO:HD3	1:P:965:MET:HE2	1.68	0.75
1:A:349:ILE:HG21	1:A:743:UNK:O	1.87	0.75
1:E:781:ILE:HG22	1:E:782:SER:H	1.52	0.75
1:F:781:ILE:HG22	1:F:782:SER:H	1.52	0.75
1:G:920:ILE:HD12	1:G:924:GLN:HG3	1.69	0.75
1:I:945:THR:HG23	1:I:948:ASP:OD1	1.87	0.75
1:K:945:THR:HG23	1:K:948:ASP:OD1	1.87	0.75
1:M:815:PRO:HD3	1:M:965:MET:HE2	1.68	0.75
1:P:920:ILE:HD12	1:P:924:GLN:HG3	1.69	0.75
1:D:327:VAL:HG12	1:D:802:ALA:HB3	1.67	0.75
1:G:312:LEU:HD11	1:H:857:GLY:O	1.86	0.75
1:L:349:ILE:HG21	1:L:743:UNK:O	1.87	0.75
1:L:945:THR:HG23	1:L:948:ASP:OD1	1.87	0.75
1:M:945:THR:HG23	1:M:948:ASP:OD1	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:781:ILE:HG22	1:D:782:SER:H	1.52	0.74
1:N:854:VAL:CG1	1:N:862:VAL:HB	2.15	0.74
1:P:349:ILE:HG21	1:P:743:UNK:O	1.87	0.74
1:P:781:ILE:HG22	1:P:782:SER:H	1.52	0.74
1:J:894:ILE:CD1	1:K:852:LEU:HD11	2.15	0.74
1:L:327:VAL:HG12	1:L:802:ALA:HB3	1.67	0.74
1:N:781:ILE:HG22	1:N:782:SER:H	1.52	0.74
1:N:945:THR:HG23	1:N:948:ASP:OD1	1.87	0.74
1:O:349:ILE:HG21	1:O:743:UNK:O	1.87	0.74
1:P:945:THR:HG23	1:P:948:ASP:OD1	1.87	0.74
1:D:815:PRO:HD3	1:D:965:MET:HE2	1.68	0.74
1:G:349:ILE:HG21	1:G:743:UNK:O	1.87	0.74
1:G:945:THR:HG23	1:G:948:ASP:OD1	1.87	0.74
1:H:327:VAL:HG12	1:H:802:ALA:HB3	1.67	0.74
1:L:757:LEU:HD23	1:L:799:ILE:HB	1.68	0.74
1:F:757:LEU:HD23	1:F:799:ILE:HB	1.68	0.74
1:K:316:THR:HG21	1:L:339:ARG:HD2	1.68	0.74
1:O:920:ILE:HD12	1:O:924:GLN:HG3	1.69	0.74
1:P:757:LEU:HD23	1:P:799:ILE:HB	1.68	0.74
1:H:757:LEU:HD23	1:H:799:ILE:HB	1.68	0.74
1:I:815:PRO:HD3	1:I:965:MET:HE2	1.68	0.74
1:I:856:ARG:HD3	1:P:891:MET:HE1	1.55	0.74
1:J:757:LEU:HD23	1:J:799:ILE:HB	1.68	0.74
1:C:349:ILE:HG21	1:C:743:UNK:O	1.87	0.74
1:J:312:LEU:HD21	1:K:858:GLU:CB	2.16	0.74
1:G:305:PHE:CE2	1:G:938:MET:HG3	2.23	0.74
1:K:757:LEU:HD23	1:K:799:ILE:HB	1.68	0.74
1:O:305:PHE:CE2	1:O:938:MET:HG3	2.23	0.74
1:A:305:PHE:CE2	1:A:938:MET:HG3	2.23	0.74
1:D:920:ILE:HD12	1:D:924:GLN:HG3	1.69	0.74
1:E:945:THR:HG23	1:E:948:ASP:OD1	1.87	0.74
1:F:920:ILE:HD12	1:F:924:GLN:HG3	1.69	0.74
1:J:781:ILE:HG22	1:J:782:SER:H	1.52	0.74
1:N:903:LYS:HZ3	1:O:839:PRO:CB	1.96	0.74
1:B:945:THR:HG23	1:B:948:ASP:OD1	1.87	0.74
1:C:305:PHE:CE2	1:C:938:MET:HG3	2.23	0.74
1:C:864:PRO:HB2	1:C:866:ILE:O	1.88	0.74
1:E:349:ILE:HG21	1:E:743:UNK:O	1.87	0.74
1:E:864:PRO:HB2	1:E:866:ILE:O	1.88	0.74
1:H:864:PRO:HB2	1:H:866:ILE:O	1.88	0.74
1:J:864:PRO:HB2	1:J:866:ILE:O	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:305:PHE:CE2	1:L:938:MET:HG3	2.23	0.74
1:N:920:ILE:HD12	1:N:924:GLN:HG3	1.69	0.74
1:A:864:PRO:HB2	1:A:866:ILE:O	1.88	0.74
1:C:939:ARG:O	1:C:939:ARG:HG2	1.88	0.74
1:F:305:PHE:CE2	1:F:938:MET:HG3	2.23	0.74
1:I:305:PHE:CE2	1:I:938:MET:HG3	2.23	0.74
1:J:920:ILE:HD12	1:J:924:GLN:HG3	1.69	0.74
1:K:864:PRO:HB2	1:K:866:ILE:O	1.88	0.74
1:M:864:PRO:HB2	1:M:866:ILE:O	1.88	0.74
1:B:864:PRO:HB2	1:B:866:ILE:O	1.88	0.73
1:C:920:ILE:HD12	1:C:924:GLN:HG3	1.69	0.73
1:F:864:PRO:HB2	1:F:866:ILE:O	1.88	0.73
1:G:815:PRO:HD3	1:G:965:MET:HE2	1.68	0.73
1:G:939:ARG:HG2	1:G:939:ARG:O	1.88	0.73
1:H:945:THR:HG23	1:H:948:ASP:OD1	1.87	0.73
1:J:945:THR:HG23	1:J:948:ASP:OD1	1.87	0.73
1:K:815:PRO:HD3	1:K:965:MET:HE2	1.68	0.73
1:M:939:ARG:HG2	1:M:939:ARG:O	1.88	0.73
1:D:305:PHE:CE2	1:D:938:MET:HG3	2.23	0.73
1:E:305:PHE:CE2	1:E:938:MET:HG3	2.23	0.73
1:I:886:ILE:HD13	1:J:856:ARG:HB3	1.67	0.73
1:O:864:PRO:HB2	1:O:866:ILE:O	1.88	0.73
1:A:945:THR:HG23	1:A:948:ASP:OD1	1.87	0.73
1:B:920:ILE:HD12	1:B:924:GLN:HG3	1.69	0.73
1:D:939:ARG:O	1:D:939:ARG:HG2	1.88	0.73
1:J:310:ARG:HD3	1:K:858:GLU:HG3	1.69	0.73
1:B:305:PHE:CE2	1:B:938:MET:HG3	2.23	0.73
1:C:894:ILE:CD1	1:D:852:LEU:HD11	2.13	0.73
1:F:945:THR:HG23	1:F:948:ASP:OD1	1.87	0.73
1:G:864:PRO:HB2	1:G:866:ILE:O	1.88	0.73
1:I:920:ILE:HD12	1:I:924:GLN:HG3	1.69	0.73
1:J:305:PHE:CE2	1:J:938:MET:HG3	2.23	0.73
1:N:923:ARG:HG3	1:N:923:ARG:HH11	1.54	0.73
1:A:781:ILE:HG22	1:A:782:SER:H	1.52	0.73
1:A:923:ARG:HG3	1:A:923:ARG:HH11	1.54	0.73
1:I:864:PRO:HB2	1:I:866:ILE:O	1.88	0.73
1:N:864:PRO:HB2	1:N:866:ILE:O	1.88	0.73
1:C:815:PRO:HD3	1:C:965:MET:HE2	1.68	0.73
1:D:785:LYS:HG3	1:M:785:LYS:CE	2.18	0.73
1:F:891:MET:CE	1:G:856:ARG:CZ	2.63	0.73
1:M:920:ILE:HD12	1:M:924:GLN:HG3	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:939:ARG:O	1:F:939:ARG:HG2	1.88	0.73
1:H:923:ARG:HH11	1:H:923:ARG:HG3	1.54	0.73
1:I:781:ILE:HG22	1:I:782:SER:H	1.52	0.73
1:L:864:PRO:HB2	1:L:866:ILE:O	1.88	0.73
1:P:939:ARG:HG2	1:P:939:ARG:O	1.88	0.73
1:A:745:UNK:O	1:A:795:ARG:NH1	2.22	0.73
1:D:349:ILE:HG21	1:D:743:UNK:O	1.87	0.73
1:E:745:UNK:O	1:E:795:ARG:NH1	2.22	0.73
1:K:349:ILE:HG21	1:K:743:UNK:O	1.87	0.73
1:K:899:VAL:HG23	1:L:841:ASP:HA	1.71	0.73
1:K:923:ARG:HH11	1:K:923:ARG:HG3	1.54	0.73
1:L:781:ILE:HG22	1:L:782:SER:H	1.52	0.73
1:B:781:ILE:HG22	1:B:782:SER:H	1.52	0.73
1:D:864:PRO:HB2	1:D:866:ILE:O	1.88	0.73
1:J:939:ARG:HG2	1:J:939:ARG:O	1.88	0.73
1:L:939:ARG:O	1:L:939:ARG:HG2	1.88	0.73
1:M:745:UNK:O	1:M:795:ARG:NH1	2.22	0.73
1:P:305:PHE:CE2	1:P:938:MET:HG3	2.23	0.73
1:G:730:UNK:CA	1:K:729:UNK:O	2.37	0.73
1:H:305:PHE:CE2	1:H:938:MET:HG3	2.23	0.73
1:I:903:LYS:HD2	1:J:841:ASP:OD2	1.88	0.73
1:J:745:UNK:O	1:J:795:ARG:NH1	2.22	0.73
1:L:745:UNK:O	1:L:795:ARG:NH1	2.22	0.73
1:M:305:PHE:CE2	1:M:938:MET:HG3	2.23	0.73
1:O:923:ARG:HH11	1:O:923:ARG:HG3	1.54	0.73
1:B:923:ARG:HH11	1:B:923:ARG:HG3	1.54	0.72
1:C:781:ILE:HG22	1:C:782:SER:H	1.52	0.72
1:K:305:PHE:CE2	1:K:938:MET:HG3	2.23	0.72
1:N:305:PHE:CE2	1:N:938:MET:HG3	2.23	0.72
1:O:945:THR:HG23	1:O:948:ASP:OD1	1.87	0.72
1:I:939:ARG:O	1:I:939:ARG:HG2	1.88	0.72
1:K:920:ILE:HD12	1:K:924:GLN:HG3	1.69	0.72
1:K:939:ARG:O	1:K:939:ARG:HG2	1.88	0.72
1:P:864:PRO:HB2	1:P:866:ILE:O	1.88	0.72
1:C:745:UNK:O	1:C:795:ARG:NH1	2.22	0.72
1:D:945:THR:HG23	1:D:948:ASP:OD1	1.87	0.72
1:H:745:UNK:O	1:H:795:ARG:NH1	2.22	0.72
1:I:923:ARG:HG3	1:I:923:ARG:HH11	1.54	0.72
1:I:929:ILE:HD11	1:J:852:LEU:CD1	2.19	0.72
1:M:923:ARG:HH11	1:M:923:ARG:HG3	1.54	0.72
1:N:745:UNK:O	1:N:795:ARG:NH1	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:923:ARG:HH11	1:C:923:ARG:HG3	1.54	0.72
1:H:781:ILE:HG22	1:H:782:SER:H	1.52	0.72
1:F:745:UNK:O	1:F:795:ARG:NH1	2.22	0.72
1:K:903:LYS:HE2	1:K:903:LYS:N	2.05	0.72
1:C:945:THR:HG23	1:C:948:ASP:OD1	1.87	0.72
1:D:745:UNK:O	1:D:795:ARG:NH1	2.22	0.72
1:G:903:LYS:N	1:G:903:LYS:HE2	2.05	0.72
1:I:903:LYS:HE2	1:I:903:LYS:N	2.05	0.72
1:A:939:ARG:O	1:A:939:ARG:HG2	1.88	0.72
1:B:745:UNK:O	1:B:795:ARG:NH1	2.22	0.72
1:B:903:LYS:N	1:B:903:LYS:HE2	2.05	0.72
1:E:923:ARG:HH11	1:E:923:ARG:HG3	1.54	0.72
1:H:903:LYS:HE2	1:H:903:LYS:N	2.05	0.72
1:L:923:ARG:HH11	1:L:923:ARG:HG3	1.54	0.72
1:N:903:LYS:HE2	1:N:903:LYS:N	2.05	0.72
1:F:808:ARG:NH1	1:F:808:ARG:HB2	2.05	0.72
1:F:923:ARG:HG3	1:F:923:ARG:HH11	1.54	0.72
1:G:745:UNK:O	1:G:795:ARG:NH1	2.22	0.72
1:H:808:ARG:NH1	1:H:808:ARG:HB2	2.05	0.72
1:L:290:ILE:C	1:L:290:ILE:HD12	2.15	0.72
1:O:314:ASP:O	1:P:340:TYR:CE2	2.43	0.72
1:O:903:LYS:N	1:O:903:LYS:HE2	2.05	0.72
1:P:923:ARG:HH11	1:P:923:ARG:HG3	1.54	0.72
1:A:903:LYS:HE2	1:A:903:LYS:N	2.05	0.71
1:B:939:ARG:HG2	1:B:939:ARG:O	1.88	0.71
1:D:290:ILE:C	1:D:290:ILE:HD12	2.15	0.71
1:H:290:ILE:C	1:H:290:ILE:HD12	2.15	0.71
1:H:939:ARG:O	1:H:939:ARG:HG2	1.88	0.71
1:J:290:ILE:C	1:J:290:ILE:HD12	2.15	0.71
1:J:898:TYR:HD2	1:K:848:ALA:HB2	1.52	0.71
1:K:290:ILE:C	1:K:290:ILE:HD12	2.15	0.71
1:K:745:UNK:O	1:K:795:ARG:NH1	2.22	0.71
1:O:808:ARG:NH1	1:O:808:ARG:HB2	2.05	0.71
1:O:939:ARG:HG2	1:O:939:ARG:O	1.88	0.71
1:P:745:UNK:O	1:P:795:ARG:NH1	2.22	0.71
1:F:903:LYS:HE2	1:F:903:LYS:N	2.05	0.71
1:J:923:ARG:HH11	1:J:923:ARG:HG3	1.54	0.71
1:M:290:ILE:C	1:M:290:ILE:HD12	2.15	0.71
1:M:903:LYS:HE2	1:M:903:LYS:N	2.05	0.71
1:O:745:UNK:O	1:O:795:ARG:NH1	2.22	0.71
1:B:729:UNK:C	1:P:730:UNK:CB	2.68	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:897:TYR:OH	1:B:957:GLU:HG2	1.90	0.71
1:C:903:LYS:HE2	1:C:903:LYS:N	2.05	0.71
1:N:939:ARG:O	1:N:939:ARG:HG2	1.88	0.71
1:P:808:ARG:NH1	1:P:808:ARG:HB2	2.05	0.71
1:A:791:THR:O	1:P:738:UNK:HA	1.90	0.71
1:A:808:ARG:NH1	1:A:808:ARG:HB2	2.05	0.71
1:I:897:TYR:OH	1:I:957:GLU:HG2	1.90	0.71
1:P:903:LYS:HE2	1:P:903:LYS:N	2.05	0.71
1:B:290:ILE:C	1:B:290:ILE:HD12	2.15	0.71
1:B:891:MET:HE1	1:C:856:ARG:CZ	2.20	0.71
1:F:898:TYR:HD2	1:G:848:ALA:HB2	1.53	0.71
1:K:808:ARG:HB2	1:K:808:ARG:NH1	2.05	0.71
1:L:897:TYR:OH	1:L:957:GLU:HG2	1.90	0.71
1:N:808:ARG:HB2	1:N:808:ARG:NH1	2.05	0.71
1:C:808:ARG:HB2	1:C:808:ARG:NH1	2.05	0.71
1:E:897:TYR:OH	1:E:957:GLU:HG2	1.90	0.71
1:E:903:LYS:HE2	1:E:903:LYS:N	2.05	0.71
1:G:290:ILE:C	1:G:290:ILE:HD12	2.15	0.71
1:I:808:ARG:NH1	1:I:808:ARG:HB2	2.05	0.71
1:P:290:ILE:C	1:P:290:ILE:HD12	2.16	0.71
1:A:290:ILE:HD12	1:A:290:ILE:C	2.15	0.71
1:B:808:ARG:NH1	1:B:808:ARG:HB2	2.05	0.71
1:D:785:LYS:CA	1:M:785:LYS:HG2	2.21	0.71
1:D:808:ARG:NH1	1:D:808:ARG:HB2	2.05	0.71
1:I:290:ILE:HD12	1:I:290:ILE:C	2.15	0.71
1:I:745:UNK:O	1:I:795:ARG:NH1	2.22	0.71
1:I:886:ILE:HB	1:J:856:ARG:CD	2.18	0.71
1:J:808:ARG:NH1	1:J:808:ARG:HB2	2.05	0.71
1:F:290:ILE:C	1:F:290:ILE:HD12	2.15	0.71
1:G:808:ARG:NH1	1:G:808:ARG:HB2	2.05	0.71
1:L:808:ARG:NH1	1:L:808:ARG:HB2	2.05	0.71
1:M:897:TYR:OH	1:M:957:GLU:HG2	1.90	0.71
1:L:853:ARG:HH12	1:L:856:ARG:HH21	1.39	0.71
1:L:891:MET:HE1	1:M:856:ARG:CZ	2.21	0.71
1:M:853:ARG:HH12	1:M:856:ARG:HH21	1.39	0.71
1:M:902:ARG:NH2	1:N:837:ASP:OD2	2.23	0.71
1:N:897:TYR:OH	1:N:957:GLU:HG2	1.90	0.71
1:A:897:TYR:OH	1:A:957:GLU:HG2	1.90	0.71
1:B:853:ARG:HH12	1:B:856:ARG:HH21	1.39	0.71
1:D:903:LYS:N	1:D:903:LYS:HE2	2.05	0.71
1:E:939:ARG:HG2	1:E:939:ARG:O	1.88	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:897:TYR:OH	1:J:957:GLU:HG2	1.90	0.71
1:M:808:ARG:NH1	1:M:808:ARG:HB2	2.05	0.71
1:N:853:ARG:HH12	1:N:856:ARG:HH21	1.39	0.71
1:E:853:ARG:HH12	1:E:856:ARG:HH21	1.39	0.70
1:A:778:GLN:O	1:A:779:GLN:HB2	1.91	0.70
1:B:778:GLN:O	1:B:779:GLN:HB2	1.92	0.70
1:C:897:TYR:OH	1:C:957:GLU:HG2	1.90	0.70
1:D:923:ARG:HH11	1:D:923:ARG:HG3	1.54	0.70
1:E:290:ILE:C	1:E:290:ILE:HD12	2.15	0.70
1:G:853:ARG:NH1	1:G:856:ARG:HH21	1.89	0.70
1:I:853:ARG:NH1	1:I:856:ARG:HH21	1.89	0.70
1:I:853:ARG:HH12	1:I:856:ARG:HH21	1.39	0.70
1:J:903:LYS:N	1:J:903:LYS:HE2	2.05	0.70
1:K:853:ARG:NH1	1:K:856:ARG:HH21	1.89	0.70
1:C:853:ARG:HH12	1:C:856:ARG:HH21	1.39	0.70
1:E:853:ARG:NH1	1:E:856:ARG:HH21	1.89	0.70
1:G:312:LEU:CD2	1:H:858:GLU:HG3	2.14	0.70
1:G:923:ARG:HH11	1:G:923:ARG:HG3	1.54	0.70
1:H:897:TYR:OH	1:H:957:GLU:HG2	1.90	0.70
1:I:778:GLN:O	1:I:779:GLN:HB2	1.92	0.70
1:L:903:LYS:HE2	1:L:903:LYS:N	2.05	0.70
1:N:290:ILE:C	1:N:290:ILE:HD12	2.15	0.70
1:A:853:ARG:HH12	1:A:856:ARG:HH21	1.39	0.70
1:C:290:ILE:C	1:C:290:ILE:HD12	2.15	0.70
1:D:853:ARG:NH1	1:D:856:ARG:HH21	1.89	0.70
1:D:897:TYR:OH	1:D:957:GLU:HG2	1.90	0.70
1:G:897:TYR:OH	1:G:957:GLU:HG2	1.90	0.70
1:O:853:ARG:NH1	1:O:856:ARG:HH21	1.89	0.70
1:O:897:TYR:OH	1:O:957:GLU:HG2	1.90	0.70
1:P:778:GLN:O	1:P:779:GLN:HB2	1.92	0.70
1:A:853:ARG:NH1	1:A:856:ARG:HH21	1.89	0.70
1:E:753:GLY:N	1:E:795:ARG:NH1	2.40	0.70
1:O:290:ILE:C	1:O:290:ILE:HD12	2.15	0.70
1:O:778:GLN:CD	1:P:354:UNK:CB	2.64	0.70
1:A:753:GLY:N	1:A:795:ARG:NH1	2.40	0.70
1:D:753:GLY:N	1:D:795:ARG:NH1	2.40	0.70
1:I:753:GLY:N	1:I:795:ARG:NH1	2.40	0.70
1:J:753:GLY:N	1:J:795:ARG:NH1	2.40	0.70
1:K:869:GLU:HA	1:K:872:ARG:NH1	2.07	0.70
1:M:753:GLY:N	1:M:795:ARG:NH1	2.40	0.70
1:P:853:ARG:HH12	1:P:856:ARG:HH21	1.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:808:ARG:NH1	1:E:808:ARG:HB2	2.05	0.70
1:F:853:ARG:NH1	1:F:856:ARG:HH21	1.89	0.70
1:M:853:ARG:NH1	1:M:856:ARG:HH21	1.89	0.70
1:N:869:GLU:HA	1:N:872:ARG:NH1	2.07	0.70
1:J:853:ARG:HH12	1:J:856:ARG:HH21	1.39	0.70
1:K:897:TYR:OH	1:K:957:GLU:HG2	1.90	0.70
1:L:778:GLN:O	1:L:779:GLN:HB2	1.92	0.70
1:L:853:ARG:NH1	1:L:856:ARG:HH21	1.89	0.70
1:P:869:GLU:HA	1:P:872:ARG:NH1	2.07	0.70
1:C:316:THR:HG21	1:D:339:ARG:CD	2.22	0.70
1:C:853:ARG:NH1	1:C:856:ARG:HH21	1.89	0.70
1:E:930:ARG:HG3	1:E:930:ARG:HH11	1.57	0.70
1:F:897:TYR:OH	1:F:957:GLU:HG2	1.90	0.70
1:N:309:SER:HB2	1:N:320:GLY:HA3	1.74	0.70
1:A:869:GLU:HA	1:A:872:ARG:NH1	2.07	0.70
1:B:853:ARG:NH1	1:B:856:ARG:HH21	1.89	0.70
1:D:309:SER:HB2	1:D:320:GLY:HA3	1.74	0.70
1:F:853:ARG:HH12	1:F:856:ARG:HH21	1.39	0.70
1:P:753:GLY:N	1:P:795:ARG:NH1	2.40	0.70
1:C:930:ARG:HH11	1:C:930:ARG:HG3	1.57	0.69
1:F:753:GLY:N	1:F:795:ARG:NH1	2.40	0.69
1:O:778:GLN:O	1:O:779:GLN:HB2	1.91	0.69
1:B:309:SER:HB2	1:B:320:GLY:HA3	1.74	0.69
1:B:753:GLY:N	1:B:795:ARG:NH1	2.40	0.69
1:D:869:GLU:HA	1:D:872:ARG:NH1	2.07	0.69
1:G:778:GLN:O	1:G:779:GLN:HB2	1.92	0.69
1:H:853:ARG:HH12	1:H:856:ARG:HH21	1.39	0.69
1:M:903:LYS:HZ3	1:N:839:PRO:HB2	1.55	0.69
1:O:753:GLY:N	1:O:795:ARG:NH1	2.40	0.69
1:O:930:ARG:HH11	1:O:930:ARG:HG3	1.57	0.69
1:P:897:TYR:OH	1:P:957:GLU:HG2	1.90	0.69
1:D:930:ARG:HH11	1:D:930:ARG:HG3	1.57	0.69
1:E:309:SER:HB2	1:E:320:GLY:HA3	1.74	0.69
1:H:309:SER:HB2	1:H:320:GLY:HA3	1.74	0.69
1:J:778:GLN:O	1:J:779:GLN:HB2	1.92	0.69
1:K:753:GLY:N	1:K:795:ARG:NH1	2.40	0.69
1:K:853:ARG:HH12	1:K:856:ARG:HH21	1.39	0.69
1:P:309:SER:HB2	1:P:320:GLY:HA3	1.74	0.69
1:G:350:TYR:H	1:G:360:UNK:CB	2.06	0.69
1:G:853:ARG:HH12	1:G:856:ARG:HH21	1.39	0.69
1:H:852:LEU:H	1:H:852:LEU:HD22	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:309:SER:HB2	1:J:320:GLY:HA3	1.74	0.69
1:J:898:TYR:HD2	1:K:848:ALA:CB	2.04	0.69
1:N:809:PHE:O	1:N:811:ARG:N	2.26	0.69
1:O:853:ARG:HH12	1:O:856:ARG:HH21	1.39	0.69
1:A:930:ARG:HH11	1:A:930:ARG:HG3	1.57	0.69
1:C:891:MET:HG3	1:D:852:LEU:HB3	1.74	0.69
1:D:778:GLN:O	1:D:779:GLN:HB2	1.91	0.69
1:D:853:ARG:HH12	1:D:856:ARG:HH21	1.39	0.69
1:E:350:TYR:H	1:E:360:UNK:CB	2.06	0.69
1:I:930:ARG:HH11	1:I:930:ARG:HG3	1.57	0.69
1:N:753:GLY:N	1:N:795:ARG:NH1	2.40	0.69
1:C:309:SER:HB2	1:C:320:GLY:HA3	1.74	0.69
1:C:753:GLY:N	1:C:795:ARG:NH1	2.40	0.69
1:E:890:ALA:HB1	1:E:949:ALA:HB2	1.75	0.69
1:H:853:ARG:NH1	1:H:856:ARG:HH21	1.89	0.69
1:J:930:ARG:HH11	1:J:930:ARG:HG3	1.57	0.69
1:L:309:SER:HB2	1:L:320:GLY:HA3	1.74	0.69
1:M:890:ALA:HB1	1:M:949:ALA:HB2	1.75	0.69
1:N:853:ARG:NH1	1:N:856:ARG:HH21	1.89	0.69
1:P:930:ARG:HG3	1:P:930:ARG:HH11	1.57	0.69
1:A:852:LEU:HD22	1:A:852:LEU:H	1.58	0.69
1:B:350:TYR:H	1:B:360:UNK:CB	2.05	0.69
1:D:809:PHE:O	1:D:811:ARG:N	2.26	0.69
1:D:852:LEU:HD22	1:D:852:LEU:H	1.58	0.69
1:F:309:SER:HB2	1:F:320:GLY:HA3	1.74	0.69
1:F:809:PHE:O	1:F:811:ARG:N	2.26	0.69
1:H:753:GLY:N	1:H:795:ARG:NH1	2.40	0.69
1:K:350:TYR:H	1:K:360:UNK:CB	2.06	0.69
1:O:316:THR:HG21	1:P:339:ARG:HD2	0.78	0.69
1:O:869:GLU:HA	1:O:872:ARG:NH1	2.07	0.69
1:P:350:TYR:H	1:P:360:UNK:CB	2.06	0.69
1:A:309:SER:HB2	1:A:320:GLY:HA3	1.74	0.69
1:A:789:THR:O	1:P:740:UNK:CA	2.35	0.69
1:C:809:PHE:O	1:C:811:ARG:N	2.26	0.69
1:E:739:UNK:O	1:L:790:ALA:HA	1.92	0.69
1:E:778:GLN:O	1:E:779:GLN:HB2	1.91	0.69
1:F:869:GLU:HA	1:F:872:ARG:NH1	2.07	0.69
1:G:753:GLY:N	1:G:795:ARG:NH1	2.40	0.69
1:H:350:TYR:H	1:H:360:UNK:CB	2.06	0.69
1:H:809:PHE:O	1:H:811:ARG:N	2.26	0.69
1:I:809:PHE:O	1:I:811:ARG:N	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:869:GLU:HA	1:J:872:ARG:NH1	2.07	0.69
1:K:852:LEU:H	1:K:852:LEU:HD22	1.58	0.69
1:M:852:LEU:H	1:M:852:LEU:HD22	1.58	0.69
1:M:869:GLU:HA	1:M:872:ARG:NH1	2.07	0.69
1:N:350:TYR:H	1:N:360:UNK:CB	2.06	0.69
1:N:852:LEU:HD22	1:N:852:LEU:H	1.58	0.69
1:A:350:TYR:H	1:A:360:UNK:CB	2.06	0.69
1:J:853:ARG:NH1	1:J:856:ARG:HH21	1.89	0.69
1:J:890:ALA:HB1	1:J:949:ALA:HB2	1.75	0.69
1:K:809:PHE:O	1:K:811:ARG:N	2.26	0.69
1:L:753:GLY:N	1:L:795:ARG:NH1	2.40	0.69
1:L:930:ARG:HH11	1:L:930:ARG:HG3	1.57	0.69
1:M:809:PHE:O	1:M:811:ARG:N	2.26	0.69
1:P:890:ALA:HB1	1:P:949:ALA:HB2	1.75	0.69
1:C:350:TYR:H	1:C:360:UNK:CB	2.06	0.69
1:C:852:LEU:H	1:C:852:LEU:HD22	1.58	0.69
1:C:869:GLU:HA	1:C:872:ARG:NH1	2.07	0.69
1:D:345:ALA:HB3	1:D:348:ALA:HB2	1.75	0.69
1:E:809:PHE:O	1:E:811:ARG:N	2.26	0.69
1:F:852:LEU:HD22	1:F:852:LEU:H	1.58	0.69
1:I:891:MET:CE	1:J:856:ARG:NH2	2.46	0.69
1:N:778:GLN:O	1:N:779:GLN:HB2	1.92	0.69
1:O:809:PHE:O	1:O:811:ARG:N	2.26	0.69
1:F:778:GLN:O	1:F:779:GLN:HB2	1.92	0.68
1:G:890:ALA:HB1	1:G:949:ALA:HB2	1.75	0.68
1:G:930:ARG:HH11	1:G:930:ARG:HG3	1.57	0.68
1:H:345:ALA:HB3	1:H:348:ALA:HB2	1.75	0.68
1:I:350:TYR:H	1:I:360:UNK:CB	2.06	0.68
1:I:852:LEU:HD22	1:I:852:LEU:H	1.58	0.68
1:I:869:GLU:HA	1:I:872:ARG:NH1	2.07	0.68
1:M:930:ARG:HG3	1:M:930:ARG:HH11	1.57	0.68
1:O:309:SER:HB2	1:O:320:GLY:HA3	1.74	0.68
1:O:891:MET:HG3	1:P:852:LEU:HG	1.75	0.68
1:P:853:ARG:NH1	1:P:856:ARG:HH21	1.89	0.68
1:B:869:GLU:HA	1:B:872:ARG:NH1	2.07	0.68
1:C:345:ALA:HB3	1:C:348:ALA:HB2	1.75	0.68
1:C:890:ALA:HB1	1:C:949:ALA:HB2	1.75	0.68
1:D:899:VAL:HG23	1:E:841:ASP:HA	1.76	0.68
1:G:869:GLU:HA	1:G:872:ARG:NH1	2.07	0.68
1:I:309:SER:HB2	1:I:320:GLY:HA3	1.74	0.68
1:I:890:ALA:HB1	1:I:949:ALA:HB2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:345:ALA:HB3	1:K:348:ALA:HB2	1.75	0.68
1:K:903:LYS:HD2	1:L:841:ASP:OD1	1.92	0.68
1:L:852:LEU:HD22	1:L:852:LEU:H	1.58	0.68
1:P:345:ALA:HB3	1:P:348:ALA:HB2	1.75	0.68
1:P:852:LEU:H	1:P:852:LEU:HD22	1.58	0.68
1:D:350:TYR:H	1:D:360:UNK:CB	2.06	0.68
1:D:785:LYS:HG3	1:M:785:LYS:HG3	0.70	0.68
1:L:809:PHE:O	1:L:811:ARG:N	2.26	0.68
1:N:345:ALA:HB3	1:N:348:ALA:HB2	1.75	0.68
1:O:852:LEU:HD22	1:O:852:LEU:H	1.58	0.68
1:B:345:ALA:HB3	1:B:348:ALA:HB2	1.75	0.68
1:F:345:ALA:HB3	1:F:348:ALA:HB2	1.75	0.68
1:I:894:ILE:HD11	1:J:852:LEU:CG	2.23	0.68
1:J:809:PHE:O	1:J:811:ARG:N	2.26	0.68
1:L:350:TYR:H	1:L:360:UNK:CB	2.06	0.68
1:C:778:GLN:O	1:C:779:GLN:HB2	1.92	0.68
1:F:350:TYR:H	1:F:360:UNK:CB	2.06	0.68
1:J:345:ALA:HB3	1:J:348:ALA:HB2	1.75	0.68
1:M:345:ALA:HB3	1:M:348:ALA:HB2	1.75	0.68
1:M:783:ILE:HD12	1:M:783:ILE:N	2.09	0.68
1:P:783:ILE:HD12	1:P:783:ILE:N	2.09	0.68
1:A:809:PHE:O	1:A:811:ARG:N	2.26	0.68
1:B:809:PHE:O	1:B:811:ARG:N	2.26	0.68
1:H:778:GLN:O	1:H:779:GLN:HB2	1.91	0.68
1:L:345:ALA:HB3	1:L:348:ALA:HB2	1.75	0.68
1:M:778:GLN:O	1:M:779:GLN:HB2	1.91	0.68
1:M:867:PRO:CB	1:M:870:ILE:HD13	2.21	0.68
1:A:783:ILE:N	1:A:783:ILE:HD12	2.09	0.68
1:A:890:ALA:HB1	1:A:949:ALA:HB2	1.75	0.68
1:D:785:LYS:CB	1:M:785:LYS:O	2.42	0.68
1:E:345:ALA:HB3	1:E:348:ALA:HB2	1.75	0.68
1:G:809:PHE:O	1:G:811:ARG:N	2.26	0.68
1:K:783:ILE:HD12	1:K:783:ILE:N	2.09	0.68
1:L:869:GLU:HA	1:L:872:ARG:NH1	2.07	0.68
1:L:890:ALA:HB1	1:L:949:ALA:HB2	1.75	0.68
1:P:809:PHE:O	1:P:811:ARG:N	2.26	0.68
1:D:867:PRO:CB	1:D:870:ILE:HD13	2.21	0.68
1:K:930:ARG:HH11	1:K:930:ARG:HG3	1.57	0.68
1:M:309:SER:HB2	1:M:320:GLY:HA3	1.74	0.68
1:N:783:ILE:HD12	1:N:783:ILE:N	2.09	0.68
1:O:295:GLU:CD	1:O:295:GLU:H	2.02	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:852:LEU:H	1:B:852:LEU:HD22	1.58	0.68
1:B:890:ALA:HB1	1:B:949:ALA:HB2	1.75	0.68
1:D:295:GLU:CD	1:D:295:GLU:H	2.02	0.68
1:B:295:GLU:CD	1:B:295:GLU:H	2.02	0.68
1:B:869:GLU:HG2	1:B:870:ILE:HD12	1.76	0.68
1:F:890:ALA:HB1	1:F:949:ALA:HB2	1.75	0.68
1:F:930:ARG:HH11	1:F:930:ARG:HG3	1.57	0.68
1:A:339:ARG:CD	1:H:316:THR:HG21	2.21	0.67
1:E:741:UNK:N	1:L:788:ILE:HG22	2.09	0.67
1:E:869:GLU:HA	1:E:872:ARG:NH1	2.07	0.67
1:F:783:ILE:HD12	1:F:783:ILE:N	2.09	0.67
1:H:295:GLU:H	1:H:295:GLU:CD	2.02	0.67
1:H:890:ALA:HB1	1:H:949:ALA:HB2	1.75	0.67
1:I:869:GLU:HG2	1:I:870:ILE:HD12	1.77	0.67
1:J:312:LEU:HD11	1:K:858:GLU:CA	2.22	0.67
1:J:350:TYR:H	1:J:360:UNK:CB	2.06	0.67
1:K:347:ARG:H	1:K:347:ARG:HD3	1.59	0.67
1:M:347:ARG:H	1:M:347:ARG:HD3	1.59	0.67
1:O:350:TYR:H	1:O:360:UNK:CB	2.06	0.67
1:P:347:ARG:H	1:P:347:ARG:HD3	1.59	0.67
1:B:347:ARG:H	1:B:347:ARG:HD3	1.59	0.67
1:C:295:GLU:H	1:C:295:GLU:CD	2.02	0.67
1:G:345:ALA:HB3	1:G:348:ALA:HB2	1.75	0.67
1:I:295:GLU:H	1:I:295:GLU:CD	2.02	0.67
1:K:309:SER:HB2	1:K:320:GLY:HA3	1.74	0.67
1:K:778:GLN:O	1:K:779:GLN:HB2	1.91	0.67
1:N:347:ARG:HD3	1:N:347:ARG:H	1.59	0.67
1:N:930:ARG:HH11	1:N:930:ARG:HG3	1.57	0.67
1:B:783:ILE:HD12	1:B:783:ILE:N	2.09	0.67
1:B:930:ARG:HH11	1:B:930:ARG:HG3	1.57	0.67
1:D:738:UNK:HA	1:M:791:THR:O	1.93	0.67
1:G:869:GLU:HG2	1:G:870:ILE:HD12	1.76	0.67
1:I:898:TYR:CD2	1:J:848:ALA:CB	2.58	0.67
1:J:783:ILE:HD12	1:J:783:ILE:N	2.09	0.67
1:M:350:TYR:H	1:M:360:UNK:CB	2.06	0.67
1:N:867:PRO:CB	1:N:870:ILE:HD13	2.21	0.67
1:D:783:ILE:N	1:D:783:ILE:HD12	2.09	0.67
1:G:295:GLU:CD	1:G:295:GLU:H	2.02	0.67
1:G:852:LEU:HD22	1:G:852:LEU:H	1.58	0.67
1:H:869:GLU:HA	1:H:872:ARG:NH1	2.07	0.67
1:I:783:ILE:N	1:I:783:ILE:HD12	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:317:ARG:HH21	1:J:779:GLN:CD	2.03	0.67
1:J:852:LEU:H	1:J:852:LEU:HD22	1.58	0.67
1:L:783:ILE:N	1:L:783:ILE:HD12	2.09	0.67
1:M:920:ILE:CD1	1:M:924:GLN:HG3	2.25	0.67
1:O:783:ILE:N	1:O:783:ILE:HD12	2.09	0.67
1:A:920:ILE:CD1	1:A:924:GLN:HG3	2.25	0.67
1:C:785:LYS:CG	1:N:785:LYS:HG3	2.25	0.67
1:C:867:PRO:CB	1:C:870:ILE:HD13	2.21	0.67
1:D:890:ALA:HB1	1:D:949:ALA:HB2	1.75	0.67
1:E:347:ARG:H	1:E:347:ARG:HD3	1.59	0.67
1:E:869:GLU:HG2	1:E:870:ILE:HD12	1.76	0.67
1:G:783:ILE:N	1:G:783:ILE:HD12	2.09	0.67
1:J:920:ILE:CD1	1:J:924:GLN:HG3	2.25	0.67
1:O:890:ALA:HB1	1:O:949:ALA:HB2	1.75	0.67
1:B:788:ILE:CG2	1:O:741:UNK:N	2.48	0.67
1:C:347:ARG:H	1:C:347:ARG:HD3	1.59	0.67
1:E:295:GLU:CD	1:E:295:GLU:H	2.02	0.67
1:E:920:ILE:CD1	1:E:924:GLN:HG3	2.25	0.67
1:F:317:ARG:HH21	1:F:779:GLN:CD	2.03	0.67
1:G:920:ILE:CD1	1:G:924:GLN:HG3	2.25	0.67
1:J:295:GLU:CD	1:J:295:GLU:H	2.02	0.67
1:K:869:GLU:HG2	1:K:870:ILE:HD12	1.77	0.67
1:A:295:GLU:H	1:A:295:GLU:CD	2.02	0.67
1:A:347:ARG:HD3	1:A:347:ARG:H	1.59	0.67
1:G:317:ARG:HH21	1:G:779:GLN:CD	2.03	0.67
1:H:930:ARG:HG3	1:H:930:ARG:HH11	1.57	0.67
1:I:345:ALA:HB3	1:I:348:ALA:HB2	1.75	0.67
1:I:886:ILE:HD13	1:J:856:ARG:CB	2.24	0.67
1:K:890:ALA:HB1	1:K:949:ALA:HB2	1.75	0.67
1:L:295:GLU:H	1:L:295:GLU:CD	2.02	0.67
1:N:869:GLU:HG2	1:N:870:ILE:HD12	1.77	0.67
1:N:890:ALA:HB1	1:N:949:ALA:HB2	1.75	0.67
1:P:295:GLU:CD	1:P:295:GLU:H	2.02	0.67
1:B:920:ILE:CD1	1:B:924:GLN:HG3	2.25	0.67
1:G:867:PRO:CB	1:G:870:ILE:HD13	2.21	0.67
1:I:856:ARG:HD3	1:P:891:MET:HE2	1.76	0.67
1:J:312:LEU:CD2	1:K:858:GLU:HB3	2.24	0.67
1:K:956:MET:O	1:K:959:THR:HG23	1.95	0.67
1:L:317:ARG:HH21	1:L:779:GLN:CD	2.03	0.67
1:O:920:ILE:CD1	1:O:924:GLN:HG3	2.25	0.67
1:B:317:ARG:HH21	1:B:779:GLN:CD	2.02	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:867:PRO:CB	1:B:870:ILE:HD13	2.21	0.67
1:H:347:ARG:H	1:H:347:ARG:HD3	1.59	0.67
1:H:783:ILE:HD12	1:H:783:ILE:N	2.09	0.67
1:J:347:ARG:H	1:J:347:ARG:HD3	1.59	0.67
1:L:869:GLU:HG2	1:L:870:ILE:HD12	1.76	0.67
1:L:920:ILE:CD1	1:L:924:GLN:HG3	2.25	0.67
1:O:347:ARG:HD3	1:O:347:ARG:H	1.59	0.67
1:C:317:ARG:HH21	1:C:779:GLN:CD	2.03	0.67
1:C:783:ILE:HD12	1:C:783:ILE:N	2.09	0.67
1:C:956:MET:O	1:C:959:THR:HG23	1.95	0.67
1:E:852:LEU:H	1:E:852:LEU:HD22	1.58	0.67
1:F:347:ARG:HD3	1:F:347:ARG:H	1.59	0.67
1:F:867:PRO:CB	1:F:870:ILE:HD13	2.21	0.67
1:G:309:SER:HB2	1:G:320:GLY:HA3	1.74	0.67
1:J:869:GLU:HG2	1:J:870:ILE:HD12	1.76	0.67
1:M:295:GLU:CD	1:M:295:GLU:H	2.02	0.67
1:O:345:ALA:HB3	1:O:348:ALA:HB2	1.75	0.67
1:O:867:PRO:CB	1:O:870:ILE:HD13	2.21	0.67
1:O:902:ARG:NH1	1:P:839:PRO:HA	2.10	0.67
1:A:317:ARG:HH21	1:A:779:GLN:CD	2.03	0.66
1:A:785:LYS:HE3	1:P:785:LYS:HE3	1.76	0.66
1:C:920:ILE:CD1	1:C:924:GLN:HG3	2.25	0.66
1:D:869:GLU:HG2	1:D:870:ILE:HD12	1.77	0.66
1:H:317:ARG:HH21	1:H:779:GLN:CD	2.02	0.66
1:K:317:ARG:HH21	1:K:779:GLN:CD	2.02	0.66
1:A:785:LYS:HG2	1:P:785:LYS:CB	2.25	0.66
1:D:891:MET:HE2	1:E:852:LEU:HB3	1.77	0.66
1:E:783:ILE:HD12	1:E:783:ILE:N	2.09	0.66
1:F:295:GLU:H	1:F:295:GLU:CD	2.02	0.66
1:F:956:MET:O	1:F:959:THR:HG23	1.95	0.66
1:G:730:UNK:C	1:K:729:UNK:O	2.42	0.66
1:N:295:GLU:H	1:N:295:GLU:CD	2.02	0.66
1:P:317:ARG:HH21	1:P:779:GLN:CD	2.03	0.66
1:D:347:ARG:HD3	1:D:347:ARG:H	1.59	0.66
1:G:956:MET:O	1:G:959:THR:HG23	1.95	0.66
1:H:920:ILE:CD1	1:H:924:GLN:HG3	2.25	0.66
1:K:867:PRO:CB	1:K:870:ILE:HD13	2.21	0.66
1:N:920:ILE:CD1	1:N:924:GLN:HG3	2.25	0.66
1:P:867:PRO:CB	1:P:870:ILE:HD13	2.21	0.66
1:D:317:ARG:HH21	1:D:779:GLN:CD	2.02	0.66
1:H:956:MET:O	1:H:959:THR:HG23	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:920:ILE:CD1	1:I:924:GLN:HG3	2.25	0.66
1:I:956:MET:O	1:I:959:THR:HG23	1.95	0.66
1:L:347:ARG:HD3	1:L:347:ARG:H	1.59	0.66
1:O:869:GLU:HG2	1:O:870:ILE:HD12	1.76	0.66
1:D:920:ILE:CD1	1:D:924:GLN:HG3	2.25	0.66
1:G:347:ARG:HD3	1:G:347:ARG:H	1.59	0.66
1:K:295:GLU:H	1:K:295:GLU:CD	2.02	0.66
1:M:869:GLU:HG2	1:M:870:ILE:HD12	1.77	0.66
1:C:869:GLU:HG2	1:C:870:ILE:HD12	1.76	0.66
1:F:920:ILE:CD1	1:F:924:GLN:HG3	2.25	0.66
1:I:852:LEU:HD11	1:P:894:ILE:CD1	2.15	0.66
1:N:903:LYS:HZ3	1:O:839:PRO:HB3	1.60	0.66
1:O:317:ARG:HH21	1:O:779:GLN:CD	2.03	0.66
1:A:345:ALA:HB3	1:A:348:ALA:HB2	1.75	0.66
1:I:317:ARG:HH21	1:I:779:GLN:CD	2.03	0.66
1:M:317:ARG:HH21	1:M:779:GLN:CD	2.03	0.66
1:M:956:MET:O	1:M:959:THR:HG23	1.95	0.66
1:N:956:MET:O	1:N:959:THR:HG23	1.95	0.66
1:D:785:LYS:HG2	1:M:785:LYS:C	2.21	0.66
1:E:267:GLN:O	1:E:271:GLU:HG2	1.96	0.66
1:I:347:ARG:HD3	1:I:347:ARG:H	1.59	0.66
1:N:267:GLN:O	1:N:271:GLU:HG2	1.96	0.66
1:G:267:GLN:O	1:G:271:GLU:HG2	1.96	0.66
1:H:869:GLU:HG2	1:H:870:ILE:HD12	1.77	0.66
1:I:856:ARG:NH1	1:P:891:MET:HE1	2.10	0.66
1:J:956:MET:O	1:J:959:THR:HG23	1.95	0.66
1:P:920:ILE:CD1	1:P:924:GLN:HG3	2.25	0.66
1:L:267:GLN:O	1:L:271:GLU:HG2	1.96	0.66
1:L:956:MET:O	1:L:959:THR:HG23	1.95	0.66
1:N:317:ARG:HH21	1:N:779:GLN:CD	2.03	0.66
1:A:729:UNK:O	1:I:729:UNK:O	2.14	0.65
1:E:317:ARG:HH21	1:E:779:GLN:CD	2.02	0.65
1:I:848:ALA:HB2	1:P:898:TYR:CD2	2.31	0.65
1:K:774:GLU:CD	1:K:781:ILE:HA	2.21	0.65
1:K:920:ILE:CD1	1:K:924:GLN:HG3	2.25	0.65
1:A:867:PRO:CB	1:A:870:ILE:HD13	2.21	0.65
1:D:956:MET:O	1:D:959:THR:HG23	1.95	0.65
1:G:359:UNK:CB	1:K:732:UNK:HA	2.26	0.65
1:B:956:MET:O	1:B:959:THR:HG23	1.95	0.65
1:K:267:GLN:O	1:K:271:GLU:HG2	1.96	0.65
1:O:956:MET:O	1:O:959:THR:HG23	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:GLN:O	1:A:271:GLU:HG2	1.96	0.65
1:F:267:GLN:O	1:F:271:GLU:HG2	1.96	0.65
1:N:746:UNK:O	1:N:792:LEU:HD11	1.97	0.65
1:N:774:GLU:CD	1:N:781:ILE:HA	2.22	0.65
1:C:774:GLU:CD	1:C:781:ILE:HA	2.21	0.65
1:C:789:THR:O	1:N:740:UNK:HA	1.96	0.65
1:D:267:GLN:O	1:D:271:GLU:HG2	1.96	0.65
1:H:267:GLN:O	1:H:271:GLU:HG2	1.96	0.65
1:H:774:GLU:CD	1:H:781:ILE:HA	2.21	0.65
1:I:891:MET:HE3	1:J:856:ARG:NH1	2.10	0.65
1:J:774:GLU:CD	1:J:781:ILE:HA	2.22	0.65
1:B:267:GLN:O	1:B:271:GLU:HG2	1.96	0.65
1:C:267:GLN:O	1:C:271:GLU:HG2	1.96	0.65
1:F:869:GLU:HG2	1:F:870:ILE:HD12	1.77	0.65
1:I:267:GLN:O	1:I:271:GLU:HG2	1.96	0.65
1:I:746:UNK:O	1:I:792:LEU:HD11	1.97	0.65
1:M:267:GLN:O	1:M:271:GLU:HG2	1.96	0.65
1:P:869:GLU:HG2	1:P:870:ILE:HD12	1.77	0.65
1:F:774:GLU:CD	1:F:781:ILE:HA	2.21	0.65
1:G:332:VAL:O	1:G:333:ALA:HB3	1.97	0.65
1:I:350:TYR:CD1	1:I:351:THR:N	2.65	0.65
1:O:332:VAL:O	1:O:333:ALA:HB3	1.97	0.65
1:P:267:GLN:O	1:P:271:GLU:HG2	1.96	0.65
1:A:869:GLU:HG2	1:A:870:ILE:HD12	1.77	0.65
1:E:774:GLU:CD	1:E:781:ILE:HA	2.21	0.65
1:G:774:GLU:CD	1:G:781:ILE:HA	2.22	0.65
1:H:746:UNK:O	1:H:792:LEU:HD11	1.97	0.65
1:J:267:GLN:O	1:J:271:GLU:HG2	1.96	0.65
1:J:350:TYR:CD1	1:J:351:THR:N	2.65	0.65
1:P:746:UNK:O	1:P:792:LEU:HD11	1.97	0.65
1:A:332:VAL:O	1:A:333:ALA:HB3	1.97	0.65
1:A:350:TYR:CD1	1:A:351:THR:N	2.65	0.65
1:B:774:GLU:CD	1:B:781:ILE:HA	2.21	0.65
1:F:313:PRO:O	1:G:343:ASN:ND2	2.30	0.65
1:F:746:UNK:O	1:F:792:LEU:HD11	1.97	0.65
1:H:867:PRO:CB	1:H:870:ILE:HD13	2.21	0.65
1:K:350:TYR:CD1	1:K:351:THR:N	2.65	0.65
1:P:956:MET:O	1:P:959:THR:HG23	1.95	0.65
1:A:746:UNK:O	1:A:792:LEU:HD11	1.97	0.65
1:A:956:MET:O	1:A:959:THR:HG23	1.95	0.65
1:E:350:TYR:CD1	1:E:351:THR:N	2.65	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:746:UNK:O	1:E:792:LEU:HD11	1.97	0.65
1:L:746:UNK:O	1:L:792:LEU:HD11	1.97	0.65
1:O:350:TYR:CD1	1:O:351:THR:N	2.65	0.65
1:O:746:UNK:O	1:O:792:LEU:HD11	1.97	0.65
1:B:332:VAL:O	1:B:333:ALA:HB3	1.97	0.64
1:B:898:TYR:HB2	1:B:925:LEU:HD23	1.80	0.64
1:D:774:GLU:CD	1:D:781:ILE:HA	2.22	0.64
1:E:956:MET:O	1:E:959:THR:HG23	1.95	0.64
1:J:956:MET:HA	1:J:959:THR:CG2	2.28	0.64
1:P:956:MET:HA	1:P:959:THR:CG2	2.28	0.64
1:A:956:MET:HA	1:A:959:THR:CG2	2.28	0.64
1:B:350:TYR:CD1	1:B:351:THR:N	2.65	0.64
1:C:350:TYR:CD1	1:C:351:THR:N	2.65	0.64
1:E:867:PRO:CB	1:E:870:ILE:HD13	2.21	0.64
1:F:332:VAL:O	1:F:333:ALA:HB3	1.97	0.64
1:M:350:TYR:CD1	1:M:351:THR:N	2.65	0.64
1:N:903:LYS:NZ	1:O:839:PRO:HB2	2.11	0.64
1:O:774:GLU:CD	1:O:781:ILE:HA	2.22	0.64
1:B:746:UNK:O	1:B:792:LEU:HD11	1.97	0.64
1:F:898:TYR:HB2	1:F:925:LEU:HD23	1.80	0.64
1:G:350:TYR:CD1	1:G:351:THR:N	2.65	0.64
1:H:785:LYS:HG2	1:I:785:LYS:HG3	1.77	0.64
1:I:895:GLU:OE1	1:J:849:ARG:CG	2.45	0.64
1:I:956:MET:HA	1:I:959:THR:CG2	2.28	0.64
1:J:867:PRO:CB	1:J:870:ILE:HD13	2.21	0.64
1:K:308:VAL:HB	1:K:933:GLU:OE1	1.98	0.64
1:L:774:GLU:CD	1:L:781:ILE:HA	2.22	0.64
1:O:956:MET:HA	1:O:959:THR:CG2	2.28	0.64
1:D:350:TYR:CD1	1:D:351:THR:N	2.65	0.64
1:D:746:UNK:O	1:D:792:LEU:HD11	1.97	0.64
1:H:350:TYR:CD1	1:H:351:THR:N	2.65	0.64
1:J:746:UNK:O	1:J:792:LEU:HD11	1.97	0.64
1:J:840:ASP:OD1	1:J:843:ILE:HG22	1.98	0.64
1:K:746:UNK:O	1:K:792:LEU:HD11	1.97	0.64
1:M:746:UNK:O	1:M:792:LEU:HD11	1.97	0.64
1:M:774:GLU:CD	1:M:781:ILE:HA	2.21	0.64
1:N:840:ASP:OD1	1:N:843:ILE:HG22	1.98	0.64
1:P:350:TYR:CD1	1:P:351:THR:N	2.65	0.64
1:P:840:ASP:OD1	1:P:843:ILE:HG22	1.98	0.64
1:D:332:VAL:O	1:D:333:ALA:HB3	1.97	0.64
1:L:956:MET:HA	1:L:959:THR:CG2	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:956:MET:HA	1:M:959:THR:CG2	2.27	0.64
1:O:267:GLN:O	1:O:271:GLU:HG2	1.96	0.64
1:D:885:VAL:HG13	1:E:856:ARG:HB2	1.79	0.64
1:E:308:VAL:HB	1:E:933:GLU:OE1	1.97	0.64
1:J:332:VAL:O	1:J:333:ALA:HB3	1.97	0.64
1:O:840:ASP:OD1	1:O:843:ILE:HG22	1.98	0.64
1:P:774:GLU:CD	1:P:781:ILE:HA	2.21	0.64
1:B:840:ASP:OD1	1:B:843:ILE:HG22	1.98	0.64
1:C:332:VAL:O	1:C:333:ALA:HB3	1.97	0.64
1:C:956:MET:HA	1:C:959:THR:CG2	2.28	0.64
1:E:840:ASP:OD1	1:E:843:ILE:HG22	1.98	0.64
1:F:350:TYR:CD1	1:F:351:THR:N	2.65	0.64
1:G:746:UNK:O	1:G:792:LEU:HD11	1.97	0.64
1:J:308:VAL:HB	1:J:933:GLU:OE1	1.98	0.64
1:N:898:TYR:HB2	1:N:925:LEU:HD23	1.80	0.64
1:P:332:VAL:O	1:P:333:ALA:HB3	1.97	0.64
1:A:774:GLU:CD	1:A:781:ILE:HA	2.21	0.64
1:C:746:UNK:O	1:C:792:LEU:HD11	1.97	0.64
1:C:840:ASP:OD1	1:C:843:ILE:HG22	1.98	0.64
1:E:884:PRO:HA	1:E:942:PRO:O	1.98	0.64
1:F:781:ILE:HG22	1:F:782:SER:N	2.13	0.64
1:F:884:PRO:HA	1:F:942:PRO:O	1.98	0.64
1:G:840:ASP:OD1	1:G:843:ILE:HG22	1.98	0.64
1:I:308:VAL:HB	1:I:933:GLU:OE1	1.98	0.64
1:I:774:GLU:CD	1:I:781:ILE:HA	2.21	0.64
1:K:956:MET:HA	1:K:959:THR:CG2	2.28	0.64
1:N:350:TYR:CD1	1:N:351:THR:N	2.65	0.64
1:A:308:VAL:HB	1:A:933:GLU:OE1	1.98	0.64
1:D:840:ASP:OD1	1:D:843:ILE:HG22	1.98	0.64
1:G:884:PRO:HA	1:G:942:PRO:O	1.98	0.64
1:G:956:MET:HA	1:G:959:THR:CG2	2.28	0.64
1:H:308:VAL:HB	1:H:933:GLU:OE1	1.97	0.64
1:N:308:VAL:HB	1:N:933:GLU:OE1	1.98	0.64
1:E:739:UNK:CB	1:L:791:THR:H	2.11	0.64
1:G:318:LEU:HD21	1:H:855:ARG:HE	1.61	0.64
1:H:840:ASP:OD1	1:H:843:ILE:HG22	1.98	0.64
1:H:884:PRO:HA	1:H:942:PRO:O	1.98	0.64
1:J:884:PRO:HA	1:J:942:PRO:O	1.98	0.64
1:K:884:PRO:HA	1:K:942:PRO:O	1.98	0.64
1:L:350:TYR:CD1	1:L:351:THR:N	2.65	0.64
1:N:956:MET:HA	1:N:959:THR:CG2	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:928:LEU:HD22	1:O:956:MET:HE1	1.80	0.64
1:F:308:VAL:HB	1:F:933:GLU:OE1	1.97	0.63
1:L:867:PRO:CB	1:L:870:ILE:HD13	2.21	0.63
1:B:956:MET:HA	1:B:959:THR:CG2	2.28	0.63
1:C:308:VAL:HB	1:C:933:GLU:OE1	1.97	0.63
1:D:781:ILE:HG22	1:D:782:SER:N	2.13	0.63
1:F:928:LEU:HD22	1:F:956:MET:HE1	1.80	0.63
1:G:898:TYR:HB2	1:G:925:LEU:HD23	1.80	0.63
1:H:332:VAL:O	1:H:333:ALA:HB3	1.97	0.63
1:J:781:ILE:HG22	1:J:782:SER:N	2.13	0.63
1:M:781:ILE:HG22	1:M:782:SER:N	2.13	0.63
1:A:884:PRO:HA	1:A:942:PRO:O	1.98	0.63
1:E:956:MET:HA	1:E:959:THR:CG2	2.28	0.63
1:F:840:ASP:OD1	1:F:843:ILE:HG22	1.98	0.63
1:G:308:VAL:HB	1:G:933:GLU:OE1	1.97	0.63
1:H:928:LEU:HD22	1:H:956:MET:HE1	1.81	0.63
1:H:956:MET:HA	1:H:959:THR:CG2	2.28	0.63
1:I:332:VAL:O	1:I:333:ALA:HB3	1.97	0.63
1:I:781:ILE:HG22	1:I:782:SER:N	2.13	0.63
1:I:898:TYR:HB2	1:I:925:LEU:HD23	1.80	0.63
1:M:928:LEU:HD22	1:M:956:MET:HE1	1.80	0.63
1:N:884:PRO:HA	1:N:942:PRO:O	1.98	0.63
1:C:785:LYS:HG3	1:N:785:LYS:HG2	1.80	0.63
1:C:898:TYR:HB2	1:C:925:LEU:HD23	1.80	0.63
1:C:928:LEU:HD22	1:C:956:MET:HE1	1.81	0.63
1:I:856:ARG:NH1	1:P:888:GLU:HG2	2.00	0.63
1:K:898:TYR:HB2	1:K:925:LEU:HD23	1.80	0.63
1:L:840:ASP:OD1	1:L:843:ILE:HG22	1.98	0.63
1:N:332:VAL:O	1:N:333:ALA:HB3	1.97	0.63
1:N:891:MET:CE	1:O:852:LEU:HB3	2.15	0.63
1:P:308:VAL:HB	1:P:933:GLU:OE1	1.98	0.63
1:I:335:SER:HA	1:I:759:ASP:OD2	1.99	0.63
1:J:335:SER:HA	1:J:759:ASP:OD2	1.99	0.63
1:K:335:SER:HA	1:K:759:ASP:OD2	1.99	0.63
1:K:781:ILE:HG22	1:K:782:SER:N	2.13	0.63
1:L:928:LEU:HD22	1:L:956:MET:HE1	1.81	0.63
1:B:884:PRO:HA	1:B:942:PRO:O	1.98	0.63
1:C:891:MET:CE	1:D:856:ARG:CD	2.64	0.63
1:L:308:VAL:HB	1:L:933:GLU:OE1	1.98	0.63
1:A:840:ASP:OD1	1:A:843:ILE:HG22	1.98	0.63
1:C:884:PRO:HA	1:C:942:PRO:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:956:MET:HA	1:D:959:THR:CG2	2.28	0.63
1:E:332:VAL:O	1:E:333:ALA:HB3	1.97	0.63
1:F:808:ARG:HB2	1:F:808:ARG:CZ	2.29	0.63
1:J:808:ARG:HB2	1:J:808:ARG:CZ	2.29	0.63
1:K:332:VAL:O	1:K:333:ALA:HB3	1.97	0.63
1:M:840:ASP:OD1	1:M:843:ILE:HG22	1.98	0.63
1:P:928:LEU:HD22	1:P:956:MET:HE1	1.80	0.63
1:B:808:ARG:HB2	1:B:808:ARG:CZ	2.29	0.63
1:H:335:SER:HA	1:H:759:ASP:OD2	1.99	0.63
1:H:898:TYR:HB2	1:H:925:LEU:HD23	1.80	0.63
1:I:840:ASP:OD1	1:I:843:ILE:HG22	1.98	0.63
1:I:928:LEU:HD22	1:I:956:MET:HE1	1.80	0.63
1:J:929:ILE:HD11	1:K:852:LEU:CD1	2.29	0.63
1:N:928:LEU:HD22	1:N:956:MET:HE1	1.81	0.63
1:O:335:SER:HA	1:O:759:ASP:OD2	1.99	0.63
1:A:808:ARG:HB2	1:A:808:ARG:CZ	2.29	0.63
1:D:808:ARG:HB2	1:D:808:ARG:CZ	2.29	0.63
1:E:739:UNK:C	1:L:789:THR:O	2.45	0.63
1:E:808:ARG:HB2	1:E:808:ARG:CZ	2.29	0.63
1:L:332:VAL:O	1:L:333:ALA:HB3	1.97	0.63
1:M:332:VAL:O	1:M:333:ALA:HB3	1.97	0.63
1:O:308:VAL:HB	1:O:933:GLU:OE1	1.98	0.63
1:P:273:ALA:HA	1:P:278:ILE:HD12	1.81	0.63
1:P:335:SER:HA	1:P:759:ASP:OD2	1.99	0.63
1:B:335:SER:HA	1:B:759:ASP:OD2	1.99	0.62
1:D:898:TYR:HB2	1:D:925:LEU:HD23	1.80	0.62
1:F:902:ARG:NH1	1:G:844:ASP:CG	2.51	0.62
1:G:273:ALA:HA	1:G:278:ILE:HD12	1.81	0.62
1:I:786:ALA:HB3	1:I:788:ILE:HD11	1.82	0.62
1:J:273:ALA:HA	1:J:278:ILE:HD12	1.81	0.62
1:K:840:ASP:OD1	1:K:843:ILE:HG22	1.98	0.62
1:N:781:ILE:HG22	1:N:782:SER:N	2.13	0.62
1:O:781:ILE:HG22	1:O:782:SER:N	2.13	0.62
1:O:898:TYR:HB2	1:O:925:LEU:HD23	1.80	0.62
1:P:781:ILE:HG22	1:P:782:SER:N	2.13	0.62
1:D:273:ALA:HA	1:D:278:ILE:HD12	1.81	0.62
1:D:786:ALA:HB3	1:D:788:ILE:HD11	1.82	0.62
1:J:898:TYR:HB2	1:J:925:LEU:HD23	1.80	0.62
1:L:781:ILE:HG22	1:L:782:SER:N	2.13	0.62
1:O:808:ARG:HB2	1:O:808:ARG:CZ	2.29	0.62
1:A:886:ILE:N	1:A:886:ILE:CD1	2.62	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:ALA:HA	1:B:278:ILE:HD12	1.81	0.62
1:B:308:VAL:HB	1:B:933:GLU:OE1	1.97	0.62
1:C:808:ARG:HB2	1:C:808:ARG:CZ	2.29	0.62
1:D:771:VAL:HG23	1:D:781:ILE:HD13	1.82	0.62
1:D:884:PRO:HA	1:D:942:PRO:O	1.98	0.62
1:E:335:SER:HA	1:E:759:ASP:OD2	1.99	0.62
1:E:786:ALA:HB3	1:E:788:ILE:HD11	1.82	0.62
1:L:884:PRO:HA	1:L:942:PRO:O	1.98	0.62
1:M:308:VAL:HB	1:M:933:GLU:OE1	1.98	0.62
1:M:786:ALA:HB3	1:M:788:ILE:HD11	1.82	0.62
1:N:808:ARG:HB2	1:N:808:ARG:CZ	2.29	0.62
1:P:884:PRO:HA	1:P:942:PRO:O	1.98	0.62
1:A:786:ALA:HB3	1:A:788:ILE:HD11	1.82	0.62
1:F:956:MET:HA	1:F:959:THR:CG2	2.28	0.62
1:H:273:ALA:HA	1:H:278:ILE:HD12	1.81	0.62
1:J:786:ALA:HB3	1:J:788:ILE:HD11	1.82	0.62
1:L:273:ALA:HA	1:L:278:ILE:HD12	1.81	0.62
1:M:808:ARG:HB2	1:M:808:ARG:CZ	2.29	0.62
1:O:771:VAL:HG23	1:O:781:ILE:HD13	1.82	0.62
1:O:786:ALA:HB3	1:O:788:ILE:HD11	1.82	0.62
1:A:771:VAL:HG23	1:A:781:ILE:HD13	1.82	0.62
1:A:898:TYR:HB2	1:A:925:LEU:HD23	1.80	0.62
1:B:886:ILE:N	1:B:886:ILE:CD1	2.63	0.62
1:E:273:ALA:HA	1:E:278:ILE:HD12	1.81	0.62
1:G:335:SER:HA	1:G:759:ASP:OD2	1.99	0.62
1:G:808:ARG:HB2	1:G:808:ARG:CZ	2.29	0.62
1:I:273:ALA:HA	1:I:278:ILE:HD12	1.81	0.62
1:K:928:LEU:HD22	1:K:956:MET:HE1	1.80	0.62
1:M:273:ALA:HA	1:M:278:ILE:HD12	1.81	0.62
1:M:898:TYR:HB2	1:M:925:LEU:HD23	1.80	0.62
1:B:781:ILE:HG22	1:B:782:SER:N	2.13	0.62
1:B:786:ALA:HB3	1:B:788:ILE:HD11	1.82	0.62
1:C:781:ILE:HG22	1:C:782:SER:N	2.13	0.62
1:D:335:SER:HA	1:D:759:ASP:OD2	1.99	0.62
1:E:886:ILE:N	1:E:886:ILE:CD1	2.62	0.62
1:G:786:ALA:HB3	1:G:788:ILE:HD11	1.81	0.62
1:H:781:ILE:HG22	1:H:782:SER:N	2.13	0.62
1:L:335:SER:HA	1:L:759:ASP:OD2	1.99	0.62
1:L:808:ARG:HB2	1:L:808:ARG:CZ	2.29	0.62
1:O:884:PRO:HA	1:O:942:PRO:O	1.98	0.62
1:O:926:GLU:OE2	2:P:1001:ADP:H4'	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:928:LEU:HD22	1:A:956:MET:HE1	1.81	0.62
1:C:335:SER:HA	1:C:759:ASP:OD2	1.99	0.62
1:D:928:LEU:HD22	1:D:956:MET:HE1	1.81	0.62
1:I:771:VAL:HG23	1:I:781:ILE:HD13	1.82	0.62
1:I:884:PRO:HA	1:I:942:PRO:O	1.98	0.62
1:L:860:GLU:C	1:L:862:VAL:H	2.08	0.62
1:M:884:PRO:HA	1:M:942:PRO:O	1.98	0.62
1:N:771:VAL:HG23	1:N:781:ILE:HD13	1.82	0.62
1:P:808:ARG:HB2	1:P:808:ARG:CZ	2.29	0.62
1:P:898:TYR:HB2	1:P:925:LEU:HD23	1.80	0.62
1:A:273:ALA:HA	1:A:278:ILE:HD12	1.81	0.62
1:A:335:SER:HA	1:A:759:ASP:OD2	1.99	0.62
1:C:771:VAL:HG23	1:C:781:ILE:HD13	1.82	0.62
1:D:308:VAL:HB	1:D:933:GLU:OE1	1.98	0.62
1:D:860:GLU:C	1:D:862:VAL:H	2.08	0.62
1:D:886:ILE:N	1:D:886:ILE:CD1	2.62	0.62
1:G:771:VAL:HG23	1:G:781:ILE:HD13	1.82	0.62
1:H:808:ARG:HB2	1:H:808:ARG:CZ	2.29	0.62
1:K:771:VAL:HG23	1:K:781:ILE:HD13	1.82	0.62
1:L:886:ILE:N	1:L:886:ILE:CD1	2.63	0.62
1:L:898:TYR:HB2	1:L:925:LEU:HD23	1.80	0.62
1:M:771:VAL:HG23	1:M:781:ILE:HD13	1.82	0.62
1:O:886:ILE:N	1:O:886:ILE:CD1	2.62	0.62
1:A:785:LYS:HE3	1:P:785:LYS:CE	2.30	0.62
1:E:898:TYR:HB2	1:E:925:LEU:HD23	1.80	0.62
1:E:928:LEU:HD22	1:E:956:MET:HE1	1.81	0.62
1:I:886:ILE:N	1:I:886:ILE:CD1	2.62	0.62
1:J:886:ILE:N	1:J:886:ILE:CD1	2.62	0.62
1:K:808:ARG:HB2	1:K:808:ARG:CZ	2.29	0.62
1:N:335:SER:HA	1:N:759:ASP:OD2	1.99	0.62
1:N:886:ILE:N	1:N:886:ILE:CD1	2.63	0.62
1:D:785:LYS:CA	1:M:785:LYS:CG	2.77	0.62
1:E:860:GLU:C	1:E:862:VAL:H	2.08	0.62
1:N:273:ALA:HA	1:N:278:ILE:HD12	1.81	0.62
1:N:786:ALA:HB3	1:N:788:ILE:HD11	1.82	0.62
1:O:316:THR:CB	1:P:339:ARG:CD	2.78	0.62
1:P:860:GLU:C	1:P:862:VAL:H	2.08	0.62
1:A:844:ASP:OD2	1:H:902:ARG:NH1	2.31	0.61
1:E:781:ILE:HG22	1:E:782:SER:N	2.13	0.61
1:F:273:ALA:HA	1:F:278:ILE:HD12	1.81	0.61
1:H:786:ALA:HB3	1:H:788:ILE:HD11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:867:PRO:CB	1:I:870:ILE:HD13	2.21	0.61
1:J:891:MET:HE1	1:K:856:ARG:NH2	2.13	0.61
1:J:928:LEU:HD22	1:J:956:MET:HE1	1.81	0.61
1:K:902:ARG:HG2	1:K:902:ARG:HH11	1.65	0.61
1:K:903:LYS:HD2	1:L:841:ASP:CG	2.25	0.61
1:P:771:VAL:HG23	1:P:781:ILE:HD13	1.82	0.61
1:A:781:ILE:HG22	1:A:782:SER:N	2.13	0.61
1:F:771:VAL:HG23	1:F:781:ILE:HD13	1.82	0.61
1:G:886:ILE:N	1:G:886:ILE:CD1	2.62	0.61
1:H:886:ILE:N	1:H:886:ILE:CD1	2.62	0.61
1:M:886:ILE:N	1:M:886:ILE:CD1	2.62	0.61
1:P:886:ILE:N	1:P:886:ILE:CD1	2.63	0.61
1:A:792:LEU:HD22	1:P:792:LEU:HD22	1.82	0.61
1:F:886:ILE:N	1:F:886:ILE:CD1	2.62	0.61
1:H:771:VAL:HG23	1:H:781:ILE:HD13	1.82	0.61
1:M:335:SER:HA	1:M:759:ASP:OD2	1.99	0.61
1:M:891:MET:HE2	1:N:852:LEU:HB3	1.81	0.61
1:N:860:GLU:C	1:N:862:VAL:H	2.08	0.61
1:N:902:ARG:HH11	1:N:902:ARG:HG2	1.65	0.61
1:A:825:LEU:O	1:A:828:ARG:HB2	2.01	0.61
1:C:860:GLU:C	1:C:862:VAL:H	2.08	0.61
1:D:891:MET:HG3	1:E:852:LEU:HG	1.81	0.61
1:F:825:LEU:O	1:F:828:ARG:HB2	2.01	0.61
1:I:808:ARG:HB2	1:I:808:ARG:CZ	2.29	0.61
1:K:273:ALA:HA	1:K:278:ILE:HD12	1.81	0.61
1:A:730:UNK:CB	1:I:730:UNK:N	2.63	0.61
1:B:928:LEU:HD22	1:B:956:MET:HE1	1.81	0.61
1:D:316:THR:HG21	1:E:339:ARG:HD2	1.83	0.61
1:D:902:ARG:HG2	1:D:902:ARG:HH11	1.65	0.61
1:G:928:LEU:HD22	1:G:956:MET:HE1	1.81	0.61
1:K:825:LEU:O	1:K:828:ARG:HB2	2.01	0.61
1:K:886:ILE:N	1:K:886:ILE:CD1	2.62	0.61
1:P:825:LEU:O	1:P:828:ARG:HB2	2.01	0.61
1:O:825:LEU:O	1:O:828:ARG:HB2	2.01	0.61
1:C:902:ARG:HG2	1:C:902:ARG:HH11	1.65	0.61
1:E:771:VAL:HG23	1:E:781:ILE:HD13	1.82	0.61
1:F:335:SER:HA	1:F:759:ASP:OD2	1.99	0.61
1:F:860:GLU:C	1:F:862:VAL:H	2.08	0.61
1:G:740:UNK:HA	1:J:789:THR:O	2.01	0.61
1:G:781:ILE:HG22	1:G:782:SER:N	2.13	0.61
1:G:825:LEU:O	1:G:828:ARG:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:312:LEU:HD11	1:J:858:GLU:HA	1.83	0.61
1:K:902:ARG:NH1	1:L:839:PRO:HA	2.16	0.61
1:L:771:VAL:HG23	1:L:781:ILE:HD13	1.82	0.61
1:L:786:ALA:HB3	1:L:788:ILE:HD11	1.82	0.61
1:L:902:ARG:HG2	1:L:902:ARG:HH11	1.65	0.61
1:O:273:ALA:HA	1:O:278:ILE:HD12	1.81	0.61
1:B:778:GLN:O	1:B:779:GLN:CB	2.49	0.61
1:B:825:LEU:O	1:B:828:ARG:HB2	2.01	0.61
1:B:860:GLU:C	1:B:862:VAL:H	2.08	0.61
1:B:897:TYR:CG	1:B:953:ILE:HG21	2.36	0.61
1:C:853:ARG:NH2	1:C:860:GLU:HG3	2.16	0.61
1:C:886:ILE:N	1:C:886:ILE:CD1	2.62	0.61
1:G:897:TYR:CG	1:G:953:ILE:HG21	2.36	0.61
1:I:825:LEU:O	1:I:828:ARG:HB2	2.01	0.61
1:J:853:ARG:NH2	1:J:860:GLU:HG3	2.16	0.61
1:L:317:ARG:HH11	1:L:317:ARG:HG3	1.66	0.61
1:N:853:ARG:NH2	1:N:860:GLU:HG3	2.16	0.61
1:N:897:TYR:CG	1:N:953:ILE:HG21	2.36	0.61
1:O:853:ARG:NH2	1:O:860:GLU:HG3	2.16	0.61
1:O:897:TYR:CG	1:O:953:ILE:HG21	2.36	0.61
1:P:897:TYR:CG	1:P:953:ILE:HG21	2.36	0.61
1:B:902:ARG:NH1	1:C:844:ASP:OD1	2.33	0.61
1:D:778:GLN:O	1:D:779:GLN:CB	2.49	0.61
1:K:853:ARG:NH2	1:K:860:GLU:HG3	2.16	0.61
1:M:778:GLN:O	1:M:779:GLN:CB	2.49	0.61
1:P:778:GLN:O	1:P:779:GLN:CB	2.49	0.61
1:P:786:ALA:HB3	1:P:788:ILE:HD11	1.82	0.61
1:P:902:ARG:HG2	1:P:902:ARG:HH11	1.65	0.61
1:A:853:ARG:NH2	1:A:860:GLU:HG3	2.16	0.61
1:A:902:ARG:HG2	1:A:902:ARG:HH11	1.65	0.61
1:B:317:ARG:HG3	1:B:317:ARG:HH11	1.66	0.61
1:D:825:LEU:O	1:D:828:ARG:HB2	2.01	0.61
1:D:897:TYR:CG	1:D:953:ILE:HG21	2.36	0.61
1:E:897:TYR:CG	1:E:953:ILE:HG21	2.36	0.61
1:F:786:ALA:HB3	1:F:788:ILE:HD11	1.82	0.61
1:I:778:GLN:O	1:I:779:GLN:CB	2.49	0.61
1:J:860:GLU:C	1:J:862:VAL:H	2.08	0.61
1:J:897:TYR:CG	1:J:953:ILE:HG21	2.36	0.61
1:K:860:GLU:C	1:K:862:VAL:H	2.08	0.61
1:M:317:ARG:HG3	1:M:317:ARG:HH11	1.66	0.61
1:B:902:ARG:HG2	1:B:902:ARG:HH11	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:902:ARG:HH11	1:C:844:ASP:CG	2.09	0.60
1:C:273:ALA:HA	1:C:278:ILE:HD12	1.81	0.60
1:C:825:LEU:O	1:C:828:ARG:HB2	2.01	0.60
1:M:853:ARG:NH2	1:M:860:GLU:HG3	2.16	0.60
1:M:897:TYR:CG	1:M:953:ILE:HG21	2.36	0.60
1:O:860:GLU:C	1:O:862:VAL:H	2.08	0.60
1:O:902:ARG:HG2	1:O:902:ARG:HH11	1.65	0.60
1:P:853:ARG:NH2	1:P:860:GLU:HG3	2.16	0.60
1:A:778:GLN:O	1:A:779:GLN:CB	2.49	0.60
1:C:897:TYR:CG	1:C:953:ILE:HG21	2.36	0.60
1:E:853:ARG:NH2	1:E:860:GLU:HG3	2.16	0.60
1:F:853:ARG:NH2	1:F:860:GLU:HG3	2.16	0.60
1:G:860:GLU:C	1:G:862:VAL:H	2.08	0.60
1:H:897:TYR:CG	1:H:953:ILE:HG21	2.36	0.60
1:H:902:ARG:HG2	1:H:902:ARG:HH11	1.65	0.60
1:I:860:GLU:C	1:I:862:VAL:H	2.08	0.60
1:J:825:LEU:O	1:J:828:ARG:HB2	2.01	0.60
1:N:825:LEU:O	1:N:828:ARG:HB2	2.01	0.60
1:N:894:ILE:HG13	1:N:895:GLU:N	2.16	0.60
1:N:930:ARG:HG3	1:N:930:ARG:NH1	2.16	0.60
1:O:316:THR:HB	1:P:339:ARG:HG2	1.83	0.60
1:B:771:VAL:HG23	1:B:781:ILE:HD13	1.82	0.60
1:D:902:ARG:NH1	1:E:839:PRO:HA	2.16	0.60
1:F:902:ARG:HH11	1:F:902:ARG:HG2	1.65	0.60
1:H:853:ARG:NH2	1:H:860:GLU:HG3	2.16	0.60
1:C:786:ALA:HB3	1:C:788:ILE:HD11	1.82	0.60
1:E:902:ARG:HG2	1:E:902:ARG:HH11	1.65	0.60
1:G:317:ARG:HH11	1:G:317:ARG:HG3	1.66	0.60
1:G:853:ARG:NH2	1:G:860:GLU:HG3	2.16	0.60
1:I:902:ARG:HG2	1:I:902:ARG:HH11	1.65	0.60
1:K:897:TYR:CG	1:K:953:ILE:HG21	2.36	0.60
1:L:897:TYR:CG	1:L:953:ILE:HG21	2.36	0.60
1:B:853:ARG:NH2	1:B:860:GLU:HG3	2.16	0.60
1:F:897:TYR:CG	1:F:953:ILE:HG21	2.36	0.60
1:H:778:GLN:O	1:H:779:GLN:CB	2.49	0.60
1:H:860:GLU:C	1:H:862:VAL:H	2.08	0.60
1:J:771:VAL:HG23	1:J:781:ILE:HD13	1.82	0.60
1:J:902:ARG:HH11	1:J:902:ARG:HG2	1.65	0.60
1:K:778:GLN:O	1:K:779:GLN:CB	2.49	0.60
1:L:825:LEU:O	1:L:828:ARG:HB2	2.01	0.60
1:L:930:ARG:HG3	1:L:930:ARG:NH1	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:825:LEU:O	1:M:828:ARG:HB2	2.01	0.60
1:O:778:GLN:O	1:O:779:GLN:CB	2.49	0.60
1:A:860:GLU:C	1:A:862:VAL:H	2.08	0.60
1:A:897:TYR:CG	1:A:953:ILE:HG21	2.36	0.60
1:D:317:ARG:HH11	1:D:317:ARG:HG3	1.66	0.60
1:J:894:ILE:HG13	1:J:895:GLU:N	2.16	0.60
1:K:786:ALA:HB3	1:K:788:ILE:HD11	1.82	0.60
1:L:778:GLN:O	1:L:779:GLN:CB	2.49	0.60
1:M:316:THR:HG21	1:N:339:ARG:CD	2.32	0.60
1:P:317:ARG:HG3	1:P:317:ARG:HH11	1.66	0.60
1:B:894:ILE:HG13	1:B:895:GLU:N	2.16	0.60
1:G:791:THR:O	1:J:738:UNK:HA	2.02	0.60
1:G:902:ARG:HG2	1:G:902:ARG:HH11	1.65	0.60
1:D:853:ARG:NH2	1:D:860:GLU:HG3	2.16	0.60
1:E:825:LEU:O	1:E:828:ARG:HB2	2.01	0.60
1:F:778:GLN:O	1:F:779:GLN:CB	2.49	0.60
1:G:318:LEU:HD21	1:H:855:ARG:NE	2.15	0.60
1:H:825:LEU:O	1:H:828:ARG:HB2	2.01	0.60
1:I:848:ALA:HB2	1:P:898:TYR:HD2	1.64	0.60
1:L:312:LEU:HD21	1:M:858:GLU:CB	2.32	0.60
1:F:930:ARG:HG3	1:F:930:ARG:NH1	2.17	0.60
1:K:949:ALA:O	1:K:953:ILE:HG12	2.02	0.60
1:M:930:ARG:HG3	1:M:930:ARG:NH1	2.17	0.60
1:M:949:ALA:O	1:M:953:ILE:HG12	2.02	0.60
1:N:317:ARG:HH11	1:N:317:ARG:HG3	1.66	0.60
1:N:778:GLN:O	1:N:779:GLN:CB	2.49	0.60
1:C:317:ARG:HH11	1:C:317:ARG:HG3	1.66	0.60
1:F:786:ALA:HB3	1:F:788:ILE:CD1	2.32	0.60
1:I:888:GLU:HG2	1:J:856:ARG:HH22	1.67	0.60
1:M:786:ALA:HB3	1:M:788:ILE:CD1	2.32	0.60
1:C:778:GLN:O	1:C:779:GLN:CB	2.49	0.59
1:E:778:GLN:O	1:E:779:GLN:CB	2.49	0.59
1:I:317:ARG:HH11	1:I:317:ARG:HG3	1.66	0.59
1:I:930:ARG:HG3	1:I:930:ARG:NH1	2.17	0.59
1:L:894:ILE:HG13	1:L:895:GLU:N	2.16	0.59
1:M:860:GLU:C	1:M:862:VAL:H	2.08	0.59
1:O:894:ILE:HG13	1:O:895:GLU:N	2.16	0.59
1:C:894:ILE:HG13	1:C:895:GLU:N	2.16	0.59
1:E:786:ALA:HB3	1:E:788:ILE:CD1	2.32	0.59
1:G:786:ALA:HB3	1:G:788:ILE:CD1	2.32	0.59
1:G:949:ALA:O	1:G:953:ILE:HG12	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:786:ALA:HB3	1:I:788:ILE:CD1	2.32	0.59
1:I:894:ILE:HG13	1:I:895:GLU:N	2.16	0.59
1:J:317:ARG:HH11	1:J:317:ARG:HG3	1.66	0.59
1:J:786:ALA:HB3	1:J:788:ILE:CD1	2.32	0.59
1:J:930:ARG:HG3	1:J:930:ARG:NH1	2.16	0.59
1:M:902:ARG:HG2	1:M:902:ARG:HH11	1.65	0.59
1:M:903:LYS:NZ	1:N:839:PRO:HB2	2.17	0.59
1:N:786:ALA:HB3	1:N:788:ILE:CD1	2.32	0.59
1:A:317:ARG:HH11	1:A:317:ARG:HG3	1.66	0.59
1:A:930:ARG:HG3	1:A:930:ARG:NH1	2.17	0.59
1:C:268:ILE:HG22	1:C:272:LEU:HD11	1.85	0.59
1:D:894:ILE:HG13	1:D:895:GLU:N	2.17	0.59
1:D:930:ARG:HG3	1:D:930:ARG:NH1	2.17	0.59
1:F:268:ILE:HG22	1:F:272:LEU:HD11	1.85	0.59
1:F:317:ARG:HH11	1:F:317:ARG:HG3	1.66	0.59
1:J:778:GLN:O	1:J:779:GLN:CB	2.49	0.59
1:O:268:ILE:HG22	1:O:272:LEU:HD11	1.85	0.59
1:O:930:ARG:HG3	1:O:930:ARG:NH1	2.17	0.59
1:P:894:ILE:HG13	1:P:895:GLU:N	2.16	0.59
1:A:785:LYS:CG	1:P:785:LYS:CB	2.79	0.59
1:A:856:ARG:CZ	1:H:891:MET:HE1	2.32	0.59
1:A:949:ALA:O	1:A:953:ILE:HG12	2.02	0.59
1:C:895:GLU:O	1:C:899:VAL:HG12	2.03	0.59
1:D:949:ALA:O	1:D:953:ILE:HG12	2.02	0.59
1:E:930:ARG:HG3	1:E:930:ARG:NH1	2.17	0.59
1:I:843:ILE:HG23	1:I:844:ASP:N	2.18	0.59
1:I:929:ILE:CD1	1:J:852:LEU:CD1	2.78	0.59
1:L:853:ARG:NH2	1:L:860:GLU:HG3	2.16	0.59
1:N:891:MET:HG3	1:O:852:LEU:CB	2.32	0.59
1:C:786:ALA:HB3	1:C:788:ILE:CD1	2.32	0.59
1:E:949:ALA:O	1:E:953:ILE:HG12	2.02	0.59
1:G:789:THR:O	1:J:739:UNK:O	2.20	0.59
1:H:786:ALA:HB3	1:H:788:ILE:CD1	2.32	0.59
1:H:894:ILE:HG13	1:H:895:GLU:N	2.16	0.59
1:I:895:GLU:O	1:I:899:VAL:HG12	2.03	0.59
1:J:949:ALA:O	1:J:953:ILE:HG12	2.02	0.59
1:K:317:ARG:HH11	1:K:317:ARG:HG3	1.66	0.59
1:K:786:ALA:HB3	1:K:788:ILE:CD1	2.32	0.59
1:O:317:ARG:HH11	1:O:317:ARG:HG3	1.66	0.59
1:O:895:GLU:O	1:O:899:VAL:HG12	2.03	0.59
1:B:898:TYR:CD2	1:C:848:ALA:HB2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:843:ILE:HG23	1:E:844:ASP:N	2.18	0.59
1:I:903:LYS:HD2	1:J:841:ASP:CG	2.28	0.59
1:K:894:ILE:HG13	1:K:895:GLU:N	2.16	0.59
1:L:786:ALA:HB3	1:L:788:ILE:CD1	2.32	0.59
1:M:894:ILE:HG13	1:M:895:GLU:N	2.16	0.59
1:N:843:ILE:HG23	1:N:844:ASP:N	2.18	0.59
1:P:949:ALA:O	1:P:953:ILE:HG12	2.02	0.59
1:B:843:ILE:HG23	1:B:844:ASP:N	2.18	0.59
1:B:949:ALA:O	1:B:953:ILE:HG12	2.02	0.59
1:D:268:ILE:HG22	1:D:272:LEU:HD11	1.85	0.59
1:G:930:ARG:HG3	1:G:930:ARG:NH1	2.17	0.59
1:I:897:TYR:CG	1:I:953:ILE:HG21	2.36	0.59
1:J:843:ILE:HG23	1:J:844:ASP:N	2.18	0.59
1:K:268:ILE:HG22	1:K:272:LEU:HD11	1.85	0.59
1:P:268:ILE:HG22	1:P:272:LEU:HD11	1.85	0.59
1:A:869:GLU:H	1:A:869:GLU:CD	2.11	0.59
1:B:268:ILE:HG22	1:B:272:LEU:HD11	1.85	0.59
1:G:843:ILE:HG23	1:G:844:ASP:N	2.18	0.59
1:H:317:ARG:HG3	1:H:317:ARG:HH11	1.66	0.59
1:H:949:ALA:O	1:H:953:ILE:HG12	2.02	0.59
1:I:902:ARG:HH11	1:J:844:ASP:CG	2.10	0.59
1:K:843:ILE:HG23	1:K:844:ASP:N	2.18	0.59
1:L:268:ILE:HG22	1:L:272:LEU:HD11	1.85	0.59
1:L:949:ALA:O	1:L:953:ILE:HG12	2.02	0.59
1:N:869:GLU:CD	1:N:869:GLU:H	2.11	0.59
1:N:895:GLU:O	1:N:899:VAL:HG12	2.03	0.59
1:P:786:ALA:HB3	1:P:788:ILE:CD1	2.32	0.59
1:A:268:ILE:HG22	1:A:272:LEU:HD11	1.85	0.59
1:A:786:ALA:HB3	1:A:788:ILE:CD1	2.32	0.59
1:A:894:ILE:HG13	1:A:895:GLU:N	2.16	0.59
1:B:869:GLU:H	1:B:869:GLU:CD	2.11	0.59
1:E:317:ARG:HG3	1:E:317:ARG:HH11	1.66	0.59
1:E:768:ASP:O	1:E:771:VAL:HG13	2.03	0.59
1:P:869:GLU:CD	1:P:869:GLU:H	2.11	0.59
1:A:768:ASP:O	1:A:771:VAL:HG13	2.03	0.59
1:C:768:ASP:O	1:C:771:VAL:HG13	2.03	0.59
1:D:895:GLU:O	1:D:899:VAL:HG12	2.03	0.59
1:G:778:GLN:O	1:G:779:GLN:CB	2.49	0.59
1:H:268:ILE:HG22	1:H:272:LEU:HD11	1.84	0.59
1:I:853:ARG:NH2	1:I:860:GLU:HG3	2.16	0.59
1:I:869:GLU:CD	1:I:869:GLU:H	2.11	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:768:ASP:O	1:J:771:VAL:HG13	2.03	0.59
1:A:317:ARG:NH2	1:A:319:ARG:HB2	2.18	0.58
1:C:317:ARG:NH2	1:C:319:ARG:HB2	2.18	0.58
1:C:843:ILE:HG23	1:C:844:ASP:N	2.18	0.58
1:D:786:ALA:HB3	1:D:788:ILE:CD1	2.32	0.58
1:F:894:ILE:HG13	1:F:895:GLU:N	2.16	0.58
1:G:894:ILE:HG13	1:G:895:GLU:N	2.16	0.58
1:G:895:GLU:O	1:G:899:VAL:HG12	2.03	0.58
1:J:317:ARG:NH2	1:J:319:ARG:HB2	2.18	0.58
1:J:869:GLU:H	1:J:869:GLU:CD	2.11	0.58
1:L:843:ILE:HG23	1:L:844:ASP:N	2.18	0.58
1:O:891:MET:HE2	1:P:852:LEU:HB3	1.85	0.58
1:A:895:GLU:O	1:A:899:VAL:HG12	2.03	0.58
1:D:768:ASP:O	1:D:771:VAL:HG13	2.03	0.58
1:D:785:LYS:HG3	1:M:785:LYS:HE3	1.85	0.58
1:E:895:GLU:O	1:E:899:VAL:HG12	2.03	0.58
1:F:949:ALA:O	1:F:953:ILE:HG12	2.02	0.58
1:I:949:ALA:O	1:I:953:ILE:HG12	2.02	0.58
1:K:768:ASP:O	1:K:771:VAL:HG13	2.03	0.58
1:O:768:ASP:O	1:O:771:VAL:HG13	2.03	0.58
1:P:843:ILE:HG23	1:P:844:ASP:N	2.18	0.58
1:B:786:ALA:HB3	1:B:788:ILE:CD1	2.32	0.58
1:B:788:ILE:HG23	1:O:741:UNK:CB	2.33	0.58
1:F:898:TYR:HD2	1:G:848:ALA:CB	2.15	0.58
1:J:895:GLU:O	1:J:899:VAL:HG12	2.03	0.58
1:K:869:GLU:CD	1:K:869:GLU:H	2.11	0.58
1:M:311:LYS:HD3	1:M:317:ARG:HA	1.86	0.58
1:M:843:ILE:HG23	1:M:844:ASP:N	2.18	0.58
1:M:895:GLU:O	1:M:899:VAL:HG12	2.03	0.58
1:O:786:ALA:HB3	1:O:788:ILE:CD1	2.32	0.58
1:O:949:ALA:O	1:O:953:ILE:HG12	2.02	0.58
1:C:949:ALA:O	1:C:953:ILE:HG12	2.02	0.58
1:F:869:GLU:CD	1:F:869:GLU:H	2.11	0.58
1:J:268:ILE:HG22	1:J:272:LEU:HD11	1.85	0.58
1:K:316:THR:HG21	1:L:339:ARG:CD	2.33	0.58
1:N:317:ARG:NH2	1:N:319:ARG:HB2	2.18	0.58
1:P:895:GLU:O	1:P:899:VAL:HG12	2.03	0.58
1:A:746:UNK:C	1:A:795:ARG:CZ	2.82	0.58
1:A:843:ILE:HG23	1:A:844:ASP:N	2.18	0.58
1:E:746:UNK:C	1:E:795:ARG:CZ	2.82	0.58
1:F:317:ARG:NH2	1:F:319:ARG:HB2	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:785:LYS:HG3	1:J:785:LYS:HG2	1.83	0.58
1:H:869:GLU:CD	1:H:869:GLU:H	2.11	0.58
1:I:317:ARG:NH2	1:I:319:ARG:HB2	2.18	0.58
1:K:746:UNK:C	1:K:795:ARG:CZ	2.82	0.58
1:M:869:GLU:H	1:M:869:GLU:CD	2.11	0.58
1:O:869:GLU:H	1:O:869:GLU:CD	2.11	0.58
1:P:311:LYS:HD3	1:P:317:ARG:HA	1.86	0.58
1:G:769:ARG:HB2	1:G:769:ARG:NH1	2.17	0.58
1:H:746:UNK:C	1:H:795:ARG:CZ	2.82	0.58
1:H:895:GLU:O	1:H:899:VAL:HG12	2.03	0.58
1:O:315:GLY:HA2	1:P:340:TYR:OH	2.03	0.58
1:O:843:ILE:HG23	1:O:844:ASP:N	2.18	0.58
1:C:311:LYS:HD3	1:C:317:ARG:HA	1.86	0.58
1:D:317:ARG:NH2	1:D:319:ARG:HB2	2.18	0.58
1:D:869:GLU:H	1:D:869:GLU:CD	2.11	0.58
1:E:317:ARG:NH2	1:E:319:ARG:HB2	2.18	0.58
1:G:268:ILE:HG22	1:G:272:LEU:HD11	1.85	0.58
1:L:317:ARG:NH2	1:L:319:ARG:HB2	2.18	0.58
1:L:895:GLU:O	1:L:899:VAL:HG12	2.03	0.58
1:N:768:ASP:O	1:N:771:VAL:HG13	2.03	0.58
1:A:891:MET:HG3	1:B:852:LEU:HG	1.85	0.58
1:D:746:UNK:C	1:D:795:ARG:CZ	2.82	0.58
1:D:843:ILE:HG23	1:D:844:ASP:N	2.18	0.58
1:E:268:ILE:HG22	1:E:272:LEU:HD11	1.85	0.58
1:E:894:ILE:HG13	1:E:895:GLU:N	2.16	0.58
1:J:746:UNK:C	1:J:795:ARG:CZ	2.82	0.58
1:O:317:ARG:NH2	1:O:319:ARG:HB2	2.18	0.58
1:P:317:ARG:NH2	1:P:319:ARG:HB2	2.18	0.58
1:F:843:ILE:HG23	1:F:844:ASP:N	2.18	0.58
1:G:317:ARG:NH2	1:G:319:ARG:HB2	2.18	0.58
1:G:768:ASP:O	1:G:771:VAL:HG13	2.03	0.58
1:I:268:ILE:HG22	1:I:272:LEU:HD11	1.85	0.58
1:I:310:ARG:NH1	1:J:858:GLU:HG3	2.18	0.58
1:I:311:LYS:HD3	1:I:317:ARG:HA	1.86	0.58
1:J:898:TYR:CD2	1:K:848:ALA:CB	2.79	0.58
1:K:895:GLU:O	1:K:899:VAL:HG12	2.03	0.58
1:M:268:ILE:HG22	1:M:272:LEU:HD11	1.85	0.58
1:P:930:ARG:HG3	1:P:930:ARG:NH1	2.17	0.58
1:C:746:UNK:C	1:C:795:ARG:CZ	2.82	0.58
1:D:311:LYS:HD3	1:D:317:ARG:HA	1.86	0.58
1:K:317:ARG:NH2	1:K:319:ARG:HB2	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:768:ASP:O	1:M:771:VAL:HG13	2.03	0.58
1:N:268:ILE:HG22	1:N:272:LEU:HD11	1.85	0.58
1:B:895:GLU:O	1:B:899:VAL:HG12	2.03	0.57
1:C:332:VAL:CG2	1:C:334:LYS:HE2	2.34	0.57
1:E:311:LYS:HD3	1:E:317:ARG:HA	1.86	0.57
1:F:332:VAL:CG2	1:F:334:LYS:HE2	2.34	0.57
1:H:768:ASP:O	1:H:771:VAL:HG13	2.03	0.57
1:K:290:ILE:HD11	1:K:297:LYS:CE	2.34	0.57
1:K:902:ARG:HG3	1:L:839:PRO:HB3	1.85	0.57
1:L:311:LYS:HD3	1:L:317:ARG:HA	1.86	0.57
1:B:317:ARG:NH2	1:B:319:ARG:HB2	2.18	0.57
1:C:316:THR:HG21	1:D:339:ARG:HD3	1.86	0.57
1:D:928:LEU:HB2	1:D:956:MET:HE1	1.86	0.57
1:H:311:LYS:HD3	1:H:317:ARG:HA	1.86	0.57
1:L:869:GLU:H	1:L:869:GLU:CD	2.11	0.57
1:M:317:ARG:NH2	1:M:319:ARG:HB2	2.18	0.57
1:N:949:ALA:O	1:N:953:ILE:HG12	2.02	0.57
1:P:768:ASP:O	1:P:771:VAL:HG13	2.03	0.57
1:A:839:PRO:HA	1:H:902:ARG:NH1	2.19	0.57
1:F:768:ASP:O	1:F:771:VAL:HG13	2.03	0.57
1:F:895:GLU:O	1:F:899:VAL:HG12	2.03	0.57
1:H:317:ARG:NH2	1:H:319:ARG:HB2	2.18	0.57
1:I:928:LEU:HB2	1:I:956:MET:HE1	1.87	0.57
1:O:746:UNK:C	1:O:795:ARG:CZ	2.82	0.57
1:P:746:UNK:C	1:P:795:ARG:CZ	2.82	0.57
1:P:928:LEU:HB2	1:P:956:MET:HE1	1.86	0.57
1:A:769:ARG:HB2	1:A:769:ARG:NH1	2.17	0.57
1:D:332:VAL:CG2	1:D:334:LYS:HE2	2.34	0.57
1:G:332:VAL:CG2	1:G:334:LYS:HE2	2.34	0.57
1:G:746:UNK:C	1:G:795:ARG:CZ	2.82	0.57
1:I:746:UNK:C	1:I:795:ARG:CZ	2.82	0.57
1:K:769:ARG:HB2	1:K:769:ARG:NH1	2.17	0.57
1:L:768:ASP:O	1:L:771:VAL:HG13	2.03	0.57
1:M:332:VAL:CG2	1:M:334:LYS:HE2	2.34	0.57
1:M:928:LEU:HB2	1:M:956:MET:HE1	1.87	0.57
1:N:891:MET:CE	1:O:852:LEU:CB	2.79	0.57
1:O:332:VAL:CG2	1:O:334:LYS:HE2	2.34	0.57
1:A:928:LEU:HB2	1:A:956:MET:HE1	1.87	0.57
1:B:746:UNK:C	1:B:795:ARG:CZ	2.82	0.57
1:B:768:ASP:O	1:B:771:VAL:HG13	2.03	0.57
1:E:869:GLU:H	1:E:869:GLU:CD	2.11	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:311:LYS:HD3	1:G:317:ARG:HA	1.86	0.57
1:I:768:ASP:O	1:I:771:VAL:HG13	2.03	0.57
1:J:894:ILE:HD11	1:K:852:LEU:CD1	2.24	0.57
1:K:332:VAL:CG2	1:K:334:LYS:HE2	2.34	0.57
1:P:332:VAL:CG2	1:P:334:LYS:HE2	2.34	0.57
1:F:891:MET:HE2	1:G:856:ARG:HD3	1.81	0.57
1:G:312:LEU:CD2	1:H:858:GLU:CG	2.77	0.57
1:H:350:TYR:CD1	1:H:350:TYR:C	2.83	0.57
1:I:332:VAL:CG2	1:I:334:LYS:HE2	2.35	0.57
1:I:350:TYR:CD1	1:I:350:TYR:C	2.83	0.57
1:M:746:UNK:C	1:M:795:ARG:CZ	2.82	0.57
1:D:350:TYR:CD1	1:D:350:TYR:C	2.83	0.57
1:E:928:LEU:HB2	1:E:956:MET:HE1	1.86	0.57
1:F:746:UNK:C	1:F:795:ARG:CZ	2.82	0.57
1:H:930:ARG:HG3	1:H:930:ARG:NH1	2.17	0.57
1:J:332:VAL:CG2	1:J:334:LYS:HE2	2.34	0.57
1:J:928:LEU:HB2	1:J:956:MET:HE1	1.87	0.57
1:K:928:LEU:HB2	1:K:956:MET:HE1	1.87	0.57
1:L:350:TYR:CD1	1:L:350:TYR:C	2.83	0.57
1:N:746:UNK:C	1:N:795:ARG:CZ	2.82	0.57
1:O:311:LYS:HD3	1:O:317:ARG:HA	1.86	0.57
1:O:928:LEU:HB2	1:O:956:MET:HE1	1.87	0.57
1:A:332:VAL:CG2	1:A:334:LYS:HE2	2.34	0.57
1:C:313:PRO:O	1:D:343:ASN:ND2	2.38	0.57
1:C:869:GLU:CD	1:C:869:GLU:H	2.11	0.57
1:D:308:VAL:HG13	1:D:309:SER:N	2.20	0.57
1:F:769:ARG:HB2	1:F:769:ARG:NH1	2.17	0.57
1:H:332:VAL:CG2	1:H:334:LYS:HE2	2.35	0.57
1:H:843:ILE:HG23	1:H:844:ASP:N	2.18	0.57
1:H:928:LEU:HB2	1:H:956:MET:HE1	1.86	0.57
1:I:856:ARG:CZ	1:P:891:MET:CE	2.75	0.57
1:J:308:VAL:HG13	1:J:309:SER:N	2.20	0.57
1:O:271:GLU:O	1:O:274:LYS:HB2	2.05	0.57
1:O:308:VAL:HG13	1:O:309:SER:N	2.20	0.57
1:I:903:LYS:O	1:I:904:SER:OG	2.22	0.57
1:I:955:LEU:O	1:I:959:THR:HG22	2.05	0.57
1:K:308:VAL:HG13	1:K:309:SER:N	2.20	0.57
1:M:769:ARG:HB2	1:M:769:ARG:NH1	2.17	0.57
1:N:290:ILE:HD11	1:N:297:LYS:CE	2.34	0.57
1:N:311:LYS:HD3	1:N:317:ARG:HA	1.86	0.57
1:A:311:LYS:HD3	1:A:317:ARG:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:903:LYS:O	1:A:904:SER:OG	2.22	0.57
1:B:271:GLU:O	1:B:274:LYS:HB2	2.05	0.57
1:B:765:SER:O	1:B:767:ARG:N	2.38	0.57
1:D:316:THR:HG21	1:E:339:ARG:CD	2.35	0.57
1:F:350:TYR:CD1	1:F:350:TYR:C	2.83	0.57
1:G:271:GLU:O	1:G:274:LYS:HB2	2.05	0.57
1:I:271:GLU:O	1:I:274:LYS:HB2	2.05	0.57
1:I:310:ARG:NH1	1:J:858:GLU:CD	2.61	0.57
1:J:891:MET:HE1	1:K:856:ARG:NE	2.14	0.57
1:J:955:LEU:O	1:J:959:THR:HG22	2.05	0.57
1:K:765:SER:O	1:K:767:ARG:N	2.38	0.57
1:L:308:VAL:HG13	1:L:309:SER:N	2.20	0.57
1:L:955:LEU:O	1:L:959:THR:HG22	2.05	0.57
1:M:308:VAL:HG13	1:M:309:SER:N	2.20	0.57
1:B:332:VAL:CG2	1:B:334:LYS:HE2	2.34	0.56
1:C:308:VAL:HG13	1:C:309:SER:N	2.20	0.56
1:C:350:TYR:CD1	1:C:350:TYR:C	2.83	0.56
1:D:815:PRO:HG2	1:D:816:PHE:HD1	1.71	0.56
1:E:815:PRO:HG2	1:E:816:PHE:HD1	1.70	0.56
1:E:955:LEU:O	1:E:959:THR:HG22	2.05	0.56
1:F:955:LEU:O	1:F:959:THR:HG22	2.05	0.56
1:G:928:LEU:HB2	1:G:956:MET:HE1	1.87	0.56
1:H:271:GLU:O	1:H:274:LYS:HB2	2.05	0.56
1:J:929:ILE:CD1	1:K:852:LEU:HD13	2.34	0.56
1:L:332:VAL:CG2	1:L:334:LYS:HE2	2.35	0.56
1:L:765:SER:O	1:L:767:ARG:N	2.38	0.56
1:M:765:SER:O	1:M:767:ARG:N	2.38	0.56
1:M:891:MET:HG3	1:N:852:LEU:CG	2.31	0.56
1:N:271:GLU:O	1:N:274:LYS:HB2	2.05	0.56
1:N:928:LEU:HB2	1:N:956:MET:HE1	1.87	0.56
1:N:955:LEU:O	1:N:959:THR:HG22	2.05	0.56
1:O:888:GLU:HG2	1:P:856:ARG:NH1	2.17	0.56
1:A:955:LEU:O	1:A:959:THR:HG22	2.05	0.56
1:B:308:VAL:HG13	1:B:309:SER:N	2.20	0.56
1:B:311:LYS:HD3	1:B:317:ARG:HA	1.86	0.56
1:B:730:UNK:N	1:P:730:UNK:CB	2.68	0.56
1:E:332:VAL:CG2	1:E:334:LYS:HE2	2.34	0.56
1:F:903:LYS:O	1:F:904:SER:OG	2.22	0.56
1:G:903:LYS:O	1:G:904:SER:OG	2.22	0.56
1:G:955:LEU:O	1:G:959:THR:HG22	2.05	0.56
1:L:746:UNK:C	1:L:795:ARG:CZ	2.82	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:928:LEU:HB2	1:L:956:MET:HE1	1.86	0.56
1:N:350:TYR:CD1	1:N:350:TYR:C	2.83	0.56
1:A:844:ASP:OD2	1:H:902:ARG:HG2	2.05	0.56
1:C:271:GLU:O	1:C:274:LYS:HB2	2.05	0.56
1:C:769:ARG:HB2	1:C:769:ARG:NH1	2.17	0.56
1:D:785:LYS:HB3	1:M:785:LYS:O	2.04	0.56
1:E:308:VAL:HG13	1:E:309:SER:N	2.20	0.56
1:E:350:TYR:CD1	1:E:350:TYR:C	2.83	0.56
1:E:765:SER:O	1:E:767:ARG:N	2.38	0.56
1:F:311:LYS:HD3	1:F:317:ARG:HA	1.86	0.56
1:G:290:ILE:HD11	1:G:297:LYS:CE	2.34	0.56
1:G:765:SER:O	1:G:767:ARG:N	2.38	0.56
1:G:869:GLU:H	1:G:869:GLU:CD	2.11	0.56
1:H:815:PRO:HG2	1:H:816:PHE:HD1	1.70	0.56
1:H:903:LYS:O	1:H:904:SER:OG	2.22	0.56
1:I:765:SER:O	1:I:767:ARG:N	2.38	0.56
1:K:350:TYR:CD1	1:K:350:TYR:C	2.83	0.56
1:L:271:GLU:O	1:L:274:LYS:HB2	2.05	0.56
1:P:308:VAL:HG13	1:P:309:SER:N	2.20	0.56
1:P:955:LEU:O	1:P:959:THR:HG22	2.05	0.56
1:A:350:TYR:CD1	1:A:350:TYR:C	2.83	0.56
1:B:350:TYR:CD1	1:B:350:TYR:C	2.83	0.56
1:B:928:LEU:HB2	1:B:956:MET:HE1	1.87	0.56
1:E:741:UNK:CA	1:L:788:ILE:HG22	2.36	0.56
1:H:955:LEU:O	1:H:959:THR:HG22	2.05	0.56
1:K:311:LYS:HD3	1:K:317:ARG:HA	1.86	0.56
1:M:815:PRO:HG2	1:M:816:PHE:HD1	1.71	0.56
1:N:765:SER:O	1:N:767:ARG:N	2.38	0.56
1:O:923:ARG:HG3	1:O:923:ARG:NH1	2.20	0.56
1:P:350:TYR:CD1	1:P:350:TYR:C	2.83	0.56
1:P:815:PRO:HG2	1:P:816:PHE:HD1	1.70	0.56
1:A:271:GLU:O	1:A:274:LYS:HB2	2.05	0.56
1:A:815:PRO:HG2	1:A:816:PHE:HD1	1.70	0.56
1:B:955:LEU:O	1:B:959:THR:HG22	2.05	0.56
1:C:928:LEU:HB2	1:C:956:MET:HE1	1.87	0.56
1:D:271:GLU:O	1:D:274:LYS:HB2	2.05	0.56
1:E:271:GLU:O	1:E:274:LYS:HB2	2.05	0.56
1:I:308:VAL:HG13	1:I:309:SER:N	2.20	0.56
1:K:955:LEU:O	1:K:959:THR:HG22	2.05	0.56
1:L:923:ARG:HG3	1:L:923:ARG:NH1	2.20	0.56
1:M:955:LEU:O	1:M:959:THR:HG22	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:765:SER:O	1:O:767:ARG:N	2.38	0.56
1:P:765:SER:O	1:P:767:ARG:N	2.38	0.56
1:D:765:SER:O	1:D:767:ARG:N	2.38	0.56
1:D:783:ILE:HG21	1:M:788:ILE:HD13	1.88	0.56
1:E:923:ARG:HG3	1:E:923:ARG:NH1	2.20	0.56
1:G:923:ARG:HG3	1:G:923:ARG:NH1	2.20	0.56
1:J:311:LYS:HD3	1:J:317:ARG:HA	1.86	0.56
1:J:765:SER:O	1:J:767:ARG:N	2.38	0.56
1:J:815:PRO:HG2	1:J:816:PHE:HD1	1.70	0.56
1:J:923:ARG:HG3	1:J:923:ARG:NH1	2.20	0.56
1:M:333:ALA:HA	2:M:1001:ADP:O1A	2.06	0.56
1:C:955:LEU:O	1:C:959:THR:HG22	2.05	0.56
1:E:333:ALA:HA	2:E:1001:ADP:O1A	2.06	0.56
1:F:765:SER:O	1:F:767:ARG:N	2.38	0.56
1:J:350:TYR:CD1	1:J:350:TYR:C	2.83	0.56
1:M:271:GLU:O	1:M:274:LYS:HB2	2.05	0.56
1:M:350:TYR:CD1	1:M:350:TYR:C	2.83	0.56
1:N:332:VAL:CG2	1:N:334:LYS:HE2	2.34	0.56
1:O:350:TYR:CD1	1:O:350:TYR:C	2.83	0.56
1:O:815:PRO:HG2	1:O:816:PHE:HD1	1.70	0.56
1:A:308:VAL:HG13	1:A:309:SER:N	2.20	0.56
1:F:271:GLU:O	1:F:274:LYS:HB2	2.05	0.56
1:F:290:ILE:HD11	1:F:297:LYS:CE	2.34	0.56
1:G:350:TYR:CD1	1:G:350:TYR:C	2.83	0.56
1:I:333:ALA:HA	2:I:1001:ADP:O1A	2.06	0.56
1:L:891:MET:HE1	1:M:856:ARG:NH1	2.20	0.56
1:M:290:ILE:HD11	1:M:297:LYS:CE	2.34	0.56
1:A:333:ALA:HA	2:A:1001:ADP:O1A	2.06	0.56
1:A:765:SER:O	1:A:767:ARG:N	2.38	0.56
1:H:765:SER:O	1:H:767:ARG:N	2.38	0.56
1:J:333:ALA:HA	2:J:1001:ADP:O1A	2.06	0.56
1:J:902:ARG:NH1	1:K:844:ASP:OD2	2.38	0.56
1:M:283:VAL:C	1:M:285:SER:H	2.14	0.56
1:N:923:ARG:HG3	1:N:923:ARG:NH1	2.20	0.56
1:P:923:ARG:HG3	1:P:923:ARG:NH1	2.20	0.56
1:B:283:VAL:C	1:B:285:SER:H	2.14	0.56
1:B:902:ARG:NH1	1:C:844:ASP:OD2	2.36	0.56
1:F:308:VAL:HG13	1:F:309:SER:N	2.20	0.56
1:G:308:VAL:HG13	1:G:309:SER:N	2.20	0.56
1:H:308:VAL:HG13	1:H:309:SER:N	2.20	0.56
1:H:923:ARG:HG3	1:H:923:ARG:NH1	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:890:ALA:O	1:A:893:GLU:N	2.40	0.55
1:A:923:ARG:HG3	1:A:923:ARG:NH1	2.20	0.55
1:B:930:ARG:HG3	1:B:930:ARG:NH1	2.16	0.55
1:D:283:VAL:C	1:D:285:SER:H	2.14	0.55
1:J:856:ARG:HG3	1:J:860:GLU:OE2	2.07	0.55
1:K:283:VAL:C	1:K:285:SER:H	2.14	0.55
1:M:890:ALA:O	1:M:893:GLU:N	2.40	0.55
1:B:333:ALA:HA	2:B:1001:ADP:O1A	2.06	0.55
1:B:769:ARG:HB2	1:B:769:ARG:NH1	2.17	0.55
1:C:923:ARG:HG3	1:C:923:ARG:NH1	2.20	0.55
1:D:856:ARG:HG3	1:D:860:GLU:OE2	2.07	0.55
1:H:283:VAL:C	1:H:285:SER:H	2.14	0.55
1:H:890:ALA:O	1:H:893:GLU:N	2.39	0.55
1:I:310:ARG:NH2	1:J:857:GLY:C	2.65	0.55
1:J:271:GLU:O	1:J:274:LYS:HB2	2.05	0.55
1:K:271:GLU:O	1:K:274:LYS:HB2	2.05	0.55
1:N:815:PRO:HG2	1:N:816:PHE:HD1	1.70	0.55
1:C:283:VAL:C	1:C:285:SER:H	2.14	0.55
1:D:730:UNK:CB	1:N:730:UNK:CA	2.84	0.55
1:E:283:VAL:C	1:E:285:SER:H	2.14	0.55
1:H:769:ARG:HB2	1:H:769:ARG:NH1	2.17	0.55
1:L:815:PRO:HG2	1:L:816:PHE:HD1	1.70	0.55
1:N:308:VAL:HG13	1:N:309:SER:N	2.20	0.55
1:C:765:SER:O	1:C:767:ARG:N	2.38	0.55
1:D:333:ALA:HA	2:D:1001:ADP:O1A	2.06	0.55
1:E:739:UNK:C	1:L:790:ALA:HA	2.37	0.55
1:E:811:ARG:HD3	1:E:813:LYS:HB2	1.89	0.55
1:F:333:ALA:HA	2:F:1001:ADP:O1A	2.06	0.55
1:F:928:LEU:HB2	1:F:956:MET:HE1	1.86	0.55
1:K:811:ARG:HD3	1:K:813:LYS:HB2	1.89	0.55
1:K:903:LYS:O	1:K:904:SER:OG	2.22	0.55
1:M:811:ARG:HD3	1:M:813:LYS:HB2	1.89	0.55
1:M:856:ARG:HG3	1:M:860:GLU:OE2	2.07	0.55
1:O:290:ILE:HD11	1:O:297:LYS:CE	2.34	0.55
1:P:271:GLU:O	1:P:274:LYS:HB2	2.05	0.55
1:P:333:ALA:HA	2:P:1001:ADP:O1A	2.06	0.55
1:A:283:VAL:C	1:A:285:SER:H	2.14	0.55
1:D:903:LYS:O	1:D:904:SER:OG	2.22	0.55
1:F:316:THR:HG21	1:G:339:ARG:HD3	1.89	0.55
1:G:333:ALA:HA	2:G:1001:ADP:O1A	2.06	0.55
1:G:856:ARG:HG3	1:G:860:GLU:OE2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:290:ILE:HD11	1:H:297:LYS:CE	2.34	0.55
1:H:789:THR:O	1:I:740:UNK:HA	2.07	0.55
1:I:769:ARG:HB2	1:I:769:ARG:NH1	2.17	0.55
1:K:333:ALA:HA	2:K:1001:ADP:O1A	2.06	0.55
1:K:815:PRO:HG2	1:K:816:PHE:HD1	1.70	0.55
1:O:333:ALA:HA	2:O:1001:ADP:O1A	2.06	0.55
1:O:856:ARG:HG3	1:O:860:GLU:OE2	2.07	0.55
1:A:785:LYS:HB3	1:P:785:LYS:HB3	1.89	0.55
1:B:856:ARG:HG3	1:B:860:GLU:OE2	2.07	0.55
1:H:856:ARG:HG3	1:H:860:GLU:OE2	2.07	0.55
1:I:811:ARG:HD3	1:I:813:LYS:HB2	1.89	0.55
1:J:890:ALA:O	1:J:893:GLU:N	2.40	0.55
1:L:283:VAL:C	1:L:285:SER:H	2.14	0.55
1:O:890:ALA:O	1:O:893:GLU:N	2.40	0.55
1:A:792:LEU:CD2	1:P:792:LEU:HD22	2.36	0.55
1:A:856:ARG:HG3	1:A:860:GLU:OE2	2.07	0.55
1:B:815:PRO:HG2	1:B:816:PHE:HD1	1.71	0.55
1:F:815:PRO:HG2	1:F:816:PHE:HD1	1.70	0.55
1:I:283:VAL:C	1:I:285:SER:H	2.14	0.55
1:J:310:ARG:NH2	1:K:857:GLY:C	2.64	0.55
1:O:955:LEU:O	1:O:959:THR:HG22	2.05	0.55
1:C:333:ALA:HA	2:C:1001:ADP:O1A	2.06	0.55
1:C:890:ALA:O	1:C:893:GLU:N	2.40	0.55
1:D:290:ILE:HD11	1:D:297:LYS:CE	2.34	0.55
1:J:283:VAL:C	1:J:285:SER:H	2.14	0.55
1:L:902:ARG:NH1	1:M:844:ASP:OD1	2.40	0.55
1:C:811:ARG:HD3	1:C:813:LYS:HB2	1.89	0.55
1:C:891:MET:CE	1:D:856:ARG:CZ	2.81	0.55
1:C:898:TYR:HD2	1:D:848:ALA:HB2	1.72	0.55
1:J:310:ARG:CZ	1:K:857:GLY:O	2.55	0.55
1:A:811:ARG:HD3	1:A:813:LYS:HB2	1.89	0.55
1:D:899:VAL:CG2	1:E:841:ASP:HA	2.37	0.55
1:I:856:ARG:HG3	1:I:860:GLU:OE2	2.07	0.55
1:I:923:ARG:HG3	1:I:923:ARG:NH1	2.20	0.55
1:K:903:LYS:HZ1	1:L:840:ASP:C	2.15	0.55
1:N:333:ALA:HA	2:N:1001:ADP:O1A	2.06	0.55
1:N:890:ALA:O	1:N:893:GLU:N	2.39	0.55
1:P:856:ARG:HG3	1:P:860:GLU:OE2	2.06	0.55
1:P:890:ALA:O	1:P:893:GLU:N	2.40	0.55
1:B:923:ARG:HG3	1:B:923:ARG:NH1	2.20	0.54
1:D:955:LEU:O	1:D:959:THR:HG22	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:741:UNK:CB	1:L:788:ILE:CB	2.85	0.54
1:E:856:ARG:HG3	1:E:860:GLU:OE2	2.07	0.54
1:G:283:VAL:C	1:G:285:SER:H	2.14	0.54
1:I:815:PRO:HG2	1:I:816:PHE:HD1	1.70	0.54
1:K:923:ARG:HG3	1:K:923:ARG:NH1	2.20	0.54
1:K:930:ARG:HG3	1:K:930:ARG:NH1	2.17	0.54
1:L:333:ALA:HA	2:L:1001:ADP:O1A	2.06	0.54
1:N:856:ARG:HG3	1:N:860:GLU:OE2	2.07	0.54
1:P:811:ARG:HD3	1:P:813:LYS:HB2	1.89	0.54
1:E:769:ARG:HB2	1:E:769:ARG:NH1	2.17	0.54
1:G:890:ALA:O	1:G:893:GLU:N	2.40	0.54
1:J:769:ARG:HB2	1:J:769:ARG:NH1	2.17	0.54
1:K:890:ALA:O	1:K:893:GLU:N	2.40	0.54
1:L:856:ARG:HG3	1:L:860:GLU:OE2	2.07	0.54
1:P:903:LYS:O	1:P:904:SER:OG	2.22	0.54
1:C:930:ARG:HG3	1:C:930:ARG:NH1	2.16	0.54
1:K:856:ARG:HG3	1:K:860:GLU:OE2	2.07	0.54
1:L:946:ARG:HB2	1:L:946:ARG:HH11	1.73	0.54
1:N:903:LYS:O	1:N:904:SER:OG	2.22	0.54
1:O:811:ARG:HD3	1:O:813:LYS:HB2	1.89	0.54
1:P:946:ARG:HH11	1:P:946:ARG:HB2	1.73	0.54
1:A:785:LYS:CE	1:P:785:LYS:HE3	2.37	0.54
1:B:890:ALA:O	1:B:893:GLU:N	2.39	0.54
1:D:890:ALA:O	1:D:893:GLU:N	2.40	0.54
1:F:856:ARG:HG3	1:F:860:GLU:OE2	2.07	0.54
1:N:811:ARG:HD3	1:N:813:LYS:HB2	1.89	0.54
1:O:283:VAL:C	1:O:285:SER:H	2.14	0.54
1:B:811:ARG:HD3	1:B:813:LYS:HB2	1.89	0.54
1:C:815:PRO:HG2	1:C:816:PHE:HD1	1.70	0.54
1:C:856:ARG:HG3	1:C:860:GLU:OE2	2.07	0.54
1:E:890:ALA:O	1:E:893:GLU:N	2.40	0.54
1:E:946:ARG:HH11	1:E:946:ARG:HB2	1.73	0.54
1:F:283:VAL:C	1:F:285:SER:H	2.14	0.54
1:H:333:ALA:HA	2:H:1001:ADP:O1A	2.06	0.54
1:I:890:ALA:O	1:I:893:GLU:N	2.40	0.54
1:A:946:ARG:HB2	1:A:946:ARG:HH11	1.73	0.54
1:B:902:ARG:NH1	1:C:844:ASP:CG	2.65	0.54
1:D:811:ARG:HD3	1:D:813:LYS:HB2	1.89	0.54
1:G:811:ARG:HD3	1:G:813:LYS:HB2	1.89	0.54
1:N:283:VAL:C	1:N:285:SER:H	2.14	0.54
1:N:946:ARG:HB2	1:N:946:ARG:HH11	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:897:TYR:HE2	1:A:901:MET:SD	2.31	0.54
1:G:815:PRO:HG2	1:G:816:PHE:HD1	1.70	0.54
1:H:897:TYR:HE2	1:H:901:MET:SD	2.31	0.54
1:B:897:TYR:HE2	1:B:901:MET:SD	2.31	0.54
1:C:316:THR:HG21	1:D:339:ARG:HD2	1.90	0.54
1:H:811:ARG:HD3	1:H:813:LYS:HB2	1.89	0.54
1:H:946:ARG:HH11	1:H:946:ARG:HB2	1.73	0.54
1:J:310:ARG:NH1	1:K:858:GLU:HG3	2.23	0.54
1:L:897:TYR:HE2	1:L:901:MET:SD	2.31	0.54
1:M:316:THR:HG21	1:N:339:ARG:HD2	1.90	0.54
1:O:946:ARG:HB2	1:O:946:ARG:HH11	1.73	0.54
1:A:894:ILE:HG22	1:A:949:ALA:HB1	1.90	0.54
1:B:329:ASP:CG	1:B:808:ARG:HG3	2.33	0.54
1:D:329:ASP:CG	1:D:808:ARG:HG3	2.33	0.54
1:F:329:ASP:CG	1:F:808:ARG:HG3	2.33	0.54
1:L:894:ILE:HG22	1:L:949:ALA:HB1	1.90	0.54
1:P:283:VAL:C	1:P:285:SER:H	2.14	0.54
1:D:894:ILE:HG22	1:D:949:ALA:HB1	1.90	0.53
1:F:923:ARG:HG3	1:F:923:ARG:NH1	2.20	0.53
1:F:928:LEU:HD22	1:F:956:MET:CE	2.38	0.53
1:G:897:TYR:HE2	1:G:901:MET:SD	2.31	0.53
1:I:894:ILE:CD1	1:J:852:LEU:CD1	2.71	0.53
1:I:897:TYR:HE2	1:I:901:MET:SD	2.31	0.53
1:J:290:ILE:HD11	1:J:297:LYS:CE	2.34	0.53
1:J:746:UNK:C	1:J:795:ARG:NH2	2.72	0.53
1:J:811:ARG:HD3	1:J:813:LYS:HB2	1.89	0.53
1:J:894:ILE:HG22	1:J:949:ALA:HB1	1.90	0.53
1:L:811:ARG:HD3	1:L:813:LYS:HB2	1.89	0.53
1:N:897:TYR:HE2	1:N:901:MET:SD	2.31	0.53
1:A:928:LEU:HD22	1:A:956:MET:CE	2.38	0.53
1:B:928:LEU:HD22	1:B:956:MET:CE	2.38	0.53
1:C:852:LEU:O	1:C:853:ARG:C	2.52	0.53
1:D:746:UNK:C	1:D:795:ARG:NH2	2.72	0.53
1:F:897:TYR:HE2	1:F:901:MET:SD	2.31	0.53
1:H:774:GLU:OE1	1:H:781:ILE:HA	2.09	0.53
1:J:897:TYR:HE2	1:J:901:MET:SD	2.31	0.53
1:L:329:ASP:CG	1:L:808:ARG:HG3	2.33	0.53
1:L:928:LEU:HD22	1:L:956:MET:CE	2.38	0.53
1:M:746:UNK:C	1:M:795:ARG:NH2	2.72	0.53
1:O:928:LEU:HD22	1:O:956:MET:CE	2.38	0.53
1:C:897:TYR:HE2	1:C:901:MET:SD	2.31	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:897:TYR:HE2	1:D:901:MET:SD	2.31	0.53
1:G:894:ILE:HG22	1:G:949:ALA:HB1	1.90	0.53
1:I:329:ASP:CG	1:I:808:ARG:HG3	2.33	0.53
1:J:310:ARG:NH1	1:K:858:GLU:CD	2.66	0.53
1:J:946:ARG:HH11	1:J:946:ARG:HB2	1.73	0.53
1:L:746:UNK:C	1:L:795:ARG:NH2	2.72	0.53
1:L:890:ALA:O	1:L:893:GLU:N	2.40	0.53
1:M:774:GLU:OE1	1:M:781:ILE:HA	2.09	0.53
1:C:946:ARG:HB2	1:C:946:ARG:HH11	1.73	0.53
1:E:329:ASP:CG	1:E:808:ARG:HG3	2.33	0.53
1:I:894:ILE:HD13	1:J:852:LEU:HD11	1.84	0.53
1:J:928:LEU:HD22	1:J:956:MET:CE	2.38	0.53
1:N:928:LEU:HD22	1:N:956:MET:CE	2.38	0.53
1:O:746:UNK:C	1:O:795:ARG:NH2	2.72	0.53
1:O:774:GLU:OE1	1:O:781:ILE:HA	2.09	0.53
1:O:852:LEU:O	1:O:853:ARG:C	2.52	0.53
1:A:329:ASP:CG	1:A:808:ARG:HG3	2.33	0.53
1:B:946:ARG:HH11	1:B:946:ARG:HB2	1.73	0.53
1:D:946:ARG:HB2	1:D:946:ARG:HH11	1.73	0.53
1:F:946:ARG:HB2	1:F:946:ARG:HH11	1.73	0.53
1:M:946:ARG:HH11	1:M:946:ARG:HB2	1.73	0.53
1:P:897:TYR:HE2	1:P:901:MET:SD	2.31	0.53
1:D:774:GLU:OE1	1:D:781:ILE:HA	2.09	0.53
1:F:811:ARG:HD3	1:F:813:LYS:HB2	1.89	0.53
1:F:894:ILE:HG22	1:F:949:ALA:HB1	1.90	0.53
1:H:852:LEU:O	1:H:853:ARG:C	2.52	0.53
1:I:852:LEU:O	1:I:853:ARG:C	2.52	0.53
1:I:894:ILE:HG22	1:I:949:ALA:HB1	1.90	0.53
1:J:852:LEU:O	1:J:853:ARG:C	2.52	0.53
1:K:774:GLU:OE1	1:K:781:ILE:HA	2.09	0.53
1:M:897:TYR:HE2	1:M:901:MET:SD	2.31	0.53
1:A:746:UNK:C	1:A:795:ARG:NH2	2.72	0.53
1:A:843:ILE:HG23	1:A:844:ASP:H	1.74	0.53
1:C:278:ILE:HG23	1:C:279:VAL:N	2.24	0.53
1:C:928:LEU:HD22	1:C:956:MET:CE	2.38	0.53
1:E:894:ILE:HG22	1:E:949:ALA:HB1	1.90	0.53
1:E:903:LYS:O	1:E:904:SER:OG	2.22	0.53
1:F:843:ILE:HG23	1:F:844:ASP:H	1.74	0.53
1:G:774:GLU:OE1	1:G:781:ILE:HA	2.09	0.53
1:H:746:UNK:C	1:H:795:ARG:NH2	2.72	0.53
1:I:290:ILE:HD11	1:I:297:LYS:CE	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:928:LEU:HD22	1:K:956:MET:CE	2.38	0.53
1:K:928:LEU:HD13	1:K:956:MET:HE2	1.91	0.53
1:N:885:VAL:HG13	1:O:856:ARG:CB	2.24	0.53
1:B:278:ILE:HG23	1:B:279:VAL:N	2.24	0.53
1:B:746:UNK:C	1:B:795:ARG:NH2	2.72	0.53
1:C:746:UNK:C	1:C:795:ARG:NH2	2.72	0.53
1:F:928:LEU:HD13	1:F:956:MET:HE2	1.91	0.53
1:G:746:UNK:C	1:G:795:ARG:NH2	2.72	0.53
1:H:329:ASP:CG	1:H:808:ARG:HG3	2.34	0.53
1:I:843:ILE:HG23	1:I:844:ASP:H	1.74	0.53
1:I:928:LEU:HD13	1:I:956:MET:HE2	1.91	0.53
1:I:946:ARG:HB2	1:I:946:ARG:HH11	1.73	0.53
1:J:329:ASP:CG	1:J:808:ARG:HG3	2.34	0.53
1:K:746:UNK:C	1:K:795:ARG:NH2	2.72	0.53
1:M:329:ASP:CG	1:M:808:ARG:HG3	2.33	0.53
1:M:894:ILE:HG22	1:M:949:ALA:HB1	1.90	0.53
1:O:897:TYR:HE2	1:O:901:MET:SD	2.31	0.53
1:P:769:ARG:HB2	1:P:769:ARG:NH1	2.17	0.53
1:B:852:LEU:O	1:B:853:ARG:C	2.52	0.53
1:B:902:ARG:HG2	1:C:844:ASP:OD2	2.08	0.53
1:B:928:LEU:HD13	1:B:956:MET:HE2	1.91	0.53
1:C:290:ILE:HD11	1:C:297:LYS:CE	2.34	0.53
1:C:869:GLU:HG2	1:C:870:ILE:CD1	2.39	0.53
1:C:894:ILE:HG22	1:C:949:ALA:HB1	1.90	0.53
1:D:278:ILE:HG23	1:D:279:VAL:N	2.24	0.53
1:D:852:LEU:O	1:D:853:ARG:C	2.52	0.53
1:E:746:UNK:C	1:E:795:ARG:NH2	2.72	0.53
1:E:928:LEU:HD13	1:E:956:MET:HE2	1.91	0.53
1:G:329:ASP:CG	1:G:808:ARG:HG3	2.33	0.53
1:G:790:ALA:HA	1:J:739:UNK:O	2.09	0.53
1:G:946:ARG:HB2	1:G:946:ARG:HH11	1.73	0.53
1:I:746:UNK:C	1:I:795:ARG:NH2	2.72	0.53
1:I:869:GLU:HG2	1:I:870:ILE:CD1	2.39	0.53
1:I:895:GLU:CD	1:J:849:ARG:HB2	2.34	0.53
1:J:848:ALA:O	1:J:849:ARG:C	2.52	0.53
1:L:769:ARG:HB2	1:L:769:ARG:NH1	2.17	0.53
1:L:774:GLU:OE1	1:L:781:ILE:HA	2.09	0.53
1:L:843:ILE:HG23	1:L:844:ASP:H	1.74	0.53
1:M:843:ILE:HG23	1:M:844:ASP:H	1.74	0.53
1:O:903:LYS:O	1:O:904:SER:OG	2.22	0.53
1:C:329:ASP:CG	1:C:808:ARG:HG3	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:891:MET:HG3	1:D:852:LEU:CB	2.39	0.53
1:E:843:ILE:HG23	1:E:844:ASP:H	1.74	0.53
1:E:852:LEU:O	1:E:853:ARG:C	2.52	0.53
1:F:746:UNK:C	1:F:795:ARG:NH2	2.72	0.53
1:G:928:LEU:HD22	1:G:956:MET:CE	2.39	0.53
1:K:848:ALA:O	1:K:849:ARG:C	2.52	0.53
1:K:946:ARG:HH11	1:K:946:ARG:HB2	1.73	0.53
1:L:290:ILE:HD11	1:L:297:LYS:CE	2.34	0.53
1:M:278:ILE:HG23	1:M:279:VAL:N	2.24	0.53
1:O:329:ASP:CG	1:O:808:ARG:HG3	2.33	0.53
1:O:894:ILE:HG22	1:O:949:ALA:HB1	1.90	0.53
1:P:329:ASP:CG	1:P:808:ARG:HG3	2.33	0.53
1:P:746:UNK:C	1:P:795:ARG:NH2	2.72	0.53
1:D:869:GLU:HG2	1:D:870:ILE:CD1	2.39	0.52
1:D:923:ARG:HG3	1:D:923:ARG:NH1	2.20	0.52
1:E:278:ILE:HG23	1:E:279:VAL:N	2.24	0.52
1:I:928:LEU:HD22	1:I:956:MET:CE	2.38	0.52
1:J:928:LEU:HD13	1:J:956:MET:HE2	1.91	0.52
1:K:897:TYR:HE2	1:K:901:MET:SD	2.31	0.52
1:L:869:GLU:HG2	1:L:870:ILE:CD1	2.39	0.52
1:N:329:ASP:CG	1:N:808:ARG:HG3	2.34	0.52
1:N:894:ILE:HG22	1:N:949:ALA:HB1	1.90	0.52
1:P:928:LEU:HD22	1:P:956:MET:CE	2.38	0.52
1:A:290:ILE:HD11	1:A:297:LYS:CE	2.34	0.52
1:A:774:GLU:OE1	1:A:781:ILE:HA	2.09	0.52
1:B:290:ILE:HD11	1:B:297:LYS:CE	2.34	0.52
1:C:804:PRO:HD2	1:C:807:GLY:O	2.10	0.52
1:C:848:ALA:O	1:C:849:ARG:C	2.52	0.52
1:E:928:LEU:HD22	1:E:956:MET:CE	2.38	0.52
1:F:774:GLU:OE1	1:F:781:ILE:HA	2.09	0.52
1:F:848:ALA:O	1:F:849:ARG:C	2.52	0.52
1:G:848:ALA:O	1:G:849:ARG:C	2.52	0.52
1:G:852:LEU:O	1:G:853:ARG:C	2.52	0.52
1:J:774:GLU:OE1	1:J:781:ILE:HA	2.09	0.52
1:J:804:PRO:HD2	1:J:807:GLY:O	2.10	0.52
1:J:843:ILE:HG23	1:J:844:ASP:H	1.74	0.52
1:K:329:ASP:CG	1:K:808:ARG:HG3	2.33	0.52
1:K:894:ILE:HG22	1:K:949:ALA:HB1	1.90	0.52
1:M:903:LYS:O	1:M:904:SER:OG	2.22	0.52
1:N:746:UNK:C	1:N:795:ARG:NH2	2.72	0.52
1:A:278:ILE:HG23	1:A:279:VAL:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:928:LEU:HD22	1:D:956:MET:CE	2.38	0.52
1:E:804:PRO:HD2	1:E:807:GLY:O	2.10	0.52
1:E:897:TYR:HE2	1:E:901:MET:SD	2.31	0.52
1:L:848:ALA:O	1:L:849:ARG:C	2.52	0.52
1:L:852:LEU:O	1:L:853:ARG:C	2.52	0.52
1:M:928:LEU:HD13	1:M:956:MET:HE2	1.91	0.52
1:P:804:PRO:HD2	1:P:807:GLY:O	2.10	0.52
1:P:869:GLU:HG2	1:P:870:ILE:CD1	2.39	0.52
1:A:804:PRO:HD2	1:A:807:GLY:O	2.10	0.52
1:D:769:ARG:HB2	1:D:769:ARG:NH1	2.17	0.52
1:E:774:GLU:OE1	1:E:781:ILE:HA	2.09	0.52
1:F:278:ILE:HG23	1:F:279:VAL:N	2.24	0.52
1:G:869:GLU:HG2	1:G:870:ILE:CD1	2.39	0.52
1:G:899:VAL:HG23	1:H:841:ASP:HA	1.90	0.52
1:M:848:ALA:O	1:M:849:ARG:C	2.52	0.52
1:N:869:GLU:HG2	1:N:870:ILE:CD1	2.39	0.52
1:O:928:LEU:HD13	1:O:956:MET:HE2	1.91	0.52
1:A:848:ALA:O	1:A:849:ARG:C	2.52	0.52
1:A:869:GLU:HG2	1:A:870:ILE:CD1	2.39	0.52
1:B:774:GLU:OE1	1:B:781:ILE:HA	2.09	0.52
1:F:852:LEU:O	1:F:853:ARG:C	2.52	0.52
1:G:843:ILE:HG23	1:G:844:ASP:H	1.74	0.52
1:H:804:PRO:HD2	1:H:807:GLY:O	2.10	0.52
1:I:774:GLU:OE1	1:I:781:ILE:HA	2.09	0.52
1:J:310:ARG:HD3	1:K:858:GLU:CG	2.39	0.52
1:K:278:ILE:HG23	1:K:279:VAL:N	2.24	0.52
1:L:278:ILE:HG23	1:L:279:VAL:N	2.24	0.52
1:M:903:LYS:NZ	1:N:839:PRO:CB	2.73	0.52
1:M:928:LEU:HD22	1:M:956:MET:CE	2.38	0.52
1:N:774:GLU:OE1	1:N:781:ILE:HA	2.09	0.52
1:N:928:LEU:HD13	1:N:956:MET:HE2	1.91	0.52
1:O:804:PRO:HD2	1:O:807:GLY:O	2.10	0.52
1:P:928:LEU:HD13	1:P:956:MET:HE2	1.91	0.52
1:D:804:PRO:HD2	1:D:807:GLY:O	2.10	0.52
1:D:928:LEU:HD13	1:D:956:MET:HE2	1.91	0.52
1:E:290:ILE:HD11	1:E:297:LYS:CE	2.34	0.52
1:E:346:PRO:HG2	1:E:755:TYR:HE1	1.75	0.52
1:H:928:LEU:HD22	1:H:956:MET:CE	2.38	0.52
1:I:804:PRO:HD2	1:I:807:GLY:O	2.10	0.52
1:J:278:ILE:HG23	1:J:279:VAL:N	2.24	0.52
1:K:804:PRO:HD2	1:K:807:GLY:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:774:GLU:OE1	1:C:781:ILE:HA	2.09	0.52
1:D:268:ILE:HG22	1:D:272:LEU:CD1	2.40	0.52
1:D:346:PRO:HG2	1:D:755:TYR:HE1	1.75	0.52
1:G:837:ASP:O	1:G:837:ASP:CG	2.53	0.52
1:K:903:LYS:NZ	1:L:840:ASP:C	2.68	0.52
1:M:852:LEU:O	1:M:853:ARG:C	2.52	0.52
1:N:268:ILE:HG22	1:N:272:LEU:CD1	2.40	0.52
1:N:278:ILE:HG23	1:N:279:VAL:N	2.24	0.52
1:N:848:ALA:O	1:N:849:ARG:C	2.52	0.52
1:N:852:LEU:O	1:N:853:ARG:C	2.52	0.52
1:A:346:PRO:HG2	1:A:755:TYR:HE1	1.75	0.52
1:E:837:ASP:CG	1:E:837:ASP:O	2.53	0.52
1:F:890:ALA:O	1:F:893:GLU:N	2.40	0.52
1:F:902:ARG:NH1	1:G:844:ASP:OD2	2.43	0.52
1:I:346:PRO:HG2	1:I:755:TYR:HE1	1.75	0.52
1:I:837:ASP:CG	1:I:837:ASP:O	2.53	0.52
1:J:332:VAL:O	1:J:333:ALA:CB	2.58	0.52
1:M:346:PRO:HG2	1:M:755:TYR:HE1	1.75	0.52
1:M:804:PRO:HD2	1:M:807:GLY:O	2.10	0.52
1:N:843:ILE:HG23	1:N:844:ASP:H	1.74	0.52
1:O:346:PRO:HG2	1:O:755:TYR:HE1	1.75	0.52
1:O:837:ASP:O	1:O:837:ASP:CG	2.53	0.52
1:A:928:LEU:HD13	1:A:956:MET:HE2	1.91	0.52
1:B:268:ILE:HG22	1:B:272:LEU:CD1	2.40	0.52
1:C:738:UNK:CB	1:C:746:UNK:C	2.88	0.52
1:C:837:ASP:CG	1:C:837:ASP:O	2.53	0.52
1:C:902:ARG:NH1	1:D:844:ASP:OD1	2.43	0.52
1:F:804:PRO:HD2	1:F:807:GLY:O	2.10	0.52
1:H:268:ILE:HG22	1:H:272:LEU:CD1	2.40	0.52
1:H:278:ILE:HG23	1:H:279:VAL:N	2.24	0.52
1:I:738:UNK:CB	1:I:746:UNK:C	2.88	0.52
1:I:856:ARG:NH1	1:P:891:MET:CE	2.72	0.52
1:J:738:UNK:CB	1:J:746:UNK:C	2.88	0.52
1:K:843:ILE:HG23	1:K:844:ASP:H	1.74	0.52
1:N:738:UNK:CB	1:N:746:UNK:C	2.88	0.52
1:O:778:GLN:NE2	1:P:354:UNK:CB	2.72	0.52
1:P:774:GLU:OE1	1:P:781:ILE:HA	2.08	0.52
1:B:346:PRO:HG2	1:B:755:TYR:HE1	1.75	0.52
1:B:848:ALA:O	1:B:849:ARG:C	2.52	0.52
1:B:929:ILE:HD11	1:C:852:LEU:HD13	1.92	0.52
1:C:843:ILE:HG23	1:C:844:ASP:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:903:LYS:O	1:C:904:SER:OG	2.22	0.52
1:D:960:LEU:HD23	1:D:963:ILE:HD12	1.92	0.52
1:G:332:VAL:O	1:G:333:ALA:CB	2.58	0.52
1:G:789:THR:CA	1:J:740:UNK:HA	2.40	0.52
1:H:928:LEU:HD13	1:H:956:MET:HE2	1.91	0.52
1:I:268:ILE:HG22	1:I:272:LEU:CD1	2.40	0.52
1:K:738:UNK:CB	1:K:746:UNK:C	2.88	0.52
1:K:902:ARG:NH1	1:L:844:ASP:OD2	2.35	0.52
1:L:346:PRO:HG2	1:L:755:TYR:HE1	1.75	0.52
1:O:278:ILE:HG23	1:O:279:VAL:N	2.24	0.52
1:P:278:ILE:HG23	1:P:279:VAL:N	2.24	0.52
1:A:738:UNK:CB	1:A:746:UNK:C	2.88	0.51
1:C:309:SER:HB2	1:C:320:GLY:CA	2.41	0.51
1:C:346:PRO:HG2	1:C:755:TYR:HE1	1.75	0.51
1:C:960:LEU:HD23	1:C:963:ILE:HD12	1.92	0.51
1:D:332:VAL:O	1:D:333:ALA:CB	2.58	0.51
1:D:837:ASP:CG	1:D:837:ASP:O	2.53	0.51
1:D:848:ALA:O	1:D:849:ARG:C	2.52	0.51
1:G:278:ILE:HG23	1:G:279:VAL:N	2.24	0.51
1:G:309:SER:HB2	1:G:320:GLY:CA	2.40	0.51
1:H:738:UNK:CB	1:H:746:UNK:C	2.88	0.51
1:K:346:PRO:HG2	1:K:755:TYR:HE1	1.75	0.51
1:M:837:ASP:CG	1:M:837:ASP:O	2.53	0.51
1:M:923:ARG:HG3	1:M:923:ARG:NH1	2.20	0.51
1:N:309:SER:HB2	1:N:320:GLY:CA	2.41	0.51
1:N:769:ARG:HB2	1:N:769:ARG:NH1	2.17	0.51
1:O:888:GLU:CG	1:P:856:ARG:HH12	2.20	0.51
1:B:837:ASP:CG	1:B:837:ASP:O	2.53	0.51
1:B:960:LEU:HD23	1:B:963:ILE:HD12	1.92	0.51
1:F:755:TYR:CD1	1:F:755:TYR:N	2.78	0.51
1:G:804:PRO:HD2	1:G:807:GLY:O	2.10	0.51
1:G:960:LEU:HD23	1:G:963:ILE:HD12	1.92	0.51
1:H:869:GLU:HG2	1:H:870:ILE:CD1	2.39	0.51
1:I:278:ILE:HG23	1:I:279:VAL:N	2.24	0.51
1:I:848:ALA:O	1:I:849:ARG:C	2.52	0.51
1:J:309:SER:HB2	1:J:320:GLY:CA	2.41	0.51
1:J:869:GLU:HG2	1:J:870:ILE:CD1	2.39	0.51
1:L:928:LEU:HD13	1:L:956:MET:HE2	1.91	0.51
1:O:309:SER:HB2	1:O:320:GLY:CA	2.41	0.51
1:P:268:ILE:HG22	1:P:272:LEU:CD1	2.40	0.51
1:P:894:ILE:HG22	1:P:949:ALA:HB1	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:VAL:O	1:A:333:ALA:CB	2.58	0.51
1:B:804:PRO:HD2	1:B:807:GLY:O	2.10	0.51
1:C:928:LEU:HD13	1:C:956:MET:HE2	1.91	0.51
1:F:346:PRO:HG2	1:F:755:TYR:HE1	1.75	0.51
1:F:891:MET:CE	1:G:856:ARG:NH1	2.73	0.51
1:G:268:ILE:HG22	1:G:272:LEU:CD1	2.40	0.51
1:J:837:ASP:CG	1:J:837:ASP:O	2.53	0.51
1:K:332:VAL:O	1:K:333:ALA:CB	2.58	0.51
1:N:346:PRO:HG2	1:N:755:TYR:HE1	1.75	0.51
1:O:332:VAL:O	1:O:333:ALA:CB	2.58	0.51
1:O:843:ILE:HG23	1:O:844:ASP:H	1.74	0.51
1:A:852:LEU:O	1:A:853:ARG:C	2.52	0.51
1:B:738:UNK:CB	1:B:746:UNK:C	2.88	0.51
1:E:268:ILE:HG22	1:E:272:LEU:CD1	2.40	0.51
1:E:869:GLU:HG2	1:E:870:ILE:CD1	2.39	0.51
1:F:332:VAL:O	1:F:333:ALA:CB	2.58	0.51
1:G:791:THR:O	1:J:738:UNK:CA	2.58	0.51
1:H:870:ILE:HD12	1:H:870:ILE:N	2.26	0.51
1:I:844:ASP:CG	1:P:902:ARG:HH11	2.19	0.51
1:I:870:ILE:HD12	1:I:870:ILE:N	2.26	0.51
1:I:960:LEU:HD23	1:I:963:ILE:HD12	1.92	0.51
1:L:804:PRO:HD2	1:L:807:GLY:O	2.10	0.51
1:L:837:ASP:CG	1:L:837:ASP:O	2.53	0.51
1:M:332:VAL:O	1:M:333:ALA:CB	2.58	0.51
1:N:804:PRO:HD2	1:N:807:GLY:O	2.10	0.51
1:O:316:THR:CB	1:P:339:ARG:HD3	2.40	0.51
1:O:960:LEU:HD23	1:O:963:ILE:HD12	1.92	0.51
1:P:346:PRO:HG2	1:P:755:TYR:HE1	1.75	0.51
1:B:788:ILE:CG2	1:O:741:UNK:CB	2.89	0.51
1:D:738:UNK:CB	1:D:746:UNK:C	2.88	0.51
1:D:870:ILE:HD12	1:D:870:ILE:N	2.26	0.51
1:E:870:ILE:HD12	1:E:870:ILE:N	2.26	0.51
1:F:268:ILE:HG22	1:F:272:LEU:CD1	2.40	0.51
1:F:837:ASP:CG	1:F:837:ASP:O	2.53	0.51
1:H:848:ALA:O	1:H:849:ARG:C	2.52	0.51
1:H:894:ILE:HG22	1:H:949:ALA:HB1	1.90	0.51
1:I:313:PRO:HG2	1:I:314:ASP:H	1.76	0.51
1:J:960:LEU:HD23	1:J:963:ILE:HD12	1.92	0.51
1:K:309:SER:HB2	1:K:320:GLY:CA	2.41	0.51
1:K:874:TYR:C	1:K:874:TYR:CD1	2.89	0.51
1:L:309:SER:HB2	1:L:320:GLY:CA	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:960:LEU:HD23	1:N:963:ILE:HD12	1.92	0.51
1:O:738:UNK:CB	1:O:746:UNK:C	2.88	0.51
1:O:869:GLU:HG2	1:O:870:ILE:CD1	2.39	0.51
1:P:313:PRO:HG2	1:P:314:ASP:H	1.76	0.51
1:P:837:ASP:CG	1:P:837:ASP:O	2.53	0.51
1:P:852:LEU:O	1:P:853:ARG:C	2.52	0.51
1:B:894:ILE:HG22	1:B:949:ALA:HB1	1.90	0.51
1:C:332:VAL:O	1:C:333:ALA:CB	2.58	0.51
1:G:785:LYS:O	1:G:786:ALA:CB	2.59	0.51
1:H:332:VAL:O	1:H:333:ALA:CB	2.58	0.51
1:H:346:PRO:HG2	1:H:755:TYR:HE1	1.75	0.51
1:K:785:LYS:O	1:K:786:ALA:CB	2.59	0.51
1:C:313:PRO:HG2	1:C:314:ASP:H	1.76	0.51
1:C:891:MET:HE2	1:D:856:ARG:HD3	1.90	0.51
1:E:313:PRO:HG2	1:E:314:ASP:H	1.76	0.51
1:E:314:ASP:O	1:F:340:TYR:CE2	2.64	0.51
1:E:785:LYS:O	1:E:786:ALA:CB	2.59	0.51
1:F:874:TYR:CD1	1:F:874:TYR:C	2.89	0.51
1:G:874:TYR:CD1	1:G:874:TYR:C	2.89	0.51
1:H:837:ASP:CG	1:H:837:ASP:O	2.53	0.51
1:K:268:ILE:HG22	1:K:272:LEU:CD1	2.40	0.51
1:K:852:LEU:O	1:K:853:ARG:C	2.52	0.51
1:N:874:TYR:CD1	1:N:874:TYR:C	2.89	0.51
1:P:309:SER:HB2	1:P:320:GLY:CA	2.41	0.51
1:P:843:ILE:HG23	1:P:844:ASP:H	1.74	0.51
1:A:785:LYS:O	1:A:786:ALA:CB	2.59	0.51
1:A:837:ASP:CG	1:A:837:ASP:O	2.53	0.51
1:A:960:LEU:HD23	1:A:963:ILE:HD12	1.92	0.51
1:B:870:ILE:HD12	1:B:870:ILE:N	2.26	0.51
1:E:738:UNK:CB	1:E:746:UNK:C	2.88	0.51
1:F:870:ILE:HD12	1:F:870:ILE:N	2.26	0.51
1:G:755:TYR:CD1	1:G:755:TYR:N	2.79	0.51
1:G:928:LEU:HD13	1:G:956:MET:HE2	1.91	0.51
1:L:738:UNK:CB	1:L:746:UNK:C	2.88	0.51
1:M:738:UNK:CB	1:M:746:UNK:C	2.88	0.51
1:O:268:ILE:HG22	1:O:272:LEU:CD1	2.40	0.51
1:P:738:UNK:CB	1:P:746:UNK:C	2.88	0.51
1:P:848:ALA:O	1:P:849:ARG:C	2.52	0.51
1:A:268:ILE:HG22	1:A:272:LEU:CD1	2.40	0.51
1:A:755:TYR:CD1	1:A:755:TYR:N	2.79	0.51
1:D:874:TYR:CD1	1:D:874:TYR:C	2.89	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:960:LEU:HD23	1:E:963:ILE:HD12	1.92	0.51
1:G:312:LEU:HD22	1:H:858:GLU:HB3	1.92	0.51
1:H:874:TYR:C	1:H:874:TYR:CD1	2.89	0.51
1:J:870:ILE:HD12	1:J:870:ILE:N	2.26	0.51
1:L:870:ILE:HD12	1:L:870:ILE:N	2.26	0.51
1:O:313:PRO:HG2	1:O:314:ASP:H	1.76	0.51
1:O:870:ILE:HD12	1:O:870:ILE:N	2.26	0.51
1:D:313:PRO:HG2	1:D:314:ASP:H	1.76	0.51
1:D:755:TYR:CD1	1:D:755:TYR:N	2.79	0.51
1:E:848:ALA:O	1:E:849:ARG:C	2.52	0.51
1:G:346:PRO:HG2	1:G:755:TYR:HE1	1.75	0.51
1:L:313:PRO:HG2	1:L:314:ASP:H	1.76	0.51
1:L:903:LYS:O	1:L:904:SER:OG	2.22	0.51
1:O:755:TYR:CD1	1:O:755:TYR:N	2.79	0.51
1:P:755:TYR:CD1	1:P:755:TYR:N	2.79	0.51
1:P:870:ILE:HD12	1:P:870:ILE:N	2.26	0.51
1:B:898:TYR:HD2	1:C:848:ALA:HB2	1.74	0.50
1:F:738:UNK:CB	1:F:746:UNK:C	2.88	0.50
1:F:785:LYS:O	1:F:786:ALA:CB	2.59	0.50
1:G:738:UNK:CB	1:G:746:UNK:C	2.88	0.50
1:H:350:TYR:HD1	1:H:351:THR:N	2.09	0.50
1:I:311:LYS:HE2	1:I:317:ARG:HG3	1.94	0.50
1:K:311:LYS:HE2	1:K:317:ARG:HG3	1.94	0.50
1:L:268:ILE:HG22	1:L:272:LEU:CD1	2.40	0.50
1:L:312:LEU:CD2	1:M:858:GLU:HB3	2.41	0.50
1:L:874:TYR:CD1	1:L:874:TYR:C	2.89	0.50
1:N:313:PRO:HG2	1:N:314:ASP:H	1.76	0.50
1:N:870:ILE:HD12	1:N:870:ILE:N	2.26	0.50
1:O:848:ALA:O	1:O:849:ARG:C	2.52	0.50
1:P:809:PHE:HB2	1:P:818:GLN:CD	2.36	0.50
1:B:843:ILE:HG23	1:B:844:ASP:H	1.74	0.50
1:B:869:GLU:HG2	1:B:870:ILE:CD1	2.39	0.50
1:C:268:ILE:HG22	1:C:272:LEU:CD1	2.40	0.50
1:G:809:PHE:HB2	1:G:818:GLN:CD	2.36	0.50
1:G:870:ILE:HD12	1:G:870:ILE:N	2.26	0.50
1:J:268:ILE:HG22	1:J:272:LEU:CD1	2.40	0.50
1:J:346:PRO:HG2	1:J:755:TYR:HE1	1.75	0.50
1:J:874:TYR:CD1	1:J:874:TYR:C	2.89	0.50
1:K:755:TYR:CD1	1:K:755:TYR:N	2.78	0.50
1:K:837:ASP:CG	1:K:837:ASP:O	2.53	0.50
1:M:309:SER:HB2	1:M:320:GLY:CA	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:785:LYS:O	1:M:786:ALA:CB	2.59	0.50
1:M:960:LEU:HD23	1:M:963:ILE:HD12	1.92	0.50
1:P:960:LEU:HD23	1:P:963:ILE:HD12	1.92	0.50
1:A:313:PRO:HG2	1:A:314:ASP:H	1.76	0.50
1:A:874:TYR:CD1	1:A:874:TYR:C	2.89	0.50
1:B:809:PHE:HB2	1:B:818:GLN:CD	2.36	0.50
1:D:843:ILE:HG23	1:D:844:ASP:H	1.74	0.50
1:E:874:TYR:CD1	1:E:874:TYR:C	2.89	0.50
1:H:791:THR:HG22	1:H:791:THR:O	2.12	0.50
1:K:869:GLU:HG2	1:K:870:ILE:CD1	2.39	0.50
1:L:311:LYS:HE2	1:L:317:ARG:HG3	1.94	0.50
1:L:332:VAL:O	1:L:333:ALA:CB	2.58	0.50
1:N:332:VAL:O	1:N:333:ALA:CB	2.58	0.50
1:N:958:TYR:CD1	1:N:958:TYR:C	2.90	0.50
1:P:785:LYS:O	1:P:786:ALA:CB	2.59	0.50
1:B:874:TYR:CD1	1:B:874:TYR:C	2.89	0.50
1:C:755:TYR:CD1	1:C:755:TYR:N	2.79	0.50
1:C:785:LYS:O	1:C:786:ALA:CB	2.59	0.50
1:D:309:SER:HB2	1:D:320:GLY:CA	2.40	0.50
1:D:350:TYR:HD1	1:D:351:THR:N	2.10	0.50
1:E:809:PHE:HB2	1:E:818:GLN:CD	2.36	0.50
1:E:863:ALA:CB	1:E:864:PRO:HD2	2.36	0.50
1:E:958:TYR:CD1	1:E:958:TYR:C	2.90	0.50
1:H:843:ILE:HG23	1:H:844:ASP:H	1.74	0.50
1:I:809:PHE:HB2	1:I:818:GLN:CD	2.36	0.50
1:I:894:ILE:HD11	1:J:852:LEU:HD21	1.93	0.50
1:I:929:ILE:HG12	1:J:852:LEU:CD1	2.42	0.50
1:M:874:TYR:CD1	1:M:874:TYR:C	2.89	0.50
1:N:311:LYS:HE2	1:N:317:ARG:HG3	1.94	0.50
1:N:785:LYS:O	1:N:786:ALA:CB	2.59	0.50
1:O:785:LYS:O	1:O:786:ALA:CB	2.59	0.50
1:D:958:TYR:C	1:D:958:TYR:CD1	2.90	0.50
1:F:791:THR:O	1:F:791:THR:HG22	2.12	0.50
1:I:350:TYR:HD1	1:I:351:THR:N	2.09	0.50
1:J:887:SER:C	1:J:889:GLU:N	2.67	0.50
1:L:958:TYR:C	1:L:958:TYR:CD1	2.90	0.50
1:M:313:PRO:HG2	1:M:314:ASP:H	1.76	0.50
1:M:842:LYS:HG3	1:M:843:ILE:N	2.27	0.50
1:N:809:PHE:HB2	1:N:818:GLN:CD	2.36	0.50
1:N:837:ASP:CG	1:N:837:ASP:O	2.53	0.50
1:O:958:TYR:C	1:O:958:TYR:CD1	2.90	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:332:VAL:O	1:P:333:ALA:CB	2.58	0.50
1:P:874:TYR:C	1:P:874:TYR:CD1	2.89	0.50
1:B:327:VAL:O	1:B:327:VAL:HG23	2.12	0.50
1:F:311:LYS:HE2	1:F:317:ARG:HG3	1.94	0.50
1:F:960:LEU:HD23	1:F:963:ILE:HD12	1.92	0.50
1:H:809:PHE:HB2	1:H:818:GLN:CD	2.36	0.50
1:H:958:TYR:CD1	1:H:958:TYR:C	2.90	0.50
1:K:960:LEU:HD23	1:K:963:ILE:HD12	1.92	0.50
1:L:755:TYR:CD1	1:L:755:TYR:N	2.79	0.50
1:L:769:ARG:O	1:L:770:SER:C	2.55	0.50
1:L:960:LEU:HD23	1:L:963:ILE:HD12	1.92	0.50
1:M:809:PHE:HB2	1:M:818:GLN:CD	2.36	0.50
1:O:902:ARG:HH12	1:P:839:PRO:HA	1.75	0.50
1:A:809:PHE:HB2	1:A:818:GLN:CD	2.36	0.50
1:A:870:ILE:HD12	1:A:870:ILE:N	2.26	0.50
1:A:887:SER:C	1:A:889:GLU:N	2.67	0.50
1:C:327:VAL:HG23	1:C:327:VAL:O	2.12	0.50
1:C:874:TYR:C	1:C:874:TYR:CD1	2.89	0.50
1:D:311:LYS:HE2	1:D:317:ARG:HG3	1.94	0.50
1:D:893:GLU:HG3	1:D:946:ARG:HG3	1.94	0.50
1:E:755:TYR:CD1	1:E:755:TYR:N	2.79	0.50
1:E:878:ALA:C	1:E:880:LYS:H	2.20	0.50
1:F:352:SER:O	1:F:354:UNK:N	2.45	0.50
1:F:809:PHE:HB2	1:F:818:GLN:CD	2.36	0.50
1:F:842:LYS:HG3	1:F:843:ILE:N	2.27	0.50
1:G:327:VAL:HG23	1:G:327:VAL:O	2.12	0.50
1:G:336:GLN:HE21	1:G:340:TYR:HE1	1.60	0.50
1:H:313:PRO:HG2	1:H:314:ASP:H	1.76	0.50
1:H:946:ARG:HB2	1:H:946:ARG:NH1	2.27	0.50
1:I:874:TYR:CD1	1:I:874:TYR:C	2.89	0.50
1:K:809:PHE:HB2	1:K:818:GLN:CD	2.36	0.50
1:K:946:ARG:HB2	1:K:946:ARG:NH1	2.27	0.50
1:L:893:GLU:HG3	1:L:946:ARG:HG3	1.94	0.50
1:M:755:TYR:CD1	1:M:755:TYR:N	2.79	0.50
1:M:769:ARG:O	1:M:770:SER:C	2.55	0.50
1:M:869:GLU:HG2	1:M:870:ILE:CD1	2.39	0.50
1:M:870:ILE:HD12	1:M:870:ILE:N	2.26	0.50
1:M:903:LYS:HE2	1:M:903:LYS:CA	2.42	0.50
1:N:878:ALA:C	1:N:880:LYS:H	2.20	0.50
1:N:887:SER:C	1:N:889:GLU:N	2.67	0.50
1:P:352:SER:O	1:P:354:UNK:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:SER:O	1:A:354:UNK:N	2.45	0.50
1:B:311:LYS:HE2	1:B:317:ARG:HG3	1.94	0.50
1:B:332:VAL:O	1:B:333:ALA:CB	2.58	0.50
1:B:958:TYR:CD1	1:B:958:TYR:C	2.90	0.50
1:C:769:ARG:O	1:C:770:SER:C	2.55	0.50
1:C:870:ILE:HD12	1:C:870:ILE:N	2.26	0.50
1:D:785:LYS:O	1:D:786:ALA:CB	2.59	0.50
1:F:313:PRO:HG2	1:F:314:ASP:H	1.76	0.50
1:F:946:ARG:HB2	1:F:946:ARG:NH1	2.27	0.50
1:H:309:SER:HB2	1:H:320:GLY:CA	2.41	0.50
1:H:960:LEU:HD23	1:H:963:ILE:HD12	1.92	0.50
1:I:352:SER:O	1:I:354:UNK:N	2.45	0.50
1:I:958:TYR:CD1	1:I:958:TYR:C	2.90	0.50
1:J:755:TYR:CD1	1:J:755:TYR:N	2.79	0.50
1:J:769:ARG:O	1:J:770:SER:C	2.55	0.50
1:J:809:PHE:HB2	1:J:818:GLN:CD	2.36	0.50
1:K:903:LYS:HE2	1:K:903:LYS:CA	2.42	0.50
1:M:946:ARG:HB2	1:M:946:ARG:NH1	2.27	0.50
1:M:958:TYR:CD1	1:M:958:TYR:C	2.90	0.50
1:N:893:GLU:HG3	1:N:946:ARG:HG3	1.94	0.50
1:N:946:ARG:HB2	1:N:946:ARG:NH1	2.27	0.50
1:O:311:LYS:HE2	1:O:317:ARG:HG3	1.94	0.50
1:O:352:SER:O	1:O:354:UNK:N	2.45	0.50
1:P:290:ILE:HD11	1:P:297:LYS:CE	2.34	0.50
1:P:958:TYR:CD1	1:P:958:TYR:C	2.90	0.50
1:B:309:SER:HB2	1:B:320:GLY:CA	2.40	0.50
1:B:352:SER:O	1:B:354:UNK:N	2.45	0.50
1:B:755:TYR:CD1	1:B:755:TYR:N	2.79	0.50
1:B:785:LYS:O	1:B:786:ALA:CB	2.59	0.50
1:B:893:GLU:HG3	1:B:946:ARG:HG3	1.94	0.50
1:C:347:ARG:HB2	1:C:754:GLY:HA2	1.94	0.50
1:C:352:SER:O	1:C:354:UNK:N	2.45	0.50
1:C:809:PHE:HB2	1:C:818:GLN:CD	2.36	0.50
1:C:898:TYR:CD2	1:D:848:ALA:HB2	2.46	0.50
1:C:946:ARG:HB2	1:C:946:ARG:NH1	2.27	0.50
1:E:295:GLU:CD	1:E:295:GLU:N	2.70	0.50
1:E:312:LEU:HD21	1:F:858:GLU:HA	1.94	0.50
1:E:791:THR:HG22	1:E:791:THR:O	2.12	0.50
1:F:309:SER:HB2	1:F:320:GLY:CA	2.41	0.50
1:G:789:THR:H	1:J:740:UNK:C	2.25	0.50
1:H:769:ARG:O	1:H:770:SER:C	2.55	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:336:GLN:HE21	1:I:340:TYR:HE1	1.60	0.50
1:J:313:PRO:HG2	1:J:314:ASP:H	1.76	0.50
1:K:753:GLY:HA2	1:K:795:ARG:HH11	1.77	0.50
1:L:785:LYS:O	1:L:786:ALA:CB	2.59	0.50
1:M:347:ARG:HB2	1:M:754:GLY:HA2	1.94	0.50
1:P:327:VAL:HG23	1:P:327:VAL:O	2.12	0.50
1:A:753:GLY:HA2	1:A:795:ARG:HH11	1.77	0.49
1:A:769:ARG:O	1:A:770:SER:C	2.55	0.49
1:A:946:ARG:HB2	1:A:946:ARG:NH1	2.27	0.49
1:B:791:THR:HG22	1:B:791:THR:O	2.12	0.49
1:C:958:TYR:CD1	1:C:958:TYR:C	2.90	0.49
1:D:352:SER:O	1:D:354:UNK:N	2.45	0.49
1:F:317:ARG:HG2	1:F:318:LEU:N	2.27	0.49
1:F:878:ALA:C	1:F:880:LYS:H	2.20	0.49
1:G:842:LYS:HG3	1:G:843:ILE:N	2.27	0.49
1:G:893:GLU:HG3	1:G:946:ARG:HG3	1.94	0.49
1:H:753:GLY:HA2	1:H:795:ARG:HH11	1.77	0.49
1:H:785:LYS:O	1:H:786:ALA:CB	2.59	0.49
1:I:309:SER:HB2	1:I:320:GLY:CA	2.41	0.49
1:I:753:GLY:HA2	1:I:795:ARG:HH11	1.77	0.49
1:J:878:ALA:C	1:J:880:LYS:H	2.20	0.49
1:L:946:ARG:HB2	1:L:946:ARG:NH1	2.27	0.49
1:M:268:ILE:HG22	1:M:272:LEU:CD1	2.40	0.49
1:M:295:GLU:CD	1:M:295:GLU:N	2.70	0.49
1:N:791:THR:O	1:N:791:THR:HG22	2.12	0.49
1:O:315:GLY:HA2	1:P:340:TYR:CZ	2.47	0.49
1:P:946:ARG:HB2	1:P:946:ARG:NH1	2.27	0.49
1:C:878:ALA:C	1:C:880:LYS:H	2.20	0.49
1:C:903:LYS:HE2	1:C:903:LYS:CA	2.42	0.49
1:D:946:ARG:HB2	1:D:946:ARG:NH1	2.27	0.49
1:E:327:VAL:O	1:E:327:VAL:HG23	2.12	0.49
1:E:946:ARG:HB2	1:E:946:ARG:NH1	2.27	0.49
1:F:327:VAL:HG23	1:F:327:VAL:O	2.12	0.49
1:F:753:GLY:HA2	1:F:795:ARG:HH11	1.77	0.49
1:F:869:GLU:HG2	1:F:870:ILE:CD1	2.39	0.49
1:G:311:LYS:HE2	1:G:317:ARG:HG3	1.94	0.49
1:G:946:ARG:HB2	1:G:946:ARG:NH1	2.27	0.49
1:H:327:VAL:HG23	1:H:327:VAL:O	2.12	0.49
1:H:352:SER:O	1:H:354:UNK:N	2.45	0.49
1:H:755:TYR:CD1	1:H:755:TYR:N	2.79	0.49
1:I:791:THR:O	1:I:791:THR:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:338:LEU:N	1:K:338:LEU:HD23	2.28	0.49
1:K:878:ALA:C	1:K:880:LYS:H	2.20	0.49
1:K:958:TYR:CD1	1:K:958:TYR:C	2.90	0.49
1:L:791:THR:O	1:L:791:THR:HG22	2.12	0.49
1:L:881:ASN:C	1:L:882:ILE:HD13	2.38	0.49
1:N:738:UNK:CB	1:N:792:LEU:HD11	2.43	0.49
1:N:891:MET:SD	1:O:852:LEU:HB2	2.52	0.49
1:O:769:ARG:HB2	1:O:769:ARG:NH1	2.17	0.49
1:P:329:ASP:OD1	1:P:808:ARG:HG3	2.13	0.49
1:P:893:GLU:HG3	1:P:946:ARG:HG3	1.94	0.49
1:A:878:ALA:C	1:A:880:LYS:H	2.20	0.49
1:B:842:LYS:HG3	1:B:843:ILE:N	2.27	0.49
1:C:791:THR:HG22	1:C:791:THR:O	2.12	0.49
1:C:887:SER:C	1:C:889:GLU:N	2.67	0.49
1:C:893:GLU:HG3	1:C:946:ARG:HG3	1.94	0.49
1:D:785:LYS:CE	1:M:785:LYS:HE3	2.37	0.49
1:D:791:THR:O	1:D:791:THR:HG22	2.12	0.49
1:E:309:SER:HB2	1:E:320:GLY:CA	2.41	0.49
1:E:329:ASP:OD1	1:E:808:ARG:HG3	2.13	0.49
1:E:347:ARG:HB2	1:E:754:GLY:HA2	1.94	0.49
1:F:336:GLN:HE21	1:F:340:TYR:HE1	1.60	0.49
1:F:958:TYR:CD1	1:F:958:TYR:C	2.90	0.49
1:G:887:SER:C	1:G:889:GLU:N	2.67	0.49
1:J:311:LYS:HE2	1:J:317:ARG:HG3	1.94	0.49
1:J:785:LYS:O	1:J:786:ALA:CB	2.59	0.49
1:K:317:ARG:HG2	1:K:318:LEU:N	2.27	0.49
1:K:851:ILE:O	1:K:852:LEU:C	2.56	0.49
1:K:870:ILE:HD12	1:K:870:ILE:N	2.26	0.49
1:K:881:ASN:C	1:K:882:ILE:HD13	2.38	0.49
1:L:809:PHE:HB2	1:L:818:GLN:CD	2.36	0.49
1:L:926:GLU:O	1:L:929:ILE:HB	2.13	0.49
1:M:887:SER:C	1:M:889:GLU:N	2.67	0.49
1:N:338:LEU:N	1:N:338:LEU:HD23	2.28	0.49
1:N:842:LYS:HG3	1:N:843:ILE:N	2.27	0.49
1:O:317:ARG:HG2	1:O:318:LEU:N	2.27	0.49
1:O:329:ASP:OD1	1:O:808:ARG:HG3	2.13	0.49
1:O:809:PHE:HB2	1:O:818:GLN:CD	2.36	0.49
1:P:881:ASN:C	1:P:882:ILE:HD13	2.38	0.49
1:A:329:ASP:OD1	1:A:808:ARG:HG3	2.13	0.49
1:A:347:ARG:HB2	1:A:754:GLY:HA2	1.94	0.49
1:A:738:UNK:CB	1:A:792:LEU:HD11	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:881:ASN:C	1:A:882:ILE:HD13	2.38	0.49
1:A:958:TYR:C	1:A:958:TYR:CD1	2.90	0.49
1:B:313:PRO:HG2	1:B:314:ASP:H	1.76	0.49
1:C:926:GLU:O	1:C:929:ILE:HB	2.13	0.49
1:D:809:PHE:HB2	1:D:818:GLN:CD	2.36	0.49
1:E:738:UNK:CB	1:E:792:LEU:HD11	2.43	0.49
1:E:753:GLY:HA2	1:E:795:ARG:HH11	1.77	0.49
1:E:881:ASN:C	1:E:882:ILE:HD13	2.38	0.49
1:E:903:LYS:HE2	1:E:903:LYS:CA	2.42	0.49
1:G:738:UNK:CB	1:G:792:LEU:HD11	2.43	0.49
1:G:753:GLY:HA2	1:G:795:ARG:HH11	1.77	0.49
1:G:878:ALA:C	1:G:880:LYS:H	2.20	0.49
1:H:738:UNK:CB	1:H:792:LEU:HD11	2.43	0.49
1:I:332:VAL:O	1:I:333:ALA:CB	2.58	0.49
1:I:785:LYS:O	1:I:786:ALA:CB	2.59	0.49
1:J:317:ARG:HG2	1:J:318:LEU:N	2.27	0.49
1:J:338:LEU:HD23	1:J:338:LEU:N	2.28	0.49
1:J:881:ASN:C	1:J:882:ILE:HD13	2.38	0.49
1:K:893:GLU:HG3	1:K:946:ARG:HG3	1.94	0.49
1:L:338:LEU:N	1:L:338:LEU:HD23	2.28	0.49
1:M:329:ASP:OD1	1:M:808:ARG:HG3	2.13	0.49
1:M:352:SER:O	1:M:354:UNK:N	2.45	0.49
1:O:874:TYR:CD1	1:O:874:TYR:C	2.89	0.49
1:O:878:ALA:C	1:O:880:LYS:H	2.20	0.49
1:O:881:ASN:C	1:O:882:ILE:HD13	2.38	0.49
1:O:893:GLU:HG3	1:O:946:ARG:HG3	1.94	0.49
1:A:311:LYS:HE2	1:A:317:ARG:HG3	1.94	0.49
1:B:311:LYS:HG2	1:B:318:LEU:N	2.28	0.49
1:B:338:LEU:HD23	1:B:338:LEU:N	2.28	0.49
1:C:317:ARG:HG2	1:C:318:LEU:N	2.27	0.49
1:C:738:UNK:CB	1:C:792:LEU:HD11	2.43	0.49
1:D:295:GLU:CD	1:D:295:GLU:N	2.70	0.49
1:D:338:LEU:N	1:D:338:LEU:HD23	2.28	0.49
1:D:851:ILE:O	1:D:852:LEU:C	2.56	0.49
1:E:332:VAL:O	1:E:333:ALA:CB	2.58	0.49
1:E:769:ARG:O	1:E:770:SER:C	2.55	0.49
1:F:311:LYS:HG2	1:F:318:LEU:N	2.28	0.49
1:H:887:SER:C	1:H:889:GLU:N	2.67	0.49
1:H:893:GLU:HG3	1:H:946:ARG:HG3	1.94	0.49
1:I:304:LEU:HA	1:I:755:TYR:CE2	2.48	0.49
1:I:738:UNK:CB	1:I:792:LEU:HD11	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:347:ARG:HB2	1:J:754:GLY:HA2	1.95	0.49
1:M:327:VAL:O	1:M:327:VAL:HG23	2.12	0.49
1:M:891:MET:HG3	1:N:852:LEU:CB	2.42	0.49
1:N:317:ARG:HG2	1:N:318:LEU:N	2.27	0.49
1:N:769:ARG:O	1:N:770:SER:C	2.55	0.49
1:O:350:TYR:HD1	1:O:351:THR:N	2.09	0.49
1:C:329:ASP:OD1	1:C:808:ARG:HG3	2.13	0.49
1:D:327:VAL:HG23	1:D:327:VAL:O	2.12	0.49
1:F:926:GLU:O	1:F:929:ILE:HB	2.13	0.49
1:G:311:LYS:HG2	1:G:318:LEU:N	2.28	0.49
1:H:347:ARG:HB2	1:H:754:GLY:HA2	1.94	0.49
1:H:785:LYS:CG	1:I:785:LYS:CB	2.91	0.49
1:I:317:ARG:HG2	1:I:318:LEU:N	2.27	0.49
1:I:338:LEU:N	1:I:338:LEU:HD23	2.28	0.49
1:J:311:LYS:HG2	1:J:318:LEU:N	2.28	0.49
1:J:352:SER:O	1:J:354:UNK:N	2.45	0.49
1:K:295:GLU:CD	1:K:295:GLU:N	2.70	0.49
1:K:329:ASP:OD1	1:K:808:ARG:HG3	2.13	0.49
1:K:738:UNK:CB	1:K:792:LEU:HD11	2.43	0.49
1:K:842:LYS:HG3	1:K:843:ILE:N	2.27	0.49
1:L:329:ASP:OD1	1:L:808:ARG:HG3	2.13	0.49
1:L:738:UNK:CB	1:L:792:LEU:HD11	2.43	0.49
1:N:903:LYS:HE2	1:N:903:LYS:CA	2.42	0.49
1:O:769:ARG:O	1:O:770:SER:C	2.55	0.49
1:P:812:MET:SD	1:P:812:MET:N	2.78	0.49
1:P:851:ILE:O	1:P:852:LEU:C	2.56	0.49
1:P:878:ALA:C	1:P:880:LYS:H	2.20	0.49
1:A:311:LYS:HG2	1:A:318:LEU:N	2.28	0.49
1:A:791:THR:O	1:A:791:THR:HG22	2.12	0.49
1:A:842:LYS:HG3	1:A:843:ILE:N	2.27	0.49
1:B:878:ALA:C	1:B:880:LYS:H	2.20	0.49
1:B:881:ASN:C	1:B:882:ILE:HD13	2.38	0.49
1:B:926:GLU:O	1:B:929:ILE:HB	2.13	0.49
1:C:311:LYS:HE2	1:C:317:ARG:HG3	1.94	0.49
1:D:878:ALA:C	1:D:880:LYS:H	2.20	0.49
1:F:295:GLU:CD	1:F:295:GLU:N	2.70	0.49
1:F:757:LEU:CD2	1:F:799:ILE:HB	2.42	0.49
1:F:903:LYS:HE2	1:F:903:LYS:CA	2.42	0.49
1:G:313:PRO:HG2	1:G:314:ASP:H	1.76	0.49
1:G:741:UNK:CB	1:J:788:ILE:CG2	2.86	0.49
1:G:958:TYR:C	1:G:958:TYR:CD1	2.90	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:295:GLU:CD	1:H:295:GLU:N	2.70	0.49
1:H:336:GLN:HE21	1:H:340:TYR:HE1	1.60	0.49
1:I:327:VAL:HG23	1:I:327:VAL:O	2.12	0.49
1:I:946:ARG:HB2	1:I:946:ARG:NH1	2.27	0.49
1:K:352:SER:O	1:K:354:UNK:N	2.45	0.49
1:L:317:ARG:HG2	1:L:318:LEU:N	2.27	0.49
1:L:947:GLU:O	1:L:950:ARG:HB3	2.13	0.49
1:M:311:LYS:HE2	1:M:317:ARG:HG3	1.94	0.49
1:M:881:ASN:C	1:M:882:ILE:HD13	2.37	0.49
1:N:881:ASN:C	1:N:882:ILE:HD13	2.38	0.49
1:P:769:ARG:O	1:P:770:SER:C	2.55	0.49
1:P:842:LYS:HG3	1:P:843:ILE:N	2.27	0.49
1:A:336:GLN:HE21	1:A:340:TYR:HE1	1.60	0.49
1:A:893:GLU:HG3	1:A:946:ARG:HG3	1.94	0.49
1:C:336:GLN:HE21	1:C:340:TYR:HE1	1.60	0.49
1:C:350:TYR:HD1	1:C:351:THR:N	2.09	0.49
1:C:842:LYS:HG3	1:C:843:ILE:N	2.27	0.49
1:C:947:GLU:O	1:C:950:ARG:HB3	2.13	0.49
1:D:347:ARG:HB2	1:D:754:GLY:HA2	1.94	0.49
1:D:903:LYS:HE2	1:D:903:LYS:CA	2.42	0.49
1:E:338:LEU:N	1:E:338:LEU:HD23	2.28	0.49
1:F:738:UNK:CB	1:F:792:LEU:HD11	2.43	0.49
1:F:769:ARG:O	1:F:770:SER:C	2.55	0.49
1:F:851:ILE:O	1:F:852:LEU:C	2.56	0.49
1:G:352:SER:O	1:G:354:UNK:N	2.45	0.49
1:H:317:ARG:HG2	1:H:318:LEU:N	2.27	0.49
1:I:329:ASP:OD1	1:I:808:ARG:HG3	2.13	0.49
1:I:757:LEU:CD2	1:I:799:ILE:HB	2.42	0.49
1:I:903:LYS:HE2	1:I:903:LYS:CA	2.42	0.49
1:J:310:ARG:CD	1:K:858:GLU:HG3	2.40	0.49
1:J:926:GLU:O	1:J:929:ILE:HB	2.13	0.49
1:K:769:ARG:O	1:K:770:SER:C	2.55	0.49
1:K:791:THR:HG22	1:K:791:THR:O	2.12	0.49
1:L:311:LYS:HG2	1:L:318:LEU:N	2.28	0.49
1:M:753:GLY:HA2	1:M:795:ARG:HH11	1.77	0.49
1:N:295:GLU:CD	1:N:295:GLU:N	2.70	0.49
1:N:352:SER:O	1:N:354:UNK:N	2.45	0.49
1:N:753:GLY:HA2	1:N:795:ARG:HH11	1.78	0.49
1:O:903:LYS:HE2	1:O:903:LYS:CA	2.42	0.49
1:O:926:GLU:O	1:O:929:ILE:HB	2.13	0.49
1:P:336:GLN:HE21	1:P:340:TYR:HE1	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:VAL:HG23	1:A:327:VAL:O	2.12	0.49
1:A:350:TYR:HD1	1:A:351:THR:N	2.09	0.49
1:B:903:LYS:HE2	1:B:903:LYS:CA	2.42	0.49
1:D:881:ASN:C	1:D:882:ILE:HD13	2.38	0.49
1:F:891:MET:HG3	1:G:852:LEU:HB3	1.94	0.49
1:F:898:TYR:CE2	1:G:848:ALA:HB2	2.46	0.49
1:G:791:THR:O	1:G:791:THR:HG22	2.12	0.49
1:H:785:LYS:HG2	1:I:785:LYS:C	2.36	0.49
1:H:851:ILE:O	1:H:852:LEU:C	2.56	0.49
1:H:903:LYS:HE2	1:H:903:LYS:CA	2.42	0.49
1:H:926:GLU:O	1:H:929:ILE:HB	2.13	0.49
1:I:311:LYS:HG2	1:I:318:LEU:N	2.28	0.49
1:I:893:GLU:HG3	1:I:946:ARG:HG3	1.94	0.49
1:J:738:UNK:CB	1:J:792:LEU:HD11	2.43	0.49
1:J:946:ARG:HB2	1:J:946:ARG:NH1	2.27	0.49
1:K:304:LEU:HA	1:K:755:TYR:CE2	2.48	0.49
1:K:313:PRO:HG2	1:K:314:ASP:H	1.76	0.49
1:K:327:VAL:HG23	1:K:327:VAL:O	2.12	0.49
1:L:327:VAL:HG23	1:L:327:VAL:O	2.12	0.49
1:L:352:SER:O	1:L:354:UNK:N	2.45	0.49
1:L:903:LYS:HE2	1:L:903:LYS:CA	2.42	0.49
1:L:936:ALA:HA	1:L:948:ASP:OD2	2.13	0.49
1:M:317:ARG:HG2	1:M:318:LEU:N	2.27	0.49
1:M:791:THR:O	1:M:791:THR:HG22	2.12	0.49
1:M:893:GLU:HG3	1:M:946:ARG:HG3	1.94	0.49
1:N:336:GLN:HE21	1:N:340:TYR:HE1	1.60	0.49
1:N:347:ARG:HB2	1:N:754:GLY:HA2	1.95	0.49
1:N:936:ALA:HA	1:N:948:ASP:OD2	2.13	0.49
1:O:316:THR:OG1	1:P:339:ARG:CD	2.57	0.49
1:O:347:ARG:HB2	1:O:754:GLY:HA2	1.95	0.49
1:O:757:LEU:CD2	1:O:799:ILE:HB	2.42	0.49
1:P:753:GLY:HA2	1:P:795:ARG:HH11	1.77	0.49
1:P:926:GLU:O	1:P:929:ILE:HB	2.13	0.49
1:A:926:GLU:O	1:A:929:ILE:HB	2.13	0.49
1:C:881:ASN:C	1:C:882:ILE:HD13	2.38	0.49
1:D:304:LEU:HA	1:D:755:TYR:CE2	2.48	0.49
1:D:936:ALA:HA	1:D:948:ASP:OD2	2.13	0.49
1:E:310:ARG:CZ	1:F:857:GLY:O	2.61	0.49
1:G:317:ARG:HG2	1:G:318:LEU:N	2.27	0.49
1:G:338:LEU:HD23	1:G:338:LEU:N	2.28	0.49
1:G:903:LYS:HE2	1:G:903:LYS:CA	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:947:GLU:O	1:G:950:ARG:HB3	2.13	0.49
1:H:311:LYS:HE2	1:H:317:ARG:HG3	1.94	0.49
1:H:311:LYS:HG2	1:H:318:LEU:N	2.28	0.49
1:I:769:ARG:O	1:I:770:SER:C	2.55	0.49
1:J:336:GLN:HE21	1:J:340:TYR:HE1	1.60	0.49
1:J:903:LYS:HE2	1:J:903:LYS:CA	2.42	0.49
1:J:958:TYR:CD1	1:J:958:TYR:C	2.90	0.49
1:K:903:LYS:HD2	1:L:841:ASP:OD2	2.13	0.49
1:M:738:UNK:CB	1:M:792:LEU:HD11	2.43	0.49
1:N:304:LEU:HA	1:N:755:TYR:CE2	2.48	0.49
1:N:311:LYS:HG2	1:N:318:LEU:N	2.28	0.49
1:N:327:VAL:HG23	1:N:327:VAL:O	2.12	0.49
1:N:350:TYR:HD1	1:N:351:THR:N	2.09	0.49
1:O:327:VAL:HG23	1:O:327:VAL:O	2.12	0.49
1:O:753:GLY:HA2	1:O:795:ARG:HH11	1.78	0.49
1:O:791:THR:O	1:O:791:THR:HG22	2.12	0.49
1:O:947:GLU:O	1:O:950:ARG:HB3	2.13	0.49
1:P:311:LYS:HE2	1:P:317:ARG:HG3	1.94	0.49
1:B:946:ARG:HB2	1:B:946:ARG:NH1	2.27	0.48
1:D:311:LYS:HG2	1:D:318:LEU:N	2.28	0.48
1:D:769:ARG:O	1:D:770:SER:C	2.55	0.48
1:E:311:LYS:HG2	1:E:318:LEU:N	2.28	0.48
1:F:893:GLU:HG3	1:F:946:ARG:HG3	1.94	0.48
1:G:295:GLU:CD	1:G:295:GLU:N	2.70	0.48
1:G:769:ARG:O	1:G:770:SER:C	2.55	0.48
1:H:842:LYS:HG3	1:H:843:ILE:N	2.27	0.48
1:H:936:ALA:HA	1:H:948:ASP:OD2	2.13	0.48
1:I:347:ARG:HB2	1:I:754:GLY:HA2	1.94	0.48
1:J:936:ALA:HA	1:J:948:ASP:OD2	2.13	0.48
1:K:350:TYR:HD1	1:K:351:THR:N	2.09	0.48
1:L:304:LEU:HA	1:L:755:TYR:CE2	2.48	0.48
1:L:757:LEU:CD2	1:L:799:ILE:HB	2.42	0.48
1:M:304:LEU:HA	1:M:755:TYR:CE2	2.48	0.48
1:M:336:GLN:HE21	1:M:340:TYR:HE1	1.60	0.48
1:M:338:LEU:N	1:M:338:LEU:HD23	2.28	0.48
1:N:890:ALA:HB1	1:N:949:ALA:CB	2.43	0.48
1:N:926:GLU:O	1:N:929:ILE:HB	2.13	0.48
1:O:946:ARG:HB2	1:O:946:ARG:NH1	2.27	0.48
1:P:338:LEU:N	1:P:338:LEU:HD23	2.28	0.48
1:A:309:SER:HB2	1:A:320:GLY:CA	2.41	0.48
1:A:338:LEU:N	1:A:338:LEU:HD23	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:GLN:HE21	1:B:340:TYR:HE1	1.60	0.48
1:B:887:SER:C	1:B:889:GLU:N	2.67	0.48
1:D:753:GLY:HA2	1:D:795:ARG:HH11	1.77	0.48
1:F:338:LEU:N	1:F:338:LEU:HD23	2.28	0.48
1:F:890:ALA:HB1	1:F:949:ALA:CB	2.43	0.48
1:G:304:LEU:HA	1:G:755:TYR:CE2	2.48	0.48
1:G:329:ASP:OD1	1:G:808:ARG:HG3	2.13	0.48
1:G:890:ALA:HB1	1:G:949:ALA:CB	2.43	0.48
1:G:926:GLU:O	1:G:929:ILE:HB	2.13	0.48
1:I:947:GLU:O	1:I:950:ARG:HB3	2.13	0.48
1:J:327:VAL:O	1:J:327:VAL:HG23	2.12	0.48
1:J:791:THR:O	1:J:791:THR:HG22	2.12	0.48
1:L:842:LYS:HG3	1:L:843:ILE:N	2.27	0.48
1:M:890:ALA:HB1	1:M:949:ALA:CB	2.43	0.48
1:N:947:GLU:O	1:N:950:ARG:HB3	2.13	0.48
1:O:936:ALA:HA	1:O:948:ASP:OD2	2.13	0.48
1:P:317:ARG:HG2	1:P:318:LEU:N	2.27	0.48
1:P:887:SER:C	1:P:889:GLU:N	2.67	0.48
1:A:903:LYS:HE2	1:A:903:LYS:CA	2.42	0.48
1:B:317:ARG:HG2	1:B:318:LEU:N	2.27	0.48
1:B:738:UNK:CB	1:B:792:LEU:HD11	2.43	0.48
1:B:936:ALA:HA	1:B:948:ASP:OD2	2.13	0.48
1:C:311:LYS:HG2	1:C:318:LEU:N	2.28	0.48
1:D:329:ASP:OD1	1:D:808:ARG:HG3	2.13	0.48
1:E:842:LYS:HG3	1:E:843:ILE:N	2.27	0.48
1:H:881:ASN:C	1:H:882:ILE:HD13	2.38	0.48
1:J:753:GLY:HA2	1:J:795:ARG:HH11	1.77	0.48
1:K:936:ALA:HA	1:K:948:ASP:OD2	2.13	0.48
1:L:878:ALA:C	1:L:880:LYS:H	2.20	0.48
1:O:338:LEU:N	1:O:338:LEU:HD23	2.28	0.48
1:O:738:UNK:CB	1:O:792:LEU:HD11	2.43	0.48
1:P:304:LEU:HA	1:P:755:TYR:CE2	2.48	0.48
1:P:347:ARG:HB2	1:P:754:GLY:HA2	1.94	0.48
1:P:738:UNK:CB	1:P:792:LEU:HD11	2.43	0.48
1:P:936:ALA:HA	1:P:948:ASP:OD2	2.13	0.48
1:B:329:ASP:OD1	1:B:808:ARG:HG3	2.13	0.48
1:B:769:ARG:O	1:B:770:SER:C	2.55	0.48
1:B:947:GLU:O	1:B:950:ARG:HB3	2.13	0.48
1:C:851:ILE:O	1:C:852:LEU:C	2.56	0.48
1:E:317:ARG:HG2	1:E:318:LEU:N	2.27	0.48
1:E:926:GLU:O	1:E:929:ILE:HB	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:947:GLU:O	1:J:950:ARG:HB3	2.13	0.48
1:M:812:MET:SD	1:M:812:MET:N	2.78	0.48
1:A:882:ILE:HG21	1:A:940:LEU:HA	1.96	0.48
1:B:851:ILE:O	1:B:852:LEU:C	2.56	0.48
1:B:890:ALA:HB1	1:B:949:ALA:CB	2.43	0.48
1:B:903:LYS:O	1:B:904:SER:OG	2.22	0.48
1:C:338:LEU:N	1:C:338:LEU:HD23	2.28	0.48
1:C:753:GLY:HA2	1:C:795:ARG:HH11	1.77	0.48
1:D:926:GLU:O	1:D:929:ILE:HB	2.13	0.48
1:E:352:SER:O	1:E:354:UNK:N	2.45	0.48
1:E:890:ALA:HB1	1:E:949:ALA:CB	2.43	0.48
1:E:936:ALA:HA	1:E:948:ASP:OD2	2.13	0.48
1:F:304:LEU:HA	1:F:755:TYR:CE2	2.48	0.48
1:F:732:UNK:HA	1:L:359:UNK:CB	2.43	0.48
1:G:757:LEU:CD2	1:G:799:ILE:HB	2.42	0.48
1:H:878:ALA:C	1:H:880:LYS:H	2.20	0.48
1:H:890:ALA:HB1	1:H:949:ALA:CB	2.43	0.48
1:J:893:GLU:HG3	1:J:946:ARG:HG3	1.94	0.48
1:L:753:GLY:HA2	1:L:795:ARG:HH11	1.77	0.48
1:M:350:TYR:HD1	1:M:351:THR:N	2.09	0.48
1:O:304:LEU:HA	1:O:755:TYR:CE2	2.48	0.48
1:O:891:MET:HG3	1:P:852:LEU:CG	2.43	0.48
1:P:791:THR:O	1:P:791:THR:HG22	2.12	0.48
1:A:295:GLU:CD	1:A:295:GLU:N	2.70	0.48
1:A:304:LEU:HA	1:A:755:TYR:CE2	2.48	0.48
1:B:890:ALA:O	1:B:891:MET:C	2.57	0.48
1:C:808:ARG:NH1	1:C:808:ARG:CB	2.77	0.48
1:C:882:ILE:HG21	1:C:940:LEU:HA	1.96	0.48
1:C:890:ALA:O	1:C:891:MET:C	2.57	0.48
1:D:317:ARG:HG2	1:D:318:LEU:N	2.27	0.48
1:D:947:GLU:O	1:D:950:ARG:HB3	2.13	0.48
1:E:311:LYS:HE2	1:E:317:ARG:HG3	1.94	0.48
1:F:891:MET:HE1	1:G:856:ARG:NH1	2.20	0.48
1:G:851:ILE:O	1:G:852:LEU:C	2.56	0.48
1:G:881:ASN:C	1:G:882:ILE:HD13	2.38	0.48
1:H:289:ALA:O	1:H:290:ILE:C	2.57	0.48
1:H:304:LEU:HA	1:H:755:TYR:CE2	2.48	0.48
1:H:882:ILE:HG21	1:H:940:LEU:HA	1.96	0.48
1:I:886:ILE:CD1	1:I:886:ILE:H	2.27	0.48
1:I:890:ALA:HB1	1:I:949:ALA:CB	2.43	0.48
1:I:936:ALA:HA	1:I:948:ASP:OD2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:842:LYS:HG3	1:J:843:ILE:N	2.27	0.48
1:L:347:ARG:HB2	1:L:754:GLY:HA2	1.95	0.48
1:M:903:LYS:NZ	1:N:840:ASP:N	2.61	0.48
1:M:947:GLU:O	1:M:950:ARG:HB3	2.13	0.48
1:P:903:LYS:HE2	1:P:903:LYS:CA	2.42	0.48
1:A:317:ARG:HG2	1:A:318:LEU:N	2.27	0.48
1:B:304:LEU:HA	1:B:755:TYR:CE2	2.48	0.48
1:B:347:ARG:HB2	1:B:754:GLY:HA2	1.94	0.48
1:C:304:LEU:HA	1:C:755:TYR:CE2	2.48	0.48
1:D:738:UNK:CB	1:D:792:LEU:HD11	2.43	0.48
1:E:336:GLN:HE21	1:E:340:TYR:HE1	1.60	0.48
1:E:882:ILE:HG21	1:E:940:LEU:HA	1.96	0.48
1:E:893:GLU:HG3	1:E:946:ARG:HG3	1.94	0.48
1:F:347:ARG:HB2	1:F:754:GLY:HA2	1.95	0.48
1:G:312:LEU:CD2	1:H:858:GLU:CB	2.92	0.48
1:G:347:ARG:HB2	1:G:754:GLY:HA2	1.95	0.48
1:G:350:TYR:HD1	1:G:351:THR:N	2.09	0.48
1:G:890:ALA:O	1:G:891:MET:C	2.57	0.48
1:H:947:GLU:O	1:H:950:ARG:HB3	2.13	0.48
1:I:755:TYR:CD1	1:I:755:TYR:N	2.79	0.48
1:I:842:LYS:HG3	1:I:843:ILE:N	2.27	0.48
1:I:881:ASN:C	1:I:882:ILE:HD13	2.38	0.48
1:J:329:ASP:OD1	1:J:808:ARG:HG3	2.13	0.48
1:J:890:ALA:HB1	1:J:949:ALA:CB	2.43	0.48
1:O:882:ILE:HG21	1:O:940:LEU:HA	1.96	0.48
1:O:886:ILE:CD1	1:O:886:ILE:H	2.27	0.48
1:P:295:GLU:CD	1:P:295:GLU:N	2.70	0.48
1:P:757:LEU:CD2	1:P:799:ILE:HB	2.42	0.48
1:A:289:ALA:O	1:A:290:ILE:C	2.57	0.48
1:A:851:ILE:O	1:A:852:LEU:C	2.56	0.48
1:A:947:GLU:O	1:A:950:ARG:HB3	2.13	0.48
1:B:312:LEU:CD1	1:C:858:GLU:HA	2.38	0.48
1:E:740:UNK:C	1:L:789:THR:OG1	2.57	0.48
1:E:851:ILE:O	1:E:852:LEU:C	2.56	0.48
1:E:890:ALA:O	1:E:891:MET:C	2.57	0.48
1:F:881:ASN:C	1:F:882:ILE:HD13	2.38	0.48
1:F:936:ALA:HA	1:F:948:ASP:OD2	2.13	0.48
1:G:785:LYS:CG	1:J:785:LYS:HG2	2.43	0.48
1:H:890:ALA:O	1:H:891:MET:C	2.57	0.48
1:I:926:GLU:O	1:I:929:ILE:HB	2.13	0.48
1:K:882:ILE:HG21	1:K:940:LEU:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:882:ILE:HG21	1:P:940:LEU:HA	1.96	0.48
1:P:886:ILE:CD1	1:P:886:ILE:H	2.27	0.48
1:P:947:GLU:O	1:P:950:ARG:HB3	2.13	0.48
1:A:936:ALA:HA	1:A:948:ASP:OD2	2.13	0.48
1:B:289:ALA:O	1:B:290:ILE:C	2.57	0.48
1:B:753:GLY:HA2	1:B:795:ARG:HH11	1.77	0.48
1:C:729:UNK:O	1:O:729:UNK:O	2.32	0.48
1:D:886:ILE:CD1	1:D:886:ILE:H	2.27	0.48
1:F:887:SER:C	1:F:889:GLU:N	2.67	0.48
1:H:338:LEU:N	1:H:338:LEU:HD23	2.28	0.48
1:I:878:ALA:C	1:I:880:LYS:H	2.20	0.48
1:K:947:GLU:O	1:K:950:ARG:HB3	2.13	0.48
1:N:890:ALA:O	1:N:891:MET:C	2.57	0.48
1:O:280:ASP:O	1:O:283:VAL:HG22	2.14	0.48
1:O:311:LYS:HG2	1:O:318:LEU:N	2.28	0.48
1:O:887:SER:C	1:O:889:GLU:N	2.67	0.48
1:P:289:ALA:O	1:P:290:ILE:C	2.57	0.48
1:P:890:ALA:O	1:P:891:MET:C	2.57	0.48
1:A:890:ALA:HB1	1:A:949:ALA:CB	2.43	0.48
1:C:886:ILE:CD1	1:C:886:ILE:H	2.27	0.48
1:D:842:LYS:HG3	1:D:843:ILE:N	2.27	0.48
1:E:280:ASP:O	1:E:283:VAL:HG22	2.14	0.48
1:F:329:ASP:OD1	1:F:808:ARG:HG3	2.13	0.48
1:F:882:ILE:HG21	1:F:940:LEU:HA	1.96	0.48
1:F:947:GLU:O	1:F:950:ARG:HB3	2.13	0.48
1:I:851:ILE:O	1:I:852:LEU:C	2.56	0.48
1:J:757:LEU:CD2	1:J:799:ILE:HB	2.42	0.48
1:J:882:ILE:HG21	1:J:940:LEU:HA	1.96	0.48
1:K:926:GLU:O	1:K:929:ILE:HB	2.13	0.48
1:L:336:GLN:HE21	1:L:340:TYR:HE1	1.60	0.48
1:M:882:ILE:HG21	1:M:940:LEU:HA	1.96	0.48
1:N:329:ASP:OD1	1:N:808:ARG:HG3	2.13	0.48
1:O:295:GLU:CD	1:O:295:GLU:N	2.70	0.48
1:O:316:THR:CG2	1:P:339:ARG:HD3	2.41	0.48
1:P:311:LYS:HG2	1:P:318:LEU:N	2.28	0.48
1:B:757:LEU:CD2	1:B:799:ILE:HB	2.42	0.47
1:D:336:GLN:HE21	1:D:340:TYR:HE1	1.60	0.47
1:D:890:ALA:HB1	1:D:949:ALA:CB	2.43	0.47
1:E:812:MET:SD	1:E:812:MET:N	2.78	0.47
1:H:280:ASP:O	1:H:283:VAL:HG22	2.14	0.47
1:H:329:ASP:OD1	1:H:808:ARG:HG3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:757:LEU:CD2	1:H:799:ILE:HB	2.42	0.47
1:J:304:LEU:HA	1:J:755:TYR:CE2	2.48	0.47
1:K:289:ALA:O	1:K:290:ILE:C	2.57	0.47
1:K:336:GLN:HE21	1:K:340:TYR:HE1	1.60	0.47
1:L:350:TYR:HD1	1:L:351:THR:N	2.09	0.47
1:L:851:ILE:O	1:L:852:LEU:C	2.56	0.47
1:M:878:ALA:C	1:M:880:LYS:H	2.20	0.47
1:M:926:GLU:O	1:M:929:ILE:HB	2.13	0.47
1:M:936:ALA:HA	1:M:948:ASP:OD2	2.13	0.47
1:O:336:GLN:HE21	1:O:340:TYR:HE1	1.60	0.47
1:O:842:LYS:HG3	1:O:843:ILE:N	2.27	0.47
1:O:890:ALA:O	1:O:891:MET:C	2.57	0.47
1:A:890:ALA:O	1:A:891:MET:C	2.57	0.47
1:E:304:LEU:HA	1:E:755:TYR:CE2	2.48	0.47
1:E:887:SER:C	1:E:889:GLU:N	2.67	0.47
1:G:936:ALA:HA	1:G:948:ASP:OD2	2.13	0.47
1:K:311:LYS:HG2	1:K:318:LEU:N	2.28	0.47
1:K:347:ARG:HB2	1:K:754:GLY:HA2	1.94	0.47
1:M:280:ASP:O	1:M:283:VAL:HG22	2.14	0.47
1:M:289:ALA:O	1:M:290:ILE:C	2.57	0.47
1:M:742:UNK:O	1:M:743:UNK:CB	2.62	0.47
1:D:289:ALA:O	1:D:290:ILE:C	2.57	0.47
1:F:812:MET:SD	1:F:812:MET:N	2.78	0.47
1:G:886:ILE:CD1	1:G:886:ILE:H	2.27	0.47
1:H:808:ARG:NH1	1:H:808:ARG:CB	2.77	0.47
1:I:317:ARG:HG3	1:I:317:ARG:NH1	2.30	0.47
1:K:317:ARG:HG3	1:K:317:ARG:NH1	2.30	0.47
1:L:289:ALA:O	1:L:290:ILE:C	2.57	0.47
1:L:882:ILE:HG21	1:L:940:LEU:HA	1.96	0.47
1:B:317:ARG:HH21	1:B:779:GLN:CG	2.28	0.47
1:D:280:ASP:O	1:D:283:VAL:HG22	2.14	0.47
1:F:289:ALA:O	1:F:290:ILE:C	2.57	0.47
1:F:808:ARG:NH1	1:F:808:ARG:CB	2.77	0.47
1:H:886:ILE:CD1	1:H:886:ILE:H	2.27	0.47
1:B:280:ASP:O	1:B:283:VAL:HG22	2.14	0.47
1:B:350:TYR:HD1	1:B:351:THR:N	2.09	0.47
1:C:936:ALA:HA	1:C:948:ASP:OD2	2.13	0.47
1:E:350:TYR:HD1	1:E:351:THR:N	2.09	0.47
1:F:350:TYR:HD1	1:F:351:THR:N	2.09	0.47
1:G:317:ARG:HH21	1:G:779:GLN:CG	2.28	0.47
1:G:742:UNK:O	1:G:743:UNK:CB	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:280:ASP:O	1:I:283:VAL:HG22	2.14	0.47
1:J:295:GLU:CD	1:J:295:GLU:N	2.70	0.47
1:O:289:ALA:O	1:O:290:ILE:C	2.57	0.47
1:B:317:ARG:HG3	1:B:317:ARG:NH1	2.30	0.47
1:E:742:UNK:O	1:E:743:UNK:CB	2.62	0.47
1:F:322:ILE:HD13	1:F:931:LEU:HD23	1.97	0.47
1:G:882:ILE:HG21	1:G:940:LEU:HA	1.96	0.47
1:H:828:ARG:HG3	1:H:828:ARG:NH1	2.30	0.47
1:J:280:ASP:O	1:J:283:VAL:HG22	2.14	0.47
1:J:890:ALA:O	1:J:891:MET:C	2.57	0.47
1:K:886:ILE:CD1	1:K:886:ILE:H	2.27	0.47
1:L:310:ARG:NH1	1:M:858:GLU:OE2	2.48	0.47
1:A:280:ASP:O	1:A:283:VAL:HG22	2.14	0.47
1:C:322:ILE:HD13	1:C:931:LEU:HD23	1.97	0.47
1:C:925:LEU:O	1:C:929:ILE:HG13	2.15	0.47
1:D:317:ARG:HG3	1:D:317:ARG:NH1	2.30	0.47
1:D:742:UNK:O	1:D:743:UNK:CB	2.62	0.47
1:E:317:ARG:HG3	1:E:317:ARG:NH1	2.30	0.47
1:E:947:GLU:O	1:E:950:ARG:HB3	2.13	0.47
1:F:317:ARG:HH21	1:F:779:GLN:CG	2.28	0.47
1:F:886:ILE:CD1	1:F:886:ILE:H	2.27	0.47
1:F:890:ALA:O	1:F:891:MET:C	2.57	0.47
1:G:350:TYR:C	1:G:350:TYR:HD1	2.23	0.47
1:G:729:UNK:C	1:K:730:UNK:O	2.63	0.47
1:G:828:ARG:HG3	1:G:828:ARG:NH1	2.30	0.47
1:H:317:ARG:HH21	1:H:779:GLN:CG	2.28	0.47
1:H:925:LEU:O	1:H:929:ILE:HG13	2.15	0.47
1:I:295:GLU:CD	1:I:295:GLU:N	2.70	0.47
1:I:322:ILE:HD13	1:I:931:LEU:HD23	1.97	0.47
1:I:742:UNK:O	1:I:743:UNK:CB	2.62	0.47
1:I:819:ILE:HG22	1:I:821:LEU:HG	1.97	0.47
1:K:828:ARG:HG3	1:K:828:ARG:NH1	2.30	0.47
1:K:890:ALA:O	1:K:891:MET:C	2.57	0.47
1:K:925:LEU:O	1:K:929:ILE:HG13	2.15	0.47
1:L:322:ILE:HD13	1:L:931:LEU:HD23	1.97	0.47
1:L:356:UNK:O	1:L:357:UNK:O	2.33	0.47
1:L:890:ALA:HB1	1:L:949:ALA:CB	2.43	0.47
1:L:890:ALA:O	1:L:891:MET:C	2.57	0.47
1:M:356:UNK:O	1:M:357:UNK:O	2.33	0.47
1:N:742:UNK:O	1:N:743:UNK:CB	2.63	0.47
1:O:317:ARG:HG3	1:O:317:ARG:NH1	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:742:UNK:O	1:O:743:UNK:CB	2.62	0.47
1:O:890:ALA:HB1	1:O:949:ALA:CB	2.43	0.47
1:P:280:ASP:O	1:P:283:VAL:HG22	2.14	0.47
1:A:738:UNK:HA	1:P:791:THR:O	2.14	0.47
1:A:819:ILE:HG22	1:A:821:LEU:HG	1.97	0.47
1:B:886:ILE:CD1	1:B:886:ILE:H	2.27	0.47
1:D:356:UNK:O	1:D:357:UNK:O	2.33	0.47
1:D:808:ARG:NH1	1:D:808:ARG:CB	2.77	0.47
1:E:886:ILE:CD1	1:E:886:ILE:H	2.27	0.47
1:G:808:ARG:NH1	1:G:808:ARG:CB	2.77	0.47
1:H:317:ARG:HG3	1:H:317:ARG:NH1	2.30	0.47
1:J:350:TYR:HD1	1:J:351:THR:N	2.09	0.47
1:J:891:MET:HE3	1:K:856:ARG:NH1	2.30	0.47
1:K:742:UNK:O	1:K:743:UNK:CB	2.63	0.47
1:K:903:LYS:HZ2	1:L:841:ASP:N	2.12	0.47
1:L:268:ILE:O	1:L:272:LEU:HD13	2.15	0.47
1:L:887:SER:C	1:L:889:GLU:N	2.67	0.47
1:M:819:ILE:HG22	1:M:821:LEU:HG	1.97	0.47
1:N:280:ASP:O	1:N:283:VAL:HG22	2.14	0.47
1:O:828:ARG:HG3	1:O:828:ARG:NH1	2.30	0.47
1:P:322:ILE:HD13	1:P:931:LEU:HD23	1.97	0.47
1:P:350:TYR:C	1:P:350:TYR:HD1	2.23	0.47
1:P:742:UNK:O	1:P:743:UNK:CB	2.63	0.47
1:A:350:TYR:C	1:A:350:TYR:HD1	2.23	0.47
1:B:770:SER:OG	1:B:771:VAL:N	2.48	0.47
1:B:808:ARG:NH1	1:B:808:ARG:CB	2.77	0.47
1:C:280:ASP:O	1:C:283:VAL:HG22	2.14	0.47
1:C:289:ALA:O	1:C:290:ILE:C	2.57	0.47
1:C:828:ARG:HG3	1:C:828:ARG:NH1	2.30	0.47
1:D:350:TYR:C	1:D:350:TYR:HD1	2.23	0.47
1:D:819:ILE:HG22	1:D:821:LEU:HG	1.97	0.47
1:I:268:ILE:O	1:I:272:LEU:HD13	2.15	0.47
1:I:887:SER:C	1:I:889:GLU:N	2.67	0.47
1:J:289:ALA:O	1:J:290:ILE:C	2.57	0.47
1:J:828:ARG:HG3	1:J:828:ARG:NH1	2.30	0.47
1:K:280:ASP:O	1:K:283:VAL:HG22	2.14	0.47
1:L:886:ILE:CD1	1:L:886:ILE:H	2.27	0.47
1:M:311:LYS:HG2	1:M:318:LEU:N	2.28	0.47
1:M:322:ILE:HD13	1:M:931:LEU:HD23	1.97	0.47
1:M:851:ILE:O	1:M:852:LEU:C	2.56	0.47
1:O:819:ILE:HG22	1:O:821:LEU:HG	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:925:LEU:O	1:O:929:ILE:HG13	2.15	0.47
1:P:819:ILE:HG22	1:P:821:LEU:HG	1.97	0.47
1:A:757:LEU:CD2	1:A:799:ILE:HB	2.42	0.47
1:B:929:ILE:CD1	1:C:852:LEU:HD13	2.45	0.47
1:C:742:UNK:O	1:C:743:UNK:CB	2.63	0.47
1:D:316:THR:HG21	1:E:339:ARG:HH11	1.80	0.47
1:D:757:LEU:CD2	1:D:799:ILE:HB	2.42	0.47
1:E:356:UNK:O	1:E:357:UNK:O	2.33	0.47
1:E:808:ARG:NH1	1:E:808:ARG:CB	2.77	0.47
1:F:742:UNK:O	1:F:743:UNK:CB	2.63	0.47
1:F:925:LEU:O	1:F:929:ILE:HG13	2.15	0.47
1:G:268:ILE:O	1:G:272:LEU:HD13	2.15	0.47
1:H:268:ILE:O	1:H:272:LEU:HD13	2.15	0.47
1:J:742:UNK:O	1:J:743:UNK:CB	2.62	0.47
1:J:886:ILE:CD1	1:J:886:ILE:H	2.27	0.47
1:K:356:UNK:O	1:K:357:UNK:O	2.33	0.47
1:K:891:MET:HE1	1:L:856:ARG:CZ	2.44	0.47
1:L:742:UNK:O	1:L:743:UNK:CB	2.62	0.47
1:L:828:ARG:HG3	1:L:828:ARG:NH1	2.30	0.47
1:M:890:ALA:O	1:M:891:MET:C	2.57	0.47
1:N:882:ILE:HG21	1:N:940:LEU:HA	1.96	0.47
1:P:925:LEU:O	1:P:929:ILE:HG13	2.15	0.47
1:A:828:ARG:HG3	1:A:828:ARG:NH1	2.30	0.46
1:A:886:ILE:CD1	1:A:886:ILE:H	2.27	0.46
1:B:268:ILE:O	1:B:272:LEU:HD13	2.15	0.46
1:C:295:GLU:CD	1:C:295:GLU:N	2.70	0.46
1:C:317:ARG:HH21	1:C:779:GLN:CG	2.28	0.46
1:D:322:ILE:HD13	1:D:931:LEU:HD23	1.97	0.46
1:D:882:ILE:HG21	1:D:940:LEU:HA	1.96	0.46
1:E:757:LEU:CD2	1:E:799:ILE:HB	2.42	0.46
1:E:819:ILE:HG22	1:E:821:LEU:HG	1.97	0.46
1:F:268:ILE:O	1:F:272:LEU:HD13	2.15	0.46
1:F:280:ASP:O	1:F:283:VAL:HG22	2.14	0.46
1:F:356:UNK:O	1:F:357:UNK:O	2.33	0.46
1:I:848:ALA:CB	1:P:898:TYR:HD2	2.26	0.46
1:J:317:ARG:HH21	1:J:779:GLN:CG	2.28	0.46
1:J:828:ARG:N	1:J:828:ARG:HD2	2.30	0.46
1:K:898:TYR:HD2	1:L:848:ALA:HB2	1.80	0.46
1:L:280:ASP:O	1:L:283:VAL:HG22	2.14	0.46
1:L:317:ARG:HG3	1:L:317:ARG:NH1	2.30	0.46
1:N:851:ILE:O	1:N:852:LEU:C	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:925:LEU:O	1:A:929:ILE:HG13	2.15	0.46
1:B:322:ILE:HD13	1:B:931:LEU:HD23	1.97	0.46
1:B:925:LEU:O	1:B:929:ILE:HG13	2.15	0.46
1:D:317:ARG:HH21	1:D:779:GLN:CG	2.28	0.46
1:D:925:LEU:O	1:D:929:ILE:HG13	2.15	0.46
1:F:853:ARG:O	1:F:856:ARG:HG2	2.16	0.46
1:G:828:ARG:N	1:G:828:ARG:HD2	2.30	0.46
1:H:853:ARG:O	1:H:856:ARG:HG2	2.16	0.46
1:I:890:ALA:O	1:I:891:MET:C	2.57	0.46
1:I:925:LEU:O	1:I:929:ILE:HG13	2.15	0.46
1:J:268:ILE:O	1:J:272:LEU:HD13	2.15	0.46
1:L:312:LEU:HD22	1:M:858:GLU:HB3	1.96	0.46
1:L:325:LEU:HB3	1:L:832:ILE:HG12	1.98	0.46
1:N:350:TYR:C	1:N:350:TYR:HD1	2.23	0.46
1:O:770:SER:OG	1:O:771:VAL:N	2.48	0.46
1:B:809:PHE:N	1:B:809:PHE:CD1	2.84	0.46
1:C:350:TYR:C	1:C:350:TYR:HD1	2.23	0.46
1:C:356:UNK:O	1:C:357:UNK:O	2.33	0.46
1:C:853:ARG:O	1:C:856:ARG:HG2	2.16	0.46
1:D:325:LEU:HB3	1:D:832:ILE:HG12	1.98	0.46
1:G:289:ALA:O	1:G:290:ILE:C	2.57	0.46
1:G:819:ILE:HG22	1:G:821:LEU:HG	1.97	0.46
1:H:356:UNK:O	1:H:357:UNK:O	2.33	0.46
1:H:742:UNK:O	1:H:743:UNK:CB	2.62	0.46
1:H:822:PRO:HA	1:H:823:PRO:HD2	1.81	0.46
1:I:310:ARG:CZ	1:J:858:GLU:HG3	2.45	0.46
1:I:317:ARG:HH21	1:I:779:GLN:CG	2.28	0.46
1:I:882:ILE:HG21	1:I:940:LEU:HA	1.96	0.46
1:J:356:UNK:O	1:J:357:UNK:O	2.33	0.46
1:J:819:ILE:HG22	1:J:821:LEU:HG	1.97	0.46
1:J:851:ILE:O	1:J:852:LEU:C	2.56	0.46
1:K:757:LEU:CD2	1:K:799:ILE:HB	2.42	0.46
1:K:819:ILE:HG22	1:K:821:LEU:HG	1.97	0.46
1:N:325:LEU:HB3	1:N:832:ILE:HG12	1.98	0.46
1:N:770:SER:OG	1:N:771:VAL:N	2.48	0.46
1:P:268:ILE:O	1:P:272:LEU:HD13	2.15	0.46
1:A:317:ARG:HH21	1:A:779:GLN:CG	2.28	0.46
1:A:317:ARG:HG3	1:A:317:ARG:NH1	2.30	0.46
1:B:742:UNK:O	1:B:743:UNK:CB	2.62	0.46
1:C:317:ARG:HG3	1:C:317:ARG:NH1	2.30	0.46
1:D:268:ILE:O	1:D:272:LEU:HD13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:809:PHE:CD1	1:D:809:PHE:N	2.84	0.46
1:E:317:ARG:HH21	1:E:779:GLN:CG	2.28	0.46
1:G:322:ILE:HD13	1:G:931:LEU:HD23	1.97	0.46
1:G:325:LEU:HB3	1:G:832:ILE:HG12	1.98	0.46
1:G:853:ARG:O	1:G:856:ARG:HG2	2.16	0.46
1:H:819:ILE:HG22	1:H:821:LEU:HG	1.97	0.46
1:J:325:LEU:HB3	1:J:832:ILE:HG12	1.98	0.46
1:K:268:ILE:O	1:K:272:LEU:HD13	2.15	0.46
1:K:317:ARG:HH21	1:K:779:GLN:CG	2.28	0.46
1:L:317:ARG:HH21	1:L:779:GLN:CG	2.28	0.46
1:L:828:ARG:N	1:L:828:ARG:HD2	2.30	0.46
1:L:894:ILE:HD11	1:M:852:LEU:HD11	1.97	0.46
1:M:268:ILE:O	1:M:272:LEU:HD13	2.15	0.46
1:N:268:ILE:O	1:N:272:LEU:HD13	2.15	0.46
1:N:356:UNK:O	1:N:357:UNK:O	2.33	0.46
1:N:819:ILE:HG22	1:N:821:LEU:HG	1.97	0.46
1:P:317:ARG:HH21	1:P:779:GLN:CG	2.28	0.46
1:P:356:UNK:O	1:P:357:UNK:O	2.33	0.46
1:P:808:ARG:NH1	1:P:808:ARG:CB	2.77	0.46
1:B:356:UNK:O	1:B:357:UNK:O	2.33	0.46
1:B:788:ILE:HG22	1:O:741:UNK:CA	2.43	0.46
1:C:290:ILE:C	1:C:290:ILE:CD1	2.84	0.46
1:D:783:ILE:HG21	1:M:788:ILE:CD1	2.45	0.46
1:D:853:ARG:O	1:D:856:ARG:HG2	2.16	0.46
1:E:322:ILE:HD13	1:E:931:LEU:HD23	1.97	0.46
1:E:828:ARG:NH1	1:E:828:ARG:HG3	2.30	0.46
1:F:325:LEU:HB3	1:F:832:ILE:HG12	1.98	0.46
1:F:809:PHE:N	1:F:809:PHE:CD1	2.84	0.46
1:G:280:ASP:O	1:G:283:VAL:HG22	2.14	0.46
1:G:809:PHE:N	1:G:809:PHE:CD1	2.84	0.46
1:H:332:VAL:HG23	1:H:334:LYS:HG3	1.98	0.46
1:H:350:TYR:C	1:H:350:TYR:HD1	2.23	0.46
1:H:828:ARG:HD2	1:H:828:ARG:N	2.30	0.46
1:I:356:UNK:O	1:I:357:UNK:O	2.33	0.46
1:I:836:ILE:HD11	1:I:965:MET:HG2	1.98	0.46
1:J:332:VAL:HG23	1:J:334:LYS:HG3	1.98	0.46
1:J:770:SER:OG	1:J:771:VAL:N	2.48	0.46
1:J:853:ARG:O	1:J:856:ARG:HG2	2.16	0.46
1:K:770:SER:OG	1:K:771:VAL:N	2.48	0.46
1:M:317:ARG:HG3	1:M:317:ARG:NH1	2.30	0.46
1:N:322:ILE:HD13	1:N:931:LEU:HD23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:853:ARG:O	1:N:856:ARG:HG2	2.16	0.46
1:A:742:UNK:O	1:A:743:UNK:CB	2.63	0.46
1:A:809:PHE:N	1:A:809:PHE:CD1	2.84	0.46
1:A:841:ASP:OD2	1:H:903:LYS:HD2	2.16	0.46
1:A:853:ARG:O	1:A:856:ARG:HG2	2.16	0.46
1:C:325:LEU:HB3	1:C:832:ILE:HG12	1.98	0.46
1:C:770:SER:OG	1:C:771:VAL:N	2.48	0.46
1:D:890:ALA:O	1:D:891:MET:C	2.57	0.46
1:D:920:ILE:CG2	1:D:921:THR:N	2.79	0.46
1:E:289:ALA:O	1:E:290:ILE:C	2.57	0.46
1:F:836:ILE:HD11	1:F:965:MET:HG2	1.98	0.46
1:G:770:SER:OG	1:G:771:VAL:N	2.48	0.46
1:I:770:SER:OG	1:I:771:VAL:N	2.48	0.46
1:I:812:MET:SD	1:I:812:MET:N	2.78	0.46
1:I:920:ILE:CG2	1:I:921:THR:N	2.79	0.46
1:M:925:LEU:O	1:M:929:ILE:HG13	2.15	0.46
1:N:289:ALA:O	1:N:290:ILE:C	2.57	0.46
1:N:925:LEU:O	1:N:929:ILE:HG13	2.15	0.46
1:O:325:LEU:HB3	1:O:832:ILE:HG12	1.98	0.46
1:P:770:SER:OG	1:P:771:VAL:N	2.48	0.46
1:P:828:ARG:HG3	1:P:828:ARG:NH1	2.30	0.46
1:P:836:ILE:HD11	1:P:965:MET:HG2	1.98	0.46
1:B:325:LEU:HB3	1:B:832:ILE:HG12	1.98	0.46
1:B:882:ILE:HG21	1:B:940:LEU:HA	1.96	0.46
1:E:925:LEU:O	1:E:929:ILE:HG13	2.15	0.46
1:G:290:ILE:C	1:G:290:ILE:CD1	2.84	0.46
1:G:897:TYR:C	1:G:897:TYR:CD2	2.94	0.46
1:H:325:LEU:HB3	1:H:832:ILE:HG12	1.98	0.46
1:I:289:ALA:O	1:I:290:ILE:C	2.57	0.46
1:I:853:ARG:O	1:I:856:ARG:HG2	2.16	0.46
1:M:350:TYR:C	1:M:350:TYR:HD1	2.23	0.46
1:M:897:TYR:CD2	1:M:897:TYR:C	2.94	0.46
1:N:897:TYR:CD2	1:N:897:TYR:C	2.94	0.46
1:O:327:VAL:HA	1:O:802:ALA:O	2.16	0.46
1:O:356:UNK:O	1:O:357:UNK:O	2.33	0.46
1:P:350:TYR:HD1	1:P:351:THR:N	2.09	0.46
1:A:268:ILE:O	1:A:272:LEU:HD13	2.15	0.46
1:A:332:VAL:HG23	1:A:334:LYS:HG3	1.98	0.46
1:B:295:GLU:CD	1:B:295:GLU:N	2.70	0.46
1:B:819:ILE:HG22	1:B:821:LEU:HG	1.97	0.46
1:C:809:PHE:N	1:C:809:PHE:CD1	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:897:TYR:CD2	1:C:897:TYR:C	2.94	0.46
1:D:836:ILE:HD11	1:D:965:MET:HG2	1.98	0.46
1:E:332:VAL:HG23	1:E:334:LYS:HG3	1.98	0.46
1:F:770:SER:OG	1:F:771:VAL:N	2.48	0.46
1:G:327:VAL:HA	1:G:802:ALA:O	2.16	0.46
1:G:334:LYS:HB2	2:G:1001:ADP:O1B	2.16	0.46
1:G:356:UNK:O	1:G:357:UNK:O	2.33	0.46
1:H:322:ILE:HD13	1:H:931:LEU:HD23	1.97	0.46
1:I:325:LEU:HB3	1:I:832:ILE:HG12	1.98	0.46
1:J:925:LEU:O	1:J:929:ILE:HG13	2.15	0.46
1:K:325:LEU:HB3	1:K:832:ILE:HG12	1.98	0.46
1:K:853:ARG:O	1:K:856:ARG:HG2	2.16	0.46
1:L:809:PHE:CD1	1:L:809:PHE:N	2.84	0.46
1:M:277:ASP:O	1:M:278:ILE:C	2.59	0.46
1:M:325:LEU:HB3	1:M:832:ILE:HG12	1.98	0.46
1:N:317:ARG:HH21	1:N:779:GLN:CG	2.28	0.46
1:O:851:ILE:O	1:O:852:LEU:C	2.56	0.46
1:P:325:LEU:HB3	1:P:832:ILE:HG12	1.98	0.46
1:A:836:ILE:HD11	1:A:965:MET:HG2	1.98	0.46
1:B:332:VAL:HG23	1:B:334:LYS:HG3	1.98	0.46
1:B:337:ILE:O	1:B:338:LEU:C	2.59	0.46
1:B:828:ARG:NH1	1:B:828:ARG:HG3	2.30	0.46
1:B:897:TYR:C	1:B:897:TYR:CD2	2.94	0.46
1:B:939:ARG:C	1:B:940:LEU:HG	2.41	0.46
1:C:268:ILE:O	1:C:272:LEU:HD13	2.15	0.46
1:D:332:VAL:HG23	1:D:334:LYS:HG3	1.98	0.46
1:D:334:LYS:HB2	2:D:1001:ADP:O1B	2.16	0.46
1:D:770:SER:OG	1:D:771:VAL:N	2.48	0.46
1:E:277:ASP:O	1:E:278:ILE:C	2.59	0.46
1:E:325:LEU:HB3	1:E:832:ILE:HG12	1.98	0.46
1:E:334:LYS:HB2	2:E:1001:ADP:O1B	2.16	0.46
1:E:809:PHE:N	1:E:809:PHE:CD1	2.84	0.46
1:F:277:ASP:O	1:F:278:ILE:C	2.59	0.46
1:G:312:LEU:HD13	1:H:858:GLU:HA	1.90	0.46
1:G:317:ARG:HG3	1:G:317:ARG:NH1	2.30	0.46
1:G:925:LEU:O	1:G:929:ILE:HG13	2.15	0.46
1:H:327:VAL:HA	1:H:802:ALA:O	2.16	0.46
1:I:310:ARG:NH1	1:J:858:GLU:CG	2.79	0.46
1:J:327:VAL:HA	1:J:802:ALA:O	2.16	0.46
1:K:860:GLU:C	1:K:862:VAL:N	2.74	0.46
1:L:836:ILE:HD11	1:L:965:MET:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:853:ARG:O	1:L:856:ARG:HG2	2.16	0.46
1:M:316:THR:HG21	1:N:339:ARG:HD3	1.98	0.46
1:N:327:VAL:HA	1:N:802:ALA:O	2.16	0.46
1:A:356:UNK:O	1:A:357:UNK:O	2.33	0.46
1:C:277:ASP:O	1:C:278:ILE:C	2.59	0.46
1:C:327:VAL:HA	1:C:802:ALA:O	2.16	0.46
1:C:334:LYS:HB2	2:C:1001:ADP:O1B	2.16	0.46
1:D:828:ARG:HG3	1:D:828:ARG:NH1	2.30	0.46
1:E:319:ARG:HG2	1:E:320:GLY:N	2.31	0.46
1:E:327:VAL:HA	1:E:802:ALA:O	2.16	0.46
1:E:853:ARG:O	1:E:856:ARG:HG2	2.16	0.46
1:F:327:VAL:HA	1:F:802:ALA:O	2.16	0.46
1:H:283:VAL:C	1:H:285:SER:N	2.74	0.46
1:H:897:TYR:C	1:H:897:TYR:CD2	2.94	0.46
1:I:897:TYR:C	1:I:897:TYR:CD2	2.94	0.46
1:J:322:ILE:HD13	1:J:931:LEU:HD23	1.97	0.46
1:L:278:ILE:HD11	1:L:874:TYR:OH	2.16	0.46
1:L:819:ILE:HG22	1:L:821:LEU:HG	1.97	0.46
1:L:925:LEU:O	1:L:929:ILE:HG13	2.15	0.46
1:M:770:SER:OG	1:M:771:VAL:N	2.48	0.46
1:M:828:ARG:NH1	1:M:828:ARG:HG3	2.30	0.46
1:M:939:ARG:C	1:M:940:LEU:HG	2.41	0.46
1:N:886:ILE:CD1	1:N:886:ILE:H	2.27	0.46
1:O:920:ILE:CG2	1:O:921:THR:N	2.79	0.46
1:P:828:ARG:HD2	1:P:828:ARG:N	2.30	0.46
1:B:278:ILE:HD11	1:B:874:TYR:OH	2.16	0.45
1:B:283:VAL:C	1:B:285:SER:N	2.74	0.45
1:B:334:LYS:HB2	2:B:1001:ADP:O1B	2.16	0.45
1:C:819:ILE:HG22	1:C:821:LEU:HG	1.97	0.45
1:D:327:VAL:HA	1:D:802:ALA:O	2.16	0.45
1:E:268:ILE:O	1:E:272:LEU:HD13	2.15	0.45
1:E:278:ILE:HD11	1:E:874:TYR:OH	2.16	0.45
1:G:290:ILE:HA	2:G:1001:ADP:C2	2.52	0.45
1:H:290:ILE:HA	2:H:1001:ADP:C2	2.52	0.45
1:I:278:ILE:HD11	1:I:874:TYR:OH	2.16	0.45
1:K:322:ILE:HD13	1:K:931:LEU:HD23	1.97	0.45
1:L:327:VAL:HA	1:L:802:ALA:O	2.16	0.45
1:L:939:ARG:C	1:L:940:LEU:HG	2.41	0.45
1:M:886:ILE:CD1	1:M:886:ILE:H	2.27	0.45
1:N:283:VAL:C	1:N:285:SER:N	2.75	0.45
1:O:317:ARG:HH21	1:O:779:GLN:CG	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ASP:O	1:A:278:ILE:C	2.59	0.45
1:A:290:ILE:HA	2:A:1001:ADP:C2	2.52	0.45
1:A:897:TYR:C	1:A:897:TYR:CD2	2.94	0.45
1:D:828:ARG:N	1:D:828:ARG:HD2	2.30	0.45
1:E:350:TYR:C	1:E:350:TYR:HD1	2.23	0.45
1:E:770:SER:OG	1:E:771:VAL:N	2.48	0.45
1:H:277:ASP:O	1:H:278:ILE:C	2.59	0.45
1:I:327:VAL:HA	1:I:802:ALA:O	2.16	0.45
1:I:753:GLY:CA	1:I:795:ARG:HH11	2.30	0.45
1:I:860:GLU:C	1:I:862:VAL:N	2.74	0.45
1:J:939:ARG:C	1:J:940:LEU:HG	2.41	0.45
1:L:768:ASP:O	1:L:771:VAL:CG1	2.65	0.45
1:L:770:SER:OG	1:L:771:VAL:N	2.48	0.45
1:N:278:ILE:HD11	1:N:874:TYR:OH	2.16	0.45
1:N:860:GLU:C	1:N:862:VAL:N	2.74	0.45
1:N:920:ILE:CG2	1:N:921:THR:N	2.79	0.45
1:O:332:VAL:HG23	1:O:334:LYS:HG3	1.98	0.45
1:O:334:LYS:HB2	2:O:1001:ADP:O1B	2.16	0.45
1:O:939:ARG:C	1:O:940:LEU:HG	2.41	0.45
1:P:890:ALA:HB1	1:P:949:ALA:CB	2.43	0.45
1:A:334:LYS:HB2	2:A:1001:ADP:O1B	2.16	0.45
1:B:327:VAL:HA	1:B:802:ALA:O	2.16	0.45
1:B:350:TYR:C	1:B:350:TYR:HD1	2.23	0.45
1:B:753:GLY:CA	1:B:795:ARG:HH11	2.30	0.45
1:B:853:ARG:O	1:B:856:ARG:HG2	2.16	0.45
1:B:878:ALA:HA	1:B:882:ILE:HG12	1.99	0.45
1:E:753:GLY:CA	1:E:795:ARG:HH11	2.30	0.45
1:F:939:ARG:C	1:F:940:LEU:HG	2.41	0.45
1:G:283:VAL:C	1:G:285:SER:N	2.75	0.45
1:G:753:GLY:CA	1:G:795:ARG:HH11	2.30	0.45
1:G:768:ASP:O	1:G:771:VAL:CG1	2.65	0.45
1:I:310:ARG:HD3	1:J:858:GLU:HG3	1.98	0.45
1:I:878:ALA:HA	1:I:882:ILE:HG12	1.99	0.45
1:I:902:ARG:HG2	1:J:844:ASP:OD2	2.16	0.45
1:J:278:ILE:HD11	1:J:874:TYR:OH	2.16	0.45
1:J:290:ILE:HA	2:J:1001:ADP:C2	2.52	0.45
1:K:290:ILE:HA	2:K:1001:ADP:C2	2.52	0.45
1:K:327:VAL:HA	1:K:802:ALA:O	2.16	0.45
1:K:768:ASP:O	1:K:771:VAL:CG1	2.65	0.45
1:L:753:GLY:CA	1:L:795:ARG:HH11	2.30	0.45
1:M:808:ARG:NH1	1:M:808:ARG:CB	2.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:878:ALA:HA	1:M:882:ILE:HG12	1.98	0.45
1:N:828:ARG:N	1:N:828:ARG:HD2	2.30	0.45
1:N:836:ILE:HD11	1:N:965:MET:HG2	1.98	0.45
1:O:268:ILE:O	1:O:272:LEU:HD13	2.15	0.45
1:O:290:ILE:HA	2:O:1001:ADP:C2	2.52	0.45
1:A:278:ILE:HD11	1:A:874:TYR:OH	2.16	0.45
1:A:322:ILE:HD13	1:A:931:LEU:HD23	1.97	0.45
1:A:770:SER:OG	1:A:771:VAL:N	2.48	0.45
1:B:290:ILE:HA	2:B:1001:ADP:C2	2.52	0.45
1:B:768:ASP:O	1:B:771:VAL:CG1	2.65	0.45
1:B:894:ILE:HD11	1:C:852:LEU:HD11	1.98	0.45
1:B:929:ILE:HD11	1:C:852:LEU:CD1	2.46	0.45
1:C:757:LEU:CD2	1:C:799:ILE:HB	2.42	0.45
1:D:290:ILE:HA	2:D:1001:ADP:C2	2.52	0.45
1:D:337:ILE:O	1:D:338:LEU:C	2.59	0.45
1:F:290:ILE:C	1:F:290:ILE:CD1	2.84	0.45
1:F:317:ARG:HG3	1:F:317:ARG:NH1	2.30	0.45
1:F:334:LYS:HB2	2:F:1001:ADP:O1B	2.16	0.45
1:F:860:GLU:C	1:F:862:VAL:N	2.74	0.45
1:G:902:ARG:HH11	1:G:902:ARG:CG	2.30	0.45
1:G:939:ARG:C	1:G:940:LEU:HG	2.41	0.45
1:I:894:ILE:HD11	1:J:852:LEU:CD2	2.46	0.45
1:L:319:ARG:HG2	1:L:320:GLY:N	2.31	0.45
1:L:332:VAL:HG23	1:L:334:LYS:HG3	1.98	0.45
1:L:808:ARG:NH1	1:L:808:ARG:CB	2.77	0.45
1:M:278:ILE:HD11	1:M:874:TYR:OH	2.16	0.45
1:M:317:ARG:HH21	1:M:779:GLN:CG	2.28	0.45
1:M:334:LYS:HB2	2:M:1001:ADP:O1B	2.16	0.45
1:M:809:PHE:N	1:M:809:PHE:CD1	2.84	0.45
1:N:290:ILE:HA	2:N:1001:ADP:C2	2.52	0.45
1:N:755:TYR:CD1	1:N:755:TYR:N	2.79	0.45
1:O:283:VAL:C	1:O:285:SER:N	2.75	0.45
1:O:753:GLY:CA	1:O:795:ARG:HH11	2.30	0.45
1:O:860:GLU:C	1:O:862:VAL:N	2.74	0.45
1:O:897:TYR:CD2	1:O:897:TYR:C	2.94	0.45
1:P:853:ARG:O	1:P:856:ARG:HG2	2.16	0.45
1:A:327:VAL:HA	1:A:802:ALA:O	2.16	0.45
1:C:290:ILE:HA	2:C:1001:ADP:C2	2.52	0.45
1:C:836:ILE:HD11	1:C:965:MET:HG2	1.98	0.45
1:C:860:GLU:C	1:C:862:VAL:N	2.74	0.45
1:C:939:ARG:C	1:C:940:LEU:HG	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:278:ILE:HD11	1:D:874:TYR:OH	2.16	0.45
1:E:828:ARG:N	1:E:828:ARG:HD2	2.30	0.45
1:F:332:VAL:HG23	1:F:334:LYS:HG3	1.98	0.45
1:F:350:TYR:C	1:F:350:TYR:HD1	2.23	0.45
1:G:730:UNK:CB	1:K:730:UNK:C	2.93	0.45
1:H:290:ILE:C	1:H:290:ILE:CD1	2.84	0.45
1:I:828:ARG:HG3	1:I:828:ARG:NH1	2.30	0.45
1:J:317:ARG:HG3	1:J:317:ARG:NH1	2.30	0.45
1:J:897:TYR:CD2	1:J:897:TYR:C	2.94	0.45
1:K:283:VAL:C	1:K:285:SER:N	2.74	0.45
1:L:290:ILE:HA	2:L:1001:ADP:C2	2.52	0.45
1:M:290:ILE:HA	2:M:1001:ADP:C2	2.52	0.45
1:M:768:ASP:O	1:M:771:VAL:CG1	2.65	0.45
1:M:853:ARG:O	1:M:856:ARG:HG2	2.16	0.45
1:P:290:ILE:HA	2:P:1001:ADP:C2	2.52	0.45
1:P:327:VAL:HA	1:P:802:ALA:O	2.16	0.45
1:P:337:ILE:O	1:P:338:LEU:C	2.59	0.45
1:P:897:TYR:C	1:P:897:TYR:CD2	2.94	0.45
1:C:768:ASP:O	1:C:771:VAL:CG1	2.65	0.45
1:F:319:ARG:HG2	1:F:320:GLY:N	2.31	0.45
1:F:828:ARG:N	1:F:828:ARG:HD2	2.30	0.45
1:F:920:ILE:CG2	1:F:921:THR:N	2.79	0.45
1:G:277:ASP:O	1:G:278:ILE:C	2.59	0.45
1:I:332:VAL:HG23	1:I:334:LYS:HG3	1.98	0.45
1:I:809:PHE:N	1:I:809:PHE:CD1	2.84	0.45
1:I:831:LEU:HD22	1:I:959:THR:HG21	1.99	0.45
1:J:878:ALA:HA	1:J:882:ILE:HG12	1.99	0.45
1:L:350:TYR:C	1:L:350:TYR:HD1	2.23	0.45
1:L:739:UNK:O	1:L:740:UNK:CB	2.65	0.45
1:M:337:ILE:O	1:M:338:LEU:C	2.59	0.45
1:N:878:ALA:HA	1:N:882:ILE:HG12	1.99	0.45
1:O:831:LEU:HD22	1:O:959:THR:HG21	1.99	0.45
1:O:836:ILE:HD11	1:O:965:MET:HG2	1.98	0.45
1:O:853:ARG:O	1:O:856:ARG:HG2	2.16	0.45
1:P:278:ILE:HD11	1:P:874:TYR:OH	2.16	0.45
1:P:332:VAL:HG23	1:P:334:LYS:HG3	1.98	0.45
1:A:753:GLY:CA	1:A:795:ARG:HH11	2.30	0.45
1:A:939:ARG:C	1:A:940:LEU:HG	2.41	0.45
1:B:739:UNK:O	1:B:740:UNK:CB	2.65	0.45
1:D:319:ARG:HG2	1:D:320:GLY:N	2.31	0.45
1:D:878:ALA:HA	1:D:882:ILE:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:278:ILE:HD11	1:F:874:TYR:OH	2.16	0.45
1:G:278:ILE:HD11	1:G:874:TYR:OH	2.16	0.45
1:H:768:ASP:O	1:H:771:VAL:CG1	2.65	0.45
1:H:836:ILE:HD11	1:H:965:MET:HG2	1.98	0.45
1:I:939:ARG:C	1:I:940:LEU:HG	2.41	0.45
1:K:277:ASP:O	1:K:278:ILE:C	2.59	0.45
1:K:878:ALA:HA	1:K:882:ILE:HG12	1.99	0.45
1:K:920:ILE:CG2	1:K:921:THR:N	2.79	0.45
1:M:831:LEU:HD22	1:M:959:THR:HG21	1.99	0.45
1:N:332:VAL:HG23	1:N:334:LYS:HG3	1.98	0.45
1:O:322:ILE:HD13	1:O:931:LEU:HD23	1.97	0.45
1:O:768:ASP:O	1:O:771:VAL:CG1	2.65	0.45
1:C:828:ARG:N	1:C:828:ARG:HD2	2.30	0.45
1:E:290:ILE:HA	2:E:1001:ADP:C2	2.52	0.45
1:E:939:ARG:C	1:E:940:LEU:HG	2.41	0.45
1:F:739:UNK:O	1:F:740:UNK:CB	2.65	0.45
1:F:897:TYR:CD2	1:F:897:TYR:C	2.94	0.45
1:G:831:LEU:HD22	1:G:959:THR:HG21	1.99	0.45
1:G:878:ALA:HA	1:G:882:ILE:HG12	1.99	0.45
1:I:283:VAL:C	1:I:285:SER:N	2.75	0.45
1:I:334:LYS:HB2	2:I:1001:ADP:O1B	2.16	0.45
1:K:898:TYR:CD2	1:L:848:ALA:HB2	2.52	0.45
1:K:939:ARG:C	1:K:940:LEU:HG	2.41	0.45
1:L:334:LYS:HB2	2:L:1001:ADP:O1B	2.16	0.45
1:O:809:PHE:N	1:O:809:PHE:CD1	2.84	0.45
1:B:828:ARG:N	1:B:828:ARG:HD2	2.30	0.45
1:B:836:ILE:HD11	1:B:965:MET:HG2	1.98	0.45
1:C:753:GLY:CA	1:C:795:ARG:HH11	2.30	0.45
1:C:878:ALA:HA	1:C:882:ILE:HG12	1.99	0.45
1:D:887:SER:C	1:D:889:GLU:N	2.67	0.45
1:E:836:ILE:HD11	1:E:965:MET:HG2	1.98	0.45
1:F:819:ILE:HG22	1:F:821:LEU:HG	1.97	0.45
1:F:828:ARG:HG3	1:F:828:ARG:NH1	2.30	0.45
1:H:334:LYS:HB2	2:H:1001:ADP:O1B	2.16	0.45
1:I:290:ILE:HA	2:I:1001:ADP:C2	2.52	0.45
1:I:739:UNK:O	1:I:740:UNK:CB	2.65	0.45
1:K:278:ILE:HD11	1:K:874:TYR:OH	2.16	0.45
1:K:897:TYR:C	1:K:897:TYR:CD2	2.94	0.45
1:M:332:VAL:HG23	1:M:334:LYS:HG3	1.98	0.45
1:O:278:ILE:HD11	1:O:874:TYR:OH	2.16	0.45
1:O:739:UNK:O	1:O:740:UNK:CB	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:808:ARG:NH1	1:A:808:ARG:CB	2.77	0.45
1:A:920:ILE:CG2	1:A:921:THR:N	2.79	0.45
1:E:337:ILE:O	1:E:338:LEU:C	2.59	0.45
1:F:290:ILE:HA	2:F:1001:ADP:C2	2.52	0.45
1:I:768:ASP:O	1:I:771:VAL:CG1	2.65	0.45
1:I:852:LEU:HB3	1:P:891:MET:HG3	1.97	0.45
1:J:277:ASP:O	1:J:278:ILE:C	2.59	0.45
1:J:283:VAL:C	1:J:285:SER:N	2.74	0.45
1:J:350:TYR:C	1:J:350:TYR:HD1	2.23	0.45
1:J:809:PHE:N	1:J:809:PHE:CD1	2.84	0.45
1:K:888:GLU:HG2	1:L:856:ARG:HH12	1.82	0.45
1:M:290:ILE:C	1:M:290:ILE:CD1	2.84	0.45
1:M:822:PRO:HA	1:M:823:PRO:HD2	1.80	0.45
1:N:334:LYS:HB2	2:N:1001:ADP:O1B	2.16	0.45
1:P:739:UNK:O	1:P:740:UNK:CB	2.65	0.45
1:F:746:UNK:O	1:F:792:LEU:CD1	2.65	0.44
1:F:753:GLY:CA	1:F:795:ARG:HH11	2.30	0.44
1:F:902:ARG:HH11	1:F:902:ARG:CG	2.30	0.44
1:G:739:UNK:O	1:G:740:UNK:CB	2.65	0.44
1:H:278:ILE:HD11	1:H:874:TYR:OH	2.16	0.44
1:H:809:PHE:N	1:H:809:PHE:CD1	2.84	0.44
1:H:878:ALA:HA	1:H:882:ILE:HG12	1.98	0.44
1:K:332:VAL:HG23	1:K:334:LYS:HG3	1.98	0.44
1:K:831:LEU:HD22	1:K:959:THR:HG21	1.99	0.44
1:K:890:ALA:HB1	1:K:949:ALA:CB	2.43	0.44
1:L:283:VAL:C	1:L:285:SER:N	2.75	0.44
1:M:888:GLU:HG2	1:N:856:ARG:HH12	1.82	0.44
1:O:337:ILE:O	1:O:338:LEU:C	2.59	0.44
1:A:768:ASP:O	1:A:771:VAL:CG1	2.65	0.44
1:A:852:LEU:O	1:A:855:ARG:HB3	2.18	0.44
1:B:831:LEU:HD22	1:B:959:THR:HG21	1.99	0.44
1:D:897:TYR:C	1:D:897:TYR:CD2	2.94	0.44
1:D:939:ARG:C	1:D:940:LEU:HG	2.41	0.44
1:E:897:TYR:C	1:E:897:TYR:CD2	2.94	0.44
1:F:852:LEU:O	1:F:855:ARG:HB3	2.18	0.44
1:F:878:ALA:HA	1:F:882:ILE:HG12	1.99	0.44
1:H:791:THR:O	1:I:738:UNK:HA	2.16	0.44
1:K:753:GLY:CA	1:K:795:ARG:HH11	2.30	0.44
1:M:319:ARG:HG2	1:M:320:GLY:N	2.31	0.44
1:N:753:GLY:CA	1:N:795:ARG:HH11	2.30	0.44
1:N:768:ASP:O	1:N:771:VAL:CG1	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:878:ALA:HA	1:O:882:ILE:HG12	1.99	0.44
1:O:885:VAL:HG13	1:P:856:ARG:HB2	1.99	0.44
1:P:809:PHE:N	1:P:809:PHE:CD1	2.84	0.44
1:P:852:LEU:O	1:P:855:ARG:HB3	2.18	0.44
1:A:319:ARG:HG2	1:A:320:GLY:N	2.31	0.44
1:A:783:ILE:N	1:A:783:ILE:CD1	2.79	0.44
1:A:860:GLU:C	1:A:862:VAL:N	2.74	0.44
1:C:278:ILE:HD11	1:C:874:TYR:OH	2.16	0.44
1:C:890:ALA:HB1	1:C:949:ALA:CB	2.43	0.44
1:D:277:ASP:O	1:D:278:ILE:C	2.59	0.44
1:D:753:GLY:CA	1:D:795:ARG:HH11	2.30	0.44
1:F:337:ILE:O	1:F:338:LEU:C	2.59	0.44
1:G:319:ARG:HG2	1:G:320:GLY:N	2.31	0.44
1:G:836:ILE:HD11	1:G:965:MET:HG2	1.98	0.44
1:H:319:ARG:HG2	1:H:320:GLY:N	2.31	0.44
1:H:739:UNK:O	1:H:740:UNK:CB	2.65	0.44
1:I:350:TYR:C	1:I:350:TYR:HD1	2.23	0.44
1:J:831:LEU:HD22	1:J:959:THR:HG21	1.99	0.44
1:J:836:ILE:HD11	1:J:965:MET:HG2	1.98	0.44
1:J:852:LEU:O	1:J:855:ARG:HB3	2.17	0.44
1:K:334:LYS:HB2	2:K:1001:ADP:O1B	2.16	0.44
1:K:808:ARG:NH1	1:K:808:ARG:CB	2.77	0.44
1:K:852:LEU:O	1:K:855:ARG:HB3	2.18	0.44
1:N:319:ARG:HG2	1:N:320:GLY:N	2.31	0.44
1:P:317:ARG:HG3	1:P:317:ARG:NH1	2.30	0.44
1:P:939:ARG:C	1:P:940:LEU:HG	2.41	0.44
1:A:325:LEU:HB3	1:A:832:ILE:HG12	1.98	0.44
1:C:852:LEU:O	1:C:855:ARG:HB3	2.17	0.44
1:E:860:GLU:C	1:E:862:VAL:N	2.74	0.44
1:F:729:UNK:C	1:L:730:UNK:CB	2.95	0.44
1:J:920:ILE:CG2	1:J:921:THR:N	2.79	0.44
1:M:327:VAL:HA	1:M:802:ALA:O	2.16	0.44
1:M:757:LEU:CD2	1:M:799:ILE:HB	2.42	0.44
1:N:337:ILE:O	1:N:338:LEU:C	2.59	0.44
1:N:828:ARG:HG3	1:N:828:ARG:NH1	2.30	0.44
1:O:808:ARG:NH1	1:O:808:ARG:CB	2.77	0.44
1:O:885:VAL:CG1	1:P:856:ARG:HB2	2.47	0.44
1:P:334:LYS:HB2	2:P:1001:ADP:O1B	2.16	0.44
1:D:283:VAL:C	1:D:285:SER:N	2.75	0.44
1:E:739:UNK:O	1:E:740:UNK:CB	2.65	0.44
1:E:878:ALA:HA	1:E:882:ILE:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:753:GLY:CA	1:H:795:ARG:HH11	2.30	0.44
1:I:852:LEU:O	1:I:855:ARG:HB3	2.17	0.44
1:J:334:LYS:HB2	2:J:1001:ADP:O1B	2.16	0.44
1:K:836:ILE:HD11	1:K:965:MET:HG2	1.98	0.44
1:N:809:PHE:N	1:N:809:PHE:CD1	2.84	0.44
1:O:350:TYR:C	1:O:350:TYR:HD1	2.23	0.44
1:P:902:ARG:HH11	1:P:902:ARG:CG	2.30	0.44
1:C:332:VAL:HG23	1:C:334:LYS:HG3	1.98	0.44
1:D:746:UNK:O	1:D:792:LEU:CD1	2.65	0.44
1:E:283:VAL:C	1:E:285:SER:N	2.75	0.44
1:E:312:LEU:HD11	1:F:858:GLU:HA	1.99	0.44
1:E:332:VAL:HG22	1:E:334:LYS:HE2	2.00	0.44
1:E:831:LEU:HD22	1:E:959:THR:HG21	1.99	0.44
1:E:852:LEU:O	1:E:855:ARG:HB3	2.17	0.44
1:G:849:ARG:HD3	1:G:853:ARG:HG3	2.00	0.44
1:G:852:LEU:O	1:G:855:ARG:HB3	2.18	0.44
1:G:929:ILE:CD1	1:H:852:LEU:CD1	2.96	0.44
1:H:770:SER:OG	1:H:771:VAL:N	2.48	0.44
1:J:310:ARG:CZ	1:K:858:GLU:HG3	2.47	0.44
1:J:768:ASP:O	1:J:771:VAL:CG1	2.65	0.44
1:J:902:ARG:HH11	1:J:902:ARG:CG	2.30	0.44
1:K:350:TYR:C	1:K:350:TYR:HD1	2.23	0.44
1:K:828:ARG:N	1:K:828:ARG:HD2	2.30	0.44
1:M:332:VAL:HG22	1:M:334:LYS:HE2	2.00	0.44
1:M:753:GLY:CA	1:M:795:ARG:HH11	2.30	0.44
1:M:836:ILE:HD11	1:M:965:MET:HG2	1.98	0.44
1:M:843:ILE:O	1:M:847:VAL:HG23	2.18	0.44
1:P:283:VAL:C	1:P:285:SER:N	2.74	0.44
1:A:878:ALA:HA	1:A:882:ILE:HG12	1.99	0.44
1:G:332:VAL:HG23	1:G:334:LYS:HG3	1.98	0.44
1:H:852:LEU:O	1:H:855:ARG:HB3	2.17	0.44
1:H:939:ARG:C	1:H:940:LEU:HG	2.41	0.44
1:I:808:ARG:NH1	1:I:808:ARG:CB	2.77	0.44
1:J:332:VAL:HG22	1:J:334:LYS:HE2	2.00	0.44
1:J:337:ILE:O	1:J:338:LEU:C	2.59	0.44
1:K:739:UNK:O	1:K:740:UNK:CB	2.65	0.44
1:L:746:UNK:O	1:L:792:LEU:CD1	2.65	0.44
1:L:852:LEU:O	1:L:855:ARG:HB3	2.18	0.44
1:L:878:ALA:HA	1:L:882:ILE:HG12	1.99	0.44
1:L:897:TYR:CD2	1:L:897:TYR:C	2.94	0.44
1:M:828:ARG:N	1:M:828:ARG:HD2	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:852:LEU:O	1:M:855:ARG:HB3	2.18	0.44
1:P:860:GLU:C	1:P:862:VAL:N	2.74	0.44
1:A:828:ARG:N	1:A:828:ARG:HD2	2.30	0.44
1:B:843:ILE:O	1:B:847:VAL:HG23	2.18	0.44
1:H:337:ILE:O	1:H:338:LEU:C	2.59	0.44
1:I:843:ILE:O	1:I:847:VAL:HG23	2.18	0.44
1:J:739:UNK:O	1:J:740:UNK:CB	2.65	0.44
1:K:843:ILE:O	1:K:847:VAL:HG23	2.18	0.44
1:K:903:LYS:NZ	1:L:841:ASP:N	2.65	0.44
1:N:939:ARG:C	1:N:940:LEU:HG	2.41	0.44
1:P:277:ASP:O	1:P:278:ILE:C	2.59	0.44
1:P:843:ILE:O	1:P:847:VAL:HG23	2.18	0.44
1:P:901:MET:HE1	1:P:956:MET:CE	2.48	0.44
1:A:332:VAL:HG22	1:A:334:LYS:HE2	2.00	0.44
1:E:901:MET:HE1	1:E:956:MET:CE	2.48	0.44
1:F:332:VAL:HG22	1:F:334:LYS:HE2	2.00	0.44
1:I:828:ARG:N	1:I:828:ARG:HD2	2.30	0.44
1:K:337:ILE:O	1:K:338:LEU:C	2.59	0.44
1:L:901:MET:HE1	1:L:956:MET:CE	2.48	0.44
1:M:283:VAL:C	1:M:285:SER:N	2.74	0.44
1:M:860:GLU:C	1:M:862:VAL:N	2.74	0.44
1:N:901:MET:HE1	1:N:956:MET:CE	2.48	0.44
1:O:277:ASP:O	1:O:278:ILE:C	2.59	0.44
1:P:753:GLY:CA	1:P:795:ARG:HH11	2.30	0.44
1:P:768:ASP:O	1:P:771:VAL:CG1	2.65	0.44
1:A:337:ILE:O	1:A:338:LEU:C	2.59	0.43
1:B:901:MET:HE1	1:B:956:MET:CE	2.48	0.43
1:D:831:LEU:HD22	1:D:959:THR:HG21	1.99	0.43
1:E:768:ASP:O	1:E:771:VAL:CG1	2.65	0.43
1:E:843:ILE:O	1:E:847:VAL:HG23	2.18	0.43
1:E:874:TYR:C	1:E:874:TYR:HD1	2.26	0.43
1:H:831:LEU:HD22	1:H:959:THR:HG21	1.99	0.43
1:I:901:MET:HE1	1:I:956:MET:CE	2.48	0.43
1:J:874:TYR:C	1:J:874:TYR:HD1	2.26	0.43
1:L:312:LEU:CD2	1:M:858:GLU:CB	2.96	0.43
1:L:831:LEU:HD22	1:L:959:THR:HG21	1.99	0.43
1:O:332:VAL:HG22	1:O:334:LYS:HE2	2.00	0.43
1:O:852:LEU:O	1:O:855:ARG:HB3	2.18	0.43
1:A:901:MET:HE1	1:A:956:MET:CE	2.48	0.43
1:A:902:ARG:HH11	1:A:902:ARG:CG	2.30	0.43
1:B:783:ILE:O	1:B:790:ALA:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:901:MET:HE1	1:D:956:MET:CE	2.48	0.43
1:F:831:LEU:HD22	1:F:959:THR:HG21	1.99	0.43
1:F:902:ARG:HG2	1:G:844:ASP:OD2	2.18	0.43
1:H:902:ARG:HH11	1:H:902:ARG:CG	2.30	0.43
1:H:920:ILE:CG2	1:H:921:THR:N	2.79	0.43
1:I:849:ARG:HD3	1:I:853:ARG:HG3	2.00	0.43
1:J:753:GLY:CA	1:J:795:ARG:HH11	2.30	0.43
1:L:843:ILE:O	1:L:847:VAL:HG23	2.18	0.43
1:L:902:ARG:HH11	1:L:902:ARG:CG	2.30	0.43
1:L:929:ILE:HD11	1:M:852:LEU:CD1	2.49	0.43
1:N:277:ASP:O	1:N:278:ILE:C	2.59	0.43
1:N:757:LEU:CD2	1:N:799:ILE:HB	2.42	0.43
1:N:831:LEU:HD22	1:N:959:THR:HG21	1.99	0.43
1:O:901:MET:HE1	1:O:956:MET:CE	2.48	0.43
1:C:337:ILE:O	1:C:338:LEU:C	2.59	0.43
1:C:831:LEU:HD22	1:C:959:THR:HG21	1.99	0.43
1:D:843:ILE:O	1:D:847:VAL:HG23	2.18	0.43
1:E:740:UNK:C	1:L:789:THR:N	2.68	0.43
1:F:901:MET:HE1	1:F:956:MET:CE	2.48	0.43
1:I:290:ILE:C	1:I:290:ILE:CD1	2.84	0.43
1:J:901:MET:HE1	1:J:956:MET:CE	2.48	0.43
1:J:903:LYS:O	1:J:904:SER:OG	2.22	0.43
1:K:849:ARG:HD3	1:K:853:ARG:HG3	2.00	0.43
1:N:317:ARG:HG3	1:N:317:ARG:NH1	2.30	0.43
1:O:783:ILE:O	1:O:790:ALA:HB3	2.18	0.43
1:P:878:ALA:HA	1:P:882:ILE:HG12	1.99	0.43
1:P:920:ILE:CG2	1:P:921:THR:N	2.79	0.43
1:A:341:VAL:HG12	1:A:757:LEU:HD11	2.01	0.43
1:A:812:MET:O	1:A:813:LYS:C	2.62	0.43
1:A:831:LEU:HD22	1:A:959:THR:HG21	1.99	0.43
1:A:874:TYR:C	1:A:874:TYR:HD1	2.27	0.43
1:B:332:VAL:HG22	1:B:334:LYS:HE2	2.00	0.43
1:B:842:LYS:HE2	1:B:846:GLU:HG3	2.01	0.43
1:B:852:LEU:O	1:B:855:ARG:HB3	2.18	0.43
1:B:874:TYR:C	1:B:874:TYR:HD1	2.26	0.43
1:C:812:MET:O	1:C:813:LYS:C	2.62	0.43
1:C:874:TYR:C	1:C:874:TYR:HD1	2.26	0.43
1:C:901:MET:HE1	1:C:956:MET:CE	2.48	0.43
1:D:768:ASP:O	1:D:771:VAL:CG1	2.65	0.43
1:G:920:ILE:CG2	1:G:921:THR:N	2.79	0.43
1:H:332:VAL:HG22	1:H:334:LYS:HE2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:277:ASP:O	1:I:278:ILE:C	2.59	0.43
1:I:319:ARG:HG2	1:I:320:GLY:N	2.30	0.43
1:I:332:VAL:HG22	1:I:334:LYS:HE2	2.00	0.43
1:I:842:LYS:HE2	1:I:846:GLU:HG3	2.01	0.43
1:J:783:ILE:O	1:J:790:ALA:HB3	2.19	0.43
1:K:899:VAL:HG21	1:L:841:ASP:HB3	2.00	0.43
1:L:277:ASP:O	1:L:278:ILE:C	2.59	0.43
1:M:739:UNK:O	1:M:740:UNK:CB	2.65	0.43
1:P:746:UNK:O	1:P:792:LEU:CD1	2.65	0.43
1:P:842:LYS:HE2	1:P:846:GLU:HG3	2.01	0.43
1:A:283:VAL:C	1:A:285:SER:N	2.74	0.43
1:B:746:UNK:O	1:B:792:LEU:CD1	2.65	0.43
1:D:739:UNK:O	1:D:740:UNK:CB	2.65	0.43
1:D:849:ARG:HD3	1:D:853:ARG:HG3	2.00	0.43
1:D:860:GLU:C	1:D:862:VAL:N	2.74	0.43
1:E:783:ILE:O	1:E:790:ALA:HB3	2.19	0.43
1:E:902:ARG:HH11	1:E:902:ARG:CG	2.30	0.43
1:F:768:ASP:O	1:F:771:VAL:CG1	2.65	0.43
1:F:849:ARG:HD3	1:F:853:ARG:HG3	2.00	0.43
1:G:842:LYS:HE2	1:G:846:GLU:HG3	2.01	0.43
1:I:337:ILE:O	1:I:338:LEU:C	2.59	0.43
1:I:746:UNK:O	1:I:792:LEU:CD1	2.65	0.43
1:I:783:ILE:O	1:I:790:ALA:HB3	2.18	0.43
1:J:808:ARG:NH1	1:J:808:ARG:CB	2.77	0.43
1:K:812:MET:O	1:K:813:LYS:C	2.62	0.43
1:K:902:ARG:HH11	1:L:844:ASP:CG	2.21	0.43
1:L:337:ILE:O	1:L:338:LEU:C	2.59	0.43
1:L:783:ILE:O	1:L:790:ALA:HB3	2.19	0.43
1:M:783:ILE:O	1:M:790:ALA:HB3	2.19	0.43
1:M:901:MET:HE1	1:M:956:MET:CE	2.48	0.43
1:N:843:ILE:O	1:N:847:VAL:HG23	2.18	0.43
1:N:852:LEU:O	1:N:855:ARG:HB3	2.18	0.43
1:O:842:LYS:HE2	1:O:846:GLU:HG3	2.01	0.43
1:O:843:ILE:O	1:O:847:VAL:HG23	2.18	0.43
1:O:849:ARG:HD3	1:O:853:ARG:HG3	2.00	0.43
1:O:891:MET:HG3	1:P:852:LEU:CB	2.48	0.43
1:O:902:ARG:HH11	1:O:902:ARG:CG	2.30	0.43
1:P:290:ILE:C	1:P:290:ILE:CD1	2.84	0.43
1:B:277:ASP:O	1:B:278:ILE:C	2.59	0.43
1:C:783:ILE:O	1:C:790:ALA:HB3	2.19	0.43
1:F:341:VAL:HG12	1:F:757:LEU:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:809:PHE:N	1:K:809:PHE:CD1	2.84	0.43
1:K:899:VAL:CG2	1:L:841:ASP:HB3	2.49	0.43
1:M:805:LYS:N	1:M:818:GLN:O	2.32	0.43
1:M:902:ARG:HH11	1:M:902:ARG:CG	2.30	0.43
1:O:341:VAL:HG12	1:O:757:LEU:HD11	2.01	0.43
1:B:920:ILE:CG2	1:B:921:THR:N	2.79	0.43
1:C:746:UNK:O	1:C:792:LEU:CD1	2.65	0.43
1:C:842:LYS:HE2	1:C:846:GLU:HG3	2.01	0.43
1:C:902:ARG:HH11	1:C:902:ARG:CG	2.30	0.43
1:D:884:PRO:HA	1:D:942:PRO:C	2.44	0.43
1:E:746:UNK:O	1:E:792:LEU:CD1	2.65	0.43
1:E:886:ILE:HD12	1:E:886:ILE:H	1.82	0.43
1:F:843:ILE:O	1:F:847:VAL:HG23	2.18	0.43
1:G:901:MET:HE1	1:G:956:MET:CE	2.48	0.43
1:J:843:ILE:O	1:J:847:VAL:HG23	2.18	0.43
1:K:887:SER:C	1:K:889:GLU:N	2.67	0.43
1:L:295:GLU:CD	1:L:295:GLU:N	2.70	0.43
1:M:812:MET:O	1:M:813:LYS:C	2.62	0.43
1:N:808:ARG:NH1	1:N:808:ARG:CB	2.77	0.43
1:N:902:ARG:HH11	1:N:902:ARG:CG	2.30	0.43
1:O:812:MET:SD	1:O:812:MET:N	2.78	0.43
1:O:884:PRO:HA	1:O:942:PRO:C	2.44	0.43
1:A:848:ALA:HB2	1:H:898:TYR:CD2	2.53	0.43
1:B:884:PRO:HA	1:B:942:PRO:C	2.44	0.43
1:B:902:ARG:HH11	1:B:902:ARG:CG	2.30	0.43
1:C:341:VAL:HG12	1:C:757:LEU:HD11	2.01	0.43
1:D:842:LYS:HE2	1:D:846:GLU:HG3	2.01	0.43
1:E:920:ILE:CG2	1:E:921:THR:N	2.79	0.43
1:F:283:VAL:C	1:F:285:SER:N	2.75	0.43
1:G:312:LEU:HD21	1:H:858:GLU:CB	2.48	0.43
1:G:822:PRO:HA	1:G:823:PRO:HD2	1.81	0.43
1:H:812:MET:O	1:H:813:LYS:C	2.62	0.43
1:I:812:MET:O	1:I:813:LYS:C	2.62	0.43
1:L:341:VAL:HG12	1:L:757:LEU:HD11	2.01	0.43
1:L:874:TYR:C	1:L:874:TYR:HD1	2.26	0.43
1:N:341:VAL:HG12	1:N:757:LEU:HD11	2.01	0.43
1:A:792:LEU:HD22	1:P:792:LEU:CD2	2.46	0.43
1:A:843:ILE:O	1:A:847:VAL:HG23	2.18	0.43
1:D:785:LYS:CB	1:M:785:LYS:CB	2.59	0.43
1:D:805:LYS:N	1:D:818:GLN:O	2.32	0.43
1:D:886:ILE:HD12	1:D:886:ILE:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:341:VAL:HG12	1:G:757:LEU:HD11	2.01	0.43
1:K:884:PRO:HA	1:K:942:PRO:C	2.44	0.43
1:M:341:VAL:HG12	1:M:757:LEU:HD11	2.01	0.43
1:M:884:PRO:HA	1:M:942:PRO:C	2.44	0.43
1:N:842:LYS:HE2	1:N:846:GLU:HG3	2.01	0.43
1:O:874:TYR:C	1:O:874:TYR:HD1	2.27	0.43
1:B:898:TYR:CB	1:B:925:LEU:HD23	2.49	0.43
1:C:785:LYS:CG	1:N:785:LYS:CG	2.83	0.43
1:C:920:ILE:CG2	1:C:921:THR:N	2.79	0.43
1:D:268:ILE:O	1:D:271:GLU:HB2	2.19	0.43
1:D:783:ILE:O	1:D:790:ALA:HB3	2.18	0.43
1:G:783:ILE:O	1:G:790:ALA:HB3	2.19	0.43
1:H:842:LYS:HE2	1:H:846:GLU:HG3	2.01	0.43
1:J:268:ILE:O	1:J:271:GLU:HB2	2.19	0.43
1:O:278:ILE:HG23	1:O:279:VAL:H	1.84	0.43
1:O:316:THR:CB	1:P:339:ARG:HG2	2.47	0.43
1:P:812:MET:O	1:P:813:LYS:C	2.62	0.43
1:A:746:UNK:O	1:A:792:LEU:CD1	2.65	0.42
1:A:842:LYS:HE2	1:A:846:GLU:HG3	2.01	0.42
1:A:848:ALA:HB2	1:H:898:TYR:HD2	1.83	0.42
1:B:812:MET:O	1:B:813:LYS:C	2.62	0.42
1:B:822:PRO:HA	1:B:823:PRO:HD2	1.80	0.42
1:C:730:UNK:CB	1:O:729:UNK:CA	2.97	0.42
1:C:791:THR:O	1:N:738:UNK:HA	2.19	0.42
1:E:268:ILE:O	1:E:271:GLU:HB2	2.19	0.42
1:E:812:MET:O	1:E:813:LYS:C	2.62	0.42
1:F:884:PRO:HA	1:F:942:PRO:C	2.44	0.42
1:G:337:ILE:O	1:G:338:LEU:C	2.59	0.42
1:G:836:ILE:HD11	1:G:965:MET:CG	2.49	0.42
1:H:809:PHE:C	1:H:811:ARG:N	2.77	0.42
1:H:836:ILE:HD11	1:H:965:MET:CG	2.49	0.42
1:H:898:TYR:CB	1:H:925:LEU:HD23	2.49	0.42
1:I:278:ILE:HG23	1:I:279:VAL:H	1.84	0.42
1:J:341:VAL:HG12	1:J:757:LEU:HD11	2.01	0.42
1:K:842:LYS:HE2	1:K:846:GLU:HG3	2.01	0.42
1:K:902:ARG:HH11	1:K:902:ARG:CG	2.30	0.42
1:N:849:ARG:HD3	1:N:853:ARG:HG3	2.00	0.42
1:P:783:ILE:O	1:P:790:ALA:HB3	2.19	0.42
1:P:831:LEU:HD22	1:P:959:THR:HG21	1.99	0.42
1:P:874:TYR:C	1:P:874:TYR:HD1	2.26	0.42
1:P:884:PRO:HA	1:P:942:PRO:C	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:841:ASP:O	1:A:842:LYS:C	2.62	0.42
1:B:836:ILE:HD11	1:B:965:MET:CG	2.49	0.42
1:B:929:ILE:CD1	1:C:852:LEU:CD1	2.97	0.42
1:C:332:VAL:HG22	1:C:334:LYS:HE2	2.00	0.42
1:C:843:ILE:O	1:C:847:VAL:HG23	2.18	0.42
1:E:842:LYS:HE2	1:E:846:GLU:HG3	2.01	0.42
1:G:789:THR:H	1:J:740:UNK:CA	2.33	0.42
1:G:812:MET:O	1:G:813:LYS:C	2.62	0.42
1:G:958:TYR:O	1:G:959:THR:C	2.63	0.42
1:H:785:LYS:CG	1:I:785:LYS:HB3	2.49	0.42
1:H:884:PRO:HA	1:H:942:PRO:C	2.44	0.42
1:I:341:VAL:HG12	1:I:757:LEU:HD11	2.01	0.42
1:M:849:ARG:HD3	1:M:853:ARG:HG3	2.00	0.42
1:O:268:ILE:O	1:O:271:GLU:HB2	2.19	0.42
1:A:783:ILE:O	1:A:790:ALA:HB3	2.18	0.42
1:A:844:ASP:CG	1:H:902:ARG:HH11	2.25	0.42
1:C:809:PHE:C	1:C:811:ARG:N	2.77	0.42
1:C:849:ARG:HD3	1:C:853:ARG:HG3	2.00	0.42
1:C:958:TYR:O	1:C:959:THR:C	2.63	0.42
1:D:809:PHE:C	1:D:811:ARG:N	2.77	0.42
1:D:852:LEU:O	1:D:855:ARG:HB3	2.17	0.42
1:E:763:LYS:HB3	1:E:763:LYS:HE2	1.89	0.42
1:E:805:LYS:N	1:E:818:GLN:O	2.32	0.42
1:F:842:LYS:HE2	1:F:846:GLU:HG3	2.01	0.42
1:F:958:TYR:O	1:F:959:THR:C	2.62	0.42
1:G:332:VAL:HG22	1:G:334:LYS:HE2	2.00	0.42
1:H:901:MET:HE1	1:H:956:MET:CE	2.48	0.42
1:I:268:ILE:O	1:I:271:GLU:HB2	2.19	0.42
1:J:842:LYS:HE2	1:J:846:GLU:HG3	2.01	0.42
1:K:901:MET:HE1	1:K:956:MET:CE	2.48	0.42
1:L:822:PRO:HA	1:L:823:PRO:HD2	1.80	0.42
1:N:739:UNK:O	1:N:740:UNK:CB	2.65	0.42
1:N:812:MET:O	1:N:813:LYS:C	2.62	0.42
1:N:854:VAL:HG21	1:N:862:VAL:HG11	2.02	0.42
1:N:874:TYR:C	1:N:874:TYR:HD1	2.26	0.42
1:N:898:TYR:CB	1:N:925:LEU:HD23	2.49	0.42
1:O:836:ILE:HD11	1:O:965:MET:CG	2.49	0.42
1:P:332:VAL:HG22	1:P:334:LYS:HE2	2.00	0.42
1:A:898:TYR:CB	1:A:925:LEU:HD23	2.49	0.42
1:B:317:ARG:CG	1:B:318:LEU:N	2.83	0.42
1:B:854:VAL:HG21	1:B:862:VAL:HG11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:898:TYR:CB	1:C:925:LEU:HD23	2.49	0.42
1:D:812:MET:O	1:D:813:LYS:C	2.62	0.42
1:D:836:ILE:HD11	1:D:965:MET:CG	2.49	0.42
1:E:317:ARG:CG	1:E:318:LEU:N	2.83	0.42
1:E:740:UNK:C	1:L:789:THR:HG1	2.27	0.42
1:E:836:ILE:HD11	1:E:965:MET:CG	2.49	0.42
1:F:278:ILE:HG23	1:F:279:VAL:H	1.84	0.42
1:F:812:MET:O	1:F:813:LYS:C	2.62	0.42
1:G:843:ILE:O	1:G:847:VAL:HG23	2.18	0.42
1:H:268:ILE:O	1:H:271:GLU:HB2	2.19	0.42
1:H:278:ILE:HG23	1:H:279:VAL:H	1.84	0.42
1:H:785:LYS:HB3	1:I:785:LYS:HB3	2.01	0.42
1:H:805:LYS:N	1:H:818:GLN:O	2.32	0.42
1:H:843:ILE:O	1:H:847:VAL:HG23	2.18	0.42
1:H:849:ARG:HD3	1:H:853:ARG:HG3	2.00	0.42
1:I:293:TYR:O	1:I:297:LYS:HG3	2.20	0.42
1:I:874:TYR:C	1:I:874:TYR:HD1	2.27	0.42
1:J:317:ARG:CG	1:J:318:LEU:N	2.83	0.42
1:J:812:MET:SD	1:J:812:MET:N	2.78	0.42
1:J:822:PRO:HA	1:J:823:PRO:HD2	1.81	0.42
1:K:290:ILE:C	1:K:290:ILE:CD1	2.84	0.42
1:L:332:VAL:HG22	1:L:334:LYS:HE2	2.00	0.42
1:M:809:PHE:C	1:M:811:ARG:N	2.78	0.42
1:N:765:SER:C	1:N:767:ARG:N	2.78	0.42
1:O:887:SER:O	1:O:888:GLU:C	2.63	0.42
1:O:958:TYR:O	1:O:959:THR:C	2.62	0.42
1:P:849:ARG:HD3	1:P:853:ARG:HG3	2.00	0.42
1:A:278:ILE:HG23	1:A:279:VAL:H	1.84	0.42
1:B:849:ARG:HD3	1:B:853:ARG:HG3	2.00	0.42
1:E:841:ASP:O	1:E:842:LYS:C	2.62	0.42
1:E:884:PRO:HA	1:E:942:PRO:C	2.44	0.42
1:F:854:VAL:HG21	1:F:862:VAL:HG11	2.02	0.42
1:H:308:VAL:HG13	1:H:309:SER:H	1.85	0.42
1:H:317:ARG:CG	1:H:318:LEU:N	2.83	0.42
1:H:746:UNK:O	1:H:792:LEU:CD1	2.65	0.42
1:H:765:SER:C	1:H:767:ARG:N	2.78	0.42
1:H:854:VAL:HG21	1:H:862:VAL:HG11	2.02	0.42
1:I:310:ARG:CZ	1:J:857:GLY:O	2.66	0.42
1:I:729:UNK:O	1:I:730:UNK:O	2.38	0.42
1:J:746:UNK:O	1:J:792:LEU:CD1	2.65	0.42
1:J:812:MET:O	1:J:813:LYS:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:849:ARG:HD3	1:J:853:ARG:HG3	2.00	0.42
1:J:887:SER:O	1:J:888:GLU:C	2.63	0.42
1:J:958:TYR:O	1:J:959:THR:C	2.62	0.42
1:K:836:ILE:HD11	1:K:965:MET:CG	2.49	0.42
1:L:779:GLN:C	1:L:794:ALA:HB3	2.45	0.42
1:L:812:MET:O	1:L:813:LYS:C	2.62	0.42
1:L:841:ASP:O	1:L:842:LYS:C	2.62	0.42
1:L:849:ARG:HD3	1:L:853:ARG:HG3	2.00	0.42
1:L:920:ILE:CG2	1:L:921:THR:N	2.79	0.42
1:M:765:SER:C	1:M:767:ARG:N	2.78	0.42
1:M:887:SER:O	1:M:888:GLU:C	2.63	0.42
1:M:920:ILE:CG2	1:M:921:THR:N	2.79	0.42
1:N:332:VAL:HG22	1:N:334:LYS:HE2	2.00	0.42
1:N:746:UNK:O	1:N:792:LEU:CD1	2.65	0.42
1:N:783:ILE:N	1:N:783:ILE:CD1	2.79	0.42
1:N:836:ILE:HD11	1:N:965:MET:CG	2.49	0.42
1:N:841:ASP:O	1:N:842:LYS:C	2.62	0.42
1:N:884:PRO:HA	1:N:942:PRO:C	2.44	0.42
1:O:765:SER:C	1:O:767:ARG:N	2.78	0.42
1:O:898:TYR:CB	1:O:925:LEU:HD23	2.49	0.42
1:P:729:UNK:O	1:P:730:UNK:O	2.38	0.42
1:P:841:ASP:O	1:P:842:LYS:C	2.62	0.42
1:A:809:PHE:C	1:A:811:ARG:N	2.77	0.42
1:B:283:VAL:CG2	1:B:284:ASP:N	2.83	0.42
1:B:308:VAL:HG13	1:B:309:SER:H	1.85	0.42
1:B:729:UNK:O	1:B:730:UNK:O	2.38	0.42
1:B:860:GLU:C	1:B:862:VAL:N	2.74	0.42
1:B:861:VAL:O	1:B:861:VAL:HG12	2.20	0.42
1:D:854:VAL:HG21	1:D:862:VAL:HG11	2.02	0.42
1:E:293:TYR:O	1:E:297:LYS:HG3	2.20	0.42
1:E:849:ARG:HD3	1:E:853:ARG:HG3	2.00	0.42
1:E:861:VAL:O	1:E:861:VAL:HG12	2.20	0.42
1:G:884:PRO:HA	1:G:942:PRO:C	2.44	0.42
1:H:874:TYR:C	1:H:874:TYR:HD1	2.26	0.42
1:I:779:GLN:C	1:I:794:ALA:HB3	2.45	0.42
1:K:278:ILE:HG23	1:K:279:VAL:H	1.84	0.42
1:K:809:PHE:C	1:K:811:ARG:N	2.78	0.42
1:K:958:TYR:O	1:K:959:THR:C	2.62	0.42
1:M:278:ILE:HG23	1:M:279:VAL:H	1.84	0.42
1:M:841:ASP:O	1:M:842:LYS:C	2.62	0.42
1:N:887:SER:O	1:N:888:GLU:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:958:TYR:O	1:N:959:THR:C	2.62	0.42
1:O:729:UNK:O	1:O:730:UNK:O	2.38	0.42
1:O:779:GLN:C	1:O:794:ALA:HB3	2.45	0.42
1:P:765:SER:C	1:P:767:ARG:N	2.78	0.42
1:A:268:ILE:O	1:A:271:GLU:HB2	2.19	0.42
1:A:785:LYS:CG	1:P:785:LYS:HB3	2.49	0.42
1:B:887:SER:O	1:B:888:GLU:C	2.63	0.42
1:C:729:UNK:O	1:C:730:UNK:O	2.38	0.42
1:C:809:PHE:HB2	1:C:818:GLN:NE2	2.35	0.42
1:D:278:ILE:HG23	1:D:279:VAL:H	1.84	0.42
1:D:317:ARG:CG	1:D:318:LEU:N	2.83	0.42
1:D:809:PHE:HB2	1:D:818:GLN:NE2	2.35	0.42
1:E:809:PHE:C	1:E:811:ARG:N	2.77	0.42
1:F:765:SER:C	1:F:767:ARG:N	2.78	0.42
1:F:836:ILE:HD11	1:F:965:MET:CG	2.49	0.42
1:G:809:PHE:C	1:G:811:ARG:N	2.78	0.42
1:H:729:UNK:O	1:H:730:UNK:O	2.38	0.42
1:H:886:ILE:HD12	1:H:886:ILE:H	1.82	0.42
1:I:772:ILE:O	1:I:773:HIS:C	2.63	0.42
1:J:729:UNK:O	1:J:730:UNK:O	2.38	0.42
1:J:779:GLN:C	1:J:794:ALA:HB3	2.45	0.42
1:J:929:ILE:CD1	1:K:852:LEU:CD1	2.94	0.42
1:K:283:VAL:CG2	1:K:284:ASP:N	2.83	0.42
1:K:293:TYR:O	1:K:297:LYS:HG3	2.20	0.42
1:K:765:SER:C	1:K:767:ARG:N	2.78	0.42
1:K:854:VAL:HG21	1:K:862:VAL:HG11	2.02	0.42
1:L:765:SER:C	1:L:767:ARG:N	2.78	0.42
1:L:884:PRO:HA	1:L:942:PRO:C	2.44	0.42
1:M:308:VAL:HG13	1:M:309:SER:H	1.85	0.42
1:M:317:ARG:CG	1:M:318:LEU:N	2.83	0.42
1:N:783:ILE:O	1:N:790:ALA:HB3	2.18	0.42
1:A:312:LEU:HD11	1:B:858:GLU:HA	2.01	0.42
1:B:763:LYS:HE2	1:B:763:LYS:HB3	1.89	0.42
1:B:809:PHE:HB2	1:B:818:GLN:NE2	2.35	0.42
1:C:268:ILE:O	1:C:271:GLU:HB2	2.19	0.42
1:C:861:VAL:O	1:C:861:VAL:HG12	2.20	0.42
1:C:953:ILE:HG12	1:C:953:ILE:H	1.61	0.42
1:D:730:UNK:N	1:N:730:UNK:CB	2.82	0.42
1:D:956:MET:HA	1:D:959:THR:HG23	2.02	0.42
1:F:763:LYS:HE2	1:F:763:LYS:HB3	1.89	0.42
1:G:278:ILE:HG23	1:G:279:VAL:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:312:LEU:HD22	1:H:858:GLU:CB	2.49	0.42
1:G:887:SER:O	1:G:888:GLU:C	2.63	0.42
1:H:861:VAL:O	1:H:861:VAL:HG12	2.20	0.42
1:I:765:SER:C	1:I:767:ARG:N	2.78	0.42
1:I:809:PHE:HB2	1:I:818:GLN:NE2	2.35	0.42
1:I:884:PRO:HA	1:I:942:PRO:C	2.44	0.42
1:K:317:ARG:CG	1:K:318:LEU:N	2.83	0.42
1:K:874:TYR:C	1:K:874:TYR:HD1	2.27	0.42
1:M:958:TYR:O	1:M:959:THR:C	2.62	0.42
1:N:767:ARG:O	1:N:770:SER:OG	2.34	0.42
1:N:809:PHE:C	1:N:811:ARG:N	2.77	0.42
1:O:809:PHE:C	1:O:811:ARG:N	2.78	0.42
1:O:841:ASP:O	1:O:842:LYS:C	2.62	0.42
1:O:854:VAL:HG21	1:O:862:VAL:HG11	2.02	0.42
1:P:293:TYR:O	1:P:297:LYS:HG3	2.20	0.42
1:P:958:TYR:O	1:P:959:THR:C	2.62	0.42
1:A:849:ARG:HD3	1:A:853:ARG:HG3	2.00	0.42
1:C:779:GLN:C	1:C:794:ALA:HB3	2.45	0.42
1:D:293:TYR:O	1:D:297:LYS:HG3	2.20	0.42
1:D:815:PRO:O	1:D:819:ILE:HG13	2.20	0.42
1:D:861:VAL:O	1:D:861:VAL:HG12	2.20	0.42
1:E:283:VAL:CG2	1:E:284:ASP:N	2.83	0.42
1:F:779:GLN:C	1:F:794:ALA:HB3	2.45	0.42
1:F:783:ILE:O	1:F:790:ALA:HB3	2.19	0.42
1:F:956:MET:HA	1:F:959:THR:HG23	2.02	0.42
1:H:293:TYR:O	1:H:297:LYS:HG3	2.20	0.42
1:H:783:ILE:O	1:H:790:ALA:HB3	2.19	0.42
1:I:861:VAL:O	1:I:861:VAL:HG12	2.20	0.42
1:J:809:PHE:C	1:J:811:ARG:N	2.78	0.42
1:K:268:ILE:O	1:K:271:GLU:HB2	2.19	0.42
1:K:783:ILE:O	1:K:790:ALA:HB3	2.19	0.42
1:L:293:TYR:O	1:L:297:LYS:HG3	2.20	0.42
1:L:772:ILE:O	1:L:773:HIS:C	2.63	0.42
1:L:805:LYS:N	1:L:818:GLN:O	2.32	0.42
1:L:809:PHE:HB2	1:L:818:GLN:NE2	2.35	0.42
1:L:958:TYR:O	1:L:959:THR:C	2.63	0.42
1:M:861:VAL:O	1:M:861:VAL:HG12	2.20	0.42
1:N:809:PHE:HB2	1:N:818:GLN:NE2	2.35	0.42
1:O:812:MET:O	1:O:813:LYS:C	2.62	0.42
1:P:772:ILE:O	1:P:773:HIS:C	2.63	0.42
1:P:809:PHE:HB2	1:P:818:GLN:NE2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:779:GLN:C	1:A:794:ALA:HB3	2.45	0.42
1:A:809:PHE:HB2	1:A:818:GLN:NE2	2.35	0.42
1:A:897:TYR:O	1:A:898:TYR:C	2.63	0.42
1:A:958:TYR:O	1:A:959:THR:C	2.62	0.42
1:B:268:ILE:O	1:B:271:GLU:HB2	2.19	0.42
1:B:293:TYR:O	1:B:297:LYS:HG3	2.20	0.42
1:B:729:UNK:O	1:P:729:UNK:C	2.63	0.42
1:D:740:UNK:HA	1:M:789:THR:OG1	2.19	0.42
1:F:772:ILE:O	1:F:773:HIS:C	2.63	0.42
1:G:283:VAL:CG2	1:G:284:ASP:N	2.83	0.42
1:G:785:LYS:HG2	1:J:785:LYS:CG	2.50	0.42
1:H:341:VAL:HG12	1:H:757:LEU:HD11	2.01	0.42
1:H:887:SER:O	1:H:888:GLU:C	2.63	0.42
1:I:283:VAL:CG2	1:I:284:ASP:N	2.83	0.42
1:I:822:PRO:HA	1:I:823:PRO:HD2	1.81	0.42
1:K:308:VAL:HG13	1:K:309:SER:H	1.85	0.42
1:L:283:VAL:CG2	1:L:284:ASP:N	2.83	0.42
1:L:729:UNK:O	1:L:730:UNK:O	2.38	0.42
1:L:854:VAL:HG21	1:L:862:VAL:HG11	2.02	0.42
1:M:268:ILE:O	1:M:271:GLU:HB2	2.19	0.42
1:M:293:TYR:O	1:M:297:LYS:HG3	2.20	0.42
1:N:268:ILE:O	1:N:271:GLU:HB2	2.19	0.42
1:N:278:ILE:HG23	1:N:279:VAL:H	1.84	0.42
1:P:809:PHE:C	1:P:811:ARG:N	2.77	0.42
1:A:283:VAL:CG2	1:A:284:ASP:N	2.83	0.41
1:C:278:ILE:HG23	1:C:279:VAL:H	1.84	0.41
1:C:283:VAL:CG2	1:C:284:ASP:N	2.83	0.41
1:C:317:ARG:CG	1:C:318:LEU:N	2.83	0.41
1:C:836:ILE:HD11	1:C:965:MET:CG	2.49	0.41
1:E:341:VAL:HG12	1:E:757:LEU:HD11	2.01	0.41
1:E:887:SER:O	1:E:888:GLU:C	2.63	0.41
1:F:729:UNK:O	1:F:730:UNK:O	2.38	0.41
1:F:809:PHE:C	1:F:811:ARG:N	2.77	0.41
1:G:841:ASP:O	1:G:842:LYS:C	2.62	0.41
1:G:861:VAL:HG12	1:G:861:VAL:O	2.20	0.41
1:G:874:TYR:C	1:G:874:TYR:HD1	2.26	0.41
1:H:809:PHE:HB2	1:H:818:GLN:NE2	2.35	0.41
1:H:841:ASP:O	1:H:842:LYS:C	2.62	0.41
1:I:809:PHE:C	1:I:811:ARG:N	2.78	0.41
1:I:836:ILE:HD11	1:I:965:MET:CG	2.49	0.41
1:I:902:ARG:HG2	1:J:844:ASP:CG	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:278:ILE:HG23	1:J:279:VAL:H	1.84	0.41
1:J:836:ILE:HD11	1:J:965:MET:CG	2.49	0.41
1:K:332:VAL:HG22	1:K:334:LYS:HE2	2.00	0.41
1:K:809:PHE:HB2	1:K:818:GLN:NE2	2.35	0.41
1:K:815:PRO:O	1:K:819:ILE:HG13	2.20	0.41
1:L:278:ILE:HG23	1:L:279:VAL:H	1.84	0.41
1:L:836:ILE:HD11	1:L:965:MET:CG	2.49	0.41
1:L:887:SER:O	1:L:888:GLU:C	2.63	0.41
1:M:836:ILE:HD11	1:M:965:MET:CG	2.49	0.41
1:M:842:LYS:HE2	1:M:846:GLU:HG3	2.01	0.41
1:M:874:TYR:C	1:M:874:TYR:HD1	2.27	0.41
1:O:746:UNK:O	1:O:792:LEU:CD1	2.65	0.41
1:O:809:PHE:HB2	1:O:818:GLN:NE2	2.35	0.41
1:P:319:ARG:HG2	1:P:320:GLY:N	2.31	0.41
1:P:815:PRO:O	1:P:819:ILE:HG13	2.20	0.41
1:A:739:UNK:O	1:A:740:UNK:CB	2.65	0.41
1:A:884:PRO:HA	1:A:942:PRO:C	2.44	0.41
1:B:341:VAL:HG12	1:B:757:LEU:HD11	2.01	0.41
1:B:958:TYR:O	1:B:959:THR:C	2.62	0.41
1:C:293:TYR:O	1:C:297:LYS:HG3	2.20	0.41
1:C:841:ASP:O	1:C:842:LYS:C	2.62	0.41
1:D:315:GLY:O	1:D:316:THR:C	2.63	0.41
1:D:332:VAL:HG22	1:D:334:LYS:HE2	2.00	0.41
1:D:729:UNK:O	1:D:730:UNK:O	2.38	0.41
1:D:765:SER:C	1:D:767:ARG:N	2.78	0.41
1:D:822:PRO:HA	1:D:823:PRO:HD2	1.81	0.41
1:D:902:ARG:HH11	1:D:902:ARG:CG	2.30	0.41
1:D:953:ILE:HG12	1:D:953:ILE:H	1.61	0.41
1:E:278:ILE:HG23	1:E:279:VAL:H	1.84	0.41
1:E:308:VAL:HG13	1:E:309:SER:H	1.85	0.41
1:F:268:ILE:O	1:F:271:GLU:HB2	2.19	0.41
1:F:317:ARG:CG	1:F:318:LEU:N	2.83	0.41
1:F:809:PHE:HB2	1:F:818:GLN:NE2	2.35	0.41
1:F:815:PRO:O	1:F:819:ILE:HG13	2.20	0.41
1:F:897:TYR:O	1:F:898:TYR:C	2.63	0.41
1:G:268:ILE:O	1:G:271:GLU:HB2	2.19	0.41
1:G:293:TYR:O	1:G:297:LYS:HG3	2.20	0.41
1:G:317:ARG:CG	1:G:318:LEU:N	2.83	0.41
1:G:765:SER:C	1:G:767:ARG:N	2.78	0.41
1:J:283:VAL:CG2	1:J:284:ASP:N	2.83	0.41
1:J:765:SER:C	1:J:767:ARG:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:805:LYS:N	1:J:818:GLN:O	2.32	0.41
1:J:815:PRO:O	1:J:819:ILE:HG13	2.20	0.41
1:K:729:UNK:O	1:K:730:UNK:O	2.38	0.41
1:K:861:VAL:O	1:K:861:VAL:HG12	2.20	0.41
1:L:809:PHE:C	1:L:811:ARG:N	2.78	0.41
1:M:958:TYR:C	1:M:960:LEU:N	2.78	0.41
1:N:729:UNK:O	1:N:730:UNK:O	2.38	0.41
1:O:315:GLY:O	1:O:316:THR:C	2.63	0.41
1:O:317:ARG:CG	1:O:318:LEU:N	2.83	0.41
1:O:763:LYS:HE2	1:O:763:LYS:HB3	1.89	0.41
1:P:854:VAL:HG21	1:P:862:VAL:HG11	2.02	0.41
1:P:861:VAL:O	1:P:861:VAL:HG12	2.20	0.41
1:P:897:TYR:O	1:P:898:TYR:C	2.63	0.41
1:A:315:GLY:O	1:A:316:THR:C	2.63	0.41
1:A:805:LYS:N	1:A:818:GLN:O	2.32	0.41
1:A:836:ILE:HD11	1:A:965:MET:CG	2.49	0.41
1:D:283:VAL:CG2	1:D:284:ASP:N	2.83	0.41
1:D:779:GLN:C	1:D:794:ALA:HB3	2.45	0.41
1:E:729:UNK:O	1:E:730:UNK:O	2.38	0.41
1:F:874:TYR:C	1:F:874:TYR:HD1	2.27	0.41
1:G:836:ILE:HD11	1:G:965:MET:CB	2.51	0.41
1:H:283:VAL:CG2	1:H:284:ASP:N	2.83	0.41
1:H:815:PRO:O	1:H:819:ILE:HG13	2.20	0.41
1:I:958:TYR:O	1:I:959:THR:C	2.62	0.41
1:J:841:ASP:O	1:J:842:LYS:C	2.62	0.41
1:K:822:PRO:HA	1:K:823:PRO:HD2	1.81	0.41
1:L:842:LYS:HE2	1:L:846:GLU:HG3	2.01	0.41
1:M:729:UNK:O	1:M:730:UNK:O	2.38	0.41
1:M:779:GLN:C	1:M:794:ALA:HB3	2.45	0.41
1:O:772:ILE:O	1:O:773:HIS:C	2.63	0.41
1:O:861:VAL:O	1:O:861:VAL:HG12	2.20	0.41
1:O:956:MET:HA	1:O:959:THR:HG23	2.02	0.41
1:P:341:VAL:HG12	1:P:757:LEU:HD11	2.01	0.41
1:A:293:TYR:O	1:A:297:LYS:HG3	2.20	0.41
1:B:809:PHE:C	1:B:811:ARG:N	2.77	0.41
1:B:836:ILE:HD11	1:B:965:MET:CB	2.51	0.41
1:C:822:PRO:HA	1:C:823:PRO:HD2	1.81	0.41
1:C:884:PRO:HA	1:C:942:PRO:C	2.44	0.41
1:D:308:VAL:HG13	1:D:309:SER:H	1.85	0.41
1:D:341:VAL:HG12	1:D:757:LEU:HD11	2.01	0.41
1:D:772:ILE:O	1:D:773:HIS:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:958:TYR:O	1:D:959:THR:C	2.63	0.41
1:E:284:ASP:CB	1:E:865:LYS:HG3	2.51	0.41
1:F:315:GLY:O	1:F:316:THR:C	2.63	0.41
1:F:861:VAL:HG12	1:F:861:VAL:O	2.20	0.41
1:G:809:PHE:HB2	1:G:818:GLN:NE2	2.35	0.41
1:H:772:ILE:O	1:H:773:HIS:C	2.63	0.41
1:H:836:ILE:HD11	1:H:965:MET:CB	2.51	0.41
1:H:958:TYR:O	1:H:959:THR:C	2.62	0.41
1:I:815:PRO:O	1:I:819:ILE:HG13	2.20	0.41
1:I:836:ILE:HD11	1:I:965:MET:CB	2.51	0.41
1:I:854:VAL:HG21	1:I:862:VAL:HG11	2.02	0.41
1:J:293:TYR:O	1:J:297:LYS:HG3	2.20	0.41
1:J:884:PRO:HA	1:J:942:PRO:C	2.44	0.41
1:K:841:ASP:O	1:K:842:LYS:C	2.62	0.41
1:L:836:ILE:HD11	1:L:965:MET:CB	2.51	0.41
1:M:772:ILE:O	1:M:773:HIS:C	2.63	0.41
1:N:308:VAL:HG13	1:N:309:SER:H	1.85	0.41
1:N:836:ILE:HD11	1:N:965:MET:CB	2.50	0.41
1:O:283:VAL:CG2	1:O:284:ASP:N	2.83	0.41
1:O:836:ILE:HD11	1:O:965:MET:CB	2.51	0.41
1:P:268:ILE:O	1:P:271:GLU:HB2	2.19	0.41
1:P:278:ILE:HG23	1:P:279:VAL:H	1.84	0.41
1:P:315:GLY:O	1:P:316:THR:C	2.63	0.41
1:A:772:ILE:O	1:A:773:HIS:C	2.63	0.41
1:A:815:PRO:O	1:A:819:ILE:HG13	2.20	0.41
1:B:772:ILE:O	1:B:773:HIS:C	2.63	0.41
1:B:805:LYS:N	1:B:818:GLN:O	2.32	0.41
1:B:897:TYR:O	1:B:898:TYR:C	2.63	0.41
1:C:739:UNK:O	1:C:740:UNK:CB	2.65	0.41
1:C:854:VAL:HG21	1:C:862:VAL:HG11	2.02	0.41
1:D:836:ILE:HD11	1:D:965:MET:CB	2.51	0.41
1:E:779:GLN:C	1:E:794:ALA:HB3	2.45	0.41
1:F:308:VAL:HG13	1:F:309:SER:H	1.85	0.41
1:F:825:LEU:C	1:F:825:LEU:HD23	2.46	0.41
1:F:841:ASP:O	1:F:842:LYS:C	2.62	0.41
1:H:284:ASP:CB	1:H:865:LYS:HG3	2.51	0.41
1:I:841:ASP:O	1:I:842:LYS:C	2.62	0.41
1:K:284:ASP:CB	1:K:865:LYS:HG3	2.51	0.41
1:K:848:ALA:O	1:K:852:LEU:HD22	2.21	0.41
1:L:315:GLY:O	1:L:316:THR:O	2.39	0.41
1:M:809:PHE:HB2	1:M:818:GLN:NE2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:854:VAL:HG21	1:M:862:VAL:HG11	2.02	0.41
1:M:899:VAL:HG23	1:N:841:ASP:HA	2.03	0.41
1:N:317:ARG:CG	1:N:318:LEU:N	2.83	0.41
1:P:284:ASP:CB	1:P:865:LYS:HG3	2.51	0.41
1:P:779:GLN:C	1:P:794:ALA:HB3	2.45	0.41
1:A:836:ILE:HD11	1:A:965:MET:CB	2.51	0.41
1:B:313:PRO:HG2	1:B:314:ASP:N	2.36	0.41
1:B:779:GLN:C	1:B:794:ALA:HB3	2.45	0.41
1:B:815:PRO:O	1:B:819:ILE:HG13	2.20	0.41
1:D:785:LYS:HB2	1:M:785:LYS:O	2.20	0.41
1:D:825:LEU:HD23	1:D:825:LEU:C	2.46	0.41
1:D:841:ASP:O	1:D:842:LYS:C	2.62	0.41
1:D:874:TYR:C	1:D:874:TYR:HD1	2.26	0.41
1:E:313:PRO:HG2	1:E:314:ASP:N	2.36	0.41
1:E:854:VAL:HG21	1:E:862:VAL:HG11	2.02	0.41
1:F:943:ILE:O	1:F:945:THR:N	2.54	0.41
1:G:313:PRO:HG2	1:G:314:ASP:N	2.36	0.41
1:G:779:GLN:C	1:G:794:ALA:HB3	2.45	0.41
1:H:779:GLN:C	1:H:794:ALA:HB3	2.45	0.41
1:I:308:VAL:HG13	1:I:309:SER:H	1.85	0.41
1:I:315:GLY:O	1:I:316:THR:C	2.63	0.41
1:I:315:GLY:O	1:I:316:THR:O	2.39	0.41
1:I:317:ARG:CG	1:I:318:LEU:N	2.83	0.41
1:I:897:TYR:O	1:I:898:TYR:C	2.63	0.41
1:I:929:ILE:CG1	1:J:852:LEU:CD1	2.97	0.41
1:K:315:GLY:O	1:K:316:THR:O	2.39	0.41
1:K:319:ARG:HG2	1:K:320:GLY:N	2.31	0.41
1:K:779:GLN:C	1:K:794:ALA:HB3	2.45	0.41
1:L:814:ASN:C	1:L:816:PHE:N	2.79	0.41
1:L:956:MET:HA	1:L:959:THR:HG23	2.02	0.41
1:M:284:ASP:CB	1:M:865:LYS:HG3	2.51	0.41
1:N:284:ASP:CB	1:N:865:LYS:HG3	2.51	0.41
1:N:812:MET:SD	1:N:812:MET:N	2.78	0.41
1:N:886:ILE:HD12	1:N:886:ILE:H	1.82	0.41
1:N:956:MET:HA	1:N:959:THR:HG23	2.02	0.41
1:O:319:ARG:HG2	1:O:320:GLY:N	2.31	0.41
1:O:828:ARG:N	1:O:828:ARG:HD2	2.31	0.41
1:P:283:VAL:CG2	1:P:284:ASP:N	2.83	0.41
1:P:317:ARG:CG	1:P:318:LEU:N	2.83	0.41
1:P:765:SER:O	1:P:766:ASP:C	2.64	0.41
1:P:943:ILE:O	1:P:945:THR:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:PRO:HG2	1:A:314:ASP:N	2.36	0.41
1:A:315:GLY:O	1:A:316:THR:O	2.39	0.41
1:A:317:ARG:CG	1:A:318:LEU:N	2.83	0.41
1:A:739:UNK:HA	1:A:744:UNK:O	2.21	0.41
1:A:765:SER:O	1:A:766:ASP:C	2.64	0.41
1:A:854:VAL:HG21	1:A:862:VAL:HG11	2.02	0.41
1:B:312:LEU:HD21	1:C:858:GLU:CB	2.51	0.41
1:C:848:ALA:O	1:C:852:LEU:HD22	2.21	0.41
1:D:958:TYR:C	1:D:960:LEU:N	2.78	0.41
1:E:814:ASN:C	1:E:816:PHE:N	2.79	0.41
1:E:836:ILE:HD11	1:E:965:MET:CB	2.51	0.41
1:E:943:ILE:O	1:E:945:THR:N	2.54	0.41
1:F:315:GLY:O	1:F:316:THR:O	2.39	0.41
1:G:729:UNK:O	1:G:730:UNK:O	2.38	0.41
1:J:814:ASN:C	1:J:816:PHE:N	2.79	0.41
1:K:341:VAL:HG12	1:K:757:LEU:HD11	2.01	0.41
1:L:739:UNK:HA	1:L:744:UNK:O	2.21	0.41
1:L:825:LEU:C	1:L:825:LEU:HD23	2.46	0.41
1:L:848:ALA:O	1:L:852:LEU:HD22	2.21	0.41
1:M:313:PRO:HG2	1:M:314:ASP:N	2.36	0.41
1:M:815:PRO:O	1:M:819:ILE:HG13	2.20	0.41
1:N:848:ALA:O	1:N:852:LEU:HD22	2.21	0.41
1:N:897:TYR:O	1:N:898:TYR:C	2.63	0.41
1:P:308:VAL:HG13	1:P:309:SER:H	1.85	0.41
1:P:836:ILE:HD11	1:P:965:MET:CG	2.49	0.41
1:A:763:LYS:HB3	1:A:763:LYS:HE2	1.89	0.41
1:B:315:GLY:O	1:B:316:THR:C	2.63	0.41
1:C:284:ASP:CB	1:C:865:LYS:HG3	2.51	0.41
1:C:765:SER:C	1:C:767:ARG:N	2.78	0.41
1:C:815:PRO:O	1:C:819:ILE:HG13	2.20	0.41
1:E:739:UNK:HA	1:E:744:UNK:O	2.21	0.41
1:F:316:THR:OG1	1:F:317:ARG:N	2.53	0.41
1:F:848:ALA:O	1:F:852:LEU:HD22	2.21	0.41
1:G:746:UNK:O	1:G:792:LEU:CD1	2.65	0.41
1:H:315:GLY:O	1:H:316:THR:C	2.63	0.41
1:I:739:UNK:HA	1:I:744:UNK:O	2.21	0.41
1:J:765:SER:O	1:J:766:ASP:C	2.64	0.41
1:J:772:ILE:O	1:J:773:HIS:C	2.63	0.41
1:J:848:ALA:O	1:J:852:LEU:HD22	2.21	0.41
1:J:854:VAL:HG21	1:J:862:VAL:HG11	2.02	0.41
1:K:814:ASN:C	1:K:816:PHE:N	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:739:UNK:HA	1:M:744:UNK:O	2.21	0.41
1:M:765:SER:O	1:M:766:ASP:C	2.64	0.41
1:N:765:SER:O	1:N:766:ASP:C	2.64	0.41
1:N:779:GLN:C	1:N:794:ALA:HB3	2.45	0.41
1:P:315:GLY:O	1:P:316:THR:O	2.39	0.41
1:A:284:ASP:CB	1:A:865:LYS:HG3	2.51	0.41
1:A:308:VAL:HG13	1:A:309:SER:H	1.85	0.41
1:A:316:THR:OG1	1:A:317:ARG:N	2.53	0.41
1:A:887:SER:O	1:A:888:GLU:C	2.63	0.41
1:B:765:SER:C	1:B:767:ARG:N	2.78	0.41
1:B:943:ILE:O	1:B:945:THR:N	2.54	0.41
1:C:812:MET:SD	1:C:812:MET:N	2.78	0.41
1:E:958:TYR:O	1:E:959:THR:C	2.62	0.41
1:F:814:ASN:C	1:F:816:PHE:N	2.79	0.41
1:F:836:ILE:HD11	1:F:965:MET:CB	2.51	0.41
1:G:334:LYS:HB2	1:G:334:LYS:HE3	1.95	0.41
1:G:854:VAL:HG21	1:G:862:VAL:HG11	2.02	0.41
1:I:312:LEU:HD21	1:J:858:GLU:HB3	2.02	0.41
1:I:313:PRO:HG2	1:I:314:ASP:N	2.36	0.41
1:I:943:ILE:O	1:I:945:THR:N	2.54	0.41
1:I:956:MET:HA	1:I:959:THR:HG23	2.02	0.41
1:J:315:GLY:O	1:J:316:THR:C	2.63	0.41
1:J:315:GLY:O	1:J:316:THR:O	2.39	0.41
1:J:836:ILE:HD11	1:J:965:MET:CB	2.51	0.41
1:J:903:LYS:N	1:J:903:LYS:CE	2.82	0.41
1:K:739:UNK:HA	1:K:744:UNK:O	2.21	0.41
1:K:765:SER:O	1:K:766:ASP:C	2.64	0.41
1:K:769:ARG:HH11	1:K:769:ARG:CG	2.33	0.41
1:K:772:ILE:O	1:K:773:HIS:C	2.63	0.41
1:K:825:LEU:C	1:K:825:LEU:HD23	2.46	0.41
1:K:899:VAL:HG23	1:L:841:ASP:CA	2.47	0.41
1:K:943:ILE:O	1:K:945:THR:N	2.54	0.41
1:L:268:ILE:O	1:L:271:GLU:HB2	2.19	0.41
1:L:317:ARG:CG	1:L:318:LEU:N	2.83	0.41
1:M:814:ASN:C	1:M:816:PHE:N	2.79	0.41
1:M:956:MET:HA	1:M:959:THR:HG23	2.02	0.41
1:N:313:PRO:HG2	1:N:314:ASP:N	2.36	0.41
1:N:815:PRO:O	1:N:819:ILE:HG13	2.20	0.41
1:O:293:TYR:O	1:O:297:LYS:HG3	2.20	0.41
1:A:825:LEU:HD23	1:A:825:LEU:C	2.46	0.41
1:A:848:ALA:O	1:A:852:LEU:HD22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:GLY:O	1:C:316:THR:O	2.39	0.41
1:D:315:GLY:O	1:D:316:THR:O	2.39	0.41
1:D:769:ARG:HH11	1:D:769:ARG:CG	2.33	0.41
1:E:315:GLY:O	1:E:316:THR:O	2.39	0.41
1:E:848:ALA:O	1:E:852:LEU:HD22	2.21	0.41
1:G:315:GLY:O	1:G:316:THR:O	2.39	0.41
1:G:860:GLU:C	1:G:862:VAL:N	2.74	0.41
1:G:956:MET:HA	1:G:959:THR:HG23	2.02	0.41
1:G:958:TYR:C	1:G:960:LEU:N	2.78	0.41
1:H:825:LEU:HD23	1:H:825:LEU:C	2.46	0.41
1:H:956:MET:HA	1:H:959:THR:HG23	2.02	0.41
1:J:739:UNK:HA	1:J:744:UNK:O	2.21	0.41
1:J:809:PHE:HB2	1:J:818:GLN:NE2	2.35	0.41
1:L:815:PRO:O	1:L:819:ILE:HG13	2.20	0.41
1:L:861:VAL:HG12	1:L:861:VAL:O	2.20	0.41
1:M:283:VAL:CG2	1:M:284:ASP:N	2.83	0.41
1:M:943:ILE:O	1:M:945:THR:N	2.54	0.41
1:N:283:VAL:CG2	1:N:284:ASP:N	2.83	0.41
1:N:330:PRO:HD3	1:N:807:GLY:O	2.21	0.41
1:A:729:UNK:O	1:A:730:UNK:O	2.38	0.40
1:A:861:VAL:O	1:A:861:VAL:HG12	2.20	0.40
1:B:765:SER:O	1:B:766:ASP:C	2.64	0.40
1:D:330:PRO:HD3	1:D:807:GLY:O	2.21	0.40
1:D:814:ASN:C	1:D:816:PHE:N	2.79	0.40
1:E:815:PRO:O	1:E:819:ILE:HG13	2.20	0.40
1:E:825:LEU:C	1:E:825:LEU:HD23	2.46	0.40
1:F:279:VAL:HG13	1:F:938:MET:CE	2.51	0.40
1:F:283:VAL:CG2	1:F:284:ASP:N	2.83	0.40
1:F:330:PRO:HD3	1:F:807:GLY:O	2.21	0.40
1:F:881:ASN:OD1	1:F:881:ASN:N	2.54	0.40
1:G:765:SER:O	1:G:766:ASP:C	2.64	0.40
1:H:958:TYR:C	1:H:960:LEU:N	2.78	0.40
1:I:317:ARG:NH2	1:I:779:GLN:CD	2.77	0.40
1:I:814:ASN:C	1:I:816:PHE:N	2.79	0.40
1:J:956:MET:HA	1:J:959:THR:HG23	2.02	0.40
1:K:313:PRO:HG2	1:K:314:ASP:N	2.36	0.40
1:K:836:ILE:HD11	1:K:965:MET:CB	2.51	0.40
1:K:956:MET:HA	1:K:959:THR:HG23	2.02	0.40
1:L:308:VAL:HG13	1:L:309:SER:H	1.85	0.40
1:L:765:SER:O	1:L:766:ASP:C	2.64	0.40
1:L:769:ARG:HH11	1:L:769:ARG:CG	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:886:ILE:HD12	1:L:886:ILE:H	1.82	0.40
1:M:825:LEU:HD23	1:M:825:LEU:C	2.46	0.40
1:N:293:TYR:O	1:N:297:LYS:HG3	2.20	0.40
1:N:316:THR:OG1	1:N:317:ARG:N	2.53	0.40
1:N:825:LEU:HD23	1:N:825:LEU:C	2.46	0.40
1:N:943:ILE:O	1:N:945:THR:N	2.54	0.40
1:A:848:ALA:O	1:A:852:LEU:CD2	2.70	0.40
1:B:812:MET:SD	1:B:812:MET:N	2.78	0.40
1:B:825:LEU:HD23	1:B:825:LEU:C	2.46	0.40
1:B:848:ALA:O	1:B:852:LEU:CD2	2.70	0.40
1:C:315:GLY:O	1:C:316:THR:C	2.63	0.40
1:E:765:SER:O	1:E:766:ASP:C	2.64	0.40
1:E:897:TYR:O	1:E:898:TYR:C	2.63	0.40
1:F:739:UNK:HA	1:F:744:UNK:O	2.21	0.40
1:G:929:ILE:HD11	1:H:852:LEU:CD1	2.52	0.40
1:H:330:PRO:HD3	1:H:807:GLY:O	2.21	0.40
1:I:356:UNK:C	1:I:357:UNK:O	2.70	0.40
1:J:284:ASP:CB	1:J:865:LYS:HG3	2.51	0.40
1:K:958:TYR:C	1:K:960:LEU:N	2.78	0.40
1:L:284:ASP:CB	1:L:865:LYS:HG3	2.51	0.40
1:L:313:PRO:HG2	1:L:314:ASP:N	2.36	0.40
1:M:836:ILE:HD11	1:M:965:MET:CB	2.51	0.40
1:M:881:ASN:OD1	1:M:881:ASN:N	2.54	0.40
1:N:315:GLY:O	1:N:316:THR:C	2.63	0.40
1:O:848:ALA:O	1:O:852:LEU:HD22	2.21	0.40
1:P:848:ALA:O	1:P:852:LEU:CD2	2.70	0.40
1:A:356:UNK:C	1:A:357:UNK:O	2.70	0.40
1:A:765:SER:C	1:A:767:ARG:N	2.78	0.40
1:A:891:MET:HE2	1:B:852:LEU:HB3	2.03	0.40
1:A:943:ILE:O	1:A:945:THR:N	2.54	0.40
1:B:317:ARG:NH2	1:B:779:GLN:CD	2.77	0.40
1:B:841:ASP:O	1:B:842:LYS:C	2.62	0.40
1:C:739:UNK:HA	1:C:744:UNK:O	2.21	0.40
1:C:765:SER:O	1:C:766:ASP:C	2.64	0.40
1:C:825:LEU:HD23	1:C:825:LEU:C	2.46	0.40
1:C:848:ALA:O	1:C:852:LEU:CD2	2.70	0.40
1:C:958:TYR:C	1:C:960:LEU:N	2.78	0.40
1:E:315:GLY:O	1:E:316:THR:C	2.63	0.40
1:E:765:SER:C	1:E:767:ARG:N	2.78	0.40
1:E:772:ILE:O	1:E:773:HIS:C	2.63	0.40
1:E:956:MET:HA	1:E:959:THR:HG23	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:284:ASP:CB	1:F:865:LYS:HG3	2.51	0.40
1:F:293:TYR:O	1:F:297:LYS:HG3	2.20	0.40
1:F:788:ILE:HG22	1:K:741:UNK:CB	2.50	0.40
1:G:772:ILE:O	1:G:773:HIS:C	2.63	0.40
1:G:943:ILE:O	1:G:945:THR:N	2.54	0.40
1:H:313:PRO:HG2	1:H:314:ASP:N	2.36	0.40
1:H:897:TYR:O	1:H:898:TYR:C	2.63	0.40
1:H:943:ILE:O	1:H:945:THR:N	2.54	0.40
1:I:284:ASP:CB	1:I:865:LYS:HG3	2.51	0.40
1:I:848:ALA:O	1:I:852:LEU:CD2	2.70	0.40
1:J:308:VAL:HG13	1:J:309:SER:H	1.85	0.40
1:J:356:UNK:C	1:J:357:UNK:O	2.70	0.40
1:J:825:LEU:HD23	1:J:825:LEU:C	2.46	0.40
1:K:279:VAL:HG13	1:K:938:MET:CE	2.52	0.40
1:K:887:SER:O	1:K:888:GLU:C	2.63	0.40
1:L:330:PRO:HD3	1:L:807:GLY:O	2.21	0.40
1:N:315:GLY:O	1:N:316:THR:O	2.39	0.40
1:O:284:ASP:CB	1:O:865:LYS:HG3	2.51	0.40
1:O:330:PRO:HD3	1:O:807:GLY:O	2.21	0.40
1:A:814:ASN:C	1:A:816:PHE:N	2.79	0.40
1:B:284:ASP:CB	1:B:865:LYS:HG3	2.51	0.40
1:C:313:PRO:HG2	1:C:314:ASP:N	2.36	0.40
1:C:316:THR:OG1	1:C:317:ARG:N	2.53	0.40
1:C:881:ASN:OD1	1:C:881:ASN:N	2.54	0.40
1:D:814:ASN:O	1:D:816:PHE:N	2.55	0.40
1:D:961:LYS:HA	1:D:961:LYS:HD2	1.87	0.40
1:E:279:VAL:HG13	1:E:938:MET:CE	2.52	0.40
1:E:881:ASN:OD1	1:E:881:ASN:N	2.54	0.40
1:F:313:PRO:HG2	1:F:314:ASP:N	2.36	0.40
1:F:828:ARG:HD2	1:F:828:ARG:HA	1.89	0.40
1:G:284:ASP:CB	1:G:865:LYS:HG3	2.51	0.40
1:G:315:GLY:O	1:G:316:THR:C	2.63	0.40
1:G:739:UNK:HA	1:G:744:UNK:O	2.21	0.40
1:H:820:ASP:O	1:H:820:ASP:CG	2.65	0.40
1:J:861:VAL:HG12	1:J:861:VAL:O	2.20	0.40
1:K:746:UNK:CB	1:K:792:LEU:CD1	3.00	0.40
1:L:897:TYR:O	1:L:898:TYR:C	2.63	0.40
1:M:315:GLY:O	1:M:316:THR:C	2.63	0.40
1:N:739:UNK:HA	1:N:744:UNK:O	2.21	0.40
1:N:772:ILE:O	1:N:773:HIS:C	2.63	0.40
1:N:953:ILE:HG12	1:N:953:ILE:H	1.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:739:UNK:HA	1:O:744:UNK:O	2.21	0.40
1:O:815:PRO:O	1:O:819:ILE:HG13	2.20	0.40
1:O:958:TYR:C	1:O:960:LEU:N	2.78	0.40
1:P:739:UNK:HA	1:P:744:UNK:O	2.21	0.40
1:P:769:ARG:HH11	1:P:769:ARG:CG	2.34	0.40
1:P:848:ALA:O	1:P:852:LEU:HD22	2.21	0.40
1:P:887:SER:O	1:P:888:GLU:C	2.63	0.40
1:B:356:UNK:C	1:B:357:UNK:O	2.70	0.40
1:B:746:UNK:CB	1:B:792:LEU:CD1	3.00	0.40
1:C:310:ARG:HD2	1:C:310:ARG:O	2.22	0.40
1:C:729:UNK:C	1:O:729:UNK:O	2.70	0.40
1:C:772:ILE:O	1:C:773:HIS:C	2.63	0.40
1:C:820:ASP:O	1:C:820:ASP:CG	2.65	0.40
1:D:848:ALA:O	1:D:852:LEU:HD22	2.21	0.40
1:D:881:ASN:OD1	1:D:881:ASN:N	2.54	0.40
1:D:899:VAL:HG21	1:E:841:ASP:HB3	2.04	0.40
1:E:310:ARG:HD2	1:E:310:ARG:O	2.22	0.40
1:E:820:ASP:O	1:E:820:ASP:CG	2.65	0.40
1:F:765:SER:O	1:F:766:ASP:C	2.64	0.40
1:F:805:LYS:N	1:F:818:GLN:O	2.32	0.40
1:F:886:ILE:HD12	1:F:886:ILE:H	1.82	0.40
1:G:848:ALA:O	1:G:852:LEU:HD22	2.21	0.40
1:H:310:ARG:HD2	1:H:310:ARG:O	2.22	0.40
1:H:860:GLU:C	1:H:862:VAL:N	2.74	0.40
1:I:887:SER:O	1:I:888:GLU:C	2.63	0.40
1:J:330:PRO:HD3	1:J:807:GLY:O	2.21	0.40
1:J:903:LYS:HD2	1:K:841:ASP:OD2	2.22	0.40
1:K:330:PRO:HD3	1:K:807:GLY:O	2.21	0.40
1:K:881:ASN:OD1	1:K:881:ASN:N	2.54	0.40
1:M:848:ALA:O	1:M:852:LEU:HD22	2.21	0.40
1:N:861:VAL:O	1:N:861:VAL:HG12	2.20	0.40
1:O:279:VAL:HG13	1:O:938:MET:CE	2.52	0.40
1:O:313:PRO:HG2	1:O:314:ASP:N	2.36	0.40
1:O:943:ILE:O	1:O:945:THR:N	2.54	0.40
1:P:310:ARG:HD2	1:P:310:ARG:O	2.22	0.40
1:P:805:LYS:N	1:P:818:GLN:O	2.32	0.40
1:P:958:TYR:C	1:P:960:LEU:N	2.78	0.40

All (38) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:PRO:CB	1:M:264:GLU:OE2[1_654]	0.81	1.39
1:B:264:GLU:OE1	1:K:264:GLU:OE1[1_564]	1.20	1.00
1:B:264:GLU:OE2	1:K:264:GLU:CB[1_564]	1.39	0.81
1:B:264:GLU:CD	1:K:264:GLU:OE1[1_564]	1.45	0.75
1:F:264:GLU:OE1	1:O:264:GLU:OE1[1_546]	1.50	0.70
1:A:263:PRO:CA	1:M:264:GLU:OE2[1_654]	1.61	0.59
1:B:264:GLU:CB	1:K:264:GLU:OE2[1_564]	1.61	0.59
1:B:264:GLU:CD	1:K:264:GLU:CD[1_564]	1.63	0.57
1:B:264:GLU:CA	1:K:264:GLU:OE1[1_564]	1.71	0.49
1:E:263:PRO:C	1:I:264:GLU:OE2[1_456]	1.71	0.49
1:B:264:GLU:OE2	1:K:264:GLU:CA[1_564]	1.75	0.45
1:E:264:GLU:OE1	1:I:264:GLU:CB[1_456]	1.75	0.45
1:B:264:GLU:CG	1:K:264:GLU:OE1[1_564]	1.76	0.44
1:K:274:LYS:CE	1:P:859:SER:OG[1_546]	1.76	0.44
1:B:264:GLU:OE1	1:K:264:GLU:CA[1_564]	1.77	0.43
1:A:263:PRO:CB	1:M:264:GLU:CD[1_654]	1.80	0.40
1:E:264:GLU:OE1	1:I:264:GLU:CG[1_456]	1.81	0.39
1:B:264:GLU:OE1	1:K:264:GLU:CD[1_564]	1.84	0.36
1:E:263:PRO:O	1:I:264:GLU:OE2[1_456]	1.85	0.35
1:E:263:PRO:CB	1:I:264:GLU:OE2[1_456]	1.86	0.34
1:B:264:GLU:CB	1:K:264:GLU:OE1[1_564]	1.88	0.32
1:B:264:GLU:CD	1:K:264:GLU:CA[1_564]	1.91	0.29
1:B:264:GLU:CB	1:K:264:GLU:CD[1_564]	1.94	0.26
1:F:264:GLU:OE1	1:O:264:GLU:CD[1_546]	1.94	0.26
1:B:274:LYS:CD	1:G:859:SER:OG[1_564]	2.00	0.20
1:K:274:LYS:CD	1:P:859:SER:OG[1_546]	2.01	0.19
1:B:264:GLU:CD	1:K:264:GLU:CB[1_564]	2.05	0.15
1:A:263:PRO:C	1:M:264:GLU:OE2[1_654]	2.06	0.14
1:E:263:PRO:CA	1:I:264:GLU:OE2[1_456]	2.10	0.10
1:B:264:GLU:CG	1:K:264:GLU:CD[1_564]	2.11	0.09
1:C:859:SER:OG	1:F:274:LYS:CE[1_564]	2.11	0.09
1:F:264:GLU:OE1	1:O:264:GLU:CA[1_546]	2.11	0.09
1:B:264:GLU:OE1	1:K:264:GLU:N[1_564]	2.15	0.05
1:A:263:PRO:CG	1:M:264:GLU:OE2[1_654]	2.16	0.04
1:A:264:GLU:OE1	1:M:264:GLU:CG[1_654]	2.16	0.04
1:B:264:GLU:OE1	1:K:264:GLU:CG[1_564]	2.17	0.03
1:B:264:GLU:CD	1:K:264:GLU:CG[1_564]	2.18	0.02
1:B:264:GLU:CA	1:K:264:GLU:CD[1_564]	2.18	0.02

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	284/338 (84%)	209 (74%)	52 (18%)	23 (8%)	1	10
1	B	284/338 (84%)	209 (74%)	52 (18%)	23 (8%)	1	10
1	C	284/338 (84%)	209 (74%)	52 (18%)	23 (8%)	1	10
1	D	284/338 (84%)	209 (74%)	52 (18%)	23 (8%)	1	10
1	E	284/338 (84%)	209 (74%)	52 (18%)	23 (8%)	1	10
1	F	284/338 (84%)	209 (74%)	52 (18%)	23 (8%)	1	10
1	G	284/338 (84%)	209 (74%)	52 (18%)	23 (8%)	1	10
1	H	284/338 (84%)	209 (74%)	52 (18%)	23 (8%)	1	10
1	I	284/338 (84%)	209 (74%)	52 (18%)	23 (8%)	1	10
1	J	284/338 (84%)	209 (74%)	52 (18%)	23 (8%)	1	10
1	K	284/338 (84%)	209 (74%)	52 (18%)	23 (8%)	1	10
1	L	284/338 (84%)	209 (74%)	52 (18%)	23 (8%)	1	10
1	M	284/338 (84%)	209 (74%)	52 (18%)	23 (8%)	1	10
1	N	284/338 (84%)	209 (74%)	52 (18%)	23 (8%)	1	10
1	O	284/338 (84%)	209 (74%)	52 (18%)	23 (8%)	1	10
1	P	284/338 (84%)	209 (74%)	52 (18%)	23 (8%)	1	10
All	All	4544/5408 (84%)	3344 (74%)	832 (18%)	368 (8%)	1	10

All (368) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	316	THR
1	A	766	ASP
1	A	786	ALA
1	A	810	ASN
1	B	316	THR
1	B	766	ASP

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Mol	Chain	Res	Type
1	B	786	ALA
1	B	810	ASN
1	C	316	THR
1	C	766	ASP
1	C	786	ALA
1	C	810	ASN
1	D	316	THR
1	D	766	ASP
1	D	786	ALA
1	D	810	ASN
1	E	316	THR
1	E	766	ASP
1	E	786	ALA
1	E	810	ASN
1	F	316	THR
1	F	766	ASP
1	F	786	ALA
1	F	810	ASN
1	G	316	THR
1	G	766	ASP
1	G	786	ALA
1	G	810	ASN
1	H	316	THR
1	H	766	ASP
1	H	786	ALA
1	H	810	ASN
1	I	316	THR
1	I	766	ASP
1	I	786	ALA
1	I	810	ASN
1	J	316	THR
1	J	766	ASP
1	J	786	ALA
1	J	810	ASN
1	K	316	THR
1	K	766	ASP
1	K	786	ALA
1	K	810	ASN
1	L	316	THR
1	L	766	ASP
1	L	786	ALA
1	L	810	ASN

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Mol	Chain	Res	Type
1	M	316	THR
1	M	766	ASP
1	M	786	ALA
1	M	810	ASN
1	N	316	THR
1	N	766	ASP
1	N	786	ALA
1	N	810	ASN
1	O	316	THR
1	O	766	ASP
1	O	786	ALA
1	O	810	ASN
1	P	316	THR
1	P	766	ASP
1	P	786	ALA
1	P	810	ASN
1	A	346	PRO
1	A	779	GLN
1	A	811	ARG
1	A	813	LYS
1	A	839	PRO
1	A	840	ASP
1	A	853	ARG
1	A	944	VAL
1	B	346	PRO
1	B	779	GLN
1	B	811	ARG
1	B	813	LYS
1	B	839	PRO
1	B	840	ASP
1	B	853	ARG
1	B	944	VAL
1	C	346	PRO
1	C	779	GLN
1	C	813	LYS
1	C	839	PRO
1	C	840	ASP
1	C	853	ARG
1	C	944	VAL
1	D	346	PRO
1	D	779	GLN
1	D	811	ARG

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Mol	Chain	Res	Type
1	D	813	LYS
1	D	839	PRO
1	D	840	ASP
1	D	853	ARG
1	D	944	VAL
1	E	346	PRO
1	E	779	GLN
1	E	811	ARG
1	E	813	LYS
1	E	839	PRO
1	E	840	ASP
1	E	853	ARG
1	E	944	VAL
1	F	346	PRO
1	F	779	GLN
1	F	813	LYS
1	F	839	PRO
1	F	840	ASP
1	F	853	ARG
1	F	944	VAL
1	G	346	PRO
1	G	779	GLN
1	G	811	ARG
1	G	813	LYS
1	G	839	PRO
1	G	840	ASP
1	G	853	ARG
1	G	944	VAL
1	H	346	PRO
1	H	779	GLN
1	H	813	LYS
1	H	839	PRO
1	H	840	ASP
1	H	853	ARG
1	H	944	VAL
1	I	346	PRO
1	I	779	GLN
1	I	811	ARG
1	I	813	LYS
1	I	839	PRO
1	I	840	ASP
1	I	853	ARG

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Mol	Chain	Res	Type
1	I	944	VAL
1	J	346	PRO
1	J	779	GLN
1	J	811	ARG
1	J	813	LYS
1	J	839	PRO
1	J	840	ASP
1	J	853	ARG
1	J	944	VAL
1	K	346	PRO
1	K	779	GLN
1	K	811	ARG
1	K	813	LYS
1	K	839	PRO
1	K	840	ASP
1	K	853	ARG
1	K	944	VAL
1	L	346	PRO
1	L	779	GLN
1	L	811	ARG
1	L	813	LYS
1	L	839	PRO
1	L	840	ASP
1	L	853	ARG
1	L	944	VAL
1	M	346	PRO
1	M	779	GLN
1	M	813	LYS
1	M	839	PRO
1	M	840	ASP
1	M	853	ARG
1	M	944	VAL
1	N	346	PRO
1	N	779	GLN
1	N	811	ARG
1	N	813	LYS
1	N	839	PRO
1	N	840	ASP
1	N	853	ARG
1	N	944	VAL
1	O	346	PRO
1	O	779	GLN

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Mol	Chain	Res	Type
1	O	811	ARG
1	O	813	LYS
1	O	839	PRO
1	O	840	ASP
1	O	853	ARG
1	O	944	VAL
1	P	346	PRO
1	P	779	GLN
1	P	813	LYS
1	P	839	PRO
1	P	840	ASP
1	P	853	ARG
1	P	944	VAL
1	A	289	ALA
1	A	309	SER
1	B	289	ALA
1	B	309	SER
1	C	289	ALA
1	C	309	SER
1	C	811	ARG
1	D	289	ALA
1	D	309	SER
1	E	289	ALA
1	E	309	SER
1	F	289	ALA
1	F	309	SER
1	F	811	ARG
1	G	289	ALA
1	G	309	SER
1	H	289	ALA
1	H	309	SER
1	H	811	ARG
1	I	289	ALA
1	I	309	SER
1	J	289	ALA
1	J	309	SER
1	K	289	ALA
1	K	309	SER
1	L	289	ALA
1	L	309	SER
1	M	289	ALA
1	M	309	SER

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Mol	Chain	Res	Type
1	M	811	ARG
1	N	289	ALA
1	N	309	SER
1	O	289	ALA
1	O	309	SER
1	P	289	ALA
1	P	309	SER
1	P	811	ARG
1	A	842	LYS
1	A	941	SER
1	B	842	LYS
1	B	941	SER
1	C	842	LYS
1	C	941	SER
1	D	842	LYS
1	D	941	SER
1	E	842	LYS
1	E	941	SER
1	F	842	LYS
1	F	941	SER
1	G	842	LYS
1	G	941	SER
1	H	842	LYS
1	H	941	SER
1	I	842	LYS
1	I	941	SER
1	J	842	LYS
1	J	941	SER
1	K	842	LYS
1	K	941	SER
1	L	842	LYS
1	L	941	SER
1	M	842	LYS
1	M	941	SER
1	N	842	LYS
1	N	941	SER
1	O	842	LYS
1	O	941	SER
1	P	842	LYS
1	P	941	SER
1	A	317	ARG
1	A	940	LEU

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Mol	Chain	Res	Type
1	B	317	ARG
1	B	940	LEU
1	C	317	ARG
1	C	940	LEU
1	D	317	ARG
1	D	940	LEU
1	E	317	ARG
1	E	940	LEU
1	F	317	ARG
1	F	940	LEU
1	G	317	ARG
1	G	940	LEU
1	H	317	ARG
1	H	940	LEU
1	I	317	ARG
1	I	940	LEU
1	J	317	ARG
1	J	940	LEU
1	K	317	ARG
1	K	940	LEU
1	L	317	ARG
1	L	940	LEU
1	M	317	ARG
1	M	940	LEU
1	N	317	ARG
1	N	940	LEU
1	O	317	ARG
1	O	940	LEU
1	P	317	ARG
1	P	940	LEU
1	A	306	GLY
1	A	903	LYS
1	B	306	GLY
1	B	903	LYS
1	C	306	GLY
1	C	903	LYS
1	D	306	GLY
1	D	903	LYS
1	E	306	GLY
1	E	903	LYS
1	F	903	LYS
1	G	306	GLY

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Mol	Chain	Res	Type
1	G	903	LYS
1	H	306	GLY
1	H	903	LYS
1	I	306	GLY
1	I	903	LYS
1	J	306	GLY
1	J	903	LYS
1	K	306	GLY
1	K	903	LYS
1	L	903	LYS
1	M	306	GLY
1	M	903	LYS
1	N	306	GLY
1	N	903	LYS
1	O	306	GLY
1	O	903	LYS
1	P	306	GLY
1	P	903	LYS
1	A	861	VAL
1	B	861	VAL
1	C	861	VAL
1	D	861	VAL
1	E	861	VAL
1	F	306	GLY
1	F	861	VAL
1	G	861	VAL
1	H	861	VAL
1	I	861	VAL
1	J	861	VAL
1	K	861	VAL
1	L	306	GLY
1	L	861	VAL
1	M	861	VAL
1	N	861	VAL
1	O	861	VAL
1	P	861	VAL
1	H	278	ILE
1	A	278	ILE
1	B	278	ILE
1	C	278	ILE
1	D	278	ILE
1	E	278	ILE

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Mol	Chain	Res	Type
1	F	278	ILE
1	G	278	ILE
1	I	278	ILE
1	J	278	ILE
1	K	278	ILE
1	L	278	ILE
1	M	278	ILE
1	N	278	ILE
1	O	278	ILE
1	P	278	ILE
1	A	854	VAL
1	B	854	VAL
1	C	854	VAL
1	D	854	VAL
1	E	854	VAL
1	F	854	VAL
1	G	854	VAL
1	H	854	VAL
1	I	854	VAL
1	J	854	VAL
1	K	854	VAL
1	L	854	VAL
1	M	854	VAL
1	N	854	VAL
1	O	854	VAL
1	P	854	VAL

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	246/260 (95%)	205 (83%)	41 (17%)	2	13
1	B	246/260 (95%)	205 (83%)	41 (17%)	2	13
1	C	246/260 (95%)	205 (83%)	41 (17%)	2	13
1	D	246/260 (95%)	205 (83%)	41 (17%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	246/260 (95%)	205 (83%)	41 (17%)	2	13
1	F	246/260 (95%)	205 (83%)	41 (17%)	2	13
1	G	246/260 (95%)	205 (83%)	41 (17%)	2	13
1	H	246/260 (95%)	206 (84%)	40 (16%)	2	14
1	I	246/260 (95%)	205 (83%)	41 (17%)	2	13
1	J	246/260 (95%)	206 (84%)	40 (16%)	2	14
1	K	246/260 (95%)	205 (83%)	41 (17%)	2	13
1	L	246/260 (95%)	205 (83%)	41 (17%)	2	13
1	M	246/260 (95%)	205 (83%)	41 (17%)	2	13
1	N	246/260 (95%)	205 (83%)	41 (17%)	2	13
1	O	246/260 (95%)	205 (83%)	41 (17%)	2	13
1	P	246/260 (95%)	205 (83%)	41 (17%)	2	13
All	All	3936/4160 (95%)	3282 (83%)	654 (17%)	2	13

All (654) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	276	LYS
1	A	283	VAL
1	A	290	ILE
1	A	314	ASP
1	A	318	LEU
1	A	319	ARG
1	A	338	LEU
1	A	347	ARG
1	A	350	TYR
1	A	351	THR
1	A	755	TYR
1	A	760	GLU
1	A	767	ARG
1	A	769	ARG
1	A	771	VAL
1	A	778	GLN
1	A	783	ILE
1	A	788	ILE
1	A	791	THR
1	A	792	LEU
1	A	809	PHE

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Mol	Chain	Res	Type
1	A	824	THR
1	A	828	ARG
1	A	849	ARG
1	A	854	VAL
1	A	860	GLU
1	A	869	GLU
1	A	882	ILE
1	A	886	ILE
1	A	887	SER
1	A	894	ILE
1	A	902	ARG
1	A	939	ARG
1	A	941	SER
1	A	942	PRO
1	A	944	VAL
1	A	945	THR
1	A	953	ILE
1	A	957	GLU
1	A	959	THR
1	A	962	GLN
1	B	276	LYS
1	B	283	VAL
1	B	290	ILE
1	B	314	ASP
1	B	318	LEU
1	B	319	ARG
1	B	338	LEU
1	B	347	ARG
1	B	350	TYR
1	B	351	THR
1	B	755	TYR
1	B	760	GLU
1	B	767	ARG
1	B	769	ARG
1	B	771	VAL
1	B	778	GLN
1	B	783	ILE
1	B	788	ILE
1	B	791	THR
1	B	792	LEU
1	B	809	PHE
1	B	824	THR

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Mol	Chain	Res	Type
1	B	828	ARG
1	B	849	ARG
1	B	854	VAL
1	B	860	GLU
1	B	869	GLU
1	B	882	ILE
1	B	886	ILE
1	B	887	SER
1	B	894	ILE
1	B	902	ARG
1	B	939	ARG
1	B	941	SER
1	B	942	PRO
1	B	944	VAL
1	B	945	THR
1	B	953	ILE
1	B	957	GLU
1	B	959	THR
1	B	962	GLN
1	C	276	LYS
1	C	283	VAL
1	C	290	ILE
1	C	314	ASP
1	C	318	LEU
1	C	319	ARG
1	C	338	LEU
1	C	347	ARG
1	C	350	TYR
1	C	351	THR
1	C	755	TYR
1	C	760	GLU
1	C	767	ARG
1	C	769	ARG
1	C	771	VAL
1	C	778	GLN
1	C	783	ILE
1	C	788	ILE
1	C	791	THR
1	C	792	LEU
1	C	809	PHE
1	C	824	THR
1	C	828	ARG

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Mol	Chain	Res	Type
1	C	849	ARG
1	C	854	VAL
1	C	860	GLU
1	C	869	GLU
1	C	882	ILE
1	C	886	ILE
1	C	887	SER
1	C	894	ILE
1	C	902	ARG
1	C	939	ARG
1	C	941	SER
1	C	942	PRO
1	C	944	VAL
1	C	945	THR
1	C	953	ILE
1	C	957	GLU
1	C	959	THR
1	C	962	GLN
1	D	276	LYS
1	D	283	VAL
1	D	290	ILE
1	D	314	ASP
1	D	318	LEU
1	D	319	ARG
1	D	338	LEU
1	D	347	ARG
1	D	350	TYR
1	D	351	THR
1	D	755	TYR
1	D	760	GLU
1	D	767	ARG
1	D	769	ARG
1	D	771	VAL
1	D	778	GLN
1	D	783	ILE
1	D	788	ILE
1	D	791	THR
1	D	792	LEU
1	D	809	PHE
1	D	824	THR
1	D	828	ARG
1	D	849	ARG

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Mol	Chain	Res	Type
1	D	854	VAL
1	D	860	GLU
1	D	869	GLU
1	D	882	ILE
1	D	886	ILE
1	D	887	SER
1	D	894	ILE
1	D	902	ARG
1	D	939	ARG
1	D	941	SER
1	D	942	PRO
1	D	944	VAL
1	D	945	THR
1	D	953	ILE
1	D	957	GLU
1	D	959	THR
1	D	962	GLN
1	E	276	LYS
1	E	283	VAL
1	E	290	ILE
1	E	314	ASP
1	E	318	LEU
1	E	319	ARG
1	E	338	LEU
1	E	347	ARG
1	E	350	TYR
1	E	351	THR
1	E	755	TYR
1	E	760	GLU
1	E	767	ARG
1	E	769	ARG
1	E	771	VAL
1	E	778	GLN
1	E	783	ILE
1	E	788	ILE
1	E	791	THR
1	E	792	LEU
1	E	809	PHE
1	E	824	THR
1	E	828	ARG
1	E	849	ARG
1	E	854	VAL

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Mol	Chain	Res	Type
1	E	860	GLU
1	E	869	GLU
1	E	882	ILE
1	E	886	ILE
1	E	887	SER
1	E	894	ILE
1	E	902	ARG
1	E	939	ARG
1	E	941	SER
1	E	942	PRO
1	E	944	VAL
1	E	945	THR
1	E	953	ILE
1	E	957	GLU
1	E	959	THR
1	E	962	GLN
1	F	276	LYS
1	F	283	VAL
1	F	290	ILE
1	F	314	ASP
1	F	318	LEU
1	F	319	ARG
1	F	338	LEU
1	F	347	ARG
1	F	350	TYR
1	F	351	THR
1	F	755	TYR
1	F	760	GLU
1	F	767	ARG
1	F	769	ARG
1	F	771	VAL
1	F	778	GLN
1	F	783	ILE
1	F	788	ILE
1	F	791	THR
1	F	792	LEU
1	F	809	PHE
1	F	824	THR
1	F	828	ARG
1	F	849	ARG
1	F	854	VAL
1	F	860	GLU

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Mol	Chain	Res	Type
1	F	869	GLU
1	F	882	ILE
1	F	886	ILE
1	F	887	SER
1	F	894	ILE
1	F	902	ARG
1	F	939	ARG
1	F	941	SER
1	F	942	PRO
1	F	944	VAL
1	F	945	THR
1	F	953	ILE
1	F	957	GLU
1	F	959	THR
1	F	962	GLN
1	G	276	LYS
1	G	283	VAL
1	G	290	ILE
1	G	314	ASP
1	G	318	LEU
1	G	319	ARG
1	G	338	LEU
1	G	347	ARG
1	G	350	TYR
1	G	351	THR
1	G	755	TYR
1	G	760	GLU
1	G	767	ARG
1	G	769	ARG
1	G	771	VAL
1	G	778	GLN
1	G	783	ILE
1	G	788	ILE
1	G	791	THR
1	G	792	LEU
1	G	809	PHE
1	G	824	THR
1	G	828	ARG
1	G	849	ARG
1	G	854	VAL
1	G	860	GLU
1	G	869	GLU

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Mol	Chain	Res	Type
1	G	882	ILE
1	G	886	ILE
1	G	887	SER
1	G	894	ILE
1	G	902	ARG
1	G	939	ARG
1	G	941	SER
1	G	942	PRO
1	G	944	VAL
1	G	945	THR
1	G	953	ILE
1	G	957	GLU
1	G	959	THR
1	G	962	GLN
1	H	276	LYS
1	H	283	VAL
1	H	290	ILE
1	H	314	ASP
1	H	318	LEU
1	H	319	ARG
1	H	338	LEU
1	H	347	ARG
1	H	350	TYR
1	H	351	THR
1	H	755	TYR
1	H	760	GLU
1	H	767	ARG
1	H	769	ARG
1	H	771	VAL
1	H	778	GLN
1	H	783	ILE
1	H	788	ILE
1	H	791	THR
1	H	792	LEU
1	H	809	PHE
1	H	824	THR
1	H	828	ARG
1	H	849	ARG
1	H	854	VAL
1	H	860	GLU
1	H	869	GLU
1	H	882	ILE

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Mol	Chain	Res	Type
1	H	886	ILE
1	H	887	SER
1	H	894	ILE
1	H	902	ARG
1	H	939	ARG
1	H	941	SER
1	H	944	VAL
1	H	945	THR
1	H	953	ILE
1	H	957	GLU
1	H	959	THR
1	H	962	GLN
1	I	276	LYS
1	I	283	VAL
1	I	290	ILE
1	I	314	ASP
1	I	318	LEU
1	I	319	ARG
1	I	338	LEU
1	I	347	ARG
1	I	350	TYR
1	I	351	THR
1	I	755	TYR
1	I	760	GLU
1	I	767	ARG
1	I	769	ARG
1	I	771	VAL
1	I	778	GLN
1	I	783	ILE
1	I	788	ILE
1	I	791	THR
1	I	792	LEU
1	I	809	PHE
1	I	824	THR
1	I	828	ARG
1	I	849	ARG
1	I	854	VAL
1	I	860	GLU
1	I	869	GLU
1	I	882	ILE
1	I	886	ILE
1	I	887	SER

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Mol	Chain	Res	Type
1	I	894	ILE
1	I	902	ARG
1	I	939	ARG
1	I	941	SER
1	I	942	PRO
1	I	944	VAL
1	I	945	THR
1	I	953	ILE
1	I	957	GLU
1	I	959	THR
1	I	962	GLN
1	J	276	LYS
1	J	283	VAL
1	J	290	ILE
1	J	314	ASP
1	J	318	LEU
1	J	319	ARG
1	J	338	LEU
1	J	347	ARG
1	J	350	TYR
1	J	351	THR
1	J	755	TYR
1	J	760	GLU
1	J	767	ARG
1	J	769	ARG
1	J	771	VAL
1	J	778	GLN
1	J	783	ILE
1	J	788	ILE
1	J	791	THR
1	J	792	LEU
1	J	809	PHE
1	J	824	THR
1	J	828	ARG
1	J	849	ARG
1	J	854	VAL
1	J	860	GLU
1	J	869	GLU
1	J	882	ILE
1	J	886	ILE
1	J	887	SER
1	J	894	ILE

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Mol	Chain	Res	Type
1	J	902	ARG
1	J	939	ARG
1	J	941	SER
1	J	944	VAL
1	J	945	THR
1	J	953	ILE
1	J	957	GLU
1	J	959	THR
1	J	962	GLN
1	K	276	LYS
1	K	283	VAL
1	K	290	ILE
1	K	314	ASP
1	K	318	LEU
1	K	319	ARG
1	K	338	LEU
1	K	347	ARG
1	K	350	TYR
1	K	351	THR
1	K	755	TYR
1	K	760	GLU
1	K	767	ARG
1	K	769	ARG
1	K	771	VAL
1	K	778	GLN
1	K	783	ILE
1	K	788	ILE
1	K	791	THR
1	K	792	LEU
1	K	809	PHE
1	K	824	THR
1	K	828	ARG
1	K	849	ARG
1	K	854	VAL
1	K	860	GLU
1	K	869	GLU
1	K	882	ILE
1	K	886	ILE
1	K	887	SER
1	K	894	ILE
1	K	902	ARG
1	K	939	ARG

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Mol	Chain	Res	Type
1	K	941	SER
1	K	942	PRO
1	K	944	VAL
1	K	945	THR
1	K	953	ILE
1	K	957	GLU
1	K	959	THR
1	K	962	GLN
1	L	276	LYS
1	L	283	VAL
1	L	290	ILE
1	L	314	ASP
1	L	318	LEU
1	L	319	ARG
1	L	338	LEU
1	L	347	ARG
1	L	350	TYR
1	L	351	THR
1	L	755	TYR
1	L	760	GLU
1	L	767	ARG
1	L	769	ARG
1	L	771	VAL
1	L	778	GLN
1	L	783	ILE
1	L	788	ILE
1	L	791	THR
1	L	792	LEU
1	L	809	PHE
1	L	824	THR
1	L	828	ARG
1	L	849	ARG
1	L	854	VAL
1	L	860	GLU
1	L	869	GLU
1	L	882	ILE
1	L	886	ILE
1	L	887	SER
1	L	894	ILE
1	L	902	ARG
1	L	939	ARG
1	L	941	SER

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Mol	Chain	Res	Type
1	L	942	PRO
1	L	944	VAL
1	L	945	THR
1	L	953	ILE
1	L	957	GLU
1	L	959	THR
1	L	962	GLN
1	M	276	LYS
1	M	283	VAL
1	M	290	ILE
1	M	314	ASP
1	M	318	LEU
1	M	319	ARG
1	M	338	LEU
1	M	347	ARG
1	M	350	TYR
1	M	351	THR
1	M	755	TYR
1	M	760	GLU
1	M	767	ARG
1	M	769	ARG
1	M	771	VAL
1	M	778	GLN
1	M	783	ILE
1	M	788	ILE
1	M	791	THR
1	M	792	LEU
1	M	809	PHE
1	M	824	THR
1	M	828	ARG
1	M	849	ARG
1	M	854	VAL
1	M	860	GLU
1	M	869	GLU
1	M	882	ILE
1	M	886	ILE
1	M	887	SER
1	M	894	ILE
1	M	902	ARG
1	M	939	ARG
1	M	941	SER
1	M	942	PRO

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Mol	Chain	Res	Type
1	M	944	VAL
1	M	945	THR
1	M	953	ILE
1	M	957	GLU
1	M	959	THR
1	M	962	GLN
1	N	276	LYS
1	N	283	VAL
1	N	290	ILE
1	N	314	ASP
1	N	318	LEU
1	N	319	ARG
1	N	338	LEU
1	N	347	ARG
1	N	350	TYR
1	N	351	THR
1	N	755	TYR
1	N	760	GLU
1	N	767	ARG
1	N	769	ARG
1	N	771	VAL
1	N	778	GLN
1	N	783	ILE
1	N	788	ILE
1	N	791	THR
1	N	792	LEU
1	N	809	PHE
1	N	824	THR
1	N	828	ARG
1	N	849	ARG
1	N	854	VAL
1	N	860	GLU
1	N	869	GLU
1	N	882	ILE
1	N	886	ILE
1	N	887	SER
1	N	894	ILE
1	N	902	ARG
1	N	939	ARG
1	N	941	SER
1	N	942	PRO
1	N	944	VAL

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Mol	Chain	Res	Type
1	N	945	THR
1	N	953	ILE
1	N	957	GLU
1	N	959	THR
1	N	962	GLN
1	O	276	LYS
1	O	283	VAL
1	O	290	ILE
1	O	314	ASP
1	O	318	LEU
1	O	319	ARG
1	O	338	LEU
1	O	347	ARG
1	O	350	TYR
1	O	351	THR
1	O	755	TYR
1	O	760	GLU
1	O	767	ARG
1	O	769	ARG
1	O	771	VAL
1	O	778	GLN
1	O	783	ILE
1	O	788	ILE
1	O	791	THR
1	O	792	LEU
1	O	809	PHE
1	O	824	THR
1	O	828	ARG
1	O	849	ARG
1	O	854	VAL
1	O	860	GLU
1	O	869	GLU
1	O	882	ILE
1	O	886	ILE
1	O	887	SER
1	O	894	ILE
1	O	902	ARG
1	O	939	ARG
1	O	941	SER
1	O	942	PRO
1	O	944	VAL
1	O	945	THR

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Mol	Chain	Res	Type
1	O	953	ILE
1	O	957	GLU
1	O	959	THR
1	O	962	GLN
1	P	276	LYS
1	P	283	VAL
1	P	290	ILE
1	P	314	ASP
1	P	318	LEU
1	P	319	ARG
1	P	338	LEU
1	P	347	ARG
1	P	350	TYR
1	P	351	THR
1	P	755	TYR
1	P	760	GLU
1	P	767	ARG
1	P	769	ARG
1	P	771	VAL
1	P	778	GLN
1	P	783	ILE
1	P	788	ILE
1	P	791	THR
1	P	792	LEU
1	P	809	PHE
1	P	824	THR
1	P	828	ARG
1	P	849	ARG
1	P	854	VAL
1	P	860	GLU
1	P	869	GLU
1	P	882	ILE
1	P	886	ILE
1	P	887	SER
1	P	894	ILE
1	P	902	ARG
1	P	939	ARG
1	P	941	SER
1	P	942	PRO
1	P	944	VAL
1	P	945	THR
1	P	953	ILE

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Continued from previous page...

Mol	Chain	Res	Type
1	P	957	GLU
1	P	959	THR
1	P	962	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	336	GLN
1	A	778	GLN
1	A	779	GLN
1	A	793	ASN
1	A	924	GLN
1	A	962	GLN
1	B	336	GLN
1	B	778	GLN
1	B	779	GLN
1	B	793	ASN
1	B	962	GLN
1	C	336	GLN
1	C	779	GLN
1	C	793	ASN
1	C	962	GLN
1	D	336	GLN
1	D	778	GLN
1	D	779	GLN
1	D	793	ASN
1	D	962	GLN
1	E	336	GLN
1	E	778	GLN
1	E	779	GLN
1	E	924	GLN
1	E	962	GLN
1	F	336	GLN
1	F	778	GLN
1	F	779	GLN
1	F	793	ASN
1	F	962	GLN
1	G	336	GLN
1	G	778	GLN
1	G	779	GLN
1	G	924	GLN
1	G	962	GLN

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Mol	Chain	Res	Type
1	H	336	GLN
1	H	778	GLN
1	H	779	GLN
1	H	793	ASN
1	H	962	GLN
1	I	336	GLN
1	I	778	GLN
1	I	779	GLN
1	I	793	ASN
1	I	924	GLN
1	I	962	GLN
1	J	336	GLN
1	J	779	GLN
1	J	793	ASN
1	J	924	GLN
1	J	962	GLN
1	K	336	GLN
1	K	778	GLN
1	K	779	GLN
1	K	924	GLN
1	K	962	GLN
1	L	336	GLN
1	L	778	GLN
1	L	779	GLN
1	L	793	ASN
1	L	962	GLN
1	M	336	GLN
1	M	778	GLN
1	M	779	GLN
1	M	924	GLN
1	M	962	GLN
1	N	336	GLN
1	N	778	GLN
1	N	779	GLN
1	N	962	GLN
1	O	336	GLN
1	O	778	GLN
1	O	779	GLN
1	O	793	ASN
1	O	850	HIS
1	O	962	GLN
1	P	336	GLN

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Mol	Chain	Res	Type
1	P	779	GLN
1	P	793	ASN
1	P	962	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 16 are monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ADP	E	1001	3	28,29,29	1.26	2 (7%)	43,45,45	1.87	10 (23%)
2	ADP	L	1001	3	28,29,29	1.25	2 (7%)	43,45,45	1.87	10 (23%)
2	ADP	D	1001	3	28,29,29	1.26	2 (7%)	43,45,45	1.87	10 (23%)
2	ADP	O	1001	3	28,29,29	1.26	2 (7%)	43,45,45	1.87	10 (23%)
2	ADP	P	1001	3	28,29,29	1.26	2 (7%)	43,45,45	1.86	10 (23%)
2	ADP	I	1001	3	28,29,29	1.25	2 (7%)	43,45,45	1.86	10 (23%)
2	ADP	A	1001	3	28,29,29	1.25	2 (7%)	43,45,45	1.87	10 (23%)
2	ADP	H	1001	3	28,29,29	1.25	2 (7%)	43,45,45	1.86	10 (23%)
2	ADP	N	1001	3	28,29,29	1.24	2 (7%)	43,45,45	1.87	10 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	J	1001	3	28,29,29	1.26	2 (7%)	43,45,45	1.86	10 (23%)
2	ADP	G	1001	3	28,29,29	1.26	2 (7%)	43,45,45	1.87	10 (23%)
2	ADP	C	1001	3	28,29,29	1.24	2 (7%)	43,45,45	1.87	10 (23%)
2	ADP	K	1001	3	28,29,29	1.25	2 (7%)	43,45,45	1.86	10 (23%)
2	ADP	B	1001	3	28,29,29	1.25	2 (7%)	43,45,45	1.86	10 (23%)
2	ADP	M	1001	3	28,29,29	1.25	2 (7%)	43,45,45	1.87	10 (23%)
2	ADP	F	1001	3	28,29,29	1.25	2 (7%)	43,45,45	1.86	10 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	E	1001	3	-	2/16/32/32	0/3/3/3
2	ADP	L	1001	3	-	2/16/32/32	0/3/3/3
2	ADP	D	1001	3	-	2/16/32/32	0/3/3/3
2	ADP	O	1001	3	-	2/16/32/32	0/3/3/3
2	ADP	P	1001	3	-	2/16/32/32	0/3/3/3
2	ADP	I	1001	3	-	2/16/32/32	0/3/3/3
2	ADP	A	1001	3	-	2/16/32/32	0/3/3/3
2	ADP	H	1001	3	-	2/16/32/32	0/3/3/3
2	ADP	N	1001	3	-	2/16/32/32	0/3/3/3
2	ADP	J	1001	3	-	2/16/32/32	0/3/3/3
2	ADP	G	1001	3	-	2/16/32/32	0/3/3/3
2	ADP	C	1001	3	-	2/16/32/32	0/3/3/3
2	ADP	K	1001	3	-	2/16/32/32	0/3/3/3
2	ADP	B	1001	3	-	2/16/32/32	0/3/3/3
2	ADP	M	1001	3	-	2/16/32/32	0/3/3/3
2	ADP	F	1001	3	-	2/16/32/32	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	1001	ADP	PA-O3A	3.96	1.63	1.59
2	G	1001	ADP	PA-O3A	3.94	1.63	1.59
2	E	1001	ADP	PA-O3A	3.94	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	1001	ADP	PA-O3A	3.92	1.63	1.59
2	M	1001	ADP	PA-O3A	3.91	1.63	1.59
2	D	1001	ADP	PA-O3A	3.89	1.63	1.59
2	B	1001	ADP	PA-O3A	3.89	1.63	1.59
2	F	1001	ADP	PA-O3A	3.88	1.63	1.59
2	J	1001	ADP	PA-O3A	3.88	1.63	1.59
2	K	1001	ADP	PA-O3A	3.87	1.63	1.59
2	A	1001	ADP	PA-O3A	3.86	1.63	1.59
2	L	1001	ADP	PA-O3A	3.85	1.63	1.59
2	H	1001	ADP	PA-O3A	3.83	1.63	1.59
2	I	1001	ADP	PA-O3A	3.83	1.63	1.59
2	N	1001	ADP	PA-O3A	3.83	1.63	1.59
2	C	1001	ADP	PA-O3A	3.80	1.63	1.59
2	P	1001	ADP	C5-N7	-2.74	1.34	1.39
2	J	1001	ADP	C5-N7	-2.73	1.34	1.39
2	H	1001	ADP	C5-N7	-2.73	1.34	1.39
2	D	1001	ADP	C5-N7	-2.73	1.34	1.39
2	F	1001	ADP	C5-N7	-2.72	1.34	1.39
2	I	1001	ADP	C5-N7	-2.72	1.34	1.39
2	A	1001	ADP	C5-N7	-2.71	1.34	1.39
2	L	1001	ADP	C5-N7	-2.71	1.34	1.39
2	E	1001	ADP	C5-N7	-2.70	1.34	1.39
2	K	1001	ADP	C5-N7	-2.70	1.34	1.39
2	O	1001	ADP	C5-N7	-2.70	1.34	1.39
2	M	1001	ADP	C5-N7	-2.69	1.34	1.39
2	G	1001	ADP	C5-N7	-2.69	1.34	1.39
2	C	1001	ADP	C5-N7	-2.68	1.34	1.39
2	B	1001	ADP	C5-N7	-2.67	1.34	1.39
2	N	1001	ADP	C5-N7	-2.66	1.34	1.39

All (160) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1001	ADP	C5-C4-N3	-5.26	119.47	126.72
2	O	1001	ADP	C5-C4-N3	-5.25	119.49	126.72
2	G	1001	ADP	C5-C4-N3	-5.25	119.49	126.72
2	D	1001	ADP	C5-C4-N3	-5.25	119.49	126.72
2	E	1001	ADP	C5-C4-N3	-5.24	119.50	126.72
2	M	1001	ADP	C5-C4-N3	-5.24	119.50	126.72
2	A	1001	ADP	C5-C4-N3	-5.24	119.50	126.72
2	L	1001	ADP	C5-C4-N3	-5.23	119.51	126.72
2	B	1001	ADP	C5-C4-N3	-5.23	119.52	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	1001	ADP	C5-C4-N3	-5.23	119.52	126.72
2	K	1001	ADP	C5-C4-N3	-5.22	119.52	126.72
2	H	1001	ADP	C5-C4-N3	-5.22	119.53	126.72
2	J	1001	ADP	C5-C4-N3	-5.22	119.53	126.72
2	P	1001	ADP	C5-C4-N3	-5.22	119.53	126.72
2	I	1001	ADP	C5-C4-N3	-5.21	119.54	126.72
2	F	1001	ADP	C5-C4-N3	-5.21	119.54	126.72
2	N	1001	ADP	N3-C2-N1	-4.64	121.56	128.58
2	O	1001	ADP	N3-C2-N1	-4.64	121.56	128.58
2	L	1001	ADP	N3-C2-N1	-4.63	121.57	128.58
2	M	1001	ADP	N3-C2-N1	-4.63	121.57	128.58
2	P	1001	ADP	N3-C2-N1	-4.63	121.58	128.58
2	D	1001	ADP	N3-C2-N1	-4.63	121.58	128.58
2	K	1001	ADP	N3-C2-N1	-4.63	121.58	128.58
2	H	1001	ADP	N3-C2-N1	-4.62	121.59	128.58
2	B	1001	ADP	N3-C2-N1	-4.62	121.59	128.58
2	A	1001	ADP	N3-C2-N1	-4.61	121.61	128.58
2	G	1001	ADP	N3-C2-N1	-4.61	121.61	128.58
2	C	1001	ADP	N3-C2-N1	-4.61	121.61	128.58
2	F	1001	ADP	N3-C2-N1	-4.60	121.62	128.58
2	E	1001	ADP	N3-C2-N1	-4.60	121.62	128.58
2	J	1001	ADP	N3-C2-N1	-4.60	121.63	128.58
2	I	1001	ADP	N3-C2-N1	-4.56	121.68	128.58
2	C	1001	ADP	N3-C4-N9	4.46	134.75	127.17
2	B	1001	ADP	N3-C4-N9	4.45	134.74	127.17
2	M	1001	ADP	N3-C4-N9	4.45	134.74	127.17
2	N	1001	ADP	N3-C4-N9	4.45	134.74	127.17
2	E	1001	ADP	N3-C4-N9	4.45	134.74	127.17
2	D	1001	ADP	N3-C4-N9	4.45	134.73	127.17
2	A	1001	ADP	N3-C4-N9	4.45	134.73	127.17
2	J	1001	ADP	N3-C4-N9	4.44	134.72	127.17
2	G	1001	ADP	N3-C4-N9	4.44	134.72	127.17
2	P	1001	ADP	N3-C4-N9	4.44	134.71	127.17
2	L	1001	ADP	N3-C4-N9	4.44	134.71	127.17
2	F	1001	ADP	N3-C4-N9	4.43	134.70	127.17
2	O	1001	ADP	N3-C4-N9	4.43	134.70	127.17
2	I	1001	ADP	N3-C4-N9	4.43	134.70	127.17
2	K	1001	ADP	N3-C4-N9	4.42	134.69	127.17
2	H	1001	ADP	N3-C4-N9	4.42	134.68	127.17
2	L	1001	ADP	C5-N7-C8	3.71	109.27	103.45
2	H	1001	ADP	C5-N7-C8	3.70	109.26	103.45
2	J	1001	ADP	C5-N7-C8	3.69	109.26	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1001	ADP	C2-N3-C4	3.69	120.84	111.83
2	M	1001	ADP	C5-N7-C8	3.69	109.25	103.45
2	O	1001	ADP	C5-N7-C8	3.69	109.24	103.45
2	M	1001	ADP	C2-N3-C4	3.69	120.83	111.83
2	N	1001	ADP	C2-N3-C4	3.69	120.83	111.83
2	L	1001	ADP	C2-N3-C4	3.68	120.83	111.83
2	G	1001	ADP	C5-N7-C8	3.68	109.24	103.45
2	P	1001	ADP	C2-N3-C4	3.68	120.83	111.83
2	C	1001	ADP	C2-N3-C4	3.68	120.82	111.83
2	F	1001	ADP	C5-N7-C8	3.68	109.23	103.45
2	I	1001	ADP	C5-N7-C8	3.68	109.23	103.45
2	K	1001	ADP	C5-N7-C8	3.68	109.23	103.45
2	A	1001	ADP	C2-N3-C4	3.68	120.81	111.83
2	D	1001	ADP	C5-N7-C8	3.68	109.23	103.45
2	G	1001	ADP	C2-N3-C4	3.68	120.81	111.83
2	F	1001	ADP	C2-N3-C4	3.68	120.81	111.83
2	A	1001	ADP	C5-N7-C8	3.68	109.23	103.45
2	C	1001	ADP	C5-N7-C8	3.68	109.23	103.45
2	B	1001	ADP	C2-N3-C4	3.67	120.81	111.83
2	O	1001	ADP	C2-N3-C4	3.67	120.80	111.83
2	K	1001	ADP	C2-N3-C4	3.67	120.79	111.83
2	E	1001	ADP	C5-N7-C8	3.67	109.22	103.45
2	P	1001	ADP	C5-N7-C8	3.67	109.22	103.45
2	H	1001	ADP	C2-N3-C4	3.67	120.79	111.83
2	J	1001	ADP	C2-N3-C4	3.67	120.79	111.83
2	E	1001	ADP	C2-N3-C4	3.67	120.79	111.83
2	I	1001	ADP	C2-N3-C4	3.66	120.76	111.83
2	N	1001	ADP	C5-N7-C8	3.65	109.19	103.45
2	B	1001	ADP	C5-N7-C8	3.64	109.17	103.45
2	G	1001	ADP	C4-C5-N7	-2.71	107.48	110.58
2	O	1001	ADP	C4-C5-N7	-2.71	107.49	110.58
2	C	1001	ADP	C4-C5-N7	-2.70	107.49	110.58
2	M	1001	ADP	C4-C5-N7	-2.70	107.50	110.58
2	K	1001	ADP	C4-C5-N7	-2.69	107.51	110.58
2	D	1001	ADP	C4-C5-N7	-2.69	107.51	110.58
2	J	1001	ADP	C4-C5-N7	-2.68	107.52	110.58
2	H	1001	ADP	C4-C5-N7	-2.68	107.52	110.58
2	L	1001	ADP	C4-C5-N7	-2.67	107.52	110.58
2	A	1001	ADP	C4-C5-N7	-2.67	107.53	110.58
2	E	1001	ADP	C4-C5-N7	-2.67	107.53	110.58
2	F	1001	ADP	C4-C5-N7	-2.66	107.54	110.58
2	I	1001	ADP	C4-C5-N7	-2.65	107.55	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	ADP	C4-C5-N7	-2.65	107.55	110.58
2	P	1001	ADP	C4-C5-N7	-2.65	107.55	110.58
2	N	1001	ADP	C4-C5-N7	-2.65	107.56	110.58
2	L	1001	ADP	O4'-C4'-C3'	2.63	110.37	105.15
2	E	1001	ADP	O4'-C4'-C3'	2.63	110.37	105.15
2	K	1001	ADP	O4'-C4'-C3'	2.63	110.36	105.15
2	C	1001	ADP	O4'-C4'-C3'	2.63	110.36	105.15
2	J	1001	ADP	O4'-C4'-C3'	2.62	110.36	105.15
2	B	1001	ADP	O4'-C4'-C3'	2.62	110.35	105.15
2	I	1001	ADP	O4'-C4'-C3'	2.62	110.34	105.15
2	D	1001	ADP	O4'-C4'-C3'	2.61	110.34	105.15
2	A	1001	ADP	O4'-C4'-C3'	2.61	110.33	105.15
2	P	1001	ADP	O4'-C4'-C3'	2.61	110.33	105.15
2	N	1001	ADP	O4'-C4'-C3'	2.61	110.33	105.15
2	O	1001	ADP	O4'-C4'-C3'	2.61	110.33	105.15
2	H	1001	ADP	O4'-C4'-C3'	2.60	110.32	105.15
2	F	1001	ADP	O4'-C4'-C3'	2.60	110.31	105.15
2	G	1001	ADP	O4'-C4'-C3'	2.60	110.31	105.15
2	M	1001	ADP	O4'-C4'-C3'	2.59	110.30	105.15
2	L	1001	ADP	N9-C8-N7	-2.33	110.62	113.94
2	I	1001	ADP	N9-C8-N7	-2.33	110.64	113.94
2	O	1001	ADP	N9-C8-N7	-2.32	110.65	113.94
2	M	1001	ADP	N9-C8-N7	-2.31	110.66	113.94
2	C	1001	ADP	N9-C8-N7	-2.31	110.66	113.94
2	P	1001	ADP	N9-C8-N7	-2.31	110.66	113.94
2	A	1001	ADP	N9-C8-N7	-2.30	110.67	113.94
2	E	1001	ADP	N9-C8-N7	-2.30	110.67	113.94
2	F	1001	ADP	N9-C8-N7	-2.30	110.67	113.94
2	J	1001	ADP	N9-C8-N7	-2.30	110.67	113.94
2	N	1001	ADP	N9-C8-N7	-2.30	110.67	113.94
2	H	1001	ADP	N9-C8-N7	-2.30	110.68	113.94
2	K	1001	ADP	N9-C8-N7	-2.29	110.68	113.94
2	D	1001	ADP	N9-C8-N7	-2.29	110.68	113.94
2	G	1001	ADP	N9-C8-N7	-2.29	110.69	113.94
2	B	1001	ADP	N9-C8-N7	-2.27	110.72	113.94
2	H	1001	ADP	PA-O5'-C5'	-2.24	108.53	121.35
2	E	1001	ADP	PA-O5'-C5'	-2.24	108.54	121.35
2	O	1001	ADP	PA-O5'-C5'	-2.24	108.54	121.35
2	G	1001	ADP	PA-O5'-C5'	-2.23	108.55	121.35
2	D	1001	ADP	PA-O5'-C5'	-2.23	108.55	121.35
2	M	1001	ADP	PA-O5'-C5'	-2.23	108.55	121.35
2	B	1001	ADP	PA-O5'-C5'	-2.23	108.56	121.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	1001	ADP	PA-O5'-C5'	-2.23	108.56	121.35
2	A	1001	ADP	PA-O5'-C5'	-2.23	108.56	121.35
2	K	1001	ADP	PA-O5'-C5'	-2.23	108.57	121.35
2	I	1001	ADP	PA-O5'-C5'	-2.23	108.57	121.35
2	C	1001	ADP	PA-O5'-C5'	-2.23	108.57	121.35
2	P	1001	ADP	PA-O5'-C5'	-2.23	108.57	121.35
2	F	1001	ADP	PA-O5'-C5'	-2.23	108.58	121.35
2	J	1001	ADP	PA-O5'-C5'	-2.23	108.58	121.35
2	N	1001	ADP	PA-O5'-C5'	-2.23	108.59	121.35
2	K	1001	ADP	C5'-C4'-C3'	-2.17	107.39	115.21
2	I	1001	ADP	C5'-C4'-C3'	-2.17	107.39	115.21
2	C	1001	ADP	C5'-C4'-C3'	-2.17	107.40	115.21
2	L	1001	ADP	C5'-C4'-C3'	-2.17	107.41	115.21
2	F	1001	ADP	C5'-C4'-C3'	-2.17	107.41	115.21
2	M	1001	ADP	C5'-C4'-C3'	-2.17	107.41	115.21
2	N	1001	ADP	C5'-C4'-C3'	-2.17	107.41	115.21
2	P	1001	ADP	C5'-C4'-C3'	-2.17	107.41	115.21
2	A	1001	ADP	C5'-C4'-C3'	-2.17	107.42	115.21
2	J	1001	ADP	C5'-C4'-C3'	-2.16	107.42	115.21
2	D	1001	ADP	C5'-C4'-C3'	-2.16	107.42	115.21
2	H	1001	ADP	C5'-C4'-C3'	-2.16	107.43	115.21
2	B	1001	ADP	C5'-C4'-C3'	-2.16	107.43	115.21
2	E	1001	ADP	C5'-C4'-C3'	-2.16	107.43	115.21
2	O	1001	ADP	C5'-C4'-C3'	-2.16	107.45	115.21
2	G	1001	ADP	C5'-C4'-C3'	-2.15	107.46	115.21

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	ADP	C2'-C1'-N9-C8
2	B	1001	ADP	C2'-C1'-N9-C8
2	C	1001	ADP	C2'-C1'-N9-C8
2	D	1001	ADP	C2'-C1'-N9-C8
2	E	1001	ADP	C2'-C1'-N9-C8
2	F	1001	ADP	C2'-C1'-N9-C8
2	H	1001	ADP	C2'-C1'-N9-C8
2	I	1001	ADP	C2'-C1'-N9-C8
2	J	1001	ADP	C2'-C1'-N9-C8
2	K	1001	ADP	C2'-C1'-N9-C8
2	L	1001	ADP	C2'-C1'-N9-C8
2	M	1001	ADP	C2'-C1'-N9-C8

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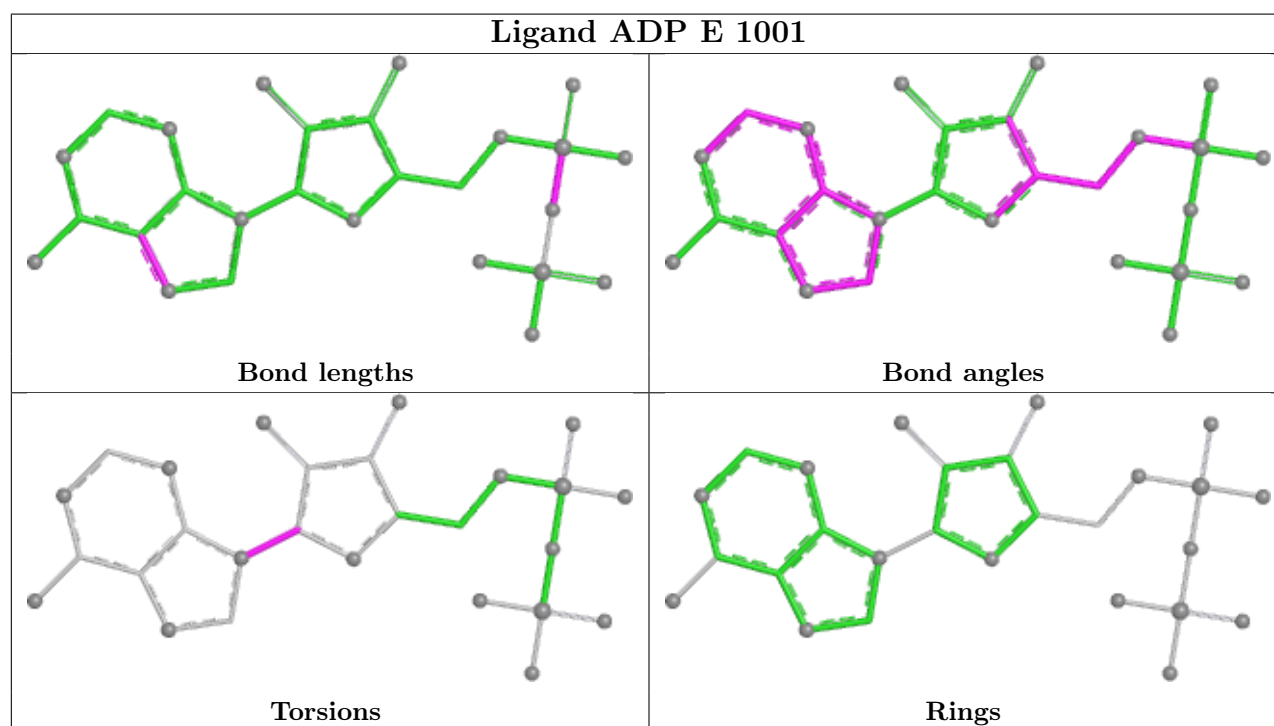
Mol	Chain	Res	Type	Atoms
2	P	1001	ADP	C2'-C1'-N9-C8
2	A	1001	ADP	C2'-C1'-N9-C4
2	B	1001	ADP	C2'-C1'-N9-C4
2	C	1001	ADP	C2'-C1'-N9-C4
2	D	1001	ADP	C2'-C1'-N9-C4
2	E	1001	ADP	C2'-C1'-N9-C4
2	F	1001	ADP	C2'-C1'-N9-C4
2	G	1001	ADP	C2'-C1'-N9-C4
2	H	1001	ADP	C2'-C1'-N9-C4
2	I	1001	ADP	C2'-C1'-N9-C4
2	J	1001	ADP	C2'-C1'-N9-C4
2	K	1001	ADP	C2'-C1'-N9-C4
2	L	1001	ADP	C2'-C1'-N9-C4
2	M	1001	ADP	C2'-C1'-N9-C4
2	N	1001	ADP	C2'-C1'-N9-C4
2	O	1001	ADP	C2'-C1'-N9-C4
2	P	1001	ADP	C2'-C1'-N9-C4
2	G	1001	ADP	C2'-C1'-N9-C8
2	N	1001	ADP	C2'-C1'-N9-C8
2	O	1001	ADP	C2'-C1'-N9-C8

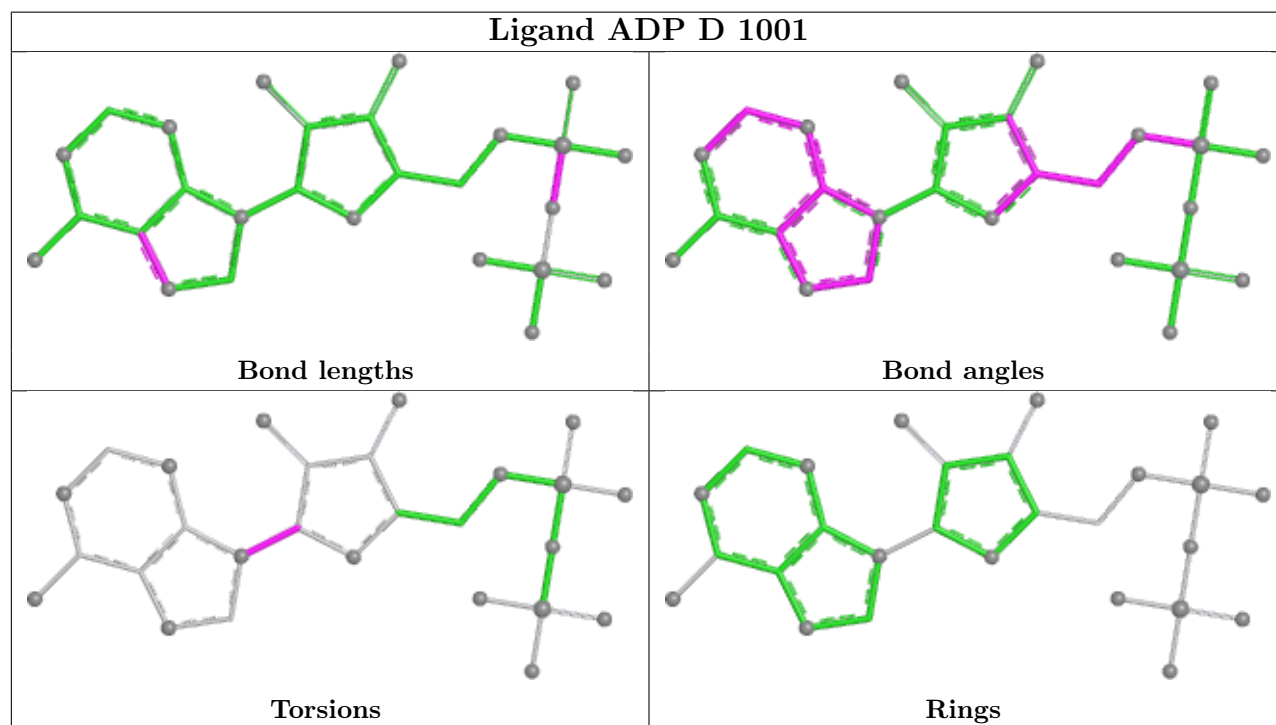
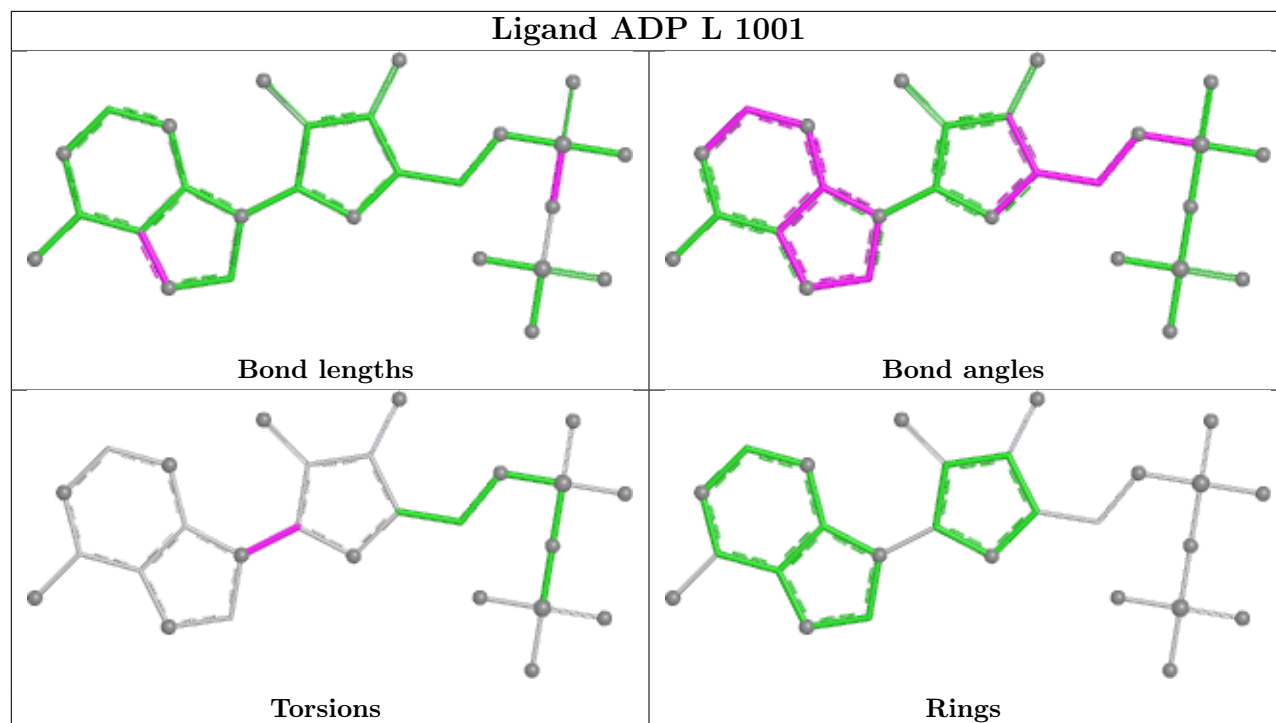
There are no ring outliers.

16 monomers are involved in 50 short contacts:

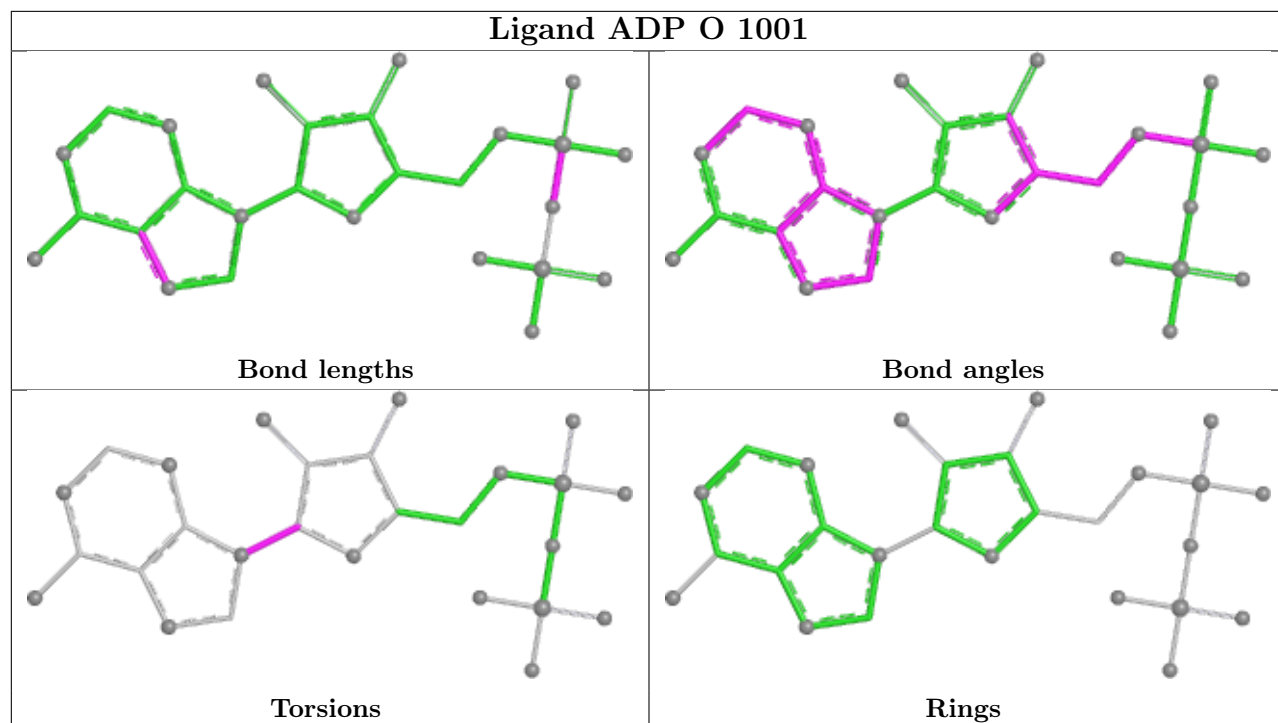
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1001	ADP	3	0
2	L	1001	ADP	3	0
2	D	1001	ADP	3	0
2	O	1001	ADP	3	0
2	P	1001	ADP	4	0
2	I	1001	ADP	3	0
2	A	1001	ADP	3	0
2	H	1001	ADP	3	0
2	N	1001	ADP	3	0
2	J	1001	ADP	3	0
2	G	1001	ADP	3	0
2	C	1001	ADP	3	0
2	K	1001	ADP	4	0
2	B	1001	ADP	3	0
2	M	1001	ADP	3	0
2	F	1001	ADP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

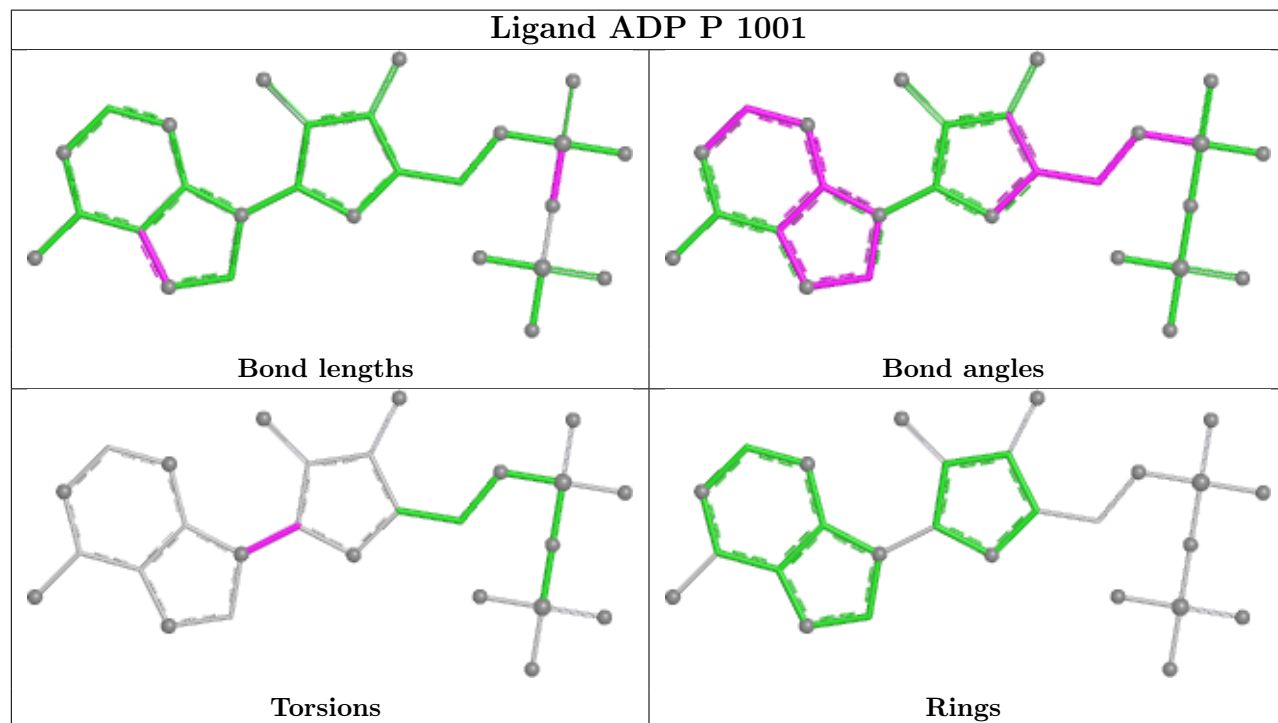


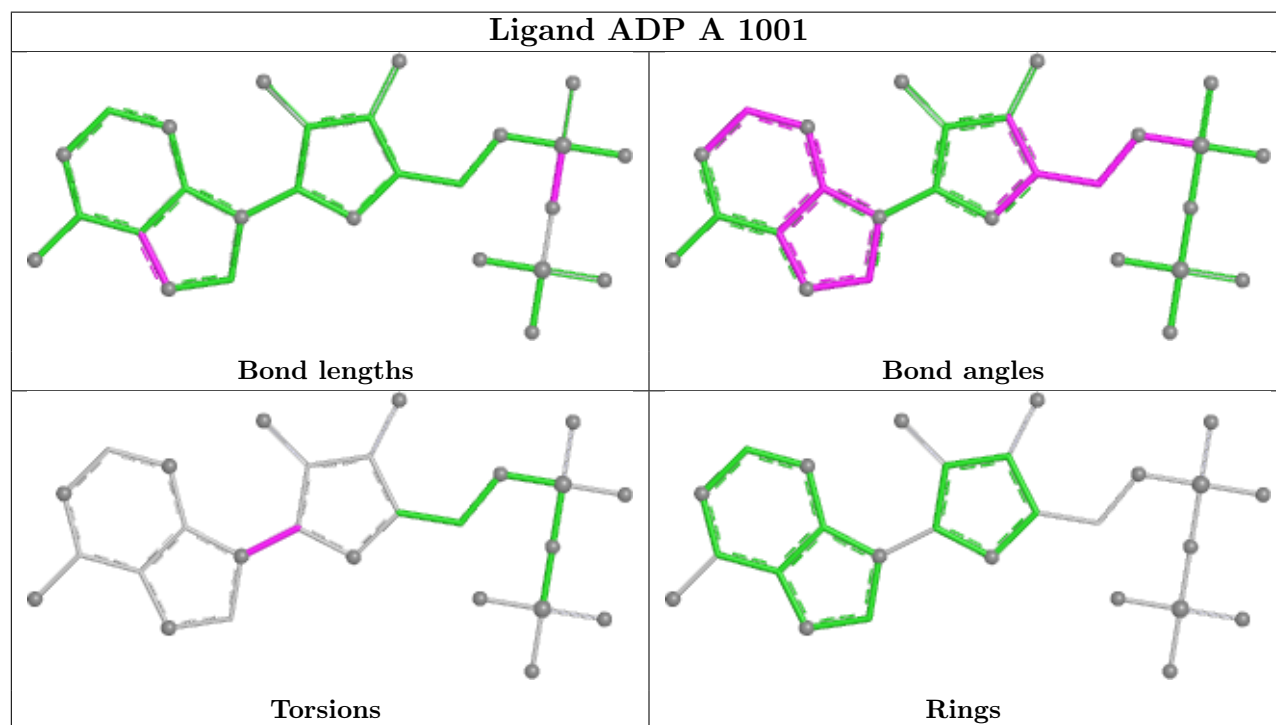
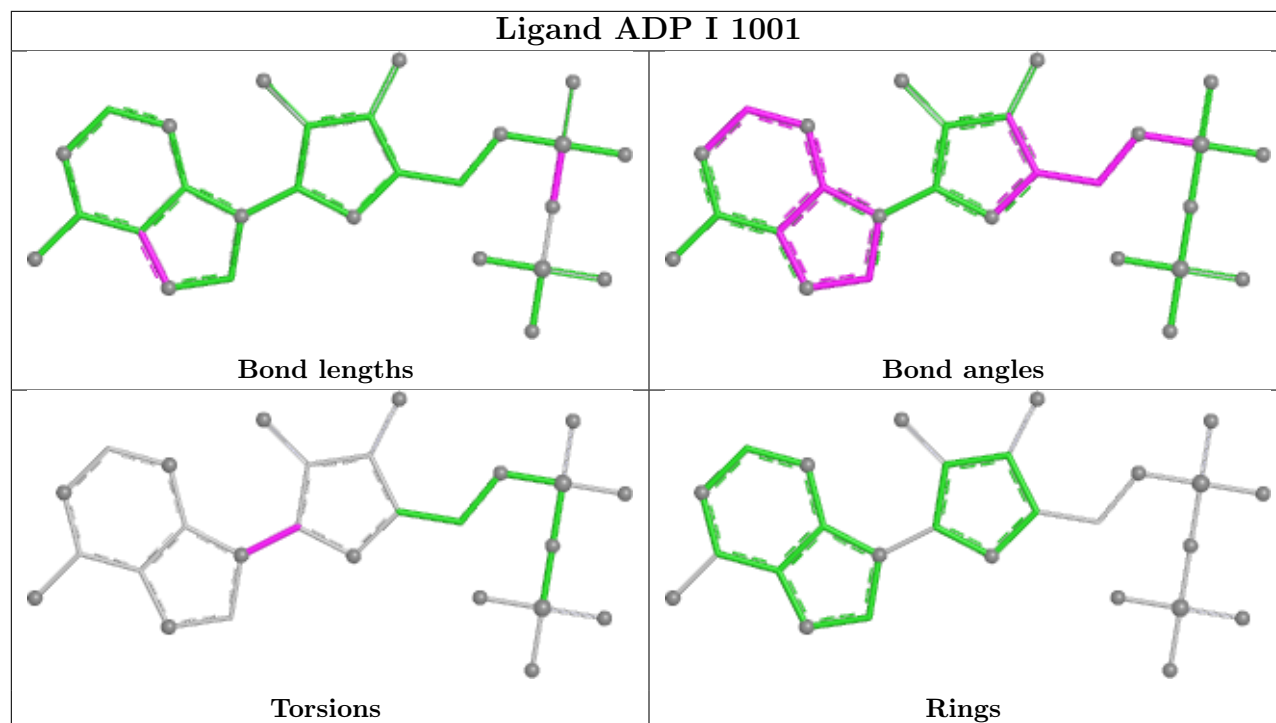


Ligand ADP O 1001

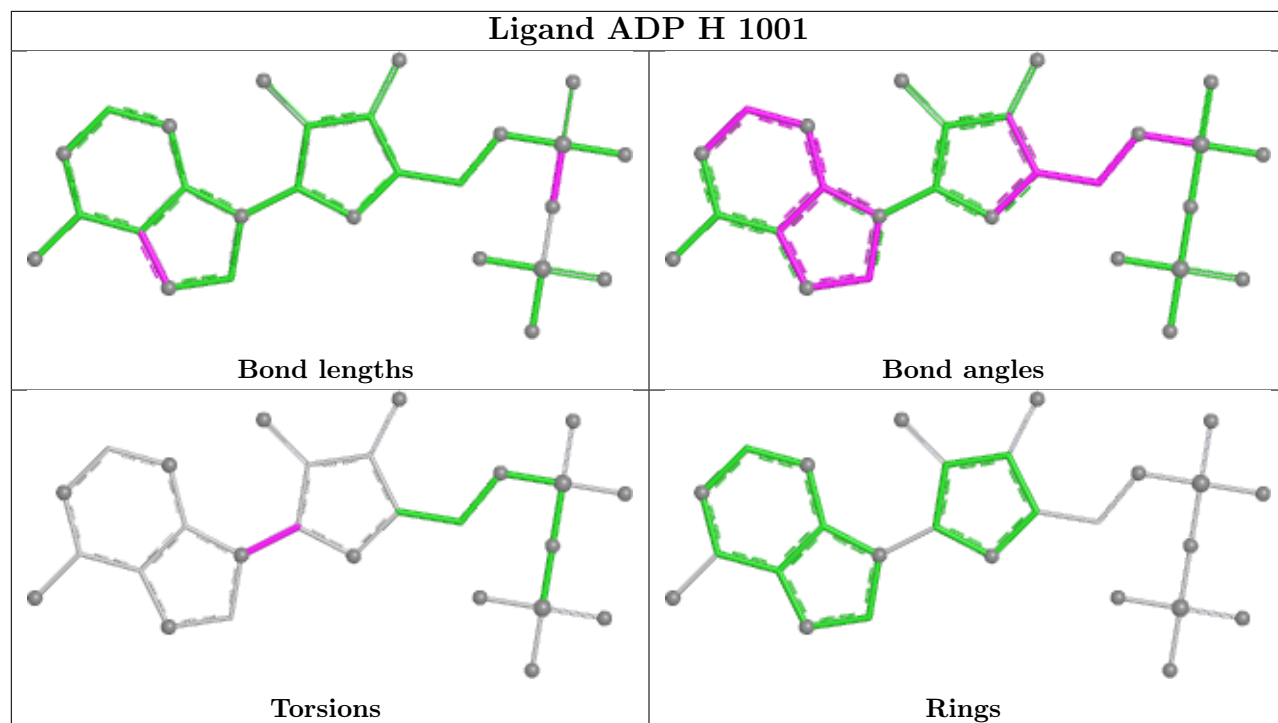


Ligand ADP P 1001

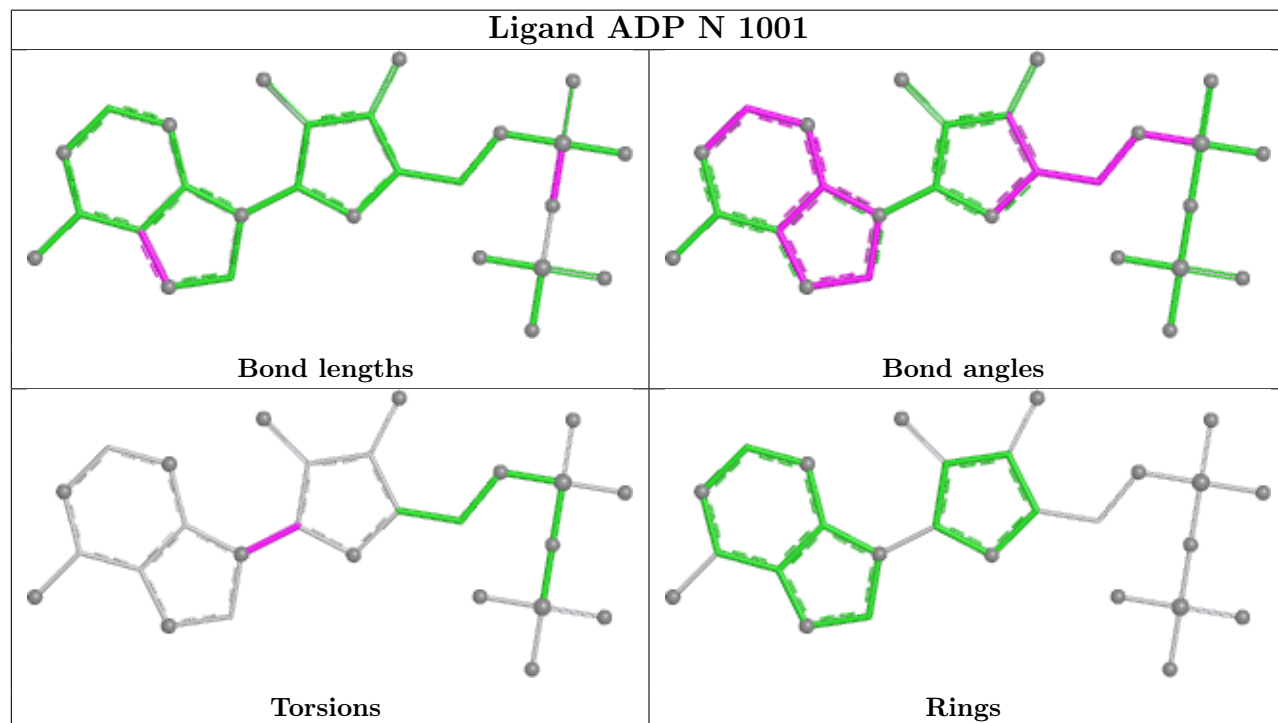


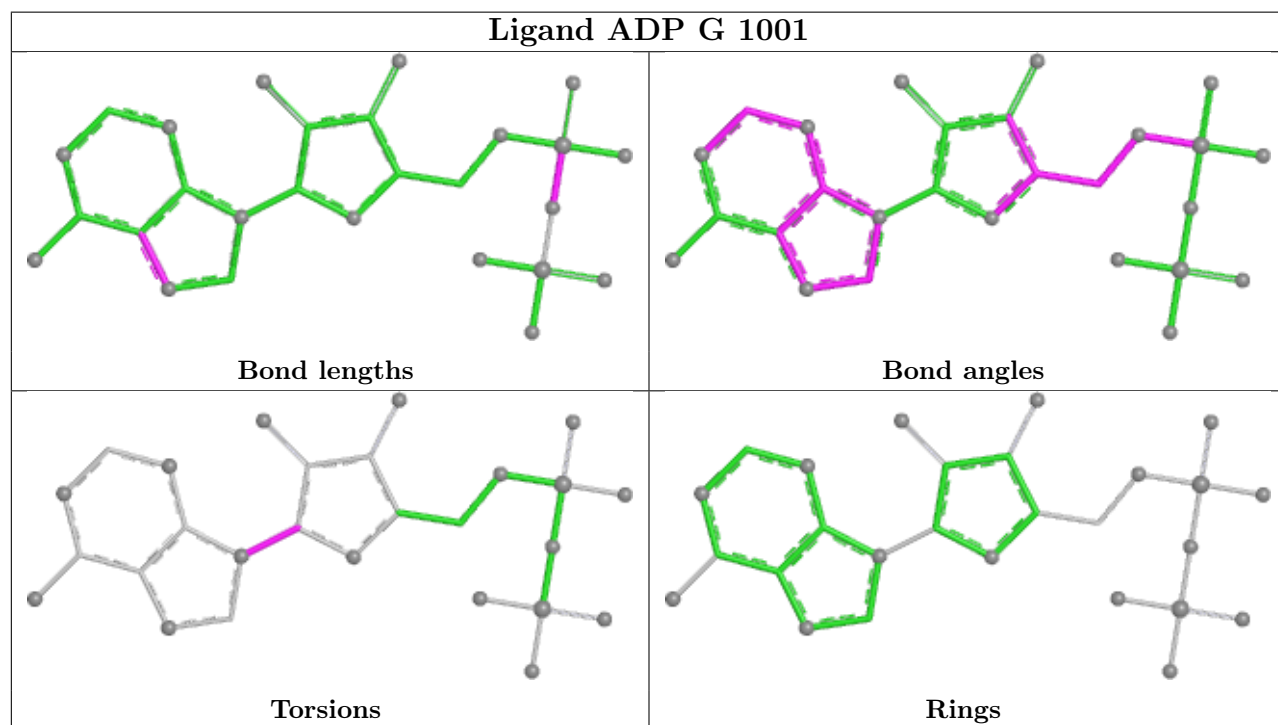
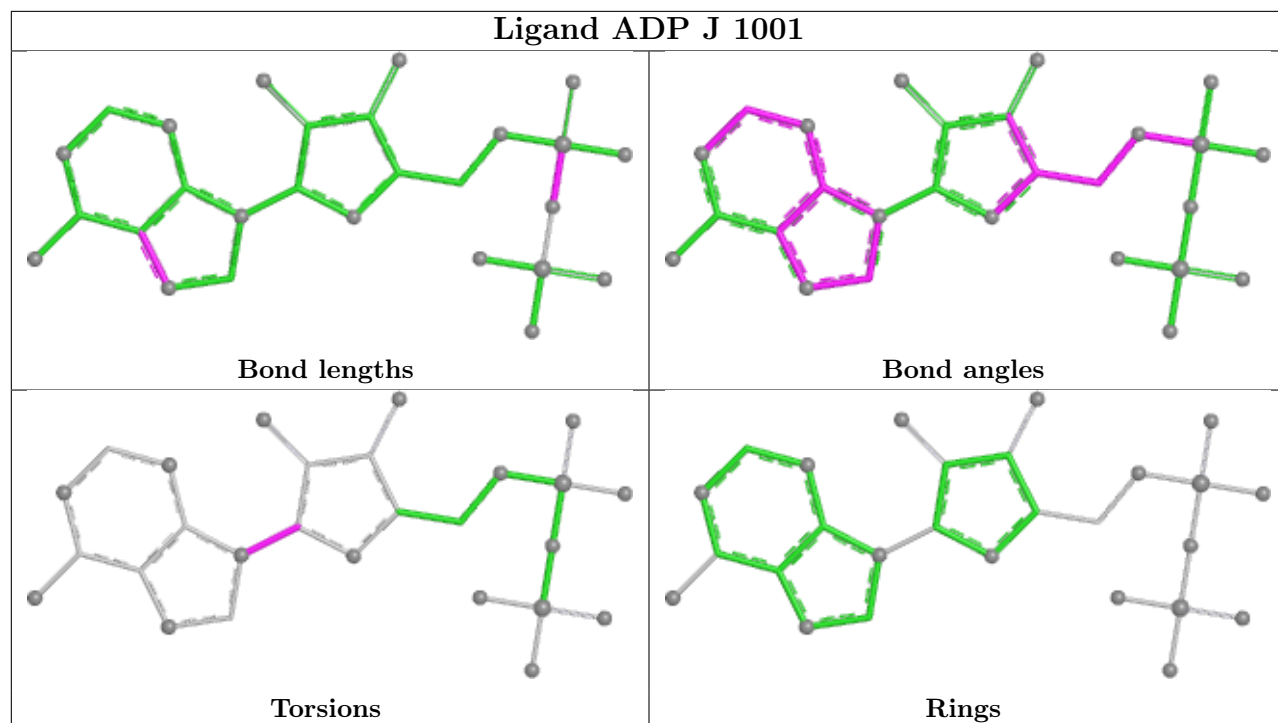


Ligand ADP H 1001

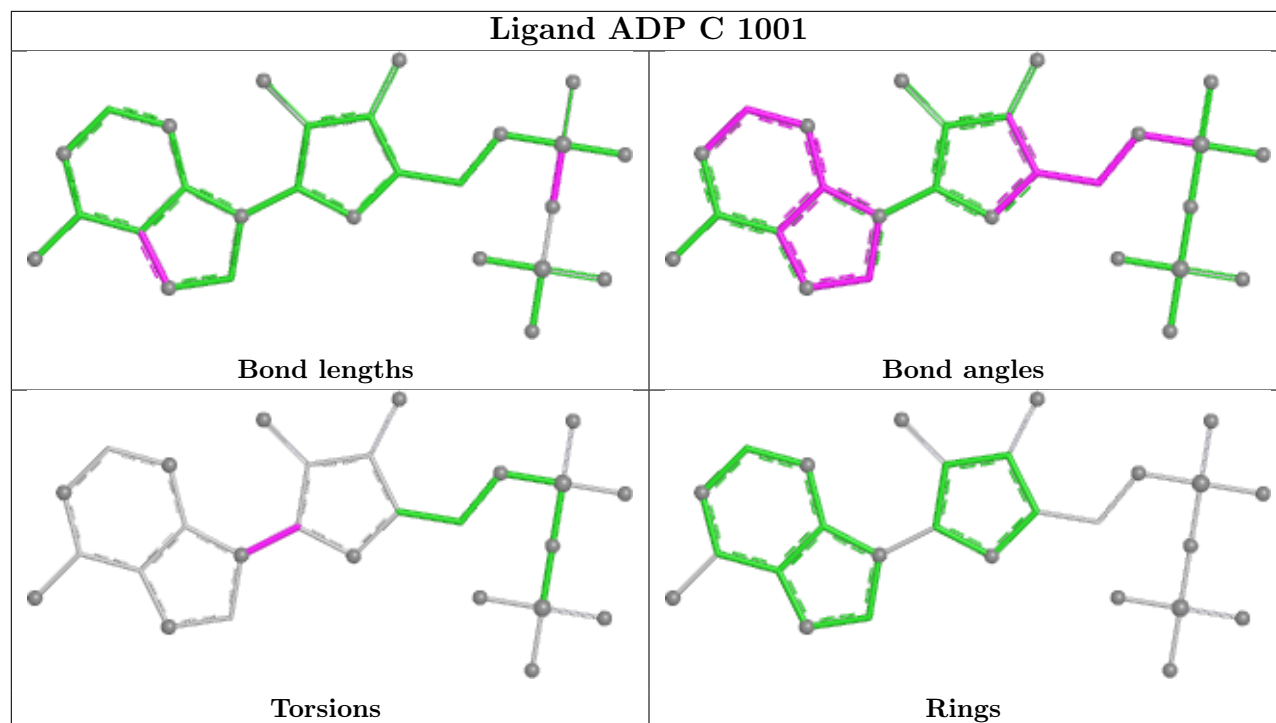


Ligand ADP N 1001

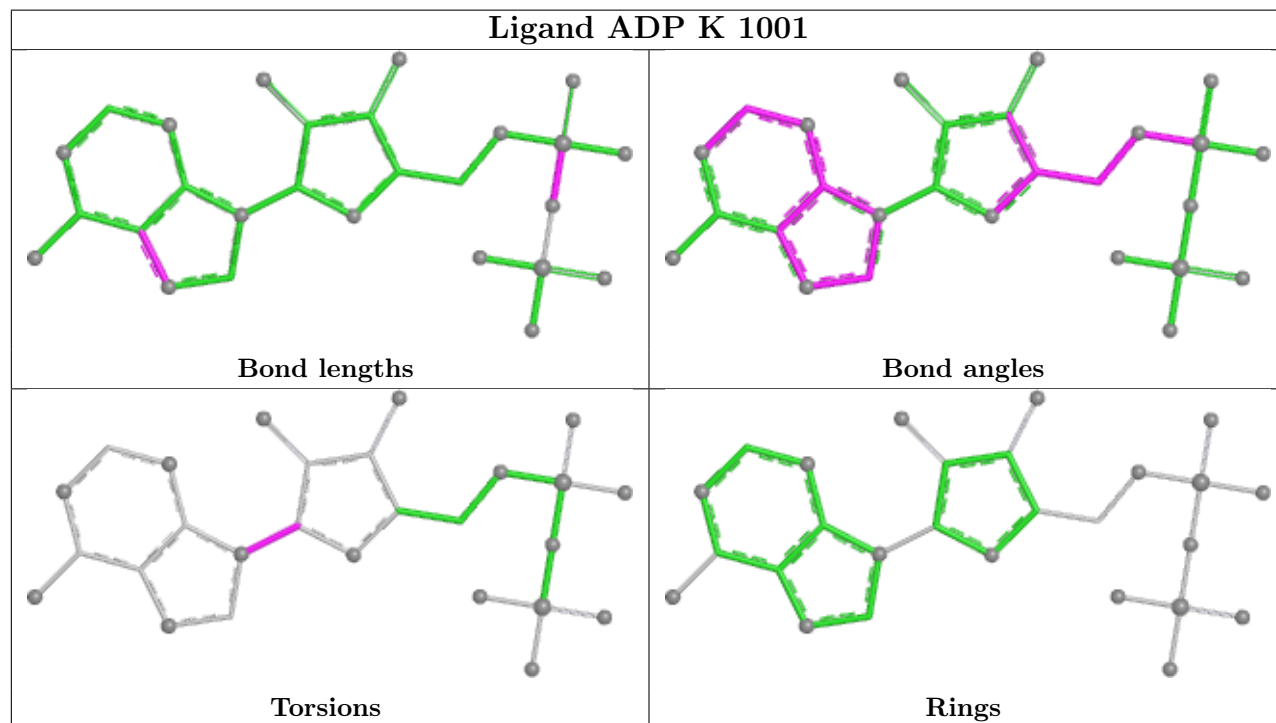




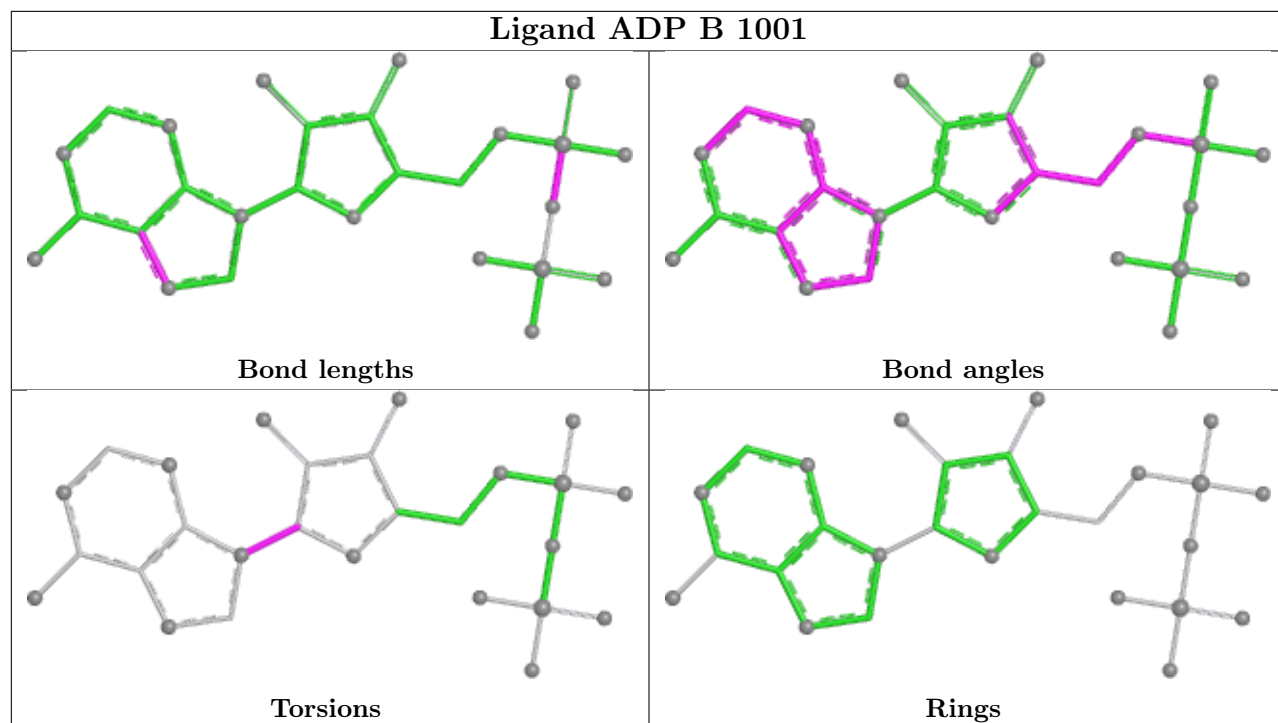
Ligand ADP C 1001



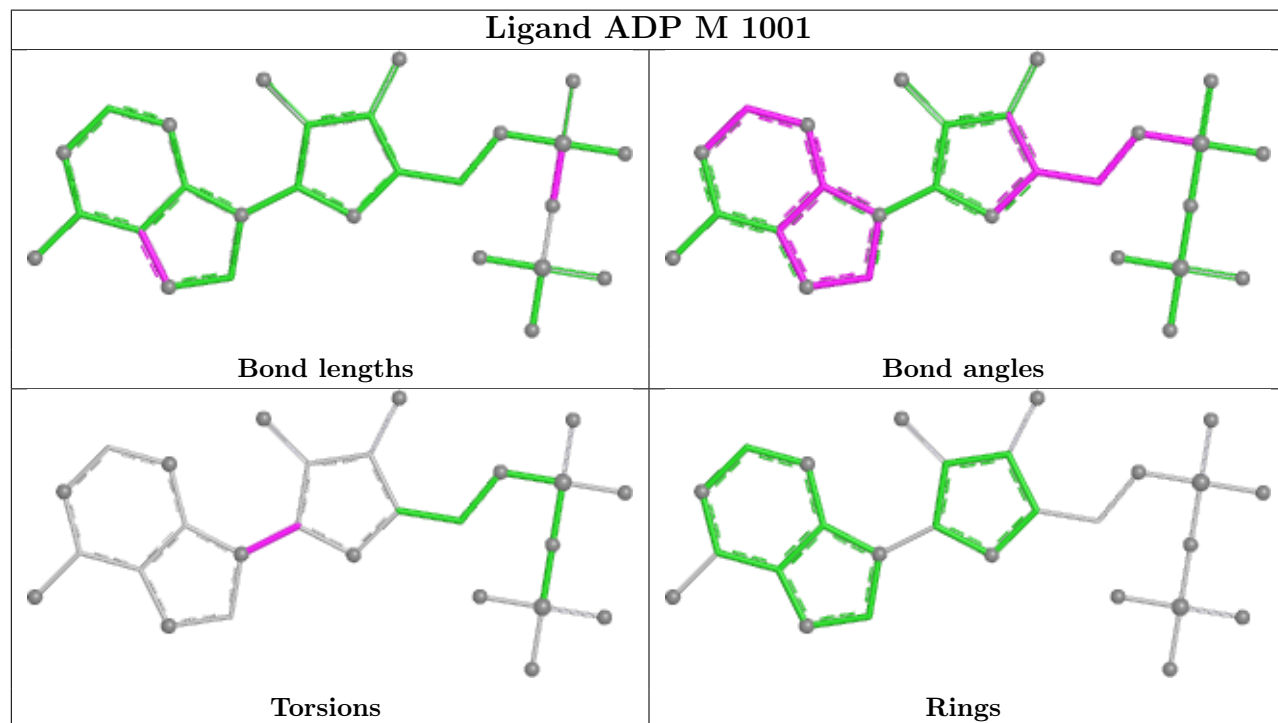
Ligand ADP K 1001

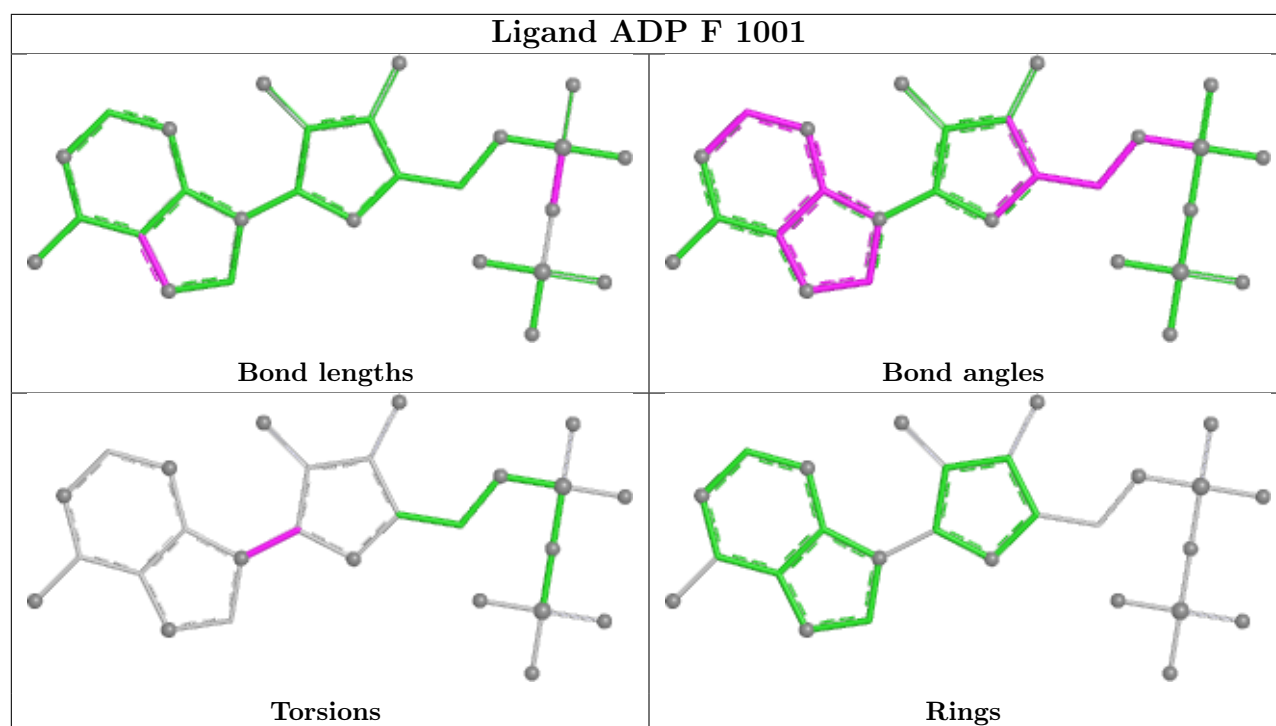


Ligand ADP B 1001



Ligand ADP M 1001





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 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	289/338 (85%)	1.08	37 (12%) 7 11	21, 84, 146, 251	0
1	B	289/338 (85%)	0.61	15 (5%) 33 25	21, 84, 146, 251	0
1	C	289/338 (85%)	0.63	14 (4%) 35 26	21, 84, 146, 251	0
1	D	289/338 (85%)	0.88	19 (6%) 24 21	21, 84, 146, 251	0
1	E	289/338 (85%)	0.91	28 (9%) 13 15	21, 84, 146, 251	0
1	F	289/338 (85%)	0.75	16 (5%) 30 23	21, 84, 146, 251	0
1	G	289/338 (85%)	1.18	46 (15%) 5 8	21, 84, 146, 251	0
1	H	289/338 (85%)	0.89	18 (6%) 26 22	21, 84, 146, 251	0
1	I	289/338 (85%)	0.78	20 (6%) 23 20	21, 84, 146, 251	0
1	J	289/338 (85%)	0.94	29 (10%) 12 15	21, 84, 146, 251	0
1	K	289/338 (85%)	0.83	17 (5%) 28 23	21, 84, 146, 251	0
1	L	289/338 (85%)	1.31	53 (18%) 3 6	21, 84, 146, 251	0
1	M	289/338 (85%)	0.90	26 (8%) 15 16	21, 84, 146, 251	0
1	N	289/338 (85%)	1.16	41 (14%) 6 9	21, 84, 146, 251	0
1	O	289/338 (85%)	1.33	62 (21%) 2 4	21, 84, 146, 251	0
1	P	289/338 (85%)	0.70	14 (4%) 35 26	21, 84, 146, 251	0
All	All	4624/5408 (85%)	0.93	455 (9%) 13 15	21, 84, 146, 251	0

All (455) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	315	GLY	6.7
1	F	857	GLY	5.9
1	N	891	MET	5.6
1	L	857	GLY	5.4
1	A	807	GLY	5.3

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Mol	Chain	Res	Type	RSRZ
1	L	314	ASP	5.3
1	P	857	GLY	5.2
1	N	857	GLY	5.2
1	B	810	ASN	5.1
1	K	857	GLY	5.0
1	L	884	PRO	4.7
1	G	314	ASP	4.7
1	H	810	ASN	4.6
1	J	964	ALA	4.6
1	M	810	ASN	4.6
1	O	810	ASN	4.5
1	J	852	LEU	4.4
1	L	932	SER	4.4
1	L	941	SER	4.4
1	N	316	THR	4.3
1	B	857	GLY	4.2
1	G	877	TYR	4.2
1	O	796	THR	4.2
1	L	933	GLU	4.2
1	G	871	LEU	4.1
1	E	315	GLY	4.1
1	G	878	ALA	4.1
1	K	272	LEU	4.0
1	L	315	GLY	4.0
1	E	857	GLY	3.9
1	C	857	GLY	3.9
1	G	861	VAL	3.9
1	H	803	ASN	3.8
1	C	314	ASP	3.8
1	F	859	SER	3.8
1	M	857	GLY	3.7
1	J	855	ARG	3.7
1	O	754	GLY	3.7
1	J	803	ASN	3.7
1	O	791	THR	3.6
1	L	349	ILE	3.6
1	E	807	GLY	3.6
1	J	859	SER	3.6
1	N	315	GLY	3.6
1	O	347	ARG	3.6
1	J	854	VAL	3.5
1	L	310	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	J	848	ALA	3.5
1	L	878	ALA	3.5
1	N	279	VAL	3.5
1	O	793	ASN	3.5
1	N	885	VAL	3.4
1	G	941	SER	3.4
1	E	861	VAL	3.4
1	J	810	ASN	3.4
1	E	810	ASN	3.4
1	A	854	VAL	3.4
1	N	817	GLU	3.4
1	I	891	MET	3.4
1	K	810	ASN	3.4
1	N	926	GLU	3.3
1	M	790	ALA	3.3
1	G	874	TYR	3.3
1	O	781	ILE	3.3
1	A	857	GLY	3.3
1	I	315	GLY	3.3
1	J	861	VAL	3.2
1	J	351	THR	3.2
1	E	854	VAL	3.2
1	G	845	SER	3.2
1	O	920	ILE	3.2
1	G	279	VAL	3.2
1	N	306	GLY	3.2
1	B	316	THR	3.2
1	L	791	THR	3.2
1	L	794	ALA	3.2
1	M	775	ALA	3.2
1	L	760	GLU	3.2
1	H	332	VAL	3.2
1	N	788	ILE	3.1
1	O	783	ILE	3.1
1	O	780	THR	3.1
1	G	884	PRO	3.1
1	L	789	THR	3.1
1	G	272	LEU	3.1
1	L	877	TYR	3.1
1	L	885	VAL	3.1
1	G	763	LYS	3.1
1	C	315	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	O	807	GLY	3.1
1	C	794	ALA	3.0
1	G	852	LEU	3.0
1	N	883	HIS	3.0
1	E	965	MET	3.0
1	L	308	VAL	3.0
1	O	820	ASP	3.0
1	E	859	SER	3.0
1	N	854	VAL	3.0
1	C	810	ASN	3.0
1	O	777	GLU	3.0
1	N	886	ILE	3.0
1	A	820	ASP	3.0
1	D	762	ASP	3.0
1	N	884	PRO	2.9
1	J	857	GLY	2.9
1	C	861	VAL	2.9
1	D	810	ASN	2.9
1	A	264	GLU	2.9
1	F	777	GLU	2.9
1	A	317	ARG	2.9
1	E	855	ARG	2.9
1	O	269	ILE	2.9
1	F	810	ASN	2.9
1	F	858	GLU	2.9
1	O	308	VAL	2.9
1	D	314	ASP	2.9
1	O	794	ALA	2.9
1	B	812	MET	2.9
1	E	837	ASP	2.8
1	L	870	ILE	2.8
1	E	927	ALA	2.8
1	M	332	VAL	2.8
1	O	803	ASN	2.8
1	N	943	ILE	2.8
1	O	809	PHE	2.8
1	L	783	ILE	2.8
1	D	803	ASN	2.8
1	E	314	ASP	2.8
1	J	764	MET	2.8
1	J	310	ARG	2.8
1	O	823	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	J	315	GLY	2.8
1	N	858	GLU	2.8
1	L	876	ALA	2.8
1	O	964	ALA	2.8
1	B	858	GLU	2.8
1	G	810	ASN	2.8
1	K	796	THR	2.8
1	P	941	SER	2.8
1	K	794	ALA	2.8
1	O	792	LEU	2.7
1	F	854	VAL	2.7
1	G	305	PHE	2.7
1	O	940	LEU	2.7
1	J	836	ILE	2.7
1	G	857	GLY	2.7
1	L	318	LEU	2.7
1	P	922	ALA	2.7
1	L	768	ASP	2.7
1	I	855	ARG	2.7
1	N	273	ALA	2.7
1	O	817	GLU	2.7
1	P	810	ASN	2.7
1	O	859	SER	2.7
1	N	308	VAL	2.7
1	I	790	ALA	2.7
1	A	316	THR	2.7
1	J	858	GLU	2.7
1	O	789	THR	2.7
1	I	311	LYS	2.7
1	J	314	ASP	2.7
1	O	857	GLY	2.7
1	A	271	GLU	2.7
1	G	858	GLU	2.7
1	D	352	SER	2.7
1	K	308	VAL	2.6
1	E	841	ASP	2.6
1	E	876	ALA	2.6
1	O	756	ALA	2.6
1	O	816	PHE	2.6
1	C	941	SER	2.6
1	E	839	PRO	2.6
1	H	331	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	N	314	ASP	2.6
1	G	938	MET	2.6
1	L	776	LEU	2.6
1	O	784	SER	2.6
1	F	778	GLN	2.6
1	M	753	GLY	2.6
1	A	835	LEU	2.6
1	L	925	LEU	2.6
1	P	318	LEU	2.6
1	K	288	PRO	2.6
1	L	753	GLY	2.6
1	L	940	LEU	2.6
1	E	860	GLU	2.6
1	F	784	SER	2.6
1	L	836	ILE	2.6
1	G	789	THR	2.6
1	N	898	TYR	2.6
1	G	882	ILE	2.6
1	M	329	ASP	2.6
1	M	820	ASP	2.6
1	F	890	ALA	2.6
1	N	962	GLN	2.6
1	G	315	GLY	2.6
1	B	317	ARG	2.5
1	O	834	VAL	2.5
1	L	871	LEU	2.5
1	L	346	PRO	2.5
1	B	315	GLY	2.5
1	I	857	GLY	2.5
1	D	921	THR	2.5
1	E	874	TYR	2.5
1	O	770	SER	2.5
1	O	266	GLU	2.5
1	P	947	GLU	2.5
1	L	812	MET	2.5
1	L	841	ASP	2.5
1	G	313	PRO	2.5
1	N	331	GLY	2.5
1	G	788	ILE	2.5
1	F	892	GLU	2.5
1	E	289	ALA	2.5
1	E	964	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	O	884	PRO	2.5
1	H	309	SER	2.5
1	J	774	GLU	2.5
1	G	943	ILE	2.5
1	M	315	GLY	2.5
1	C	317	ARG	2.5
1	J	791	THR	2.5
1	A	836	ILE	2.5
1	L	810	ASN	2.5
1	J	802	ALA	2.5
1	O	804	PRO	2.5
1	A	841	ASP	2.5
1	F	314	ASP	2.5
1	I	347	ARG	2.5
1	O	776	LEU	2.5
1	O	811	ARG	2.5
1	D	891	MET	2.5
1	H	942	PRO	2.4
1	H	308	VAL	2.4
1	E	264	GLU	2.4
1	I	876	ALA	2.4
1	M	792	LEU	2.4
1	A	839	PRO	2.4
1	G	859	SER	2.4
1	L	771	VAL	2.4
1	A	775	ALA	2.4
1	L	779	GLN	2.4
1	F	316	THR	2.4
1	L	316	THR	2.4
1	H	820	ASP	2.4
1	L	319	ARG	2.4
1	O	323	HIS	2.4
1	B	778	GLN	2.4
1	D	942	PRO	2.4
1	M	825	LEU	2.4
1	A	874	TYR	2.4
1	A	898	TYR	2.4
1	L	874	TYR	2.4
1	D	774	GLU	2.4
1	D	858	GLU	2.4
1	E	808	ARG	2.4
1	A	862	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	K	894	ILE	2.4
1	G	855	ARG	2.4
1	K	858	GLU	2.4
1	O	778	GLN	2.3
1	A	810	ASN	2.3
1	E	942	PRO	2.3
1	D	859	SER	2.3
1	G	932	SER	2.3
1	L	881	ASN	2.3
1	I	894	ILE	2.3
1	N	894	ILE	2.3
1	H	780	THR	2.3
1	O	877	TYR	2.3
1	N	800	ALA	2.3
1	A	804	PRO	2.3
1	M	839	PRO	2.3
1	A	791	THR	2.3
1	F	824	THR	2.3
1	L	279	VAL	2.3
1	L	780	THR	2.3
1	M	347	ARG	2.3
1	H	876	ALA	2.3
1	G	820	ASP	2.3
1	G	864	PRO	2.3
1	O	753	GLY	2.3
1	A	861	VAL	2.3
1	I	319	ARG	2.3
1	L	938	MET	2.3
1	A	962	GLN	2.3
1	G	286	ILE	2.3
1	D	315	GLY	2.3
1	N	861	VAL	2.3
1	I	803	ASN	2.3
1	G	298	LYS	2.3
1	J	801	ALA	2.3
1	J	922	ALA	2.3
1	D	760	GLU	2.3
1	G	847	VAL	2.3
1	M	331	GLY	2.3
1	N	330	PRO	2.3
1	A	894	ILE	2.3
1	F	964	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	263	PRO	2.3
1	G	844	ASP	2.3
1	J	965	MET	2.3
1	O	284	ASP	2.3
1	O	812	MET	2.3
1	N	922	ALA	2.2
1	I	859	SER	2.2
1	B	965	MET	2.2
1	H	764	MET	2.2
1	I	331	GLY	2.2
1	O	798	VAL	2.2
1	H	825	LEU	2.2
1	N	318	LEU	2.2
1	H	311	LYS	2.2
1	N	859	SER	2.2
1	A	767	ARG	2.2
1	C	263	PRO	2.2
1	K	315	GLY	2.2
1	O	304	LEU	2.2
1	H	819	ILE	2.2
1	L	786	ALA	2.2
1	L	936	ALA	2.2
1	A	859	SER	2.2
1	H	941	SER	2.2
1	K	859	SER	2.2
1	O	774	GLU	2.2
1	N	839	PRO	2.2
1	N	942	PRO	2.2
1	A	789	THR	2.2
1	K	791	THR	2.2
1	N	810	ASN	2.2
1	G	903	LYS	2.2
1	I	844	ASP	2.2
1	O	759	ASP	2.2
1	O	785	LYS	2.2
1	D	309	SER	2.2
1	O	760	GLU	2.2
1	L	943	ILE	2.2
1	O	886	ILE	2.2
1	O	943	ILE	2.2
1	B	921	THR	2.2
1	K	789	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	O	814	ASN	2.2
1	E	329	ASP	2.2
1	K	965	MET	2.2
1	N	938	MET	2.2
1	M	779	GLN	2.2
1	M	308	VAL	2.2
1	E	843	ILE	2.2
1	B	838	GLU	2.2
1	G	860	GLU	2.2
1	L	263	PRO	2.2
1	M	816	PHE	2.2
1	O	965	MET	2.2
1	B	811	ARG	2.1
1	D	820	ASP	2.1
1	G	329	ASP	2.1
1	I	314	ASP	2.1
1	M	808	ARG	2.1
1	N	317	ARG	2.1
1	G	755	TYR	2.1
1	J	332	VAL	2.1
1	P	774	GLU	2.1
1	G	780	THR	2.1
1	J	812	MET	2.1
1	G	790	ALA	2.1
1	M	319	ARG	2.1
1	D	778	GLN	2.1
1	M	841	ASP	2.1
1	N	758	ILE	2.1
1	P	315	GLY	2.1
1	C	264	GLU	2.1
1	G	933	GLU	2.1
1	O	888	GLU	2.1
1	I	316	THR	2.1
1	A	319	ARG	2.1
1	D	814	ASN	2.1
1	P	317	ARG	2.1
1	A	845	SER	2.1
1	C	321	ASP	2.1
1	E	766	ASP	2.1
1	G	768	ASP	2.1
1	I	841	ASP	2.1
1	O	837	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	340	TYR	2.1
1	A	331	GLY	2.1
1	L	777	GLU	2.1
1	E	824	THR	2.1
1	D	794	ALA	2.1
1	B	943	ILE	2.1
1	K	803	ASN	2.1
1	O	818	GLN	2.1
1	C	854	VAL	2.1
1	O	277	ASP	2.1
1	P	841	ASP	2.1
1	A	901	MET	2.1
1	L	764	MET	2.1
1	E	869	GLU	2.1
1	H	933	GLU	2.1
1	A	788	ILE	2.1
1	F	352	SER	2.1
1	L	803	ASN	2.1
1	M	809	PHE	2.1
1	M	814	ASN	2.1
1	I	898	TYR	2.1
1	M	330	PRO	2.1
1	O	942	PRO	2.1
1	P	884	PRO	2.1
1	O	838	GLU	2.1
1	F	347	ARG	2.1
1	K	317	ARG	2.1
1	J	282	ILE	2.1
1	O	790	ALA	2.1
1	G	291	TYR	2.0
1	H	299	GLY	2.0
1	L	306	GLY	2.0
1	O	340	TYR	2.0
1	N	815	PRO	2.0
1	G	939	ARG	2.0
1	G	948	ASP	2.0
1	M	768	ASP	2.0
1	A	920	ILE	2.0
1	B	888	GLU	2.0
1	I	266	GLU	2.0
1	M	876	ALA	2.0
1	N	949	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	M	965	MET	2.0
1	A	753	GLY	2.0
1	J	278	ILE	2.0
1	L	317	ARG	2.0
1	O	868	HIS	2.0
1	O	939	ARG	2.0
1	P	310	ARG	2.0
1	C	837	ASP	2.0
1	J	820	ASP	2.0
1	L	838	GLU	2.0
1	N	830	ASP	2.0
1	I	852	LEU	2.0
1	N	778	GLN	2.0
1	A	919	PRO	2.0
1	D	319	ARG	2.0
1	G	269	ILE	2.0
1	N	310	ARG	2.0
1	P	263	PRO	2.0
1	A	760	GLU	2.0
1	E	858	GLU	2.0
1	H	816	PHE	2.0
1	J	264	GLU	2.0
1	L	312	LEU	2.0
1	L	774	GLU	2.0
1	N	940	LEU	2.0
1	P	858	GLU	2.0
1	A	289	ALA	2.0
1	A	941	SER	2.0
1	B	766	ASP	2.0
1	C	948	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

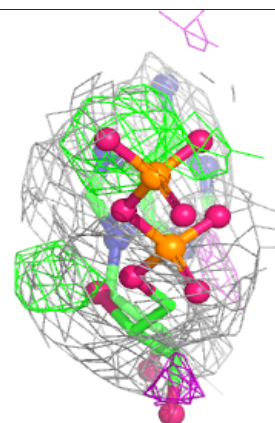
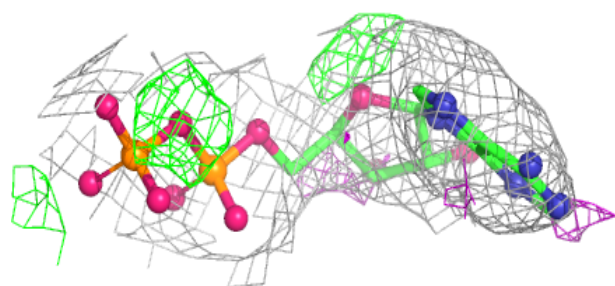
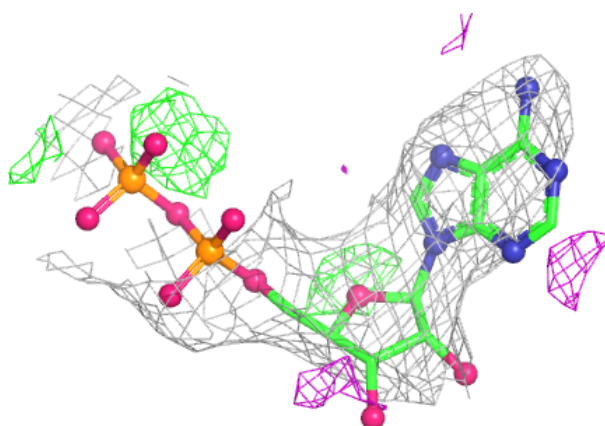
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	L	1002	1/1	0.19	0.42	81,81,81,81	0
3	MG	D	1002	1/1	0.21	0.45	81,81,81,81	0
3	MG	I	1002	1/1	0.33	0.43	81,81,81,81	0
3	MG	A	1002	1/1	0.39	0.30	81,81,81,81	0
3	MG	N	1002	1/1	0.41	0.27	81,81,81,81	0
3	MG	G	1002	1/1	0.44	0.37	81,81,81,81	0
3	MG	C	1002	1/1	0.54	0.23	81,81,81,81	0
3	MG	J	1002	1/1	0.59	0.14	81,81,81,81	0
3	MG	P	1002	1/1	0.59	0.35	81,81,81,81	0
3	MG	M	1002	1/1	0.64	0.34	81,81,81,81	0
3	MG	B	1002	1/1	0.65	0.28	81,81,81,81	0
3	MG	O	1002	1/1	0.67	0.26	81,81,81,81	0
3	MG	K	1002	1/1	0.69	0.18	81,81,81,81	0
3	MG	F	1002	1/1	0.72	0.29	81,81,81,81	0
3	MG	H	1002	1/1	0.77	0.33	81,81,81,81	0
3	MG	E	1002	1/1	0.78	0.17	81,81,81,81	0
2	ADP	A	1001	27/27	0.85	0.18	72,72,72,72	0
2	ADP	L	1001	27/27	0.85	0.17	72,72,72,72	0
2	ADP	D	1001	27/27	0.86	0.16	72,72,72,72	0
2	ADP	J	1001	27/27	0.87	0.16	72,72,72,72	0
2	ADP	H	1001	27/27	0.87	0.17	72,72,72,72	0
2	ADP	G	1001	27/27	0.88	0.19	72,72,72,72	0
2	ADP	N	1001	27/27	0.88	0.14	72,72,72,72	0
2	ADP	M	1001	27/27	0.89	0.14	72,72,72,72	0
2	ADP	E	1001	27/27	0.89	0.15	72,72,72,72	0
2	ADP	I	1001	27/27	0.89	0.15	72,72,72,72	0
2	ADP	K	1001	27/27	0.90	0.15	72,72,72,72	0
2	ADP	P	1001	27/27	0.90	0.13	72,72,72,72	0
2	ADP	C	1001	27/27	0.91	0.13	72,72,72,72	0
2	ADP	O	1001	27/27	0.92	0.14	72,72,72,72	0
2	ADP	B	1001	27/27	0.92	0.12	72,72,72,72	0
2	ADP	F	1001	27/27	0.92	0.12	72,72,72,72	0

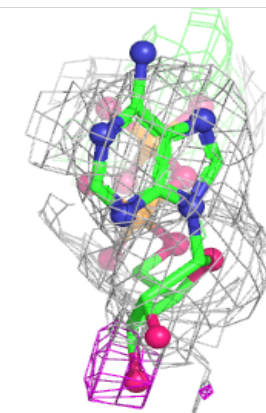
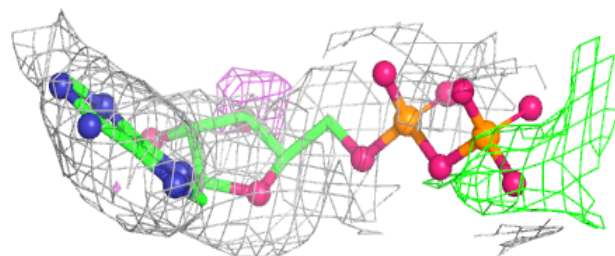
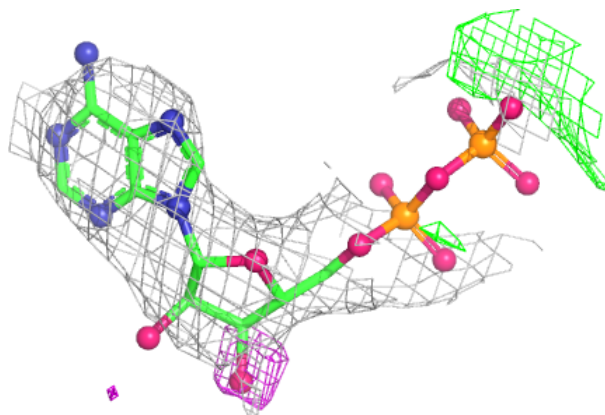
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ADP A 1001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

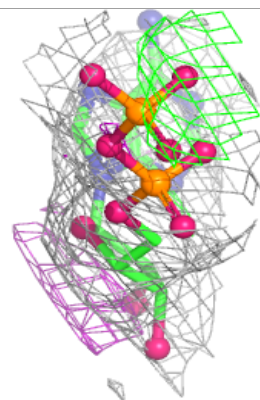
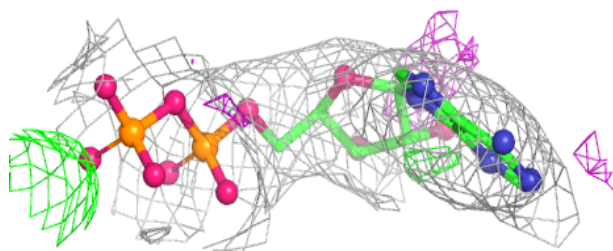
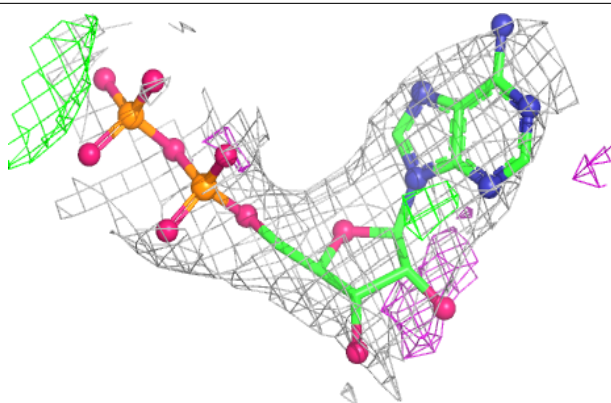
**Electron density around ADP L 1001:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

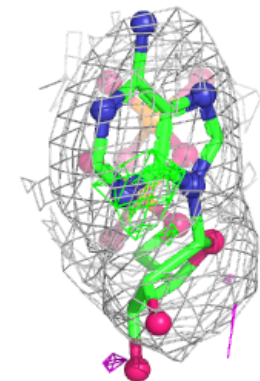
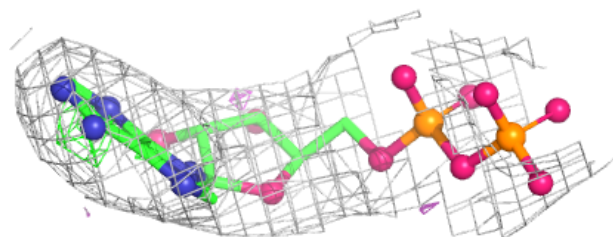
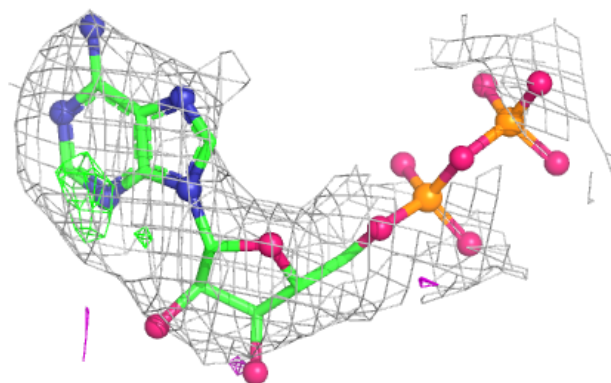


Electron density around ADP D 1001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

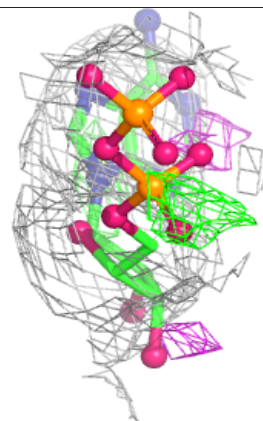
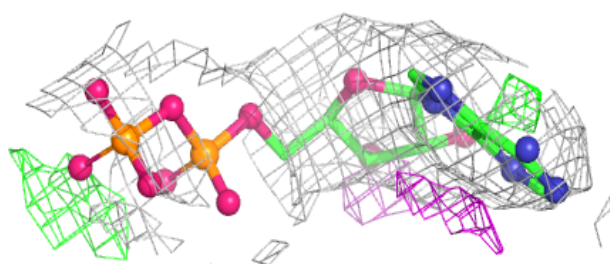
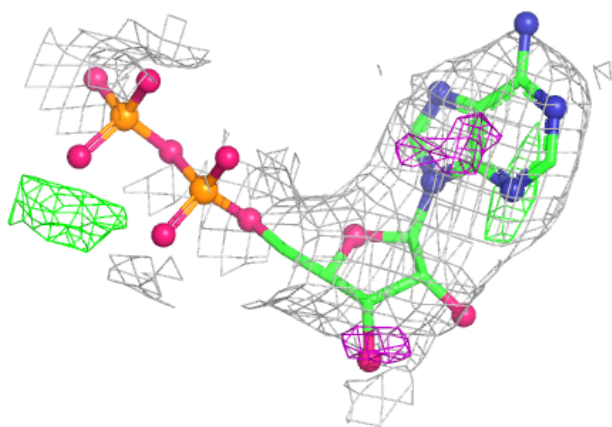
**Electron density around ADP J 1001:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

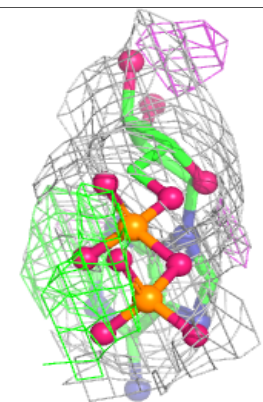
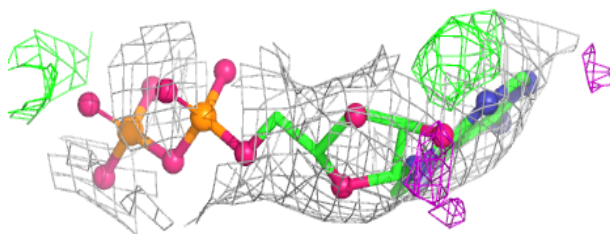
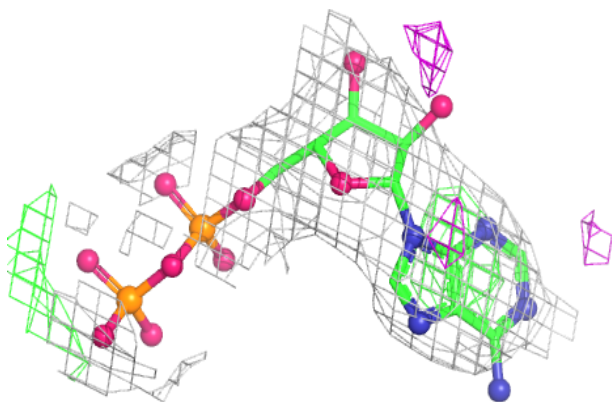


Electron density around ADP H 1001:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

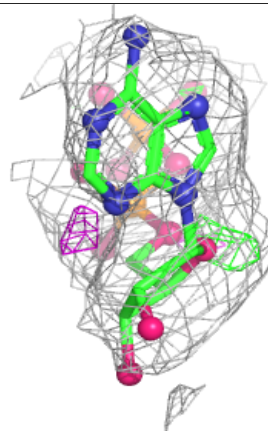
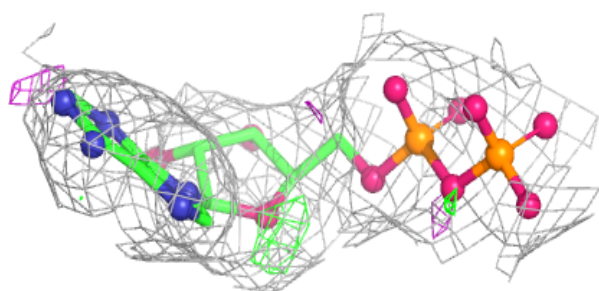
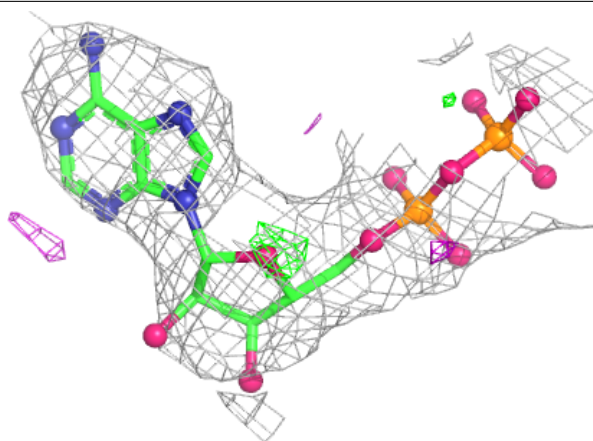
**Electron density around ADP G 1001:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

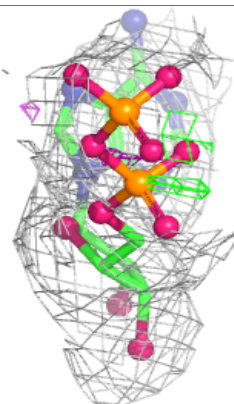
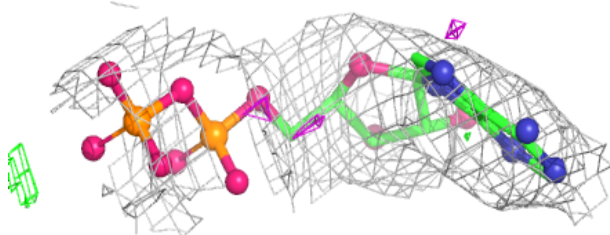
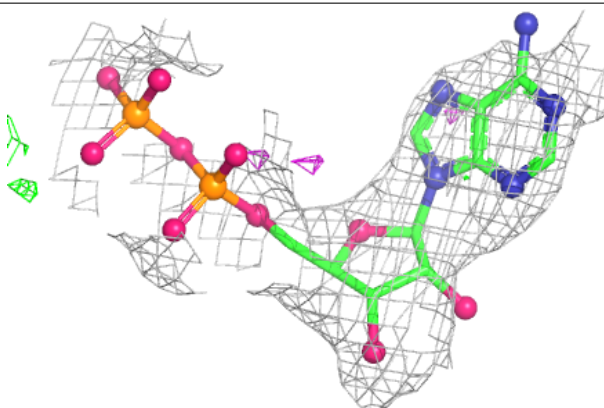


Electron density around ADP N 1001:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

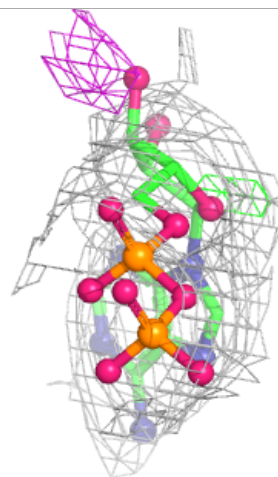
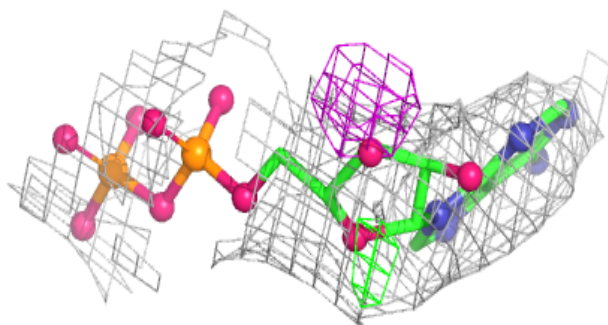
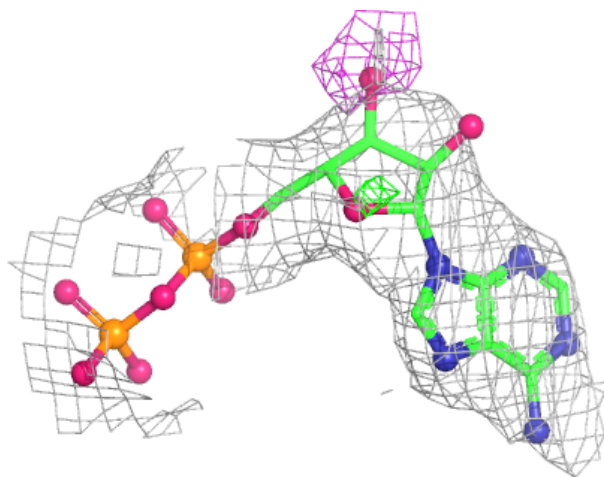
**Electron density around ADP M 1001:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



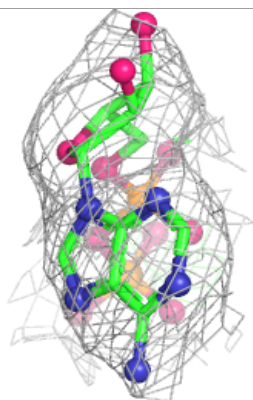
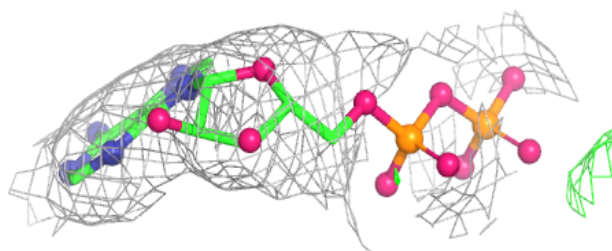
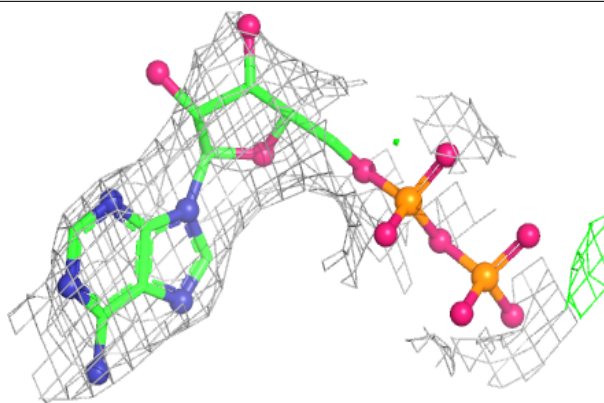
Electron density around ADP E 1001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

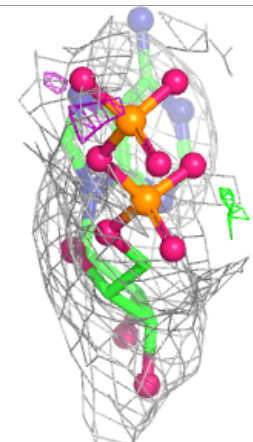
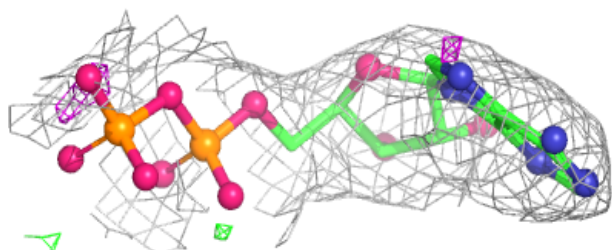
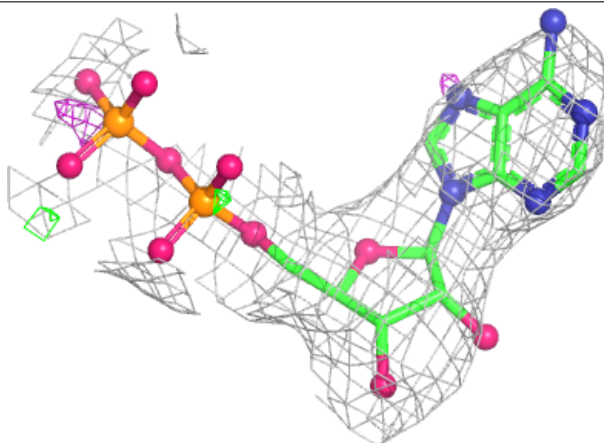


Electron density around ADP I 1001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

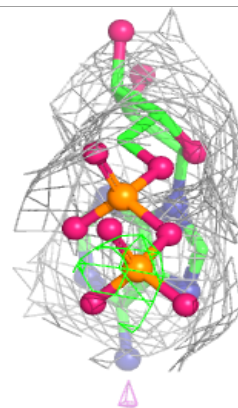
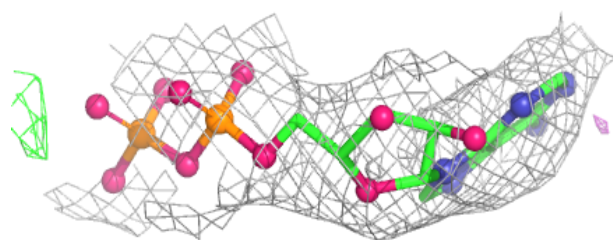
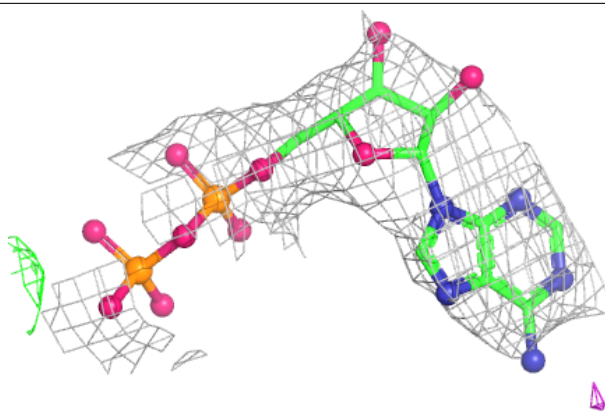
**Electron density around ADP K 1001:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



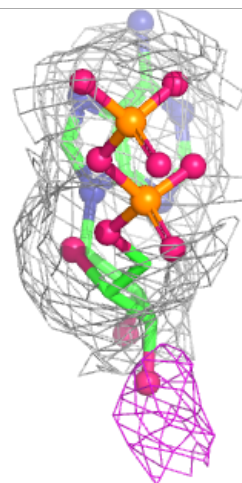
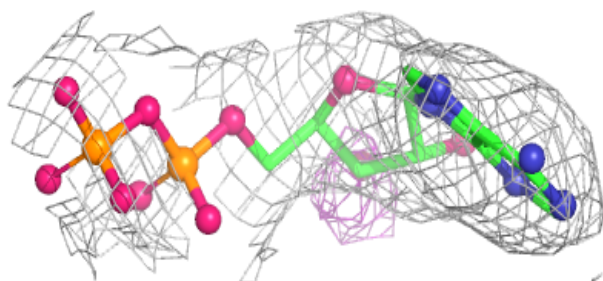
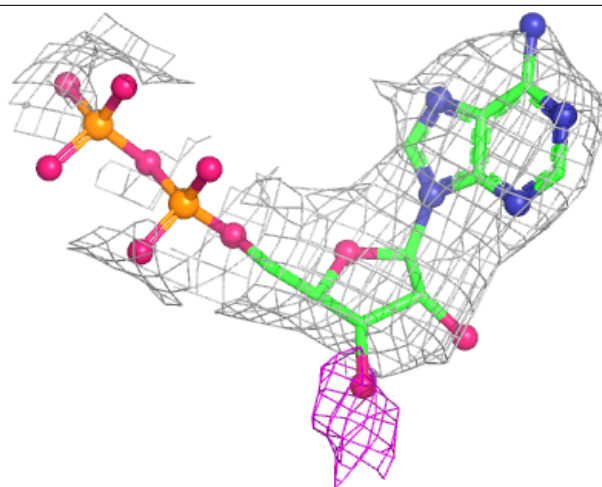
Electron density around ADP P 1001:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
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and green (positive)



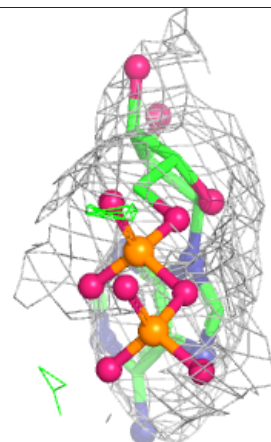
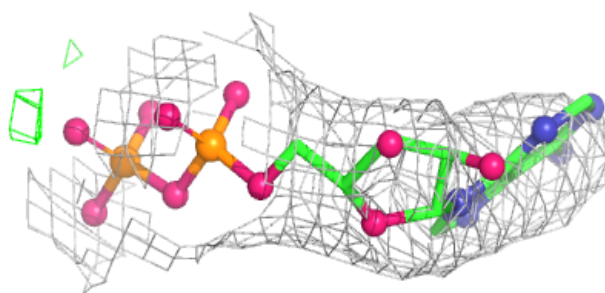
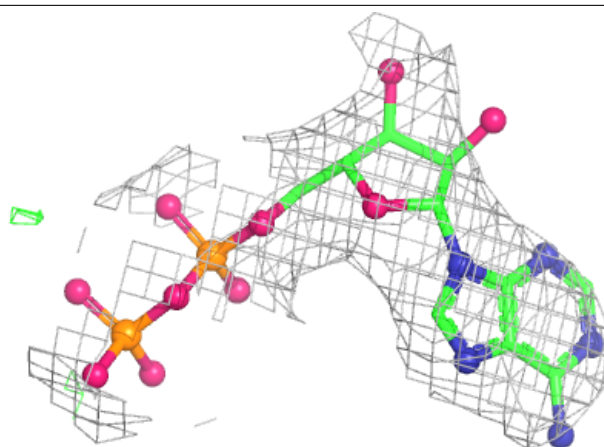
Electron density around ADP C 1001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



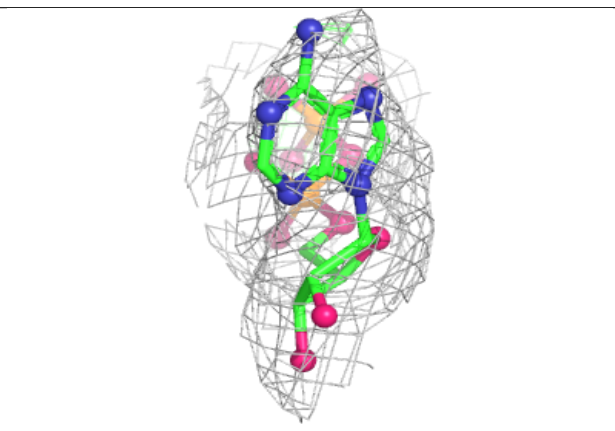
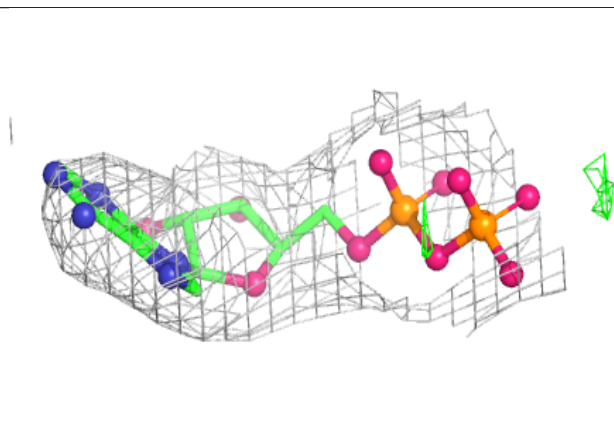
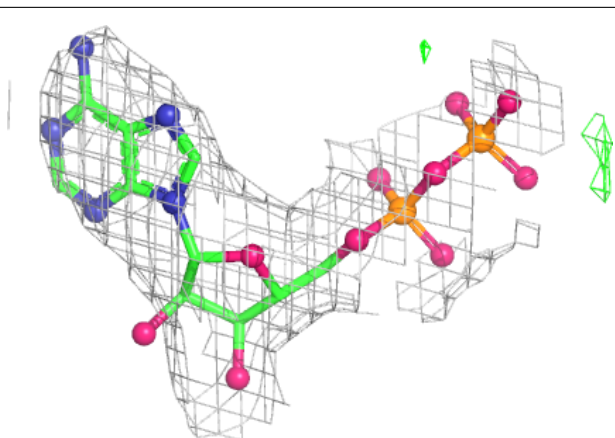
Electron density around ADP O 1001:

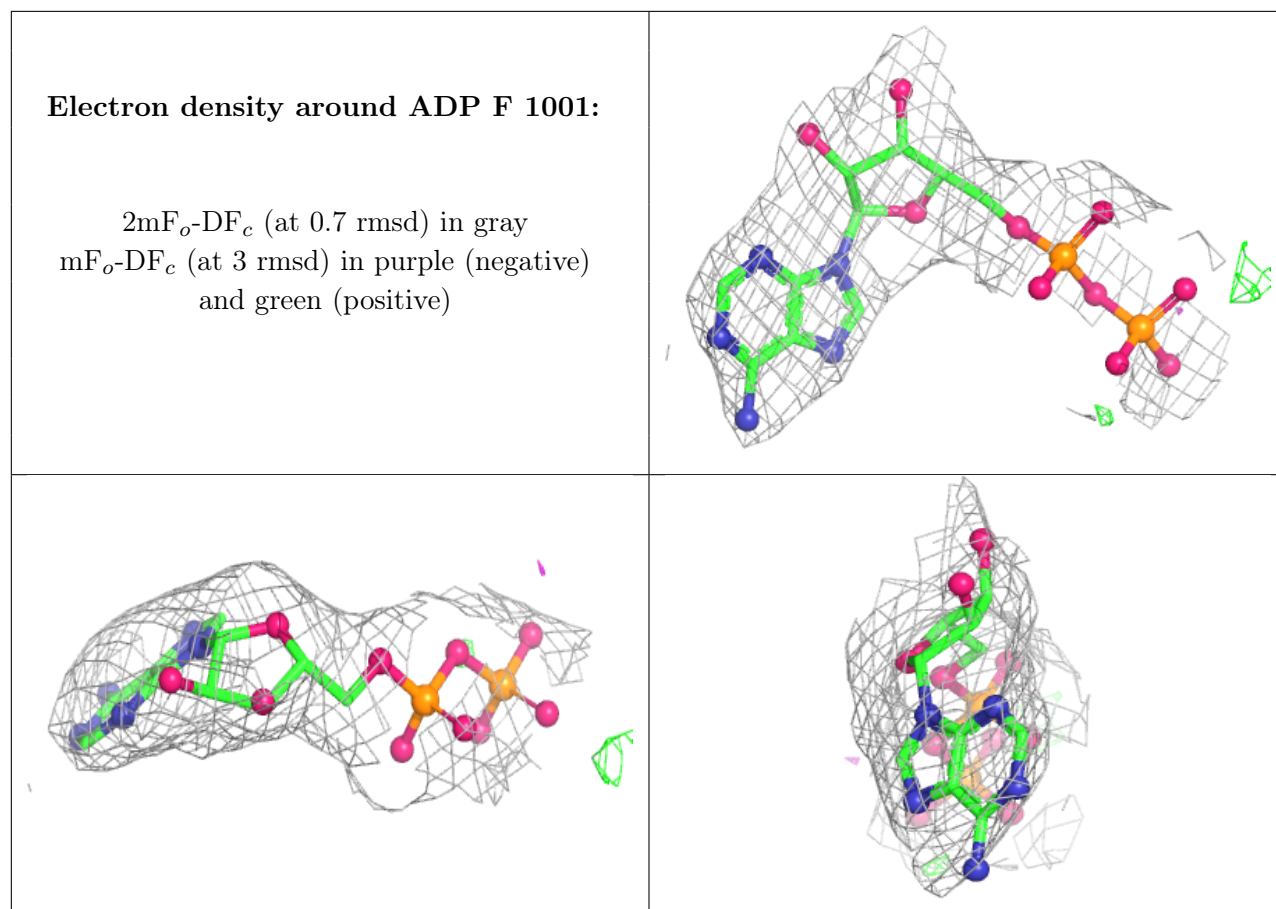
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ADP B 1001:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.