Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:41 PM GMT

PDB ID	:	4V81
Title	:	The crystal structure of yeast CCT reveals intrinsic asymmetry of eukaryotic cytosolic chaperonins
Authors	:	Dekker, C.; Roe, S.M.; McCormack, E.A.; Beuron, F.; Pearl, L.H.; Willison, K.R.
Deposited on	:	2010-10-17
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

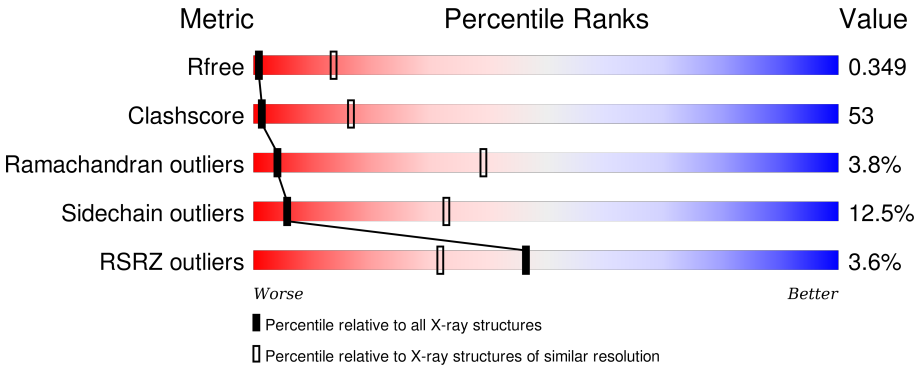
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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}	91344	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	559	2% 52% 39% 6%
1	I	559	5% 53% 38% 6%
1	a	559	3% 89% 8%
1	i	559	3% 89% 8%
2	B	527	% 36% 49% 11%

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Mol	Chain	Length	Quality of chain
2	J	527	4% 34% 51% 12%
2	b	527	2% 82% 14%
2	j	527	% 82% 14%
3	C	590	2% 45% 37% 5% 13%
3	K	590	3% 46% 36% 5% 13%
3	c	590	3% 79% 7% 13%
3	k	590	2% 79% 8% 13%
4	D	528	3% 50% 43% 6%
4	L	528	5% 50% 43% 5%
4	d	528	3% 91% 8%
4	l	528	4% 91% 8%
5	E	562	3% 48% 39% 6% 7%
5	M	562	6% 48% 39% 6% 7%
5	e	562	4% 84% 9% 7%
5	m	562	3% 84% 9% 7%
6	F	546	5% 35% 50% 12%
6	N	546	3% 37% 49% 11%
6	f	546	4% 83% 14%
6	n	546	4% 84% 14%
7	G	550	2% 43% 41% 8% 7%
7	O	550	4% 45% 40% 8% 7%
7	g	550	3% 83% 10% 7%
7	o	550	4% 83% 10% 7%
8	H	568	2% 46% 39% 7% 8%
8	P	568	7% 47% 38% 7% 8%

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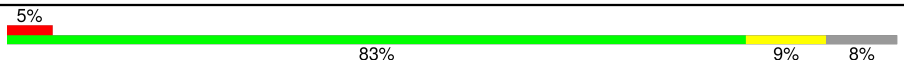
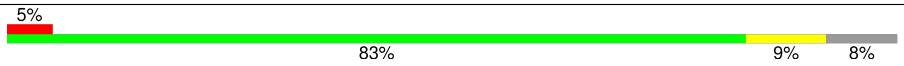
Mol	Chain	Length	Quality of chain
8	h	568	
8	p	568	

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
10	BEF	B	602	-	-	-	X
10	BEF	C	1102	-	-	X	-
10	BEF	E	602	-	-	-	X
10	BEF	F	602	-	-	X	-
10	BEF	G	602	-	-	-	X
10	BEF	N	602	-	-	X	-
9	ADP	A	601	X	-	-	-
9	ADP	B	601	X	-	-	-
9	ADP	C	1101	X	-	-	-
9	ADP	D	601	X	-	-	-
9	ADP	E	601	X	-	-	-
9	ADP	G	601	X	-	-	-
9	ADP	H	601	X	-	-	-
9	ADP	J	601	X	-	-	-
9	ADP	M	601	X	-	-	-
9	ADP	N	601	X	-	-	-
9	ADP	P	601	X	-	-	-
9	ADP	a	1601	X	-	-	-
9	ADP	b	1601	X	-	-	-
9	ADP	e	1601	X	-	-	-
9	ADP	f	1601	X	-	-	-
9	ADP	g	1601	X	-	-	-
9	ADP	h	1601	X	-	-	-
9	ADP	k	2101	X	-	-	-
9	ADP	m	1601	X	-	-	-
9	ADP	n	1601	X	-	-	-
9	ADP	p	1601	X	-	-	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 111235 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 T-complex protein 1 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	544	Total	C	N	O	S	0	0	0
			3492	2146	600	732	14			
1	I	544	Total	C	N	O	S	0	0	0
			3492	2146	600	732	14			
1	a	544	Total	C	N	O	S	0	0	0
			3492	2146	600	732	14			
1	i	544	Total	C	N	O	S	0	0	0
			3492	2146	600	732	14			

- Molecule 2 is a protein called T-complex protein 1 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	513	Total	C	N	O	S	0	0	0
			3459	2125	597	728	9			
2	J	513	Total	C	N	O	S	0	0	0
			3459	2125	597	728	9			
2	b	513	Total	C	N	O	S	0	0	0
			3460	2126	597	728	9			
2	j	513	Total	C	N	O	S	0	0	0
			3457	2123	597	728	9			

- Molecule 3 is a protein called T-complex protein 1 subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	514	Total	C	N	O	S	0	0	0
			3392	2104	590	685	13			
3	K	514	Total	C	N	O	S	0	0	0
			3393	2104	590	685	14			
3	c	514	Total	C	N	O	S	0	0	0
			3395	2106	590	685	14			
3	k	514	Total	C	N	O	S	0	0	0
			3395	2106	590	685	14			

There are 224 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1001	GLY	-	SEE REMARK 999	UNP P39077
C	1002	SER	-	SEE REMARK 999	UNP P39077
C	1003	GLY	-	SEE REMARK 999	UNP P39077
C	1004	SER	-	SEE REMARK 999	UNP P39077
C	1005	GLY	-	SEE REMARK 999	UNP P39077
C	1006	TRP	-	SEE REMARK 999	UNP P39077
C	1007	SER	-	SEE REMARK 999	UNP P39077
C	1008	HIS	-	SEE REMARK 999	UNP P39077
C	1009	PRO	-	SEE REMARK 999	UNP P39077
C	1010	GLN	-	SEE REMARK 999	UNP P39077
C	1011	PHE	-	SEE REMARK 999	UNP P39077
C	1012	GLU	-	SEE REMARK 999	UNP P39077
C	1013	LYS	-	SEE REMARK 999	UNP P39077
C	1014	GLY	-	SEE REMARK 999	UNP P39077
C	1015	SER	-	SEE REMARK 999	UNP P39077
C	1016	GLY	-	SEE REMARK 999	UNP P39077
C	1017	LYS	-	SEE REMARK 999	UNP P39077
C	1018	ARG	-	SEE REMARK 999	UNP P39077
C	1019	ARG	-	SEE REMARK 999	UNP P39077
C	1020	TRP	-	SEE REMARK 999	UNP P39077
C	1021	LYS	-	SEE REMARK 999	UNP P39077
C	1022	LYS	-	SEE REMARK 999	UNP P39077
C	1023	ASN	-	SEE REMARK 999	UNP P39077
C	1024	PHE	-	SEE REMARK 999	UNP P39077
C	1025	ILE	-	SEE REMARK 999	UNP P39077
C	1026	ALA	-	SEE REMARK 999	UNP P39077
C	1027	VAL	-	SEE REMARK 999	UNP P39077
C	1028	SER	-	SEE REMARK 999	UNP P39077
C	1029	ALA	-	SEE REMARK 999	UNP P39077
C	1030	ALA	-	SEE REMARK 999	UNP P39077
C	1031	ASN	-	SEE REMARK 999	UNP P39077
C	1032	ARG	-	SEE REMARK 999	UNP P39077
C	1033	PHE	-	SEE REMARK 999	UNP P39077
C	1034	LYS	-	SEE REMARK 999	UNP P39077
C	1035	LYS	-	SEE REMARK 999	UNP P39077
C	1036	ILE	-	SEE REMARK 999	UNP P39077
C	1037	SER	-	SEE REMARK 999	UNP P39077
C	1038	SER	-	SEE REMARK 999	UNP P39077
C	1039	SER	-	SEE REMARK 999	UNP P39077
C	1040	GLY	-	SEE REMARK 999	UNP P39077
C	1041	ALA	-	SEE REMARK 999	UNP P39077
C	1042	LEU	-	SEE REMARK 999	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1043	GLY	-	SEE REMARK 999	UNP P39077
C	1044	SER	-	SEE REMARK 999	UNP P39077
C	1045	GLY	-	SEE REMARK 999	UNP P39077
C	1046	HIS	-	SEE REMARK 999	UNP P39077
C	1047	HIS	-	SEE REMARK 999	UNP P39077
C	1048	HIS	-	SEE REMARK 999	UNP P39077
C	1049	HIS	-	SEE REMARK 999	UNP P39077
C	1050	HIS	-	SEE REMARK 999	UNP P39077
C	1051	HIS	-	SEE REMARK 999	UNP P39077
C	1052	HIS	-	SEE REMARK 999	UNP P39077
C	1053	HIS	-	SEE REMARK 999	UNP P39077
C	1054	GLY	-	SEE REMARK 999	UNP P39077
C	1055	SER	-	SEE REMARK 999	UNP P39077
C	1056	GLY	-	SEE REMARK 999	UNP P39077
K	1001	GLY	-	SEE REMARK 999	UNP P39077
K	1002	SER	-	SEE REMARK 999	UNP P39077
K	1003	GLY	-	SEE REMARK 999	UNP P39077
K	1004	SER	-	SEE REMARK 999	UNP P39077
K	1005	GLY	-	SEE REMARK 999	UNP P39077
K	1006	TRP	-	SEE REMARK 999	UNP P39077
K	1007	SER	-	SEE REMARK 999	UNP P39077
K	1008	HIS	-	SEE REMARK 999	UNP P39077
K	1009	PRO	-	SEE REMARK 999	UNP P39077
K	1010	GLN	-	SEE REMARK 999	UNP P39077
K	1011	PHE	-	SEE REMARK 999	UNP P39077
K	1012	GLU	-	SEE REMARK 999	UNP P39077
K	1013	LYS	-	SEE REMARK 999	UNP P39077
K	1014	GLY	-	SEE REMARK 999	UNP P39077
K	1015	SER	-	SEE REMARK 999	UNP P39077
K	1016	GLY	-	SEE REMARK 999	UNP P39077
K	1017	LYS	-	SEE REMARK 999	UNP P39077
K	1018	ARG	-	SEE REMARK 999	UNP P39077
K	1019	ARG	-	SEE REMARK 999	UNP P39077
K	1020	TRP	-	SEE REMARK 999	UNP P39077
K	1021	LYS	-	SEE REMARK 999	UNP P39077
K	1022	LYS	-	SEE REMARK 999	UNP P39077
K	1023	ASN	-	SEE REMARK 999	UNP P39077
K	1024	PHE	-	SEE REMARK 999	UNP P39077
K	1025	ILE	-	SEE REMARK 999	UNP P39077
K	1026	ALA	-	SEE REMARK 999	UNP P39077
K	1027	VAL	-	SEE REMARK 999	UNP P39077
K	1028	SER	-	SEE REMARK 999	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
K	1029	ALA	-	SEE REMARK 999	UNP P39077
K	1030	ALA	-	SEE REMARK 999	UNP P39077
K	1031	ASN	-	SEE REMARK 999	UNP P39077
K	1032	ARG	-	SEE REMARK 999	UNP P39077
K	1033	PHE	-	SEE REMARK 999	UNP P39077
K	1034	LYS	-	SEE REMARK 999	UNP P39077
K	1035	LYS	-	SEE REMARK 999	UNP P39077
K	1036	ILE	-	SEE REMARK 999	UNP P39077
K	1037	SER	-	SEE REMARK 999	UNP P39077
K	1038	SER	-	SEE REMARK 999	UNP P39077
K	1039	SER	-	SEE REMARK 999	UNP P39077
K	1040	GLY	-	SEE REMARK 999	UNP P39077
K	1041	ALA	-	SEE REMARK 999	UNP P39077
K	1042	LEU	-	SEE REMARK 999	UNP P39077
K	1043	GLY	-	SEE REMARK 999	UNP P39077
K	1044	SER	-	SEE REMARK 999	UNP P39077
K	1045	GLY	-	SEE REMARK 999	UNP P39077
K	1046	HIS	-	SEE REMARK 999	UNP P39077
K	1047	HIS	-	SEE REMARK 999	UNP P39077
K	1048	HIS	-	SEE REMARK 999	UNP P39077
K	1049	HIS	-	SEE REMARK 999	UNP P39077
K	1050	HIS	-	SEE REMARK 999	UNP P39077
K	1051	HIS	-	SEE REMARK 999	UNP P39077
K	1052	HIS	-	SEE REMARK 999	UNP P39077
K	1053	HIS	-	SEE REMARK 999	UNP P39077
K	1054	GLY	-	SEE REMARK 999	UNP P39077
K	1055	SER	-	SEE REMARK 999	UNP P39077
K	1056	GLY	-	SEE REMARK 999	UNP P39077
c	2001	GLY	-	SEE REMARK 999	UNP P39077
c	2002	SER	-	SEE REMARK 999	UNP P39077
c	2003	GLY	-	SEE REMARK 999	UNP P39077
c	2004	SER	-	SEE REMARK 999	UNP P39077
c	2005	GLY	-	SEE REMARK 999	UNP P39077
c	2006	TRP	-	SEE REMARK 999	UNP P39077
c	2007	SER	-	SEE REMARK 999	UNP P39077
c	2008	HIS	-	SEE REMARK 999	UNP P39077
c	2009	PRO	-	SEE REMARK 999	UNP P39077
c	2010	GLN	-	SEE REMARK 999	UNP P39077
c	2011	PHE	-	SEE REMARK 999	UNP P39077
c	2012	GLU	-	SEE REMARK 999	UNP P39077
c	2013	LYS	-	SEE REMARK 999	UNP P39077
c	2014	GLY	-	SEE REMARK 999	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
c	2015	SER	-	SEE REMARK 999	UNP P39077
c	2016	GLY	-	SEE REMARK 999	UNP P39077
c	2017	LYS	-	SEE REMARK 999	UNP P39077
c	2018	ARG	-	SEE REMARK 999	UNP P39077
c	2019	ARG	-	SEE REMARK 999	UNP P39077
c	2020	TRP	-	SEE REMARK 999	UNP P39077
c	2021	LYS	-	SEE REMARK 999	UNP P39077
c	2022	LYS	-	SEE REMARK 999	UNP P39077
c	2023	ASN	-	SEE REMARK 999	UNP P39077
c	2024	PHE	-	SEE REMARK 999	UNP P39077
c	2025	ILE	-	SEE REMARK 999	UNP P39077
c	2026	ALA	-	SEE REMARK 999	UNP P39077
c	2027	VAL	-	SEE REMARK 999	UNP P39077
c	2028	SER	-	SEE REMARK 999	UNP P39077
c	2029	ALA	-	SEE REMARK 999	UNP P39077
c	2030	ALA	-	SEE REMARK 999	UNP P39077
c	2031	ASN	-	SEE REMARK 999	UNP P39077
c	2032	ARG	-	SEE REMARK 999	UNP P39077
c	2033	PHE	-	SEE REMARK 999	UNP P39077
c	2034	LYS	-	SEE REMARK 999	UNP P39077
c	2035	LYS	-	SEE REMARK 999	UNP P39077
c	2036	ILE	-	SEE REMARK 999	UNP P39077
c	2037	SER	-	SEE REMARK 999	UNP P39077
c	2038	SER	-	SEE REMARK 999	UNP P39077
c	2039	SER	-	SEE REMARK 999	UNP P39077
c	2040	GLY	-	SEE REMARK 999	UNP P39077
c	2041	ALA	-	SEE REMARK 999	UNP P39077
c	2042	LEU	-	SEE REMARK 999	UNP P39077
c	2043	GLY	-	SEE REMARK 999	UNP P39077
c	2044	SER	-	SEE REMARK 999	UNP P39077
c	2045	GLY	-	SEE REMARK 999	UNP P39077
c	2046	HIS	-	SEE REMARK 999	UNP P39077
c	2047	HIS	-	SEE REMARK 999	UNP P39077
c	2048	HIS	-	SEE REMARK 999	UNP P39077
c	2049	HIS	-	SEE REMARK 999	UNP P39077
c	2050	HIS	-	SEE REMARK 999	UNP P39077
c	2051	HIS	-	SEE REMARK 999	UNP P39077
c	2052	HIS	-	SEE REMARK 999	UNP P39077
c	2053	HIS	-	SEE REMARK 999	UNP P39077
c	2054	GLY	-	SEE REMARK 999	UNP P39077
c	2055	SER	-	SEE REMARK 999	UNP P39077
c	2056	GLY	-	SEE REMARK 999	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
k	2001	GLY	-	SEE REMARK 999	UNP P39077
k	2002	SER	-	SEE REMARK 999	UNP P39077
k	2003	GLY	-	SEE REMARK 999	UNP P39077
k	2004	SER	-	SEE REMARK 999	UNP P39077
k	2005	GLY	-	SEE REMARK 999	UNP P39077
k	2006	TRP	-	SEE REMARK 999	UNP P39077
k	2007	SER	-	SEE REMARK 999	UNP P39077
k	2008	HIS	-	SEE REMARK 999	UNP P39077
k	2009	PRO	-	SEE REMARK 999	UNP P39077
k	2010	GLN	-	SEE REMARK 999	UNP P39077
k	2011	PHE	-	SEE REMARK 999	UNP P39077
k	2012	GLU	-	SEE REMARK 999	UNP P39077
k	2013	LYS	-	SEE REMARK 999	UNP P39077
k	2014	GLY	-	SEE REMARK 999	UNP P39077
k	2015	SER	-	SEE REMARK 999	UNP P39077
k	2016	GLY	-	SEE REMARK 999	UNP P39077
k	2017	LYS	-	SEE REMARK 999	UNP P39077
k	2018	ARG	-	SEE REMARK 999	UNP P39077
k	2019	ARG	-	SEE REMARK 999	UNP P39077
k	2020	TRP	-	SEE REMARK 999	UNP P39077
k	2021	LYS	-	SEE REMARK 999	UNP P39077
k	2022	LYS	-	SEE REMARK 999	UNP P39077
k	2023	ASN	-	SEE REMARK 999	UNP P39077
k	2024	PHE	-	SEE REMARK 999	UNP P39077
k	2025	ILE	-	SEE REMARK 999	UNP P39077
k	2026	ALA	-	SEE REMARK 999	UNP P39077
k	2027	VAL	-	SEE REMARK 999	UNP P39077
k	2028	SER	-	SEE REMARK 999	UNP P39077
k	2029	ALA	-	SEE REMARK 999	UNP P39077
k	2030	ALA	-	SEE REMARK 999	UNP P39077
k	2031	ASN	-	SEE REMARK 999	UNP P39077
k	2032	ARG	-	SEE REMARK 999	UNP P39077
k	2033	PHE	-	SEE REMARK 999	UNP P39077
k	2034	LYS	-	SEE REMARK 999	UNP P39077
k	2035	LYS	-	SEE REMARK 999	UNP P39077
k	2036	ILE	-	SEE REMARK 999	UNP P39077
k	2037	SER	-	SEE REMARK 999	UNP P39077
k	2038	SER	-	SEE REMARK 999	UNP P39077
k	2039	SER	-	SEE REMARK 999	UNP P39077
k	2040	GLY	-	SEE REMARK 999	UNP P39077
k	2041	ALA	-	SEE REMARK 999	UNP P39077
k	2042	LEU	-	SEE REMARK 999	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
k	2043	GLY	-	SEE REMARK 999	UNP P39077
k	2044	SER	-	SEE REMARK 999	UNP P39077
k	2045	GLY	-	SEE REMARK 999	UNP P39077
k	2046	HIS	-	SEE REMARK 999	UNP P39077
k	2047	HIS	-	SEE REMARK 999	UNP P39077
k	2048	HIS	-	SEE REMARK 999	UNP P39077
k	2049	HIS	-	SEE REMARK 999	UNP P39077
k	2050	HIS	-	SEE REMARK 999	UNP P39077
k	2051	HIS	-	SEE REMARK 999	UNP P39077
k	2052	HIS	-	SEE REMARK 999	UNP P39077
k	2053	HIS	-	SEE REMARK 999	UNP P39077
k	2054	GLY	-	SEE REMARK 999	UNP P39077
k	2055	SER	-	SEE REMARK 999	UNP P39077
k	2056	GLY	-	SEE REMARK 999	UNP P39077

- Molecule 4 is a protein called T-complex protein 1 subunit delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	522	Total	C	N	O	S	0	0	0
			3398	2092	609	686	11			
4	L	522	Total	C	N	O	S	0	0	0
			3398	2092	609	686	11			
4	d	522	Total	C	N	O	S	0	0	0
			3398	2092	609	686	11			
4	l	522	Total	C	N	O	S	0	0	0
			3398	2092	609	686	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	345	ASP	GLY	ENGINEERED MUTATION	UNP P39078
L	345	ASP	GLY	ENGINEERED MUTATION	UNP P39078
d	1345	ASP	GLY	ENGINEERED MUTATION	UNP P39078
l	1345	ASP	GLY	ENGINEERED MUTATION	UNP P39078

- Molecule 5 is a protein called T-complex protein 1 subunit epsilon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	525	Total	C	N	O	S	0	0	0
			3437	2110	599	720	8			
5	M	525	Total	C	N	O	S	0	0	0
			3437	2110	599	720	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	e	525	Total	C	N	O	S	0	0	0
			3437	2110	599	720	8			
5	m	525	Total	C	N	O	S	0	0	0
			3437	2110	599	720	8			

- Molecule 6 is a protein called T-complex protein 1 subunit zeta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	533	Total	C	N	O	S	0	0	0
			3631	2253	629	740	9			
6	N	533	Total	C	N	O	S	0	0	0
			3628	2250	629	740	9			
6	f	533	Total	C	N	O	S	0	0	0
			3633	2255	630	739	9			
6	n	533	Total	C	N	O	S	0	0	0
			3629	2252	629	739	9			

- Molecule 7 is a protein called T-complex protein 1 subunit eta.

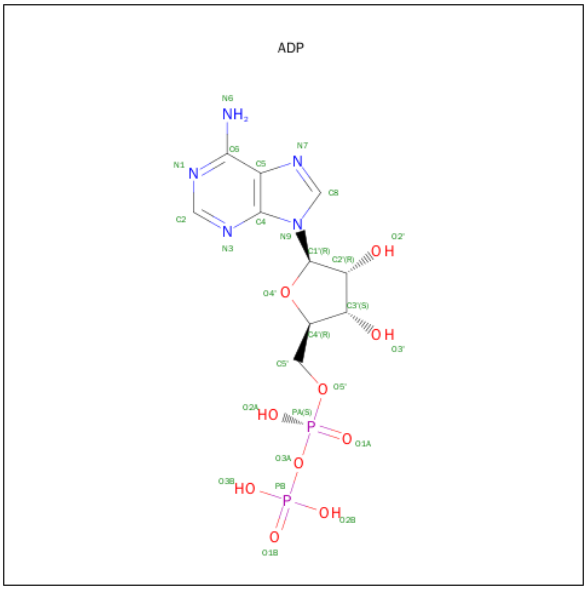
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	509	Total	C	N	O	S	0	0	0
			3317	2055	583	669	10			
7	O	509	Total	C	N	O	S	0	0	0
			3314	2052	583	669	10			
7	g	509	Total	C	N	O	S	0	0	0
			3314	2052	583	669	10			
7	o	509	Total	C	N	O	S	0	0	0
			3314	2052	583	669	10			

- Molecule 8 is a protein called T-complex protein 1 subunit theta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	525	Total	C	N	O	S	0	0	0
			3487	2161	608	705	13			
8	P	525	Total	C	N	O	S	0	0	0
			3487	2161	608	705	13			
8	h	525	Total	C	N	O	S	0	0	0
			3485	2159	608	705	13			
8	p	525	Total	C	N	O	S	0	0	0
			3487	2161	608	705	13			

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:

$C_{10}H_{15}N_5O_{10}P_2$).



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

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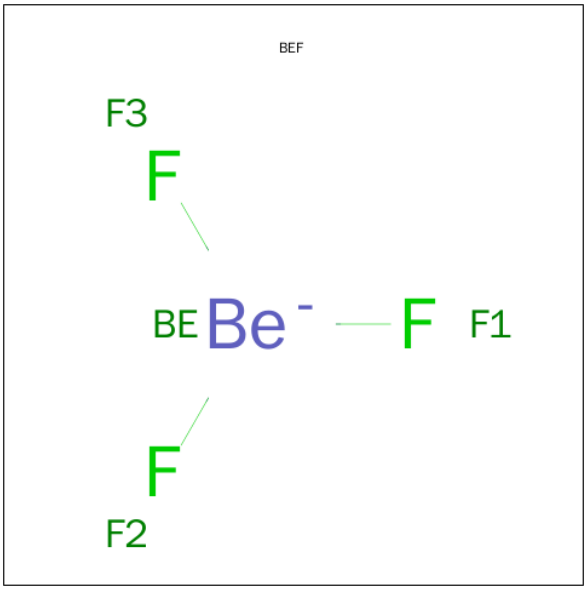
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	a	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	b	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	e	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	f	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	g	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	h	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	k	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	l	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	m	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	n	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	p	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 10 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total Be F 4 1 3	0	0
10	B	1	Total Be F 4 1 3	0	0
10	C	1	Total Be F 4 1 3	0	0
10	D	1	Total Be F 4 1 3	0	0
10	E	1	Total Be F 4 1 3	0	0
10	F	1	Total Be F 4 1 3	0	0
10	G	1	Total Be F 4 1 3	0	0
10	H	1	Total Be F 4 1 3	0	0
10	J	1	Total Be F 4 1 3	0	0
10	L	1	Total Be F 4 1 3	0	0
10	M	1	Total Be F 4 1 3	0	0
10	N	1	Total Be F 4 1 3	0	0
10	P	1	Total Be F 4 1 3	0	0
10	a	1	Total Be F 4 1 3	0	0
10	b	1	Total Be F 4 1 3	0	0
10	e	1	Total Be F 4 1 3	0	0
10	f	1	Total Be F 4 1 3	0	0
10	g	1	Total Be F 4 1 3	0	0
10	h	1	Total Be F 4 1 3	0	0
10	k	1	Total Be F 4 1 3	0	0
10	l	1	Total Be F 4 1 3	0	0
10	m	1	Total Be F 4 1 3	0	0

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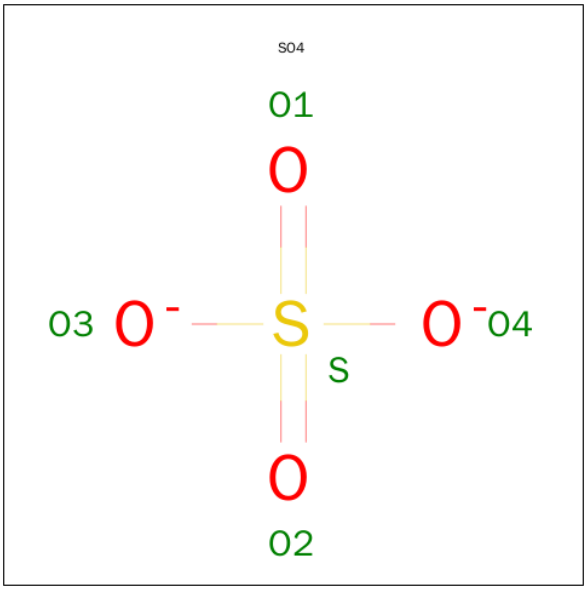
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	n	1	Total Be F 4 1 3	0	0
10	p	1	Total Be F 4 1 3	0	0

- Molecule 11 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	I	1	Total O S 5 4 1	0	0
11	K	1	Total O S 5 4 1	0	0
11	O	1	Total O S 5 4 1	0	0
11	c	1	Total O S 5 4 1	0	0
11	d	1	Total O S 5 4 1	0	0
11	i	1	Total O S 5 4 1	0	0
11	j	1	Total O S 5 4 1	0	0
11	o	1	Total O S 5 4 1	0	0

- Molecule 12 is water.

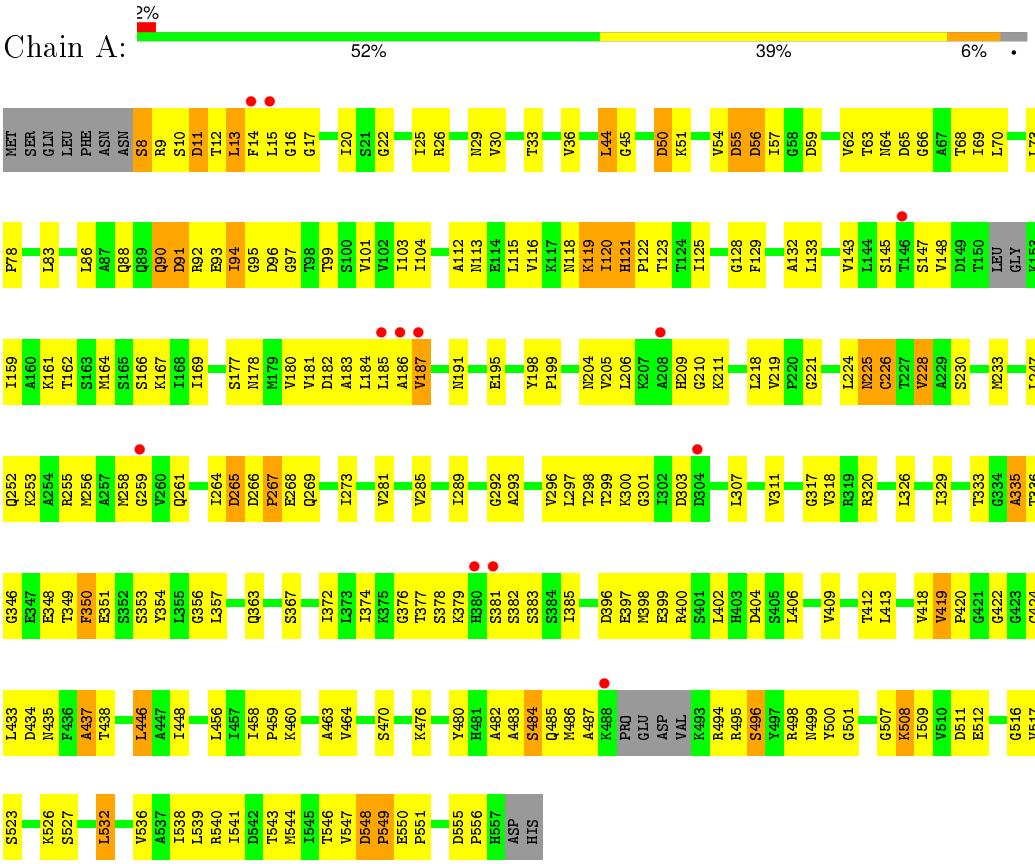
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	1	Total O 1 1	0	0
12	E	1	Total O 1 1	0	0
12	G	1	Total O 1 1	0	0
12	M	1	Total O 1 1	0	0
12	e	1	Total O 1 1	0	0
12	g	1	Total O 1 1	0	0
12	m	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

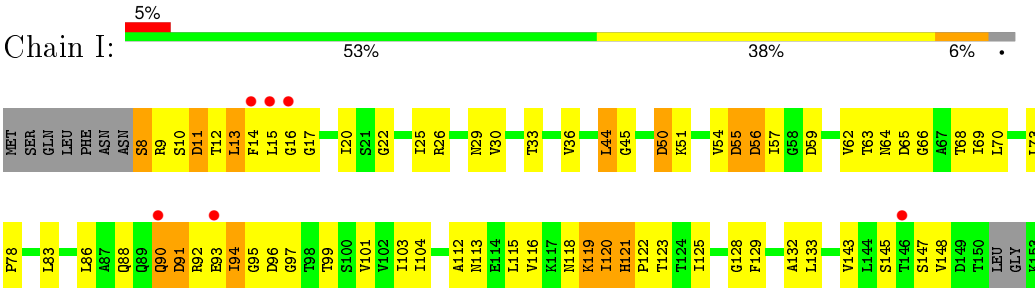
- Molecule 1: T-complex protein 1 subunit alpha

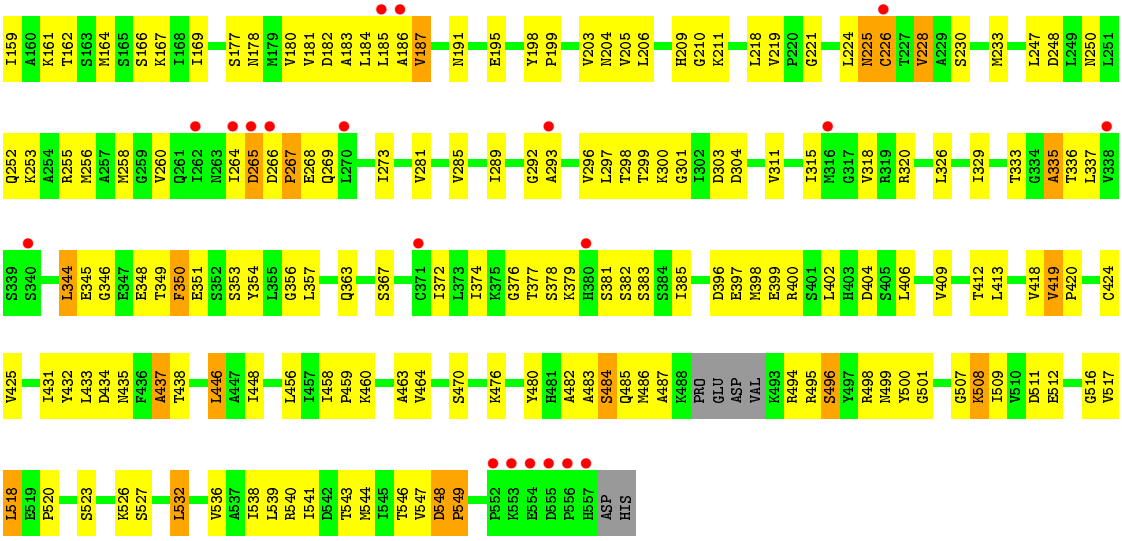
Chain A:



- Molecule 1: T-complex protein 1 subunit alpha

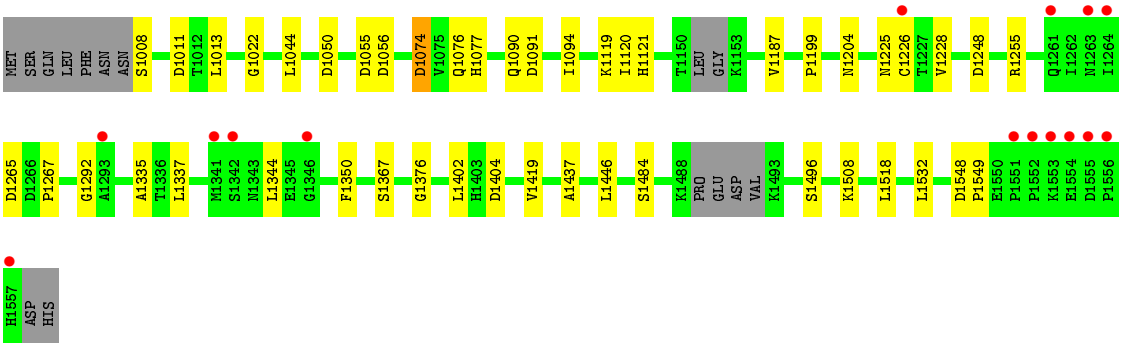
Chain I:





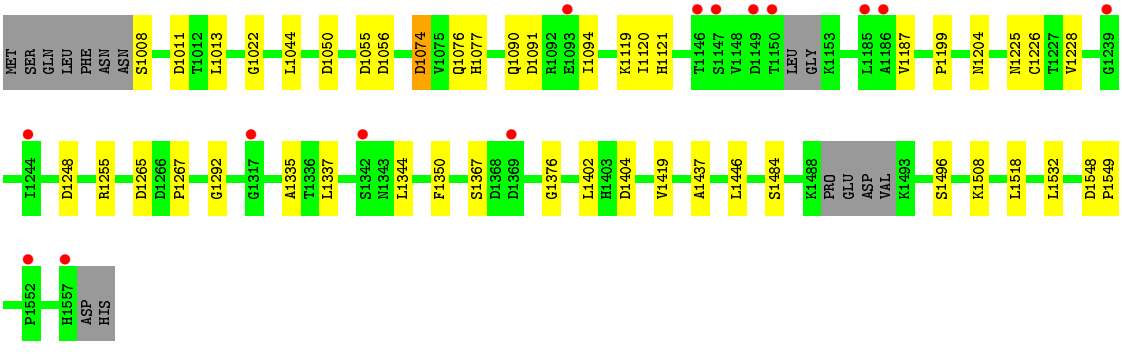
• Molecule 1: T-complex protein 1 subunit alpha

Chain a:



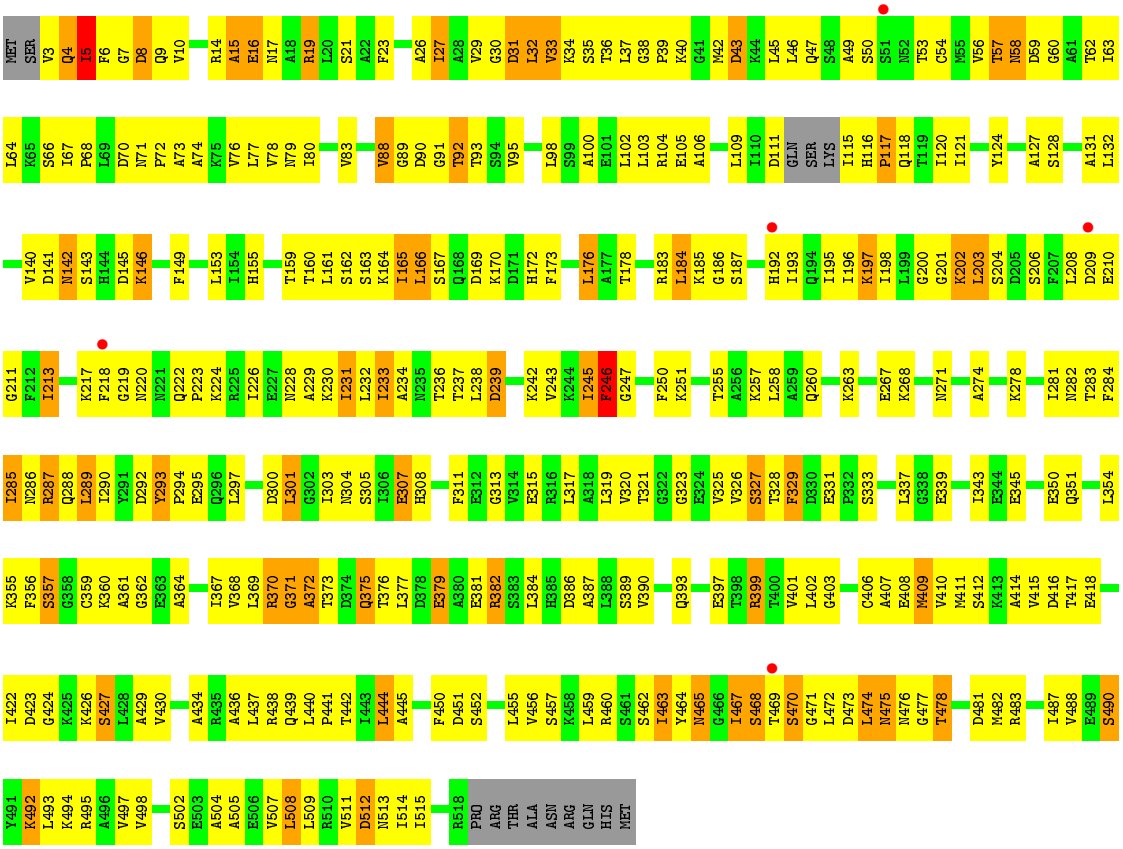
• Molecule 1: T-complex protein 1 subunit alpha

Chain i:



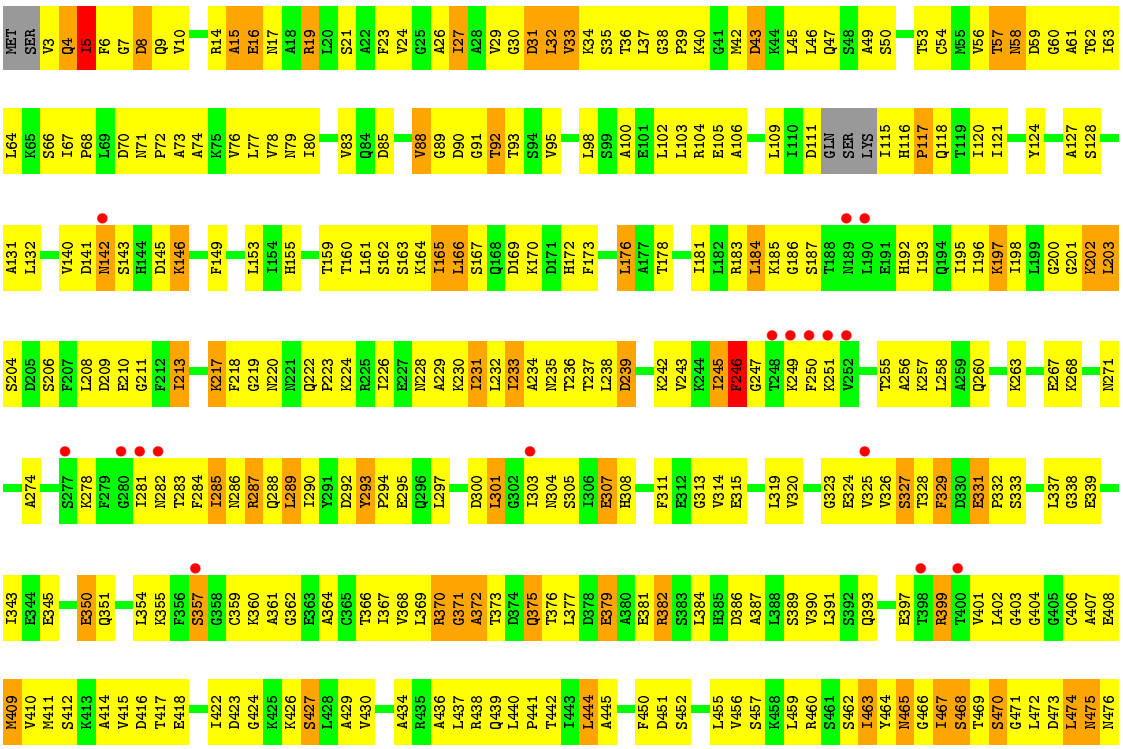
• Molecule 2: T-complex protein 1 subunit beta

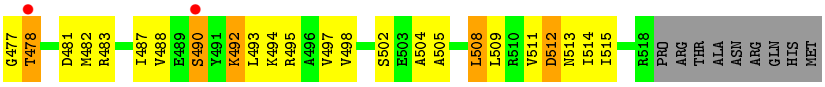
Chain B:



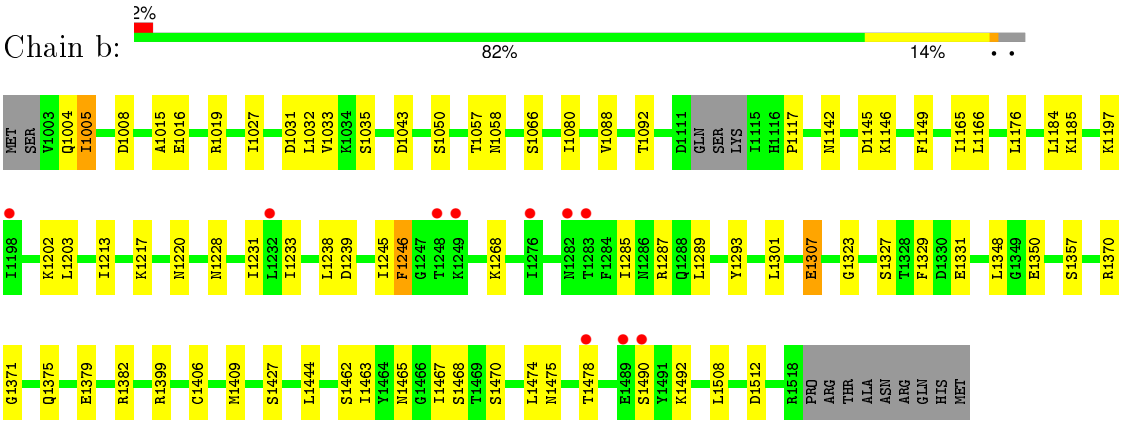
• Molecule 2: T-complex protein 1 subunit beta

Chain J:

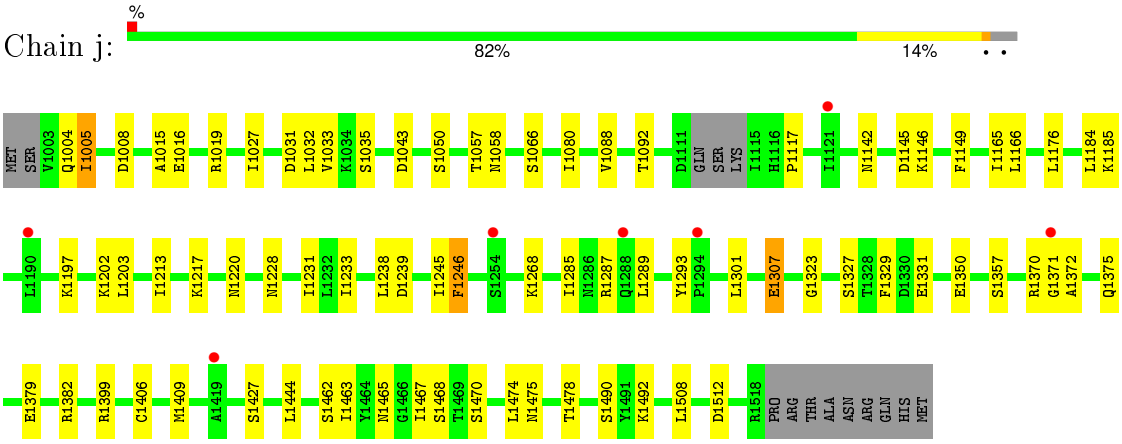




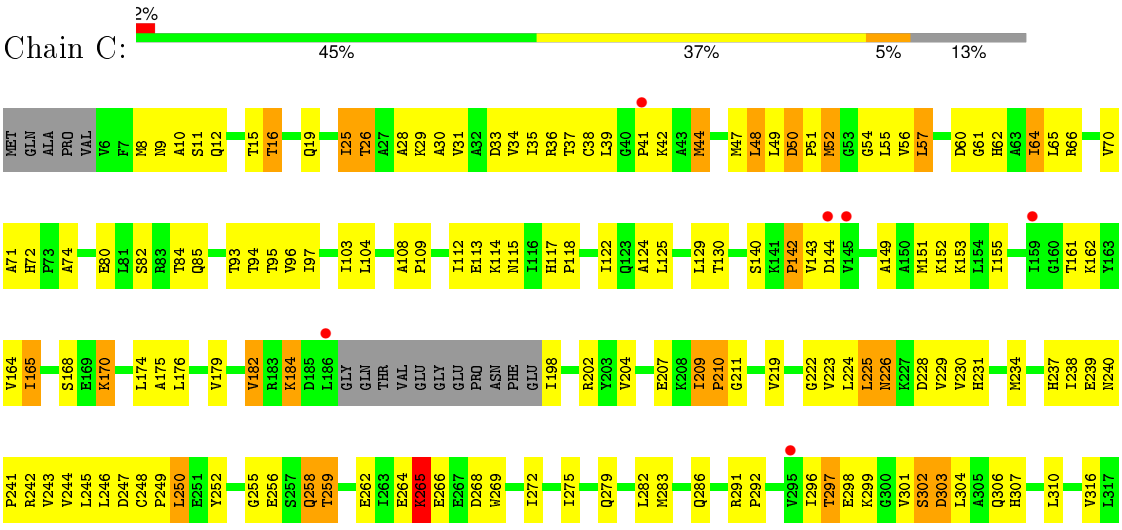
• Molecule 2: T-complex protein 1 subunit beta

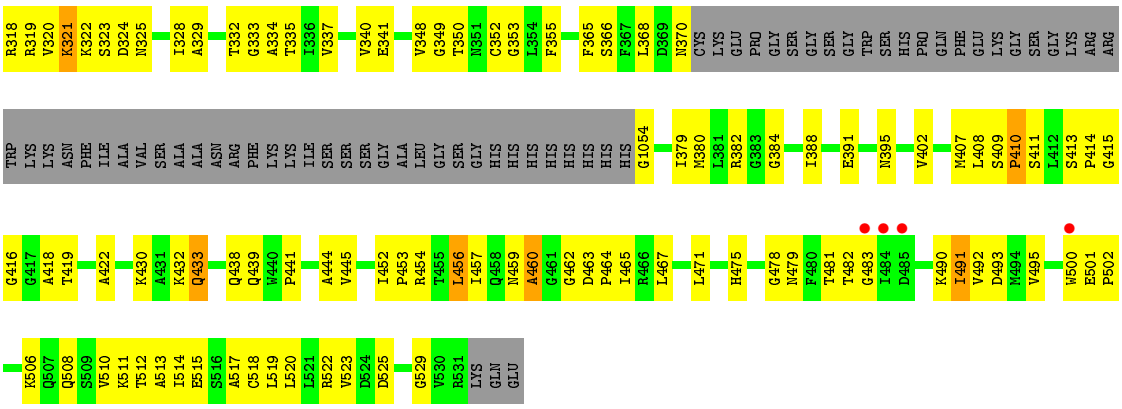


• Molecule 2: T-complex protein 1 subunit beta



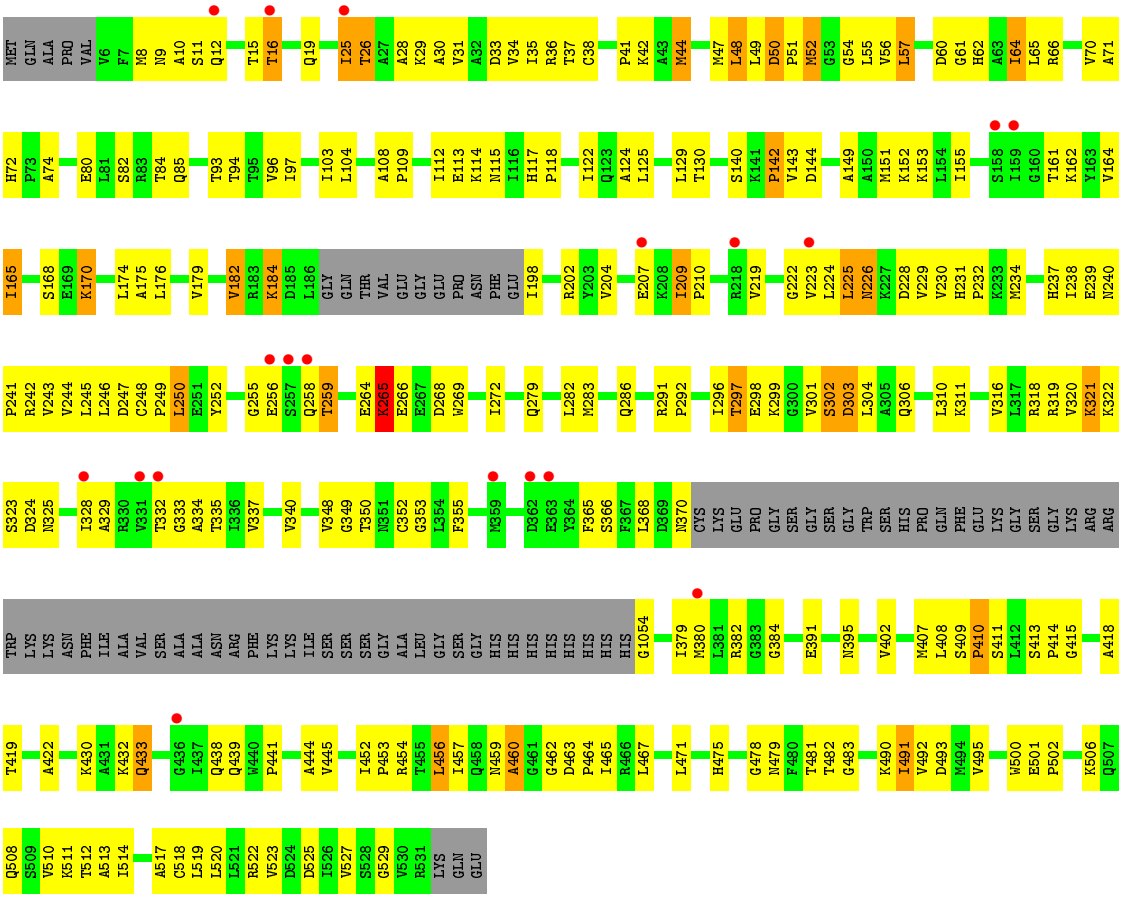
• Molecule 3: T-complex protein 1 subunit gamma





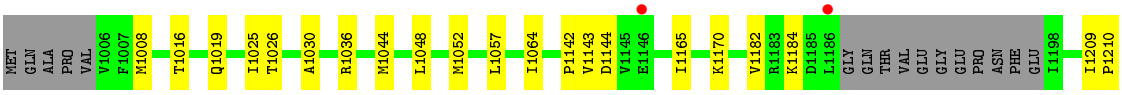
• Molecule 3: T-complex protein 1 subunit gamma

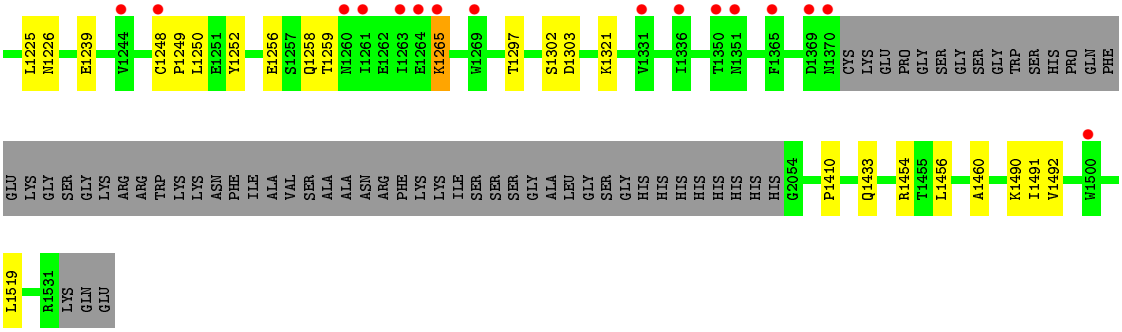
Chain K:



• Molecule 3: T-complex protein 1 subunit gamma

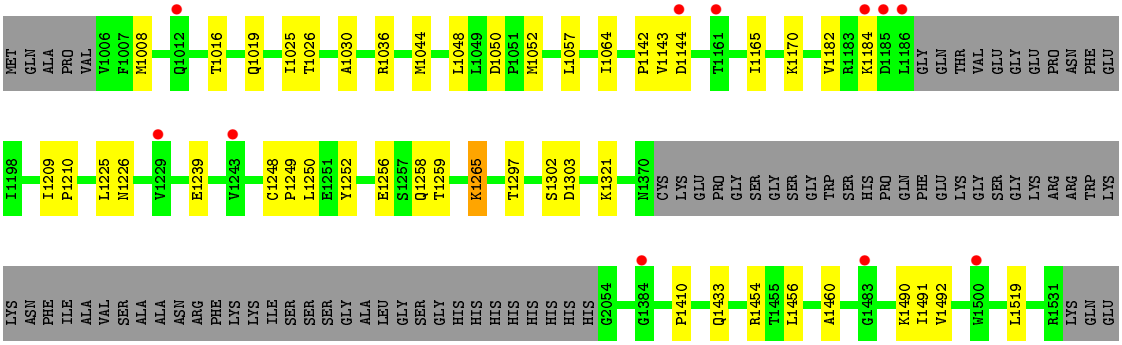
Chain c:





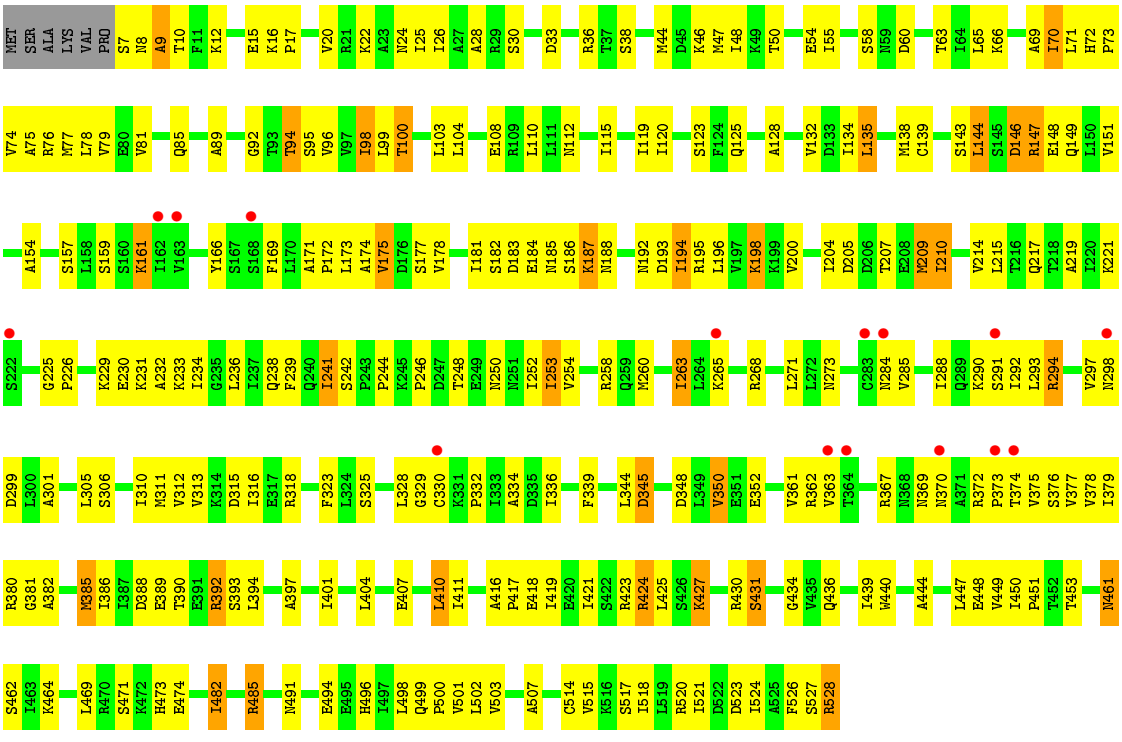
• Molecule 3: T-complex protein 1 subunit gamma

Chain k:



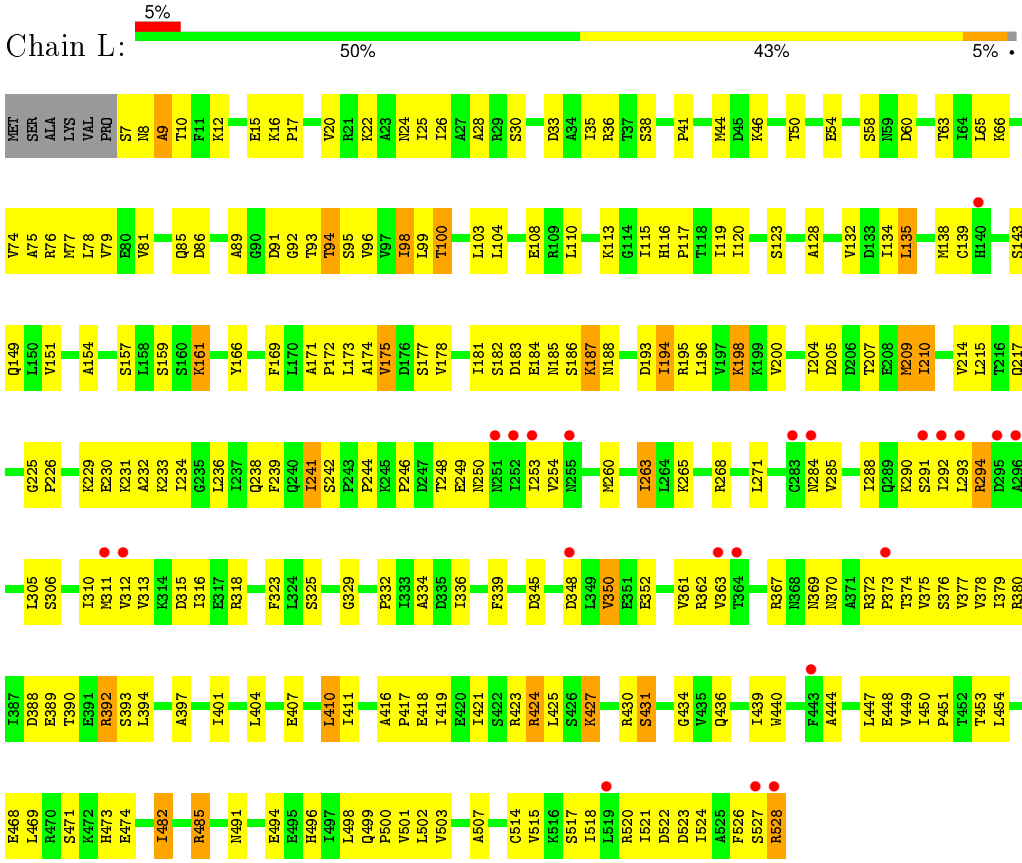
• Molecule 4: T-complex protein 1 subunit delta

Chain D:



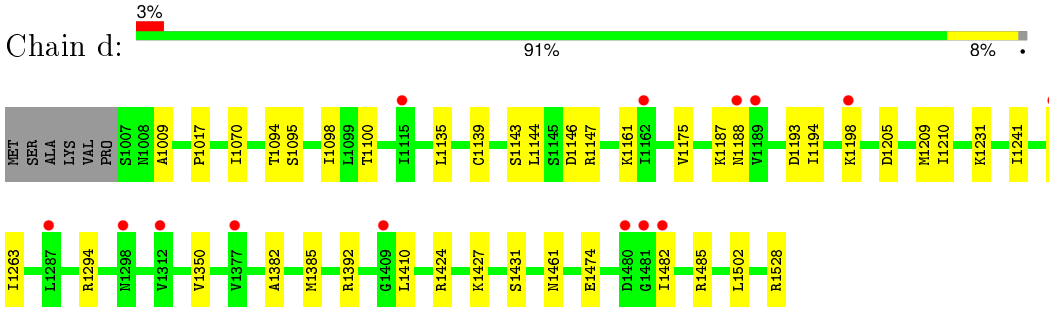
• Molecule 4: T-complex protein 1 subunit delta

Chain L:



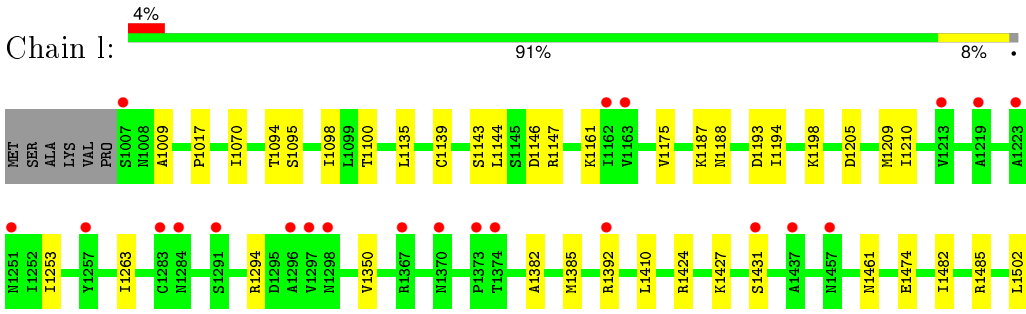
• Molecule 4: T-complex protein 1 subunit delta

Chain d:



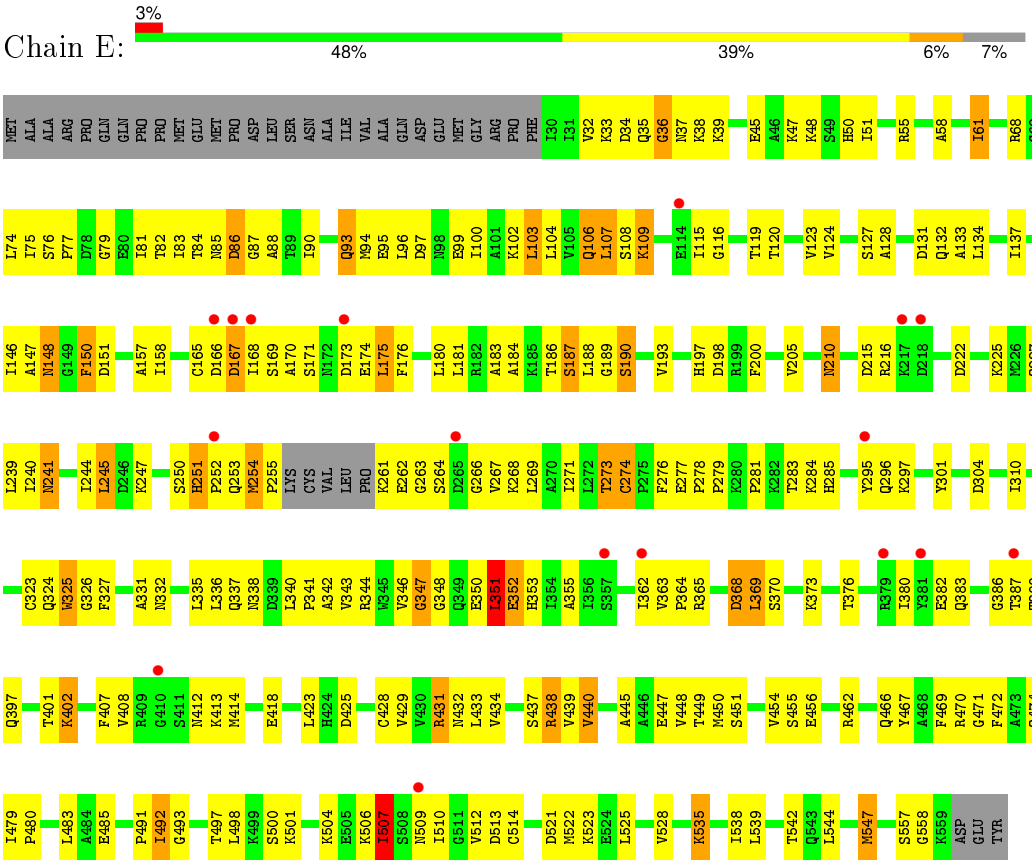
• Molecule 4: T-complex protein 1 subunit delta

Chain l:



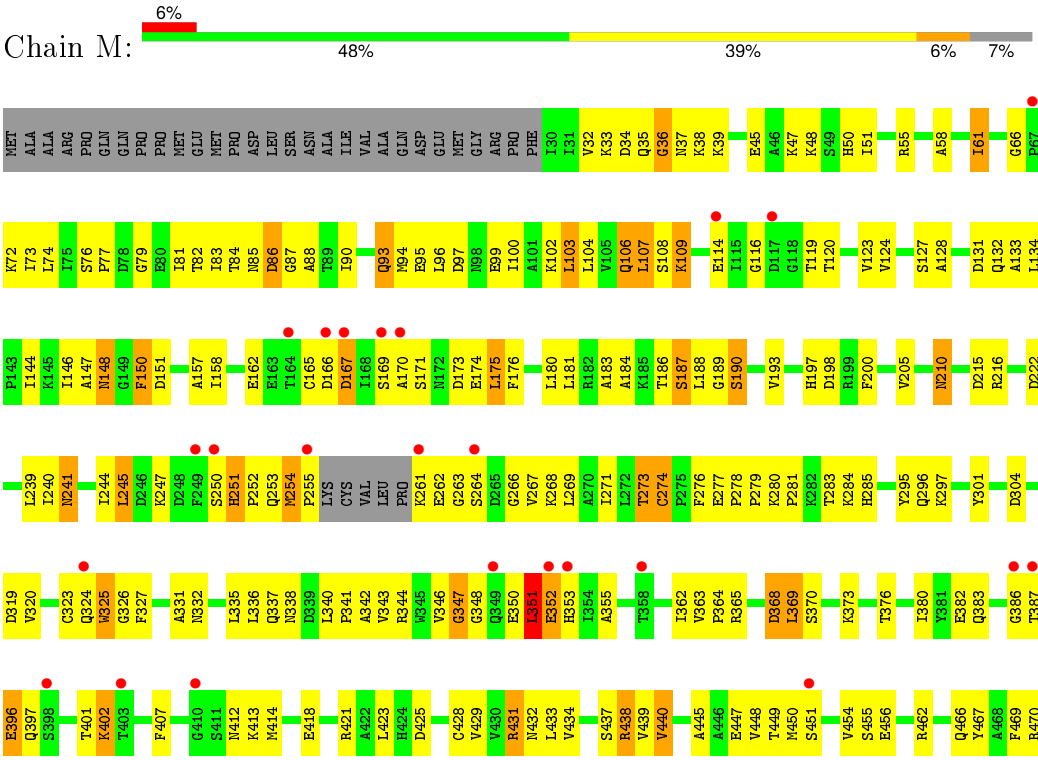
• Molecule 5: T-complex protein 1 subunit epsilon

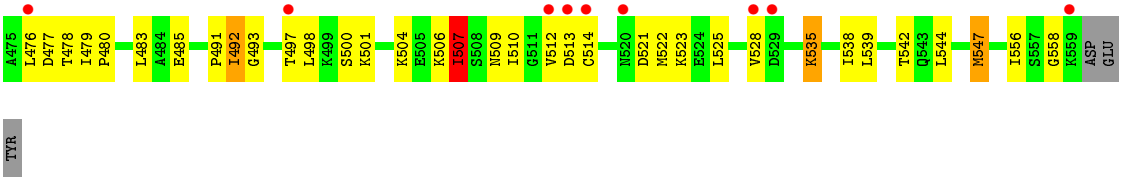
Chain E:



• Molecule 5: T-complex protein 1 subunit epsilon

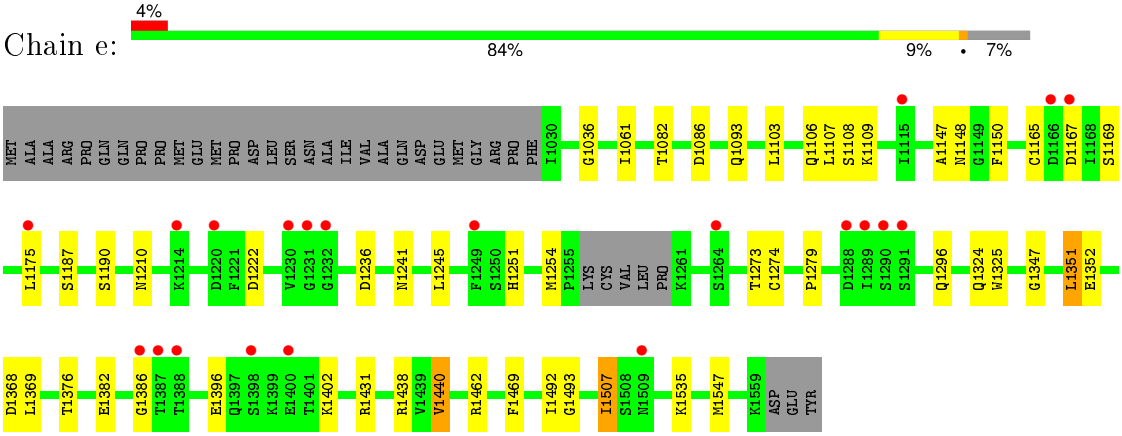
Chain M:





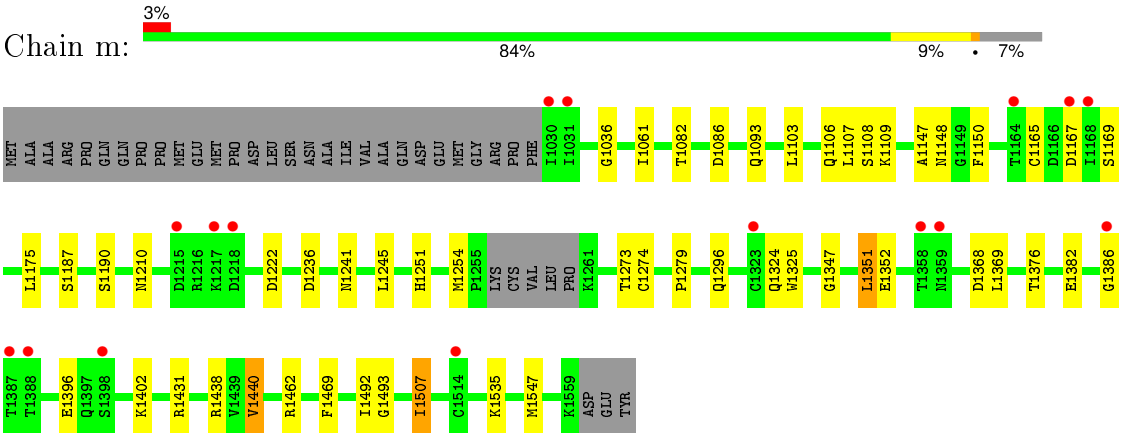
• Molecule 5: T-complex protein 1 subunit epsilon

Chain e:



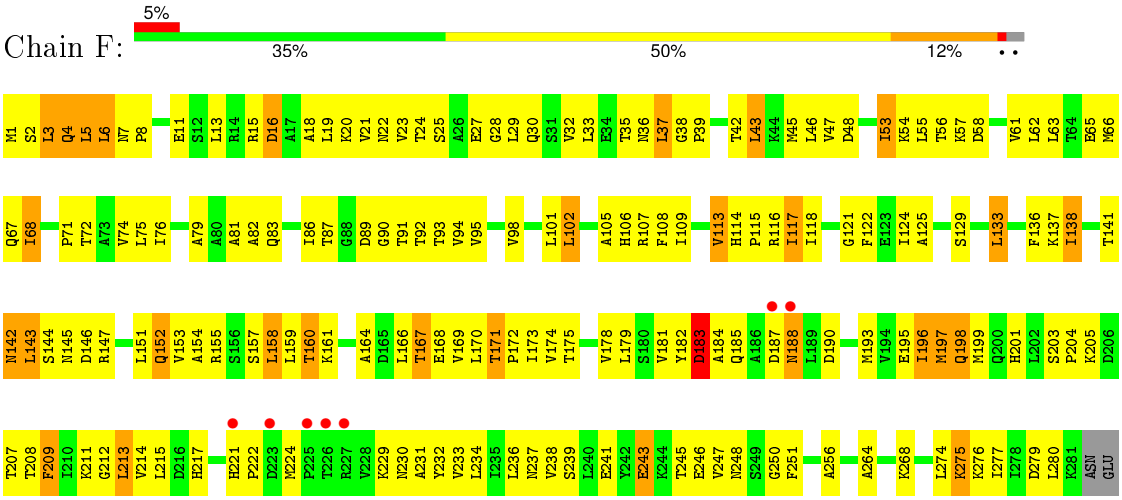
• Molecule 5: T-complex protein 1 subunit epsilon

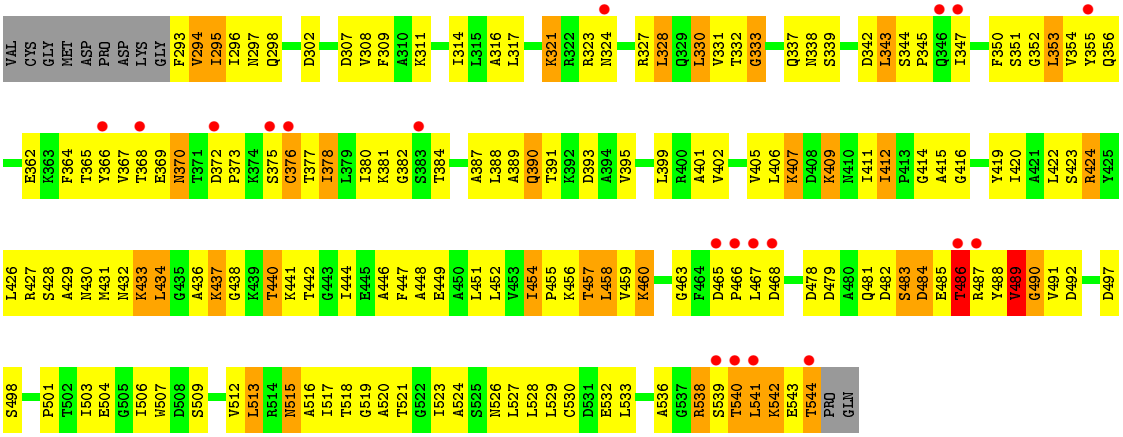
Chain m:



• Molecule 6: T-complex protein 1 subunit zeta

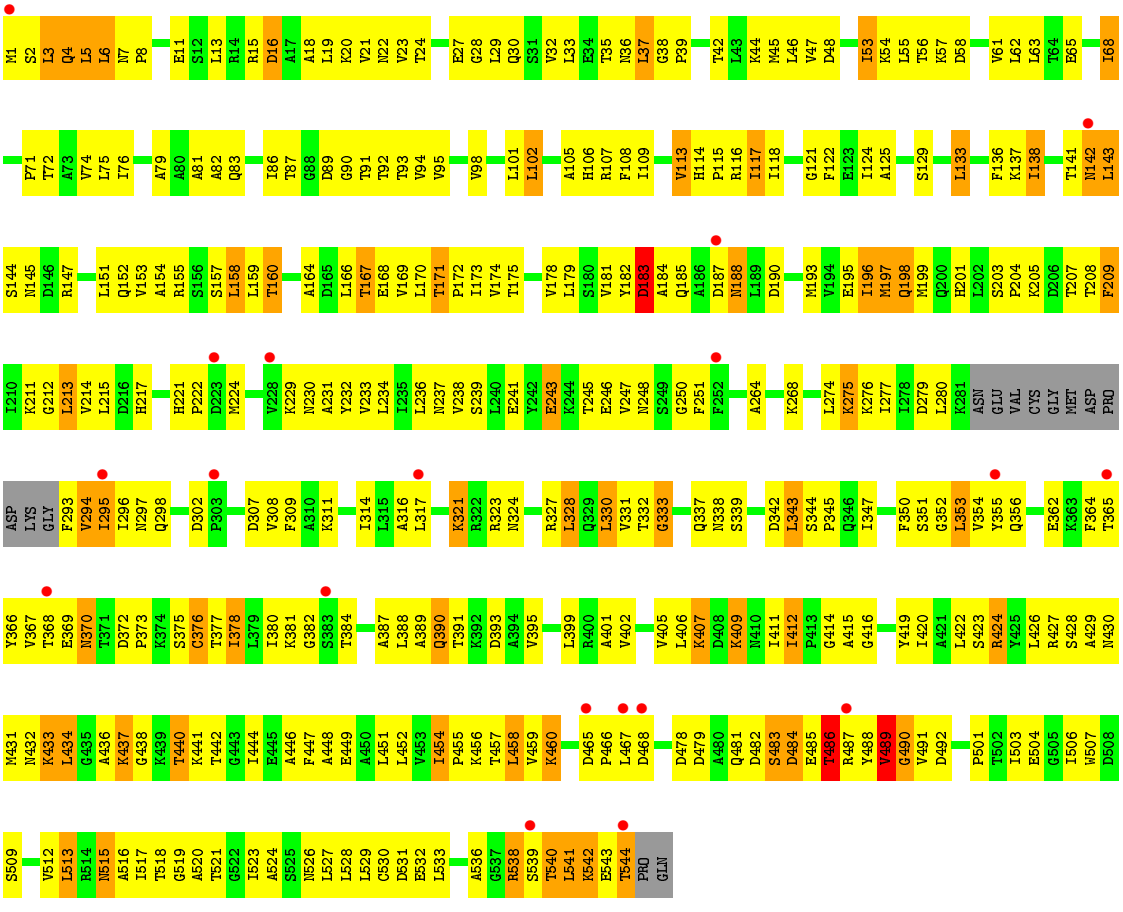
Chain F:





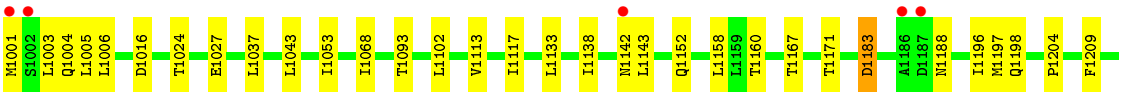
• Molecule 6: T-complex protein 1 subunit zeta

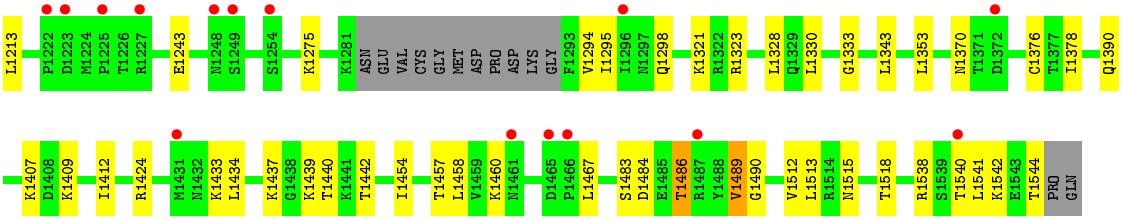
Chain N:



• Molecule 6: T-complex protein 1 subunit zeta

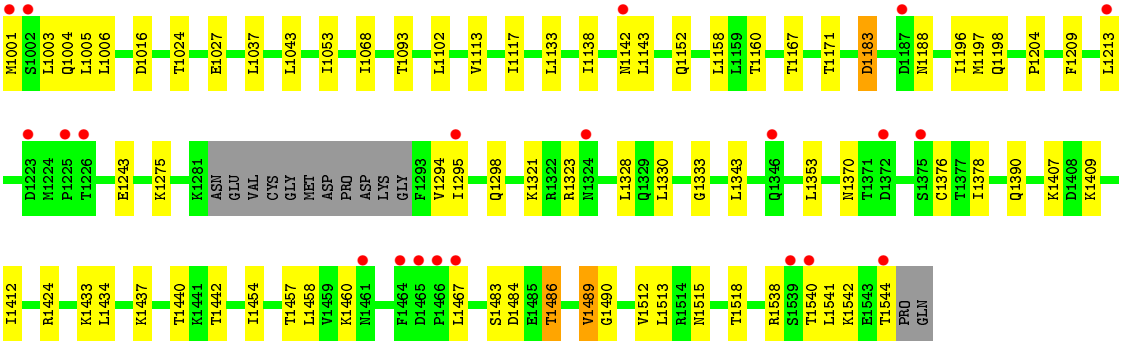
Chain f:





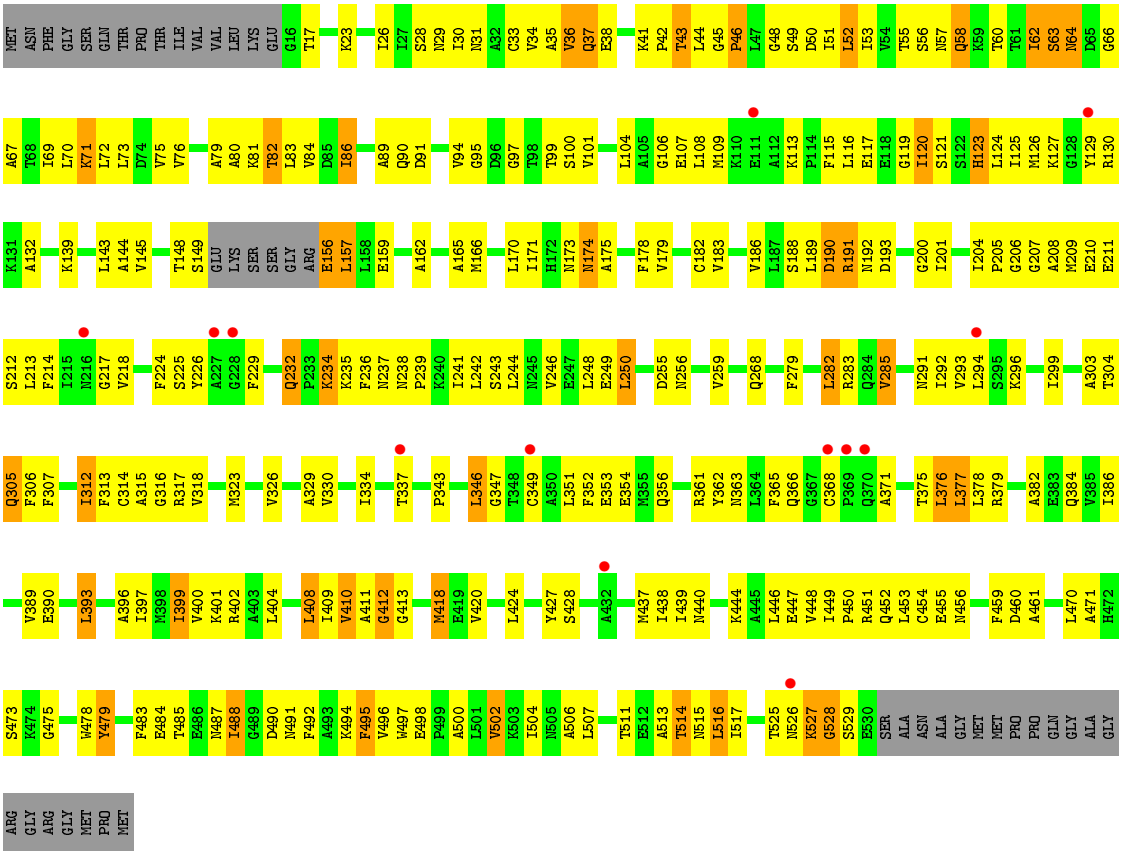
• Molecule 6: T-complex protein 1 subunit zeta

Chain n:



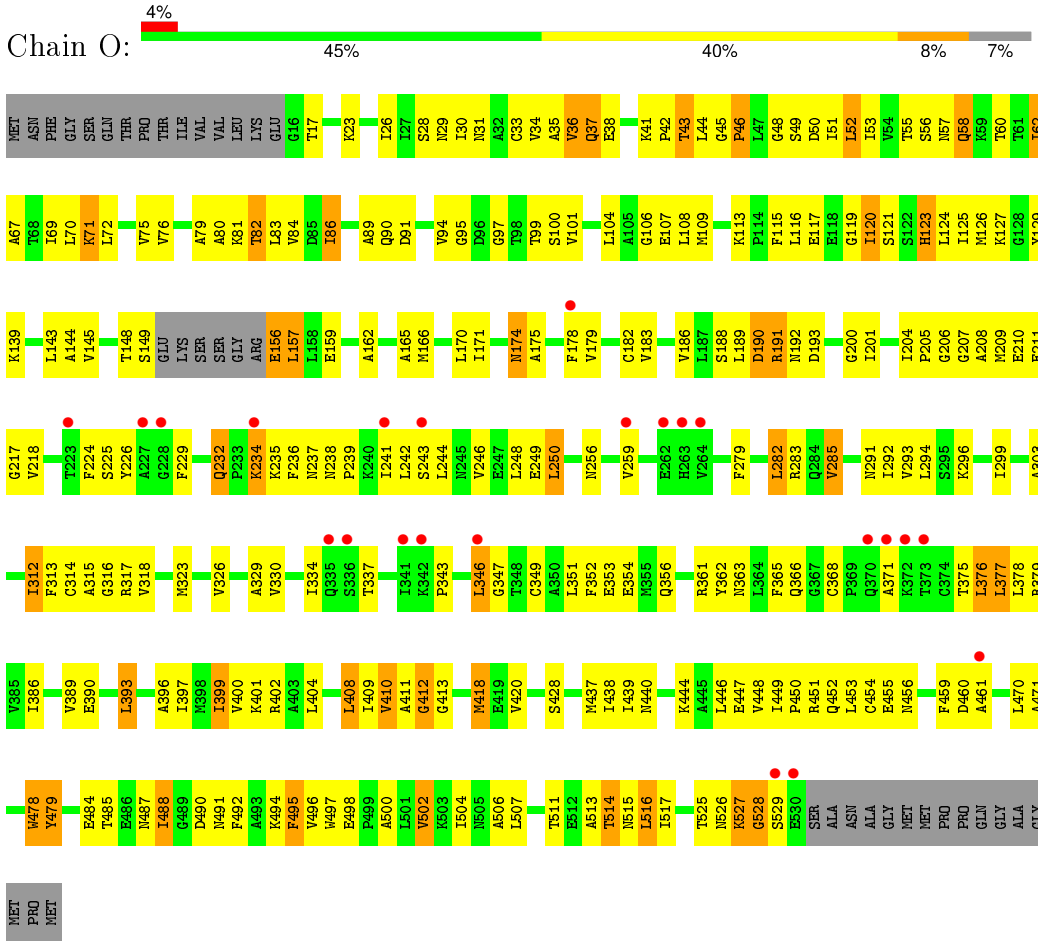
• Molecule 7: T-complex protein 1 subunit eta

Chain G:



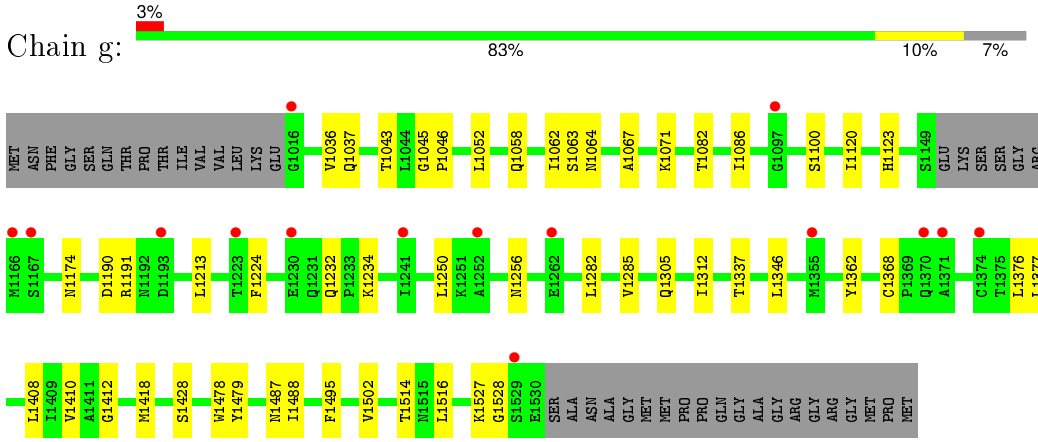
• Molecule 7: T-complex protein 1 subunit eta

Chain O:



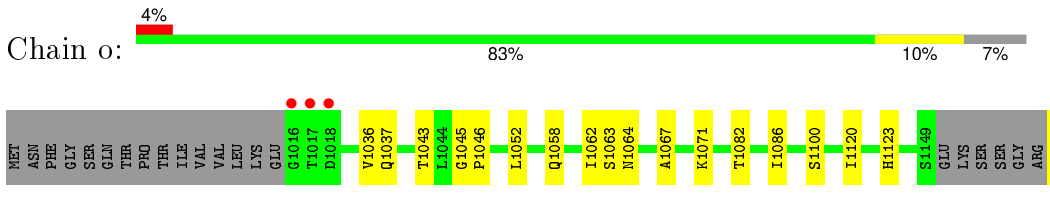
• Molecule 7: T-complex protein 1 subunit eta

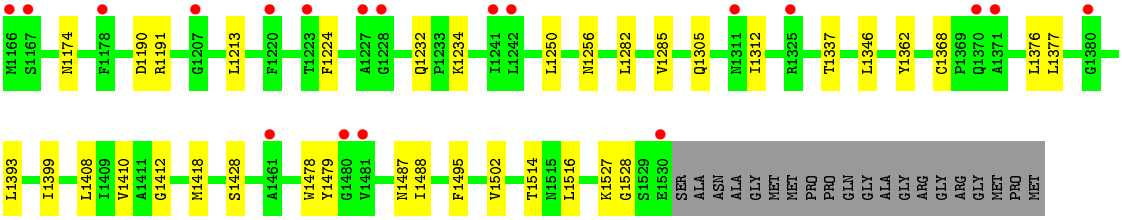
Chain g:



• Molecule 7: T-complex protein 1 subunit eta

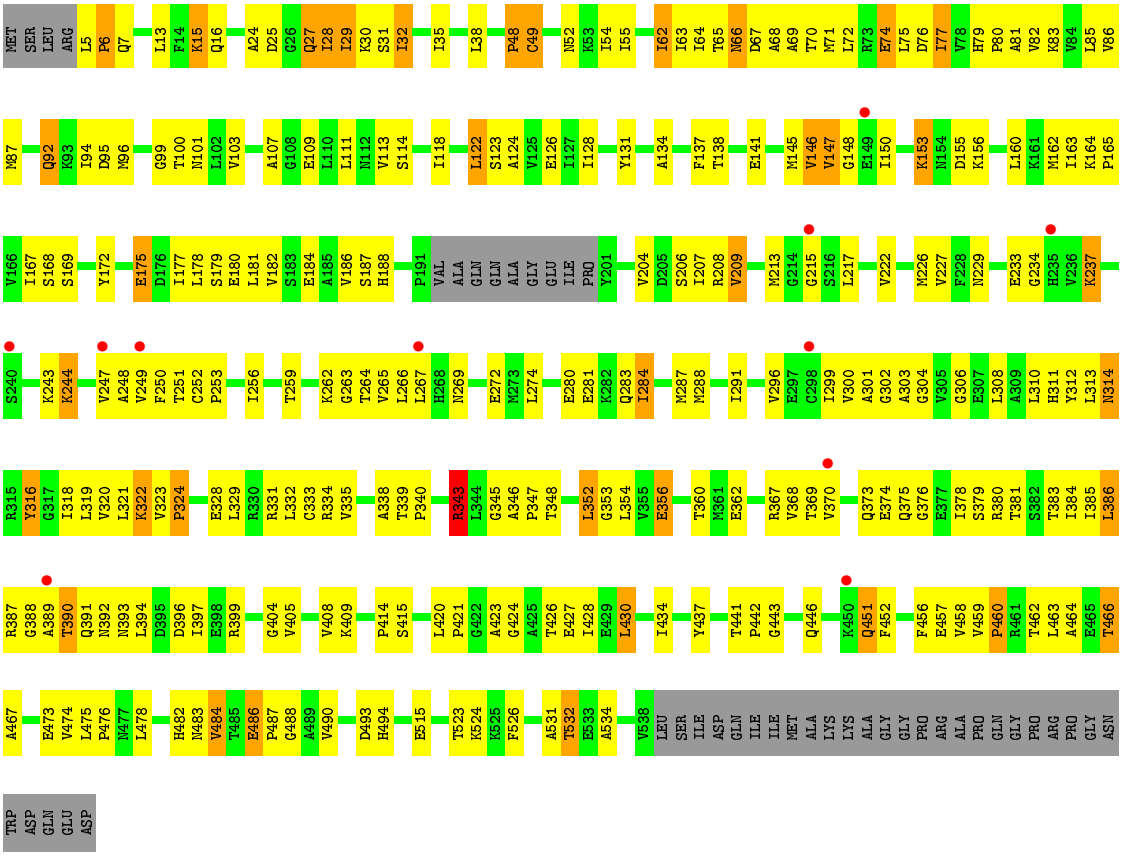
Chain o:





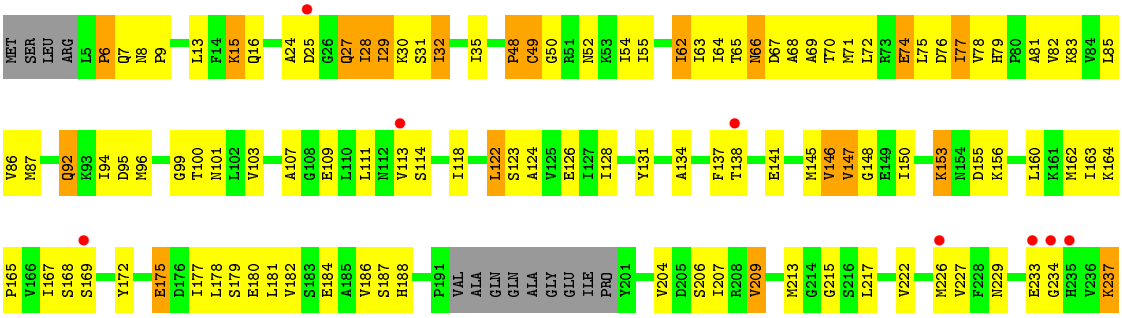
• Molecule 8: T-complex protein 1 subunit theta

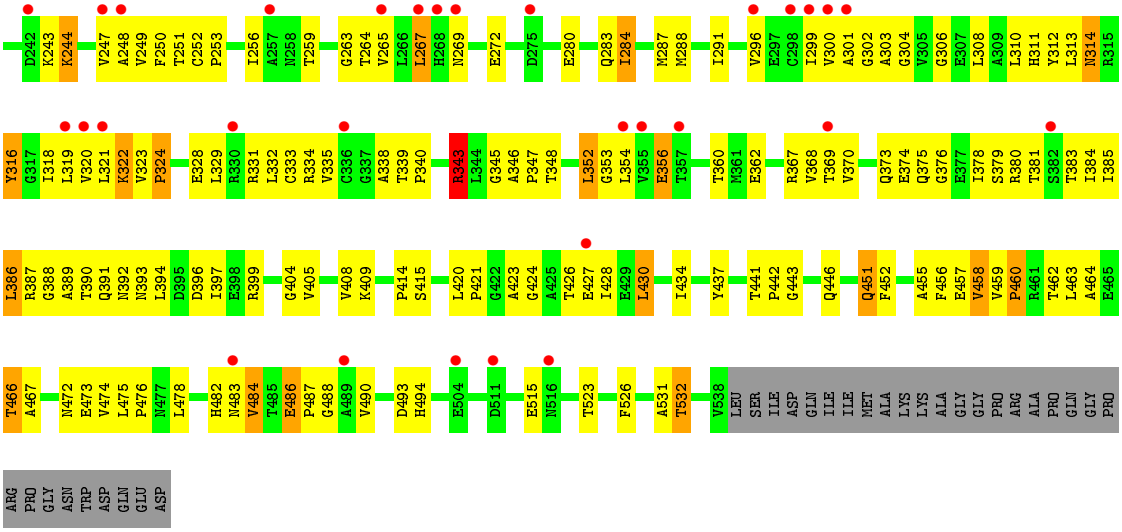
Chain H:



• Molecule 8: T-complex protein 1 subunit theta

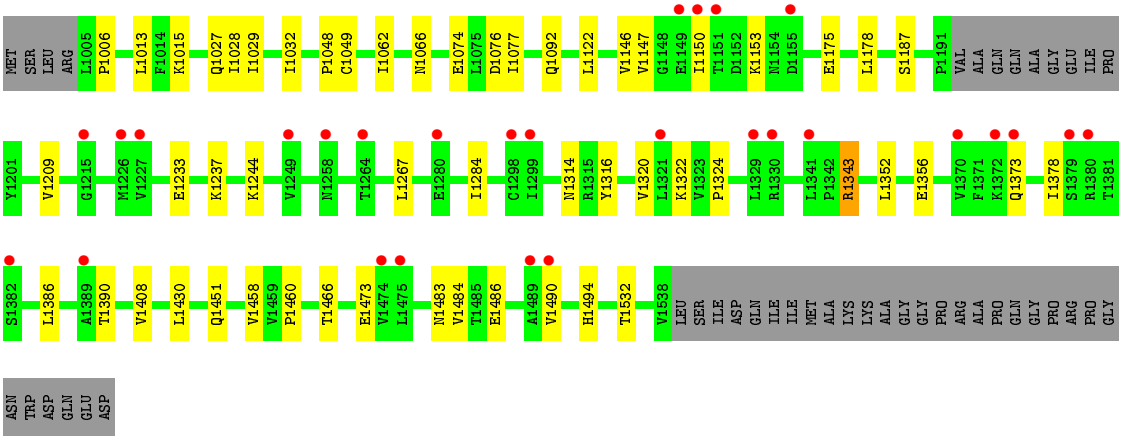
Chain P:





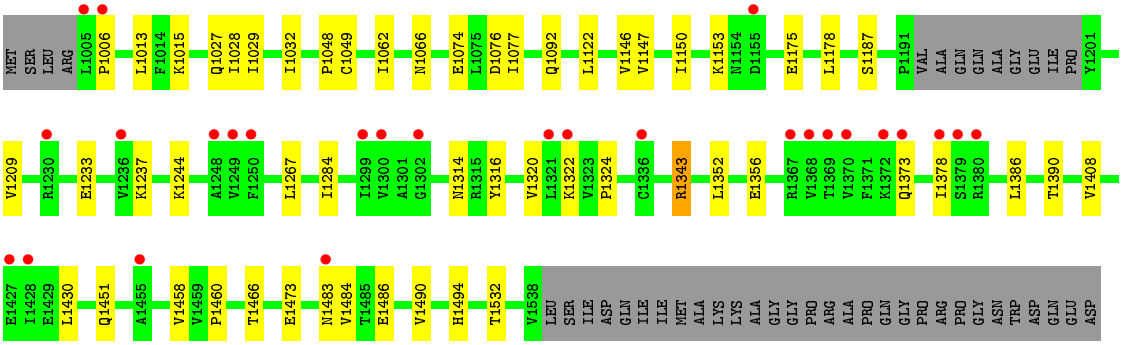
• Molecule 8: T-complex protein 1 subunit theta

Chain h:



• Molecule 8: T-complex protein 1 subunit theta

Chain p:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	159.10Å 162.54Å 268.10Å 85.23° 81.15° 61.17°	Depositor
Resolution (Å)	89.95 – 3.80 89.95 – 3.80	Depositor EDS
% Data completeness (in resolution range)	91.6 (89.95-3.80) 91.2 (89.95-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 3.78Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.307 , 0.344 0.318 , 0.349	Depositor DCC
R_{free} test set	10483 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	112.3	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 193.3	EDS
Estimated twinning fraction	0.024 for -h,-h+k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 209673 reflections	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	111235	wwPDB-VP
Average B, all atoms (Å^2)	141.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.01% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: BEF, SO4, ADP

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	0.23	0/3515	0.47	1/4835 (0.0%)
1	I	0.23	0/3515	0.47	1/4835 (0.0%)
1	a	0.23	0/3515	0.47	1/4835 (0.0%)
1	i	0.23	0/3515	0.47	1/4835 (0.0%)
2	B	0.26	0/3480	0.49	0/4754
2	J	0.26	0/3480	0.49	0/4754
2	b	0.26	0/3481	0.49	0/4755
2	j	0.26	0/3478	0.49	0/4751
3	C	0.23	0/3421	0.46	0/4689
3	K	0.23	0/3422	0.46	0/4690
3	c	0.23	0/3424	0.46	0/4693
3	k	0.23	0/3424	0.46	0/4693
4	D	0.23	0/3421	0.46	2/4683 (0.0%)
4	L	0.23	0/3421	0.45	1/4683 (0.0%)
4	d	0.23	0/3421	0.45	1/4683 (0.0%)
4	l	0.23	0/3421	0.45	1/4683 (0.0%)
5	E	0.23	0/3466	0.46	0/4739
5	M	0.23	0/3466	0.46	0/4739
5	e	0.23	0/3466	0.46	0/4739
5	m	0.23	0/3466	0.46	0/4739
6	F	0.26	0/3663	0.52	1/5008 (0.0%)
6	N	0.26	0/3660	0.52	1/5004 (0.0%)
6	f	0.26	0/3665	0.52	1/5009 (0.0%)
6	n	0.26	0/3661	0.52	1/5005 (0.0%)
7	G	0.23	0/3342	0.46	0/4578
7	O	0.23	0/3339	0.45	0/4574
7	g	0.23	0/3339	0.45	0/4574
7	o	0.23	0/3339	0.45	0/4574
8	H	0.22	0/3522	0.42	0/4825
8	P	0.22	0/3522	0.42	0/4825
8	h	0.22	0/3519	0.42	0/4820
8	p	0.22	0/3522	0.42	0/4825

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	0.24	0/111311	0.47	13/152428 (0.0%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	437	ALA	CB-CA-C	8.54	122.92	110.10
1	i	1437	ALA	CB-CA-C	8.53	122.89	110.10
1	A	437	ALA	CB-CA-C	8.53	122.89	110.10
1	a	1437	ALA	CB-CA-C	8.52	122.88	110.10
4	L	350	VAL	N-CA-C	-6.53	93.36	111.00
4	d	1350	VAL	N-CA-C	-6.53	93.37	111.00
4	l	1350	VAL	N-CA-C	-6.53	93.37	111.00
4	D	350	VAL	N-CA-C	-6.52	93.41	111.00
6	F	275	LYS	O-C-N	-5.79	113.43	122.70
6	n	1275	LYS	O-C-N	-5.77	113.47	122.70
6	f	1275	LYS	O-C-N	-5.77	113.47	122.70
6	N	275	LYS	O-C-N	-5.76	113.49	122.70
4	D	345	ASP	CB-CG-OD2	5.18	122.96	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3492	0	3026	298	0
1	I	3492	0	3026	291	0
1	a	3492	0	3026	0	0
1	i	3492	0	3026	0	0
2	B	3459	0	3146	476	0
2	J	3459	0	3146	479	0
2	b	3460	0	3148	0	0
2	j	3457	0	3139	0	0
3	C	3392	0	3019	295	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	3393	0	3022	272	0
3	c	3395	0	3029	0	0
3	k	3395	0	3029	0	0
4	D	3398	0	3010	337	0
4	L	3398	0	3010	315	0
4	d	3398	0	3010	0	0
4	l	3398	0	3010	0	0
5	E	3437	0	2943	285	0
5	M	3437	0	2943	289	0
5	e	3437	0	2943	0	0
5	m	3437	0	2943	0	0
6	F	3631	0	3330	640	0
6	N	3628	0	3321	629	0
6	f	3633	0	3333	0	0
6	n	3629	0	3322	0	0
7	G	3317	0	2920	382	0
7	O	3314	0	2911	375	0
7	g	3314	0	2911	0	0
7	o	3314	0	2911	0	0
8	H	3487	0	3109	296	0
8	P	3487	0	3109	273	0
8	h	3485	0	3103	0	0
8	p	3487	0	3109	0	0
9	A	27	0	11	3	0
9	B	27	0	11	8	0
9	C	27	0	12	7	0
9	D	27	0	11	8	0
9	E	27	0	11	2	0
9	F	27	0	11	6	0
9	G	27	0	11	5	0
9	H	27	0	12	3	0
9	J	27	0	11	5	0
9	L	27	0	11	7	0
9	M	27	0	11	6	0
9	N	27	0	11	6	0
9	P	27	0	12	5	0
9	a	27	0	11	0	0
9	b	27	0	11	0	0
9	e	27	0	12	0	0
9	f	27	0	11	0	0
9	g	27	0	11	0	0
9	h	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	k	27	0	11	0	0
9	l	27	0	11	0	0
9	m	27	0	11	0	0
9	n	27	0	11	0	0
9	p	27	0	12	0	0
10	A	4	0	0	0	0
10	B	4	0	0	0	0
10	C	4	0	0	3	0
10	D	4	0	0	0	0
10	E	4	0	0	0	0
10	F	4	0	0	2	0
10	G	4	0	0	0	0
10	H	4	0	0	0	0
10	J	4	0	0	0	0
10	L	4	0	0	1	0
10	M	4	0	0	0	0
10	N	4	0	0	3	0
10	P	4	0	0	0	0
10	a	4	0	0	0	0
10	b	4	0	0	0	0
10	e	4	0	0	0	0
10	f	4	0	0	0	0
10	g	4	0	0	0	0
10	h	4	0	0	0	0
10	k	4	0	0	0	0
10	l	4	0	0	0	0
10	m	4	0	0	0	0
10	n	4	0	0	0	0
10	p	4	0	0	0	0
11	I	5	0	0	0	0
11	K	5	0	0	0	0
11	O	5	0	0	0	0
11	c	5	0	0	0	0
11	d	5	0	0	0	0
11	i	5	0	0	0	0
11	j	5	0	0	0	0
11	o	5	0	0	0	0
12	B	1	0	0	0	0
12	E	1	0	0	0	0
12	G	1	0	0	0	0
12	M	1	0	0	0	0
12	e	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	g	1	0	0	0	0
12	m	1	0	0	0	0
All	All	111235	0	98253	5533	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 53.

All (5533) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:GLN:HA	2:B:5:ILE:CG1	1.37	1.53
2:J:4:GLN:HA	2:J:5:ILE:CG1	1.37	1.48
6:N:36:ASN:HB3	6:N:57:LYS:NZ	1.28	1.46
6:F:151:LEU:CD1	6:F:175:THR:CG2	1.90	1.46
6:N:151:LEU:CD1	6:N:175:THR:CG2	1.90	1.46
6:N:434:LEU:HD22	6:N:441:LYS:CB	1.45	1.46
8:H:6:PRO:HG3	4:L:71:LEU:CB	1.43	1.45
6:F:541:LEU:CB	6:F:542:LYS:HA	1.31	1.44
6:F:434:LEU:HD22	6:F:441:LYS:CB	1.45	1.43
6:F:151:LEU:HD13	6:F:175:THR:CG2	0.95	1.43
6:F:36:ASN:HB3	6:F:57:LYS:NZ	1.28	1.43
6:N:151:LEU:HD13	6:N:175:THR:CG2	0.95	1.41
7:G:189:LEU:HA	7:G:190:ASP:CB	1.23	1.41
6:N:541:LEU:CB	6:N:542:LYS:HA	1.30	1.41
6:N:352:GLY:CA	6:N:369:GLU:O	1.70	1.39
6:F:352:GLY:CA	6:F:369:GLU:O	1.70	1.39
7:O:189:LEU:HA	7:O:190:ASP:CB	1.23	1.39
4:D:71:LEU:CB	8:P:6:PRO:HG3	1.51	1.38
6:F:541:LEU:HB2	6:F:542:LYS:CA	1.51	1.37
6:F:117:ILE:CD1	5:M:34:ASP:HA	1.51	1.35
2:J:4:GLN:CA	2:J:5:ILE:HG12	1.59	1.33
2:B:4:GLN:CA	2:B:5:ILE:HG12	1.59	1.32
6:N:541:LEU:HB2	6:N:542:LYS:CA	1.51	1.31
6:N:151:LEU:CD1	6:N:175:THR:HG21	1.54	1.30
6:F:151:LEU:CD1	6:F:175:THR:HG21	1.54	1.29
8:H:6:PRO:CG	4:L:71:LEU:CB	2.10	1.29
7:O:516:LEU:C	7:O:516:LEU:HD22	1.54	1.28
1:A:184:LEU:HD21	1:A:198:TYR:CD2	1.67	1.27
1:I:184:LEU:HD21	1:I:198:TYR:CD2	1.67	1.27
2:J:361:ALA:N	2:J:362:GLY:HA2	1.31	1.27
1:I:250:ASN:HB2	1:I:300:LYS:CB	1.62	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:36:ASN:CB	6:F:57:LYS:HZ3	1.48	1.26
1:A:250:ASN:HB2	1:A:300:LYS:CB	1.62	1.26
6:F:352:GLY:HA3	6:F:369:GLU:C	1.54	1.25
7:O:235:LYS:HA	7:O:352:PHE:O	1.35	1.25
2:B:361:ALA:N	2:B:362:GLY:HA2	1.31	1.25
7:G:235:LYS:HA	7:G:352:PHE:O	1.35	1.25
6:N:352:GLY:HA3	6:N:369:GLU:C	1.54	1.25
6:N:352:GLY:O	6:N:367:VAL:CG1	1.85	1.25
2:B:463:ILE:O	2:B:467:ILE:CG1	1.85	1.24
6:N:94:VAL:O	6:N:98:VAL:CG2	1.85	1.24
4:D:521:ILE:HA	7:G:50:ASP:O	1.37	1.24
6:F:352:GLY:O	6:F:367:VAL:CG1	1.85	1.23
6:F:151:LEU:CD1	6:F:175:THR:HG23	1.60	1.23
6:F:94:VAL:O	6:F:98:VAL:CG2	1.85	1.23
7:O:189:LEU:CA	7:O:190:ASP:CB	2.14	1.23
2:J:463:ILE:O	2:J:467:ILE:CG1	1.85	1.23
2:J:463:ILE:O	2:J:467:ILE:HG12	1.05	1.22
2:B:463:ILE:O	2:B:467:ILE:HG12	1.06	1.22
6:F:90:GLY:O	6:F:94:VAL:HG23	1.40	1.22
7:G:516:LEU:HD22	7:G:516:LEU:C	1.54	1.22
1:I:184:LEU:HD21	1:I:198:TYR:CG	1.75	1.21
7:G:189:LEU:CA	7:G:190:ASP:CB	2.14	1.21
4:L:521:ILE:HA	7:O:50:ASP:O	1.37	1.21
1:A:184:LEU:HD21	1:A:198:TYR:CG	1.75	1.20
6:F:478:ASP:O	6:F:482:ASP:CB	1.90	1.20
6:N:478:ASP:O	6:N:482:ASP:CB	1.90	1.19
4:D:71:LEU:CB	8:P:6:PRO:CG	2.20	1.19
4:D:521:ILE:HD11	7:G:62:ILE:HD11	1.20	1.19
7:G:189:LEU:CA	7:G:190:ASP:HB3	1.71	1.19
6:N:90:GLY:O	6:N:94:VAL:HG23	1.40	1.18
6:N:151:LEU:CD1	6:N:175:THR:HG23	1.60	1.18
7:O:189:LEU:CA	7:O:190:ASP:HB3	1.71	1.18
4:L:524:ILE:HA	7:O:52:LEU:O	1.41	1.17
4:L:524:ILE:HG12	7:O:52:LEU:CB	1.72	1.17
3:C:457:ILE:HD13	3:C:467:LEU:HD13	1.26	1.17
2:J:4:GLN:HA	2:J:5:ILE:CB	1.73	1.16
6:N:36:ASN:CB	6:N:57:LYS:HZ3	1.59	1.16
8:H:54:ILE:HG13	8:H:64:ILE:HG12	1.21	1.15
2:B:4:GLN:HA	2:B:5:ILE:CB	1.73	1.15
5:E:273:THR:HG22	5:E:364:PRO:HA	1.29	1.15
6:F:94:VAL:O	6:F:98:VAL:HG23	0.98	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:228:VAL:HG22	1:I:363:GLN:HE22	1.03	1.14
4:D:524:ILE:HG12	7:G:52:LEU:CB	1.77	1.14
4:L:524:ILE:CG1	7:O:52:LEU:HB3	1.77	1.14
7:O:191:ARG:HE	7:O:191:ARG:HA	1.12	1.14
6:F:434:LEU:CD2	6:F:441:LYS:CB	2.26	1.13
6:N:501:PRO:HB3	6:N:506:ILE:HB	1.27	1.13
6:N:94:VAL:O	6:N:98:VAL:HG23	0.98	1.13
3:K:230:VAL:HG11	3:K:302:SER:OG	1.49	1.13
3:C:230:VAL:HG11	3:C:302:SER:OG	1.49	1.13
6:N:434:LEU:CD2	6:N:441:LYS:CB	2.27	1.12
5:E:34:ASP:HA	6:N:117:ILE:CD1	1.78	1.12
7:G:94:VAL:HG21	7:G:502:VAL:HG22	1.17	1.12
4:D:520:ARG:O	7:G:49:SER:HB3	1.47	1.12
1:A:228:VAL:HG22	1:A:363:GLN:HE22	1.03	1.12
6:F:166:LEU:O	6:F:167:THR:HG23	1.48	1.12
6:N:478:ASP:O	6:N:482:ASP:HB2	1.47	1.12
2:B:200:GLY:HA3	2:B:369:LEU:HD23	1.30	1.12
7:O:94:VAL:HG21	7:O:502:VAL:HG22	1.17	1.11
6:N:166:LEU:O	6:N:167:THR:HG23	1.48	1.11
8:P:206:SER:HB2	8:P:381:THR:HG22	1.32	1.11
6:N:434:LEU:HD23	6:N:434:LEU:H	0.98	1.11
5:M:273:THR:HG22	5:M:364:PRO:HA	1.29	1.11
6:F:434:LEU:HD23	6:F:434:LEU:H	0.98	1.11
2:J:357:SER:HB3	2:J:360:LYS:CB	1.79	1.11
4:D:521:ILE:CD1	7:G:62:ILE:HD11	1.79	1.11
4:L:521:ILE:HD11	7:O:62:ILE:HD11	1.28	1.11
8:P:54:ILE:HG13	8:P:64:ILE:HG12	1.21	1.11
6:F:274:LEU:HD21	6:F:308:VAL:HG11	1.31	1.11
6:N:274:LEU:HD21	6:N:308:VAL:HG11	1.31	1.11
6:F:53:ILE:HD12	6:F:53:ILE:O	1.49	1.10
2:B:357:SER:HB3	2:B:360:LYS:CB	1.79	1.10
2:B:422:ILE:HB	2:B:427:SER:HB2	1.28	1.10
6:F:478:ASP:O	6:F:482:ASP:HB2	1.47	1.10
2:J:200:GLY:HA3	2:J:369:LEU:HD23	1.30	1.10
6:N:143:LEU:HD13	6:N:145:ASN:H	0.94	1.10
1:A:494:ARG:CB	1:A:495:ARG:CA	2.29	1.10
2:J:29:VAL:O	2:J:33:VAL:HG22	1.50	1.10
6:N:53:ILE:O	6:N:53:ILE:HD12	1.49	1.09
2:B:29:VAL:O	2:B:33:VAL:HG22	1.50	1.09
1:I:494:ARG:CB	1:I:495:ARG:CA	2.30	1.09
6:F:83:GLN:HG3	6:F:94:VAL:HG21	1.32	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:ARG:CB	1:A:10:SER:CA	2.30	1.09
6:N:3:LEU:N	6:N:4:GLN:HB2	1.68	1.09
1:I:9:ARG:CB	1:I:10:SER:CA	2.30	1.09
7:G:191:ARG:HE	7:G:191:ARG:HA	1.12	1.09
3:K:457:ILE:HD13	3:K:467:LEU:HD13	1.26	1.09
5:M:273:THR:CG2	5:M:364:PRO:HA	1.81	1.09
2:J:422:ILE:HB	2:J:427:SER:HB2	1.28	1.09
7:O:189:LEU:HA	7:O:190:ASP:HB2	1.26	1.08
4:L:521:ILE:HD11	7:O:62:ILE:CD1	1.82	1.08
4:L:521:ILE:CD1	7:O:62:ILE:HD11	1.82	1.08
6:F:3:LEU:N	6:F:4:GLN:HB2	1.68	1.08
5:E:186:THR:HG21	5:E:528:VAL:O	1.51	1.08
5:E:273:THR:CG2	5:E:364:PRO:HA	1.81	1.08
6:N:352:GLY:HA3	6:N:369:GLU:O	0.90	1.08
5:M:186:THR:HG21	5:M:528:VAL:O	1.51	1.08
3:C:264:GLU:O	3:C:265:LYS:HG3	1.54	1.08
4:D:521:ILE:HD11	7:G:62:ILE:CD1	1.82	1.08
1:I:90:GLN:HG3	1:I:101:VAL:HG21	1.27	1.08
1:A:90:GLN:HG3	1:A:101:VAL:HG21	1.27	1.08
8:H:206:SER:HB2	8:H:381:THR:HG22	1.32	1.08
4:D:524:ILE:CG1	7:G:52:LEU:HB3	1.84	1.07
5:E:34:ASP:HA	6:N:117:ILE:HD11	1.11	1.07
4:L:250:ASN:HA	7:O:259:VAL:HG12	1.35	1.07
6:F:539:SER:HB3	6:F:542:LYS:HD2	1.37	1.07
6:F:352:GLY:HA3	6:F:369:GLU:O	0.90	1.07
6:F:143:LEU:HD13	6:F:145:ASN:H	0.93	1.07
2:J:242:LYS:NZ	2:J:247:GLY:O	1.86	1.07
8:H:237:LYS:HB3	8:H:314:ASN:CB	1.84	1.07
7:G:189:LEU:HA	7:G:190:ASP:HB2	1.26	1.07
6:N:539:SER:HB3	6:N:542:LYS:HD2	1.37	1.07
4:D:72:HIS:HB2	4:D:75:ALA:HB3	1.35	1.07
8:P:237:LYS:HB3	8:P:314:ASN:CB	1.85	1.07
6:F:501:PRO:HB3	6:F:506:ILE:HB	1.27	1.07
2:B:5:ILE:O	3:C:71:ALA:N	1.87	1.06
7:G:188:SER:O	7:G:190:ASP:HB2	1.54	1.06
1:A:93:GLU:CB	1:A:94:ILE:HD12	1.86	1.06
8:H:482:HIS:O	8:H:484:VAL:N	1.89	1.06
2:B:242:LYS:NZ	2:B:247:GLY:O	1.86	1.06
6:N:83:GLN:HG3	6:N:94:VAL:HG21	1.32	1.06
6:F:489:VAL:O	6:F:490:GLY:O	1.72	1.06
1:I:93:GLU:CB	1:I:94:ILE:HD12	1.85	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:513:ASN:O	2:B:514:ILE:HD13	1.56	1.05
6:N:489:VAL:O	6:N:490:GLY:O	1.72	1.05
6:N:430:ASN:HA	6:N:433:LYS:HG2	1.05	1.05
1:A:9:ARG:CB	1:A:10:SER:HA	1.84	1.05
7:O:188:SER:O	7:O:190:ASP:HB2	1.54	1.05
8:P:482:HIS:O	8:P:484:VAL:N	1.89	1.05
6:F:133:LEU:HD12	6:F:422:LEU:HD21	1.37	1.05
1:A:517:VAL:O	1:A:518:LEU:HG	1.56	1.05
6:F:430:ASN:HA	6:F:433:LYS:HG2	1.05	1.05
1:I:9:ARG:CB	1:I:10:SER:HA	1.83	1.05
6:F:434:LEU:N	6:F:434:LEU:HD23	1.62	1.04
1:I:494:ARG:CB	1:I:495:ARG:HA	1.87	1.04
8:H:243:LYS:O	8:H:244:LYS:HG2	1.57	1.04
6:F:430:ASN:HA	6:F:433:LYS:CG	1.86	1.04
8:P:237:LYS:HB3	8:P:314:ASN:HB2	1.39	1.04
1:I:517:VAL:O	1:I:518:LEU:HG	1.56	1.04
2:J:513:ASN:O	2:J:514:ILE:HD13	1.56	1.04
7:G:226:TYR:CD1	7:G:229:PHE:O	2.10	1.04
3:K:264:GLU:O	3:K:265:LYS:HG3	1.54	1.04
4:L:520:ARG:O	7:O:49:SER:HB3	1.57	1.04
6:N:430:ASN:HA	6:N:433:LYS:CG	1.86	1.04
8:H:237:LYS:HB3	8:H:314:ASN:HB2	1.39	1.04
5:M:401:THR:O	5:M:402:LYS:HE2	1.58	1.04
6:N:430:ASN:O	6:N:433:LYS:HB2	1.55	1.03
6:N:5:LEU:HA	6:N:6:LEU:CB	1.86	1.03
8:P:243:LYS:O	8:P:244:LYS:HG2	1.57	1.03
3:K:302:SER:O	3:K:303:ASP:HB2	1.59	1.03
6:F:5:LEU:HA	6:F:6:LEU:CB	1.86	1.03
5:M:184:ALA:O	5:M:188:LEU:N	1.91	1.03
4:D:524:ILE:HA	7:G:52:LEU:O	1.56	1.03
1:A:494:ARG:CB	1:A:495:ARG:HA	1.86	1.03
6:N:434:LEU:HD23	6:N:434:LEU:N	1.62	1.03
6:F:430:ASN:O	6:F:433:LYS:HB2	1.55	1.03
2:B:361:ALA:N	2:B:362:GLY:CA	2.22	1.03
4:L:72:HIS:HB2	4:L:75:ALA:HB3	1.35	1.03
6:F:2:SER:C	6:F:4:GLN:HB2	1.77	1.03
2:B:142:ASN:HB2	2:B:143:SER:HA	1.41	1.03
7:O:226:TYR:CD1	7:O:229:PHE:O	2.10	1.03
5:E:401:THR:O	5:E:402:LYS:HE2	1.58	1.02
6:N:2:SER:C	6:N:4:GLN:HB2	1.77	1.02
6:N:133:LEU:HD12	6:N:422:LEU:HD21	1.37	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:228:VAL:HG22	1:I:363:GLN:NE2	1.75	1.02
5:E:350:GLU:O	5:E:352:GLU:N	1.92	1.02
5:M:350:GLU:O	5:M:352:GLU:N	1.92	1.02
6:F:158:LEU:HD12	6:F:158:LEU:O	1.60	1.02
6:N:352:GLY:O	6:N:367:VAL:HG13	1.57	1.01
2:J:361:ALA:N	2:J:362:GLY:CA	2.22	1.01
1:A:228:VAL:HG22	1:A:363:GLN:NE2	1.75	1.01
5:E:184:ALA:O	5:E:188:LEU:N	1.91	1.01
6:F:352:GLY:O	6:F:367:VAL:HG13	1.57	1.01
7:G:42:PRO:O	7:G:48:GLY:HA2	1.59	1.01
6:F:167:THR:HB	6:F:169:VAL:N	1.76	1.00
6:N:167:THR:HB	6:N:169:VAL:N	1.76	1.00
6:N:158:LEU:O	6:N:158:LEU:HD12	1.60	1.00
3:C:298:GLU:C	3:C:319:ARG:CB	2.30	1.00
2:J:4:GLN:CA	2:J:5:ILE:HG23	1.91	1.00
3:C:234:MET:HB3	3:C:310:LEU:HD22	1.44	1.00
4:L:134:ILE:HD11	4:L:424:ARG:HD3	1.41	1.00
6:N:143:LEU:HD13	6:N:145:ASN:N	1.76	1.00
3:K:298:GLU:C	3:K:319:ARG:CB	2.30	1.00
7:O:42:PRO:O	7:O:48:GLY:HA2	1.59	0.99
6:F:434:LEU:HA	6:F:441:LYS:CB	1.93	0.99
2:B:4:GLN:CA	2:B:5:ILE:HG23	1.91	0.99
6:F:143:LEU:HD13	6:F:145:ASN:N	1.75	0.99
6:N:434:LEU:HA	6:N:441:LYS:CB	1.92	0.99
6:F:434:LEU:O	6:F:438:GLY:N	1.95	0.99
6:N:434:LEU:O	6:N:438:GLY:N	1.95	0.99
6:F:540:THR:O	6:F:542:LYS:HG2	1.62	0.99
7:O:516:LEU:HD13	7:O:517:ILE:HG12	1.44	0.99
1:I:9:ARG:CB	1:I:10:SER:C	2.31	0.99
3:C:302:SER:O	3:C:303:ASP:HB2	1.59	0.99
2:J:142:ASN:HB2	2:J:143:SER:HA	1.41	0.99
6:F:16:ASP:HA	6:F:19:LEU:HD12	1.44	0.99
2:B:490:SER:O	2:B:493:LEU:HG	1.63	0.99
7:G:516:LEU:HD13	7:G:517:ILE:HG12	1.44	0.98
2:J:490:SER:O	2:J:493:LEU:HG	1.63	0.98
7:O:516:LEU:C	7:O:516:LEU:CD2	2.30	0.98
1:A:9:ARG:CB	1:A:10:SER:C	2.31	0.98
4:D:70:ILE:HG12	4:D:70:ILE:O	1.63	0.98
3:K:265:LYS:NZ	3:K:268:ASP:HB3	1.79	0.98
8:H:423:ALA:HA	9:H:601:ADP:H2'	1.45	0.98
6:N:540:THR:O	6:N:542:LYS:HG2	1.62	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:124:ALA:O	8:H:128:ILE:HG13	1.63	0.98
6:F:540:THR:C	6:F:541:LEU:HD22	1.84	0.98
4:D:134:ILE:HD11	4:D:424:ARG:HD3	1.41	0.98
2:J:8:ASP:HB3	2:J:9:GLN:HA	1.43	0.98
6:N:540:THR:C	6:N:541:LEU:HD22	1.84	0.97
2:B:8:ASP:HB3	2:B:9:GLN:HA	1.43	0.97
2:J:260:GLN:HA	2:J:263:LYS:HD2	1.46	0.97
3:C:265:LYS:NZ	3:C:268:ASP:HB3	1.79	0.97
7:O:516:LEU:CD1	7:O:517:ILE:HG12	1.94	0.97
4:L:524:ILE:CA	7:O:52:LEU:O	2.12	0.97
6:N:3:LEU:HD12	6:N:5:LEU:HD23	1.46	0.97
4:L:70:ILE:HG12	4:L:70:ILE:O	1.63	0.97
7:G:94:VAL:CG2	7:G:502:VAL:HG22	1.93	0.97
2:B:260:GLN:HA	2:B:263:LYS:HD2	1.46	0.97
6:F:43:LEU:HD23	6:F:57:LYS:HB2	1.44	0.97
6:N:16:ASP:HA	6:N:19:LEU:HD12	1.44	0.97
6:F:434:LEU:CA	6:F:441:LYS:CB	2.43	0.97
6:F:117:ILE:HD11	5:M:34:ASP:CA	1.93	0.97
3:K:234:MET:HB3	3:K:310:LEU:HD22	1.44	0.97
3:K:298:GLU:O	3:K:319:ARG:CB	2.13	0.97
1:A:184:LEU:CD2	1:A:198:TYR:CD2	2.49	0.96
2:J:202:LYS:O	2:J:370:ARG:HA	1.64	0.96
2:J:4:GLN:CA	2:J:5:ILE:CG1	2.30	0.96
2:B:202:LYS:O	2:B:370:ARG:HA	1.64	0.96
7:O:94:VAL:CG2	7:O:502:VAL:HG22	1.93	0.96
5:M:88:ALA:HB2	5:M:119:THR:HB	1.46	0.96
5:E:88:ALA:HB2	5:E:119:THR:HB	1.46	0.96
6:N:434:LEU:CA	6:N:441:LYS:CB	2.43	0.96
4:D:254:VAL:HG22	8:H:265:VAL:HA	1.47	0.96
7:G:43:THR:HG22	7:G:64:ASN:HB3	1.45	0.96
5:M:66:GLY:H	9:M:601:ADP:H5'1	1.30	0.96
3:K:269:TRP:HH2	6:N:248:ASN:H	0.97	0.96
2:J:514:ILE:HD12	3:K:47:MET:HB3	1.48	0.96
6:N:154:ALA:CB	6:N:402:VAL:HG23	1.96	0.96
3:C:298:GLU:O	3:C:319:ARG:CB	2.13	0.96
7:G:516:LEU:CD1	7:G:517:ILE:HG12	1.94	0.96
6:F:154:ALA:CB	6:F:402:VAL:HG23	1.96	0.96
6:F:117:ILE:CD1	5:M:34:ASP:CA	2.43	0.95
6:F:117:ILE:HD11	5:M:34:ASP:HA	0.97	0.95
7:O:90:GLN:HG3	7:O:101:VAL:HG21	1.48	0.95
8:P:124:ALA:O	8:P:128:ILE:HG13	1.63	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:3:LEU:HD12	6:F:5:LEU:HD23	1.46	0.95
6:F:43:LEU:CD2	6:F:57:LYS:HB2	1.96	0.95
6:N:36:ASN:CB	6:N:57:LYS:NZ	2.24	0.95
1:I:184:LEU:CD2	1:I:198:TYR:CD2	2.49	0.95
1:A:494:ARG:CB	1:A:495:ARG:C	2.35	0.95
7:O:235:LYS:CA	7:O:352:PHE:O	2.15	0.95
4:D:521:ILE:CA	7:G:50:ASP:O	2.14	0.95
1:I:494:ARG:CB	1:I:495:ARG:C	2.35	0.95
7:O:43:THR:HG22	7:O:64:ASN:HB3	1.45	0.94
6:N:541:LEU:CB	6:N:542:LYS:CA	2.22	0.94
2:J:263:LYS:NZ	3:K:266:GLU:HB3	1.81	0.94
6:F:465:ASP:HA	6:F:466:PRO:C	1.88	0.94
3:C:335:THR:HB	8:H:237:LYS:HE2	1.48	0.94
6:N:465:ASP:HA	6:N:466:PRO:C	1.88	0.94
5:E:253:GLN:CB	5:E:254:MET:CB	2.46	0.94
8:H:316:TYR:H	8:H:316:TYR:HD2	1.15	0.94
5:M:253:GLN:CB	5:M:254:MET:CB	2.46	0.94
8:P:316:TYR:H	8:P:316:TYR:HD2	1.15	0.94
5:M:107:LEU:HD22	5:M:544:LEU:HG	1.49	0.94
4:D:523:ASP:O	7:G:51:ILE:HG23	1.67	0.94
1:A:494:ARG:CB	1:A:496:SER:N	2.30	0.94
2:J:70:ASP:HB2	6:N:5:LEU:HD22	1.49	0.94
6:F:420:ILE:CG2	6:F:482:ASP:OD1	2.15	0.94
1:I:494:ARG:CB	1:I:496:SER:N	2.30	0.94
7:G:235:LYS:CA	7:G:352:PHE:O	2.15	0.93
7:G:516:LEU:CD2	7:G:516:LEU:C	2.30	0.93
7:O:191:ARG:NE	7:O:192:ASN:H	1.65	0.93
8:H:237:LYS:CB	8:H:314:ASN:HB3	1.98	0.93
6:N:420:ILE:CG2	6:N:482:ASP:OD1	2.15	0.93
2:B:4:GLN:CA	2:B:5:ILE:CG1	2.30	0.93
6:N:434:LEU:CD2	6:N:434:LEU:N	2.30	0.93
7:G:516:LEU:HD22	7:G:517:ILE:N	1.83	0.93
2:J:251:LYS:H	6:N:251:PHE:HA	1.32	0.93
7:O:513:ALA:O	7:O:516:LEU:HD13	1.68	0.93
2:J:127:ALA:HB2	2:J:430:VAL:HG22	1.51	0.93
8:P:237:LYS:CB	8:P:314:ASN:HB3	1.98	0.93
3:K:57:LEU:HD23	3:K:57:LEU:N	1.83	0.93
4:D:524:ILE:HG12	7:G:52:LEU:HB3	0.94	0.93
3:C:42:LYS:CB	3:C:460:ALA:HA	1.98	0.93
2:B:459:LEU:HD22	2:B:472:LEU:HG	1.51	0.93
3:K:42:LYS:CB	3:K:460:ALA:HA	1.98	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:434:LEU:N	6:F:434:LEU:CD2	2.30	0.93
6:N:53:ILE:C	6:N:53:ILE:HD12	1.89	0.93
6:F:424:ARG:HE	6:F:424:ARG:HA	1.33	0.93
1:A:433:LEU:O	1:A:437:ALA:N	2.01	0.93
7:G:513:ALA:O	7:G:516:LEU:HD13	1.68	0.93
7:G:471:ALA:O	7:G:475:GLY:CA	2.17	0.93
6:F:195:GLU:HB3	6:F:377:THR:HG22	1.51	0.93
6:F:409:LYS:HD3	6:F:409:LYS:H	1.34	0.93
2:J:459:LEU:HD22	2:J:472:LEU:HG	1.51	0.93
7:G:191:ARG:NE	7:G:192:ASN:H	1.65	0.92
4:L:523:ASP:O	7:O:51:ILE:HG23	1.69	0.92
1:I:433:LEU:O	1:I:437:ALA:N	2.01	0.92
1:I:350:PHE:HE2	1:I:354:TYR:HB2	1.34	0.92
3:C:57:LEU:N	3:C:57:LEU:HD23	1.83	0.92
6:N:424:ARG:HE	6:N:424:ARG:HA	1.33	0.92
2:B:442:THR:HG23	2:B:452:SER:HB2	1.50	0.92
7:O:471:ALA:O	7:O:475:GLY:N	2.02	0.92
6:N:409:LYS:HD3	6:N:409:LYS:H	1.34	0.92
4:L:210:ILE:HB	4:L:376:SER:O	1.69	0.92
6:F:434:LEU:CD2	6:F:434:LEU:H	1.80	0.92
7:O:516:LEU:HD22	7:O:517:ILE:N	1.83	0.92
2:J:442:THR:HG23	2:J:452:SER:HB2	1.50	0.92
6:F:541:LEU:CB	6:F:542:LYS:CA	2.22	0.92
4:D:254:VAL:HG11	4:D:260:MET:SD	2.09	0.92
5:E:107:LEU:HD22	5:E:544:LEU:HG	1.49	0.92
4:L:254:VAL:HG11	4:L:260:MET:SD	2.09	0.92
6:N:195:GLU:HB3	6:N:377:THR:HG22	1.51	0.92
7:G:90:GLN:HG3	7:G:101:VAL:HG21	1.48	0.92
8:H:209:VAL:HG22	8:H:386:LEU:HD11	1.52	0.92
7:O:471:ALA:O	7:O:475:GLY:CA	2.17	0.92
1:A:250:ASN:CB	1:A:300:LYS:CB	2.47	0.91
1:A:228:VAL:CG2	1:A:363:GLN:HE22	1.82	0.91
6:F:53:ILE:C	6:F:53:ILE:HD12	1.89	0.91
1:I:228:VAL:CG2	1:I:363:GLN:HE22	1.82	0.91
2:B:127:ALA:HB2	2:B:430:VAL:HG22	1.51	0.91
2:B:21:SER:HG	1:I:8:SER:N	1.67	0.91
5:E:166:ASP:N	5:E:167:ASP:HB2	1.86	0.91
4:D:210:ILE:HB	4:D:376:SER:O	1.69	0.91
6:N:36:ASN:HB3	6:N:57:LYS:HZ1	1.29	0.91
6:N:151:LEU:HD13	6:N:175:THR:HG23	0.91	0.91
2:J:3:VAL:O	2:J:5:ILE:HG21	1.71	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:250:ASN:CB	1:I:300:LYS:CB	2.47	0.91
7:G:471:ALA:O	7:G:475:GLY:N	2.02	0.91
4:L:521:ILE:CA	7:O:50:ASP:O	2.18	0.91
2:B:29:VAL:O	2:B:33:VAL:CG2	2.19	0.91
2:J:27:ILE:HD12	2:J:104:ARG:HH11	1.36	0.91
2:B:27:ILE:HD12	2:B:104:ARG:HH11	1.36	0.91
8:H:113:VAL:HG12	8:H:451:GLN:HG3	1.53	0.91
6:N:434:LEU:N	6:N:441:LYS:CB	2.34	0.90
6:F:159:LEU:HA	6:F:164:ALA:CB	2.01	0.90
2:J:422:ILE:CG2	2:J:427:SER:HB3	2.02	0.90
3:C:264:GLU:C	3:C:265:LYS:HG3	1.91	0.90
2:B:3:VAL:O	2:B:5:ILE:HG21	1.71	0.90
7:G:191:ARG:NE	7:G:191:ARG:HA	1.85	0.90
8:P:237:LYS:CB	8:P:314:ASN:CB	2.49	0.90
6:N:354:VAL:HG13	6:N:367:VAL:HG22	1.53	0.90
6:F:209:PHE:HE2	6:F:376:CYS:HG	0.92	0.90
8:H:463:LEU:O	8:H:466:THR:OG1	1.87	0.90
7:O:316:GLY:O	7:O:317:ARG:HB3	1.71	0.90
1:A:350:PHE:HE2	1:A:354:TYR:HB2	1.34	0.90
6:N:159:LEU:HA	6:N:164:ALA:CB	2.01	0.90
2:B:3:VAL:O	2:B:5:ILE:HD13	1.72	0.90
6:F:434:LEU:N	6:F:441:LYS:CB	2.34	0.90
8:P:463:LEU:O	8:P:466:THR:OG1	1.87	0.90
3:C:265:LYS:HZ3	3:C:268:ASP:HB3	1.35	0.89
6:F:354:VAL:HG13	6:F:367:VAL:HG22	1.53	0.89
5:M:32:VAL:HG22	5:M:33:LYS:H	1.34	0.89
7:O:191:ARG:HA	7:O:191:ARG:NE	1.85	0.89
2:J:70:ASP:CB	6:N:5:LEU:HD22	2.02	0.89
6:F:109:ILE:HG13	5:M:39:LYS:HZ3	1.35	0.89
8:P:209:VAL:HG22	8:P:386:LEU:HD11	1.52	0.89
5:M:166:ASP:N	5:M:167:ASP:HB2	1.85	0.89
2:B:422:ILE:CG2	2:B:427:SER:HB3	2.02	0.89
3:K:41:PRO:HA	3:K:161:THR:CG2	2.02	0.89
2:B:4:GLN:HA	2:B:5:ILE:HG12	0.90	0.89
6:F:151:LEU:HD13	6:F:175:THR:HG23	0.91	0.89
2:J:29:VAL:O	2:J:33:VAL:CG2	2.19	0.89
1:A:156:LEU:HD13	1:A:185:LEU:HD11	1.54	0.89
7:G:316:GLY:O	7:G:317:ARG:HB3	1.71	0.89
8:H:6:PRO:CB	4:L:71:LEU:CB	2.51	0.89
4:L:521:ILE:CG1	7:O:62:ILE:HD11	2.01	0.89
3:C:41:PRO:HA	3:C:161:THR:CG2	2.02	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:242:LYS:CE	2:B:247:GLY:H	1.86	0.89
6:N:83:GLN:CG	6:N:94:VAL:HG21	2.02	0.89
2:B:72:PRO:HB3	3:C:47:MET:HE3	1.55	0.89
6:F:452:LEU:C	6:F:455:PRO:HD2	1.93	0.89
8:P:113:VAL:HG12	8:P:451:GLN:HG3	1.54	0.88
2:J:3:VAL:O	2:J:5:ILE:HD13	1.72	0.88
6:N:430:ASN:CA	6:N:433:LYS:HG2	2.00	0.88
1:I:90:GLN:CG	1:I:101:VAL:HG21	2.03	0.88
8:P:6:PRO:HB2	8:P:7:GLN:HG3	1.55	0.88
6:N:143:LEU:CD1	6:N:145:ASN:H	1.85	0.88
2:J:242:LYS:CE	2:J:247:GLY:H	1.86	0.88
5:E:174:GLU:O	5:E:175:LEU:HG	1.74	0.88
2:J:4:GLN:HA	2:J:5:ILE:HG12	0.89	0.88
1:I:350:PHE:CE2	1:I:354:TYR:HB2	2.09	0.88
6:N:452:LEU:C	6:N:455:PRO:HD2	1.93	0.88
8:H:388:GLY:HA3	8:H:394:LEU:HD21	1.53	0.88
6:F:83:GLN:CG	6:F:94:VAL:HG21	2.02	0.88
5:M:173:ASP:HB3	5:M:437:SER:CB	2.04	0.88
5:E:32:VAL:HG22	5:E:33:LYS:H	1.34	0.88
3:K:265:LYS:HZ3	3:K:268:ASP:HB3	1.34	0.88
6:N:209:PHE:HE2	6:N:376:CYS:HG	0.92	0.88
1:A:90:GLN:CG	1:A:101:VAL:HG21	2.03	0.88
5:M:174:GLU:O	5:M:175:LEU:HG	1.74	0.88
6:N:541:LEU:HB3	6:N:542:LYS:HA	1.56	0.88
6:N:330:LEU:HD12	6:N:375:SER:HB3	1.57	0.88
8:H:237:LYS:CB	8:H:314:ASN:CB	2.49	0.88
5:E:320:VAL:HG22	5:E:341:PRO:HD2	1.56	0.88
6:F:330:LEU:HD12	6:F:375:SER:HB3	1.56	0.87
2:B:514:ILE:HD12	3:C:47:MET:HB3	1.56	0.87
7:G:188:SER:C	7:G:190:ASP:HB2	1.95	0.87
1:I:156:LEU:HD13	1:I:185:LEU:HD11	1.54	0.87
3:K:230:VAL:CG1	3:K:302:SER:OG	2.22	0.87
3:C:230:VAL:CG1	3:C:302:SER:OG	2.22	0.87
2:B:474:LEU:HG	9:B:601:ADP:C2	2.09	0.87
3:K:269:TRP:CZ3	6:N:247:VAL:HB	2.09	0.87
6:F:430:ASN:CA	6:F:433:LYS:HG2	2.00	0.87
3:C:329:ALA:HB1	3:C:334:ALA:O	1.73	0.87
7:O:188:SER:C	7:O:190:ASP:HB2	1.95	0.87
2:J:285:ILE:HD11	2:J:289:LEU:HD23	1.56	0.87
6:N:362:GLU:HG2	6:N:364:PHE:CE2	2.10	0.87
7:G:43:THR:CG2	7:G:64:ASN:HB3	2.05	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:38:GLY:H	9:F:601:ADP:H5'1	1.36	0.87
5:E:173:ASP:HB3	5:E:437:SER:CB	2.04	0.87
7:O:170:LEU:O	7:O:170:LEU:HD23	1.75	0.87
1:A:350:PHE:CE2	1:A:354:TYR:HB2	2.09	0.86
2:B:285:ILE:HD11	2:B:289:LEU:HD23	1.56	0.86
8:H:204:VAL:HG13	8:H:405:VAL:HG12	1.57	0.86
6:N:5:LEU:HA	6:N:6:LEU:HB3	1.57	0.86
6:N:5:LEU:HB2	6:N:6:LEU:O	1.75	0.86
7:O:43:THR:CG2	7:O:64:ASN:HB3	2.05	0.86
6:F:143:LEU:CD1	6:F:145:ASN:H	1.85	0.86
3:K:15:THR:O	3:K:16:THR:O	1.93	0.86
8:P:388:GLY:HA3	8:P:394:LEU:HD21	1.54	0.86
2:J:208:LEU:HD13	2:J:366:THR:HG22	1.56	0.86
6:F:362:GLU:HG2	6:F:364:PHE:CE2	2.10	0.86
6:F:117:ILE:HG12	5:M:33:LYS:HE2	1.56	0.86
3:K:264:GLU:C	3:K:265:LYS:HG3	1.91	0.86
7:O:148:THR:O	7:O:149:SER:HB3	1.75	0.86
3:C:129:LEU:HG	3:C:514:ILE:HG21	1.57	0.86
8:P:24:ALA:HA	8:P:531:ALA:O	1.76	0.86
3:K:129:LEU:HG	3:K:514:ILE:HG21	1.57	0.86
8:H:6:PRO:HB2	8:H:7:GLN:HG3	1.55	0.86
6:F:154:ALA:CB	6:F:402:VAL:CG2	2.54	0.86
6:F:411:ILE:HG22	6:F:412:ILE:H	1.39	0.86
6:F:151:LEU:HD13	6:F:175:THR:HG21	0.86	0.85
6:F:541:LEU:HB3	6:F:542:LYS:HA	1.56	0.85
5:E:401:THR:C	5:E:402:LYS:HG3	1.96	0.85
5:M:320:VAL:HG22	5:M:341:PRO:HD2	1.56	0.85
6:N:411:ILE:HG22	6:N:412:ILE:H	1.39	0.85
7:G:516:LEU:HD22	7:G:516:LEU:O	1.76	0.85
6:F:5:LEU:HA	6:F:6:LEU:HB3	1.57	0.85
4:L:72:HIS:CB	4:L:75:ALA:HB3	2.05	0.85
5:E:166:ASP:CA	5:E:167:ASP:HB2	2.06	0.85
3:C:15:THR:O	3:C:16:THR:O	1.93	0.85
3:K:329:ALA:HB1	3:K:334:ALA:O	1.73	0.85
4:L:185:ASN:N	4:L:186:SER:C	2.30	0.85
7:G:189:LEU:O	7:G:189:LEU:HD12	1.77	0.85
6:F:5:LEU:HB2	6:F:6:LEU:O	1.75	0.85
6:N:154:ALA:CB	6:N:402:VAL:CG2	2.54	0.85
2:J:208:LEU:HD11	2:J:364:ALA:HB1	1.59	0.85
6:N:243:GLU:HA	6:N:243:GLU:OE2	1.76	0.85
4:D:520:ARG:O	7:G:49:SER:CB	2.23	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:185:ASN:N	4:D:186:SER:C	2.30	0.85
2:B:211:GLY:HA3	2:B:355:LYS:O	1.77	0.85
2:B:422:ILE:CB	2:B:427:SER:HB2	2.07	0.85
4:D:72:HIS:CB	4:D:75:ALA:HB3	2.05	0.85
2:B:245:ILE:O	2:B:246:PHE:CD2	2.30	0.85
6:N:75:LEU:HD13	6:N:527:LEU:HD21	1.59	0.85
2:B:208:LEU:HD11	2:B:364:ALA:HB1	1.59	0.85
7:G:148:THR:O	7:G:149:SER:HB3	1.75	0.85
6:N:151:LEU:HD13	6:N:175:THR:HG21	0.86	0.85
6:N:224:MET:HE1	6:N:316:ALA:H	1.42	0.85
1:A:88:GLN:O	1:A:92:ARG:HD2	1.76	0.85
2:J:422:ILE:CB	2:J:427:SER:HB2	2.07	0.85
1:A:93:GLU:CB	1:A:94:ILE:CD1	2.55	0.85
2:J:72:PRO:O	2:J:76:VAL:HG23	1.76	0.85
8:H:346:ALA:N	8:H:347:PRO:HD3	1.92	0.85
8:H:24:ALA:HA	8:H:531:ALA:O	1.76	0.85
2:B:72:PRO:O	2:B:76:VAL:HG23	1.76	0.84
5:E:104:LEU:HD21	5:E:123:VAL:HG13	1.58	0.84
5:M:166:ASP:CA	5:M:167:ASP:HB2	2.07	0.84
4:L:285:VAL:HA	4:L:311:MET:O	1.78	0.84
8:P:204:VAL:HG13	8:P:405:VAL:HG12	1.57	0.84
7:O:189:LEU:HD12	7:O:189:LEU:O	1.77	0.84
7:O:516:LEU:HD22	7:O:516:LEU:O	1.76	0.84
4:L:521:ILE:CD1	7:O:62:ILE:CD1	2.48	0.84
4:D:330:CYS:CB	4:D:345:ASP:OD1	2.25	0.84
7:O:189:LEU:CA	7:O:190:ASP:HB2	1.94	0.84
6:N:3:LEU:N	6:N:4:GLN:CB	2.41	0.84
2:J:245:ILE:O	2:J:246:PHE:CD2	2.30	0.84
6:F:75:LEU:HD13	6:F:527:LEU:HD21	1.59	0.84
7:O:109:MET:CG	7:O:514:THR:HG22	2.08	0.84
4:D:330:CYS:CB	4:D:345:ASP:CG	2.45	0.84
1:I:158:ASN:HB3	1:I:516:GLY:O	1.77	0.84
7:G:170:LEU:O	7:G:170:LEU:HD23	1.75	0.84
1:I:88:GLN:O	1:I:92:ARG:HD2	1.76	0.84
7:O:186:VAL:HG21	7:O:400:VAL:CG2	2.08	0.84
6:N:424:ARG:HG2	6:N:483:SER:HA	1.60	0.84
4:D:285:VAL:HA	4:D:311:MET:O	1.78	0.84
4:D:250:ASN:HA	7:G:259:VAL:HG12	1.60	0.84
6:F:36:ASN:HB3	6:F:57:LYS:HZ1	1.41	0.84
4:D:71:LEU:CB	8:P:6:PRO:CB	2.55	0.84
1:I:93:GLU:CB	1:I:94:ILE:CD1	2.54	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:524:ILE:HG12	7:O:52:LEU:HB3	0.87	0.84
2:B:329:PHE:CD2	2:B:329:PHE:C	2.51	0.84
6:F:35:THR:HG22	6:F:42:THR:O	1.78	0.84
2:J:361:ALA:H	2:J:362:GLY:HA2	1.01	0.83
6:N:415:ALA:HB2	6:N:506:ILE:HG21	1.57	0.83
4:D:524:ILE:CA	7:G:52:LEU:O	2.24	0.83
5:M:401:THR:C	5:M:402:LYS:HG3	1.97	0.83
5:M:104:LEU:HD21	5:M:123:VAL:HG13	1.58	0.83
4:D:185:ASN:CB	4:D:186:SER:HB2	2.08	0.83
7:O:94:VAL:HG21	7:O:502:VAL:CG2	2.06	0.83
6:F:3:LEU:N	6:F:4:GLN:CB	2.41	0.83
2:B:88:VAL:HG13	2:B:393:GLN:HE22	1.43	0.83
5:E:84:THR:HG22	5:E:86:ASP:H	1.42	0.83
7:G:109:MET:CG	7:G:514:THR:HG22	2.08	0.83
4:L:151:VAL:HG22	4:L:175:VAL:HG21	1.58	0.83
6:F:539:SER:CB	6:F:542:LYS:HD2	2.09	0.83
2:B:320:VAL:HG21	2:B:337:LEU:CB	2.09	0.83
4:D:254:VAL:HG21	8:H:265:VAL:HG22	1.60	0.83
8:P:346:ALA:N	8:P:347:PRO:HD3	1.92	0.83
1:A:264:ILE:HD11	7:G:259:VAL:HG23	1.61	0.83
6:N:382:GLY:HA3	6:N:388:LEU:HD21	1.61	0.83
7:G:186:VAL:HG21	7:G:400:VAL:CG2	2.08	0.83
6:N:56:THR:HB	6:N:390:GLN:NE2	1.94	0.83
6:N:35:THR:HG22	6:N:42:THR:O	1.78	0.83
6:N:539:SER:CB	6:N:542:LYS:HD2	2.09	0.83
3:K:430:LYS:O	3:K:433:GLN:HG3	1.78	0.83
7:G:186:VAL:HG21	7:G:400:VAL:HG21	1.59	0.83
7:O:175:ALA:O	7:O:179:VAL:HG23	1.79	0.83
7:O:189:LEU:HA	7:O:190:ASP:HB3	0.83	0.83
6:F:415:ALA:HB2	6:F:506:ILE:HG21	1.58	0.83
2:B:37:LEU:HA	9:B:601:ADP:H5'1	1.61	0.83
6:F:243:GLU:OE2	6:F:243:GLU:HA	1.76	0.83
5:M:84:THR:HG22	5:M:86:ASP:H	1.42	0.83
4:D:521:ILE:CD1	7:G:62:ILE:CD1	2.50	0.82
7:G:175:ALA:O	7:G:179:VAL:HG23	1.79	0.82
2:J:211:GLY:HA3	2:J:355:LYS:O	1.77	0.82
5:M:173:ASP:HB3	5:M:437:SER:HB2	1.60	0.82
2:J:329:PHE:CD2	2:J:329:PHE:C	2.51	0.82
3:K:306:GLN:HA	3:K:316:VAL:HG11	1.62	0.82
4:L:185:ASN:CB	4:L:186:SER:HB2	2.08	0.82
6:F:382:GLY:HA3	6:F:388:LEU:HD21	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ASN:HB3	1:A:516:GLY:O	1.77	0.82
2:J:4:GLN:CA	2:J:5:ILE:CB	2.57	0.82
6:F:56:THR:HB	6:F:390:GLN:NE2	1.94	0.82
2:B:4:GLN:CA	2:B:5:ILE:CG2	2.57	0.82
2:J:4:GLN:CA	2:J:5:ILE:CG2	2.57	0.82
6:F:3:LEU:HA	6:F:5:LEU:HG	1.60	0.82
2:J:88:VAL:HG13	2:J:393:GLN:HE22	1.43	0.82
2:J:176:LEU:HD23	2:J:208:LEU:HB2	1.60	0.82
4:D:99:LEU:O	4:D:103:LEU:HB2	1.79	0.82
2:J:320:VAL:HG21	2:J:337:LEU:CB	2.09	0.82
2:B:361:ALA:H	2:B:362:GLY:HA2	1.01	0.82
4:D:521:ILE:HG23	7:G:51:ILE:HA	1.61	0.82
3:C:306:GLN:HA	3:C:316:VAL:HG11	1.62	0.82
4:D:134:ILE:HD11	4:D:424:ARG:CD	2.09	0.82
7:O:186:VAL:HG21	7:O:400:VAL:HG21	1.59	0.82
3:C:493:ASP:HB3	3:C:495:VAL:HG12	1.62	0.82
1:I:12:THR:HG21	5:M:97:ASP:H	1.45	0.82
4:D:151:VAL:HG22	4:D:175:VAL:HG21	1.58	0.82
7:G:189:LEU:HA	7:G:190:ASP:HB3	0.83	0.82
6:N:540:THR:C	6:N:541:LEU:CD2	2.47	0.82
3:C:430:LYS:O	3:C:433:GLN:HG3	1.79	0.82
4:D:521:ILE:HG23	7:G:50:ASP:O	1.80	0.82
7:O:191:ARG:CD	7:O:192:ASN:H	1.92	0.81
7:G:191:ARG:CD	7:G:192:ASN:H	1.92	0.81
8:H:74:GLU:HA	8:H:74:GLU:OE1	1.78	0.81
6:F:430:ASN:O	6:F:433:LYS:N	2.12	0.81
2:J:361:ALA:H	2:J:362:GLY:CA	1.86	0.81
4:D:246:PRO:HB2	4:D:250:ASN:OD1	1.80	0.81
2:J:249:LYS:O	6:N:250:GLY:N	2.12	0.81
2:B:4:GLN:N	2:B:5:ILE:HG23	1.96	0.81
6:F:478:ASP:O	6:F:482:ASP:HB3	1.80	0.81
7:G:94:VAL:HG21	7:G:502:VAL:CG2	2.06	0.81
4:L:134:ILE:HD11	4:L:424:ARG:CD	2.09	0.81
6:F:424:ARG:HG2	6:F:483:SER:HA	1.60	0.81
5:M:166:ASP:CB	5:M:167:ASP:HB2	2.11	0.81
3:K:506:LYS:HA	3:K:506:LYS:HE2	1.63	0.81
8:P:74:GLU:HA	8:P:74:GLU:OE1	1.79	0.81
6:N:430:ASN:O	6:N:433:LYS:N	2.12	0.81
6:F:143:LEU:HA	6:F:145:ASN:N	1.95	0.81
5:M:401:THR:O	5:M:402:LYS:HG3	1.81	0.81
5:M:368:ASP:O	5:M:370:SER:N	2.13	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:540:THR:C	6:F:541:LEU:CD2	2.47	0.81
8:P:206:SER:CB	8:P:381:THR:HG22	2.11	0.81
6:N:3:LEU:HA	6:N:5:LEU:HG	1.60	0.81
5:E:173:ASP:HB3	5:E:437:SER:HB2	1.60	0.81
2:J:426:LYS:O	2:J:429:ALA:HB3	1.81	0.81
2:B:4:GLN:HA	2:B:5:ILE:CG2	2.11	0.81
2:J:4:GLN:N	2:J:5:ILE:HG23	1.96	0.81
6:N:2:SER:HA	6:N:3:LEU:HB2	1.63	0.81
6:F:5:LEU:HA	6:F:6:LEU:HB2	1.62	0.81
5:E:401:THR:O	5:E:402:LYS:HG3	1.81	0.81
5:E:166:ASP:CB	5:E:167:ASP:HB2	2.10	0.81
2:B:426:LYS:O	2:B:429:ALA:HB3	1.81	0.81
7:G:171:ILE:HG23	7:G:178:PHE:CD2	2.16	0.81
7:G:145:VAL:O	7:G:408:LEU:HA	1.80	0.81
6:N:541:LEU:N	6:N:541:LEU:HD22	1.95	0.81
3:K:41:PRO:HA	3:K:161:THR:HG22	1.63	0.81
3:K:493:ASP:HB3	3:K:495:VAL:HG12	1.62	0.81
4:L:99:LEU:O	4:L:103:LEU:HB2	1.79	0.81
4:D:499:GLN:HE22	9:D:601:ADP:H2'	1.45	0.81
6:N:452:LEU:O	6:N:455:PRO:HD2	1.80	0.81
7:O:120:ILE:H	7:O:120:ILE:HD13	1.46	0.81
2:J:4:GLN:HA	2:J:5:ILE:CG2	2.11	0.81
2:J:263:LYS:HZ3	3:K:266:GLU:HB3	1.43	0.81
8:P:360:THR:HG22	8:P:369:THR:HG22	1.63	0.81
7:O:171:ILE:HG23	7:O:178:PHE:CD2	2.16	0.81
2:B:4:GLN:CA	2:B:5:ILE:CB	2.58	0.81
7:G:232:GLN:CG	7:G:313:PHE:HA	2.10	0.81
5:E:368:ASP:O	5:E:370:SER:N	2.13	0.81
4:D:71:LEU:CB	8:P:6:PRO:HB3	2.12	0.80
6:F:195:GLU:HG2	6:F:197:MET:SD	2.21	0.80
2:B:176:LEU:HD23	2:B:208:LEU:HB2	1.60	0.80
7:G:248:LEU:CB	7:G:299:ILE:HD12	2.11	0.80
6:N:143:LEU:HA	6:N:145:ASN:N	1.95	0.80
4:L:246:PRO:HB2	4:L:250:ASN:OD1	1.80	0.80
2:B:242:LYS:HB2	3:C:269:TRP:HZ2	1.45	0.80
1:A:517:VAL:O	1:A:518:LEU:CG	2.28	0.80
8:H:360:THR:HG22	8:H:369:THR:HG22	1.63	0.80
3:K:457:ILE:CD1	3:K:467:LEU:HD13	2.11	0.80
1:I:264:ILE:HD11	7:O:259:VAL:HG23	1.62	0.80
7:G:412:GLY:O	7:G:491:ASN:ND2	2.14	0.80
5:E:245:LEU:HD13	5:E:247:LYS:H	1.47	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:224:LEU:CD1	1:I:226:CYS:HB2	2.11	0.80
2:J:4:GLN:C	2:J:5:ILE:HG23	2.02	0.80
6:F:541:LEU:N	6:F:541:LEU:HD22	1.95	0.80
1:I:9:ARG:CB	1:I:10:SER:O	2.30	0.80
6:F:452:LEU:O	6:F:455:PRO:HD2	1.80	0.80
7:O:145:VAL:O	7:O:408:LEU:HA	1.81	0.80
7:G:189:LEU:CA	7:G:190:ASP:HB2	1.94	0.80
4:D:521:ILE:CG1	7:G:62:ILE:HD11	2.11	0.80
4:L:72:HIS:O	4:L:76:ARG:CB	2.30	0.80
5:E:401:THR:O	5:E:402:LYS:CG	2.30	0.80
6:F:215:LEU:HB3	6:F:217:HIS:HD2	1.46	0.80
4:D:230:GLU:O	4:D:348:ASP:O	2.00	0.80
1:I:517:VAL:O	1:I:518:LEU:CG	2.28	0.80
7:O:248:LEU:CB	7:O:299:ILE:HD12	2.11	0.80
8:H:206:SER:CB	8:H:381:THR:HG22	2.11	0.80
5:M:401:THR:O	5:M:402:LYS:CG	2.30	0.80
2:J:132:LEU:HD21	2:J:495:ARG:HG3	1.64	0.80
2:J:250:PHE:HA	6:N:250:GLY:O	1.81	0.80
4:D:323:PHE:HA	4:D:374:THR:HG21	1.64	0.80
2:B:361:ALA:H	2:B:362:GLY:CA	1.86	0.80
5:E:401:THR:O	5:E:402:LYS:CE	2.30	0.80
6:N:195:GLU:HG2	6:N:197:MET:SD	2.21	0.80
3:C:506:LYS:HA	3:C:506:LYS:HE2	1.63	0.80
4:L:336:ILE:O	4:L:336:ILE:HG22	1.81	0.80
7:O:232:GLN:CG	7:O:313:PHE:HA	2.10	0.80
2:B:233:ILE:O	2:B:325:VAL:HB	1.82	0.80
6:N:5:LEU:HA	6:N:6:LEU:HB2	1.62	0.80
1:A:224:LEU:CD1	1:A:226:CYS:HB2	2.11	0.80
7:G:191:ARG:NE	7:G:192:ASN:N	2.30	0.79
6:F:2:SER:HA	6:F:3:LEU:HB2	1.63	0.79
4:D:72:HIS:O	4:D:76:ARG:CB	2.30	0.79
6:F:276:LYS:O	6:F:279:ASP:CB	2.30	0.79
7:O:191:ARG:NE	7:O:192:ASN:N	2.30	0.79
8:P:24:ALA:O	8:P:28:ILE:CG1	2.30	0.79
7:O:412:GLY:O	7:O:491:ASN:ND2	2.14	0.79
2:B:463:ILE:C	2:B:467:ILE:HG12	2.01	0.79
1:A:9:ARG:CB	1:A:10:SER:O	2.30	0.79
7:G:191:ARG:HE	7:G:191:ARG:CA	1.94	0.79
8:H:24:ALA:O	8:H:28:ILE:HG12	1.82	0.79
6:N:276:LYS:O	6:N:279:ASP:CB	2.30	0.79
6:N:46:LEU:N	6:N:54:LYS:O	2.14	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:188:SER:O	7:G:190:ASP:CB	2.28	0.79
8:H:49:CYS:O	8:H:466:THR:HB	1.83	0.79
5:M:509:ASN:HB3	5:M:521:ASP:HB3	1.64	0.79
3:C:82:SER:HB2	3:C:97:ILE:HD11	1.64	0.79
2:B:4:GLN:C	2:B:5:ILE:HG23	2.02	0.79
3:K:264:GLU:O	3:K:265:LYS:CG	2.30	0.79
6:N:215:LEU:HB3	6:N:217:HIS:HD2	1.46	0.79
2:J:463:ILE:C	2:J:467:ILE:HG12	2.01	0.79
8:P:49:CYS:O	8:P:466:THR:HB	1.82	0.79
2:B:295:GLU:C	6:F:337:GLN:HE22	1.86	0.79
1:I:180:VAL:HG13	1:I:406:LEU:HD23	1.63	0.79
2:B:3:VAL:O	2:B:5:ILE:CD1	2.30	0.79
6:N:478:ASP:O	6:N:482:ASP:HB3	1.80	0.79
1:I:93:GLU:C	1:I:94:ILE:HD12	2.03	0.79
4:L:250:ASN:HA	7:O:259:VAL:CG1	2.12	0.79
8:H:24:ALA:O	8:H:28:ILE:CG1	2.30	0.79
3:K:82:SER:HB2	3:K:97:ILE:HD11	1.64	0.79
2:B:475:ASN:H	2:B:475:ASN:HD22	1.28	0.79
4:L:230:GLU:O	4:L:348:ASP:O	2.00	0.79
2:J:3:VAL:O	2:J:5:ILE:CG2	2.30	0.79
6:F:433:LYS:CG	6:F:444:ILE:HG21	2.13	0.79
7:O:191:ARG:HE	7:O:191:ARG:CA	1.94	0.79
2:J:233:ILE:O	2:J:325:VAL:HB	1.82	0.79
7:O:455:GLU:HG3	7:O:461:ALA:CB	2.13	0.79
2:J:475:ASN:HD22	2:J:475:ASN:H	1.28	0.79
7:G:120:ILE:HD13	7:G:120:ILE:H	1.46	0.79
2:B:3:VAL:O	2:B:5:ILE:CG2	2.30	0.79
4:D:524:ILE:HG23	7:G:52:LEU:O	1.82	0.79
2:B:132:LEU:HD21	2:B:495:ARG:HG3	1.64	0.79
7:O:125:ILE:HA	7:O:438:ILE:HG12	1.65	0.79
2:J:37:LEU:HA	9:J:601:ADP:H5'1	1.65	0.79
2:B:206:SER:HB3	2:B:368:VAL:HG13	1.65	0.79
1:A:180:VAL:HG13	1:A:406:LEU:HD23	1.63	0.79
6:F:117:ILE:HD12	5:M:34:ASP:O	1.81	0.79
6:N:501:PRO:HB3	6:N:506:ILE:CB	2.11	0.79
3:C:457:ILE:CD1	3:C:467:LEU:HD13	2.11	0.79
6:N:53:ILE:CD1	6:N:53:ILE:O	2.30	0.79
2:B:70:ASP:HB2	6:F:5:LEU:HD22	1.65	0.79
5:M:253:GLN:CA	5:M:254:MET:CB	2.61	0.79
3:C:41:PRO:HA	3:C:161:THR:HG22	1.63	0.79
7:O:378:LEU:HD11	7:O:393:LEU:HD12	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:THR:HG21	5:E:68:ARG:HE	1.46	0.79
5:M:245:LEU:HD13	5:M:247:LYS:H	1.47	0.79
2:B:3:VAL:O	2:B:5:ILE:CG1	2.32	0.78
6:N:433:LYS:CG	6:N:444:ILE:HG21	2.13	0.78
8:P:24:ALA:O	8:P:28:ILE:HG12	1.82	0.78
2:J:3:VAL:O	2:J:5:ILE:CD1	2.30	0.78
7:O:191:ARG:CA	7:O:191:ARG:NE	2.46	0.78
2:J:3:VAL:O	2:J:5:ILE:CG1	2.31	0.78
7:O:188:SER:O	7:O:190:ASP:CB	2.28	0.78
7:O:191:ARG:CZ	7:O:192:ASN:H	1.97	0.78
6:F:501:PRO:HB3	6:F:506:ILE:CB	2.12	0.78
4:D:336:ILE:O	4:D:336:ILE:HG22	1.81	0.78
6:N:36:ASN:HA	6:N:57:LYS:HD2	1.66	0.78
5:E:253:GLN:CA	5:E:254:MET:CB	2.61	0.78
4:L:323:PHE:HA	4:L:374:THR:HG21	1.64	0.78
1:A:12:THR:HG21	5:E:97:ASP:H	1.47	0.78
8:H:206:SER:HB2	8:H:381:THR:CG2	2.13	0.78
7:G:191:ARG:NE	7:G:191:ARG:CA	2.46	0.78
5:M:401:THR:O	5:M:402:LYS:CE	2.30	0.78
5:E:166:ASP:HB3	5:E:167:ASP:HB2	1.66	0.78
6:N:35:THR:CG2	6:N:42:THR:O	2.32	0.78
2:J:329:PHE:O	2:J:329:PHE:HD2	1.67	0.78
2:J:469:THR:O	2:J:470:SER:HB2	1.82	0.78
6:N:331:VAL:HG12	6:N:332:THR:HG23	1.65	0.78
6:F:331:VAL:HG12	6:F:332:THR:HG23	1.65	0.78
6:N:221:HIS:HB2	6:N:224:MET:HG3	1.66	0.78
5:E:509:ASN:HB3	5:E:521:ASP:HB3	1.64	0.78
8:H:6:PRO:HB3	4:L:71:LEU:CB	2.11	0.78
2:B:72:PRO:HB3	3:C:47:MET:CE	2.13	0.78
7:G:455:GLU:HG3	7:G:461:ALA:CB	2.13	0.78
4:D:292:ILE:H	4:D:293:LEU:HA	1.48	0.78
2:J:208:LEU:HD12	2:J:209:ASP:H	1.48	0.78
7:G:212:SER:HB3	7:G:378:LEU:HA	1.66	0.78
6:F:36:ASN:HA	6:F:57:LYS:HD2	1.66	0.77
2:B:492:LYS:HE2	2:B:493:LEU:H	1.48	0.77
5:M:88:ALA:HB1	5:M:109:LYS:NZ	2.00	0.77
5:M:166:ASP:HB3	5:M:167:ASP:HB2	1.66	0.77
4:D:241:ILE:O	4:D:299:ASP:HB2	1.83	0.77
4:L:292:ILE:H	4:L:293:LEU:HA	1.48	0.77
6:F:151:LEU:HD12	6:F:175:THR:HG21	1.65	0.77
4:L:521:ILE:HG23	7:O:51:ILE:HA	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:GLU:C	1:A:94:ILE:HD12	2.03	0.77
6:N:395:VAL:O	6:N:399:LEU:HB2	1.85	0.77
4:L:241:ILE:O	4:L:299:ASP:HB2	1.83	0.77
7:G:191:ARG:CZ	7:G:192:ASN:H	1.97	0.77
7:G:378:LEU:HD11	7:G:393:LEU:HD12	1.65	0.77
6:N:539:SER:CB	6:N:542:LYS:CD	2.62	0.77
3:C:264:GLU:O	3:C:265:LYS:CG	2.30	0.77
3:C:42:LYS:O	3:C:459:ASN:HB3	1.85	0.77
2:B:208:LEU:HD12	2:B:209:ASP:H	1.48	0.77
7:O:212:SER:HB3	7:O:378:LEU:HA	1.66	0.77
2:B:469:THR:O	2:B:470:SER:HB2	1.82	0.77
3:C:452:ILE:O	3:C:456:LEU:HB2	1.84	0.77
6:F:224:MET:HE1	6:F:316:ALA:H	1.49	0.77
1:I:123:THR:HG21	5:M:68:ARG:HE	1.49	0.77
2:B:463:ILE:O	2:B:467:ILE:N	2.18	0.77
6:F:395:VAL:O	6:F:399:LEU:HB2	1.85	0.77
8:P:430:LEU:O	8:P:434:ILE:HG12	1.84	0.77
7:G:125:ILE:HA	7:G:438:ILE:HG12	1.65	0.77
6:N:430:ASN:O	6:N:433:LYS:CB	2.33	0.77
6:F:420:ILE:HA	6:F:423:SER:HB3	1.67	0.77
2:J:492:LYS:HE2	2:J:493:LEU:H	1.48	0.77
2:B:329:PHE:O	2:B:329:PHE:HD2	1.67	0.77
6:F:35:THR:CG2	6:F:42:THR:O	2.32	0.77
7:G:30:ILE:HD12	7:G:109:MET:HB3	1.65	0.77
5:E:449:THR:HG22	5:E:507:ILE:HB	1.65	0.77
3:K:452:ILE:O	3:K:456:LEU:HB2	1.84	0.77
1:I:184:LEU:O	1:I:184:LEU:HD23	1.85	0.77
4:D:292:ILE:N	4:D:293:LEU:HA	1.98	0.77
6:F:46:LEU:N	6:F:54:LYS:O	2.14	0.77
7:G:513:ALA:O	7:G:516:LEU:CD1	2.33	0.76
4:L:416:ALA:HB3	4:L:417:PRO:HD3	1.66	0.76
6:F:221:HIS:HB2	6:F:224:MET:HG3	1.66	0.76
6:N:420:ILE:HA	6:N:423:SER:HB3	1.67	0.76
8:P:206:SER:HB2	8:P:381:THR:CG2	2.13	0.76
2:B:70:ASP:CB	6:F:5:LEU:HD22	2.15	0.76
5:E:348:GLY:O	5:E:351:LEU:CD1	2.33	0.76
4:D:416:ALA:HB3	4:D:417:PRO:HD3	1.66	0.76
4:L:184:GLU:CA	4:L:186:SER:O	2.33	0.76
5:M:509:ASN:OD1	5:M:523:LYS:HB2	1.86	0.76
8:H:430:LEU:O	8:H:434:ILE:HG12	1.84	0.76
6:F:539:SER:CB	6:F:542:LYS:CD	2.62	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:513:ALA:O	7:O:516:LEU:CD1	2.33	0.76
4:L:292:ILE:N	4:L:293:LEU:HA	1.98	0.76
2:J:412:SER:O	2:J:416:ASP:HB2	1.86	0.76
8:H:237:LYS:HB2	8:H:314:ASN:HB3	1.65	0.76
4:D:334:ALA:HB3	7:G:305:GLN:HB2	1.64	0.76
1:A:431:ILE:HG12	1:A:482:ALA:HB2	1.68	0.76
6:F:430:ASN:O	6:F:433:LYS:CB	2.33	0.76
2:J:463:ILE:O	2:J:467:ILE:N	2.18	0.76
6:N:478:ASP:O	6:N:482:ASP:N	2.19	0.76
5:M:348:GLY:O	5:M:351:LEU:CD1	2.33	0.76
2:B:412:SER:O	2:B:416:ASP:HB2	1.86	0.76
5:M:449:THR:HG22	5:M:507:ILE:HB	1.65	0.76
3:K:42:LYS:O	3:K:459:ASN:HB3	1.85	0.76
6:F:526:ASN:HA	6:F:529:LEU:HD12	1.67	0.76
5:E:509:ASN:OD1	5:E:523:LYS:HB2	1.86	0.76
4:L:36:ARG:HE	4:L:98:ILE:HG23	1.51	0.76
4:L:268:ARG:HA	4:L:271:LEU:HD23	1.68	0.76
1:A:184:LEU:HD23	1:A:184:LEU:O	1.85	0.76
2:J:422:ILE:CG2	2:J:427:SER:CB	2.63	0.76
3:K:56:VAL:C	3:K:57:LEU:HD23	2.06	0.76
6:F:159:LEU:HA	6:F:164:ALA:HB1	1.68	0.76
7:G:447:GLU:O	7:G:450:PRO:HD2	1.86	0.76
5:M:73:ILE:HG12	5:M:83:ILE:HG12	1.67	0.76
1:A:169:ILE:HD11	1:A:398:MET:HA	1.68	0.76
2:B:201:GLY:H	6:F:86:ILE:HD12	1.49	0.76
8:P:237:LYS:HB2	8:P:314:ASN:HB3	1.65	0.76
2:J:493:LEU:HD12	2:J:494:LYS:N	2.01	0.76
7:O:471:ALA:O	7:O:475:GLY:HA3	1.85	0.76
7:O:30:ILE:HD12	7:O:109:MET:HB3	1.65	0.76
2:B:473:ASP:OD2	2:B:476:ASN:O	2.04	0.76
2:J:473:ASP:OD2	2:J:476:ASN:O	2.04	0.76
6:N:352:GLY:O	6:N:367:VAL:HG12	1.86	0.76
2:B:422:ILE:CG2	2:B:427:SER:CB	2.63	0.76
5:E:88:ALA:HB1	5:E:109:LYS:NZ	2.00	0.76
1:I:350:PHE:HD2	1:I:351:GLU:N	1.83	0.76
6:N:159:LEU:HA	6:N:164:ALA:HB1	1.68	0.76
7:O:448:VAL:HG12	7:O:452:GLN:HE22	1.51	0.76
7:O:447:GLU:O	7:O:450:PRO:HD2	1.86	0.76
6:F:352:GLY:O	6:F:367:VAL:HG12	1.86	0.76
6:N:159:LEU:HA	6:N:164:ALA:HB2	1.66	0.76
4:D:184:GLU:CA	4:D:186:SER:O	2.33	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:72:PRO:HG3	3:C:49:LEU:HD11	1.68	0.75
6:F:213:LEU:HD23	6:F:377:THR:HG23	1.68	0.75
3:C:129:LEU:HB2	3:C:514:ILE:HD13	1.69	0.75
7:O:238:ASN:N	7:O:239:PRO:HD3	2.01	0.75
6:F:478:ASP:O	6:F:482:ASP:N	2.19	0.75
5:E:187:SER:OG	5:E:429:VAL:HG21	1.86	0.75
8:P:316:TYR:CD2	8:P:316:TYR:N	2.54	0.75
6:N:526:ASN:HA	6:N:529:LEU:HD12	1.68	0.75
5:E:73:ILE:HG12	5:E:83:ILE:HG12	1.67	0.75
1:I:543:THR:HB	5:M:72:LYS:HD3	1.67	0.75
2:B:493:LEU:HD12	2:B:494:LYS:N	2.01	0.75
6:F:154:ALA:HB2	6:F:402:VAL:CG2	2.16	0.75
2:B:208:LEU:HD12	2:B:209:ASP:N	2.01	0.75
1:A:226:CYS:SG	1:A:318:VAL:CG1	2.75	0.75
2:J:165:ILE:HG12	6:N:529:LEU:HD13	1.68	0.75
3:C:56:VAL:C	3:C:57:LEU:HD23	2.06	0.75
7:G:238:ASN:N	7:G:239:PRO:HD3	2.01	0.75
1:A:221:GLY:HA2	1:A:382:SER:HB2	1.68	0.75
2:J:208:LEU:HD12	2:J:209:ASP:N	2.01	0.75
3:K:104:LEU:HD11	3:K:520:LEU:HD12	1.69	0.75
8:P:72:LEU:HD13	8:P:86:VAL:HG22	1.69	0.75
6:N:154:ALA:HB2	6:N:402:VAL:CG2	2.16	0.75
3:K:129:LEU:HB2	3:K:514:ILE:HD13	1.69	0.75
7:G:448:VAL:HG12	7:G:452:GLN:HE22	1.51	0.75
1:A:456:LEU:O	1:A:460:LYS:HG2	1.86	0.75
5:E:39:LYS:HZ3	6:N:109:ILE:HG13	1.51	0.75
4:D:36:ARG:HE	4:D:98:ILE:HG23	1.51	0.75
1:A:8:SER:N	2:J:21:SER:HG	1.84	0.75
6:F:53:ILE:CD1	6:F:53:ILE:O	2.30	0.75
6:F:465:ASP:HA	6:F:466:PRO:O	1.86	0.75
6:F:159:LEU:HA	6:F:164:ALA:HB2	1.66	0.75
7:G:377:LEU:HD13	7:G:377:LEU:H	1.51	0.75
1:I:431:ILE:HG12	1:I:482:ALA:HB2	1.68	0.75
3:K:306:GLN:O	3:K:310:LEU:HG	1.87	0.74
6:N:395:VAL:O	6:N:399:LEU:CB	2.35	0.74
7:G:33:CYS:SG	7:G:83:LEU:HD11	2.27	0.74
7:O:413:GLY:HA3	7:O:491:ASN:HD21	1.52	0.74
2:B:295:GLU:HB2	6:F:337:GLN:NE2	2.02	0.74
6:N:13:LEU:HD13	6:N:21:VAL:HG21	1.69	0.74
1:A:543:THR:HB	5:E:72:LYS:HD3	1.67	0.74
5:M:492:ILE:H	5:M:492:ILE:HD12	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:117:ILE:HD12	5:M:34:ASP:HA	1.64	0.74
3:C:306:GLN:O	3:C:310:LEU:HG	1.87	0.74
7:G:471:ALA:O	7:G:475:GLY:HA3	1.85	0.74
1:I:226:CYS:SG	1:I:318:VAL:CG1	2.75	0.74
7:O:488:ILE:H	7:O:488:ILE:HD12	1.52	0.74
4:D:268:ARG:HA	4:D:271:LEU:HD23	1.68	0.74
1:I:221:GLY:HA2	1:I:382:SER:HB2	1.68	0.74
1:I:115:LEU:HD21	1:I:446:LEU:HD22	1.69	0.74
8:P:114:SER:O	8:P:118:ILE:HG13	1.87	0.74
8:H:72:LEU:HD13	8:H:86:VAL:HG22	1.69	0.74
8:P:204:VAL:CG1	8:P:405:VAL:HG12	2.16	0.74
5:M:187:SER:OG	5:M:429:VAL:HG21	1.86	0.74
1:A:350:PHE:HD2	1:A:351:GLU:N	1.83	0.74
3:C:104:LEU:HD11	3:C:520:LEU:HD12	1.69	0.74
1:A:357:LEU:HB2	1:A:378:SER:HB3	1.69	0.74
4:D:119:ILE:HG23	4:D:436:GLN:HA	1.68	0.74
6:F:43:LEU:HD21	6:F:161:LYS:HA	1.68	0.74
4:L:25:ILE:HD13	4:L:108:GLU:HB2	1.70	0.74
6:F:3:LEU:HD12	6:F:5:LEU:CD2	2.17	0.74
6:F:395:VAL:O	6:F:399:LEU:CB	2.35	0.74
2:B:451:ASP:O	2:B:455:LEU:HB2	1.88	0.74
2:B:4:GLN:O	3:C:72:HIS:HB2	1.87	0.74
2:J:422:ILE:HG22	2:J:427:SER:HB3	1.68	0.74
7:O:33:CYS:SG	7:O:83:LEU:HD11	2.27	0.74
6:N:201:HIS:HB3	6:N:381:LYS:NZ	2.03	0.74
5:M:355:ALA:HB3	6:N:222:PRO:HG2	1.68	0.74
8:H:204:VAL:CG1	8:H:405:VAL:HG12	2.16	0.74
7:G:109:MET:SD	7:G:514:THR:CG2	2.76	0.74
7:G:498:GLU:OE2	9:G:601:ADP:H1'	1.88	0.74
2:B:422:ILE:HG22	2:B:427:SER:HB3	1.68	0.74
2:B:242:LYS:HE2	2:B:246:PHE:HA	1.69	0.74
2:J:451:ASP:O	2:J:455:LEU:HB2	1.88	0.74
7:G:330:VAL:HG12	7:G:347:GLY:HA3	1.69	0.74
1:I:169:ILE:HD11	1:I:398:MET:HA	1.68	0.74
3:C:329:ALA:O	3:C:333:GLY:N	2.21	0.74
7:G:488:ILE:HD12	7:G:488:ILE:H	1.52	0.74
6:F:13:LEU:HD13	6:F:21:VAL:HG21	1.69	0.74
6:N:155:ARG:CB	6:N:171:THR:CG2	2.66	0.73
2:B:242:LYS:CE	2:B:247:GLY:N	2.50	0.73
3:C:501:GLU:OE2	9:C:1101:ADP:H3'	1.87	0.73
8:P:345:GLY:C	8:P:347:PRO:HD3	2.08	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:44:LEU:HD12	7:O:452:GLN:HB2	1.68	0.73
7:G:44:LEU:HD12	7:G:452:GLN:HB2	1.68	0.73
1:I:187:VAL:CG2	1:I:383:SER:HB3	2.18	0.73
1:I:63:THR:HG22	1:I:65:ASP:H	1.52	0.73
6:F:138:ILE:HG22	6:F:138:ILE:O	1.87	0.73
6:N:465:ASP:HA	6:N:466:PRO:O	1.86	0.73
6:N:213:LEU:HD23	6:N:377:THR:HG23	1.68	0.73
7:G:413:GLY:HA3	7:G:491:ASN:HD21	1.52	0.73
4:L:336:ILE:CG2	4:L:336:ILE:O	2.35	0.73
2:B:232:LEU:HB3	2:B:283:THR:HG22	1.68	0.73
1:A:115:LEU:HD21	1:A:446:LEU:HD22	1.69	0.73
4:L:120:ILE:HG12	4:L:439:ILE:HG21	1.68	0.73
4:D:421:ILE:O	4:D:425:LEU:HG	1.88	0.73
8:H:316:TYR:N	8:H:316:TYR:CD2	2.54	0.73
7:O:143:LEU:HD13	7:O:411:ALA:HB3	1.70	0.73
7:O:377:LEU:H	7:O:377:LEU:HD13	1.51	0.73
6:N:138:ILE:O	6:N:138:ILE:HG22	1.87	0.73
1:I:456:LEU:O	1:I:460:LYS:HG2	1.86	0.73
6:N:166:LEU:O	6:N:167:THR:CG2	2.33	0.73
8:H:316:TYR:N	8:H:316:TYR:HD2	1.87	0.73
7:O:330:VAL:HG12	7:O:347:GLY:HA3	1.69	0.73
2:J:232:LEU:HB3	2:J:283:THR:HG22	1.68	0.73
4:D:336:ILE:CG2	4:D:336:ILE:O	2.35	0.73
1:A:30:VAL:O	1:A:33:THR:HG22	1.87	0.73
8:P:163:ILE:HG23	8:P:179:SER:HB2	1.71	0.73
1:A:63:THR:HG22	1:A:65:ASP:H	1.52	0.73
8:P:77:ILE:HD13	8:P:77:ILE:H	1.53	0.73
4:L:485:ARG:H	4:L:485:ARG:HD2	1.54	0.73
1:I:357:LEU:HB2	1:I:378:SER:HB3	1.69	0.73
1:I:267:PRO:HA	1:I:268:GLU:CB	2.19	0.73
7:G:479:TYR:HA	7:G:490:ASP:HA	1.70	0.73
4:D:25:ILE:HD13	4:D:108:GLU:HB2	1.70	0.73
3:K:329:ALA:O	3:K:333:GLY:N	2.21	0.73
1:A:187:VAL:CG2	1:A:383:SER:HB3	2.18	0.73
4:D:120:ILE:HG12	4:D:439:ILE:HG21	1.68	0.73
8:H:114:SER:O	8:H:118:ILE:HG13	1.87	0.73
6:N:3:LEU:HD12	6:N:5:LEU:CD2	2.17	0.73
2:J:242:LYS:HE2	2:J:246:PHE:HA	1.69	0.73
2:B:285:ILE:CD1	2:B:289:LEU:HD23	2.19	0.73
4:D:183:ASP:O	4:D:187:LYS:HG2	1.88	0.73
8:P:204:VAL:HG21	8:P:409:LYS:CB	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:109:MET:SD	7:O:514:THR:CG2	2.76	0.73
5:M:142:HIS:O	5:M:146:ILE:HG13	1.89	0.73
6:F:155:ARG:CB	6:F:171:THR:CG2	2.66	0.73
6:F:193:MET:CE	6:F:330:LEU:HD11	2.19	0.73
2:J:242:LYS:CE	2:J:247:GLY:N	2.50	0.73
8:H:345:GLY:C	8:H:347:PRO:HD3	2.08	0.73
6:F:201:HIS:HB3	6:F:381:LYS:NZ	2.03	0.73
8:H:77:ILE:H	8:H:77:ILE:HD13	1.53	0.73
2:B:71:ASN:OD1	2:B:73:ALA:N	2.22	0.73
6:N:193:MET:CE	6:N:330:LEU:HD11	2.19	0.73
8:P:54:ILE:CG1	8:P:64:ILE:HG12	2.13	0.73
4:D:254:VAL:CG2	8:H:265:VAL:HG22	2.18	0.73
4:L:183:ASP:O	4:L:187:LYS:HG2	1.88	0.73
3:K:518:CYS:O	3:K:522:ARG:HG3	1.89	0.73
2:J:57:THR:HG21	2:J:382:ARG:HD3	1.71	0.73
2:J:285:ILE:CD1	2:J:289:LEU:HD23	2.19	0.73
6:N:411:ILE:HG22	6:N:412:ILE:N	2.04	0.73
4:D:258:ARG:HD2	8:H:283:GLN:HE21	1.54	0.73
5:E:142:HIS:O	5:E:146:ILE:HG13	1.89	0.73
6:N:167:THR:HB	6:N:168:GLU:C	2.09	0.72
6:N:193:MET:HE3	6:N:330:LEU:HD11	1.71	0.72
2:B:411:MET:HB2	2:B:437:LEU:HD13	1.70	0.72
7:G:55:THR:HG21	7:G:72:LEU:HB3	1.70	0.72
5:M:479:ILE:O	5:M:483:LEU:HB2	1.89	0.72
1:I:17:GLY:HA3	5:M:95:GLU:OE2	1.88	0.72
7:G:143:LEU:HD13	7:G:411:ALA:HB3	1.70	0.72
5:E:479:ILE:O	5:E:483:LEU:HB2	1.89	0.72
3:C:518:CYS:O	3:C:522:ARG:HG3	1.89	0.72
5:E:492:ILE:HD11	2:J:115:ILE:HG12	1.71	0.72
6:F:540:THR:HB	6:F:541:LEU:HD22	1.72	0.72
6:F:143:LEU:CD2	6:F:145:ASN:HB3	2.19	0.72
8:H:234:GLY:HA2	8:H:310:LEU:HD11	1.69	0.72
4:L:421:ILE:O	4:L:425:LEU:HG	1.89	0.72
8:P:28:ILE:O	8:P:32:ILE:HB	1.89	0.72
8:H:63:ILE:HD12	8:H:74:GLU:HG3	1.70	0.72
6:F:167:THR:HB	6:F:168:GLU:C	2.09	0.72
8:H:6:PRO:HG2	4:L:71:LEU:HA	1.71	0.72
6:N:352:GLY:C	6:N:369:GLU:O	2.27	0.72
4:L:524:ILE:HG23	7:O:52:LEU:O	1.88	0.72
6:F:5:LEU:CA	6:F:6:LEU:CB	2.66	0.72
1:I:122:PRO:HG3	5:M:70:LEU:HD11	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:119:ILE:HG23	4:L:436:GLN:HA	1.68	0.72
7:O:479:TYR:HA	7:O:490:ASP:HA	1.70	0.72
2:J:5:ILE:O	3:K:70:VAL:HA	1.88	0.72
6:F:352:GLY:C	6:F:369:GLU:O	2.27	0.72
2:J:263:LYS:NZ	3:K:266:GLU:CB	2.53	0.72
6:F:108:PHE:CZ	6:F:118:ILE:HG13	2.25	0.72
2:B:475:ASN:ND2	2:B:475:ASN:N	2.38	0.72
5:E:492:ILE:H	5:E:492:ILE:HD12	1.52	0.72
6:N:540:THR:HB	6:N:541:LEU:HD22	1.72	0.72
2:J:411:MET:HB2	2:J:437:LEU:HD13	1.70	0.72
2:J:242:LYS:HB2	3:K:269:TRP:HZ2	1.55	0.72
8:P:234:GLY:HA2	8:P:310:LEU:HD11	1.69	0.72
1:I:156:LEU:HD22	1:I:181:VAL:HG13	1.71	0.72
1:I:30:VAL:O	1:I:33:THR:HG22	1.87	0.72
6:F:420:ILE:HG21	6:F:482:ASP:OD1	1.89	0.72
7:G:191:ARG:HD3	7:G:192:ASN:H	1.55	0.72
2:B:164:LYS:O	2:B:166:LEU:N	2.22	0.72
8:H:204:VAL:HG21	8:H:409:LYS:CB	2.19	0.72
7:O:205:PRO:HA	7:O:386:ILE:HD11	1.71	0.72
7:G:232:GLN:HG2	7:G:313:PHE:HA	1.72	0.72
2:J:71:ASN:OD1	2:J:73:ALA:N	2.22	0.72
2:J:4:GLN:HG2	3:K:72:HIS:HB2	1.72	0.72
6:N:143:LEU:CD2	6:N:145:ASN:HB3	2.19	0.72
6:F:411:ILE:HG22	6:F:412:ILE:N	2.04	0.72
2:J:164:LYS:O	2:J:166:LEU:N	2.22	0.72
3:C:114:LYS:HA	3:C:115:ASN:CB	2.20	0.72
1:A:267:PRO:HA	1:A:268:GLU:CB	2.19	0.72
3:C:322:LYS:HG3	3:C:323:SER:H	1.55	0.72
3:K:322:LYS:HG3	3:K:323:SER:H	1.55	0.72
2:J:198:ILE:O	2:J:377:LEU:HD21	1.89	0.72
4:D:207:THR:HG22	4:D:380:ARG:H	1.54	0.72
2:J:357:SER:O	2:J:360:LYS:CB	2.38	0.72
2:B:357:SER:O	2:B:360:LYS:CB	2.38	0.72
4:L:207:THR:HG22	4:L:380:ARG:H	1.54	0.72
7:O:56:SER:HA	7:O:57:ASN:O	1.90	0.71
3:C:291:ARG:N	3:C:292:PRO:HD3	2.05	0.71
6:F:166:LEU:O	6:F:167:THR:CG2	2.33	0.71
8:H:28:ILE:O	8:H:32:ILE:HB	1.89	0.71
8:H:163:ILE:HG23	8:H:179:SER:HB2	1.70	0.71
4:D:404:LEU:O	4:D:407:GLU:O	2.08	0.71
6:N:108:PHE:CZ	6:N:118:ILE:HG13	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:251:LYS:H	6:F:251:PHE:HA	1.55	0.71
6:N:151:LEU:HD12	6:N:175:THR:HG21	1.66	0.71
7:G:56:SER:HA	7:G:57:ASN:O	1.90	0.71
7:G:43:THR:HB	7:G:99:THR:HG21	1.72	0.71
2:J:373:THR:O	2:J:376:THR:HG22	1.91	0.71
8:P:63:ILE:HD12	8:P:74:GLU:HG3	1.70	0.71
3:K:51:PRO:O	3:K:52:MET:HG3	1.90	0.71
7:O:55:THR:HG21	7:O:72:LEU:HB3	1.71	0.71
2:B:4:GLN:HG2	3:C:72:HIS:HB2	1.72	0.71
6:N:539:SER:HB3	6:N:542:LYS:CD	2.15	0.71
1:I:184:LEU:HD23	1:I:184:LEU:C	2.10	0.71
4:L:210:ILE:O	4:L:375:VAL:CG1	2.39	0.71
2:B:345:GLU:O	2:B:351:GLN:CB	2.39	0.71
5:M:558:GLY:HA2	6:N:48:ASP:HB2	1.72	0.71
6:N:203:SER:O	6:N:205:LYS:N	2.24	0.71
6:N:5:LEU:CB	6:N:6:LEU:O	2.38	0.71
7:G:226:TYR:CE1	7:G:229:PHE:O	2.44	0.71
3:K:225:LEU:HD13	3:K:320:VAL:HG13	1.73	0.71
6:N:154:ALA:HB1	6:N:402:VAL:HG23	1.73	0.71
3:C:51:PRO:O	3:C:52:MET:HG3	1.90	0.71
7:G:232:GLN:HG3	7:G:313:PHE:HA	1.73	0.71
5:E:319:ASP:O	5:E:340:LEU:HB2	1.91	0.71
1:I:16:GLY:HA3	1:I:548:ASP:HB3	1.73	0.71
4:D:71:LEU:HA	8:P:6:PRO:HG2	1.73	0.71
1:A:184:LEU:HD23	1:A:184:LEU:C	2.10	0.71
7:O:226:TYR:CE1	7:O:229:PHE:O	2.44	0.71
1:A:350:PHE:HD2	1:A:351:GLU:H	1.37	0.71
5:M:319:ASP:O	5:M:340:LEU:HB2	1.91	0.71
4:D:328:LEU:CB	4:D:345:ASP:OD2	2.38	0.71
2:B:57:THR:HG21	2:B:382:ARG:HD3	1.71	0.71
4:D:485:ARG:H	4:D:485:ARG:HD2	1.54	0.71
7:O:232:GLN:HG2	7:O:313:PHE:HA	1.72	0.71
1:A:12:THR:HG22	1:A:13:LEU:HD23	1.73	0.71
6:N:433:LYS:HG3	6:N:444:ILE:HG21	1.73	0.71
1:I:101:VAL:HG22	1:I:527:SER:HB2	1.71	0.71
1:I:418:VAL:HG12	1:I:419:VAL:H	1.56	0.71
2:B:373:THR:O	2:B:376:THR:HG22	1.91	0.71
3:K:114:LYS:HA	3:K:115:ASN:CB	2.20	0.71
1:A:230:SER:O	1:A:233:MET:HG3	1.91	0.71
1:A:16:GLY:HA3	1:A:548:ASP:HB3	1.73	0.71
1:A:418:VAL:HG12	1:A:419:VAL:H	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:243:LYS:C	8:H:244:LYS:HG2	2.12	0.71
4:L:134:ILE:CD1	4:L:424:ARG:HD3	2.20	0.71
1:I:350:PHE:C	1:I:351:GLU:OE2	2.30	0.71
2:B:198:ILE:O	2:B:377:LEU:HD21	1.89	0.71
4:D:46:LYS:HG3	8:H:532:THR:HG23	1.71	0.71
3:K:269:TRP:HZ3	6:N:247:VAL:HB	1.54	0.70
6:F:209:PHE:HE2	6:F:376:CYS:SG	2.10	0.70
6:N:209:PHE:HE2	6:N:376:CYS:SG	2.10	0.70
7:O:232:GLN:HG3	7:O:313:PHE:HA	1.73	0.70
2:J:475:ASN:N	2:J:475:ASN:ND2	2.38	0.70
2:J:237:THR:H	2:J:287:ARG:HD2	1.56	0.70
6:F:203:SER:O	6:F:205:LYS:N	2.24	0.70
6:F:5:LEU:CB	6:F:6:LEU:O	2.38	0.70
1:I:94:ILE:HG22	1:I:96:ASP:H	1.56	0.70
2:B:30:GLY:HA2	2:B:33:VAL:HG23	1.73	0.70
2:B:242:LYS:NZ	2:B:247:GLY:H	1.90	0.70
4:D:210:ILE:O	4:D:375:VAL:CG1	2.39	0.70
8:P:291:ILE:HD11	8:P:345:GLY:HA2	1.74	0.70
2:B:131:ALA:HB1	2:B:411:MET:HB3	1.73	0.70
2:B:237:THR:H	2:B:287:ARG:HD2	1.56	0.70
8:P:243:LYS:C	8:P:244:LYS:HG2	2.12	0.70
3:K:225:LEU:HD13	3:K:320:VAL:CG1	2.22	0.70
6:F:154:ALA:HB1	6:F:402:VAL:HG23	1.73	0.70
2:B:295:GLU:OE1	6:F:339:SER:HB3	1.91	0.70
4:D:482:ILE:H	4:D:482:ILE:HD13	1.57	0.70
6:N:420:ILE:HG21	6:N:482:ASP:OD1	1.89	0.70
6:N:5:LEU:CA	6:N:6:LEU:CB	2.66	0.70
6:F:16:ASP:HA	6:F:19:LEU:CD1	2.20	0.70
7:O:43:THR:HB	7:O:99:THR:HG21	1.72	0.70
1:I:12:THR:HG22	1:I:13:LEU:HD23	1.73	0.70
2:B:475:ASN:ND2	2:B:475:ASN:H	1.89	0.70
8:H:333:CYS:SG	8:H:340:PRO:HD3	2.32	0.70
4:L:521:ILE:CG2	7:O:52:LEU:H	2.05	0.70
2:B:30:GLY:HA2	2:B:33:VAL:CG2	2.22	0.70
3:C:225:LEU:HD13	3:C:320:VAL:CG1	2.22	0.70
5:M:253:GLN:N	5:M:254:MET:CB	2.54	0.70
7:O:396:ALA:O	7:O:399:ILE:HG22	1.92	0.70
5:M:509:ASN:O	5:M:522:MET:N	2.24	0.70
2:J:345:GLU:O	2:J:351:GLN:CB	2.39	0.70
8:H:6:PRO:CG	4:L:71:LEU:CA	2.69	0.70
7:G:58:GLN:NE2	8:P:6:PRO:O	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:VAL:HG22	1:A:527:SER:HB2	1.71	0.70
6:F:245:THR:OG1	6:F:247:VAL:HG22	1.91	0.70
5:M:104:LEU:HA	5:M:107:LEU:HD23	1.73	0.70
4:D:184:GLU:HA	4:D:186:SER:O	1.91	0.70
2:J:39:PRO:HA	2:J:163:SER:HA	1.74	0.70
4:D:207:THR:HG22	4:D:380:ARG:N	2.06	0.70
4:L:404:LEU:O	4:L:407:GLU:O	2.08	0.70
2:J:295:GLU:C	6:N:337:GLN:HE22	1.94	0.70
2:J:131:ALA:HB1	2:J:411:MET:HB3	1.73	0.70
6:N:7:ASN:OD1	6:N:8:PRO:N	2.25	0.70
6:N:245:THR:OG1	6:N:247:VAL:HG22	1.91	0.70
1:A:350:PHE:C	1:A:351:GLU:OE2	2.30	0.70
3:K:125:LEU:HD22	3:K:445:VAL:HG23	1.74	0.70
5:E:509:ASN:O	5:E:522:MET:N	2.24	0.70
8:P:333:CYS:SG	8:P:340:PRO:HD3	2.32	0.70
8:H:475:LEU:HB2	8:H:476:PRO:HD3	1.74	0.70
3:K:291:ARG:N	3:K:292:PRO:HD3	2.05	0.70
4:L:482:ILE:H	4:L:482:ILE:HD13	1.57	0.70
6:F:37:LEU:HD13	6:F:458:LEU:HA	1.73	0.70
2:J:242:LYS:NZ	2:J:247:GLY:H	1.90	0.70
1:A:156:LEU:HD22	1:A:181:VAL:HG13	1.71	0.70
4:L:184:GLU:HA	4:L:186:SER:O	1.91	0.70
1:I:12:THR:HB	1:I:13:LEU:HB2	1.74	0.70
4:L:207:THR:HG22	4:L:380:ARG:N	2.06	0.70
5:E:319:ASP:O	5:E:340:LEU:CB	2.40	0.70
2:B:83:VAL:HG21	3:C:384:GLY:O	1.91	0.70
7:O:121:SER:HB2	7:O:124:LEU:HD23	1.74	0.70
2:J:206:SER:HB3	2:J:368:VAL:HG13	1.73	0.70
2:B:3:VAL:C	2:B:5:ILE:CG2	2.61	0.70
2:J:3:VAL:C	2:J:5:ILE:CG2	2.61	0.70
4:L:521:ILE:HG12	7:O:62:ILE:HD11	1.73	0.70
6:F:113:VAL:HB	6:F:118:ILE:HD11	1.73	0.70
6:N:113:VAL:HB	6:N:118:ILE:HD11	1.73	0.70
2:B:31:ASP:C	2:B:31:ASP:OD1	2.30	0.70
6:N:434:LEU:O	6:N:437:LYS:C	2.30	0.69
6:F:36:ASN:CB	6:F:57:LYS:NZ	2.24	0.69
6:N:158:LEU:O	6:N:158:LEU:CD1	2.39	0.69
2:B:263:LYS:NZ	3:C:266:GLU:HB3	2.06	0.69
6:F:154:ALA:HB2	6:F:402:VAL:HG23	1.73	0.69
5:E:253:GLN:N	5:E:254:MET:CB	2.54	0.69
7:G:205:PRO:HA	7:G:386:ILE:HD11	1.71	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:31:ASP:C	2:J:31:ASP:OD1	2.30	0.69
8:P:475:LEU:HB2	8:P:476:PRO:HD3	1.74	0.69
7:G:121:SER:HB2	7:G:124:LEU:HD23	1.74	0.69
6:F:433:LYS:HG3	6:F:444:ILE:HG13	1.74	0.69
7:O:191:ARG:HD3	7:O:192:ASN:H	1.55	0.69
2:B:422:ILE:HB	2:B:427:SER:CB	2.15	0.69
3:C:299:LYS:CA	3:C:319:ARG:CB	2.70	0.69
5:M:35:GLN:CD	5:M:36:GLY:HA3	2.13	0.69
6:N:37:LEU:HD13	6:N:458:LEU:HA	1.74	0.69
2:B:414:ALA:O	2:B:417:THR:HG22	1.92	0.69
6:F:434:LEU:O	6:F:437:LYS:C	2.30	0.69
5:E:104:LEU:HA	5:E:107:LEU:HD23	1.73	0.69
2:B:328:THR:O	2:B:329:PHE:CG	2.46	0.69
1:A:299:THR:HG23	1:A:326:LEU:HD12	1.74	0.69
4:L:166:TYR:O	4:L:169:PHE:HB3	1.92	0.69
6:N:353:LEU:O	6:N:367:VAL:CG1	2.40	0.69
3:C:265:LYS:NZ	3:C:268:ASP:CB	2.55	0.69
8:P:237:LYS:HB3	8:P:314:ASN:HB3	1.63	0.69
4:D:254:VAL:HG22	8:H:264:THR:O	1.92	0.69
2:J:328:THR:O	2:J:329:PHE:CG	2.45	0.69
1:I:224:LEU:HD11	1:I:226:CYS:HB2	1.75	0.69
6:F:321:LYS:HA	6:F:321:LYS:HE3	1.75	0.69
6:N:433:LYS:HG3	6:N:444:ILE:HG13	1.74	0.69
4:L:521:ILE:HG21	7:O:52:LEU:H	1.56	0.69
3:C:416:GLY:HA2	9:C:1101:ADP:H2'	1.74	0.69
4:D:169:PHE:O	4:D:173:LEU:HD13	1.92	0.69
3:C:225:LEU:HD13	3:C:320:VAL:HG13	1.73	0.69
4:D:265:LYS:NZ	8:H:343:ARG:HD3	2.07	0.69
1:I:299:THR:HG23	1:I:326:LEU:HD12	1.75	0.69
2:J:311:PHE:O	2:J:315:GLU:HG2	1.93	0.69
1:I:230:SER:O	1:I:233:MET:HG3	1.91	0.69
2:J:30:GLY:HA2	2:J:33:VAL:CG2	2.22	0.69
4:D:134:ILE:CD1	4:D:424:ARG:HD3	2.20	0.69
2:J:459:LEU:HB2	2:J:472:LEU:HD21	1.73	0.69
7:O:148:THR:O	7:O:149:SER:CB	2.40	0.69
7:O:109:MET:HG2	7:O:514:THR:HG22	1.74	0.69
4:D:404:LEU:HD22	4:D:410:LEU:HG	1.74	0.69
2:B:32:LEU:CD1	6:F:532:GLU:OE2	2.41	0.69
8:H:153:LYS:H	8:H:153:LYS:HD2	1.56	0.69
6:F:167:THR:HA	6:F:168:GLU:HB3	1.75	0.69
6:N:433:LYS:HG2	6:N:444:ILE:HG21	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:539:SER:HB3	6:F:542:LYS:CD	2.15	0.69
4:D:15:GLU:O	4:D:523:ASP:OD2	2.11	0.69
8:H:335:VAL:HG13	8:H:379:SER:HB3	1.75	0.69
2:B:257:LYS:HA	2:B:260:GLN:HB3	1.75	0.69
1:I:350:PHE:HD2	1:I:351:GLU:H	1.37	0.69
5:E:166:ASP:HB3	5:E:167:ASP:CB	2.23	0.69
7:G:148:THR:O	7:G:149:SER:CB	2.40	0.69
8:H:291:ILE:HD11	8:H:345:GLY:HA2	1.73	0.69
8:H:346:ALA:N	8:H:347:PRO:CD	2.56	0.69
2:J:328:THR:O	2:J:329:PHE:CD1	2.46	0.69
2:J:475:ASN:H	2:J:475:ASN:ND2	1.89	0.69
2:B:32:LEU:HG	6:F:532:GLU:OE1	1.92	0.69
4:D:166:TYR:O	4:D:169:PHE:HB3	1.92	0.69
4:D:159:SER:O	4:D:161:LYS:HD3	1.93	0.69
8:P:153:LYS:H	8:P:153:LYS:HD2	1.56	0.69
5:E:35:GLN:CD	5:E:36:GLY:HA3	2.13	0.69
6:F:433:LYS:HG3	6:F:444:ILE:HG21	1.73	0.69
3:C:467:LEU:O	3:C:471:LEU:HB2	1.93	0.69
3:K:299:LYS:CA	3:K:319:ARG:CB	2.70	0.69
5:E:544:LEU:HD23	6:F:384:THR:HG21	1.73	0.69
5:M:319:ASP:O	5:M:340:LEU:CB	2.40	0.69
7:G:396:ALA:O	7:G:399:ILE:HG22	1.92	0.69
6:F:354:VAL:HG22	6:F:367:VAL:HG13	1.75	0.69
2:J:30:GLY:HA2	2:J:33:VAL:HG23	1.73	0.69
4:L:520:ARG:O	7:O:49:SER:CB	2.36	0.69
6:F:158:LEU:O	6:F:158:LEU:CD1	2.39	0.69
3:K:299:LYS:N	3:K:319:ARG:CB	2.55	0.69
2:B:459:LEU:HB2	2:B:472:LEU:HD21	1.73	0.69
6:F:209:PHE:HB2	6:F:378:ILE:HB	1.75	0.69
3:C:125:LEU:HD22	3:C:445:VAL:HG23	1.74	0.69
6:F:353:LEU:O	6:F:367:VAL:CG1	2.40	0.68
2:J:360:LYS:C	2:J:362:GLY:HA2	2.12	0.68
7:G:94:VAL:HG13	7:G:95:GLY:H	1.59	0.68
3:K:467:LEU:O	3:K:471:LEU:HB2	1.93	0.68
1:A:94:ILE:HG22	1:A:96:ASP:H	1.56	0.68
2:B:39:PRO:HA	2:B:163:SER:HA	1.74	0.68
1:A:224:LEU:HD11	1:A:226:CYS:HB2	1.75	0.68
7:G:450:PRO:HA	7:G:453:LEU:HD12	1.75	0.68
1:A:94:ILE:HG12	1:A:523:SER:HA	1.75	0.68
3:C:299:LYS:N	3:C:319:ARG:CB	2.55	0.68
6:N:154:ALA:HB2	6:N:402:VAL:HG23	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:251:HIS:O	5:E:253:GLN:N	2.25	0.68
2:B:328:THR:O	2:B:329:PHE:CD1	2.46	0.68
8:P:346:ALA:N	8:P:347:PRO:CD	2.56	0.68
1:A:12:THR:HB	1:A:13:LEU:HB2	1.74	0.68
5:M:74:LEU:HG	5:M:93:GLN:HB3	1.75	0.68
2:J:83:VAL:HG21	3:K:384:GLY:O	1.92	0.68
8:P:6:PRO:HB3	8:P:7:GLN:HA	1.75	0.68
6:F:420:ILE:HG22	6:F:482:ASP:OD1	1.94	0.68
2:J:30:GLY:CA	2:J:33:VAL:HG23	2.24	0.68
8:P:316:TYR:N	8:P:316:TYR:HD2	1.87	0.68
4:L:169:PHE:O	4:L:173:LEU:HD13	1.92	0.68
2:J:4:GLN:CB	2:J:5:ILE:HG12	2.24	0.68
6:N:330:LEU:HB2	6:N:375:SER:OG	1.93	0.68
4:D:71:LEU:CA	8:P:6:PRO:CG	2.71	0.68
2:J:422:ILE:HG22	2:J:424:GLY:N	2.08	0.68
6:N:141:THR:HB	6:N:409:LYS:HG3	1.75	0.68
1:A:66:GLY:O	1:A:69:ILE:HG22	1.94	0.68
4:L:404:LEU:HD22	4:L:410:LEU:HG	1.74	0.68
4:L:159:SER:O	4:L:161:LYS:HD3	1.93	0.68
6:F:433:LYS:HG2	6:F:444:ILE:HG21	1.74	0.68
6:N:354:VAL:HG22	6:N:367:VAL:HG13	1.75	0.68
6:F:233:VAL:HG13	6:F:351:SER:HB3	1.76	0.68
2:B:30:GLY:CA	2:B:33:VAL:HG23	2.24	0.68
6:F:141:THR:HB	6:F:409:LYS:HG3	1.75	0.68
2:J:285:ILE:HD11	2:J:289:LEU:CD2	2.24	0.68
7:G:109:MET:HG2	7:G:514:THR:HG22	1.74	0.68
5:E:74:LEU:HG	5:E:93:GLN:HB3	1.75	0.68
2:J:402:LEU:HD21	2:J:483:ARG:HG3	1.74	0.68
6:F:7:ASN:OD1	6:F:8:PRO:N	2.25	0.68
8:P:24:ALA:HB2	8:P:531:ALA:HB1	1.76	0.68
4:D:184:GLU:C	4:D:186:SER:O	2.32	0.68
8:H:283:GLN:O	8:H:287:MET:HG2	1.93	0.68
8:H:249:VAL:HG22	8:H:300:VAL:HB	1.75	0.68
5:M:166:ASP:HB3	5:M:167:ASP:CB	2.23	0.68
2:J:295:GLU:OE2	6:N:338:ASN:HB2	1.92	0.68
2:B:402:LEU:HD21	2:B:483:ARG:HG3	1.74	0.68
2:J:414:ALA:O	2:J:417:THR:HG22	1.92	0.68
4:D:461:ASN:HB3	4:D:464:LYS:HG2	1.75	0.68
4:D:178:VAL:HG11	4:D:401:ILE:HD11	1.76	0.68
6:N:154:ALA:O	6:N:157:SER:OG	2.12	0.68
4:D:181:ILE:HD13	4:D:373:PRO:O	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:ARG:NH2	2:B:512:ASP:H	1.92	0.68
1:A:289:ILE:HA	1:A:293:ALA:HB2	1.76	0.68
4:L:178:VAL:HG11	4:L:401:ILE:HD11	1.76	0.68
4:L:15:GLU:O	4:L:523:ASP:OD2	2.11	0.68
8:H:291:ILE:HD12	8:H:347:PRO:CG	2.24	0.68
8:H:131:TYR:HD2	8:H:452:PHE:HD2	1.42	0.68
3:K:250:LEU:HG	3:K:301:VAL:CB	2.23	0.68
6:F:43:LEU:HD23	6:F:57:LYS:CB	2.20	0.68
4:L:521:ILE:HG23	7:O:50:ASP:O	1.94	0.68
5:E:34:ASP:O	6:N:117:ILE:HD12	1.94	0.68
3:K:332:THR:HB	3:K:349:GLY:HA3	1.76	0.68
8:P:291:ILE:HD12	8:P:347:PRO:CG	2.24	0.68
7:O:409:ILE:HG22	7:O:410:VAL:H	1.59	0.68
3:C:250:LEU:HG	3:C:301:VAL:CB	2.23	0.68
6:N:167:THR:HA	6:N:168:GLU:HB3	1.75	0.67
8:H:6:PRO:HB3	8:H:7:GLN:HA	1.76	0.67
6:F:352:GLY:O	6:F:353:LEU:C	2.33	0.67
7:O:94:VAL:HG13	7:O:95:GLY:H	1.59	0.67
7:O:42:PRO:O	7:O:48:GLY:CA	2.40	0.67
2:J:257:LYS:HA	2:J:260:GLN:HB3	1.75	0.67
2:B:285:ILE:HD11	2:B:289:LEU:CD2	2.24	0.67
4:L:184:GLU:C	4:L:186:SER:O	2.32	0.67
1:I:66:GLY:O	1:I:69:ILE:HG22	1.94	0.67
6:F:352:GLY:O	6:F:367:VAL:HG11	1.91	0.67
6:F:330:LEU:HB2	6:F:375:SER:OG	1.93	0.67
6:N:423:SER:O	6:N:427:ARG:HG3	1.94	0.67
5:E:88:ALA:HB1	5:E:109:LYS:HZ1	1.60	0.67
3:C:332:THR:HB	3:C:349:GLY:HA3	1.76	0.67
7:G:241:ILE:HB	7:G:330:VAL:HG11	1.77	0.67
7:G:448:VAL:HG12	7:G:452:GLN:NE2	2.09	0.67
7:G:492:PHE:HA	7:G:497:TRP:HE1	1.59	0.67
2:B:311:PHE:O	2:B:315:GLU:HG2	1.93	0.67
6:N:501:PRO:CB	6:N:506:ILE:HB	2.17	0.67
8:P:249:VAL:HG22	8:P:300:VAL:HB	1.76	0.67
2:B:243:VAL:HG12	2:B:245:ILE:H	1.59	0.67
6:F:170:LEU:O	6:F:173:ILE:HG22	1.94	0.67
3:C:94:THR:HG23	10:C:1102:BEF:F1	1.82	0.67
7:O:241:ILE:HB	7:O:330:VAL:HG11	1.77	0.67
4:D:241:ILE:H	4:D:241:ILE:HD12	1.60	0.67
7:O:450:PRO:HA	7:O:453:LEU:HD12	1.75	0.67
1:I:64:ASN:ND2	1:I:166:SER:O	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:289:ILE:HA	1:I:293:ALA:HB2	1.76	0.67
8:H:54:ILE:CG1	8:H:64:ILE:HG12	2.13	0.67
2:B:237:THR:N	2:B:287:ARG:HG3	2.10	0.67
2:B:422:ILE:HG22	2:B:424:GLY:N	2.08	0.67
2:J:422:ILE:HB	2:J:427:SER:CB	2.15	0.67
1:I:94:ILE:HG12	1:I:523:SER:HA	1.75	0.67
6:N:209:PHE:HB2	6:N:378:ILE:HB	1.75	0.67
8:P:283:GLN:O	8:P:287:MET:HG2	1.93	0.67
4:D:521:ILE:CG2	7:G:50:ASP:O	2.42	0.67
5:E:34:ASP:CA	6:N:117:ILE:CD1	2.66	0.67
1:A:64:ASN:ND2	1:A:166:SER:O	2.27	0.67
7:G:162:ALA:HB3	7:G:179:VAL:HG13	1.77	0.67
4:L:100:THR:HG22	4:L:515:VAL:HG13	1.77	0.67
2:B:295:GLU:OE2	6:F:338:ASN:HB2	1.93	0.67
6:N:321:LYS:HA	6:N:321:LYS:HE3	1.75	0.67
4:D:69:ALA:O	8:H:15:LYS:HE2	1.94	0.67
6:N:485:GLU:HB3	6:N:488:TYR:CB	2.24	0.67
5:M:251:HIS:O	5:M:253:GLN:N	2.24	0.67
6:F:224:MET:CE	6:F:316:ALA:H	2.06	0.67
3:K:108:ALA:N	3:K:109:PRO:HD2	2.10	0.67
1:I:66:GLY:H	1:I:99:THR:HG22	1.60	0.67
2:J:19:ARG:NH2	2:J:512:ASP:H	1.92	0.67
8:H:334:ARG:HG2	8:H:380:ARG:HB3	1.77	0.67
6:F:151:LEU:HB3	6:F:175:THR:OG1	1.95	0.67
8:P:335:VAL:HG13	8:P:379:SER:HB3	1.75	0.67
6:N:170:LEU:O	6:N:173:ILE:HG22	1.94	0.67
4:D:100:THR:HG22	4:D:515:VAL:HG13	1.77	0.67
7:G:282:LEU:HD22	7:G:307:PHE:HB3	1.76	0.67
1:A:66:GLY:H	1:A:99:THR:HG22	1.60	0.67
1:I:348:GLU:CB	1:I:349:THR:HA	2.25	0.67
7:O:492:PHE:HA	7:O:497:TRP:HE1	1.59	0.67
6:F:485:GLU:HB3	6:F:488:TYR:CB	2.25	0.67
6:N:16:ASP:HA	6:N:19:LEU:CD1	2.20	0.67
4:L:181:ILE:HD13	4:L:373:PRO:O	1.94	0.67
2:B:34:LYS:O	2:B:36:THR:N	2.27	0.67
7:O:282:LEU:HD22	7:O:307:PHE:HB3	1.76	0.67
6:N:280:LEU:HD23	6:N:280:LEU:H	1.60	0.67
4:L:461:ASN:HB3	4:L:464:LYS:HG2	1.75	0.67
8:H:6:PRO:O	7:O:58:GLN:NE2	2.28	0.67
6:F:423:SER:O	6:F:427:ARG:HG3	1.94	0.67
7:O:162:ALA:HB3	7:O:179:VAL:HG13	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:187:ASP:O	6:N:188:ASN:CB	2.43	0.67
4:D:528:ARG:HE	4:D:528:ARG:H	1.43	0.67
6:F:187:ASP:O	6:F:188:ASN:CB	2.43	0.67
1:I:250:ASN:CG	1:I:250:ASN:O	2.32	0.67
4:D:233:LYS:HA	4:D:345:ASP:O	1.95	0.67
5:E:355:ALA:HB3	6:F:222:PRO:HG2	1.76	0.67
8:P:334:ARG:HG2	8:P:380:ARG:HB3	1.77	0.67
4:L:9:ALA:HB1	7:O:76:VAL:H	1.60	0.67
3:C:467:LEU:HD21	3:C:491:ILE:HG21	1.78	0.66
6:F:195:GLU:OE1	6:F:197:MET:SD	2.53	0.66
1:I:397:GLU:HG2	1:I:400:ARG:HH11	1.61	0.66
4:L:24:ASN:HD21	4:L:524:ILE:HD11	1.60	0.66
7:G:91:ASP:O	7:G:95:GLY:HA2	1.95	0.66
6:N:224:MET:CE	6:N:316:ALA:H	2.06	0.66
7:O:448:VAL:HG12	7:O:452:GLN:NE2	2.09	0.66
2:J:237:THR:N	2:J:287:ARG:HG3	2.10	0.66
7:O:108:LEU:HD11	7:O:511:THR:HG22	1.77	0.66
1:A:507:GLY:O	1:A:508:LYS:CB	2.43	0.66
2:B:360:LYS:C	2:B:362:GLY:HA2	2.12	0.66
4:D:24:ASN:HD21	4:D:524:ILE:HD11	1.60	0.66
2:J:409:MET:HE2	2:J:409:MET:HA	1.76	0.66
3:K:467:LEU:HD21	3:K:491:ILE:HG21	1.77	0.66
3:K:265:LYS:NZ	3:K:268:ASP:CB	2.55	0.66
8:H:24:ALA:HB2	8:H:531:ALA:HB1	1.76	0.66
2:B:329:PHE:C	2:B:329:PHE:HD2	1.96	0.66
7:G:483:PHE:CB	9:G:601:ADP:HN62	2.08	0.66
9:D:601:ADP:O3'	9:D:601:ADP:H8	1.78	0.66
2:B:206:SER:CB	2:B:368:VAL:HG13	2.26	0.66
4:L:241:ILE:H	4:L:241:ILE:HD12	1.60	0.66
8:P:131:TYR:HD2	8:P:452:PHE:HD2	1.42	0.66
1:A:118:ASN:C	1:A:119:LYS:HD2	2.16	0.66
1:A:348:GLU:CB	1:A:349:THR:HA	2.25	0.66
6:F:543:GLU:O	6:F:544:THR:C	2.33	0.66
4:L:24:ASN:HA	4:L:74:VAL:HG21	1.77	0.66
7:O:317:ARG:O	7:O:317:ARG:HG3	1.94	0.66
7:G:410:VAL:HG12	7:G:498:GLU:O	1.95	0.66
2:J:49:ALA:HB1	6:N:538:ARG:HB2	1.78	0.66
7:G:343:PRO:HA	7:G:346:LEU:HD21	1.78	0.66
2:B:4:GLN:CB	2:B:5:ILE:HG12	2.24	0.66
6:N:541:LEU:HB3	6:N:543:GLU:H	1.60	0.66
6:N:352:GLY:O	6:N:353:LEU:C	2.33	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:463:ILE:O	2:J:467:ILE:CA	2.44	0.66
2:J:422:ILE:O	2:J:423:ASP:CG	2.34	0.66
7:G:317:ARG:O	7:G:317:ARG:HG3	1.95	0.66
2:B:165:ILE:HG12	6:F:529:LEU:HD13	1.76	0.66
8:H:204:VAL:HG13	8:H:405:VAL:CG1	2.25	0.66
4:D:44:MET:HG3	8:H:531:ALA:HB3	1.77	0.66
1:I:431:ILE:HG12	1:I:482:ALA:CB	2.25	0.66
2:B:255:THR:HA	2:B:258:LEU:HD13	1.77	0.66
1:A:397:GLU:HG2	1:A:400:ARG:HH11	1.61	0.66
4:L:528:ARG:H	4:L:528:ARG:HE	1.43	0.66
2:B:23:PHE:HA	2:B:103:LEU:HD13	1.77	0.66
4:L:233:LYS:HA	4:L:345:ASP:O	1.95	0.66
7:O:516:LEU:HD11	7:O:517:ILE:HG12	1.75	0.66
4:L:254:VAL:HG22	8:P:265:VAL:HA	1.77	0.66
6:F:451:LEU:O	6:F:455:PRO:CD	2.44	0.66
6:N:75:LEU:HD22	6:N:527:LEU:HD11	1.78	0.66
4:D:252:ILE:HB	8:H:262:LYS:O	1.96	0.66
6:F:541:LEU:HB3	6:F:543:GLU:H	1.60	0.66
6:N:233:VAL:HG13	6:N:351:SER:HB3	1.76	0.66
8:P:6:PRO:CB	8:P:7:GLN:HA	2.26	0.66
3:K:297:THR:O	3:K:319:ARG:HA	1.96	0.66
2:B:444:LEU:HD21	9:B:601:ADP:H1'	1.78	0.66
7:G:409:ILE:HG22	7:G:410:VAL:H	1.59	0.66
7:O:410:VAL:HG12	7:O:498:GLU:O	1.95	0.66
7:O:91:ASP:O	7:O:95:GLY:HA2	1.95	0.66
5:M:350:GLU:HA	5:M:352:GLU:OE2	1.96	0.66
1:A:65:ASP:HB3	1:A:68:THR:OG1	1.96	0.66
1:A:54:VAL:HG12	1:A:56:ASP:H	1.60	0.66
7:G:108:LEU:HD11	7:G:511:THR:HG22	1.77	0.66
5:M:55:ARG:HG3	5:M:131:ASP:OD2	1.96	0.66
1:I:118:ASN:C	1:I:119:LYS:HD2	2.16	0.66
7:O:75:VAL:HG21	7:O:84:VAL:HG21	1.78	0.66
2:J:3:VAL:O	2:J:5:ILE:HG12	1.96	0.66
6:N:151:LEU:HB3	6:N:175:THR:OG1	1.95	0.66
8:H:6:PRO:CB	8:H:7:GLN:HA	2.26	0.66
6:N:420:ILE:HG22	6:N:482:ASP:OD1	1.94	0.66
2:J:243:VAL:HG12	2:J:245:ILE:H	1.60	0.66
8:P:24:ALA:CA	8:P:531:ALA:O	2.43	0.66
6:F:280:LEU:H	6:F:280:LEU:HD23	1.59	0.66
1:A:431:ILE:HG12	1:A:482:ALA:CB	2.25	0.66
1:A:183:ALA:HB1	1:A:383:SER:CB	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:94:ILE:HD12	8:P:95:ASP:H	1.61	0.66
5:E:55:ARG:HG3	5:E:131:ASP:OD2	1.96	0.66
7:G:70:LEU:HB3	7:G:84:VAL:HG13	1.78	0.66
2:J:255:THR:HA	2:J:258:LEU:HD13	1.77	0.66
1:A:250:ASN:O	1:A:250:ASN:CG	2.32	0.65
5:M:66:GLY:N	9:M:601:ADP:H5'1	2.07	0.65
7:O:90:GLN:CG	7:O:101:VAL:HG21	2.24	0.65
3:C:108:ALA:N	3:C:109:PRO:HD2	2.10	0.65
6:N:543:GLU:O	6:N:544:THR:C	2.33	0.65
6:F:193:MET:HE2	6:F:330:LEU:HD11	1.76	0.65
6:N:195:GLU:OE1	6:N:197:MET:SD	2.53	0.65
6:F:75:LEU:HD22	6:F:527:LEU:HD11	1.78	0.65
2:J:263:LYS:HZ1	3:K:266:GLU:CB	2.09	0.65
6:F:154:ALA:O	6:F:157:SER:OG	2.12	0.65
6:N:451:LEU:O	6:N:455:PRO:CD	2.44	0.65
4:D:185:ASN:N	4:D:186:SER:O	2.30	0.65
2:J:300:ASP:O	2:J:301:LEU:CB	2.44	0.65
8:H:94:ILE:HD12	8:H:95:ASP:H	1.61	0.65
2:B:5:ILE:HG13	2:B:6:PHE:N	2.09	0.65
6:N:353:LEU:O	6:N:367:VAL:HG13	1.97	0.65
2:J:319:LEU:HD21	2:J:357:SER:OG	1.97	0.65
2:J:492:LYS:HE2	2:J:493:LEU:N	2.12	0.65
4:D:254:VAL:CG2	8:H:265:VAL:HA	2.25	0.65
1:I:183:ALA:HB1	1:I:383:SER:CB	2.26	0.65
6:N:540:THR:HB	6:N:541:LEU:CD2	2.25	0.65
2:B:422:ILE:O	2:B:423:ASP:CG	2.34	0.65
3:K:269:TRP:HH2	6:N:248:ASN:N	1.82	0.65
3:K:57:LEU:N	3:K:57:LEU:CD2	2.57	0.65
8:H:24:ALA:CA	8:H:531:ALA:O	2.43	0.65
4:D:297:VAL:HB	4:D:298:ASN:HA	1.78	0.65
6:N:53:ILE:CD1	6:N:53:ILE:C	2.62	0.65
2:J:459:LEU:HD22	2:J:472:LEU:CG	2.26	0.65
4:L:297:VAL:HB	4:L:298:ASN:HA	1.78	0.65
1:I:65:ASP:HB3	1:I:68:THR:OG1	1.96	0.65
3:C:122:ILE:HD13	3:C:522:ARG:HG2	1.79	0.65
2:B:402:LEU:HD11	2:B:483:ARG:HE	1.62	0.65
7:G:75:VAL:HG21	7:G:84:VAL:HG21	1.78	0.65
8:H:250:PHE:HE2	8:H:299:ILE:HD12	1.62	0.65
8:P:250:PHE:HE2	8:P:299:ILE:HD12	1.61	0.65
2:J:5:ILE:HG13	2:J:6:PHE:N	2.09	0.65
8:P:300:VAL:HG11	8:P:332:LEU:HD21	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:393:GLN:HB3	2:J:492:LYS:HE3	1.79	0.65
1:I:187:VAL:HG23	1:I:383:SER:HB3	1.79	0.65
1:I:507:GLY:O	1:I:508:LYS:CB	2.43	0.65
3:K:255:GLY:H	3:K:259:THR:HG21	1.62	0.65
2:J:23:PHE:HA	2:J:103:LEU:HD13	1.77	0.65
6:F:540:THR:HB	6:F:541:LEU:CD2	2.25	0.65
6:N:540:THR:O	6:N:542:LYS:CG	2.44	0.65
4:D:330:CYS:CB	4:D:345:ASP:OD2	2.44	0.65
7:G:86:ILE:HA	7:G:89:ALA:HB3	1.79	0.65
7:O:70:LEU:HB3	7:O:84:VAL:HG13	1.78	0.65
1:I:54:VAL:HG12	1:I:56:ASP:H	1.60	0.65
7:O:56:SER:HA	7:O:57:ASN:C	2.17	0.65
2:B:319:LEU:HD21	2:B:357:SER:OG	1.97	0.65
4:D:24:ASN:HA	4:D:74:VAL:HG21	1.77	0.65
2:J:409:MET:HB3	2:J:463:ILE:HD13	1.78	0.65
2:B:8:ASP:CB	2:B:9:GLN:HA	2.22	0.65
6:F:174:VAL:HG13	6:F:399:LEU:HD13	1.77	0.65
4:L:154:ALA:HB2	4:L:175:VAL:HG13	1.79	0.65
4:D:217:GLN:NE2	4:D:316:ILE:HA	2.12	0.65
2:B:278:LYS:HA	2:B:333:SER:HB3	1.79	0.65
7:G:446:LEU:HD21	7:G:507:LEU:HD23	1.78	0.65
4:L:38:SER:HB3	4:L:46:LYS:HZ3	1.61	0.65
6:F:539:SER:HB2	6:F:542:LYS:CD	2.27	0.65
2:J:230:LYS:HA	2:J:337:LEU:O	1.97	0.65
5:E:350:GLU:HA	5:E:352:GLU:OE2	1.96	0.65
3:C:297:THR:O	3:C:319:ARG:HA	1.96	0.65
2:J:27:ILE:CD1	2:J:104:ARG:HH11	2.09	0.65
3:C:161:THR:H	3:C:165:ILE:HG13	1.62	0.65
7:O:83:LEU:HD23	7:O:86:ILE:HD11	1.78	0.65
7:G:454:CYS:HB2	7:G:461:ALA:CB	2.27	0.65
2:J:402:LEU:HD11	2:J:483:ARG:HE	1.62	0.65
2:B:21:SER:OG	1:I:8:SER:N	2.30	0.64
4:L:185:ASN:N	4:L:186:SER:O	2.30	0.64
4:L:38:SER:HB3	4:L:46:LYS:NZ	2.12	0.64
2:J:45:LEU:HB2	6:N:533:LEU:CB	2.27	0.64
4:L:214:VAL:HG22	4:L:362:ARG:HG2	1.80	0.64
2:B:463:ILE:O	2:B:467:ILE:CA	2.44	0.64
4:D:521:ILE:HG21	7:G:52:LEU:H	1.61	0.64
4:L:524:ILE:HG23	7:O:52:LEU:HD22	1.80	0.64
1:A:45:GLY:H	9:A:601:ADP:H5'1	1.63	0.64
2:B:492:LYS:HE2	2:B:493:LEU:N	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:226:PRO:HB2	4:D:311:MET:HG2	1.79	0.64
2:B:206:SER:HB2	2:B:368:VAL:HG22	1.78	0.64
2:J:197:LYS:HB3	2:J:381:GLU:OE1	1.97	0.64
4:D:38:SER:HB3	4:D:46:LYS:NZ	2.12	0.64
7:O:446:LEU:HD21	7:O:507:LEU:HD23	1.78	0.64
3:C:255:GLY:H	3:C:259:THR:HG21	1.62	0.64
6:F:241:GLU:HA	6:F:302:ASP:OD2	1.98	0.64
3:K:124:ALA:HB1	3:K:441:PRO:HB2	1.79	0.64
2:B:300:ASP:O	2:B:301:LEU:CB	2.44	0.64
7:G:235:LYS:CB	7:G:352:PHE:O	2.46	0.64
6:N:143:LEU:HD22	6:N:145:ASN:HB3	1.79	0.64
3:K:269:TRP:CH2	6:N:248:ASN:N	2.60	0.64
7:G:90:GLN:CG	7:G:101:VAL:HG21	2.24	0.64
4:L:410:LEU:HD13	4:L:498:LEU:HD22	1.78	0.64
4:L:217:GLN:NE2	4:L:316:ILE:HA	2.12	0.64
4:D:239:PHE:H	4:D:288:ILE:HD12	1.62	0.64
6:N:419:TYR:CZ	6:N:513:LEU:HD21	2.32	0.64
6:F:419:TYR:CZ	6:F:513:LEU:HD21	2.32	0.64
2:J:357:SER:C	2:J:360:LYS:CB	2.66	0.64
2:B:230:LYS:HA	2:B:337:LEU:O	1.98	0.64
2:J:408:GLU:HG2	2:J:440:LEU:HB3	1.78	0.64
6:F:53:ILE:CD1	6:F:53:ILE:C	2.62	0.64
2:B:8:ASP:HA	2:B:10:VAL:HG23	1.80	0.64
7:G:83:LEU:HD23	7:G:86:ILE:HD11	1.78	0.64
1:A:187:VAL:HG23	1:A:383:SER:HB3	1.79	0.64
5:E:39:LYS:HE2	6:N:109:ILE:O	1.96	0.64
6:F:434:LEU:O	6:F:438:GLY:CA	2.45	0.64
1:A:184:LEU:HD21	1:A:198:TYR:CB	2.28	0.64
6:N:414:GLY:O	6:N:415:ALA:HB3	1.97	0.64
7:G:42:PRO:O	7:G:48:GLY:CA	2.40	0.64
2:B:393:GLN:HB3	2:B:492:LYS:HE3	1.79	0.64
4:L:226:PRO:HB2	4:L:311:MET:HG2	1.80	0.64
7:O:239:PRO:HA	7:O:291:ASN:HD21	1.63	0.64
2:B:232:LEU:HD21	2:B:325:VAL:HG21	1.79	0.64
2:J:232:LEU:HD21	2:J:325:VAL:HG21	1.80	0.64
2:J:295:GLU:HB2	6:N:337:GLN:NE2	2.12	0.64
8:P:168:SER:HB3	8:P:175:GLU:HB3	1.80	0.64
4:L:239:PHE:H	4:L:288:ILE:HD12	1.62	0.64
7:G:56:SER:HA	7:G:57:ASN:C	2.16	0.64
2:B:409:MET:HB3	2:B:463:ILE:HD13	1.78	0.64
4:D:134:ILE:HD11	4:D:424:ARG:CG	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:8:ASP:HA	2:J:10:VAL:HG23	1.79	0.64
6:N:174:VAL:HG13	6:N:399:LEU:HD13	1.78	0.64
5:E:166:ASP:H	5:E:167:ASP:HB2	1.60	0.64
7:G:239:PRO:HA	7:G:291:ASN:HD21	1.63	0.64
1:A:218:LEU:HD22	1:A:219:VAL:H	1.63	0.64
3:K:122:ILE:HD13	3:K:522:ARG:HG2	1.79	0.64
4:D:410:LEU:HD13	4:D:498:LEU:HD22	1.78	0.64
4:D:214:VAL:HG22	4:D:362:ARG:HG2	1.80	0.64
6:N:434:LEU:O	6:N:438:GLY:CA	2.45	0.64
7:G:516:LEU:HD11	7:G:517:ILE:HG12	1.75	0.64
4:L:134:ILE:HD11	4:L:424:ARG:CG	2.28	0.64
3:K:161:THR:H	3:K:165:ILE:HG13	1.62	0.64
7:G:109:MET:HG2	7:G:514:THR:CG2	2.28	0.64
7:O:454:CYS:HB2	7:O:461:ALA:CB	2.27	0.64
7:O:343:PRO:HA	7:O:346:LEU:HD21	1.78	0.64
6:F:353:LEU:O	6:F:367:VAL:HG13	1.97	0.64
7:O:191:ARG:CD	7:O:192:ASN:N	2.61	0.64
2:J:201:GLY:H	6:N:86:ILE:HD12	1.63	0.64
5:M:66:GLY:H	9:M:601:ADP:C5'	2.05	0.64
3:C:93:THR:HG22	10:C:1102:BEF:F2	1.87	0.64
7:O:86:ILE:HA	7:O:89:ALA:HB3	1.79	0.64
4:D:499:GLN:NE2	9:D:601:ADP:H2'	2.12	0.64
2:B:197:LYS:HB3	2:B:381:GLU:OE1	1.97	0.64
6:N:538:ARG:HH11	6:N:538:ARG:CG	2.11	0.64
2:B:4:GLN:HB2	3:C:71:ALA:HB3	1.80	0.64
6:N:83:GLN:HG3	6:N:94:VAL:CG2	2.18	0.64
1:A:517:VAL:C	1:A:518:LEU:HG	2.18	0.64
4:D:154:ALA:HB2	4:D:175:VAL:HG13	1.79	0.64
2:J:465:ASN:OD1	2:J:465:ASN:C	2.36	0.64
4:L:367:ARG:C	4:L:369:ASN:H	2.01	0.64
6:N:352:GLY:O	6:N:367:VAL:HG11	1.91	0.64
6:F:331:VAL:O	6:F:332:THR:OG1	2.12	0.64
2:J:411:MET:O	2:J:415:VAL:HG23	1.98	0.64
5:E:33:LYS:HE2	6:N:117:ILE:HG12	1.79	0.64
5:M:401:THR:O	5:M:402:LYS:CB	2.46	0.64
7:O:317:ARG:O	7:O:317:ARG:CG	2.46	0.64
6:F:23:VAL:HG11	6:F:106:HIS:CB	2.28	0.64
1:I:66:GLY:N	1:I:99:THR:HG22	2.12	0.64
1:A:66:GLY:N	1:A:99:THR:HG22	2.12	0.64
5:E:128:ALA:HB2	5:E:478:THR:HG21	1.80	0.64
2:J:278:LYS:HA	2:J:333:SER:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:223:VAL:HG12	3:C:224:LEU:H	1.63	0.64
2:B:357:SER:C	2:B:360:LYS:CB	2.66	0.63
5:M:166:ASP:H	5:M:167:ASP:HB2	1.60	0.63
2:J:329:PHE:HD2	2:J:329:PHE:C	1.95	0.63
8:P:430:LEU:HD13	8:P:434:ILE:HD11	1.79	0.63
1:I:540:ARG:O	5:M:70:LEU:HB3	1.98	0.63
3:C:124:ALA:HB1	3:C:441:PRO:HB2	1.79	0.63
2:J:251:LYS:N	6:N:251:PHE:HA	2.10	0.63
4:D:210:ILE:O	4:D:375:VAL:HG13	1.98	0.63
1:I:218:LEU:HD22	1:I:219:VAL:H	1.63	0.63
6:F:538:ARG:HH11	6:F:538:ARG:CG	2.11	0.63
3:C:391:GLU:O	3:C:395:ASN:HB2	1.99	0.63
2:B:411:MET:O	2:B:415:VAL:HG23	1.98	0.63
3:K:335:THR:HB	8:P:237:LYS:HE2	1.80	0.63
7:G:317:ARG:O	7:G:317:ARG:CG	2.46	0.63
7:O:235:LYS:CB	7:O:352:PHE:O	2.46	0.63
6:N:159:LEU:O	6:N:160:THR:CB	2.46	0.63
4:D:252:ILE:O	8:H:263:GLY:HA2	1.99	0.63
6:N:241:GLU:HA	6:N:302:ASP:OD2	1.98	0.63
6:N:433:LYS:HB3	6:N:441:LYS:HA	1.80	0.63
6:N:539:SER:HB2	6:N:542:LYS:CD	2.27	0.63
2:B:408:GLU:HG2	2:B:440:LEU:HB3	1.78	0.63
6:F:83:GLN:HG3	6:F:94:VAL:CG2	2.18	0.63
8:H:300:VAL:HG11	8:H:332:LEU:HD21	1.79	0.63
3:C:35:ILE:HD11	3:C:65:LEU:HG	1.80	0.63
6:F:106:HIS:O	6:F:109:ILE:HG12	1.97	0.63
1:I:158:ASN:ND2	1:I:516:GLY:HA2	2.13	0.63
7:O:282:LEU:HD21	7:O:306:PHE:HB2	1.80	0.63
8:H:430:LEU:HD13	8:H:434:ILE:HD11	1.79	0.63
6:N:331:VAL:O	6:N:332:THR:OG1	2.12	0.63
6:F:330:LEU:CB	6:F:375:SER:OG	2.47	0.63
2:B:236:THR:OG1	2:B:327:SER:HA	1.99	0.63
6:F:143:LEU:HD22	6:F:145:ASN:HB3	1.79	0.63
8:P:204:VAL:HG13	8:P:405:VAL:CG1	2.25	0.63
7:O:237:ASN:C	7:O:239:PRO:HD3	2.18	0.63
1:I:115:LEU:HD13	1:I:125:ILE:HD11	1.81	0.63
5:E:283:THR:HG22	5:E:284:LYS:H	1.64	0.63
6:N:330:LEU:CB	6:N:375:SER:OG	2.47	0.63
7:O:189:LEU:N	7:O:190:ASP:HB2	2.14	0.63
2:J:210:GLU:OE1	2:J:357:SER:O	2.17	0.63
7:G:191:ARG:CZ	7:G:192:ASN:N	2.61	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:517:VAL:C	1:I:518:LEU:HG	2.18	0.63
2:J:492:LYS:H	2:J:492:LYS:NZ	1.97	0.63
6:F:159:LEU:O	6:F:160:THR:CB	2.46	0.63
7:O:109:MET:HG2	7:O:514:THR:CG2	2.28	0.63
7:O:109:MET:SD	7:O:514:THR:HG22	2.39	0.63
6:N:106:HIS:O	6:N:109:ILE:HG12	1.97	0.63
5:M:283:THR:HG22	5:M:284:LYS:H	1.64	0.63
1:I:55:ASP:HA	7:O:527:LYS:HB3	1.80	0.63
2:B:465:ASN:OD1	2:B:465:ASN:C	2.36	0.63
2:B:3:VAL:O	2:B:5:ILE:HG12	1.96	0.63
2:B:230:LYS:H	2:B:281:ILE:HG22	1.62	0.63
7:G:191:ARG:CD	7:G:192:ASN:N	2.61	0.63
5:M:104:LEU:CD2	5:M:123:VAL:HG13	2.27	0.63
7:G:498:GLU:HG2	9:G:601:ADP:O2'	1.99	0.63
7:O:304:THR:HA	7:O:307:PHE:HE2	1.63	0.63
2:J:34:LYS:O	2:J:36:THR:N	2.27	0.63
6:N:23:VAL:HG11	6:N:106:HIS:CB	2.28	0.63
8:H:168:SER:HB3	8:H:175:GLU:HB3	1.80	0.63
1:A:458:ILE:HB	1:A:459:PRO:HD3	1.81	0.63
4:D:367:ARG:C	4:D:369:ASN:H	2.01	0.63
6:F:203:SER:C	6:F:205:LYS:H	2.03	0.63
1:I:228:VAL:CG2	1:I:363:GLN:NE2	2.49	0.63
2:J:422:ILE:HG21	2:J:427:SER:HB3	1.79	0.63
6:F:414:GLY:O	6:F:415:ALA:HB3	1.98	0.63
6:N:108:PHE:CE2	6:N:118:ILE:HG13	2.34	0.63
4:L:528:ARG:NE	4:L:528:ARG:H	1.97	0.63
2:J:98:LEU:O	2:J:102:LEU:HB2	1.99	0.63
5:M:128:ALA:HB2	5:M:478:THR:HG21	1.80	0.63
5:M:383:GLN:O	5:M:391:ARG:CB	2.47	0.63
2:B:210:GLU:OE1	2:B:357:SER:O	2.17	0.62
2:J:246:PHE:CD1	2:J:246:PHE:C	2.73	0.62
7:G:237:ASN:C	7:G:239:PRO:HD3	2.18	0.62
7:G:304:THR:HA	7:G:307:PHE:HE2	1.63	0.62
1:A:115:LEU:HD13	1:A:125:ILE:HD11	1.81	0.62
4:L:292:ILE:HG13	4:L:293:LEU:HA	1.81	0.62
4:D:528:ARG:H	4:D:528:ARG:NE	1.97	0.62
7:O:79:ALA:O	7:O:82:THR:HG22	1.99	0.62
2:J:230:LYS:H	2:J:281:ILE:HG22	1.62	0.62
5:E:273:THR:HG22	5:E:363:VAL:O	1.99	0.62
3:K:35:ILE:HD11	3:K:65:LEU:HG	1.80	0.62
6:F:109:ILE:HG13	5:M:39:LYS:NZ	2.11	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:GLY:HA3	2:B:474:LEU:CD1	2.29	0.62
1:A:158:ASN:ND2	1:A:516:GLY:HA2	2.13	0.62
7:G:409:ILE:HG22	7:G:410:VAL:N	2.14	0.62
2:J:436:ALA:O	2:J:439:GLN:HB3	1.99	0.62
8:P:227:VAL:HG21	8:P:385:ILE:HD11	1.81	0.62
8:H:227:VAL:HG21	8:H:385:ILE:HD11	1.81	0.62
7:O:214:PHE:HD1	7:O:376:LEU:HB3	1.64	0.62
6:F:481:GLN:O	6:F:489:VAL:HG21	1.99	0.62
7:G:126:MET:HE3	7:G:515:ASN:HA	1.82	0.62
4:L:375:VAL:HG12	4:L:376:SER:H	1.64	0.62
5:E:174:GLU:O	5:E:175:LEU:CG	2.47	0.62
7:G:109:MET:SD	7:G:514:THR:HG22	2.39	0.62
2:J:38:GLY:HA3	2:J:474:LEU:CD1	2.29	0.62
4:D:292:ILE:HG13	4:D:293:LEU:HA	1.82	0.62
5:E:337:GLN:C	5:E:338:ASN:HD22	2.03	0.62
3:K:223:VAL:HG12	3:K:224:LEU:H	1.63	0.62
1:A:184:LEU:CD2	1:A:198:TYR:CG	2.69	0.62
2:B:246:PHE:C	2:B:246:PHE:CD1	2.73	0.62
7:G:226:TYR:CE1	7:G:229:PHE:C	2.73	0.62
5:E:401:THR:O	5:E:402:LYS:CB	2.46	0.62
4:L:210:ILE:O	4:L:375:VAL:HG13	1.98	0.62
6:N:173:ILE:HD11	6:N:209:PHE:HB3	1.82	0.62
8:P:24:ALA:O	8:P:28:ILE:HG13	1.99	0.62
4:D:185:ASN:H	4:D:186:SER:C	2.02	0.62
7:O:409:ILE:HG22	7:O:410:VAL:N	2.14	0.62
8:P:227:VAL:HG22	8:P:370:VAL:HG12	1.81	0.62
3:K:391:GLU:O	3:K:395:ASN:HB2	1.98	0.62
8:H:375:GLN:N	8:H:376:GLY:HA3	2.14	0.62
2:B:98:LEU:O	2:B:102:LEU:HB2	1.99	0.62
5:M:88:ALA:HB1	5:M:109:LYS:HZ1	1.64	0.62
5:M:483:LEU:HD11	9:M:601:ADP:O4'	1.99	0.62
1:I:224:LEU:HD13	1:I:226:CYS:HB2	1.81	0.62
2:J:236:THR:OG1	2:J:327:SER:HA	1.99	0.62
8:H:227:VAL:HG22	8:H:370:VAL:HG12	1.81	0.62
3:C:142:PRO:HB3	3:C:410:PRO:HB2	1.81	0.62
8:H:441:THR:O	8:H:446:GLN:HG2	2.00	0.62
6:F:540:THR:O	6:F:542:LYS:CG	2.44	0.62
1:I:184:LEU:CD2	1:I:198:TYR:CG	2.69	0.62
2:B:464:TYR:O	2:B:467:ILE:HD11	2.00	0.62
6:F:501:PRO:CB	6:F:506:ILE:HB	2.17	0.62
6:N:481:GLN:O	6:N:489:VAL:HG21	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:226:TYR:CE1	7:O:229:PHE:C	2.73	0.62
2:J:375:GLN:NE2	6:N:75:LEU:HD12	2.14	0.62
3:K:495:VAL:HG23	3:K:500:TRP:HH2	1.65	0.62
7:G:282:LEU:HD21	7:G:306:PHE:HB2	1.80	0.62
1:A:224:LEU:HD13	1:A:226:CYS:HB2	1.81	0.62
1:A:470:SER:H	3:K:115:ASN:CB	2.13	0.62
7:G:214:PHE:HD1	7:G:376:LEU:HB3	1.64	0.62
1:I:480:TYR:O	1:I:483:ALA:HB3	2.00	0.62
3:K:31:VAL:HG11	3:K:70:VAL:HG11	1.81	0.62
6:F:155:ARG:CB	6:F:171:THR:HG21	2.30	0.62
7:G:189:LEU:N	7:G:190:ASP:HB2	2.14	0.62
6:F:353:LEU:HB2	6:F:368:THR:OG1	2.00	0.62
6:N:92:THR:CG2	10:N:602:BEF:F3	2.37	0.62
4:D:375:VAL:HG12	4:D:376:SER:H	1.64	0.62
7:G:413:GLY:HA3	7:G:491:ASN:ND2	2.15	0.62
3:K:223:VAL:HG11	3:K:328:ILE:CG1	2.29	0.62
2:B:436:ALA:O	2:B:439:GLN:HB3	2.00	0.62
1:I:458:ILE:HB	1:I:459:PRO:HD3	1.81	0.62
5:E:133:ALA:O	5:E:137:ILE:HG13	1.99	0.62
5:E:210:ASN:H	5:E:210:ASN:HD22	1.48	0.62
5:M:273:THR:HG22	5:M:363:VAL:O	1.99	0.62
3:K:264:GLU:C	3:K:265:LYS:CG	2.62	0.62
2:B:492:LYS:H	2:B:492:LYS:NZ	1.97	0.62
2:J:8:ASP:CB	2:J:9:GLN:HA	2.22	0.62
7:O:43:THR:HG22	7:O:64:ASN:CB	2.27	0.62
8:H:131:TYR:CD2	8:H:452:PHE:HD2	2.17	0.62
3:C:223:VAL:HG11	3:C:328:ILE:CG1	2.29	0.62
1:A:122:PRO:HG3	5:E:70:LEU:HD11	1.82	0.62
3:C:62:HIS:O	3:C:66:ARG:HG3	2.00	0.62
5:E:383:GLN:O	5:E:391:ARG:CB	2.47	0.62
3:C:462:GLY:O	3:C:464:PRO:HD3	1.99	0.62
5:E:348:GLY:O	5:E:351:LEU:HD11	2.00	0.62
1:I:233:MET:HG2	1:I:311:VAL:HG22	1.82	0.62
5:M:50:HIS:HB3	5:M:100:ILE:HG21	1.82	0.62
3:K:142:PRO:HB3	3:K:410:PRO:HB2	1.81	0.62
4:D:521:ILE:HG23	7:G:51:ILE:CA	2.29	0.61
8:H:335:VAL:HG22	8:H:379:SER:HB2	1.82	0.61
8:P:109:GLU:O	8:P:113:VAL:HG23	2.00	0.61
8:H:24:ALA:O	8:H:28:ILE:HG13	1.99	0.61
3:C:495:VAL:HG23	3:C:500:TRP:HH2	1.65	0.61
7:G:307:PHE:HD1	7:G:312:ILE:HG23	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:39:LYS:NZ	6:N:109:ILE:HG13	2.14	0.61
1:I:266:ASP:N	1:I:267:PRO:HD2	2.15	0.61
5:M:133:ALA:O	5:M:137:ILE:HG13	1.99	0.61
6:N:229:LYS:HA	6:N:353:LEU:HD23	1.82	0.61
6:F:515:ASN:HD22	6:F:516:ALA:N	1.99	0.61
5:E:183:ALA:O	5:E:187:SER:HB2	2.00	0.61
5:M:348:GLY:O	5:M:351:LEU:HD11	2.00	0.61
3:C:50:ASP:HB2	3:C:51:PRO:HD2	1.82	0.61
5:E:104:LEU:CD2	5:E:123:VAL:HG13	2.27	0.61
1:I:187:VAL:HG21	1:I:383:SER:HB3	1.83	0.61
1:A:118:ASN:O	1:A:119:LYS:HG2	2.00	0.61
8:P:441:THR:O	8:P:446:GLN:HG2	1.99	0.61
6:F:133:LEU:HD12	6:F:422:LEU:CD2	2.24	0.61
6:N:353:LEU:HB2	6:N:368:THR:OG1	2.00	0.61
7:G:79:ALA:O	7:G:82:THR:HG22	1.99	0.61
1:A:228:VAL:CG2	1:A:363:GLN:NE2	2.49	0.61
1:I:90:GLN:OE1	1:I:96:ASP:O	2.17	0.61
2:B:263:LYS:HZ3	3:C:266:GLU:HB3	1.62	0.61
3:K:50:ASP:HB2	3:K:51:PRO:HD2	1.82	0.61
5:M:174:GLU:O	5:M:175:LEU:CG	2.47	0.61
7:G:165:ALA:HB2	7:G:399:ILE:HG21	1.82	0.61
7:O:239:PRO:HD2	7:O:349:CYS:O	2.01	0.61
7:O:413:GLY:HA3	7:O:491:ASN:ND2	2.15	0.61
1:I:118:ASN:O	1:I:119:LYS:HG2	2.00	0.61
2:J:509:LEU:O	2:J:509:LEU:HD23	2.00	0.61
3:C:31:VAL:HG11	3:C:70:VAL:HG11	1.81	0.61
6:N:203:SER:C	6:N:205:LYS:H	2.03	0.61
7:O:191:ARG:CZ	7:O:192:ASN:N	2.61	0.61
5:E:433:LEU:HD11	5:E:439:VAL:HG13	1.82	0.61
6:F:108:PHE:CE2	6:F:118:ILE:HG13	2.34	0.61
5:M:337:GLN:C	5:M:338:ASN:HD22	2.03	0.61
7:G:37:GLN:HE21	7:G:38:GLU:N	1.98	0.61
1:A:233:MET:HG2	1:A:311:VAL:HG22	1.82	0.61
3:K:512:THR:HG23	8:P:389:ALA:HB1	1.82	0.61
8:P:375:GLN:N	8:P:376:GLY:HA3	2.14	0.61
6:N:36:ASN:HB3	6:N:57:LYS:HZ3	0.81	0.61
6:F:433:LYS:HB3	6:F:441:LYS:HA	1.80	0.61
2:B:437:LEU:O	2:B:441:PRO:HD2	2.01	0.61
5:E:273:THR:HG22	5:E:364:PRO:CA	2.20	0.61
6:N:454:ILE:N	6:N:455:PRO:CD	2.64	0.61
7:G:239:PRO:HD2	7:G:349:CYS:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:524:ILE:CG2	7:G:52:LEU:O	2.47	0.61
3:K:462:GLY:O	3:K:464:PRO:HD3	1.99	0.61
6:N:178:VAL:O	6:N:182:TYR:N	2.34	0.61
8:H:109:GLU:O	8:H:113:VAL:HG23	2.00	0.61
3:C:41:PRO:HA	3:C:161:THR:HG21	1.82	0.61
6:F:454:ILE:N	6:F:455:PRO:CD	2.64	0.61
3:K:149:ALA:HA	3:K:152:LYS:HG3	1.83	0.61
1:A:540:ARG:O	5:E:70:LEU:HB3	2.00	0.61
2:J:203:LEU:O	2:J:204:SER:CB	2.49	0.61
8:P:335:VAL:HG22	8:P:379:SER:HB2	1.82	0.61
6:F:7:ASN:OD1	6:F:8:PRO:HD2	1.99	0.61
5:M:183:ALA:O	5:M:187:SER:HB2	2.00	0.61
3:C:149:ALA:HA	3:C:152:LYS:HG3	1.83	0.61
7:O:307:PHE:HD1	7:O:312:ILE:HG23	1.64	0.61
8:P:131:TYR:CD2	8:P:452:PHE:HD2	2.17	0.61
1:A:218:LEU:HD13	1:A:219:VAL:N	2.16	0.61
1:I:70:LEU:HD23	1:I:73:LEU:HD22	1.83	0.61
1:I:348:GLU:N	1:I:349:THR:HB	2.16	0.61
6:F:437:LYS:HE2	6:F:437:LYS:HA	1.83	0.61
7:G:43:THR:HG22	7:G:64:ASN:CB	2.27	0.61
6:F:178:VAL:O	6:F:182:TYR:N	2.34	0.61
6:F:173:ILE:HD11	6:F:209:PHE:HB3	1.82	0.61
4:D:499:GLN:HE22	9:D:601:ADP:C2'	2.13	0.61
1:I:218:LEU:HD13	1:I:219:VAL:N	2.16	0.61
1:A:266:ASP:N	1:A:267:PRO:HD2	2.15	0.61
1:A:348:GLU:N	1:A:349:THR:HB	2.16	0.61
3:K:96:VAL:HG13	3:K:513:ALA:HB2	1.83	0.61
1:I:258:MET:HA	1:I:258:MET:HE3	1.82	0.61
2:J:3:VAL:C	2:J:5:ILE:HG23	2.21	0.61
6:N:437:LYS:HA	6:N:437:LYS:HE2	1.83	0.61
6:F:98:VAL:HG22	6:F:520:ALA:HA	1.83	0.61
6:N:7:ASN:OD1	6:N:8:PRO:CD	2.49	0.61
6:N:7:ASN:OD1	6:N:8:PRO:HD2	1.99	0.61
2:B:72:PRO:CB	3:C:47:MET:CE	2.79	0.61
3:C:299:LYS:HA	3:C:319:ARG:CB	2.31	0.61
6:F:108:PHE:CE2	6:F:118:ILE:HG21	2.36	0.61
4:D:485:ARG:NH2	9:D:601:ADP:HN62	1.99	0.61
3:K:62:HIS:O	3:K:66:ARG:HG3	2.00	0.61
2:J:464:TYR:O	2:J:467:ILE:HD11	2.00	0.61
7:G:94:VAL:HG13	7:G:95:GLY:N	2.16	0.61
3:K:54:GLY:O	3:K:56:VAL:HG23	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:35:THR:CG2	6:N:42:THR:H	2.14	0.61
1:A:73:LEU:O	1:A:74:ASP:HB3	2.01	0.61
2:B:3:VAL:C	2:B:5:ILE:HG23	2.21	0.60
1:I:184:LEU:HD21	1:I:198:TYR:CB	2.28	0.60
6:F:478:ASP:C	6:F:482:ASP:HB2	2.21	0.60
8:H:138:THR:HG22	8:H:434:ILE:HD12	1.83	0.60
6:N:458:LEU:HD12	6:N:458:LEU:O	2.01	0.60
3:C:142:PRO:HG3	3:C:411:SER:HA	1.83	0.60
1:A:480:TYR:O	1:A:483:ALA:HB3	2.00	0.60
2:B:509:LEU:HD23	2:B:509:LEU:O	2.00	0.60
2:B:424:GLY:O	2:B:427:SER:CB	2.49	0.60
2:J:30:GLY:C	2:J:33:VAL:HG23	2.22	0.60
2:J:424:GLY:O	2:J:427:SER:CB	2.49	0.60
6:N:465:ASP:CA	6:N:466:PRO:C	2.68	0.60
2:B:232:LEU:HD22	2:B:233:ILE:N	2.16	0.60
2:J:295:GLU:OE1	6:N:339:SER:HB3	2.01	0.60
1:I:233:MET:HE2	1:I:315:ILE:O	2.01	0.60
3:K:142:PRO:HG3	3:K:411:SER:HA	1.83	0.60
8:P:269:ASN:H	8:P:272:GLU:HG3	1.66	0.60
6:F:198:GLN:HE21	6:F:198:GLN:N	1.99	0.60
6:N:133:LEU:HD12	6:N:422:LEU:CD2	2.24	0.60
6:N:515:ASN:HD22	6:N:516:ALA:N	1.99	0.60
6:F:478:ASP:O	6:F:482:ASP:CA	2.49	0.60
2:B:422:ILE:HG21	2:B:427:SER:HB3	1.79	0.60
2:B:397:GLU:OE1	2:B:399:ARG:HG3	2.01	0.60
2:B:459:LEU:HD22	2:B:472:LEU:CG	2.26	0.60
2:B:27:ILE:CD1	2:B:104:ARG:HH11	2.09	0.60
6:F:35:THR:CG2	6:F:42:THR:H	2.14	0.60
7:G:420:VAL:O	7:G:424:LEU:HG	2.01	0.60
5:M:100:ILE:HA	5:M:103:LEU:HD12	1.83	0.60
6:F:264:ALA:O	6:F:268:LYS:HG2	2.02	0.60
6:F:229:LYS:HA	6:F:353:LEU:HD23	1.82	0.60
2:J:357:SER:CB	2:J:360:LYS:CB	2.69	0.60
5:M:433:LEU:HD11	5:M:439:VAL:HG13	1.82	0.60
2:J:38:GLY:HA3	2:J:474:LEU:HD11	1.83	0.60
1:I:73:LEU:O	1:I:74:ASP:HB3	2.00	0.60
6:F:458:LEU:HD12	6:F:458:LEU:O	2.01	0.60
5:E:50:HIS:HB3	5:E:100:ILE:HG21	1.82	0.60
3:C:512:THR:HG23	8:H:389:ALA:HB1	1.83	0.60
6:F:151:LEU:O	6:F:171:THR:CG2	2.50	0.60
7:O:94:VAL:HG13	7:O:95:GLY:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:299:LYS:HA	3:K:319:ARG:CB	2.31	0.60
3:K:15:THR:O	3:K:16:THR:C	2.39	0.60
6:N:108:PHE:CE2	6:N:118:ILE:HG21	2.36	0.60
4:L:284:ASN:O	4:L:310:ILE:HG23	2.01	0.60
4:D:284:ASN:O	4:D:310:ILE:HG23	2.01	0.60
3:K:9:ASN:ND2	3:K:10:ALA:N	2.50	0.60
7:O:174:ASN:OD1	7:O:174:ASN:N	2.33	0.60
2:B:384:LEU:O	2:B:387:ALA:HB3	2.01	0.60
7:O:516:LEU:CD2	7:O:516:LEU:O	2.46	0.60
6:N:98:VAL:HG22	6:N:520:ALA:HA	1.83	0.60
6:F:7:ASN:OD1	6:F:8:PRO:CD	2.49	0.60
1:A:90:GLN:OE1	1:A:96:ASP:O	2.17	0.60
6:N:160:THR:H	6:N:164:ALA:HB3	1.67	0.60
6:N:61:VAL:HG12	6:N:62:LEU:HD23	1.84	0.60
7:G:293:VAL:HG13	7:G:312:ILE:HD11	1.84	0.60
1:I:113:ASN:HA	1:I:116:VAL:HG22	1.83	0.60
1:I:65:ASP:O	1:I:69:ILE:HB	2.01	0.60
8:P:182:VAL:O	8:P:186:VAL:HG23	2.02	0.60
3:K:223:VAL:HG11	3:K:328:ILE:HG13	1.83	0.60
3:C:9:ASN:ND2	3:C:10:ALA:N	2.50	0.60
6:N:430:ASN:HA	6:N:433:LYS:CB	2.32	0.60
6:N:233:VAL:HG12	6:N:294:VAL:HG22	1.84	0.60
2:B:326:VAL:HG13	3:C:304:LEU:HD22	1.83	0.60
2:B:200:GLY:O	2:B:371:GLY:N	2.28	0.60
3:C:266:GLU:CD	3:C:266:GLU:H	2.05	0.60
2:B:487:ILE:HD12	9:B:601:ADP:N6	2.17	0.60
8:H:182:VAL:O	8:H:186:VAL:HG23	2.02	0.60
6:N:198:GLN:N	6:N:198:GLN:HE21	1.99	0.60
2:J:397:GLU:OE1	2:J:399:ARG:HG3	2.02	0.60
6:N:155:ARG:CB	6:N:171:THR:HG21	2.30	0.60
6:F:125:ALA:HB2	6:F:444:ILE:HG23	1.82	0.60
6:F:233:VAL:HG12	6:F:294:VAL:HG22	1.84	0.60
2:J:437:LEU:O	2:J:441:PRO:HD2	2.00	0.60
4:L:524:ILE:CG2	7:O:52:LEU:O	2.50	0.60
6:F:485:GLU:HB2	6:F:488:TYR:O	2.01	0.60
7:O:37:GLN:HE21	7:O:38:GLU:N	1.98	0.60
7:G:109:MET:CG	7:G:514:THR:CG2	2.79	0.60
1:A:187:VAL:HG21	1:A:383:SER:HB3	1.83	0.60
3:C:96:VAL:HG13	3:C:513:ALA:HB2	1.83	0.60
6:N:264:ALA:O	6:N:268:LYS:HG2	2.02	0.60
5:M:210:ASN:H	5:M:210:ASN:HD22	1.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:389:ALA:O	6:N:393:ASP:OD2	2.20	0.60
7:G:208:ALA:HB3	7:G:211:GLU:HG3	1.84	0.60
2:J:384:LEU:O	2:J:387:ALA:HB3	2.01	0.60
6:N:151:LEU:CG	6:N:175:THR:HG23	2.32	0.60
6:N:38:GLY:H	9:N:601:ADP:H5'1	1.66	0.60
3:C:229:VAL:HG12	3:C:230:VAL:N	2.17	0.60
3:K:457:ILE:CD1	3:K:467:LEU:HD22	2.31	0.60
3:C:42:LYS:CB	3:C:460:ALA:CA	2.75	0.60
2:B:27:ILE:HD12	2:B:104:ARG:HD2	1.84	0.60
6:F:170:LEU:HA	6:F:173:ILE:HG22	1.84	0.60
8:P:459:VAL:O	8:P:463:LEU:HD23	2.02	0.60
6:F:61:VAL:HG12	6:F:62:LEU:HD23	1.84	0.60
1:A:183:ALA:HB1	1:A:383:SER:OG	2.02	0.60
8:P:162:MET:O	8:P:165:PRO:HD2	2.02	0.60
2:B:203:LEU:O	2:B:204:SER:CB	2.49	0.60
5:M:273:THR:HG21	5:M:364:PRO:HA	1.78	0.60
2:B:30:GLY:C	2:B:33:VAL:HG23	2.22	0.60
7:G:191:ARG:HD3	7:G:192:ASN:N	2.16	0.60
3:C:54:GLY:O	3:C:56:VAL:HG23	2.01	0.60
4:L:210:ILE:O	4:L:375:VAL:HG12	2.02	0.60
7:O:165:ALA:HB2	7:O:399:ILE:HG21	1.82	0.60
1:I:183:ALA:HB1	1:I:383:SER:OG	2.02	0.60
4:D:38:SER:HB3	4:D:46:LYS:HZ3	1.65	0.60
8:P:153:LYS:H	8:P:153:LYS:CD	2.15	0.60
6:F:389:ALA:O	6:F:393:ASP:OD2	2.20	0.60
5:E:323:CYS:O	5:E:344:ARG:HA	2.02	0.60
6:F:430:ASN:C	6:F:433:LYS:H	2.05	0.59
6:F:352:GLY:O	6:F:353:LEU:O	2.20	0.59
3:K:229:VAL:HG12	3:K:230:VAL:N	2.17	0.59
3:C:258:GLN:O	8:H:264:THR:HB	2.02	0.59
3:C:15:THR:O	3:C:16:THR:C	2.39	0.59
1:A:333:THR:HB	1:A:357:LEU:H	1.67	0.59
8:H:162:MET:O	8:H:165:PRO:HD2	2.02	0.59
8:P:362:GLU:HG2	8:P:367:ARG:HA	1.82	0.59
4:D:71:LEU:HA	8:P:6:PRO:CG	2.31	0.59
6:N:478:ASP:C	6:N:482:ASP:HB2	2.20	0.59
3:C:457:ILE:CD1	3:C:467:LEU:HD22	2.31	0.59
6:F:415:ALA:CB	6:F:506:ILE:HG21	2.30	0.59
6:N:485:GLU:HB2	6:N:488:TYR:O	2.01	0.59
7:O:293:VAL:HG13	7:O:312:ILE:HD11	1.83	0.59
1:I:333:THR:HB	1:I:357:LEU:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:50:ASP:CG	1:I:64:ASN:HB2	2.23	0.59
5:M:281:PRO:HD2	5:M:285:HIS:HB3	1.84	0.59
6:N:167:THR:HB	6:N:169:VAL:H	1.66	0.59
6:N:151:LEU:O	6:N:171:THR:CG2	2.50	0.59
7:O:189:LEU:CD1	7:O:189:LEU:O	2.50	0.59
1:I:97:GLY:O	1:I:101:VAL:HG23	2.02	0.59
5:M:351:LEU:HD13	5:M:351:LEU:H	1.67	0.59
3:K:42:LYS:CB	3:K:460:ALA:CA	2.75	0.59
6:F:92:THR:HG21	10:F:602:BEF:F3	1.92	0.59
8:P:138:THR:HG22	8:P:434:ILE:HD12	1.83	0.59
5:M:74:LEU:CD1	5:M:93:GLN:HB3	2.33	0.59
5:E:39:LYS:HZ3	6:N:109:ILE:CG1	2.15	0.59
1:A:65:ASP:O	1:A:69:ILE:HB	2.01	0.59
6:F:201:HIS:HB3	6:F:381:LYS:CE	2.32	0.59
8:H:153:LYS:H	8:H:153:LYS:CD	2.15	0.59
8:H:177:ILE:O	8:H:180:GLU:HB2	2.03	0.59
2:B:213:ILE:HD12	2:B:213:ILE:H	1.67	0.59
7:G:174:ASN:OD1	7:G:174:ASN:N	2.34	0.59
7:O:401:LYS:HG3	7:O:402:ARG:N	2.17	0.59
6:F:430:ASN:HA	6:F:433:LYS:CB	2.32	0.59
6:N:478:ASP:O	6:N:482:ASP:CA	2.49	0.59
1:A:97:GLY:O	1:A:101:VAL:HG23	2.02	0.59
3:C:57:LEU:CD2	3:C:57:LEU:N	2.57	0.59
4:L:44:MET:HG3	8:P:531:ALA:HB3	1.83	0.59
4:L:185:ASN:H	4:L:186:SER:C	2.02	0.59
7:O:109:MET:CG	7:O:514:THR:CG2	2.79	0.59
5:M:368:ASP:O	5:M:369:LEU:C	2.41	0.59
4:D:81:VAL:HG22	7:G:382:ALA:HB2	1.84	0.59
1:A:113:ASN:HA	1:A:116:VAL:HG22	1.83	0.59
5:M:55:ARG:HH21	5:M:134:LEU:HD13	1.67	0.59
4:D:238:GLN:HB2	4:D:290:LYS:HE3	1.84	0.59
8:P:177:ILE:O	8:P:180:GLU:HB2	2.03	0.59
8:P:146:VAL:HG13	8:P:147:VAL:H	1.68	0.59
3:C:275:ILE:HA	8:H:274:LEU:HD21	1.84	0.59
6:F:485:GLU:HG3	6:F:489:VAL:HB	1.85	0.59
1:I:159:ILE:HD11	1:I:418:VAL:HG11	1.84	0.59
1:I:418:VAL:HG12	1:I:419:VAL:N	2.17	0.59
4:L:254:VAL:O	4:L:254:VAL:HG23	2.01	0.59
8:H:459:VAL:O	8:H:463:LEU:HD23	2.02	0.59
3:K:41:PRO:HA	3:K:161:THR:HG21	1.82	0.59
1:A:70:LEU:HD23	1:A:73:LEU:HD22	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:201:HIS:HB3	6:F:381:LYS:HZ3	1.66	0.59
3:C:223:VAL:HG11	3:C:328:ILE:HG13	1.83	0.59
8:H:362:GLU:HG2	8:H:367:ARG:HA	1.82	0.59
4:L:12:LYS:HD3	4:L:526:PHE:O	2.01	0.59
6:N:125:ALA:HB2	6:N:444:ILE:HG23	1.82	0.59
5:E:368:ASP:O	5:E:369:LEU:C	2.41	0.59
8:P:322:LYS:O	8:P:324:PRO:HD3	2.02	0.59
4:D:12:LYS:HD3	4:D:526:PHE:O	2.01	0.59
5:E:241:ASN:ND2	5:E:241:ASN:O	2.34	0.59
5:M:32:VAL:HG22	5:M:33:LYS:N	2.13	0.59
1:A:50:ASP:CG	1:A:64:ASN:HB2	2.23	0.59
5:E:351:LEU:HD13	5:E:351:LEU:H	1.67	0.59
3:K:266:GLU:H	3:K:266:GLU:CD	2.05	0.59
2:J:27:ILE:HD12	2:J:104:ARG:HD2	1.83	0.59
4:L:336:ILE:HG23	4:L:339:PHE:HB3	1.85	0.59
4:D:336:ILE:HG23	4:D:339:PHE:HB3	1.85	0.59
1:I:73:LEU:O	1:I:74:ASP:CB	2.50	0.59
1:A:73:LEU:O	1:A:74:ASP:CB	2.50	0.59
8:H:269:ASN:H	8:H:272:GLU:HG3	1.66	0.59
3:K:414:PRO:O	3:K:418:ALA:HB3	2.03	0.59
4:D:379:ILE:H	4:D:379:ILE:HD12	1.68	0.59
8:H:322:LYS:O	8:H:324:PRO:HD3	2.02	0.59
6:N:540:THR:O	6:N:541:LEU:HD23	2.03	0.59
4:D:521:ILE:CG2	7:G:52:LEU:H	2.15	0.59
7:O:191:ARG:HD3	7:O:192:ASN:N	2.16	0.59
2:B:326:VAL:HG22	3:C:304:LEU:HD22	1.85	0.59
7:G:238:ASN:N	7:G:239:PRO:CD	2.66	0.59
1:A:164:MET:O	1:A:167:LYS:CB	2.51	0.59
5:E:74:LEU:CD1	5:E:93:GLN:HB3	2.32	0.59
6:N:201:HIS:HB3	6:N:381:LYS:CE	2.33	0.59
2:J:32:LEU:CD1	6:N:532:GLU:OE2	2.51	0.59
8:H:94:ILE:HD12	8:H:95:ASP:N	2.18	0.59
6:N:352:GLY:O	6:N:353:LEU:O	2.20	0.59
6:F:109:ILE:O	5:M:39:LYS:HE2	2.02	0.59
4:D:330:CYS:N	4:D:345:ASP:OD2	2.36	0.59
4:D:103:LEU:HD13	4:D:515:VAL:HG21	1.85	0.59
2:J:232:LEU:HD22	2:J:233:ILE:N	2.17	0.59
5:E:335:LEU:HD22	5:E:340:LEU:HD11	1.84	0.59
5:E:240:ILE:HG12	5:E:244:ILE:CG2	2.32	0.59
3:C:414:PRO:O	3:C:418:ALA:HB3	2.03	0.59
6:F:433:LYS:HG3	6:F:444:ILE:CG1	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:43:LEU:CD2	6:F:57:LYS:CB	2.78	0.59
3:C:264:GLU:C	3:C:265:LYS:CG	2.62	0.59
5:M:544:LEU:HD23	6:N:384:THR:HG21	1.85	0.59
6:N:201:HIS:HB3	6:N:381:LYS:HE2	1.85	0.59
3:C:112:ILE:C	3:C:114:LYS:H	2.06	0.59
3:C:508:GLN:HG2	8:H:215:GLY:HA2	1.85	0.59
8:H:288:MET:CE	8:H:313:LEU:HG	2.33	0.59
7:O:484:GLU:CB	7:O:485:THR:HA	2.32	0.59
8:H:217:LEU:HA	8:H:387:ARG:O	2.03	0.59
5:E:373:LYS:HE2	6:F:311:LYS:NZ	2.18	0.59
5:E:281:PRO:HD2	5:E:285:HIS:HB3	1.84	0.59
6:F:57:LYS:HG2	6:F:57:LYS:O	2.03	0.58
3:C:265:LYS:O	3:C:268:ASP:OD1	2.21	0.58
5:M:350:GLU:C	5:M:352:GLU:N	2.55	0.58
6:F:160:THR:H	6:F:164:ALA:HB3	1.67	0.58
5:E:55:ARG:HH21	5:E:134:LEU:HD13	1.67	0.58
5:E:100:ILE:HA	5:E:103:LEU:HD12	1.83	0.58
3:C:151:MET:O	3:C:155:ILE:HG12	2.04	0.58
4:L:128:ALA:O	4:L:132:VAL:HG23	2.03	0.58
4:L:334:ALA:HB3	7:O:305:GLN:HB2	1.84	0.58
6:N:433:LYS:HG3	6:N:444:ILE:CG1	2.33	0.58
7:G:189:LEU:O	7:G:189:LEU:CD1	2.50	0.58
2:J:463:ILE:HG13	2:J:468:SER:HA	1.85	0.58
6:N:485:GLU:HG3	6:N:489:VAL:HB	1.85	0.58
5:E:544:LEU:HD23	6:F:384:THR:CG2	2.33	0.58
6:F:33:LEU:HD21	6:F:63:LEU:HD21	1.85	0.58
7:O:455:GLU:CG	7:O:461:ALA:CB	2.81	0.58
8:P:94:ILE:HD12	8:P:95:ASP:N	2.18	0.58
1:A:17:GLY:HA3	5:E:95:GLU:OE2	2.03	0.58
3:K:151:MET:O	3:K:155:ILE:HG12	2.04	0.58
6:N:424:ARG:NE	6:N:424:ARG:HA	2.12	0.58
6:F:280:LEU:HD13	6:F:343:LEU:HD21	1.85	0.58
7:O:125:ILE:HG22	7:O:129:TYR:CE2	2.38	0.58
3:K:112:ILE:C	3:K:114:LYS:H	2.06	0.58
6:N:201:HIS:CB	6:N:381:LYS:HE2	2.34	0.58
1:I:55:ASP:HB2	1:I:59:ASP:HB2	1.85	0.58
2:J:213:ILE:H	2:J:213:ILE:HD12	1.67	0.58
5:M:240:ILE:HG12	5:M:244:ILE:CG2	2.32	0.58
2:B:357:SER:CB	2:B:360:LYS:CB	2.69	0.58
2:B:422:ILE:CB	2:B:427:SER:CB	2.79	0.58
6:F:465:ASP:CA	6:F:466:PRO:C	2.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:253:GLN:H	5:E:254:MET:CB	2.16	0.58
4:D:147:ARG:HG2	4:D:148:GLU:N	2.18	0.58
4:L:298:ASN:HB3	4:L:299:ASP:HA	1.84	0.58
3:K:452:ILE:HB	3:K:453:PRO:HD3	1.85	0.58
1:I:164:MET:O	1:I:167:LYS:CB	2.51	0.58
4:D:110:LEU:HD13	4:D:439:ILE:HD12	1.85	0.58
8:P:217:LEU:HA	8:P:387:ARG:O	2.03	0.58
8:H:48:PRO:HA	8:H:169:SER:O	2.04	0.58
8:P:222:VAL:HG22	8:P:384:ILE:HG23	1.86	0.58
6:N:155:ARG:CB	6:N:171:THR:OG1	2.52	0.58
4:D:254:VAL:O	4:D:254:VAL:HG23	2.02	0.58
6:F:109:ILE:CG1	5:M:39:LYS:HZ3	2.13	0.58
5:M:335:LEU:HD22	5:M:340:LEU:HD11	1.84	0.58
2:J:373:THR:CG2	2:J:375:GLN:HG2	2.34	0.58
3:C:452:ILE:HB	3:C:453:PRO:HD3	1.85	0.58
1:A:333:THR:HG22	1:A:377:THR:HG22	1.86	0.58
4:L:238:GLN:HB2	4:L:290:LYS:HE3	1.84	0.58
7:G:218:VAL:HA	7:G:375:THR:HG21	1.86	0.58
8:H:69:ALA:HB2	8:H:100:THR:HB	1.85	0.58
6:N:57:LYS:O	6:N:57:LYS:HG2	2.03	0.58
2:B:407:ALA:O	2:B:410:VAL:HG12	2.03	0.58
2:B:463:ILE:O	2:B:467:ILE:CB	2.52	0.58
4:D:521:ILE:HG12	7:G:62:ILE:HD11	1.86	0.58
1:A:159:ILE:HD11	1:A:418:VAL:HG11	1.84	0.58
3:C:296:ILE:HG23	3:C:320:VAL:HG21	1.85	0.58
8:H:427:GLU:HG2	8:H:459:VAL:HG21	1.85	0.58
2:B:38:GLY:HA3	2:B:474:LEU:HD11	1.84	0.58
4:D:182:SER:HB2	4:D:187:LYS:HE2	1.85	0.58
2:B:373:THR:CG2	2:B:375:GLN:HG2	2.34	0.58
6:F:32:VAL:HB	6:F:33:LEU:HD22	1.86	0.58
7:G:125:ILE:HG22	7:G:129:TYR:CE2	2.38	0.58
6:F:201:HIS:CB	6:F:381:LYS:HE2	2.34	0.58
6:F:201:HIS:HB3	6:F:381:LYS:HE2	1.85	0.58
2:J:32:LEU:HG	6:N:532:GLU:OE1	2.04	0.58
4:D:128:ALA:O	4:D:132:VAL:HG23	2.03	0.58
1:A:247:LEU:O	1:A:298:THR:HA	2.04	0.58
5:M:323:CYS:O	5:M:344:ARG:HA	2.02	0.58
6:N:175:THR:O	6:N:179:LEU:HG	2.04	0.58
6:F:541:LEU:HB2	6:F:542:LYS:CB	2.32	0.58
6:F:125:ALA:HA	6:F:426:LEU:HD21	1.85	0.58
4:D:104:LEU:HD11	4:D:518:ILE:HD12	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:200:GLY:O	2:J:371:GLY:N	2.28	0.58
5:M:253:GLN:H	5:M:254:MET:CB	2.16	0.58
4:D:210:ILE:O	4:D:375:VAL:HG12	2.02	0.58
2:B:159:THR:HG21	2:B:488:VAL:H	1.69	0.58
2:B:285:ILE:HD13	2:B:285:ILE:N	2.19	0.58
6:N:33:LEU:HD21	6:N:63:LEU:HD21	1.85	0.58
6:N:56:THR:HG22	6:N:390:GLN:HB2	1.86	0.58
4:D:171:ALA:HB3	4:D:172:PRO:HD3	1.86	0.58
1:A:463:ALA:HB1	1:A:470:SER:HB2	1.86	0.58
6:N:343:LEU:HG	6:N:344:SER:HB3	1.85	0.58
7:O:376:LEU:HD23	7:O:376:LEU:H	1.69	0.58
7:G:376:LEU:HD23	7:G:376:LEU:H	1.69	0.58
7:O:126:MET:HE3	7:O:515:ASN:HA	1.86	0.58
5:M:448:VAL:HG21	5:M:498:LEU:HD13	1.86	0.58
6:F:401:ALA:O	6:F:405:VAL:HG23	2.04	0.58
7:O:208:ALA:HB3	7:O:211:GLU:HG3	1.84	0.58
6:F:151:LEU:O	6:F:171:THR:HG22	2.04	0.58
6:F:155:ARG:CB	6:F:171:THR:OG1	2.52	0.58
6:N:433:LYS:C	6:N:441:LYS:CB	2.72	0.58
6:F:433:LYS:C	6:F:441:LYS:CB	2.72	0.58
8:H:68:ALA:H	8:H:101:ASN:HD21	1.49	0.58
3:C:514:ILE:HA	3:C:517:ALA:HB3	1.86	0.58
4:D:258:ARG:HD2	8:H:283:GLN:NE2	2.19	0.58
7:G:401:LYS:HG3	7:G:402:ARG:N	2.17	0.58
1:I:247:LEU:O	1:I:298:THR:HA	2.04	0.58
8:P:288:MET:CE	8:P:313:LEU:HG	2.32	0.58
6:N:125:ALA:HA	6:N:426:LEU:HD21	1.86	0.58
6:F:540:THR:O	6:F:541:LEU:HD23	2.03	0.58
6:N:415:ALA:CB	6:N:506:ILE:HG21	2.30	0.58
4:L:16:LYS:O	4:L:20:VAL:HG23	2.04	0.58
5:E:273:THR:HG21	5:E:364:PRO:HA	1.78	0.58
1:I:93:GLU:CA	1:I:94:ILE:HD12	2.34	0.58
3:K:296:ILE:HG23	3:K:320:VAL:HG21	1.85	0.58
6:N:447:PHE:CE2	6:N:451:LEU:HD11	2.39	0.58
1:A:209:HIS:HE1	7:G:89:ALA:HB2	1.69	0.58
6:F:343:LEU:HG	6:F:344:SER:HB3	1.85	0.58
1:I:333:THR:HG22	1:I:377:THR:HG22	1.86	0.58
4:D:215:LEU:HB3	4:D:217:GLN:HG2	1.86	0.58
4:D:89:ALA:HB1	4:D:503:VAL:HG22	1.85	0.58
7:O:218:VAL:HA	7:O:375:THR:HG21	1.86	0.58
4:L:521:ILE:HG23	7:O:51:ILE:CA	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:88:VAL:HA	2:B:393:GLN:NE2	2.19	0.58
6:N:411:ILE:CG2	6:N:412:ILE:H	2.16	0.58
4:L:182:SER:HB2	4:L:187:LYS:HE2	1.85	0.58
6:N:32:VAL:HB	6:N:33:LEU:HD22	1.86	0.58
8:P:138:THR:HG22	8:P:434:ILE:CD1	2.34	0.58
8:H:138:THR:HG22	8:H:434:ILE:CD1	2.34	0.58
3:C:255:GLY:N	3:C:259:THR:HG21	2.18	0.58
4:L:65:LEU:HD13	4:L:79:VAL:HG13	1.85	0.58
1:A:55:ASP:HB2	1:A:59:ASP:HB2	1.85	0.58
7:G:484:GLU:CB	7:G:485:THR:HA	2.32	0.58
8:H:222:VAL:HG22	8:H:384:ILE:HG23	1.86	0.58
6:N:401:ALA:O	6:N:405:VAL:HG23	2.04	0.58
4:D:291:SER:HA	4:D:315:ASP:HA	1.86	0.58
8:P:69:ALA:HB2	8:P:100:THR:HB	1.85	0.58
8:P:213:MET:HE2	8:P:391:GLN:HG3	1.84	0.58
6:F:203:SER:C	6:F:205:LYS:N	2.58	0.57
2:J:407:ALA:O	2:J:410:VAL:HG12	2.03	0.57
1:A:93:GLU:CA	1:A:94:ILE:HD12	2.34	0.57
3:K:265:LYS:O	3:K:268:ASP:OD1	2.21	0.57
3:C:320:VAL:O	3:C:321:LYS:C	2.41	0.57
8:P:48:PRO:HA	8:P:169:SER:O	2.04	0.57
6:N:451:LEU:HD12	6:N:451:LEU:H	1.69	0.57
2:J:285:ILE:HD13	2:J:285:ILE:N	2.19	0.57
2:B:375:GLN:NE2	6:F:75:LEU:HD12	2.19	0.57
4:L:103:LEU:HD13	4:L:515:VAL:HG21	1.85	0.57
7:O:238:ASN:N	7:O:239:PRO:CD	2.66	0.57
5:M:68:ARG:HD3	5:M:514:CYS:HB3	1.85	0.57
8:P:68:ALA:H	8:P:101:ASN:HD21	1.49	0.57
4:L:110:LEU:HD13	4:L:439:ILE:HD12	1.84	0.57
4:L:379:ILE:H	4:L:379:ILE:HD12	1.68	0.57
2:B:250:PHE:HA	6:F:250:GLY:O	2.04	0.57
8:H:146:VAL:HG13	8:H:147:VAL:H	1.68	0.57
7:O:516:LEU:HD13	7:O:517:ILE:N	2.20	0.57
2:B:30:GLY:O	2:B:33:VAL:HG23	2.04	0.57
6:N:221:HIS:HD2	6:N:224:MET:SD	2.27	0.57
1:I:350:PHE:CE2	1:I:354:TYR:CB	2.85	0.57
7:G:393:LEU:HD22	7:G:397:ILE:HG13	1.85	0.57
4:D:171:ALA:O	4:D:175:VAL:HG22	2.04	0.57
3:K:255:GLY:N	3:K:259:THR:HG21	2.18	0.57
4:L:305:LEU:HD21	4:L:312:VAL:HG21	1.85	0.57
6:F:175:THR:O	6:F:179:LEU:HG	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:167:THR:CA	6:N:168:GLU:HB3	2.35	0.57
6:N:430:ASN:C	6:N:433:LYS:HB2	2.24	0.57
6:N:231:ALA:HB1	6:N:293:PHE:N	2.18	0.57
4:D:16:LYS:O	4:D:20:VAL:HG23	2.04	0.57
5:M:273:THR:HG22	5:M:364:PRO:CA	2.20	0.57
2:J:30:GLY:O	2:J:33:VAL:HG23	2.04	0.57
1:A:418:VAL:HG12	1:A:419:VAL:N	2.17	0.57
3:K:320:VAL:O	3:K:321:LYS:C	2.41	0.57
2:J:142:ASN:CB	2:J:143:SER:HA	2.18	0.57
2:B:263:LYS:HB3	2:B:267:GLU:OE2	2.04	0.57
1:A:433:LEU:O	1:A:437:ALA:HB3	2.05	0.57
6:F:447:PHE:CD2	6:F:451:LEU:HD11	2.39	0.57
6:F:451:LEU:HD12	6:F:451:LEU:H	1.69	0.57
5:M:267:VAL:HA	5:M:319:ASP:OD2	2.04	0.57
4:L:147:ARG:HG2	4:L:148:GLU:N	2.18	0.57
4:L:171:ALA:HB3	4:L:172:PRO:HD3	1.86	0.57
6:F:221:HIS:HD2	6:F:224:MET:SD	2.27	0.57
4:D:305:LEU:HD21	4:D:312:VAL:HG21	1.85	0.57
7:G:294:LEU:HD23	7:G:315:ALA:HB3	1.87	0.57
3:K:279:GLN:O	3:K:283:MET:HG2	2.05	0.57
4:D:65:LEU:HD13	4:D:79:VAL:HG13	1.85	0.57
6:F:167:THR:HG21	6:F:169:VAL:HG23	1.86	0.57
6:N:430:ASN:C	6:N:433:LYS:H	2.05	0.57
2:B:463:ILE:HG13	2:B:468:SER:HA	1.85	0.57
7:G:516:LEU:HD13	7:G:517:ILE:N	2.20	0.57
1:I:90:GLN:HG3	1:I:101:VAL:CG2	2.19	0.57
2:B:72:PRO:CB	3:C:47:MET:HE1	2.33	0.57
6:N:170:LEU:HA	6:N:173:ILE:HG22	1.84	0.57
2:B:373:THR:HG22	2:B:376:THR:N	2.20	0.57
7:O:83:LEU:O	7:O:86:ILE:HG13	2.04	0.57
7:G:83:LEU:O	7:G:86:ILE:HG13	2.04	0.57
7:G:282:LEU:O	7:G:285:VAL:HG12	2.05	0.57
7:G:455:GLU:CG	7:G:461:ALA:CB	2.81	0.57
9:L:601:ADP:O3B	9:L:601:ADP:H5'2	2.04	0.57
5:M:241:ASN:ND2	5:M:241:ASN:O	2.34	0.57
2:J:116:HIS:HE1	2:J:118:GLN:CB	2.18	0.57
3:C:402:VAL:HG13	3:C:502:PRO:HG2	1.86	0.57
6:N:151:LEU:O	6:N:171:THR:HG22	2.04	0.57
6:F:231:ALA:HB1	6:F:293:PHE:N	2.18	0.57
3:K:353:GLY:H	3:K:370:ASN:HB3	1.70	0.57
6:N:447:PHE:CD2	6:N:451:LEU:HD11	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:373:THR:HG22	2:J:376:THR:N	2.20	0.57
4:L:171:ALA:O	4:L:175:VAL:HG22	2.05	0.57
4:D:298:ASN:HB3	4:D:299:ASP:HA	1.84	0.57
3:C:9:ASN:HD22	3:C:10:ALA:H	1.53	0.57
4:L:89:ALA:HB1	4:L:503:VAL:HG22	1.85	0.57
6:F:167:THR:CA	6:F:168:GLU:HB3	2.34	0.57
6:F:193:MET:HE3	6:F:330:LEU:HD11	1.86	0.57
2:B:329:PHE:CD2	2:B:329:PHE:O	2.53	0.57
6:F:58:ASP:O	6:F:62:LEU:HG	2.04	0.57
5:M:509:ASN:CG	5:M:523:LYS:HB2	2.24	0.57
3:C:113:GLU:HB2	1:I:460:LYS:HD2	1.86	0.57
2:J:206:SER:CB	2:J:368:VAL:HG13	2.34	0.57
2:J:68:PRO:HG2	6:N:536:ALA:HB2	1.86	0.57
1:A:182:ASP:O	1:A:186:ALA:HB3	2.05	0.57
8:H:486:GLU:H	8:H:487:PRO:HA	1.69	0.57
6:F:430:ASN:C	6:F:433:LYS:HB2	2.24	0.57
2:B:40:LYS:HZ1	6:F:117:ILE:HG13	1.68	0.57
7:G:51:ILE:HG22	7:G:53:ILE:HG23	1.87	0.57
7:G:516:LEU:O	7:G:516:LEU:CD2	2.46	0.57
5:M:352:GLU:HA	6:N:222:PRO:HG3	1.86	0.57
2:J:88:VAL:HA	2:J:393:GLN:NE2	2.19	0.57
8:H:204:VAL:CG2	8:H:409:LYS:CB	2.82	0.57
4:D:328:LEU:C	4:D:345:ASP:OD2	2.43	0.57
7:O:393:LEU:HD22	7:O:397:ILE:HG13	1.85	0.57
6:F:56:THR:HG22	6:F:390:GLN:HB2	1.86	0.57
4:L:41:PRO:HG2	9:L:601:ADP:C6	2.40	0.57
1:I:329:ILE:HD13	1:I:374:ILE:HD12	1.87	0.57
6:N:108:PHE:O	6:N:113:VAL:HG23	2.04	0.57
4:L:215:LEU:HB3	4:L:217:GLN:HG2	1.86	0.57
4:L:291:SER:HA	4:L:315:ASP:HA	1.86	0.57
7:O:494:LYS:O	7:O:495:PHE:CB	2.52	0.57
6:N:167:THR:HG21	6:N:169:VAL:HG23	1.86	0.57
6:N:485:GLU:O	6:N:488:TYR:CB	2.52	0.57
1:I:433:LEU:O	1:I:437:ALA:HB3	2.05	0.57
6:F:108:PHE:O	6:F:113:VAL:HG23	2.04	0.57
2:B:43:ASP:O	6:F:530:CYS:HA	2.04	0.57
4:D:120:ILE:HA	4:D:123:SER:HB3	1.87	0.57
6:N:280:LEU:HD13	6:N:343:LEU:HD21	1.85	0.57
7:O:294:LEU:HD23	7:O:315:ALA:HB3	1.86	0.57
5:E:448:VAL:HG21	5:E:498:LEU:HD13	1.86	0.57
6:N:169:VAL:C	6:N:172:PRO:HD2	2.26	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:54:ILE:HG13	8:P:64:ILE:CG1	2.15	0.57
2:J:263:LYS:HB3	2:J:267:GLU:OE2	2.04	0.57
1:A:264:ILE:O	1:A:265:ASP:HB3	2.05	0.57
4:L:110:LEU:HD13	4:L:439:ILE:HG23	1.87	0.57
1:I:33:THR:OG1	1:I:83:LEU:HD11	2.05	0.57
3:K:355:PHE:HB2	3:K:368:LEU:HD13	1.87	0.57
5:M:255:PRO:HG3	5:M:336:LEU:HA	1.87	0.57
1:A:252:GLN:HG3	1:A:253:LYS:N	2.20	0.57
2:J:463:ILE:O	2:J:467:ILE:CB	2.52	0.57
6:F:6:LEU:CD1	6:F:7:ASN:H	2.18	0.57
4:L:177:SER:O	4:L:181:ILE:HG12	2.05	0.57
6:F:38:GLY:N	9:F:601:ADP:H5'1	2.15	0.57
6:N:58:ASP:O	6:N:62:LEU:HG	2.04	0.57
6:N:56:THR:O	6:N:62:LEU:HD21	2.05	0.57
6:N:45:MET:HA	6:N:54:LYS:O	2.05	0.57
2:J:91:GLY:HA2	9:J:601:ADP:O2A	2.05	0.57
5:E:68:ARG:HD3	5:E:514:CYS:HB3	1.85	0.57
1:I:183:ALA:HB1	1:I:383:SER:HB2	1.87	0.57
5:E:267:VAL:HA	5:E:319:ASP:OD2	2.04	0.57
3:K:223:VAL:HG12	3:K:224:LEU:N	2.20	0.57
3:K:402:VAL:HG13	3:K:502:PRO:HG2	1.86	0.57
8:P:300:VAL:HG13	8:P:321:LEU:HB3	1.87	0.56
2:B:245:ILE:O	2:B:246:PHE:HD2	1.87	0.56
3:C:353:GLY:H	3:C:370:ASN:HB3	1.70	0.56
6:F:447:PHE:CE2	6:F:451:LEU:HD11	2.39	0.56
6:F:452:LEU:O	6:F:455:PRO:CD	2.51	0.56
1:A:33:THR:OG1	1:A:83:LEU:HD11	2.05	0.56
2:J:159:THR:HG21	2:J:488:VAL:H	1.69	0.56
1:I:252:GLN:HG3	1:I:253:LYS:N	2.20	0.56
2:B:230:LYS:H	2:B:281:ILE:CG2	2.18	0.56
5:E:32:VAL:HG22	5:E:33:LYS:N	2.14	0.56
5:M:352:GLU:HA	6:N:222:PRO:CG	2.35	0.56
7:G:43:THR:CG2	7:G:64:ASN:CB	2.83	0.56
6:F:29:LEU:O	6:F:33:LEU:HD23	2.05	0.56
5:M:74:LEU:CG	5:M:93:GLN:HB3	2.35	0.56
4:D:36:ARG:HE	4:D:98:ILE:CG2	2.18	0.56
1:A:548:ASP:N	1:A:548:ASP:OD2	2.37	0.56
2:J:213:ILE:HG23	2:J:354:LEU:CD2	2.35	0.56
6:N:428:SER:O	6:N:431:MET:HG2	2.06	0.56
6:F:169:VAL:C	6:F:172:PRO:HD2	2.26	0.56
4:L:104:LEU:HD11	4:L:518:ILE:HD12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:51:ILE:HG22	7:O:53:ILE:HG23	1.87	0.56
3:K:302:SER:O	3:K:303:ASP:CB	2.40	0.56
1:I:264:ILE:O	1:I:265:ASP:HB3	2.05	0.56
2:J:245:ILE:O	2:J:246:PHE:HD2	1.87	0.56
3:K:321:LYS:HB3	3:K:324:ASP:HB2	1.87	0.56
8:P:427:GLU:HG2	8:P:459:VAL:HG21	1.85	0.56
6:N:452:LEU:O	6:N:455:PRO:CD	2.51	0.56
3:K:514:ILE:HA	3:K:517:ALA:HB3	1.86	0.56
7:O:109:MET:SD	7:O:514:THR:HB	2.45	0.56
6:F:56:THR:O	6:F:62:LEU:HD21	2.05	0.56
5:E:509:ASN:CG	5:E:523:LYS:HB2	2.24	0.56
3:K:118:PRO:O	3:K:122:ILE:HG13	2.05	0.56
8:H:284:ILE:O	8:H:288:MET:HG2	2.06	0.56
1:A:55:ASP:HA	7:G:527:LYS:HB3	1.86	0.56
5:M:252:PRO:HA	5:M:255:PRO:C	2.26	0.56
2:J:239:ASP:OD1	2:J:290:ILE:HB	2.06	0.56
6:F:428:SER:O	6:F:431:MET:HG2	2.05	0.56
3:C:80:GLU:O	3:C:84:THR:HG23	2.05	0.56
5:E:428:CYS:HA	5:E:431:ARG:HG3	1.88	0.56
4:L:7:SER:HA	7:O:35:ALA:HB1	1.86	0.56
6:N:6:LEU:CD1	6:N:7:ASN:H	2.18	0.56
8:P:204:VAL:CG2	8:P:409:LYS:CB	2.82	0.56
3:C:149:ALA:O	3:C:153:LYS:HG2	2.05	0.56
1:A:266:ASP:N	1:A:267:PRO:CD	2.68	0.56
2:B:213:ILE:HG23	2:B:354:LEU:CD2	2.35	0.56
8:H:52:ASN:OD1	8:H:66:ASN:HB2	2.06	0.56
7:G:494:LYS:O	7:G:495:PHE:CB	2.52	0.56
3:K:226:ASN:OD1	3:K:365:PHE:HA	2.06	0.56
8:P:486:GLU:H	8:P:487:PRO:HA	1.69	0.56
3:C:279:GLN:O	3:C:283:MET:HG2	2.05	0.56
8:H:300:VAL:HG13	8:H:321:LEU:HB3	1.87	0.56
6:F:485:GLU:O	6:F:488:TYR:CB	2.52	0.56
1:I:159:ILE:O	1:I:162:THR:HG22	2.06	0.56
4:L:209:MET:HA	4:L:377:VAL:HG12	1.86	0.56
4:D:485:ARG:N	4:D:485:ARG:HD2	2.20	0.56
4:D:110:LEU:HD13	4:D:439:ILE:HG23	1.87	0.56
7:G:71:LYS:HD2	7:G:72:LEU:HD12	1.88	0.56
2:J:237:THR:CB	2:J:288:GLN:O	2.54	0.56
3:K:80:GLU:O	3:K:84:THR:HG23	2.05	0.56
5:E:255:PRO:HG3	5:E:336:LEU:HA	1.87	0.56
1:I:463:ALA:HB1	1:I:470:SER:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:116:HIS:HE1	2:B:118:GLN:CB	2.18	0.56
8:P:52:ASN:OD1	8:P:66:ASN:HB2	2.06	0.56
3:C:355:PHE:HB2	3:C:368:LEU:HD13	1.87	0.56
2:B:319:LEU:HD22	2:B:320:VAL:HG13	1.88	0.56
2:B:237:THR:CB	2:B:288:GLN:O	2.54	0.56
1:A:422:GLY:HA2	9:A:601:ADP:N3	2.20	0.56
3:C:335:THR:O	3:C:337:VAL:HG23	2.06	0.56
3:K:335:THR:O	3:K:337:VAL:HG23	2.06	0.56
2:B:242:LYS:HD3	3:C:269:TRP:CZ2	2.39	0.56
8:H:68:ALA:O	8:H:72:LEU:HG	2.05	0.56
2:B:450:PHE:CB	2:B:455:LEU:HD22	2.36	0.56
4:D:372:ARG:N	4:D:373:PRO:HD3	2.21	0.56
2:J:375:GLN:HE22	6:N:75:LEU:HB2	1.70	0.56
5:M:84:THR:HG22	5:M:86:ASP:N	2.18	0.56
7:O:282:LEU:O	7:O:285:VAL:HG12	2.05	0.56
7:O:121:SER:HB3	7:O:123:HIS:CE1	2.41	0.56
8:P:123:SER:OG	8:P:126:GLU:HG3	2.06	0.56
3:C:12:GLN:NE2	3:C:529:GLY:HA2	2.21	0.56
2:B:45:LEU:CD2	2:B:56:VAL:HG22	2.35	0.56
6:N:541:LEU:HB2	6:N:542:LYS:HA	0.59	0.56
6:N:143:LEU:CD1	6:N:145:ASN:CG	2.74	0.56
6:F:143:LEU:HA	6:F:144:SER:C	2.24	0.56
6:F:415:ALA:O	6:F:491:VAL:HG23	2.06	0.56
6:F:154:ALA:HB2	6:F:402:VAL:HG22	1.87	0.56
7:O:43:THR:CG2	7:O:64:ASN:CB	2.83	0.56
6:F:424:ARG:HG2	6:F:483:SER:CA	2.34	0.56
4:D:177:SER:O	4:D:181:ILE:HG12	2.05	0.56
6:N:29:LEU:O	6:N:33:LEU:HD23	2.05	0.56
1:I:209:HIS:HE1	7:O:89:ALA:HB2	1.71	0.56
3:K:149:ALA:O	3:K:153:LYS:HG2	2.05	0.56
3:K:9:ASN:HD22	3:K:10:ALA:H	1.53	0.56
8:P:284:ILE:O	8:P:288:MET:HG2	2.05	0.56
4:D:219:ALA:HB1	4:D:221:LYS:NZ	2.20	0.56
2:J:16:GLU:HG3	2:J:17:ASN:H	1.70	0.56
7:G:323:MET:HA	7:G:326:VAL:HG22	1.88	0.56
1:A:76:GLN:O	1:A:77:HIS:HB3	2.06	0.56
6:N:203:SER:C	6:N:205:LYS:N	2.58	0.56
3:K:264:GLU:O	3:K:265:LYS:CB	2.54	0.56
2:J:37:LEU:HB2	2:J:444:LEU:HD13	1.87	0.56
4:L:242:SER:O	4:L:244:PRO:HD3	2.06	0.56
1:A:183:ALA:HB1	1:A:383:SER:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:120:ILE:HA	4:L:123:SER:HB3	1.87	0.56
3:C:118:PRO:O	3:C:122:ILE:HG13	2.05	0.56
2:B:32:LEU:HD12	6:F:532:GLU:OE2	2.05	0.56
7:G:23:LYS:HA	7:G:26:ILE:CG2	2.36	0.56
4:L:219:ALA:HB1	4:L:221:LYS:NZ	2.20	0.56
5:M:428:CYS:HA	5:M:431:ARG:HG3	1.88	0.56
2:J:47:GLN:OE1	2:J:54:CYS:HB3	2.05	0.56
2:B:239:ASP:OD1	2:B:290:ILE:HB	2.06	0.56
6:F:541:LEU:HB2	6:F:542:LYS:HA	0.60	0.56
6:N:92:THR:HG21	10:N:602:BEF:F3	1.95	0.56
2:B:326:VAL:CG1	3:C:304:LEU:HD22	2.36	0.56
7:O:41:LYS:N	7:O:42:PRO:CD	2.69	0.56
6:F:424:ARG:NH1	6:F:479:ASP:CB	2.69	0.56
2:J:450:PHE:CB	2:J:455:LEU:HD22	2.36	0.56
8:P:25:ASP:HA	8:P:28:ILE:HG13	1.87	0.56
9:D:601:ADP:O3'	9:D:601:ADP:C8	2.59	0.56
1:A:187:VAL:HB	1:A:382:SER:N	2.21	0.56
6:N:47:VAL:HG12	6:N:48:ASP:H	1.71	0.56
7:G:121:SER:HB3	7:G:123:HIS:CE1	2.41	0.56
2:J:402:LEU:HD21	2:J:483:ARG:CG	2.36	0.56
7:G:420:VAL:HG23	7:G:446:LEU:HD13	1.88	0.56
3:C:223:VAL:HG12	3:C:224:LEU:N	2.20	0.56
8:P:323:VAL:O	8:P:323:VAL:HG23	2.06	0.56
6:N:540:THR:O	6:N:541:LEU:CD2	2.54	0.56
2:J:230:LYS:H	2:J:281:ILE:CG2	2.18	0.56
1:A:159:ILE:O	1:A:162:THR:HG22	2.06	0.56
2:B:37:LEU:HB2	2:B:444:LEU:HD13	1.87	0.56
2:B:63:ILE:HG23	2:B:64:LEU:HG	1.88	0.56
8:H:25:ASP:HA	8:H:28:ILE:HG13	1.87	0.56
8:H:29:ILE:CG2	8:H:30:LYS:N	2.69	0.56
2:J:63:ILE:HG23	2:J:64:LEU:HG	1.88	0.56
4:D:242:SER:O	4:D:244:PRO:HD3	2.06	0.56
1:I:266:ASP:N	1:I:267:PRO:CD	2.68	0.56
4:L:527:SER:HB3	4:L:528:ARG:HH21	1.71	0.56
7:O:323:MET:HA	7:O:326:VAL:HG22	1.88	0.56
2:B:47:GLN:OE1	2:B:54:CYS:HB3	2.05	0.56
1:I:76:GLN:O	1:I:77:HIS:HB3	2.06	0.56
2:J:5:ILE:O	3:K:71:ALA:N	2.39	0.55
1:A:252:GLN:HG3	1:A:253:LYS:H	1.71	0.55
1:I:517:VAL:O	1:I:518:LEU:CD2	2.54	0.55
4:L:372:ARG:N	4:L:373:PRO:HD3	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:475:ASN:N	2:B:475:ASN:HD22	1.92	0.55
5:E:74:LEU:CG	5:E:93:GLN:HB3	2.35	0.55
1:A:329:ILE:HD13	1:A:374:ILE:HD12	1.87	0.55
1:I:187:VAL:HB	1:I:382:SER:N	2.21	0.55
5:E:35:GLN:OE1	5:E:36:GLY:HA3	2.06	0.55
2:B:402:LEU:HD11	2:B:483:ARG:HG3	1.88	0.55
5:E:252:PRO:HA	5:E:255:PRO:C	2.26	0.55
5:M:181:LEU:HA	5:M:205:VAL:HG21	1.89	0.55
2:B:16:GLU:HG3	2:B:17:ASN:H	1.71	0.55
4:L:394:LEU:HA	4:L:397:ALA:HB3	1.88	0.55
1:A:517:VAL:O	1:A:518:LEU:CD2	2.54	0.55
5:E:350:GLU:C	5:E:352:GLU:N	2.55	0.55
3:C:321:LYS:HB3	3:C:324:ASP:HB2	1.87	0.55
6:N:209:PHE:CZ	6:N:211:LYS:HD2	2.41	0.55
3:K:482:THR:HA	3:K:493:ASP:HA	1.87	0.55
6:F:45:MET:HA	6:F:54:LYS:O	2.05	0.55
2:B:115:ILE:HG12	5:M:492:ILE:HD11	1.88	0.55
1:I:182:ASP:O	1:I:186:ALA:HB3	2.05	0.55
3:C:226:ASN:OD1	3:C:365:PHE:HA	2.06	0.55
6:N:68:ILE:HD13	6:N:74:VAL:HG22	1.89	0.55
1:A:500:TYR:HA	1:A:511:ASP:HA	1.89	0.55
6:F:47:VAL:HG12	6:F:48:ASP:H	1.70	0.55
6:F:151:LEU:CG	6:F:175:THR:HG23	2.31	0.55
7:G:58:GLN:HA	7:G:58:GLN:NE2	2.22	0.55
5:M:273:THR:CG2	5:M:364:PRO:CA	2.72	0.55
6:F:5:LEU:CB	6:F:6:LEU:C	2.75	0.55
6:N:489:VAL:O	6:N:490:GLY:C	2.41	0.55
2:J:511:VAL:HB	2:J:514:ILE:HD11	1.88	0.55
5:E:351:LEU:N	5:E:351:LEU:HD13	2.22	0.55
5:M:351:LEU:HD13	5:M:351:LEU:N	2.22	0.55
4:D:209:MET:HA	4:D:377:VAL:HG12	1.86	0.55
1:A:350:PHE:CE2	1:A:354:TYR:CB	2.85	0.55
3:K:506:LYS:O	3:K:510:VAL:HG23	2.06	0.55
8:P:68:ALA:O	8:P:72:LEU:HG	2.06	0.55
3:C:322:LYS:HG3	3:C:323:SER:N	2.21	0.55
4:D:411:ILE:HG13	4:D:501:VAL:HG22	1.87	0.55
5:E:181:LEU:HA	5:E:205:VAL:HG21	1.88	0.55
6:F:68:ILE:HD13	6:F:74:VAL:HG22	1.89	0.55
1:I:273:ILE:HG21	5:M:295:TYR:CE2	2.41	0.55
2:B:3:VAL:C	2:B:5:ILE:HG21	2.25	0.55
6:F:540:THR:O	6:F:541:LEU:CD2	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:319:LEU:HD22	2:J:320:VAL:HG13	1.88	0.55
4:L:521:ILE:HD11	7:O:62:ILE:HD12	1.82	0.55
8:P:29:ILE:CG2	8:P:30:LYS:N	2.69	0.55
2:B:402:LEU:HD21	2:B:483:ARG:CG	2.36	0.55
7:O:492:PHE:HA	7:O:497:TRP:NE1	2.21	0.55
7:O:23:LYS:HA	7:O:26:ILE:CG2	2.36	0.55
1:I:484:SER:OG	1:I:498:ARG:CB	2.55	0.55
1:A:252:GLN:HB2	1:A:303:ASP:HB2	1.89	0.55
6:N:415:ALA:O	6:N:491:VAL:HG23	2.06	0.55
2:J:460:ARG:O	2:J:463:ILE:HG22	2.07	0.55
4:L:524:ILE:HG22	4:L:524:ILE:O	2.06	0.55
6:N:424:ARG:NH1	6:N:479:ASP:CB	2.69	0.55
6:N:5:LEU:CB	6:N:6:LEU:C	2.75	0.55
6:F:143:LEU:CD1	6:F:145:ASN:CG	2.74	0.55
6:N:160:THR:H	6:N:164:ALA:CB	2.20	0.55
3:C:104:LEU:HD21	3:C:517:ALA:HA	1.89	0.55
7:G:109:MET:SD	7:G:514:THR:HB	2.45	0.55
6:N:35:THR:HG22	6:N:42:THR:H	1.72	0.55
2:J:402:LEU:HD11	2:J:483:ARG:HG3	1.88	0.55
7:G:294:LEU:CD2	7:G:315:ALA:HB3	2.37	0.55
1:I:252:GLN:HG3	1:I:253:LYS:H	1.71	0.55
3:C:47:MET:HE2	3:C:49:LEU:HD21	1.87	0.55
6:F:209:PHE:CZ	6:F:211:LYS:HD2	2.41	0.55
4:L:298:ASN:CB	4:L:299:ASP:HA	2.37	0.55
4:L:485:ARG:N	4:L:485:ARG:HD2	2.20	0.55
4:D:207:THR:HB	4:D:378:VAL:O	2.07	0.55
2:J:45:LEU:CD2	2:J:56:VAL:HG22	2.36	0.55
7:O:126:MET:HE2	7:O:126:MET:HA	1.88	0.55
1:I:76:GLN:O	1:I:77:HIS:CB	2.55	0.55
8:P:328:GLU:HG3	8:P:331:ARG:HH12	1.72	0.55
5:M:470:ARG:O	5:M:474:GLN:HG3	2.07	0.55
1:A:484:SER:OG	1:A:498:ARG:CB	2.55	0.55
7:O:115:PHE:O	7:O:119:GLY:HA3	2.07	0.55
8:H:323:VAL:O	8:H:323:VAL:HG23	2.06	0.55
6:N:143:LEU:HA	6:N:144:SER:C	2.24	0.55
7:G:41:LYS:N	7:G:42:PRO:CD	2.69	0.55
6:F:214:VAL:O	6:F:215:LEU:HD23	2.06	0.55
6:F:160:THR:H	6:F:164:ALA:CB	2.20	0.55
6:F:92:THR:CG2	10:F:602:BEF:F3	2.44	0.55
3:K:104:LEU:HD21	3:K:517:ALA:HA	1.89	0.55
1:A:92:ARG:HB3	5:E:388:THR:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:34:VAL:O	7:G:38:GLU:HG2	2.06	0.55
3:C:482:THR:HA	3:C:493:ASP:HA	1.87	0.55
8:P:146:VAL:C	8:P:148:GLY:H	2.10	0.55
3:K:508:GLN:HG2	8:P:215:GLY:HA2	1.89	0.55
4:D:394:LEU:HA	4:D:397:ALA:HB3	1.89	0.55
2:J:4:GLN:N	2:J:5:ILE:HG12	2.19	0.55
2:J:3:VAL:C	2:J:5:ILE:HG21	2.24	0.55
2:B:460:ARG:O	2:B:463:ILE:HG22	2.07	0.55
3:C:264:GLU:O	3:C:265:LYS:CB	2.54	0.55
2:B:514:ILE:CD1	3:C:47:MET:HB3	2.35	0.55
6:N:195:GLU:CG	6:N:197:MET:SD	2.94	0.55
6:N:214:VAL:O	6:N:215:LEU:HD23	2.07	0.55
5:E:173:ASP:HB3	5:E:437:SER:HB3	1.87	0.55
2:J:173:PHE:HA	2:J:176:LEU:HD12	1.89	0.55
8:P:24:ALA:CB	8:P:531:ALA:HB1	2.37	0.55
4:L:81:VAL:HG22	7:O:382:ALA:HB2	1.89	0.55
7:O:386:ILE:O	7:O:389:VAL:HB	2.07	0.55
2:J:475:ASN:HD22	2:J:475:ASN:N	1.92	0.55
3:K:322:LYS:HG3	3:K:323:SER:N	2.21	0.55
4:L:207:THR:HB	4:L:378:VAL:O	2.07	0.55
4:L:410:LEU:HD22	4:L:498:LEU:HB3	1.89	0.55
6:N:277:ILE:HG21	6:N:295:ILE:HG13	1.89	0.55
2:B:229:ALA:HB3	2:B:339:GLU:O	2.07	0.55
6:N:171:THR:O	6:N:175:THR:CB	2.55	0.55
6:N:541:LEU:HB2	6:N:542:LYS:CB	2.32	0.55
6:F:353:LEU:N	6:F:369:GLU:HB3	2.22	0.55
6:F:372:ASP:N	6:F:373:PRO:HD3	2.22	0.55
4:D:375:VAL:HG12	4:D:376:SER:N	2.22	0.55
2:B:173:PHE:HA	2:B:176:LEU:HD12	1.89	0.55
2:J:39:PRO:HA	2:J:163:SER:CA	2.37	0.55
7:O:71:LYS:HD2	7:O:72:LEU:HD12	1.88	0.55
5:M:35:GLN:OE1	5:M:36:GLY:HA3	2.06	0.55
6:N:538:ARG:HG3	6:N:538:ARG:HH11	1.71	0.55
3:C:275:ILE:CA	8:H:274:LEU:HD21	2.37	0.55
3:K:523:VAL:HA	8:P:52:ASN:O	2.06	0.55
6:F:406:LEU:C	6:F:407:LYS:HE3	2.27	0.55
2:B:95:VAL:HG22	2:B:497:VAL:HG22	1.89	0.55
6:F:277:ILE:HG21	6:F:295:ILE:HG13	1.89	0.55
7:O:58:GLN:HA	7:O:58:GLN:NE2	2.22	0.55
6:N:372:ASP:N	6:N:373:PRO:HD3	2.22	0.55
1:I:252:GLN:HB2	1:I:303:ASP:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:88:ALA:CB	5:E:109:LYS:NZ	2.68	0.55
7:O:455:GLU:HG3	7:O:461:ALA:HB2	1.88	0.55
6:F:199:MET:O	6:F:381:LYS:CE	2.55	0.55
4:L:411:ILE:HG13	4:L:501:VAL:HG22	1.87	0.55
3:C:124:ALA:HB1	3:C:441:PRO:CB	2.37	0.55
6:F:538:ARG:HG3	6:F:538:ARG:HH11	1.71	0.55
8:H:123:SER:OG	8:H:126:GLU:HG3	2.06	0.55
6:N:353:LEU:N	6:N:369:GLU:HB3	2.22	0.54
2:J:210:GLU:HB3	2:J:357:SER:O	2.07	0.54
4:D:524:ILE:O	4:D:524:ILE:HG22	2.07	0.54
2:B:422:ILE:HG21	2:B:427:SER:CB	2.36	0.54
7:G:191:ARG:HB3	7:G:193:ASP:O	2.07	0.54
2:J:127:ALA:CB	2:J:430:VAL:HG22	2.31	0.54
1:A:94:ILE:HD11	1:A:526:LYS:HB2	1.89	0.54
3:C:370:ASN:OD1	3:C:1054:GLY:HA2	2.07	0.54
4:D:196:LEU:HD22	4:D:377:VAL:CG2	2.37	0.54
6:N:33:LEU:N	6:N:33:LEU:HD22	2.22	0.54
4:L:499:GLN:HE22	9:L:601:ADP:H1'	1.72	0.54
1:A:460:LYS:HD2	3:K:113:GLU:HB2	1.89	0.54
4:D:214:VAL:HG13	4:D:362:ARG:HG2	1.89	0.54
7:G:440:ASN:O	7:G:444:LYS:HD3	2.08	0.54
3:K:432:LYS:HA	3:K:439:GLN:HE21	1.72	0.54
6:F:171:THR:O	6:F:175:THR:CB	2.55	0.54
6:N:424:ARG:HG2	6:N:483:SER:CA	2.34	0.54
4:D:70:ILE:HA	8:H:15:LYS:HZ3	1.72	0.54
2:B:511:VAL:HB	2:B:514:ILE:HD11	1.88	0.54
6:F:215:LEU:HB3	6:F:217:HIS:CD2	2.36	0.54
6:N:75:LEU:HD21	6:N:523:ILE:HG23	1.89	0.54
6:N:199:MET:O	6:N:381:LYS:CE	2.55	0.54
1:I:548:ASP:OD2	1:I:548:ASP:N	2.37	0.54
2:J:505:ALA:O	2:J:509:LEU:HB2	2.07	0.54
7:O:294:LEU:CD2	7:O:315:ALA:HB3	2.36	0.54
2:B:192:HIS:CD2	2:B:193:ILE:HG23	2.42	0.54
4:D:418:GLU:HG2	4:D:450:ILE:HB	1.89	0.54
4:L:418:GLU:HG2	4:L:450:ILE:HB	1.89	0.54
2:B:4:GLN:N	2:B:5:ILE:HG12	2.19	0.54
6:N:501:PRO:O	6:N:504:GLU:N	2.39	0.54
1:A:90:GLN:NE2	1:A:527:SER:HB3	2.22	0.54
6:F:75:LEU:HD21	6:F:523:ILE:HG23	1.89	0.54
5:E:84:THR:HG23	5:E:418:GLU:OE2	2.08	0.54
8:H:138:THR:HG21	8:H:452:PHE:HE1	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:326:VAL:HG13	3:K:304:LEU:HD22	1.90	0.54
4:D:527:SER:HB3	4:D:528:ARG:HH21	1.71	0.54
7:O:420:VAL:HG23	7:O:446:LEU:HD13	1.88	0.54
6:F:324:ASN:O	6:F:328:LEU:N	2.33	0.54
3:K:12:GLN:NE2	3:K:529:GLY:HA2	2.21	0.54
5:E:470:ARG:O	5:E:474:GLN:HG3	2.07	0.54
6:N:155:ARG:CB	6:N:171:THR:HG23	2.38	0.54
2:B:326:VAL:CG2	3:C:304:LEU:HD22	2.37	0.54
1:A:412:THR:OG1	1:A:520:PRO:HG3	2.08	0.54
4:D:196:LEU:HD22	4:D:377:VAL:HG22	1.89	0.54
5:M:173:ASP:HB3	5:M:437:SER:HB3	1.87	0.54
2:B:289:LEU:HD13	2:B:294:PRO:HG3	1.90	0.54
7:O:397:ILE:O	7:O:400:VAL:HG22	2.07	0.54
2:J:31:ASP:OD1	2:J:32:LEU:N	2.40	0.54
4:L:46:LYS:HG3	8:P:532:THR:HG23	1.89	0.54
4:L:214:VAL:HG13	4:L:362:ARG:HG2	1.89	0.54
2:J:284:PHE:HB3	2:J:305:SER:HB3	1.89	0.54
2:J:95:VAL:HG22	2:J:497:VAL:HG22	1.89	0.54
4:L:28:ALA:HB1	4:L:78:LEU:HD11	1.89	0.54
3:C:262:GLU:H	8:H:266:LEU:HD11	1.73	0.54
2:J:196:ILE:O	2:J:367:ILE:HA	2.07	0.54
2:B:284:PHE:HB3	2:B:305:SER:HB3	1.89	0.54
6:N:488:TYR:O	6:N:489:VAL:CB	2.56	0.54
3:K:370:ASN:OD1	3:K:1054:GLY:HA2	2.07	0.54
3:K:334:ALA:HB2	3:K:349:GLY:N	2.23	0.54
6:F:33:LEU:HD22	6:F:33:LEU:N	2.21	0.54
7:O:34:VAL:O	7:O:38:GLU:HG2	2.06	0.54
6:F:35:THR:HG22	6:F:42:THR:H	1.72	0.54
1:A:267:PRO:HB3	1:A:268:GLU:C	2.28	0.54
1:I:500:TYR:HA	1:I:511:ASP:HA	1.89	0.54
5:M:476:LEU:HD11	5:M:538:ILE:HD11	1.90	0.54
1:A:44:LEU:HD21	1:A:103:ILE:HD12	1.89	0.54
7:G:115:PHE:O	7:G:119:GLY:HA3	2.07	0.54
2:J:192:HIS:CD2	2:J:193:ILE:HG23	2.42	0.54
2:B:504:ALA:O	2:B:508:LEU:HB3	2.07	0.54
6:N:434:LEU:O	6:N:438:GLY:HA2	2.08	0.54
2:J:70:ASP:HB3	6:N:5:LEU:HD22	1.87	0.54
2:B:455:LEU:HG	2:B:472:LEU:HD13	1.90	0.54
1:I:350:PHE:HE2	1:I:354:TYR:CB	2.16	0.54
2:J:27:ILE:HA	2:J:100:ALA:HB1	1.88	0.54
7:G:397:ILE:O	7:G:400:VAL:HG22	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:131:TYR:HD2	8:H:452:PHE:CD2	2.24	0.54
3:C:515:GLU:OE2	8:H:390:THR:HG22	2.08	0.54
8:P:288:MET:HE2	8:P:313:LEU:HG	1.89	0.54
1:A:76:GLN:O	1:A:77:HIS:CB	2.55	0.54
3:C:241:PRO:O	3:C:350:THR:HG23	2.08	0.54
7:O:440:ASN:O	7:O:444:LYS:HD3	2.08	0.54
1:I:532:LEU:HD22	1:I:536:VAL:HG23	1.90	0.54
6:N:406:LEU:C	6:N:407:LYS:HE3	2.27	0.54
4:D:28:ALA:HB1	4:D:78:LEU:HD11	1.89	0.54
6:F:434:LEU:O	6:F:438:GLY:HA2	2.08	0.54
2:J:245:ILE:O	2:J:246:PHE:CB	2.56	0.54
8:H:237:LYS:HB2	8:H:314:ASN:CB	2.31	0.54
6:F:501:PRO:O	6:F:504:GLU:N	2.39	0.54
2:J:514:ILE:CD1	3:K:47:MET:HB3	2.30	0.54
5:E:350:GLU:O	5:E:351:LEU:C	2.46	0.54
5:M:88:ALA:CB	5:M:109:LYS:NZ	2.68	0.54
2:B:459:LEU:CD2	2:B:472:LEU:HG	2.33	0.54
2:J:445:ALA:HB2	2:J:455:LEU:HD23	1.90	0.54
2:J:455:LEU:HG	2:J:472:LEU:HD13	1.90	0.54
6:N:451:LEU:O	6:N:455:PRO:HD3	2.07	0.54
3:C:334:ALA:HB2	3:C:349:GLY:N	2.23	0.54
7:O:241:ILE:HG12	7:O:292:ILE:HG23	1.89	0.54
8:P:131:TYR:HD2	8:P:452:PHE:CD2	2.24	0.54
1:I:431:ILE:HG13	1:I:435:ASN:HD22	1.73	0.54
2:B:505:ALA:O	2:B:509:LEU:HB2	2.07	0.54
4:D:273:ASN:HD22	7:G:268:GLN:HE22	1.56	0.54
6:F:155:ARG:CB	6:F:171:THR:HG23	2.38	0.54
6:N:125:ALA:CA	6:N:426:LEU:HD21	2.38	0.54
2:B:40:LYS:HA	6:F:116:ARG:HG3	1.90	0.54
2:J:359:CYS:CB	2:J:360:LYS:HA	2.38	0.54
2:J:242:LYS:HE2	2:J:247:GLY:H	1.69	0.54
6:F:481:GLN:O	6:F:485:GLU:HG2	2.07	0.54
1:A:350:PHE:CD2	1:A:351:GLU:N	2.72	0.54
3:C:506:LYS:O	3:C:510:VAL:HG23	2.06	0.54
1:I:12:THR:HB	5:M:96:LEU:HA	1.90	0.54
7:G:206:GLY:O	7:G:379:ARG:HD2	2.07	0.54
7:G:455:GLU:HG3	7:G:461:ALA:HB2	1.88	0.54
8:P:138:THR:HG21	8:P:452:PHE:HE1	1.72	0.54
3:K:124:ALA:HB1	3:K:441:PRO:CB	2.37	0.54
2:B:213:ILE:HG23	2:B:354:LEU:HD23	1.90	0.54
7:O:208:ALA:HB1	7:O:210:GLU:OE1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:236:LEU:O	6:F:297:ASN:HA	2.08	0.54
2:B:359:CYS:CB	2:B:360:LYS:HA	2.38	0.54
6:F:488:TYR:O	6:F:489:VAL:CB	2.56	0.54
5:M:188:LEU:CB	5:M:197:HIS:HB2	2.38	0.54
6:N:154:ALA:HB2	6:N:402:VAL:HG22	1.87	0.54
7:O:377:LEU:H	7:O:377:LEU:CD1	2.19	0.54
4:D:110:LEU:CD1	4:D:439:ILE:HG23	2.38	0.54
2:B:49:ALA:HB1	6:F:538:ARG:HB2	1.90	0.54
2:J:213:ILE:HG23	2:J:354:LEU:HD23	1.90	0.54
2:B:45:LEU:HB2	6:F:533:LEU:CB	2.38	0.54
6:N:15:ARG:O	6:N:18:ALA:HB3	2.08	0.54
6:F:43:LEU:HD22	6:F:57:LYS:HB2	1.84	0.54
2:B:210:GLU:HB3	2:B:357:SER:O	2.07	0.54
2:B:409:MET:CE	2:B:409:MET:HA	2.38	0.54
4:L:521:ILE:CG2	7:O:50:ASP:O	2.55	0.54
3:C:457:ILE:HD11	3:C:467:LEU:HD22	1.90	0.54
1:I:90:GLN:NE2	1:I:527:SER:HB3	2.22	0.54
6:F:16:ASP:O	6:F:19:LEU:HB2	2.08	0.54
8:H:252:CYS:HB2	8:H:343:ARG:H	1.73	0.54
2:B:27:ILE:HA	2:B:100:ALA:HB1	1.88	0.54
2:J:289:LEU:O	2:J:289:LEU:HD12	2.08	0.54
2:J:289:LEU:HD13	2:J:294:PRO:HG3	1.90	0.54
8:H:24:ALA:CB	8:H:531:ALA:O	2.56	0.54
5:E:355:ALA:HB2	5:E:362:ILE:HD11	1.90	0.54
7:G:492:PHE:HA	7:G:497:TRP:NE1	2.21	0.54
1:I:458:ILE:N	1:I:458:ILE:HD12	2.24	0.54
7:G:208:ALA:HB1	7:G:210:GLU:OE1	2.08	0.54
7:G:174:ASN:ND2	7:G:209:MET:SD	2.80	0.54
5:E:61:ILE:O	5:E:61:ILE:HD13	2.08	0.54
1:A:184:LEU:CD2	1:A:184:LEU:C	2.76	0.53
6:N:481:GLN:O	6:N:485:GLU:HG2	2.08	0.53
6:N:16:ASP:O	6:N:19:LEU:HB2	2.08	0.53
5:E:88:ALA:CB	5:E:119:THR:HB	2.29	0.53
4:L:196:LEU:HD22	4:L:377:VAL:HG22	1.89	0.53
6:F:105:ALA:C	6:F:107:ARG:H	2.10	0.53
6:F:451:LEU:O	6:F:455:PRO:HD3	2.07	0.53
8:P:24:ALA:CB	8:P:531:ALA:O	2.56	0.53
4:D:258:ARG:CD	8:H:283:GLN:HE21	2.20	0.53
7:G:386:ILE:O	7:G:389:VAL:HB	2.07	0.53
4:D:485:ARG:HH22	9:D:601:ADP:HN62	1.55	0.53
7:G:377:LEU:H	7:G:377:LEU:CD1	2.19	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:VAL:HG13	1:A:70:LEU:HD22	1.89	0.53
1:I:267:PRO:HB3	1:I:268:GLU:C	2.28	0.53
7:G:75:VAL:HG11	7:G:80:ALA:HB1	1.89	0.53
8:H:288:MET:HE2	8:H:313:LEU:HG	1.90	0.53
2:J:504:ALA:O	2:J:508:LEU:HB3	2.07	0.53
4:D:423:ARG:HH12	4:D:473:HIS:CD2	2.26	0.53
3:K:241:PRO:O	3:K:350:THR:HG23	2.08	0.53
6:F:183:ASP:OD1	6:F:183:ASP:N	2.41	0.53
8:H:354:LEU:H	8:H:354:LEU:HD23	1.73	0.53
8:H:213:MET:HE2	8:H:391:GLN:HG3	1.89	0.53
6:N:57:LYS:O	6:N:57:LYS:NZ	2.40	0.53
6:F:125:ALA:CA	6:F:426:LEU:HD21	2.38	0.53
1:I:363:GLN:HA	1:I:372:ILE:HA	1.90	0.53
2:J:422:ILE:HG21	2:J:427:SER:CB	2.36	0.53
4:L:196:LEU:HD22	4:L:377:VAL:CG2	2.37	0.53
4:L:375:VAL:HG12	4:L:376:SER:N	2.22	0.53
4:D:410:LEU:HD22	4:D:498:LEU:HB3	1.89	0.53
7:G:420:VAL:CG2	7:G:446:LEU:HD13	2.38	0.53
1:A:20:ILE:CB	1:A:25:ILE:HG12	2.38	0.53
2:B:196:ILE:O	2:B:367:ILE:HA	2.09	0.53
8:P:354:LEU:H	8:P:354:LEU:HD23	1.74	0.53
6:N:236:LEU:O	6:N:297:ASN:HA	2.08	0.53
1:I:94:ILE:HD11	1:I:526:LYS:HB2	1.89	0.53
1:I:412:THR:OG1	1:I:520:PRO:HG3	2.08	0.53
2:J:459:LEU:CD2	2:J:472:LEU:HG	2.33	0.53
2:B:39:PRO:HA	2:B:163:SER:CA	2.37	0.53
8:H:24:ALA:CB	8:H:531:ALA:HB1	2.37	0.53
1:I:158:ASN:CG	1:I:516:GLY:HA2	2.28	0.53
2:B:198:ILE:O	2:B:377:LEU:CD2	2.55	0.53
1:I:63:THR:HG22	1:I:65:ASP:N	2.22	0.53
2:B:31:ASP:OD1	2:B:32:LEU:N	2.40	0.53
7:O:75:VAL:HG11	7:O:80:ALA:HB1	1.89	0.53
6:N:406:LEU:HB3	6:N:407:LYS:NZ	2.24	0.53
8:P:428:ILE:HD13	8:P:478:LEU:HD13	1.89	0.53
5:E:476:LEU:HD11	5:E:538:ILE:HD11	1.90	0.53
6:F:117:ILE:CG1	5:M:33:LYS:HE2	2.34	0.53
3:K:457:ILE:HD11	3:K:467:LEU:HD22	1.90	0.53
5:M:350:GLU:O	5:M:351:LEU:C	2.46	0.53
5:M:84:THR:HG23	5:M:418:GLU:OE2	2.08	0.53
4:L:110:LEU:CD1	4:L:439:ILE:HG23	2.38	0.53
2:J:49:ALA:HB2	6:N:536:ALA:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:229:ASN:HA	8:P:368:VAL:HG22	1.90	0.53
8:P:420:LEU:HD23	8:P:421:PRO:N	2.24	0.53
5:E:81:ILE:HG22	5:E:414:MET:HE1	1.89	0.53
2:J:229:ALA:HB3	2:J:339:GLU:O	2.07	0.53
2:B:319:LEU:CD2	2:B:357:SER:OG	2.57	0.53
2:B:201:GLY:N	6:F:86:ILE:HD12	2.21	0.53
2:B:127:ALA:CB	2:B:430:VAL:HG22	2.31	0.53
7:G:225:SER:HB3	7:G:314:CYS:O	2.09	0.53
6:F:35:THR:HG21	6:F:42:THR:O	2.08	0.53
7:O:206:GLY:O	7:O:379:ARG:HD2	2.07	0.53
1:A:431:ILE:HG13	1:A:435:ASN:HD22	1.73	0.53
5:M:93:GLN:NE2	5:M:93:GLN:HA	2.23	0.53
2:B:124:TYR:O	2:B:128:SER:HB2	2.08	0.53
5:M:471:GLY:HA2	5:M:474:GLN:OE1	2.08	0.53
1:A:532:LEU:HD22	1:A:536:VAL:HG23	1.90	0.53
3:C:432:LYS:HA	3:C:439:GLN:HE21	1.72	0.53
4:L:491:ASN:HB2	4:L:494:GLU:OE1	2.09	0.53
7:G:201:ILE:HG21	7:G:390:GLU:HG3	1.90	0.53
6:N:183:ASP:N	6:N:183:ASP:OD1	2.41	0.53
8:H:420:LEU:HD23	8:H:421:PRO:N	2.24	0.53
6:F:416:GLY:HA2	6:F:419:TYR:CD2	2.44	0.53
6:F:437:LYS:HE2	6:F:437:LYS:CA	2.33	0.53
6:F:36:ASN:HA	6:F:57:LYS:CD	2.38	0.53
7:O:191:ARG:HB3	7:O:193:ASP:O	2.08	0.53
2:J:30:GLY:CA	2:J:33:VAL:CG2	2.86	0.53
6:F:105:ALA:HA	6:F:108:PHE:CD2	2.44	0.53
1:A:158:ASN:CG	1:A:516:GLY:HA2	2.28	0.53
4:D:77:MET:CE	7:G:384:GLN:HB2	2.39	0.53
4:L:36:ARG:HE	4:L:98:ILE:CG2	2.18	0.53
1:A:63:THR:HG22	1:A:65:ASP:N	2.22	0.53
2:J:124:TYR:O	2:J:128:SER:HB2	2.08	0.53
1:I:20:ILE:CB	1:I:25:ILE:HG12	2.38	0.53
4:L:423:ARG:HH12	4:L:473:HIS:CD2	2.26	0.53
8:H:27:GLN:O	8:H:31:SER:N	2.33	0.53
3:K:422:ALA:HA	3:K:475:HIS:CE1	2.44	0.53
6:N:143:LEU:HD11	6:N:145:ASN:CG	2.29	0.53
4:L:249:GLU:O	7:O:259:VAL:HG12	2.09	0.53
3:C:269:TRP:HH2	6:F:248:ASN:H	1.56	0.53
5:M:350:GLU:C	5:M:352:GLU:H	2.11	0.53
6:F:45:MET:HA	6:F:55:LEU:HA	1.91	0.53
6:N:105:ALA:HA	6:N:108:PHE:CD2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:45:LEU:HD12	6:N:533:LEU:HD13	1.91	0.53
5:E:58:ALA:CB	5:E:127:SER:HB3	2.39	0.53
5:M:58:ALA:CB	5:M:127:SER:HB3	2.39	0.53
5:E:100:ILE:O	5:E:103:LEU:HB2	2.08	0.53
3:K:413:SER:HB3	3:K:419:THR:HG21	1.91	0.53
5:M:227:GLN:O	5:M:407:PHE:HA	2.09	0.53
1:I:44:LEU:HD21	1:I:103:ILE:HD12	1.89	0.53
2:J:43:ASP:O	6:N:530:CYS:HA	2.09	0.53
5:E:273:THR:CG2	5:E:364:PRO:CA	2.72	0.53
6:F:5:LEU:CA	6:F:6:LEU:HB2	2.34	0.53
8:P:243:LYS:C	8:P:244:LYS:CG	2.77	0.53
5:E:188:LEU:CB	5:E:197:HIS:HB2	2.38	0.53
6:N:76:ILE:CG2	6:N:95:VAL:HG13	2.39	0.53
2:B:376:THR:HA	2:B:379:GLU:HB2	1.91	0.53
1:I:498:ARG:O	1:I:499:ASN:CB	2.56	0.53
5:M:81:ILE:HG22	5:M:414:MET:HE1	1.91	0.53
7:O:201:ILE:HG21	7:O:390:GLU:HG3	1.90	0.53
6:F:15:ARG:O	6:F:18:ALA:HB3	2.08	0.53
6:N:171:THR:N	6:N:172:PRO:CD	2.71	0.53
1:I:184:LEU:CD2	1:I:184:LEU:C	2.76	0.53
4:D:524:ILE:HG23	7:G:52:LEU:HD22	1.91	0.53
2:J:409:MET:CE	2:J:409:MET:HA	2.38	0.53
1:A:363:GLN:HA	1:A:372:ILE:HA	1.90	0.53
8:H:237:LYS:HB3	8:H:314:ASN:HB3	1.63	0.53
4:D:263:ILE:HD13	4:D:263:ILE:O	2.09	0.53
2:B:91:GLY:HA2	9:B:601:ADP:PA	2.48	0.53
6:N:35:THR:HG21	6:N:42:THR:O	2.08	0.53
2:J:39:PRO:HD2	2:J:474:LEU:HD12	1.91	0.53
5:E:58:ALA:HB3	5:E:127:SER:HB3	1.91	0.53
6:N:324:ASN:O	6:N:328:LEU:N	2.33	0.53
8:P:67:ASP:HB3	8:P:70:THR:OG1	2.08	0.53
6:F:167:THR:HB	6:F:169:VAL:H	1.66	0.53
6:F:171:THR:N	6:F:172:PRO:CD	2.71	0.53
9:N:601:ADP:C8	9:N:601:ADP:O2'	2.62	0.53
3:C:269:TRP:CZ3	6:F:247:VAL:HB	2.44	0.53
7:G:43:THR:HB	7:G:99:THR:CG2	2.40	0.53
6:F:195:GLU:CG	6:F:197:MET:SD	2.94	0.53
2:B:289:LEU:HD12	2:B:289:LEU:O	2.08	0.53
6:N:276:LYS:O	6:N:279:ASP:N	2.42	0.53
6:F:345:PRO:O	6:F:347:ILE:HG13	2.09	0.53
1:I:541:ILE:HD13	5:M:73:ILE:HG13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:164:LYS:O	2:J:165:ILE:C	2.48	0.53
1:I:544:MET:HG2	1:I:546:THR:HG23	1.90	0.53
6:N:345:PRO:O	6:N:347:ILE:HG13	2.09	0.53
4:D:491:ASN:HB2	4:D:494:GLU:OE1	2.09	0.53
5:M:61:ILE:O	5:M:61:ILE:HD13	2.08	0.53
3:C:422:ALA:HA	3:C:475:HIS:CE1	2.44	0.53
7:O:225:SER:HB3	7:O:314:CYS:O	2.09	0.52
2:J:263:LYS:HZ1	3:K:266:GLU:HB3	1.66	0.52
8:P:252:CYS:HB2	8:P:343:ARG:H	1.73	0.52
4:D:195:ARG:O	4:D:196:LEU:HD23	2.10	0.52
2:B:39:PRO:HD2	2:B:474:LEU:HD12	1.91	0.52
5:M:310:ILE:HD11	5:M:331:ALA:HB1	1.91	0.52
7:G:307:PHE:CD1	7:G:312:ILE:HG23	2.44	0.52
2:J:64:LEU:HD23	2:J:67:ILE:HD12	1.91	0.52
7:O:377:LEU:O	7:O:377:LEU:HD22	2.09	0.52
1:A:544:MET:HG2	1:A:546:THR:HG23	1.90	0.52
8:H:146:VAL:C	8:H:148:GLY:H	2.10	0.52
5:E:471:GLY:HA2	5:E:474:GLN:OE1	2.08	0.52
6:N:167:THR:OG1	6:N:169:VAL:HB	2.09	0.52
6:N:231:ALA:O	6:N:351:SER:OG	2.22	0.52
6:F:352:GLY:CA	6:F:369:GLU:C	2.48	0.52
8:H:243:LYS:C	8:H:244:LYS:CG	2.77	0.52
2:B:445:ALA:HB2	2:B:455:LEU:HD23	1.90	0.52
8:P:423:ALA:HA	9:P:601:ADP:H2'	1.90	0.52
7:G:241:ILE:HG12	7:G:292:ILE:HG23	1.89	0.52
6:N:45:MET:HA	6:N:55:LEU:HA	1.91	0.52
6:N:105:ALA:C	6:N:107:ARG:H	2.10	0.52
2:B:102:LEU:HD21	2:B:124:TYR:HD2	1.75	0.52
5:M:100:ILE:O	5:M:103:LEU:HB2	2.08	0.52
2:J:106:ALA:HB1	2:J:509:LEU:HD11	1.91	0.52
4:L:310:ILE:HG22	4:L:312:VAL:HG23	1.92	0.52
1:A:498:ARG:O	1:A:499:ASN:CB	2.57	0.52
1:I:501:GLY:HA3	1:I:512:GLU:CG	2.39	0.52
8:H:328:GLU:HG3	8:H:331:ARG:HH12	1.72	0.52
5:E:48:LYS:O	5:E:51:ILE:HG22	2.09	0.52
6:N:129:SER:HB2	6:N:426:LEU:HD23	1.91	0.52
7:G:66:GLY:HA2	7:G:69:ILE:HG22	1.92	0.52
2:B:88:VAL:HG13	2:B:393:GLN:NE2	2.21	0.52
5:E:84:THR:HG22	5:E:86:ASP:N	2.19	0.52
4:L:241:ILE:HD13	4:L:292:ILE:HG23	1.92	0.52
5:E:74:LEU:HG	5:E:93:GLN:CB	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:36:VAL:HG13	1:I:70:LEU:HD22	1.89	0.52
7:O:420:VAL:CG2	7:O:446:LEU:HD13	2.38	0.52
5:E:498:LEU:HD11	5:E:512:VAL:HG23	1.91	0.52
8:H:428:ILE:HD13	8:H:478:LEU:HD13	1.90	0.52
6:N:171:THR:O	6:N:175:THR:OG1	2.24	0.52
6:F:129:SER:HB2	6:F:426:LEU:HD23	1.91	0.52
2:B:407:ALA:O	2:B:411:MET:HG2	2.10	0.52
2:J:514:ILE:HG22	2:J:515:ILE:N	2.24	0.52
4:L:69:ALA:O	8:P:15:LYS:HE2	2.09	0.52
5:M:355:ALA:HB2	5:M:362:ILE:HD11	1.90	0.52
3:K:320:VAL:CG1	3:K:324:ASP:HB3	2.40	0.52
5:M:544:LEU:HD23	6:N:384:THR:CG2	2.40	0.52
8:P:463:LEU:HD11	9:P:601:ADP:H8	1.73	0.52
6:F:76:ILE:CG2	6:F:95:VAL:HG13	2.39	0.52
1:A:458:ILE:HD12	1:A:458:ILE:N	2.24	0.52
2:J:102:LEU:O	2:J:105:GLU:HB2	2.10	0.52
5:M:498:LEU:HD11	5:M:512:VAL:HG23	1.91	0.52
6:F:406:LEU:HB3	6:F:407:LYS:NZ	2.24	0.52
4:D:198:LYS:H	4:D:198:LYS:HD3	1.74	0.52
2:J:319:LEU:CD2	2:J:357:SER:OG	2.57	0.52
7:G:516:LEU:HD13	7:G:517:ILE:H	1.75	0.52
8:H:54:ILE:HG13	8:H:64:ILE:CG1	2.15	0.52
7:O:91:ASP:O	7:O:95:GLY:CA	2.57	0.52
5:E:186:THR:HG23	5:E:187:SER:N	2.24	0.52
6:F:143:LEU:HD11	6:F:145:ASN:CG	2.29	0.52
2:J:245:ILE:O	2:J:246:PHE:CG	2.62	0.52
5:E:166:ASP:N	5:E:167:ASP:CB	2.66	0.52
8:P:138:THR:HG21	8:P:452:PHE:CE1	2.45	0.52
8:P:160:LEU:HA	8:P:163:ILE:HG22	1.92	0.52
8:H:160:LEU:HA	8:H:163:ILE:HG22	1.92	0.52
2:J:102:LEU:HD21	2:J:124:TYR:CD2	2.45	0.52
5:M:58:ALA:HB3	5:M:127:SER:HB3	1.91	0.52
2:B:102:LEU:HD21	2:B:124:TYR:CD2	2.45	0.52
5:M:48:LYS:O	5:M:51:ILE:HG22	2.09	0.52
6:N:436:ALA:HA	6:N:437:LYS:HE2	1.92	0.52
3:C:320:VAL:CG1	3:C:324:ASP:HB3	2.40	0.52
4:L:195:ARG:O	4:L:196:LEU:HD23	2.10	0.52
4:L:263:ILE:O	4:L:263:ILE:HD13	2.09	0.52
2:B:295:GLU:HB2	6:F:337:GLN:CD	2.29	0.52
2:B:106:ALA:HB1	2:B:509:LEU:HD11	1.91	0.52
3:C:413:SER:HB3	3:C:419:THR:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:85:GLN:NE2	4:L:507:ALA:HB2	2.25	0.52
5:E:37:ASN:HD22	6:N:114:HIS:CD2	2.27	0.52
3:C:341:GLU:OE1	8:H:281:GLU:OE1	2.28	0.52
7:G:91:ASP:O	7:G:95:GLY:CA	2.57	0.52
2:B:30:GLY:CA	2:B:33:VAL:CG2	2.86	0.52
2:B:245:ILE:O	2:B:246:PHE:CB	2.56	0.52
3:C:320:VAL:O	3:C:321:LYS:O	2.28	0.52
2:J:376:THR:HA	2:J:379:GLU:HB2	1.91	0.52
1:I:226:CYS:SG	1:I:318:VAL:HG12	2.50	0.52
7:O:307:PHE:CD1	7:O:312:ILE:HG23	2.44	0.52
4:D:292:ILE:HG13	4:D:293:LEU:CA	2.40	0.52
4:D:94:THR:O	4:D:98:ILE:HG12	2.10	0.52
4:D:135:LEU:HD11	4:D:411:ILE:HD11	1.92	0.52
2:J:102:LEU:HD21	2:J:124:TYR:HD2	1.74	0.52
2:J:159:THR:HG21	2:J:488:VAL:N	2.25	0.52
4:D:219:ALA:HB1	4:D:221:LYS:HZ3	1.74	0.52
2:B:153:LEU:HB3	2:B:178:THR:HG22	1.92	0.52
8:H:229:ASN:HA	8:H:368:VAL:HG22	1.91	0.52
3:K:60:ASP:OD1	3:K:93:THR:HG21	2.10	0.52
7:G:243:SER:HB2	7:G:334:ILE:HD13	1.92	0.52
6:F:515:ASN:ND2	6:F:516:ALA:N	2.58	0.52
2:J:407:ALA:O	2:J:411:MET:HG2	2.10	0.52
6:F:420:ILE:CB	6:F:482:ASP:OD1	2.58	0.52
6:N:420:ILE:CB	6:N:482:ASP:OD1	2.58	0.52
2:B:245:ILE:O	2:B:246:PHE:CG	2.62	0.52
1:A:147:SER:OG	1:A:418:VAL:HB	2.10	0.52
6:F:16:ASP:CA	6:F:19:LEU:HD12	2.28	0.52
2:J:256:ALA:HB1	3:K:266:GLU:OE2	2.10	0.52
5:M:88:ALA:HB1	5:M:109:LYS:HZ2	1.72	0.52
2:B:64:LEU:HD23	2:B:67:ILE:HD12	1.91	0.52
4:L:449:VAL:O	4:L:453:THR:HG23	2.10	0.52
7:G:303:ALA:O	7:G:307:PHE:HD2	1.93	0.52
2:J:231:ILE:HD13	2:J:282:ASN:HB2	1.92	0.52
8:H:138:THR:HG21	8:H:452:PHE:CE1	2.45	0.52
5:M:74:LEU:HG	5:M:93:GLN:CB	2.39	0.52
4:D:178:VAL:CG1	4:D:401:ILE:HD11	2.40	0.52
2:B:68:PRO:HG2	6:F:536:ALA:HB2	1.92	0.52
4:D:85:GLN:NE2	4:D:507:ALA:HB2	2.25	0.52
7:G:156:GLU:OE1	7:G:157:LEU:HB2	2.10	0.52
1:A:344:LEU:CD1	1:A:345:GLU:H	2.23	0.52
6:N:36:ASN:HA	6:N:57:LYS:CD	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:57:LYS:O	6:F:57:LYS:NZ	2.40	0.52
6:N:193:MET:HE2	6:N:330:LEU:HD11	1.92	0.52
6:N:367:VAL:HG12	6:N:369:GLU:O	2.10	0.52
6:F:353:LEU:O	6:F:367:VAL:HG12	2.09	0.52
4:L:521:ILE:CD1	7:O:62:ILE:HD12	2.36	0.52
4:L:20:VAL:HG13	4:L:524:ILE:HD12	1.92	0.52
2:J:371:GLY:O	2:J:372:ALA:C	2.49	0.52
6:N:143:LEU:CD1	6:N:145:ASN:OD1	2.58	0.52
2:B:514:ILE:HG22	2:B:515:ILE:N	2.24	0.52
6:N:488:TYR:O	6:N:489:VAL:HB	2.10	0.52
2:J:141:ASP:CG	2:J:142:ASN:H	2.13	0.52
3:C:165:ILE:HA	3:C:168:SER:HB3	1.91	0.52
7:O:303:ALA:O	7:O:307:PHE:HD2	1.92	0.52
4:D:241:ILE:HD13	4:D:292:ILE:HG23	1.91	0.52
4:L:292:ILE:HG13	4:L:293:LEU:CA	2.40	0.52
6:F:137:LYS:O	6:F:138:ILE:HB	2.10	0.52
6:N:342:ASP:O	6:N:345:PRO:HD3	2.10	0.52
7:G:424:LEU:O	7:G:427:TYR:N	2.43	0.52
2:B:102:LEU:O	2:B:105:GLU:HB2	2.10	0.52
7:O:243:SER:HB2	7:O:334:ILE:HD13	1.92	0.52
1:A:501:GLY:HA3	1:A:512:GLU:CG	2.39	0.52
5:E:450:MET:HE3	5:E:454:VAL:HG23	1.92	0.52
6:N:416:GLY:HA2	6:N:419:TYR:CD2	2.44	0.52
7:O:516:LEU:HD13	7:O:517:ILE:H	1.75	0.52
6:F:143:LEU:HD13	6:F:145:ASN:CB	2.40	0.52
8:H:243:LYS:HB3	8:H:244:LYS:CE	2.40	0.52
2:B:159:THR:HG21	2:B:488:VAL:N	2.25	0.52
4:L:94:THR:O	4:L:98:ILE:HG12	2.10	0.52
5:E:93:GLN:NE2	5:E:93:GLN:HA	2.23	0.52
2:J:198:ILE:O	2:J:377:LEU:CD2	2.55	0.52
4:D:419:ILE:O	4:D:423:ARG:HG3	2.09	0.52
4:L:419:ILE:O	4:L:423:ARG:HG3	2.10	0.52
1:A:345:GLU:CD	1:A:346:GLY:HA2	2.30	0.52
5:M:450:MET:HE3	5:M:454:VAL:HG23	1.92	0.52
1:I:345:GLU:CD	1:I:346:GLY:HA2	2.30	0.52
8:H:67:ASP:HB3	8:H:70:THR:OG1	2.08	0.52
6:F:167:THR:OG1	6:F:169:VAL:HB	2.09	0.51
3:C:491:ILE:H	3:C:491:ILE:HD13	1.75	0.51
6:F:143:LEU:CD1	6:F:145:ASN:OD1	2.58	0.51
6:F:488:TYR:O	6:F:489:VAL:HG12	2.10	0.51
8:P:463:LEU:CD1	9:P:601:ADP:H8	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:92:THR:OG1	9:F:601:ADP:O2B	2.28	0.51
3:C:104:LEU:CD1	3:C:520:LEU:HD12	2.39	0.51
4:L:226:PRO:CB	4:L:311:MET:HG2	2.40	0.51
2:J:250:PHE:CA	6:N:250:GLY:O	2.56	0.51
6:F:276:LYS:O	6:F:279:ASP:N	2.43	0.51
5:E:509:ASN:O	5:E:521:ASP:HA	2.09	0.51
7:G:377:LEU:O	7:G:377:LEU:HD22	2.09	0.51
6:N:201:HIS:HB3	6:N:381:LYS:HZ3	1.74	0.51
2:J:45:LEU:HB2	6:N:533:LEU:HB2	1.92	0.51
4:D:310:ILE:HG22	4:D:312:VAL:HG23	1.91	0.51
6:N:406:LEU:HD22	6:N:407:LYS:HZ1	1.75	0.51
1:A:549:PRO:HA	5:E:77:PRO:O	2.10	0.51
2:B:319:LEU:HD11	2:B:355:LYS:O	2.10	0.51
6:F:485:GLU:O	6:F:486:THR:C	2.48	0.51
6:F:488:TYR:O	6:F:489:VAL:HB	2.10	0.51
2:B:141:ASP:CG	2:B:142:ASN:H	2.13	0.51
7:O:225:SER:O	7:O:226:TYR:HB3	2.10	0.51
5:E:197:HIS:O	5:E:200:PHE:N	2.44	0.51
2:B:43:ASP:OD1	6:F:529:LEU:HD22	2.11	0.51
4:D:226:PRO:CB	4:D:311:MET:HG2	2.40	0.51
7:O:242:LEU:HB2	7:O:293:VAL:HG12	1.93	0.51
5:E:310:ILE:HD11	5:E:331:ALA:HB1	1.91	0.51
5:E:431:ARG:O	5:E:434:VAL:HG12	2.10	0.51
2:J:153:LEU:HB3	2:J:178:THR:HG22	1.92	0.51
6:F:356:GLN:CB	6:F:365:THR:HG22	2.40	0.51
6:N:92:THR:HG23	10:N:602:BEF:F3	2.00	0.51
3:K:49:LEU:HD21	3:K:55:LEU:HD23	1.92	0.51
5:E:197:HIS:O	5:E:198:ASP:C	2.49	0.51
6:F:39:PRO:HA	6:F:160:THR:CB	2.40	0.51
4:L:147:ARG:HG2	4:L:148:GLU:H	1.74	0.51
7:O:413:GLY:CA	7:O:491:ASN:HD21	2.22	0.51
6:F:342:ASP:O	6:F:345:PRO:HD3	2.10	0.51
6:N:138:ILE:O	6:N:138:ILE:CG2	2.58	0.51
3:K:250:LEU:HD23	3:K:250:LEU:N	2.26	0.51
5:M:431:ARG:O	5:M:434:VAL:HG12	2.10	0.51
8:P:304:GLY:N	8:P:323:VAL:HG11	2.26	0.51
6:N:356:GLN:CB	6:N:365:THR:HG22	2.40	0.51
3:C:38:CYS:HA	3:C:44:MET:H	1.75	0.51
4:D:192:ASN:HB2	7:G:361:ARG:HH21	1.76	0.51
6:F:129:SER:O	6:F:422:LEU:HD23	2.10	0.51
5:M:186:THR:HG23	5:M:187:SER:N	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:242:LYS:HE2	2:B:247:GLY:H	1.69	0.51
6:N:488:TYR:O	6:N:489:VAL:HG12	2.10	0.51
5:M:197:HIS:O	5:M:198:ASP:C	2.49	0.51
2:J:88:VAL:HG13	2:J:393:GLN:NE2	2.21	0.51
3:K:165:ILE:HA	3:K:168:SER:HB3	1.91	0.51
2:B:164:LYS:O	2:B:165:ILE:C	2.48	0.51
7:G:418:MET:HE3	7:G:447:GLU:HG2	1.93	0.51
8:H:163:ILE:CG2	8:H:179:SER:HB2	2.40	0.51
5:E:76:SER:HB2	5:E:79:GLY:H	1.75	0.51
5:M:76:SER:HB2	5:M:79:GLY:H	1.75	0.51
4:D:8:ASN:C	4:D:10:THR:H	2.14	0.51
2:J:319:LEU:HD11	2:J:355:LYS:O	2.10	0.51
6:N:424:ARG:HD3	6:N:483:SER:OG	2.11	0.51
6:F:143:LEU:HD13	6:F:145:ASN:OD1	2.10	0.51
5:M:197:HIS:O	5:M:200:PHE:N	2.44	0.51
5:M:166:ASP:N	5:M:167:ASP:CB	2.66	0.51
5:E:341:PRO:O	5:E:343:VAL:HG23	2.11	0.51
6:F:92:THR:OG1	9:F:601:ADP:O3B	2.28	0.51
4:D:147:ARG:HG2	4:D:148:GLU:H	1.74	0.51
7:G:242:LEU:HB2	7:G:293:VAL:HG12	1.92	0.51
2:J:93:THR:HG21	9:J:601:ADP:O3B	2.10	0.51
1:A:12:THR:HB	5:E:96:LEU:HA	1.91	0.51
8:H:452:PHE:CE1	8:H:456:PHE:HE2	2.28	0.51
4:D:390:THR:O	4:D:394:LEU:HD23	2.10	0.51
8:P:31:SER:O	8:P:35:ILE:HG12	2.11	0.51
6:F:354:VAL:HA	6:F:367:VAL:HA	1.93	0.51
6:N:143:LEU:HD13	6:N:145:ASN:CB	2.40	0.51
3:K:47:MET:HE2	3:K:49:LEU:HD21	1.93	0.51
7:G:225:SER:O	7:G:226:TYR:HB3	2.10	0.51
8:P:243:LYS:HB3	8:P:244:LYS:CE	2.41	0.51
8:P:15:LYS:HE3	8:P:16:GLN:N	2.26	0.51
3:K:320:VAL:O	3:K:321:LYS:O	2.28	0.51
1:I:350:PHE:CD2	1:I:351:GLU:N	2.72	0.51
6:N:209:PHE:HB2	6:N:378:ILE:CB	2.40	0.51
3:K:104:LEU:CD1	3:K:520:LEU:HD12	2.39	0.51
6:N:56:THR:OG1	6:N:61:VAL:HG11	2.10	0.51
3:C:153:LYS:HD3	3:C:500:TRP:CD1	2.46	0.51
5:M:509:ASN:O	5:M:521:ASP:HA	2.09	0.51
2:J:46:LEU:HD11	2:J:63:ILE:HA	1.93	0.51
4:D:298:ASN:CB	4:D:299:ASP:HA	2.37	0.51
8:P:163:ILE:CG2	8:P:179:SER:HB2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:402:LEU:CD1	2:B:483:ARG:HE	2.24	0.51
7:G:126:MET:CE	7:G:126:MET:HA	2.40	0.51
7:G:126:MET:HE2	7:G:126:MET:HA	1.92	0.51
6:F:114:HIS:HA	5:M:37:ASN:HB2	1.92	0.51
1:A:258:MET:HE3	1:A:258:MET:HA	1.93	0.51
6:N:167:THR:HG22	6:N:168:GLU:HB3	1.93	0.51
6:N:151:LEU:CD2	6:N:175:THR:HG23	2.41	0.51
2:B:371:GLY:O	2:B:372:ALA:C	2.49	0.51
2:B:442:THR:HG23	2:B:452:SER:CB	2.34	0.51
4:D:449:VAL:O	4:D:453:THR:HG23	2.10	0.51
7:G:292:ILE:HA	7:G:313:PHE:O	2.10	0.51
1:A:226:CYS:SG	1:A:318:VAL:HG12	2.50	0.51
5:M:506:LYS:C	5:M:507:ILE:HD12	2.31	0.51
5:E:55:ARG:NH2	5:E:134:LEU:HD13	2.26	0.51
8:P:250:PHE:CE2	8:P:299:ILE:HD12	2.45	0.51
7:O:126:MET:CE	7:O:126:MET:HA	2.40	0.51
7:O:156:GLU:OE1	7:O:157:LEU:HB2	2.10	0.51
5:E:227:GLN:O	5:E:407:PHE:HA	2.09	0.51
7:O:459:PHE:HB3	7:O:460:ASP:HB3	1.93	0.51
3:K:38:CYS:HA	3:K:44:MET:H	1.75	0.51
6:F:167:THR:HG22	6:F:168:GLU:HB3	1.93	0.51
6:N:437:LYS:CA	6:N:437:LYS:HE2	2.33	0.51
6:F:436:ALA:HA	6:F:437:LYS:HE2	1.92	0.51
6:N:230:ASN:H	6:N:353:LEU:HD23	1.76	0.51
6:N:354:VAL:HA	6:N:367:VAL:HA	1.93	0.51
6:N:515:ASN:ND2	6:N:516:ALA:N	2.58	0.51
6:N:143:LEU:HD13	6:N:145:ASN:OD1	2.10	0.51
3:K:491:ILE:H	3:K:491:ILE:HD13	1.75	0.51
3:C:335:THR:CB	8:H:237:LYS:HE2	2.30	0.51
1:I:147:SER:OG	1:I:418:VAL:HB	2.10	0.51
3:K:266:GLU:CD	3:K:266:GLU:N	2.64	0.51
6:N:39:PRO:HA	6:N:160:THR:CB	2.41	0.51
3:C:60:ASP:OD1	3:C:93:THR:HG21	2.10	0.51
2:B:375:GLN:HE22	6:F:75:LEU:HB2	1.75	0.51
3:C:109:PRO:O	3:C:113:GLU:HG2	2.11	0.51
4:D:221:LYS:HE2	4:D:225:GLY:CA	2.41	0.51
6:N:129:SER:O	6:N:422:LEU:HD23	2.10	0.51
6:F:367:VAL:HG12	6:F:369:GLU:O	2.10	0.51
2:J:422:ILE:HG22	2:J:424:GLY:H	1.75	0.51
6:N:16:ASP:CA	6:N:19:LEU:HD12	2.28	0.51
8:P:29:ILE:O	8:P:32:ILE:HG22	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:483:LEU:HD11	9:E:601:ADP:H1'	1.92	0.51
3:K:153:LYS:HD3	3:K:500:TRP:CD1	2.46	0.51
3:K:109:PRO:O	3:K:113:GLU:HG2	2.11	0.51
1:I:221:GLY:HA3	1:I:374:ILE:O	2.11	0.51
1:I:104:ILE:HG12	1:I:458:ILE:HD11	1.93	0.51
8:H:304:GLY:N	8:H:323:VAL:HG11	2.26	0.51
4:L:8:ASN:C	4:L:10:THR:H	2.14	0.51
5:M:45:GLU:C	5:M:47:LYS:H	2.14	0.51
6:N:484:ASP:OD1	6:N:484:ASP:N	2.44	0.51
1:I:225:ASN:HD22	1:I:225:ASN:C	2.13	0.51
6:F:151:LEU:CD2	6:F:175:THR:HG23	2.41	0.51
6:F:230:ASN:H	6:F:353:LEU:HD23	1.76	0.51
7:O:62:ILE:O	7:O:63:SER:HB3	2.11	0.51
3:C:269:TRP:HZ3	6:F:247:VAL:HB	1.76	0.51
1:A:159:ILE:HD12	1:A:412:THR:HG21	1.93	0.51
1:A:351:GLU:O	1:A:353:SER:N	2.44	0.51
5:M:90:ILE:O	5:M:94:MET:HG2	2.11	0.51
7:O:292:ILE:HA	7:O:313:PHE:O	2.10	0.51
4:L:390:THR:O	4:L:394:LEU:HD23	2.10	0.51
4:L:450:ILE:HB	4:L:451:PRO:HD3	1.93	0.51
5:M:513:ASP:OD2	5:M:525:LEU:HD13	2.11	0.51
6:N:433:LYS:O	6:N:436:ALA:O	2.30	0.50
6:F:433:LYS:O	6:F:436:ALA:O	2.30	0.50
6:F:90:GLY:O	6:F:94:VAL:CG2	2.34	0.50
7:O:66:GLY:HA2	7:O:69:ILE:HG22	1.92	0.50
2:J:242:LYS:HE3	2:J:247:GLY:N	2.25	0.50
3:C:266:GLU:CD	3:C:266:GLU:N	2.64	0.50
6:F:424:ARG:HD3	6:F:483:SER:OG	2.11	0.50
2:B:46:LEU:HD11	2:B:63:ILE:HA	1.93	0.50
2:J:271:ASN:ND2	2:J:328:THR:OG1	2.44	0.50
6:F:56:THR:OG1	6:F:61:VAL:HG11	2.10	0.50
2:J:46:LEU:HD11	2:J:63:ILE:HD12	1.93	0.50
8:P:452:PHE:CE1	8:P:456:PHE:HE2	2.28	0.50
3:C:242:ARG:CB	3:C:292:PRO:HA	2.42	0.50
4:L:135:LEU:HD11	4:L:411:ILE:HD11	1.92	0.50
7:O:115:PHE:CD1	7:O:437:MET:HB3	2.46	0.50
4:L:198:LYS:HD3	4:L:198:LYS:H	1.74	0.50
4:L:229:LYS:CB	4:L:232:ALA:HB2	2.42	0.50
2:J:3:VAL:HB	2:J:4:GLN:OE1	2.12	0.50
6:N:353:LEU:O	6:N:367:VAL:HG12	2.09	0.50
4:D:20:VAL:HG13	4:D:524:ILE:HD12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:485:GLU:O	6:N:486:THR:C	2.48	0.50
1:I:351:GLU:O	1:I:353:SER:N	2.44	0.50
5:M:341:PRO:O	5:M:343:VAL:HG23	2.11	0.50
6:N:137:LYS:O	6:N:138:ILE:HB	2.10	0.50
3:K:242:ARG:CB	3:K:292:PRO:HA	2.42	0.50
5:E:513:ASP:OD2	5:E:525:LEU:HD13	2.11	0.50
1:A:225:ASN:HD22	1:A:225:ASN:C	2.14	0.50
6:F:484:ASP:OD1	6:F:484:ASP:N	2.44	0.50
4:D:30:SER:O	4:D:33:ASP:HB2	2.11	0.50
8:H:226:MET:HA	8:H:383:THR:OG1	2.11	0.50
6:N:440:THR:O	6:N:444:ILE:HG12	2.12	0.50
2:B:490:SER:HB2	2:B:492:LYS:NZ	2.26	0.50
5:M:88:ALA:CB	5:M:119:THR:HB	2.29	0.50
2:B:34:LYS:O	2:B:37:LEU:HG	2.12	0.50
8:P:287:MET:O	8:P:291:ILE:HG12	2.12	0.50
4:D:115:ILE:HG21	4:D:439:ILE:HG13	1.94	0.50
5:M:556:ILE:HG23	6:N:47:VAL:HB	1.93	0.50
7:O:346:LEU:HD23	7:O:346:LEU:H	1.76	0.50
4:L:418:GLU:HG3	4:L:447:LEU:O	2.11	0.50
8:P:31:SER:CB	8:P:79:HIS:HE1	2.24	0.50
4:L:386:ILE:C	4:L:388:ASP:H	2.15	0.50
2:B:3:VAL:HB	2:B:4:GLN:OE1	2.12	0.50
6:F:541:LEU:HB3	6:F:543:GLU:N	2.26	0.50
5:E:273:THR:O	5:E:274:CYS:CB	2.59	0.50
5:M:364:PRO:O	5:M:365:ARG:CB	2.59	0.50
8:H:49:CYS:O	8:H:466:THR:CB	2.57	0.50
7:O:171:ILE:O	7:O:171:ILE:HG22	2.12	0.50
1:A:221:GLY:HA3	1:A:374:ILE:O	2.11	0.50
6:N:538:ARG:NH1	6:N:538:ARG:CG	2.72	0.50
5:M:131:ASP:O	5:M:134:LEU:HB3	2.12	0.50
2:B:367:ILE:HG23	2:B:367:ILE:O	2.11	0.50
3:K:475:HIS:O	3:K:478:GLY:O	2.28	0.50
4:L:198:LYS:HD3	4:L:198:LYS:N	2.27	0.50
1:I:379:LYS:N	1:I:379:LYS:HD2	2.26	0.50
3:K:170:LYS:C	3:K:170:LYS:HD3	2.32	0.50
3:K:465:ILE:HD12	3:K:465:ILE:N	2.26	0.50
6:N:167:THR:HA	6:N:168:GLU:CB	2.40	0.50
6:N:124:ILE:HB	6:N:444:ILE:HD12	1.94	0.50
6:F:440:THR:O	6:F:444:ILE:HG12	2.12	0.50
5:E:364:PRO:O	5:E:365:ARG:CB	2.59	0.50
6:N:489:VAL:O	6:N:489:VAL:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:SER:HB3	1:A:418:VAL:O	2.11	0.50
1:I:147:SER:HB3	1:I:418:VAL:O	2.11	0.50
1:I:159:ILE:HD12	1:I:412:THR:HG21	1.93	0.50
2:B:292:ASP:HA	2:B:295:GLU:CD	2.32	0.50
5:E:506:LYS:C	5:E:507:ILE:HD12	2.31	0.50
1:A:161:LYS:HA	1:A:164:MET:HG2	1.93	0.50
5:M:55:ARG:NH2	5:M:134:LEU:HD13	2.26	0.50
5:E:210:ASN:N	5:E:210:ASN:HD22	2.08	0.50
4:D:450:ILE:HB	4:D:451:PRO:HD3	1.93	0.50
3:C:475:HIS:O	3:C:478:GLY:O	2.28	0.50
1:A:379:LYS:HD2	1:A:379:LYS:N	2.26	0.50
5:E:171:SER:HA	5:E:438:ARG:HA	1.93	0.50
4:L:430:ARG:O	4:L:431:SER:C	2.50	0.50
2:B:3:VAL:C	2:B:5:ILE:HG12	2.32	0.50
6:N:436:ALA:HA	6:N:437:LYS:CE	2.42	0.50
2:J:464:TYR:HA	2:J:467:ILE:CD1	2.42	0.50
2:J:422:ILE:O	2:J:423:ASP:OD2	2.30	0.50
6:F:209:PHE:HB2	6:F:378:ILE:CB	2.40	0.50
2:B:46:LEU:HD11	2:B:63:ILE:HD12	1.93	0.50
2:B:271:ASN:ND2	2:B:328:THR:OG1	2.44	0.50
7:G:455:GLU:CG	7:G:461:ALA:HB3	2.42	0.50
4:L:178:VAL:CG1	4:L:401:ILE:HD11	2.40	0.50
3:C:250:LEU:N	3:C:250:LEU:HD23	2.26	0.50
1:I:129:PHE:HB3	1:I:532:LEU:HD21	1.93	0.50
7:G:459:PHE:HB3	7:G:460:ASP:HB3	1.93	0.50
3:C:465:ILE:N	3:C:465:ILE:HD12	2.26	0.50
6:F:167:THR:HA	6:F:168:GLU:CB	2.40	0.50
6:N:430:ASN:O	6:N:433:LYS:CA	2.60	0.50
6:N:193:MET:HB3	6:N:330:LEU:HD12	1.94	0.50
2:B:422:ILE:O	2:B:423:ASP:OD2	2.30	0.50
7:G:191:ARG:NH1	7:G:192:ASN:HB2	2.27	0.50
3:C:49:LEU:HD21	3:C:55:LEU:HD23	1.93	0.50
2:B:507:VAL:HG13	3:C:57:LEU:HD12	1.94	0.50
6:N:409:LYS:HD3	6:N:409:LYS:N	2.16	0.50
6:F:411:ILE:CG2	6:F:412:ILE:H	2.16	0.50
5:E:90:ILE:O	5:E:94:MET:HG2	2.11	0.50
8:H:31:SER:O	8:H:35:ILE:HG12	2.11	0.50
8:H:31:SER:CB	8:H:79:HIS:HE1	2.25	0.50
8:H:79:HIS:ND1	8:H:81:ALA:HB3	2.27	0.50
1:I:344:LEU:CD1	1:I:345:GLU:H	2.23	0.50
6:F:387:ALA:O	6:F:391:THR:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:60:ASP:HB3	4:D:63:THR:OG1	2.12	0.50
5:M:535:LYS:O	5:M:539:LEU:HG	2.11	0.50
6:F:436:ALA:HA	6:F:437:LYS:CE	2.42	0.50
2:B:131:ALA:HB2	2:B:415:VAL:CG2	2.42	0.50
7:O:193:ASP:OD1	7:O:193:ASP:O	2.30	0.50
2:B:423:ASP:O	2:B:423:ASP:OD1	2.30	0.50
7:G:193:ASP:OD1	7:G:193:ASP:O	2.30	0.50
6:F:489:VAL:O	6:F:489:VAL:HG13	2.11	0.50
2:J:490:SER:HB2	2:J:492:LYS:NZ	2.26	0.50
8:H:29:ILE:O	8:H:32:ILE:HG22	2.11	0.50
2:B:231:ILE:HD13	2:B:282:ASN:HB2	1.92	0.50
4:L:115:ILE:HG21	4:L:439:ILE:HG13	1.94	0.50
8:H:259:THR:HG21	8:H:263:GLY:HA3	1.94	0.50
7:G:75:VAL:O	7:G:81:LYS:HE3	2.12	0.50
1:A:104:ILE:HG12	1:A:458:ILE:HD11	1.93	0.50
7:O:23:LYS:HA	7:O:26:ILE:HG22	1.93	0.50
7:G:115:PHE:CD1	7:G:437:MET:HB3	2.46	0.50
6:N:387:ALA:O	6:N:391:THR:HG23	2.12	0.50
3:C:170:LYS:HD3	3:C:170:LYS:C	2.32	0.50
4:L:30:SER:O	4:L:33:ASP:HB2	2.11	0.50
7:O:57:ASN:O	7:O:58:GLN:NE2	2.45	0.50
6:N:232:TYR:HA	6:N:351:SER:OG	2.12	0.50
2:B:464:TYR:HA	2:B:467:ILE:CD1	2.42	0.50
2:B:236:THR:HA	2:B:287:ARG:HD2	1.94	0.50
8:H:15:LYS:HE3	8:H:16:GLN:N	2.26	0.50
4:L:195:ARG:O	4:L:376:SER:HA	2.12	0.50
6:N:195:GLU:OE1	6:N:197:MET:HE2	2.11	0.50
4:D:229:LYS:CB	4:D:232:ALA:HB2	2.42	0.50
1:I:92:ARG:HB3	5:M:388:THR:HA	1.93	0.50
7:G:483:PHE:CB	9:G:601:ADP:N6	2.74	0.50
5:M:509:ASN:HB3	5:M:521:ASP:CB	2.36	0.50
2:J:235:ASN:ND2	3:K:304:LEU:HD21	2.27	0.50
7:G:23:LYS:HA	7:G:26:ILE:HG22	1.93	0.50
4:D:418:GLU:HG3	4:D:447:LEU:O	2.11	0.50
5:M:264:SER:O	5:M:266:GLY:O	2.30	0.50
8:P:83:LYS:O	8:P:87:MET:HG2	2.12	0.50
4:D:430:ARG:O	4:D:431:SER:C	2.50	0.50
3:K:29:LYS:O	3:K:33:ASP:HB2	2.12	0.50
5:E:45:GLU:C	5:E:47:LYS:H	2.14	0.50
2:J:242:LYS:HE2	2:J:247:GLY:N	2.26	0.49
2:B:164:LYS:O	2:B:167:SER:N	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:36:VAL:HG22	7:O:83:LEU:HD13	1.93	0.49
2:J:34:LYS:O	2:J:37:LEU:HG	2.12	0.49
2:J:195:ILE:HG21	2:J:381:GLU:HB2	1.93	0.49
7:O:75:VAL:O	7:O:81:LYS:HE3	2.12	0.49
7:O:214:PHE:CD1	7:O:376:LEU:HB3	2.46	0.49
4:L:221:LYS:HE2	4:L:225:GLY:CA	2.41	0.49
1:I:77:HIS:CG	1:I:78:PRO:HD2	2.47	0.49
6:F:406:LEU:O	6:F:406:LEU:HD23	2.12	0.49
4:D:198:LYS:N	4:D:198:LYS:HD3	2.27	0.49
5:M:132:GLN:HA	5:M:132:GLN:HE21	1.77	0.49
7:G:117:GLU:CD	7:G:117:GLU:H	2.15	0.49
8:P:226:MET:HA	8:P:383:THR:OG1	2.11	0.49
2:B:4:GLN:O	3:C:72:HIS:CB	2.60	0.49
6:F:171:THR:O	6:F:175:THR:OG1	2.24	0.49
6:N:491:VAL:HG12	6:N:492:ASP:N	2.27	0.49
6:F:2:SER:C	6:F:3:LEU:HD22	2.32	0.49
6:N:215:LEU:HB3	6:N:217:HIS:CD2	2.36	0.49
6:F:23:VAL:HG22	6:F:102:LEU:CD1	2.42	0.49
2:B:60:GLY:H	2:B:93:THR:CG2	2.25	0.49
5:E:509:ASN:HB3	5:E:521:ASP:CB	2.36	0.49
8:P:72:LEU:HA	8:P:75:LEU:HB2	1.94	0.49
7:G:346:LEU:HD23	7:G:346:LEU:H	1.76	0.49
6:N:406:LEU:HD23	6:N:406:LEU:O	2.12	0.49
1:A:129:PHE:HB3	1:A:532:LEU:HD21	1.93	0.49
3:C:29:LYS:O	3:C:33:ASP:HB2	2.12	0.49
8:P:259:THR:HG21	8:P:263:GLY:HA3	1.94	0.49
7:O:117:GLU:CD	7:O:117:GLU:H	2.15	0.49
5:M:325:TRP:CG	5:M:326:GLY:N	2.80	0.49
8:H:83:LYS:O	8:H:87:MET:HG2	2.12	0.49
6:F:43:LEU:CD2	6:F:161:LYS:HA	2.40	0.49
6:N:229:LYS:C	6:N:231:ALA:H	2.16	0.49
6:F:193:MET:HB3	6:F:330:LEU:HD12	1.94	0.49
2:J:131:ALA:HB2	2:J:415:VAL:CG2	2.42	0.49
5:M:364:PRO:HG3	6:N:307:ASP:CB	2.41	0.49
8:H:249:VAL:HG13	8:H:300:VAL:O	2.13	0.49
6:N:154:ALA:O	6:N:157:SER:CB	2.60	0.49
6:F:213:LEU:HD23	6:F:377:THR:CG2	2.40	0.49
8:H:287:MET:O	8:H:291:ILE:HG12	2.12	0.49
7:G:236:PHE:O	7:G:351:LEU:HA	2.12	0.49
2:J:42:MET:HB3	6:N:531:ASP:HB2	1.95	0.49
2:J:236:THR:HA	2:J:287:ARG:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:124:ALA:HB2	3:K:438:GLN:HE22	1.77	0.49
3:C:124:ALA:HB2	3:C:438:GLN:HE22	1.77	0.49
8:P:301:ALA:O	8:P:323:VAL:HA	2.11	0.49
6:F:121:GLY:O	6:F:444:ILE:HD13	2.12	0.49
6:F:124:ILE:HB	6:F:444:ILE:HD12	1.94	0.49
8:P:249:VAL:HG13	8:P:300:VAL:O	2.12	0.49
5:M:273:THR:O	5:M:274:CYS:CB	2.59	0.49
4:L:246:PRO:HB2	4:L:250:ASN:CG	2.33	0.49
3:K:16:THR:HA	3:K:525:ASP:HB3	1.95	0.49
7:O:304:THR:HA	7:O:307:PHE:CE2	2.46	0.49
2:B:195:ILE:HG21	2:B:381:GLU:HB2	1.93	0.49
1:A:8:SER:N	2:J:21:SER:OG	2.43	0.49
1:I:161:LYS:HA	1:I:164:MET:HG2	1.93	0.49
7:G:214:PHE:CD1	7:G:376:LEU:HB3	2.46	0.49
6:F:71:PRO:HG2	6:F:533:LEU:HD12	1.94	0.49
1:A:77:HIS:CG	1:A:78:PRO:HD2	2.47	0.49
8:H:301:ALA:O	8:H:323:VAL:HA	2.11	0.49
7:O:470:LEU:O	7:O:473:SER:OG	2.29	0.49
2:B:160:THR:HG21	2:B:390:VAL:HG21	1.94	0.49
2:J:170:LYS:HB2	2:J:170:LYS:NZ	2.28	0.49
2:B:409:MET:HA	2:B:409:MET:HE1	1.93	0.49
2:J:423:ASP:OD1	2:J:423:ASP:O	2.30	0.49
2:B:242:LYS:HE3	2:B:247:GLY:N	2.25	0.49
5:E:350:GLU:C	5:E:352:GLU:H	2.11	0.49
3:C:103:ILE:HD12	3:C:445:VAL:HG22	1.95	0.49
2:B:274:ALA:HB1	2:B:329:PHE:HA	1.94	0.49
5:E:84:THR:CG2	5:E:86:ASP:H	2.20	0.49
7:G:36:VAL:HG22	7:G:83:LEU:HD13	1.93	0.49
6:F:280:LEU:N	6:F:280:LEU:HD23	2.27	0.49
5:E:131:ASP:O	5:E:134:LEU:HB3	2.12	0.49
6:N:446:ALA:HA	6:N:449:GLU:HG3	1.95	0.49
5:E:535:LYS:O	5:E:539:LEU:HG	2.11	0.49
6:F:446:ALA:HA	6:F:449:GLU:HG3	1.95	0.49
5:M:171:SER:HA	5:M:438:ARG:HA	1.93	0.49
6:F:430:ASN:O	6:F:433:LYS:CA	2.60	0.49
7:O:191:ARG:NH1	7:O:192:ASN:HB2	2.27	0.49
6:N:2:SER:C	6:N:3:LEU:HD22	2.32	0.49
8:H:482:HIS:C	8:H:484:VAL:N	2.65	0.49
6:F:154:ALA:O	6:F:157:SER:CB	2.60	0.49
1:A:433:LEU:O	1:A:437:ALA:CB	2.61	0.49
1:I:433:LEU:O	1:I:437:ALA:CB	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:317:ARG:O	7:G:317:ARG:CD	2.61	0.49
7:O:236:PHE:O	7:O:351:LEU:HA	2.12	0.49
6:N:458:LEU:HD12	6:N:458:LEU:C	2.33	0.49
1:I:45:GLY:C	1:I:166:SER:HB2	2.33	0.49
8:H:250:PHE:CE2	8:H:299:ILE:HD12	2.45	0.49
2:J:502:SER:HA	2:J:505:ALA:HB3	1.94	0.49
1:I:501:GLY:HA3	1:I:512:GLU:HG2	1.95	0.49
8:P:79:HIS:ND1	8:P:81:ALA:HB3	2.27	0.49
5:E:132:GLN:HE21	5:E:132:GLN:HA	1.77	0.49
2:B:4:GLN:C	2:B:5:ILE:CG2	2.73	0.49
2:J:5:ILE:HD12	2:J:7:GLY:H	1.78	0.49
3:C:229:VAL:HG11	3:C:234:MET:HE2	1.95	0.49
1:A:96:ASP:OD1	9:A:601:ADP:O1B	2.31	0.49
2:J:72:PRO:HB3	3:K:47:MET:HE3	1.95	0.49
8:P:463:LEU:HD11	9:P:601:ADP:C8	2.48	0.49
8:H:29:ILE:HG22	8:H:30:LYS:N	2.28	0.49
6:F:61:VAL:O	6:F:65:GLU:HB2	2.13	0.49
3:C:430:LYS:O	3:C:433:GLN:CG	2.57	0.49
6:N:23:VAL:HG22	6:N:102:LEU:CD1	2.42	0.49
6:F:237:ASN:HA	6:F:297:ASN:OD1	2.13	0.49
2:J:183:ARG:O	2:J:184:LEU:CB	2.60	0.49
5:E:264:SER:O	5:E:266:GLY:O	2.30	0.49
2:J:3:VAL:C	2:J:5:ILE:HG12	2.32	0.49
6:F:232:TYR:HA	6:F:351:SER:OG	2.12	0.49
7:G:516:LEU:HD22	7:G:517:ILE:CA	2.42	0.49
3:K:103:ILE:HD12	3:K:445:VAL:HG22	1.95	0.49
1:I:12:THR:CG2	5:M:97:ASP:H	2.18	0.49
7:O:455:GLU:CG	7:O:461:ALA:HB3	2.42	0.49
4:D:46:LYS:HG3	8:H:532:THR:CG2	2.40	0.49
2:J:292:ASP:HA	2:J:295:GLU:CD	2.32	0.49
8:P:79:HIS:CE1	8:P:81:ALA:HB3	2.48	0.49
5:E:148:ASN:HA	5:E:151:ASP:HB2	1.95	0.49
7:G:57:ASN:O	7:G:58:GLN:NE2	2.45	0.49
6:F:117:ILE:HD12	5:M:34:ASP:C	2.33	0.49
7:O:29:ASN:OD1	7:O:79:ALA:HB2	2.12	0.49
2:B:464:TYR:HA	2:B:467:ILE:HD11	1.94	0.49
2:J:427:SER:O	2:J:430:VAL:HB	2.12	0.49
7:G:43:THR:HG21	7:G:64:ASN:O	2.13	0.49
4:L:209:MET:HE3	4:L:375:VAL:HG11	1.95	0.49
4:D:195:ARG:O	4:D:376:SER:HA	2.12	0.49
7:O:317:ARG:CD	7:O:317:ARG:O	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:13:LEU:HD22	1:I:14:PHE:H	1.78	0.49
4:L:77:MET:HE1	7:O:384:GLN:HB2	1.94	0.49
7:G:44:LEU:C	7:G:46:PRO:HD2	2.33	0.49
6:F:138:ILE:CG2	6:F:138:ILE:O	2.58	0.49
6:F:199:MET:O	6:F:381:LYS:HE2	2.13	0.49
7:G:143:LEU:HD22	7:G:411:ALA:HB2	1.94	0.49
8:H:163:ILE:HG23	8:H:179:SER:CB	2.42	0.49
2:B:32:LEU:HD11	6:F:532:GLU:CD	2.33	0.49
2:B:32:LEU:HG	6:F:532:GLU:CD	2.33	0.49
6:N:405:VAL:HG22	6:N:509:SER:HB2	1.94	0.49
5:E:558:GLY:HA2	6:F:48:ASP:HB2	1.94	0.49
5:E:157:ALA:HA	5:E:450:MET:HE1	1.95	0.49
8:H:356:GLU:HB2	8:H:374:GLU:HA	1.95	0.49
6:N:355:TYR:O	6:N:366:TYR:O	2.31	0.49
2:B:183:ARG:O	2:B:184:LEU:CB	2.60	0.49
2:J:160:THR:HG21	2:J:390:VAL:HG21	1.94	0.49
6:N:121:GLY:O	6:N:444:ILE:HD13	2.12	0.49
6:F:16:ASP:N	6:F:16:ASP:OD1	2.36	0.49
2:J:459:LEU:HD13	2:J:472:LEU:CD2	2.43	0.49
8:P:49:CYS:O	8:P:466:THR:CB	2.57	0.49
2:B:382:ARG:HH11	2:B:382:ARG:HG3	1.78	0.49
3:K:430:LYS:O	3:K:433:GLN:CG	2.57	0.49
7:G:413:GLY:CA	7:G:491:ASN:HD21	2.22	0.49
2:B:233:ILE:O	2:B:325:VAL:N	2.46	0.49
7:O:44:LEU:HB2	7:O:456:ASN:ND2	2.28	0.49
7:O:44:LEU:C	7:O:46:PRO:HD2	2.33	0.49
1:A:116:VAL:HG12	1:A:120:ILE:HG22	1.95	0.49
4:D:135:LEU:CD1	4:D:411:ILE:HD11	2.43	0.49
3:C:409:SER:C	3:C:411:SER:H	2.17	0.49
1:I:132:ALA:HB2	1:I:448:ILE:HD13	1.94	0.49
7:G:127:LYS:C	7:G:127:LYS:HD3	2.34	0.49
7:O:127:LYS:HD3	7:O:127:LYS:C	2.34	0.49
2:B:170:LYS:HB2	2:B:170:LYS:NZ	2.28	0.49
5:M:148:ASN:HA	5:M:151:ASP:HB2	1.95	0.49
7:G:62:ILE:O	7:G:63:SER:HB3	2.11	0.48
2:J:464:TYR:HA	2:J:467:ILE:HD11	1.94	0.48
2:J:514:ILE:HG22	2:J:515:ILE:H	1.78	0.48
2:J:263:LYS:NZ	3:K:266:GLU:CG	2.76	0.48
4:D:254:VAL:CG2	4:D:254:VAL:O	2.61	0.48
3:K:41:PRO:CA	3:K:161:THR:HG21	2.43	0.48
2:J:60:GLY:H	2:J:93:THR:CG2	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:HIS:CE1	5:E:68:ARG:HG3	2.48	0.48
1:A:14:PHE:CB	1:A:15:LEU:HA	2.43	0.48
1:I:164:MET:CE	1:I:169:ILE:HB	2.43	0.48
4:L:204:ILE:O	4:L:207:THR:HG23	2.13	0.48
4:L:135:LEU:CD1	4:L:411:ILE:HD11	2.43	0.48
8:P:334:ARG:HD3	8:P:380:ARG:HH11	1.78	0.48
5:M:157:ALA:HA	5:M:450:MET:HE1	1.95	0.48
4:L:325:SER:O	4:L:329:GLY:N	2.46	0.48
1:A:132:ALA:HB2	1:A:448:ILE:HD13	1.94	0.48
2:B:5:ILE:HD12	2:B:7:GLY:H	1.78	0.48
2:J:463:ILE:CG2	2:J:464:TYR:N	2.76	0.48
1:A:10:SER:O	1:A:11:ASP:O	2.31	0.48
1:A:45:GLY:C	1:A:166:SER:HB2	2.33	0.48
6:F:491:VAL:HG12	6:F:492:ASP:N	2.27	0.48
2:B:514:ILE:HG22	2:B:515:ILE:H	1.78	0.48
2:B:263:LYS:HZ1	3:C:266:GLU:HG2	1.78	0.48
6:F:160:THR:N	6:F:164:ALA:CB	2.76	0.48
8:P:29:ILE:HG22	8:P:30:LYS:N	2.28	0.48
3:C:16:THR:HA	3:C:525:ASP:HB3	1.95	0.48
2:J:274:ALA:HB1	2:J:329:PHE:HA	1.94	0.48
7:O:145:VAL:O	7:O:408:LEU:CA	2.58	0.48
7:G:107:GLU:HG2	7:G:448:VAL:HG21	1.95	0.48
1:A:164:MET:CE	1:A:169:ILE:HB	2.43	0.48
2:J:382:ARG:HG3	2:J:382:ARG:HH11	1.78	0.48
8:H:334:ARG:HD3	8:H:380:ARG:HH11	1.78	0.48
3:C:414:PRO:O	3:C:419:THR:HG23	2.14	0.48
5:E:547:MET:SD	6:F:387:ALA:HA	2.53	0.48
7:G:470:LEU:O	7:G:473:SER:OG	2.30	0.48
8:P:356:GLU:HB2	8:P:374:GLU:HA	1.95	0.48
5:M:193:VAL:HG12	5:M:193:VAL:O	2.14	0.48
5:E:189:GLY:O	5:E:190:SER:CB	2.61	0.48
6:N:433:LYS:O	6:N:436:ALA:C	2.52	0.48
6:F:229:LYS:C	6:F:231:ALA:H	2.16	0.48
7:G:29:ASN:OD1	7:G:79:ALA:HB2	2.12	0.48
1:I:264:ILE:HD12	1:I:264:ILE:O	2.13	0.48
8:H:72:LEU:HA	8:H:75:LEU:HB2	1.94	0.48
4:D:254:VAL:HG13	8:H:264:THR:O	2.14	0.48
2:B:459:LEU:HD13	2:B:472:LEU:CD2	2.43	0.48
6:N:160:THR:N	6:N:164:ALA:CB	2.76	0.48
2:B:57:THR:HG21	2:B:382:ARG:NH1	2.28	0.48
6:F:275:LYS:O	6:F:276:LYS:C	2.52	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:377:LEU:HD12	2:B:377:LEU:H	1.78	0.48
1:A:13:LEU:HD22	1:A:14:PHE:H	1.78	0.48
7:G:44:LEU:HB2	7:G:456:ASN:ND2	2.28	0.48
6:N:199:MET:O	6:N:381:LYS:HE2	2.13	0.48
1:I:540:ARG:HA	5:M:70:LEU:HD22	1.95	0.48
3:K:409:SER:C	3:K:411:SER:H	2.17	0.48
8:P:443:GLY:O	8:P:446:GLN:HG3	2.13	0.48
3:K:9:ASN:HD22	3:K:10:ALA:N	2.11	0.48
5:M:240:ILE:HG12	5:M:244:ILE:HG21	1.94	0.48
4:L:60:ASP:HB3	4:L:63:THR:OG1	2.12	0.48
6:N:353:LEU:H	6:N:369:GLU:HB3	1.77	0.48
5:M:32:VAL:CG2	5:M:33:LYS:H	2.15	0.48
2:B:467:ILE:HA	2:B:468:SER:HA	1.59	0.48
6:N:83:GLN:CD	6:N:94:VAL:HG21	2.34	0.48
2:B:427:SER:O	2:B:430:VAL:HB	2.12	0.48
4:D:260:MET:O	4:D:263:ILE:HG22	2.13	0.48
6:N:395:VAL:O	6:N:399:LEU:HB3	2.14	0.48
7:O:97:GLY:O	7:O:101:VAL:HG23	2.14	0.48
2:J:442:THR:HG23	2:J:452:SER:CB	2.34	0.48
5:M:84:THR:CG2	5:M:86:ASP:H	2.20	0.48
4:D:204:ILE:O	4:D:207:THR:HG23	2.13	0.48
3:C:9:ASN:HD22	3:C:10:ALA:N	2.11	0.48
6:F:405:VAL:HG22	6:F:509:SER:HB2	1.94	0.48
7:O:217:GLY:HA3	7:O:366:GLN:HA	1.95	0.48
2:B:118:GLN:O	2:B:121:ILE:HG12	2.14	0.48
4:D:8:ASN:OD1	4:D:8:ASN:O	2.31	0.48
8:H:348:THR:O	8:H:352:LEU:HD23	2.13	0.48
8:P:248:ALA:HB2	8:P:352:LEU:HD13	1.95	0.48
4:D:386:ILE:C	4:D:388:ASP:H	2.15	0.48
7:O:516:LEU:HD22	7:O:517:ILE:CA	2.42	0.48
1:I:10:SER:O	1:I:11:ASP:O	2.31	0.48
8:P:237:LYS:HB2	8:P:314:ASN:CB	2.31	0.48
6:F:105:ALA:C	6:F:107:ARG:N	2.67	0.48
6:N:61:VAL:O	6:N:65:GLU:HB2	2.13	0.48
1:I:12:THR:CB	5:M:96:LEU:HA	2.43	0.48
2:J:250:PHE:HA	6:N:250:GLY:C	2.32	0.48
2:J:57:THR:HG21	2:J:382:ARG:NH1	2.28	0.48
7:G:214:PHE:O	7:G:214:PHE:CG	2.67	0.48
2:B:502:SER:HA	2:B:505:ALA:HB3	1.94	0.48
3:C:9:ASN:ND2	3:C:10:ALA:H	2.11	0.48
8:H:85:LEU:HD13	8:H:107:ALA:HB1	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:31:SER:HB2	8:H:79:HIS:HE1	1.78	0.48
8:P:27:GLN:O	8:P:31:SER:N	2.33	0.48
6:F:355:TYR:O	6:F:366:TYR:O	2.31	0.48
2:B:463:ILE:CG2	2:B:464:TYR:N	2.76	0.48
4:D:523:ASP:O	7:G:51:ILE:CG2	2.53	0.48
6:N:486:THR:O	6:N:487:ARG:CB	2.62	0.48
4:D:265:LYS:HZ2	8:H:343:ARG:HD3	1.74	0.48
4:D:246:PRO:HB2	4:D:250:ASN:CG	2.33	0.48
7:G:171:ILE:O	7:G:171:ILE:HG22	2.12	0.48
4:L:81:VAL:HG21	4:L:514:CYS:SG	2.54	0.48
7:O:108:LEU:O	7:O:108:LEU:HD23	2.13	0.48
4:L:291:SER:HA	4:L:315:ASP:CA	2.44	0.48
6:F:47:VAL:HG12	6:F:48:ASP:N	2.28	0.48
6:N:430:ASN:HA	6:N:433:LYS:HB2	1.96	0.48
2:J:438:ARG:O	2:J:441:PRO:HG2	2.14	0.48
1:A:494:ARG:CB	1:A:496:SER:H	2.21	0.48
6:F:486:THR:O	6:F:487:ARG:CB	2.62	0.48
4:L:72:HIS:CD2	8:P:15:LYS:NZ	2.82	0.48
5:E:351:LEU:HD22	5:E:352:GLU:N	2.29	0.48
2:J:206:SER:HB2	2:J:368:VAL:HG22	1.94	0.48
4:L:367:ARG:C	4:L:369:ASN:N	2.67	0.48
8:H:443:GLY:O	8:H:446:GLN:HG3	2.13	0.48
6:F:406:LEU:HD22	6:F:407:LYS:HZ1	1.78	0.48
4:D:448:GLU:C	4:D:451:PRO:HD2	2.34	0.48
6:N:237:ASN:HA	6:N:297:ASN:OD1	2.13	0.48
8:P:85:LEU:HD13	8:P:107:ALA:HB1	1.95	0.48
7:O:500:ALA:O	7:O:504:ILE:HG13	2.14	0.48
5:M:215:ASP:O	5:M:216:ARG:CB	2.62	0.48
5:E:215:ASP:O	5:E:216:ARG:CB	2.62	0.48
2:J:314:VAL:HG11	3:K:232:PRO:HD3	1.95	0.48
2:J:59:ASP:HB3	2:J:62:THR:OG1	2.14	0.48
8:H:65:THR:HG22	8:H:396:ASP:OD1	2.14	0.48
6:N:429:ALA:O	6:N:433:LYS:HD3	2.14	0.48
6:F:433:LYS:O	6:F:436:ALA:C	2.52	0.48
6:N:332:THR:HB	6:N:351:SER:HA	1.96	0.48
6:N:414:GLY:O	6:N:415:ALA:CB	2.62	0.48
8:H:310:LEU:HD13	8:H:314:ASN:OD1	2.14	0.48
6:N:485:GLU:CG	6:N:489:VAL:HB	2.44	0.48
5:M:250:SER:HB3	5:M:342:ALA:O	2.14	0.48
7:G:97:GLY:O	7:G:101:VAL:HG23	2.14	0.48
8:P:48:PRO:HB3	8:P:172:TYR:CD1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:LEU:O	1:A:156:LEU:HD23	2.14	0.48
1:A:92:ARG:HG2	5:E:388:THR:CB	2.43	0.48
6:F:22:ASN:O	6:F:72:THR:HG21	2.14	0.48
7:O:107:GLU:HG2	7:O:448:VAL:HG21	1.95	0.48
6:F:429:ALA:O	6:F:433:LYS:HD3	2.14	0.48
6:N:2:SER:HA	6:N:3:LEU:CB	2.35	0.48
3:K:268:ASP:O	3:K:272:ILE:HG12	2.14	0.48
5:M:401:THR:C	5:M:402:LYS:CG	2.70	0.48
5:M:351:LEU:HD22	5:M:352:GLU:N	2.29	0.48
2:B:263:LYS:NZ	3:C:266:GLU:CB	2.77	0.48
7:O:43:THR:HB	7:O:99:THR:CG2	2.39	0.48
2:J:285:ILE:HD13	2:J:285:ILE:H	1.78	0.48
4:D:44:MET:HG3	8:H:531:ALA:CB	2.41	0.48
3:C:479:ASN:HB3	3:C:482:THR:OG1	2.14	0.48
7:G:241:ILE:HG12	7:G:292:ILE:CG2	2.44	0.48
2:J:233:ILE:O	2:J:325:VAL:N	2.46	0.48
2:J:377:LEU:H	2:J:377:LEU:HD12	1.78	0.48
6:F:458:LEU:HD12	6:F:458:LEU:C	2.33	0.48
5:M:373:LYS:HE2	6:N:311:LYS:HZ3	1.79	0.48
4:L:91:ASP:OD1	10:L:602:BEF:F1	2.22	0.48
5:E:193:VAL:O	5:E:193:VAL:HG12	2.14	0.48
8:P:65:THR:HG22	8:P:396:ASP:OD1	2.14	0.48
6:N:541:LEU:HB3	6:N:543:GLU:N	2.26	0.48
6:F:332:THR:HB	6:F:351:SER:HA	1.96	0.48
6:F:353:LEU:H	6:F:369:GLU:HB3	1.77	0.48
6:F:83:GLN:CD	6:F:94:VAL:HG21	2.34	0.48
3:C:471:LEU:HG	3:C:491:ILE:HG13	1.96	0.48
3:C:268:ASP:O	3:C:272:ILE:HG12	2.14	0.48
1:A:94:ILE:HD12	1:A:94:ILE:N	2.29	0.48
1:I:351:GLU:C	1:I:353:SER:N	2.66	0.48
4:L:254:VAL:O	4:L:254:VAL:CG2	2.61	0.48
1:A:264:ILE:HD12	1:A:264:ILE:O	2.14	0.48
7:G:145:VAL:O	7:G:408:LEU:CA	2.58	0.48
7:G:455:GLU:N	7:G:461:ALA:HB2	2.29	0.48
1:I:116:VAL:HG12	1:I:120:ILE:HG22	1.95	0.48
8:P:163:ILE:HG23	8:P:179:SER:CB	2.42	0.48
5:E:133:ALA:HB2	5:E:150:PHE:HE2	1.79	0.48
7:O:174:ASN:ND2	7:O:209:MET:SD	2.80	0.48
8:H:48:PRO:HB3	8:H:172:TYR:CD1	2.49	0.48
1:A:501:GLY:HA3	1:A:512:GLU:HG2	1.95	0.48
5:E:325:TRP:CG	5:E:326:GLY:N	2.80	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:167:THR:CB	6:F:169:VAL:N	2.64	0.47
3:K:471:LEU:HG	3:K:491:ILE:HG13	1.96	0.47
8:P:310:LEU:HD13	8:P:314:ASN:OD1	2.14	0.47
1:A:162:THR:HG21	1:A:518:LEU:O	2.13	0.47
1:I:162:THR:HG21	1:I:518:LEU:O	2.13	0.47
5:M:355:ALA:CB	6:N:222:PRO:HG2	2.43	0.47
3:C:225:LEU:HD13	3:C:320:VAL:HG11	1.96	0.47
3:K:225:LEU:HD13	3:K:320:VAL:HG11	1.96	0.47
2:B:88:VAL:CG1	2:B:393:GLN:HE22	2.22	0.47
4:L:260:MET:O	4:L:263:ILE:HG22	2.13	0.47
3:C:39:LEU:CB	9:C:1101:ADP:O2A	2.62	0.47
6:N:454:ILE:N	6:N:455:PRO:HD2	2.29	0.47
5:E:85:ASN:ND2	9:E:601:ADP:O3B	2.46	0.47
4:D:81:VAL:HG21	4:D:514:CYS:SG	2.54	0.47
2:B:282:ASN:ND2	2:B:303:ILE:HB	2.29	0.47
4:L:298:ASN:HB3	4:L:299:ASP:CA	2.43	0.47
6:N:47:VAL:HG12	6:N:48:ASP:N	2.28	0.47
2:B:32:LEU:CD1	6:F:532:GLU:CD	2.82	0.47
6:N:71:PRO:HG2	6:N:533:LEU:HD12	1.94	0.47
7:O:214:PHE:O	7:O:214:PHE:CG	2.67	0.47
2:B:124:TYR:N	2:B:124:TYR:HD1	2.12	0.47
7:G:208:ALA:O	7:G:211:GLU:HB2	2.14	0.47
7:O:115:PHE:CE1	7:O:437:MET:HB3	2.49	0.47
8:H:79:HIS:CE1	8:H:81:ALA:HB3	2.48	0.47
4:L:8:ASN:OD1	4:L:8:ASN:O	2.31	0.47
8:P:396:ASP:HA	8:P:399:ARG:HH11	1.79	0.47
7:G:500:ALA:O	7:G:504:ILE:HG13	2.14	0.47
8:H:6:PRO:CG	4:L:71:LEU:HA	2.35	0.47
2:J:410:VAL:HB	2:J:468:SER:OG	2.13	0.47
5:E:32:VAL:CG2	5:E:33:LYS:H	2.15	0.47
6:N:86:ILE:HG23	6:N:87:THR:HG23	1.96	0.47
6:F:414:GLY:O	6:F:415:ALA:CB	2.62	0.47
2:B:242:LYS:HE2	2:B:247:GLY:N	2.26	0.47
5:E:250:SER:HB3	5:E:342:ALA:O	2.14	0.47
5:E:175:LEU:O	5:E:175:LEU:HD12	2.14	0.47
3:K:129:LEU:HD23	3:K:510:VAL:HG12	1.96	0.47
7:O:241:ILE:HG12	7:O:292:ILE:CG2	2.44	0.47
7:G:120:ILE:HG23	8:P:472:ASN:ND2	2.30	0.47
4:D:298:ASN:HB3	4:D:299:ASP:CA	2.43	0.47
4:L:434:GLY:HA3	4:L:436:GLN:OE1	2.14	0.47
8:H:167:ILE:HD11	8:H:182:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:237:THR:N	2:J:287:ARG:HD2	2.28	0.47
4:D:174:ALA:O	4:D:178:VAL:HG23	2.13	0.47
7:G:108:LEU:O	7:G:108:LEU:HD23	2.13	0.47
8:H:248:ALA:HB2	8:H:352:LEU:HD13	1.95	0.47
8:P:248:ALA:HB2	8:P:352:LEU:CD1	2.44	0.47
5:E:277:GLU:CB	5:E:278:PRO:HD2	2.44	0.47
2:J:319:LEU:HD23	2:J:319:LEU:C	2.35	0.47
2:B:422:ILE:HG22	2:B:424:GLY:H	1.75	0.47
1:I:14:PHE:CB	1:I:15:LEU:HA	2.43	0.47
3:K:479:ASN:HB3	3:K:482:THR:OG1	2.14	0.47
5:E:74:LEU:HD12	5:E:93:GLN:HB3	1.96	0.47
7:O:143:LEU:HD22	7:O:411:ALA:HB2	1.94	0.47
3:K:117:HIS:HE1	8:P:50:GLY:O	1.97	0.47
6:N:105:ALA:C	6:N:107:ARG:N	2.67	0.47
2:J:124:TYR:N	2:J:124:TYR:CD1	2.82	0.47
1:A:540:ARG:HA	5:E:70:LEU:HD22	1.95	0.47
3:K:84:THR:HG21	8:P:389:ALA:HA	1.97	0.47
5:E:428:CYS:O	5:E:431:ARG:HG3	2.15	0.47
1:A:258:MET:HE2	1:A:259:GLY:H	1.79	0.47
3:K:170:LYS:O	3:K:170:LYS:HD3	2.14	0.47
8:H:248:ALA:HB2	8:H:352:LEU:CD1	2.44	0.47
2:B:59:ASP:HB3	2:B:62:THR:OG1	2.14	0.47
4:L:350:VAL:HG22	4:L:363:VAL:HG13	1.97	0.47
9:N:601:ADP:H8	9:N:601:ADP:O2'	1.97	0.47
1:I:94:ILE:HD12	1:I:94:ILE:N	2.29	0.47
8:H:423:ALA:CA	9:H:601:ADP:H2'	2.31	0.47
2:J:263:LYS:HZ1	3:K:266:GLU:HG2	1.78	0.47
7:O:43:THR:HG21	7:O:64:ASN:O	2.13	0.47
6:N:213:LEU:HD23	6:N:377:THR:CG2	2.40	0.47
5:M:175:LEU:O	5:M:175:LEU:HD12	2.14	0.47
3:K:495:VAL:HG23	3:K:500:TRP:CH2	2.48	0.47
2:J:282:ASN:ND2	2:J:303:ILE:HB	2.29	0.47
2:J:63:ILE:CG2	2:J:64:LEU:HG	2.44	0.47
2:J:469:THR:CG2	2:J:481:ASP:HB2	2.44	0.47
3:K:112:ILE:HG13	3:K:113:GLU:N	2.29	0.47
1:I:221:GLY:HA2	1:I:382:SER:CB	2.42	0.47
4:D:367:ARG:C	4:D:369:ASN:N	2.67	0.47
2:J:118:GLN:O	2:J:121:ILE:HG12	2.14	0.47
4:L:448:GLU:C	4:L:451:PRO:HD2	2.34	0.47
7:G:235:LYS:CB	7:G:353:GLU:HA	2.44	0.47
2:B:410:VAL:HB	2:B:468:SER:OG	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:457:ILE:HG22	3:C:462:GLY:O	2.14	0.47
2:B:514:ILE:HG23	3:C:47:MET:O	2.14	0.47
3:C:47:MET:HG2	3:C:48:LEU:N	2.30	0.47
1:A:419:VAL:CG1	1:A:425:VAL:HG21	2.44	0.47
8:H:243:LYS:HB3	8:H:244:LYS:NZ	2.29	0.47
8:P:243:LYS:HB3	8:P:244:LYS:NZ	2.29	0.47
6:F:424:ARG:NE	6:F:424:ARG:HA	2.12	0.47
2:J:289:LEU:HD21	2:J:304:ASN:OD1	2.15	0.47
2:B:285:ILE:HD13	2:B:285:ILE:H	1.78	0.47
2:B:289:LEU:HD21	2:B:304:ASN:OD1	2.15	0.47
4:D:81:VAL:HA	7:G:382:ALA:HB2	1.96	0.47
7:O:452:GLN:HA	7:O:455:GLU:HB2	1.96	0.47
4:L:292:ILE:N	4:L:293:LEU:CA	2.73	0.47
3:K:108:ALA:O	3:K:112:ILE:HG23	2.15	0.47
6:N:108:PHE:CE1	6:N:118:ILE:HG13	2.50	0.47
2:J:402:LEU:CD1	2:J:483:ARG:HE	2.24	0.47
5:E:150:PHE:CD1	5:E:472:PHE:CE2	3.03	0.47
5:M:133:ALA:HB2	5:M:150:PHE:HE2	1.79	0.47
8:H:164:LYS:HB3	8:H:165:PRO:HD3	1.96	0.47
4:D:12:LYS:HZ2	7:G:73:LEU:CD2	2.28	0.47
3:K:414:PRO:O	3:K:419:THR:HG23	2.14	0.47
7:G:217:GLY:O	7:G:375:THR:HG22	2.15	0.47
6:F:406:LEU:HB3	6:F:407:LYS:HZ2	1.80	0.47
8:P:31:SER:HB2	8:P:79:HIS:HE1	1.78	0.47
8:P:348:THR:O	8:P:352:LEU:HD23	2.13	0.47
3:C:184:LYS:HA	3:C:198:ILE:C	2.35	0.47
5:M:189:GLY:O	5:M:190:SER:CB	2.61	0.47
3:K:174:LEU:HG	3:K:219:VAL:HG22	1.96	0.47
2:B:93:THR:OG1	9:B:601:ADP:O2A	2.31	0.47
6:N:280:LEU:HD23	6:N:280:LEU:N	2.27	0.47
5:M:150:PHE:CD1	5:M:472:PHE:CE2	3.03	0.47
1:I:145:SER:O	1:I:148:VAL:HG23	2.15	0.47
6:N:246:GLU:H	6:N:246:GLU:CD	2.18	0.47
2:B:463:ILE:HD11	2:B:468:SER:OG	2.15	0.47
4:D:24:ASN:ND2	4:D:524:ILE:HD11	2.29	0.47
4:D:521:ILE:CB	7:G:50:ASP:O	2.61	0.47
2:J:463:ILE:HD11	2:J:468:SER:OG	2.15	0.47
7:O:51:ILE:HB	7:O:69:ILE:HD11	1.96	0.47
6:F:86:ILE:HG23	6:F:87:THR:HG23	1.96	0.47
6:N:3:LEU:N	6:N:3:LEU:HD22	2.30	0.47
3:K:457:ILE:HG22	3:K:462:GLY:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:3:LEU:N	6:F:3:LEU:HD22	2.30	0.47
6:F:485:GLU:CG	6:F:489:VAL:HB	2.44	0.47
2:B:142:ASN:CB	2:B:143:SER:HA	2.18	0.47
5:E:88:ALA:HB1	5:E:109:LYS:HZ2	1.77	0.47
6:F:424:ARG:HE	6:F:424:ARG:CA	2.17	0.47
1:I:156:LEU:HD23	1:I:156:LEU:O	2.14	0.47
6:N:22:ASN:O	6:N:72:THR:HG21	2.14	0.47
7:G:204:ILE:O	7:G:379:ARG:HD3	2.14	0.47
7:G:279:PHE:O	7:G:282:LEU:HD12	2.15	0.47
7:G:292:ILE:N	7:G:312:ILE:HG13	2.30	0.47
7:G:291:ASN:C	7:G:312:ILE:HG13	2.34	0.47
6:N:275:LYS:O	6:N:276:LYS:C	2.52	0.47
2:J:60:GLY:O	2:J:63:ILE:HG22	2.15	0.47
3:C:112:ILE:HG13	3:C:113:GLU:N	2.29	0.47
3:C:108:ALA:O	3:C:112:ILE:HG23	2.15	0.47
3:C:117:HIS:CG	3:C:118:PRO:HD2	2.50	0.47
2:B:124:TYR:N	2:B:124:TYR:CD1	2.82	0.47
3:K:142:PRO:HG3	3:K:411:SER:CA	2.44	0.47
7:G:217:GLY:HA3	7:G:366:GLN:HA	1.95	0.47
2:J:403:GLY:O	2:J:482:MET:HG3	2.14	0.47
8:H:35:ILE:HD13	8:H:82:VAL:HA	1.95	0.47
8:H:396:ASP:HA	8:H:399:ARG:HH11	1.79	0.47
8:H:99:GLY:O	8:H:103:VAL:HG23	2.15	0.47
4:D:352:GLU:HA	4:D:361:VAL:HA	1.95	0.47
3:C:174:LEU:HG	3:C:219:VAL:HG22	1.96	0.47
6:F:246:GLU:H	6:F:246:GLU:CD	2.18	0.47
3:K:175:ALA:O	3:K:179:VAL:HG23	2.14	0.47
3:K:25:ILE:HD13	3:K:26:THR:N	2.30	0.47
3:K:184:LYS:HA	3:K:198:ILE:C	2.35	0.47
3:C:407:MET:HE1	3:C:408:LEU:HD23	1.97	0.47
4:D:350:VAL:HG22	4:D:363:VAL:HG13	1.97	0.47
7:O:94:VAL:CG1	7:O:95:GLY:H	2.28	0.47
6:N:16:ASP:N	6:N:16:ASP:OD1	2.36	0.47
2:B:27:ILE:HG12	2:B:27:ILE:O	2.15	0.47
1:A:351:GLU:C	1:A:353:SER:N	2.66	0.47
3:C:41:PRO:CA	3:C:161:THR:HG21	2.43	0.47
6:N:76:ILE:HG21	6:N:95:VAL:HG13	1.96	0.47
2:B:328:THR:O	2:B:329:PHE:CB	2.62	0.47
5:E:84:THR:CG2	5:E:85:ASN:N	2.78	0.47
7:G:409:ILE:CG2	7:G:410:VAL:H	2.28	0.47
2:B:232:LEU:HD22	2:B:233:ILE:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:455:GLU:N	7:O:461:ALA:HB2	2.29	0.47
3:K:117:HIS:CG	3:K:118:PRO:HD2	2.50	0.47
3:K:9:ASN:ND2	3:K:10:ALA:H	2.11	0.47
7:O:217:GLY:HA3	7:O:365:PHE:O	2.15	0.47
5:M:428:CYS:O	5:M:431:ARG:HG3	2.14	0.47
3:C:262:GLU:H	8:H:266:LEU:CD1	2.28	0.47
5:M:547:MET:SD	6:N:387:ALA:HA	2.55	0.47
3:C:25:ILE:HD13	3:C:26:THR:N	2.30	0.47
5:E:176:PHE:O	5:E:180:LEU:HD23	2.15	0.47
6:F:430:ASN:HA	6:F:433:LYS:HB2	1.96	0.47
4:L:523:ASP:O	7:O:51:ILE:CG2	2.53	0.47
4:L:134:ILE:HD12	4:L:421:ILE:HD13	1.95	0.47
2:J:494:LYS:HA	2:J:494:LYS:HD2	1.79	0.47
6:F:454:ILE:HB	6:F:455:PRO:HD3	1.97	0.47
2:B:403:GLY:O	2:B:482:MET:HG3	2.14	0.47
3:C:348:VAL:HG12	3:C:349:GLY:N	2.30	0.47
3:K:348:VAL:HG12	3:K:349:GLY:N	2.30	0.47
7:O:455:GLU:HG3	7:O:461:ALA:HB3	1.97	0.47
1:A:12:THR:CB	5:E:96:LEU:HA	2.44	0.47
4:L:92:GLY:O	4:L:96:VAL:HG23	2.15	0.47
3:C:202:ARG:O	3:C:204:VAL:O	2.32	0.47
4:D:178:VAL:CB	4:D:401:ILE:HD11	2.45	0.47
4:L:174:ALA:O	4:L:178:VAL:HG23	2.13	0.47
4:L:461:ASN:HD22	4:L:462:SER:N	2.13	0.47
3:C:142:PRO:HG3	3:C:411:SER:CA	2.44	0.47
1:A:480:TYR:O	1:A:483:ALA:CB	2.63	0.47
8:P:35:ILE:HD13	8:P:82:VAL:HA	1.95	0.47
5:M:277:GLU:CB	5:M:278:PRO:HD2	2.44	0.47
2:J:324:GLU:H	3:K:311:LYS:NZ	2.12	0.47
3:K:246:LEU:O	3:K:247:ASP:HB3	2.15	0.47
8:P:99:GLY:O	8:P:103:VAL:HG23	2.15	0.47
4:L:352:GLU:HA	4:L:361:VAL:HA	1.95	0.47
8:H:6:PRO:CB	8:H:7:GLN:HG3	2.38	0.47
2:B:319:LEU:C	2:B:319:LEU:HD23	2.35	0.47
2:B:438:ARG:O	2:B:441:PRO:HG2	2.14	0.47
1:I:419:VAL:CG1	1:I:425:VAL:HG21	2.44	0.47
2:J:263:LYS:HZ1	3:K:266:GLU:CG	2.26	0.47
6:F:141:THR:CB	6:F:409:LYS:HG3	2.45	0.47
2:B:165:ILE:HD13	6:F:526:ASN:HB2	1.97	0.47
7:O:279:PHE:O	7:O:282:LEU:HD12	2.15	0.47
7:O:291:ASN:C	7:O:312:ILE:HG13	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:292:ILE:N	4:D:293:LEU:CA	2.73	0.47
1:I:29:ASN:HD22	1:I:538:ILE:HG23	1.80	0.47
4:D:434:GLY:HA3	4:D:436:GLN:OE1	2.14	0.47
5:M:210:ASN:N	5:M:210:ASN:HD22	2.08	0.47
3:C:275:ILE:O	8:H:274:LEU:HD21	2.15	0.47
5:E:240:ILE:HG12	5:E:244:ILE:HG21	1.94	0.47
7:G:217:GLY:HA3	7:G:365:PHE:O	2.15	0.47
7:O:354:GLU:HA	7:O:363:ASN:HA	1.97	0.47
5:E:262:GLU:HA	5:E:263:GLY:HA2	1.67	0.47
2:J:477:GLY:O	2:J:478:THR:CB	2.62	0.47
7:O:235:LYS:CB	7:O:353:GLU:HA	2.44	0.46
4:D:521:ILE:CD1	7:G:62:ILE:HD12	2.44	0.46
2:J:30:GLY:HA2	2:J:33:VAL:HG21	1.97	0.46
6:F:395:VAL:O	6:F:399:LEU:HB3	2.14	0.46
5:M:84:THR:CG2	5:M:85:ASN:N	2.78	0.46
7:O:204:ILE:O	7:O:379:ARG:HD3	2.14	0.46
3:K:202:ARG:O	3:K:204:VAL:O	2.32	0.46
4:D:496:HIS:O	4:D:498:LEU:HD12	2.15	0.46
1:A:16:GLY:CA	1:A:548:ASP:HB3	2.44	0.46
8:H:442:PRO:HA	8:H:446:GLN:HE21	1.80	0.46
1:I:480:TYR:O	1:I:483:ALA:CB	2.63	0.46
7:G:115:PHE:CE1	7:G:437:MET:HB3	2.49	0.46
1:A:128:GLY:O	1:A:448:ILE:HD13	2.15	0.46
7:G:354:GLU:HA	7:G:363:ASN:HA	1.97	0.46
1:A:145:SER:O	1:A:148:VAL:HG23	2.15	0.46
7:G:17:THR:HG22	7:G:526:ASN:HD22	1.80	0.46
6:F:422:LEU:HD13	6:F:517:ILE:HD11	1.98	0.46
6:F:332:THR:HB	6:F:350:PHE:O	2.15	0.46
6:N:515:ASN:C	6:N:515:ASN:HD22	2.18	0.46
3:K:229:VAL:HG12	3:K:230:VAL:H	1.80	0.46
6:N:143:LEU:HD13	6:N:145:ASN:CG	2.36	0.46
6:N:143:LEU:HD21	6:N:145:ASN:HB3	1.97	0.46
2:B:513:ASN:O	2:B:514:ILE:CD1	2.46	0.46
1:A:143:VAL:HG12	1:A:419:VAL:HG22	1.97	0.46
6:F:454:ILE:N	6:F:455:PRO:HD2	2.29	0.46
2:B:444:LEU:HD21	9:B:601:ADP:C1'	2.46	0.46
2:B:42:MET:HE3	6:F:529:LEU:O	2.15	0.46
6:F:76:ILE:HG21	6:F:95:VAL:HG13	1.96	0.46
7:O:83:LEU:HD23	7:O:86:ILE:CD1	2.45	0.46
7:G:304:THR:HA	7:G:307:PHE:CE2	2.46	0.46
8:P:167:ILE:HD11	8:P:182:VAL:HG21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:202:ARG:HH21	3:K:323:SER:HB3	1.81	0.46
1:A:16:GLY:HA3	1:A:548:ASP:CB	2.44	0.46
3:C:250:LEU:CG	3:C:301:VAL:CB	2.92	0.46
5:E:103:LEU:HA	5:E:106:GLN:HE21	1.81	0.46
7:O:208:ALA:O	7:O:211:GLU:HB2	2.14	0.46
5:M:176:PHE:O	5:M:180:LEU:HD23	2.15	0.46
5:E:301:TYR:HA	5:E:304:ASP:OD2	2.15	0.46
3:C:175:ALA:O	3:C:179:VAL:HG23	2.15	0.46
7:O:60:THR:O	7:O:60:THR:HG23	2.15	0.46
4:L:194:ILE:O	4:L:194:ILE:HG12	2.15	0.46
2:B:26:ALA:HB1	2:B:77:LEU:HD11	1.98	0.46
6:N:166:LEU:HG	6:N:167:THR:OG1	2.15	0.46
2:B:408:GLU:CD	2:B:440:LEU:HD23	2.36	0.46
6:N:427:ARG:HG2	6:N:448:ALA:CB	2.46	0.46
6:N:16:ASP:HA	6:N:19:LEU:CG	2.45	0.46
6:F:195:GLU:OE1	6:F:197:MET:HE2	2.15	0.46
6:N:454:ILE:HB	6:N:455:PRO:HD3	1.97	0.46
6:F:362:GLU:CG	6:F:364:PHE:CE2	2.93	0.46
4:L:147:ARG:O	4:L:151:VAL:HG23	2.16	0.46
4:D:77:MET:HE1	7:G:384:GLN:HB2	1.97	0.46
7:O:292:ILE:N	7:O:312:ILE:HG13	2.30	0.46
2:B:469:THR:CG2	2:B:481:ASP:HB2	2.44	0.46
5:M:114:GLU:HB3	6:N:201:HIS:CE1	2.50	0.46
4:L:178:VAL:CB	4:L:401:ILE:HD11	2.45	0.46
2:J:124:TYR:N	2:J:124:TYR:HD1	2.12	0.46
8:P:442:PRO:HA	8:P:446:GLN:HE21	1.80	0.46
3:C:170:LYS:HD3	3:C:170:LYS:O	2.14	0.46
8:H:184:GLU:O	8:H:188:HIS:HD2	1.97	0.46
5:M:301:TYR:HA	5:M:304:ASP:OD2	2.15	0.46
2:B:360:LYS:HA	2:B:361:ALA:HA	1.69	0.46
7:G:51:ILE:HB	7:G:69:ILE:HD11	1.96	0.46
6:F:143:LEU:HD13	6:F:145:ASN:CG	2.36	0.46
2:B:242:LYS:HA	3:C:269:TRP:HE1	1.81	0.46
6:F:16:ASP:HA	6:F:19:LEU:CG	2.45	0.46
4:D:134:ILE:HD12	4:D:421:ILE:HD13	1.95	0.46
4:L:254:VAL:HG22	8:P:264:THR:O	2.16	0.46
2:B:58:ASN:ND2	2:B:58:ASN:C	2.69	0.46
1:I:92:ARG:HG2	5:M:388:THR:CB	2.46	0.46
2:J:328:THR:O	2:J:329:PHE:CB	2.62	0.46
7:G:144:ALA:HA	7:G:409:ILE:O	2.14	0.46
9:D:601:ADP:C3'	9:D:601:ADP:C8	2.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:162:SER:O	2:J:163:SER:CB	2.64	0.46
2:J:165:ILE:HD13	6:N:526:ASN:HB2	1.98	0.46
4:D:92:GLY:O	4:D:96:VAL:HG23	2.15	0.46
5:M:114:GLU:HG2	6:N:201:HIS:ND1	2.31	0.46
7:O:80:ALA:O	7:O:84:VAL:HG23	2.16	0.46
8:P:164:LYS:HB3	8:P:165:PRO:HD3	1.96	0.46
7:O:217:GLY:O	7:O:375:THR:HG22	2.15	0.46
8:P:487:PRO:HA	8:P:488:GLY:HA3	1.69	0.46
6:F:370:ASN:N	6:F:370:ASN:HD22	2.14	0.46
2:B:477:GLY:O	2:B:478:THR:CB	2.62	0.46
8:P:6:PRO:CB	8:P:7:GLN:CA	2.93	0.46
3:K:47:MET:HG2	3:K:48:LEU:N	2.30	0.46
3:K:51:PRO:O	3:K:52:MET:CG	2.63	0.46
1:A:351:GLU:C	1:A:353:SER:H	2.17	0.46
8:H:32:ILE:O	8:H:32:ILE:HD13	2.16	0.46
4:D:234:ILE:HG22	4:D:236:LEU:HD22	1.97	0.46
7:G:83:LEU:HD23	7:G:86:ILE:CD1	2.45	0.46
7:O:236:PHE:O	7:O:239:PRO:CG	2.64	0.46
7:O:454:CYS:HB3	7:O:461:ALA:HA	1.98	0.46
7:G:454:CYS:HB3	7:G:461:ALA:HA	1.98	0.46
5:M:74:LEU:HD12	5:M:93:GLN:HB3	1.96	0.46
2:J:164:LYS:O	2:J:167:SER:N	2.40	0.46
4:D:461:ASN:HD22	4:D:462:SER:N	2.13	0.46
7:G:80:ALA:O	7:G:84:VAL:HG23	2.16	0.46
4:L:239:PHE:C	4:L:290:LYS:HG3	2.36	0.46
4:L:284:ASN:O	4:L:310:ILE:CG2	2.63	0.46
3:K:402:VAL:HG13	3:K:502:PRO:CG	2.45	0.46
8:P:184:GLU:O	8:P:188:HIS:HD2	1.97	0.46
2:J:331:GLU:HA	2:J:332:PRO:HD3	1.79	0.46
6:F:166:LEU:HG	6:F:167:THR:OG1	2.15	0.46
2:J:411:MET:CE	2:J:498:VAL:HG21	2.45	0.46
6:F:420:ILE:HB	6:F:482:ASP:OD1	2.16	0.46
2:B:286:ASN:HD22	2:B:287:ARG:N	2.14	0.46
3:C:229:VAL:HG12	3:C:230:VAL:H	1.80	0.46
2:J:40:LYS:HZ1	6:N:117:ILE:HG13	1.80	0.46
6:N:5:LEU:CA	6:N:6:LEU:HB2	2.35	0.46
4:L:77:MET:CE	7:O:384:GLN:HB2	2.45	0.46
7:O:144:ALA:HA	7:O:409:ILE:O	2.15	0.46
6:F:343:LEU:HA	6:F:344:SER:HA	1.48	0.46
1:A:29:ASN:HD22	1:A:538:ILE:HG23	1.81	0.46
4:L:496:HIS:O	4:L:498:LEU:HD12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:17:THR:HG22	7:O:526:ASN:HD22	1.80	0.46
7:O:200:GLY:O	7:O:375:THR:HA	2.16	0.46
4:D:291:SER:HA	4:D:315:ASP:CA	2.44	0.46
2:B:224:LYS:O	2:B:343:ILE:HA	2.16	0.46
2:J:4:GLN:C	2:J:5:ILE:CG2	2.73	0.46
6:N:233:VAL:HG13	6:N:351:SER:CB	2.43	0.46
2:J:242:LYS:HD3	3:K:269:TRP:CZ2	2.50	0.46
8:P:457:GLU:C	8:P:460:PRO:HD2	2.36	0.46
2:B:60:GLY:O	2:B:63:ILE:HG22	2.15	0.46
2:B:63:ILE:CG2	2:B:64:LEU:HG	2.44	0.46
3:C:129:LEU:HD23	3:C:510:VAL:HG12	1.96	0.46
8:P:32:ILE:O	8:P:32:ILE:HD13	2.16	0.46
7:G:207:GLY:HA3	7:G:379:ARG:HH11	1.81	0.46
7:G:491:ASN:OD1	7:G:496:VAL:CG2	2.64	0.46
8:H:94:ILE:H	8:H:94:ILE:HG13	1.50	0.46
4:L:392:ARG:HD3	4:L:393:SER:N	2.31	0.46
7:G:60:THR:HG23	7:G:60:THR:O	2.15	0.46
6:N:332:THR:HB	6:N:350:PHE:O	2.15	0.46
6:F:233:VAL:HG13	6:F:351:SER:CB	2.43	0.46
2:J:408:GLU:CD	2:J:440:LEU:HD23	2.36	0.46
6:F:427:ARG:HG2	6:F:448:ALA:CB	2.46	0.46
3:K:298:GLU:HA	3:K:320:VAL:H	1.81	0.46
1:I:351:GLU:C	1:I:353:SER:H	2.17	0.46
8:H:457:GLU:C	8:H:460:PRO:HD2	2.36	0.46
6:N:122:PHE:HD1	6:N:447:PHE:HD1	1.63	0.46
4:D:182:SER:HB2	4:D:187:LYS:CE	2.46	0.46
7:O:33:CYS:SG	7:O:106:GLY:HA2	2.56	0.46
5:E:84:THR:HG22	5:E:85:ASN:N	2.31	0.46
7:G:33:CYS:SG	7:G:106:GLY:HA2	2.56	0.46
7:O:491:ASN:OD1	7:O:496:VAL:CG2	2.64	0.46
6:F:458:LEU:HG	6:F:459:VAL:HG23	1.97	0.46
6:N:458:LEU:HG	6:N:459:VAL:HG23	1.97	0.46
7:G:200:GLY:O	7:G:375:THR:HA	2.15	0.46
4:L:234:ILE:HG22	4:L:236:LEU:HD22	1.97	0.46
3:K:407:MET:HE1	3:K:408:LEU:HD23	1.97	0.46
8:H:464:ALA:HB1	8:H:474:VAL:HG21	1.98	0.46
5:E:269:LEU:HD22	5:E:269:LEU:N	2.31	0.46
7:O:234:LYS:HD3	7:O:234:LYS:HA	1.34	0.46
7:G:296:LYS:HA	7:G:318:VAL:HG23	1.97	0.46
6:F:330:LEU:O	6:F:372:ASP:O	2.34	0.46
2:J:242:LYS:HA	3:K:269:TRP:HE1	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:143:VAL:HG12	1:I:419:VAL:HG22	1.97	0.46
5:M:184:ALA:O	5:M:188:LEU:CB	2.64	0.46
4:D:417:PRO:O	4:D:421:ILE:HG12	2.16	0.46
2:B:162:SER:O	2:B:163:SER:CB	2.63	0.46
4:D:344:LEU:O	4:D:345:ASP:OD1	2.33	0.46
2:J:295:GLU:HB2	6:N:337:GLN:CD	2.35	0.46
3:K:142:PRO:HB3	3:K:410:PRO:O	2.15	0.46
5:E:239:LEU:HD23	5:E:240:ILE:N	2.31	0.46
4:D:392:ARG:HD3	4:D:393:SER:N	2.31	0.46
2:J:26:ALA:HB1	2:J:77:LEU:HD11	1.97	0.46
3:C:246:LEU:O	3:C:247:ASP:HB3	2.15	0.46
1:A:486:MET:CB	1:A:487:ALA:HB2	2.46	0.46
4:L:144:LEU:HD23	4:L:144:LEU:N	2.31	0.46
4:D:469:LEU:C	4:D:471:SER:H	2.19	0.46
6:N:141:THR:CG2	6:N:142:ASN:N	2.78	0.46
9:C:1101:ADP:O3'	9:C:1101:ADP:C8	2.69	0.46
3:C:95:THR:HG23	9:C:1101:ADP:O1A	2.15	0.46
6:F:454:ILE:O	6:F:457:THR:OG1	2.30	0.46
8:H:291:ILE:HD12	8:H:347:PRO:HG3	1.97	0.46
7:O:396:ALA:O	7:O:397:ILE:C	2.55	0.46
7:G:236:PHE:O	7:G:239:PRO:CG	2.64	0.46
7:G:291:ASN:HA	7:G:312:ILE:HB	1.97	0.46
1:I:224:LEU:CD1	1:I:226:CYS:CB	2.90	0.46
4:L:241:ILE:N	4:L:241:ILE:HD12	2.30	0.46
7:O:418:MET:HE3	7:O:447:GLU:HG2	1.98	0.46
1:A:218:LEU:HD23	1:A:385:ILE:HG12	1.98	0.46
4:L:120:ILE:CG1	4:L:439:ILE:HG21	2.44	0.46
2:J:286:ASN:HD22	2:J:287:ARG:N	2.14	0.46
4:D:161:LYS:HD2	4:D:161:LYS:HA	1.66	0.46
4:L:9:ALA:CB	7:O:76:VAL:H	2.27	0.46
8:H:175:GLU:H	8:H:175:GLU:HG3	1.45	0.46
4:D:284:ASN:O	4:D:310:ILE:CG2	2.63	0.46
1:A:210:GLY:O	1:A:211:LYS:CB	2.64	0.46
4:D:144:LEU:N	4:D:144:LEU:HD23	2.31	0.46
6:F:540:THR:CB	6:F:541:LEU:HD22	2.44	0.45
4:D:521:ILE:CG2	7:G:51:ILE:HA	2.40	0.45
4:L:24:ASN:ND2	4:L:524:ILE:HD11	2.30	0.45
8:H:386:LEU:H	8:H:386:LEU:HD12	1.81	0.45
8:P:169:SER:HB2	9:P:601:ADP:O2A	2.15	0.45
2:J:219:GLY:HA3	2:J:304:ASN:ND2	2.31	0.45
4:D:185:ASN:H	4:D:187:LYS:N	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:72:THR:O	6:F:75:LEU:HB3	2.16	0.45
6:F:243:GLU:OE2	6:F:243:GLU:CA	2.52	0.45
1:I:12:THR:HA	1:I:13:LEU:HA	1.69	0.45
2:J:58:ASN:ND2	2:J:58:ASN:C	2.69	0.45
7:G:452:GLN:HA	7:G:455:GLU:HB2	1.96	0.45
1:I:66:GLY:CA	1:I:99:THR:HG22	2.47	0.45
5:M:103:LEU:HA	5:M:106:GLN:HE21	1.80	0.45
2:J:203:LEU:O	2:J:204:SER:OG	2.30	0.45
5:M:239:LEU:HD23	5:M:240:ILE:N	2.31	0.45
6:F:296:ILE:HD12	6:F:328:LEU:HD22	1.99	0.45
6:N:153:VAL:CB	6:N:507:TRP:CB	2.94	0.45
6:F:43:LEU:HD21	6:F:161:LYS:CA	2.42	0.45
2:B:210:GLU:CB	2:B:357:SER:O	2.65	0.45
3:C:335:THR:HB	8:H:237:LYS:CE	2.34	0.45
1:A:420:PRO:O	1:A:424:CYS:HB3	2.16	0.45
1:I:420:PRO:O	1:I:424:CYS:HB3	2.16	0.45
1:I:433:LEU:O	1:I:437:ALA:CA	2.65	0.45
1:I:336:THR:HB	1:I:354:TYR:HD1	1.80	0.45
2:J:27:ILE:O	2:J:27:ILE:HG12	2.15	0.45
6:F:160:THR:N	6:F:164:ALA:HB3	2.31	0.45
8:P:426:THR:HG23	8:P:427:GLU:N	2.31	0.45
4:L:182:SER:HB2	4:L:187:LYS:CE	2.46	0.45
4:D:325:SER:O	4:D:329:GLY:N	2.47	0.45
4:L:499:GLN:HA	4:L:500:PRO:HD3	1.86	0.45
4:D:98:ILE:HG12	4:D:98:ILE:H	1.57	0.45
6:N:337:GLN:HG2	6:N:347:ILE:CD1	2.46	0.45
4:D:239:PHE:C	4:D:290:LYS:HG3	2.36	0.45
2:B:116:HIS:HA	2:B:117:PRO:HD3	1.74	0.45
2:B:116:HIS:CE1	2:B:118:GLN:CB	2.99	0.45
4:D:418:GLU:HG2	4:D:451:PRO:HD3	1.98	0.45
6:N:296:ILE:HG12	6:N:317:LEU:HB2	1.98	0.45
1:A:256:MET:HE3	1:A:261:GLN:HA	1.97	0.45
4:L:50:THR:HG22	4:L:54:GLU:N	2.30	0.45
5:M:396:GLU:HA	5:M:397:GLN:HA	1.53	0.45
7:O:296:LYS:HA	7:O:318:VAL:HG23	1.97	0.45
7:O:329:ALA:HA	7:O:371:ALA:HB1	1.98	0.45
4:D:50:THR:HG22	4:D:54:GLU:N	2.31	0.45
6:F:167:THR:CB	6:F:168:GLU:HB3	2.47	0.45
2:B:411:MET:CE	2:B:498:VAL:HG21	2.46	0.45
6:N:415:ALA:HA	9:N:601:ADP:H1'	1.97	0.45
6:N:420:ILE:HB	6:N:482:ASP:OD1	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:471:LEU:HD12	3:K:491:ILE:HG21	1.98	0.45
6:F:489:VAL:O	6:F:490:GLY:C	2.41	0.45
6:N:221:HIS:HB2	6:N:224:MET:CG	2.43	0.45
2:B:492:LYS:H	2:B:492:LYS:HZ1	1.63	0.45
8:P:252:CYS:HB2	8:P:343:ARG:N	2.32	0.45
6:F:159:LEU:CA	6:F:164:ALA:HB2	2.41	0.45
8:H:426:THR:HG23	8:H:427:GLU:N	2.31	0.45
2:J:293:TYR:O	2:J:297:LEU:HD23	2.17	0.45
6:N:79:ALA:HB1	6:N:523:ILE:HD11	1.98	0.45
1:A:69:ILE:O	1:A:73:LEU:HD13	2.15	0.45
3:C:142:PRO:HB3	3:C:410:PRO:O	2.15	0.45
1:I:128:GLY:O	1:I:448:ILE:HD13	2.15	0.45
3:C:174:LEU:HG	3:C:219:VAL:CG2	2.47	0.45
4:D:194:ILE:O	4:D:194:ILE:HG12	2.15	0.45
1:I:210:GLY:O	1:I:211:LYS:CB	2.64	0.45
2:J:210:GLU:CB	2:J:357:SER:O	2.64	0.45
3:K:230:VAL:HG21	3:K:303:ASP:H	1.80	0.45
3:C:64:ILE:HG22	3:C:65:LEU:N	2.31	0.45
1:I:419:VAL:HG13	1:I:425:VAL:HG21	1.98	0.45
6:N:221:HIS:CD2	6:N:224:MET:SD	3.09	0.45
8:P:386:LEU:H	8:P:386:LEU:HD12	1.81	0.45
6:F:122:PHE:HD1	6:F:447:PHE:HD1	1.63	0.45
7:O:400:VAL:O	7:O:404:LEU:HB2	2.17	0.45
7:O:241:ILE:HD12	7:O:330:VAL:HG21	1.98	0.45
1:I:120:ILE:O	1:I:120:ILE:HD13	2.16	0.45
1:I:458:ILE:H	1:I:458:ILE:HD12	1.82	0.45
3:K:508:GLN:CG	8:P:215:GLY:HA2	2.46	0.45
4:L:30:SER:HA	4:L:33:ASP:CG	2.37	0.45
5:M:269:LEU:HD22	5:M:269:LEU:N	2.31	0.45
1:I:205:VAL:C	1:I:206:LEU:HD23	2.36	0.45
1:I:86:LEU:HD21	1:I:101:VAL:HG12	1.99	0.45
3:K:64:ILE:HG22	3:K:65:LEU:N	2.32	0.45
2:J:88:VAL:HG12	2:J:89:GLY:N	2.32	0.45
8:H:101:ASN:N	9:H:601:ADP:O2B	2.43	0.45
4:L:185:ASN:H	4:L:187:LYS:N	2.14	0.45
8:H:291:ILE:HD12	8:H:347:PRO:HG2	1.96	0.45
7:G:165:ALA:CB	7:G:399:ILE:HG21	2.46	0.45
7:G:282:LEU:HD23	7:G:303:ALA:O	2.17	0.45
6:F:337:GLN:HG2	6:F:347:ILE:CD1	2.46	0.45
2:J:234:ALA:HA	2:J:325:VAL:HB	1.99	0.45
4:D:292:ILE:CG1	4:D:293:LEU:HA	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:GLY:CA	1:A:99:THR:HG22	2.47	0.45
3:C:202:ARG:HH21	3:C:323:SER:HB3	1.81	0.45
2:J:386:ASP:O	2:J:390:VAL:HG23	2.17	0.45
8:P:247:VAL:HG22	8:P:248:ALA:N	2.32	0.45
8:H:329:LEU:HD23	8:H:329:LEU:O	2.17	0.45
5:E:297:LYS:HA	5:E:297:LYS:HD2	1.66	0.45
2:B:4:GLN:CB	3:C:71:ALA:HB3	2.45	0.45
5:E:439:VAL:HB	5:E:528:VAL:HG13	1.99	0.45
5:M:439:VAL:HB	5:M:528:VAL:HG13	1.99	0.45
1:A:86:LEU:HD21	1:A:101:VAL:HG12	1.99	0.45
3:C:298:GLU:HA	3:C:320:VAL:H	1.81	0.45
6:N:399:LEU:HD12	6:N:399:LEU:O	2.17	0.45
6:F:141:THR:CG2	6:F:142:ASN:N	2.78	0.45
6:F:173:ILE:HD11	6:F:209:PHE:N	2.32	0.45
7:O:317:ARG:HD2	7:O:317:ARG:O	2.16	0.45
1:A:336:THR:HB	1:A:354:TYR:HD1	1.80	0.45
7:G:317:ARG:HD2	7:G:317:ARG:O	2.16	0.45
4:L:226:PRO:CG	4:L:311:MET:HG2	2.47	0.45
4:D:226:PRO:CG	4:D:311:MET:HG2	2.47	0.45
5:M:84:THR:HG22	5:M:85:ASN:N	2.31	0.45
7:O:207:GLY:HA3	7:O:379:ARG:HH11	1.81	0.45
2:J:232:LEU:HD22	2:J:233:ILE:H	1.80	0.45
1:I:69:ILE:O	1:I:73:LEU:HD13	2.16	0.45
6:N:108:PHE:C	6:N:108:PHE:CD1	2.90	0.45
1:A:55:ASP:O	1:A:57:ILE:N	2.50	0.45
5:E:189:GLY:O	5:E:190:SER:HB2	2.17	0.45
6:F:238:VAL:HG22	6:F:239:SER:N	2.32	0.45
8:P:96:MET:CB	8:P:515:GLU:OE1	2.65	0.45
2:J:456:VAL:HG13	2:J:457:SER:N	2.32	0.45
1:A:205:VAL:C	1:A:206:LEU:HD23	2.36	0.45
8:P:464:ALA:HB1	8:P:474:VAL:HG21	1.98	0.45
1:I:486:MET:CB	1:I:487:ALA:HB2	2.46	0.45
6:N:238:VAL:HG22	6:N:239:SER:N	2.32	0.45
8:H:96:MET:CB	8:H:515:GLU:OE1	2.65	0.45
3:C:230:VAL:HG21	3:C:303:ASP:H	1.80	0.45
2:B:30:GLY:HA2	2:B:33:VAL:HG21	1.97	0.45
7:O:226:TYR:CE1	7:O:229:PHE:CB	3.00	0.45
9:C:1101:ADP:O1A	10:C:1102:BEF:F3	2.24	0.45
6:F:108:PHE:CE1	6:F:118:ILE:HG13	2.50	0.45
6:N:173:ILE:HD11	6:N:209:PHE:N	2.32	0.45
6:N:72:THR:O	6:N:75:LEU:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:103:LEU:HD22	4:D:515:VAL:HG21	1.99	0.45
8:P:63:ILE:HD12	8:P:74:GLU:CG	2.45	0.45
7:O:291:ASN:HA	7:O:312:ILE:HB	1.97	0.45
4:L:299:ASP:OD1	4:L:301:ALA:HB3	2.16	0.45
9:L:601:ADP:H2'	9:L:601:ADP:N3	2.31	0.45
8:P:71:MET:O	8:P:75:LEU:HG	2.17	0.45
1:I:164:MET:HE3	1:I:169:ILE:HB	1.99	0.45
2:J:45:LEU:HB2	6:N:533:LEU:HB3	1.95	0.45
3:C:222:GLY:HA3	3:C:368:LEU:O	2.17	0.45
6:F:296:ILE:HG12	6:F:317:LEU:HB2	1.98	0.45
1:A:532:LEU:O	1:A:536:VAL:HG23	2.16	0.45
2:B:386:ASP:O	2:B:390:VAL:HG23	2.17	0.45
4:L:469:LEU:C	4:L:471:SER:H	2.19	0.45
6:F:436:ALA:HA	6:F:437:LYS:HA	1.66	0.45
6:N:540:THR:CB	6:N:541:LEU:HD22	2.44	0.45
6:N:491:VAL:HG12	6:N:492:ASP:H	1.82	0.45
6:F:515:ASN:HD22	6:F:515:ASN:C	2.18	0.45
3:C:471:LEU:HD12	3:C:491:ILE:HG21	1.98	0.45
2:B:219:GLY:HA3	2:B:304:ASN:ND2	2.31	0.45
2:B:293:TYR:O	2:B:297:LEU:HD23	2.17	0.45
2:J:469:THR:O	2:J:470:SER:CB	2.59	0.45
1:I:55:ASP:O	1:I:57:ILE:N	2.50	0.45
3:K:10:ALA:HA	3:K:11:SER:HA	1.59	0.45
3:C:414:PRO:HG2	3:C:481:THR:CG2	2.47	0.45
8:H:247:VAL:HG22	8:H:248:ALA:N	2.32	0.45
4:L:313:VAL:HG11	4:L:361:VAL:HG21	1.99	0.45
6:F:207:THR:HB	6:F:380:ILE:HA	1.99	0.45
7:G:249:GLU:O	7:G:250:LEU:C	2.55	0.45
6:N:167:THR:CA	6:N:168:GLU:CB	2.95	0.45
6:N:166:LEU:CD2	6:N:205:LYS:HA	2.47	0.45
6:N:330:LEU:O	6:N:372:ASP:O	2.34	0.45
6:F:117:ILE:HG12	5:M:33:LYS:CE	2.39	0.45
3:K:229:VAL:HG11	3:K:234:MET:HE2	1.98	0.45
2:J:40:LYS:HA	6:N:116:ARG:HG3	1.99	0.45
2:J:88:VAL:CG1	2:J:393:GLN:HE22	2.22	0.45
6:N:178:VAL:HG21	6:N:402:VAL:CG1	2.47	0.45
6:F:92:THR:OG1	9:F:601:ADP:PB	2.74	0.45
5:M:267:VAL:HG12	5:M:268:LYS:N	2.32	0.45
7:G:170:LEU:O	7:G:170:LEU:CD2	2.58	0.45
7:O:438:ILE:HD12	7:O:438:ILE:N	2.32	0.45
1:I:62:VAL:O	1:I:397:GLU:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ILE:HG22	1:A:26:ARG:N	2.32	0.45
1:A:129:PHE:CD2	1:A:129:PHE:N	2.84	0.45
6:N:296:ILE:HD12	6:N:328:LEU:HD22	1.99	0.45
3:C:219:VAL:HG13	3:C:379:ILE:HD12	1.99	0.45
6:N:207:THR:HB	6:N:380:ILE:HA	1.99	0.45
5:E:500:SER:O	5:E:504:LYS:HG2	2.17	0.45
5:M:456:GLU:HA	5:M:456:GLU:OE2	2.17	0.45
5:M:500:SER:O	5:M:504:LYS:HG2	2.17	0.45
2:B:74:ALA:O	2:B:78:VAL:HG23	2.17	0.45
2:B:222:GLN:HB3	2:B:223:PRO:HD2	1.98	0.45
6:N:539:SER:HB2	6:N:542:LYS:HD3	1.99	0.45
8:H:332:LEU:O	8:H:335:VAL:HB	2.17	0.45
8:H:335:VAL:HG13	8:H:379:SER:CB	2.46	0.45
6:F:491:VAL:HG12	6:F:492:ASP:H	1.82	0.45
8:H:252:CYS:HB2	8:H:343:ARG:N	2.32	0.45
6:F:399:LEU:O	6:F:399:LEU:HD12	2.17	0.45
5:E:84:THR:HA	5:E:418:GLU:OE1	2.17	0.45
7:G:159:GLU:O	7:G:179:VAL:HG11	2.17	0.45
8:H:62:ILE:HD13	8:H:63:ILE:N	2.32	0.45
7:O:204:ILE:HA	7:O:205:PRO:HD3	1.79	0.45
6:F:342:ASP:CG	6:F:345:PRO:HG2	2.38	0.45
2:B:368:VAL:O	2:B:377:LEU:HD23	2.17	0.45
1:A:120:ILE:HD13	1:A:120:ILE:O	2.16	0.45
8:P:134:ALA:O	8:P:138:THR:HG23	2.17	0.45
1:I:218:LEU:HD23	1:I:385:ILE:HG12	1.98	0.45
2:J:32:LEU:HD12	6:N:532:GLU:OE2	2.17	0.45
5:E:150:PHE:CD1	5:E:472:PHE:HE2	2.35	0.45
3:C:402:VAL:HG13	3:C:502:PRO:CG	2.45	0.45
3:K:222:GLY:HA3	3:K:368:LEU:O	2.17	0.45
5:E:255:PRO:HG3	5:E:336:LEU:CB	2.47	0.45
4:L:418:GLU:HG2	4:L:451:PRO:HD3	1.98	0.45
1:I:129:PHE:N	1:I:129:PHE:CD2	2.84	0.45
2:J:222:GLN:HB3	2:J:223:PRO:HD2	1.98	0.45
2:B:456:VAL:HG13	2:B:457:SER:N	2.32	0.45
6:N:167:THR:CB	6:N:168:GLU:HB3	2.47	0.44
6:N:422:LEU:HD13	6:N:517:ILE:HD11	1.98	0.44
6:F:539:SER:HB2	6:F:542:LYS:HD3	2.00	0.44
6:F:231:ALA:O	6:F:351:SER:OG	2.22	0.44
2:B:411:MET:H	2:B:411:MET:HG2	1.53	0.44
6:F:83:GLN:OE1	6:F:515:ASN:ND2	2.50	0.44
4:L:524:ILE:CB	7:O:52:LEU:O	2.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:184:ALA:O	5:E:188:LEU:CB	2.64	0.44
4:L:181:ILE:HD11	4:L:375:VAL:HG23	1.98	0.44
6:F:122:PHE:CD1	6:F:447:PHE:HD1	2.35	0.44
6:N:122:PHE:CD1	6:N:447:PHE:HD1	2.35	0.44
7:O:109:MET:SD	7:O:514:THR:CB	3.05	0.44
5:E:84:THR:O	5:E:90:ILE:HD11	2.18	0.44
3:C:495:VAL:HG23	3:C:500:TRP:CH2	2.49	0.44
4:D:147:ARG:O	4:D:151:VAL:HG23	2.16	0.44
1:A:120:ILE:HG21	1:A:125:ILE:CG1	2.47	0.44
4:D:299:ASP:OD1	4:D:301:ALA:HB3	2.16	0.44
7:G:438:ILE:HD12	7:G:438:ILE:N	2.32	0.44
7:O:123:HIS:N	7:O:123:HIS:ND1	2.65	0.44
3:K:250:LEU:CG	3:K:301:VAL:CB	2.92	0.44
4:D:238:GLN:HE22	4:D:318:ARG:NH1	2.15	0.44
2:B:203:LEU:O	2:B:204:SER:OG	2.30	0.44
8:P:428:ILE:CD1	8:P:478:LEU:HD13	2.48	0.44
6:F:433:LYS:HG3	6:F:444:ILE:CG2	2.46	0.44
6:N:90:GLY:O	6:N:94:VAL:CG2	2.34	0.44
4:L:521:ILE:CG2	7:O:52:LEU:N	2.78	0.44
2:J:370:ARG:O	2:J:372:ALA:N	2.50	0.44
1:A:419:VAL:HG13	1:A:425:VAL:HG21	1.98	0.44
1:A:433:LEU:O	1:A:437:ALA:CA	2.64	0.44
6:N:214:VAL:HG22	6:N:377:THR:OG1	2.18	0.44
2:B:37:LEU:CB	2:B:444:LEU:HD13	2.47	0.44
5:E:387:THR:HA	5:E:388:THR:HA	1.61	0.44
7:G:109:MET:SD	7:G:514:THR:CB	3.05	0.44
7:O:159:GLU:O	7:O:179:VAL:HG11	2.17	0.44
5:M:84:THR:HA	5:M:418:GLU:OE1	2.17	0.44
8:P:62:ILE:HD13	8:P:63:ILE:N	2.32	0.44
7:G:241:ILE:HD12	7:G:330:VAL:HG21	1.98	0.44
7:O:241:ILE:HD12	7:O:330:VAL:CG2	2.48	0.44
5:E:271:ILE:CB	5:E:362:ILE:HA	2.48	0.44
5:M:73:ILE:O	5:M:74:LEU:HD22	2.17	0.44
1:A:221:GLY:HA2	1:A:382:SER:CB	2.42	0.44
3:K:414:PRO:HG2	3:K:481:THR:CG2	2.47	0.44
8:H:256:ILE:HD13	8:H:280:GLU:OE1	2.17	0.44
1:I:112:ALA:HB1	1:I:539:LEU:HD21	1.98	0.44
6:F:153:VAL:CB	6:F:507:TRP:CB	2.94	0.44
6:N:330:LEU:HB3	6:N:375:SER:OG	2.17	0.44
3:K:457:ILE:HD13	3:K:467:LEU:CD1	2.19	0.44
5:E:351:LEU:HD22	5:E:352:GLU:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:370:ASN:O	4:D:373:PRO:HD3	2.18	0.44
6:F:108:PHE:CD1	6:F:108:PHE:C	2.90	0.44
5:M:340:LEU:H	5:M:340:LEU:HD23	1.81	0.44
7:G:452:GLN:CD	7:G:452:GLN:H	2.21	0.44
5:E:267:VAL:HG12	5:E:268:LYS:N	2.32	0.44
8:H:428:ILE:CD1	8:H:478:LEU:HD13	2.48	0.44
5:M:450:MET:HE3	5:M:454:VAL:CG2	2.47	0.44
5:M:189:GLY:O	5:M:190:SER:HB2	2.17	0.44
2:J:224:LYS:O	2:J:343:ILE:HA	2.16	0.44
7:O:244:LEU:HB3	7:O:246:VAL:HG22	1.99	0.44
7:G:329:ALA:HA	7:G:371:ALA:HB1	1.98	0.44
8:P:332:LEU:O	8:P:335:VAL:HB	2.17	0.44
1:I:91:ASP:HA	1:I:95:GLY:HA2	2.00	0.44
1:A:90:GLN:HE21	1:A:527:SER:HB3	1.83	0.44
4:L:417:PRO:O	4:L:421:ILE:HG12	2.16	0.44
4:D:209:MET:HE3	4:D:375:VAL:HG11	2.00	0.44
6:N:159:LEU:CA	6:N:164:ALA:HB2	2.41	0.44
8:P:209:VAL:CG2	8:P:386:LEU:HD11	2.35	0.44
2:B:42:MET:HE3	2:B:42:MET:HA	2.00	0.44
8:H:134:ALA:O	8:H:138:THR:HG23	2.17	0.44
8:P:101:ASN:N	8:P:101:ASN:HD22	2.16	0.44
5:E:340:LEU:HD23	5:E:340:LEU:H	1.81	0.44
2:B:417:THR:HG23	2:B:418:GLU:N	2.33	0.44
1:I:54:VAL:HG12	1:I:56:ASP:N	2.29	0.44
3:C:515:GLU:CD	8:H:389:ALA:HB3	2.38	0.44
4:D:12:LYS:HZ2	7:G:73:LEU:HD22	1.82	0.44
5:E:37:ASN:HB2	6:N:114:HIS:HA	2.00	0.44
4:D:313:VAL:HG11	4:D:361:VAL:HG21	1.99	0.44
6:F:101:LEU:HD23	6:F:101:LEU:O	2.17	0.44
6:N:101:LEU:HD23	6:N:101:LEU:O	2.17	0.44
8:H:6:PRO:CB	8:H:7:GLN:CA	2.93	0.44
6:F:36:ASN:HB3	6:F:57:LYS:HZ3	0.68	0.44
6:F:330:LEU:HB3	6:F:375:SER:OG	2.17	0.44
3:C:463:ASP:O	3:C:467:LEU:HB2	2.18	0.44
2:J:243:VAL:HG12	2:J:245:ILE:N	2.29	0.44
7:G:226:TYR:CE1	7:G:229:PHE:CB	3.00	0.44
4:L:134:ILE:HB	4:L:421:ILE:CD1	2.48	0.44
6:N:141:THR:CB	6:N:409:LYS:HG3	2.45	0.44
4:L:370:ASN:O	4:L:373:PRO:HD3	2.18	0.44
4:D:181:ILE:HD11	4:D:375:VAL:HG23	1.98	0.44
8:P:113:VAL:CG1	8:P:451:GLN:HG3	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:89:ASP:OD1	9:F:601:ADP:O1B	2.35	0.44
7:O:170:LEU:CD2	7:O:170:LEU:O	2.58	0.44
5:M:340:LEU:HA	5:M:341:PRO:HD3	1.83	0.44
7:O:186:VAL:HG21	7:O:400:VAL:HG22	1.98	0.44
7:G:241:ILE:HD12	7:G:330:VAL:CG2	2.48	0.44
1:A:120:ILE:CG2	1:A:121:HIS:N	2.81	0.44
1:I:183:ALA:CB	1:I:383:SER:HB2	2.47	0.44
5:E:276:PHE:HB3	5:E:327:PHE:HA	2.00	0.44
1:A:62:VAL:O	1:A:397:GLU:HG3	2.17	0.44
4:L:238:GLN:HE22	4:L:318:ARG:NH1	2.15	0.44
4:L:219:ALA:HB1	4:L:221:LYS:HZ3	1.83	0.44
8:H:424:GLY:O	8:H:428:ILE:HG13	2.18	0.44
6:F:114:HIS:CD2	5:M:37:ASN:HD22	2.35	0.44
5:M:373:LYS:HE2	6:N:311:LYS:NZ	2.31	0.44
2:J:74:ALA:O	2:J:78:VAL:HG23	2.17	0.44
8:P:155:ASP:HB3	8:P:156:LYS:H	1.48	0.44
8:P:256:ILE:HD13	8:P:280:GLU:OE1	2.17	0.44
5:E:456:GLU:HA	5:E:456:GLU:OE2	2.17	0.44
6:N:503:ILE:O	6:N:503:ILE:HG22	2.18	0.44
8:P:329:LEU:HD23	8:P:329:LEU:O	2.17	0.44
7:G:244:LEU:HB3	7:G:246:VAL:HG22	1.99	0.44
6:F:166:LEU:CD2	6:F:205:LYS:HA	2.47	0.44
6:N:430:ASN:CA	6:N:433:LYS:HB2	2.48	0.44
5:E:429:VAL:O	5:E:432:ASN:HB2	2.18	0.44
1:I:90:GLN:HE21	1:I:527:SER:HB3	1.83	0.44
2:B:389:SER:O	2:B:393:GLN:HG3	2.17	0.44
2:J:8:ASP:OD1	2:J:8:ASP:N	2.51	0.44
8:H:113:VAL:CG1	8:H:451:GLN:HG3	2.37	0.44
6:N:209:PHE:CE2	6:N:376:CYS:SG	2.97	0.44
2:B:36:THR:HG22	2:B:42:MET:O	2.18	0.44
5:M:314:LYS:HZ1	5:M:338:ASN:HA	1.82	0.44
2:J:250:PHE:CB	6:N:250:GLY:O	2.65	0.44
7:O:454:CYS:HB2	7:O:461:ALA:HB1	1.98	0.44
1:I:538:ILE:HA	1:I:541:ILE:HD12	2.00	0.44
1:I:120:ILE:CG2	1:I:121:HIS:N	2.81	0.44
1:I:17:GLY:HA2	1:I:546:THR:O	2.18	0.44
1:I:16:GLY:CA	1:I:548:ASP:HB3	2.44	0.44
1:A:17:GLY:HA2	1:A:546:THR:O	2.18	0.44
1:I:532:LEU:O	1:I:536:VAL:HG23	2.16	0.44
4:D:273:ASN:ND2	7:G:268:GLN:HE22	2.15	0.44
3:K:219:VAL:HG13	3:K:379:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:186:GLY:HA2	2:B:187:SER:HA	1.47	0.44
1:A:112:ALA:HB1	1:A:539:LEU:HD21	1.98	0.44
4:D:7:SER:HA	7:G:35:ALA:HB1	2.00	0.44
6:N:83:GLN:OE1	6:N:515:ASN:ND2	2.51	0.44
3:C:306:GLN:C	3:C:310:LEU:HG	2.37	0.44
1:I:419:VAL:HA	1:I:420:PRO:HD3	1.86	0.44
8:P:15:LYS:HG3	8:P:16:GLN:H	1.83	0.44
5:M:351:LEU:HD22	5:M:352:GLU:H	1.83	0.44
6:N:195:GLU:HG2	6:N:197:MET:CE	2.48	0.44
2:B:482:MET:SD	2:B:487:ILE:HB	2.58	0.44
6:F:79:ALA:HB1	6:F:523:ILE:HD11	1.98	0.44
7:G:396:ALA:O	7:G:397:ILE:C	2.55	0.44
2:J:231:ILE:H	2:J:231:ILE:HG12	1.60	0.44
1:A:120:ILE:HG21	1:A:125:ILE:HG12	2.00	0.44
1:I:120:ILE:HG21	1:I:125:ILE:CG1	2.48	0.44
3:C:114:LYS:CA	3:C:115:ASN:CB	2.94	0.44
5:E:535:LYS:C	5:E:535:LYS:HD2	2.38	0.44
6:N:124:ILE:HB	6:N:444:ILE:CD1	2.48	0.44
6:N:422:LEU:O	6:N:426:LEU:HB2	2.17	0.44
8:H:243:LYS:HA	8:H:243:LYS:HD3	1.87	0.44
4:D:134:ILE:HB	4:D:421:ILE:CD1	2.48	0.44
6:F:174:VAL:O	6:F:178:VAL:HG23	2.18	0.44
1:A:350:PHE:HE2	1:A:354:TYR:CB	2.16	0.44
4:D:234:ILE:HB	4:D:345:ASP:HB2	2.00	0.44
7:O:162:ALA:CB	7:O:179:VAL:HG13	2.47	0.44
7:O:282:LEU:HD23	7:O:303:ALA:O	2.17	0.44
2:J:37:LEU:CB	2:J:444:LEU:HD13	2.47	0.44
5:E:492:ILE:CD1	2:J:115:ILE:HG12	2.45	0.44
7:G:123:HIS:N	7:G:123:HIS:ND1	2.65	0.44
1:A:458:ILE:H	1:A:458:ILE:HD12	1.82	0.44
5:M:255:PRO:HG3	5:M:336:LEU:CB	2.47	0.44
2:J:482:MET:SD	2:J:487:ILE:HB	2.57	0.44
2:J:92:THR:HA	2:J:95:VAL:HG23	2.00	0.44
8:H:393:ASN:O	8:H:397:ILE:HG13	2.18	0.44
6:N:370:ASN:N	6:N:370:ASN:HD22	2.14	0.44
3:C:28:ALA:HB2	3:C:74:ALA:O	2.18	0.44
6:F:167:THR:CA	6:F:168:GLU:CB	2.95	0.44
6:F:190:ASP:O	6:F:193:MET:HG2	2.18	0.44
2:B:237:THR:N	2:B:287:ARG:HD2	2.28	0.44
6:N:143:LEU:CD1	6:N:145:ASN:CB	2.96	0.44
3:K:483:GLY:O	3:K:491:ILE:HB	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:VAL:HG11	1:A:425:VAL:HG22	1.99	0.44
2:J:389:SER:O	2:J:393:GLN:HG3	2.17	0.44
6:F:178:VAL:HG21	6:F:402:VAL:CG1	2.47	0.44
3:K:50:ASP:OD1	3:K:54:GLY:HA3	2.18	0.44
2:B:459:LEU:HD13	2:B:472:LEU:HD23	2.00	0.44
5:E:107:LEU:CD2	5:E:544:LEU:HG	2.35	0.44
2:J:100:ALA:O	2:J:104:ARG:HG3	2.18	0.44
1:A:185:LEU:HD23	1:A:185:LEU:HA	1.85	0.44
6:F:451:LEU:O	6:F:455:PRO:CG	2.66	0.44
7:G:400:VAL:O	7:G:404:LEU:HB2	2.17	0.44
4:D:485:ARG:H	4:D:485:ARG:CD	2.27	0.44
7:O:382:ALA:O	7:O:386:ILE:HG13	2.18	0.44
2:B:231:ILE:HG22	2:B:232:LEU:H	1.83	0.44
2:B:234:ALA:HA	2:B:325:VAL:HB	1.99	0.44
7:O:454:CYS:CB	7:O:461:ALA:HA	2.48	0.44
1:I:267:PRO:CA	1:I:268:GLU:CB	2.95	0.44
1:A:267:PRO:CA	1:A:268:GLU:CB	2.95	0.44
1:I:16:GLY:HA3	1:I:548:ASP:CB	2.45	0.44
6:N:280:LEU:CD1	6:N:343:LEU:HD11	2.48	0.44
2:J:401:VAL:HG22	2:J:402:LEU:N	2.33	0.44
5:M:150:PHE:CD1	5:M:472:PHE:HE2	2.35	0.44
4:L:379:ILE:HD12	4:L:379:ILE:N	2.33	0.44
3:K:350:THR:HG22	3:K:350:THR:O	2.18	0.44
1:A:129:PHE:CB	1:A:532:LEU:HD21	2.48	0.44
6:F:238:VAL:HG22	6:F:239:SER:H	1.83	0.44
6:F:422:LEU:O	6:F:426:LEU:HB2	2.17	0.43
8:P:6:PRO:CB	8:P:7:GLN:HG3	2.38	0.43
7:G:62:ILE:HG23	7:G:62:ILE:O	2.17	0.43
7:O:62:ILE:O	7:O:62:ILE:HG23	2.17	0.43
3:C:467:LEU:HD21	3:C:491:ILE:CG2	2.46	0.43
3:C:523:VAL:HG22	8:H:54:ILE:CD1	2.48	0.43
1:I:143:VAL:HG11	1:I:425:VAL:HG22	1.99	0.43
3:K:35:ILE:C	3:K:37:THR:H	2.21	0.43
8:H:71:MET:O	8:H:75:LEU:HG	2.17	0.43
6:F:195:GLU:OE1	6:F:197:MET:CE	2.65	0.43
2:B:100:ALA:O	2:B:104:ARG:HG3	2.18	0.43
6:F:105:ALA:HA	6:F:108:PHE:CE2	2.54	0.43
8:P:291:ILE:HD12	8:P:347:PRO:HG2	1.96	0.43
7:G:303:ALA:O	7:G:307:PHE:CD2	2.70	0.43
7:G:454:CYS:HB2	7:G:461:ALA:HB1	1.98	0.43
1:I:120:ILE:HG21	1:I:125:ILE:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:142:HIS:CD2	5:E:144:ILE:HB	2.53	0.43
5:E:314:LYS:HZ1	5:E:338:ASN:HA	1.83	0.43
6:N:342:ASP:CG	6:N:345:PRO:HG2	2.38	0.43
2:B:102:LEU:HD23	2:B:102:LEU:C	2.39	0.43
5:M:132:GLN:HA	5:M:132:GLN:NE2	2.32	0.43
3:K:174:LEU:HG	3:K:219:VAL:CG2	2.47	0.43
4:D:125:GLN:HB2	7:G:173:ASN:ND2	2.32	0.43
7:O:249:GLU:O	7:O:250:LEU:C	2.55	0.43
5:E:346:VAL:O	5:E:347:GLY:C	2.57	0.43
3:K:28:ALA:HB2	3:K:74:ALA:O	2.18	0.43
6:N:190:ASP:O	6:N:193:MET:HG2	2.18	0.43
2:B:370:ARG:O	2:B:372:ALA:N	2.50	0.43
3:K:467:LEU:HD21	3:K:491:ILE:CG2	2.46	0.43
8:H:15:LYS:HG3	8:H:16:GLN:H	1.83	0.43
3:C:35:ILE:C	3:C:37:THR:H	2.22	0.43
3:K:48:LEU:HD21	3:K:64:ILE:HD13	1.99	0.43
2:B:88:VAL:HG12	2:B:89:GLY:N	2.32	0.43
9:M:601:ADP:C8	9:M:601:ADP:C4'	3.01	0.43
3:C:51:PRO:O	3:C:52:MET:CG	2.63	0.43
5:M:276:PHE:HB3	5:M:327:PHE:HA	2.00	0.43
7:G:30:ILE:O	7:G:33:CYS:HB3	2.19	0.43
1:A:12:THR:CG2	5:E:97:ASP:H	2.24	0.43
4:L:94:THR:HG23	9:L:601:ADP:O3B	2.18	0.43
3:K:114:LYS:CA	3:K:115:ASN:CB	2.94	0.43
6:N:234:LEU:HD12	6:N:280:LEU:HD11	2.00	0.43
7:O:492:PHE:CB	7:O:497:TRP:HZ2	2.31	0.43
7:G:346:LEU:HD23	7:G:346:LEU:N	2.33	0.43
3:C:441:PRO:O	3:C:444:ALA:HB3	2.18	0.43
6:F:538:ARG:CG	6:F:538:ARG:NH1	2.72	0.43
1:I:25:ILE:HG22	1:I:26:ARG:N	2.32	0.43
5:E:450:MET:HE3	5:E:454:VAL:CG2	2.47	0.43
4:L:236:LEU:O	4:L:332:PRO:HA	2.18	0.43
3:C:219:VAL:O	3:C:219:VAL:HG12	2.18	0.43
5:E:396:GLU:HA	5:E:397:GLN:HA	1.53	0.43
6:N:83:GLN:HB2	6:N:91:THR:HG22	2.00	0.43
4:L:517:SER:O	4:L:521:ILE:HG13	2.19	0.43
3:C:457:ILE:HD13	3:C:467:LEU:CD1	2.19	0.43
1:I:494:ARG:CB	1:I:496:SER:H	2.21	0.43
3:K:463:ASP:O	3:K:467:LEU:HB2	2.18	0.43
3:C:48:LEU:HD21	3:C:64:ILE:HD13	1.99	0.43
3:C:318:ARG:O	3:C:319:ARG:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:147:ARG:HH22	6:F:409:LYS:HA	1.84	0.43
9:B:601:ADP:O1A	9:B:601:ADP:O3'	2.29	0.43
6:N:362:GLU:CG	6:N:364:PHE:CE2	2.93	0.43
4:D:184:GLU:HA	4:D:187:LYS:HG2	2.00	0.43
7:O:165:ALA:CB	7:O:399:ILE:HG21	2.46	0.43
7:O:409:ILE:CG2	7:O:410:VAL:H	2.28	0.43
6:F:280:LEU:CD1	6:F:343:LEU:HD11	2.48	0.43
7:O:452:GLN:H	7:O:452:GLN:CD	2.21	0.43
2:J:36:THR:HG22	2:J:42:MET:O	2.18	0.43
7:G:448:VAL:HA	7:G:451:ARG:HB2	2.00	0.43
6:N:105:ALA:HA	6:N:108:PHE:CE2	2.54	0.43
8:P:250:PHE:N	8:P:250:PHE:CD2	2.86	0.43
3:C:10:ALA:HA	3:C:11:SER:HA	1.59	0.43
3:C:508:GLN:CG	8:H:215:GLY:HA2	2.46	0.43
1:A:532:LEU:HD22	1:A:536:VAL:CG2	2.48	0.43
8:P:311:HIS:CG	8:P:312:TYR:N	2.86	0.43
3:K:209:ILE:HG23	3:K:382:ARG:HA	1.99	0.43
4:D:146:ASP:HB2	4:D:149:GLN:HB2	2.00	0.43
3:C:162:LYS:C	3:C:164:VAL:H	2.22	0.43
8:P:338:ALA:N	8:P:353:GLY:HA3	2.33	0.43
6:N:11:GLU:OE2	6:N:11:GLU:N	2.52	0.43
2:J:146:LYS:HD3	2:J:146:LYS:N	2.33	0.43
8:P:393:ASN:O	8:P:397:ILE:HG13	2.18	0.43
5:M:346:VAL:O	5:M:347:GLY:C	2.57	0.43
2:B:5:ILE:O	3:C:70:VAL:HA	2.18	0.43
6:F:171:THR:CB	6:F:172:PRO:HD3	2.48	0.43
6:N:171:THR:CB	6:N:172:PRO:HD3	2.48	0.43
4:D:518:ILE:HA	4:D:521:ILE:HD12	2.01	0.43
7:G:82:THR:HG21	7:G:517:ILE:HD11	1.99	0.43
3:K:310:LEU:HD21	3:K:316:VAL:HG22	1.99	0.43
4:L:72:HIS:CD2	8:P:15:LYS:HZ2	2.37	0.43
5:M:271:ILE:CB	5:M:362:ILE:HA	2.48	0.43
6:N:221:HIS:HA	6:N:222:PRO:HD3	1.92	0.43
3:K:318:ARG:O	3:K:319:ARG:C	2.56	0.43
6:F:214:VAL:HG22	6:F:377:THR:OG1	2.18	0.43
1:I:351:GLU:OE2	1:I:351:GLU:N	2.51	0.43
6:N:195:GLU:OE1	6:N:197:MET:CE	2.65	0.43
6:N:195:GLU:CD	6:N:197:MET:SD	2.97	0.43
6:F:209:PHE:HZ	6:F:211:LYS:HD2	1.83	0.43
3:C:129:LEU:HD21	3:C:511:LYS:HA	2.00	0.43
7:G:454:CYS:CB	7:G:461:ALA:HA	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:242:SER:HB3	4:D:298:ASN:HB2	2.00	0.43
1:A:538:ILE:HA	1:A:541:ILE:HD12	2.00	0.43
5:M:142:HIS:CD2	5:M:144:ILE:HB	2.53	0.43
2:J:32:LEU:HG	6:N:532:GLU:CD	2.37	0.43
4:L:161:LYS:HD2	4:L:161:LYS:HA	1.66	0.43
7:G:492:PHE:CB	7:G:497:TRP:HZ2	2.31	0.43
1:A:118:ASN:O	1:A:119:LYS:CG	2.65	0.43
6:N:185:GLN:HB3	6:N:407:LYS:HD3	2.00	0.43
2:B:146:LYS:HD3	2:B:146:LYS:N	2.33	0.43
8:H:311:HIS:CG	8:H:312:TYR:N	2.86	0.43
8:P:467:ALA:HB2	8:P:493:ASP:CB	2.49	0.43
7:O:51:ILE:HD12	7:O:69:ILE:HD11	2.01	0.43
2:J:422:ILE:CB	2:J:427:SER:CB	2.79	0.43
1:I:86:LEU:C	1:I:86:LEU:HD23	2.39	0.43
2:J:515:ILE:O	3:K:48:LEU:HA	2.19	0.43
2:J:459:LEU:HD13	2:J:472:LEU:HD23	2.00	0.43
1:A:177:SER:O	1:A:181:VAL:HG23	2.19	0.43
3:C:61:GLY:CA	3:C:94:THR:HG22	2.49	0.43
4:D:248:THR:O	4:D:250:ASN:OD1	2.37	0.43
3:C:152:LYS:HG2	3:C:176:LEU:HG	2.01	0.43
2:B:226:ILE:HG13	2:B:282:ASN:OD1	2.18	0.43
7:O:452:GLN:O	7:O:456:ASN:N	2.49	0.43
5:M:73:ILE:HG12	5:M:83:ILE:CG1	2.44	0.43
1:I:187:VAL:CG1	1:I:382:SER:H	2.31	0.43
1:I:73:LEU:O	1:I:74:ASP:OD1	2.36	0.43
1:I:460:LYS:O	1:I:464:VAL:HG23	2.18	0.43
8:H:333:CYS:SG	8:H:339:THR:HA	2.59	0.43
4:D:461:ASN:CB	4:D:464:LYS:HG2	2.47	0.43
8:H:250:PHE:N	8:H:250:PHE:CD2	2.86	0.43
1:I:54:VAL:HB	7:O:525:THR:HA	2.00	0.43
2:J:102:LEU:HD23	2:J:102:LEU:C	2.39	0.43
3:K:9:ASN:HB2	8:P:78:VAL:HG13	2.00	0.43
5:E:373:LYS:HE2	6:F:311:LYS:HZ3	1.83	0.43
6:F:324:ASN:HA	6:F:327:ARG:HB2	2.00	0.43
4:D:30:SER:HA	4:D:33:ASP:CG	2.37	0.43
8:H:464:ALA:HB2	8:H:474:VAL:HG11	2.00	0.43
2:B:169:ASP:HB2	2:B:172:HIS:HB2	2.00	0.43
4:D:66:LYS:HA	4:D:66:LYS:HD2	1.62	0.43
7:O:130:ARG:HE	7:O:130:ARG:HA	1.84	0.43
4:L:22:LYS:O	4:L:26:ILE:HG13	2.19	0.43
6:F:430:ASN:C	6:F:432:ASN:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:229:VAL:HG11	3:C:234:MET:CE	2.49	0.43
5:E:33:LYS:HG2	5:E:33:LYS:O	2.19	0.43
6:N:527:LEU:HD23	6:N:527:LEU:HA	1.71	0.43
7:O:83:LEU:HA	7:O:86:ILE:HD11	2.01	0.43
7:G:162:ALA:CB	7:G:179:VAL:HG13	2.47	0.43
2:J:329:PHE:CD2	2:J:329:PHE:O	2.53	0.43
7:G:166:MET:O	7:G:171:ILE:HB	2.18	0.43
7:G:382:ALA:O	7:G:386:ILE:HG13	2.18	0.43
3:K:152:LYS:HG2	3:K:176:LEU:HG	2.01	0.43
1:A:224:LEU:CD1	1:A:226:CYS:CB	2.90	0.43
6:F:221:HIS:CD2	6:F:224:MET:SD	3.09	0.43
5:E:73:ILE:O	5:E:74:LEU:HD22	2.18	0.43
1:A:187:VAL:CG1	1:A:382:SER:H	2.30	0.43
1:A:460:LYS:O	1:A:464:VAL:HG23	2.18	0.43
8:P:333:CYS:SG	8:P:339:THR:HA	2.59	0.43
2:B:401:VAL:HG22	2:B:402:LEU:N	2.33	0.43
1:A:54:VAL:HG12	1:A:56:ASP:N	2.30	0.43
5:E:127:SER:O	5:E:128:ALA:C	2.57	0.43
2:B:45:LEU:HD12	6:F:533:LEU:HD13	2.00	0.43
5:M:431:ARG:HA	5:M:434:VAL:HG12	2.01	0.43
8:P:424:GLY:O	8:P:428:ILE:HG13	2.18	0.43
8:P:420:LEU:HD23	8:P:421:PRO:HD2	2.01	0.43
8:P:35:ILE:HG23	8:P:85:LEU:HD12	2.01	0.43
6:F:114:HIS:ND1	6:F:115:PRO:HD2	2.34	0.43
8:H:155:ASP:HB3	8:H:156:LYS:H	1.48	0.43
7:G:130:ARG:HA	7:G:130:ARG:HE	1.84	0.43
3:C:209:ILE:HG23	3:C:382:ARG:HA	2.00	0.43
4:L:146:ASP:HB2	4:L:149:GLN:HB2	2.01	0.43
5:M:262:GLU:HA	5:M:263:GLY:HA2	1.67	0.43
6:F:419:TYR:O	6:F:422:LEU:HB2	2.19	0.43
7:G:516:LEU:CD2	7:G:517:ILE:N	2.68	0.43
3:K:306:GLN:C	3:K:310:LEU:HG	2.37	0.43
5:M:429:VAL:O	5:M:432:ASN:HB2	2.18	0.43
1:A:86:LEU:C	1:A:86:LEU:HD23	2.39	0.43
1:A:90:GLN:HG3	1:A:101:VAL:CG2	2.19	0.43
2:B:490:SER:HB2	2:B:492:LYS:CE	2.49	0.43
8:H:101:ASN:HD22	8:H:101:ASN:N	2.16	0.43
2:B:8:ASP:N	2:B:8:ASP:OD1	2.51	0.43
1:A:350:PHE:O	1:A:351:GLU:OE2	2.36	0.43
6:F:390:GLN:HE21	6:F:390:GLN:HA	1.84	0.43
7:O:132:ALA:HB2	7:O:439:ILE:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:55:THR:HG21	7:O:72:LEU:HD23	2.01	0.43
2:J:417:THR:HG23	2:J:418:GLU:N	2.33	0.43
4:D:461:ASN:HB3	4:D:464:LYS:CG	2.48	0.43
7:O:139:LYS:CB	7:O:420:VAL:HG12	2.49	0.43
3:C:341:GLU:OE2	8:H:281:GLU:OE2	2.37	0.43
4:L:58:SER:HA	4:L:392:ARG:HH12	1.84	0.43
3:C:174:LEU:HD21	3:C:379:ILE:HG21	2.01	0.43
4:L:469:LEU:HA	4:L:469:LEU:HD23	1.87	0.43
8:H:523:THR:HA	8:H:526:PHE:HD2	1.83	0.43
8:H:467:ALA:HB2	8:H:493:ASP:CB	2.49	0.43
1:A:396:ASP:O	1:A:399:GLU:HB3	2.19	0.43
1:A:434:ASP:O	1:A:438:THR:HG23	2.19	0.43
5:M:33:LYS:O	5:M:33:LYS:HG2	2.19	0.43
4:L:523:ASP:C	7:O:51:ILE:HG23	2.37	0.43
6:F:420:ILE:CG2	6:F:482:ASP:CG	2.86	0.43
5:E:364:PRO:HG3	6:F:307:ASP:CB	2.49	0.43
2:B:326:VAL:HG13	3:C:304:LEU:CD2	2.48	0.43
3:C:310:LEU:HD21	3:C:316:VAL:HG22	1.99	0.43
8:P:335:VAL:HG23	8:P:381:THR:OG1	2.19	0.43
8:H:335:VAL:HG23	8:H:381:THR:OG1	2.19	0.43
2:B:243:VAL:HG12	2:B:245:ILE:N	2.29	0.43
5:M:447:GLU:HG2	5:M:479:ILE:HB	2.01	0.43
7:O:101:VAL:HG22	7:O:506:ALA:HA	2.01	0.43
6:F:195:GLU:HG2	6:F:197:MET:CE	2.48	0.43
6:N:160:THR:N	6:N:164:ALA:HB3	2.31	0.43
6:N:32:VAL:HA	6:N:44:LYS:HZ2	1.84	0.43
2:J:60:GLY:H	2:J:93:THR:HG22	1.83	0.43
1:A:431:ILE:HG21	1:A:482:ALA:HA	2.01	0.43
1:I:187:VAL:O	1:I:381:SER:CA	2.67	0.43
1:A:66:GLY:HA3	1:A:99:THR:HG22	2.01	0.43
1:I:267:PRO:HB2	1:I:269:GLN:CB	2.49	0.43
1:I:129:PHE:CB	1:I:532:LEU:HD21	2.48	0.43
6:N:114:HIS:ND1	6:N:115:PRO:HD2	2.34	0.43
4:D:58:SER:HA	4:D:392:ARG:HH12	1.84	0.43
1:I:256:MET:HE3	1:I:260:VAL:O	2.19	0.43
5:M:87:GLY:HA3	5:M:120:THR:HG22	2.01	0.43
7:G:234:LYS:HA	7:G:234:LYS:HD3	1.34	0.43
2:J:350:GLU:HG2	2:J:350:GLU:H	1.37	0.43
4:D:55:ILE:HD12	8:H:80:PRO:HB3	2.01	0.43
6:F:429:ALA:O	6:F:432:ASN:HB2	2.19	0.43
6:F:433:LYS:HB3	6:F:444:ILE:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:82:THR:HG21	7:O:517:ILE:HD11	1.99	0.43
7:G:51:ILE:HD12	7:G:69:ILE:HD11	2.01	0.43
6:F:83:GLN:HB2	6:F:91:THR:HG22	2.00	0.43
2:J:243:VAL:CG1	2:J:245:ILE:HG13	2.49	0.43
3:C:35:ILE:CD1	3:C:65:LEU:HG	2.47	0.43
8:P:482:HIS:C	8:P:484:VAL:N	2.65	0.43
4:D:134:ILE:HB	4:D:421:ILE:HD13	2.01	0.43
5:M:483:LEU:HD21	9:M:601:ADP:H1'	2.00	0.43
1:A:351:GLU:N	1:A:351:GLU:OE2	2.52	0.43
6:N:451:LEU:O	6:N:455:PRO:CG	2.66	0.43
1:I:177:SER:O	1:I:181:VAL:HG23	2.19	0.43
4:D:325:SER:HB3	4:D:332:PRO:CG	2.49	0.43
5:E:447:GLU:HG2	5:E:479:ILE:HB	2.01	0.43
5:M:84:THR:O	5:M:90:ILE:HD11	2.18	0.43
4:L:103:LEU:HD22	4:L:515:VAL:HG21	1.99	0.43
5:E:245:LEU:HD22	5:E:245:LEU:HA	1.80	0.43
6:F:234:LEU:HD12	6:F:280:LEU:HD11	2.00	0.43
2:J:58:ASN:HD21	2:J:93:THR:HG21	1.84	0.43
3:C:108:ALA:N	3:C:109:PRO:CD	2.81	0.43
7:G:55:THR:HG21	7:G:72:LEU:HD23	2.01	0.43
6:N:113:VAL:CB	6:N:118:ILE:HD11	2.47	0.43
4:L:461:ASN:HB3	4:L:464:LYS:CG	2.48	0.43
6:F:185:GLN:HB3	6:F:407:LYS:HD3	2.00	0.43
2:B:92:THR:HA	2:B:95:VAL:HG23	2.00	0.43
1:A:129:PHE:HD2	1:A:129:PHE:N	2.17	0.43
6:N:324:ASN:HA	6:N:327:ARG:HB2	2.00	0.43
1:A:345:GLU:HA	1:A:346:GLY:HA2	1.67	0.43
3:K:219:VAL:O	3:K:219:VAL:HG12	2.18	0.43
7:G:17:THR:HG21	7:G:525:THR:O	2.19	0.43
5:E:87:GLY:HA3	5:E:120:THR:HG22	2.01	0.43
6:F:81:ALA:O	6:F:82:ALA:C	2.57	0.43
7:G:113:LYS:O	7:G:116:LEU:HB2	2.19	0.43
6:F:503:ILE:O	6:F:503:ILE:HG22	2.18	0.43
6:N:81:ALA:O	6:N:82:ALA:C	2.57	0.43
4:D:22:LYS:O	4:D:26:ILE:HG13	2.19	0.43
3:K:282:LEU:O	3:K:286:GLN:HG3	2.19	0.43
6:N:151:LEU:O	6:N:171:THR:HG21	2.19	0.43
6:N:426:LEU:HD22	6:N:426:LEU:HA	1.86	0.43
2:J:440:LEU:N	2:J:441:PRO:HD2	2.33	0.43
2:J:467:ILE:HA	2:J:468:SER:HA	1.59	0.43
6:N:420:ILE:O	6:N:424:ARG:N	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:483:GLY:O	3:C:491:ILE:HB	2.18	0.43
6:F:5:LEU:HB3	6:F:6:LEU:C	2.39	0.43
6:N:174:VAL:O	6:N:178:VAL:HG23	2.18	0.43
3:C:50:ASP:OD1	3:C:54:GLY:HA3	2.18	0.43
2:J:294:PRO:HA	2:J:297:LEU:HB2	2.00	0.43
5:M:310:ILE:HG23	5:M:335:LEU:HD23	2.01	0.43
4:L:184:GLU:HA	4:L:187:LYS:HG2	2.00	0.43
4:L:226:PRO:HD2	4:L:311:MET:HG2	2.01	0.43
4:D:328:LEU:O	4:D:345:ASP:CG	2.57	0.43
4:D:241:ILE:HD12	4:D:241:ILE:N	2.30	0.43
6:F:221:HIS:HB2	6:F:224:MET:CG	2.43	0.43
2:J:165:ILE:HG12	6:N:529:LEU:CD1	2.43	0.43
8:H:77:ILE:CD1	8:H:77:ILE:H	2.26	0.43
2:B:32:LEU:HD11	6:F:532:GLU:OE2	2.17	0.43
7:O:17:THR:HG21	7:O:525:THR:O	2.19	0.43
3:K:441:PRO:O	3:K:444:ALA:HB3	2.18	0.43
4:L:221:LYS:HE3	4:L:306:SER:CB	2.49	0.43
2:J:47:GLN:HE22	2:J:53:THR:N	2.17	0.43
3:C:350:THR:HG22	3:C:350:THR:O	2.18	0.43
8:H:420:LEU:HD23	8:H:421:PRO:HD2	2.01	0.43
4:L:423:ARG:O	4:L:427:LYS:HG2	2.19	0.43
4:L:389:GLU:O	4:L:392:ARG:HD3	2.19	0.43
8:P:464:ALA:HB2	8:P:474:VAL:HG11	2.00	0.43
1:I:434:ASP:O	1:I:438:THR:HG23	2.19	0.43
2:J:169:ASP:HB2	2:J:172:HIS:HB2	2.00	0.43
4:D:253:ILE:HG12	4:D:253:ILE:H	1.64	0.43
1:I:281:VAL:O	1:I:285:VAL:HG23	2.19	0.43
2:B:308:HIS:CE1	2:B:313:GLY:HA3	2.54	0.43
6:F:28:GLY:C	6:F:30:GLN:H	2.22	0.43
2:J:319:LEU:O	2:J:319:LEU:HD23	2.19	0.42
2:B:319:LEU:O	2:B:319:LEU:HD23	2.19	0.42
2:B:440:LEU:N	2:B:441:PRO:HD2	2.33	0.42
6:N:92:THR:OG1	9:N:601:ADP:O2B	2.35	0.42
6:F:143:LEU:CD1	6:F:145:ASN:CB	2.96	0.42
4:L:138:MET:HE1	4:L:416:ALA:HB1	2.01	0.42
4:L:134:ILE:HB	4:L:421:ILE:HD13	2.01	0.42
6:N:147:ARG:HH22	6:N:409:LYS:HA	1.84	0.42
7:G:101:VAL:HG22	7:G:506:ALA:HA	2.01	0.42
2:J:218:PHE:HA	2:J:304:ASN:O	2.19	0.42
2:B:294:PRO:HA	2:B:297:LEU:HB2	2.00	0.42
7:G:178:PHE:CZ	7:G:389:VAL:HG13	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:77:MET:O	4:L:81:VAL:HG23	2.18	0.42
7:G:282:LEU:HD12	7:G:283:ARG:N	2.34	0.42
7:O:236:PHE:O	7:O:239:PRO:HG3	2.19	0.42
8:P:137:PHE:HE2	8:P:434:ILE:HA	1.84	0.42
1:I:543:THR:O	5:M:72:LYS:HB3	2.19	0.42
8:H:302:GLY:HA2	8:H:324:PRO:HD2	2.01	0.42
1:A:546:THR:HA	5:E:75:ILE:HB	2.01	0.42
5:E:431:ARG:HA	5:E:434:VAL:HG12	2.00	0.42
3:K:237:HIS:C	3:K:238:ILE:HG13	2.40	0.42
8:H:35:ILE:HG23	8:H:85:LEU:HD12	2.01	0.42
5:E:132:GLN:NE2	5:E:132:GLN:HA	2.33	0.42
3:C:282:LEU:O	3:C:286:GLN:HG3	2.19	0.42
8:P:318:ILE:HG22	8:P:319:LEU:O	2.19	0.42
3:K:162:LYS:C	3:K:164:VAL:H	2.22	0.42
5:M:477:ASP:O	5:M:480:PRO:HD2	2.19	0.42
6:N:419:TYR:O	6:N:422:LEU:HB2	2.19	0.42
6:F:430:ASN:CA	6:F:433:LYS:HB2	2.48	0.42
6:N:233:VAL:HG12	6:N:294:VAL:CG2	2.49	0.42
6:N:352:GLY:C	6:N:367:VAL:HG12	2.40	0.42
6:N:352:GLY:CA	6:N:369:GLU:C	2.48	0.42
4:D:517:SER:O	4:D:521:ILE:HG13	2.19	0.42
4:L:518:ILE:HA	4:L:521:ILE:HD12	2.01	0.42
6:F:143:LEU:HD21	6:F:145:ASN:HB3	1.97	0.42
2:B:494:LYS:HD2	2:B:494:LYS:HA	1.79	0.42
6:N:16:ASP:O	6:N:20:LYS:N	2.46	0.42
8:P:48:PRO:HG3	8:P:169:SER:HA	2.02	0.42
4:D:236:LEU:O	4:D:332:PRO:HA	2.18	0.42
7:O:36:VAL:CG2	7:O:37:GLN:N	2.83	0.42
7:O:178:PHE:CZ	7:O:389:VAL:HG13	2.53	0.42
4:D:436:GLN:CD	4:D:436:GLN:H	2.22	0.42
1:I:66:GLY:HA3	1:I:99:THR:HG22	2.01	0.42
4:L:436:GLN:CD	4:L:436:GLN:H	2.22	0.42
2:J:287:ARG:H	2:J:287:ARG:HG2	1.58	0.42
2:J:120:ILE:HG23	2:J:124:TYR:CE1	2.54	0.42
5:M:127:SER:O	5:M:128:ALA:C	2.57	0.42
4:D:423:ARG:O	4:D:427:LYS:HG2	2.19	0.42
7:G:117:GLU:CD	7:G:117:GLU:N	2.73	0.42
5:E:263:GLY:HA3	5:E:380:ILE:O	2.19	0.42
4:L:200:VAL:HA	4:L:381:GLY:O	2.18	0.42
5:E:485:GLU:HB2	5:E:491:PRO:HG3	2.01	0.42
4:D:200:VAL:HA	4:D:381:GLY:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:466:GLN:HG3	5:E:467:TYR:CD2	2.54	0.42
6:N:430:ASN:C	6:N:432:ASN:H	2.22	0.42
5:E:273:THR:HG21	5:E:364:PRO:CA	2.47	0.42
1:I:363:GLN:HE21	1:I:363:GLN:HB2	1.66	0.42
2:B:236:THR:HA	2:B:287:ARG:CD	2.50	0.42
3:C:228:ASP:OD2	3:C:229:VAL:N	2.53	0.42
4:D:72:HIS:CD2	8:H:15:LYS:NZ	2.87	0.42
2:J:513:ASN:O	2:J:514:ILE:CD1	2.46	0.42
2:J:490:SER:HB2	2:J:492:LYS:CE	2.49	0.42
4:D:254:VAL:HG22	8:H:265:VAL:CA	2.34	0.42
6:F:195:GLU:CD	6:F:197:MET:SD	2.97	0.42
5:M:320:VAL:HG22	5:M:341:PRO:CD	2.40	0.42
4:D:232:ALA:O	4:D:234:ILE:HD12	2.19	0.42
6:F:527:LEU:HA	6:F:527:LEU:HD23	1.71	0.42
7:O:86:ILE:HG13	7:O:86:ILE:H	1.58	0.42
7:G:236:PHE:O	7:G:239:PRO:HD3	2.19	0.42
7:G:236:PHE:O	7:G:239:PRO:HG3	2.19	0.42
2:J:226:ILE:HG13	2:J:282:ASN:OD1	2.18	0.42
1:A:482:ALA:O	1:A:485:GLN:O	2.37	0.42
3:C:291:ARG:N	3:C:292:PRO:CD	2.80	0.42
7:O:346:LEU:HD23	7:O:346:LEU:N	2.33	0.42
8:P:177:ILE:O	8:P:181:LEU:HD12	2.19	0.42
1:A:17:GLY:HA2	1:A:547:VAL:HA	2.01	0.42
8:P:486:GLU:N	8:P:487:PRO:HA	2.34	0.42
8:H:35:ILE:CD1	8:H:82:VAL:HA	2.49	0.42
8:P:35:ILE:HD13	8:P:82:VAL:HG22	2.00	0.42
5:M:477:ASP:C	5:M:480:PRO:HD2	2.39	0.42
3:K:61:GLY:CA	3:K:94:THR:HG22	2.49	0.42
5:M:297:LYS:HD2	5:M:297:LYS:HA	1.66	0.42
8:H:338:ALA:N	8:H:353:GLY:HA3	2.33	0.42
2:J:3:VAL:HB	2:J:4:GLN:CD	2.40	0.42
6:N:433:LYS:HB3	6:N:444:ILE:HG13	2.00	0.42
6:F:433:LYS:CG	6:F:444:ILE:HG13	2.48	0.42
3:K:229:VAL:HG11	3:K:234:MET:CE	2.49	0.42
3:K:228:ASP:OD2	3:K:229:VAL:N	2.52	0.42
2:B:326:VAL:HG11	3:C:304:LEU:HD13	2.01	0.42
2:B:372:ALA:HA	6:F:519:GLY:HA2	2.01	0.42
8:P:335:VAL:HG13	8:P:379:SER:CB	2.46	0.42
6:F:6:LEU:HD12	6:F:7:ASN:H	1.85	0.42
4:L:248:THR:O	4:L:250:ASN:OD1	2.37	0.42
8:H:306:GLY:O	8:H:310:LEU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:485:GLU:O	6:F:488:TYR:N	2.53	0.42
2:J:76:VAL:O	2:J:79:ASN:HB2	2.20	0.42
3:K:320:VAL:HG12	3:K:324:ASP:HB3	2.01	0.42
6:F:209:PHE:CE2	6:F:376:CYS:SG	2.97	0.42
2:B:218:PHE:HA	2:B:304:ASN:O	2.19	0.42
4:D:77:MET:O	4:D:81:VAL:HG23	2.18	0.42
7:O:448:VAL:HA	7:O:451:ARG:HB2	2.00	0.42
4:L:242:SER:HB3	4:L:298:ASN:HB2	2.00	0.42
8:H:137:PHE:HE2	8:H:434:ILE:HA	1.84	0.42
4:L:94:THR:O	4:L:96:VAL:N	2.52	0.42
1:A:183:ALA:CB	1:A:383:SER:HB2	2.47	0.42
6:F:136:PHE:O	6:F:138:ILE:HG13	2.19	0.42
1:I:17:GLY:HA2	1:I:547:VAL:HA	2.01	0.42
8:P:296:VAL:HG11	8:P:299:ILE:HD11	2.01	0.42
1:A:178:ASN:HD21	1:A:182:ASP:CG	2.23	0.42
1:I:133:LEU:HG	1:I:532:LEU:HD12	2.01	0.42
4:L:325:SER:HB3	4:L:332:PRO:CG	2.49	0.42
5:M:535:LYS:C	5:M:535:LYS:HD2	2.38	0.42
6:N:238:VAL:HG22	6:N:239:SER:H	1.83	0.42
5:E:477:ASP:C	5:E:480:PRO:HD2	2.39	0.42
1:A:281:VAL:O	1:A:285:VAL:HG23	2.19	0.42
1:I:296:VAL:O	1:I:297:LEU:HD23	2.19	0.42
1:A:301:GLY:HA2	1:A:320:ARG:H	1.84	0.42
1:I:301:GLY:HA2	1:I:320:ARG:H	1.84	0.42
6:N:171:THR:N	6:N:172:PRO:HD2	2.33	0.42
6:F:124:ILE:HB	6:F:444:ILE:CD1	2.48	0.42
2:B:415:VAL:HB	2:B:434:ALA:HB2	2.02	0.42
6:N:5:LEU:HB3	6:N:6:LEU:C	2.39	0.42
5:E:350:GLU:O	5:E:353:HIS:N	2.52	0.42
3:C:298:GLU:HG3	3:C:325:ASN:HD22	1.84	0.42
7:O:41:LYS:N	7:O:42:PRO:HD2	2.34	0.42
2:J:132:LEU:HD21	2:J:495:ARG:CG	2.43	0.42
6:F:147:ARG:O	6:F:147:ARG:HG3	2.20	0.42
6:N:147:ARG:HG3	6:N:147:ARG:O	2.20	0.42
3:C:415:GLY:HA3	3:C:501:GLU:OE1	2.20	0.42
2:B:159:THR:CG2	2:B:487:ILE:HA	2.50	0.42
3:C:243:VAL:O	3:C:348:VAL:HG13	2.19	0.42
3:C:332:THR:HB	3:C:349:GLY:CA	2.49	0.42
3:K:129:LEU:HD21	3:K:511:LYS:HA	2.00	0.42
3:K:243:VAL:O	3:K:348:VAL:HG13	2.19	0.42
7:O:455:GLU:CG	7:O:461:ALA:HB2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:404:GLY:HA2	9:J:601:ADP:N3	2.34	0.42
1:A:187:VAL:O	1:A:381:SER:CA	2.67	0.42
1:I:431:ILE:HG21	1:I:482:ALA:HA	2.01	0.42
4:L:439:ILE:O	4:L:439:ILE:HG22	2.19	0.42
8:P:77:ILE:H	8:P:77:ILE:CD1	2.26	0.42
8:P:269:ASN:O	8:P:272:GLU:HB2	2.19	0.42
2:J:213:ILE:HG23	2:J:354:LEU:HD21	2.02	0.42
1:I:178:ASN:HD21	1:I:182:ASP:CG	2.23	0.42
1:I:532:LEU:HD22	1:I:536:VAL:CG2	2.48	0.42
4:D:389:GLU:O	4:D:392:ARG:HD3	2.19	0.42
5:E:269:LEU:HD22	5:E:269:LEU:H	1.84	0.42
3:K:286:GLN:OE1	3:K:340:VAL:HG22	2.19	0.42
1:A:296:VAL:O	1:A:297:LEU:HD23	2.19	0.42
1:I:476:LYS:C	1:I:509:ILE:HD11	2.40	0.42
5:E:445:ALA:CB	5:E:510:ILE:O	2.67	0.42
6:F:230:ASN:N	6:F:353:LEU:HD23	2.35	0.42
2:J:415:VAL:HB	2:J:434:ALA:HB2	2.02	0.42
4:L:521:ILE:HD13	7:O:52:LEU:HB2	2.00	0.42
6:N:6:LEU:HD13	6:N:7:ASN:H	1.85	0.42
3:C:47:MET:CE	3:C:49:LEU:HD21	2.49	0.42
1:I:351:GLU:H	1:I:354:TYR:HD2	1.68	0.42
7:G:83:LEU:HA	7:G:86:ILE:HD11	2.01	0.42
7:O:282:LEU:HD12	7:O:283:ARG:N	2.34	0.42
2:J:231:ILE:HG22	2:J:232:LEU:H	1.83	0.42
4:D:94:THR:O	4:D:96:VAL:N	2.52	0.42
1:I:115:LEU:HD23	1:I:115:LEU:HA	1.80	0.42
8:P:163:ILE:HD11	8:P:404:GLY:CA	2.50	0.42
4:L:178:VAL:HG11	4:L:401:ILE:CD1	2.48	0.42
8:P:94:ILE:H	8:P:94:ILE:HG13	1.50	0.42
8:H:296:VAL:HG11	8:H:299:ILE:HD11	2.01	0.42
3:C:140:SER:HB2	3:C:411:SER:HB2	2.02	0.42
3:K:9:ASN:HB2	8:P:78:VAL:CG1	2.50	0.42
5:M:280:LYS:HA	5:M:281:PRO:HD3	1.80	0.42
8:H:177:ILE:O	8:H:181:LEU:HD12	2.20	0.42
2:J:116:HIS:CE1	2:J:118:GLN:CB	2.99	0.42
5:E:476:LEU:HD13	5:E:476:LEU:HA	1.89	0.42
4:L:234:ILE:N	4:L:234:ILE:HD12	2.35	0.42
7:O:117:GLU:CD	7:O:117:GLU:N	2.73	0.42
5:M:269:LEU:HD22	5:M:269:LEU:H	1.85	0.42
5:M:263:GLY:HA3	5:M:380:ILE:O	2.20	0.42
5:M:466:GLN:HG3	5:M:467:TYR:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:GLU:HA	1:A:551:PRO:HD3	1.88	0.42
6:F:11:GLU:OE2	6:F:11:GLU:N	2.52	0.42
7:O:113:LYS:O	7:O:116:LEU:HB2	2.19	0.42
5:M:445:ALA:CB	5:M:510:ILE:O	2.67	0.42
8:H:318:ILE:HG22	8:H:319:LEU:O	2.19	0.42
2:B:3:VAL:HB	2:B:4:GLN:CD	2.40	0.42
6:F:53:ILE:CG1	6:F:53:ILE:O	2.68	0.42
3:C:34:VAL:HG12	3:C:35:ILE:N	2.35	0.42
2:J:511:VAL:O	2:J:513:ASN:N	2.49	0.42
3:K:47:MET:CE	3:K:49:LEU:HD21	2.49	0.42
5:M:362:ILE:N	5:M:362:ILE:HD12	2.34	0.42
3:C:320:VAL:HG12	3:C:324:ASP:HB3	2.02	0.42
4:D:138:MET:HE1	4:D:416:ALA:HB1	2.01	0.42
2:J:27:ILE:HG21	2:J:104:ARG:HD2	2.02	0.42
8:P:459:VAL:O	8:P:462:THR:HG22	2.20	0.42
2:B:60:GLY:H	2:B:93:THR:HG22	1.84	0.42
3:C:104:LEU:CD2	3:C:517:ALA:HA	2.49	0.42
3:K:104:LEU:CD2	3:K:517:ALA:HA	2.49	0.42
8:H:24:ALA:HB2	8:H:531:ALA:O	2.20	0.42
7:O:30:ILE:O	7:O:33:CYS:HB3	2.19	0.42
8:P:291:ILE:HD12	8:P:347:PRO:HG3	1.97	0.42
6:N:56:THR:HB	6:N:390:GLN:HE22	1.79	0.42
4:D:499:GLN:HA	4:D:500:PRO:HD3	1.86	0.42
2:J:232:LEU:CD1	2:J:234:ALA:HB2	2.50	0.42
1:A:12:THR:HA	1:A:13:LEU:HA	1.69	0.42
7:G:450:PRO:O	7:G:453:LEU:HB2	2.20	0.42
2:J:236:THR:HA	2:J:287:ARG:CD	2.50	0.42
2:B:49:ALA:HB2	6:F:536:ALA:O	2.20	0.42
5:E:116:GLY:HA3	5:E:428:CYS:CB	2.50	0.42
4:D:221:LYS:HE2	4:D:221:LYS:HB2	1.94	0.42
4:D:221:LYS:HE3	4:D:306:SER:CB	2.49	0.42
1:I:129:PHE:N	1:I:129:PHE:HD2	2.17	0.42
8:P:420:LEU:HD23	8:P:421:PRO:CD	2.50	0.42
3:K:207:GLU:HB2	3:K:380:MET:HA	2.02	0.42
6:F:456:LYS:O	6:F:460:LYS:N	2.53	0.42
6:N:422:LEU:CD1	6:N:517:ILE:HD11	2.50	0.42
6:F:117:ILE:HD12	5:M:34:ASP:CA	2.31	0.42
2:J:424:GLY:O	2:J:427:SER:OG	2.33	0.42
1:A:91:ASP:HA	1:A:95:GLY:HA2	2.00	0.42
2:B:243:VAL:CG1	2:B:245:ILE:HG13	2.49	0.42
1:A:143:VAL:CG1	1:A:420:PRO:HD2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:507:VAL:HG21	3:C:388:ILE:HG12	2.01	0.42
4:D:99:LEU:HA	4:D:449:VAL:HG11	2.02	0.42
4:D:81:VAL:HG22	7:G:382:ALA:CB	2.49	0.42
5:M:170:ALA:N	5:M:523:LYS:HZ1	2.18	0.42
3:K:456:LEU:HD22	3:K:456:LEU:HA	1.79	0.42
2:J:161:LEU:HD22	2:J:166:LEU:HD11	2.01	0.42
3:K:527:VAL:HG11	8:P:75:LEU:HD21	2.02	0.42
4:D:439:ILE:HG22	4:D:439:ILE:O	2.19	0.42
7:O:507:LEU:C	7:O:507:LEU:HD13	2.40	0.42
2:B:120:ILE:HG23	2:B:124:TYR:CE1	2.54	0.42
8:P:302:GLY:HA2	8:P:324:PRO:HD2	2.01	0.42
8:H:420:LEU:HD23	8:H:421:PRO:CD	2.50	0.42
8:H:35:ILE:HD13	8:H:82:VAL:HG22	2.00	0.42
3:C:182:VAL:HG23	3:C:184:LYS:HG3	2.02	0.42
3:C:286:GLN:OE1	3:C:340:VAL:HG22	2.19	0.42
1:A:335:ALA:HB2	1:A:356:GLY:CA	2.49	0.42
8:P:523:THR:HA	8:P:526:PHE:HD2	1.83	0.42
3:C:207:GLU:HB2	3:C:380:MET:HA	2.02	0.42
1:I:396:ASP:O	1:I:399:GLU:HB3	2.19	0.42
6:F:171:THR:N	6:F:172:PRO:HD2	2.33	0.42
2:J:424:GLY:H	2:J:427:SER:HB3	1.85	0.42
5:M:350:GLU:O	5:M:353:HIS:N	2.52	0.42
2:J:459:LEU:HD11	2:J:471:GLY:C	2.40	0.42
2:B:155:HIS:O	2:B:159:THR:HG23	2.20	0.42
3:C:103:ILE:CG2	3:C:517:ALA:HB1	2.50	0.42
5:M:268:LYS:O	5:M:319:ASP:N	2.53	0.42
6:N:243:GLU:CA	6:N:243:GLU:OE2	2.52	0.42
4:D:226:PRO:HD2	4:D:311:MET:HG2	2.01	0.42
7:G:109:MET:SD	7:G:514:THR:HG21	2.59	0.42
7:O:409:ILE:CG2	7:O:410:VAL:N	2.82	0.42
7:G:455:GLU:CG	7:G:461:ALA:HB2	2.49	0.42
7:G:132:ALA:HB2	7:G:439:ILE:HD13	2.01	0.42
7:O:104:LEU:O	7:O:108:LEU:HB2	2.20	0.42
1:I:54:VAL:C	1:I:56:ASP:H	2.23	0.42
3:C:241:PRO:O	3:C:350:THR:HA	2.20	0.42
6:F:356:GLN:HA	6:F:365:THR:HA	2.02	0.42
6:N:356:GLN:HA	6:N:365:THR:HA	2.02	0.42
4:D:60:ASP:N	4:D:392:ARG:NH2	2.68	0.42
4:L:60:ASP:N	4:L:392:ARG:NH2	2.68	0.42
1:A:256:MET:H	7:G:255:ASP:CB	2.32	0.42
8:P:256:ILE:HD11	8:P:308:LEU:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:477:ASP:O	5:E:480:PRO:HD2	2.19	0.42
3:C:237:HIS:C	3:C:238:ILE:HG13	2.39	0.42
2:J:308:HIS:CE1	2:J:313:GLY:HA3	2.54	0.42
1:I:335:ALA:HB2	1:I:356:GLY:CA	2.50	0.42
4:D:9:ALA:HB1	7:G:76:VAL:H	1.85	0.42
4:L:113:LYS:HB2	4:L:113:LYS:HE3	1.86	0.42
6:F:133:LEU:HD12	6:F:422:LEU:HD11	2.02	0.42
6:F:422:LEU:CD1	6:F:517:ILE:HD11	2.50	0.42
6:N:230:ASN:N	6:N:353:LEU:HD23	2.35	0.42
6:F:332:THR:O	6:F:333:GLY:C	2.58	0.42
1:I:250:ASN:HD21	1:I:252:GLN:HG2	1.85	0.42
5:M:273:THR:HG21	5:M:364:PRO:CA	2.47	0.42
2:B:422:ILE:HG22	2:B:424:GLY:CA	2.50	0.42
6:N:53:ILE:O	6:N:53:ILE:CG1	2.68	0.42
2:J:245:ILE:O	2:J:246:PHE:HB3	2.19	0.42
2:B:459:LEU:HD11	2:B:471:GLY:C	2.40	0.42
2:B:459:LEU:CD1	2:B:471:GLY:O	2.68	0.42
1:I:350:PHE:O	1:I:351:GLU:OE2	2.36	0.42
5:M:332:ASN:HA	5:M:335:LEU:HD12	2.02	0.42
4:L:226:PRO:CD	4:L:311:MET:HG2	2.50	0.42
7:O:182:CYS:SG	7:O:183:VAL:N	2.93	0.42
7:G:83:LEU:HA	7:G:86:ILE:CD1	2.50	0.42
7:O:166:MET:O	7:O:171:ILE:HB	2.18	0.42
2:B:232:LEU:CD1	2:B:234:ALA:HB2	2.50	0.42
5:E:362:ILE:N	5:E:362:ILE:HD12	2.34	0.42
1:A:543:THR:O	5:E:72:LYS:HB3	2.20	0.42
1:A:73:LEU:O	1:A:74:ASP:OD1	2.36	0.42
4:L:485:ARG:H	4:L:485:ARG:CD	2.27	0.42
2:J:57:THR:HG21	2:J:382:ARG:CD	2.46	0.42
1:A:118:ASN:C	1:A:119:LYS:CD	2.88	0.42
7:G:139:LYS:CB	7:G:420:VAL:HG12	2.49	0.42
8:H:48:PRO:HG3	8:H:169:SER:HA	2.01	0.42
2:B:47:GLN:HE22	2:B:53:THR:N	2.17	0.42
6:F:68:ILE:HD13	6:F:74:VAL:HG13	2.02	0.42
3:K:85:GLN:NE2	3:K:508:GLN:OE1	2.53	0.42
4:L:232:ALA:O	4:L:234:ILE:HD12	2.19	0.42
8:H:256:ILE:HD11	8:H:308:LEU:HD13	2.02	0.42
6:F:309:PHE:HB3	6:F:314:ILE:O	2.20	0.42
1:I:549:PRO:HA	5:M:77:PRO:O	2.20	0.42
6:N:309:PHE:HB3	6:N:314:ILE:O	2.20	0.42
6:N:433:LYS:HG3	6:N:444:ILE:CG2	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:434:LEU:HD23	6:N:441:LYS:CB	2.40	0.41
3:C:303:ASP:HB3	3:C:304:LEU:H	1.46	0.41
1:I:143:VAL:CG1	1:I:420:PRO:HD2	2.50	0.41
3:K:298:GLU:HG3	3:K:325:ASN:HD22	1.84	0.41
4:L:265:LYS:NZ	8:P:343:ARG:HD3	2.36	0.41
2:B:162:SER:O	2:B:163:SER:OG	2.30	0.41
2:B:58:ASN:HD21	2:B:93:THR:HG21	1.84	0.41
4:D:234:ILE:N	4:D:234:ILE:HD12	2.35	0.41
7:O:145:VAL:O	7:O:409:ILE:N	2.52	0.41
2:J:474:LEU:HG	9:J:601:ADP:C2	2.55	0.41
2:B:197:LYS:C	2:B:198:ILE:HD12	2.41	0.41
7:O:450:PRO:O	7:O:453:LEU:HB2	2.20	0.41
1:A:219:VAL:HG12	1:A:221:GLY:N	2.34	0.41
1:I:219:VAL:HG12	1:I:221:GLY:N	2.35	0.41
8:P:163:ILE:HG12	8:P:182:VAL:HG11	2.01	0.41
1:A:267:PRO:HB2	1:A:269:GLN:CB	2.49	0.41
8:H:186:VAL:HA	8:H:207:ILE:HD11	2.02	0.41
2:B:15:ALA:O	2:B:19:ARG:HG2	2.20	0.41
1:A:54:VAL:C	1:A:56:ASP:H	2.23	0.41
7:G:507:LEU:HD13	7:G:507:LEU:C	2.40	0.41
4:D:379:ILE:N	4:D:379:ILE:HD12	2.33	0.41
6:N:429:ALA:O	6:N:432:ASN:HB2	2.19	0.41
2:B:424:GLY:H	2:B:427:SER:HB3	1.85	0.41
2:B:72:PRO:CG	3:C:47:MET:HE1	2.50	0.41
6:N:485:GLU:O	6:N:488:TYR:N	2.53	0.41
6:N:196:ILE:HG22	6:N:378:ILE:HG23	2.02	0.41
8:H:32:ILE:HD11	8:H:111:LEU:C	2.41	0.41
6:F:63:LEU:HD11	6:F:95:VAL:HG21	2.03	0.41
7:O:109:MET:SD	7:O:514:THR:HG21	2.59	0.41
7:G:182:CYS:SG	7:G:183:VAL:N	2.93	0.41
7:G:396:ALA:O	7:G:400:VAL:HG13	2.20	0.41
5:M:418:GLU:OE2	5:M:418:GLU:HA	2.20	0.41
2:J:38:GLY:HA3	2:J:474:LEU:HD12	2.02	0.41
1:I:482:ALA:O	1:I:485:GLN:O	2.37	0.41
5:E:268:LYS:O	5:E:319:ASP:N	2.53	0.41
7:G:104:LEU:O	7:G:108:LEU:HB2	2.20	0.41
2:J:105:GLU:O	2:J:109:LEU:HD23	2.21	0.41
4:D:65:LEU:HA	4:D:65:LEU:HD23	1.84	0.41
3:K:355:PHE:HE2	3:K:366:SER:HB3	1.84	0.41
6:F:533:LEU:HD23	6:F:533:LEU:N	2.35	0.41
7:G:23:LYS:O	7:G:26:ILE:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:81:ILE:N	5:E:81:ILE:HD12	2.35	0.41
5:M:81:ILE:HD12	5:M:81:ILE:N	2.35	0.41
3:K:174:LEU:HD21	3:K:379:ILE:HG21	2.01	0.41
6:N:456:LYS:O	6:N:460:LYS:N	2.53	0.41
5:E:38:LYS:HA	5:E:38:LYS:HD2	1.70	0.41
1:A:476:LYS:C	1:A:509:ILE:HD11	2.40	0.41
7:G:528:GLY:HA3	7:G:529:SER:C	2.41	0.41
6:N:133:LEU:HD12	6:N:422:LEU:HD11	2.02	0.41
6:N:539:SER:O	6:N:540:THR:C	2.58	0.41
2:B:320:VAL:HG21	2:B:337:LEU:CA	2.51	0.41
4:D:521:ILE:HG23	7:G:50:ASP:C	2.40	0.41
8:H:54:ILE:CG2	8:H:55:ILE:N	2.83	0.41
3:C:229:VAL:CG1	3:C:230:VAL:N	2.84	0.41
2:J:422:ILE:HG22	2:J:424:GLY:CA	2.50	0.41
2:B:492:LYS:O	2:B:495:ARG:HB3	2.20	0.41
2:J:492:LYS:H	2:J:492:LYS:HZ3	1.65	0.41
2:J:492:LYS:O	2:J:495:ARG:HB3	2.21	0.41
2:J:263:LYS:NZ	3:K:266:GLU:HG2	2.35	0.41
4:L:263:ILE:C	4:L:265:LYS:H	2.23	0.41
5:E:167:ASP:HB3	5:E:168:ILE:H	1.58	0.41
2:B:27:ILE:HG21	2:B:104:ARG:HD2	2.02	0.41
1:A:351:GLU:H	1:A:354:TYR:HD2	1.68	0.41
8:P:24:ALA:HB2	8:P:531:ALA:O	2.20	0.41
3:K:103:ILE:CG2	3:K:517:ALA:HB1	2.50	0.41
3:K:244:VAL:HG22	3:K:348:VAL:HG22	2.03	0.41
2:B:57:THR:HG21	2:B:382:ARG:CD	2.46	0.41
8:P:62:ILE:HG23	8:P:392:ASN:OD1	2.20	0.41
7:O:236:PHE:O	7:O:239:PRO:HD3	2.19	0.41
7:O:303:ALA:O	7:O:307:PHE:CD2	2.70	0.41
2:J:474:LEU:HD23	2:J:474:LEU:N	2.35	0.41
6:F:221:HIS:HA	6:F:222:PRO:HD3	1.92	0.41
5:E:73:ILE:HG12	5:E:83:ILE:CG1	2.44	0.41
2:J:197:LYS:C	2:J:198:ILE:HD12	2.41	0.41
4:D:411:ILE:O	4:D:498:LEU:HB3	2.21	0.41
2:J:45:LEU:HD23	2:J:56:VAL:HG13	2.02	0.41
3:K:140:SER:HB2	3:K:411:SER:HB2	2.02	0.41
8:H:269:ASN:O	8:H:272:GLU:HB2	2.19	0.41
2:J:159:THR:CG2	2:J:487:ILE:HA	2.49	0.41
7:O:23:LYS:O	7:O:26:ILE:HG22	2.20	0.41
1:A:498:ARG:O	1:A:499:ASN:HB3	2.20	0.41
2:J:160:THR:HG21	2:J:390:VAL:HG11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:415:GLY:HA3	3:K:501:GLU:OE1	2.20	0.41
5:M:485:GLU:HB2	5:M:491:PRO:HG3	2.01	0.41
8:P:92:GLN:HB3	8:P:92:GLN:HE21	1.63	0.41
6:F:524:ALA:O	6:F:528:LEU:HG	2.21	0.41
5:M:423:LEU:C	5:M:425:ASP:N	2.73	0.41
1:A:273:ILE:HG21	5:E:295:TYR:CE2	2.54	0.41
6:N:167:THR:CB	6:N:169:VAL:N	2.64	0.41
6:N:415:ALA:HB2	6:N:506:ILE:HD13	2.03	0.41
6:N:89:ASP:OD1	9:N:601:ADP:O3B	2.38	0.41
6:N:89:ASP:OD1	6:N:90:GLY:N	2.43	0.41
2:J:466:GLY:C	2:J:467:ILE:HG13	2.41	0.41
2:B:326:VAL:O	2:B:327:SER:HB3	2.21	0.41
3:C:230:VAL:O	3:C:231:HIS:CG	2.74	0.41
2:B:127:ALA:HB1	2:B:430:VAL:HG13	2.02	0.41
2:J:246:PHE:CD1	2:J:247:GLY:N	2.89	0.41
2:B:246:PHE:CD1	2:B:247:GLY:N	2.89	0.41
2:B:76:VAL:O	2:B:79:ASN:HB2	2.20	0.41
6:N:181:VAL:O	6:N:184:ALA:HB3	2.20	0.41
2:B:161:LEU:HD22	2:B:166:LEU:HD11	2.01	0.41
5:M:86:ASP:O	5:M:90:ILE:HG13	2.20	0.41
2:J:162:SER:O	2:J:163:SER:OG	2.30	0.41
1:A:541:ILE:HD11	5:E:83:ILE:HD13	2.02	0.41
6:F:137:LYS:O	6:F:138:ILE:CB	2.68	0.41
6:N:136:PHE:O	6:N:138:ILE:HG13	2.19	0.41
8:P:213:MET:CE	8:P:391:GLN:HG3	2.51	0.41
8:H:146:VAL:HG22	8:H:147:VAL:N	2.35	0.41
1:I:345:GLU:HA	1:I:346:GLY:HA2	1.67	0.41
8:P:35:ILE:CD1	8:P:82:VAL:HA	2.50	0.41
5:M:451:SER:O	5:M:455:SER:HB2	2.20	0.41
6:N:28:GLY:C	6:N:30:GLN:H	2.22	0.41
5:M:99:GLU:O	5:M:102:LYS:HB2	2.20	0.41
5:E:99:GLU:O	5:E:102:LYS:HB2	2.20	0.41
6:F:171:THR:O	6:F:175:THR:N	2.45	0.41
1:A:94:ILE:HG22	1:A:95:GLY:N	2.36	0.41
2:J:242:LYS:HD2	2:J:243:VAL:N	2.35	0.41
5:E:352:GLU:H	5:E:352:GLU:HG3	1.59	0.41
6:N:182:TYR:C	6:N:184:ALA:N	2.73	0.41
6:N:154:ALA:HB3	6:N:402:VAL:CG2	2.47	0.41
6:F:178:VAL:HG11	6:F:402:VAL:HG12	2.03	0.41
6:F:466:PRO:O	6:F:468:ASP:N	2.54	0.41
1:A:156:LEU:HD21	1:A:409:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:32:ILE:HD11	8:P:111:LEU:C	2.41	0.41
6:N:390:GLN:HE21	6:N:390:GLN:HA	1.84	0.41
7:G:452:GLN:O	7:G:456:ASN:N	2.49	0.41
8:H:163:ILE:HG12	8:H:182:VAL:HG11	2.01	0.41
5:E:310:ILE:HG23	5:E:335:LEU:HD23	2.01	0.41
4:D:305:LEU:HD23	4:D:305:LEU:C	2.41	0.41
2:B:45:LEU:HB2	6:F:533:LEU:HB2	2.03	0.41
5:M:116:GLY:HA3	5:M:428:CYS:CB	2.50	0.41
8:H:213:MET:CE	8:H:391:GLN:HG3	2.51	0.41
5:E:412:ASN:C	5:E:414:MET:H	2.24	0.41
3:K:182:VAL:HG23	3:K:184:LYS:HG3	2.02	0.41
6:F:212:GLY:HA2	6:F:370:ASN:OD1	2.21	0.41
5:M:120:THR:O	5:M:124:VAL:HG23	2.20	0.41
2:J:217:LYS:HE2	2:J:217:LYS:HB3	1.75	0.41
6:F:488:TYR:O	6:F:489:VAL:CG1	2.69	0.41
5:E:250:SER:O	5:E:251:HIS:O	2.38	0.41
2:B:459:LEU:HD22	2:B:472:LEU:CD1	2.51	0.41
2:J:459:LEU:CD1	2:J:471:GLY:O	2.68	0.41
4:L:183:ASP:O	4:L:187:LYS:HA	2.21	0.41
4:D:183:ASP:O	4:D:187:LYS:HA	2.21	0.41
2:B:57:THR:HB	2:B:379:GLU:HG3	2.03	0.41
7:O:33:CYS:HA	7:O:83:LEU:CD1	2.51	0.41
8:H:63:ILE:HD12	8:H:74:GLU:CG	2.45	0.41
7:O:488:ILE:H	7:O:488:ILE:CD1	2.21	0.41
6:N:137:LYS:O	6:N:138:ILE:CB	2.69	0.41
4:L:461:ASN:HD22	4:L:462:SER:H	1.68	0.41
2:B:105:GLU:O	2:B:109:LEU:HD23	2.21	0.41
4:L:305:LEU:HD23	4:L:305:LEU:C	2.41	0.41
2:J:116:HIS:HA	2:J:117:PRO:HD3	1.74	0.41
4:L:85:GLN:O	4:L:89:ALA:HB3	2.21	0.41
2:J:155:HIS:O	2:J:159:THR:HG23	2.20	0.41
3:C:355:PHE:HE2	3:C:366:SER:HB3	1.84	0.41
2:B:45:LEU:HD23	2:B:56:VAL:HG13	2.02	0.41
2:J:196:ILE:HD12	2:J:196:ILE:N	2.36	0.41
4:D:273:ASN:HD22	7:G:268:GLN:NE2	2.17	0.41
4:L:198:LYS:H	4:L:198:LYS:CD	2.33	0.41
3:C:184:LYS:HA	3:C:198:ILE:CA	2.51	0.41
3:K:184:LYS:HA	3:K:198:ILE:CA	2.51	0.41
7:G:28:SER:HA	7:G:31:ASN:OD1	2.21	0.41
8:P:455:ALA:O	8:P:458:VAL:HG23	2.21	0.41
5:E:497:THR:O	5:E:501:LYS:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:423:LEU:C	5:E:425:ASP:N	2.73	0.41
5:M:38:LYS:HD2	5:M:38:LYS:HA	1.70	0.41
6:F:233:VAL:HG12	6:F:294:VAL:CG2	2.49	0.41
6:N:420:ILE:CG2	6:N:482:ASP:CG	2.86	0.41
3:K:230:VAL:O	3:K:231:HIS:CG	2.74	0.41
7:G:41:LYS:N	7:G:42:PRO:HD2	2.34	0.41
2:B:88:VAL:HG12	2:B:90:ASP:H	1.85	0.41
8:H:251:THR:O	8:H:252:CYS:C	2.59	0.41
5:M:107:LEU:CD2	5:M:544:LEU:HG	2.34	0.41
8:H:459:VAL:HB	8:H:460:PRO:HD3	2.02	0.41
6:F:105:ALA:O	6:F:107:ARG:N	2.54	0.41
6:N:447:PHE:CE1	6:N:521:THR:HG22	2.56	0.41
3:C:244:VAL:HG22	3:C:348:VAL:HG22	2.03	0.41
6:N:63:LEU:HD11	6:N:95:VAL:HG21	2.02	0.41
5:E:418:GLU:HA	5:E:418:GLU:OE2	2.20	0.41
7:G:36:VAL:CG2	7:G:37:GLN:N	2.83	0.41
5:M:84:THR:HG21	5:M:421:ARG:HD3	2.03	0.41
8:H:62:ILE:HG23	8:H:392:ASN:OD1	2.20	0.41
7:G:449:ILE:CB	7:G:450:PRO:HD3	2.50	0.41
5:E:338:ASN:HB2	5:E:340:LEU:HD22	2.02	0.41
1:A:233:MET:HE1	1:A:317:GLY:N	2.35	0.41
4:L:464:LYS:O	4:L:468:GLU:HG3	2.20	0.41
2:J:109:LEU:C	2:J:111:ASP:H	2.24	0.41
2:B:213:ILE:HG23	2:B:354:LEU:HD21	2.01	0.41
8:H:487:PRO:HA	8:H:488:GLY:HA3	1.69	0.41
1:I:498:ARG:O	1:I:499:ASN:HB3	2.20	0.41
1:A:344:LEU:HD12	1:A:345:GLU:H	1.85	0.41
7:G:356:GLN:HG2	7:G:361:ARG:HD3	2.03	0.41
2:B:160:THR:HG21	2:B:390:VAL:HG11	2.01	0.41
5:E:158:ILE:CB	5:E:539:LEU:HD21	2.51	0.41
6:N:207:THR:O	6:N:208:THR:HG23	2.21	0.41
7:O:356:GLN:HG2	7:O:361:ARG:HD3	2.03	0.41
6:F:497:ASP:CG	6:F:498:SER:N	2.74	0.41
8:H:92:GLN:HE21	8:H:92:GLN:HB3	1.63	0.41
6:N:6:LEU:HD12	6:N:7:ASN:H	1.85	0.41
2:J:422:ILE:HA	2:J:422:ILE:HD13	1.93	0.41
4:D:72:HIS:HA	4:D:73:PRO:HD3	1.96	0.41
2:B:242:LYS:HD2	2:B:243:VAL:N	2.35	0.41
3:K:321:LYS:O	3:K:324:ASP:HB2	2.21	0.41
6:F:141:THR:HG23	6:F:142:ASN:N	2.36	0.41
8:P:386:LEU:N	8:P:386:LEU:HD12	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:129:LEU:HD13	3:C:130:THR:N	2.36	0.41
4:L:185:ASN:CB	4:L:186:SER:CB	2.92	0.41
7:G:182:CYS:O	7:G:186:VAL:HG23	2.21	0.41
7:G:399:ILE:O	7:G:399:ILE:HD13	2.21	0.41
6:N:533:LEU:HD23	6:N:533:LEU:N	2.35	0.41
3:C:85:GLN:NE2	3:C:508:GLN:OE1	2.53	0.41
8:H:486:GLU:N	8:H:487:PRO:HA	2.34	0.41
1:A:133:LEU:HG	1:A:532:LEU:HD12	2.02	0.41
6:N:212:GLY:HA2	6:N:370:ASN:OD1	2.21	0.41
6:N:524:ALA:O	6:N:528:LEU:HG	2.21	0.41
5:E:557:SER:OG	6:F:67:GLN:N	2.53	0.41
4:L:66:LYS:HA	4:L:66:LYS:HD2	1.62	0.41
5:M:497:THR:O	5:M:501:LYS:HG2	2.20	0.41
2:B:5:ILE:CD1	2:B:7:GLY:H	2.34	0.41
2:J:5:ILE:CD1	2:J:7:GLY:H	2.34	0.41
6:F:151:LEU:O	6:F:171:THR:HG21	2.19	0.41
6:N:444:ILE:HG12	6:N:444:ILE:H	1.66	0.41
6:N:331:VAL:O	6:N:332:THR:CB	2.68	0.41
2:J:320:VAL:HG21	2:J:337:LEU:CA	2.51	0.41
1:A:250:ASN:HD21	1:A:252:GLN:HG2	1.85	0.41
2:J:127:ALA:HB1	2:J:430:VAL:HG13	2.02	0.41
8:P:306:GLY:O	8:P:310:LEU:HB2	2.20	0.41
6:N:488:TYR:O	6:N:489:VAL:CG1	2.69	0.41
2:B:142:ASN:CB	2:B:143:SER:CA	2.95	0.41
2:B:397:GLU:HG2	2:B:492:LYS:HZ3	1.86	0.41
6:F:16:ASP:O	6:F:20:LYS:N	2.46	0.41
6:F:16:ASP:HA	6:F:19:LEU:HB2	2.02	0.41
8:H:75:LEU:HA	8:H:75:LEU:HD23	1.93	0.41
6:F:181:VAL:O	6:F:184:ALA:HB3	2.20	0.41
6:F:182:TYR:C	6:F:184:ALA:N	2.73	0.41
6:N:466:PRO:O	6:N:468:ASP:N	2.54	0.41
5:E:250:SER:O	5:E:251:HIS:CG	2.74	0.41
8:P:48:PRO:CA	8:P:169:SER:O	2.68	0.41
6:F:447:PHE:CE1	6:F:521:THR:HG22	2.56	0.41
5:M:338:ASN:HB2	5:M:340:LEU:HD22	2.02	0.41
6:N:75:LEU:HD23	6:N:76:ILE:N	2.36	0.41
7:O:182:CYS:O	7:O:186:VAL:HG23	2.21	0.41
7:O:399:ILE:HD13	7:O:399:ILE:O	2.21	0.41
7:O:396:ALA:O	7:O:400:VAL:HG13	2.20	0.41
1:A:209:HIS:HE1	7:G:89:ALA:CB	2.34	0.41
6:N:56:THR:HB	6:N:390:GLN:CD	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:99:LEU:HA	4:L:449:VAL:HG11	2.02	0.41
4:L:454:LEU:CD1	9:L:601:ADP:H8	2.34	0.41
4:L:35:ILE:HG22	4:L:98:ILE:HD11	2.03	0.41
4:D:108:GLU:O	4:D:112:ASN:N	2.50	0.41
8:H:163:ILE:HD11	8:H:404:GLY:CA	2.50	0.41
6:N:105:ALA:O	6:N:108:PHE:CD2	2.74	0.41
2:J:326:VAL:O	2:J:327:SER:HB3	2.21	0.41
4:L:157:SER:C	4:L:159:SER:H	2.24	0.41
2:J:14:ARG:O	2:J:15:ALA:HB3	2.21	0.41
1:I:51:LYS:O	1:I:62:VAL:HA	2.20	0.41
1:A:51:LYS:O	1:A:62:VAL:HA	2.20	0.41
1:I:118:ASN:O	1:I:119:LYS:CG	2.65	0.41
2:J:45:LEU:HD12	6:N:533:LEU:HB3	2.02	0.41
3:K:223:VAL:HG11	3:K:328:ILE:HG12	2.03	0.41
5:M:472:PHE:HZ	5:M:542:THR:HG22	1.86	0.41
8:H:146:VAL:HG22	8:H:148:GLY:H	1.86	0.41
3:K:241:PRO:O	3:K:350:THR:HA	2.20	0.41
5:E:412:ASN:O	5:E:413:LYS:CB	2.69	0.41
1:I:344:LEU:HD12	1:I:345:GLU:H	1.85	0.41
5:M:158:ILE:CB	5:M:539:LEU:HD21	2.51	0.41
4:D:385:MET:HA	4:D:388:ASP:OD2	2.21	0.41
6:F:207:THR:O	6:F:208:THR:HG23	2.21	0.41
6:F:152:GLN:HG2	6:F:153:VAL:N	2.32	0.41
8:H:38:LEU:HD23	8:H:38:LEU:HA	1.92	0.41
4:D:48:ILE:CD1	8:H:534:ALA:HB3	2.51	0.41
8:P:253:PRO:HA	8:P:303:ALA:O	2.21	0.41
5:E:225:LYS:HG3	5:E:225:LYS:O	2.21	0.41
8:P:267:LEU:HD23	8:P:267:LEU:N	2.36	0.41
8:P:8:ASN:HA	8:P:9:PRO:HD3	1.90	0.41
6:N:539:SER:HB2	6:N:542:LYS:CG	2.51	0.41
6:N:332:THR:O	6:N:333:GLY:C	2.58	0.41
6:F:331:VAL:O	6:F:332:THR:CB	2.68	0.41
6:F:352:GLY:C	6:F:367:VAL:HG12	2.40	0.41
7:O:516:LEU:HD11	7:O:517:ILE:CG1	2.48	0.41
7:O:191:ARG:C	7:O:191:ARG:NE	2.75	0.41
8:P:54:ILE:CG2	8:P:55:ILE:N	2.83	0.41
1:I:94:ILE:HG22	1:I:95:GLY:N	2.36	0.41
2:J:242:LYS:HB2	3:K:269:TRP:CZ2	2.45	0.41
2:B:245:ILE:O	2:B:246:PHE:HB3	2.19	0.41
5:M:355:ALA:HB2	5:M:362:ILE:CD1	2.51	0.41
7:G:43:THR:HG23	7:G:64:ASN:HB3	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:178:VAL:HG11	6:N:402:VAL:HG12	2.03	0.41
2:J:459:LEU:HD22	2:J:472:LEU:CD1	2.51	0.41
8:H:386:LEU:N	8:H:386:LEU:HD12	2.36	0.41
8:H:459:VAL:O	8:H:462:THR:HG22	2.20	0.41
6:F:23:VAL:O	6:F:25:SER:N	2.54	0.41
6:F:113:VAL:CB	6:F:118:ILE:HD11	2.47	0.41
3:K:129:LEU:HD13	3:K:130:THR:N	2.36	0.41
7:O:83:LEU:HA	7:O:86:ILE:CD1	2.50	0.41
4:D:226:PRO:CD	4:D:311:MET:HG2	2.50	0.41
7:G:145:VAL:O	7:G:409:ILE:N	2.52	0.41
4:D:123:SER:OG	4:D:440:TRP:HA	2.21	0.41
6:N:105:ALA:O	6:N:107:ARG:N	2.54	0.41
1:A:397:GLU:HA	1:A:400:ARG:HH11	1.86	0.41
7:O:214:PHE:O	7:O:214:PHE:CD2	2.74	0.41
7:G:214:PHE:O	7:G:214:PHE:CD2	2.74	0.41
8:P:146:VAL:HG22	8:P:148:GLY:N	2.36	0.41
8:H:48:PRO:CA	8:H:169:SER:O	2.68	0.41
4:L:219:ALA:HB1	4:L:221:LYS:HZ1	1.85	0.41
3:K:238:ILE:O	3:K:241:PRO:HG3	2.21	0.41
1:I:203:VAL:O	1:I:205:VAL:HG23	2.21	0.41
5:E:120:THR:O	5:E:124:VAL:HG23	2.20	0.41
8:H:253:PRO:HA	8:H:303:ALA:O	2.21	0.41
8:P:141:GLU:O	8:P:145:MET:HG2	2.21	0.41
3:C:240:ASN:HA	3:C:352:CYS:O	2.21	0.41
3:K:240:ASN:HA	3:K:352:CYS:O	2.21	0.41
2:J:186:GLY:HA2	2:J:187:SER:HA	1.47	0.41
8:H:437:TYR:C	8:H:437:TYR:CD2	2.95	0.41
1:I:191:ASN:HA	1:I:195:GLU:O	2.21	0.41
5:E:451:SER:O	5:E:455:SER:HB2	2.20	0.41
8:H:414:PRO:HA	8:H:415:SER:HA	1.60	0.41
6:F:420:ILE:HG22	6:F:482:ASP:CG	2.41	0.40
3:C:306:GLN:O	3:C:307:HIS:C	2.59	0.40
6:F:6:LEU:HD13	6:F:7:ASN:H	1.85	0.40
4:L:425:LEU:HD12	4:L:444:ALA:HA	2.03	0.40
3:K:245:LEU:HA	3:K:296:ILE:O	2.21	0.40
2:J:88:VAL:HG12	2:J:90:ASP:H	1.86	0.40
4:D:425:LEU:HD12	4:D:444:ALA:HA	2.03	0.40
5:M:250:SER:O	5:M:251:HIS:O	2.38	0.40
8:P:459:VAL:HB	8:P:460:PRO:HD3	2.02	0.40
6:F:105:ALA:O	6:F:108:PHE:CD2	2.74	0.40
7:G:33:CYS:HA	7:G:83:LEU:CD1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:71:ASP:OD2	5:M:85:ASN:HB2	2.21	0.40
4:D:292:ILE:HG13	4:D:294:ARG:N	2.36	0.40
1:A:431:ILE:CG2	1:A:432:TYR:N	2.84	0.40
1:I:431:ILE:CG2	1:I:432:TYR:N	2.84	0.40
8:P:186:VAL:HA	8:P:207:ILE:HD11	2.02	0.40
4:L:411:ILE:O	4:L:498:LEU:HB3	2.21	0.40
2:B:109:LEU:C	2:B:111:ASP:H	2.24	0.40
8:P:146:VAL:HG22	8:P:147:VAL:N	2.35	0.40
8:P:122:LEU:HD23	8:P:126:GLU:OE1	2.21	0.40
6:N:68:ILE:HD13	6:N:74:VAL:HG13	2.02	0.40
7:O:28:SER:HA	7:O:31:ASN:OD1	2.21	0.40
1:A:198:TYR:CE2	1:A:413:LEU:CB	3.05	0.40
7:G:94:VAL:CG1	7:G:95:GLY:H	2.28	0.40
2:J:372:ALA:HA	6:N:519:GLY:HA2	2.02	0.40
5:E:115:ILE:CB	5:E:432:ASN:HD21	2.35	0.40
6:F:158:LEU:CG	6:F:158:LEU:O	2.69	0.40
6:N:158:LEU:O	6:N:158:LEU:CG	2.69	0.40
5:M:338:ASN:HD22	5:M:338:ASN:N	2.16	0.40
6:N:411:ILE:CG2	6:N:412:ILE:N	2.75	0.40
6:F:75:LEU:HD23	6:F:76:ILE:N	2.36	0.40
6:F:56:THR:HB	6:F:390:GLN:CD	2.42	0.40
6:F:56:THR:HB	6:F:390:GLN:HE22	1.79	0.40
1:A:115:LEU:HA	1:A:115:LEU:HD23	1.80	0.40
4:L:292:ILE:HG13	4:L:294:ARG:N	2.36	0.40
5:E:355:ALA:HB2	5:E:362:ILE:CD1	2.51	0.40
7:G:129:TYR:O	7:G:132:ALA:HB3	2.21	0.40
4:L:454:LEU:HD13	9:L:601:ADP:H8	1.86	0.40
4:L:94:THR:C	4:L:96:VAL:H	2.25	0.40
4:D:94:THR:C	4:D:96:VAL:H	2.25	0.40
4:L:123:SER:OG	4:L:440:TRP:HA	2.21	0.40
5:E:332:ASN:HA	5:E:335:LEU:HD12	2.02	0.40
6:F:459:VAL:O	6:F:463:GLY:N	2.54	0.40
5:E:35:GLN:CD	5:E:36:GLY:CA	2.86	0.40
2:J:140:VAL:HG23	2:J:483:ARG:NH2	2.36	0.40
2:J:15:ALA:O	2:J:19:ARG:HG2	2.21	0.40
1:I:397:GLU:HA	1:I:400:ARG:HH11	1.86	0.40
7:O:528:GLY:HA3	7:O:529:SER:C	2.41	0.40
1:A:191:ASN:HA	1:A:195:GLU:O	2.21	0.40
8:P:437:TYR:CD2	8:P:437:TYR:C	2.95	0.40
2:B:317:LEU:O	2:B:321:THR:N	2.50	0.40
1:I:198:TYR:CE2	1:I:413:LEU:CB	3.05	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:72:HIS:HA	4:L:73:PRO:HD3	1.96	0.40
5:E:88:ALA:CB	5:E:109:LYS:HZ1	2.32	0.40
6:F:146:ASP:O	6:F:147:ARG:C	2.59	0.40
3:C:56:VAL:CA	3:C:57:LEU:HD23	2.50	0.40
8:P:251:THR:O	8:P:252:CYS:C	2.59	0.40
8:H:209:VAL:CG2	8:H:386:LEU:HD11	2.36	0.40
2:J:24:VAL:HA	2:J:27:ILE:CG2	2.51	0.40
6:F:196:ILE:HG22	6:F:378:ILE:HG23	2.02	0.40
8:H:49:CYS:O	8:H:466:THR:CG2	2.69	0.40
5:E:261:LYS:O	5:E:341:PRO:HG3	2.21	0.40
1:I:156:LEU:HD21	1:I:409:VAL:HG13	2.02	0.40
2:B:164:LYS:O	2:B:166:LEU:HD23	2.22	0.40
2:B:474:LEU:HD23	2:B:474:LEU:N	2.35	0.40
5:M:276:PHE:HZ	5:M:310:ILE:HG12	1.86	0.40
5:M:261:LYS:O	5:M:341:PRO:HG3	2.21	0.40
5:M:387:THR:HA	5:M:388:THR:HA	1.61	0.40
5:E:86:ASP:O	5:E:90:ILE:HG13	2.20	0.40
5:E:170:ALA:N	5:E:523:LYS:HZ1	2.19	0.40
8:P:75:LEU:HD23	8:P:75:LEU:HA	1.94	0.40
4:D:120:ILE:CG1	4:D:439:ILE:HG21	2.43	0.40
4:D:135:LEU:HD22	4:D:135:LEU:HA	1.87	0.40
6:N:342:ASP:O	6:N:343:LEU:C	2.59	0.40
6:F:198:GLN:HE21	6:F:198:GLN:H	1.66	0.40
8:P:146:VAL:HG22	8:P:148:GLY:H	1.86	0.40
4:L:65:LEU:HB3	4:L:79:VAL:HG13	2.04	0.40
6:N:370:ASN:N	6:N:370:ASN:ND2	2.70	0.40
5:E:557:SER:CB	6:F:66:MET:HA	2.52	0.40
4:D:47:MET:O	8:H:534:ALA:N	2.53	0.40
1:A:555:ASP:HA	1:A:556:PRO:HD3	1.90	0.40
5:M:162:GLU:OE2	5:M:162:GLU:N	2.55	0.40
2:J:181:ILE:HG21	2:J:391:LEU:O	2.21	0.40
2:J:61:ALA:HB2	2:J:85:ASP:HB2	2.02	0.40
8:H:141:GLU:O	8:H:145:MET:HG2	2.21	0.40
8:H:5:LEU:HA	8:H:6:PRO:HD3	1.87	0.40
2:J:360:LYS:HA	2:J:361:ALA:HA	1.70	0.40
2:J:201:GLY:O	2:J:202:LYS:CB	2.69	0.40
7:G:191:ARG:NE	7:G:191:ARG:C	2.75	0.40
3:C:245:LEU:HA	3:C:296:ILE:O	2.21	0.40
2:B:88:VAL:HG11	2:B:493:LEU:HB2	2.04	0.40
6:N:16:ASP:HA	6:N:19:LEU:HB2	2.02	0.40
5:E:107:LEU:HD12	5:E:107:LEU:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:41:PRO:HD3	9:C:1101:ADP:N3	2.36	0.40
6:F:118:ILE:HG22	6:F:122:PHE:CD2	2.57	0.40
8:H:111:LEU:HD21	8:H:524:LYS:HA	2.04	0.40
7:G:413:GLY:HA2	9:G:601:ADP:C2	2.57	0.40
5:E:245:LEU:CD1	5:E:247:LYS:H	2.25	0.40
2:B:295:GLU:CB	6:F:337:GLN:NE2	2.79	0.40
7:O:129:TYR:O	7:O:132:ALA:HB3	2.21	0.40
4:D:292:ILE:HG13	4:D:293:LEU:C	2.42	0.40
4:L:292:ILE:CG1	4:L:293:LEU:HA	2.47	0.40
7:O:449:ILE:CB	7:O:450:PRO:HD3	2.50	0.40
3:K:112:ILE:C	3:K:114:LYS:N	2.74	0.40
3:C:113:GLU:OE1	1:I:460:LYS:NZ	2.47	0.40
7:O:478:TRP:O	7:O:479:TYR:CB	2.69	0.40
5:E:276:PHE:HZ	5:E:310:ILE:HG12	1.86	0.40
2:B:140:VAL:HG23	2:B:483:ARG:NH2	2.36	0.40
2:B:14:ARG:O	2:B:15:ALA:HB3	2.21	0.40
2:B:354:LEU:HD13	2:B:356:PHE:CE2	2.56	0.40
5:E:428:CYS:HA	5:E:431:ARG:CG	2.52	0.40
8:H:122:LEU:HD23	8:H:126:GLU:OE1	2.22	0.40
2:B:196:ILE:HD12	2:B:196:ILE:N	2.36	0.40
5:M:412:ASN:O	5:M:413:LYS:CB	2.69	0.40
5:E:297:LYS:HB3	6:F:256:ALA:CB	2.52	0.40
8:P:414:PRO:HA	8:P:415:SER:HA	1.60	0.40
4:L:86:ASP:HB2	4:L:93:THR:HG22	2.03	0.40
6:N:331:VAL:HG23	6:N:375:SER:OG	2.21	0.40
6:F:331:VAL:HG23	6:F:375:SER:OG	2.21	0.40
2:J:320:VAL:HB	2:J:338:GLY:H	1.87	0.40
1:I:303:ASP:OD1	1:I:304:ASP:N	2.55	0.40
4:L:20:VAL:HG21	4:L:522:ASP:O	2.22	0.40
2:B:201:GLY:O	2:B:202:LYS:CB	2.69	0.40
7:O:94:VAL:CG1	7:O:95:GLY:N	2.83	0.40
3:K:34:VAL:HG12	3:K:35:ILE:N	2.35	0.40
4:D:263:ILE:C	4:D:265:LYS:H	2.23	0.40
7:G:204:ILE:HA	7:G:205:PRO:HD3	1.79	0.40
6:F:342:ASP:O	6:F:343:LEU:C	2.59	0.40
2:J:164:LYS:O	2:J:166:LEU:HD23	2.22	0.40
3:C:112:ILE:C	3:C:114:LYS:N	2.74	0.40
1:A:307:LEU:O	1:A:311:VAL:N	2.53	0.40
4:D:157:SER:C	4:D:159:SER:H	2.24	0.40
2:J:402:LEU:CD2	2:J:483:ARG:HG3	2.46	0.40
5:E:472:PHE:HZ	5:E:542:THR:HG22	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:354:LEU:HD13	2:B:356:PHE:HE2	1.87	0.40
3:C:413:SER:HA	3:C:414:PRO:HD3	1.90	0.40
4:L:65:LEU:HA	4:L:65:LEU:HD23	1.83	0.40
5:M:412:ASN:C	5:M:414:MET:H	2.24	0.40
8:H:208:ARG:O	8:H:383:THR:HA	2.22	0.40
4:L:116:HIS:HA	4:L:117:PRO:HD3	1.99	0.40
5:E:237:SER:HB3	5:E:408:VAL:HA	2.04	0.40
3:C:210:PRO:HB2	3:C:211:GLY:H	1.63	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	538/559 (96%)	441 (82%)	78 (14%)	19 (4%)	4	42
1	I	538/559 (96%)	441 (82%)	78 (14%)	19 (4%)	4	42
1	a	538/559 (96%)	441 (82%)	78 (14%)	19 (4%)	4	42
1	i	538/559 (96%)	441 (82%)	78 (14%)	19 (4%)	4	42
2	B	509/527 (97%)	417 (82%)	67 (13%)	25 (5%)	3	32
2	J	509/527 (97%)	417 (82%)	67 (13%)	25 (5%)	3	32
2	b	509/527 (97%)	417 (82%)	68 (13%)	24 (5%)	3	33
2	j	509/527 (97%)	417 (82%)	67 (13%)	25 (5%)	3	32
3	C	508/590 (86%)	420 (83%)	68 (13%)	20 (4%)	4	38
3	K	508/590 (86%)	421 (83%)	67 (13%)	20 (4%)	4	38
3	c	508/590 (86%)	419 (82%)	70 (14%)	19 (4%)	4	40
3	k	508/590 (86%)	420 (83%)	68 (13%)	20 (4%)	4	38
4	D	520/528 (98%)	429 (82%)	79 (15%)	12 (2%)	8	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	L	520/528 (98%)	429 (82%)	79 (15%)	12 (2%)	8	51
4	d	520/528 (98%)	429 (82%)	79 (15%)	12 (2%)	8	51
4	l	520/528 (98%)	429 (82%)	79 (15%)	12 (2%)	8	51
5	E	521/562 (93%)	443 (85%)	59 (11%)	19 (4%)	4	41
5	M	521/562 (93%)	443 (85%)	59 (11%)	19 (4%)	4	41
5	e	521/562 (93%)	442 (85%)	60 (12%)	19 (4%)	4	41
5	m	521/562 (93%)	443 (85%)	59 (11%)	19 (4%)	4	41
6	F	529/546 (97%)	429 (81%)	82 (16%)	18 (3%)	5	43
6	N	529/546 (97%)	429 (81%)	82 (16%)	18 (3%)	5	43
6	f	529/546 (97%)	429 (81%)	82 (16%)	18 (3%)	5	43
6	n	529/546 (97%)	429 (81%)	82 (16%)	18 (3%)	5	43
7	G	505/550 (92%)	424 (84%)	60 (12%)	21 (4%)	3	36
7	O	505/550 (92%)	424 (84%)	60 (12%)	21 (4%)	3	36
7	g	505/550 (92%)	424 (84%)	60 (12%)	21 (4%)	3	36
7	o	505/550 (92%)	424 (84%)	60 (12%)	21 (4%)	3	36
8	H	521/568 (92%)	439 (84%)	58 (11%)	24 (5%)	3	34
8	P	521/568 (92%)	439 (84%)	58 (11%)	24 (5%)	3	34
8	h	521/568 (92%)	439 (84%)	58 (11%)	24 (5%)	3	34
8	p	521/568 (92%)	439 (84%)	58 (11%)	24 (5%)	3	34
All	All	16604/17720 (94%)	13767 (83%)	2207 (13%)	630 (4%)	4	39

All (630) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	5	ILE
2	B	165	ILE
2	B	184	LEU
2	B	185	LYS
2	B	307	GLU
2	B	370	ARG
2	B	470	SER
3	C	16	THR
3	C	210	PRO
3	C	252	TYR
3	C	303	ASP

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Mol	Chain	Res	Type
4	D	205	ASP
4	D	427	LYS
5	E	167	ASP
5	E	351	LEU
5	E	369	LEU
6	F	160	THR
6	F	353	LEU
6	F	460	LYS
6	F	489	VAL
6	F	490	GLY
7	G	46	PRO
7	G	190	ASP
7	G	213	LEU
7	G	487	ASN
7	G	495	PHE
8	H	147	VAL
8	H	483	ASN
8	H	490	VAL
2	J	5	ILE
2	J	165	ILE
2	J	184	LEU
2	J	185	LYS
2	J	307	GLU
2	J	370	ARG
2	J	470	SER
3	K	16	THR
3	K	210	PRO
3	K	252	TYR
3	K	303	ASP
4	L	205	ASP
4	L	427	LYS
5	M	167	ASP
5	M	351	LEU
5	M	369	LEU
6	N	160	THR
6	N	353	LEU
6	N	460	LYS
6	N	489	VAL
6	N	490	GLY
7	O	46	PRO
7	O	190	ASP
7	O	213	LEU

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Mol	Chain	Res	Type
7	O	487	ASN
7	O	495	PHE
8	P	147	VAL
8	P	483	ASN
8	P	490	VAL
2	b	1005	ILE
2	b	1165	ILE
2	b	1184	LEU
2	b	1185	LYS
2	b	1307	GLU
2	b	1370	ARG
2	b	1470	SER
3	c	1016	THR
3	c	1210	PRO
3	c	1252	TYR
3	c	1303	ASP
4	d	1205	ASP
4	d	1427	LYS
5	e	1167	ASP
5	e	1351	LEU
5	e	1369	LEU
6	f	1160	THR
6	f	1353	LEU
6	f	1460	LYS
6	f	1489	VAL
6	f	1490	GLY
7	g	1046	PRO
7	g	1190	ASP
7	g	1213	LEU
7	g	1487	ASN
7	g	1495	PHE
8	h	1006	PRO
8	h	1147	VAL
8	h	1483	ASN
8	h	1490	VAL
2	j	1005	ILE
2	j	1165	ILE
2	j	1184	LEU
2	j	1185	LYS
2	j	1307	GLU
2	j	1370	ARG
2	j	1470	SER

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Mol	Chain	Res	Type
3	k	1016	THR
3	k	1210	PRO
3	k	1252	TYR
3	k	1303	ASP
4	l	1205	ASP
4	l	1427	LYS
5	m	1167	ASP
5	m	1351	LEU
5	m	1369	LEU
6	n	1160	THR
6	n	1353	LEU
6	n	1460	LYS
6	n	1489	VAL
6	n	1490	GLY
7	o	1046	PRO
7	o	1190	ASP
7	o	1213	LEU
7	o	1487	ASN
7	o	1495	PHE
8	p	1147	VAL
8	p	1483	ASN
8	p	1490	VAL
1	A	11	ASP
1	A	56	ASP
1	A	94	ILE
1	A	265	ASP
1	A	508	LYS
2	B	35	SER
2	B	50	SER
2	B	142	ASN
2	B	220	ASN
2	B	323	GLY
2	B	371	GLY
3	C	19	GLN
3	C	36	ARG
3	C	144	ASP
3	C	258	GLN
3	C	321	LYS
3	C	454	ARG
4	D	188	ASN
4	D	485	ARG
5	E	251	HIS

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Mol	Chain	Res	Type
5	E	347	GLY
5	E	402	LYS
5	E	438	ARG
6	F	138	ILE
6	F	298	GLN
6	F	333	GLY
6	F	467	LEU
6	F	486	THR
7	G	45	GLY
7	G	224	PHE
7	G	256	ASN
7	G	478	TRP
7	G	502	VAL
1	I	11	ASP
1	I	56	ASP
1	I	94	ILE
1	I	265	ASP
1	I	508	LYS
2	J	35	SER
2	J	50	SER
2	J	142	ASN
2	J	220	ASN
2	J	323	GLY
2	J	371	GLY
3	K	19	GLN
3	K	36	ARG
3	K	144	ASP
3	K	258	GLN
3	K	321	LYS
3	K	454	ARG
4	L	188	ASN
4	L	485	ARG
5	M	251	HIS
5	M	347	GLY
5	M	402	LYS
5	M	438	ARG
6	N	138	ILE
6	N	298	GLN
6	N	333	GLY
6	N	467	LEU
6	N	486	THR
7	O	45	GLY

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Mol	Chain	Res	Type
7	O	224	PHE
7	O	256	ASN
7	O	478	TRP
7	O	502	VAL
1	a	1011	ASP
1	a	1056	ASP
1	a	1094	ILE
1	a	1265	ASP
1	a	1508	LYS
2	b	1035	SER
2	b	1050	SER
2	b	1142	ASN
2	b	1220	ASN
2	b	1323	GLY
2	b	1371	GLY
3	c	1019	GLN
3	c	1036	ARG
3	c	1144	ASP
3	c	1258	GLN
3	c	1321	LYS
3	c	1454	ARG
4	d	1188	ASN
4	d	1485	ARG
5	e	1251	HIS
5	e	1347	GLY
5	e	1402	LYS
5	e	1438	ARG
6	f	1138	ILE
6	f	1298	GLN
6	f	1333	GLY
6	f	1467	LEU
6	f	1486	THR
7	g	1045	GLY
7	g	1224	PHE
7	g	1256	ASN
7	g	1478	TRP
7	g	1502	VAL
1	i	1011	ASP
1	i	1056	ASP
1	i	1094	ILE
1	i	1265	ASP
1	i	1508	LYS

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Mol	Chain	Res	Type
2	j	1035	SER
2	j	1050	SER
2	j	1142	ASN
2	j	1220	ASN
2	j	1323	GLY
2	j	1371	GLY
3	k	1019	GLN
3	k	1036	ARG
3	k	1144	ASP
3	k	1258	GLN
3	k	1321	LYS
3	k	1454	ARG
4	l	1188	ASN
4	l	1485	ARG
5	m	1251	HIS
5	m	1347	GLY
5	m	1402	LYS
5	m	1438	ARG
6	n	1138	ILE
6	n	1298	GLN
6	n	1333	GLY
6	n	1467	LEU
6	n	1486	THR
7	o	1045	GLY
7	o	1224	PHE
7	o	1256	ASN
7	o	1478	TRP
7	o	1502	VAL
1	A	335	ALA
1	A	337	LEU
2	B	15	ALA
2	B	301	LEU
2	B	467	ILE
2	B	478	THR
3	C	52	MET
3	C	256	GLU
3	C	460	ALA
3	C	490	LYS
4	D	17	PRO
4	D	143	SER
4	D	474	GLU
5	E	36	GLY

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Mol	Chain	Res	Type
5	E	190	SER
6	F	204	PRO
7	G	63	SER
7	G	250	LEU
7	G	362	TYR
8	H	6	PRO
8	H	13	LEU
8	H	48	PRO
8	H	146	VAL
8	H	150	ILE
8	H	178	LEU
8	H	343	ARG
8	H	378	ILE
8	H	458	VAL
8	H	460	PRO
8	H	486	GLU
1	I	335	ALA
1	I	337	LEU
2	J	15	ALA
2	J	301	LEU
2	J	467	ILE
2	J	478	THR
3	K	52	MET
3	K	256	GLU
3	K	460	ALA
3	K	490	LYS
4	L	17	PRO
4	L	143	SER
4	L	474	GLU
5	M	36	GLY
5	M	190	SER
6	N	204	PRO
7	O	63	SER
7	O	250	LEU
7	O	362	TYR
8	P	6	PRO
8	P	13	LEU
8	P	48	PRO
8	P	146	VAL
8	P	150	ILE
8	P	178	LEU
8	P	343	ARG

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Mol	Chain	Res	Type
8	P	378	ILE
8	P	458	VAL
8	P	460	PRO
8	P	486	GLU
1	a	1335	ALA
1	a	1337	LEU
2	b	1015	ALA
2	b	1301	LEU
2	b	1467	ILE
2	b	1478	THR
3	c	1052	MET
3	c	1256	GLU
3	c	1460	ALA
3	c	1490	LYS
4	d	1017	PRO
4	d	1143	SER
4	d	1474	GLU
5	e	1036	GLY
5	e	1190	SER
6	f	1204	PRO
7	g	1063	SER
7	g	1250	LEU
7	g	1362	TYR
8	h	1013	LEU
8	h	1048	PRO
8	h	1146	VAL
8	h	1150	ILE
8	h	1178	LEU
8	h	1343	ARG
8	h	1378	ILE
8	h	1458	VAL
8	h	1460	PRO
8	h	1486	GLU
1	i	1335	ALA
1	i	1337	LEU
2	j	1015	ALA
2	j	1301	LEU
2	j	1467	ILE
2	j	1478	THR
3	k	1052	MET
3	k	1256	GLU
3	k	1460	ALA

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Mol	Chain	Res	Type
3	k	1490	LYS
4	l	1017	PRO
4	l	1143	SER
4	l	1474	GLU
5	m	1036	GLY
5	m	1190	SER
6	n	1204	PRO
7	o	1063	SER
7	o	1250	LEU
7	o	1362	TYR
8	p	1006	PRO
8	p	1013	LEU
8	p	1048	PRO
8	p	1146	VAL
8	p	1150	ILE
8	p	1178	LEU
8	p	1343	ARG
8	p	1378	ILE
8	p	1458	VAL
8	p	1460	PRO
8	p	1486	GLU
1	A	74	ASP
1	A	121	HIS
1	A	267	PRO
1	A	518	LEU
2	B	16	GLU
2	B	202	LYS
2	B	246	PHE
2	B	327	SER
3	C	265	LYS
4	D	9	ALA
4	D	95	SER
4	D	382	ALA
5	E	274	CYS
5	E	462	ARG
6	F	167	THR
6	F	343	LEU
7	G	368	CYS
7	G	428	SER
8	H	122	LEU
8	H	233	GLU
8	H	356	GLU

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Mol	Chain	Res	Type
8	H	373	GLN
1	I	74	ASP
1	I	121	HIS
1	I	267	PRO
1	I	518	LEU
2	J	16	GLU
2	J	202	LYS
2	J	246	PHE
2	J	327	SER
3	K	265	LYS
4	L	9	ALA
4	L	95	SER
4	L	382	ALA
5	M	274	CYS
5	M	462	ARG
6	N	167	THR
6	N	343	LEU
7	O	368	CYS
7	O	428	SER
8	P	122	LEU
8	P	233	GLU
8	P	356	GLU
8	P	373	GLN
1	a	1074	ASP
1	a	1121	HIS
1	a	1267	PRO
1	a	1518	LEU
2	b	1016	GLU
2	b	1202	LYS
2	b	1246	PHE
2	b	1327	SER
3	c	1265	LYS
4	d	1009	ALA
4	d	1095	SER
4	d	1382	ALA
5	e	1274	CYS
5	e	1462	ARG
6	f	1167	THR
6	f	1343	LEU
7	g	1368	CYS
7	g	1428	SER
8	h	1122	LEU

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Mol	Chain	Res	Type
8	h	1233	GLU
8	h	1356	GLU
8	h	1373	GLN
1	i	1074	ASP
1	i	1121	HIS
1	i	1267	PRO
1	i	1518	LEU
2	j	1016	GLU
2	j	1202	LYS
2	j	1246	PHE
2	j	1327	SER
3	k	1265	LYS
4	l	1009	ALA
4	l	1095	SER
4	l	1382	ALA
5	m	1274	CYS
5	m	1462	ARG
6	n	1167	THR
6	n	1343	LEU
7	o	1368	CYS
7	o	1428	SER
8	p	1122	LEU
8	p	1233	GLU
8	p	1356	GLU
8	p	1373	GLN
1	A	199	PRO
1	A	367	SER
2	B	293	TYR
3	C	30	ALA
3	C	249	PRO
4	D	294	ARG
4	D	431	SER
5	E	147	ALA
5	E	279	PRO
5	E	376	THR
6	F	24	THR
6	F	188	ASN
7	G	337	THR
8	H	49	CYS
8	H	322	LYS
1	I	199	PRO
1	I	367	SER

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Mol	Chain	Res	Type
2	J	293	TYR
3	K	30	ALA
3	K	249	PRO
4	L	294	ARG
4	L	431	SER
5	M	147	ALA
5	M	279	PRO
5	M	376	THR
6	N	24	THR
6	N	188	ASN
7	O	337	THR
8	P	49	CYS
8	P	322	LYS
1	a	1199	PRO
1	a	1367	SER
2	b	1293	TYR
3	c	1030	ALA
3	c	1249	PRO
4	d	1294	ARG
4	d	1431	SER
5	e	1147	ALA
5	e	1279	PRO
5	e	1376	THR
6	f	1024	THR
6	f	1188	ASN
7	g	1337	THR
8	h	1049	CYS
8	h	1322	LYS
1	i	1199	PRO
1	i	1367	SER
2	j	1293	TYR
3	k	1030	ALA
3	k	1249	PRO
4	l	1294	ARG
4	l	1431	SER
5	m	1147	ALA
5	m	1279	PRO
5	m	1376	THR
6	n	1024	THR
6	n	1188	ASN
7	o	1337	THR
8	p	1049	CYS

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Mol	Chain	Res	Type
8	p	1322	LYS
1	A	55	ASP
1	A	77	HIS
2	B	372	ALA
5	E	254	MET
6	F	183	ASP
7	G	67	ALA
7	G	479	TYR
8	H	187	SER
8	H	484	VAL
1	I	55	ASP
1	I	77	HIS
2	J	372	ALA
5	M	254	MET
6	N	183	ASP
7	O	67	ALA
7	O	479	TYR
8	P	187	SER
8	P	484	VAL
1	a	1055	ASP
1	a	1077	HIS
5	e	1254	MET
6	f	1183	ASP
7	g	1067	ALA
7	g	1479	TYR
8	h	1187	SER
8	h	1484	VAL
1	i	1055	ASP
1	i	1077	HIS
2	j	1372	ALA
5	m	1254	MET
6	n	1183	ASP
7	o	1067	ALA
7	o	1479	TYR
8	p	1187	SER
8	p	1484	VAL
1	A	22	GLY
1	A	376	GLY
1	A	549	PRO
2	B	117	PRO
3	C	410	PRO
5	E	493	GLY

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Mol	Chain	Res	Type
8	H	284	ILE
8	H	324	PRO
1	I	22	GLY
1	I	376	GLY
1	I	549	PRO
2	J	117	PRO
3	K	410	PRO
5	M	493	GLY
8	P	284	ILE
8	P	324	PRO
1	a	1022	GLY
1	a	1376	GLY
1	a	1549	PRO
2	b	1117	PRO
3	c	1410	PRO
5	e	1493	GLY
8	h	1284	ILE
8	h	1324	PRO
1	i	1022	GLY
1	i	1376	GLY
1	i	1549	PRO
2	j	1117	PRO
3	k	1410	PRO
5	m	1493	GLY
8	p	1284	ILE
8	p	1324	PRO
1	A	292	GLY
2	B	88	VAL
5	E	440	VAL
1	I	292	GLY
2	J	88	VAL
5	M	440	VAL
1	a	1292	GLY
2	b	1088	VAL
5	e	1440	VAL
1	i	1292	GLY
2	j	1088	VAL
5	m	1440	VAL
7	G	412	GLY
7	G	528	GLY
7	O	412	GLY
7	O	528	GLY

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Mol	Chain	Res	Type
7	g	1412	GLY
7	g	1528	GLY
7	o	1412	GLY
7	o	1528	GLY
3	C	142	PRO
5	E	386	GLY
6	F	412	ILE
7	G	62	ILE
3	K	142	PRO
5	M	386	GLY
6	N	412	ILE
6	N	512	VAL
7	O	62	ILE
3	c	1142	PRO
5	e	1386	GLY
6	f	1412	ILE
7	g	1062	ILE
3	k	1142	PRO
5	m	1386	GLY
6	n	1412	ILE
7	o	1062	ILE
3	C	50	ASP
5	E	507	ILE
6	F	512	VAL
3	K	50	ASP
5	M	507	ILE
5	e	1507	ILE
6	f	1512	VAL
3	k	1050	ASP
5	m	1507	ILE
6	n	1512	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	301/471 (64%)	274 (91%)	27 (9%)	12 49
1	I	301/471 (64%)	274 (91%)	27 (9%)	12 49
1	a	301/471 (64%)	274 (91%)	27 (9%)	12 49
1	i	301/471 (64%)	274 (91%)	27 (9%)	12 49
2	B	320/441 (73%)	263 (82%)	57 (18%)	2 17
2	J	320/441 (73%)	263 (82%)	57 (18%)	2 17
2	b	320/441 (73%)	262 (82%)	58 (18%)	2 16
2	j	319/441 (72%)	262 (82%)	57 (18%)	2 16
3	C	295/497 (59%)	268 (91%)	27 (9%)	11 48
3	K	296/497 (60%)	269 (91%)	27 (9%)	12 48
3	c	297/497 (60%)	270 (91%)	27 (9%)	12 48
3	k	297/497 (60%)	270 (91%)	27 (9%)	12 48
4	D	290/454 (64%)	261 (90%)	29 (10%)	9 43
4	L	290/454 (64%)	261 (90%)	29 (10%)	9 43
4	d	290/454 (64%)	261 (90%)	29 (10%)	9 43
4	l	290/454 (64%)	261 (90%)	29 (10%)	9 43
5	E	293/483 (61%)	257 (88%)	36 (12%)	6 34
5	M	293/483 (61%)	257 (88%)	36 (12%)	6 34
5	e	293/483 (61%)	257 (88%)	36 (12%)	6 34
5	m	293/483 (61%)	257 (88%)	36 (12%)	6 34
6	F	334/463 (72%)	273 (82%)	61 (18%)	2 15
6	N	333/463 (72%)	273 (82%)	60 (18%)	2 16
6	f	334/463 (72%)	272 (81%)	62 (19%)	2 14
6	n	333/463 (72%)	272 (82%)	61 (18%)	2 15
7	G	275/454 (61%)	241 (88%)	34 (12%)	6 33
7	O	274/454 (60%)	240 (88%)	34 (12%)	6 33
7	g	274/454 (60%)	240 (88%)	34 (12%)	6 33
7	o	274/454 (60%)	240 (88%)	34 (12%)	6 33
8	H	307/473 (65%)	276 (90%)	31 (10%)	9 43
8	P	307/473 (65%)	276 (90%)	31 (10%)	9 43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	h	306/473 (65%)	275 (90%)	31 (10%)	9 43
8	p	307/473 (65%)	276 (90%)	31 (10%)	9 43
All	All	9658/14944 (65%)	8449 (88%)	1209 (12%)	6 33

All (1209) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	13	LEU
1	A	44	LEU
1	A	50	ASP
1	A	74	ASP
1	A	76	GLN
1	A	90	GLN
1	A	91	ASP
1	A	119	LYS
1	A	120	ILE
1	A	187	VAL
1	A	204	ASN
1	A	225	ASN
1	A	226	CYS
1	A	228	VAL
1	A	248	ASP
1	A	255	ARG
1	A	344	LEU
1	A	350	PHE
1	A	402	LEU
1	A	404	ASP
1	A	419	VAL
1	A	446	LEU
1	A	484	SER
1	A	496	SER
1	A	532	LEU
1	A	548	ASP
2	B	4	GLN
2	B	5	ILE
2	B	8	ASP
2	B	19	ARG
2	B	27	ILE
2	B	31	ASP
2	B	32	LEU

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Mol	Chain	Res	Type
2	B	33	VAL
2	B	43	ASP
2	B	57	THR
2	B	58	ASN
2	B	66	SER
2	B	80	ILE
2	B	92	THR
2	B	145	ASP
2	B	146	LYS
2	B	149	PHE
2	B	166	LEU
2	B	176	LEU
2	B	197	LYS
2	B	203	LEU
2	B	213	ILE
2	B	217	LYS
2	B	228	ASN
2	B	231	ILE
2	B	233	ILE
2	B	238	LEU
2	B	239	ASP
2	B	245	ILE
2	B	246	PHE
2	B	268	LYS
2	B	285	ILE
2	B	287	ARG
2	B	289	LEU
2	B	307	GLU
2	B	329	PHE
2	B	331	GLU
2	B	350	GLU
2	B	357	SER
2	B	375	GLN
2	B	379	GLU
2	B	382	ARG
2	B	399	ARG
2	B	406	CYS
2	B	409	MET
2	B	427	SER
2	B	444	LEU
2	B	462	SER
2	B	463	ILE

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Mol	Chain	Res	Type
2	B	465	ASN
2	B	468	SER
2	B	474	LEU
2	B	475	ASN
2	B	490	SER
2	B	492	LYS
2	B	508	LEU
2	B	512	ASP
3	C	8	MET
3	C	25	ILE
3	C	26	THR
3	C	44	MET
3	C	48	LEU
3	C	57	LEU
3	C	64	ILE
3	C	143	VAL
3	C	165	ILE
3	C	170	LYS
3	C	182	VAL
3	C	184	LYS
3	C	209	ILE
3	C	225	LEU
3	C	226	ASN
3	C	239	GLU
3	C	248	CYS
3	C	250	LEU
3	C	259	THR
3	C	265	LYS
3	C	297	THR
3	C	302	SER
3	C	433	GLN
3	C	456	LEU
3	C	491	ILE
3	C	492	VAL
3	C	519	LEU
4	D	70	ILE
4	D	94	THR
4	D	98	ILE
4	D	100	THR
4	D	135	LEU
4	D	139	CYS
4	D	144	LEU

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Mol	Chain	Res	Type
4	D	146	ASP
4	D	147	ARG
4	D	161	LYS
4	D	175	VAL
4	D	187	LYS
4	D	193	ASP
4	D	194	ILE
4	D	198	LYS
4	D	209	MET
4	D	210	ILE
4	D	231	LYS
4	D	241	ILE
4	D	253	ILE
4	D	263	ILE
4	D	385	MET
4	D	392	ARG
4	D	410	LEU
4	D	424	ARG
4	D	461	ASN
4	D	482	ILE
4	D	502	LEU
4	D	528	ARG
5	E	61	ILE
5	E	82	THR
5	E	86	ASP
5	E	93	GLN
5	E	103	LEU
5	E	106	GLN
5	E	107	LEU
5	E	108	SER
5	E	109	LYS
5	E	148	ASN
5	E	150	PHE
5	E	165	CYS
5	E	169	SER
5	E	175	LEU
5	E	187	SER
5	E	210	ASN
5	E	222	ASP
5	E	236	ASP
5	E	241	ASN
5	E	245	LEU

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Mol	Chain	Res	Type
5	E	273	THR
5	E	296	GLN
5	E	324	GLN
5	E	325	TRP
5	E	351	LEU
5	E	352	GLU
5	E	368	ASP
5	E	382	GLU
5	E	396	GLU
5	E	431	ARG
5	E	440	VAL
5	E	469	PHE
5	E	492	ILE
5	E	507	ILE
5	E	535	LYS
5	E	547	MET
6	F	1	MET
6	F	3	LEU
6	F	4	GLN
6	F	5	LEU
6	F	6	LEU
6	F	16	ASP
6	F	27	GLU
6	F	37	LEU
6	F	43	LEU
6	F	53	ILE
6	F	68	ILE
6	F	93	THR
6	F	102	LEU
6	F	113	VAL
6	F	117	ILE
6	F	133	LEU
6	F	142	ASN
6	F	143	LEU
6	F	152	GLN
6	F	158	LEU
6	F	171	THR
6	F	183	ASP
6	F	196	ILE
6	F	197	MET
6	F	198	GLN
6	F	209	PHE

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Mol	Chain	Res	Type
6	F	213	LEU
6	F	243	GLU
6	F	294	VAL
6	F	295	ILE
6	F	321	LYS
6	F	323	ARG
6	F	328	LEU
6	F	330	LEU
6	F	370	ASN
6	F	376	CYS
6	F	378	ILE
6	F	390	GLN
6	F	407	LYS
6	F	409	LYS
6	F	424	ARG
6	F	433	LYS
6	F	434	LEU
6	F	437	LYS
6	F	440	THR
6	F	442	THR
6	F	454	ILE
6	F	457	THR
6	F	458	LEU
6	F	483	SER
6	F	484	ASP
6	F	486	THR
6	F	489	VAL
6	F	513	LEU
6	F	515	ASN
6	F	518	THR
6	F	538	ARG
6	F	540	THR
6	F	541	LEU
6	F	542	LYS
6	F	544	THR
7	G	36	VAL
7	G	37	GLN
7	G	43	THR
7	G	52	LEU
7	G	58	GLN
7	G	64	ASN
7	G	71	LYS

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Mol	Chain	Res	Type
7	G	82	THR
7	G	86	ILE
7	G	100	SER
7	G	120	ILE
7	G	123	HIS
7	G	156	GLU
7	G	157	LEU
7	G	174	ASN
7	G	191	ARG
7	G	232	GLN
7	G	234	LYS
7	G	282	LEU
7	G	285	VAL
7	G	305	GLN
7	G	312	ILE
7	G	346	LEU
7	G	376	LEU
7	G	377	LEU
7	G	393	LEU
7	G	399	ILE
7	G	408	LEU
7	G	410	VAL
7	G	418	MET
7	G	488	ILE
7	G	514	THR
7	G	516	LEU
7	G	527	LYS
8	H	15	LYS
8	H	27	GLN
8	H	28	ILE
8	H	29	ILE
8	H	32	ILE
8	H	62	ILE
8	H	66	ASN
8	H	74	GLU
8	H	76	ASP
8	H	77	ILE
8	H	92	GLN
8	H	153	LYS
8	H	175	GLU
8	H	209	VAL
8	H	237	LYS

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Mol	Chain	Res	Type
8	H	244	LYS
8	H	267	LEU
8	H	314	ASN
8	H	316	TYR
8	H	320	VAL
8	H	343	ARG
8	H	352	LEU
8	H	386	LEU
8	H	390	THR
8	H	408	VAL
8	H	430	LEU
8	H	451	GLN
8	H	466	THR
8	H	473	GLU
8	H	494	HIS
8	H	532	THR
1	I	8	SER
1	I	13	LEU
1	I	44	LEU
1	I	50	ASP
1	I	74	ASP
1	I	76	GLN
1	I	90	GLN
1	I	91	ASP
1	I	119	LYS
1	I	120	ILE
1	I	187	VAL
1	I	204	ASN
1	I	225	ASN
1	I	226	CYS
1	I	228	VAL
1	I	248	ASP
1	I	255	ARG
1	I	344	LEU
1	I	350	PHE
1	I	402	LEU
1	I	404	ASP
1	I	419	VAL
1	I	446	LEU
1	I	484	SER
1	I	496	SER
1	I	532	LEU

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Mol	Chain	Res	Type
1	I	548	ASP
2	J	4	GLN
2	J	5	ILE
2	J	8	ASP
2	J	19	ARG
2	J	27	ILE
2	J	31	ASP
2	J	32	LEU
2	J	33	VAL
2	J	43	ASP
2	J	57	THR
2	J	58	ASN
2	J	66	SER
2	J	80	ILE
2	J	92	THR
2	J	145	ASP
2	J	146	LYS
2	J	149	PHE
2	J	166	LEU
2	J	176	LEU
2	J	197	LYS
2	J	203	LEU
2	J	213	ILE
2	J	217	LYS
2	J	228	ASN
2	J	231	ILE
2	J	233	ILE
2	J	238	LEU
2	J	239	ASP
2	J	245	ILE
2	J	246	PHE
2	J	268	LYS
2	J	285	ILE
2	J	287	ARG
2	J	289	LEU
2	J	307	GLU
2	J	329	PHE
2	J	331	GLU
2	J	350	GLU
2	J	357	SER
2	J	375	GLN
2	J	379	GLU

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Mol	Chain	Res	Type
2	J	382	ARG
2	J	399	ARG
2	J	406	CYS
2	J	409	MET
2	J	427	SER
2	J	444	LEU
2	J	462	SER
2	J	463	ILE
2	J	465	ASN
2	J	468	SER
2	J	474	LEU
2	J	475	ASN
2	J	490	SER
2	J	492	LYS
2	J	508	LEU
2	J	512	ASP
3	K	8	MET
3	K	25	ILE
3	K	26	THR
3	K	44	MET
3	K	48	LEU
3	K	57	LEU
3	K	64	ILE
3	K	143	VAL
3	K	165	ILE
3	K	170	LYS
3	K	182	VAL
3	K	184	LYS
3	K	209	ILE
3	K	225	LEU
3	K	226	ASN
3	K	239	GLU
3	K	248	CYS
3	K	250	LEU
3	K	259	THR
3	K	265	LYS
3	K	297	THR
3	K	302	SER
3	K	433	GLN
3	K	456	LEU
3	K	491	ILE
3	K	492	VAL

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Mol	Chain	Res	Type
3	K	519	LEU
4	L	70	ILE
4	L	94	THR
4	L	98	ILE
4	L	100	THR
4	L	135	LEU
4	L	139	CYS
4	L	144	LEU
4	L	146	ASP
4	L	147	ARG
4	L	161	LYS
4	L	175	VAL
4	L	187	LYS
4	L	193	ASP
4	L	194	ILE
4	L	198	LYS
4	L	209	MET
4	L	210	ILE
4	L	231	LYS
4	L	241	ILE
4	L	253	ILE
4	L	263	ILE
4	L	385	MET
4	L	392	ARG
4	L	410	LEU
4	L	424	ARG
4	L	461	ASN
4	L	482	ILE
4	L	502	LEU
4	L	528	ARG
5	M	61	ILE
5	M	82	THR
5	M	86	ASP
5	M	93	GLN
5	M	103	LEU
5	M	106	GLN
5	M	107	LEU
5	M	108	SER
5	M	109	LYS
5	M	148	ASN
5	M	150	PHE
5	M	165	CYS

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Mol	Chain	Res	Type
5	M	169	SER
5	M	175	LEU
5	M	187	SER
5	M	210	ASN
5	M	222	ASP
5	M	236	ASP
5	M	241	ASN
5	M	245	LEU
5	M	273	THR
5	M	296	GLN
5	M	324	GLN
5	M	325	TRP
5	M	351	LEU
5	M	352	GLU
5	M	368	ASP
5	M	382	GLU
5	M	396	GLU
5	M	431	ARG
5	M	440	VAL
5	M	469	PHE
5	M	492	ILE
5	M	507	ILE
5	M	535	LYS
5	M	547	MET
6	N	1	MET
6	N	3	LEU
6	N	4	GLN
6	N	5	LEU
6	N	6	LEU
6	N	16	ASP
6	N	27	GLU
6	N	37	LEU
6	N	53	ILE
6	N	68	ILE
6	N	93	THR
6	N	102	LEU
6	N	113	VAL
6	N	117	ILE
6	N	133	LEU
6	N	142	ASN
6	N	143	LEU
6	N	152	GLN

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Mol	Chain	Res	Type
6	N	158	LEU
6	N	171	THR
6	N	183	ASP
6	N	196	ILE
6	N	197	MET
6	N	198	GLN
6	N	209	PHE
6	N	213	LEU
6	N	243	GLU
6	N	294	VAL
6	N	295	ILE
6	N	321	LYS
6	N	323	ARG
6	N	328	LEU
6	N	330	LEU
6	N	370	ASN
6	N	376	CYS
6	N	378	ILE
6	N	390	GLN
6	N	407	LYS
6	N	409	LYS
6	N	424	ARG
6	N	433	LYS
6	N	434	LEU
6	N	437	LYS
6	N	440	THR
6	N	442	THR
6	N	454	ILE
6	N	457	THR
6	N	458	LEU
6	N	483	SER
6	N	484	ASP
6	N	486	THR
6	N	489	VAL
6	N	513	LEU
6	N	515	ASN
6	N	518	THR
6	N	538	ARG
6	N	540	THR
6	N	541	LEU
6	N	542	LYS
6	N	544	THR

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Mol	Chain	Res	Type
7	O	36	VAL
7	O	37	GLN
7	O	43	THR
7	O	52	LEU
7	O	58	GLN
7	O	64	ASN
7	O	71	LYS
7	O	82	THR
7	O	86	ILE
7	O	100	SER
7	O	120	ILE
7	O	123	HIS
7	O	156	GLU
7	O	157	LEU
7	O	174	ASN
7	O	191	ARG
7	O	232	GLN
7	O	234	LYS
7	O	282	LEU
7	O	285	VAL
7	O	305	GLN
7	O	312	ILE
7	O	346	LEU
7	O	376	LEU
7	O	377	LEU
7	O	393	LEU
7	O	399	ILE
7	O	408	LEU
7	O	410	VAL
7	O	418	MET
7	O	488	ILE
7	O	514	THR
7	O	516	LEU
7	O	527	LYS
8	P	15	LYS
8	P	27	GLN
8	P	28	ILE
8	P	29	ILE
8	P	32	ILE
8	P	62	ILE
8	P	66	ASN
8	P	74	GLU

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Mol	Chain	Res	Type
8	P	76	ASP
8	P	77	ILE
8	P	92	GLN
8	P	153	LYS
8	P	175	GLU
8	P	209	VAL
8	P	237	LYS
8	P	244	LYS
8	P	267	LEU
8	P	314	ASN
8	P	316	TYR
8	P	320	VAL
8	P	343	ARG
8	P	352	LEU
8	P	386	LEU
8	P	390	THR
8	P	408	VAL
8	P	430	LEU
8	P	451	GLN
8	P	466	THR
8	P	473	GLU
8	P	494	HIS
8	P	532	THR
1	a	1008	SER
1	a	1013	LEU
1	a	1044	LEU
1	a	1050	ASP
1	a	1074	ASP
1	a	1076	GLN
1	a	1090	GLN
1	a	1091	ASP
1	a	1119	LYS
1	a	1120	ILE
1	a	1187	VAL
1	a	1204	ASN
1	a	1225	ASN
1	a	1226	CYS
1	a	1228	VAL
1	a	1248	ASP
1	a	1255	ARG
1	a	1344	LEU
1	a	1350	PHE

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Mol	Chain	Res	Type
1	a	1402	LEU
1	a	1404	ASP
1	a	1419	VAL
1	a	1446	LEU
1	a	1484	SER
1	a	1496	SER
1	a	1532	LEU
1	a	1548	ASP
2	b	1004	GLN
2	b	1005	ILE
2	b	1008	ASP
2	b	1019	ARG
2	b	1027	ILE
2	b	1031	ASP
2	b	1032	LEU
2	b	1033	VAL
2	b	1043	ASP
2	b	1057	THR
2	b	1058	ASN
2	b	1066	SER
2	b	1080	ILE
2	b	1092	THR
2	b	1145	ASP
2	b	1146	LYS
2	b	1149	PHE
2	b	1166	LEU
2	b	1176	LEU
2	b	1197	LYS
2	b	1203	LEU
2	b	1213	ILE
2	b	1217	LYS
2	b	1228	ASN
2	b	1231	ILE
2	b	1233	ILE
2	b	1238	LEU
2	b	1239	ASP
2	b	1245	ILE
2	b	1246	PHE
2	b	1268	LYS
2	b	1285	ILE
2	b	1287	ARG
2	b	1289	LEU

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Mol	Chain	Res	Type
2	b	1307	GLU
2	b	1329	PHE
2	b	1331	GLU
2	b	1348	LEU
2	b	1350	GLU
2	b	1357	SER
2	b	1375	GLN
2	b	1379	GLU
2	b	1382	ARG
2	b	1399	ARG
2	b	1406	CYS
2	b	1409	MET
2	b	1427	SER
2	b	1444	LEU
2	b	1462	SER
2	b	1463	ILE
2	b	1465	ASN
2	b	1468	SER
2	b	1474	LEU
2	b	1475	ASN
2	b	1490	SER
2	b	1492	LYS
2	b	1508	LEU
2	b	1512	ASP
3	c	1008	MET
3	c	1025	ILE
3	c	1026	THR
3	c	1044	MET
3	c	1048	LEU
3	c	1057	LEU
3	c	1064	ILE
3	c	1143	VAL
3	c	1165	ILE
3	c	1170	LYS
3	c	1182	VAL
3	c	1184	LYS
3	c	1209	ILE
3	c	1225	LEU
3	c	1226	ASN
3	c	1239	GLU
3	c	1248	CYS
3	c	1250	LEU

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Mol	Chain	Res	Type
3	c	1259	THR
3	c	1265	LYS
3	c	1297	THR
3	c	1302	SER
3	c	1433	GLN
3	c	1456	LEU
3	c	1491	ILE
3	c	1492	VAL
3	c	1519	LEU
4	d	1070	ILE
4	d	1094	THR
4	d	1098	ILE
4	d	1100	THR
4	d	1135	LEU
4	d	1139	CYS
4	d	1144	LEU
4	d	1146	ASP
4	d	1147	ARG
4	d	1161	LYS
4	d	1175	VAL
4	d	1187	LYS
4	d	1193	ASP
4	d	1194	ILE
4	d	1198	LYS
4	d	1209	MET
4	d	1210	ILE
4	d	1231	LYS
4	d	1241	ILE
4	d	1253	ILE
4	d	1263	ILE
4	d	1385	MET
4	d	1392	ARG
4	d	1410	LEU
4	d	1424	ARG
4	d	1461	ASN
4	d	1482	ILE
4	d	1502	LEU
4	d	1528	ARG
5	e	1061	ILE
5	e	1082	THR
5	e	1086	ASP
5	e	1093	GLN

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Mol	Chain	Res	Type
5	e	1103	LEU
5	e	1106	GLN
5	e	1107	LEU
5	e	1108	SER
5	e	1109	LYS
5	e	1148	ASN
5	e	1150	PHE
5	e	1165	CYS
5	e	1169	SER
5	e	1175	LEU
5	e	1187	SER
5	e	1210	ASN
5	e	1222	ASP
5	e	1236	ASP
5	e	1241	ASN
5	e	1245	LEU
5	e	1273	THR
5	e	1296	GLN
5	e	1324	GLN
5	e	1325	TRP
5	e	1351	LEU
5	e	1352	GLU
5	e	1368	ASP
5	e	1382	GLU
5	e	1396	GLU
5	e	1431	ARG
5	e	1440	VAL
5	e	1469	PHE
5	e	1492	ILE
5	e	1507	ILE
5	e	1535	LYS
5	e	1547	MET
6	f	1001	MET
6	f	1003	LEU
6	f	1004	GLN
6	f	1005	LEU
6	f	1006	LEU
6	f	1016	ASP
6	f	1027	GLU
6	f	1037	LEU
6	f	1043	LEU
6	f	1053	ILE

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Mol	Chain	Res	Type
6	f	1068	ILE
6	f	1093	THR
6	f	1102	LEU
6	f	1113	VAL
6	f	1117	ILE
6	f	1133	LEU
6	f	1142	ASN
6	f	1143	LEU
6	f	1152	GLN
6	f	1158	LEU
6	f	1171	THR
6	f	1183	ASP
6	f	1196	ILE
6	f	1197	MET
6	f	1198	GLN
6	f	1209	PHE
6	f	1213	LEU
6	f	1243	GLU
6	f	1294	VAL
6	f	1295	ILE
6	f	1321	LYS
6	f	1323	ARG
6	f	1328	LEU
6	f	1330	LEU
6	f	1370	ASN
6	f	1376	CYS
6	f	1378	ILE
6	f	1390	GLN
6	f	1407	LYS
6	f	1409	LYS
6	f	1424	ARG
6	f	1433	LYS
6	f	1434	LEU
6	f	1437	LYS
6	f	1439	LYS
6	f	1440	THR
6	f	1442	THR
6	f	1454	ILE
6	f	1457	THR
6	f	1458	LEU
6	f	1483	SER
6	f	1484	ASP

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Mol	Chain	Res	Type
6	f	1486	THR
6	f	1489	VAL
6	f	1513	LEU
6	f	1515	ASN
6	f	1518	THR
6	f	1538	ARG
6	f	1540	THR
6	f	1541	LEU
6	f	1542	LYS
6	f	1544	THR
7	g	1036	VAL
7	g	1037	GLN
7	g	1043	THR
7	g	1052	LEU
7	g	1058	GLN
7	g	1064	ASN
7	g	1071	LYS
7	g	1082	THR
7	g	1086	ILE
7	g	1100	SER
7	g	1120	ILE
7	g	1123	HIS
7	g	1156	GLU
7	g	1157	LEU
7	g	1174	ASN
7	g	1191	ARG
7	g	1232	GLN
7	g	1234	LYS
7	g	1282	LEU
7	g	1285	VAL
7	g	1305	GLN
7	g	1312	ILE
7	g	1346	LEU
7	g	1376	LEU
7	g	1377	LEU
7	g	1393	LEU
7	g	1399	ILE
7	g	1408	LEU
7	g	1410	VAL
7	g	1418	MET
7	g	1488	ILE
7	g	1514	THR

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Mol	Chain	Res	Type
7	g	1516	LEU
7	g	1527	LYS
8	h	1015	LYS
8	h	1027	GLN
8	h	1028	ILE
8	h	1029	ILE
8	h	1032	ILE
8	h	1062	ILE
8	h	1066	ASN
8	h	1074	GLU
8	h	1076	ASP
8	h	1077	ILE
8	h	1092	GLN
8	h	1153	LYS
8	h	1175	GLU
8	h	1209	VAL
8	h	1237	LYS
8	h	1244	LYS
8	h	1267	LEU
8	h	1314	ASN
8	h	1316	TYR
8	h	1320	VAL
8	h	1343	ARG
8	h	1352	LEU
8	h	1386	LEU
8	h	1390	THR
8	h	1408	VAL
8	h	1430	LEU
8	h	1451	GLN
8	h	1466	THR
8	h	1473	GLU
8	h	1494	HIS
8	h	1532	THR
1	i	1008	SER
1	i	1013	LEU
1	i	1044	LEU
1	i	1050	ASP
1	i	1074	ASP
1	i	1076	GLN
1	i	1090	GLN
1	i	1091	ASP
1	i	1119	LYS

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Mol	Chain	Res	Type
1	i	1120	ILE
1	i	1187	VAL
1	i	1204	ASN
1	i	1225	ASN
1	i	1226	CYS
1	i	1228	VAL
1	i	1248	ASP
1	i	1255	ARG
1	i	1344	LEU
1	i	1350	PHE
1	i	1402	LEU
1	i	1404	ASP
1	i	1419	VAL
1	i	1446	LEU
1	i	1484	SER
1	i	1496	SER
1	i	1532	LEU
1	i	1548	ASP
2	j	1004	GLN
2	j	1005	ILE
2	j	1008	ASP
2	j	1019	ARG
2	j	1027	ILE
2	j	1031	ASP
2	j	1032	LEU
2	j	1033	VAL
2	j	1043	ASP
2	j	1057	THR
2	j	1058	ASN
2	j	1066	SER
2	j	1080	ILE
2	j	1092	THR
2	j	1145	ASP
2	j	1146	LYS
2	j	1149	PHE
2	j	1166	LEU
2	j	1176	LEU
2	j	1197	LYS
2	j	1203	LEU
2	j	1213	ILE
2	j	1217	LYS
2	j	1228	ASN

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Mol	Chain	Res	Type
2	j	1231	ILE
2	j	1233	ILE
2	j	1238	LEU
2	j	1239	ASP
2	j	1245	ILE
2	j	1246	PHE
2	j	1268	LYS
2	j	1285	ILE
2	j	1287	ARG
2	j	1289	LEU
2	j	1307	GLU
2	j	1329	PHE
2	j	1331	GLU
2	j	1350	GLU
2	j	1357	SER
2	j	1375	GLN
2	j	1379	GLU
2	j	1382	ARG
2	j	1399	ARG
2	j	1406	CYS
2	j	1409	MET
2	j	1427	SER
2	j	1444	LEU
2	j	1462	SER
2	j	1463	ILE
2	j	1465	ASN
2	j	1468	SER
2	j	1474	LEU
2	j	1475	ASN
2	j	1490	SER
2	j	1492	LYS
2	j	1508	LEU
2	j	1512	ASP
3	k	1008	MET
3	k	1025	ILE
3	k	1026	THR
3	k	1044	MET
3	k	1048	LEU
3	k	1057	LEU
3	k	1064	ILE
3	k	1143	VAL
3	k	1165	ILE

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Mol	Chain	Res	Type
3	k	1170	LYS
3	k	1182	VAL
3	k	1184	LYS
3	k	1209	ILE
3	k	1225	LEU
3	k	1226	ASN
3	k	1239	GLU
3	k	1248	CYS
3	k	1250	LEU
3	k	1259	THR
3	k	1265	LYS
3	k	1297	THR
3	k	1302	SER
3	k	1433	GLN
3	k	1456	LEU
3	k	1491	ILE
3	k	1492	VAL
3	k	1519	LEU
4	l	1070	ILE
4	l	1094	THR
4	l	1098	ILE
4	l	1100	THR
4	l	1135	LEU
4	l	1139	CYS
4	l	1144	LEU
4	l	1146	ASP
4	l	1147	ARG
4	l	1161	LYS
4	l	1175	VAL
4	l	1187	LYS
4	l	1193	ASP
4	l	1194	ILE
4	l	1198	LYS
4	l	1209	MET
4	l	1210	ILE
4	l	1231	LYS
4	l	1241	ILE
4	l	1253	ILE
4	l	1263	ILE
4	l	1385	MET
4	l	1392	ARG
4	l	1410	LEU

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Mol	Chain	Res	Type
4	l	1424	ARG
4	l	1461	ASN
4	l	1482	ILE
4	l	1502	LEU
4	l	1528	ARG
5	m	1061	ILE
5	m	1082	THR
5	m	1086	ASP
5	m	1093	GLN
5	m	1103	LEU
5	m	1106	GLN
5	m	1107	LEU
5	m	1108	SER
5	m	1109	LYS
5	m	1148	ASN
5	m	1150	PHE
5	m	1165	CYS
5	m	1169	SER
5	m	1175	LEU
5	m	1187	SER
5	m	1210	ASN
5	m	1222	ASP
5	m	1236	ASP
5	m	1241	ASN
5	m	1245	LEU
5	m	1273	THR
5	m	1296	GLN
5	m	1324	GLN
5	m	1325	TRP
5	m	1351	LEU
5	m	1352	GLU
5	m	1368	ASP
5	m	1382	GLU
5	m	1396	GLU
5	m	1431	ARG
5	m	1440	VAL
5	m	1469	PHE
5	m	1492	ILE
5	m	1507	ILE
5	m	1535	LYS
5	m	1547	MET
6	n	1001	MET

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Mol	Chain	Res	Type
6	n	1003	LEU
6	n	1004	GLN
6	n	1005	LEU
6	n	1006	LEU
6	n	1016	ASP
6	n	1027	GLU
6	n	1037	LEU
6	n	1043	LEU
6	n	1053	ILE
6	n	1068	ILE
6	n	1093	THR
6	n	1102	LEU
6	n	1113	VAL
6	n	1117	ILE
6	n	1133	LEU
6	n	1142	ASN
6	n	1143	LEU
6	n	1152	GLN
6	n	1158	LEU
6	n	1171	THR
6	n	1183	ASP
6	n	1196	ILE
6	n	1197	MET
6	n	1198	GLN
6	n	1209	PHE
6	n	1213	LEU
6	n	1243	GLU
6	n	1294	VAL
6	n	1295	ILE
6	n	1321	LYS
6	n	1323	ARG
6	n	1328	LEU
6	n	1330	LEU
6	n	1370	ASN
6	n	1376	CYS
6	n	1378	ILE
6	n	1390	GLN
6	n	1407	LYS
6	n	1409	LYS
6	n	1424	ARG
6	n	1433	LYS
6	n	1434	LEU

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Mol	Chain	Res	Type
6	n	1437	LYS
6	n	1440	THR
6	n	1442	THR
6	n	1454	ILE
6	n	1457	THR
6	n	1458	LEU
6	n	1483	SER
6	n	1484	ASP
6	n	1486	THR
6	n	1489	VAL
6	n	1513	LEU
6	n	1515	ASN
6	n	1518	THR
6	n	1538	ARG
6	n	1540	THR
6	n	1541	LEU
6	n	1542	LYS
6	n	1544	THR
7	o	1036	VAL
7	o	1037	GLN
7	o	1043	THR
7	o	1052	LEU
7	o	1058	GLN
7	o	1064	ASN
7	o	1071	LYS
7	o	1082	THR
7	o	1086	ILE
7	o	1100	SER
7	o	1120	ILE
7	o	1123	HIS
7	o	1156	GLU
7	o	1157	LEU
7	o	1174	ASN
7	o	1191	ARG
7	o	1232	GLN
7	o	1234	LYS
7	o	1282	LEU
7	o	1285	VAL
7	o	1305	GLN
7	o	1312	ILE
7	o	1346	LEU
7	o	1376	LEU

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Mol	Chain	Res	Type
7	o	1377	LEU
7	o	1393	LEU
7	o	1399	ILE
7	o	1408	LEU
7	o	1410	VAL
7	o	1418	MET
7	o	1488	ILE
7	o	1514	THR
7	o	1516	LEU
7	o	1527	LYS
8	p	1015	LYS
8	p	1027	GLN
8	p	1028	ILE
8	p	1029	ILE
8	p	1032	ILE
8	p	1062	ILE
8	p	1066	ASN
8	p	1074	GLU
8	p	1076	ASP
8	p	1077	ILE
8	p	1092	GLN
8	p	1153	LYS
8	p	1175	GLU
8	p	1209	VAL
8	p	1237	LYS
8	p	1244	LYS
8	p	1267	LEU
8	p	1314	ASN
8	p	1316	TYR
8	p	1320	VAL
8	p	1343	ARG
8	p	1352	LEU
8	p	1386	LEU
8	p	1390	THR
8	p	1408	VAL
8	p	1430	LEU
8	p	1451	GLN
8	p	1466	THR
8	p	1473	GLU
8	p	1494	HIS
8	p	1532	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (306) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	90	GLN
1	A	121	HIS
1	A	178	ASN
1	A	204	ASN
1	A	209	HIS
1	A	250	ASN
1	A	252	GLN
1	A	363	GLN
1	A	391	ASN
1	A	435	ASN
2	B	4	GLN
2	B	9	GLN
2	B	58	ASN
2	B	116	HIS
2	B	228	ASN
2	B	260	GLN
2	B	271	ASN
2	B	286	ASN
2	B	375	GLN
2	B	385	HIS
2	B	393	GLN
2	B	439	GLN
2	B	475	ASN
3	C	9	ASN
3	C	59	ASN
3	C	85	GLN
3	C	166	HIS
3	C	281	GLN
3	C	325	ASN
3	C	433	GLN
3	C	439	GLN
3	C	508	GLN
4	D	59	ASN
4	D	72	HIS
4	D	217	GLN
4	D	238	GLN
4	D	259	GLN
4	D	384	ASN
4	D	461	ASN
4	D	499	GLN
5	E	37	ASN

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Mol	Chain	Res	Type
5	E	50	HIS
5	E	93	GLN
5	E	106	GLN
5	E	132	GLN
5	E	210	ASN
5	E	324	GLN
5	E	338	ASN
5	E	466	GLN
5	E	553	ASN
6	F	104	GLN
6	F	110	GLN
6	F	198	GLN
6	F	200	GLN
6	F	217	HIS
6	F	221	HIS
6	F	312	HIS
6	F	515	ASN
7	G	37	GLN
7	G	58	GLN
7	G	232	GLN
7	G	268	GLN
7	G	305	GLN
7	G	491	ASN
8	H	27	GLN
8	H	66	ASN
8	H	79	HIS
8	H	92	GLN
8	H	101	ASN
8	H	188	HIS
8	H	283	GLN
8	H	373	GLN
8	H	446	GLN
8	H	451	GLN
1	I	64	ASN
1	I	90	GLN
1	I	121	HIS
1	I	178	ASN
1	I	204	ASN
1	I	209	HIS
1	I	225	ASN
1	I	250	ASN
1	I	252	GLN

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Mol	Chain	Res	Type
1	I	363	GLN
1	I	391	ASN
1	I	435	ASN
2	J	4	GLN
2	J	9	GLN
2	J	58	ASN
2	J	116	HIS
2	J	228	ASN
2	J	235	ASN
2	J	260	GLN
2	J	271	ASN
2	J	286	ASN
2	J	375	GLN
2	J	393	GLN
2	J	439	GLN
2	J	475	ASN
3	K	9	ASN
3	K	12	GLN
3	K	59	ASN
3	K	85	GLN
3	K	117	HIS
3	K	166	HIS
3	K	270	ASN
3	K	281	GLN
3	K	325	ASN
3	K	433	GLN
3	K	439	GLN
3	K	508	GLN
4	L	59	ASN
4	L	72	HIS
4	L	217	GLN
4	L	238	GLN
4	L	259	GLN
4	L	384	ASN
4	L	461	ASN
4	L	499	GLN
5	M	37	ASN
5	M	50	HIS
5	M	93	GLN
5	M	132	GLN
5	M	142	HIS
5	M	210	ASN

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Mol	Chain	Res	Type
5	M	324	GLN
5	M	338	ASN
5	M	466	GLN
6	N	104	GLN
6	N	110	GLN
6	N	198	GLN
6	N	200	GLN
6	N	217	HIS
6	N	221	HIS
6	N	312	HIS
6	N	515	ASN
7	O	37	GLN
7	O	58	GLN
7	O	231	GLN
7	O	232	GLN
7	O	305	GLN
7	O	491	ASN
8	P	27	GLN
8	P	66	ASN
8	P	79	HIS
8	P	92	GLN
8	P	101	ASN
8	P	188	HIS
8	P	283	GLN
8	P	373	GLN
8	P	446	GLN
8	P	451	GLN
1	a	1064	ASN
1	a	1090	GLN
1	a	1121	HIS
1	a	1178	ASN
1	a	1204	ASN
1	a	1209	HIS
1	a	1250	ASN
1	a	1252	GLN
1	a	1363	GLN
1	a	1391	ASN
1	a	1435	ASN
2	b	1004	GLN
2	b	1009	GLN
2	b	1058	ASN
2	b	1116	HIS

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Mol	Chain	Res	Type
2	b	1228	ASN
2	b	1235	ASN
2	b	1260	GLN
2	b	1271	ASN
2	b	1286	ASN
2	b	1375	GLN
2	b	1393	GLN
2	b	1439	GLN
2	b	1475	ASN
3	c	1009	ASN
3	c	1012	GLN
3	c	1059	ASN
3	c	1085	GLN
3	c	1117	HIS
3	c	1166	HIS
3	c	1270	ASN
3	c	1281	GLN
3	c	1325	ASN
3	c	1433	GLN
3	c	1439	GLN
3	c	1508	GLN
4	d	1059	ASN
4	d	1072	HIS
4	d	1217	GLN
4	d	1238	GLN
4	d	1259	GLN
4	d	1384	ASN
4	d	1461	ASN
4	d	1499	GLN
5	e	1037	ASN
5	e	1050	HIS
5	e	1093	GLN
5	e	1132	GLN
5	e	1142	HIS
5	e	1210	ASN
5	e	1324	GLN
5	e	1338	ASN
5	e	1466	GLN
6	f	1110	GLN
6	f	1198	GLN
6	f	1200	GLN
6	f	1217	HIS

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Mol	Chain	Res	Type
6	f	1221	HIS
6	f	1312	HIS
6	f	1515	ASN
7	g	1037	GLN
7	g	1058	GLN
7	g	1232	GLN
7	g	1305	GLN
7	g	1356	GLN
7	g	1491	ASN
8	h	1027	GLN
8	h	1066	ASN
8	h	1079	HIS
8	h	1092	GLN
8	h	1101	ASN
8	h	1188	HIS
8	h	1373	GLN
8	h	1446	GLN
8	h	1451	GLN
8	h	1472	ASN
1	i	1064	ASN
1	i	1090	GLN
1	i	1121	HIS
1	i	1178	ASN
1	i	1204	ASN
1	i	1209	HIS
1	i	1250	ASN
1	i	1252	GLN
1	i	1363	GLN
1	i	1391	ASN
1	i	1435	ASN
2	j	1004	GLN
2	j	1009	GLN
2	j	1058	ASN
2	j	1116	HIS
2	j	1228	ASN
2	j	1235	ASN
2	j	1260	GLN
2	j	1271	ASN
2	j	1286	ASN
2	j	1375	GLN
2	j	1393	GLN
2	j	1439	GLN

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Mol	Chain	Res	Type
2	j	1475	ASN
3	k	1009	ASN
3	k	1012	GLN
3	k	1085	GLN
3	k	1117	HIS
3	k	1166	HIS
3	k	1270	ASN
3	k	1281	GLN
3	k	1325	ASN
3	k	1433	GLN
3	k	1439	GLN
3	k	1508	GLN
4	l	1059	ASN
4	l	1072	HIS
4	l	1217	GLN
4	l	1238	GLN
4	l	1259	GLN
4	l	1384	ASN
4	l	1461	ASN
4	l	1499	GLN
5	m	1037	ASN
5	m	1050	HIS
5	m	1093	GLN
5	m	1132	GLN
5	m	1210	ASN
5	m	1296	GLN
5	m	1324	GLN
5	m	1338	ASN
5	m	1466	GLN
5	m	1553	ASN
6	n	1104	GLN
6	n	1110	GLN
6	n	1198	GLN
6	n	1200	GLN
6	n	1217	HIS
6	n	1221	HIS
6	n	1312	HIS
6	n	1515	ASN
7	o	1037	GLN
7	o	1058	GLN
7	o	1231	GLN
7	o	1232	GLN

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Mol	Chain	Res	Type
7	o	1305	GLN
7	o	1491	ASN
8	p	1027	GLN
8	p	1066	ASN
8	p	1079	HIS
8	p	1092	GLN
8	p	1101	ASN
8	p	1188	HIS
8	p	1283	GLN
8	p	1373	GLN
8	p	1446	GLN
8	p	1451	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

56 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
9	ADP	A	601	10	22,29,29	2.06	8 (36%)	27,45,45	2.99	10 (37%)
10	BEF	A	602	9	0,3,3	0.00	-	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	ADP	B	601	10	22,29,29	2.08	9 (40%)	27,45,45	2.96	9 (33%)
10	BEF	B	602	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	C	1101	-	22,29,29	2.01	8 (36%)	27,45,45	2.79	5 (18%)
10	BEF	C	1102	-	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	D	601	-	22,29,29	1.99	8 (36%)	27,45,45	2.85	8 (29%)
10	BEF	D	602	-	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	E	601	10	22,29,29	2.07	9 (40%)	27,45,45	3.00	8 (29%)
10	BEF	E	602	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	F	601	-	22,29,29	2.06	9 (40%)	27,45,45	2.87	9 (33%)
10	BEF	F	602	-	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	G	601	-	22,29,29	2.09	8 (36%)	27,45,45	3.03	10 (37%)
10	BEF	G	602	-	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	H	601	-	22,29,29	2.02	8 (36%)	27,45,45	2.89	7 (25%)
10	BEF	H	602	-	0,3,3	0.00	-	0,3,3	0.00	-
11	SO4	I	600	-	4,4,4	0.18	0	6,6,6	0.12	0
9	ADP	J	601	10	22,29,29	2.03	9 (40%)	27,45,45	3.12	11 (40%)
10	BEF	J	602	9	0,3,3	0.00	-	0,3,3	0.00	-
11	SO4	K	1101	-	4,4,4	0.21	0	6,6,6	0.17	0
9	ADP	L	601	-	22,29,29	2.02	8 (36%)	27,45,45	2.80	8 (29%)
10	BEF	L	602	-	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	M	601	-	22,29,29	2.00	9 (40%)	27,45,45	2.92	8 (29%)
10	BEF	M	602	-	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	N	601	10	22,29,29	2.05	8 (36%)	27,45,45	2.94	10 (37%)
10	BEF	N	602	9	0,3,3	0.00	-	0,3,3	0.00	-
11	SO4	O	600	-	4,4,4	0.10	0	6,6,6	0.12	0
9	ADP	P	601	-	22,29,29	2.02	8 (36%)	27,45,45	2.90	11 (40%)
10	BEF	P	602	-	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	a	1601	-	22,29,29	2.02	8 (36%)	27,45,45	3.00	10 (37%)
10	BEF	a	1602	-	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	b	1601	10	22,29,29	2.03	9 (40%)	27,45,45	2.85	11 (40%)
10	BEF	b	1602	9	0,3,3	0.00	-	0,3,3	0.00	-
11	SO4	c	2101	-	4,4,4	0.20	0	6,6,6	0.18	0
11	SO4	d	1600	-	4,4,4	0.18	0	6,6,6	0.14	0
9	ADP	e	1601	-	22,29,29	2.03	8 (36%)	27,45,45	2.84	8 (29%)
10	BEF	e	1602	-	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	f	1601	-	22,29,29	2.05	8 (36%)	27,45,45	3.04	10 (37%)
10	BEF	f	1602	-	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	g	1601	-	22,29,29	2.06	8 (36%)	27,45,45	2.85	9 (33%)
10	BEF	g	1602	-	0,3,3	0.00	-	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	ADP	h	1601	10	22,29,29	2.04	9 (40%)	27,45,45	2.72	9 (33%)
10	BEF	h	1602	9	0,3,3	0.00	-	0,3,3	0.00	-
11	SO4	i	1600	-	4,4,4	0.18	0	6,6,6	0.29	0
11	SO4	j	1600	-	4,4,4	0.21	0	6,6,6	0.15	0
9	ADP	k	2101	10	22,29,29	2.03	9 (40%)	27,45,45	3.04	9 (33%)
10	BEF	k	2102	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	l	1601	10	22,29,29	2.05	8 (36%)	27,45,45	2.94	9 (33%)
10	BEF	l	1602	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	m	1601	-	22,29,29	2.06	9 (40%)	27,45,45	2.83	8 (29%)
10	BEF	m	1602	-	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	n	1601	-	22,29,29	2.01	9 (40%)	27,45,45	2.86	10 (37%)
10	BEF	n	1602	-	0,3,3	0.00	-	0,3,3	0.00	-
11	SO4	o	1600	-	4,4,4	0.23	0	6,6,6	0.13	0
9	ADP	p	1601	10	22,29,29	2.07	8 (36%)	27,45,45	2.85	11 (40%)
10	BEF	p	1602	9	0,3,3	0.00	-	0,3,3	0.00	-

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
9	ADP	A	601	10	2/2/6/6	0/12/32/32	0/3/3/3
10	BEF	A	602	9	-	0/0/0/0	0/0/0/0
9	ADP	B	601	10	2/2/6/6	0/12/32/32	0/3/3/3
10	BEF	B	602	9	-	0/0/0/0	0/0/0/0
9	ADP	C	1101	-	2/2/6/6	0/12/32/32	0/3/3/3
10	BEF	C	1102	-	-	0/0/0/0	0/0/0/0
9	ADP	D	601	-	2/2/6/6	0/12/32/32	0/3/3/3
10	BEF	D	602	-	-	0/0/0/0	0/0/0/0
9	ADP	E	601	10	1/1/6/6	0/12/32/32	0/3/3/3
10	BEF	E	602	9	-	0/0/0/0	0/0/0/0
9	ADP	F	601	-	-	0/12/32/32	0/3/3/3
10	BEF	F	602	-	-	0/0/0/0	0/0/0/0
9	ADP	G	601	-	1/1/6/6	0/12/32/32	0/3/3/3
10	BEF	G	602	-	-	0/0/0/0	0/0/0/0
9	ADP	H	601	-	1/1/6/6	0/12/32/32	0/3/3/3
10	BEF	H	602	-	-	0/0/0/0	0/0/0/0
11	SO4	I	600	-	-	0/0/0/0	0/0/0/0
9	ADP	J	601	10	2/2/6/6	0/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	BEF	J	602	9	-	0/0/0/0	0/0/0/0
11	SO4	K	1101	-	-	0/0/0/0	0/0/0/0
9	ADP	L	601	-	-	0/12/32/32	0/3/3/3
10	BEF	L	602	-	-	0/0/0/0	0/0/0/0
9	ADP	M	601	-	2/2/6/6	0/12/32/32	0/3/3/3
10	BEF	M	602	-	-	0/0/0/0	0/0/0/0
9	ADP	N	601	10	2/2/6/6	0/12/32/32	0/3/3/3
10	BEF	N	602	9	-	0/0/0/0	0/0/0/0
11	SO4	O	600	-	-	0/0/0/0	0/0/0/0
9	ADP	P	601	-	1/1/6/6	0/12/32/32	0/3/3/3
10	BEF	P	602	-	-	0/0/0/0	0/0/0/0
9	ADP	a	1601	-	2/2/6/6	0/12/32/32	0/3/3/3
10	BEF	a	1602	-	-	0/0/0/0	0/0/0/0
9	ADP	b	1601	10	2/2/6/6	0/12/32/32	0/3/3/3
10	BEF	b	1602	9	-	0/0/0/0	0/0/0/0
11	SO4	c	2101	-	-	0/0/0/0	0/0/0/0
11	SO4	d	1600	-	-	0/0/0/0	0/0/0/0
9	ADP	e	1601	-	2/2/6/6	0/12/32/32	0/3/3/3
10	BEF	e	1602	-	-	0/0/0/0	0/0/0/0
9	ADP	f	1601	-	2/2/6/6	0/12/32/32	0/3/3/3
10	BEF	f	1602	-	-	0/0/0/0	0/0/0/0
9	ADP	g	1601	-	1/1/6/6	0/12/32/32	0/3/3/3
10	BEF	g	1602	-	-	0/0/0/0	0/0/0/0
9	ADP	h	1601	10	1/1/6/6	0/12/32/32	0/3/3/3
10	BEF	h	1602	9	-	0/0/0/0	0/0/0/0
11	SO4	i	1600	-	-	0/0/0/0	0/0/0/0
11	SO4	j	1600	-	-	0/0/0/0	0/0/0/0
9	ADP	k	2101	10	2/2/6/6	0/12/32/32	0/3/3/3
10	BEF	k	2102	9	-	0/0/0/0	0/0/0/0
9	ADP	l	1601	10	-	0/12/32/32	0/3/3/3
10	BEF	l	1602	9	-	0/0/0/0	0/0/0/0
9	ADP	m	1601	-	2/2/6/6	0/12/32/32	0/3/3/3
10	BEF	m	1602	-	-	0/0/0/0	0/0/0/0
9	ADP	n	1601	-	1/1/6/6	0/12/32/32	0/3/3/3
10	BEF	n	1602	-	-	0/0/0/0	0/0/0/0
11	SO4	o	1600	-	-	0/0/0/0	0/0/0/0
9	ADP	p	1601	10	1/1/6/6	0/12/32/32	0/3/3/3
10	BEF	p	1602	9	-	0/0/0/0	0/0/0/0

All (202) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	H	601	ADP	C5-C4	-2.68	1.34	1.40
9	F	601	ADP	C5-C4	-2.66	1.34	1.40
9	e	1601	ADP	C5-C4	-2.60	1.34	1.40
9	g	1601	ADP	C5-C4	-2.60	1.34	1.40
9	a	1601	ADP	C5-C4	-2.56	1.34	1.40
9	C	1101	ADP	C5-C4	-2.55	1.34	1.40
9	E	601	ADP	C5-C4	-2.54	1.34	1.40
9	J	601	ADP	C5-C4	-2.53	1.34	1.40
9	P	601	ADP	C5-C4	-2.51	1.34	1.40
9	h	1601	ADP	C5-C4	-2.50	1.34	1.40
9	D	601	ADP	C5-C4	-2.49	1.34	1.40
9	p	1601	ADP	C5-C4	-2.48	1.34	1.40
9	B	601	ADP	C5-C4	-2.48	1.34	1.40
9	l	1601	ADP	C5-C4	-2.47	1.34	1.40
9	m	1601	ADP	C5-C4	-2.46	1.34	1.40
9	M	601	ADP	C5-C4	-2.45	1.35	1.40
9	b	1601	ADP	C5-C4	-2.44	1.35	1.40
9	k	2101	ADP	C5-C4	-2.44	1.35	1.40
9	n	1601	ADP	C5-C4	-2.44	1.35	1.40
9	p	1601	ADP	PB-O3B	-2.44	1.46	1.54
9	G	601	ADP	C5-C4	-2.44	1.35	1.40
9	E	601	ADP	PB-O3B	-2.43	1.46	1.54
9	N	601	ADP	C5-C4	-2.42	1.35	1.40
9	A	601	ADP	PB-O3B	-2.37	1.46	1.54
9	l	1601	ADP	PB-O3B	-2.37	1.46	1.54
9	k	2101	ADP	PB-O3B	-2.35	1.46	1.54
9	L	601	ADP	C5-C4	-2.35	1.35	1.40
9	L	601	ADP	PB-O3B	-2.34	1.46	1.54
9	B	601	ADP	PB-O3B	-2.33	1.46	1.54
9	G	601	ADP	PB-O3B	-2.32	1.46	1.54
9	m	1601	ADP	PB-O3B	-2.32	1.46	1.54
9	A	601	ADP	C5-C4	-2.31	1.35	1.40
9	J	601	ADP	PB-O3B	-2.31	1.46	1.54
9	H	601	ADP	PB-O3B	-2.31	1.46	1.54
9	F	601	ADP	PB-O3B	-2.30	1.46	1.54
9	C	1101	ADP	PB-O3B	-2.28	1.46	1.54
9	e	1601	ADP	PB-O3B	-2.27	1.46	1.54
9	g	1601	ADP	PB-O3B	-2.26	1.46	1.54
9	P	601	ADP	PB-O3B	-2.26	1.46	1.54
9	h	1601	ADP	PB-O3B	-2.25	1.46	1.54
9	M	601	ADP	PB-O3B	-2.24	1.46	1.54
9	a	1601	ADP	PB-O3B	-2.24	1.46	1.54
9	b	1601	ADP	PB-O3B	-2.21	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	601	ADP	PB-O3B	-2.20	1.46	1.54
9	f	1601	ADP	C5-C4	-2.17	1.35	1.40
9	B	601	ADP	PA-O2A	-2.17	1.45	1.54
9	f	1601	ADP	PB-O3B	-2.15	1.47	1.54
9	N	601	ADP	PB-O3B	-2.14	1.47	1.54
9	M	601	ADP	PA-O2A	-2.13	1.45	1.54
9	m	1601	ADP	PA-O2A	-2.06	1.46	1.54
9	b	1601	ADP	PA-O2A	-2.06	1.46	1.54
9	h	1601	ADP	PA-O2A	-2.04	1.46	1.54
9	n	1601	ADP	PB-O3B	-2.03	1.47	1.54
9	k	2101	ADP	PA-O2A	-2.03	1.46	1.54
9	J	601	ADP	PA-O2A	-2.02	1.46	1.54
9	n	1601	ADP	PA-O2A	-2.02	1.46	1.54
9	F	601	ADP	PA-O2A	-2.00	1.46	1.54
9	e	1601	ADP	C2-N3	2.02	1.35	1.32
9	g	1601	ADP	C8-N7	2.02	1.38	1.34
9	J	601	ADP	C2-N3	2.03	1.35	1.32
9	E	601	ADP	C2-N3	2.04	1.35	1.32
9	h	1601	ADP	C2-N3	2.06	1.35	1.32
9	P	601	ADP	C2-N3	2.08	1.35	1.32
9	H	601	ADP	C2-N3	2.09	1.35	1.32
9	E	601	ADP	O4'-C1'	2.10	1.43	1.41
9	k	2101	ADP	C2-N3	2.11	1.35	1.32
9	a	1601	ADP	C8-N7	2.11	1.38	1.34
9	G	601	ADP	C8-N7	2.11	1.38	1.34
9	b	1601	ADP	C2-N3	2.14	1.36	1.32
9	l	1601	ADP	C2-N3	2.14	1.36	1.32
9	F	601	ADP	C2-N3	2.15	1.36	1.32
9	L	601	ADP	C8-N7	2.15	1.38	1.34
9	k	2101	ADP	C8-N7	2.16	1.38	1.34
9	L	601	ADP	C2-N3	2.16	1.36	1.32
9	B	601	ADP	C2-N3	2.17	1.36	1.32
9	a	1601	ADP	C2-N3	2.18	1.36	1.32
9	C	1101	ADP	C2-N3	2.18	1.36	1.32
9	P	601	ADP	C8-N7	2.19	1.38	1.34
9	h	1601	ADP	C8-N7	2.20	1.38	1.34
9	H	601	ADP	C8-N7	2.20	1.38	1.34
9	D	601	ADP	C8-N7	2.20	1.38	1.34
9	M	601	ADP	C2-N3	2.20	1.36	1.32
9	p	1601	ADP	C8-N7	2.21	1.38	1.34
9	b	1601	ADP	C8-N7	2.23	1.38	1.34
9	g	1601	ADP	C2-N3	2.23	1.36	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	601	ADP	C8-N7	2.24	1.38	1.34
9	N	601	ADP	C8-N7	2.25	1.38	1.34
9	e	1601	ADP	C8-N7	2.25	1.38	1.34
9	D	601	ADP	C2-N3	2.26	1.36	1.32
9	l	1601	ADP	C8-N7	2.27	1.39	1.34
9	F	601	ADP	C8-N7	2.27	1.39	1.34
9	C	1101	ADP	C8-N7	2.27	1.39	1.34
9	B	601	ADP	C8-N7	2.28	1.39	1.34
9	p	1601	ADP	C2-N3	2.28	1.36	1.32
9	n	1601	ADP	C8-N7	2.28	1.39	1.34
9	n	1601	ADP	C2-N3	2.29	1.36	1.32
9	J	601	ADP	C8-N7	2.29	1.39	1.34
9	A	601	ADP	C2-N3	2.29	1.36	1.32
9	m	1601	ADP	C8-N7	2.30	1.39	1.34
9	N	601	ADP	C2-N3	2.30	1.36	1.32
9	A	601	ADP	C8-N7	2.35	1.39	1.34
9	E	601	ADP	C8-N7	2.36	1.39	1.34
9	m	1601	ADP	C2-N3	2.37	1.36	1.32
9	G	601	ADP	C2-N3	2.39	1.36	1.32
9	f	1601	ADP	C8-N7	2.40	1.39	1.34
9	f	1601	ADP	C2-N3	2.47	1.36	1.32
9	C	1101	ADP	PB-O2B	2.74	1.64	1.54
9	A	601	ADP	PB-O2B	2.79	1.64	1.54
9	h	1601	ADP	PB-O2B	2.81	1.64	1.54
9	b	1601	ADP	PB-O2B	2.82	1.64	1.54
9	D	601	ADP	PB-O2B	2.84	1.64	1.54
9	J	601	ADP	PB-O2B	2.87	1.65	1.54
9	f	1601	ADP	PB-O2B	2.88	1.65	1.54
9	P	601	ADP	PB-O2B	2.90	1.65	1.54
9	n	1601	ADP	PB-O2B	2.90	1.65	1.54
9	N	601	ADP	PB-O2B	2.90	1.65	1.54
9	p	1601	ADP	PB-O2B	2.92	1.65	1.54
9	H	601	ADP	PB-O2B	2.93	1.65	1.54
9	M	601	ADP	PB-O2B	2.93	1.65	1.54
9	E	601	ADP	PB-O2B	2.94	1.65	1.54
9	F	601	ADP	PB-O2B	2.97	1.65	1.54
9	l	1601	ADP	PB-O2B	3.00	1.65	1.54
9	k	2101	ADP	PB-O2B	3.01	1.65	1.54
9	e	1601	ADP	PB-O2B	3.01	1.65	1.54
9	L	601	ADP	PB-O2B	3.02	1.65	1.54
9	m	1601	ADP	PB-O2B	3.04	1.65	1.54
9	a	1601	ADP	PB-O2B	3.05	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	601	ADP	PB-O2B	3.16	1.66	1.54
9	g	1601	ADP	PB-O2B	3.17	1.66	1.54
9	G	601	ADP	PB-O2B	3.19	1.66	1.54
9	D	601	ADP	C6-N6	3.32	1.45	1.34
9	E	601	ADP	C6-N6	3.37	1.45	1.34
9	A	601	ADP	C6-N6	3.39	1.45	1.34
9	G	601	ADP	C6-N6	3.39	1.45	1.34
9	g	1601	ADP	C6-N6	3.40	1.45	1.34
9	F	601	ADP	C6-N6	3.41	1.45	1.34
9	a	1601	ADP	C6-N6	3.41	1.45	1.34
9	H	601	ADP	C6-N6	3.44	1.45	1.34
9	N	601	ADP	C6-N6	3.44	1.45	1.34
9	L	601	ADP	C6-N6	3.45	1.45	1.34
9	J	601	ADP	C6-N6	3.45	1.45	1.34
9	C	1101	ADP	C6-N6	3.45	1.45	1.34
9	e	1601	ADP	C6-N6	3.45	1.45	1.34
9	m	1601	ADP	C6-N6	3.46	1.45	1.34
9	b	1601	ADP	C6-N6	3.47	1.45	1.34
9	P	601	ADP	C6-N6	3.48	1.45	1.34
9	M	601	ADP	C6-N6	3.48	1.45	1.34
9	B	601	ADP	C6-N6	3.49	1.45	1.34
9	h	1601	ADP	C6-N6	3.51	1.45	1.34
9	k	2101	ADP	C6-N6	3.51	1.45	1.34
9	n	1601	ADP	C6-N6	3.53	1.45	1.34
9	f	1601	ADP	C6-N6	3.56	1.45	1.34
9	p	1601	ADP	C6-N6	3.56	1.45	1.34
9	l	1601	ADP	C6-N6	3.57	1.46	1.34
9	D	601	ADP	PA-O1A	3.69	1.64	1.51
9	J	601	ADP	PA-O1A	3.71	1.64	1.51
9	p	1601	ADP	PA-O1A	3.72	1.64	1.51
9	L	601	ADP	PA-O1A	3.74	1.64	1.51
9	M	601	ADP	PA-O1A	3.76	1.64	1.51
9	B	601	ADP	PA-O1A	3.76	1.64	1.51
9	l	1601	ADP	PA-O1A	3.76	1.64	1.51
9	e	1601	ADP	PA-O1A	3.77	1.65	1.51
9	m	1601	ADP	PA-O1A	3.78	1.65	1.51
9	b	1601	ADP	PA-O1A	3.79	1.65	1.51
9	n	1601	ADP	PA-O1A	3.81	1.65	1.51
9	f	1601	ADP	PA-O1A	3.81	1.65	1.51
9	E	601	ADP	PA-O1A	3.82	1.65	1.51
9	h	1601	ADP	PA-O1A	3.84	1.65	1.51
9	N	601	ADP	PA-O1A	3.85	1.65	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	1101	ADP	PA-O1A	3.85	1.65	1.51
9	a	1601	ADP	PA-O1A	3.86	1.65	1.51
9	H	601	ADP	PA-O1A	3.86	1.65	1.51
9	g	1601	ADP	PA-O1A	3.88	1.65	1.51
9	P	601	ADP	PA-O1A	3.88	1.65	1.51
9	F	601	ADP	PA-O1A	3.90	1.65	1.51
9	k	2101	ADP	PA-O1A	3.91	1.65	1.51
9	D	601	ADP	PB-O1B	3.98	1.64	1.51
9	A	601	ADP	PA-O1A	4.01	1.65	1.51
9	C	1101	ADP	PB-O1B	4.02	1.64	1.51
9	n	1601	ADP	PB-O1B	4.05	1.64	1.51
9	a	1601	ADP	PB-O1B	4.09	1.64	1.51
9	P	601	ADP	PB-O1B	4.10	1.64	1.51
9	m	1601	ADP	PB-O1B	4.11	1.64	1.51
9	e	1601	ADP	PB-O1B	4.12	1.64	1.51
9	L	601	ADP	PB-O1B	4.13	1.64	1.51
9	H	601	ADP	PB-O1B	4.15	1.64	1.51
9	M	601	ADP	PB-O1B	4.15	1.64	1.51
9	G	601	ADP	PB-O1B	4.16	1.64	1.51
9	G	601	ADP	PA-O1A	4.17	1.66	1.51
9	b	1601	ADP	PB-O1B	4.20	1.65	1.51
9	A	601	ADP	PB-O1B	4.25	1.65	1.51
9	g	1601	ADP	PB-O1B	4.26	1.65	1.51
9	J	601	ADP	PB-O1B	4.27	1.65	1.51
9	B	601	ADP	PB-O1B	4.27	1.65	1.51
9	F	601	ADP	PB-O1B	4.28	1.65	1.51
9	f	1601	ADP	PB-O1B	4.35	1.65	1.51
9	k	2101	ADP	PB-O1B	4.37	1.65	1.51
9	h	1601	ADP	PB-O1B	4.37	1.65	1.51
9	E	601	ADP	PB-O1B	4.37	1.65	1.51
9	l	1601	ADP	PB-O1B	4.38	1.65	1.51
9	N	601	ADP	PB-O1B	4.38	1.65	1.51
9	p	1601	ADP	PB-O1B	4.49	1.65	1.51

All (218) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	J	601	ADP	N3-C2-N1	-12.45	119.36	128.89
9	H	601	ADP	N3-C2-N1	-12.17	119.58	128.89
9	l	1601	ADP	N3-C2-N1	-11.93	119.76	128.89
9	a	1601	ADP	N3-C2-N1	-11.81	119.86	128.89
9	P	601	ADP	N3-C2-N1	-11.67	119.96	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	E	601	ADP	N3-C2-N1	-11.66	119.97	128.89
9	M	601	ADP	N3-C2-N1	-11.63	119.99	128.89
9	C	1101	ADP	N3-C2-N1	-11.63	119.99	128.89
9	k	2101	ADP	N3-C2-N1	-11.58	120.03	128.89
9	L	601	ADP	N3-C2-N1	-11.56	120.04	128.89
9	p	1601	ADP	N3-C2-N1	-11.54	120.06	128.89
9	F	601	ADP	N3-C2-N1	-11.53	120.06	128.89
9	D	601	ADP	N3-C2-N1	-11.52	120.07	128.89
9	h	1601	ADP	N3-C2-N1	-11.49	120.10	128.89
9	B	601	ADP	N3-C2-N1	-11.43	120.14	128.89
9	m	1601	ADP	N3-C2-N1	-11.43	120.14	128.89
9	e	1601	ADP	N3-C2-N1	-11.39	120.17	128.89
9	A	601	ADP	N3-C2-N1	-11.31	120.23	128.89
9	N	601	ADP	N3-C2-N1	-11.25	120.28	128.89
9	f	1601	ADP	N3-C2-N1	-11.15	120.36	128.89
9	n	1601	ADP	N3-C2-N1	-11.11	120.39	128.89
9	G	601	ADP	N3-C2-N1	-10.98	120.49	128.89
9	g	1601	ADP	N3-C2-N1	-10.94	120.52	128.89
9	b	1601	ADP	N3-C2-N1	-10.91	120.54	128.89
9	G	601	ADP	PA-O3A-PB	-6.43	111.12	132.67
9	k	2101	ADP	C4'-O4'-C1'	-5.64	103.53	109.72
9	e	1601	ADP	PA-O3A-PB	-5.56	114.03	132.67
9	E	601	ADP	PA-O3A-PB	-5.54	114.09	132.67
9	a	1601	ADP	PA-O3A-PB	-5.52	114.15	132.67
9	N	601	ADP	PA-O3A-PB	-5.46	114.36	132.67
9	m	1601	ADP	PA-O3A-PB	-5.15	115.39	132.67
9	C	1101	ADP	PA-O3A-PB	-5.06	115.70	132.67
9	f	1601	ADP	PA-O3A-PB	-4.97	116.02	132.67
9	b	1601	ADP	PA-O3A-PB	-4.81	116.55	132.67
9	A	601	ADP	PA-O3A-PB	-4.79	116.60	132.67
9	B	601	ADP	PA-O3A-PB	-4.79	116.62	132.67
9	g	1601	ADP	C2'-C1'-N9	-4.77	107.00	114.29
9	n	1601	ADP	PA-O3A-PB	-4.65	117.06	132.67
9	H	601	ADP	PA-O3A-PB	-4.57	117.35	132.67
9	g	1601	ADP	PA-O3A-PB	-4.55	117.40	132.67
9	G	601	ADP	C2'-C1'-N9	-4.54	107.36	114.29
9	l	1601	ADP	PA-O3A-PB	-4.48	117.64	132.67
9	J	601	ADP	PA-O3A-PB	-4.31	118.20	132.67
9	P	601	ADP	PA-O3A-PB	-4.27	118.35	132.67
9	F	601	ADP	PA-O3A-PB	-4.22	118.52	132.67
9	L	601	ADP	PA-O3A-PB	-4.16	118.72	132.67
9	M	601	ADP	C4'-O4'-C1'	-4.08	105.24	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	k	2101	ADP	PA-O3A-PB	-4.04	119.11	132.67
9	A	601	ADP	C4'-O4'-C1'	-4.01	105.31	109.72
9	p	1601	ADP	PA-O3A-PB	-3.70	120.26	132.67
9	a	1601	ADP	C4'-O4'-C1'	-3.53	105.84	109.72
9	h	1601	ADP	PA-O3A-PB	-3.50	120.93	132.67
9	k	2101	ADP	C2'-C1'-N9	-3.49	108.96	114.29
9	M	601	ADP	PA-O3A-PB	-3.44	121.12	132.67
9	D	601	ADP	PA-O3A-PB	-3.43	121.17	132.67
9	G	601	ADP	C4'-O4'-C1'	-3.38	106.01	109.72
9	f	1601	ADP	C2'-C1'-N9	-3.31	109.23	114.29
9	P	601	ADP	C2'-C1'-N9	-3.28	109.27	114.29
9	A	601	ADP	C2'-C1'-N9	-3.28	109.28	114.29
9	J	601	ADP	C2'-C1'-N9	-3.26	109.31	114.29
9	E	601	ADP	C2'-C1'-N9	-3.18	109.43	114.29
9	n	1601	ADP	C2'-C1'-N9	-3.13	109.52	114.29
9	B	601	ADP	C2'-C1'-N9	-3.09	109.58	114.29
9	p	1601	ADP	O4'-C4'-C3'	-2.95	99.20	105.15
9	J	601	ADP	C4'-O4'-C1'	-2.93	106.50	109.72
9	P	601	ADP	O4'-C4'-C3'	-2.85	99.40	105.15
9	f	1601	ADP	C4'-O4'-C1'	-2.83	106.61	109.72
9	P	601	ADP	C4'-O4'-C1'	-2.80	106.64	109.72
9	e	1601	ADP	C2'-C1'-N9	-2.80	110.02	114.29
9	F	601	ADP	C2'-C1'-N9	-2.78	110.05	114.29
9	b	1601	ADP	O4'-C4'-C3'	-2.63	99.84	105.15
9	h	1601	ADP	O4'-C4'-C3'	-2.62	99.87	105.15
9	G	601	ADP	O4'-C4'-C3'	-2.58	99.96	105.15
9	l	1601	ADP	C2'-C1'-N9	-2.47	110.51	114.29
9	B	601	ADP	C4'-O4'-C1'	-2.39	107.10	109.72
9	n	1601	ADP	C4'-O4'-C1'	-2.38	107.10	109.72
9	J	601	ADP	O4'-C4'-C3'	-2.32	100.47	105.15
9	b	1601	ADP	C4'-O4'-C1'	-2.30	107.19	109.72
9	g	1601	ADP	C4'-O4'-C1'	-2.29	107.21	109.72
9	H	601	ADP	O4'-C4'-C3'	-2.27	100.58	105.15
9	H	601	ADP	C2'-C1'-N9	-2.26	110.84	114.29
9	g	1601	ADP	O4'-C4'-C3'	-2.25	100.61	105.15
9	F	601	ADP	C4'-O4'-C1'	-2.20	107.30	109.72
9	p	1601	ADP	C4'-O4'-C1'	-2.18	107.32	109.72
9	N	601	ADP	C4-C5-N7	-2.17	107.48	109.48
9	a	1601	ADP	C2'-C1'-N9	-2.14	111.02	114.29
9	b	1601	ADP	C2'-C1'-N9	-2.14	111.03	114.29
9	n	1601	ADP	C4-C5-N7	-2.11	107.53	109.48
9	m	1601	ADP	C4-C5-N7	-2.08	107.57	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	p	1601	ADP	C4-C5-N7	-2.01	107.63	109.48
9	h	1601	ADP	O2'-C2'-C3'	2.01	118.37	111.83
9	h	1601	ADP	O5'-C5'-C4'	2.05	116.66	109.12
9	E	601	ADP	O5'-C5'-C4'	2.05	116.67	109.12
9	g	1601	ADP	O5'-C5'-C4'	2.07	116.73	109.12
9	k	2101	ADP	O2'-C2'-C3'	2.07	118.55	111.83
9	G	601	ADP	O2'-C2'-C3'	2.07	118.55	111.83
9	B	601	ADP	O2'-C2'-C3'	2.10	118.65	111.83
9	e	1601	ADP	O5'-C5'-C4'	2.12	116.94	109.12
9	G	601	ADP	O3'-C3'-C2'	2.13	118.75	111.83
9	F	601	ADP	O3'-C3'-C4'	2.13	117.44	111.05
9	n	1601	ADP	O5'-C5'-C4'	2.13	116.98	109.12
9	N	601	ADP	O2'-C2'-C3'	2.16	118.84	111.83
9	G	601	ADP	O5'-C5'-C4'	2.16	117.07	109.12
9	p	1601	ADP	O5'-C5'-C4'	2.17	117.13	109.12
9	p	1601	ADP	O2'-C2'-C3'	2.18	118.90	111.83
9	P	601	ADP	O2'-C2'-C3'	2.18	118.92	111.83
9	H	601	ADP	O2'-C2'-C3'	2.21	119.00	111.83
9	D	601	ADP	O3'-C3'-C2'	2.21	119.02	111.83
9	A	601	ADP	O3'-C3'-C2'	2.23	119.09	111.83
9	L	601	ADP	O3'-C3'-C2'	2.25	119.15	111.83
9	D	601	ADP	O2'-C2'-C3'	2.28	119.23	111.83
9	P	601	ADP	O5'-C5'-C4'	2.28	117.52	109.12
9	a	1601	ADP	O3A-PA-O5'	2.28	108.98	102.94
9	P	601	ADP	O4'-C4'-C5'	2.29	117.53	109.32
9	m	1601	ADP	O3A-PA-O5'	2.30	109.03	102.94
9	a	1601	ADP	O3'-C3'-C2'	2.33	119.41	111.83
9	a	1601	ADP	O2'-C2'-C3'	2.34	119.42	111.83
9	A	601	ADP	O3A-PA-O5'	2.38	109.24	102.94
9	m	1601	ADP	O5'-C5'-C4'	2.38	117.88	109.12
9	J	601	ADP	O3'-C3'-C2'	2.38	119.57	111.83
9	g	1601	ADP	O3'-C3'-C2'	2.39	119.59	111.83
9	e	1601	ADP	O2'-C2'-C3'	2.39	119.60	111.83
9	k	2101	ADP	O3'-C3'-C2'	2.42	119.68	111.83
9	p	1601	ADP	O4'-C4'-C5'	2.42	117.98	109.32
9	F	601	ADP	O3A-PA-O5'	2.42	109.36	102.94
9	k	2101	ADP	O3A-PA-O5'	2.44	109.40	102.94
9	C	1101	ADP	O3'-C3'-C2'	2.44	119.76	111.83
9	H	601	ADP	O3'-C3'-C2'	2.46	119.82	111.83
9	N	601	ADP	O4'-C1'-N9	2.47	113.28	108.10
9	C	1101	ADP	O3'-C3'-C4'	2.47	118.47	111.05
9	b	1601	ADP	O2'-C2'-C3'	2.48	119.89	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	P	601	ADP	O3'-C3'-C2'	2.49	119.92	111.83
9	g	1601	ADP	O3'-C3'-C4'	2.50	118.55	111.05
9	A	601	ADP	O2'-C2'-C3'	2.51	120.00	111.83
9	b	1601	ADP	O3'-C3'-C2'	2.52	120.03	111.83
9	h	1601	ADP	O4'-C4'-C5'	2.54	118.40	109.32
9	l	1601	ADP	O3A-PA-O5'	2.55	109.70	102.94
9	L	601	ADP	O5'-C5'-C4'	2.56	118.55	109.12
9	G	601	ADP	O3'-C3'-C4'	2.59	118.82	111.05
9	P	601	ADP	O3A-PA-O5'	2.59	109.82	102.94
9	h	1601	ADP	O3A-PA-O5'	2.59	109.82	102.94
9	L	601	ADP	O3'-C3'-C4'	2.61	118.89	111.05
9	e	1601	ADP	O3'-C3'-C2'	2.61	120.33	111.83
9	a	1601	ADP	O5'-C5'-C4'	2.63	118.80	109.12
9	N	601	ADP	O3'-C3'-C2'	2.63	120.38	111.83
9	J	601	ADP	O2'-C2'-C3'	2.64	120.41	111.83
9	f	1601	ADP	O3'-C3'-C2'	2.64	120.42	111.83
9	a	1601	ADP	O3'-C3'-C4'	2.65	118.99	111.05
9	F	601	ADP	O2'-C2'-C3'	2.65	120.44	111.83
9	h	1601	ADP	O3'-C3'-C2'	2.66	120.47	111.83
9	M	601	ADP	O3'-C3'-C2'	2.66	120.47	111.83
9	L	601	ADP	O2'-C2'-C3'	2.67	120.52	111.83
9	L	601	ADP	O3A-PA-O5'	2.68	110.04	102.94
9	f	1601	ADP	O4'-C1'-N9	2.69	113.72	108.10
9	l	1601	ADP	O3'-C3'-C2'	2.71	120.64	111.83
9	D	601	ADP	O3'-C3'-C4'	2.72	119.22	111.05
9	b	1601	ADP	O3A-PA-O5'	2.74	110.21	102.94
9	E	601	ADP	O2'-C2'-C3'	2.77	120.85	111.83
9	l	1601	ADP	O5'-C5'-C4'	2.78	119.37	109.12
9	C	1101	ADP	O4'-C4'-C5'	2.79	119.28	109.32
9	M	601	ADP	O3A-PA-O5'	2.79	110.35	102.94
9	F	601	ADP	O4'-C4'-C5'	2.80	119.35	109.32
9	m	1601	ADP	O3'-C3'-C2'	2.81	120.97	111.83
9	L	601	ADP	O4'-C4'-C5'	2.81	119.38	109.32
9	M	601	ADP	O5'-C5'-C4'	2.82	119.50	109.12
9	l	1601	ADP	O2'-C2'-C3'	2.86	121.11	111.83
9	p	1601	ADP	O3A-PA-O5'	2.86	110.52	102.94
9	e	1601	ADP	O4'-C4'-C5'	2.86	119.56	109.32
9	N	601	ADP	O5'-C5'-C4'	2.88	119.73	109.12
9	E	601	ADP	O4'-C4'-C5'	2.89	119.67	109.32
9	h	1601	ADP	O3'-C3'-C4'	2.90	119.75	111.05
9	A	601	ADP	O5'-C5'-C4'	2.90	119.81	109.12
9	n	1601	ADP	O3'-C3'-C4'	2.91	119.77	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	N	601	ADP	O4'-C4'-C5'	2.91	119.74	109.32
9	J	601	ADP	O3A-PA-O5'	2.94	110.74	102.94
9	n	1601	ADP	O3A-PA-O5'	2.95	110.75	102.94
9	E	601	ADP	O3'-C3'-C2'	2.95	121.43	111.83
9	m	1601	ADP	O4'-C4'-C5'	2.96	119.92	109.32
9	b	1601	ADP	O3'-C3'-C4'	2.97	119.95	111.05
9	e	1601	ADP	O3'-C3'-C4'	2.99	120.03	111.05
9	P	601	ADP	O3'-C3'-C4'	3.00	120.05	111.05
9	n	1601	ADP	O3'-C3'-C2'	3.00	121.59	111.83
9	J	601	ADP	O3'-C3'-C4'	3.01	120.08	111.05
9	b	1601	ADP	O4'-C4'-C5'	3.03	120.16	109.32
9	B	601	ADP	O4'-C4'-C5'	3.06	120.27	109.32
9	l	1601	ADP	O3'-C3'-C4'	3.07	120.25	111.05
9	k	2101	ADP	O3'-C3'-C4'	3.07	120.26	111.05
9	A	601	ADP	O4'-C4'-C5'	3.09	120.37	109.32
9	l	1601	ADP	O4'-C4'-C5'	3.09	120.37	109.32
9	B	601	ADP	O3A-PA-O5'	3.10	111.16	102.94
9	b	1601	ADP	O5'-C5'-C4'	3.16	120.78	109.12
9	p	1601	ADP	O3'-C3'-C2'	3.17	122.13	111.83
9	F	601	ADP	O5'-C5'-C4'	3.18	120.85	109.12
9	B	601	ADP	O5'-C5'-C4'	3.19	120.90	109.12
9	J	601	ADP	O5'-C5'-C4'	3.23	121.01	109.12
9	n	1601	ADP	O4'-C4'-C5'	3.24	120.89	109.32
9	M	601	ADP	O3'-C3'-C4'	3.24	120.77	111.05
9	p	1601	ADP	O3'-C3'-C4'	3.27	120.87	111.05
9	H	601	ADP	O3'-C3'-C4'	3.28	120.88	111.05
9	J	601	ADP	O4'-C4'-C5'	3.29	121.07	109.32
9	G	601	ADP	O4'-C4'-C5'	3.29	121.10	109.32
9	g	1601	ADP	O4'-C4'-C5'	3.30	121.12	109.32
9	D	601	ADP	O3A-PA-O5'	3.32	111.75	102.94
9	N	601	ADP	O3A-PA-O5'	3.32	111.75	102.94
9	m	1601	ADP	O3'-C3'-C4'	3.39	121.22	111.05
9	M	601	ADP	O4'-C4'-C5'	3.39	121.45	109.32
9	N	601	ADP	O3'-C3'-C4'	3.45	121.39	111.05
9	f	1601	ADP	O3A-PA-O5'	3.46	112.12	102.94
9	f	1601	ADP	O5'-C5'-C4'	3.51	122.05	109.12
9	B	601	ADP	O3'-C3'-C4'	3.51	121.59	111.05
9	f	1601	ADP	O3'-C3'-C4'	3.52	121.60	111.05
9	A	601	ADP	O3'-C3'-C4'	3.52	121.62	111.05
9	f	1601	ADP	O4'-C4'-C5'	3.53	121.95	109.32
9	k	2101	ADP	O4'-C4'-C5'	3.61	122.25	109.32
9	a	1601	ADP	O4'-C4'-C5'	3.62	122.28	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	D	601	ADP	O5'-C5'-C4'	3.74	122.90	109.12
9	D	601	ADP	O4'-C4'-C5'	3.80	122.90	109.32
9	E	601	ADP	O3'-C3'-C4'	3.99	123.03	111.05

All (34) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	J	601	ADP	C4'
9	J	601	ADP	C3'
9	a	1601	ADP	C4'
9	a	1601	ADP	C3'
9	P	601	ADP	C4'
9	n	1601	ADP	C2'
9	m	1601	ADP	C4'
9	m	1601	ADP	C3'
9	p	1601	ADP	C4'
9	A	601	ADP	C4'
9	A	601	ADP	C3'
9	e	1601	ADP	C4'
9	e	1601	ADP	C3'
9	g	1601	ADP	C3'
9	b	1601	ADP	C4'
9	b	1601	ADP	C3'
9	B	601	ADP	C4'
9	B	601	ADP	C3'
9	H	601	ADP	C4'
9	M	601	ADP	C4'
9	M	601	ADP	C3'
9	C	1101	ADP	C4'
9	C	1101	ADP	C3'
9	N	601	ADP	C2'
9	N	601	ADP	C3'
9	D	601	ADP	C4'
9	D	601	ADP	C3'
9	E	601	ADP	C4'
9	G	601	ADP	C3'
9	f	1601	ADP	C2'
9	f	1601	ADP	C3'
9	h	1601	ADP	C4'
9	k	2101	ADP	C4'
9	k	2101	ADP	C3'

There are no torsion outliers.

There are no ring outliers.

17 monomers are involved in 79 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	601	ADP	3	0
9	B	601	ADP	8	0
9	C	1101	ADP	7	0
10	C	1102	BEF	3	0
9	D	601	ADP	8	0
9	E	601	ADP	2	0
9	F	601	ADP	6	0
10	F	602	BEF	2	0
9	G	601	ADP	5	0
9	H	601	ADP	3	0
9	J	601	ADP	5	0
9	L	601	ADP	7	0
10	L	602	BEF	1	0
9	M	601	ADP	6	0
9	N	601	ADP	6	0
10	N	602	BEF	3	0
9	P	601	ADP	5	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 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, 95^{th} 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	544/559 (97%)	0.03	13 (2%) 62 46	72, 134, 206, 254	0
1	I	544/559 (97%)	0.05	26 (4%) 34 22	72, 134, 206, 254	0
1	a	544/559 (97%)	-0.06	15 (2%) 56 40	72, 134, 206, 254	0
1	i	544/559 (97%)	-0.03	14 (2%) 59 43	72, 134, 206, 254	0
2	B	513/527 (97%)	-0.08	5 (0%) 84 72	47, 120, 192, 236	0
2	J	513/527 (97%)	0.08	19 (3%) 45 30	47, 120, 192, 236	0
2	b	513/527 (97%)	-0.07	10 (1%) 70 54	47, 120, 192, 236	0
2	j	513/527 (97%)	-0.06	7 (1%) 78 63	47, 120, 192, 236	0
3	C	514/590 (87%)	0.09	10 (1%) 70 54	73, 141, 205, 295	0
3	K	514/590 (87%)	0.04	19 (3%) 45 30	73, 141, 205, 295	0
3	c	514/590 (87%)	0.06	18 (3%) 48 32	73, 141, 205, 295	0
3	k	514/590 (87%)	-0.05	11 (2%) 67 51	73, 141, 205, 295	0
4	D	522/528 (98%)	0.03	15 (2%) 55 38	70, 149, 232, 297	0
4	L	522/528 (98%)	0.10	27 (5%) 31 21	70, 149, 232, 297	0
4	d	522/528 (98%)	0.04	15 (2%) 55 38	70, 149, 232, 297	0
4	l	522/528 (98%)	0.12	22 (4%) 40 26	70, 149, 232, 297	0
5	E	525/562 (93%)	0.08	17 (3%) 51 35	56, 138, 238, 297	0
5	M	525/562 (93%)	0.25	34 (6%) 22 13	56, 138, 238, 297	0
5	e	525/562 (93%)	0.05	21 (4%) 42 28	56, 138, 238, 297	0
5	m	525/562 (93%)	-0.03	16 (3%) 54 37	56, 138, 238, 297	0
6	F	533/546 (97%)	0.13	27 (5%) 32 21	42, 116, 214, 301	0
6	N	533/546 (97%)	0.08	19 (3%) 46 32	42, 116, 214, 301	0
6	f	533/546 (97%)	0.10	20 (3%) 44 30	42, 116, 214, 301	0
6	n	533/546 (97%)	0.08	21 (3%) 43 29	42, 116, 214, 301	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
7	G	509/550 (92%)	0.06	13 (2%)	59	43	65, 136, 207, 264	0
7	O	509/550 (92%)	0.16	24 (4%)	35	23	65, 136, 207, 264	0
7	g	509/550 (92%)	-0.02	16 (3%)	52	36	65, 136, 207, 264	0
7	o	509/550 (92%)	0.12	23 (4%)	37	24	65, 136, 207, 264	0
8	H	525/568 (92%)	0.04	11 (2%)	67	51	70, 148, 236, 294	0
8	P	525/568 (92%)	0.29	38 (7%)	18	11	70, 148, 236, 294	0
8	h	525/568 (92%)	0.18	28 (5%)	30	20	70, 148, 236, 294	0
8	p	525/568 (92%)	0.14	27 (5%)	32	21	70, 148, 236, 294	0
All	All	16740/17720 (94%)	0.06	601 (3%)	46	32	42, 136, 217, 301	0

All (601) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	e	1387	THR	13.8
5	M	387	THR	12.1
7	o	1228	GLY	11.4
5	m	1387	THR	10.0
6	n	1539	SER	8.8
1	a	1552	PRO	8.8
5	e	1388	THR	8.2
6	F	223	ASP	8.2
5	m	1398	SER	7.9
4	D	283	CYS	7.6
6	n	1001	MET	7.3
6	F	539	SER	7.2
7	O	530	GLU	6.8
6	N	223	ASP	6.3
5	M	388	THR	6.1
4	L	251	ASN	6.0
6	n	1466	PRO	6.0
1	I	556	PRO	5.8
7	o	1227	ALA	5.7
4	L	292	ILE	5.6
6	F	187	ASP	5.6
7	G	228	GLY	5.6
6	n	1467	LEU	5.6
7	o	1207	GLY	5.5
5	m	1358	THR	5.5
4	L	252	ILE	5.4

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Mol	Chain	Res	Type	RSRZ
6	n	1002	SER	5.4
5	M	249	PHE	5.4
6	f	1487	ARG	5.4
1	a	1342	SER	5.4
1	I	14	PHE	5.3
6	N	487	ARG	5.3
7	O	371	ALA	5.3
3	K	258	GLN	5.2
6	f	1465	ASP	5.2
4	l	1284	ASN	5.2
7	O	373	THR	5.1
1	i	1146	THR	5.1
3	K	257	SER	5.0
1	a	1341	MET	5.0
6	F	368	THR	5.0
5	M	169	SER	5.0
7	g	1371	ALA	4.9
4	l	1374	THR	4.9
8	P	235	HIS	4.9
7	O	529	SER	4.8
6	f	1466	PRO	4.8
1	I	186	ALA	4.8
6	n	1372	ASP	4.8
7	O	372	LYS	4.8
4	L	298	ASN	4.8
4	D	364	THR	4.7
1	A	15	LEU	4.7
4	D	374	THR	4.7
8	p	1379	SER	4.7
5	e	1509	ASN	4.6
5	e	1166	ASP	4.6
3	C	484	ILE	4.6
4	d	1298	ASN	4.5
7	g	1370	GLN	4.4
6	F	540	THR	4.4
8	P	138	THR	4.4
7	G	369	PRO	4.4
1	i	1149	ASP	4.4
7	O	228	GLY	4.4
6	N	252	PHE	4.4
1	a	1553	LYS	4.3
4	l	1283	CYS	4.3

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Mol	Chain	Res	Type	RSRZ
3	C	483	GLY	4.3
3	C	500	TRP	4.3
5	M	164	THR	4.3
3	c	1351	ASN	4.3
6	N	544	THR	4.3
6	F	467	LEU	4.3
5	M	398	SER	4.3
2	j	1294	PRO	4.3
1	I	555	ASP	4.3
8	P	355	VAL	4.3
6	F	468	ASP	4.2
5	E	381	TYR	4.2
5	e	1290	SER	4.2
4	L	364	THR	4.2
8	p	1006	PRO	4.2
8	P	336	CYS	4.2
6	n	1544	THR	4.1
4	D	291	SER	4.1
5	m	1388	THR	4.1
4	L	283	CYS	4.1
7	O	370	GLN	4.1
8	P	321	LEU	4.1
4	L	291	SER	4.0
7	G	227	ALA	4.0
6	F	487	ARG	4.0
5	M	410	GLY	4.0
8	P	300	VAL	4.0
4	l	1257	TYR	4.0
8	h	1370	VAL	4.0
8	P	248	ALA	4.0
5	e	1291	SER	3.9
6	F	466	PRO	3.9
1	I	380	HIS	3.9
1	I	557	HIS	3.9
3	K	362	ASP	3.9
1	I	270	LEU	3.9
5	m	1217	LYS	3.9
3	C	485	ASP	3.8
2	J	282	ASN	3.8
4	L	373	PRO	3.8
5	e	1289	ILE	3.8
8	P	268	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
4	l	1298	ASN	3.8
5	M	514	CYS	3.8
8	P	257	ALA	3.8
6	n	1223	ASP	3.8
6	N	539	SER	3.7
4	L	284	ASN	3.7
2	J	249	LYS	3.7
5	M	386	GLY	3.7
4	L	253	ILE	3.7
6	N	1	MET	3.7
6	F	225	PRO	3.7
6	N	368	THR	3.7
4	L	297	VAL	3.7
8	H	370	VAL	3.7
1	a	1554	GLU	3.6
4	L	219	ALA	3.6
4	d	1480	ASP	3.6
3	c	1146	GLU	3.6
7	o	1530	GLU	3.6
5	m	1168	ILE	3.6
6	f	1186	ALA	3.6
3	c	1336	ILE	3.5
3	c	1370	ASN	3.5
4	L	293	LEU	3.5
5	M	349	GLN	3.5
7	o	1165	ALA	3.5
6	N	468	ASP	3.5
8	P	267	LEU	3.5
8	h	1249	VAL	3.5
8	H	149	GLU	3.5
4	l	1297	VAL	3.5
3	c	1365	PHE	3.5
4	D	163	VAL	3.5
2	J	250	PHE	3.5
1	I	264	ILE	3.5
2	J	490	SER	3.5
3	k	1500	TRP	3.4
4	L	363	VAL	3.4
4	l	1163	VAL	3.4
8	p	1336	CYS	3.4
5	M	358	THR	3.4
6	F	188	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
8	P	483	ASN	3.4
4	D	222	SER	3.4
2	J	478	THR	3.4
4	L	528	ARG	3.4
7	o	1223	THR	3.4
5	m	1167	ASP	3.4
6	n	1142	ASN	3.4
8	h	1329	LEU	3.4
4	l	1162	ILE	3.4
3	C	186	LEU	3.4
1	I	16	GLY	3.4
5	m	1359	ASN	3.4
1	I	554	GLU	3.3
7	G	368	CYS	3.3
8	h	1258	ASN	3.3
6	f	1248	ASN	3.3
7	O	263	HIS	3.3
6	f	1222	PRO	3.3
5	M	451	SER	3.3
8	p	1322	LYS	3.3
1	I	266	ASP	3.3
6	n	1187	ASP	3.3
8	p	1455	ALA	3.3
8	p	1249	VAL	3.3
8	P	234	GLY	3.3
6	f	1254	SER	3.3
3	c	1260	ASN	3.3
6	F	372	ASP	3.3
6	N	365	THR	3.3
8	p	1372	LYS	3.3
3	K	359	MET	3.3
3	c	1264	GLU	3.3
1	I	146	THR	3.3
1	I	15	LEU	3.3
7	g	1167	SER	3.3
5	e	1386	GLY	3.2
1	I	552	PRO	3.2
6	f	1223	ASP	3.2
4	d	1188	ASN	3.2
4	D	298	ASN	3.2
5	e	1231	GLY	3.2
3	c	1269	TRP	3.2

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Mol	Chain	Res	Type	RSRZ
3	c	1369	ASP	3.2
1	a	1263	ASN	3.2
7	g	1016	GLY	3.2
2	b	1282	ASN	3.2
1	I	338	VAL	3.2
4	L	312	VAL	3.2
2	j	1419	ALA	3.2
8	p	1321	LEU	3.2
3	k	1012	GLN	3.1
8	h	1155	ASP	3.1
7	O	227	ALA	3.1
8	p	1378	ILE	3.1
7	o	1166	MET	3.1
2	b	1283	THR	3.1
1	a	1226	CYS	3.1
4	l	1296	ALA	3.1
5	M	166	ASP	3.1
5	E	218	ASP	3.1
6	f	1461	ASN	3.1
7	g	1166	MET	3.1
6	f	1187	ASP	3.1
4	l	1007	SER	3.1
4	L	311	MET	3.1
8	h	1330	ARG	3.1
1	I	553	LYS	3.1
8	P	275	ASP	3.0
1	a	1557	HIS	3.0
7	g	1252	ALA	3.0
4	l	1219	ALA	3.0
1	A	146	THR	3.0
2	J	303	ILE	3.0
7	O	264	VAL	3.0
8	p	1300	VAL	3.0
2	J	252	VAL	3.0
4	d	1255	ASN	3.0
6	N	355	TYR	3.0
5	E	357	SER	3.0
8	h	1227	VAL	3.0
1	I	185	LEU	3.0
7	o	1017	THR	3.0
6	n	1465	ASP	3.0
3	K	331	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
8	P	269	ASN	3.0
3	c	1265	LYS	3.0
3	K	218	ARG	2.9
4	D	330	CYS	2.9
1	I	340	SER	2.9
3	k	1384	GLY	2.9
3	C	145	VAL	2.9
8	h	1372	LYS	2.9
3	K	223	VAL	2.9
5	E	362	ILE	2.9
5	e	1288	ASP	2.9
6	F	227	ARG	2.9
8	H	298	CYS	2.9
6	f	1372	ASP	2.9
7	g	1223	THR	2.9
8	H	450	LYS	2.9
7	o	1220	PHE	2.9
8	p	1236	VAL	2.9
7	G	337	THR	2.9
6	F	541	LEU	2.9
5	E	295	TYR	2.8
6	F	375	SER	2.8
1	I	371	CYS	2.8
3	k	1184	LYS	2.8
6	f	1001	MET	2.8
2	J	398	THR	2.8
6	F	226	THR	2.8
1	i	1317	GLY	2.8
1	i	1186	ALA	2.8
3	K	256	GLU	2.8
7	g	1165	ALA	2.8
5	m	1323	CYS	2.8
2	J	400	THR	2.8
5	M	512	VAL	2.8
6	F	324	ASN	2.8
6	F	346	GLN	2.8
4	l	1291	SER	2.8
7	O	259	VAL	2.8
4	l	1251	ASN	2.8
8	P	330	ARG	2.8
2	B	51	SER	2.8
2	B	218	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
8	H	235	HIS	2.8
3	C	41	PRO	2.8
2	b	1232	LEU	2.8
1	a	1555	ASP	2.8
5	m	1215	ASP	2.8
5	m	1386	GLY	2.8
4	L	348	ASP	2.8
4	D	284	ASN	2.7
7	O	306	PHE	2.8
4	L	296	ALA	2.7
8	h	1150	ILE	2.7
1	i	1552	PRO	2.7
3	k	1243	VAL	2.7
7	G	294	LEU	2.7
8	h	1490	VAL	2.7
7	O	461	ALA	2.7
3	k	1144	ASP	2.7
1	A	380	HIS	2.7
7	o	1480	GLY	2.7
3	k	1185	ASP	2.7
1	I	293	ALA	2.7
6	n	1461	ASN	2.7
6	F	544	THR	2.7
1	A	14	PHE	2.7
3	K	16	THR	2.7
5	m	1031	ILE	2.7
4	l	1437	ALA	2.7
1	I	262	ILE	2.7
5	e	1264	SER	2.7
1	a	1551	PRO	2.7
5	M	520	ASN	2.7
8	h	1373	GLN	2.7
5	M	170	ALA	2.6
7	g	1241	ILE	2.6
8	h	1151	THR	2.6
4	l	1370	ASN	2.6
6	n	1324	ASN	2.6
6	N	383	SER	2.6
6	n	1346	GLN	2.6
8	P	427	GLU	2.6
5	e	1230	VAL	2.6
5	e	1398	SER	2.6

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Mol	Chain	Res	Type	RSRZ
6	f	1249	SER	2.6
8	h	1489	ALA	2.6
3	K	363	GLU	2.6
8	h	1226	MET	2.6
5	M	67	PRO	2.6
8	p	1373	GLN	2.6
4	D	370	ASN	2.6
7	g	1355	MET	2.6
8	p	1368	VAL	2.6
1	i	1342	SER	2.6
8	P	296	VAL	2.6
6	F	465	ASP	2.6
8	h	1379	SER	2.6
1	A	304	ASP	2.6
1	a	1346	GLY	2.6
3	K	25	ILE	2.6
3	K	159	ILE	2.6
4	l	1367	ARG	2.6
5	E	387	THR	2.6
1	I	265	ASP	2.6
4	L	527	SER	2.6
6	f	1540	THR	2.6
8	P	320	VAL	2.6
8	h	1389	ALA	2.5
7	G	111	GLU	2.5
8	p	1428	ILE	2.5
5	M	403	THR	2.5
8	p	1369	THR	2.5
2	B	192	HIS	2.5
3	c	1331	VAL	2.5
2	j	1190	LEU	2.5
3	K	207	GLU	2.5
6	f	1431	MET	2.5
8	H	267	LEU	2.5
7	G	349	CYS	2.5
3	c	1350	THR	2.5
5	M	497	THR	2.5
7	O	336	SER	2.5
8	p	1250	PHE	2.5
6	f	1002	SER	2.5
7	G	432	ALA	2.5
3	c	1248	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
8	P	298	CYS	2.5
8	P	25	ASP	2.5
4	D	162	ILE	2.5
4	L	295	ASP	2.5
4	d	1481	GLY	2.5
6	N	465	ASP	2.5
8	P	369	THR	2.5
8	P	382	SER	2.5
3	k	1483	GLY	2.5
6	N	467	LEU	2.5
5	E	173	ASP	2.5
1	A	186	ALA	2.5
6	n	1295	ILE	2.5
3	c	1186	LEU	2.4
2	J	251	LYS	2.4
1	A	208	ALA	2.4
1	i	1369	ASP	2.4
3	K	380	MET	2.4
6	F	355	TYR	2.4
8	p	1248	ALA	2.4
6	N	317	LEU	2.4
3	C	144	ASP	2.4
5	e	1232	GLY	2.4
8	P	265	VAL	2.4
1	a	1264	ILE	2.4
2	J	189	ASN	2.4
4	L	255	ASN	2.4
8	H	215	GLY	2.4
1	a	1261	GLN	2.4
2	J	190	LEU	2.4
4	d	1312	VAL	2.4
7	o	1380	GLY	2.4
1	a	1556	PRO	2.4
5	e	1175	LEU	2.4
5	M	559	LYS	2.4
8	h	1380	ARG	2.4
7	o	1242	LEU	2.4
8	h	1149	GLU	2.4
6	F	347	ILE	2.4
8	P	489	ALA	2.4
4	D	363	VAL	2.4
5	M	476	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
5	E	509	ASN	2.4
5	e	1214	LYS	2.4
6	N	228	VAL	2.4
1	i	1239	GLY	2.4
8	P	354	LEU	2.4
3	C	295	VAL	2.4
1	i	1244	ILE	2.3
3	C	159	ILE	2.3
3	c	1263	ILE	2.3
5	M	114	GLU	2.3
8	H	389	ALA	2.3
5	M	513	ASP	2.3
2	j	1371	GLY	2.3
6	F	486	THR	2.3
7	O	342	LYS	2.3
7	o	1311	ASN	2.3
7	O	241	ILE	2.3
5	E	217	LYS	2.3
6	f	1227	ARG	2.3
3	k	1229	VAL	2.3
7	g	1230	GLU	2.3
4	l	1431	SER	2.3
7	o	1325	ARG	2.3
4	L	220	ILE	2.3
6	F	366	TYR	2.3
7	o	1481	VAL	2.3
3	K	158	SER	2.3
5	M	264	SER	2.3
6	N	303	PRO	2.3
6	n	1226	THR	2.3
7	O	262	GLU	2.3
5	e	1115	ILE	2.3
5	e	1249	PHE	2.3
1	A	187	VAL	2.3
7	O	234	LYS	2.3
2	b	1198	ILE	2.3
5	m	1030	ILE	2.3
1	A	381	SER	2.3
8	P	301	ALA	2.3
2	J	281	ILE	2.3
2	J	325	VAL	2.3
5	E	166	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
5	E	167	ASP	2.3
7	o	1016	GLY	2.3
1	a	1293	ALA	2.3
6	F	221	HIS	2.3
4	d	1162	ILE	2.3
1	I	316	MET	2.3
2	J	277	SER	2.3
4	d	1253	ILE	2.3
7	O	335	GLN	2.3
7	O	341	ILE	2.3
8	h	1382	SER	2.3
1	I	93	GLU	2.3
4	d	1198	LYS	2.3
4	l	1213	VAL	2.3
1	I	90	GLN	2.3
2	b	1248	THR	2.3
7	o	1178	PHE	2.3
7	G	526	ASN	2.2
8	h	1280	GLU	2.2
1	A	259	GLY	2.2
7	G	216	ASN	2.2
6	N	187	ASP	2.2
7	o	1370	GLN	2.2
4	L	443	PHE	2.2
4	d	1189	VAL	2.2
8	H	240	SER	2.2
8	H	249	VAL	2.2
4	L	140	HIS	2.2
2	j	1254	SER	2.2
6	F	383	SER	2.2
7	O	243	SER	2.2
7	g	1262	GLU	2.2
8	p	1483	ASN	2.2
2	J	248	THR	2.2
7	G	370	GLN	2.2
5	E	410	GLY	2.2
3	c	1500	TRP	2.2
3	K	328	ILE	2.2
8	h	1299	ILE	2.2
7	o	1167	SER	2.2
1	i	1557	HIS	2.2
6	n	1213	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
8	h	1264	THR	2.2
8	p	1370	VAL	2.2
1	I	226	CYS	2.2
5	m	1164	THR	2.2
5	m	1514	CYS	2.2
1	A	488	LYS	2.2
6	n	1225	PRO	2.2
2	B	469	THR	2.2
2	B	209	ASP	2.2
8	P	169	SER	2.2
4	l	1223	ALA	2.2
5	M	255	PRO	2.2
8	h	1215	GLY	2.2
2	b	1249	LYS	2.2
5	M	250	SER	2.2
4	D	373	PRO	2.2
5	E	252	PRO	2.2
7	O	178	PHE	2.2
6	f	1296	ILE	2.2
7	O	346	LEU	2.2
8	P	319	LEU	2.2
7	g	1097	GLY	2.2
8	P	504	GLU	2.2
6	f	1142	ASN	2.2
8	p	1005	LEU	2.2
5	E	168	ILE	2.1
2	b	1478	THR	2.1
5	M	167	ASP	2.1
4	D	168	SER	2.1
3	K	436	GLY	2.1
4	l	1373	PRO	2.1
7	g	1529	SER	2.1
5	M	261	LYS	2.1
5	M	353	HIS	2.1
8	P	247	VAL	2.1
6	N	295	ILE	2.1
8	P	233	GLU	2.1
8	h	1475	LEU	2.1
6	f	1225	PRO	2.1
1	i	1147	SER	2.1
3	K	12	GLN	2.1
8	P	242	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
7	o	1461	ALA	2.1
7	o	1241	ILE	2.1
8	P	511	ASP	2.1
1	i	1185	LEU	2.1
4	l	1392	ARG	2.1
5	e	1220	ASP	2.1
8	p	1380	ARG	2.1
8	p	1230	ARG	2.1
2	j	1288	GLN	2.1
8	P	226	MET	2.1
1	i	1093	GLU	2.1
2	J	280	GLY	2.1
8	h	1341	LEU	2.1
5	E	114	GLU	2.1
3	c	1261	ILE	2.1
8	P	299	ILE	2.1
2	J	142	ASN	2.1
7	g	1193	ASP	2.1
8	H	247	VAL	2.1
8	p	1155	ASP	2.1
1	A	518	LEU	2.1
7	G	129	TYR	2.1
8	P	113	VAL	2.1
5	E	265	ASP	2.1
7	o	1018	ASP	2.1
4	L	519	LEU	2.1
4	d	1115	ILE	2.1
4	d	1377	VAL	2.1
5	e	1400	GLU	2.1
8	p	1427	GLU	2.1
2	j	1121	ILE	2.1
7	g	1374	CYS	2.1
2	J	357	SER	2.1
5	M	117	ASP	2.1
6	N	142	ASN	2.1
6	n	1375	SER	2.1
5	M	324	GLN	2.1
1	i	1150	THR	2.0
2	b	1489	GLU	2.1
2	b	1276	ILE	2.0
8	p	1299	ILE	2.0
4	D	265	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
3	k	1186	LEU	2.0
5	M	352	GLU	2.0
8	h	1298	CYS	2.0
4	d	1409	GLY	2.0
5	E	379	ARG	2.0
7	O	223	THR	2.0
8	p	1367	ARG	2.0
5	e	1167	ASP	2.0
6	F	376	CYS	2.0
8	h	1321	LEU	2.0
4	d	1482	ILE	2.0
4	L	222	SER	2.0
4	d	1287	LEU	2.0
5	M	529	ASP	2.0
3	c	1244	VAL	2.0
8	h	1474	VAL	2.0
6	n	1540	THR	2.0
5	M	528	VAL	2.0
3	k	1161	THR	2.0
6	n	1464	PHE	2.0
8	p	1302	GLY	2.0
3	K	332	THR	2.0
2	b	1490	SER	2.0
1	A	185	LEU	2.0
4	l	1457	ASN	2.0
5	m	1218	ASP	2.0
7	o	1371	ALA	2.0
8	P	516	ASN	2.0
8	P	357	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
10	BEF	B	602	4/4	0.90	0.33	3.98	210,215,215,215	0
10	BEF	E	602	4/4	0.87	0.43	3.63	240,241,242,244	0
10	BEF	G	602	4/4	0.89	0.42	2.91	236,237,238,239	0
11	SO4	d	1600	5/5	0.95	0.29	1.74	106,109,115,118	0
11	SO4	c	2101	5/5	0.95	0.28	1.46	82,98,107,111	0
10	BEF	J	602	4/4	0.81	0.29	1.31	235,236,240,246	0
11	SO4	I	600	5/5	0.94	0.28	1.06	98,103,110,113	0
10	BEF	m	1602	4/4	0.95	0.26	0.96	185,193,195,196	0
10	BEF	A	602	4/4	0.90	0.37	0.87	246,247,249,251	0
9	ADP	A	601	27/27	0.90	0.35	0.77	46,110,243,330	0
10	BEF	N	602	4/4	0.95	0.31	0.74	112,120,121,122	0
11	SO4	j	1600	5/5	0.92	0.29	0.70	79,96,98,100	0
10	BEF	a	1602	4/4	0.85	0.25	0.64	235,239,240,241	0
9	ADP	h	1601	27/27	0.94	0.33	0.63	40,139,153,188	0
10	BEF	F	602	4/4	0.97	0.27	0.61	157,163,163,171	0
11	SO4	i	1600	5/5	0.96	0.28	0.51	91,94,103,116	0
9	ADP	F	601	27/27	0.95	0.30	0.50	11,105,323,481	0
9	ADP	l	1601	27/27	0.87	0.29	0.40	62,105,189,226	0
11	SO4	K	1101	5/5	0.96	0.35	0.34	84,89,97,102	0
9	ADP	B	601	27/27	0.90	0.27	0.29	62,105,202,218	0
9	ADP	E	601	27/27	0.91	0.32	0.23	11,102,242,288	0
9	ADP	f	1601	27/27	0.90	0.28	0.14	13,50,316,499	0
10	BEF	f	1602	4/4	0.95	0.23	0.09	167,170,171,173	0
9	ADP	L	601	27/27	0.90	0.24	-0.01	102,157,212,241	0
10	BEF	e	1602	4/4	0.96	0.21	-0.03	201,205,207,207	0
9	ADP	a	1601	27/27	0.92	0.23	-0.10	50,112,239,328	0
9	ADP	N	601	27/27	0.95	0.24	-0.11	11,88,232,484	0
9	ADP	k	2101	27/27	0.95	0.28	-0.15	80,131,164,321	0
9	ADP	m	1601	27/27	0.90	0.24	-0.19	13,87,195,273	0
9	ADP	n	1601	27/27	0.93	0.26	-0.19	27,94,337,491	0
9	ADP	p	1601	27/27	0.94	0.21	-0.35	11,114,136,239	0
9	ADP	H	601	27/27	0.94	0.24	-0.35	11,112,145,153	0
9	ADP	C	1101	27/27	0.92	0.28	-0.40	38,135,163,237	0
9	ADP	J	601	27/27	0.93	0.24	-0.43	74,85,241,279	0
10	BEF	n	1602	4/4	0.97	0.23	-0.48	163,167,167,173	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
11	SO4	O	600	5/5	0.95	0.27	-0.49	78,79,92,100	0
9	ADP	e	1601	27/27	0.93	0.20	-0.54	30,116,232,274	0
9	ADP	M	601	27/27	0.87	0.26	-0.61	43,113,256,333	0
9	ADP	G	601	27/27	0.92	0.21	-0.65	12,133,240,248	0
9	ADP	P	601	27/27	0.94	0.25	-0.69	73,153,161,164	0
10	BEF	C	1102	4/4	0.91	0.21	-0.69	104,105,105,120	0
10	BEF	b	1602	4/4	0.91	0.19	-0.71	154,158,161,163	0
10	BEF	M	602	4/4	0.78	0.23	-0.72	152,158,161,170	0
9	ADP	b	1601	27/27	0.95	0.20	-0.75	44,69,220,243	0
9	ADP	g	1601	27/27	0.94	0.19	-0.78	26,159,211,215	0
11	SO4	o	1600	5/5	0.95	0.23	-0.79	107,107,115,117	0
10	BEF	g	1602	4/4	0.97	0.18	-0.85	162,165,165,166	0
9	ADP	D	601	27/27	0.94	0.20	-1.06	41,92,238,264	0
10	BEF	p	1602	4/4	0.97	0.13	-1.30	84,99,102,108	0
10	BEF	P	602	4/4	0.99	0.12	-1.78	158,158,158,162	0
10	BEF	H	602	4/4	0.99	0.11	-1.93	101,103,104,110	0
10	BEF	h	1602	4/4	0.98	0.14	-2.49	85,93,93,106	0
10	BEF	k	2102	4/4	0.94	0.09	-2.80	68,69,80,82	0
10	BEF	D	602	4/4	0.97	0.11	-3.16	81,84,91,92	0
10	BEF	l	1602	4/4	0.96	0.13	-	28,61,73,75	0
10	BEF	L	602	4/4	0.93	0.18	-	172,177,177,180	0

6.5 Other polymers (i)

There are no such residues in this entry.