Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:37 AM GMT

PDB ID	:	3EXG
Title	:	Crystal structure of the pyruvate dehydrogenase (E1p) component of human pyruvate dehydrogenase complex
Authors	:	Kato, M.; Wynn, R.M.; Chuang, J.L.; Tso, S.-C.; Machius, M.; Li, J.; Chuang, D.T.
Deposited on	:	2008-10-16
Resolution	:	3.01 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:

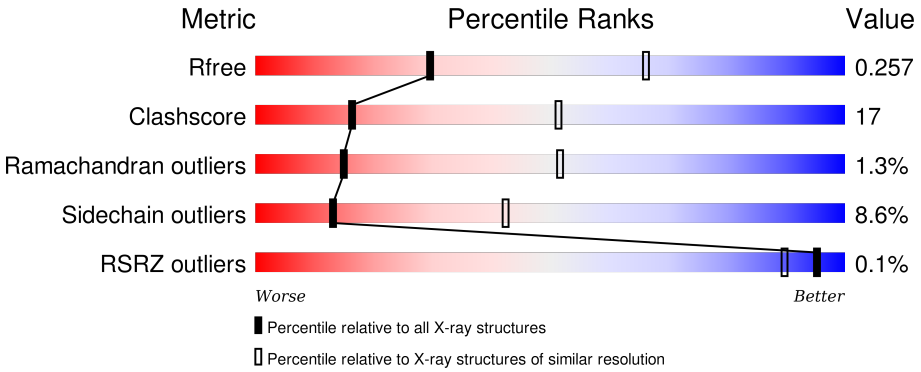
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.01 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	1773 (3.04-3.00)
Clashscore	102246	2117 (3.04-3.00)
Ramachandran outliers	100387	2050 (3.04-3.00)
Sidechain outliers	100360	2053 (3.04-3.00)
RSRZ outliers	91569	1788 (3.04-3.00)

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	1	382	54% 29% • • 12%
1	3	382	55% 28% 6% • 10%
1	5	382	61% 22% 7% • 9%
1	A	382	53% 31% 5% • 10%
1	C	382	51% 34% • • 10%

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Mol	Chain	Length	Quality of chain
1	E	382	61% 25% 5% 9%
1	G	382	60% 26% 9%
1	I	382	58% 29% 10%
1	K	382	62% 25% 9%
1	M	382	61% 25% 5% 9%
1	O	382	51% 31% 5% 13%
1	Q	382	52% 32% 6% 10%
1	S	382	57% 26% 5% 11%
1	U	382	61% 25% 5% 9%
1	W	382	59% 26% 10%
1	Y	382	61% 26% 9%
2	2	329	72% 25%
2	4	329	70% 27%
2	6	329	73% 22% 5%
2	B	329	73% 25%
2	D	329	70% 25% 5%
2	F	329	69% 28%
2	H	329	69% 27%
2	J	329	65% 33%
2	L	329	71% 25%
2	N	329	67% 29%
2	P	329	71% 25%
2	R	329	68% 28%
2	T	329	72% 23% 5%
2	V	329	71% 26%

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Mol	Chain	Length	Quality of chain
2	X	329	
2	Z	329	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 83339 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 Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2677	1684	471	500	22			
1	C	342	Total	C	N	O	S	0	0	0
			2677	1684	471	500	22			
1	E	349	Total	C	N	O	S	0	0	0
			2728	1717	481	508	22			
1	G	346	Total	C	N	O	S	0	0	0
			2712	1707	478	505	22			
1	I	344	Total	C	N	O	S	0	0	0
			2693	1694	473	504	22			
1	K	347	Total	C	N	O	S	0	0	0
			2712	1708	476	506	22			
1	M	349	Total	C	N	O	S	0	0	0
			2728	1717	481	508	22			
1	O	332	Total	C	N	O	S	0	0	0
			2580	1626	449	483	22			
1	Q	344	Total	C	N	O	S	0	0	0
			2693	1694	473	504	22			
1	S	340	Total	C	N	O	S	0	0	0
			2661	1675	466	498	22			
1	U	348	Total	C	N	O	S	0	0	0
			2723	1714	480	507	22			
1	W	345	Total	C	N	O	S	0	0	0
			2705	1702	477	504	22			
1	Y	349	Total	C	N	O	S	0	0	0
			2728	1717	481	508	22			
1	1	335	Total	C	N	O	S	0	0	0
			2614	1647	458	487	22			
1	3	342	Total	C	N	O	S	0	0	0
			2676	1683	469	502	22			
1	5	347	Total	C	N	O	S	0	0	0
			2712	1708	476	506	22			

There are 368 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	EXPRESSION TAG	UNP P08559
A	-19	GLY	-	EXPRESSION TAG	UNP P08559
A	-18	SER	-	EXPRESSION TAG	UNP P08559
A	-17	SER	-	EXPRESSION TAG	UNP P08559
A	-16	HIS	-	EXPRESSION TAG	UNP P08559
A	-15	HIS	-	EXPRESSION TAG	UNP P08559
A	-14	HIS	-	EXPRESSION TAG	UNP P08559
A	-13	HIS	-	EXPRESSION TAG	UNP P08559
A	-12	HIS	-	EXPRESSION TAG	UNP P08559
A	-11	HIS	-	EXPRESSION TAG	UNP P08559
A	-10	SER	-	EXPRESSION TAG	UNP P08559
A	-9	SER	-	EXPRESSION TAG	UNP P08559
A	-8	GLY	-	EXPRESSION TAG	UNP P08559
A	-7	LEU	-	EXPRESSION TAG	UNP P08559
A	-6	VAL	-	EXPRESSION TAG	UNP P08559
A	-5	PRO	-	EXPRESSION TAG	UNP P08559
A	-4	ARG	-	EXPRESSION TAG	UNP P08559
A	-3	GLY	-	EXPRESSION TAG	UNP P08559
A	-2	SER	-	EXPRESSION TAG	UNP P08559
A	-1	HIS	-	EXPRESSION TAG	UNP P08559
A	0	MET	-	EXPRESSION TAG	UNP P08559
A	203	ALA	SER	ENGINEERED	UNP P08559
A	271	ALA	SER	ENGINEERED	UNP P08559
C	-20	MET	-	EXPRESSION TAG	UNP P08559
C	-19	GLY	-	EXPRESSION TAG	UNP P08559
C	-18	SER	-	EXPRESSION TAG	UNP P08559
C	-17	SER	-	EXPRESSION TAG	UNP P08559
C	-16	HIS	-	EXPRESSION TAG	UNP P08559
C	-15	HIS	-	EXPRESSION TAG	UNP P08559
C	-14	HIS	-	EXPRESSION TAG	UNP P08559
C	-13	HIS	-	EXPRESSION TAG	UNP P08559
C	-12	HIS	-	EXPRESSION TAG	UNP P08559
C	-11	HIS	-	EXPRESSION TAG	UNP P08559
C	-10	SER	-	EXPRESSION TAG	UNP P08559
C	-9	SER	-	EXPRESSION TAG	UNP P08559
C	-8	GLY	-	EXPRESSION TAG	UNP P08559
C	-7	LEU	-	EXPRESSION TAG	UNP P08559
C	-6	VAL	-	EXPRESSION TAG	UNP P08559
C	-5	PRO	-	EXPRESSION TAG	UNP P08559
C	-4	ARG	-	EXPRESSION TAG	UNP P08559
C	-3	GLY	-	EXPRESSION TAG	UNP P08559
C	-2	SER	-	EXPRESSION TAG	UNP P08559

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	HIS	-	EXPRESSION TAG	UNP P08559
C	0	MET	-	EXPRESSION TAG	UNP P08559
C	203	ALA	SER	ENGINEERED	UNP P08559
C	271	ALA	SER	ENGINEERED	UNP P08559
E	-20	MET	-	EXPRESSION TAG	UNP P08559
E	-19	GLY	-	EXPRESSION TAG	UNP P08559
E	-18	SER	-	EXPRESSION TAG	UNP P08559
E	-17	SER	-	EXPRESSION TAG	UNP P08559
E	-16	HIS	-	EXPRESSION TAG	UNP P08559
E	-15	HIS	-	EXPRESSION TAG	UNP P08559
E	-14	HIS	-	EXPRESSION TAG	UNP P08559
E	-13	HIS	-	EXPRESSION TAG	UNP P08559
E	-12	HIS	-	EXPRESSION TAG	UNP P08559
E	-11	HIS	-	EXPRESSION TAG	UNP P08559
E	-10	SER	-	EXPRESSION TAG	UNP P08559
E	-9	SER	-	EXPRESSION TAG	UNP P08559
E	-8	GLY	-	EXPRESSION TAG	UNP P08559
E	-7	LEU	-	EXPRESSION TAG	UNP P08559
E	-6	VAL	-	EXPRESSION TAG	UNP P08559
E	-5	PRO	-	EXPRESSION TAG	UNP P08559
E	-4	ARG	-	EXPRESSION TAG	UNP P08559
E	-3	GLY	-	EXPRESSION TAG	UNP P08559
E	-2	SER	-	EXPRESSION TAG	UNP P08559
E	-1	HIS	-	EXPRESSION TAG	UNP P08559
E	0	MET	-	EXPRESSION TAG	UNP P08559
E	203	ALA	SER	ENGINEERED	UNP P08559
E	271	ALA	SER	ENGINEERED	UNP P08559
G	-20	MET	-	EXPRESSION TAG	UNP P08559
G	-19	GLY	-	EXPRESSION TAG	UNP P08559
G	-18	SER	-	EXPRESSION TAG	UNP P08559
G	-17	SER	-	EXPRESSION TAG	UNP P08559
G	-16	HIS	-	EXPRESSION TAG	UNP P08559
G	-15	HIS	-	EXPRESSION TAG	UNP P08559
G	-14	HIS	-	EXPRESSION TAG	UNP P08559
G	-13	HIS	-	EXPRESSION TAG	UNP P08559
G	-12	HIS	-	EXPRESSION TAG	UNP P08559
G	-11	HIS	-	EXPRESSION TAG	UNP P08559
G	-10	SER	-	EXPRESSION TAG	UNP P08559
G	-9	SER	-	EXPRESSION TAG	UNP P08559
G	-8	GLY	-	EXPRESSION TAG	UNP P08559
G	-7	LEU	-	EXPRESSION TAG	UNP P08559
G	-6	VAL	-	EXPRESSION TAG	UNP P08559

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-5	PRO	-	EXPRESSION TAG	UNP P08559
G	-4	ARG	-	EXPRESSION TAG	UNP P08559
G	-3	GLY	-	EXPRESSION TAG	UNP P08559
G	-2	SER	-	EXPRESSION TAG	UNP P08559
G	-1	HIS	-	EXPRESSION TAG	UNP P08559
G	0	MET	-	EXPRESSION TAG	UNP P08559
G	203	ALA	SER	ENGINEERED	UNP P08559
G	271	ALA	SER	ENGINEERED	UNP P08559
I	-20	MET	-	EXPRESSION TAG	UNP P08559
I	-19	GLY	-	EXPRESSION TAG	UNP P08559
I	-18	SER	-	EXPRESSION TAG	UNP P08559
I	-17	SER	-	EXPRESSION TAG	UNP P08559
I	-16	HIS	-	EXPRESSION TAG	UNP P08559
I	-15	HIS	-	EXPRESSION TAG	UNP P08559
I	-14	HIS	-	EXPRESSION TAG	UNP P08559
I	-13	HIS	-	EXPRESSION TAG	UNP P08559
I	-12	HIS	-	EXPRESSION TAG	UNP P08559
I	-11	HIS	-	EXPRESSION TAG	UNP P08559
I	-10	SER	-	EXPRESSION TAG	UNP P08559
I	-9	SER	-	EXPRESSION TAG	UNP P08559
I	-8	GLY	-	EXPRESSION TAG	UNP P08559
I	-7	LEU	-	EXPRESSION TAG	UNP P08559
I	-6	VAL	-	EXPRESSION TAG	UNP P08559
I	-5	PRO	-	EXPRESSION TAG	UNP P08559
I	-4	ARG	-	EXPRESSION TAG	UNP P08559
I	-3	GLY	-	EXPRESSION TAG	UNP P08559
I	-2	SER	-	EXPRESSION TAG	UNP P08559
I	-1	HIS	-	EXPRESSION TAG	UNP P08559
I	0	MET	-	EXPRESSION TAG	UNP P08559
I	203	ALA	SER	ENGINEERED	UNP P08559
I	271	ALA	SER	ENGINEERED	UNP P08559
K	-20	MET	-	EXPRESSION TAG	UNP P08559
K	-19	GLY	-	EXPRESSION TAG	UNP P08559
K	-18	SER	-	EXPRESSION TAG	UNP P08559
K	-17	SER	-	EXPRESSION TAG	UNP P08559
K	-16	HIS	-	EXPRESSION TAG	UNP P08559
K	-15	HIS	-	EXPRESSION TAG	UNP P08559
K	-14	HIS	-	EXPRESSION TAG	UNP P08559
K	-13	HIS	-	EXPRESSION TAG	UNP P08559
K	-12	HIS	-	EXPRESSION TAG	UNP P08559
K	-11	HIS	-	EXPRESSION TAG	UNP P08559
K	-10	SER	-	EXPRESSION TAG	UNP P08559

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-9	SER	-	EXPRESSION TAG	UNP P08559
K	-8	GLY	-	EXPRESSION TAG	UNP P08559
K	-7	LEU	-	EXPRESSION TAG	UNP P08559
K	-6	VAL	-	EXPRESSION TAG	UNP P08559
K	-5	PRO	-	EXPRESSION TAG	UNP P08559
K	-4	ARG	-	EXPRESSION TAG	UNP P08559
K	-3	GLY	-	EXPRESSION TAG	UNP P08559
K	-2	SER	-	EXPRESSION TAG	UNP P08559
K	-1	HIS	-	EXPRESSION TAG	UNP P08559
K	0	MET	-	EXPRESSION TAG	UNP P08559
K	203	ALA	SER	ENGINEERED	UNP P08559
K	271	ALA	SER	ENGINEERED	UNP P08559
M	-20	MET	-	EXPRESSION TAG	UNP P08559
M	-19	GLY	-	EXPRESSION TAG	UNP P08559
M	-18	SER	-	EXPRESSION TAG	UNP P08559
M	-17	SER	-	EXPRESSION TAG	UNP P08559
M	-16	HIS	-	EXPRESSION TAG	UNP P08559
M	-15	HIS	-	EXPRESSION TAG	UNP P08559
M	-14	HIS	-	EXPRESSION TAG	UNP P08559
M	-13	HIS	-	EXPRESSION TAG	UNP P08559
M	-12	HIS	-	EXPRESSION TAG	UNP P08559
M	-11	HIS	-	EXPRESSION TAG	UNP P08559
M	-10	SER	-	EXPRESSION TAG	UNP P08559
M	-9	SER	-	EXPRESSION TAG	UNP P08559
M	-8	GLY	-	EXPRESSION TAG	UNP P08559
M	-7	LEU	-	EXPRESSION TAG	UNP P08559
M	-6	VAL	-	EXPRESSION TAG	UNP P08559
M	-5	PRO	-	EXPRESSION TAG	UNP P08559
M	-4	ARG	-	EXPRESSION TAG	UNP P08559
M	-3	GLY	-	EXPRESSION TAG	UNP P08559
M	-2	SER	-	EXPRESSION TAG	UNP P08559
M	-1	HIS	-	EXPRESSION TAG	UNP P08559
M	0	MET	-	EXPRESSION TAG	UNP P08559
M	203	ALA	SER	ENGINEERED	UNP P08559
M	271	ALA	SER	ENGINEERED	UNP P08559
O	-20	MET	-	EXPRESSION TAG	UNP P08559
O	-19	GLY	-	EXPRESSION TAG	UNP P08559
O	-18	SER	-	EXPRESSION TAG	UNP P08559
O	-17	SER	-	EXPRESSION TAG	UNP P08559
O	-16	HIS	-	EXPRESSION TAG	UNP P08559
O	-15	HIS	-	EXPRESSION TAG	UNP P08559
O	-14	HIS	-	EXPRESSION TAG	UNP P08559

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-13	HIS	-	EXPRESSION TAG	UNP P08559
O	-12	HIS	-	EXPRESSION TAG	UNP P08559
O	-11	HIS	-	EXPRESSION TAG	UNP P08559
O	-10	SER	-	EXPRESSION TAG	UNP P08559
O	-9	SER	-	EXPRESSION TAG	UNP P08559
O	-8	GLY	-	EXPRESSION TAG	UNP P08559
O	-7	LEU	-	EXPRESSION TAG	UNP P08559
O	-6	VAL	-	EXPRESSION TAG	UNP P08559
O	-5	PRO	-	EXPRESSION TAG	UNP P08559
O	-4	ARG	-	EXPRESSION TAG	UNP P08559
O	-3	GLY	-	EXPRESSION TAG	UNP P08559
O	-2	SER	-	EXPRESSION TAG	UNP P08559
O	-1	HIS	-	EXPRESSION TAG	UNP P08559
O	0	MET	-	EXPRESSION TAG	UNP P08559
O	203	ALA	SER	ENGINEERED	UNP P08559
O	271	ALA	SER	ENGINEERED	UNP P08559
Q	-20	MET	-	EXPRESSION TAG	UNP P08559
Q	-19	GLY	-	EXPRESSION TAG	UNP P08559
Q	-18	SER	-	EXPRESSION TAG	UNP P08559
Q	-17	SER	-	EXPRESSION TAG	UNP P08559
Q	-16	HIS	-	EXPRESSION TAG	UNP P08559
Q	-15	HIS	-	EXPRESSION TAG	UNP P08559
Q	-14	HIS	-	EXPRESSION TAG	UNP P08559
Q	-13	HIS	-	EXPRESSION TAG	UNP P08559
Q	-12	HIS	-	EXPRESSION TAG	UNP P08559
Q	-11	HIS	-	EXPRESSION TAG	UNP P08559
Q	-10	SER	-	EXPRESSION TAG	UNP P08559
Q	-9	SER	-	EXPRESSION TAG	UNP P08559
Q	-8	GLY	-	EXPRESSION TAG	UNP P08559
Q	-7	LEU	-	EXPRESSION TAG	UNP P08559
Q	-6	VAL	-	EXPRESSION TAG	UNP P08559
Q	-5	PRO	-	EXPRESSION TAG	UNP P08559
Q	-4	ARG	-	EXPRESSION TAG	UNP P08559
Q	-3	GLY	-	EXPRESSION TAG	UNP P08559
Q	-2	SER	-	EXPRESSION TAG	UNP P08559
Q	-1	HIS	-	EXPRESSION TAG	UNP P08559
Q	0	MET	-	EXPRESSION TAG	UNP P08559
Q	203	ALA	SER	ENGINEERED	UNP P08559
Q	271	ALA	SER	ENGINEERED	UNP P08559
S	-20	MET	-	EXPRESSION TAG	UNP P08559
S	-19	GLY	-	EXPRESSION TAG	UNP P08559
S	-18	SER	-	EXPRESSION TAG	UNP P08559

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Chain	Residue	Modelled	Actual	Comment	Reference
S	-17	SER	-	EXPRESSION TAG	UNP P08559
S	-16	HIS	-	EXPRESSION TAG	UNP P08559
S	-15	HIS	-	EXPRESSION TAG	UNP P08559
S	-14	HIS	-	EXPRESSION TAG	UNP P08559
S	-13	HIS	-	EXPRESSION TAG	UNP P08559
S	-12	HIS	-	EXPRESSION TAG	UNP P08559
S	-11	HIS	-	EXPRESSION TAG	UNP P08559
S	-10	SER	-	EXPRESSION TAG	UNP P08559
S	-9	SER	-	EXPRESSION TAG	UNP P08559
S	-8	GLY	-	EXPRESSION TAG	UNP P08559
S	-7	LEU	-	EXPRESSION TAG	UNP P08559
S	-6	VAL	-	EXPRESSION TAG	UNP P08559
S	-5	PRO	-	EXPRESSION TAG	UNP P08559
S	-4	ARG	-	EXPRESSION TAG	UNP P08559
S	-3	GLY	-	EXPRESSION TAG	UNP P08559
S	-2	SER	-	EXPRESSION TAG	UNP P08559
S	-1	HIS	-	EXPRESSION TAG	UNP P08559
S	0	MET	-	EXPRESSION TAG	UNP P08559
S	203	ALA	SER	ENGINEERED	UNP P08559
S	271	ALA	SER	ENGINEERED	UNP P08559
U	-20	MET	-	EXPRESSION TAG	UNP P08559
U	-19	GLY	-	EXPRESSION TAG	UNP P08559
U	-18	SER	-	EXPRESSION TAG	UNP P08559
U	-17	SER	-	EXPRESSION TAG	UNP P08559
U	-16	HIS	-	EXPRESSION TAG	UNP P08559
U	-15	HIS	-	EXPRESSION TAG	UNP P08559
U	-14	HIS	-	EXPRESSION TAG	UNP P08559
U	-13	HIS	-	EXPRESSION TAG	UNP P08559
U	-12	HIS	-	EXPRESSION TAG	UNP P08559
U	-11	HIS	-	EXPRESSION TAG	UNP P08559
U	-10	SER	-	EXPRESSION TAG	UNP P08559
U	-9	SER	-	EXPRESSION TAG	UNP P08559
U	-8	GLY	-	EXPRESSION TAG	UNP P08559
U	-7	LEU	-	EXPRESSION TAG	UNP P08559
U	-6	VAL	-	EXPRESSION TAG	UNP P08559
U	-5	PRO	-	EXPRESSION TAG	UNP P08559
U	-4	ARG	-	EXPRESSION TAG	UNP P08559
U	-3	GLY	-	EXPRESSION TAG	UNP P08559
U	-2	SER	-	EXPRESSION TAG	UNP P08559
U	-1	HIS	-	EXPRESSION TAG	UNP P08559
U	0	MET	-	EXPRESSION TAG	UNP P08559
U	203	ALA	SER	ENGINEERED	UNP P08559

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Chain	Residue	Modelled	Actual	Comment	Reference
U	271	ALA	SER	ENGINEERED	UNP P08559
W	-20	MET	-	EXPRESSION TAG	UNP P08559
W	-19	GLY	-	EXPRESSION TAG	UNP P08559
W	-18	SER	-	EXPRESSION TAG	UNP P08559
W	-17	SER	-	EXPRESSION TAG	UNP P08559
W	-16	HIS	-	EXPRESSION TAG	UNP P08559
W	-15	HIS	-	EXPRESSION TAG	UNP P08559
W	-14	HIS	-	EXPRESSION TAG	UNP P08559
W	-13	HIS	-	EXPRESSION TAG	UNP P08559
W	-12	HIS	-	EXPRESSION TAG	UNP P08559
W	-11	HIS	-	EXPRESSION TAG	UNP P08559
W	-10	SER	-	EXPRESSION TAG	UNP P08559
W	-9	SER	-	EXPRESSION TAG	UNP P08559
W	-8	GLY	-	EXPRESSION TAG	UNP P08559
W	-7	LEU	-	EXPRESSION TAG	UNP P08559
W	-6	VAL	-	EXPRESSION TAG	UNP P08559
W	-5	PRO	-	EXPRESSION TAG	UNP P08559
W	-4	ARG	-	EXPRESSION TAG	UNP P08559
W	-3	GLY	-	EXPRESSION TAG	UNP P08559
W	-2	SER	-	EXPRESSION TAG	UNP P08559
W	-1	HIS	-	EXPRESSION TAG	UNP P08559
W	0	MET	-	EXPRESSION TAG	UNP P08559
W	203	ALA	SER	ENGINEERED	UNP P08559
W	271	ALA	SER	ENGINEERED	UNP P08559
Y	-20	MET	-	EXPRESSION TAG	UNP P08559
Y	-19	GLY	-	EXPRESSION TAG	UNP P08559
Y	-18	SER	-	EXPRESSION TAG	UNP P08559
Y	-17	SER	-	EXPRESSION TAG	UNP P08559
Y	-16	HIS	-	EXPRESSION TAG	UNP P08559
Y	-15	HIS	-	EXPRESSION TAG	UNP P08559
Y	-14	HIS	-	EXPRESSION TAG	UNP P08559
Y	-13	HIS	-	EXPRESSION TAG	UNP P08559
Y	-12	HIS	-	EXPRESSION TAG	UNP P08559
Y	-11	HIS	-	EXPRESSION TAG	UNP P08559
Y	-10	SER	-	EXPRESSION TAG	UNP P08559
Y	-9	SER	-	EXPRESSION TAG	UNP P08559
Y	-8	GLY	-	EXPRESSION TAG	UNP P08559
Y	-7	LEU	-	EXPRESSION TAG	UNP P08559
Y	-6	VAL	-	EXPRESSION TAG	UNP P08559
Y	-5	PRO	-	EXPRESSION TAG	UNP P08559
Y	-4	ARG	-	EXPRESSION TAG	UNP P08559
Y	-3	GLY	-	EXPRESSION TAG	UNP P08559

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	-2	SER	-	EXPRESSION TAG	UNP P08559
Y	-1	HIS	-	EXPRESSION TAG	UNP P08559
Y	0	MET	-	EXPRESSION TAG	UNP P08559
Y	203	ALA	SER	ENGINEERED	UNP P08559
Y	271	ALA	SER	ENGINEERED	UNP P08559
1	-20	MET	-	EXPRESSION TAG	UNP P08559
1	-19	GLY	-	EXPRESSION TAG	UNP P08559
1	-18	SER	-	EXPRESSION TAG	UNP P08559
1	-17	SER	-	EXPRESSION TAG	UNP P08559
1	-16	HIS	-	EXPRESSION TAG	UNP P08559
1	-15	HIS	-	EXPRESSION TAG	UNP P08559
1	-14	HIS	-	EXPRESSION TAG	UNP P08559
1	-13	HIS	-	EXPRESSION TAG	UNP P08559
1	-12	HIS	-	EXPRESSION TAG	UNP P08559
1	-11	HIS	-	EXPRESSION TAG	UNP P08559
1	-10	SER	-	EXPRESSION TAG	UNP P08559
1	-9	SER	-	EXPRESSION TAG	UNP P08559
1	-8	GLY	-	EXPRESSION TAG	UNP P08559
1	-7	LEU	-	EXPRESSION TAG	UNP P08559
1	-6	VAL	-	EXPRESSION TAG	UNP P08559
1	-5	PRO	-	EXPRESSION TAG	UNP P08559
1	-4	ARG	-	EXPRESSION TAG	UNP P08559
1	-3	GLY	-	EXPRESSION TAG	UNP P08559
1	-2	SER	-	EXPRESSION TAG	UNP P08559
1	-1	HIS	-	EXPRESSION TAG	UNP P08559
1	0	MET	-	EXPRESSION TAG	UNP P08559
1	203	ALA	SER	ENGINEERED	UNP P08559
1	271	ALA	SER	ENGINEERED	UNP P08559
3	-20	MET	-	EXPRESSION TAG	UNP P08559
3	-19	GLY	-	EXPRESSION TAG	UNP P08559
3	-18	SER	-	EXPRESSION TAG	UNP P08559
3	-17	SER	-	EXPRESSION TAG	UNP P08559
3	-16	HIS	-	EXPRESSION TAG	UNP P08559
3	-15	HIS	-	EXPRESSION TAG	UNP P08559
3	-14	HIS	-	EXPRESSION TAG	UNP P08559
3	-13	HIS	-	EXPRESSION TAG	UNP P08559
3	-12	HIS	-	EXPRESSION TAG	UNP P08559
3	-11	HIS	-	EXPRESSION TAG	UNP P08559
3	-10	SER	-	EXPRESSION TAG	UNP P08559
3	-9	SER	-	EXPRESSION TAG	UNP P08559
3	-8	GLY	-	EXPRESSION TAG	UNP P08559
3	-7	LEU	-	EXPRESSION TAG	UNP P08559

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Chain	Residue	Modelled	Actual	Comment	Reference
3	-6	VAL	-	EXPRESSION TAG	UNP P08559
3	-5	PRO	-	EXPRESSION TAG	UNP P08559
3	-4	ARG	-	EXPRESSION TAG	UNP P08559
3	-3	GLY	-	EXPRESSION TAG	UNP P08559
3	-2	SER	-	EXPRESSION TAG	UNP P08559
3	-1	HIS	-	EXPRESSION TAG	UNP P08559
3	0	MET	-	EXPRESSION TAG	UNP P08559
3	203	ALA	SER	ENGINEERED	UNP P08559
3	271	ALA	SER	ENGINEERED	UNP P08559
5	-20	MET	-	EXPRESSION TAG	UNP P08559
5	-19	GLY	-	EXPRESSION TAG	UNP P08559
5	-18	SER	-	EXPRESSION TAG	UNP P08559
5	-17	SER	-	EXPRESSION TAG	UNP P08559
5	-16	HIS	-	EXPRESSION TAG	UNP P08559
5	-15	HIS	-	EXPRESSION TAG	UNP P08559
5	-14	HIS	-	EXPRESSION TAG	UNP P08559
5	-13	HIS	-	EXPRESSION TAG	UNP P08559
5	-12	HIS	-	EXPRESSION TAG	UNP P08559
5	-11	HIS	-	EXPRESSION TAG	UNP P08559
5	-10	SER	-	EXPRESSION TAG	UNP P08559
5	-9	SER	-	EXPRESSION TAG	UNP P08559
5	-8	GLY	-	EXPRESSION TAG	UNP P08559
5	-7	LEU	-	EXPRESSION TAG	UNP P08559
5	-6	VAL	-	EXPRESSION TAG	UNP P08559
5	-5	PRO	-	EXPRESSION TAG	UNP P08559
5	-4	ARG	-	EXPRESSION TAG	UNP P08559
5	-3	GLY	-	EXPRESSION TAG	UNP P08559
5	-2	SER	-	EXPRESSION TAG	UNP P08559
5	-1	HIS	-	EXPRESSION TAG	UNP P08559
5	0	MET	-	EXPRESSION TAG	UNP P08559
5	203	ALA	SER	ENGINEERED	UNP P08559
5	271	ALA	SER	ENGINEERED	UNP P08559

- Molecule 2 is a protein called Pyruvate dehydrogenase E1 component subunit beta, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	329	Total	C	N	O	S	0	0	0
			2519	1604	427	469	19			
2	D	329	Total	C	N	O	S	0	0	0
			2519	1604	427	469	19			
2	F	329	Total	C	N	O	S	0	0	0
			2519	1604	427	469	19			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	329	Total	C	N	O	S	0	0	0
			2519	1604	427	469	19			
2	J	329	Total	C	N	O	S	0	0	0
			2519	1604	427	469	19			
2	L	329	Total	C	N	O	S	0	0	0
			2519	1604	427	469	19			
2	N	329	Total	C	N	O	S	0	0	0
			2519	1604	427	469	19			
2	P	329	Total	C	N	O	S	0	0	0
			2519	1604	427	469	19			
2	R	329	Total	C	N	O	S	0	0	0
			2519	1604	427	469	19			
2	T	329	Total	C	N	O	S	0	0	0
			2519	1604	427	469	19			
2	V	329	Total	C	N	O	S	0	0	0
			2519	1604	427	469	19			
2	X	329	Total	C	N	O	S	0	0	0
			2519	1604	427	469	19			
2	Z	329	Total	C	N	O	S	0	0	0
			2519	1604	427	469	19			
2	2	329	Total	C	N	O	S	0	0	0
			2519	1604	427	469	19			
2	4	329	Total	C	N	O	S	0	0	0
			2519	1604	427	469	19			
2	6	329	Total	C	N	O	S	0	0	0
			2519	1604	427	469	19			

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	1	Total	K	0	0
			1	1		
3	J	1	Total	K	0	0
			1	1		
3	D	1	Total	K	0	0
			1	1		
3	H	1	Total	K	0	0
			1	1		
3	B	1	Total	K	0	0
			1	1		
3	V	1	Total	K	0	0
			1	1		

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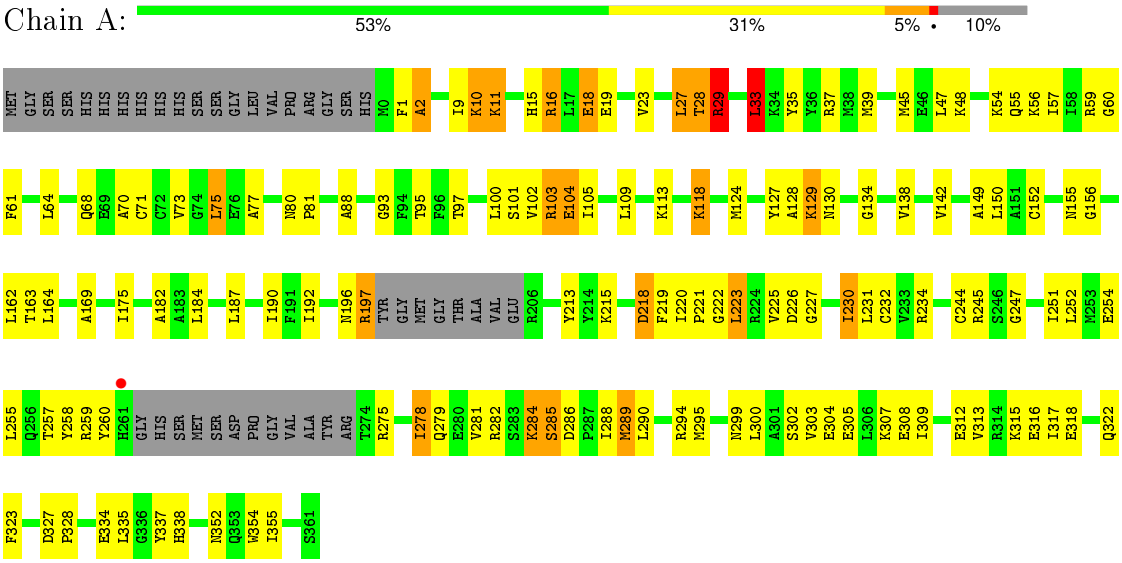
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	Z	1	Total K 1 1	0	0
3	T	1	Total K 1 1	0	0
3	6	1	Total K 1 1	0	0
3	N	1	Total K 1 1	0	0
3	X	1	Total K 1 1	0	0
3	4	1	Total K 1 1	0	0
3	R	1	Total K 1 1	0	0
3	L	1	Total K 1 1	0	0
3	2	1	Total K 1 1	0	0
3	F	1	Total K 1 1	0	0

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.

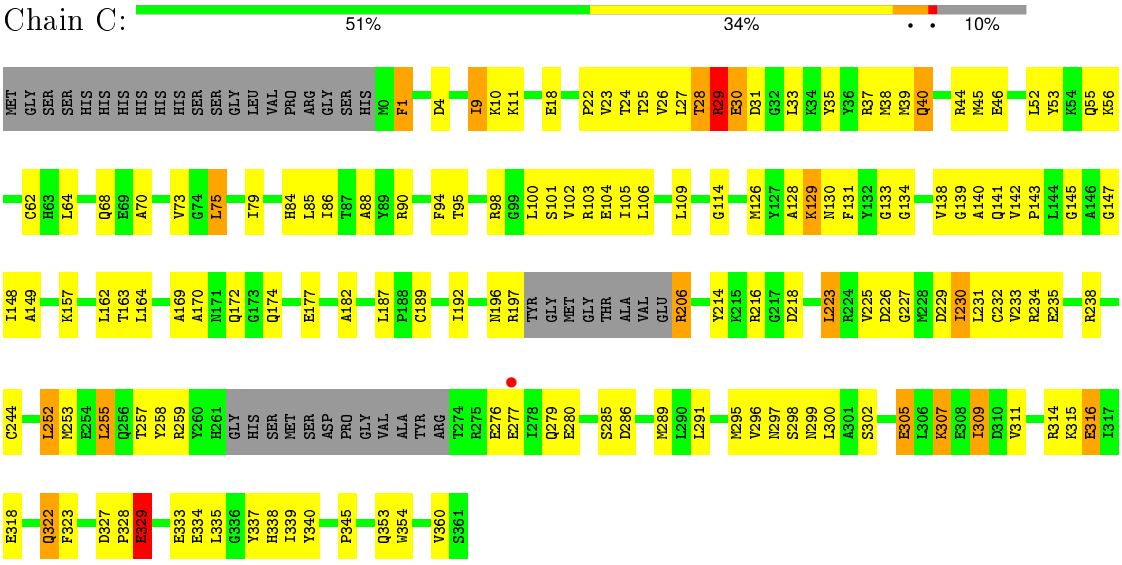
• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

Chain A:



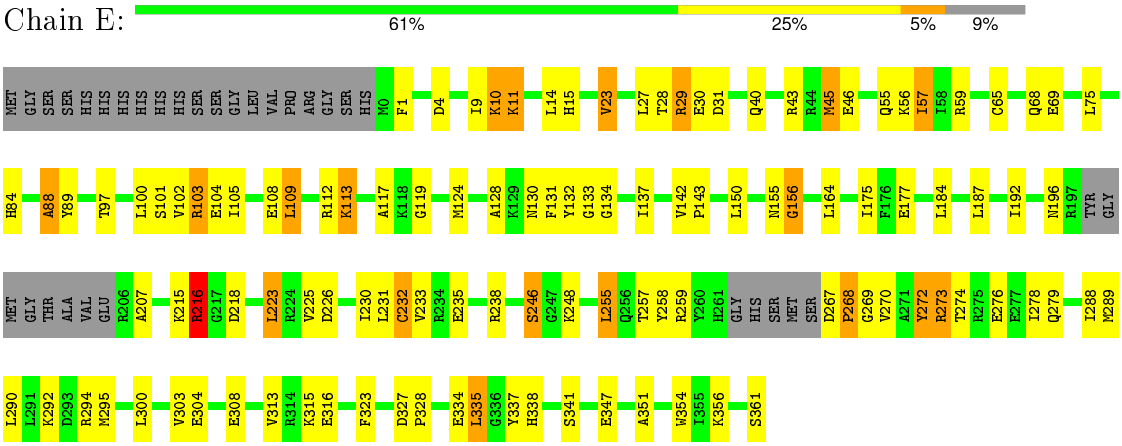
• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

Chain C:



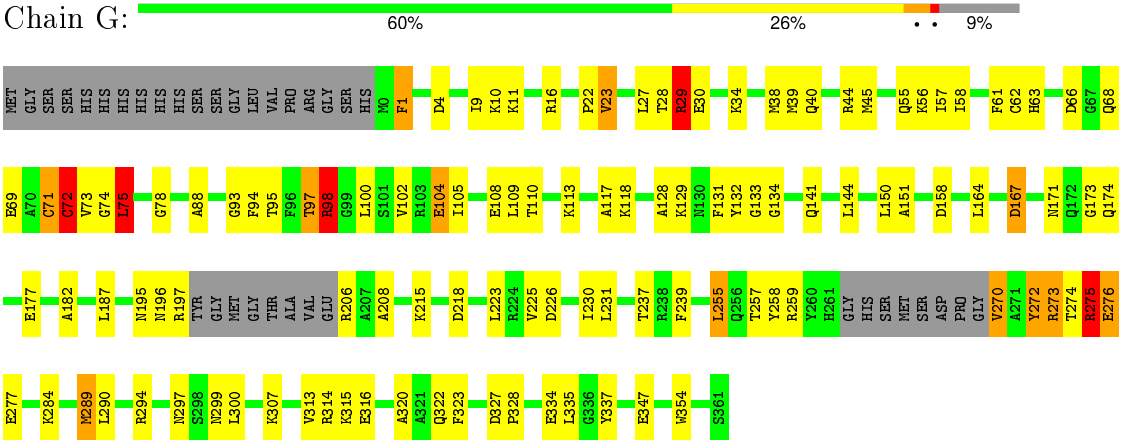
• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

Chain E:



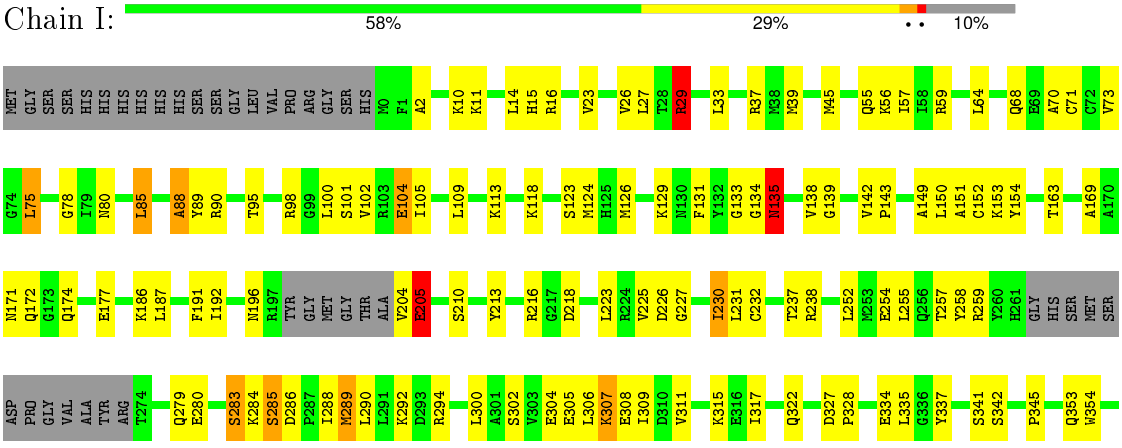
• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

Chain G:



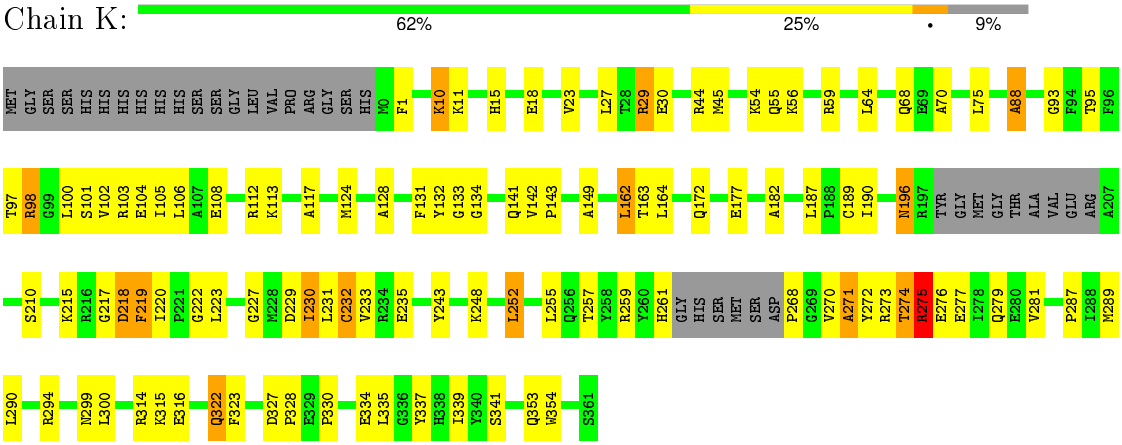
• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

Chain I:



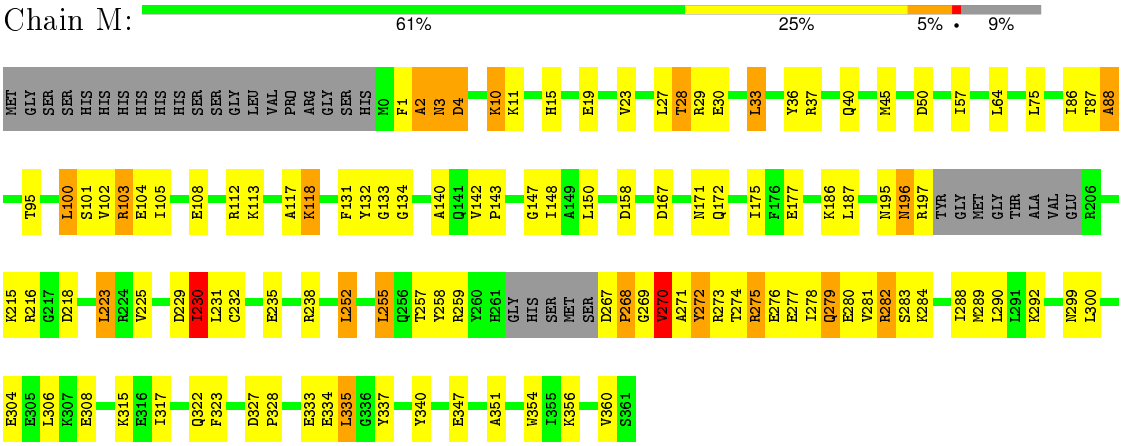
• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

Chain K:



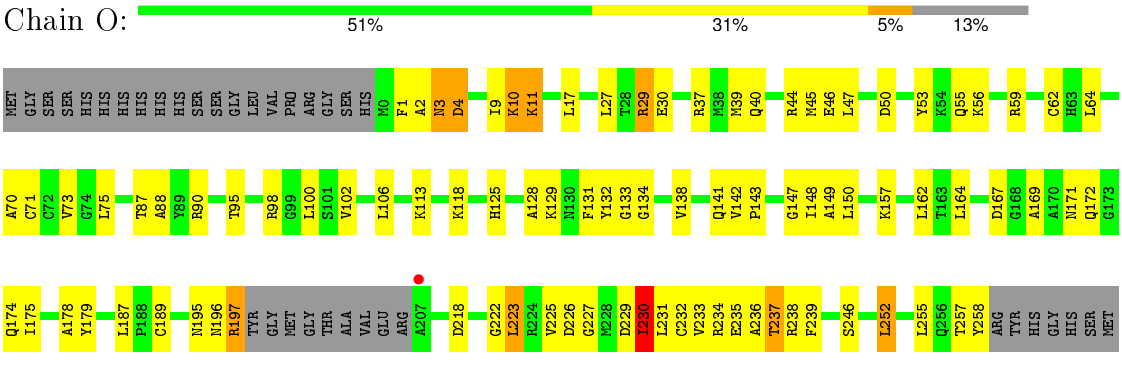
• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

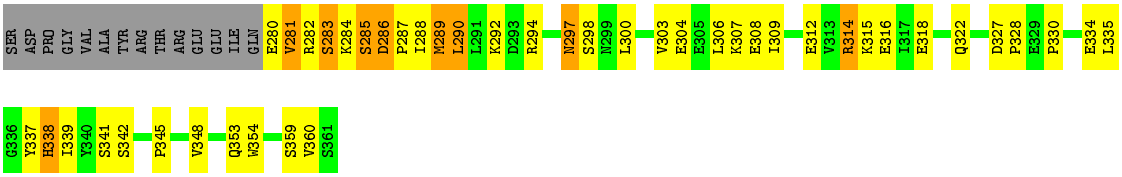
Chain M:



• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

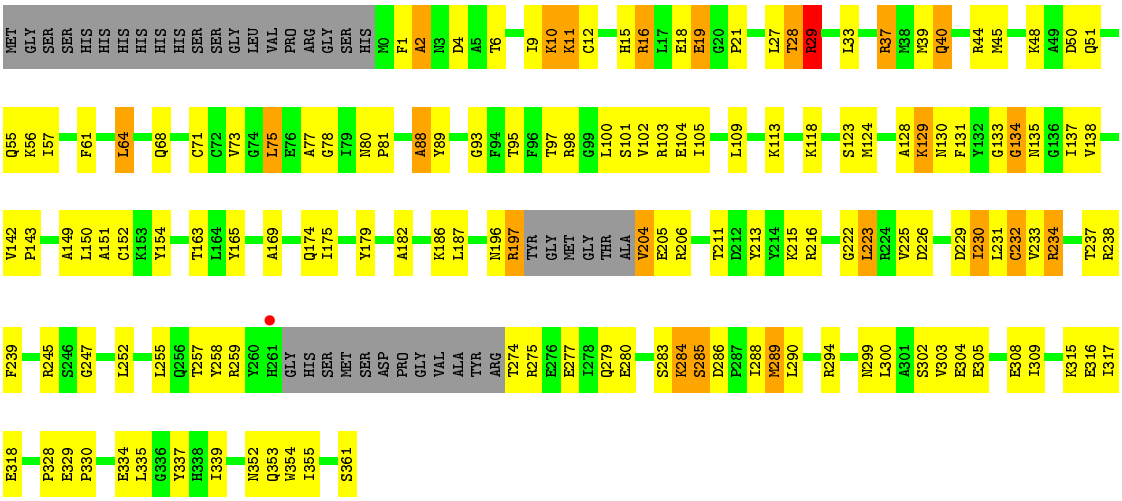
Chain O:





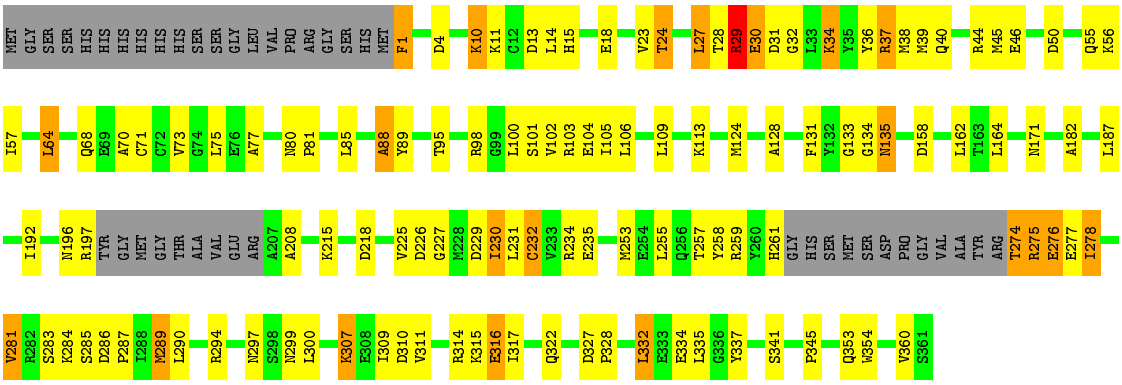
• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

Chain Q:



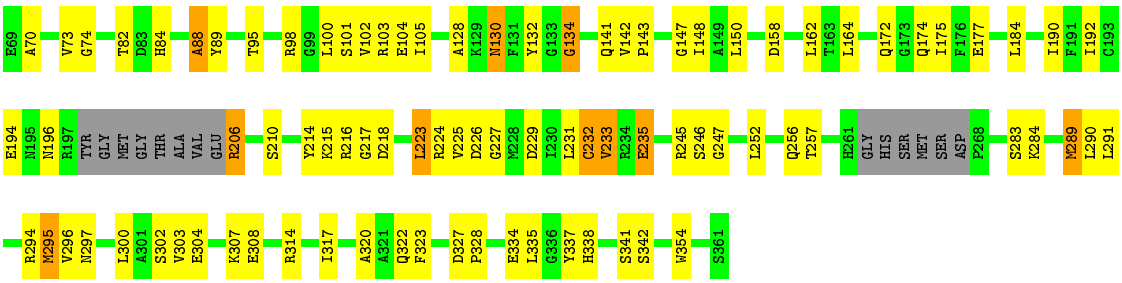
• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

Chain S:



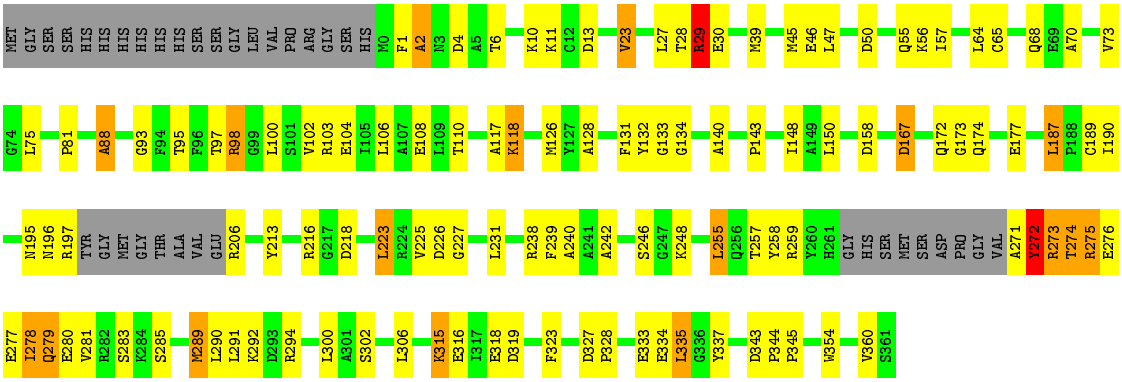
• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

Chain U:



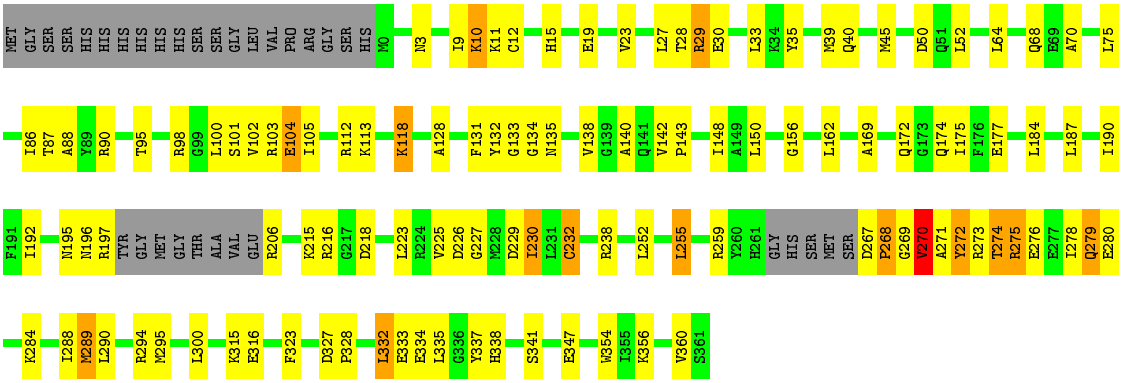
• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

Chain W:



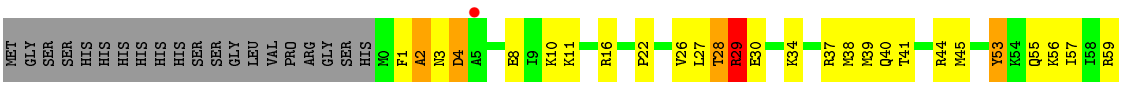
• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

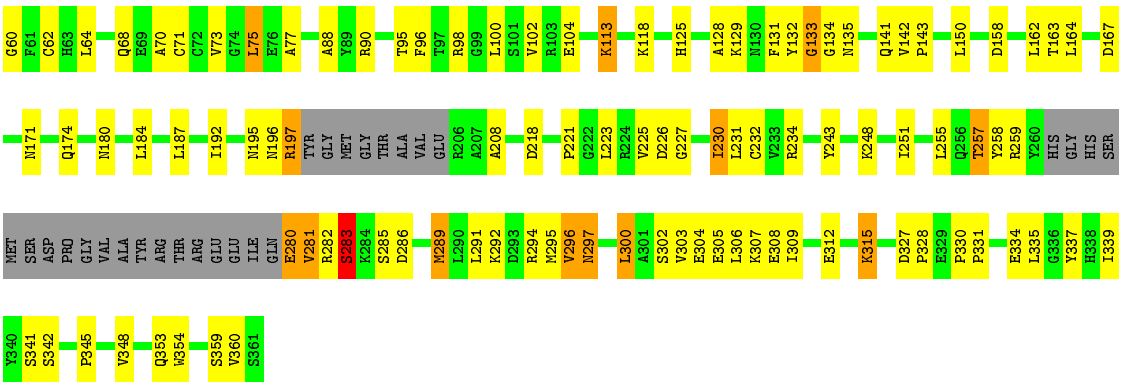
Chain Y:



• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

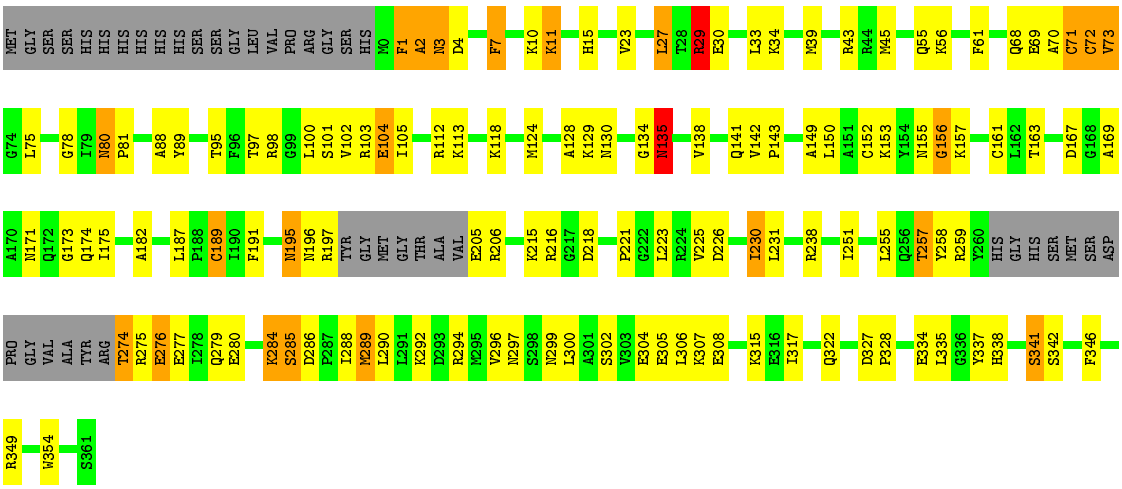
Chain 1:





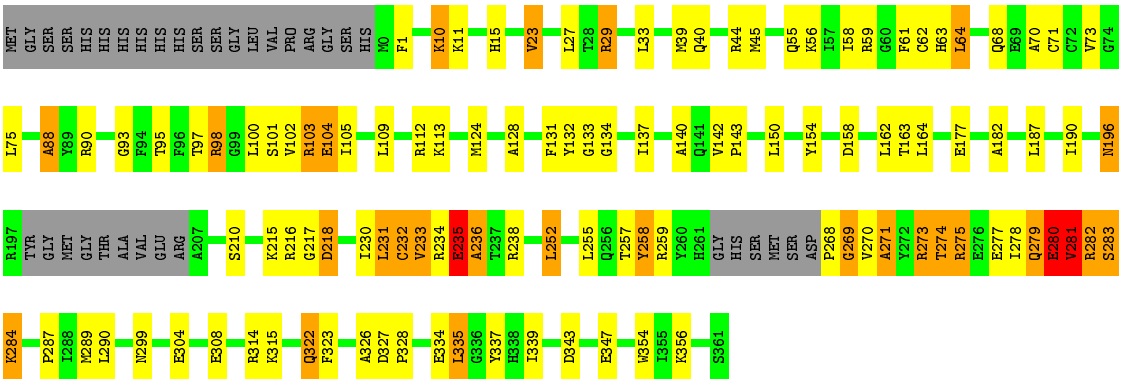
• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

Chain 3:



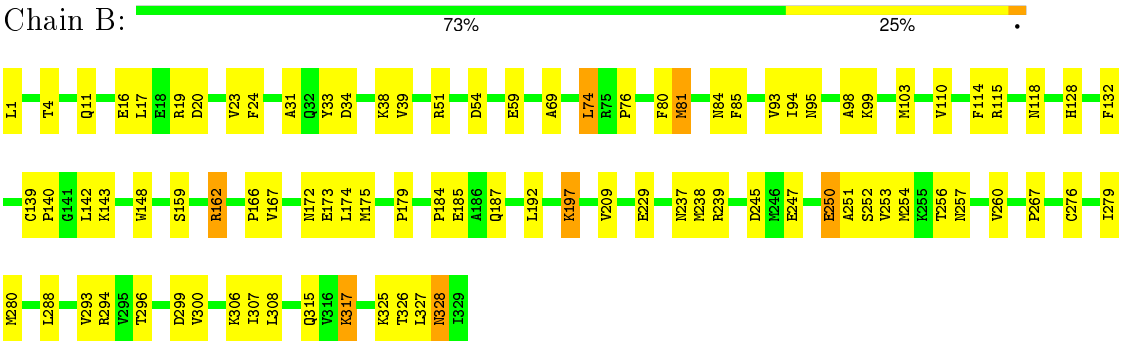
• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

Chain 5:



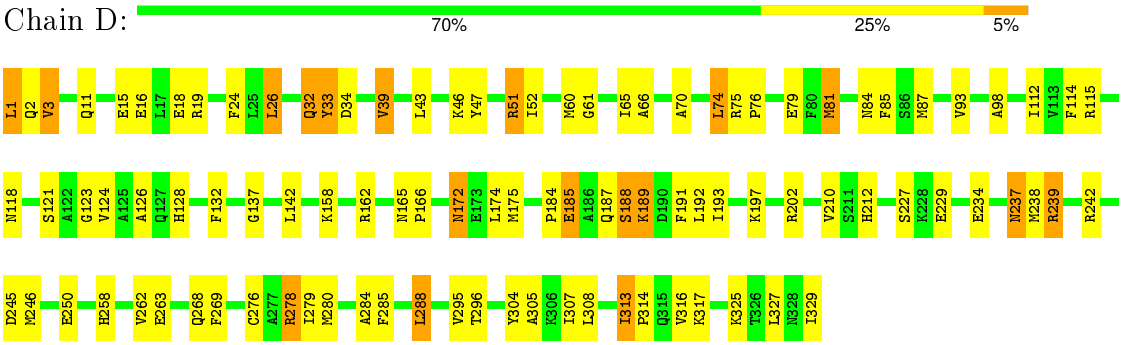
• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial

Chain B:



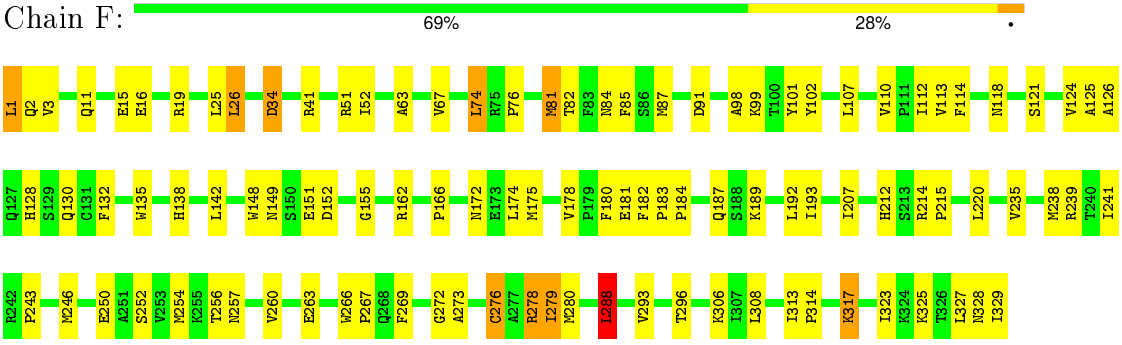
- Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial

Chain D:



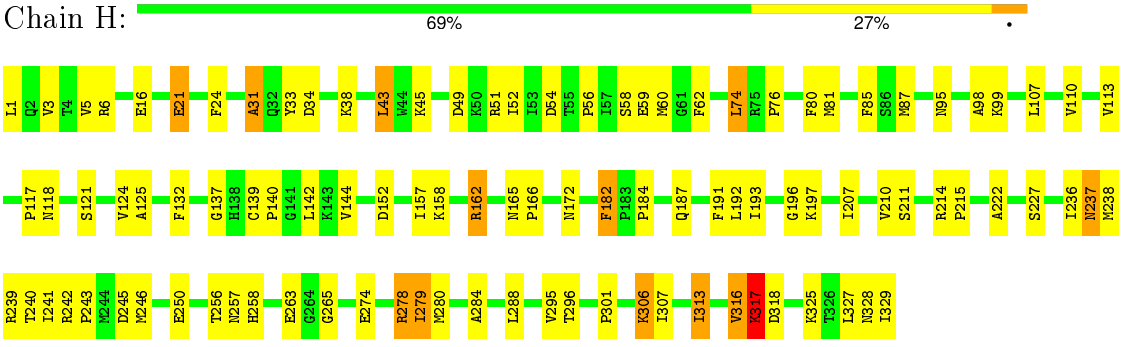
- Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial

Chain F:



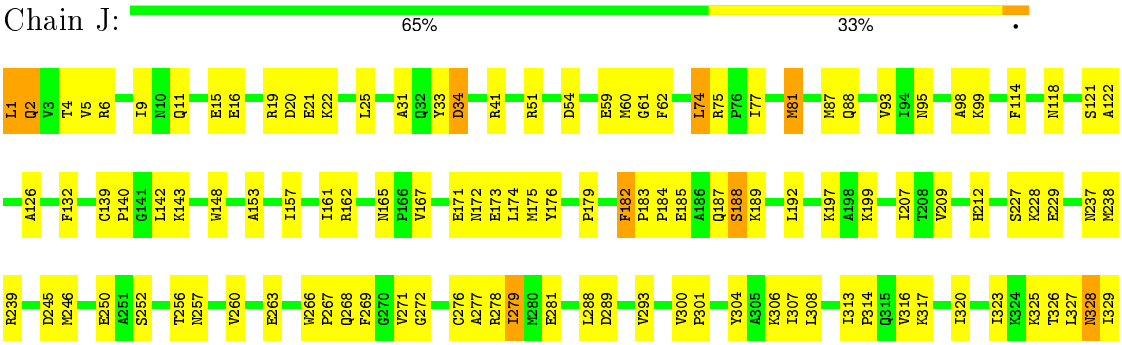
- Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial

Chain H:



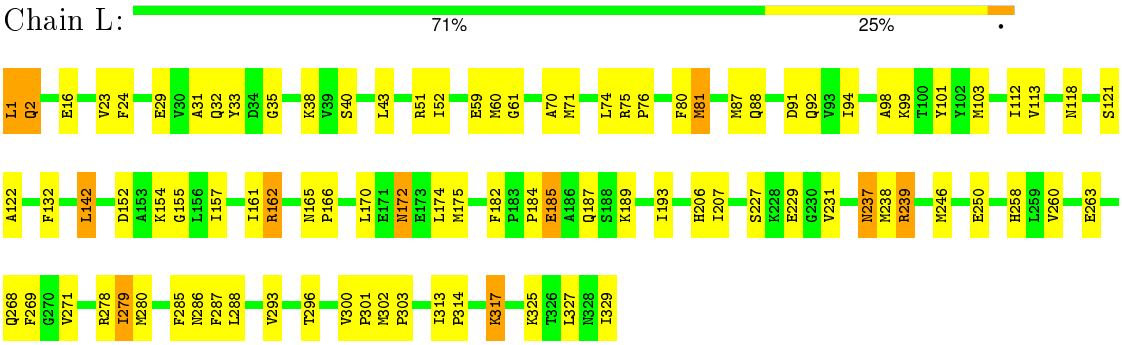
- Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial

Chain J:



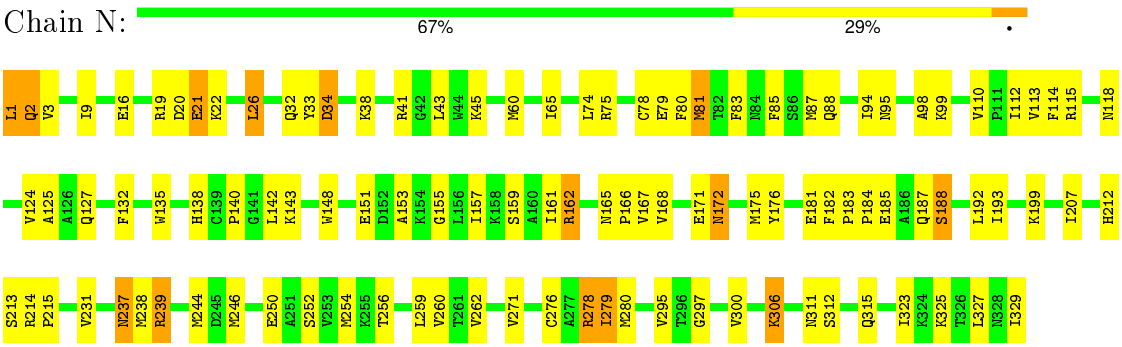
• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial

Chain L:



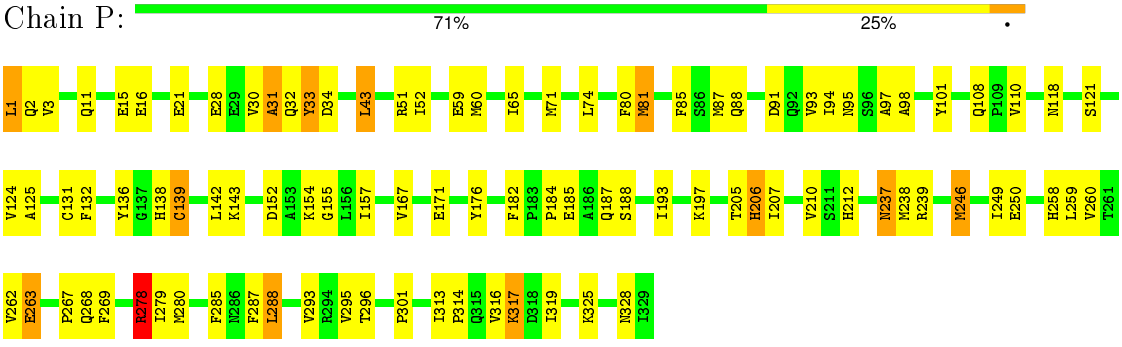
• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial

Chain N:



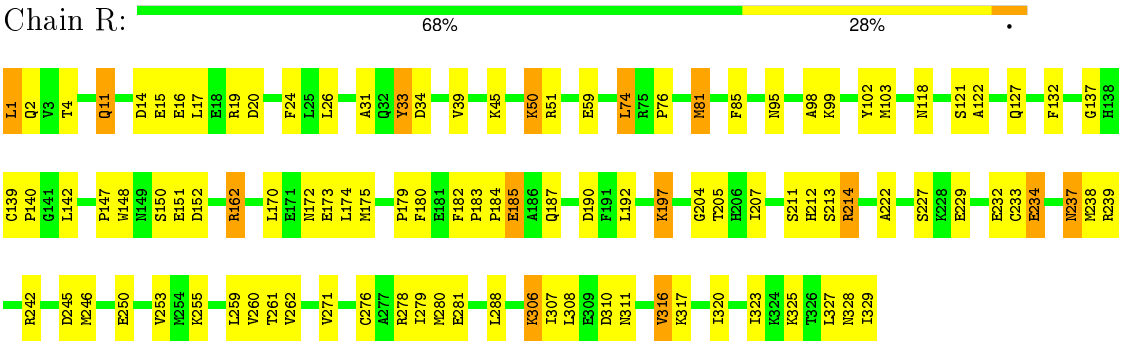
• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial

Chain P:



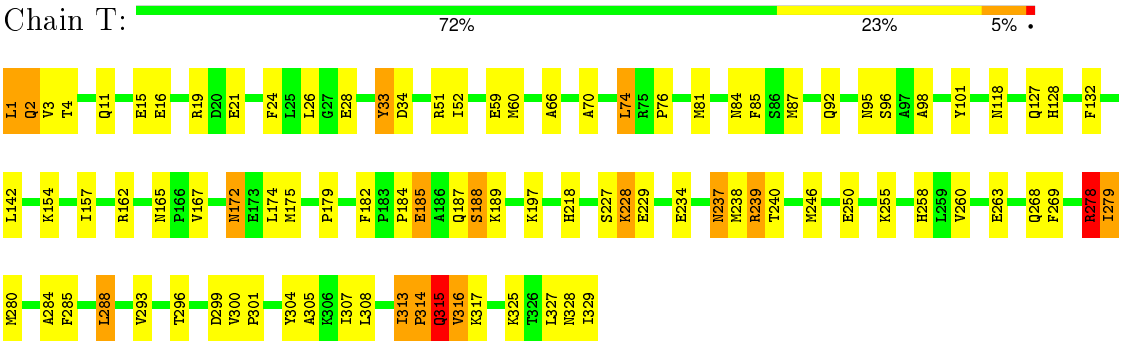
• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial

Chain R:



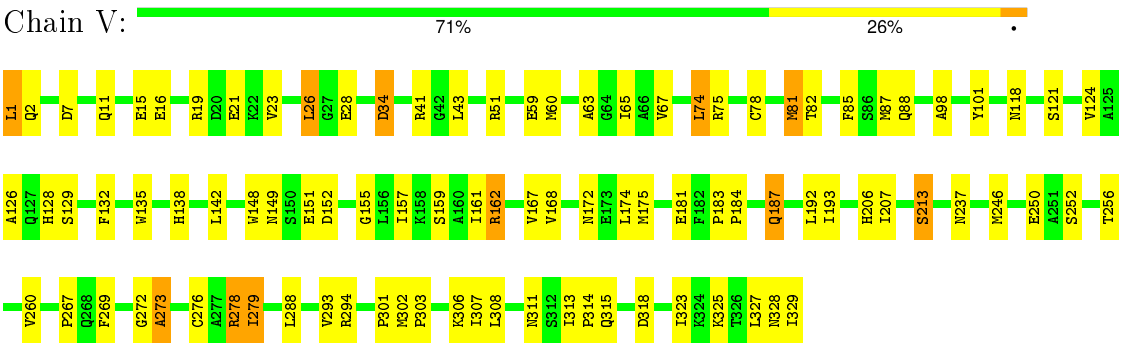
• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial

Chain T:



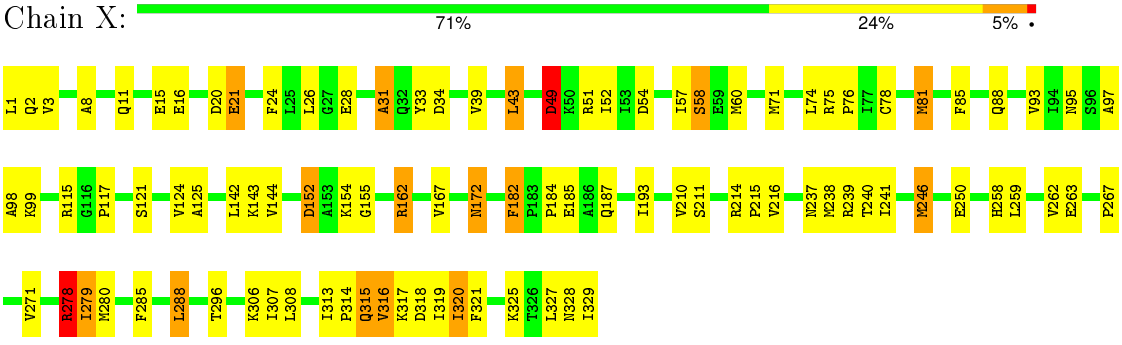
• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial

Chain V:



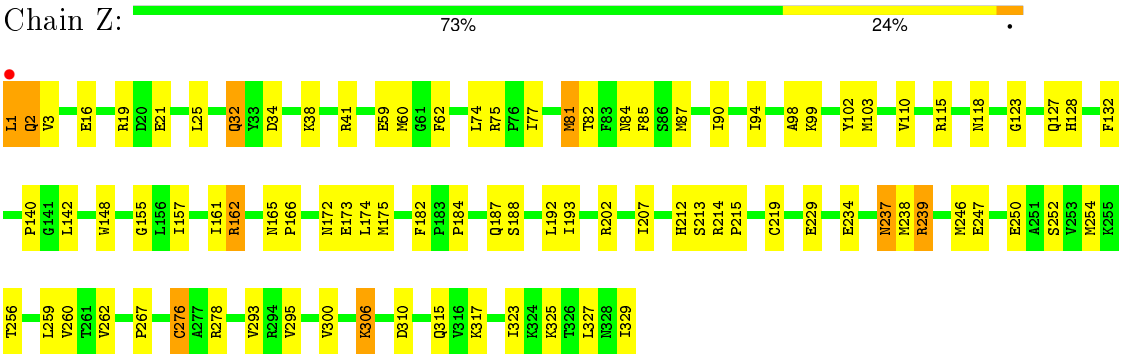
• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial

Chain X:



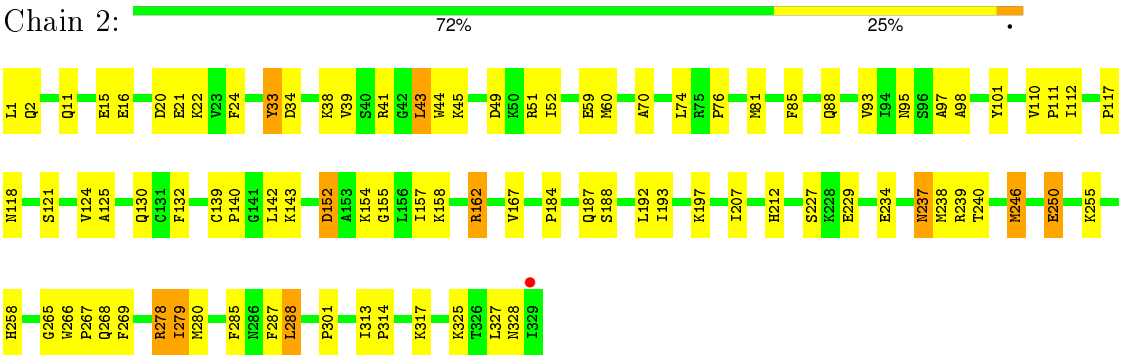
• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial

Chain Z:



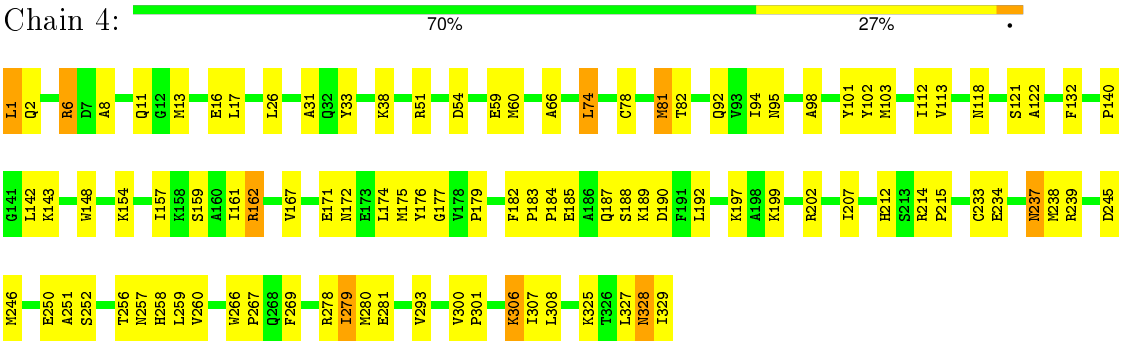
• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial

Chain 2:



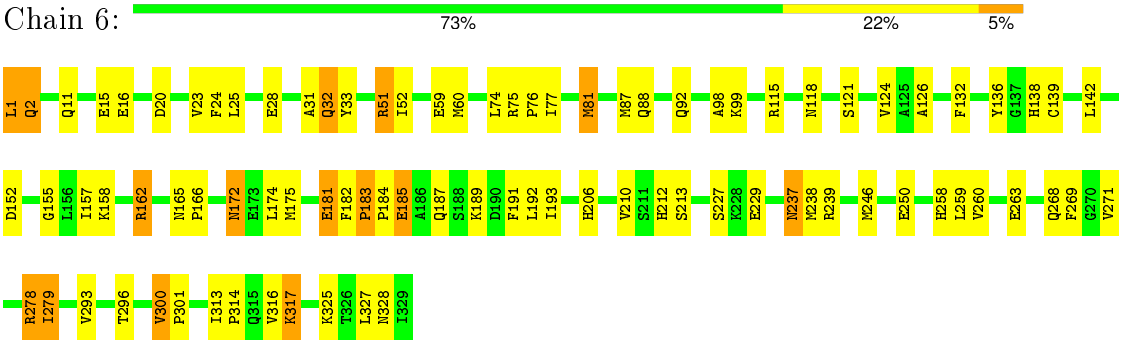
• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial

Chain 4:



• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial

Chain 6:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	119.28Å 128.29Å 228.41Å 90.14° 90.05° 90.02°	Depositor
Resolution (Å)	50.00 – 3.01 49.11 – 3.01	Depositor EDS
% Data completeness (in resolution range)	97.9 (50.00-3.01) 97.9 (49.11-3.01)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.43 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.4	Depositor
R, R_{free}	0.189 , 0.253 0.196 , 0.257	Depositor DCC
R_{free} test set	13221 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	56.5	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.429 for h,-k,-l 0.000 for -h,k,-l 0.000 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.36$	Xtriage
Outliers	0 of 262510 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	83339	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.55 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.1273e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: K

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	1	0.79	1/2663 (0.0%)	0.87	2/3583 (0.1%)
1	3	0.87	3/2725 (0.1%)	0.91	3/3666 (0.1%)
1	5	0.78	2/2764 (0.1%)	0.83	2/3720 (0.1%)
1	A	0.93	2/2727 (0.1%)	0.94	3/3669 (0.1%)
1	C	0.92	3/2727 (0.1%)	0.92	2/3669 (0.1%)
1	E	0.91	1/2780 (0.0%)	0.96	1/3742 (0.0%)
1	G	0.90	4/2763 (0.1%)	0.93	3/3718 (0.1%)
1	I	0.88	1/2743 (0.0%)	0.90	3/3691 (0.1%)
1	K	0.81	0/2764	0.85	1/3720 (0.0%)
1	M	0.90	3/2780 (0.1%)	0.93	2/3742 (0.1%)
1	O	0.81	0/2628	0.89	3/3537 (0.1%)
1	Q	0.86	1/2743 (0.0%)	0.93	5/3691 (0.1%)
1	S	0.86	0/2711	0.92	3/3648 (0.1%)
1	U	0.94	2/2775 (0.1%)	0.95	1/3734 (0.0%)
1	W	0.88	1/2756 (0.0%)	0.93	3/3708 (0.1%)
1	Y	0.93	2/2780 (0.1%)	0.93	1/3742 (0.0%)
2	2	0.90	2/2574 (0.1%)	0.93	2/3488 (0.1%)
2	4	0.87	1/2574 (0.0%)	0.93	1/3488 (0.0%)
2	6	0.90	2/2574 (0.1%)	0.94	7/3488 (0.2%)
2	B	1.00	3/2574 (0.1%)	0.98	3/3488 (0.1%)
2	D	0.95	0/2574	0.99	7/3488 (0.2%)
2	F	0.95	0/2574	0.94	3/3488 (0.1%)
2	H	0.93	1/2574 (0.0%)	0.93	1/3488 (0.0%)
2	J	0.89	1/2574 (0.0%)	0.92	2/3488 (0.1%)
2	L	0.90	0/2574	0.93	3/3488 (0.1%)
2	N	0.87	1/2574 (0.0%)	0.90	4/3488 (0.1%)
2	P	0.91	1/2574 (0.0%)	0.95	4/3488 (0.1%)
2	R	0.95	1/2574 (0.0%)	0.97	5/3488 (0.1%)
2	T	0.92	0/2574	0.96	5/3488 (0.1%)
2	V	0.91	1/2574 (0.0%)	0.94	1/3488 (0.0%)
2	X	0.90	0/2574	0.94	4/3488 (0.1%)
2	Z	0.87	2/2574 (0.1%)	0.88	3/3488 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	0.89	42/85013 (0.0%)	0.93	93/114788 (0.1%)

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Y	232	CYS	CB-SG	-10.74	1.64	1.82
1	5	232	CYS	CB-SG	-7.94	1.68	1.82
1	M	232	CYS	CB-SG	-7.92	1.68	1.82
2	B	276	CYS	CB-SG	-7.73	1.69	1.82
1	W	189	CYS	CB-SG	-7.02	1.70	1.82
1	I	283	SER	CB-OG	6.91	1.51	1.42
1	U	232	CYS	CB-SG	-6.63	1.71	1.82
2	Z	276	CYS	CB-SG	-6.60	1.71	1.82
2	N	276	CYS	CB-SG	-6.50	1.71	1.82
1	3	71	CYS	CB-SG	-6.42	1.71	1.82
1	C	305	GLU	CD-OE1	6.27	1.32	1.25
2	V	276	CYS	CB-SG	-6.25	1.71	1.82
2	R	233	CYS	CB-SG	-6.24	1.71	1.82
1	M	276	GLU	CB-CG	6.12	1.63	1.52
1	G	1	PHE	CE2-CZ	-6.07	1.25	1.37
1	C	329	GLU	CG-CD	6.01	1.60	1.51
1	C	244	CYS	CB-SG	-6.00	1.72	1.82
2	6	139	CYS	CB-SG	-5.88	1.72	1.81
1	Y	12	CYS	CB-SG	-5.77	1.72	1.81
2	P	139	CYS	CB-SG	-5.75	1.72	1.81
2	2	139	CYS	CB-SG	-5.69	1.72	1.81
2	Z	247	GLU	CG-CD	5.53	1.60	1.51
2	6	181	GLU	CG-CD	5.51	1.60	1.51
2	2	250	GLU	CG-CD	5.50	1.60	1.51
1	5	62	CYS	CB-SG	-5.46	1.73	1.81
2	J	139	CYS	CB-SG	-5.45	1.73	1.81
1	E	232	CYS	CB-SG	-5.35	1.73	1.81
2	B	315	GLN	CG-CD	5.33	1.63	1.51
1	U	62	CYS	CB-SG	-5.32	1.73	1.81
1	G	71	CYS	CB-SG	-5.26	1.73	1.81
1	M	276	GLU	CG-CD	5.23	1.59	1.51
1	1	232	CYS	CB-SG	-5.21	1.73	1.81
1	G	72	CYS	CB-SG	-5.21	1.73	1.81
1	Q	232	CYS	CB-SG	-5.18	1.73	1.81
2	H	113	VAL	CB-CG2	-5.14	1.42	1.52
1	A	244	CYS	CB-SG	-5.12	1.73	1.81
1	G	1	PHE	CG-CD1	-5.12	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	71	CYS	CB-SG	-5.05	1.73	1.81
2	B	250	GLU	CD-OE2	5.01	1.31	1.25
1	3	161	CYS	CB-SG	-5.01	1.73	1.81
2	4	33	TYR	CE1-CZ	5.01	1.45	1.38
1	3	189	CYS	CB-SG	-5.00	1.73	1.81

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	29	ARG	NE-CZ-NH1	10.01	125.31	120.30
2	P	278	ARG	NE-CZ-NH2	-9.34	115.63	120.30
2	P	278	ARG	NE-CZ-NH1	9.10	124.85	120.30
2	2	278	ARG	NE-CZ-NH2	-8.95	115.83	120.30
2	D	278	ARG	NE-CZ-NH2	-8.14	116.23	120.30
2	X	278	ARG	NE-CZ-NH1	7.78	124.19	120.30
2	T	278	ARG	NE-CZ-NH1	7.75	124.17	120.30
2	6	152	ASP	CB-CG-OD1	7.71	125.24	118.30
1	E	109	LEU	CB-CG-CD2	-7.14	98.86	111.00
1	O	90	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	Y	294	ARG	NE-CZ-NH1	-6.95	116.82	120.30
1	1	29	ARG	NE-CZ-NH1	-6.88	116.86	120.30
2	6	152	ASP	CB-CG-OD2	-6.87	112.11	118.30
2	N	239	ARG	NE-CZ-NH1	-6.75	116.93	120.30
1	W	29	ARG	NE-CZ-NH1	6.74	123.67	120.30
2	L	152	ASP	CB-CG-OD1	6.73	124.36	118.30
2	H	152	ASP	CB-CG-OD2	-6.71	112.26	118.30
2	4	6	ARG	NE-CZ-NH1	-6.63	116.99	120.30
2	D	75	ARG	NE-CZ-NH1	-6.45	117.08	120.30
2	F	26	LEU	CB-CG-CD1	-6.42	100.08	111.00
2	J	289	ASP	CB-CG-OD1	6.39	124.05	118.30
2	N	276	CYS	CA-CB-SG	-6.29	102.69	114.00
2	R	14	ASP	CB-CG-OD1	6.25	123.92	118.30
1	O	29	ARG	NE-CZ-NH1	6.20	123.40	120.30
2	D	19	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	C	29	ARG	NE-CZ-NH2	-6.13	117.23	120.30
2	N	75	ARG	NE-CZ-NH1	-6.03	117.29	120.30
1	W	187	LEU	CB-CG-CD1	-5.98	100.84	111.00
2	B	299	ASP	CB-CG-OD1	5.95	123.66	118.30
2	D	245	ASP	CB-CG-OD2	-5.94	112.96	118.30
1	A	29	ARG	NE-CZ-NH1	5.88	123.24	120.30
2	6	51	ARG	NE-CZ-NH1	-5.82	117.39	120.30
2	D	242	ARG	NE-CZ-NH1	-5.82	117.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	210	VAL	CB-CA-C	-5.81	100.36	111.40
2	P	71	MET	CG-SD-CE	5.78	109.44	100.20
2	Z	239	ARG	NE-CZ-NH1	-5.74	117.43	120.30
1	3	135	ASN	N-CA-C	-5.73	95.53	111.00
2	B	294	ARG	NE-CZ-NH2	5.72	123.16	120.30
2	6	115	ARG	NE-CZ-NH1	-5.72	117.44	120.30
1	Q	29	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	W	167	ASP	CB-CG-OD2	5.72	123.44	118.30
2	X	43	LEU	CB-CG-CD2	-5.70	101.31	111.00
1	S	29	ARG	NE-CZ-NH1	-5.66	117.47	120.30
1	O	90	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	5	64	LEU	CA-CB-CG	-5.61	102.39	115.30
2	T	299	ASP	CB-CG-OD1	5.60	123.34	118.30
1	K	162	LEU	CB-CG-CD2	-5.57	101.53	111.00
2	Z	75	ARG	NE-CZ-NH1	-5.57	117.52	120.30
1	I	29	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	S	135	ASN	N-CA-C	-5.53	96.08	111.00
1	3	71	CYS	CA-CB-SG	-5.53	104.05	114.00
2	T	314	PRO	N-CA-C	5.52	126.46	112.10
1	Q	234	ARG	NE-CZ-NH1	-5.46	117.57	120.30
2	J	6	ARG	NE-CZ-NH1	-5.45	117.58	120.30
2	2	41	ARG	NE-CZ-NH2	-5.45	117.58	120.30
2	F	276	CYS	CA-CB-SG	-5.38	104.31	114.00
2	T	19	ARG	NE-CZ-NH1	5.36	122.98	120.30
2	R	214	ARG	NE-CZ-NH1	5.34	122.97	120.30
2	6	139	CYS	CA-CB-SG	-5.34	104.39	114.00
1	S	64	LEU	CA-CB-CG	-5.33	103.03	115.30
2	L	239	ARG	NE-CZ-NH1	-5.33	117.63	120.30
1	Q	37	ARG	NE-CZ-NH1	-5.32	117.64	120.30
2	F	288	LEU	CB-CG-CD2	-5.32	101.96	111.00
2	V	288	LEU	CB-CG-CD2	-5.31	101.97	111.00
1	Q	64	LEU	CA-CB-CG	-5.30	103.10	115.30
2	N	113	VAL	CB-CA-C	-5.26	101.41	111.40
2	D	51	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	U	134	GLY	N-CA-C	-5.24	100.01	113.10
1	G	75	LEU	CB-CG-CD1	5.23	119.90	111.00
2	Z	276	CYS	CA-CB-SG	-5.21	104.61	114.00
1	M	252	LEU	CB-CG-CD1	-5.21	102.14	111.00
2	R	278	ARG	NE-CZ-NH2	-5.20	117.70	120.30
2	6	210	VAL	CB-CA-C	-5.19	101.54	111.40
1	A	64	LEU	CA-CB-CG	-5.19	103.37	115.30
2	R	316	VAL	CB-CA-C	-5.18	101.55	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	R	152	ASP	CB-CG-OD1	5.17	122.96	118.30
1	Q	134	GLY	N-CA-C	-5.16	100.20	113.10
2	L	152	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	G	98	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	5	252	LEU	CB-CG-CD1	-5.14	102.26	111.00
2	6	279	ILE	CG1-CB-CG2	-5.14	100.10	111.40
2	X	152	ASP	CB-CG-OD2	-5.13	113.69	118.30
1	G	167	ASP	CB-CG-OD2	5.12	122.91	118.30
1	M	33	LEU	CB-CG-CD2	-5.11	102.32	111.00
2	B	247	GLU	CA-CB-CG	5.09	124.59	113.40
1	I	135	ASN	N-CA-C	-5.06	97.33	111.00
2	T	239	ARG	NE-CZ-NH1	-5.06	117.77	120.30
1	1	29	ARG	CD-NE-CZ	5.06	130.68	123.60
2	P	210	VAL	CB-CA-C	-5.05	101.80	111.40
1	A	33	LEU	CA-CB-CG	-5.04	103.70	115.30
2	X	115	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	I	71	CYS	CA-CB-SG	-5.01	104.98	114.00
1	3	29	ARG	NE-CZ-NH1	5.00	122.80	120.30

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	1	2614	0	2587	120	0
1	3	2676	0	2644	123	0
1	5	2712	0	2679	115	0
1	A	2677	0	2645	136	0
1	C	2677	0	2645	116	0
1	E	2728	0	2693	93	0
1	G	2712	0	2681	103	0
1	I	2693	0	2660	88	0
1	K	2712	0	2679	97	0
1	M	2728	0	2693	97	0
1	O	2580	0	2552	119	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Q	2693	0	2660	122	0
1	S	2661	0	2630	130	0
1	U	2723	0	2692	87	0
1	W	2705	0	2672	95	0
1	Y	2728	0	2693	93	0
2	2	2519	0	2517	72	0
2	4	2519	0	2517	82	0
2	6	2519	0	2517	74	0
2	B	2519	0	2517	60	0
2	D	2519	0	2517	77	0
2	F	2519	0	2517	86	0
2	H	2519	0	2517	81	0
2	J	2519	0	2517	85	0
2	L	2519	0	2517	79	0
2	N	2519	0	2517	78	0
2	P	2519	0	2517	70	0
2	R	2519	0	2517	77	0
2	T	2519	0	2517	81	0
2	V	2519	0	2517	73	0
2	X	2519	0	2517	79	0
2	Z	2519	0	2517	70	0
3	2	1	0	0	0	0
3	4	1	0	0	0	0
3	6	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
3	J	1	0	0	0	0
3	L	1	0	0	0	0
3	N	1	0	0	0	0
3	P	1	0	0	0	0
3	R	1	0	0	0	0
3	T	1	0	0	0	0
3	V	1	0	0	0	0
3	X	1	0	0	0	0
3	Z	1	0	0	0	0
All	All	83339	0	82777	2778	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 17.

All (2778) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:231:LEU:HD12	1:O:294:ARG:NH1	1.20	1.50
1:A:289:MET:CE	1:A:290:LEU:HD23	1.60	1.30
1:G:270:VAL:HG12	1:G:273:ARG:NH2	1.51	1.22
1:M:268:PRO:HB2	1:M:270:VAL:HG23	1.21	1.17
1:1:280:GLU:HG2	1:1:281:VAL:N	1.55	1.17
2:F:246:MET:CE	2:F:279:ILE:HD13	1.73	1.16
1:A:18:GLU:HG2	1:A:19:GLU:H	1.06	1.16
1:S:28:THR:CG2	1:S:30:GLU:HB2	1.76	1.15
1:5:230:ILE:HG23	1:5:231:LEU:HD23	1.28	1.14
1:A:289:MET:HE2	1:A:290:LEU:HD23	1.14	1.13
1:S:28:THR:HG21	1:S:30:GLU:CB	1.77	1.13
1:Q:18:GLU:HG2	1:Q:19:GLU:H	1.10	1.13
1:3:69:GLU:O	1:3:73:VAL:HG23	1.47	1.12
1:Y:268:PRO:HB2	1:Y:270:VAL:HG12	1.20	1.12
1:S:278:ILE:CD1	1:S:278:ILE:H	1.60	1.12
1:S:278:ILE:HD12	1:S:278:ILE:H	1.07	1.11
1:S:28:THR:CG2	1:S:30:GLU:CB	2.29	1.11
1:O:231:LEU:CD1	1:O:294:ARG:NH1	2.17	1.07
1:5:275:ARG:HG3	1:5:275:ARG:NH1	1.58	1.07
1:S:28:THR:HG22	1:S:30:GLU:N	1.68	1.07
1:M:230:ILE:HG13	1:M:230:ILE:O	1.54	1.07
1:M:267:ASP:CB	1:M:268:PRO:HD2	1.84	1.06
1:Y:267:ASP:CB	1:Y:268:PRO:HD3	1.84	1.06
1:5:270:VAL:O	1:5:274:THR:HG23	1.52	1.06
1:1:197:ARG:HB3	1:1:197:ARG:HH11	1.20	1.05
1:A:289:MET:CE	1:A:290:LEU:CD2	2.34	1.05
1:G:272:TYR:HD1	1:G:273:ARG:N	1.53	1.04
1:U:88:ALA:O	1:U:134:GLY:HA2	1.57	1.04
1:M:268:PRO:HB2	1:M:270:VAL:CG2	1.87	1.03
2:N:279:ILE:HG22	2:N:280:MET:N	1.73	1.03
1:5:275:ARG:HH11	1:5:275:ARG:HG3	0.86	1.03
1:5:275:ARG:HH11	1:5:275:ARG:CG	1.71	1.01
1:U:327:ASP:OD1	1:U:328:PRO:HD2	1.60	1.01
1:A:197:ARG:HH11	1:A:197:ARG:HB3	1.23	1.01
1:M:267:ASP:CB	1:M:268:PRO:CD	2.39	1.00
2:N:278:ARG:HH11	2:N:278:ARG:CG	1.75	1.00
2:D:313:ILE:HG22	2:D:314:PRO:HD2	1.44	1.00
1:A:289:MET:HE2	1:A:290:LEU:CD2	1.90	0.99
2:F:246:MET:HE1	2:F:279:ILE:HD13	1.45	0.99
2:N:278:ARG:HG3	2:N:278:ARG:NH1	1.75	0.99
1:K:275:ARG:HG2	1:K:275:ARG:HH11	1.27	0.98
1:K:98:ARG:HG2	1:K:131:PHE:HB2	1.44	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:LYS:O	1:A:285:SER:HB3	1.61	0.98
1:1:196:ASN:HB3	1:1:257:THR:HG23	1.42	0.98
1:S:278:ILE:N	1:S:278:ILE:HD12	1.70	0.98
2:2:184:PRO:HA	2:2:187:GLN:HE21	1.25	0.98
2:Z:1:LEU:HD13	2:Z:2:GLN:H	1.28	0.97
2:V:313:ILE:HG23	2:V:314:PRO:HD2	1.46	0.97
1:Q:18:GLU:HG2	1:Q:19:GLU:N	1.80	0.97
1:5:29:ARG:HG3	1:5:29:ARG:HH11	1.30	0.97
1:G:272:TYR:CD1	1:G:273:ARG:N	2.33	0.96
1:3:39:MET:HG2	1:3:73:VAL:HG21	1.45	0.96
1:G:327:ASP:OD1	1:G:328:PRO:HD2	1.65	0.96
1:O:229:ASP:OD1	1:O:231:LEU:HB2	1.64	0.96
1:Y:267:ASP:CB	1:Y:268:PRO:CD	2.44	0.96
1:S:28:THR:HG21	1:S:30:GLU:HB3	1.43	0.95
1:Q:45:MET:HE3	1:Q:102:VAL:HG13	1.46	0.95
1:3:68:GLN:HE21	1:3:259:ARG:HB3	1.30	0.95
1:G:131:PHE:CE2	1:G:133:GLY:HA2	2.02	0.94
1:A:18:GLU:HG2	1:A:19:GLU:N	1.82	0.94
2:V:278:ARG:HH11	2:V:278:ARG:HG3	1.32	0.94
1:S:29:ARG:HA	1:S:300:LEU:HD22	1.49	0.94
1:E:216:ARG:HG3	1:E:216:ARG:HH11	1.30	0.93
1:C:229:ASP:O	1:C:233:VAL:HG23	1.68	0.93
1:C:68:GLN:HE21	1:C:259:ARG:HB3	1.31	0.93
2:N:278:ARG:HG3	2:N:278:ARG:HH11	1.31	0.92
2:T:278:ARG:HH11	2:T:278:ARG:HG3	1.31	0.92
1:K:11:LYS:HB3	1:K:23:VAL:HG12	1.52	0.92
1:G:270:VAL:HG12	1:G:273:ARG:HH22	1.10	0.91
1:O:231:LEU:HD12	1:O:294:ARG:HH11	1.13	0.91
1:A:16:ARG:HG2	1:A:16:ARG:HH11	1.34	0.91
2:6:98:ALA:HB2	2:6:142:LEU:HD13	1.52	0.91
1:G:98:ARG:HG2	1:G:131:PHE:HB2	1.53	0.91
1:G:196:ASN:HB3	1:G:257:THR:HG23	1.53	0.90
1:3:354:TRP:CZ2	2:6:325:LYS:HG2	2.07	0.90
1:3:68:GLN:NE2	1:3:259:ARG:HB3	1.87	0.90
2:X:278:ARG:HG3	2:X:278:ARG:HH11	1.35	0.90
1:W:68:GLN:HE21	1:W:259:ARG:HB3	1.36	0.90
2:B:118:ASN:HD21	2:B:132:PHE:H	1.16	0.90
1:E:45:MET:HE1	1:E:105:ILE:HD12	1.51	0.90
1:C:196:ASN:HB3	1:C:257:THR:HG23	1.53	0.89
1:S:28:THR:O	1:S:28:THR:HG22	1.70	0.89
1:3:113:LYS:HD2	1:3:328:PRO:HG2	1.52	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:246:MET:CE	2:F:279:ILE:CD1	2.50	0.89
2:R:212:HIS:HB3	2:R:238:MET:HE3	1.55	0.89
1:S:88:ALA:O	1:S:134:GLY:HA2	1.73	0.89
1:G:272:TYR:CD1	1:G:272:TYR:C	2.47	0.88
1:S:29:ARG:CA	1:S:300:LEU:HD22	2.02	0.88
1:S:274:THR:O	1:S:278:ILE:HD13	1.73	0.88
1:Q:289:MET:CE	1:Q:290:LEU:HD23	2.03	0.88
1:Q:284:LYS:O	1:Q:285:SER:HB3	1.71	0.88
1:K:45:MET:HE3	1:K:102:VAL:HG22	1.55	0.88
1:M:274:THR:O	1:M:277:GLU:HB3	1.74	0.88
2:4:1:LEU:HD13	2:4:2:GLN:H	1.37	0.88
1:O:197:ARG:HB3	1:O:197:ARG:HH11	1.37	0.88
1:A:197:ARG:NH1	1:A:197:ARG:HB3	1.88	0.87
1:K:334:GLU:HG2	1:K:337:TYR:CE2	2.09	0.87
1:O:231:LEU:HD12	1:O:294:ARG:HH12	1.35	0.87
2:P:184:PRO:HA	2:P:187:GLN:HE21	1.39	0.87
1:3:284:LYS:HB3	1:3:284:LYS:NZ	1.89	0.87
1:K:88:ALA:O	1:K:134:GLY:HA2	1.74	0.87
1:Y:270:VAL:HG22	1:Y:270:VAL:O	1.74	0.86
1:1:303:VAL:HG13	1:1:304:GLU:OE2	1.76	0.86
1:O:196:ASN:HB3	1:O:257:THR:HG23	1.57	0.86
1:A:16:ARG:CG	1:A:16:ARG:HH11	1.89	0.86
1:5:98:ARG:HG2	1:5:131:PHE:HB2	1.57	0.85
1:S:68:GLN:HE21	1:S:259:ARG:HB3	1.41	0.85
1:M:268:PRO:CB	1:M:270:VAL:HG23	2.07	0.85
1:M:334:GLU:HG2	1:M:337:TYR:CE2	2.12	0.85
1:W:131:PHE:CE2	1:W:133:GLY:HA2	2.10	0.85
2:H:98:ALA:HB2	2:H:142:LEU:HD13	1.59	0.85
1:5:269:GLY:O	1:5:273:ARG:HD3	1.77	0.84
1:5:182:ALA:HA	1:5:187:LEU:HD12	1.59	0.84
1:E:131:PHE:CE2	1:E:133:GLY:HA2	2.11	0.84
1:M:131:PHE:CE2	1:M:133:GLY:HA2	2.12	0.84
1:G:55:GLN:O	1:G:56:LYS:HB2	1.75	0.84
1:S:28:THR:HG21	1:S:30:GLU:HB2	1.45	0.84
2:2:184:PRO:HA	2:2:187:GLN:NE2	1.91	0.83
2:R:325:LYS:HG2	1:S:354:TRP:CZ2	2.13	0.83
1:S:277:GLU:O	1:S:281:VAL:HG23	1.77	0.83
1:M:45:MET:HE1	1:M:105:ILE:HD12	1.59	0.83
1:5:269:GLY:HA3	1:5:273:ARG:NH1	1.94	0.83
1:I:113:LYS:HD3	1:I:328:PRO:HG2	1.59	0.83
1:1:88:ALA:O	1:1:134:GLY:HA2	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:45:MET:HE1	1:K:105:ILE:HD12	1.61	0.83
1:A:45:MET:HE3	1:A:102:VAL:HG13	1.59	0.83
1:5:45:MET:HE3	1:5:102:VAL:HG22	1.61	0.83
2:F:98:ALA:HB2	2:F:142:LEU:HD13	1.60	0.83
1:U:289:MET:HE2	1:U:290:LEU:HD23	1.59	0.82
1:Y:334:GLU:HG2	1:Y:337:TYR:CE2	2.13	0.82
1:E:334:GLU:HG2	1:E:337:TYR:CE2	2.14	0.82
2:N:118:ASN:HD21	2:N:132:PHE:H	1.26	0.82
2:N:278:ARG:NH1	2:N:278:ARG:CG	2.38	0.82
1:Y:270:VAL:CG2	1:Y:270:VAL:O	2.28	0.82
1:1:68:GLN:HE21	1:1:259:ARG:HB3	1.44	0.82
1:G:272:TYR:HA	1:G:275:ARG:HD3	1.60	0.82
1:O:229:ASP:C	1:O:231:LEU:H	1.82	0.81
1:5:230:ILE:HG23	1:5:231:LEU:CD2	2.09	0.81
1:W:98:ARG:HG2	1:W:131:PHE:HB2	1.62	0.81
1:U:84:HIS:CE1	1:U:130:ASN:ND2	2.48	0.81
2:T:278:ARG:NH1	2:T:278:ARG:HG3	1.90	0.81
2:F:329:ILE:OXT	2:F:329:ILE:HG13	1.80	0.81
1:1:100:LEU:HD13	1:1:128:ALA:HB2	1.60	0.81
2:V:313:ILE:HG23	2:V:314:PRO:CD	2.10	0.81
1:W:196:ASN:HB3	1:W:257:THR:HG23	1.62	0.81
1:O:230:ILE:HD12	1:O:230:ILE:O	1.79	0.81
2:B:280:MET:HE1	2:D:276:CYS:HB3	1.62	0.81
1:1:231:LEU:HD12	1:1:294:ARG:NH1	1.95	0.81
1:K:289:MET:CE	1:K:290:LEU:HD23	2.10	0.81
2:F:1:LEU:HD13	2:F:2:GLN:H	1.46	0.81
1:Q:289:MET:HE2	1:Q:290:LEU:HD23	1.61	0.81
2:F:246:MET:HE3	2:F:279:ILE:HD13	1.62	0.80
1:K:113:LYS:HD3	1:K:328:PRO:HG2	1.63	0.80
1:U:101:SER:OG	1:U:104:GLU:HG3	1.81	0.80
1:3:274:THR:HB	1:3:276:GLU:HG3	1.63	0.80
1:W:55:GLN:O	1:W:56:LYS:HB2	1.81	0.80
1:3:258:TYR:CE2	1:3:277:GLU:OE2	2.34	0.80
2:T:313:ILE:HG22	2:T:314:PRO:HD2	1.62	0.80
2:P:11:GLN:O	2:P:15:GLU:HG3	1.81	0.80
2:X:184:PRO:HA	2:X:187:GLN:NE2	1.97	0.80
2:V:278:ARG:NH1	2:V:278:ARG:HG3	1.92	0.80
1:5:269:GLY:C	1:5:273:ARG:NH1	2.35	0.80
2:V:98:ALA:HB2	2:V:142:LEU:HD13	1.62	0.80
1:Y:268:PRO:HB2	1:Y:270:VAL:CG1	2.07	0.80
1:K:327:ASP:OD1	1:K:328:PRO:HD2	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:TRP:CZ2	2:D:325:LYS:HG2	2.18	0.79
2:N:279:ILE:CG2	2:N:280:MET:N	2.45	0.79
1:U:334:GLU:HG2	1:U:337:TYR:CE2	2.18	0.79
1:K:131:PHE:CE2	1:K:133:GLY:HA2	2.18	0.79
1:Q:29:ARG:HH11	1:Q:29:ARG:HG3	1.48	0.79
1:M:45:MET:HE3	1:M:102:VAL:HG13	1.64	0.79
1:U:88:ALA:O	1:U:134:GLY:CA	2.31	0.79
1:C:88:ALA:O	1:C:134:GLY:HA2	1.83	0.79
1:S:45:MET:HE3	1:S:102:VAL:HG13	1.63	0.79
1:5:334:GLU:HG2	1:5:337:TYR:CE2	2.18	0.79
2:L:98:ALA:HB2	2:L:142:LEU:CD1	2.12	0.78
2:6:184:PRO:HA	2:6:187:GLN:NE2	1.98	0.78
1:U:289:MET:CE	1:U:290:LEU:HD23	2.13	0.78
1:O:29:ARG:HB2	1:O:300:LEU:HD22	1.64	0.78
1:Q:68:GLN:HE21	1:Q:259:ARG:HB3	1.48	0.78
1:3:69:GLU:O	1:3:73:VAL:CG2	2.30	0.78
1:O:280:GLU:HG2	1:O:281:VAL:N	1.98	0.78
2:V:207:ILE:HD13	2:V:323:ILE:HG23	1.64	0.78
1:O:230:ILE:CD1	1:O:230:ILE:O	2.31	0.78
1:W:334:GLU:HG2	1:W:337:TYR:CE2	2.19	0.78
1:Q:197:ARG:HH11	1:Q:197:ARG:HB3	1.46	0.77
1:Y:230:ILE:HG13	1:Y:230:ILE:O	1.84	0.77
1:5:113:LYS:HD3	1:5:328:PRO:HG2	1.66	0.77
1:C:234:ARG:NE	1:C:238:ARG:NH2	2.32	0.77
1:A:289:MET:HE3	1:A:290:LEU:HD23	1.63	0.77
1:E:57:ILE:HD13	1:E:57:ILE:N	1.98	0.77
1:5:131:PHE:CE2	1:5:133:GLY:HA2	2.18	0.77
2:V:118:ASN:HD21	2:V:132:PHE:H	1.28	0.77
1:G:270:VAL:CG1	1:G:273:ARG:HH22	1.95	0.77
1:O:71:CYS:O	1:O:75:LEU:HB2	1.84	0.77
1:I:113:LYS:CD	1:I:328:PRO:HG2	2.13	0.77
1:5:88:ALA:O	1:5:134:GLY:HA2	1.84	0.77
1:U:45:MET:HE1	1:U:105:ILE:HD12	1.67	0.77
2:N:207:ILE:HD13	2:N:323:ILE:HG23	1.66	0.77
1:O:230:ILE:CG1	1:O:230:ILE:O	2.32	0.77
2:B:280:MET:CE	2:D:276:CYS:HB3	2.15	0.77
1:K:182:ALA:HA	1:K:187:LEU:HD12	1.67	0.77
2:2:121:SER:HB3	2:2:124:VAL:HG21	1.65	0.77
2:V:329:ILE:OXT	2:V:329:ILE:HG13	1.83	0.77
1:Q:29:ARG:CG	1:Q:29:ARG:HH11	1.98	0.76
1:S:37:ARG:CG	1:S:37:ARG:HH11	1.98	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:196:ASN:HB3	1:5:257:THR:HG23	1.67	0.76
1:S:28:THR:HG22	1:S:30:GLU:CA	2.15	0.76
1:M:223:LEU:N	1:M:223:LEU:HD23	2.00	0.76
2:P:118:ASN:HD21	2:P:132:PHE:H	1.31	0.76
2:V:278:ARG:CG	2:V:278:ARG:HH11	1.98	0.76
2:D:11:GLN:O	2:D:15:GLU:HG3	1.86	0.76
1:S:196:ASN:HB3	1:S:257:THR:HG23	1.66	0.76
2:F:327:LEU:O	2:F:329:ILE:HG23	1.86	0.76
1:5:277:GLU:O	1:5:281:VAL:HG23	1.86	0.76
1:G:72:CYS:HB2	1:G:97:THR:HG21	1.68	0.76
1:E:88:ALA:O	1:E:134:GLY:HA2	1.86	0.76
1:A:29:ARG:HA	1:A:300:LEU:HD22	1.68	0.76
2:B:118:ASN:HD21	2:B:132:PHE:N	1.84	0.75
2:H:184:PRO:HA	2:H:187:GLN:NE2	2.02	0.75
1:W:10:LYS:HG2	1:W:11:LYS:N	2.00	0.75
2:X:11:GLN:O	2:X:15:GLU:HG3	1.87	0.75
1:K:100:LEU:HD13	1:K:128:ALA:HB2	1.69	0.75
1:M:272:TYR:C	1:M:272:TYR:CD1	2.60	0.75
1:A:231:LEU:HD12	1:A:294:ARG:NH1	2.01	0.75
1:I:204:VAL:HG23	1:I:205:GLU:H	1.50	0.75
1:C:95:THR:CG2	1:C:100:LEU:HD22	2.15	0.75
1:G:270:VAL:CG1	1:G:273:ARG:NH2	2.43	0.75
1:A:29:ARG:CG	1:A:29:ARG:HH11	1.99	0.75
1:1:280:GLU:CG	1:1:281:VAL:N	2.40	0.74
1:O:230:ILE:HG13	1:O:230:ILE:O	1.86	0.74
1:O:229:ASP:O	1:O:231:LEU:N	2.20	0.74
1:C:253:MET:HE3	1:C:255:LEU:CD1	2.16	0.74
1:3:196:ASN:HB3	1:3:257:THR:HG23	1.69	0.74
1:5:269:GLY:CA	1:5:273:ARG:NH1	2.50	0.74
1:C:29:ARG:HD2	1:C:300:LEU:O	1.88	0.74
1:G:88:ALA:O	1:G:134:GLY:HA2	1.88	0.74
2:L:238:MET:O	2:L:239:ARG:HB2	1.86	0.74
1:G:150:LEU:HA	1:G:187:LEU:HD22	1.70	0.74
1:Q:197:ARG:HB3	1:Q:197:ARG:NH1	2.02	0.73
1:A:10:LYS:HG2	1:A:11:LYS:N	2.02	0.73
1:I:354:TRP:CZ2	2:L:325:LYS:HG2	2.23	0.73
1:A:334:GLU:HG2	1:A:337:TYR:CE2	2.23	0.73
2:J:143:LYS:HB2	2:J:167:VAL:HG22	1.69	0.73
1:5:11:LYS:HB3	1:5:23:VAL:HG13	1.69	0.73
1:Q:88:ALA:O	1:Q:134:GLY:HA2	1.87	0.73
1:1:3:ASN:O	1:1:4:ASP:HB3	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:207:ILE:HD13	2:R:323:ILE:HG23	1.70	0.73
1:K:275:ARG:HG2	1:K:275:ARG:NH1	2.01	0.73
1:C:68:GLN:NE2	1:C:259:ARG:HB3	2.03	0.73
2:J:246:MET:O	2:J:250:GLU:HG3	1.89	0.73
1:I:55:GLN:O	1:I:56:LYS:HB2	1.88	0.73
2:T:316:VAL:CG1	2:T:316:VAL:O	2.37	0.73
1:M:327:ASP:OD1	1:M:328:PRO:HD2	1.89	0.73
1:K:29:ARG:HH11	1:K:29:ARG:HG3	1.54	0.73
1:S:95:THR:CG2	1:S:100:LEU:HD22	2.18	0.73
2:V:252:SER:O	2:V:256:THR:HG23	1.89	0.73
1:3:29:ARG:HA	1:3:300:LEU:HD22	1.69	0.73
1:Y:268:PRO:CB	1:Y:270:VAL:HG12	2.10	0.72
1:M:88:ALA:O	1:M:134:GLY:HA2	1.88	0.72
1:K:196:ASN:HB3	1:K:257:THR:HG23	1.69	0.72
1:S:28:THR:CG2	1:S:30:GLU:N	2.48	0.72
1:E:142:VAL:HG21	1:E:175:ILE:HG12	1.72	0.72
2:D:313:ILE:CG2	2:D:314:PRO:HD2	2.19	0.72
2:N:110:VAL:O	2:N:166:PRO:HD3	1.88	0.72
1:3:55:GLN:O	1:3:56:LYS:HB2	1.88	0.72
1:U:354:TRP:CZ2	2:X:325:LYS:HG2	2.25	0.72
1:C:29:ARG:CA	1:C:300:LEU:HD22	2.19	0.72
1:U:74:GLY:HA3	1:U:233:VAL:CG1	2.19	0.72
1:W:88:ALA:O	1:W:134:GLY:HA2	1.90	0.72
1:5:268:PRO:O	1:5:271:ALA:HB3	1.90	0.71
2:R:99:LYS:O	2:R:103:MET:HG3	1.90	0.71
1:C:45:MET:HE3	1:C:102:VAL:HG13	1.73	0.71
2:F:1:LEU:HD13	2:F:2:GLN:N	2.03	0.71
1:3:274:THR:CB	1:3:276:GLU:HG3	2.20	0.71
1:O:100:LEU:HD13	1:O:128:ALA:HB2	1.70	0.71
1:5:270:VAL:O	1:5:274:THR:CG2	2.35	0.71
1:5:269:GLY:HA3	1:5:273:ARG:HH12	1.56	0.71
1:A:318:GLU:HG2	2:P:287:PHE:CE2	2.26	0.71
2:F:207:ILE:HD13	2:F:323:ILE:HG23	1.71	0.71
1:K:11:LYS:HB3	1:K:23:VAL:CG1	2.21	0.71
2:D:39:VAL:HG11	2:D:115:ARG:NH2	2.05	0.71
2:Z:212:HIS:HB3	2:Z:238:MET:HE3	1.73	0.71
2:P:121:SER:HB3	2:P:124:VAL:CG2	2.21	0.71
1:S:27:LEU:HD22	1:S:28:THR:N	2.05	0.71
1:C:230:ILE:HG13	1:C:230:ILE:O	1.89	0.71
1:O:45:MET:HE3	1:O:102:VAL:HG13	1.73	0.70
2:R:118:ASN:HD21	2:R:132:PHE:H	1.35	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:72:CYS:HB2	1:3:97:THR:HG21	1.73	0.70
1:G:196:ASN:HD21	1:G:259:ARG:HE	1.39	0.70
2:Z:115:ARG:HD2	2:Z:157:ILE:HD11	1.73	0.70
1:M:280:GLU:OE1	1:M:280:GLU:C	2.30	0.70
1:1:231:LEU:HD12	1:1:294:ARG:HH11	1.54	0.70
1:A:29:ARG:HH11	1:A:29:ARG:HG3	1.57	0.70
1:1:29:ARG:HH11	1:1:29:ARG:HG2	1.56	0.70
2:V:34:ASP:OD2	2:V:41:ARG:HA	1.91	0.70
2:F:118:ASN:HD21	2:F:132:PHE:H	1.39	0.70
1:O:29:ARG:HB2	1:O:300:LEU:CD2	2.21	0.70
2:H:16:GLU:OE2	2:H:162:ARG:NH1	2.25	0.70
2:P:121:SER:HB3	2:P:124:VAL:HG21	1.72	0.70
1:O:280:GLU:O	1:O:283:SER:N	2.25	0.70
2:D:185:GLU:HG2	2:D:185:GLU:O	1.88	0.69
1:1:280:GLU:HG2	1:1:281:VAL:H	1.53	0.69
1:M:131:PHE:CZ	1:M:133:GLY:HA2	2.28	0.69
1:Q:354:TRP:CZ2	2:T:325:LYS:HG2	2.27	0.69
2:N:327:LEU:O	2:N:329:ILE:HG23	1.92	0.69
1:M:196:ASN:ND2	1:M:259:ARG:HE	1.89	0.69
2:2:193:ILE:HD13	2:2:239:ARG:NH2	2.07	0.69
2:N:250:GLU:O	2:N:254:MET:HG3	1.91	0.69
2:P:184:PRO:HA	2:P:187:GLN:NE2	2.07	0.69
1:I:29:ARG:HA	1:I:300:LEU:HD22	1.73	0.69
1:I:335:LEU:O	1:I:335:LEU:HD23	1.92	0.69
1:U:11:LYS:HB3	1:U:23:VAL:CG1	2.23	0.69
1:5:64:LEU:N	1:5:64:LEU:HD23	2.06	0.69
2:F:34:ASP:OD2	2:F:41:ARG:HA	1.92	0.69
1:K:101:SER:OG	1:K:104:GLU:HG2	1.93	0.69
1:1:100:LEU:HD13	1:1:128:ALA:CB	2.22	0.69
1:S:37:ARG:CZ	1:S:309:ILE:HG23	2.22	0.69
2:D:246:MET:O	2:D:250:GLU:HG3	1.92	0.69
2:H:121:SER:HB3	2:H:124:VAL:HG21	1.74	0.69
2:Z:1:LEU:HD13	2:Z:2:GLN:N	2.06	0.69
2:Z:184:PRO:HA	2:Z:187:GLN:NE2	2.08	0.69
1:S:28:THR:O	1:S:29:ARG:C	2.29	0.69
1:S:28:THR:HG22	1:S:30:GLU:H	1.53	0.69
1:S:28:THR:HG22	1:S:30:GLU:CB	2.21	0.69
1:5:29:ARG:HH11	1:5:29:ARG:CG	2.03	0.69
1:3:29:ARG:HG2	1:3:29:ARG:HH11	1.58	0.69
2:T:327:LEU:O	2:T:329:ILE:HG23	1.93	0.69
1:I:68:GLN:NE2	1:I:259:ARG:HB3	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:131:PHE:CZ	1:E:133:GLY:HA2	2.28	0.69
1:Y:131:PHE:CE2	1:Y:133:GLY:HA2	2.28	0.69
1:U:142:VAL:HG21	1:U:175:ILE:HG12	1.75	0.69
2:T:316:VAL:HG13	2:T:316:VAL:O	1.92	0.69
2:N:19:ARG:HH11	2:N:19:ARG:HG2	1.57	0.69
2:N:252:SER:O	2:N:256:THR:HG23	1.93	0.68
1:1:197:ARG:HH11	1:1:197:ARG:CB	2.01	0.68
1:O:286:ASP:C	1:O:286:ASP:OD2	2.31	0.68
1:C:131:PHE:CE2	1:C:133:GLY:HA2	2.28	0.68
2:Z:19:ARG:HG2	2:Z:19:ARG:HH11	1.57	0.68
1:I:101:SER:OG	1:I:104:GLU:HG3	1.94	0.68
1:K:55:GLN:O	1:K:56:LYS:HB2	1.94	0.68
1:U:1:PHE:CD2	1:U:29:ARG:NH2	2.62	0.68
1:S:29:ARG:HG3	1:S:300:LEU:O	1.92	0.68
2:L:92:GLN:OE1	2:L:92:GLN:HA	1.93	0.68
1:K:268:PRO:O	1:K:271:ALA:HB3	1.94	0.68
1:5:327:ASP:OD1	1:5:328:PRO:HD2	1.94	0.68
1:5:10:LYS:HG2	1:5:11:LYS:N	2.07	0.68
1:I:257:THR:OG1	1:I:258:TYR:N	2.26	0.68
1:Q:334:GLU:HG2	1:Q:337:TYR:CE2	2.27	0.68
1:W:118:LYS:HB2	1:W:118:LYS:NZ	2.09	0.68
2:V:88:GLN:HG2	2:X:60:MET:CE	2.23	0.68
1:W:100:LEU:HD13	1:W:128:ALA:HB2	1.75	0.68
1:1:297:ASN:HD22	1:1:297:ASN:N	1.88	0.68
1:M:113:LYS:HD3	1:M:328:PRO:HG2	1.76	0.68
2:X:98:ALA:HB2	2:X:142:LEU:HD13	1.75	0.68
1:A:138:VAL:HG13	1:A:169:ALA:HB2	1.75	0.68
1:A:196:ASN:ND2	1:A:259:ARG:HD3	2.08	0.68
1:S:28:THR:CG2	1:S:30:GLU:H	2.06	0.68
1:O:231:LEU:CD1	1:O:294:ARG:HH11	1.92	0.68
2:P:237:ASN:HD22	2:P:237:ASN:C	1.96	0.68
2:4:199:LYS:HD3	2:4:239:ARG:NH2	2.08	0.68
1:W:272:TYR:HA	1:W:275:ARG:HG3	1.75	0.68
1:G:272:TYR:HA	1:G:275:ARG:CD	2.24	0.67
1:S:274:THR:O	1:S:276:GLU:N	2.27	0.67
1:M:274:THR:O	1:M:277:GLU:CB	2.42	0.67
1:S:274:THR:HB	1:S:276:GLU:CG	2.24	0.67
2:V:88:GLN:HG2	2:X:60:MET:HE1	1.76	0.67
2:F:102:TYR:CD2	2:H:301:PRO:HG2	2.29	0.67
1:K:100:LEU:CD1	1:K:128:ALA:HB2	2.23	0.67
1:O:286:ASP:OD2	1:O:287:PRO:N	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:30:GLU:OE1	1:S:30:GLU:C	2.32	0.67
1:S:88:ALA:O	1:S:134:GLY:CA	2.42	0.67
1:1:29:ARG:HA	1:1:300:LEU:HD22	1.75	0.67
2:T:33:TYR:O	2:T:34:ASP:HB2	1.95	0.67
1:3:89:TYR:HB2	1:3:124:MET:HG2	1.76	0.67
2:B:33:TYR:O	2:B:34:ASP:HB2	1.93	0.67
1:W:327:ASP:OD1	1:W:328:PRO:HD2	1.94	0.67
1:Y:196:ASN:ND2	1:Y:259:ARG:HE	1.93	0.67
1:U:74:GLY:HA3	1:U:233:VAL:HG12	1.75	0.67
2:N:157:ILE:O	2:N:161:ILE:HG13	1.95	0.67
1:O:236:ALA:O	1:O:237:THR:C	2.33	0.67
2:6:155:GLY:HA3	2:6:193:ILE:HG13	1.76	0.67
2:T:118:ASN:HD21	2:T:132:PHE:H	1.43	0.67
1:U:177:GLU:OE2	1:W:173:GLY:N	2.26	0.67
2:X:121:SER:HB3	2:X:124:VAL:HG21	1.75	0.67
1:O:284:LYS:O	1:O:285:SER:HB3	1.94	0.67
2:D:238:MET:O	2:D:239:ARG:HB2	1.93	0.67
1:3:284:LYS:CB	1:3:284:LYS:NZ	2.58	0.67
2:D:263:GLU:O	2:D:296:THR:HA	1.95	0.67
2:R:1:LEU:HD13	2:R:2:GLN:H	1.60	0.67
2:V:327:LEU:O	2:V:329:ILE:HG23	1.96	0.66
1:3:101:SER:OG	1:3:104:GLU:HG3	1.95	0.66
1:M:270:VAL:O	1:M:273:ARG:N	2.29	0.66
1:S:28:THR:HG23	1:S:30:GLU:HB2	1.74	0.66
1:K:131:PHE:CZ	1:K:133:GLY:HA2	2.30	0.66
1:3:257:THR:OG1	1:3:258:TYR:N	2.28	0.66
1:3:11:LYS:HB3	1:3:23:VAL:HG12	1.77	0.66
1:W:271:ALA:O	1:W:272:TYR:C	2.30	0.66
1:Y:223:LEU:HD23	1:Y:223:LEU:N	2.11	0.66
2:2:1:LEU:HD13	2:2:2:GLN:N	2.11	0.66
1:K:229:ASP:OD1	1:K:231:LEU:HB2	1.94	0.66
2:F:246:MET:HE3	2:F:279:ILE:CD1	2.19	0.66
1:W:196:ASN:HD21	1:W:259:ARG:HE	1.41	0.66
1:5:289:MET:CE	1:5:290:LEU:HD23	2.26	0.66
2:R:118:ASN:HD21	2:R:132:PHE:N	1.92	0.66
2:T:238:MET:O	2:T:239:ARG:HB2	1.95	0.66
1:G:334:GLU:HG2	1:G:337:TYR:CD2	2.30	0.66
1:M:272:TYR:HD1	1:M:272:TYR:C	1.97	0.66
1:M:45:MET:CE	1:M:102:VAL:HG13	2.26	0.66
2:2:238:MET:O	2:2:239:ARG:HB2	1.96	0.66
2:N:1:LEU:HD13	2:N:2:GLN:H	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:100:LEU:HD13	1:U:128:ALA:HB2	1.76	0.66
1:1:292:LYS:HG3	1:1:306:LEU:HD13	1.77	0.66
1:C:29:ARG:HA	1:C:300:LEU:HD22	1.75	0.66
1:K:232:CYS:O	1:K:233:VAL:C	2.32	0.66
1:A:352:ASN:H	1:A:355:ILE:HD12	1.61	0.66
1:5:231:LEU:HD23	1:5:231:LEU:N	2.11	0.66
1:C:197:ARG:NH2	1:C:277:GLU:OE2	2.29	0.66
1:1:327:ASP:OD1	1:1:328:PRO:HD2	1.96	0.66
2:T:185:GLU:HG2	2:T:185:GLU:O	1.93	0.65
1:5:233:VAL:O	1:5:234:ARG:C	2.33	0.65
1:G:11:LYS:HB3	1:G:23:VAL:CG1	2.26	0.65
1:Y:172:GLN:HE22	2:2:88:GLN:HE22	1.44	0.65
1:O:327:ASP:OD1	1:O:328:PRO:HD2	1.96	0.65
2:B:325:LYS:HG2	1:C:354:TRP:CZ2	2.31	0.65
1:A:230:ILE:O	1:A:230:ILE:HG13	1.96	0.65
1:K:268:PRO:O	1:K:271:ALA:CB	2.45	0.65
1:S:113:LYS:HD3	1:S:328:PRO:HG2	1.78	0.65
2:4:92:GLN:HA	2:4:92:GLN:OE1	1.96	0.65
1:W:272:TYR:C	1:W:272:TYR:CD2	2.70	0.65
1:Y:29:ARG:NH1	1:Y:300:LEU:O	2.30	0.65
2:6:278:ARG:NH1	2:6:278:ARG:HG3	2.12	0.65
1:K:274:THR:O	1:K:276:GLU:N	2.29	0.65
1:I:327:ASP:OD1	1:I:328:PRO:HD2	1.97	0.65
1:1:113:LYS:HE2	1:1:331:PRO:HD3	1.77	0.65
1:Y:195:ASN:OD1	1:Y:195:ASN:C	2.33	0.65
1:Y:327:ASP:OD1	1:Y:328:PRO:HD2	1.96	0.65
1:C:55:GLN:O	1:C:56:LYS:HB2	1.97	0.65
1:S:274:THR:O	1:S:278:ILE:CD1	2.45	0.65
1:3:11:LYS:HB3	1:3:23:VAL:CG1	2.27	0.65
2:6:184:PRO:HA	2:6:187:GLN:HE21	1.62	0.65
2:2:110:VAL:O	2:2:110:VAL:HG12	1.95	0.65
2:D:237:ASN:C	2:D:237:ASN:HD22	2.00	0.65
1:E:354:TRP:CZ2	2:H:325:LYS:HG2	2.32	0.65
1:A:286:ASP:OD2	1:A:288:ILE:HB	1.97	0.65
1:5:270:VAL:O	1:5:271:ALA:C	2.35	0.65
1:A:29:ARG:CA	1:A:300:LEU:HD22	2.26	0.65
1:W:11:LYS:HB3	1:W:23:VAL:HG12	1.79	0.65
1:3:274:THR:HB	1:3:276:GLU:CG	2.27	0.64
1:Q:29:ARG:NH1	1:Q:300:LEU:O	2.30	0.64
2:Z:34:ASP:OD2	2:Z:41:ARG:HG3	1.96	0.64
1:1:29:ARG:HH11	1:1:29:ARG:CG	2.09	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:16:GLU:OE2	2:J:162:ARG:NH1	2.30	0.64
1:3:231:LEU:HD12	1:3:294:ARG:NH1	2.12	0.64
1:3:223:LEU:H	1:3:223:LEU:HD23	1.62	0.64
1:U:225:VAL:HG12	1:U:226:ASP:N	2.11	0.64
2:P:154:LYS:O	2:P:157:ILE:HG22	1.98	0.64
1:1:291:LEU:O	1:1:295:MET:HG2	1.98	0.64
2:P:1:LEU:HD13	2:P:2:GLN:N	2.12	0.64
1:Q:204:VAL:HG23	1:Q:205:GLU:OE1	1.97	0.64
1:E:225:VAL:HG12	1:E:226:ASP:N	2.11	0.64
1:S:274:THR:C	1:S:276:GLU:N	2.47	0.64
1:Y:162:LEU:HG	1:Y:192:ILE:HD11	1.78	0.64
2:J:269:PHE:HE1	2:L:271:VAL:HA	1.63	0.64
2:2:98:ALA:HB2	2:2:142:LEU:HD13	1.78	0.64
1:A:18:GLU:CG	1:A:19:GLU:H	1.97	0.64
1:W:271:ALA:O	1:W:274:THR:N	2.30	0.64
1:G:334:GLU:HG2	1:G:337:TYR:CE2	2.32	0.64
2:J:184:PRO:HA	2:J:187:GLN:NE2	2.13	0.64
1:O:334:GLU:HG2	1:O:337:TYR:CE2	2.31	0.64
1:Q:289:MET:HE1	1:Q:290:LEU:HD23	1.77	0.64
1:A:100:LEU:HD13	1:A:128:ALA:HB2	1.79	0.64
1:O:131:PHE:CE2	1:O:133:GLY:HA2	2.33	0.64
1:1:88:ALA:O	1:1:134:GLY:CA	2.46	0.64
1:K:289:MET:HE3	1:K:290:LEU:HD23	1.80	0.64
2:Z:19:ARG:HG2	2:Z:19:ARG:NH1	2.11	0.64
2:D:191:PHE:O	2:D:192:LEU:HD12	1.97	0.64
1:G:131:PHE:CZ	1:G:133:GLY:HA2	2.32	0.64
1:A:45:MET:HE1	1:A:105:ILE:HD12	1.80	0.64
2:R:316:VAL:CG1	2:R:316:VAL:O	2.44	0.64
2:V:1:LEU:HD13	2:V:2:GLN:N	2.12	0.64
2:B:148:TRP:O	2:B:175:MET:HE2	1.97	0.64
1:1:71:CYS:O	1:1:75:LEU:HB2	1.97	0.64
1:5:268:PRO:O	1:5:271:ALA:N	2.31	0.63
1:C:101:SER:OG	1:C:104:GLU:HG3	1.98	0.63
2:N:184:PRO:HA	2:N:187:GLN:NE2	2.12	0.63
1:K:275:ARG:CG	1:K:275:ARG:HH11	2.06	0.63
1:3:274:THR:HB	1:3:276:GLU:H	1.63	0.63
2:V:19:ARG:HG2	2:V:19:ARG:HH11	1.64	0.63
2:D:172:ASN:HD22	2:D:175:MET:H	1.46	0.63
1:1:225:VAL:HG12	1:1:226:ASP:N	2.14	0.63
2:N:34:ASP:OD2	2:N:41:ARG:HG3	1.98	0.63
1:S:37:ARG:CG	1:S:37:ARG:NH1	2.59	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:98:ALA:HB2	2:R:142:LEU:HD13	1.79	0.63
1:3:100:LEU:HD13	1:3:128:ALA:HB2	1.80	0.63
1:E:101:SER:OG	1:E:104:GLU:HG3	1.97	0.63
1:U:334:GLU:HG2	1:U:337:TYR:CD2	2.34	0.63
2:L:98:ALA:HB2	2:L:142:LEU:HD13	1.79	0.63
1:5:11:LYS:HB3	1:5:23:VAL:CG1	2.29	0.63
2:T:118:ASN:HD21	2:T:132:PHE:N	1.96	0.63
1:O:297:ASN:N	1:O:297:ASN:HD22	1.97	0.63
2:L:155:GLY:HA3	2:L:193:ILE:HG13	1.78	0.63
2:F:181:GLU:O	2:F:183:PRO:HD3	1.99	0.63
1:Y:50:ASP:HB2	1:Y:64:LEU:CD1	2.29	0.63
1:K:270:VAL:HG22	1:K:273:ARG:HH12	1.64	0.63
1:C:182:ALA:HA	1:C:187:LEU:HD12	1.81	0.63
2:L:172:ASN:ND2	2:L:174:LEU:H	1.95	0.63
1:K:274:THR:O	1:K:277:GLU:N	2.31	0.63
1:C:88:ALA:O	1:C:134:GLY:CA	2.46	0.63
1:1:16:ARG:HG2	1:1:16:ARG:HH11	1.63	0.63
1:5:273:ARG:H	1:5:273:ARG:HD3	1.62	0.63
1:W:196:ASN:O	1:W:197:ARG:HB2	1.98	0.63
1:3:113:LYS:CD	1:3:328:PRO:HG2	2.28	0.63
2:4:184:PRO:HA	2:4:187:GLN:NE2	2.14	0.63
1:3:205:GLU:HG3	1:3:206:ARG:N	2.14	0.63
1:Y:45:MET:HE1	1:Y:105:ILE:HD12	1.79	0.63
2:B:172:ASN:HD22	2:B:175:MET:H	1.45	0.63
2:J:118:ASN:HD21	2:J:132:PHE:H	1.45	0.63
1:A:335:LEU:C	1:A:335:LEU:HD23	2.19	0.63
2:J:252:SER:O	2:J:256:THR:HG23	1.99	0.62
2:Z:276:CYS:HB3	2:2:280:MET:CE	2.29	0.62
1:Q:10:LYS:HG2	1:Q:11:LYS:N	2.14	0.62
1:C:257:THR:OG1	1:C:258:TYR:N	2.32	0.62
1:S:37:ARG:NH1	1:S:37:ARG:HG3	2.13	0.62
1:Q:50:ASP:HB2	1:Q:64:LEU:HD13	1.81	0.62
2:N:16:GLU:OE2	2:N:162:ARG:NH1	2.32	0.62
1:Y:88:ALA:O	1:Y:134:GLY:HA2	1.99	0.62
2:N:19:ARG:NH1	2:N:19:ARG:HG2	2.13	0.62
1:W:29:ARG:NH1	1:W:300:LEU:O	2.32	0.62
2:4:172:ASN:HD22	2:4:175:MET:H	1.47	0.62
2:X:259:LEU:CD2	2:X:279:ILE:HG13	2.29	0.62
2:N:1:LEU:HD13	2:N:2:GLN:N	2.13	0.62
1:G:68:GLN:HE21	1:G:259:ARG:HB3	1.64	0.62
1:U:84:HIS:CE1	1:U:130:ASN:HD21	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:335:LEU:O	1:Q:335:LEU:HD23	2.00	0.62
2:T:307:ILE:HG23	2:T:308:LEU:N	2.15	0.62
1:O:29:ARG:CB	1:O:300:LEU:HD22	2.29	0.62
1:Y:272:TYR:CD1	1:Y:272:TYR:C	2.72	0.62
2:6:246:MET:O	2:6:250:GLU:HG3	1.99	0.62
1:S:4:ASP:HA	1:S:300:LEU:HD21	1.82	0.62
1:Q:29:ARG:HA	1:Q:300:LEU:HD22	1.82	0.62
1:I:196:ASN:HB3	1:I:257:THR:HG23	1.80	0.62
1:3:1:PHE:HB3	1:3:299:ASN:O	1.99	0.62
2:P:316:VAL:O	2:P:317:LYS:C	2.35	0.62
1:5:268:PRO:C	1:5:270:VAL:N	2.52	0.62
1:O:100:LEU:HD13	1:O:128:ALA:CB	2.29	0.62
1:U:11:LYS:HB3	1:U:23:VAL:HG12	1.82	0.62
1:1:132:TYR:CD1	1:1:132:TYR:N	2.68	0.62
2:H:316:VAL:O	2:H:317:LYS:C	2.37	0.62
2:L:263:GLU:O	2:L:296:THR:HA	1.98	0.62
1:I:231:LEU:HD12	1:I:294:ARG:NH1	2.15	0.62
2:Z:172:ASN:HD22	2:Z:175:MET:H	1.47	0.62
1:S:27:LEU:HD22	1:S:27:LEU:C	2.19	0.62
2:H:98:ALA:HB2	2:H:142:LEU:CD1	2.29	0.62
1:Q:257:THR:OG1	1:Q:258:TYR:N	2.33	0.62
1:O:280:GLU:CG	1:O:281:VAL:N	2.62	0.62
1:A:196:ASN:HD21	1:A:259:ARG:HD3	1.64	0.62
2:X:327:LEU:O	2:X:329:ILE:HG23	2.00	0.62
2:J:172:ASN:HD22	2:J:175:MET:H	1.48	0.62
2:2:51:ARG:HH11	2:2:51:ARG:HG3	1.64	0.62
1:K:231:LEU:HD12	1:K:294:ARG:NH1	2.15	0.62
1:G:223:LEU:N	1:G:223:LEU:HD23	2.15	0.62
1:Q:274:THR:O	1:Q:277:GLU:N	2.33	0.62
1:I:45:MET:HE3	1:I:102:VAL:HG13	1.81	0.62
1:W:327:ASP:CG	1:W:328:PRO:HD2	2.20	0.61
1:3:150:LEU:HA	1:3:187:LEU:HD22	1.82	0.61
2:6:165:ASN:HB3	2:6:166:PRO:HD2	1.81	0.61
2:X:278:ARG:HG3	2:X:278:ARG:NH1	2.03	0.61
1:3:205:GLU:HG3	1:3:206:ARG:H	1.65	0.61
1:3:1:PHE:N	1:3:1:PHE:CD2	2.68	0.61
2:6:191:PHE:O	2:6:192:LEU:HD12	2.00	0.61
2:D:1:LEU:HD12	2:D:3:VAL:HG12	1.82	0.61
2:4:300:VAL:HG12	1:5:339:ILE:HD11	1.82	0.61
1:A:1:PHE:HA	1:A:299:ASN:ND2	2.14	0.61
1:3:71:CYS:O	1:3:72:CYS:C	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:39:MET:HG2	1:O:73:VAL:HG21	1.83	0.61
1:1:297:ASN:H	1:1:297:ASN:HD22	1.48	0.61
1:Y:196:ASN:O	1:Y:197:ARG:HB2	1.99	0.61
2:4:308:LEU:HD22	1:5:335:LEU:HB2	1.83	0.61
2:P:98:ALA:HB2	2:P:142:LEU:HD13	1.81	0.61
1:Q:80:ASN:HB3	1:Q:81:PRO:HD2	1.81	0.61
2:Z:300:VAL:HG12	1:1:339:ILE:HD11	1.81	0.61
1:5:70:ALA:HB2	1:5:287:PRO:HB3	1.81	0.61
1:O:197:ARG:HB3	1:O:197:ARG:NH1	2.12	0.61
1:W:271:ALA:O	1:W:273:ARG:N	2.33	0.61
1:Q:16:ARG:CG	1:Q:16:ARG:HH11	2.14	0.61
2:T:184:PRO:HA	2:T:187:GLN:NE2	2.14	0.61
1:W:271:ALA:O	1:W:274:THR:HG23	2.01	0.61
2:D:316:VAL:O	2:D:316:VAL:CG1	2.49	0.61
1:M:195:ASN:C	1:M:195:ASN:OD1	2.37	0.61
1:E:289:MET:CE	1:E:290:LEU:HD23	2.30	0.61
1:M:196:ASN:HD22	1:M:259:ARG:HE	1.47	0.61
2:R:1:LEU:CD1	2:R:2:GLN:H	2.13	0.61
2:R:316:VAL:O	2:R:316:VAL:HG12	1.99	0.61
1:I:174:GLN:HB3	2:J:60:MET:HG2	1.83	0.61
1:O:286:ASP:OD2	1:O:287:PRO:HD2	2.01	0.61
1:E:272:TYR:CE1	1:E:276:GLU:OE2	2.54	0.61
1:3:335:LEU:C	1:3:335:LEU:HD23	2.20	0.61
1:K:229:ASP:O	1:K:231:LEU:N	2.33	0.61
2:D:327:LEU:O	2:D:329:ILE:HG23	2.00	0.61
1:C:11:LYS:HB3	1:C:23:VAL:HG12	1.82	0.61
2:Z:207:ILE:HD13	2:Z:323:ILE:HG23	1.83	0.61
2:Z:250:GLU:O	2:Z:254:MET:HG3	2.00	0.61
1:S:44:ARG:HB2	1:S:317:ILE:HG13	1.83	0.61
1:S:274:THR:O	1:S:275:ARG:C	2.38	0.60
1:O:280:GLU:O	1:O:282:ARG:N	2.34	0.60
1:3:29:ARG:HH11	1:3:29:ARG:CG	2.13	0.60
1:I:335:LEU:HD23	1:I:335:LEU:C	2.21	0.60
2:L:278:ARG:HG3	2:L:278:ARG:NH1	2.15	0.60
2:V:313:ILE:CG2	2:V:314:PRO:CD	2.78	0.60
1:K:10:LYS:HG2	1:K:11:LYS:N	2.15	0.60
2:Z:246:MET:O	2:Z:250:GLU:HG3	2.00	0.60
2:R:95:ASN:ND2	2:T:87:MET:CE	2.64	0.60
1:O:289:MET:CE	1:O:290:LEU:HD23	2.31	0.60
2:N:278:ARG:HH11	2:N:278:ARG:HG2	1.65	0.60
1:O:286:ASP:OD2	1:O:287:PRO:CD	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:45:MET:HE3	1:Y:102:VAL:HG13	1.83	0.60
2:H:193:ILE:HD13	2:H:239:ARG:NH2	2.16	0.60
2:P:1:LEU:HD13	2:P:2:GLN:H	1.64	0.60
1:I:174:GLN:HB3	2:J:60:MET:CG	2.30	0.60
2:P:110:VAL:HG12	2:P:110:VAL:O	2.00	0.60
2:4:329:ILE:OXT	2:4:329:ILE:HG13	2.02	0.60
1:1:40:GLN:O	1:1:44:ARG:HG2	2.01	0.60
2:Z:327:LEU:O	2:Z:329:ILE:HG23	2.00	0.60
2:6:98:ALA:HB2	2:6:142:LEU:CD1	2.28	0.60
2:2:155:GLY:HA3	2:2:193:ILE:HG13	1.83	0.60
2:H:21:GLU:HG2	2:H:21:GLU:O	2.01	0.60
1:O:174:GLN:HB3	2:P:60:MET:HG2	1.84	0.60
2:N:325:LYS:HG2	1:O:354:TRP:CZ2	2.35	0.60
1:G:272:TYR:CA	1:G:275:ARG:HD3	2.31	0.60
1:G:274:THR:O	1:G:277:GLU:N	2.34	0.60
1:M:270:VAL:O	1:M:272:TYR:N	2.35	0.60
1:E:45:MET:HE3	1:E:102:VAL:HG22	1.84	0.60
1:S:45:MET:CE	1:S:105:ILE:HD12	2.31	0.60
2:T:258:HIS:CD2	2:T:327:LEU:HD23	2.36	0.60
1:3:78:GLY:HA2	1:3:238:ARG:HG2	1.82	0.60
1:U:70:ALA:HB3	1:U:227:GLY:O	2.01	0.60
2:B:98:ALA:HB2	2:B:142:LEU:HD13	1.83	0.60
1:W:108:GLU:OE1	1:W:117:ALA:N	2.29	0.60
1:E:177:GLU:OE2	1:G:173:GLY:N	2.35	0.60
1:A:55:GLN:O	1:A:56:LYS:HB2	2.02	0.60
1:3:7:PHE:CD2	1:3:294:ARG:HD3	2.37	0.60
1:1:53:TYR:CD2	1:1:62:CYS:HB3	2.36	0.60
2:B:238:MET:O	2:B:239:ARG:HB2	2.01	0.60
1:1:131:PHE:CE2	1:1:133:GLY:HA2	2.36	0.60
1:1:334:GLU:HG2	1:1:337:TYR:CE2	2.37	0.60
1:Q:335:LEU:HD23	1:Q:335:LEU:C	2.22	0.60
1:C:335:LEU:C	1:C:335:LEU:HD23	2.21	0.60
2:4:246:MET:O	2:4:250:GLU:HG3	2.02	0.60
1:M:3:ASN:ND2	1:M:3:ASN:O	2.34	0.60
1:G:196:ASN:O	1:G:197:ARG:HB2	2.01	0.59
2:X:278:ARG:CG	2:X:278:ARG:HH11	2.12	0.59
1:G:10:LYS:HG2	1:G:11:LYS:N	2.16	0.59
1:S:28:THR:O	1:S:30:GLU:N	2.35	0.59
2:D:258:HIS:CD2	2:D:327:LEU:HD23	2.38	0.59
2:J:4:THR:HA	2:J:179:PRO:HA	1.84	0.59
2:R:16:GLU:OE2	2:R:162:ARG:NH1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:39:MET:HG2	1:1:73:VAL:HG21	1.83	0.59
1:S:257:THR:OG1	1:S:258:TYR:N	2.35	0.59
1:I:345:PRO:HB3	1:I:360:VAL:HG12	1.84	0.59
1:E:304:GLU:O	1:E:308:GLU:HG3	2.02	0.59
1:M:15:HIS:CG	1:M:215:LYS:HG2	2.37	0.59
1:Q:61:PHE:HD2	1:Q:124:MET:HE2	1.68	0.59
1:Q:61:PHE:HD2	1:Q:124:MET:CE	2.16	0.59
1:S:345:PRO:HB3	1:S:360:VAL:HG12	1.83	0.59
1:1:280:GLU:O	1:1:283:SER:N	2.28	0.59
1:M:274:THR:O	1:M:277:GLU:N	2.35	0.59
2:H:121:SER:HB3	2:H:124:VAL:CG2	2.32	0.59
1:O:286:ASP:OD2	1:O:288:ILE:N	2.35	0.59
1:W:174:GLN:HB3	2:X:60:MET:HG2	1.84	0.59
2:4:98:ALA:HB2	2:4:142:LEU:HD13	1.83	0.59
1:3:284:LYS:HB3	1:3:284:LYS:HZ1	1.66	0.59
1:W:315:LYS:HB2	1:W:315:LYS:NZ	2.18	0.59
2:R:11:GLN:O	2:R:15:GLU:HG3	2.03	0.59
1:Y:15:HIS:CG	1:Y:215:LYS:HG2	2.38	0.59
1:A:80:ASN:HB3	1:A:81:PRO:HD2	1.84	0.59
1:O:88:ALA:HB2	1:O:141:GLN:NE2	2.18	0.59
2:D:84:ASN:ND2	2:D:128:HIS:HA	2.18	0.59
1:Q:113:LYS:HD3	1:Q:328:PRO:HG2	1.83	0.59
1:G:274:THR:O	1:G:276:GLU:N	2.35	0.59
1:1:280:GLU:O	1:1:282:ARG:N	2.35	0.59
1:O:29:ARG:CA	1:O:300:LEU:HD22	2.33	0.59
1:A:281:VAL:O	1:A:281:VAL:HG12	2.03	0.59
1:S:40:GLN:O	1:S:44:ARG:HG2	2.02	0.59
1:1:285:SER:O	1:1:286:ASP:C	2.41	0.59
1:C:334:GLU:HG2	1:C:337:TYR:CE2	2.37	0.59
1:O:236:ALA:O	1:O:239:PHE:N	2.35	0.59
1:Q:50:ASP:HB2	1:Q:64:LEU:CD1	2.33	0.59
2:J:11:GLN:O	2:J:15:GLU:HG3	2.03	0.59
2:P:268:GLN:O	2:P:269:PHE:HB2	2.03	0.59
2:H:81:MET:HB3	2:H:85:PHE:CD2	2.38	0.59
1:3:102:VAL:HG11	1:3:317:ILE:HD12	1.85	0.59
1:S:46:GLU:HA	1:S:46:GLU:OE1	2.03	0.58
2:J:1:LEU:CD1	2:J:2:GLN:H	2.16	0.58
2:F:184:PRO:HA	2:F:187:GLN:NE2	2.18	0.58
1:Y:289:MET:CE	1:Y:290:LEU:HD23	2.32	0.58
1:A:16:ARG:CG	1:A:16:ARG:NH1	2.53	0.58
1:A:29:ARG:NH1	1:A:300:LEU:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:95:ASN:HD21	2:6:87:MET:CE	2.16	0.58
1:5:270:VAL:HG12	1:5:271:ALA:N	2.17	0.58
1:M:132:TYR:CD1	1:M:148:ILE:HD13	2.38	0.58
1:O:335:LEU:C	1:O:335:LEU:HD23	2.23	0.58
1:3:29:ARG:NH1	1:3:300:LEU:O	2.37	0.58
1:S:327:ASP:OD1	1:S:328:PRO:HD2	2.04	0.58
1:3:206:ARG:NH2	2:6:32:GLN:HE22	2.00	0.58
1:E:272:TYR:CD1	1:E:272:TYR:C	2.76	0.58
1:E:272:TYR:HE1	1:E:276:GLU:OE2	1.87	0.58
1:E:267:ASP:O	1:E:270:VAL:N	2.37	0.58
1:W:57:ILE:HG22	1:W:110:THR:HG22	1.84	0.58
1:E:108:GLU:OE2	1:E:119:GLY:HA2	2.04	0.58
1:5:231:LEU:N	1:5:231:LEU:CD2	2.64	0.58
1:S:100:LEU:HD13	1:S:128:ALA:HB2	1.84	0.58
1:3:223:LEU:N	1:3:223:LEU:HD23	2.18	0.58
2:4:148:TRP:CD1	2:4:175:MET:HE2	2.38	0.58
2:X:193:ILE:HD13	2:X:239:ARG:NH2	2.17	0.58
1:S:39:MET:HG2	1:S:73:VAL:HG21	1.86	0.58
1:S:29:ARG:HB2	1:S:300:LEU:CD2	2.33	0.58
1:5:132:TYR:CD1	1:5:132:TYR:N	2.72	0.58
1:I:304:GLU:O	1:I:308:GLU:HG3	2.02	0.58
1:1:77:ALA:HB3	1:1:234:ARG:HG3	1.85	0.58
2:4:102:TYR:CG	2:6:301:PRO:HG2	2.38	0.58
1:Q:353:GLN:NE2	2:R:281:GLU:HB3	2.18	0.58
1:M:289:MET:CE	1:M:290:LEU:HD23	2.34	0.58
2:P:143:LYS:HB2	2:P:167:VAL:HG22	1.86	0.58
1:1:29:ARG:CA	1:1:300:LEU:HD22	2.33	0.58
2:2:237:ASN:HD22	2:2:237:ASN:C	2.07	0.58
2:F:276:CYS:HB3	2:H:280:MET:CE	2.33	0.58
1:S:30:GLU:CA	1:S:30:GLU:OE1	2.50	0.58
1:E:274:THR:O	1:E:278:ILE:HG12	2.04	0.58
1:E:29:ARG:NH1	1:E:300:LEU:O	2.36	0.58
2:F:172:ASN:HD22	2:F:175:MET:H	1.51	0.58
2:R:184:PRO:HG2	2:R:185:GLU:H	1.69	0.58
1:Q:165:TYR:HH	1:Q:179:TYR:HH	1.51	0.58
2:X:121:SER:HB3	2:X:124:VAL:CG2	2.34	0.58
2:L:172:ASN:HD22	2:L:174:LEU:N	2.01	0.58
1:G:223:LEU:H	1:G:223:LEU:HD23	1.69	0.58
2:R:95:ASN:ND2	2:T:87:MET:HE1	2.19	0.58
2:H:51:ARG:HG3	2:H:51:ARG:HH11	1.68	0.58
1:I:78:GLY:HA2	1:I:238:ARG:HG2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:99:LYS:HG2	2:P:301:PRO:HB3	1.84	0.58
1:Y:347:GLU:OE1	1:Y:356:LYS:HD3	2.04	0.58
2:V:121:SER:HB3	2:V:124:VAL:HG21	1.86	0.58
1:W:132:TYR:CD1	1:W:132:TYR:N	2.71	0.58
1:5:289:MET:HE3	1:5:290:LEU:HD23	1.86	0.57
2:P:278:ARG:HG3	2:P:278:ARG:NH1	2.18	0.57
2:4:17:LEU:O	2:4:51:ARG:NH2	2.37	0.57
1:1:70:ALA:HB3	1:1:227:GLY:O	2.03	0.57
1:A:45:MET:CE	1:A:102:VAL:HG13	2.31	0.57
1:3:274:THR:C	1:3:276:GLU:N	2.57	0.57
2:H:238:MET:O	2:H:239:ARG:HB2	2.03	0.57
1:W:150:LEU:HA	1:W:187:LEU:HD22	1.86	0.57
1:A:327:ASP:OD1	1:A:328:PRO:HD2	2.04	0.57
2:P:193:ILE:HD13	2:P:239:ARG:NH2	2.19	0.57
2:2:16:GLU:OE2	2:2:162:ARG:NH1	2.37	0.57
2:4:301:PRO:HB3	2:6:99:LYS:HG2	1.87	0.57
2:F:11:GLN:O	2:F:15:GLU:HG3	2.04	0.57
1:A:33:LEU:HD12	1:A:295:MET:HE1	1.86	0.57
1:S:286:ASP:HB3	1:S:289:MET:HB3	1.86	0.57
1:5:268:PRO:O	1:5:270:VAL:N	2.36	0.57
1:G:55:GLN:O	1:G:56:LYS:CB	2.47	0.57
1:Q:88:ALA:O	1:Q:134:GLY:CA	2.52	0.57
2:D:212:HIS:HB3	2:D:238:MET:HE3	1.86	0.57
2:H:316:VAL:O	2:H:318:ASP:N	2.37	0.57
2:4:143:LYS:HB2	2:4:167:VAL:HG22	1.86	0.57
1:G:274:THR:O	1:G:275:ARG:C	2.41	0.57
1:3:284:LYS:HZ2	1:3:284:LYS:HB3	1.65	0.57
1:U:337:TYR:HB3	1:U:338:HIS:CD2	2.40	0.57
2:F:102:TYR:CG	2:H:301:PRO:HG2	2.38	0.57
2:D:237:ASN:C	2:D:237:ASN:ND2	2.57	0.57
1:A:2:ALA:H	1:A:299:ASN:HD22	1.52	0.57
2:L:237:ASN:HD22	2:L:237:ASN:C	2.08	0.57
1:E:335:LEU:O	1:E:335:LEU:HG	2.02	0.57
1:O:234:ARG:HH21	1:O:238:ARG:HH22	1.51	0.57
2:4:1:LEU:CD1	2:4:2:GLN:H	2.14	0.57
2:P:118:ASN:ND2	2:P:132:PHE:H	2.02	0.57
2:2:152:ASP:HA	2:2:193:ILE:HD12	1.87	0.57
1:Y:68:GLN:HE22	1:Y:196:ASN:HD22	1.53	0.57
2:P:155:GLY:HA3	2:P:193:ILE:HG13	1.85	0.57
2:2:268:GLN:O	2:2:269:PHE:HB2	2.05	0.57
1:I:88:ALA:O	1:I:134:GLY:HA2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:268:PRO:CB	1:M:270:VAL:CG2	2.74	0.57
2:D:158:LYS:HE3	2:D:191:PHE:O	2.05	0.57
1:E:267:ASP:O	1:E:269:GLY:N	2.38	0.57
2:L:157:ILE:O	2:L:161:ILE:HG13	2.04	0.57
1:S:101:SER:OG	1:S:104:GLU:HG3	2.05	0.57
1:O:3:ASN:O	1:O:4:ASP:HB3	2.05	0.57
1:G:151:ALA:HB1	2:H:74:LEU:HD22	1.86	0.57
2:F:87:MET:CE	2:H:95:ASN:ND2	2.68	0.57
1:Q:78:GLY:HA2	1:Q:238:ARG:HG2	1.85	0.57
2:6:16:GLU:OE2	2:6:162:ARG:NH1	2.36	0.57
2:6:268:GLN:O	2:6:269:PHE:HB2	2.04	0.57
1:K:275:ARG:NH1	1:K:275:ARG:CG	2.66	0.57
2:T:278:ARG:CG	2:T:278:ARG:HH11	2.12	0.57
1:G:151:ALA:CB	2:H:74:LEU:HD22	2.35	0.57
1:5:322:GLN:HG3	1:5:323:PHE:N	2.20	0.57
2:X:16:GLU:OE2	2:X:162:ARG:NH1	2.38	0.57
2:4:252:SER:O	2:4:256:THR:HG23	2.04	0.57
1:C:29:ARG:HG3	1:C:30:GLU:N	2.17	0.57
2:L:172:ASN:ND2	2:L:174:LEU:N	2.53	0.57
2:2:154:LYS:O	2:2:157:ILE:HG22	2.05	0.57
1:S:231:LEU:HD12	1:S:294:ARG:NH1	2.20	0.57
2:L:23:VAL:HG22	2:L:75:ARG:HB2	1.87	0.57
1:5:162:LEU:CD1	1:5:190:ILE:HD12	2.35	0.57
1:O:229:ASP:C	1:O:231:LEU:N	2.47	0.56
2:P:207:ILE:HG13	2:P:258:HIS:HB2	1.85	0.56
1:O:345:PRO:HB3	1:O:360:VAL:HG12	1.85	0.56
2:D:98:ALA:HB2	2:D:142:LEU:HD13	1.86	0.56
2:P:33:TYR:O	2:P:34:ASP:HB2	2.03	0.56
1:I:29:ARG:HH11	1:I:29:ARG:HG2	1.70	0.56
2:V:51:ARG:HH11	2:V:51:ARG:HG3	1.70	0.56
2:B:19:ARG:HH11	2:B:19:ARG:HG2	1.70	0.56
1:1:45:MET:CE	1:1:102:VAL:HA	2.34	0.56
1:Q:225:VAL:HG12	1:Q:226:ASP:N	2.19	0.56
2:F:246:MET:O	2:F:250:GLU:HG3	2.04	0.56
1:C:100:LEU:HD13	1:C:128:ALA:HB2	1.87	0.56
1:A:169:ALA:O	1:A:175:ILE:HD12	2.05	0.56
1:G:74:GLY:HA2	1:G:230:ILE:HD12	1.87	0.56
1:S:334:GLU:HG2	1:S:337:TYR:CE2	2.40	0.56
2:Z:99:LYS:HG2	2:2:301:PRO:HB3	1.88	0.56
1:Y:101:SER:OG	1:Y:104:GLU:HG3	2.06	0.56
1:E:347:GLU:OE1	1:E:356:LYS:HD3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:118:ASN:HD21	2:N:132:PHE:N	2.00	0.56
1:A:196:ASN:ND2	1:A:259:ARG:CD	2.68	0.56
1:K:229:ASP:C	1:K:231:LEU:H	2.08	0.56
1:1:196:ASN:HD21	1:1:259:ARG:NE	2.04	0.56
1:K:272:TYR:C	1:K:272:TYR:CD1	2.79	0.56
1:Y:29:ARG:HH11	1:Y:29:ARG:HG2	1.71	0.56
2:T:1:LEU:HD13	2:T:2:GLN:N	2.21	0.56
2:F:325:LYS:HG2	1:G:354:TRP:CZ2	2.39	0.56
1:E:89:TYR:HB2	1:E:124:MET:HG2	1.88	0.56
1:S:29:ARG:HB2	1:S:300:LEU:HD23	1.86	0.56
1:1:141:GLN:OE1	1:1:141:GLN:N	2.37	0.56
1:Q:204:VAL:HG23	1:Q:205:GLU:H	1.70	0.56
2:V:19:ARG:NH1	2:V:19:ARG:HG2	2.21	0.56
1:Y:50:ASP:HB2	1:Y:64:LEU:HD11	1.86	0.56
2:2:11:GLN:O	2:2:15:GLU:HG3	2.05	0.56
2:N:238:MET:O	2:N:239:ARG:HB2	2.06	0.56
2:V:325:LYS:HG2	1:W:354:TRP:CZ2	2.41	0.56
1:O:10:LYS:HG2	1:O:11:LYS:N	2.20	0.56
1:O:45:MET:CE	1:O:102:VAL:HA	2.35	0.56
1:5:100:LEU:CD1	1:5:128:ALA:HB2	2.36	0.56
2:J:304:TYR:O	1:K:59:ARG:NH2	2.39	0.56
1:5:268:PRO:O	1:5:271:ALA:CB	2.54	0.56
1:G:196:ASN:HD21	1:G:259:ARG:NE	2.04	0.56
1:Q:29:ARG:NH1	1:Q:29:ARG:HG3	2.21	0.56
2:J:148:TRP:O	2:J:175:MET:HE2	2.06	0.56
2:X:81:MET:HB3	2:X:85:PHE:CD2	2.41	0.56
1:M:304:GLU:O	1:M:308:GLU:HG3	2.06	0.56
1:Q:222:GLY:HA2	1:Q:252:LEU:O	2.06	0.56
1:K:70:ALA:HB2	1:K:287:PRO:HB3	1.86	0.56
1:A:284:LYS:O	1:A:285:SER:CB	2.42	0.56
1:W:95:THR:HG23	1:W:100:LEU:HD22	1.88	0.56
2:L:98:ALA:HB2	2:L:142:LEU:HD12	1.87	0.56
1:C:253:MET:CE	1:C:255:LEU:CD1	2.84	0.56
1:Y:29:ARG:HG3	1:Y:300:LEU:O	2.05	0.56
2:J:300:VAL:HG12	1:K:339:ILE:HD11	1.87	0.56
1:Y:103:ARG:HG2	1:Y:323:PHE:CD2	2.40	0.56
2:L:260:VAL:HG22	2:L:293:VAL:HG23	1.88	0.56
2:V:149:ASN:OD1	2:V:151:GLU:HB3	2.06	0.56
2:X:320:ILE:HG22	2:X:321:PHE:N	2.20	0.56
1:I:68:GLN:HE21	1:I:259:ARG:HB3	1.70	0.56
2:4:237:ASN:HD22	2:4:237:ASN:C	2.08	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:272:GLY:O	2:V:273:ALA:C	2.44	0.56
2:T:11:GLN:O	2:T:15:GLU:HG3	2.06	0.56
1:A:275:ARG:HA	1:A:278:ILE:HD13	1.88	0.56
2:6:11:GLN:O	2:6:15:GLU:HG3	2.05	0.56
1:G:40:GLN:O	1:G:44:ARG:HG2	2.06	0.56
1:U:174:GLN:HB3	2:V:60:MET:HG2	1.88	0.56
1:U:55:GLN:O	1:U:56:LYS:HB2	2.05	0.56
1:K:196:ASN:ND2	1:K:259:ARG:HE	2.04	0.55
2:6:278:ARG:HG3	2:6:278:ARG:HH11	1.71	0.55
1:1:335:LEU:C	1:1:335:LEU:HD23	2.26	0.55
2:F:155:GLY:HA3	2:F:193:ILE:HG13	1.88	0.55
1:Q:150:LEU:HA	1:Q:187:LEU:HD22	1.88	0.55
2:V:148:TRP:O	2:V:175:MET:HE2	2.05	0.55
1:O:229:ASP:OD1	1:O:231:LEU:CB	2.48	0.55
1:A:289:MET:HE1	1:A:290:LEU:CD2	2.34	0.55
1:U:1:PHE:HD2	1:U:29:ARG:NH2	2.03	0.55
1:A:196:ASN:HB3	1:A:257:THR:HG23	1.88	0.55
1:A:225:VAL:HG12	1:A:226:ASP:N	2.20	0.55
1:Q:2:ALA:H	1:Q:299:ASN:HD22	1.54	0.55
2:B:256:THR:O	2:B:257:ASN:HB2	2.04	0.55
1:M:1:PHE:C	1:M:2:ALA:O	2.42	0.55
1:5:45:MET:HE3	1:5:102:VAL:HA	1.87	0.55
1:E:334:GLU:HG2	1:E:337:TYR:CZ	2.42	0.55
1:5:217:GLY:O	1:5:218:ASP:HB3	2.04	0.55
1:O:132:TYR:N	1:O:132:TYR:CD1	2.75	0.55
2:N:279:ILE:HG22	2:N:280:MET:H	1.66	0.55
1:W:196:ASN:HD21	1:W:259:ARG:NE	2.04	0.55
1:C:4:ASP:HA	1:C:300:LEU:HD21	1.89	0.55
2:J:301:PRO:HB3	2:L:99:LYS:HG2	1.88	0.55
1:G:16:ARG:HG2	1:G:16:ARG:HH11	1.71	0.55
2:H:24:PHE:CZ	2:H:76:PRO:HB3	2.42	0.55
1:3:80:ASN:HB3	1:3:81:PRO:HD2	1.88	0.55
1:G:94:PHE:O	1:G:98:ARG:HB2	2.06	0.55
1:3:45:MET:HE1	1:3:105:ILE:HD12	1.89	0.55
2:X:81:MET:O	2:X:117:PRO:HD2	2.07	0.55
2:Z:81:MET:HB3	2:Z:85:PHE:CE2	2.42	0.55
1:5:93:GLY:O	1:5:97:THR:HG23	2.07	0.55
1:S:71:CYS:SG	1:S:255:LEU:HD23	2.47	0.55
1:S:55:GLN:O	1:S:56:LYS:HB2	2.05	0.55
1:E:1:PHE:CD2	1:E:29:ARG:NH2	2.75	0.55
1:O:167:ASP:HB3	1:O:195:ASN:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:1:PHE:HA	1:K:299:ASN:HD21	1.71	0.55
1:G:34:LYS:HE3	1:G:38:MET:HE1	1.89	0.55
1:G:272:TYR:CD1	1:G:273:ARG:CA	2.90	0.55
1:G:272:TYR:O	1:G:274:THR:N	2.40	0.55
1:5:274:THR:O	1:5:278:ILE:HG13	2.06	0.55
1:5:112:ARG:HD2	1:5:327:ASP:O	2.06	0.55
1:3:29:ARG:CA	1:3:300:LEU:HD22	2.36	0.55
1:3:45:MET:HE3	1:3:102:VAL:HG13	1.89	0.55
1:I:223:LEU:H	1:I:223:LEU:HD23	1.72	0.55
1:W:177:GLU:OE1	2:X:58:SER:HB3	2.05	0.55
2:N:214:ARG:N	2:N:215:PRO:HD2	2.21	0.55
2:H:210:VAL:HG12	2:H:211:SER:N	2.21	0.55
1:W:345:PRO:HB3	1:W:360:VAL:HG12	1.89	0.55
1:W:167:ASP:HB3	1:W:195:ASN:HA	1.89	0.55
2:2:118:ASN:HD21	2:2:132:PHE:H	1.53	0.55
2:J:140:PRO:HB2	2:L:301:PRO:HD3	1.89	0.55
1:W:11:LYS:HB3	1:W:23:VAL:CG1	2.35	0.55
1:C:253:MET:HE3	1:C:255:LEU:HD13	1.86	0.55
1:C:29:ARG:CB	1:C:300:LEU:HD22	2.36	0.55
1:S:253:MET:HE3	1:S:255:LEU:HD11	1.87	0.55
2:4:118:ASN:HD21	2:4:132:PHE:H	1.55	0.55
2:H:237:ASN:C	2:H:237:ASN:HD22	2.11	0.55
1:K:15:HIS:CG	1:K:215:LYS:HG2	2.41	0.55
1:K:45:MET:CE	1:K:102:VAL:HA	2.36	0.55
1:G:182:ALA:HA	1:G:187:LEU:HD12	1.88	0.55
1:K:272:TYR:CD1	1:K:273:ARG:N	2.75	0.55
1:U:95:THR:CG2	1:U:100:LEU:HD22	2.37	0.55
2:R:184:PRO:HA	2:R:187:GLN:NE2	2.22	0.55
2:F:87:MET:HE3	2:H:95:ASN:ND2	2.22	0.55
1:S:182:ALA:HA	1:S:187:LEU:HD12	1.89	0.55
1:3:274:THR:C	1:3:276:GLU:H	2.10	0.54
2:T:218:HIS:O	2:T:316:VAL:HG22	2.08	0.54
1:5:100:LEU:HD13	1:5:128:ALA:HB2	1.90	0.54
2:P:171:GLU:OE1	2:P:176:TYR:OH	2.22	0.54
1:E:46:GLU:HA	1:E:46:GLU:OE1	2.07	0.54
1:C:296:VAL:O	1:C:298:SER:N	2.40	0.54
1:C:1:PHE:HA	1:C:299:ASN:ND2	2.22	0.54
1:S:229:ASP:HB3	1:S:232:CYS:SG	2.46	0.54
1:Y:150:LEU:HA	1:Y:187:LEU:HD22	1.89	0.54
1:A:260:TYR:OH	1:A:286:ASP:HA	2.08	0.54
1:C:334:GLU:HG2	1:C:337:TYR:CD2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:155:GLY:HA3	2:X:193:ILE:HG13	1.90	0.54
2:H:51:ARG:O	2:H:52:ILE:HD13	2.07	0.54
1:A:15:HIS:CG	1:A:215:LYS:HG2	2.42	0.54
1:M:279:GLN:OE1	1:M:279:GLN:CA	2.56	0.54
2:J:87:MET:HE3	2:L:91:ASP:HA	1.89	0.54
1:E:113:LYS:HD3	1:E:328:PRO:HG2	1.89	0.54
1:M:354:TRP:CZ2	2:P:325:LYS:HG2	2.42	0.54
2:R:213:SER:OG	2:R:214:ARG:N	2.41	0.54
1:U:74:GLY:HA3	1:U:233:VAL:HG11	1.88	0.54
2:N:115:ARG:HD2	2:N:157:ILE:HD11	1.88	0.54
1:Y:269:GLY:C	1:Y:271:ALA:H	2.10	0.54
2:6:118:ASN:HD21	2:6:132:PHE:H	1.54	0.54
1:3:142:VAL:HB	1:3:143:PRO:HD3	1.88	0.54
2:X:20:ASP:C	2:X:20:ASP:OD1	2.46	0.54
1:I:11:LYS:HB3	1:I:23:VAL:CG1	2.37	0.54
1:M:167:ASP:OD2	1:M:196:ASN:OD1	2.24	0.54
1:U:304:GLU:O	1:U:308:GLU:HG3	2.07	0.54
1:M:10:LYS:HG2	1:M:11:LYS:N	2.22	0.54
1:G:100:LEU:HD13	1:G:128:ALA:HB2	1.89	0.54
2:F:126:ALA:HB1	2:H:99:LYS:HD3	1.89	0.54
1:3:88:ALA:O	1:3:134:GLY:HA2	2.06	0.54
1:U:68:GLN:NE2	1:U:196:ASN:HD22	2.06	0.54
1:A:303:VAL:CG1	1:A:304:GLU:OE2	2.56	0.54
1:Q:61:PHE:CD2	1:Q:124:MET:CE	2.91	0.54
1:Q:182:ALA:HA	1:Q:187:LEU:HD12	1.90	0.54
1:C:1:PHE:HA	1:C:299:ASN:HD21	1.71	0.54
1:M:278:ILE:O	1:M:279:GLN:C	2.44	0.54
2:T:92:GLN:HA	2:T:92:GLN:OE1	2.08	0.54
1:Q:352:ASN:H	1:Q:355:ILE:HD12	1.73	0.54
2:X:31:ALA:HB3	2:X:54:ASP:CG	2.27	0.54
1:Y:11:LYS:O	1:Y:11:LYS:HG3	2.06	0.54
1:Q:138:VAL:HG13	1:Q:169:ALA:HB2	1.89	0.54
1:Q:95:THR:HG23	1:Q:100:LEU:HD22	1.88	0.54
1:M:142:VAL:HG21	1:M:175:ILE:HG12	1.90	0.54
1:M:40:GLN:HE21	1:M:288:ILE:HD13	1.72	0.54
2:V:313:ILE:CG2	2:V:314:PRO:HD2	2.26	0.54
2:B:118:ASN:ND2	2:B:132:PHE:H	1.96	0.54
1:U:9:ILE:HB	1:U:232:CYS:SG	2.48	0.54
2:F:278:ARG:HH11	2:F:278:ARG:CG	2.21	0.54
2:F:278:ARG:NH1	2:F:278:ARG:HG3	2.22	0.54
2:X:57:ILE:HG22	2:X:57:ILE:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:40:GLN:O	1:O:44:ARG:HG2	2.08	0.54
2:V:23:VAL:HG22	2:V:75:ARG:HB2	1.89	0.54
2:4:185:GLU:O	2:4:188:SER:HB3	2.08	0.54
1:C:40:GLN:O	1:C:44:ARG:HG2	2.08	0.54
2:J:325:LYS:HG2	1:K:354:TRP:CZ2	2.43	0.54
2:P:118:ASN:HD21	2:P:132:PHE:N	2.01	0.54
2:J:269:PHE:CE1	2:L:271:VAL:HA	2.42	0.54
2:B:172:ASN:ND2	2:B:174:LEU:H	2.05	0.54
1:E:289:MET:HE2	1:E:290:LEU:HD23	1.88	0.54
2:L:165:ASN:HB3	2:L:166:PRO:HD2	1.89	0.54
2:6:23:VAL:HG22	2:6:75:ARG:HB2	1.89	0.54
2:4:171:GLU:OE1	2:4:176:TYR:OH	2.23	0.54
2:R:238:MET:O	2:R:239:ARG:HB2	2.08	0.54
1:S:95:THR:HG23	1:S:100:LEU:HD22	1.89	0.54
1:K:243:TYR:CE2	1:K:248:LYS:HD2	2.43	0.54
1:O:147:GLY:HA2	2:P:65:ILE:HG23	1.89	0.54
1:A:302:SER:OG	1:A:305:GLU:HG3	2.08	0.54
1:A:285:SER:C	1:A:286:ASP:O	2.42	0.54
1:M:223:LEU:H	1:M:223:LEU:HD23	1.72	0.54
2:R:99:LYS:HG2	2:T:301:PRO:HB3	1.89	0.54
1:K:232:CYS:O	1:K:235:GLU:N	2.41	0.54
1:O:88:ALA:O	1:O:134:GLY:HA2	2.08	0.54
2:P:259:LEU:CD2	2:P:279:ILE:HG13	2.38	0.54
2:L:80:PHE:O	2:L:81:MET:C	2.46	0.54
2:R:24:PHE:CZ	2:R:76:PRO:HB3	2.43	0.54
2:V:63:ALA:O	2:V:67:VAL:HG23	2.08	0.54
1:W:289:MET:CE	1:W:290:LEU:HD23	2.37	0.54
1:W:343:ASP:HB3	1:W:344:PRO:HD2	1.89	0.54
1:G:113:LYS:HD3	1:G:328:PRO:HG2	1.90	0.53
1:W:68:GLN:NE2	1:W:259:ARG:HB3	2.15	0.53
1:I:302:SER:OG	1:I:305:GLU:HG3	2.08	0.53
1:Q:55:GLN:O	1:Q:56:LYS:HB2	2.07	0.53
1:1:37:ARG:NH2	1:1:309:ILE:HG23	2.23	0.53
2:Z:16:GLU:OE2	2:Z:162:ARG:NH1	2.40	0.53
2:F:63:ALA:O	2:F:67:VAL:HG23	2.08	0.53
2:D:165:ASN:HB3	2:D:166:PRO:HD2	1.89	0.53
2:R:172:ASN:HD22	2:R:175:MET:H	1.54	0.53
2:D:227:SER:C	2:D:229:GLU:H	2.11	0.53
2:6:172:ASN:ND2	2:6:174:LEU:N	2.56	0.53
1:G:98:ARG:HG2	1:G:131:PHE:CB	2.33	0.53
2:D:278:ARG:HG3	2:D:278:ARG:NH1	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:110:VAL:O	2:F:166:PRO:HD3	2.08	0.53
1:K:149:ALA:CB	1:K:189:CYS:HB2	2.39	0.53
1:A:164:LEU:HG	1:A:192:ILE:HB	1.90	0.53
1:M:347:GLU:OE1	1:M:356:LYS:HD3	2.08	0.53
1:5:268:PRO:O	1:5:269:GLY:C	2.44	0.53
1:S:45:MET:HE1	1:S:105:ILE:HD12	1.90	0.53
1:K:268:PRO:O	1:K:271:ALA:N	2.42	0.53
1:Y:142:VAL:HG21	1:Y:175:ILE:HG12	1.88	0.53
2:R:327:LEU:O	2:R:329:ILE:HG23	2.09	0.53
1:U:225:VAL:CG1	1:U:226:ASP:N	2.71	0.53
1:U:196:ASN:HB3	1:U:257:THR:HG23	1.90	0.53
2:V:152:ASP:HA	2:V:193:ILE:HD12	1.89	0.53
1:I:280:GLU:O	1:I:284:LYS:HB2	2.09	0.53
2:6:263:GLU:O	2:6:296:THR:HA	2.07	0.53
2:L:70:ALA:HA	2:L:74:LEU:O	2.09	0.53
1:I:29:ARG:CA	1:I:300:LEU:HD22	2.38	0.53
2:D:212:HIS:HB3	2:D:238:MET:CE	2.38	0.53
1:S:230:ILE:O	1:S:230:ILE:HG13	2.09	0.53
2:R:51:ARG:HG3	2:R:51:ARG:HH11	1.73	0.53
2:F:16:GLU:OE2	2:F:162:ARG:NH1	2.42	0.53
2:D:24:PHE:CZ	2:D:76:PRO:HB3	2.43	0.53
1:Y:29:ARG:HH11	1:Y:29:ARG:CG	2.22	0.53
1:Q:77:ALA:CB	1:Q:234:ARG:HG3	2.39	0.53
1:O:223:LEU:HD23	1:O:223:LEU:N	2.24	0.53
2:D:280:MET:HA	2:D:285:PHE:CD1	2.43	0.53
2:T:98:ALA:HB2	2:T:142:LEU:HD13	1.90	0.53
1:S:50:ASP:HB2	1:S:64:LEU:HD13	1.90	0.53
1:Q:232:CYS:O	1:Q:233:VAL:C	2.46	0.53
1:Q:286:ASP:HB3	1:Q:289:MET:HB3	1.90	0.53
1:M:102:VAL:HG11	1:M:317:ILE:HD12	1.91	0.53
2:L:154:LYS:O	2:L:157:ILE:HG22	2.08	0.53
2:B:19:ARG:NH1	2:B:19:ARG:HG2	2.23	0.53
1:I:39:MET:HG2	1:I:73:VAL:HG21	1.91	0.53
2:N:124:VAL:O	2:N:125:ALA:HB3	2.08	0.53
1:E:10:LYS:HG2	1:E:11:LYS:N	2.24	0.53
2:T:84:ASN:ND2	2:T:128:HIS:HA	2.24	0.53
2:R:102:TYR:CD2	2:T:301:PRO:HG2	2.44	0.53
2:N:81:MET:HB3	2:N:85:PHE:CE2	2.44	0.53
1:1:171:ASN:HD21	1:1:208:ALA:HB2	1.73	0.53
1:A:286:ASP:OD2	1:A:288:ILE:N	2.34	0.53
2:P:81:MET:HB3	2:P:85:PHE:CD2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:231:LEU:HD12	1:G:294:ARG:NH1	2.24	0.53
2:H:34:ASP:O	2:H:38:LYS:HA	2.08	0.53
1:Q:286:ASP:OD2	1:Q:288:ILE:HB	2.08	0.52
1:A:102:VAL:HG11	1:A:317:ILE:CD1	2.39	0.52
1:Q:29:ARG:CA	1:Q:300:LEU:HD22	2.38	0.52
2:6:278:ARG:CG	2:6:278:ARG:HH11	2.21	0.52
1:C:232:CYS:HA	1:C:235:GLU:HB2	1.90	0.52
1:E:351:ALA:HA	2:H:296:THR:O	2.09	0.52
2:B:24:PHE:CZ	2:B:76:PRO:HB3	2.44	0.52
1:A:35:TYR:O	1:A:39:MET:HG3	2.09	0.52
2:4:172:ASN:ND2	2:4:174:LEU:H	2.07	0.52
2:J:1:LEU:HD12	2:J:2:GLN:H	1.74	0.52
2:P:278:ARG:HG3	2:P:278:ARG:HH11	1.72	0.52
2:F:152:ASP:HA	2:F:193:ILE:HD12	1.91	0.52
2:4:118:ASN:HD21	2:4:132:PHE:N	2.08	0.52
2:X:20:ASP:OD1	2:X:21:GLU:N	2.42	0.52
1:O:50:ASP:HB2	1:O:64:LEU:HD13	1.92	0.52
1:I:334:GLU:HG2	1:I:337:TYR:CE2	2.44	0.52
1:W:93:GLY:O	1:W:97:THR:HG23	2.09	0.52
1:3:102:VAL:HG11	1:3:317:ILE:CD1	2.39	0.52
1:U:150:LEU:O	1:U:150:LEU:HG	2.08	0.52
2:R:246:MET:O	2:R:250:GLU:HG3	2.09	0.52
2:2:33:TYR:O	2:2:34:ASP:HB2	2.08	0.52
2:Z:118:ASN:HD21	2:Z:132:PHE:H	1.56	0.52
1:1:57:ILE:HD12	1:5:326:ALA:HB1	1.91	0.52
1:S:131:PHE:CE2	1:S:133:GLY:HA2	2.44	0.52
2:B:184:PRO:HA	2:B:187:GLN:NE2	2.25	0.52
1:O:235:GLU:O	1:O:236:ALA:C	2.47	0.52
2:2:1:LEU:C	2:2:1:LEU:HD13	2.30	0.52
1:A:95:THR:HG22	1:A:100:LEU:HB2	1.89	0.52
1:G:16:ARG:HG2	1:G:16:ARG:NH1	2.25	0.52
2:X:51:ARG:O	2:X:52:ILE:HD13	2.10	0.52
1:Y:11:LYS:HB3	1:Y:23:VAL:CG1	2.40	0.52
1:E:223:LEU:HD23	1:E:223:LEU:N	2.23	0.52
1:U:46:GLU:HA	1:U:46:GLU:OE1	2.08	0.52
1:G:174:GLN:HB3	2:H:60:MET:HG2	1.90	0.52
2:L:51:ARG:HG3	2:L:51:ARG:HH11	1.74	0.52
1:G:272:TYR:C	1:G:274:THR:N	2.63	0.52
2:D:16:GLU:OE2	2:D:162:ARG:NH1	2.41	0.52
1:W:29:ARG:CA	1:W:300:LEU:HD22	2.39	0.52
2:R:172:ASN:ND2	2:R:174:LEU:H	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:150:LEU:HA	1:I:187:LEU:HD22	1.92	0.52
2:Z:306:LYS:HG2	1:1:59:ARG:CZ	2.40	0.52
2:H:118:ASN:HD21	2:H:132:PHE:H	1.58	0.52
2:6:227:SER:C	2:6:229:GLU:H	2.13	0.52
2:T:172:ASN:ND2	2:T:174:LEU:H	2.08	0.52
2:R:271:VAL:HA	2:T:269:PHE:HE1	1.72	0.52
2:F:112:ILE:HD13	2:F:114:PHE:CZ	2.44	0.52
1:Q:68:GLN:NE2	1:Q:259:ARG:HB3	2.21	0.52
2:L:263:GLU:HG3	2:L:263:GLU:O	2.10	0.52
1:1:55:GLN:O	1:1:56:LYS:HB2	2.09	0.52
1:A:278:ILE:N	1:A:278:ILE:HD12	2.25	0.52
2:X:51:ARG:HH11	2:X:51:ARG:HG3	1.75	0.52
2:X:246:MET:O	2:X:250:GLU:HG3	2.09	0.52
2:B:84:ASN:ND2	2:B:128:HIS:HA	2.25	0.52
2:R:147:PRO:HD2	2:R:170:LEU:O	2.10	0.52
2:F:263:GLU:O	2:F:296:THR:HA	2.10	0.52
1:Q:142:VAL:HA	1:Q:163:THR:HG21	1.91	0.52
1:M:274:THR:OG1	1:M:275:ARG:N	2.42	0.52
1:Y:334:GLU:HG2	1:Y:337:TYR:CD2	2.44	0.52
2:P:152:ASP:HA	2:P:193:ILE:HD12	1.92	0.52
1:Q:225:VAL:CG1	1:Q:226:ASP:N	2.72	0.52
1:S:307:LYS:O	1:S:311:VAL:HG23	2.10	0.52
1:1:345:PRO:HB3	1:1:360:VAL:HG12	1.92	0.52
1:M:272:TYR:O	1:M:272:TYR:CD1	2.63	0.52
2:F:279:ILE:HG22	2:F:280:MET:N	2.24	0.52
1:U:95:THR:O	1:U:100:LEU:HB2	2.09	0.52
1:E:103:ARG:HG2	1:E:323:PHE:CD2	2.44	0.52
1:C:234:ARG:CD	1:C:238:ARG:NH2	2.73	0.52
1:1:4:ASP:HA	1:1:300:LEU:HD21	1.92	0.52
2:6:87:MET:HE2	2:6:132:PHE:HZ	1.75	0.52
1:S:335:LEU:C	1:S:335:LEU:HD23	2.30	0.52
2:H:327:LEU:O	2:H:329:ILE:HG23	2.10	0.52
2:4:266:TRP:HB3	2:4:267:PRO:HD2	1.91	0.52
1:G:95:THR:HG22	1:G:100:LEU:HB2	1.91	0.52
1:3:4:ASP:HA	1:3:300:LEU:HD21	1.92	0.52
1:I:223:LEU:N	1:I:223:LEU:HD23	2.24	0.52
2:T:154:LYS:O	2:T:157:ILE:HG22	2.09	0.52
1:O:142:VAL:HG21	1:O:175:ILE:HG12	1.91	0.52
1:S:105:ILE:O	1:S:109:LEU:HG	2.10	0.51
1:3:230:ILE:HG13	1:3:230:ILE:O	2.09	0.51
2:R:311:ASN:CG	1:S:332:LEU:HD11	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:225:VAL:HG12	1:O:226:ASP:N	2.25	0.51
1:Q:131:PHE:CE2	1:Q:133:GLY:HA2	2.45	0.51
2:L:278:ARG:HG3	2:L:278:ARG:HH11	1.74	0.51
1:S:38:MET:O	1:S:39:MET:C	2.47	0.51
1:W:177:GLU:CD	2:X:58:SER:HB3	2.30	0.51
1:Y:177:GLU:HG2	1:1:171:ASN:O	2.11	0.51
2:H:263:GLU:O	2:H:296:THR:HA	2.10	0.51
2:X:315:GLN:HG3	2:X:318:ASP:OD2	2.11	0.51
2:T:250:GLU:HB3	2:T:284:ALA:HB2	1.92	0.51
1:Q:93:GLY:O	1:Q:97:THR:HG23	2.09	0.51
2:N:246:MET:CE	2:N:279:ILE:HD13	2.40	0.51
1:5:29:ARG:NH1	1:5:29:ARG:HG3	2.11	0.51
2:H:184:PRO:HA	2:H:187:GLN:HE22	1.75	0.51
2:Z:184:PRO:HA	2:Z:187:GLN:HE22	1.75	0.51
2:Z:34:ASP:O	2:Z:38:LYS:HA	2.10	0.51
2:L:260:VAL:HG22	2:L:293:VAL:CG2	2.40	0.51
2:F:76:PRO:HG2	2:F:112:ILE:HG13	1.92	0.51
2:H:329:ILE:OXT	2:H:329:ILE:HG13	2.09	0.51
1:E:9:ILE:CD1	1:E:235:GLU:HG3	2.40	0.51
1:Y:229:ASP:OD1	1:Y:229:ASP:C	2.49	0.51
1:G:132:TYR:N	1:G:132:TYR:CD1	2.77	0.51
1:A:88:ALA:O	1:A:134:GLY:HA2	2.11	0.51
2:Z:155:GLY:HA3	2:Z:193:ILE:HG13	1.92	0.51
1:M:267:ASP:CB	1:M:268:PRO:HD3	2.37	0.51
1:1:95:THR:HG23	1:1:100:LEU:HD22	1.92	0.51
2:2:121:SER:HB3	2:2:124:VAL:CG2	2.36	0.51
1:3:45:MET:CE	1:3:102:VAL:HG13	2.41	0.51
1:E:11:LYS:HB3	1:E:23:VAL:HG12	1.93	0.51
2:J:260:VAL:HG22	2:J:293:VAL:CG2	2.40	0.51
2:D:33:TYR:O	2:D:34:ASP:HB2	2.10	0.51
2:H:246:MET:O	2:H:250:GLU:HG3	2.11	0.51
1:5:269:GLY:O	1:5:273:ARG:CD	2.55	0.51
1:S:253:MET:CE	1:S:255:LEU:HD11	2.39	0.51
1:A:9:ILE:HB	1:A:232:CYS:SG	2.50	0.51
2:J:238:MET:O	2:J:239:ARG:HB2	2.11	0.51
1:5:269:GLY:C	1:5:273:ARG:HH11	2.12	0.51
1:3:95:THR:HG23	1:3:100:LEU:HD22	1.92	0.51
1:Q:11:LYS:O	1:Q:11:LYS:HG3	2.09	0.51
2:4:140:PRO:HB2	2:6:301:PRO:HD3	1.93	0.51
2:D:285:PHE:O	2:D:288:LEU:HB2	2.11	0.51
1:E:11:LYS:O	1:E:11:LYS:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:315:GLN:O	2:X:316:VAL:C	2.48	0.51
2:2:143:LYS:HB2	2:2:167:VAL:HG22	1.91	0.51
2:N:98:ALA:HB2	2:N:142:LEU:HD13	1.92	0.51
1:A:222:GLY:HA2	1:A:252:LEU:O	2.11	0.51
2:T:24:PHE:CZ	2:T:76:PRO:HB3	2.46	0.51
1:S:259:ARG:NH1	1:S:261:HIS:O	2.44	0.51
1:C:28:THR:O	1:C:29:ARG:C	2.48	0.51
2:2:98:ALA:HB2	2:2:142:LEU:CD1	2.40	0.51
2:R:184:PRO:HA	2:R:187:GLN:HE21	1.76	0.51
2:F:135:TRP:O	2:F:138:HIS:HB3	2.10	0.51
2:R:20:ASP:OD1	2:R:20:ASP:C	2.48	0.51
1:Y:275:ARG:HH11	1:Y:275:ARG:HB2	1.75	0.51
1:Q:230:ILE:O	1:Q:230:ILE:HG13	2.10	0.51
1:C:307:LYS:O	1:C:311:VAL:HG23	2.11	0.51
1:M:172:GLN:HE22	2:P:88:GLN:HE22	1.58	0.51
1:C:322:GLN:HG3	1:C:323:PHE:N	2.25	0.51
2:V:16:GLU:OE2	2:V:162:ARG:NH1	2.43	0.51
1:Y:272:TYR:HD1	1:Y:272:TYR:C	2.11	0.51
1:S:232:CYS:HA	1:S:235:GLU:HB2	1.93	0.51
1:Y:10:LYS:HG2	1:Y:11:LYS:N	2.26	0.51
1:I:353:GLN:NE2	2:J:281:GLU:HB3	2.25	0.51
1:O:55:GLN:O	1:O:56:LYS:HB2	2.10	0.51
2:J:19:ARG:NH1	2:J:19:ARG:HG2	2.26	0.51
1:M:171:ASN:OD1	1:M:216:ARG:NH2	2.31	0.51
1:G:1:PHE:HA	1:G:299:ASN:HD21	1.76	0.51
1:K:277:GLU:O	1:K:281:VAL:HG23	2.10	0.51
1:3:88:ALA:HB2	1:3:141:GLN:NE2	2.25	0.51
2:V:87:MET:CE	2:X:95:ASN:ND2	2.74	0.51
2:2:234:GLU:OE1	2:2:255:LYS:NZ	2.44	0.51
1:Q:302:SER:OG	1:Q:305:GLU:HG3	2.11	0.51
1:G:289:MET:CE	1:G:290:LEU:HD23	2.41	0.51
1:5:40:GLN:O	1:5:44:ARG:HG2	2.11	0.51
1:1:280:GLU:CG	1:1:281:VAL:H	2.18	0.51
1:K:196:ASN:HD21	1:K:259:ARG:HE	1.59	0.51
2:N:329:ILE:HG13	2:N:329:ILE:OXT	2.10	0.51
2:Z:173:GLU:HG2	2:Z:173:GLU:O	2.11	0.51
1:I:286:ASP:OD2	1:I:288:ILE:HB	2.11	0.51
2:H:144:VAL:HG12	2:H:241:ILE:HB	1.92	0.51
1:A:182:ALA:HA	1:A:187:LEU:HD12	1.93	0.51
1:W:100:LEU:HD13	1:W:128:ALA:CB	2.41	0.50
1:5:150:LEU:HA	1:5:187:LEU:HD22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:118:ASN:ND2	2:N:132:PHE:H	2.03	0.50
1:Q:29:ARG:HB2	1:Q:300:LEU:HD22	1.92	0.50
1:I:29:ARG:HH11	1:I:29:ARG:CG	2.24	0.50
1:U:1:PHE:C	1:U:2:ALA:O	2.48	0.50
1:A:68:GLN:HE21	1:A:259:ARG:HB3	1.75	0.50
2:H:81:MET:HB3	2:H:85:PHE:HD2	1.74	0.50
2:Z:21:GLU:OE1	2:Z:21:GLU:N	2.44	0.50
1:A:313:VAL:O	1:A:316:GLU:HB3	2.11	0.50
1:3:15:HIS:CG	1:3:215:LYS:HG2	2.46	0.50
2:Z:127:GLN:OE1	1:1:125:HIS:HE1	1.94	0.50
1:Y:225:VAL:HB	1:Y:255:LEU:HD12	1.92	0.50
2:B:110:VAL:O	2:B:166:PRO:HD3	2.11	0.50
2:N:171:GLU:OE1	2:N:176:TYR:OH	2.23	0.50
2:J:98:ALA:HB2	2:J:142:LEU:HD13	1.92	0.50
2:T:314:PRO:O	2:T:315:GLN:HB2	2.11	0.50
1:1:29:ARG:HB2	1:1:300:LEU:CD2	2.41	0.50
2:D:18:GLU:OE2	1:E:272:TYR:CE2	2.63	0.50
2:P:238:MET:O	2:P:239:ARG:HB2	2.10	0.50
1:K:70:ALA:HB3	1:K:227:GLY:O	2.09	0.50
1:G:58:ILE:HD13	1:G:109:LEU:HB3	1.92	0.50
1:S:316:GLU:HA	1:S:316:GLU:OE1	2.10	0.50
1:Q:15:HIS:CG	1:Q:215:LYS:HG2	2.46	0.50
1:3:302:SER:OG	1:3:305:GLU:HG3	2.11	0.50
1:K:93:GLY:O	1:K:97:THR:HG23	2.12	0.50
1:S:27:LEU:CD2	1:S:28:THR:N	2.73	0.50
1:5:29:ARG:NH1	1:5:29:ARG:CG	2.70	0.50
1:O:223:LEU:HD23	1:O:223:LEU:H	1.76	0.50
1:U:132:TYR:CD1	1:U:148:ILE:HD13	2.47	0.50
1:W:103:ARG:HG2	1:W:323:PHE:CD2	2.46	0.50
1:W:140:ALA:O	1:W:143:PRO:HD2	2.11	0.50
1:A:196:ASN:HD21	1:A:259:ARG:CD	2.24	0.50
1:Q:100:LEU:HD13	1:Q:128:ALA:HB2	1.94	0.50
2:D:227:SER:C	2:D:229:GLU:N	2.64	0.50
2:6:172:ASN:HD21	2:6:174:LEU:HB2	1.75	0.50
2:J:276:CYS:HB3	2:L:280:MET:CE	2.42	0.50
2:V:28:GLU:OE2	2:V:59:GLU:OE2	2.28	0.50
1:G:71:CYS:O	1:G:75:LEU:HB2	2.11	0.50
1:3:167:ASP:HB3	1:3:195:ASN:HA	1.94	0.50
1:1:308:GLU:O	1:1:312:GLU:HG3	2.11	0.50
1:C:286:ASP:HB3	1:C:289:MET:HB2	1.92	0.50
1:Y:40:GLN:HE21	1:Y:288:ILE:HD13	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:313:VAL:O	1:E:316:GLU:HB3	2.11	0.50
2:P:118:ASN:HD21	2:P:131:CYS:HA	1.75	0.50
1:3:10:LYS:HG2	1:3:11:LYS:N	2.26	0.50
1:G:11:LYS:HB3	1:G:23:VAL:HG12	1.94	0.50
2:4:95:ASN:HD21	2:6:87:MET:HE3	1.77	0.50
1:Y:275:ARG:HB2	1:Y:275:ARG:NH1	2.26	0.50
2:J:31:ALA:HB3	2:J:54:ASP:OD2	2.12	0.50
2:J:9:ILE:HG13	2:J:153:ALA:HB1	1.93	0.50
2:6:1:LEU:HD13	2:6:2:GLN:N	2.26	0.50
2:F:51:ARG:O	2:F:52:ILE:HD13	2.11	0.50
1:U:33:LEU:HD12	1:U:295:MET:HE1	1.93	0.50
1:W:225:VAL:HG12	1:W:226:ASP:N	2.27	0.50
1:3:149:ALA:CB	1:3:189:CYS:HB2	2.41	0.50
2:F:19:ARG:HH11	2:F:19:ARG:HG2	1.76	0.50
1:I:230:ILE:O	1:I:230:ILE:HG13	2.12	0.50
1:U:320:ALA:O	1:U:323:PHE:HB3	2.12	0.50
2:Z:262:VAL:HA	2:Z:295:VAL:O	2.11	0.50
2:L:121:SER:OG	2:L:122:ALA:N	2.44	0.50
1:W:95:THR:HG22	1:W:100:LEU:HB2	1.93	0.50
1:1:3:ASN:O	1:1:4:ASP:CB	2.59	0.50
1:E:225:VAL:CG1	1:E:226:ASP:N	2.74	0.50
2:J:172:ASN:HD22	2:J:175:MET:N	2.09	0.50
1:5:95:THR:HG22	1:5:100:LEU:HB2	1.94	0.50
2:V:155:GLY:HA3	2:V:193:ILE:HG13	1.93	0.50
1:G:289:MET:HE2	1:G:290:LEU:HD23	1.93	0.50
2:L:112:ILE:CG1	2:L:113:VAL:N	2.75	0.50
2:2:124:VAL:O	2:2:125:ALA:HB3	2.12	0.50
2:N:231:VAL:HG21	2:N:329:ILE:HD11	1.93	0.50
1:5:335:LEU:O	1:5:335:LEU:HG	2.11	0.50
1:A:225:VAL:CG1	1:A:226:ASP:N	2.75	0.50
1:3:138:VAL:HG13	1:3:169:ALA:CB	2.42	0.50
1:M:335:LEU:HG	1:M:335:LEU:O	2.11	0.50
2:T:263:GLU:O	2:T:296:THR:HA	2.11	0.50
1:G:29:ARG:NH1	1:G:300:LEU:O	2.45	0.50
1:S:277:GLU:O	1:S:277:GLU:HG2	2.06	0.50
1:W:55:GLN:O	1:W:56:LYS:CB	2.54	0.50
1:Y:88:ALA:O	1:Y:134:GLY:CA	2.60	0.50
1:S:50:ASP:HB2	1:S:64:LEU:CD1	2.41	0.50
1:E:257:THR:OG1	1:E:258:TYR:N	2.44	0.50
1:C:39:MET:HG2	1:C:73:VAL:HG21	1.94	0.50
1:I:57:ILE:HD13	1:I:57:ILE:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:TYR:HA	1:C:252:LEU:HD22	1.94	0.50
1:Q:45:MET:HE1	1:Q:105:ILE:HD12	1.94	0.49
1:1:29:ARG:CG	1:1:29:ARG:NH1	2.74	0.49
1:W:29:ARG:CG	1:W:29:ARG:HH11	2.25	0.49
1:Q:113:LYS:CD	1:Q:328:PRO:HG2	2.42	0.49
1:A:281:VAL:O	1:A:281:VAL:CG1	2.60	0.49
2:Z:59:GLU:HA	2:Z:62:PHE:CE2	2.47	0.49
2:R:204:GLY:O	2:R:234:GLU:OE1	2.30	0.49
2:B:103:MET:SD	2:D:126:ALA:HB3	2.51	0.49
1:Y:278:ILE:O	1:Y:279:GLN:C	2.50	0.49
1:E:15:HIS:CG	1:E:215:LYS:HG2	2.47	0.49
1:S:1:PHE:HA	1:S:299:ASN:HD21	1.76	0.49
1:Q:289:MET:HE1	1:Q:290:LEU:CD2	2.42	0.49
1:3:284:LYS:O	1:3:285:SER:HB3	2.12	0.49
1:K:270:VAL:O	1:K:271:ALA:C	2.50	0.49
2:J:118:ASN:HD21	2:J:132:PHE:N	2.09	0.49
1:C:1:PHE:CE1	1:C:299:ASN:OD1	2.66	0.49
2:R:329:ILE:HG13	2:R:329:ILE:OXT	2.10	0.49
1:C:35:TYR:O	1:C:39:MET:HG3	2.12	0.49
2:N:237:ASN:C	2:N:237:ASN:ND2	2.65	0.49
2:P:280:MET:HA	2:P:285:PHE:CD1	2.47	0.49
2:6:24:PHE:CZ	2:6:76:PRO:HB3	2.47	0.49
2:6:51:ARG:O	2:6:52:ILE:HD13	2.13	0.49
2:N:181:GLU:O	2:N:183:PRO:HD3	2.12	0.49
1:I:138:VAL:HG13	1:I:169:ALA:HB2	1.94	0.49
2:R:102:TYR:CG	2:T:301:PRO:HG2	2.47	0.49
2:F:238:MET:O	2:F:239:ARG:HB2	2.12	0.49
1:I:307:LYS:O	1:I:311:VAL:HG23	2.12	0.49
1:Q:129:LYS:O	1:Q:130:ASN:HB2	2.12	0.49
1:C:138:VAL:HG13	1:C:169:ALA:HB2	1.94	0.49
1:G:274:THR:C	1:G:276:GLU:N	2.63	0.49
1:I:113:LYS:HG2	1:I:328:PRO:O	2.12	0.49
2:T:172:ASN:C	2:T:172:ASN:ND2	2.65	0.49
2:P:246:MET:O	2:P:250:GLU:HG3	2.12	0.49
1:3:43:ARG:HH11	1:3:43:ARG:HG2	1.76	0.49
1:U:147:GLY:HA2	2:V:65:ILE:HG23	1.95	0.49
2:V:181:GLU:O	2:V:183:PRO:HD3	2.13	0.49
1:O:29:ARG:HA	1:O:300:LEU:HD22	1.95	0.49
1:C:29:ARG:CB	1:C:300:LEU:CD2	2.90	0.49
1:I:55:GLN:O	1:I:56:LYS:CB	2.56	0.49
1:3:78:GLY:CA	1:3:238:ARG:HG2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:273:ALA:N	2:V:294:ARG:HD3	2.28	0.49
1:C:318:GLU:O	1:C:322:GLN:HB3	2.13	0.49
1:U:12:CYS:HB3	1:U:224:ARG:O	2.12	0.49
2:6:238:MET:O	2:6:239:ARG:HB2	2.12	0.49
2:L:1:LEU:HD13	2:L:2:GLN:N	2.28	0.49
1:Q:231:LEU:HD12	1:Q:294:ARG:NH1	2.28	0.49
1:Q:18:GLU:CG	1:Q:19:GLU:N	2.63	0.49
1:G:196:ASN:ND2	1:G:259:ARG:HE	2.09	0.49
2:4:1:LEU:HD13	2:4:2:GLN:N	2.15	0.49
1:S:95:THR:HG22	1:S:100:LEU:HB2	1.94	0.49
2:N:212:HIS:HB3	2:N:238:MET:CE	2.42	0.49
2:J:99:LYS:HG2	2:L:301:PRO:HB3	1.94	0.49
2:6:92:GLN:OE1	2:6:92:GLN:HA	2.12	0.49
1:M:103:ARG:HG2	1:M:323:PHE:CD2	2.47	0.49
1:C:302:SER:OG	1:C:305:GLU:HG3	2.13	0.49
1:Y:132:TYR:CD1	1:Y:148:ILE:HD13	2.48	0.49
1:I:139:GLY:HA3	1:I:172:GLN:HG3	1.94	0.49
1:S:27:LEU:CD2	1:S:27:LEU:C	2.77	0.49
2:R:325:LYS:HG2	1:S:354:TRP:CE2	2.46	0.49
1:A:100:LEU:HD13	1:A:128:ALA:CB	2.43	0.49
1:1:225:VAL:CG1	1:1:226:ASP:N	2.75	0.49
1:E:270:VAL:O	1:E:274:THR:HG23	2.13	0.49
2:4:256:THR:O	2:4:257:ASN:HB2	2.11	0.49
1:I:11:LYS:HG3	1:I:11:LYS:O	2.12	0.49
2:6:227:SER:C	2:6:229:GLU:N	2.65	0.49
2:B:99:LYS:O	2:B:103:MET:HG3	2.13	0.49
1:1:230:ILE:O	1:1:230:ILE:HG13	2.11	0.49
2:6:185:GLU:O	2:6:185:GLU:HG2	2.12	0.49
2:Z:84:ASN:ND2	2:Z:128:HIS:HA	2.27	0.49
1:Q:101:SER:OG	1:Q:104:GLU:HG3	2.13	0.49
2:B:250:GLU:O	2:B:254:MET:HG3	2.13	0.49
1:S:68:GLN:NE2	1:S:259:ARG:HB3	2.19	0.49
1:1:88:ALA:HB2	1:1:141:GLN:NE2	2.28	0.49
1:1:29:ARG:CB	1:1:300:LEU:HD22	2.43	0.49
1:K:229:ASP:C	1:K:231:LEU:N	2.65	0.49
1:E:351:ALA:O	2:H:295:VAL:HG13	2.12	0.49
1:S:24:THR:HG23	1:S:24:THR:O	2.12	0.49
1:5:154:TYR:CD1	2:6:74:LEU:HD21	2.47	0.49
2:V:126:ALA:HB1	2:X:99:LYS:HD3	1.94	0.49
2:D:304:TYR:O	2:D:305:ALA:C	2.49	0.49
2:P:313:ILE:HG23	2:P:314:PRO:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:84:HIS:CE1	1:E:130:ASN:ND2	2.80	0.49
2:N:246:MET:O	2:N:250:GLU:HG3	2.12	0.49
1:3:1:PHE:O	1:3:2:ALA:O	2.30	0.49
1:5:103:ARG:HG2	1:5:323:PHE:CD2	2.47	0.49
2:Z:87:MET:HE3	2:2:95:ASN:ND2	2.28	0.49
2:P:285:PHE:O	2:P:288:LEU:HB2	2.13	0.49
2:R:137:GLY:O	2:R:242:ARG:HD2	2.13	0.49
1:U:229:ASP:OD1	1:U:229:ASP:C	2.51	0.49
1:O:113:LYS:HB3	1:O:330:PRO:HA	1.95	0.49
1:A:18:GLU:CG	1:A:19:GLU:N	2.60	0.49
1:5:131:PHE:CZ	1:5:133:GLY:HA2	2.47	0.49
1:E:128:ALA:HB3	1:E:131:PHE:HB3	1.94	0.49
1:U:27:LEU:HD12	1:U:300:LEU:HD13	1.95	0.49
1:Y:289:MET:HE2	1:Y:290:LEU:HD23	1.93	0.49
2:D:112:ILE:O	2:D:166:PRO:HA	2.12	0.49
1:K:322:GLN:HG3	1:K:323:PHE:N	2.27	0.49
1:W:223:LEU:N	1:W:223:LEU:HD23	2.27	0.49
1:W:278:ILE:HG22	1:W:279:GLN:N	2.27	0.49
2:X:24:PHE:CZ	2:X:76:PRO:HB3	2.48	0.49
1:W:45:MET:HE3	1:W:102:VAL:HG22	1.95	0.49
2:D:118:ASN:HD21	2:D:132:PHE:H	1.60	0.49
1:E:75:LEU:HD11	1:E:255:LEU:HD21	1.94	0.49
2:X:214:ARG:HB3	2:X:215:PRO:HD3	1.94	0.49
1:A:289:MET:CE	1:A:290:LEU:HD21	2.37	0.48
1:M:269:GLY:O	1:M:270:VAL:C	2.50	0.48
1:C:258:TYR:CD1	1:C:258:TYR:C	2.86	0.48
2:6:182:PHE:O	2:6:183:PRO:C	2.51	0.48
1:K:182:ALA:HA	1:K:187:LEU:CD1	2.38	0.48
1:A:257:THR:OG1	1:A:258:TYR:N	2.45	0.48
1:U:100:LEU:HD13	1:U:128:ALA:CB	2.43	0.48
1:3:231:LEU:HD12	1:3:294:ARG:HH11	1.78	0.48
1:Y:45:MET:CE	1:Y:102:VAL:HG13	2.42	0.48
1:I:45:MET:HE1	1:I:105:ILE:HD12	1.95	0.48
1:U:68:GLN:HE22	1:U:196:ASN:HD22	1.60	0.48
1:C:340:TYR:HB3	2:D:165:ASN:ND2	2.27	0.48
2:Z:87:MET:CE	2:2:95:ASN:ND2	2.77	0.48
1:A:162:LEU:N	1:A:162:LEU:HD12	2.28	0.48
1:Y:95:THR:HG22	1:Y:100:LEU:HB2	1.96	0.48
2:Z:202:ARG:O	2:Z:234:GLU:HA	2.13	0.48
1:5:71:CYS:SG	1:5:255:LEU:HD23	2.53	0.48
2:J:157:ILE:O	2:J:161:ILE:HG13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:243:TYR:CE2	1:1:248:LYS:HD2	2.48	0.48
1:1:68:GLN:NE2	1:1:259:ARG:HB3	2.23	0.48
1:W:10:LYS:HG2	1:W:11:LYS:H	1.78	0.48
2:4:238:MET:O	2:4:239:ARG:HB2	2.14	0.48
1:3:100:LEU:HD13	1:3:128:ALA:CB	2.42	0.48
1:3:338:HIS:O	2:4:102:TYR:HA	2.12	0.48
2:Z:237:ASN:C	2:Z:237:ASN:ND2	2.67	0.48
2:Z:214:ARG:N	2:Z:215:PRO:HD2	2.28	0.48
1:I:89:TYR:HB2	1:I:124:MET:HG2	1.94	0.48
1:3:286:ASP:OD2	1:3:288:ILE:HB	2.13	0.48
2:B:253:VAL:HG11	2:B:288:LEU:HD13	1.94	0.48
2:2:93:VAL:O	2:2:97:ALA:HB3	2.13	0.48
2:V:313:ILE:CG2	2:V:314:PRO:N	2.77	0.48
1:3:289:MET:HE3	1:3:290:LEU:HD23	1.95	0.48
1:M:281:VAL:HG12	1:M:282:ARG:N	2.27	0.48
1:1:29:ARG:NH1	1:1:300:LEU:O	2.46	0.48
1:1:4:ASP:HB3	1:1:28:THR:HA	1.95	0.48
2:F:172:ASN:ND2	2:F:174:LEU:H	2.11	0.48
1:Q:9:ILE:HB	1:Q:232:CYS:SG	2.53	0.48
2:L:51:ARG:O	2:L:52:ILE:HD13	2.13	0.48
2:T:268:GLN:O	2:T:269:PHE:HB2	2.14	0.48
1:S:171:ASN:HD21	1:S:208:ALA:HB2	1.79	0.48
1:Q:149:ALA:O	1:Q:152:CYS:HB2	2.14	0.48
2:R:197:LYS:HA	2:R:245:ASP:OD2	2.13	0.48
1:A:223:LEU:HD23	1:A:223:LEU:N	2.27	0.48
1:Q:39:MET:HG2	1:Q:73:VAL:HG21	1.95	0.48
2:J:207:ILE:HD13	2:J:323:ILE:HG23	1.95	0.48
1:M:50:ASP:HB2	1:M:64:LEU:CD1	2.43	0.48
1:1:16:ARG:HG2	1:1:16:ARG:NH1	2.26	0.48
1:3:182:ALA:HA	1:3:187:LEU:HD12	1.95	0.48
2:H:238:MET:O	2:H:240:THR:N	2.45	0.48
1:I:11:LYS:HE3	1:I:11:LYS:HB2	1.71	0.48
2:N:9:ILE:HG12	2:N:153:ALA:HB1	1.95	0.48
1:1:302:SER:OG	1:1:305:GLU:HG3	2.12	0.48
1:1:174:GLN:HB3	2:2:60:MET:HG2	1.94	0.48
1:5:142:VAL:HA	1:5:163:THR:HG21	1.96	0.48
2:Z:259:LEU:HD12	2:Z:260:VAL:N	2.28	0.48
2:J:329:ILE:HG13	2:J:329:ILE:OXT	2.12	0.48
1:S:28:THR:C	1:S:30:GLU:N	2.66	0.48
1:1:257:THR:OG1	1:1:258:TYR:N	2.47	0.48
1:5:45:MET:CE	1:5:102:VAL:HA	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:95:THR:CG2	1:1:100:LEU:HD22	2.43	0.48
1:1:113:LYS:HB3	1:1:330:PRO:HA	1.95	0.48
2:2:51:ARG:NH1	2:2:51:ARG:HG3	2.27	0.48
2:T:184:PRO:HA	2:T:187:GLN:HE21	1.75	0.48
1:E:108:GLU:OE1	1:E:117:ALA:N	2.44	0.48
1:Q:77:ALA:HB3	1:Q:234:ARG:HG3	1.96	0.48
1:M:229:ASP:O	1:M:231:LEU:N	2.46	0.48
1:C:105:ILE:O	1:C:109:LEU:HG	2.14	0.48
1:Y:70:ALA:HB3	1:Y:227:GLY:O	2.12	0.48
1:Q:196:ASN:ND2	1:Q:259:ARG:HD3	2.28	0.48
2:H:182:PHE:HD2	2:H:187:GLN:HG3	1.79	0.48
1:O:39:MET:HE3	1:O:288:ILE:HG12	1.95	0.48
2:X:28:GLU:HB2	2:X:81:MET:HE3	1.95	0.48
2:X:39:VAL:O	2:X:39:VAL:HG12	2.13	0.48
1:C:162:LEU:HD12	1:C:162:LEU:N	2.29	0.48
2:L:246:MET:O	2:L:250:GLU:HG3	2.13	0.48
1:3:171:ASN:OD1	1:3:216:ARG:NH2	2.46	0.48
1:Y:354:TRP:CZ2	2:2:325:LYS:HG2	2.48	0.48
2:X:285:PHE:O	2:X:288:LEU:HB2	2.14	0.48
2:J:313:ILE:HG23	2:J:314:PRO:HD2	1.95	0.48
1:S:278:ILE:HD13	1:S:278:ILE:H	1.65	0.48
1:Q:258:TYR:C	1:Q:258:TYR:CD1	2.87	0.48
1:G:177:GLU:CD	2:H:58:SER:HB3	2.34	0.48
1:K:44:ARG:HH21	1:K:314:ARG:HE	1.62	0.48
1:K:124:MET:O	1:K:134:GLY:HA3	2.14	0.48
2:H:98:ALA:CB	2:H:142:LEU:HD13	2.39	0.48
1:M:101:SER:OG	1:M:104:GLU:HG3	2.13	0.48
2:V:88:GLN:HG2	2:X:60:MET:HE3	1.94	0.48
1:Q:335:LEU:HB2	2:T:308:LEU:HD22	1.96	0.48
1:I:10:LYS:HG2	1:I:11:LYS:N	2.28	0.48
2:L:118:ASN:HD21	2:L:132:PHE:H	1.61	0.48
2:Z:98:ALA:HB2	2:Z:142:LEU:HD13	1.96	0.48
2:4:260:VAL:HG22	2:4:293:VAL:CG2	2.44	0.48
1:A:352:ASN:HB3	2:D:295:VAL:HG22	1.94	0.48
2:F:267:PRO:HA	2:F:296:THR:HG21	1.96	0.48
2:R:140:PRO:HA	2:R:242:ARG:HH21	1.79	0.48
2:R:259:LEU:HD12	2:R:260:VAL:N	2.29	0.48
1:M:177:GLU:HG2	1:O:171:ASN:O	2.14	0.48
1:3:292:LYS:HG3	1:3:306:LEU:HD13	1.95	0.48
1:G:196:ASN:HB3	1:G:257:THR:CG2	2.36	0.47
1:S:37:ARG:HG3	1:S:37:ARG:HH11	1.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:250:GLU:HB3	2:D:284:ALA:HB2	1.96	0.47
1:I:102:VAL:HG11	1:I:317:ILE:CD1	2.43	0.47
1:Q:229:ASP:OD1	1:Q:231:LEU:HB2	2.14	0.47
1:W:45:MET:HE3	1:W:102:VAL:HG13	1.96	0.47
2:L:94:ILE:HA	2:L:94:ILE:HD13	1.64	0.47
2:R:127:GLN:NE2	2:T:95:ASN:O	2.46	0.47
2:V:308:LEU:HD22	1:W:335:LEU:HB2	1.96	0.47
1:U:45:MET:CE	1:U:102:VAL:HG13	2.44	0.47
1:U:95:THR:HG23	1:U:100:LEU:HD22	1.96	0.47
1:M:15:HIS:ND1	1:M:215:LYS:HG2	2.30	0.47
2:R:327:LEU:HA	2:R:327:LEU:HD23	1.72	0.47
2:N:81:MET:HB3	2:N:85:PHE:CD2	2.48	0.47
2:Z:127:GLN:HE21	2:2:95:ASN:HB3	1.79	0.47
2:J:34:ASP:OD2	2:J:41:ARG:HA	2.15	0.47
1:U:89:TYR:C	1:U:89:TYR:CD1	2.87	0.47
2:V:21:GLU:N	2:V:21:GLU:OE1	2.47	0.47
2:4:31:ALA:HB3	2:4:54:ASP:OD2	2.15	0.47
1:3:334:GLU:HG2	1:3:337:TYR:CE2	2.48	0.47
1:S:164:LEU:N	1:S:164:LEU:HD12	2.29	0.47
1:S:70:ALA:HB3	1:S:227:GLY:O	2.13	0.47
1:Q:75:LEU:HD12	1:Q:237:THR:OG1	2.13	0.47
1:E:100:LEU:HD13	1:E:128:ALA:HB2	1.96	0.47
1:A:102:VAL:HG11	1:A:317:ILE:HD13	1.97	0.47
1:I:29:ARG:NH1	1:I:300:LEU:O	2.47	0.47
1:I:353:GLN:HE22	2:J:281:GLU:HB3	1.79	0.47
2:F:81:MET:HB3	2:F:85:PHE:CE2	2.49	0.47
1:G:141:GLN:HA	1:G:144:LEU:HD12	1.97	0.47
2:V:184:PRO:HA	2:V:187:GLN:HE22	1.78	0.47
1:C:328:PRO:C	1:C:329:GLU:O	2.50	0.47
2:R:4:THR:HA	2:R:179:PRO:HA	1.96	0.47
1:M:197:ARG:HG2	1:M:257:THR:O	2.13	0.47
2:N:185:GLU:O	2:N:188:SER:HB3	2.14	0.47
1:C:164:LEU:HA	1:C:192:ILE:O	2.15	0.47
1:K:45:MET:HE1	1:K:105:ILE:CD1	2.38	0.47
2:P:182:PHE:HD2	2:P:187:GLN:HG2	1.79	0.47
1:E:337:TYR:HB3	1:E:338:HIS:CD2	2.49	0.47
1:U:1:PHE:O	1:U:2:ALA:O	2.32	0.47
1:Y:197:ARG:HA	1:Y:197:ARG:HD3	1.41	0.47
1:Y:196:ASN:ND2	1:Y:259:ARG:NE	2.61	0.47
2:J:256:THR:O	2:J:257:ASN:HB2	2.15	0.47
1:A:323:PHE:O	1:A:327:ASP:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:15:GLU:OE1	2:F:189:LYS:HA	2.14	0.47
1:M:11:LYS:HE3	1:M:11:LYS:HB2	1.63	0.47
2:6:263:GLU:O	2:6:263:GLU:HG3	2.14	0.47
2:P:80:PHE:O	2:P:81:MET:C	2.49	0.47
2:V:87:MET:HE1	2:X:95:ASN:ND2	2.30	0.47
2:F:220:LEU:HD23	2:F:235:VAL:HG21	1.95	0.47
1:I:95:THR:HG23	1:I:100:LEU:HD22	1.95	0.47
2:H:214:ARG:HB3	2:H:215:PRO:HD3	1.96	0.47
1:A:279:GLN:HE22	1:A:282:ARG:HH21	1.63	0.47
2:D:313:ILE:HG22	2:D:314:PRO:CD	2.29	0.47
1:A:29:ARG:NH1	1:A:29:ARG:HG3	2.28	0.47
1:C:95:THR:HG23	1:C:100:LEU:HD22	1.92	0.47
1:O:95:THR:HG23	1:O:100:LEU:HD22	1.96	0.47
2:T:182:PHE:CD2	2:T:187:GLN:HG3	2.50	0.47
1:O:233:VAL:O	1:O:234:ARG:C	2.49	0.47
1:G:74:GLY:CA	1:G:230:ILE:HD12	2.45	0.47
1:I:284:LYS:O	1:I:285:SER:HB3	2.14	0.47
2:T:172:ASN:HD22	2:T:175:MET:H	1.62	0.47
1:C:216:ARG:HG3	1:C:216:ARG:HH11	1.79	0.47
1:C:223:LEU:HD23	1:C:223:LEU:N	2.29	0.47
1:W:39:MET:HG2	1:W:73:VAL:HG21	1.94	0.47
2:B:17:LEU:HD23	2:B:23:VAL:HG12	1.96	0.47
1:C:234:ARG:CZ	1:C:238:ARG:NH2	2.78	0.47
1:1:113:LYS:HD2	1:1:328:PRO:HG2	1.97	0.47
2:T:307:ILE:CG2	2:T:308:LEU:N	2.77	0.47
2:P:212:HIS:HB3	2:P:238:MET:CE	2.43	0.47
1:W:289:MET:HE2	1:W:290:LEU:HD23	1.97	0.47
2:J:185:GLU:O	2:J:188:SER:HB3	2.14	0.47
2:N:306:LYS:HG2	1:O:59:ARG:CZ	2.45	0.47
2:B:81:MET:HB3	2:B:85:PHE:CD2	2.50	0.47
1:C:345:PRO:HB3	1:C:360:VAL:HG12	1.95	0.47
1:G:272:TYR:CD1	1:G:273:ARG:HA	2.50	0.47
1:G:272:TYR:C	1:G:274:THR:H	2.18	0.47
1:Q:45:MET:HE2	1:Q:105:ILE:HB	1.97	0.47
1:3:327:ASP:OD1	1:3:328:PRO:HD2	2.15	0.47
1:W:95:THR:CG2	1:W:100:LEU:HD22	2.44	0.47
1:5:45:MET:HE1	1:5:105:ILE:HD12	1.96	0.47
1:S:45:MET:HE2	1:S:105:ILE:HB	1.96	0.47
1:I:335:LEU:HD21	2:L:300:VAL:HG21	1.97	0.47
2:B:172:ASN:HD21	2:B:174:LEU:HB2	1.78	0.47
1:3:335:LEU:HD23	1:3:335:LEU:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:162:LEU:HD11	1:5:190:ILE:HD12	1.97	0.47
2:N:212:HIS:HB3	2:N:238:MET:HE3	1.97	0.47
1:O:44:ARG:NH1	1:O:47:LEU:HD12	2.29	0.47
2:H:110:VAL:HG12	2:H:110:VAL:O	2.14	0.47
1:I:70:ALA:HB3	1:I:227:GLY:O	2.14	0.47
2:X:1:LEU:C	2:X:1:LEU:HD13	2.35	0.47
1:G:45:MET:HE1	1:G:105:ILE:HD12	1.97	0.47
2:N:43:LEU:N	2:N:43:LEU:HD12	2.30	0.47
1:S:10:LYS:HG2	1:S:11:LYS:N	2.30	0.47
1:U:296:VAL:HG12	1:U:297:ASN:HD22	1.79	0.47
1:O:257:THR:OG1	1:O:258:TYR:N	2.46	0.47
2:6:182:PHE:HA	2:6:183:PRO:HD2	1.64	0.47
1:5:196:ASN:N	1:5:196:ASN:OD1	2.48	0.47
2:4:172:ASN:HD22	2:4:175:MET:N	2.13	0.47
2:H:33:TYR:O	2:H:34:ASP:HB2	2.15	0.47
2:H:87:MET:HE2	2:H:132:PHE:HZ	1.80	0.47
2:R:237:ASN:HD22	2:R:237:ASN:C	2.17	0.47
2:6:313:ILE:HG23	2:6:314:PRO:HD2	1.96	0.47
1:G:171:ASN:HD21	1:G:208:ALA:HB2	1.79	0.47
1:A:213:TYR:HB2	1:A:254:GLU:OE1	2.15	0.47
1:A:308:GLU:O	1:A:312:GLU:HG3	2.14	0.47
1:K:341:SER:HB2	2:L:101:TYR:CZ	2.49	0.47
1:A:129:LYS:O	1:A:130:ASN:HB2	2.14	0.47
2:J:326:THR:C	2:J:328:ASN:H	2.16	0.47
1:G:9:ILE:HD11	1:G:22:PRO:O	2.14	0.47
1:I:177:GLU:OE1	2:J:61:GLY:N	2.47	0.47
1:A:286:ASP:O	1:A:290:LEU:HG	2.14	0.47
1:K:112:ARG:HD2	1:K:327:ASP:O	2.15	0.47
1:C:253:MET:CE	1:C:255:LEU:HD13	2.44	0.47
1:W:29:ARG:HA	1:W:300:LEU:HD22	1.97	0.47
2:R:184:PRO:CG	2:R:185:GLU:H	2.28	0.47
1:1:45:MET:HE3	1:1:102:VAL:HG22	1.97	0.47
2:F:263:GLU:HG2	2:F:296:THR:HG22	1.97	0.47
2:H:137:GLY:HA2	2:H:144:VAL:HG21	1.97	0.47
2:X:214:ARG:N	2:X:215:PRO:HD2	2.30	0.47
1:5:304:GLU:O	1:5:308:GLU:HG3	2.14	0.47
1:G:225:VAL:HG12	1:G:226:ASP:N	2.30	0.47
2:L:258:HIS:CD2	2:L:327:LEU:HD23	2.49	0.47
1:C:225:VAL:CG1	1:C:226:ASP:N	2.78	0.47
1:M:28:THR:O	1:M:29:ARG:C	2.53	0.47
1:5:269:GLY:CA	1:5:273:ARG:HH11	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:184:PRO:HA	2:X:187:GLN:HE22	1.76	0.47
1:S:45:MET:HE2	1:S:105:ILE:HD12	1.96	0.47
1:Q:196:ASN:HB3	1:Q:257:THR:HG23	1.97	0.47
1:E:272:TYR:CD1	1:E:272:TYR:O	2.68	0.47
2:4:95:ASN:HD21	2:6:87:MET:HE1	1.80	0.47
1:A:150:LEU:HA	1:A:187:LEU:HD22	1.97	0.47
1:M:229:ASP:OD1	1:M:231:LEU:HB2	2.15	0.47
1:5:1:PHE:HA	1:5:299:ASN:HD21	1.80	0.47
1:C:316:GLU:HA	1:C:316:GLU:OE1	2.15	0.47
1:U:141:GLN:OE1	1:U:141:GLN:N	2.42	0.47
2:V:260:VAL:HG22	2:V:293:VAL:CG2	2.44	0.47
1:W:190:ILE:HD13	1:W:240:ALA:HB1	1.97	0.47
1:E:55:GLN:O	1:E:56:LYS:HB2	2.15	0.47
1:K:217:GLY:O	1:K:218:ASP:HB3	2.15	0.47
1:A:286:ASP:HB3	1:A:289:MET:HB3	1.97	0.46
2:Z:238:MET:O	2:Z:239:ARG:HB2	2.13	0.46
1:I:102:VAL:HG11	1:I:317:ILE:HD12	1.96	0.46
2:F:278:ARG:CG	2:F:278:ARG:NH1	2.77	0.46
1:G:45:MET:HE3	1:G:102:VAL:HG22	1.96	0.46
1:3:225:VAL:HG12	1:3:226:ASP:N	2.30	0.46
1:S:89:TYR:HB2	1:S:124:MET:HG2	1.96	0.46
2:6:88:GLN:HB3	2:6:88:GLN:HE21	1.49	0.46
1:W:70:ALA:HB3	1:W:227:GLY:O	2.15	0.46
2:R:276:CYS:HB3	2:T:280:MET:CE	2.45	0.46
1:M:108:GLU:OE1	1:M:117:ALA:N	2.47	0.46
2:B:148:TRP:CD1	2:B:175:MET:HE2	2.50	0.46
2:J:171:GLU:OE1	2:J:176:TYR:OH	2.26	0.46
1:C:11:LYS:CB	1:C:23:VAL:HG12	2.46	0.46
2:H:237:ASN:ND2	2:H:237:ASN:C	2.68	0.46
1:3:138:VAL:HG13	1:3:169:ALA:HB2	1.97	0.46
1:Q:231:LEU:HD23	1:Q:231:LEU:HA	1.43	0.46
1:E:231:LEU:HD12	1:E:294:ARG:NH1	2.31	0.46
1:K:164:LEU:N	1:K:164:LEU:HD12	2.31	0.46
2:Z:94:ILE:HD13	2:Z:94:ILE:HA	1.70	0.46
2:4:16:GLU:OE2	2:4:162:ARG:NH1	2.47	0.46
2:L:285:PHE:C	2:L:287:PHE:H	2.18	0.46
2:J:271:VAL:HA	2:L:269:PHE:HE1	1.80	0.46
2:F:250:GLU:O	2:F:254:MET:HG3	2.15	0.46
1:Q:29:ARG:CG	1:Q:29:ARG:NH1	2.66	0.46
1:1:4:ASP:CB	1:1:28:THR:HA	2.45	0.46
1:K:29:ARG:HH11	1:K:29:ARG:CG	2.25	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:237:ASN:ND2	2:P:237:ASN:C	2.67	0.46
1:Y:68:GLN:NE2	1:Y:196:ASN:HD22	2.13	0.46
1:Y:113:LYS:HD3	1:Y:328:PRO:HG2	1.97	0.46
1:3:1:PHE:C	1:3:2:ALA:O	2.53	0.46
2:H:222:ALA:HB2	2:H:316:VAL:HG12	1.96	0.46
2:H:238:MET:C	2:H:240:THR:H	2.18	0.46
2:D:118:ASN:HD21	2:D:132:PHE:N	2.13	0.46
1:S:164:LEU:HA	1:S:192:ILE:O	2.15	0.46
2:L:285:PHE:C	2:L:287:PHE:N	2.68	0.46
2:X:93:VAL:O	2:X:97:ALA:HB3	2.16	0.46
2:F:313:ILE:HG23	2:F:314:PRO:N	2.28	0.46
2:V:26:LEU:HD23	2:V:78:CYS:HA	1.97	0.46
2:B:59:GLU:OE1	2:B:59:GLU:N	2.49	0.46
1:I:85:LEU:HD23	1:I:131:PHE:CD1	2.50	0.46
1:E:292:LYS:NZ	1:E:303:VAL:HG23	2.31	0.46
2:2:81:MET:HB2	2:2:81:MET:HE3	1.85	0.46
2:F:279:ILE:HA	2:F:279:ILE:HD12	1.67	0.46
1:3:258:TYR:CZ	1:3:277:GLU:OE2	2.67	0.46
1:3:29:ARG:NH1	1:3:29:ARG:CG	2.79	0.46
1:1:286:ASP:HB3	1:1:289:MET:HB3	1.97	0.46
2:L:16:GLU:HG3	2:L:161:ILE:HD12	1.96	0.46
2:R:271:VAL:HA	2:T:269:PHE:CE1	2.50	0.46
1:O:164:LEU:H	1:O:164:LEU:HD12	1.80	0.46
1:S:106:LEU:HA	1:S:106:LEU:HD23	1.81	0.46
1:K:230:ILE:O	1:K:230:ILE:CG1	2.63	0.46
1:5:140:ALA:O	1:5:143:PRO:HD2	2.15	0.46
1:I:37:ARG:NH2	1:I:309:ILE:HG23	2.30	0.46
2:J:21:GLU:HA	2:J:51:ARG:NH2	2.30	0.46
2:N:87:MET:CE	2:P:95:ASN:ND2	2.79	0.46
1:E:142:VAL:HB	1:E:143:PRO:HD3	1.97	0.46
1:3:55:GLN:O	1:3:56:LYS:CB	2.59	0.46
1:Y:28:THR:O	1:Y:29:ARG:C	2.53	0.46
1:I:45:MET:HE3	1:I:102:VAL:HG22	1.97	0.46
1:E:29:ARG:HG2	1:E:300:LEU:O	2.16	0.46
1:C:296:VAL:C	1:C:298:SER:H	2.18	0.46
1:U:39:MET:HG2	1:U:73:VAL:HG21	1.98	0.46
2:R:39:VAL:O	2:R:39:VAL:HG12	2.13	0.46
1:1:223:LEU:H	1:1:223:LEU:HD23	1.79	0.46
2:N:311:ASN:HA	2:N:315:GLN:HE21	1.81	0.46
1:O:37:ARG:NH2	1:O:309:ILE:HG23	2.29	0.46
1:C:174:GLN:HB3	2:D:60:MET:HG3	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:121:SER:OG	2:J:122:ALA:N	2.48	0.46
1:K:222:GLY:HA2	1:K:252:LEU:O	2.16	0.46
2:Z:25:LEU:HD12	2:Z:77:ILE:O	2.15	0.46
1:U:231:LEU:HD12	1:U:294:ARG:NH1	2.30	0.46
1:W:275:ARG:CG	1:W:275:ARG:HH11	2.29	0.46
2:D:172:ASN:ND2	2:D:175:MET:H	2.12	0.46
1:O:234:ARG:HE	1:O:238:ARG:NH1	2.13	0.46
1:O:234:ARG:HE	1:O:238:ARG:HH12	1.63	0.46
2:F:313:ILE:HG13	2:F:314:PRO:HD2	1.98	0.46
2:2:81:MET:HB3	2:2:85:PHE:CD2	2.51	0.46
2:P:16:GLU:OE1	2:P:16:GLU:HA	2.15	0.46
1:M:118:LYS:HB2	1:M:118:LYS:HE2	1.80	0.46
2:X:263:GLU:O	2:X:296:THR:HA	2.16	0.46
1:W:277:GLU:O	1:W:281:VAL:HG23	2.15	0.46
1:C:147:GLY:HA2	2:D:65:ILE:HG23	1.96	0.46
2:V:135:TRP:O	2:V:138:HIS:HB3	2.15	0.46
1:O:348:VAL:HG23	1:O:359:SER:HB2	1.97	0.46
2:F:142:LEU:HA	2:F:142:LEU:HD12	1.59	0.46
1:U:334:GLU:HG2	1:U:337:TYR:CZ	2.50	0.46
1:A:95:THR:HG23	1:A:100:LEU:HD22	1.97	0.46
1:5:142:VAL:HA	1:5:163:THR:CG2	2.45	0.46
1:M:29:ARG:HG3	1:M:300:LEU:O	2.15	0.46
2:R:205:THR:HG22	2:R:255:LYS:HD3	1.98	0.46
2:V:81:MET:HB3	2:V:85:PHE:CD2	2.51	0.46
1:C:145:GLY:HA2	1:C:148:ILE:HD12	1.98	0.46
1:U:337:TYR:O	1:U:338:HIS:HB2	2.15	0.46
1:5:282:ARG:HG2	1:5:283:SER:N	2.31	0.46
1:5:162:LEU:HD12	1:5:190:ILE:HD12	1.97	0.46
1:3:142:VAL:HG21	1:3:175:ILE:HG12	1.97	0.46
2:X:280:MET:HA	2:X:285:PHE:CD1	2.51	0.46
1:U:39:MET:HE2	1:U:291:LEU:HD22	1.98	0.46
2:L:279:ILE:HD13	2:L:279:ILE:HA	1.63	0.46
2:T:279:ILE:HD12	2:T:279:ILE:HG23	1.64	0.46
1:1:162:LEU:N	1:1:162:LEU:HD12	2.30	0.46
1:Y:118:LYS:HB2	1:Y:118:LYS:HE2	1.83	0.46
1:M:140:ALA:O	1:M:143:PRO:HD2	2.16	0.46
1:S:225:VAL:HG12	1:S:226:ASP:N	2.30	0.46
1:E:101:SER:O	1:E:105:ILE:HG13	2.16	0.46
1:M:101:SER:O	1:M:105:ILE:HG13	2.15	0.46
1:E:57:ILE:HD13	1:E:57:ILE:H	1.74	0.46
2:2:212:HIS:HB3	2:2:238:MET:HE3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:10:LYS:HG2	1:U:11:LYS:N	2.31	0.46
1:W:118:LYS:HB2	1:W:118:LYS:HZ2	1.78	0.46
2:D:262:VAL:HG22	2:D:295:VAL:HB	1.98	0.46
2:2:21:GLU:HA	2:2:51:ARG:NH2	2.30	0.46
1:3:149:ALA:HB1	1:3:189:CYS:HB2	1.98	0.46
2:L:237:ASN:C	2:L:237:ASN:ND2	2.70	0.46
1:Q:1:PHE:C	1:Q:2:ALA:O	2.54	0.46
1:S:85:LEU:HD23	1:S:131:PHE:CD1	2.50	0.46
1:I:138:VAL:HG13	1:I:169:ALA:CB	2.46	0.46
2:F:124:VAL:HB	2:F:128:HIS:HB2	1.98	0.46
1:A:61:PHE:HD2	1:A:124:MET:CE	2.29	0.46
2:2:20:ASP:OD1	2:2:22:LYS:HB2	2.15	0.46
1:E:155:ASN:O	1:E:156:GLY:C	2.54	0.46
1:Q:279:GLN:O	1:Q:280:GLU:C	2.53	0.46
1:1:150:LEU:HA	1:1:187:LEU:HD22	1.98	0.46
2:L:184:PRO:HA	2:L:187:GLN:NE2	2.31	0.46
1:3:279:GLN:O	1:3:280:GLU:C	2.54	0.46
1:Q:284:LYS:HB2	1:Q:284:LYS:HE3	1.61	0.46
2:P:124:VAL:O	2:P:125:ALA:HB3	2.16	0.46
1:U:29:ARG:HA	1:U:300:LEU:HD22	1.99	0.46
2:H:74:LEU:HA	2:H:74:LEU:HD12	1.71	0.46
1:M:11:LYS:O	1:M:11:LYS:HG3	2.14	0.46
1:A:164:LEU:HD12	1:A:164:LEU:N	2.31	0.46
1:C:9:ILE:HD11	1:C:22:PRO:O	2.16	0.46
2:F:19:ARG:NH1	2:F:19:ARG:HG2	2.31	0.46
1:1:221:PRO:HG3	1:1:243:TYR:OH	2.16	0.46
2:F:214:ARG:N	2:F:215:PRO:HD2	2.31	0.46
1:A:118:LYS:HB2	1:A:118:LYS:HE2	1.43	0.46
2:4:197:LYS:HA	2:4:245:ASP:OD2	2.16	0.46
2:P:51:ARG:O	2:P:52:ILE:HD13	2.16	0.46
2:Z:252:SER:O	2:Z:256:THR:HG23	2.16	0.46
2:4:325:LYS:HG2	1:5:354:TRP:CZ2	2.51	0.46
1:A:37:ARG:CZ	1:A:309:ILE:HG23	2.46	0.46
1:C:95:THR:HG22	1:C:100:LEU:HB2	1.97	0.45
1:M:112:ARG:HD2	1:M:327:ASP:O	2.16	0.45
2:D:172:ASN:ND2	2:D:174:LEU:H	2.14	0.45
2:F:148:TRP:O	2:F:175:MET:HE2	2.16	0.45
2:2:268:GLN:O	2:2:269:PHE:CB	2.62	0.45
2:B:252:SER:O	2:B:256:THR:HG23	2.16	0.45
1:C:1:PHE:CD1	1:C:299:ASN:OD1	2.68	0.45
2:P:206:HIS:ND1	2:P:206:HIS:N	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:26:LEU:HD21	2:T:66:ALA:HB2	1.97	0.45
2:B:16:GLU:OE2	2:B:162:ARG:NH1	2.48	0.45
2:X:307:ILE:HG23	2:X:308:LEU:N	2.31	0.45
1:U:327:ASP:OD1	1:U:328:PRO:CD	2.50	0.45
1:C:131:PHE:CZ	1:C:133:GLY:HA2	2.51	0.45
1:1:297:ASN:ND2	1:1:297:ASN:N	2.61	0.45
1:W:29:ARG:HG2	1:W:29:ARG:HH11	1.81	0.45
2:4:148:TRP:O	2:4:175:MET:HE2	2.17	0.45
2:Z:140:PRO:HB2	2:2:301:PRO:HD3	1.99	0.45
2:X:81:MET:HB3	2:X:85:PHE:HD2	1.78	0.45
1:C:38:MET:O	1:C:39:MET:C	2.54	0.45
1:W:39:MET:CE	1:W:291:LEU:HD22	2.47	0.45
1:G:61:PHE:HB3	1:G:63:HIS:CE1	2.50	0.45
2:J:266:TRP:HB3	2:J:267:PRO:HD2	1.97	0.45
1:5:259:ARG:HG3	1:5:259:ARG:HH11	1.82	0.45
2:F:149:ASN:OD1	2:F:151:GLU:HB3	2.17	0.45
2:B:143:LYS:HB2	2:B:167:VAL:HG22	1.97	0.45
2:D:26:LEU:HD21	2:D:66:ALA:HB2	1.98	0.45
1:Q:37:ARG:NH2	1:Q:309:ILE:HG23	2.32	0.45
2:4:269:PHE:CE1	2:6:271:VAL:HA	2.52	0.45
1:S:30:GLU:O	1:S:30:GLU:OE1	2.33	0.45
1:O:95:THR:HG22	1:O:100:LEU:HB2	1.99	0.45
1:1:77:ALA:CB	1:1:234:ARG:HG3	2.46	0.45
2:N:199:LYS:HD3	2:N:239:ARG:NH2	2.30	0.45
2:P:28:GLU:HB2	2:P:81:MET:HE3	1.98	0.45
2:H:144:VAL:CG1	2:H:241:ILE:HB	2.47	0.45
2:J:31:ALA:HB3	2:J:54:ASP:CG	2.37	0.45
1:Y:274:THR:O	1:Y:278:ILE:HD13	2.16	0.45
2:X:313:ILE:HG23	2:X:314:PRO:HD2	1.98	0.45
1:5:55:GLN:O	1:5:56:LYS:HB2	2.16	0.45
2:L:227:SER:C	2:L:229:GLU:H	2.19	0.45
2:X:238:MET:C	2:X:240:THR:H	2.20	0.45
2:T:70:ALA:HA	2:T:74:LEU:O	2.17	0.45
2:T:237:ASN:HD22	2:T:237:ASN:C	2.18	0.45
1:O:314:ARG:HD3	1:O:314:ARG:HA	1.86	0.45
1:C:231:LEU:HD23	1:C:231:LEU:HA	1.48	0.45
2:6:20:ASP:C	2:6:20:ASP:OD1	2.55	0.45
2:N:127:GLN:OE1	1:O:125:HIS:HE1	2.00	0.45
2:Z:325:LYS:HG2	1:1:354:TRP:CZ2	2.51	0.45
1:K:108:GLU:OE1	1:K:117:ALA:N	2.41	0.45
1:G:272:TYR:CE1	1:G:273:ARG:HA	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:314:PRO:O	2:T:315:GLN:CB	2.61	0.45
2:N:19:ARG:HH11	2:N:19:ARG:CG	2.27	0.45
1:A:138:VAL:HG13	1:A:169:ALA:CB	2.45	0.45
1:O:236:ALA:O	1:O:237:THR:O	2.33	0.45
2:X:152:ASP:HA	2:X:193:ILE:HD12	1.97	0.45
2:F:278:ARG:HH11	2:F:278:ARG:HG3	1.82	0.45
2:T:172:ASN:C	2:T:172:ASN:HD22	2.19	0.45
2:F:25:LEU:HD23	2:F:52:ILE:HG23	1.98	0.45
2:B:250:GLU:O	2:B:251:ALA:C	2.55	0.45
2:X:214:ARG:O	2:X:216:VAL:N	2.50	0.45
2:V:308:LEU:HD23	2:V:308:LEU:HA	1.67	0.45
1:S:11:LYS:HB3	1:S:23:VAL:HG12	1.99	0.45
1:Q:21:PRO:HB3	1:Q:239:PHE:HB2	1.99	0.45
2:J:95:ASN:ND2	2:L:87:MET:CE	2.79	0.45
2:4:306:LYS:HG2	1:5:59:ARG:CZ	2.47	0.45
1:M:75:LEU:HD11	1:M:255:LEU:HD21	1.97	0.45
1:S:314:ARG:HH11	1:S:314:ARG:HG2	1.81	0.45
1:I:129:LYS:HD3	1:I:129:LYS:HA	1.77	0.45
1:O:149:ALA:CB	1:O:189:CYS:HB2	2.46	0.45
2:T:28:GLU:HB2	2:T:81:MET:HE3	1.99	0.45
2:J:74:LEU:HA	2:J:74:LEU:HD12	1.62	0.45
2:L:59:GLU:O	2:L:60:MET:C	2.54	0.45
1:G:272:TYR:HD1	1:G:273:ARG:CA	2.26	0.45
1:W:271:ALA:C	1:W:273:ARG:N	2.69	0.45
1:G:10:LYS:CG	1:G:11:LYS:N	2.79	0.45
1:Q:95:THR:CG2	1:Q:100:LEU:HD22	2.47	0.45
1:A:129:LYS:HD2	1:A:129:LYS:HA	1.69	0.45
2:4:214:ARG:N	2:4:215:PRO:HD2	2.32	0.45
2:D:32:GLN:HE21	2:D:32:GLN:HB2	1.58	0.45
1:O:162:LEU:HD12	1:O:162:LEU:N	2.32	0.45
1:E:65:CYS:O	1:E:68:GLN:HB2	2.16	0.45
1:G:167:ASP:HB3	1:G:195:ASN:HA	1.97	0.45
2:L:302:MET:HA	2:L:303:PRO:HD2	1.87	0.45
1:G:72:CYS:HB2	1:G:97:THR:CG2	2.43	0.45
2:D:172:ASN:C	2:D:172:ASN:ND2	2.70	0.45
2:F:87:MET:HE1	2:H:95:ASN:ND2	2.31	0.45
2:J:260:VAL:HG22	2:J:293:VAL:HG22	1.98	0.45
1:W:258:TYR:OH	1:W:278:ILE:HD12	2.16	0.45
2:L:285:PHE:O	2:L:287:PHE:N	2.49	0.45
1:S:225:VAL:CG1	1:S:226:ASP:N	2.79	0.45
2:H:191:PHE:O	2:H:192:LEU:HD12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:14:LEU:HA	1:U:14:LEU:HD23	1.57	0.45
2:P:94:ILE:HD12	2:P:139:CYS:SG	2.57	0.45
1:1:29:ARG:HB2	1:1:300:LEU:HD22	1.99	0.45
1:K:272:TYR:O	1:K:273:ARG:C	2.55	0.45
2:X:124:VAL:O	2:X:125:ALA:HB3	2.17	0.45
2:F:172:ASN:ND2	2:F:174:LEU:N	2.65	0.45
2:R:148:TRP:O	2:R:175:MET:HE2	2.16	0.45
2:J:182:PHE:O	2:J:183:PRO:C	2.54	0.45
2:X:172:ASN:C	2:X:172:ASN:HD22	2.20	0.45
1:U:223:LEU:HD23	1:U:223:LEU:N	2.32	0.45
2:N:135:TRP:O	2:N:138:HIS:HB3	2.17	0.45
1:C:75:LEU:O	1:C:79:ILE:HG12	2.16	0.45
2:R:33:TYR:O	2:R:34:ASP:HB2	2.15	0.45
2:H:31:ALA:HB3	2:H:54:ASP:OD2	2.17	0.45
1:3:112:ARG:HD3	1:3:112:ARG:HA	1.73	0.45
1:E:337:TYR:O	1:E:338:HIS:HB2	2.16	0.45
2:X:182:PHE:HD2	2:X:187:GLN:HG3	1.81	0.45
1:K:100:LEU:CD1	1:K:128:ALA:CB	2.94	0.45
1:A:335:LEU:O	1:A:335:LEU:HD23	2.17	0.45
1:Y:272:TYR:CD1	1:Y:272:TYR:O	2.70	0.45
2:D:316:VAL:O	2:D:316:VAL:HG12	2.17	0.45
1:I:174:GLN:HB3	2:J:60:MET:HG3	1.97	0.45
2:R:95:ASN:ND2	2:T:87:MET:HE3	2.31	0.45
1:1:302:SER:O	1:1:305:GLU:HB2	2.17	0.45
2:L:268:GLN:O	2:L:269:PHE:HB2	2.16	0.45
2:F:124:VAL:O	2:F:125:ALA:HB3	2.16	0.45
1:W:106:LEU:HA	1:W:106:LEU:HD23	1.79	0.45
1:3:221:PRO:O	1:3:251:ILE:HG13	2.15	0.45
2:T:227:SER:C	2:T:229:GLU:N	2.70	0.45
1:O:303:VAL:CG1	1:O:304:GLU:OE2	2.65	0.45
1:E:196:ASN:ND2	1:E:259:ARG:HE	2.15	0.45
1:W:292:LYS:HG3	1:W:306:LEU:HD13	1.99	0.45
2:2:70:ALA:HB1	2:2:111:PRO:HD2	1.99	0.45
1:K:64:LEU:HD12	1:K:261:HIS:CD2	2.52	0.45
1:5:63:HIS:C	1:5:64:LEU:HD23	2.38	0.45
2:B:325:LYS:HG2	1:C:354:TRP:CE2	2.52	0.45
2:6:32:GLN:HB2	2:6:32:GLN:HE21	1.51	0.45
2:P:268:GLN:O	2:P:269:PHE:CB	2.60	0.45
1:Y:142:VAL:HB	1:Y:143:PRO:HD3	1.99	0.45
2:L:51:ARG:NH1	2:L:51:ARG:HG3	2.31	0.45
2:R:259:LEU:CD2	2:R:279:ILE:HG13	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:9:ILE:HB	1:Y:232:CYS:SG	2.57	0.45
1:Q:154:TYR:O	2:R:50:LYS:NZ	2.50	0.45
2:R:211:SER:HB2	2:R:262:VAL:HB	1.98	0.45
1:S:29:ARG:CB	1:S:300:LEU:HD22	2.45	0.45
1:S:196:ASN:ND2	1:S:259:ARG:HD3	2.32	0.45
1:C:88:ALA:HB2	1:C:141:GLN:NE2	2.32	0.45
1:5:282:ARG:O	1:5:284:LYS:N	2.49	0.45
2:2:237:ASN:HD22	2:2:238:MET:N	2.13	0.45
1:5:289:MET:HE2	1:5:290:LEU:HD23	1.98	0.45
2:6:191:PHE:C	2:6:192:LEU:HD12	2.36	0.45
1:Q:353:GLN:HE22	2:R:281:GLU:HB3	1.82	0.45
2:L:23:VAL:CG2	2:L:75:ARG:HB2	2.47	0.45
2:X:21:GLU:HA	2:X:51:ARG:NH2	2.32	0.45
1:A:303:VAL:HG13	1:A:304:GLU:OE2	2.17	0.45
1:1:221:PRO:O	1:1:251:ILE:HG13	2.17	0.45
2:4:207:ILE:HG13	2:4:258:HIS:HB2	1.97	0.45
2:R:81:MET:HB2	2:R:81:MET:HE3	1.76	0.45
2:V:279:ILE:HD13	2:V:279:ILE:HA	1.71	0.45
1:W:47:LEU:HD23	1:W:47:LEU:HA	1.79	0.45
1:U:57:ILE:HD11	2:4:328:ASN:ND2	2.32	0.45
1:O:308:GLU:O	1:O:312:GLU:HG3	2.16	0.45
1:3:296:VAL:HG12	1:3:297:ASN:ND2	2.32	0.45
2:N:143:LYS:HB2	2:N:167:VAL:HG22	1.98	0.45
1:K:142:VAL:HA	1:K:163:THR:HG21	1.98	0.45
1:U:341:SER:HB2	2:V:101:TYR:CZ	2.52	0.45
1:S:28:THR:CG2	1:S:31:ASP:H	2.30	0.44
1:U:45:MET:CE	1:U:102:VAL:HA	2.48	0.44
1:O:95:THR:CG2	1:O:100:LEU:HD22	2.47	0.44
1:3:335:LEU:HD21	2:6:300:VAL:HG21	1.98	0.44
2:Z:207:ILE:CD1	2:Z:323:ILE:HG23	2.46	0.44
2:Z:99:LYS:O	2:Z:103:MET:HG3	2.17	0.44
1:M:1:PHE:HA	1:M:299:ASN:HD21	1.82	0.44
1:W:246:SER:OG	1:W:248:LYS:HG3	2.18	0.44
2:N:26:LEU:HD23	2:N:78:CYS:HA	1.98	0.44
1:G:320:ALA:O	1:G:323:PHE:HB3	2.18	0.44
1:O:70:ALA:HB3	1:O:227:GLY:O	2.17	0.44
1:I:15:HIS:O	1:I:16:ARG:HB2	2.17	0.44
1:A:285:SER:O	1:A:286:ASP:C	2.51	0.44
1:M:1:PHE:O	1:M:2:ALA:O	2.35	0.44
2:Z:84:ASN:HD21	2:Z:128:HIS:C	2.20	0.44
1:C:164:LEU:HD12	1:C:164:LEU:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:269:PHE:HE1	2:6:271:VAL:HA	1.82	0.44
2:V:11:GLN:O	2:V:15:GLU:HG3	2.18	0.44
1:G:57:ILE:HG22	1:G:110:THR:HG22	1.99	0.44
2:B:267:PRO:HA	2:B:296:THR:HG21	1.99	0.44
2:J:20:ASP:C	2:J:20:ASP:OD1	2.56	0.44
2:4:94:ILE:HD13	2:4:94:ILE:HA	1.70	0.44
2:B:317:LYS:HA	2:B:317:LYS:HD3	1.86	0.44
1:S:162:LEU:N	1:S:162:LEU:HD12	2.32	0.44
2:D:268:GLN:O	2:D:269:PHE:HB2	2.18	0.44
1:I:126:MET:O	1:I:133:GLY:HA2	2.17	0.44
1:5:347:GLU:OE1	1:5:356:LYS:HD3	2.17	0.44
1:S:36:TYR:OH	1:S:310:ASP:OD1	2.19	0.44
1:A:286:ASP:OD2	1:A:288:ILE:CB	2.65	0.44
1:M:270:VAL:O	1:M:273:ARG:HB3	2.17	0.44
1:K:289:MET:HE2	1:K:290:LEU:HD23	1.93	0.44
2:D:193:ILE:HD13	2:D:239:ARG:NH2	2.32	0.44
1:Y:112:ARG:HD2	1:Y:327:ASP:O	2.17	0.44
2:Z:172:ASN:ND2	2:Z:174:LEU:H	2.15	0.44
1:3:189:CYS:SG	1:3:191:PHE:CE1	3.11	0.44
1:1:53:TYR:CD2	1:1:62:CYS:CB	2.99	0.44
1:E:29:ARG:CG	1:E:300:LEU:O	2.66	0.44
1:W:132:TYR:HB3	2:X:71:MET:HE1	1.99	0.44
2:6:1:LEU:HD22	2:6:1:LEU:HA	1.76	0.44
1:G:29:ARG:CA	1:G:300:LEU:HD22	2.48	0.44
1:G:45:MET:CE	1:G:102:VAL:HA	2.47	0.44
1:1:223:LEU:N	1:1:223:LEU:HD23	2.32	0.44
2:T:279:ILE:HD13	2:T:279:ILE:HA	1.59	0.44
2:T:237:ASN:ND2	2:T:237:ASN:C	2.70	0.44
1:O:150:LEU:HA	1:O:187:LEU:HD22	1.99	0.44
1:5:101:SER:OG	1:5:104:GLU:HG3	2.17	0.44
1:E:273:ARG:HB3	1:E:273:ARG:HE	1.57	0.44
1:A:70:ALA:HB3	1:A:227:GLY:O	2.17	0.44
2:Z:123:GLY:O	1:1:60:GLY:HA3	2.17	0.44
2:6:316:VAL:O	2:6:317:LYS:C	2.55	0.44
2:2:207:ILE:HG13	2:2:258:HIS:HB2	1.99	0.44
1:3:173:GLY:N	1:5:177:GLU:OE2	2.40	0.44
2:2:313:ILE:HG22	2:2:314:PRO:N	2.33	0.44
2:N:112:ILE:HD13	2:N:114:PHE:CZ	2.51	0.44
1:A:29:ARG:CB	1:A:300:LEU:HD22	2.48	0.44
1:1:1:PHE:O	1:1:2:ALA:O	2.35	0.44
1:1:37:ARG:HH21	1:1:309:ILE:HG23	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4:ASP:HA	1:G:300:LEU:HD21	1.99	0.44
1:E:15:HIS:ND1	1:E:215:LYS:HG2	2.33	0.44
1:3:157:LYS:HD3	1:3:157:LYS:HA	1.79	0.44
1:Y:184:LEU:HA	1:Y:184:LEU:HD12	1.73	0.44
2:R:59:GLU:OE1	2:R:59:GLU:N	2.49	0.44
1:Q:40:GLN:O	1:Q:44:ARG:HG2	2.17	0.44
1:S:80:ASN:HB3	1:S:81:PRO:HD2	1.99	0.44
2:N:148:TRP:O	2:N:175:MET:HE2	2.17	0.44
1:C:84:HIS:CE1	1:C:130:ASN:ND2	2.85	0.44
2:4:202:ARG:O	2:4:234:GLU:HA	2.18	0.44
1:5:231:LEU:HD22	1:5:231:LEU:HA	1.58	0.44
1:E:334:GLU:HG2	1:E:337:TYR:CD2	2.49	0.44
1:K:29:ARG:HB2	1:K:300:LEU:HD22	2.00	0.44
1:C:55:GLN:O	1:C:56:LYS:CB	2.64	0.44
2:T:1:LEU:HD13	2:T:2:GLN:H	1.81	0.44
2:X:31:ALA:HB3	2:X:54:ASP:OD2	2.17	0.44
2:J:199:LYS:HD2	2:J:239:ARG:NH2	2.32	0.44
1:W:225:VAL:HB	1:W:255:LEU:HD12	1.99	0.44
2:6:24:PHE:CE1	2:6:76:PRO:HB3	2.52	0.44
1:3:286:ASP:HB3	1:3:289:MET:HB3	2.00	0.44
1:W:239:PHE:O	1:W:242:ALA:HB3	2.16	0.44
1:C:149:ALA:CB	1:C:189:CYS:HB2	2.47	0.44
2:B:31:ALA:HB3	2:B:54:ASP:OD2	2.17	0.44
2:D:279:ILE:HD12	2:D:279:ILE:HG23	1.75	0.44
2:J:288:LEU:HA	2:J:288:LEU:HD12	1.74	0.44
1:C:106:LEU:HA	1:C:106:LEU:HD23	1.84	0.44
2:H:278:ARG:HG3	2:H:278:ARG:NH1	2.31	0.44
1:O:341:SER:HB2	2:P:101:TYR:CZ	2.52	0.44
1:W:50:ASP:HB2	1:W:64:LEU:CD1	2.48	0.44
1:I:64:LEU:O	1:I:90:ARG:NH1	2.50	0.44
1:A:184:LEU:HD21	1:C:206:ARG:O	2.18	0.44
2:J:316:VAL:O	2:J:320:ILE:HG13	2.18	0.44
1:5:39:MET:HG2	1:5:73:VAL:HG21	1.99	0.44
1:C:253:MET:CE	1:C:255:LEU:HD11	2.48	0.44
1:I:196:ASN:HD21	1:I:259:ARG:HE	1.63	0.44
2:N:33:TYR:O	2:N:34:ASP:HB2	2.17	0.44
1:C:11:LYS:HB3	1:C:23:VAL:CG1	2.46	0.44
2:Z:102:TYR:CD2	2:2:301:PRO:HG2	2.52	0.44
2:N:213:SER:O	2:N:214:ARG:C	2.55	0.44
2:R:51:ARG:NH1	2:R:51:ARG:HG3	2.33	0.44
1:3:289:MET:CE	1:3:290:LEU:HD23	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:209:VAL:HG21	2:J:323:ILE:HD11	2.00	0.44
1:C:328:PRO:O	1:C:329:GLU:O	2.36	0.44
2:X:313:ILE:CG2	2:X:314:PRO:HD2	2.47	0.44
2:T:227:SER:C	2:T:229:GLU:H	2.21	0.44
1:3:129:LYS:O	1:3:130:ASN:HB2	2.17	0.44
2:V:43:LEU:HD12	2:V:43:LEU:N	2.33	0.44
1:Q:223:LEU:N	1:Q:223:LEU:HD23	2.33	0.44
1:A:109:LEU:HD23	1:A:109:LEU:HA	1.87	0.44
1:C:33:LEU:HD12	1:C:33:LEU:HA	1.84	0.44
2:R:227:SER:HB2	2:R:232:GLU:OE2	2.17	0.44
1:3:196:ASN:HD21	1:3:259:ARG:NE	2.16	0.44
1:S:37:ARG:HH11	1:S:37:ARG:HG2	1.78	0.44
1:K:29:ARG:HB2	1:K:300:LEU:CD2	2.48	0.44
2:V:1:LEU:HD13	2:V:2:GLN:H	1.79	0.44
1:1:71:CYS:SG	1:1:255:LEU:HD23	2.57	0.44
2:4:172:ASN:ND2	2:4:174:LEU:N	2.65	0.44
2:X:258:HIS:CD2	2:X:327:LEU:HD23	2.52	0.44
1:U:303:VAL:HG12	1:U:304:GLU:OE2	2.18	0.44
2:P:81:MET:HB3	2:P:85:PHE:HD2	1.80	0.44
2:B:17:LEU:O	2:B:51:ARG:NH2	2.47	0.44
1:K:142:VAL:HA	1:K:163:THR:CG2	2.48	0.44
2:D:279:ILE:HA	2:D:279:ILE:HD13	1.67	0.44
1:C:139:GLY:HA3	1:C:172:GLN:HG3	1.99	0.44
1:E:150:LEU:O	1:E:150:LEU:HG	2.17	0.44
2:X:49:ASP:OD1	2:X:49:ASP:N	2.50	0.44
1:M:147:GLY:HA2	2:N:65:ILE:HG23	2.00	0.44
2:4:8:ALA:O	2:4:154:LYS:HB2	2.18	0.44
1:S:341:SER:HB3	2:T:101:TYR:CE1	2.53	0.44
2:6:136:TYR:C	2:6:138:HIS:H	2.21	0.44
1:Q:109:LEU:CD2	1:Q:123:SER:HB2	2.47	0.44
1:K:132:TYR:N	1:K:132:TYR:CD1	2.86	0.44
2:F:279:ILE:CG2	2:F:280:MET:N	2.80	0.44
2:D:79:GLU:HG3	2:D:115:ARG:NH1	2.33	0.44
2:P:121:SER:HB3	2:P:124:VAL:HG22	1.96	0.44
2:R:1:LEU:CD1	2:R:2:GLN:N	2.80	0.44
2:2:118:ASN:HD21	2:2:132:PHE:N	2.14	0.44
2:F:212:HIS:HB3	2:F:238:MET:HE3	1.99	0.44
1:M:229:ASP:C	1:M:231:LEU:H	2.21	0.44
1:M:29:ARG:HA	1:M:300:LEU:HD22	2.00	0.44
1:E:150:LEU:HA	1:E:187:LEU:HD22	1.99	0.44
2:4:74:LEU:HD12	2:4:74:LEU:HA	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:164:LEU:HG	1:E:192:ILE:HB	1.99	0.44
1:E:59:ARG:NH1	2:H:306:LYS:HG2	2.33	0.44
1:I:142:VAL:HA	1:I:163:THR:HG21	1.99	0.44
1:1:142:VAL:HA	1:1:163:THR:HG21	1.99	0.44
1:1:280:GLU:C	1:1:282:ARG:N	2.71	0.44
1:5:268:PRO:C	1:5:270:VAL:H	2.20	0.44
1:M:334:GLU:HG2	1:M:337:TYR:CD2	2.53	0.44
1:O:286:ASP:CG	1:O:287:PRO:HD2	2.38	0.44
2:Z:276:CYS:HB3	2:2:280:MET:HE2	2.00	0.44
1:A:1:PHE:C	1:A:2:ALA:O	2.54	0.44
1:A:278:ILE:H	1:A:278:ILE:CD1	2.31	0.44
1:C:9:ILE:HB	1:C:232:CYS:HB3	1.99	0.44
1:A:101:SER:OG	1:A:104:GLU:HG3	2.18	0.44
2:B:4:THR:HA	2:B:179:PRO:HA	1.99	0.44
2:H:313:ILE:H	2:H:313:ILE:HG13	1.75	0.44
1:5:258:TYR:C	1:5:258:TYR:CD1	2.92	0.44
2:J:308:LEU:HA	2:J:308:LEU:HD23	1.62	0.44
1:I:14:LEU:HA	1:I:14:LEU:HD23	1.66	0.44
2:H:279:ILE:HD13	2:H:279:ILE:HA	1.71	0.44
2:L:317:LYS:HA	2:L:317:LYS:HD3	1.45	0.44
2:6:25:LEU:HD12	2:6:77:ILE:O	2.18	0.44
2:F:256:THR:O	2:F:257:ASN:HB2	2.18	0.44
2:4:103:MET:SD	2:6:126:ALA:HB3	2.58	0.44
1:A:245:ARG:C	1:A:247:GLY:H	2.21	0.44
1:W:1:PHE:HZ	1:W:302:SER:HB3	1.83	0.44
1:Y:174:GLN:HB3	2:Z:60:MET:HG2	1.99	0.44
2:F:260:VAL:HG22	2:F:293:VAL:HG22	2.00	0.44
1:3:304:GLU:O	1:3:308:GLU:HG3	2.17	0.44
1:W:231:LEU:HD12	1:W:294:ARG:NH1	2.33	0.44
1:Q:102:VAL:HG11	1:Q:317:ILE:CD1	2.48	0.43
1:C:128:ALA:HB3	1:C:131:PHE:HB3	2.00	0.43
1:Q:274:THR:O	1:Q:277:GLU:HB2	2.18	0.43
2:4:327:LEU:O	2:4:329:ILE:HG23	2.18	0.43
1:1:53:TYR:CE2	1:1:62:CYS:HB3	2.53	0.43
2:F:172:ASN:HD22	2:F:175:MET:N	2.16	0.43
1:Y:150:LEU:HG	1:Y:150:LEU:O	2.18	0.43
2:F:212:HIS:HB3	2:F:238:MET:CE	2.47	0.43
2:2:59:GLU:O	2:2:60:MET:C	2.55	0.43
2:4:202:ARG:NH1	2:4:233:CYS:O	2.47	0.43
1:S:77:ALA:CB	1:S:234:ARG:HG3	2.48	0.43
2:2:246:MET:O	2:2:250:GLU:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:239:PHE:C	1:G:239:PHE:CD1	2.91	0.43
1:3:34:LYS:HB3	1:3:34:LYS:HE3	1.86	0.43
1:C:126:MET:HE3	1:C:126:MET:HB2	1.86	0.43
2:F:288:LEU:HA	2:F:288:LEU:HD12	1.83	0.43
1:I:33:LEU:HA	1:I:33:LEU:HD12	1.78	0.43
2:4:81:MET:HE3	2:4:81:MET:HB2	1.91	0.43
2:J:126:ALA:HB3	2:L:103:MET:SD	2.58	0.43
2:N:300:VAL:HG12	1:O:339:ILE:HD11	2.00	0.43
1:5:279:GLN:O	1:5:280:GLU:C	2.56	0.43
1:C:142:VAL:HA	1:C:163:THR:CG2	2.48	0.43
1:K:113:LYS:HB3	1:K:330:PRO:HA	2.00	0.43
1:C:28:THR:O	1:C:30:GLU:N	2.51	0.43
1:5:234:ARG:CZ	1:5:238:ARG:HH22	2.31	0.43
1:Y:29:ARG:HB2	1:Y:300:LEU:CD2	2.48	0.43
2:2:51:ARG:O	2:2:52:ILE:HD13	2.18	0.43
1:Q:89:TYR:HB2	1:Q:124:MET:HG2	2.00	0.43
2:H:81:MET:O	2:H:117:PRO:HD2	2.19	0.43
2:D:142:LEU:HD12	2:D:142:LEU:HA	1.72	0.43
2:F:130:GLN:HG3	2:F:266:TRP:CH2	2.53	0.43
2:V:184:PRO:HA	2:V:187:GLN:NE2	2.33	0.43
1:G:225:VAL:HB	1:G:255:LEU:HD12	2.00	0.43
1:G:108:GLU:OE1	1:G:117:ALA:N	2.45	0.43
1:U:184:LEU:HD12	1:U:184:LEU:HA	1.82	0.43
1:Y:138:VAL:HG13	1:Y:169:ALA:HB2	2.00	0.43
2:F:269:PHE:CD1	2:H:274:GLU:HB2	2.53	0.43
2:N:88:GLN:HE22	1:O:172:GLN:HE22	1.66	0.43
1:K:274:THR:O	1:K:275:ARG:C	2.56	0.43
1:U:84:HIS:ND1	1:U:130:ASN:ND2	2.64	0.43
1:G:93:GLY:O	1:G:97:THR:HG23	2.18	0.43
2:2:238:MET:C	2:2:240:THR:H	2.21	0.43
2:T:238:MET:C	2:T:240:THR:H	2.22	0.43
1:E:272:TYR:HD1	1:E:272:TYR:C	2.18	0.43
1:1:55:GLN:O	1:1:56:LYS:CB	2.66	0.43
2:F:112:ILE:HG12	2:F:113:VAL:N	2.33	0.43
2:V:172:ASN:HD21	2:V:174:LEU:HB2	1.82	0.43
2:2:278:ARG:HA	2:2:278:ARG:HD2	1.74	0.43
2:P:108:GLN:O	2:P:108:GLN:HG3	2.18	0.43
1:I:292:LYS:HG3	1:I:306:LEU:CD1	2.48	0.43
2:V:307:ILE:O	2:V:311:ASN:ND2	2.43	0.43
2:X:26:LEU:HD23	2:X:78:CYS:HA	1.98	0.43
2:R:121:SER:OG	2:R:122:ALA:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:27:LEU:HD11	1:S:32:GLY:HA3	1.99	0.43
1:E:216:ARG:HG3	1:E:216:ARG:NH1	2.09	0.43
1:3:72:CYS:HB2	1:3:97:THR:CG2	2.45	0.43
1:Q:16:ARG:HG2	1:Q:16:ARG:HH11	1.84	0.43
1:E:29:ARG:HB2	1:E:300:LEU:HD23	2.01	0.43
2:L:118:ASN:HD21	2:L:132:PHE:N	2.17	0.43
2:V:43:LEU:CD1	2:V:43:LEU:N	2.81	0.43
2:F:317:LYS:H	2:F:317:LYS:HG3	1.51	0.43
2:J:88:GLN:HE22	1:K:172:GLN:HE22	1.66	0.43
2:D:46:LYS:HE2	2:D:47:TYR:CZ	2.53	0.43
1:M:340:TYR:HB3	2:N:165:ASN:ND2	2.34	0.43
1:Q:213:TYR:HA	1:Q:216:ARG:HG2	2.00	0.43
2:V:246:MET:O	2:V:250:GLU:HG3	2.18	0.43
1:S:27:LEU:HA	1:S:27:LEU:HD23	1.64	0.43
2:4:148:TRP:CD1	2:4:175:MET:CE	3.02	0.43
2:T:182:PHE:HD2	2:T:187:GLN:HG3	1.84	0.43
2:6:268:GLN:O	2:6:269:PHE:CB	2.63	0.43
2:T:172:ASN:ND2	2:T:174:LEU:N	2.66	0.43
1:Q:142:VAL:HG21	1:Q:175:ILE:HG12	2.00	0.43
2:T:246:MET:O	2:T:250:GLU:HG3	2.19	0.43
2:J:212:HIS:HB3	2:J:238:MET:CE	2.48	0.43
2:6:313:ILE:CG2	2:6:314:PRO:HD2	2.48	0.43
2:P:260:VAL:HG22	2:P:293:VAL:HG23	2.00	0.43
1:K:177:GLU:OE1	2:L:61:GLY:N	2.52	0.43
1:W:46:GLU:OE2	1:W:65:CYS:N	2.51	0.43
2:D:70:ALA:HA	2:D:74:LEU:O	2.18	0.43
1:Y:337:TYR:HB3	1:Y:338:HIS:CD2	2.53	0.43
2:6:182:PHE:O	2:6:183:PRO:O	2.36	0.43
1:Q:196:ASN:ND2	1:Q:259:ARG:CD	2.81	0.43
1:5:68:GLN:NE2	1:5:196:ASN:HD22	2.16	0.43
2:X:321:PHE:O	2:X:325:LYS:HB2	2.18	0.43
2:2:44:TRP:HA	2:2:52:ILE:HG13	2.01	0.43
1:A:1:PHE:O	1:A:2:ALA:O	2.36	0.43
2:H:80:PHE:O	2:H:81:MET:C	2.55	0.43
1:E:223:LEU:H	1:E:223:LEU:HD23	1.84	0.43
2:H:258:HIS:CD2	2:H:327:LEU:HD23	2.53	0.43
2:H:250:GLU:HB3	2:H:284:ALA:HB2	2.00	0.43
2:X:1:LEU:HD13	2:X:2:GLN:N	2.33	0.43
2:J:271:VAL:O	2:J:272:GLY:C	2.56	0.43
2:F:252:SER:O	2:F:256:THR:HG23	2.18	0.43
2:T:260:VAL:HG22	2:T:293:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:339:ILE:HD11	2:T:300:VAL:HG12	2.01	0.43
2:4:121:SER:OG	2:4:122:ALA:N	2.49	0.43
2:B:74:LEU:CD1	2:B:74:LEU:N	2.81	0.43
1:A:149:ALA:O	1:A:152:CYS:HB2	2.19	0.43
2:L:29:GLU:O	2:L:35:GLY:HA2	2.19	0.43
1:I:151:ALA:O	1:I:154:TYR:HB3	2.19	0.43
1:W:128:ALA:HB3	1:W:131:PHE:HB3	1.99	0.43
1:M:223:LEU:N	1:M:223:LEU:CD2	2.73	0.43
1:U:74:GLY:CA	1:U:233:VAL:HG12	2.47	0.43
2:P:59:GLU:O	2:P:60:MET:C	2.56	0.43
1:M:279:GLN:O	1:M:279:GLN:OE1	2.36	0.43
1:3:142:VAL:HA	1:3:163:THR:CG2	2.48	0.43
2:6:172:ASN:ND2	2:6:174:LEU:H	2.15	0.43
1:Q:129:LYS:HD2	1:Q:129:LYS:HA	1.81	0.43
2:T:51:ARG:O	2:T:52:ILE:HD13	2.18	0.43
2:B:209:VAL:HA	2:B:260:VAL:O	2.19	0.43
2:B:260:VAL:HG22	2:B:293:VAL:HG23	1.99	0.43
1:5:314:ARG:HD2	1:5:314:ARG:HA	1.76	0.43
2:2:285:PHE:O	2:2:288:LEU:HB2	2.18	0.43
1:C:37:ARG:NH2	1:C:309:ILE:HG23	2.33	0.43
1:M:150:LEU:HA	1:M:187:LEU:HD22	2.00	0.43
1:U:245:ARG:C	1:U:247:GLY:H	2.22	0.43
1:M:95:THR:HG23	1:M:100:LEU:HD22	2.00	0.43
1:5:45:MET:HE3	1:5:102:VAL:CG2	2.40	0.43
1:A:29:ARG:CG	1:A:29:ARG:NH1	2.68	0.43
1:A:29:ARG:HB2	1:A:300:LEU:HD22	2.00	0.43
1:K:196:ASN:ND2	1:K:259:ARG:NE	2.66	0.43
2:Z:172:ASN:HD22	2:Z:175:MET:N	2.13	0.43
1:M:3:ASN:O	1:M:4:ASP:HB3	2.19	0.43
1:O:87:THR:OG1	1:O:88:ALA:N	2.52	0.43
2:4:95:ASN:ND2	2:6:87:MET:CE	2.80	0.43
1:E:112:ARG:HD2	1:E:327:ASP:O	2.18	0.43
2:X:210:VAL:HG12	2:X:211:SER:N	2.34	0.43
1:Q:143:PRO:CG	1:Q:174:GLN:HB2	2.49	0.43
1:G:196:ASN:ND2	1:G:259:ARG:NE	2.65	0.43
2:N:207:ILE:CD1	2:N:323:ILE:HG23	2.43	0.43
2:Z:157:ILE:O	2:Z:161:ILE:HG13	2.18	0.43
1:W:118:LYS:HZ3	1:W:118:LYS:HB2	1.82	0.43
1:O:337:TYR:O	1:O:338:HIS:HB2	2.19	0.43
2:2:81:MET:O	2:2:117:PRO:HD2	2.18	0.43
1:A:61:PHE:CD2	1:A:124:MET:CE	3.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:279:GLN:O	1:5:280:GLU:O	2.36	0.43
2:L:38:LYS:HD3	2:L:38:LYS:HA	1.90	0.43
1:3:174:GLN:HB3	2:4:60:MET:CG	2.49	0.43
1:Y:341:SER:H	2:Z:165:ASN:HD21	1.66	0.43
2:4:279:ILE:HA	2:4:279:ILE:HD13	1.68	0.43
2:N:155:GLY:HA3	2:N:193:ILE:HG13	1.99	0.43
1:A:39:MET:HE3	1:A:288:ILE:HA	2.00	0.43
1:U:45:MET:HE3	1:U:102:VAL:HG13	2.01	0.43
1:Y:64:LEU:O	1:Y:90:ARG:NH1	2.52	0.43
2:Z:148:TRP:O	2:Z:175:MET:HE2	2.19	0.43
1:E:289:MET:HE1	1:E:290:LEU:HD23	1.99	0.43
1:E:267:ASP:HA	1:E:268:PRO:HD2	1.66	0.43
2:L:16:GLU:OE2	2:L:162:ARG:NH1	2.51	0.43
2:Z:102:TYR:CG	2:2:301:PRO:HG2	2.54	0.43
1:Q:1:PHE:O	1:Q:2:ALA:O	2.37	0.43
2:H:210:VAL:CG1	2:H:211:SER:N	2.81	0.43
1:Q:229:ASP:C	1:Q:231:LEU:N	2.72	0.43
2:L:327:LEU:O	2:L:329:ILE:HG23	2.19	0.43
2:L:227:SER:C	2:L:229:GLU:N	2.72	0.43
2:V:167:VAL:HG12	2:V:168:VAL:N	2.33	0.43
1:U:172:GLN:HE22	2:X:88:GLN:HE22	1.67	0.43
1:5:58:ILE:HD13	1:5:109:LEU:HB3	2.01	0.43
2:L:313:ILE:HG23	2:L:314:PRO:HD2	2.00	0.43
2:R:74:LEU:HA	2:R:74:LEU:HD12	1.83	0.43
1:A:190:ILE:HG23	1:A:251:ILE:HG23	2.00	0.43
1:3:349:ARG:HH12	2:4:281:GLU:CD	2.22	0.43
2:4:177:GLY:O	2:4:179:PRO:HD3	2.18	0.43
2:B:34:ASP:O	2:B:38:LYS:HA	2.18	0.42
1:W:289:MET:HE1	1:W:290:LEU:HD23	2.00	0.42
2:Z:87:MET:CE	2:2:95:ASN:HD21	2.32	0.42
1:Y:226:ASP:OD1	1:Y:226:ASP:C	2.56	0.42
1:E:75:LEU:HD12	1:E:233:VAL:CG1	2.49	0.42
2:H:31:ALA:HB3	2:H:54:ASP:CG	2.39	0.42
1:3:174:GLN:HB3	2:4:60:MET:HG2	2.00	0.42
1:Q:245:ARG:C	1:Q:247:GLY:H	2.21	0.42
2:J:279:ILE:HD13	2:J:279:ILE:HA	1.62	0.42
1:Q:118:LYS:HB2	1:Q:118:LYS:HE2	1.62	0.42
2:Z:32:GLN:HE21	2:Z:32:GLN:HB3	1.49	0.42
2:D:188:SER:OG	2:D:189:LYS:N	2.52	0.42
1:S:13:ASP:O	1:S:14:LEU:HD23	2.19	0.42
2:Z:2:GLN:HB3	2:Z:2:GLN:HE21	1.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:258:TYR:CE1	1:M:259:ARG:O	2.72	0.42
1:U:1:PHE:HZ	1:U:302:SER:HB3	1.85	0.42
2:J:148:TRP:CD1	2:J:175:MET:HE2	2.54	0.42
2:L:278:ARG:HH11	2:L:278:ARG:CG	2.31	0.42
1:U:55:GLN:O	1:U:56:LYS:CB	2.67	0.42
2:2:34:ASP:O	2:2:38:LYS:HA	2.19	0.42
2:N:151:GLU:OE1	2:N:183:PRO:HG2	2.18	0.42
1:K:314:ARG:HD2	1:K:314:ARG:HA	1.82	0.42
2:B:80:PHE:O	2:B:81:MET:C	2.57	0.42
1:O:162:LEU:CD1	1:O:162:LEU:N	2.82	0.42
2:L:286:ASN:ND2	2:L:286:ASN:H	2.16	0.42
2:T:59:GLU:O	2:T:60:MET:C	2.57	0.42
2:F:74:LEU:HA	2:F:74:LEU:HD12	1.65	0.42
2:L:88:GLN:HB3	2:L:88:GLN:HE21	1.39	0.42
2:6:59:GLU:O	2:6:60:MET:C	2.57	0.42
1:C:291:LEU:O	1:C:295:MET:HG2	2.19	0.42
1:C:70:ALA:HB3	1:C:227:GLY:O	2.18	0.42
1:C:140:ALA:O	1:C:143:PRO:HD2	2.18	0.42
1:1:341:SER:HB2	2:2:101:TYR:CZ	2.54	0.42
1:S:29:ARG:N	1:S:300:LEU:HD22	2.33	0.42
1:A:45:MET:CE	1:A:105:ILE:HD12	2.49	0.42
1:Q:234:ARG:O	1:Q:238:ARG:HG3	2.20	0.42
1:A:303:VAL:HG12	1:A:304:GLU:OE2	2.19	0.42
2:P:279:ILE:HA	2:P:279:ILE:HD13	1.86	0.42
2:Z:237:ASN:HD22	2:Z:237:ASN:C	2.23	0.42
2:H:59:GLU:HA	2:H:62:PHE:CE2	2.54	0.42
1:3:346:PHE:CD1	1:3:346:PHE:N	2.87	0.42
1:O:157:LYS:HA	1:O:157:LYS:HD3	1.89	0.42
1:I:191:PHE:O	1:I:252:LEU:HA	2.19	0.42
1:U:15:HIS:CG	1:U:215:LYS:HG2	2.54	0.42
1:U:215:LYS:O	1:U:217:GLY:N	2.52	0.42
2:4:6:ARG:HD3	2:4:38:LYS:O	2.19	0.42
1:O:178:ALA:O	1:O:179:TYR:C	2.56	0.42
2:4:212:HIS:HB3	2:4:238:MET:CE	2.50	0.42
1:O:334:GLU:HG2	1:O:337:TYR:CD2	2.54	0.42
1:Y:289:MET:HE2	1:Y:290:LEU:CD2	2.49	0.42
2:4:95:ASN:ND2	2:6:87:MET:HE1	2.35	0.42
1:C:177:GLU:OE1	2:D:61:GLY:N	2.50	0.42
1:S:15:HIS:CG	1:S:215:LYS:HG2	2.54	0.42
1:G:307:LYS:HA	1:G:307:LYS:HD2	1.94	0.42
1:5:33:LEU:HD12	1:5:33:LEU:HA	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:262:VAL:HG21	2:X:319:ILE:HD13	2.01	0.42
2:6:121:SER:HB3	2:6:124:VAL:CG2	2.49	0.42
1:I:75:LEU:HD21	1:I:192:ILE:HD13	2.00	0.42
2:H:165:ASN:HB3	2:H:166:PRO:HD2	2.02	0.42
2:6:259:LEU:HD12	2:6:260:VAL:N	2.34	0.42
2:6:260:VAL:HG22	2:6:293:VAL:HG23	2.00	0.42
1:I:171:ASN:OD1	1:I:216:ARG:NH2	2.48	0.42
1:K:113:LYS:HG2	1:K:328:PRO:O	2.20	0.42
1:Q:29:ARG:HG3	1:Q:300:LEU:O	2.19	0.42
1:W:88:ALA:O	1:W:134:GLY:CA	2.65	0.42
1:G:11:LYS:HB3	1:G:23:VAL:HG13	2.00	0.42
1:Q:16:ARG:NH1	1:Q:16:ARG:CG	2.77	0.42
2:4:17:LEU:HD23	2:4:17:LEU:HA	1.77	0.42
1:M:229:ASP:C	1:M:231:LEU:N	2.72	0.42
1:I:95:THR:HG22	1:I:100:LEU:HB2	2.02	0.42
1:I:142:VAL:HB	1:I:143:PRO:HD3	2.00	0.42
1:I:75:LEU:HD12	1:I:237:THR:OG1	2.20	0.42
1:E:207:ALA:HB1	2:H:56:PRO:HB3	2.01	0.42
2:X:143:LYS:HB2	2:X:167:VAL:HG22	2.01	0.42
1:A:93:GLY:O	1:A:97:THR:HG23	2.19	0.42
2:B:307:ILE:CG2	2:B:308:LEU:N	2.83	0.42
2:D:307:ILE:HG23	2:D:308:LEU:N	2.34	0.42
1:S:274:THR:HB	1:S:276:GLU:HG3	1.98	0.42
1:3:112:ARG:HD2	1:3:327:ASP:O	2.19	0.42
1:3:284:LYS:O	1:3:285:SER:CB	2.68	0.42
1:C:85:LEU:HD21	1:C:94:PHE:CD1	2.54	0.42
1:C:85:LEU:HD23	1:C:131:PHE:CD1	2.55	0.42
1:K:68:GLN:NE2	1:K:196:ASN:HD22	2.18	0.42
1:5:64:LEU:N	1:5:64:LEU:CD2	2.68	0.42
2:J:59:GLU:O	2:J:60:MET:C	2.56	0.42
2:J:59:GLU:HA	2:J:62:PHE:CE2	2.55	0.42
2:4:250:GLU:O	2:4:251:ALA:C	2.57	0.42
2:H:51:ARG:HG3	2:H:51:ARG:NH1	2.33	0.42
2:Z:84:ASN:ND2	2:Z:128:HIS:C	2.73	0.42
1:M:282:ARG:HG2	1:M:283:SER:N	2.34	0.42
2:Z:259:LEU:HD12	2:Z:260:VAL:H	1.83	0.42
1:Q:151:ALA:O	1:Q:154:TYR:HB3	2.19	0.42
1:W:1:PHE:O	1:W:2:ALA:O	2.37	0.42
2:F:241:ILE:HD12	2:F:241:ILE:HG23	1.79	0.42
1:O:106:LEU:HD23	1:O:106:LEU:HA	1.79	0.42
1:3:33:LEU:HD12	1:3:33:LEU:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:315:LYS:HB2	1:1:315:LYS:NZ	2.34	0.42
2:4:59:GLU:OE1	2:4:59:GLU:N	2.50	0.42
1:G:104:GLU:H	1:G:104:GLU:HG3	1.50	0.42
1:A:60:GLY:HA3	2:D:123:GLY:O	2.20	0.42
2:T:188:SER:OG	2:T:189:LYS:N	2.52	0.42
1:M:292:LYS:HG3	1:M:306:LEU:CD1	2.49	0.42
1:S:196:ASN:ND2	1:S:259:ARG:CD	2.83	0.42
1:C:45:MET:HE3	1:C:102:VAL:HG22	2.01	0.42
1:I:196:ASN:ND2	1:I:259:ARG:CD	2.82	0.42
1:U:3:ASN:O	1:U:4:ASP:HB3	2.20	0.42
2:X:98:ALA:HB2	2:X:142:LEU:CD1	2.48	0.42
1:5:235:GLU:O	1:5:236:ALA:C	2.57	0.42
2:D:191:PHE:C	2:D:192:LEU:HD12	2.39	0.42
1:C:11:LYS:HE3	1:C:11:LYS:HB2	1.79	0.42
1:S:289:MET:HE3	1:S:290:LEU:HD23	2.00	0.42
2:X:238:MET:O	2:X:240:THR:N	2.47	0.42
2:R:81:MET:HB3	2:R:85:PHE:HD2	1.84	0.42
2:B:307:ILE:HD13	2:B:307:ILE:HG21	1.79	0.42
1:G:215:LYS:HB2	1:G:215:LYS:HE3	1.92	0.42
2:N:21:GLU:OE1	2:N:21:GLU:N	2.49	0.42
1:Y:52:LEU:HA	1:Y:52:LEU:HD23	1.86	0.42
2:H:43:LEU:HD12	2:H:43:LEU:HA	1.75	0.42
2:Z:310:ASP:O	2:Z:315:GLN:NE2	2.52	0.42
1:C:53:TYR:CD2	1:C:62:CYS:HB2	2.55	0.42
2:P:262:VAL:HA	2:P:295:VAL:O	2.20	0.42
2:B:139:CYS:HA	2:B:140:PRO:HD2	1.86	0.42
2:2:24:PHE:CZ	2:2:76:PRO:HB3	2.54	0.42
2:2:227:SER:C	2:2:229:GLU:H	2.23	0.42
2:X:8:ALA:HB1	2:X:154:LYS:HB2	2.02	0.42
1:1:164:LEU:HA	1:1:192:ILE:O	2.19	0.42
1:1:100:LEU:CD1	1:1:128:ALA:HB2	2.41	0.42
1:5:281:VAL:O	1:5:282:ARG:O	2.37	0.42
2:V:88:GLN:HE22	1:W:172:GLN:HE22	1.66	0.42
1:O:9:ILE:CD1	1:O:235:GLU:HG3	2.50	0.42
2:4:142:LEU:HA	2:4:142:LEU:HD12	1.84	0.42
2:N:140:PRO:HB2	2:P:301:PRO:HD3	2.02	0.42
2:P:278:ARG:CG	2:P:278:ARG:HH11	2.31	0.42
2:T:280:MET:HA	2:T:285:PHE:CD1	2.55	0.42
2:4:279:ILE:HG22	2:4:280:MET:N	2.35	0.42
2:T:4:THR:HA	2:T:179:PRO:HA	2.01	0.42
2:H:5:VAL:O	2:H:6:ARG:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:137:ILE:HD13	1:5:137:ILE:HA	1.74	0.42
2:R:17:LEU:HD23	2:R:17:LEU:HA	1.78	0.42
1:C:129:LYS:HD2	1:C:129:LYS:HA	1.46	0.42
2:J:197:LYS:HA	2:J:245:ASP:OD2	2.20	0.42
2:V:269:PHE:CE1	2:X:271:VAL:HA	2.55	0.42
2:4:26:LEU:HD21	2:4:66:ALA:HB2	2.01	0.42
2:V:315:GLN:O	2:V:318:ASP:N	2.52	0.42
2:B:300:VAL:HG12	1:C:339:ILE:HD11	2.01	0.42
1:Q:329:GLU:HB3	1:Q:330:PRO:HD2	2.01	0.42
2:T:329:ILE:OXT	2:T:329:ILE:HG13	2.19	0.42
2:D:172:ASN:ND2	2:D:174:LEU:N	2.68	0.42
1:Y:50:ASP:HB2	1:Y:64:LEU:HD13	2.00	0.42
2:H:51:ARG:C	2:H:52:ILE:HD13	2.39	0.42
1:Y:75:LEU:HD11	1:Y:255:LEU:HD21	2.00	0.42
1:S:70:ALA:HB2	1:S:287:PRO:HB3	2.02	0.42
1:G:45:MET:HE3	1:G:102:VAL:HG13	2.00	0.42
1:K:132:TYR:HB3	2:L:71:MET:HE1	2.02	0.42
1:A:218:ASP:OD1	1:A:218:ASP:C	2.58	0.42
2:J:75:ARG:HH11	2:J:75:ARG:HG2	1.85	0.42
2:B:173:GLU:HG2	2:B:173:GLU:O	2.19	0.42
2:D:93:VAL:HG22	2:D:114:PHE:CZ	2.55	0.42
2:N:259:LEU:HD12	2:N:260:VAL:N	2.34	0.42
1:O:222:GLY:HA2	1:O:252:LEU:O	2.20	0.42
1:Y:267:ASP:O	1:Y:268:PRO:O	2.37	0.42
1:S:274:THR:HB	1:S:276:GLU:CB	2.49	0.42
1:Q:68:GLN:O	1:Q:71:CYS:HB2	2.20	0.42
1:C:234:ARG:NE	1:C:238:ARG:HH21	2.15	0.42
2:J:165:ASN:O	2:J:167:VAL:HG23	2.20	0.42
1:K:196:ASN:OD1	1:K:196:ASN:N	2.52	0.42
1:K:231:LEU:HB2	1:K:294:ARG:HH12	1.84	0.42
1:E:4:ASP:HA	1:E:300:LEU:HD21	2.01	0.42
1:1:142:VAL:HB	1:1:143:PRO:HD3	2.00	0.42
2:X:144:VAL:CG1	2:X:241:ILE:HB	2.50	0.42
1:A:48:LYS:HE2	1:A:48:LYS:HB2	1.83	0.42
1:1:34:LYS:HG2	1:1:38:MET:CE	2.50	0.42
2:H:157:ILE:HG23	2:H:158:LYS:N	2.35	0.42
2:T:16:GLU:OE2	2:T:162:ARG:NH1	2.52	0.42
2:D:121:SER:HB3	2:D:124:VAL:CG2	2.50	0.42
2:H:256:THR:O	2:H:257:ASN:HB2	2.19	0.42
1:1:64:LEU:O	1:1:90:ARG:HD3	2.20	0.42
2:N:262:VAL:HA	2:N:295:VAL:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:229:ASP:OD1	1:O:231:LEU:N	2.53	0.41
1:G:94:PHE:CZ	1:G:164:LEU:HD22	2.54	0.41
1:Q:29:ARG:HB2	1:Q:300:LEU:CD2	2.49	0.41
2:2:238:MET:O	2:2:240:THR:N	2.51	0.41
1:W:272:TYR:CD2	1:W:273:ARG:N	2.88	0.41
2:4:307:ILE:CG2	2:4:308:LEU:N	2.83	0.41
2:R:95:ASN:HD21	2:T:87:MET:CE	2.32	0.41
1:Q:12:CYS:SG	1:Q:225:VAL:HG22	2.60	0.41
2:J:277:ALA:O	2:J:281:GLU:HG3	2.19	0.41
2:N:237:ASN:C	2:N:237:ASN:HD22	2.24	0.41
2:R:139:CYS:HA	2:R:140:PRO:HD2	1.91	0.41
1:1:142:VAL:HA	1:1:163:THR:CG2	2.50	0.41
1:A:221:PRO:O	1:A:251:ILE:HG13	2.20	0.41
2:2:76:PRO:HG2	2:2:112:ILE:HG13	2.01	0.41
2:R:306:LYS:HD3	2:R:310:ASP:OD2	2.20	0.41
1:Y:332:LEU:O	1:Y:332:LEU:HG	2.20	0.41
2:R:253:VAL:HG11	2:R:288:LEU:HD13	2.02	0.41
1:I:225:VAL:HG12	1:I:226:ASP:N	2.35	0.41
1:Y:35:TYR:O	1:Y:39:MET:HG3	2.20	0.41
1:K:162:LEU:HD11	1:K:190:ILE:HD12	2.02	0.41
1:Q:304:GLU:O	1:Q:308:GLU:HG3	2.20	0.41
1:M:86:ILE:HG12	1:M:87:THR:N	2.35	0.41
1:Q:137:ILE:HD13	2:T:85:PHE:HE1	1.85	0.41
2:J:268:GLN:O	2:J:269:PHE:HB2	2.20	0.41
1:S:34:LYS:HE2	1:S:34:LYS:HB3	1.67	0.41
1:O:234:ARG:HE	1:O:238:ARG:NH2	2.17	0.41
2:6:212:HIS:HB3	2:6:238:MET:CE	2.51	0.41
1:M:50:ASP:HB2	1:M:64:LEU:HD11	2.01	0.41
2:F:121:SER:HB3	2:F:124:VAL:HG21	2.02	0.41
1:A:127:TYR:CD1	1:A:127:TYR:N	2.88	0.41
2:X:75:ARG:HG2	2:X:75:ARG:HH11	1.86	0.41
1:A:219:PHE:CD1	1:A:220:ILE:HG13	2.55	0.41
2:4:157:ILE:O	2:4:161:ILE:HG13	2.21	0.41
2:P:30:VAL:HG23	2:P:31:ALA:N	2.36	0.41
1:I:113:LYS:HD2	1:I:328:PRO:HG2	2.01	0.41
1:U:104:GLU:H	1:U:104:GLU:HG3	1.65	0.41
1:S:37:ARG:NH1	1:S:309:ILE:HG23	2.35	0.41
1:1:297:ASN:ND2	1:1:297:ASN:H	2.17	0.41
1:5:238:ARG:HD3	1:5:238:ARG:HH11	1.73	0.41
2:4:307:ILE:HG23	2:4:308:LEU:N	2.35	0.41
1:A:278:ILE:N	1:A:278:ILE:CD1	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:81:MET:HB3	2:Z:85:PHE:CD2	2.56	0.41
2:6:172:ASN:HD22	2:6:175:MET:H	1.67	0.41
1:M:29:ARG:CA	1:M:300:LEU:HD22	2.51	0.41
2:R:81:MET:HB3	2:R:85:PHE:CD2	2.55	0.41
2:Z:278:ARG:HA	2:Z:278:ARG:HD2	1.75	0.41
2:Z:278:ARG:HG3	2:Z:278:ARG:NH1	2.35	0.41
2:B:20:ASP:OD1	2:B:20:ASP:C	2.59	0.41
1:G:313:VAL:O	1:G:316:GLU:HB3	2.19	0.41
1:K:141:GLN:N	1:K:141:GLN:OE1	2.44	0.41
2:T:165:ASN:O	2:T:167:VAL:HG23	2.20	0.41
1:W:213:TYR:HA	1:W:216:ARG:HG2	2.02	0.41
1:3:152:CYS:O	1:3:153:LYS:C	2.57	0.41
1:O:197:ARG:CB	1:O:197:ARG:HH11	2.20	0.41
1:A:29:ARG:HB2	1:A:300:LEU:CD2	2.50	0.41
2:H:124:VAL:O	2:H:125:ALA:HB3	2.20	0.41
2:L:172:ASN:HB3	2:L:175:MET:HG2	2.01	0.41
2:L:207:ILE:HG13	2:L:258:HIS:HB2	2.02	0.41
2:T:285:PHE:O	2:T:288:LEU:HB2	2.20	0.41
1:G:66:ASP:HA	1:G:69:GLU:OE2	2.19	0.41
1:C:276:GLU:HA	1:C:279:GLN:HB2	2.03	0.41
1:A:75:LEU:HA	1:A:75:LEU:HD12	1.88	0.41
1:Y:335:LEU:HG	1:Y:335:LEU:O	2.18	0.41
1:I:289:MET:CE	1:I:290:LEU:HD23	2.51	0.41
1:E:43:ARG:NE	1:E:69:GLU:OE2	2.46	0.41
1:I:213:TYR:HB2	1:I:254:GLU:OE1	2.20	0.41
1:1:280:GLU:O	1:1:283:SER:OG	2.37	0.41
1:G:128:ALA:HB3	1:G:131:PHE:HB3	2.02	0.41
1:1:95:THR:HG22	1:1:100:LEU:HB2	2.01	0.41
2:T:313:ILE:CG2	2:T:314:PRO:HD2	2.43	0.41
2:N:34:ASP:O	2:N:38:LYS:HA	2.21	0.41
2:B:256:THR:O	2:B:257:ASN:CB	2.68	0.41
2:J:327:LEU:O	2:J:329:ILE:N	2.54	0.41
2:R:279:ILE:HA	2:R:279:ILE:HD13	1.98	0.41
2:4:31:ALA:HB3	2:4:54:ASP:CG	2.40	0.41
2:F:313:ILE:HG13	2:F:314:PRO:CD	2.50	0.41
2:J:22:LYS:HD2	2:J:74:LEU:HD12	2.02	0.41
2:P:263:GLU:O	2:P:296:THR:HA	2.21	0.41
1:1:184:LEU:HA	1:1:184:LEU:HD12	1.73	0.41
1:I:149:ALA:O	1:I:152:CYS:HB2	2.21	0.41
1:M:36:TYR:O	1:M:37:ARG:C	2.58	0.41
2:J:93:VAL:HG22	2:J:114:PHE:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:3:ASN:O	1:3:4:ASP:HB3	2.21	0.41
1:5:234:ARG:NE	1:5:238:ARG:NH2	2.68	0.41
1:1:225:VAL:CG1	1:1:226:ASP:H	2.33	0.41
1:O:234:ARG:NH2	1:O:238:ARG:HH22	2.18	0.41
1:E:9:ILE:HB	1:E:232:CYS:SG	2.61	0.41
1:O:55:GLN:O	1:O:56:LYS:CB	2.69	0.41
2:J:329:ILE:OXT	2:J:329:ILE:CG1	2.68	0.41
2:X:75:ARG:HG2	2:X:75:ARG:NH1	2.36	0.41
1:E:14:LEU:HA	1:E:14:LEU:HD23	1.77	0.41
1:C:52:LEU:HA	1:C:52:LEU:HD23	1.84	0.41
2:L:170:LEU:HD23	2:L:170:LEU:HA	1.88	0.41
2:6:81:MET:HE3	2:6:81:MET:HB2	1.97	0.41
1:U:317:ILE:HD13	1:U:317:ILE:HA	1.81	0.41
2:N:172:ASN:C	2:N:172:ASN:ND2	2.73	0.41
2:X:237:ASN:ND2	2:X:237:ASN:C	2.74	0.41
2:L:24:PHE:CZ	2:L:76:PRO:HB3	2.56	0.41
2:J:25:LEU:HD12	2:J:77:ILE:O	2.20	0.41
2:4:182:PHE:O	2:4:183:PRO:C	2.58	0.41
1:O:292:LYS:HG3	1:O:306:LEU:HD13	2.01	0.41
2:4:112:ILE:CG1	2:4:113:VAL:N	2.83	0.41
1:K:95:THR:HG22	1:K:105:ILE:HD11	2.02	0.41
2:V:142:LEU:HD12	2:V:142:LEU:HA	1.89	0.41
1:Y:269:GLY:O	1:Y:272:TYR:HB3	2.20	0.41
1:3:187:LEU:O	1:3:189:CYS:N	2.54	0.41
2:N:271:VAL:HA	2:P:269:PHE:HE1	1.85	0.41
1:Y:100:LEU:HD13	1:Y:128:ALA:HB2	2.01	0.41
2:6:28:GLU:OE2	2:6:59:GLU:OE2	2.39	0.41
1:C:53:TYR:CE2	1:C:62:CYS:HB2	2.56	0.41
2:B:197:LYS:HA	2:B:245:ASP:OD2	2.20	0.41
1:5:61:PHE:CD2	1:5:124:MET:SD	3.13	0.41
2:B:326:THR:C	2:B:328:ASN:H	2.22	0.41
1:Q:4:ASP:HB3	1:Q:28:THR:HA	2.03	0.41
2:D:81:MET:HB3	2:D:85:PHE:CD2	2.55	0.41
2:B:95:ASN:ND2	2:D:87:MET:CE	2.84	0.41
2:2:130:GLN:HG3	2:2:266:TRP:CH2	2.55	0.41
1:A:39:MET:HG2	1:A:73:VAL:HG21	2.02	0.41
1:A:337:TYR:O	1:A:338:HIS:HB2	2.21	0.41
1:1:2:ALA:HB3	1:1:300:LEU:HD23	2.02	0.41
2:F:99:LYS:HG2	2:H:301:PRO:HB3	2.02	0.41
2:J:118:ASN:ND2	2:J:132:PHE:H	2.17	0.41
1:A:55:GLN:O	1:A:56:LYS:CB	2.65	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:78:GLY:HA2	1:I:238:ARG:CG	2.51	0.41
1:S:289:MET:CE	1:S:290:LEU:HD23	2.51	0.41
2:2:157:ILE:HG23	2:2:158:LYS:N	2.34	0.41
1:U:9:ILE:H	1:U:9:ILE:HG12	1.69	0.41
2:D:278:ARG:HH11	2:D:278:ARG:HG3	1.85	0.41
1:1:57:ILE:HD12	1:5:326:ALA:CB	2.50	0.41
2:F:266:TRP:HB3	2:F:267:PRO:HD2	2.03	0.41
1:1:162:LEU:N	1:1:162:LEU:CD1	2.84	0.41
1:M:225:VAL:HB	1:M:255:LEU:HD12	2.02	0.41
2:L:59:GLU:N	2:L:59:GLU:OE1	2.51	0.41
1:K:142:VAL:HB	1:K:143:PRO:HD3	2.01	0.41
2:2:39:VAL:O	2:2:39:VAL:CG1	2.68	0.41
2:6:237:ASN:C	2:6:237:ASN:ND2	2.74	0.41
2:J:81:MET:HB2	2:J:81:MET:HE3	1.80	0.41
2:L:206:HIS:HD2	2:L:231:VAL:HA	1.86	0.41
1:5:15:HIS:CG	1:5:215:LYS:HG2	2.56	0.41
2:Z:110:VAL:O	2:Z:166:PRO:HD3	2.21	0.41
2:N:95:ASN:ND2	2:P:87:MET:CE	2.84	0.41
2:N:83:PHE:CZ	2:N:168:VAL:HG13	2.56	0.41
1:M:269:GLY:O	1:M:272:TYR:HB3	2.21	0.41
1:3:69:GLU:O	1:3:70:ALA:C	2.57	0.41
2:V:313:ILE:HG22	2:V:314:PRO:N	2.36	0.41
1:O:196:ASN:CB	1:O:257:THR:HG23	2.39	0.41
1:Q:29:ARG:CB	1:Q:300:LEU:HD22	2.49	0.41
2:6:182:PHE:CD2	2:6:187:GLN:HG3	2.56	0.41
1:Q:258:TYR:HD1	1:Q:258:TYR:C	2.24	0.41
1:A:29:ARG:HH11	1:A:29:ARG:HG2	1.83	0.41
1:K:232:CYS:HA	1:K:235:GLU:HB2	2.03	0.41
1:5:234:ARG:O	1:5:235:GLU:C	2.58	0.41
2:D:16:GLU:OE2	2:D:158:LYS:NZ	2.53	0.41
2:B:172:ASN:HD22	2:B:175:MET:N	2.13	0.41
2:D:172:ASN:HD22	2:D:172:ASN:C	2.24	0.41
1:A:80:ASN:HB3	1:A:81:PRO:CD	2.50	0.41
1:C:337:TYR:O	1:C:338:HIS:HB2	2.21	0.41
2:V:124:VAL:HB	2:V:128:HIS:HB2	2.03	0.41
1:1:45:MET:HE2	1:1:102:VAL:HG13	2.02	0.41
1:M:279:GLN:HA	1:M:279:GLN:OE1	2.20	0.41
2:L:51:ARG:C	2:L:52:ILE:HD13	2.41	0.41
2:J:9:ILE:CG1	2:J:153:ALA:HB1	2.51	0.41
2:Z:219:CYS:SG	2:Z:262:VAL:HG21	2.61	0.41
1:3:43:ARG:NH1	1:3:43:ARG:HG2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:230:ILE:O	1:K:230:ILE:HG12	2.20	0.41
1:3:129:LYS:HD2	1:3:129:LYS:HA	1.67	0.41
2:6:260:VAL:HG22	2:6:293:VAL:CG2	2.51	0.41
2:V:269:PHE:HE1	2:X:271:VAL:HA	1.85	0.41
1:1:180:ASN:O	1:1:184:LEU:HB2	2.21	0.41
1:I:152:CYS:O	1:I:153:LYS:C	2.58	0.41
1:C:25:THR:OG1	1:C:26:VAL:N	2.53	0.41
2:B:327:LEU:HD23	2:B:327:LEU:HA	1.80	0.41
1:C:157:LYS:HA	1:C:157:LYS:HD3	1.89	0.41
1:E:40:GLN:HE21	1:E:288:ILE:HD13	1.86	0.41
2:H:139:CYS:HA	2:H:140:PRO:HD2	1.65	0.41
2:N:20:ASP:OD1	2:N:22:LYS:HB2	2.21	0.41
1:1:348:VAL:HG23	1:1:359:SER:HB2	2.03	0.41
2:N:297:GLY:HA2	2:N:312:SER:O	2.21	0.41
1:E:246:SER:OG	1:E:248:LYS:HG3	2.21	0.41
2:B:94:ILE:HD13	2:B:94:ILE:HA	1.80	0.41
1:M:57:ILE:HD13	1:M:57:ILE:N	2.35	0.41
1:E:137:ILE:HA	1:E:137:ILE:HD13	1.82	0.41
2:D:184:PRO:HA	2:D:187:GLN:NE2	2.36	0.41
1:C:64:LEU:O	1:C:90:ARG:NH1	2.48	0.41
1:Y:276:GLU:O	1:Y:280:GLU:HB2	2.20	0.41
1:C:114:GLY:N	1:C:327:ASP:OD2	2.52	0.41
1:K:112:ARG:HD3	1:K:112:ARG:HA	1.94	0.41
2:T:218:HIS:HB3	2:T:316:VAL:HG23	2.03	0.41
1:Y:196:ASN:N	1:Y:196:ASN:OD1	2.48	0.41
1:Y:29:ARG:CG	1:Y:300:LEU:O	2.69	0.41
2:X:279:ILE:HG23	2:X:279:ILE:HD12	1.82	0.41
2:T:268:GLN:O	2:T:269:PHE:CB	2.69	0.41
1:O:142:VAL:HB	1:O:143:PRO:HD3	2.03	0.41
2:L:185:GLU:O	2:L:185:GLU:HG2	2.20	0.41
1:K:106:LEU:HD23	1:K:106:LEU:HA	1.88	0.41
2:4:278:ARG:NH1	2:4:278:ARG:HG3	2.36	0.41
1:E:132:TYR:N	1:E:132:TYR:CD1	2.88	0.41
2:F:308:LEU:HD23	2:F:308:LEU:HA	1.84	0.41
1:1:41:THR:HG21	1:1:96:PHE:CZ	2.56	0.41
2:N:79:GLU:HG2	2:N:80:PHE:N	2.35	0.41
1:O:53:TYR:CD2	1:O:62:CYS:HB2	2.56	0.41
2:F:178:VAL:HG12	2:F:180:PHE:CE1	2.56	0.41
2:F:272:GLY:O	2:F:273:ALA:C	2.60	0.41
1:A:142:VAL:HA	1:A:163:THR:CG2	2.51	0.41
1:A:27:LEU:HD22	1:A:28:THR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:50:ASP:HB2	1:U:64:LEU:CD1	2.51	0.41
1:3:197:ARG:HD2	1:3:257:THR:O	2.22	0.40
1:G:196:ASN:ND2	1:G:259:ARG:CD	2.84	0.40
1:G:197:ARG:HG3	1:G:258:TYR:HD2	1.85	0.40
1:W:196:ASN:ND2	1:W:259:ARG:NE	2.68	0.40
1:Y:29:ARG:HB2	1:Y:300:LEU:HD22	2.03	0.40
1:3:27:LEU:HG	1:3:231:LEU:HD21	2.02	0.40
1:W:4:ASP:HA	1:W:300:LEU:HD21	2.02	0.40
2:4:237:ASN:C	2:4:237:ASN:ND2	2.74	0.40
2:H:207:ILE:HG13	2:H:258:HIS:HB2	2.02	0.40
1:W:45:MET:CE	1:W:102:VAL:HA	2.51	0.40
2:4:26:LEU:HD23	2:4:78:CYS:HA	2.03	0.40
1:U:206:ARG:HB3	1:U:206:ARG:HH11	1.86	0.40
1:I:135:ASN:ND2	1:I:135:ASN:N	2.69	0.40
1:W:126:MET:HB2	1:W:126:MET:HE3	1.82	0.40
2:P:249:ILE:HD13	2:P:249:ILE:HG21	1.89	0.40
1:A:103:ARG:HG2	1:A:103:ARG:HH11	1.86	0.40
2:T:304:TYR:O	2:T:305:ALA:C	2.59	0.40
1:3:341:SER:HB2	2:4:101:TYR:CZ	2.56	0.40
2:D:51:ARG:O	2:D:52:ILE:HD13	2.21	0.40
2:6:258:HIS:CD2	2:6:327:LEU:HD23	2.56	0.40
1:3:155:ASN:O	1:3:156:GLY:C	2.58	0.40
1:5:45:MET:HE1	1:5:105:ILE:CD1	2.51	0.40
2:2:237:ASN:ND2	2:2:237:ASN:C	2.74	0.40
1:5:63:HIS:HB3	1:5:90:ARG:HG3	2.03	0.40
1:Q:204:VAL:HB	1:Q:211:THR:CG2	2.51	0.40
1:Y:162:LEU:CD1	1:Y:190:ILE:HD12	2.52	0.40
1:A:95:THR:CG2	1:A:100:LEU:HD22	2.52	0.40
2:2:118:ASN:ND2	2:2:132:PHE:H	2.19	0.40
2:4:259:LEU:HD22	2:4:279:ILE:HG13	2.02	0.40
2:B:307:ILE:HG23	2:B:308:LEU:N	2.37	0.40
1:M:351:ALA:O	2:P:295:VAL:HG13	2.22	0.40
1:O:46:GLU:OE1	1:O:46:GLU:HA	2.22	0.40
2:2:279:ILE:HA	2:2:279:ILE:HD13	1.83	0.40
2:R:19:ARG:HG2	2:R:19:ARG:NH1	2.36	0.40
1:O:17:LEU:HD23	1:O:17:LEU:HA	1.86	0.40
1:A:47:LEU:HA	1:A:47:LEU:HD23	1.89	0.40
1:A:77:ALA:CB	1:A:234:ARG:HG3	2.51	0.40
1:Q:318:GLU:HG2	2:2:287:PHE:CE2	2.57	0.40
2:R:150:SER:HB2	2:R:180:PHE:HB2	2.03	0.40
1:Y:33:LEU:HD12	1:Y:295:MET:HE1	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:341:SER:HB2	2:F:101:TYR:CE1	2.56	0.40
1:1:167:ASP:HB3	1:1:195:ASN:HA	2.03	0.40
2:V:157:ILE:O	2:V:161:ILE:HG13	2.20	0.40
1:O:231:LEU:O	1:O:232:CYS:C	2.56	0.40
1:W:81:PRO:HA	1:W:98:ARG:NH2	2.36	0.40
2:P:118:ASN:ND2	2:P:131:CYS:HA	2.36	0.40
2:J:118:ASN:N	2:J:171:GLU:O	2.49	0.40
2:J:172:ASN:ND2	2:J:174:LEU:N	2.69	0.40
1:S:34:LYS:HD2	1:S:38:MET:HE2	2.02	0.40
1:O:234:ARG:HE	1:O:238:ARG:HH22	1.69	0.40
1:O:113:LYS:HE2	1:O:113:LYS:HB2	1.92	0.40
2:Z:260:VAL:HG22	2:Z:293:VAL:HG23	2.03	0.40
2:V:172:ASN:ND2	2:V:172:ASN:C	2.74	0.40
2:L:286:ASN:HD22	2:L:286:ASN:H	1.68	0.40
2:B:95:ASN:ND2	2:D:87:MET:HE1	2.37	0.40
2:R:151:GLU:OE1	2:R:183:PRO:HG3	2.21	0.40
2:V:74:LEU:HD12	2:V:74:LEU:HA	1.83	0.40
1:E:109:LEU:HA	1:E:109:LEU:HD23	1.60	0.40
1:I:109:LEU:HA	1:I:109:LEU:HD23	1.85	0.40
1:I:109:LEU:CD2	1:I:123:SER:HB2	2.50	0.40
2:H:196:GLY:O	2:H:245:ASP:HB2	2.21	0.40
2:6:157:ILE:HG23	2:6:158:LYS:N	2.37	0.40
2:P:136:TYR:C	2:P:138:HIS:H	2.25	0.40
1:O:138:VAL:HG13	1:O:169:ALA:HB2	2.04	0.40
2:B:39:VAL:HG11	2:B:115:ARG:NH2	2.37	0.40
1:A:285:SER:HA	1:A:290:LEU:HD21	2.04	0.40
1:5:10:LYS:HG2	1:5:11:LYS:H	1.84	0.40
1:M:258:TYR:C	1:M:258:TYR:CD1	2.95	0.40
1:U:4:ASP:HA	1:U:300:LEU:HD21	2.03	0.40
1:1:296:VAL:HG12	1:1:297:ASN:HD22	1.84	0.40
1:W:315:LYS:HB2	1:W:315:LYS:HZ3	1.86	0.40
1:E:108:GLU:OE2	1:E:119:GLY:CA	2.69	0.40
1:W:132:TYR:CD1	1:W:148:ILE:HD13	2.57	0.40
2:6:172:ASN:HD22	2:6:174:LEU:N	2.18	0.40
1:Y:225:VAL:HG12	1:Y:226:ASP:N	2.36	0.40
2:V:43:LEU:CD1	2:V:43:LEU:H	2.34	0.40
2:Z:278:ARG:HG3	2:Z:278:ARG:HH11	1.86	0.40
1:E:341:SER:HB2	2:F:101:TYR:CZ	2.56	0.40
1:U:162:LEU:HD12	1:U:190:ILE:HD12	2.03	0.40
1:G:39:MET:HG2	1:G:73:VAL:HG21	2.04	0.40
1:C:46:GLU:HA	1:C:46:GLU:OE1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:278:ARG:HG3	2:J:278:ARG:NH1	2.36	0.40
1:E:184:LEU:HD12	1:E:184:LEU:HA	1.91	0.40
1:C:86:ILE:HG23	1:C:86:ILE:O	2.21	0.40
1:Y:86:ILE:HG12	1:Y:87:THR:N	2.37	0.40
2:D:202:ARG:O	2:D:234:GLU:HA	2.20	0.40
2:V:302:MET:HA	2:V:303:PRO:HD2	1.96	0.40
2:P:93:VAL:O	2:P:97:ALA:HB3	2.21	0.40
1:U:164:LEU:HG	1:U:192:ILE:HB	2.03	0.40
1:K:219:PHE:CD1	1:K:220:ILE:HG13	2.56	0.40
2:R:307:ILE:CG2	2:R:308:LEU:N	2.84	0.40
1:U:142:VAL:HB	1:U:143:PRO:HD3	2.03	0.40
1:3:61:PHE:HD2	1:3:124:MET:CE	2.35	0.40
1:3:1:PHE:HD2	1:3:1:PHE:H	1.69	0.40
2:J:5:VAL:HB	2:J:175:MET:O	2.22	0.40
1:1:53:TYR:C	1:1:55:GLN:N	2.74	0.40
1:O:141:GLN:N	1:O:141:GLN:OE1	2.52	0.40
1:W:57:ILE:HD13	1:W:57:ILE:N	2.35	0.40
2:V:121:SER:HB3	2:V:124:VAL:CG2	2.50	0.40
1:O:132:TYR:CD1	1:O:148:ILE:HD13	2.55	0.40
2:V:301:PRO:HB3	2:X:99:LYS:HG2	2.04	0.40
2:F:84:ASN:ND2	2:F:128:HIS:HA	2.36	0.40
1:S:341:SER:HB3	2:T:101:TYR:CZ	2.57	0.40
2:R:222:ALA:HB1	2:R:320:ILE:HG13	2.03	0.40
1:U:52:LEU:HA	1:U:52:LEU:HD23	1.94	0.40
2:2:327:LEU:HD23	2:2:327:LEU:HA	1.87	0.40
1:3:135:ASN:N	1:3:135:ASN:ND2	2.70	0.40
2:B:93:VAL:HG22	2:B:114:PHE:CZ	2.57	0.40
1:G:78:GLY:HA3	1:G:237:THR:CG2	2.52	0.40
2:T:234:GLU:OE1	2:T:255:LYS:NZ	2.47	0.40
2:H:242:ARG:HA	2:H:243:PRO:HA	1.93	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	1	329/382 (86%)	295 (90%)	25 (8%)	9 (3%)	6 30
1	3	336/382 (88%)	305 (91%)	25 (7%)	6 (2%)	11 43
1	5	341/382 (89%)	306 (90%)	22 (6%)	13 (4%)	4 21
1	A	336/382 (88%)	311 (93%)	20 (6%)	5 (2%)	13 48
1	C	336/382 (88%)	303 (90%)	28 (8%)	5 (2%)	13 48
1	E	343/382 (90%)	313 (91%)	23 (7%)	7 (2%)	9 39
1	G	340/382 (89%)	305 (90%)	29 (8%)	6 (2%)	11 43
1	I	338/382 (88%)	309 (91%)	24 (7%)	5 (2%)	13 48
1	K	341/382 (89%)	304 (89%)	31 (9%)	6 (2%)	11 43
1	M	343/382 (90%)	311 (91%)	24 (7%)	8 (2%)	8 35
1	O	326/382 (85%)	286 (88%)	32 (10%)	8 (2%)	7 32
1	Q	338/382 (88%)	314 (93%)	19 (6%)	5 (2%)	13 48
1	S	334/382 (87%)	301 (90%)	25 (8%)	8 (2%)	7 34
1	U	342/382 (90%)	313 (92%)	23 (7%)	6 (2%)	11 43
1	W	339/382 (89%)	312 (92%)	22 (6%)	5 (2%)	13 48
1	Y	343/382 (90%)	319 (93%)	19 (6%)	5 (2%)	13 48
2	2	327/329 (99%)	297 (91%)	26 (8%)	4 (1%)	16 54
2	4	327/329 (99%)	304 (93%)	23 (7%)	0	100 100
2	6	327/329 (99%)	300 (92%)	24 (7%)	3 (1%)	21 62
2	B	327/329 (99%)	307 (94%)	19 (6%)	1 (0%)	46 82
2	D	327/329 (99%)	306 (94%)	19 (6%)	2 (1%)	30 71
2	F	327/329 (99%)	304 (93%)	22 (7%)	1 (0%)	46 82
2	H	327/329 (99%)	300 (92%)	24 (7%)	3 (1%)	21 62
2	J	327/329 (99%)	302 (92%)	25 (8%)	0	100 100
2	L	327/329 (99%)	302 (92%)	24 (7%)	1 (0%)	46 82
2	N	327/329 (99%)	307 (94%)	20 (6%)	0	100 100
2	P	327/329 (99%)	292 (89%)	30 (9%)	5 (2%)	13 48
2	R	327/329 (99%)	310 (95%)	16 (5%)	1 (0%)	46 82
2	T	327/329 (99%)	308 (94%)	16 (5%)	3 (1%)	21 62
2	V	327/329 (99%)	294 (90%)	30 (9%)	3 (1%)	21 62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	X	327/329 (99%)	294 (90%)	30 (9%)	3 (1%)	21 62
2	Z	327/329 (99%)	306 (94%)	20 (6%)	1 (0%)	46 82
All	All	10637/11376 (94%)	9740 (92%)	759 (7%)	138 (1%)	15 52

All (138) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ALA
1	A	285	SER
1	E	268	PRO
1	I	2	ALA
1	K	274	THR
1	K	275	ARG
1	M	268	PRO
1	M	270	VAL
1	M	271	ALA
1	O	230	ILE
1	O	281	VAL
1	O	285	SER
2	P	43	LEU
1	Q	285	SER
1	S	275	ARG
2	T	188	SER
1	U	2	ALA
1	U	216	ARG
1	W	2	ALA
1	Y	268	PRO
1	1	2	ALA
1	1	4	ASP
1	1	281	VAL
1	1	283	SER
2	2	43	LEU
1	3	2	ALA
1	3	285	SER
1	5	235	GLU
1	5	280	GLU
1	5	282	ARG
1	5	283	SER
1	C	285	SER
1	C	297	ASN
2	D	137	GLY

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Mol	Chain	Res	Type
2	D	188	SER
1	G	29	ARG
1	G	275	ARG
2	H	317	LYS
1	I	205	GLU
1	I	285	SER
1	K	218	ASP
1	K	230	ILE
1	M	2	ALA
1	Q	2	ALA
1	Q	275	ARG
1	S	285	SER
2	T	315	GLN
1	U	130	ASN
1	U	235	GLU
1	W	272	TYR
1	Y	270	VAL
1	5	88	ALA
1	5	218	ASP
1	5	236	ALA
1	A	129	LYS
1	A	156	GLY
1	E	88	ALA
1	E	97	THR
1	G	273	ARG
1	K	88	ALA
1	K	271	ALA
1	M	88	ALA
1	O	237	THR
2	P	31	ALA
1	Q	129	LYS
1	S	88	ALA
1	S	297	ASN
2	V	273	ALA
1	W	88	ALA
1	W	218	ASP
2	X	49	ASP
1	1	133	GLY
1	1	230	ILE
1	5	216	ARG
1	5	258	TYR
1	5	271	ALA

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Mol	Chain	Res	Type
2	6	181	GLU
2	6	183	PRO
1	C	170	ALA
1	C	218	ASP
1	E	218	ASP
2	H	31	ALA
2	L	31	ALA
1	M	4	ASP
1	M	218	ASP
1	O	4	ASP
1	O	218	ASP
1	O	338	HIS
2	P	32	GLN
2	P	317	LYS
1	S	29	ARG
1	S	218	ASP
1	S	276	GLU
1	S	281	VAL
2	T	228	LYS
1	U	218	ASP
1	W	285	SER
2	X	31	ALA
1	Y	218	ASP
1	1	218	ASP
1	3	218	ASP
1	3	275	ARG
1	5	233	VAL
1	5	269	GLY
1	5	281	VAL
1	A	218	ASP
2	B	69	ALA
1	E	216	ARG
1	G	62	CYS
1	G	218	ASP
1	I	88	ALA
1	I	218	ASP
1	Q	88	ALA
1	U	88	ALA
2	V	213	SER
1	Y	140	ALA
1	1	22	PRO
1	3	276	GLU

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Mol	Chain	Res	Type
2	6	31	ALA
1	E	230	ILE
1	G	297	ASN
1	O	2	ALA
2	R	31	ALA
2	V	267	PRO
1	Y	156	GLY
1	1	296	VAL
2	2	45	LYS
2	2	267	PRO
1	3	156	GLY
2	P	267	PRO
1	C	329	GLU
1	E	156	GLY
1	M	230	ILE
2	X	267	PRO
2	Z	267	PRO
2	2	265	GLY
2	H	265	GLY
2	F	243	PRO

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1	271/310 (87%)	243 (90%)	28 (10%)	9 32
1	3	278/310 (90%)	250 (90%)	28 (10%)	9 33
1	5	281/310 (91%)	254 (90%)	27 (10%)	10 36
1	A	278/310 (90%)	250 (90%)	28 (10%)	9 33
1	C	278/310 (90%)	249 (90%)	29 (10%)	9 31
1	E	282/310 (91%)	258 (92%)	24 (8%)	13 43
1	G	281/310 (91%)	255 (91%)	26 (9%)	11 38
1	I	280/310 (90%)	255 (91%)	25 (9%)	12 41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	K	281/310 (91%)	258 (92%)	23 (8%)	14 45
1	M	282/310 (91%)	251 (89%)	31 (11%)	8 29
1	O	268/310 (86%)	239 (89%)	29 (11%)	8 29
1	Q	280/310 (90%)	249 (89%)	31 (11%)	8 28
1	S	277/310 (89%)	249 (90%)	28 (10%)	9 33
1	U	282/310 (91%)	251 (89%)	31 (11%)	8 29
1	W	280/310 (90%)	248 (89%)	32 (11%)	7 27
1	Y	282/310 (91%)	253 (90%)	29 (10%)	9 32
2	2	268/268 (100%)	252 (94%)	16 (6%)	24 60
2	4	268/268 (100%)	253 (94%)	15 (6%)	26 64
2	6	268/268 (100%)	251 (94%)	17 (6%)	22 58
2	B	268/268 (100%)	253 (94%)	15 (6%)	26 64
2	D	268/268 (100%)	249 (93%)	19 (7%)	18 53
2	F	268/268 (100%)	251 (94%)	17 (6%)	22 58
2	H	268/268 (100%)	244 (91%)	24 (9%)	12 40
2	J	268/268 (100%)	247 (92%)	21 (8%)	16 48
2	L	268/268 (100%)	251 (94%)	17 (6%)	22 58
2	N	268/268 (100%)	245 (91%)	23 (9%)	13 42
2	P	268/268 (100%)	248 (92%)	20 (8%)	17 50
2	R	268/268 (100%)	245 (91%)	23 (9%)	13 42
2	T	268/268 (100%)	247 (92%)	21 (8%)	16 48
2	V	268/268 (100%)	249 (93%)	19 (7%)	18 53
2	X	268/268 (100%)	245 (91%)	23 (9%)	13 42
2	Z	268/268 (100%)	251 (94%)	17 (6%)	22 58
All	All	8749/9248 (95%)	7993 (91%)	756 (9%)	13 42

All (756) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	11	LYS
1	A	16	ARG
1	A	18	GLU
1	A	23	VAL

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Mol	Chain	Res	Type
1	A	27	LEU
1	A	28	THR
1	A	29	ARG
1	A	33	LEU
1	A	54	LYS
1	A	57	ILE
1	A	59	ARG
1	A	75	LEU
1	A	103	ARG
1	A	104	GLU
1	A	113	LYS
1	A	118	LYS
1	A	155	ASN
1	A	197	ARG
1	A	223	LEU
1	A	230	ILE
1	A	255	LEU
1	A	278	ILE
1	A	284	LYS
1	A	289	MET
1	A	307	LYS
1	A	315	LYS
1	A	322	GLN
2	B	1	LEU
2	B	11	GLN
2	B	74	LEU
2	B	81	MET
2	B	159	SER
2	B	162	ARG
2	B	185	GLU
2	B	192	LEU
2	B	197	LYS
2	B	229	GLU
2	B	237	ASN
2	B	279	ILE
2	B	306	LYS
2	B	317	LYS
2	B	328	ASN
1	C	1	PHE
1	C	9	ILE
1	C	10	LYS
1	C	18	GLU

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Mol	Chain	Res	Type
1	C	24	THR
1	C	27	LEU
1	C	28	THR
1	C	29	ARG
1	C	30	GLU
1	C	31	ASP
1	C	40	GLN
1	C	75	LEU
1	C	98	ARG
1	C	103	ARG
1	C	129	LYS
1	C	206	ARG
1	C	223	LEU
1	C	230	ILE
1	C	252	LEU
1	C	255	LEU
1	C	280	GLU
1	C	307	LYS
1	C	309	ILE
1	C	314	ARG
1	C	315	LYS
1	C	316	GLU
1	C	322	GLN
1	C	333	GLU
1	C	353	GLN
2	D	1	LEU
2	D	2	GLN
2	D	3	VAL
2	D	26	LEU
2	D	32	GLN
2	D	33	TYR
2	D	39	VAL
2	D	43	LEU
2	D	74	LEU
2	D	81	MET
2	D	172	ASN
2	D	185	GLU
2	D	189	LYS
2	D	197	LYS
2	D	237	ASN
2	D	239	ARG
2	D	288	LEU

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Mol	Chain	Res	Type
2	D	313	ILE
2	D	317	LYS
1	E	10	LYS
1	E	11	LYS
1	E	23	VAL
1	E	27	LEU
1	E	28	THR
1	E	29	ARG
1	E	30	GLU
1	E	31	ASP
1	E	45	MET
1	E	57	ILE
1	E	103	ARG
1	E	113	LYS
1	E	216	ARG
1	E	223	LEU
1	E	238	ARG
1	E	246	SER
1	E	255	LEU
1	E	272	TYR
1	E	273	ARG
1	E	279	GLN
1	E	295	MET
1	E	315	LYS
1	E	335	LEU
1	E	361	SER
2	F	1	LEU
2	F	3	VAL
2	F	26	LEU
2	F	34	ASP
2	F	74	LEU
2	F	81	MET
2	F	82	THR
2	F	91	ASP
2	F	107	LEU
2	F	182	PHE
2	F	192	LEU
2	F	278	ARG
2	F	279	ILE
2	F	288	LEU
2	F	306	LYS
2	F	317	LYS

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Mol	Chain	Res	Type
2	F	328	ASN
1	G	23	VAL
1	G	27	LEU
1	G	28	THR
1	G	29	ARG
1	G	30	GLU
1	G	72	CYS
1	G	75	LEU
1	G	97	THR
1	G	98	ARG
1	G	104	GLU
1	G	118	LYS
1	G	129	LYS
1	G	158	ASP
1	G	206	ARG
1	G	255	LEU
1	G	270	VAL
1	G	272	TYR
1	G	275	ARG
1	G	276	GLU
1	G	284	LYS
1	G	289	MET
1	G	314	ARG
1	G	315	LYS
1	G	322	GLN
1	G	335	LEU
1	G	347	GLU
2	H	1	LEU
2	H	3	VAL
2	H	21	GLU
2	H	43	LEU
2	H	45	LYS
2	H	49	ASP
2	H	74	LEU
2	H	107	LEU
2	H	162	ARG
2	H	172	ASN
2	H	182	PHE
2	H	197	LYS
2	H	227	SER
2	H	236	ILE
2	H	237	ASN

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Mol	Chain	Res	Type
2	H	278	ARG
2	H	279	ILE
2	H	288	LEU
2	H	306	LYS
2	H	307	ILE
2	H	313	ILE
2	H	316	VAL
2	H	317	LYS
2	H	328	ASN
1	I	26	VAL
1	I	27	LEU
1	I	29	ARG
1	I	59	ARG
1	I	75	LEU
1	I	80	ASN
1	I	85	LEU
1	I	98	ARG
1	I	104	GLU
1	I	118	LYS
1	I	135	ASN
1	I	186	LYS
1	I	205	GLU
1	I	210	SER
1	I	230	ILE
1	I	232	CYS
1	I	255	LEU
1	I	279	GLN
1	I	283	SER
1	I	289	MET
1	I	307	LYS
1	I	315	LYS
1	I	322	GLN
1	I	341	SER
1	I	342	SER
2	J	1	LEU
2	J	2	GLN
2	J	33	TYR
2	J	34	ASP
2	J	74	LEU
2	J	81	MET
2	J	173	GLU
2	J	182	PHE

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Mol	Chain	Res	Type
2	J	188	SER
2	J	189	LYS
2	J	192	LEU
2	J	227	SER
2	J	228	LYS
2	J	229	GLU
2	J	237	ASN
2	J	263	GLU
2	J	279	ILE
2	J	306	LYS
2	J	307	ILE
2	J	317	LYS
2	J	328	ASN
1	K	10	LYS
1	K	18	GLU
1	K	27	LEU
1	K	29	ARG
1	K	30	GLU
1	K	54	LYS
1	K	75	LEU
1	K	98	ARG
1	K	103	ARG
1	K	196	ASN
1	K	210	SER
1	K	219	PHE
1	K	223	LEU
1	K	232	CYS
1	K	252	LEU
1	K	255	LEU
1	K	275	ARG
1	K	279	GLN
1	K	315	LYS
1	K	316	GLU
1	K	322	GLN
1	K	335	LEU
1	K	353	GLN
2	L	1	LEU
2	L	2	GLN
2	L	32	GLN
2	L	33	TYR
2	L	40	SER
2	L	43	LEU

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Mol	Chain	Res	Type
2	L	81	MET
2	L	142	LEU
2	L	162	ARG
2	L	172	ASN
2	L	182	PHE
2	L	185	GLU
2	L	189	LYS
2	L	237	ASN
2	L	279	ILE
2	L	288	LEU
2	L	317	LYS
1	M	3	ASN
1	M	10	LYS
1	M	19	GLU
1	M	23	VAL
1	M	27	LEU
1	M	28	THR
1	M	30	GLU
1	M	33	LEU
1	M	100	LEU
1	M	103	ARG
1	M	118	LYS
1	M	158	ASP
1	M	186	LYS
1	M	196	ASN
1	M	223	LEU
1	M	230	ILE
1	M	235	GLU
1	M	238	ARG
1	M	252	LEU
1	M	255	LEU
1	M	270	VAL
1	M	272	TYR
1	M	275	ARG
1	M	279	GLN
1	M	282	ARG
1	M	284	LYS
1	M	315	LYS
1	M	322	GLN
1	M	333	GLU
1	M	335	LEU
1	M	360	VAL

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Mol	Chain	Res	Type
2	N	1	LEU
2	N	2	GLN
2	N	3	VAL
2	N	21	GLU
2	N	26	LEU
2	N	32	GLN
2	N	34	ASP
2	N	45	LYS
2	N	60	MET
2	N	74	LEU
2	N	81	MET
2	N	94	ILE
2	N	159	SER
2	N	162	ARG
2	N	172	ASN
2	N	182	PHE
2	N	188	SER
2	N	192	LEU
2	N	237	ASN
2	N	244	MET
2	N	278	ARG
2	N	279	ILE
2	N	306	LYS
1	O	1	PHE
1	O	3	ASN
1	O	10	LYS
1	O	11	LYS
1	O	27	LEU
1	O	30	GLU
1	O	98	ARG
1	O	118	LYS
1	O	129	LYS
1	O	197	ARG
1	O	223	LEU
1	O	230	ILE
1	O	246	SER
1	O	252	LEU
1	O	255	LEU
1	O	283	SER
1	O	286	ASP
1	O	289	MET
1	O	290	LEU

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Mol	Chain	Res	Type
1	O	297	ASN
1	O	298	SER
1	O	307	LYS
1	O	314	ARG
1	O	315	LYS
1	O	316	GLU
1	O	318	GLU
1	O	322	GLN
1	O	342	SER
1	O	353	GLN
2	P	1	LEU
2	P	3	VAL
2	P	21	GLU
2	P	33	TYR
2	P	43	LEU
2	P	74	LEU
2	P	81	MET
2	P	91	ASP
2	P	185	GLU
2	P	188	SER
2	P	197	LYS
2	P	205	THR
2	P	206	HIS
2	P	237	ASN
2	P	246	MET
2	P	263	GLU
2	P	278	ARG
2	P	288	LEU
2	P	319	ILE
2	P	328	ASN
1	Q	6	THR
1	Q	10	LYS
1	Q	11	LYS
1	Q	16	ARG
1	Q	19	GLU
1	Q	27	LEU
1	Q	28	THR
1	Q	29	ARG
1	Q	33	LEU
1	Q	40	GLN
1	Q	48	LYS
1	Q	51	GLN

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Mol	Chain	Res	Type
1	Q	57	ILE
1	Q	75	LEU
1	Q	98	ARG
1	Q	103	ARG
1	Q	135	ASN
1	Q	186	LYS
1	Q	197	ARG
1	Q	204	VAL
1	Q	206	ARG
1	Q	223	LEU
1	Q	230	ILE
1	Q	255	LEU
1	Q	283	SER
1	Q	284	LYS
1	Q	289	MET
1	Q	303	VAL
1	Q	315	LYS
1	Q	316	GLU
1	Q	361	SER
2	R	1	LEU
2	R	11	GLN
2	R	26	LEU
2	R	33	TYR
2	R	45	LYS
2	R	50	LYS
2	R	74	LEU
2	R	81	MET
2	R	162	ARG
2	R	173	GLU
2	R	182	PHE
2	R	185	GLU
2	R	190	ASP
2	R	192	LEU
2	R	197	LYS
2	R	229	GLU
2	R	234	GLU
2	R	237	ASN
2	R	261	THR
2	R	280	MET
2	R	306	LYS
2	R	317	LYS
2	R	328	ASN

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Mol	Chain	Res	Type
1	S	1	PHE
1	S	10	LYS
1	S	18	GLU
1	S	24	THR
1	S	27	LEU
1	S	30	GLU
1	S	34	LYS
1	S	37	ARG
1	S	57	ILE
1	S	75	LEU
1	S	98	ARG
1	S	103	ARG
1	S	135	ASN
1	S	158	ASP
1	S	197	ARG
1	S	230	ILE
1	S	232	CYS
1	S	274	THR
1	S	278	ILE
1	S	283	SER
1	S	284	LYS
1	S	289	MET
1	S	307	LYS
1	S	315	LYS
1	S	316	GLU
1	S	322	GLN
1	S	332	LEU
1	S	353	GLN
2	T	1	LEU
2	T	2	GLN
2	T	3	VAL
2	T	21	GLU
2	T	33	TYR
2	T	74	LEU
2	T	96	SER
2	T	127	GLN
2	T	172	ASN
2	T	185	GLU
2	T	197	LYS
2	T	228	LYS
2	T	237	ASN
2	T	278	ARG

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Mol	Chain	Res	Type
2	T	279	ILE
2	T	288	LEU
2	T	313	ILE
2	T	315	GLN
2	T	316	VAL
2	T	317	LYS
2	T	328	ASN
1	U	3	ASN
1	U	9	ILE
1	U	10	LYS
1	U	11	LYS
1	U	23	VAL
1	U	27	LEU
1	U	28	THR
1	U	33	LEU
1	U	82	THR
1	U	98	ARG
1	U	103	ARG
1	U	158	ASP
1	U	194	GLU
1	U	206	ARG
1	U	210	SER
1	U	214	TYR
1	U	223	LEU
1	U	233	VAL
1	U	235	GLU
1	U	246	SER
1	U	252	LEU
1	U	256	GLN
1	U	283	SER
1	U	284	LYS
1	U	289	MET
1	U	295	MET
1	U	307	LYS
1	U	314	ARG
1	U	322	GLN
1	U	335	LEU
1	U	342	SER
2	V	1	LEU
2	V	7	ASP
2	V	26	LEU
2	V	34	ASP

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Mol	Chain	Res	Type
2	V	74	LEU
2	V	81	MET
2	V	82	THR
2	V	129	SER
2	V	159	SER
2	V	162	ARG
2	V	187	GLN
2	V	192	LEU
2	V	206	HIS
2	V	213	SER
2	V	237	ASN
2	V	278	ARG
2	V	279	ILE
2	V	306	LYS
2	V	328	ASN
1	W	6	THR
1	W	13	ASP
1	W	23	VAL
1	W	27	LEU
1	W	28	THR
1	W	29	ARG
1	W	30	GLU
1	W	75	LEU
1	W	98	ARG
1	W	104	GLU
1	W	118	LYS
1	W	158	ASP
1	W	206	ARG
1	W	223	LEU
1	W	238	ARG
1	W	255	LEU
1	W	272	TYR
1	W	273	ARG
1	W	274	THR
1	W	275	ARG
1	W	276	GLU
1	W	278	ILE
1	W	279	GLN
1	W	280	GLU
1	W	283	SER
1	W	289	MET
1	W	315	LYS

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Mol	Chain	Res	Type
1	W	316	GLU
1	W	318	GLU
1	W	319	ASP
1	W	333	GLU
1	W	335	LEU
2	X	3	VAL
2	X	21	GLU
2	X	33	TYR
2	X	34	ASP
2	X	43	LEU
2	X	49	ASP
2	X	58	SER
2	X	74	LEU
2	X	81	MET
2	X	162	ARG
2	X	172	ASN
2	X	182	PHE
2	X	185	GLU
2	X	246	MET
2	X	278	ARG
2	X	279	ILE
2	X	288	LEU
2	X	306	LYS
2	X	315	GLN
2	X	316	VAL
2	X	317	LYS
2	X	320	ILE
2	X	328	ASN
1	Y	3	ASN
1	Y	10	LYS
1	Y	19	GLU
1	Y	27	LEU
1	Y	29	ARG
1	Y	30	GLU
1	Y	98	ARG
1	Y	104	GLU
1	Y	118	LYS
1	Y	135	ASN
1	Y	206	ARG
1	Y	216	ARG
1	Y	230	ILE
1	Y	238	ARG

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Mol	Chain	Res	Type
1	Y	252	LEU
1	Y	255	LEU
1	Y	270	VAL
1	Y	272	TYR
1	Y	273	ARG
1	Y	274	THR
1	Y	275	ARG
1	Y	279	GLN
1	Y	284	LYS
1	Y	289	MET
1	Y	315	LYS
1	Y	316	GLU
1	Y	332	LEU
1	Y	333	GLU
1	Y	360	VAL
2	Z	1	LEU
2	Z	2	GLN
2	Z	3	VAL
2	Z	32	GLN
2	Z	74	LEU
2	Z	81	MET
2	Z	82	THR
2	Z	90	ILE
2	Z	162	ARG
2	Z	182	PHE
2	Z	188	SER
2	Z	192	LEU
2	Z	213	SER
2	Z	229	GLU
2	Z	237	ASN
2	Z	306	LYS
2	Z	317	LYS
1	1	8	GLU
1	1	10	LYS
1	1	11	LYS
1	1	26	VAL
1	1	27	LEU
1	1	28	THR
1	1	29	ARG
1	1	30	GLU
1	1	53	TYR
1	1	75	LEU

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Mol	Chain	Res	Type
1	1	98	ARG
1	1	104	GLU
1	1	113	LYS
1	1	118	LYS
1	1	129	LYS
1	1	135	ASN
1	1	158	ASP
1	1	197	ARG
1	1	257	THR
1	1	280	GLU
1	1	283	SER
1	1	289	MET
1	1	297	ASN
1	1	300	LEU
1	1	307	LYS
1	1	315	LYS
1	1	342	SER
1	1	353	GLN
2	2	33	TYR
2	2	43	LEU
2	2	49	ASP
2	2	74	LEU
2	2	140	PRO
2	2	152	ASP
2	2	162	ARG
2	2	188	SER
2	2	192	LEU
2	2	197	LYS
2	2	237	ASN
2	2	246	MET
2	2	279	ILE
2	2	288	LEU
2	2	317	LYS
2	2	328	ASN
1	3	1	PHE
1	3	3	ASN
1	3	7	PHE
1	3	11	LYS
1	3	27	LEU
1	3	29	ARG
1	3	30	GLU
1	3	72	CYS

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Mol	Chain	Res	Type
1	3	73	VAL
1	3	75	LEU
1	3	80	ASN
1	3	98	ARG
1	3	103	ARG
1	3	104	GLU
1	3	118	LYS
1	3	135	ASN
1	3	195	ASN
1	3	230	ILE
1	3	255	LEU
1	3	257	THR
1	3	274	THR
1	3	284	LYS
1	3	289	MET
1	3	307	LYS
1	3	315	LYS
1	3	322	GLN
1	3	341	SER
1	3	342	SER
2	4	1	LEU
2	4	11	GLN
2	4	13	MET
2	4	74	LEU
2	4	81	MET
2	4	82	THR
2	4	159	SER
2	4	162	ARG
2	4	189	LYS
2	4	190	ASP
2	4	192	LEU
2	4	237	ASN
2	4	279	ILE
2	4	306	LYS
2	4	328	ASN
1	5	10	LYS
1	5	23	VAL
1	5	27	LEU
1	5	29	ARG
1	5	75	LEU
1	5	98	ARG
1	5	103	ARG

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Mol	Chain	Res	Type
1	5	104	GLU
1	5	158	ASP
1	5	164	LEU
1	5	196	ASN
1	5	210	SER
1	5	231	LEU
1	5	232	CYS
1	5	235	GLU
1	5	252	LEU
1	5	273	ARG
1	5	274	THR
1	5	275	ARG
1	5	279	GLN
1	5	280	GLU
1	5	281	VAL
1	5	284	LYS
1	5	315	LYS
1	5	322	GLN
1	5	335	LEU
1	5	343	ASP
2	6	1	LEU
2	6	2	GLN
2	6	32	GLN
2	6	33	TYR
2	6	81	MET
2	6	162	ARG
2	6	172	ASN
2	6	185	GLU
2	6	189	LYS
2	6	206	HIS
2	6	213	SER
2	6	237	ASN
2	6	278	ARG
2	6	279	ILE
2	6	300	VAL
2	6	317	LYS
2	6	328	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (231) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN

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Mol	Chain	Res	Type
1	A	68	GLN
1	A	125	HIS
1	A	135	ASN
1	A	196	ASN
1	A	279	GLN
1	A	297	ASN
1	A	299	ASN
2	B	32	GLN
2	B	84	ASN
2	B	118	ASN
2	B	172	ASN
2	B	187	GLN
2	B	237	ASN
1	C	68	GLN
1	C	92	HIS
1	C	130	ASN
1	C	297	ASN
2	D	32	GLN
2	D	88	GLN
2	D	118	ASN
2	D	172	ASN
2	D	237	ASN
2	D	328	ASN
1	E	40	GLN
1	E	55	GLN
1	E	68	GLN
1	E	125	HIS
1	E	130	ASN
1	E	297	ASN
1	E	299	ASN
1	E	338	HIS
2	F	32	GLN
2	F	88	GLN
2	F	118	ASN
2	F	172	ASN
2	F	187	GLN
2	F	237	ASN
2	F	315	GLN
1	G	55	GLN
1	G	68	GLN
1	G	80	ASN
1	G	125	HIS

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Mol	Chain	Res	Type
1	G	196	ASN
1	G	297	ASN
1	G	299	ASN
2	H	2	GLN
2	H	32	GLN
2	H	88	GLN
2	H	118	ASN
2	H	172	ASN
2	H	187	GLN
2	H	206	HIS
2	H	237	ASN
1	I	40	GLN
1	I	68	GLN
1	I	125	HIS
1	I	135	ASN
1	I	297	ASN
1	I	299	ASN
1	I	353	GLN
2	J	10	ASN
2	J	88	GLN
2	J	118	ASN
2	J	172	ASN
2	J	187	GLN
2	J	237	ASN
2	J	268	GLN
1	K	40	GLN
1	K	55	GLN
1	K	63	HIS
1	K	68	GLN
1	K	80	ASN
1	K	92	HIS
1	K	125	HIS
1	K	130	ASN
1	K	297	ASN
1	K	299	ASN
2	L	88	GLN
2	L	118	ASN
2	L	172	ASN
2	L	187	GLN
2	L	206	HIS
2	L	237	ASN
2	L	286	ASN

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Mol	Chain	Res	Type
2	L	328	ASN
1	M	40	GLN
1	M	51	GLN
1	M	55	GLN
1	M	297	ASN
1	M	299	ASN
2	N	2	GLN
2	N	32	GLN
2	N	88	GLN
2	N	118	ASN
2	N	172	ASN
2	N	187	GLN
2	N	237	ASN
2	N	315	GLN
1	O	63	HIS
1	O	80	ASN
1	O	125	HIS
1	O	297	ASN
2	P	2	GLN
2	P	88	GLN
2	P	118	ASN
2	P	172	ASN
2	P	187	GLN
2	P	237	ASN
2	P	328	ASN
1	Q	51	GLN
1	Q	55	GLN
1	Q	68	GLN
1	Q	125	HIS
1	Q	135	ASN
1	Q	279	GLN
1	Q	297	ASN
1	Q	299	ASN
1	Q	353	GLN
2	R	10	ASN
2	R	32	GLN
2	R	88	GLN
2	R	95	ASN
2	R	118	ASN
2	R	172	ASN
2	R	187	GLN
2	R	237	ASN

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Mol	Chain	Res	Type
2	R	268	GLN
1	S	68	GLN
1	S	80	ASN
1	S	84	HIS
1	S	196	ASN
1	S	279	GLN
1	S	297	ASN
1	S	299	ASN
2	T	118	ASN
2	T	172	ASN
2	T	187	GLN
2	T	237	ASN
2	T	286	ASN
2	T	328	ASN
1	U	40	GLN
1	U	51	GLN
1	U	55	GLN
1	U	63	HIS
1	U	68	GLN
1	U	125	HIS
1	U	130	ASN
1	U	297	ASN
2	V	2	GLN
2	V	32	GLN
2	V	88	GLN
2	V	118	ASN
2	V	172	ASN
2	V	187	GLN
2	V	237	ASN
2	V	257	ASN
1	W	40	GLN
1	W	55	GLN
1	W	68	GLN
1	W	125	HIS
1	W	196	ASN
1	W	279	GLN
1	W	297	ASN
2	X	2	GLN
2	X	32	GLN
2	X	88	GLN
2	X	118	ASN
2	X	172	ASN

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Mol	Chain	Res	Type
2	X	187	GLN
2	X	237	ASN
2	X	268	GLN
2	X	328	ASN
1	Y	40	GLN
1	Y	68	GLN
1	Y	80	ASN
1	Y	125	HIS
1	Y	135	ASN
1	Y	297	ASN
1	Y	299	ASN
1	Y	338	HIS
2	Z	2	GLN
2	Z	32	GLN
2	Z	88	GLN
2	Z	118	ASN
2	Z	172	ASN
2	Z	187	GLN
2	Z	237	ASN
1	1	68	GLN
1	1	125	HIS
1	1	135	ASN
1	1	196	ASN
1	1	297	ASN
1	1	353	GLN
2	2	2	GLN
2	2	88	GLN
2	2	95	ASN
2	2	118	ASN
2	2	172	ASN
2	2	187	GLN
2	2	237	ASN
2	2	315	GLN
2	2	328	ASN
1	3	40	GLN
1	3	68	GLN
1	3	125	HIS
1	3	135	ASN
1	3	279	GLN
1	3	297	ASN
1	3	299	ASN
2	4	2	GLN

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Mol	Chain	Res	Type
2	4	32	GLN
2	4	88	GLN
2	4	95	ASN
2	4	118	ASN
2	4	172	ASN
2	4	187	GLN
2	4	237	ASN
2	4	328	ASN
1	5	55	GLN
1	5	68	GLN
1	5	125	HIS
1	5	297	ASN
1	5	299	ASN
2	6	32	GLN
2	6	88	GLN
2	6	118	ASN
2	6	172	ASN
2	6	187	GLN
2	6	237	ASN
2	6	328	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	1	335/382 (87%)	-0.27	1 (0%) 94 84	46, 56, 67, 88	0
1	3	342/382 (89%)	-0.36	0 100 100	45, 55, 72, 101	0
1	5	347/382 (90%)	-0.38	0 100 100	45, 56, 69, 92	0
1	A	342/382 (89%)	-0.40	1 (0%) 94 84	44, 55, 70, 101	0
1	C	342/382 (89%)	-0.31	1 (0%) 94 84	47, 56, 72, 100	0
1	E	349/382 (91%)	-0.45	0 100 100	45, 55, 67, 86	0
1	G	346/382 (90%)	-0.38	0 100 100	42, 55, 69, 86	0
1	I	344/382 (90%)	-0.35	0 100 100	44, 56, 75, 103	0
1	K	347/382 (90%)	-0.37	0 100 100	45, 56, 69, 86	0
1	M	349/382 (91%)	-0.47	0 100 100	45, 55, 66, 85	0
1	O	332/382 (86%)	-0.30	1 (0%) 94 84	45, 57, 66, 86	0
1	Q	344/382 (90%)	-0.41	1 (0%) 94 84	43, 56, 74, 98	0
1	S	340/382 (89%)	-0.32	0 100 100	47, 55, 73, 105	0
1	U	348/382 (91%)	-0.46	0 100 100	42, 55, 66, 84	0
1	W	345/382 (90%)	-0.42	0 100 100	43, 55, 70, 84	0
1	Y	349/382 (91%)	-0.43	0 100 100	46, 55, 66, 87	0
2	2	329/329 (100%)	-0.50	1 (0%) 94 84	45, 54, 63, 73	0
2	4	329/329 (100%)	-0.44	0 100 100	44, 54, 63, 73	0
2	6	329/329 (100%)	-0.47	0 100 100	45, 53, 63, 73	0
2	B	329/329 (100%)	-0.49	0 100 100	46, 53, 62, 72	0
2	D	329/329 (100%)	-0.49	0 100 100	44, 53, 61, 73	0
2	F	329/329 (100%)	-0.46	0 100 100	45, 54, 64, 76	0
2	H	329/329 (100%)	-0.46	0 100 100	45, 53, 63, 75	0
2	J	329/329 (100%)	-0.48	0 100 100	46, 54, 63, 71	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
2	L	329/329 (100%)	-0.46	0	100	100	45, 53, 62, 72	0
2	N	329/329 (100%)	-0.46	0	100	100	47, 54, 63, 73	0
2	P	329/329 (100%)	-0.51	0	100	100	44, 53, 63, 74	0
2	R	329/329 (100%)	-0.49	0	100	100	45, 53, 62, 71	0
2	T	329/329 (100%)	-0.49	0	100	100	45, 53, 62, 73	0
2	V	329/329 (100%)	-0.46	0	100	100	47, 54, 64, 77	0
2	X	329/329 (100%)	-0.46	0	100	100	45, 54, 63, 75	0
2	Z	329/329 (100%)	-0.44	1 (0%)	94	84	45, 54, 62, 73	0
All	All	10765/11376 (94%)	-0.43	7 (0%)	95	90	42, 54, 65, 105	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	261	HIS	4.2
1	1	5	ALA	3.5
1	A	261	HIS	3.4
2	2	329	ILE	2.9
2	Z	1	LEU	2.4
1	O	207	ALA	2.1
1	C	277	GLU	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
3	K	4	1016	1/1	0.97	0.18	0.08	80,80,80,80	0
3	K	6	1007	1/1	0.97	0.09	-2.35	69,69,69,69	0
3	K	J	1014	1/1	0.96	0.10	-2.68	78,78,78,78	0
3	K	D	1002	1/1	0.95	0.05	-3.15	72,72,72,72	0
3	K	F	1008	1/1	0.96	0.06	-3.20	75,75,75,75	0
3	K	V	1004	1/1	0.93	0.07	-3.27	70,70,70,70	0
3	K	N	1009	1/1	0.97	0.07	-3.45	79,79,79,79	0
3	K	H	1013	1/1	0.93	0.07	-3.71	79,79,79,79	0
3	K	T	1006	1/1	0.90	0.08	-3.74	76,76,76,76	0
3	K	L	1011	1/1	0.98	0.06	-3.76	69,69,69,69	0
3	K	B	1003	1/1	0.97	0.06	-3.77	65,65,65,65	0
3	K	X	1005	1/1	0.97	0.10	-3.96	67,67,67,67	0
3	K	2	1015	1/1	0.96	0.06	-4.15	88,88,88,88	0
3	K	R	1001	1/1	0.95	0.06	-5.49	70,70,70,70	0
3	K	P	1012	1/1	0.97	0.05	-5.70	84,84,84,84	0
3	K	Z	1010	1/1	0.97	0.07	-5.82	75,75,75,75	0

6.5 Other polymers (i)

There are no such residues in this entry.