Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2024 – 12:55 PM EST

PDB ID	:	3QIL
Title	:	Crystal structure analysis of the clathrin trimerization domain
Authors	:	Ybe, J.A.; Mishra, S.; Nix, J.
Deposited on	:	2011-01-27
Resolution	:	3.92 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

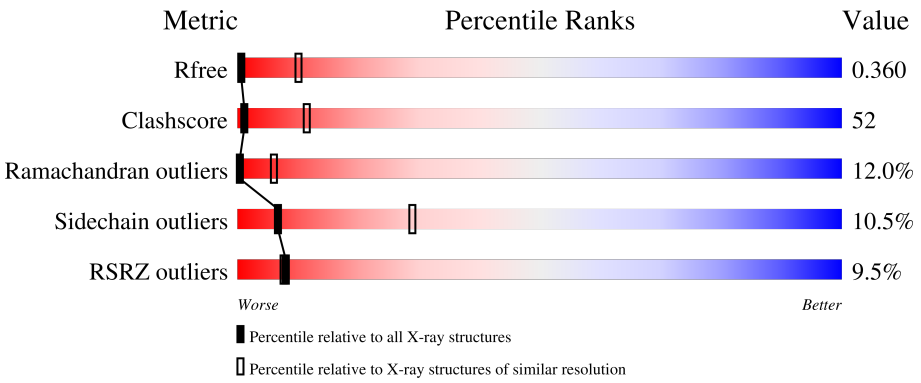
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.92 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}	130704	1019 (4.18-3.66)
Clashscore	141614	1016 (4.16-3.68)
Ramachandran outliers	138981	1039 (4.18-3.66)
Sidechain outliers	138945	1032 (4.18-3.66)
RSRZ outliers	127900	1002 (4.20-3.64)

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

Mol	Chain	Length	Quality of chain
1	A	125	4%; 41%, 41%, 16%, •
1	B	125	13%; 24%, 43%, 10%, •, 22%
1	C	125	12%; 32%, 49%, 18%, •
1	D	125	2%; 40%, 42%, 14%, •
1	E	125	12%; 32%, 35%, 10%, •, 22%

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Mol	Chain	Length	Quality of chain
1	F	125	13% 30% 54% 14%
1	G	125	3% 42% 40% 16%
1	H	125	10% 26% 42% 9% 22%
1	I	125	13% 35% 47% 16%
1	J	125	7% 45% 39% 13%
1	K	125	8% 26% 41% 10% 22%
1	L	125	13% 33% 50% 16%
1	M	125	5% 42% 40% 15%
1	N	125	10% 29% 38% 10% 22%
1	O	125	13% 29% 55% 14%
1	P	125	4% 43% 40% 14%
1	Q	125	6% 32% 35% 10% 22%
1	R	125	13% 28% 54% 17%
1	S	125	4% 44% 37% 18%
1	T	125	13% 21% 47% 10% 22%
1	U	125	10% 30% 54% 14%
1	V	125	2% 44% 37% 17%
1	W	125	10% 27% 40% 10% 22%
1	X	125	13% 33% 51% 14%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 23032 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 Clathrin heavy chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	125	1034	655	175	195	9	0	0	0
			Total	C	N	O	S			
1	B	97	811	519	127	158	7	0	0	0
			Total	C	N	O	S			
1	C	125	1034	655	175	195	9	0	0	0
			Total	C	N	O	S			
1	D	125	1034	655	175	195	9	0	0	0
			Total	C	N	O	S			
1	E	97	811	519	127	158	7	0	0	0
			Total	C	N	O	S			
1	F	125	1034	655	175	195	9	0	0	0
			Total	C	N	O	S			
1	G	125	1034	655	175	195	9	0	0	0
			Total	C	N	O	S			
1	H	97	811	519	127	158	7	0	0	0
			Total	C	N	O	S			
1	I	125	1034	655	175	195	9	0	0	0
			Total	C	N	O	S			
1	J	125	1034	655	175	195	9	0	0	0
			Total	C	N	O	S			
1	K	97	811	519	127	158	7	0	0	0
			Total	C	N	O	S			
1	L	125	1034	655	175	195	9	0	0	0
			Total	C	N	O	S			
1	M	125	1034	655	175	195	9	0	0	0
			Total	C	N	O	S			
1	N	97	811	519	127	158	7	0	0	0
			Total	C	N	O	S			
1	O	125	1034	655	175	195	9	0	0	0
			Total	C	N	O	S			
1	P	125	1034	655	175	195	9	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	Q	97	811	519	127	158	7	0	0	0
			Total	C	N	O	S			
1	R	125	1034	655	175	195	9	0	0	0
			Total	C	N	O	S			
1	S	125	1034	655	175	195	9	0	0	0
			Total	C	N	O	S			
1	T	97	811	519	127	158	7	0	0	0
			Total	C	N	O	S			
1	U	125	1034	655	175	195	9	0	0	0
			Total	C	N	O	S			
1	V	125	1034	655	175	195	9	0	0	0
			Total	C	N	O	S			
1	W	97	811	519	127	158	7	0	0	0
			Total	C	N	O	S			
1	X	125	1034	655	175	195	9	0	0	0

There are 552 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1500	MET	-	expression tag	UNP P49951
A	1501	GLY	-	expression tag	UNP P49951
A	1502	SER	-	expression tag	UNP P49951
A	1503	SER	-	expression tag	UNP P49951
A	1504	HIS	-	expression tag	UNP P49951
A	1505	HIS	-	expression tag	UNP P49951
A	1506	HIS	-	expression tag	UNP P49951
A	1507	HIS	-	expression tag	UNP P49951
A	1508	HIS	-	expression tag	UNP P49951
A	1509	HIS	-	expression tag	UNP P49951
A	1510	SER	-	expression tag	UNP P49951
A	1511	SER	-	expression tag	UNP P49951
A	1512	GLY	-	expression tag	UNP P49951
A	1513	LEU	-	expression tag	UNP P49951
A	1514	VAL	-	expression tag	UNP P49951
A	1515	PRO	-	expression tag	UNP P49951
A	1516	ARG	-	expression tag	UNP P49951
A	1517	GLY	-	expression tag	UNP P49951
A	1518	SER	-	expression tag	UNP P49951
A	1519	HIS	-	expression tag	UNP P49951
A	1520	MET	-	expression tag	UNP P49951
A	1528	ALA	CYS	engineered mutation	UNP P49951
A	1585	LEU	THR	engineered mutation	UNP P49951

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1500	MET	-	expression tag	UNP P49951
B	1501	GLY	-	expression tag	UNP P49951
B	1502	SER	-	expression tag	UNP P49951
B	1503	SER	-	expression tag	UNP P49951
B	1504	HIS	-	expression tag	UNP P49951
B	1505	HIS	-	expression tag	UNP P49951
B	1506	HIS	-	expression tag	UNP P49951
B	1507	HIS	-	expression tag	UNP P49951
B	1508	HIS	-	expression tag	UNP P49951
B	1509	HIS	-	expression tag	UNP P49951
B	1510	SER	-	expression tag	UNP P49951
B	1511	SER	-	expression tag	UNP P49951
B	1512	GLY	-	expression tag	UNP P49951
B	1513	LEU	-	expression tag	UNP P49951
B	1514	VAL	-	expression tag	UNP P49951
B	1515	PRO	-	expression tag	UNP P49951
B	1516	ARG	-	expression tag	UNP P49951
B	1517	GLY	-	expression tag	UNP P49951
B	1518	SER	-	expression tag	UNP P49951
B	1519	HIS	-	expression tag	UNP P49951
B	1520	MET	-	expression tag	UNP P49951
B	1528	ALA	CYS	engineered mutation	UNP P49951
B	1585	LEU	THR	engineered mutation	UNP P49951
C	1500	MET	-	expression tag	UNP P49951
C	1501	GLY	-	expression tag	UNP P49951
C	1502	SER	-	expression tag	UNP P49951
C	1503	SER	-	expression tag	UNP P49951
C	1504	HIS	-	expression tag	UNP P49951
C	1505	HIS	-	expression tag	UNP P49951
C	1506	HIS	-	expression tag	UNP P49951
C	1507	HIS	-	expression tag	UNP P49951
C	1508	HIS	-	expression tag	UNP P49951
C	1509	HIS	-	expression tag	UNP P49951
C	1510	SER	-	expression tag	UNP P49951
C	1511	SER	-	expression tag	UNP P49951
C	1512	GLY	-	expression tag	UNP P49951
C	1513	LEU	-	expression tag	UNP P49951
C	1514	VAL	-	expression tag	UNP P49951
C	1515	PRO	-	expression tag	UNP P49951
C	1516	ARG	-	expression tag	UNP P49951
C	1517	GLY	-	expression tag	UNP P49951
C	1518	SER	-	expression tag	UNP P49951

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1519	HIS	-	expression tag	UNP P49951
C	1520	MET	-	expression tag	UNP P49951
C	1528	ALA	CYS	engineered mutation	UNP P49951
C	1585	LEU	THR	engineered mutation	UNP P49951
D	1500	MET	-	expression tag	UNP P49951
D	1501	GLY	-	expression tag	UNP P49951
D	1502	SER	-	expression tag	UNP P49951
D	1503	SER	-	expression tag	UNP P49951
D	1504	HIS	-	expression tag	UNP P49951
D	1505	HIS	-	expression tag	UNP P49951
D	1506	HIS	-	expression tag	UNP P49951
D	1507	HIS	-	expression tag	UNP P49951
D	1508	HIS	-	expression tag	UNP P49951
D	1509	HIS	-	expression tag	UNP P49951
D	1510	SER	-	expression tag	UNP P49951
D	1511	SER	-	expression tag	UNP P49951
D	1512	GLY	-	expression tag	UNP P49951
D	1513	LEU	-	expression tag	UNP P49951
D	1514	VAL	-	expression tag	UNP P49951
D	1515	PRO	-	expression tag	UNP P49951
D	1516	ARG	-	expression tag	UNP P49951
D	1517	GLY	-	expression tag	UNP P49951
D	1518	SER	-	expression tag	UNP P49951
D	1519	HIS	-	expression tag	UNP P49951
D	1520	MET	-	expression tag	UNP P49951
D	1528	ALA	CYS	engineered mutation	UNP P49951
D	1585	LEU	THR	engineered mutation	UNP P49951
E	1500	MET	-	expression tag	UNP P49951
E	1501	GLY	-	expression tag	UNP P49951
E	1502	SER	-	expression tag	UNP P49951
E	1503	SER	-	expression tag	UNP P49951
E	1504	HIS	-	expression tag	UNP P49951
E	1505	HIS	-	expression tag	UNP P49951
E	1506	HIS	-	expression tag	UNP P49951
E	1507	HIS	-	expression tag	UNP P49951
E	1508	HIS	-	expression tag	UNP P49951
E	1509	HIS	-	expression tag	UNP P49951
E	1510	SER	-	expression tag	UNP P49951
E	1511	SER	-	expression tag	UNP P49951
E	1512	GLY	-	expression tag	UNP P49951
E	1513	LEU	-	expression tag	UNP P49951
E	1514	VAL	-	expression tag	UNP P49951

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1515	PRO	-	expression tag	UNP P49951
E	1516	ARG	-	expression tag	UNP P49951
E	1517	GLY	-	expression tag	UNP P49951
E	1518	SER	-	expression tag	UNP P49951
E	1519	HIS	-	expression tag	UNP P49951
E	1520	MET	-	expression tag	UNP P49951
E	1528	ALA	CYS	engineered mutation	UNP P49951
E	1585	LEU	THR	engineered mutation	UNP P49951
F	1500	MET	-	expression tag	UNP P49951
F	1501	GLY	-	expression tag	UNP P49951
F	1502	SER	-	expression tag	UNP P49951
F	1503	SER	-	expression tag	UNP P49951
F	1504	HIS	-	expression tag	UNP P49951
F	1505	HIS	-	expression tag	UNP P49951
F	1506	HIS	-	expression tag	UNP P49951
F	1507	HIS	-	expression tag	UNP P49951
F	1508	HIS	-	expression tag	UNP P49951
F	1509	HIS	-	expression tag	UNP P49951
F	1510	SER	-	expression tag	UNP P49951
F	1511	SER	-	expression tag	UNP P49951
F	1512	GLY	-	expression tag	UNP P49951
F	1513	LEU	-	expression tag	UNP P49951
F	1514	VAL	-	expression tag	UNP P49951
F	1515	PRO	-	expression tag	UNP P49951
F	1516	ARG	-	expression tag	UNP P49951
F	1517	GLY	-	expression tag	UNP P49951
F	1518	SER	-	expression tag	UNP P49951
F	1519	HIS	-	expression tag	UNP P49951
F	1520	MET	-	expression tag	UNP P49951
F	1528	ALA	CYS	engineered mutation	UNP P49951
F	1585	LEU	THR	engineered mutation	UNP P49951
G	1500	MET	-	expression tag	UNP P49951
G	1501	GLY	-	expression tag	UNP P49951
G	1502	SER	-	expression tag	UNP P49951
G	1503	SER	-	expression tag	UNP P49951
G	1504	HIS	-	expression tag	UNP P49951
G	1505	HIS	-	expression tag	UNP P49951
G	1506	HIS	-	expression tag	UNP P49951
G	1507	HIS	-	expression tag	UNP P49951
G	1508	HIS	-	expression tag	UNP P49951
G	1509	HIS	-	expression tag	UNP P49951
G	1510	SER	-	expression tag	UNP P49951

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Chain	Residue	Modelled	Actual	Comment	Reference
G	1511	SER	-	expression tag	UNP P49951
G	1512	GLY	-	expression tag	UNP P49951
G	1513	LEU	-	expression tag	UNP P49951
G	1514	VAL	-	expression tag	UNP P49951
G	1515	PRO	-	expression tag	UNP P49951
G	1516	ARG	-	expression tag	UNP P49951
G	1517	GLY	-	expression tag	UNP P49951
G	1518	SER	-	expression tag	UNP P49951
G	1519	HIS	-	expression tag	UNP P49951
G	1520	MET	-	expression tag	UNP P49951
G	1528	ALA	CYS	engineered mutation	UNP P49951
G	1585	LEU	THR	engineered mutation	UNP P49951
H	1500	MET	-	expression tag	UNP P49951
H	1501	GLY	-	expression tag	UNP P49951
H	1502	SER	-	expression tag	UNP P49951
H	1503	SER	-	expression tag	UNP P49951
H	1504	HIS	-	expression tag	UNP P49951
H	1505	HIS	-	expression tag	UNP P49951
H	1506	HIS	-	expression tag	UNP P49951
H	1507	HIS	-	expression tag	UNP P49951
H	1508	HIS	-	expression tag	UNP P49951
H	1509	HIS	-	expression tag	UNP P49951
H	1510	SER	-	expression tag	UNP P49951
H	1511	SER	-	expression tag	UNP P49951
H	1512	GLY	-	expression tag	UNP P49951
H	1513	LEU	-	expression tag	UNP P49951
H	1514	VAL	-	expression tag	UNP P49951
H	1515	PRO	-	expression tag	UNP P49951
H	1516	ARG	-	expression tag	UNP P49951
H	1517	GLY	-	expression tag	UNP P49951
H	1518	SER	-	expression tag	UNP P49951
H	1519	HIS	-	expression tag	UNP P49951
H	1520	MET	-	expression tag	UNP P49951
H	1528	ALA	CYS	engineered mutation	UNP P49951
H	1585	LEU	THR	engineered mutation	UNP P49951
I	1500	MET	-	expression tag	UNP P49951
I	1501	GLY	-	expression tag	UNP P49951
I	1502	SER	-	expression tag	UNP P49951
I	1503	SER	-	expression tag	UNP P49951
I	1504	HIS	-	expression tag	UNP P49951
I	1505	HIS	-	expression tag	UNP P49951
I	1506	HIS	-	expression tag	UNP P49951

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Chain	Residue	Modelled	Actual	Comment	Reference
I	1507	HIS	-	expression tag	UNP P49951
I	1508	HIS	-	expression tag	UNP P49951
I	1509	HIS	-	expression tag	UNP P49951
I	1510	SER	-	expression tag	UNP P49951
I	1511	SER	-	expression tag	UNP P49951
I	1512	GLY	-	expression tag	UNP P49951
I	1513	LEU	-	expression tag	UNP P49951
I	1514	VAL	-	expression tag	UNP P49951
I	1515	PRO	-	expression tag	UNP P49951
I	1516	ARG	-	expression tag	UNP P49951
I	1517	GLY	-	expression tag	UNP P49951
I	1518	SER	-	expression tag	UNP P49951
I	1519	HIS	-	expression tag	UNP P49951
I	1520	MET	-	expression tag	UNP P49951
I	1528	ALA	CYS	engineered mutation	UNP P49951
I	1585	LEU	THR	engineered mutation	UNP P49951
J	1500	MET	-	expression tag	UNP P49951
J	1501	GLY	-	expression tag	UNP P49951
J	1502	SER	-	expression tag	UNP P49951
J	1503	SER	-	expression tag	UNP P49951
J	1504	HIS	-	expression tag	UNP P49951
J	1505	HIS	-	expression tag	UNP P49951
J	1506	HIS	-	expression tag	UNP P49951
J	1507	HIS	-	expression tag	UNP P49951
J	1508	HIS	-	expression tag	UNP P49951
J	1509	HIS	-	expression tag	UNP P49951
J	1510	SER	-	expression tag	UNP P49951
J	1511	SER	-	expression tag	UNP P49951
J	1512	GLY	-	expression tag	UNP P49951
J	1513	LEU	-	expression tag	UNP P49951
J	1514	VAL	-	expression tag	UNP P49951
J	1515	PRO	-	expression tag	UNP P49951
J	1516	ARG	-	expression tag	UNP P49951
J	1517	GLY	-	expression tag	UNP P49951
J	1518	SER	-	expression tag	UNP P49951
J	1519	HIS	-	expression tag	UNP P49951
J	1520	MET	-	expression tag	UNP P49951
J	1528	ALA	CYS	engineered mutation	UNP P49951
J	1585	LEU	THR	engineered mutation	UNP P49951
K	1500	MET	-	expression tag	UNP P49951
K	1501	GLY	-	expression tag	UNP P49951
K	1502	SER	-	expression tag	UNP P49951

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Chain	Residue	Modelled	Actual	Comment	Reference
K	1503	SER	-	expression tag	UNP P49951
K	1504	HIS	-	expression tag	UNP P49951
K	1505	HIS	-	expression tag	UNP P49951
K	1506	HIS	-	expression tag	UNP P49951
K	1507	HIS	-	expression tag	UNP P49951
K	1508	HIS	-	expression tag	UNP P49951
K	1509	HIS	-	expression tag	UNP P49951
K	1510	SER	-	expression tag	UNP P49951
K	1511	SER	-	expression tag	UNP P49951
K	1512	GLY	-	expression tag	UNP P49951
K	1513	LEU	-	expression tag	UNP P49951
K	1514	VAL	-	expression tag	UNP P49951
K	1515	PRO	-	expression tag	UNP P49951
K	1516	ARG	-	expression tag	UNP P49951
K	1517	GLY	-	expression tag	UNP P49951
K	1518	SER	-	expression tag	UNP P49951
K	1519	HIS	-	expression tag	UNP P49951
K	1520	MET	-	expression tag	UNP P49951
K	1528	ALA	CYS	engineered mutation	UNP P49951
K	1585	LEU	THR	engineered mutation	UNP P49951
L	1500	MET	-	expression tag	UNP P49951
L	1501	GLY	-	expression tag	UNP P49951
L	1502	SER	-	expression tag	UNP P49951
L	1503	SER	-	expression tag	UNP P49951
L	1504	HIS	-	expression tag	UNP P49951
L	1505	HIS	-	expression tag	UNP P49951
L	1506	HIS	-	expression tag	UNP P49951
L	1507	HIS	-	expression tag	UNP P49951
L	1508	HIS	-	expression tag	UNP P49951
L	1509	HIS	-	expression tag	UNP P49951
L	1510	SER	-	expression tag	UNP P49951
L	1511	SER	-	expression tag	UNP P49951
L	1512	GLY	-	expression tag	UNP P49951
L	1513	LEU	-	expression tag	UNP P49951
L	1514	VAL	-	expression tag	UNP P49951
L	1515	PRO	-	expression tag	UNP P49951
L	1516	ARG	-	expression tag	UNP P49951
L	1517	GLY	-	expression tag	UNP P49951
L	1518	SER	-	expression tag	UNP P49951
L	1519	HIS	-	expression tag	UNP P49951
L	1520	MET	-	expression tag	UNP P49951
L	1528	ALA	CYS	engineered mutation	UNP P49951

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Chain	Residue	Modelled	Actual	Comment	Reference
L	1585	LEU	THR	engineered mutation	UNP P49951
M	1500	MET	-	expression tag	UNP P49951
M	1501	GLY	-	expression tag	UNP P49951
M	1502	SER	-	expression tag	UNP P49951
M	1503	SER	-	expression tag	UNP P49951
M	1504	HIS	-	expression tag	UNP P49951
M	1505	HIS	-	expression tag	UNP P49951
M	1506	HIS	-	expression tag	UNP P49951
M	1507	HIS	-	expression tag	UNP P49951
M	1508	HIS	-	expression tag	UNP P49951
M	1509	HIS	-	expression tag	UNP P49951
M	1510	SER	-	expression tag	UNP P49951
M	1511	SER	-	expression tag	UNP P49951
M	1512	GLY	-	expression tag	UNP P49951
M	1513	LEU	-	expression tag	UNP P49951
M	1514	VAL	-	expression tag	UNP P49951
M	1515	PRO	-	expression tag	UNP P49951
M	1516	ARG	-	expression tag	UNP P49951
M	1517	GLY	-	expression tag	UNP P49951
M	1518	SER	-	expression tag	UNP P49951
M	1519	HIS	-	expression tag	UNP P49951
M	1520	MET	-	expression tag	UNP P49951
M	1528	ALA	CYS	engineered mutation	UNP P49951
M	1585	LEU	THR	engineered mutation	UNP P49951
N	1500	MET	-	expression tag	UNP P49951
N	1501	GLY	-	expression tag	UNP P49951
N	1502	SER	-	expression tag	UNP P49951
N	1503	SER	-	expression tag	UNP P49951
N	1504	HIS	-	expression tag	UNP P49951
N	1505	HIS	-	expression tag	UNP P49951
N	1506	HIS	-	expression tag	UNP P49951
N	1507	HIS	-	expression tag	UNP P49951
N	1508	HIS	-	expression tag	UNP P49951
N	1509	HIS	-	expression tag	UNP P49951
N	1510	SER	-	expression tag	UNP P49951
N	1511	SER	-	expression tag	UNP P49951
N	1512	GLY	-	expression tag	UNP P49951
N	1513	LEU	-	expression tag	UNP P49951
N	1514	VAL	-	expression tag	UNP P49951
N	1515	PRO	-	expression tag	UNP P49951
N	1516	ARG	-	expression tag	UNP P49951
N	1517	GLY	-	expression tag	UNP P49951

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Chain	Residue	Modelled	Actual	Comment	Reference
N	1518	SER	-	expression tag	UNP P49951
N	1519	HIS	-	expression tag	UNP P49951
N	1520	MET	-	expression tag	UNP P49951
N	1528	ALA	CYS	engineered mutation	UNP P49951
N	1585	LEU	THR	engineered mutation	UNP P49951
O	1500	MET	-	expression tag	UNP P49951
O	1501	GLY	-	expression tag	UNP P49951
O	1502	SER	-	expression tag	UNP P49951
O	1503	SER	-	expression tag	UNP P49951
O	1504	HIS	-	expression tag	UNP P49951
O	1505	HIS	-	expression tag	UNP P49951
O	1506	HIS	-	expression tag	UNP P49951
O	1507	HIS	-	expression tag	UNP P49951
O	1508	HIS	-	expression tag	UNP P49951
O	1509	HIS	-	expression tag	UNP P49951
O	1510	SER	-	expression tag	UNP P49951
O	1511	SER	-	expression tag	UNP P49951
O	1512	GLY	-	expression tag	UNP P49951
O	1513	LEU	-	expression tag	UNP P49951
O	1514	VAL	-	expression tag	UNP P49951
O	1515	PRO	-	expression tag	UNP P49951
O	1516	ARG	-	expression tag	UNP P49951
O	1517	GLY	-	expression tag	UNP P49951
O	1518	SER	-	expression tag	UNP P49951
O	1519	HIS	-	expression tag	UNP P49951
O	1520	MET	-	expression tag	UNP P49951
O	1528	ALA	CYS	engineered mutation	UNP P49951
O	1585	LEU	THR	engineered mutation	UNP P49951
P	1500	MET	-	expression tag	UNP P49951
P	1501	GLY	-	expression tag	UNP P49951
P	1502	SER	-	expression tag	UNP P49951
P	1503	SER	-	expression tag	UNP P49951
P	1504	HIS	-	expression tag	UNP P49951
P	1505	HIS	-	expression tag	UNP P49951
P	1506	HIS	-	expression tag	UNP P49951
P	1507	HIS	-	expression tag	UNP P49951
P	1508	HIS	-	expression tag	UNP P49951
P	1509	HIS	-	expression tag	UNP P49951
P	1510	SER	-	expression tag	UNP P49951
P	1511	SER	-	expression tag	UNP P49951
P	1512	GLY	-	expression tag	UNP P49951
P	1513	LEU	-	expression tag	UNP P49951

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Chain	Residue	Modelled	Actual	Comment	Reference
P	1514	VAL	-	expression tag	UNP P49951
P	1515	PRO	-	expression tag	UNP P49951
P	1516	ARG	-	expression tag	UNP P49951
P	1517	GLY	-	expression tag	UNP P49951
P	1518	SER	-	expression tag	UNP P49951
P	1519	HIS	-	expression tag	UNP P49951
P	1520	MET	-	expression tag	UNP P49951
P	1528	ALA	CYS	engineered mutation	UNP P49951
P	1585	LEU	THR	engineered mutation	UNP P49951
Q	1500	MET	-	expression tag	UNP P49951
Q	1501	GLY	-	expression tag	UNP P49951
Q	1502	SER	-	expression tag	UNP P49951
Q	1503	SER	-	expression tag	UNP P49951
Q	1504	HIS	-	expression tag	UNP P49951
Q	1505	HIS	-	expression tag	UNP P49951
Q	1506	HIS	-	expression tag	UNP P49951
Q	1507	HIS	-	expression tag	UNP P49951
Q	1508	HIS	-	expression tag	UNP P49951
Q	1509	HIS	-	expression tag	UNP P49951
Q	1510	SER	-	expression tag	UNP P49951
Q	1511	SER	-	expression tag	UNP P49951
Q	1512	GLY	-	expression tag	UNP P49951
Q	1513	LEU	-	expression tag	UNP P49951
Q	1514	VAL	-	expression tag	UNP P49951
Q	1515	PRO	-	expression tag	UNP P49951
Q	1516	ARG	-	expression tag	UNP P49951
Q	1517	GLY	-	expression tag	UNP P49951
Q	1518	SER	-	expression tag	UNP P49951
Q	1519	HIS	-	expression tag	UNP P49951
Q	1520	MET	-	expression tag	UNP P49951
Q	1528	ALA	CYS	engineered mutation	UNP P49951
Q	1585	LEU	THR	engineered mutation	UNP P49951
R	1500	MET	-	expression tag	UNP P49951
R	1501	GLY	-	expression tag	UNP P49951
R	1502	SER	-	expression tag	UNP P49951
R	1503	SER	-	expression tag	UNP P49951
R	1504	HIS	-	expression tag	UNP P49951
R	1505	HIS	-	expression tag	UNP P49951
R	1506	HIS	-	expression tag	UNP P49951
R	1507	HIS	-	expression tag	UNP P49951
R	1508	HIS	-	expression tag	UNP P49951
R	1509	HIS	-	expression tag	UNP P49951

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Chain	Residue	Modelled	Actual	Comment	Reference
R	1510	SER	-	expression tag	UNP P49951
R	1511	SER	-	expression tag	UNP P49951
R	1512	GLY	-	expression tag	UNP P49951
R	1513	LEU	-	expression tag	UNP P49951
R	1514	VAL	-	expression tag	UNP P49951
R	1515	PRO	-	expression tag	UNP P49951
R	1516	ARG	-	expression tag	UNP P49951
R	1517	GLY	-	expression tag	UNP P49951
R	1518	SER	-	expression tag	UNP P49951
R	1519	HIS	-	expression tag	UNP P49951
R	1520	MET	-	expression tag	UNP P49951
R	1528	ALA	CYS	engineered mutation	UNP P49951
R	1585	LEU	THR	engineered mutation	UNP P49951
S	1500	MET	-	expression tag	UNP P49951
S	1501	GLY	-	expression tag	UNP P49951
S	1502	SER	-	expression tag	UNP P49951
S	1503	SER	-	expression tag	UNP P49951
S	1504	HIS	-	expression tag	UNP P49951
S	1505	HIS	-	expression tag	UNP P49951
S	1506	HIS	-	expression tag	UNP P49951
S	1507	HIS	-	expression tag	UNP P49951
S	1508	HIS	-	expression tag	UNP P49951
S	1509	HIS	-	expression tag	UNP P49951
S	1510	SER	-	expression tag	UNP P49951
S	1511	SER	-	expression tag	UNP P49951
S	1512	GLY	-	expression tag	UNP P49951
S	1513	LEU	-	expression tag	UNP P49951
S	1514	VAL	-	expression tag	UNP P49951
S	1515	PRO	-	expression tag	UNP P49951
S	1516	ARG	-	expression tag	UNP P49951
S	1517	GLY	-	expression tag	UNP P49951
S	1518	SER	-	expression tag	UNP P49951
S	1519	HIS	-	expression tag	UNP P49951
S	1520	MET	-	expression tag	UNP P49951
S	1528	ALA	CYS	engineered mutation	UNP P49951
S	1585	LEU	THR	engineered mutation	UNP P49951
T	1500	MET	-	expression tag	UNP P49951
T	1501	GLY	-	expression tag	UNP P49951
T	1502	SER	-	expression tag	UNP P49951
T	1503	SER	-	expression tag	UNP P49951
T	1504	HIS	-	expression tag	UNP P49951
T	1505	HIS	-	expression tag	UNP P49951

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Chain	Residue	Modelled	Actual	Comment	Reference
T	1506	HIS	-	expression tag	UNP P49951
T	1507	HIS	-	expression tag	UNP P49951
T	1508	HIS	-	expression tag	UNP P49951
T	1509	HIS	-	expression tag	UNP P49951
T	1510	SER	-	expression tag	UNP P49951
T	1511	SER	-	expression tag	UNP P49951
T	1512	GLY	-	expression tag	UNP P49951
T	1513	LEU	-	expression tag	UNP P49951
T	1514	VAL	-	expression tag	UNP P49951
T	1515	PRO	-	expression tag	UNP P49951
T	1516	ARG	-	expression tag	UNP P49951
T	1517	GLY	-	expression tag	UNP P49951
T	1518	SER	-	expression tag	UNP P49951
T	1519	HIS	-	expression tag	UNP P49951
T	1520	MET	-	expression tag	UNP P49951
T	1528	ALA	CYS	engineered mutation	UNP P49951
T	1585	LEU	THR	engineered mutation	UNP P49951
U	1500	MET	-	expression tag	UNP P49951
U	1501	GLY	-	expression tag	UNP P49951
U	1502	SER	-	expression tag	UNP P49951
U	1503	SER	-	expression tag	UNP P49951
U	1504	HIS	-	expression tag	UNP P49951
U	1505	HIS	-	expression tag	UNP P49951
U	1506	HIS	-	expression tag	UNP P49951
U	1507	HIS	-	expression tag	UNP P49951
U	1508	HIS	-	expression tag	UNP P49951
U	1509	HIS	-	expression tag	UNP P49951
U	1510	SER	-	expression tag	UNP P49951
U	1511	SER	-	expression tag	UNP P49951
U	1512	GLY	-	expression tag	UNP P49951
U	1513	LEU	-	expression tag	UNP P49951
U	1514	VAL	-	expression tag	UNP P49951
U	1515	PRO	-	expression tag	UNP P49951
U	1516	ARG	-	expression tag	UNP P49951
U	1517	GLY	-	expression tag	UNP P49951
U	1518	SER	-	expression tag	UNP P49951
U	1519	HIS	-	expression tag	UNP P49951
U	1520	MET	-	expression tag	UNP P49951
U	1528	ALA	CYS	engineered mutation	UNP P49951
U	1585	LEU	THR	engineered mutation	UNP P49951
V	1500	MET	-	expression tag	UNP P49951
V	1501	GLY	-	expression tag	UNP P49951

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Chain	Residue	Modelled	Actual	Comment	Reference
V	1502	SER	-	expression tag	UNP P49951
V	1503	SER	-	expression tag	UNP P49951
V	1504	HIS	-	expression tag	UNP P49951
V	1505	HIS	-	expression tag	UNP P49951
V	1506	HIS	-	expression tag	UNP P49951
V	1507	HIS	-	expression tag	UNP P49951
V	1508	HIS	-	expression tag	UNP P49951
V	1509	HIS	-	expression tag	UNP P49951
V	1510	SER	-	expression tag	UNP P49951
V	1511	SER	-	expression tag	UNP P49951
V	1512	GLY	-	expression tag	UNP P49951
V	1513	LEU	-	expression tag	UNP P49951
V	1514	VAL	-	expression tag	UNP P49951
V	1515	PRO	-	expression tag	UNP P49951
V	1516	ARG	-	expression tag	UNP P49951
V	1517	GLY	-	expression tag	UNP P49951
V	1518	SER	-	expression tag	UNP P49951
V	1519	HIS	-	expression tag	UNP P49951
V	1520	MET	-	expression tag	UNP P49951
V	1528	ALA	CYS	engineered mutation	UNP P49951
V	1585	LEU	THR	engineered mutation	UNP P49951
W	1500	MET	-	expression tag	UNP P49951
W	1501	GLY	-	expression tag	UNP P49951
W	1502	SER	-	expression tag	UNP P49951
W	1503	SER	-	expression tag	UNP P49951
W	1504	HIS	-	expression tag	UNP P49951
W	1505	HIS	-	expression tag	UNP P49951
W	1506	HIS	-	expression tag	UNP P49951
W	1507	HIS	-	expression tag	UNP P49951
W	1508	HIS	-	expression tag	UNP P49951
W	1509	HIS	-	expression tag	UNP P49951
W	1510	SER	-	expression tag	UNP P49951
W	1511	SER	-	expression tag	UNP P49951
W	1512	GLY	-	expression tag	UNP P49951
W	1513	LEU	-	expression tag	UNP P49951
W	1514	VAL	-	expression tag	UNP P49951
W	1515	PRO	-	expression tag	UNP P49951
W	1516	ARG	-	expression tag	UNP P49951
W	1517	GLY	-	expression tag	UNP P49951
W	1518	SER	-	expression tag	UNP P49951
W	1519	HIS	-	expression tag	UNP P49951
W	1520	MET	-	expression tag	UNP P49951

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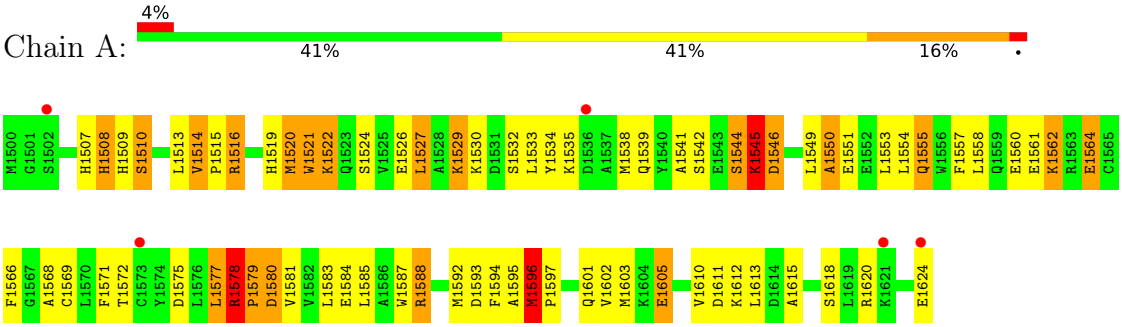
Chain	Residue	Modelled	Actual	Comment	Reference
W	1528	ALA	CYS	engineered mutation	UNP P49951
W	1585	LEU	THR	engineered mutation	UNP P49951
X	1500	MET	-	expression tag	UNP P49951
X	1501	GLY	-	expression tag	UNP P49951
X	1502	SER	-	expression tag	UNP P49951
X	1503	SER	-	expression tag	UNP P49951
X	1504	HIS	-	expression tag	UNP P49951
X	1505	HIS	-	expression tag	UNP P49951
X	1506	HIS	-	expression tag	UNP P49951
X	1507	HIS	-	expression tag	UNP P49951
X	1508	HIS	-	expression tag	UNP P49951
X	1509	HIS	-	expression tag	UNP P49951
X	1510	SER	-	expression tag	UNP P49951
X	1511	SER	-	expression tag	UNP P49951
X	1512	GLY	-	expression tag	UNP P49951
X	1513	LEU	-	expression tag	UNP P49951
X	1514	VAL	-	expression tag	UNP P49951
X	1515	PRO	-	expression tag	UNP P49951
X	1516	ARG	-	expression tag	UNP P49951
X	1517	GLY	-	expression tag	UNP P49951
X	1518	SER	-	expression tag	UNP P49951
X	1519	HIS	-	expression tag	UNP P49951
X	1520	MET	-	expression tag	UNP P49951
X	1528	ALA	CYS	engineered mutation	UNP P49951
X	1585	LEU	THR	engineered mutation	UNP P49951

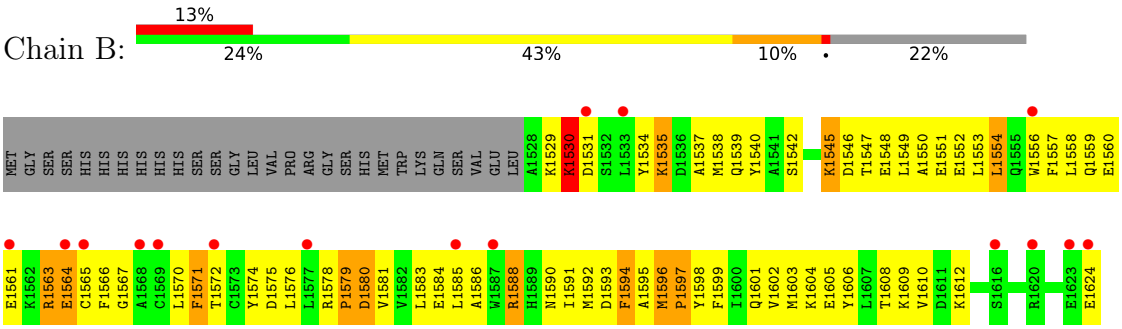
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

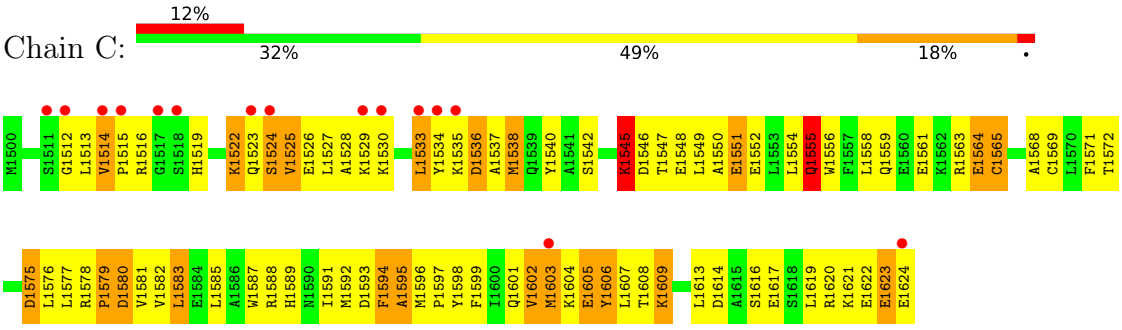
• Molecule 1: Clathrin heavy chain 1



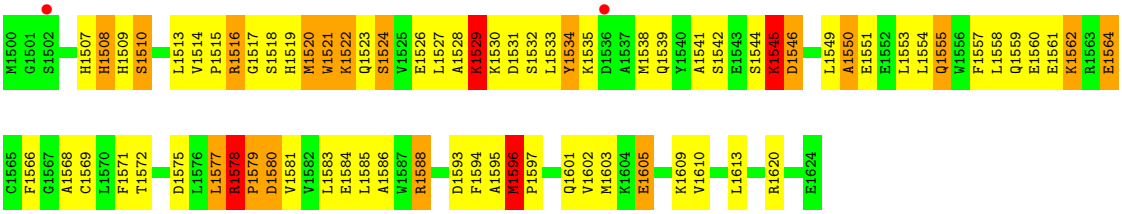
• Molecule 1: Clathrin heavy chain 1



• Molecule 1: Clathrin heavy chain 1

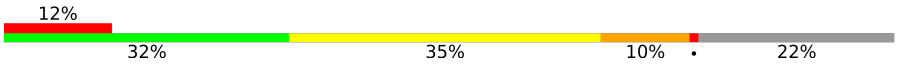


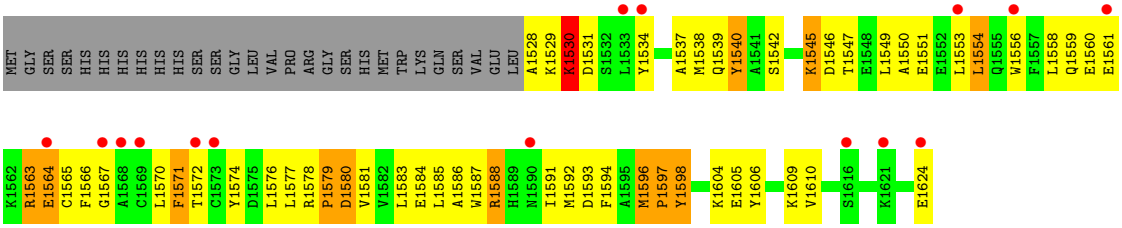
• Molecule 1: Clathrin heavy chain 1



• Molecule 1: Clathrin heavy chain 1

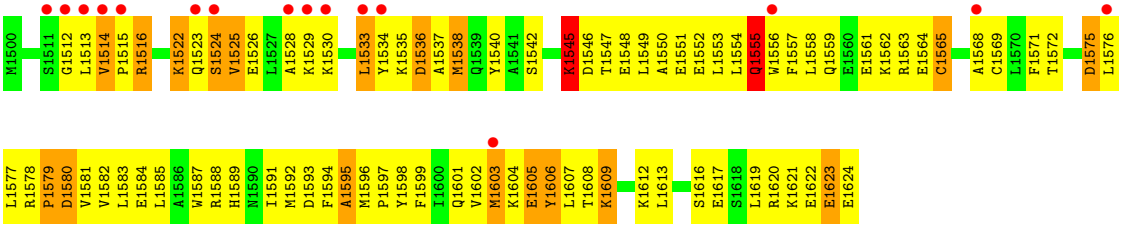
Chain E:





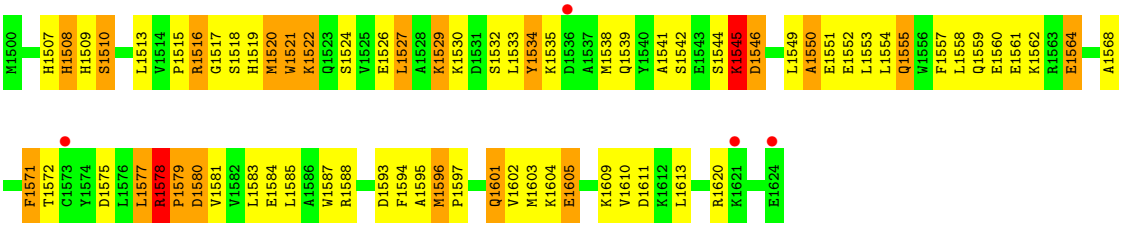
• Molecule 1: Clathrin heavy chain 1

Chain F:



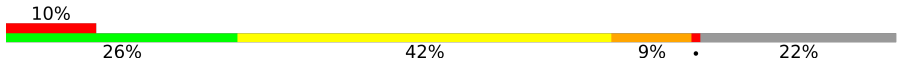
• Molecule 1: Clathrin heavy chain 1

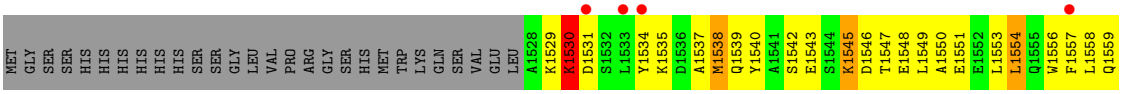
Chain G:

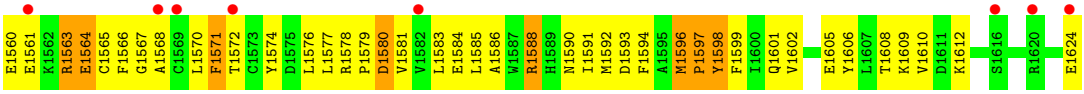


• Molecule 1: Clathrin heavy chain 1

Chain H:

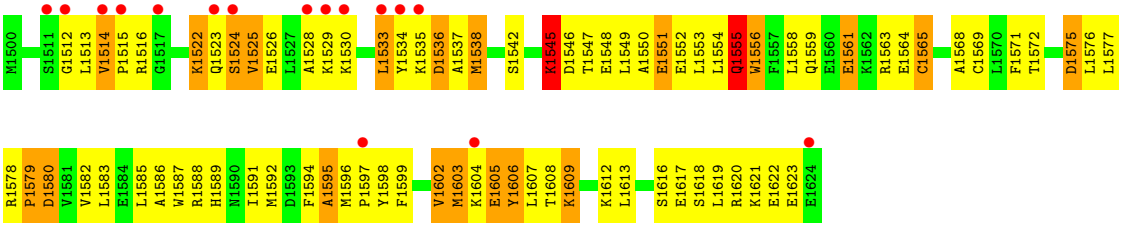






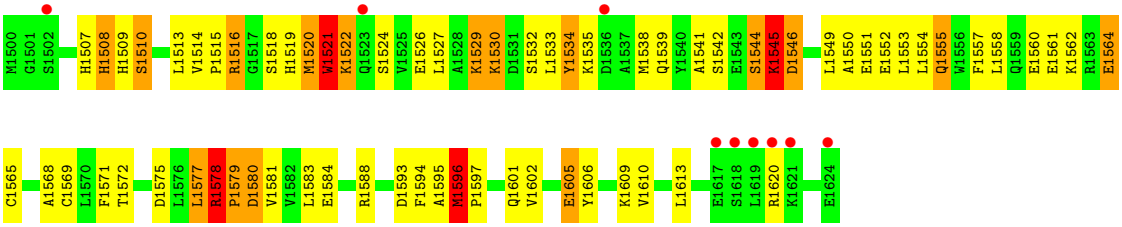
• Molecule 1: Clathrin heavy chain 1

Chain I:



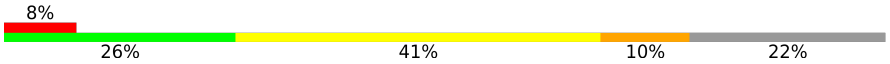
• Molecule 1: Clathrin heavy chain 1

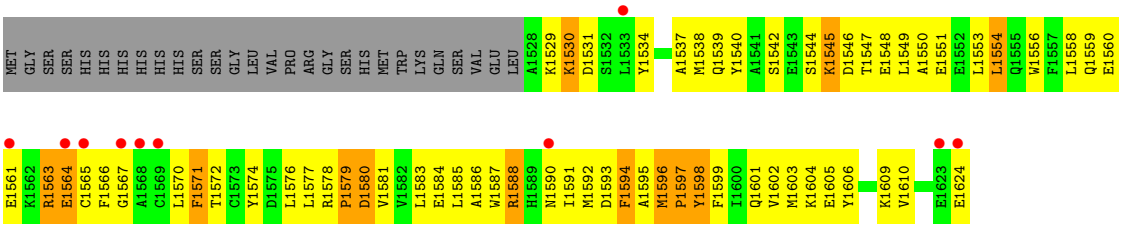
Chain J:



• Molecule 1: Clathrin heavy chain 1

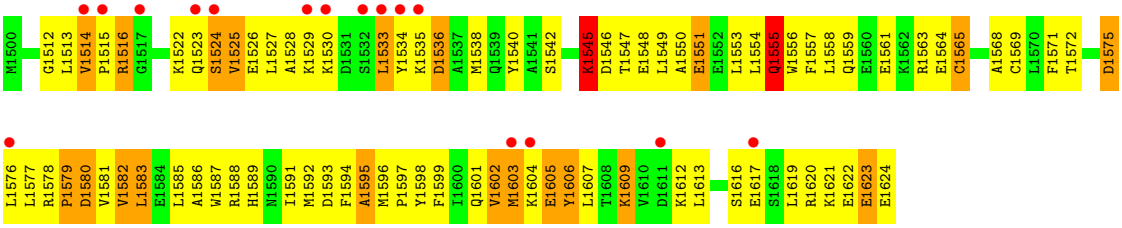
Chain K:





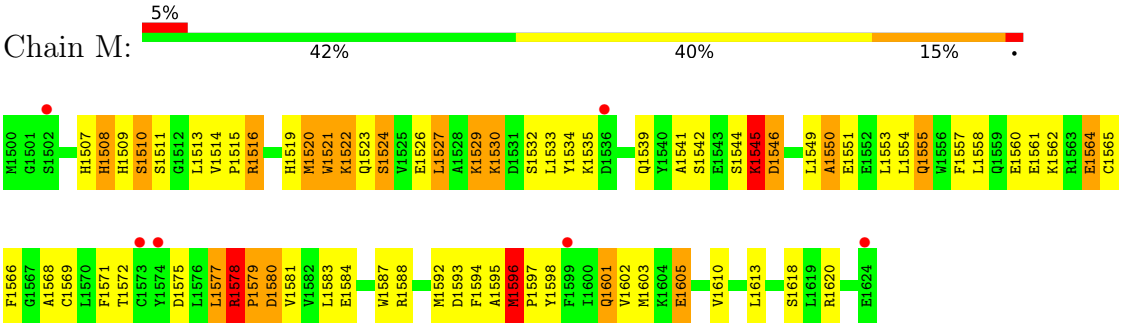
• Molecule 1: Clathrin heavy chain 1

Chain L:



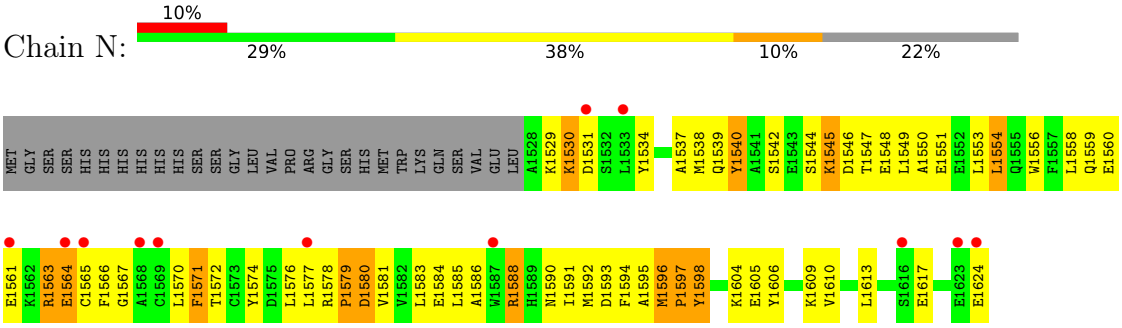
• Molecule 1: Clathrin heavy chain 1

Chain M:



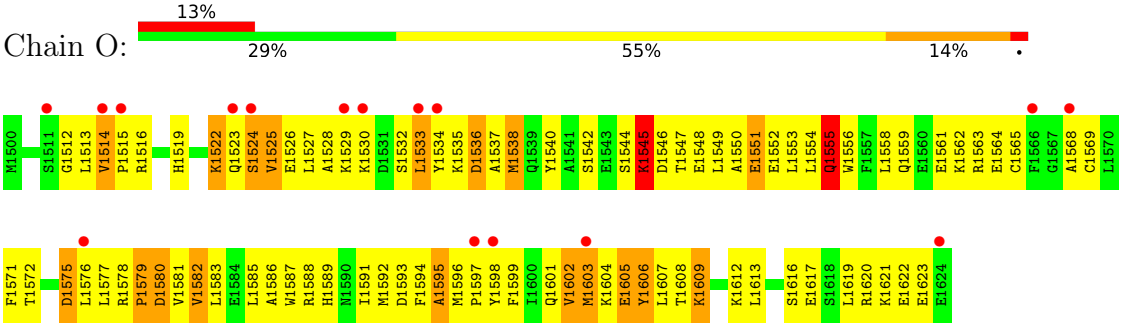
- Molecule 1: Clathrin heavy chain 1

Chain N:



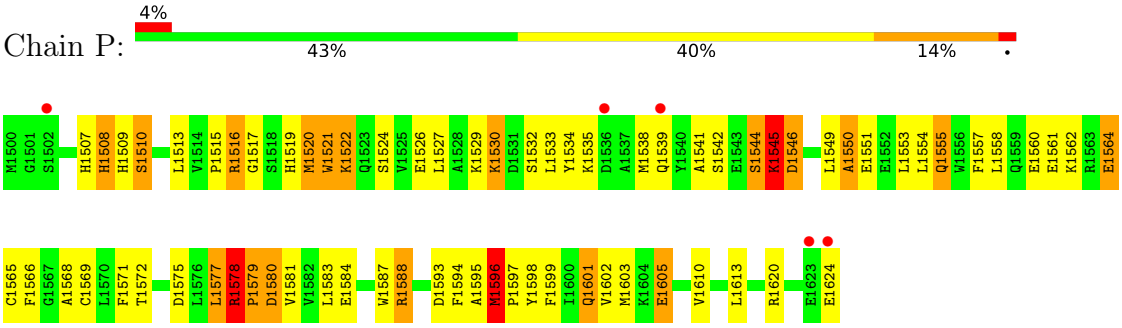
- Molecule 1: Clathrin heavy chain 1

Chain O:



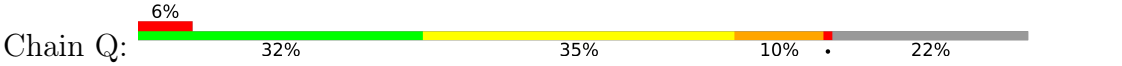
- Molecule 1: Clathrin heavy chain 1

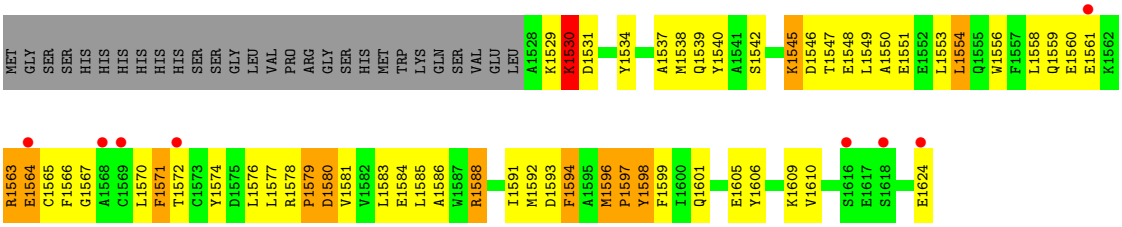
Chain P:



- Molecule 1: Clathrin heavy chain 1

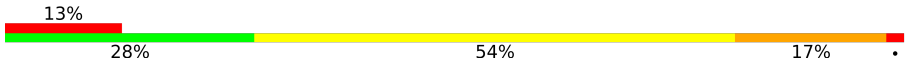
Chain Q:

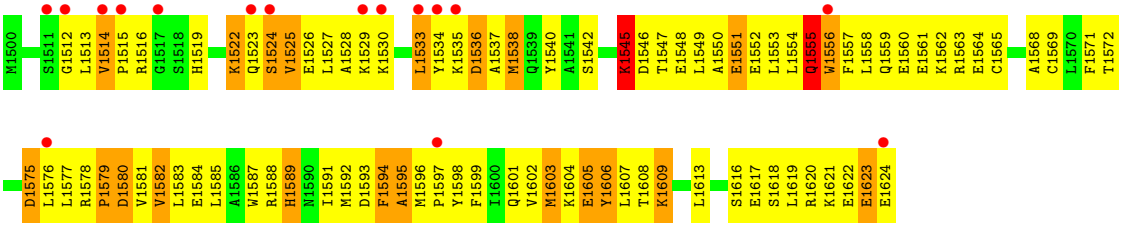




- Molecule 1: Clathrin heavy chain 1

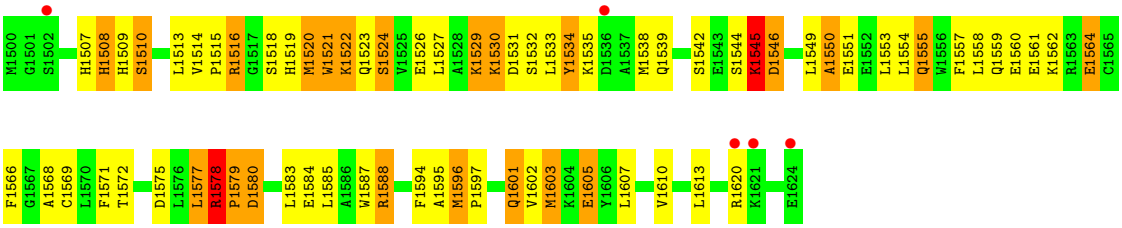
Chain R:





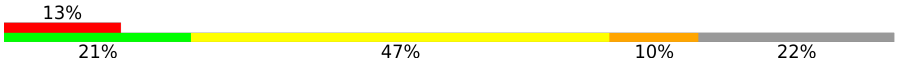
- Molecule 1: Clathrin heavy chain 1

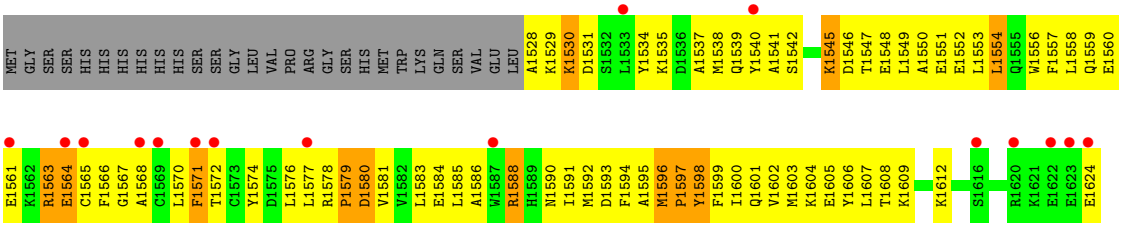
Chain S:



- Molecule 1: Clathrin heavy chain 1

Chain T:

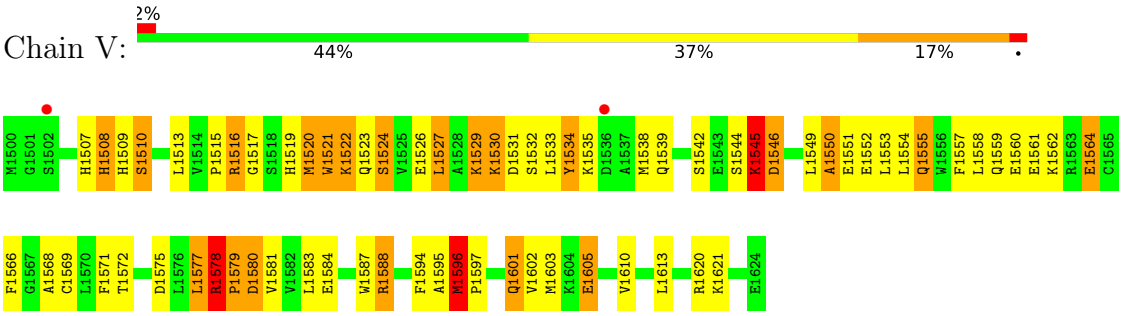




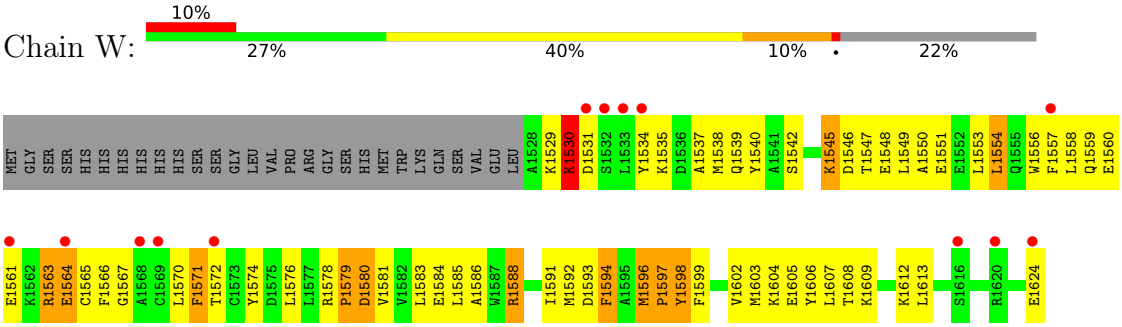
- Molecule 1: Clathrin heavy chain 1

Chain U:

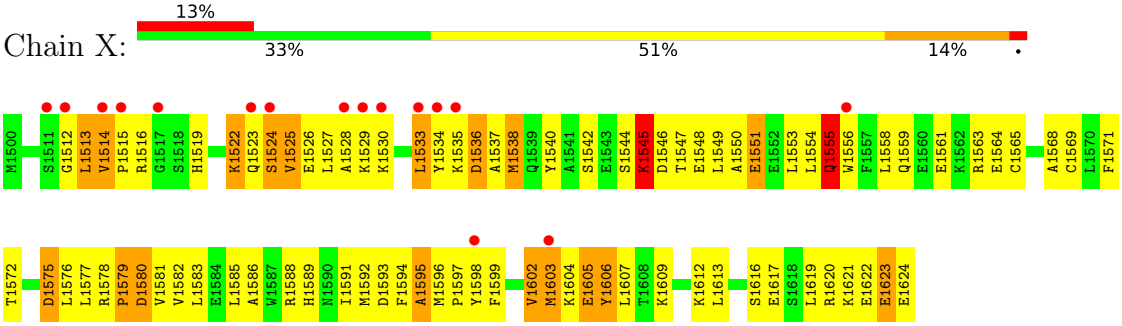
• Molecule 1: Clathrin heavy chain 1



• Molecule 1: Clathrin heavy chain 1



• Molecule 1: Clathrin heavy chain 1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	255.78Å 255.78Å 312.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	54.58 – 3.92 48.34 – 3.92	Depositor EDS
% Data completeness (in resolution range)	86.1 (54.58-3.92) 89.0 (48.34-3.92)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.68 (at 3.88Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.339 , 0.386 0.343 , 0.360	Depositor DCC
R_{free} test set	6653 reflections (9.74%)	wwPDB-VP
Wilson B-factor (Å^2)	134.3	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 500.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.458 for -2/3*h-1/3*k+2/3*l,-1/3*h-2/3*k-2/3*l,2/3*h-2/3*k+1/3*l 0.458 for -h,1/3*h-1/3*k+2/3*l,2/3*h+4/3*k+1/3*l 0.458 for -1/3*h+1/3*k-2/3*l,-k,-4/3*h-2/3*k+1/3*l 0.458 for -h,2/3*h+1/3*k-2/3*l,-2/3*h-4/3*k-1/3*l 0.458 for 1/3*h+2/3*k+2/3*l,-k,4/3*h+2/3*k-1/3*l 0.458 for -1/3*h-2/3*k-2/3*l,-2/3*h-1/3*k+2/3*l,-2/3*h+2/3*k-1/3*l 0.458 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	23032	wwPDB-VP
Average B, all atoms (Å^2)	277.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	A	0.85	2/1060 (0.2%)	0.89	1/1424 (0.1%)
1	B	0.70	0/827	0.73	0/1110
1	C	0.74	3/1060 (0.3%)	0.75	0/1424
1	D	0.81	1/1060 (0.1%)	0.90	2/1424 (0.1%)
1	E	0.82	1/827 (0.1%)	0.79	0/1110
1	F	0.71	1/1060 (0.1%)	0.76	0/1424
1	G	0.80	0/1060	0.87	2/1424 (0.1%)
1	H	0.77	0/827	0.81	0/1110
1	I	0.81	3/1060 (0.3%)	0.78	0/1424
1	J	0.82	2/1060 (0.2%)	0.88	0/1424
1	K	0.75	1/827 (0.1%)	0.74	0/1110
1	L	0.76	0/1060	0.82	1/1424 (0.1%)
1	M	0.81	0/1060	0.89	2/1424 (0.1%)
1	N	0.74	0/827	0.74	0/1110
1	O	0.73	0/1060	0.79	0/1424
1	P	0.84	2/1060 (0.2%)	0.89	2/1424 (0.1%)
1	Q	0.76	0/827	0.76	0/1110
1	R	0.74	0/1060	0.75	0/1424
1	S	0.82	0/1060	0.85	0/1424
1	T	0.74	1/827 (0.1%)	0.74	0/1110
1	U	0.74	1/1060 (0.1%)	0.76	0/1424
1	V	0.83	0/1060	0.89	1/1424 (0.1%)
1	W	0.72	0/827	0.73	0/1110
1	X	0.77	1/1060 (0.1%)	0.76	0/1424
All	All	0.78	19/23576 (0.1%)	0.81	11/31664 (0.0%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	1544	SER	CA-CB	6.89	1.63	1.52
1	I	1586	ALA	CA-CB	-6.60	1.38	1.52
1	A	1514	VAL	CA-CB	-6.34	1.41	1.54
1	K	1537	ALA	CA-CB	6.26	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	1544	SER	CA-CB	6.06	1.62	1.52
1	F	1565	CYS	CB-SG	-6.01	1.72	1.82
1	C	1565	CYS	CB-SG	-5.98	1.72	1.81
1	E	1528	ALA	CA-CB	5.81	1.64	1.52
1	C	1564	GLU	CB-CG	5.68	1.62	1.52
1	A	1544	SER	CA-CB	5.65	1.61	1.52
1	J	1514	VAL	CA-CB	-5.60	1.43	1.54
1	U	1586	ALA	CA-CB	-5.59	1.40	1.52
1	I	1565	CYS	CB-SG	-5.48	1.72	1.81
1	P	1544	SER	CB-OG	5.35	1.49	1.42
1	C	1564	GLU	CG-CD	5.32	1.59	1.51
1	T	1541	ALA	CA-CB	-5.21	1.41	1.52
1	X	1586	ALA	CA-CB	-5.19	1.41	1.52
1	I	1561	GLU	CB-CG	5.19	1.62	1.52
1	D	1529	LYS	CA-C	5.14	1.66	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	1565	CYS	CA-CB-SG	7.19	126.94	114.00
1	M	1527	LEU	CB-CG-CD2	-5.96	100.87	111.00
1	G	1527	LEU	CB-CG-CD2	-5.73	101.26	111.00
1	P	1544	SER	CA-CB-OG	5.71	126.62	111.20
1	P	1517	GLY	N-CA-C	5.41	126.63	113.10
1	V	1517	GLY	N-CA-C	5.33	126.44	113.10
1	D	1528	ALA	C-N-CA	5.28	134.90	121.70
1	G	1517	GLY	N-CA-C	5.25	126.24	113.10
1	A	1527	LEU	CA-CB-CG	5.10	127.03	115.30
1	M	1592	MET	N-CA-C	-5.04	97.39	111.00
1	D	1517	GLY	N-CA-C	5.00	125.61	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1034	0	991	87	0
1	B	811	0	788	85	0
1	C	1034	0	991	112	0
1	D	1034	0	991	97	1
1	E	811	0	788	98	0
1	F	1034	0	991	143	0
1	G	1034	0	991	93	0
1	H	811	0	788	97	0
1	I	1034	0	991	105	0
1	J	1034	0	991	81	0
1	K	811	0	788	102	0
1	L	1034	0	991	153	0
1	M	1034	0	991	85	0
1	N	811	0	788	96	0
1	O	1034	0	991	130	0
1	P	1034	0	991	87	0
1	Q	811	0	788	78	0
1	R	1034	0	991	124	0
1	S	1034	0	991	99	0
1	T	811	0	788	128	0
1	U	1034	0	991	143	1
1	V	1034	0	991	97	0
1	W	811	0	788	106	0
1	X	1034	0	991	114	0
All	All	23032	0	22160	2357	1

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 52.

All (2357) 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:T:1604:LYS:HD3	1:U:1612:LYS:NZ	1.44	1.31
1:L:1533:LEU:HD12	1:V:1588:ARG:NH2	1.58	1.18
1:E:1546:ASP:H	1:E:1550:ALA:HB2	1.07	1.16
1:V:1572:THR:HA	1:V:1578:ARG:NH2	1.60	1.16
1:M:1593:ASP:HA	1:O:1587:TRP:CZ3	1.82	1.14
1:P:1593:ASP:HA	1:R:1587:TRP:HZ3	1.04	1.12
1:L:1533:LEU:HD12	1:V:1588:ARG:HH22	1.04	1.11
1:W:1546:ASP:H	1:W:1550:ALA:HB2	1.06	1.11
1:K:1546:ASP:H	1:K:1550:ALA:HB2	1.01	1.11
1:D:1572:THR:HA	1:D:1578:ARG:NH2	1.65	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1593:ASP:HA	1:O:1587:TRP:HZ3	1.06	1.09
1:S:1572:THR:HA	1:S:1578:ARG:NH2	1.66	1.09
1:T:1604:LYS:HG3	1:U:1609:LYS:CE	1.82	1.09
1:G:1572:THR:HA	1:G:1578:ARG:NH2	1.66	1.08
1:H:1546:ASP:H	1:H:1550:ALA:HB2	1.16	1.07
1:J:1572:THR:HA	1:J:1578:ARG:NH2	1.67	1.07
1:D:1572:THR:HA	1:D:1578:ARG:HH22	1.19	1.07
1:E:1579:PRO:HG3	1:F:1599:PHE:HB3	1.35	1.07
1:N:1546:ASP:H	1:N:1550:ALA:HB2	1.18	1.06
1:T:1546:ASP:H	1:T:1550:ALA:HB2	1.17	1.06
1:P:1572:THR:HA	1:P:1578:ARG:NH2	1.74	1.02
1:G:1572:THR:HA	1:G:1578:ARG:HH22	1.15	1.01
1:T:1604:LYS:HG3	1:U:1609:LYS:HE3	1.38	1.01
1:T:1604:LYS:HE3	1:U:1609:LYS:HD3	1.41	1.00
1:T:1604:LYS:HD3	1:U:1612:LYS:HZ3	0.90	1.00
1:P:1593:ASP:HA	1:R:1587:TRP:CZ3	1.96	0.98
1:G:1554:LEU:HD22	1:G:1568:ALA:HB1	1.44	0.98
1:A:1572:THR:HA	1:A:1578:ARG:NH2	1.78	0.98
1:Q:1546:ASP:H	1:Q:1550:ALA:HB2	1.26	0.97
1:B:1546:ASP:H	1:B:1550:ALA:HB2	1.29	0.97
1:B:1578:ARG:HH22	1:B:1580:ASP:HB2	1.27	0.96
1:G:1604:LYS:HD3	1:H:1605:GLU:CD	1.84	0.96
1:D:1578:ARG:HH11	1:D:1578:ARG:HB2	1.28	0.96
1:V:1572:THR:HA	1:V:1578:ARG:HH22	1.19	0.96
1:V:1578:ARG:HB2	1:V:1578:ARG:HH11	1.29	0.96
1:K:1578:ARG:HH22	1:K:1580:ASP:HB2	1.30	0.96
1:O:1532:SER:HB2	1:S:1588:ARG:NE	1.81	0.95
1:N:1579:PRO:HG3	1:O:1599:PHE:HB3	1.51	0.93
1:T:1584:GLU:O	1:T:1588:ARG:NH1	2.02	0.93
1:J:1610:VAL:HA	1:J:1613:LEU:HD12	1.49	0.93
1:M:1610:VAL:HA	1:M:1613:LEU:HD12	1.50	0.93
1:N:1578:ARG:HH22	1:N:1580:ASP:HB2	1.32	0.92
1:G:1604:LYS:HD3	1:H:1605:GLU:OE1	1.70	0.92
1:W:1546:ASP:H	1:W:1550:ALA:CB	1.82	0.92
1:I:1525:VAL:HG12	1:I:1526:GLU:H	1.35	0.92
1:B:1591:ILE:C	1:B:1592:MET:SD	2.49	0.91
1:K:1546:ASP:N	1:K:1550:ALA:HB2	1.86	0.91
1:M:1572:THR:HA	1:M:1578:ARG:NH2	1.84	0.91
1:S:1572:THR:HA	1:S:1578:ARG:HH22	1.28	0.91
1:S:1610:VAL:HA	1:S:1613:LEU:HD12	1.53	0.91
1:L:1533:LEU:HG	1:V:1588:ARG:NH1	1.86	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:1606:TYR:HA	1:W:1609:LYS:HE2	1.53	0.90
1:E:1578:ARG:HH22	1:E:1580:ASP:HB2	1.37	0.90
1:V:1578:ARG:HB2	1:V:1578:ARG:NH1	1.86	0.90
1:P:1554:LEU:HD22	1:P:1568:ALA:HB1	1.54	0.90
1:D:1554:LEU:HD22	1:D:1568:ALA:HB1	1.51	0.89
1:L:1558:LEU:HD13	1:L:1565:CYS:HB3	1.54	0.89
1:M:1578:ARG:NH1	1:M:1578:ARG:HB2	1.88	0.89
1:P:1572:THR:HA	1:P:1578:ARG:HH22	1.36	0.89
1:C:1525:VAL:HG12	1:C:1526:GLU:H	1.37	0.89
1:L:1533:LEU:HD22	1:L:1534:TYR:H	1.36	0.89
1:E:1546:ASP:H	1:E:1550:ALA:CB	1.86	0.89
1:Q:1578:ARG:HH22	1:Q:1580:ASP:HB2	1.38	0.89
1:D:1578:ARG:HB2	1:D:1578:ARG:NH1	1.87	0.89
1:M:1578:ARG:HB2	1:M:1578:ARG:HH11	1.37	0.89
1:U:1525:VAL:HG12	1:U:1526:GLU:H	1.37	0.89
1:A:1572:THR:HA	1:A:1578:ARG:HH22	1.36	0.88
1:E:1577:LEU:HD13	1:F:1603:MET:HA	1.55	0.88
1:G:1578:ARG:HH11	1:G:1578:ARG:HB2	1.39	0.88
1:J:1578:ARG:HH11	1:J:1578:ARG:HB2	1.36	0.88
1:J:1572:THR:HA	1:J:1578:ARG:HH22	1.33	0.88
1:J:1578:ARG:HB2	1:J:1578:ARG:NH1	1.88	0.88
1:O:1591:ILE:HG22	1:O:1592:MET:H	1.38	0.87
1:F:1525:VAL:HG12	1:F:1526:GLU:H	1.38	0.87
1:G:1610:VAL:HA	1:G:1613:LEU:HD12	1.57	0.87
1:V:1572:THR:CA	1:V:1578:ARG:HH22	1.87	0.87
1:D:1610:VAL:HA	1:D:1613:LEU:HD12	1.56	0.86
1:P:1610:VAL:HA	1:P:1613:LEU:HD12	1.57	0.86
1:T:1604:LYS:CD	1:U:1612:LYS:HZ3	1.84	0.86
1:E:1556:TRP:O	1:E:1559:GLN:HG3	1.75	0.86
1:L:1595:ALA:O	1:L:1596:MET:SD	2.32	0.86
1:W:1604:LYS:HG3	1:X:1609:LYS:HE3	1.55	0.86
1:W:1546:ASP:N	1:W:1550:ALA:HB2	1.90	0.86
1:N:1556:TRP:O	1:N:1559:GLN:HG3	1.73	0.86
1:S:1554:LEU:HD22	1:S:1568:ALA:HB1	1.56	0.86
1:E:1581:VAL:O	1:E:1585:LEU:HD23	1.75	0.86
1:X:1545:LYS:HB3	1:X:1571:PHE:CZ	2.10	0.86
1:F:1545:LYS:HB3	1:F:1571:PHE:CZ	2.11	0.85
1:H:1547:THR:O	1:H:1551:GLU:HG3	1.76	0.85
1:T:1578:ARG:HH22	1:T:1580:ASP:HB2	1.40	0.85
1:I:1591:ILE:HG22	1:I:1592:MET:H	1.40	0.85
1:K:1579:PRO:HG3	1:L:1599:PHE:HB3	1.56	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1533:LEU:HD22	1:U:1534:TYR:H	1.41	0.85
1:C:1591:ILE:HG22	1:C:1592:MET:H	1.42	0.85
1:L:1516:ARG:HD2	1:W:1563:ARG:NH2	1.91	0.85
1:X:1525:VAL:HG12	1:X:1526:GLU:H	1.41	0.85
1:T:1604:LYS:CE	1:U:1609:LYS:HD3	2.06	0.84
1:U:1545:LYS:HB3	1:U:1571:PHE:CZ	2.12	0.84
1:I:1545:LYS:HB3	1:I:1571:PHE:CZ	2.13	0.84
1:L:1591:ILE:HG22	1:L:1592:MET:H	1.40	0.84
1:H:1578:ARG:HH22	1:H:1580:ASP:HB2	1.40	0.84
1:E:1579:PRO:CG	1:F:1599:PHE:HB3	2.08	0.84
1:R:1525:VAL:HG12	1:R:1526:GLU:H	1.40	0.84
1:T:1605:GLU:O	1:T:1609:LYS:HG3	1.78	0.84
1:L:1545:LYS:HB3	1:L:1571:PHE:CZ	2.13	0.84
1:W:1604:LYS:CE	1:X:1609:LYS:HD2	2.07	0.84
1:W:1578:ARG:HH22	1:W:1580:ASP:HB2	1.42	0.83
1:I:1616:SER:O	1:I:1620:ARG:HG2	1.76	0.83
1:X:1591:ILE:HG22	1:X:1592:MET:H	1.42	0.83
1:L:1533:LEU:CD1	1:V:1588:ARG:NH2	2.41	0.83
1:M:1572:THR:HA	1:M:1578:ARG:HH22	1.40	0.83
1:G:1572:THR:CA	1:G:1578:ARG:HH22	1.90	0.83
1:J:1554:LEU:HD22	1:J:1568:ALA:HB1	1.59	0.83
1:X:1545:LYS:HB3	1:X:1571:PHE:HZ	1.42	0.83
1:F:1516:ARG:HD2	1:H:1563:ARG:HH22	1.42	0.83
1:N:1577:LEU:HD13	1:O:1603:MET:HA	1.60	0.83
1:E:1584:GLU:O	1:E:1588:ARG:NH1	2.12	0.83
1:A:1610:VAL:HA	1:A:1613:LEU:HD12	1.61	0.83
1:U:1545:LYS:HB3	1:U:1571:PHE:HZ	1.43	0.83
1:F:1591:ILE:HG22	1:F:1592:MET:H	1.43	0.83
1:O:1545:LYS:HB3	1:O:1571:PHE:CZ	2.14	0.83
1:G:1554:LEU:O	1:G:1558:LEU:HD13	1.79	0.82
1:P:1578:ARG:HB2	1:P:1578:ARG:HH11	1.44	0.82
1:A:1509:HIS:O	1:A:1510:SER:HB3	1.77	0.82
1:S:1572:THR:CA	1:S:1578:ARG:HH22	1.93	0.82
1:L:1533:LEU:HG	1:V:1588:ARG:CZ	2.09	0.82
1:O:1619:LEU:HA	1:O:1622:GLU:OE2	1.79	0.82
1:Q:1566:PHE:O	1:Q:1570:LEU:HD12	1.77	0.82
1:T:1563:ARG:HD3	1:T:1563:ARG:H	1.45	0.82
1:W:1606:TYR:HA	1:W:1609:LYS:CE	2.10	0.82
1:K:1604:LYS:NZ	1:L:1613:LEU:HG	1.95	0.82
1:W:1605:GLU:O	1:W:1609:LYS:HG3	1.78	0.82
1:K:1556:TRP:O	1:K:1559:GLN:HG3	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:1604:LYS:CD	1:U:1612:LYS:NZ	2.38	0.82
1:W:1556:TRP:O	1:W:1559:GLN:HG3	1.80	0.82
1:G:1601:GLN:O	1:G:1605:GLU:HG3	1.79	0.82
1:O:1525:VAL:HG12	1:O:1526:GLU:H	1.43	0.81
1:H:1546:ASP:H	1:H:1550:ALA:CB	1.93	0.81
1:H:1556:TRP:O	1:H:1559:GLN:HG3	1.80	0.81
1:I:1533:LEU:HD22	1:I:1534:TYR:H	1.45	0.81
1:A:1578:ARG:HH11	1:A:1578:ARG:HB2	1.45	0.81
1:O:1514:VAL:HB	1:O:1515:PRO:HD3	1.63	0.81
1:B:1563:ARG:HA	1:B:1566:PHE:CD1	2.16	0.81
1:H:1584:GLU:O	1:H:1588:ARG:NH1	2.14	0.81
1:I:1558:LEU:HD13	1:I:1565:CYS:HB3	1.63	0.81
1:F:1533:LEU:HD22	1:F:1534:TYR:H	1.46	0.81
1:Q:1556:TRP:O	1:Q:1559:GLN:HG3	1.81	0.81
1:A:1578:ARG:HB2	1:A:1578:ARG:NH1	1.96	0.81
1:F:1516:ARG:HD2	1:H:1563:ARG:NH2	1.96	0.80
1:X:1533:LEU:HD22	1:X:1534:TYR:H	1.47	0.80
1:G:1578:ARG:HB2	1:G:1578:ARG:NH1	1.97	0.80
1:T:1604:LYS:HD3	1:U:1612:LYS:CE	2.11	0.80
1:I:1545:LYS:HB3	1:I:1571:PHE:HZ	1.45	0.80
1:R:1533:LEU:HD22	1:R:1534:TYR:H	1.46	0.80
1:A:1593:ASP:HA	1:C:1587:TRP:HZ3	1.45	0.80
1:K:1604:LYS:HG3	1:L:1609:LYS:HD2	1.62	0.80
1:L:1525:VAL:HG12	1:L:1526:GLU:H	1.46	0.80
1:F:1595:ALA:O	1:F:1596:MET:SD	2.39	0.80
1:T:1547:THR:O	1:T:1551:GLU:HG3	1.82	0.80
1:B:1578:ARG:NH2	1:B:1580:ASP:HB2	1.97	0.80
1:H:1563:ARG:H	1:H:1563:ARG:HD3	1.46	0.80
1:R:1545:LYS:HB3	1:R:1571:PHE:CZ	2.16	0.80
1:C:1533:LEU:HD22	1:C:1534:TYR:H	1.47	0.80
1:O:1545:LYS:HB3	1:O:1571:PHE:HZ	1.45	0.80
1:T:1604:LYS:HE3	1:U:1609:LYS:CD	2.11	0.80
1:M:1554:LEU:HD22	1:M:1568:ALA:HB1	1.64	0.79
1:C:1595:ALA:O	1:C:1596:MET:SD	2.40	0.79
1:V:1610:VAL:HA	1:V:1613:LEU:HD12	1.64	0.79
1:K:1546:ASP:HB2	1:K:1549:LEU:HB2	1.63	0.79
1:U:1514:VAL:HB	1:U:1515:PRO:HD3	1.64	0.79
1:R:1595:ALA:O	1:R:1596:MET:SD	2.41	0.79
1:O:1558:LEU:HD13	1:O:1565:CYS:HB3	1.62	0.79
1:I:1514:VAL:HB	1:I:1515:PRO:HD3	1.63	0.78
1:E:1566:PHE:O	1:E:1570:LEU:HD12	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:1556:TRP:O	1:T:1559:GLN:HG3	1.82	0.78
1:D:1572:THR:CA	1:D:1578:ARG:HH22	1.94	0.78
1:K:1578:ARG:NH2	1:K:1580:ASP:HB2	1.96	0.78
1:N:1566:PHE:O	1:N:1570:LEU:HD12	1.82	0.78
1:L:1516:ARG:HD2	1:W:1563:ARG:HH22	1.46	0.78
1:U:1591:ILE:HG22	1:U:1592:MET:H	1.47	0.78
1:E:1546:ASP:HB2	1:E:1549:LEU:HB2	1.64	0.78
1:R:1616:SER:O	1:R:1620:ARG:HG2	1.84	0.78
1:B:1605:GLU:O	1:B:1609:LYS:HG3	1.83	0.78
1:X:1585:LEU:HA	1:X:1588:ARG:HG2	1.65	0.78
1:K:1591:ILE:C	1:K:1592:MET:SD	2.62	0.77
1:U:1595:ALA:O	1:U:1596:MET:SD	2.42	0.77
1:E:1546:ASP:N	1:E:1550:ALA:HB2	1.93	0.77
1:M:1509:HIS:O	1:M:1510:SER:HB3	1.84	0.77
1:A:1601:GLN:O	1:A:1605:GLU:HG3	1.85	0.77
1:F:1514:VAL:HB	1:F:1515:PRO:HD3	1.66	0.77
1:X:1514:VAL:HB	1:X:1515:PRO:HD3	1.66	0.77
1:B:1566:PHE:O	1:B:1570:LEU:HD12	1.84	0.77
1:P:1578:ARG:HB2	1:P:1578:ARG:NH1	1.99	0.77
1:R:1545:LYS:HB3	1:R:1571:PHE:HZ	1.49	0.77
1:O:1533:LEU:HD22	1:O:1534:TYR:H	1.48	0.77
1:F:1545:LYS:HB3	1:F:1571:PHE:HZ	1.46	0.77
1:U:1561:GLU:HB3	1:U:1564:GLU:HB2	1.67	0.77
1:Q:1581:VAL:O	1:Q:1585:LEU:HD23	1.85	0.76
1:R:1514:VAL:HB	1:R:1515:PRO:HD3	1.67	0.76
1:S:1578:ARG:NH1	1:S:1578:ARG:HB2	2.00	0.76
1:I:1602:VAL:O	1:I:1602:VAL:HG12	1.85	0.76
1:N:1554:LEU:HD21	1:N:1571:PHE:HB3	1.67	0.76
1:W:1591:ILE:C	1:W:1592:MET:SD	2.63	0.76
1:D:1601:GLN:O	1:D:1605:GLU:HG3	1.85	0.76
1:X:1558:LEU:HD13	1:X:1565:CYS:SG	2.26	0.76
1:X:1558:LEU:HA	1:X:1565:CYS:SG	2.26	0.76
1:J:1509:HIS:O	1:J:1510:SER:HB3	1.84	0.76
1:L:1545:LYS:HB3	1:L:1571:PHE:HZ	1.47	0.76
1:U:1585:LEU:HA	1:U:1588:ARG:HG2	1.66	0.76
1:X:1595:ALA:O	1:X:1596:MET:SD	2.44	0.76
1:B:1550:ALA:HB1	1:B:1571:PHE:CE2	2.21	0.76
1:P:1602:VAL:HA	1:P:1605:GLU:CD	2.06	0.76
1:T:1566:PHE:O	1:T:1570:LEU:HD12	1.85	0.76
1:W:1547:THR:O	1:W:1551:GLU:HG3	1.86	0.76
1:C:1619:LEU:HA	1:C:1622:GLU:OE2	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:1554:LEU:O	1:V:1558:LEU:HD13	1.86	0.76
1:I:1547:THR:HG22	1:I:1548:GLU:H	1.50	0.76
1:E:1578:ARG:NH2	1:E:1580:ASP:HB2	2.01	0.76
1:N:1578:ARG:NH2	1:N:1580:ASP:HB2	2.00	0.76
1:B:1547:THR:O	1:B:1551:GLU:HG3	1.86	0.75
1:L:1533:LEU:CD1	1:V:1588:ARG:HH22	1.92	0.75
1:P:1521:TRP:O	1:P:1522:LYS:HB2	1.85	0.75
1:T:1554:LEU:O	1:T:1558:LEU:HD13	1.86	0.75
1:I:1591:ILE:HG22	1:I:1592:MET:N	2.02	0.75
1:L:1514:VAL:HB	1:L:1515:PRO:HD3	1.67	0.75
1:N:1577:LEU:HD11	1:O:1606:TYR:HB3	1.68	0.75
1:U:1572:THR:O	1:U:1575:ASP:HB3	1.87	0.75
1:E:1579:PRO:HB2	1:F:1599:PHE:HD1	1.51	0.75
1:R:1591:ILE:HG22	1:R:1592:MET:H	1.50	0.75
1:S:1580:ASP:O	1:S:1584:GLU:OE2	2.05	0.75
1:C:1514:VAL:HB	1:C:1515:PRO:HD3	1.66	0.75
1:C:1616:SER:O	1:C:1620:ARG:HG2	1.86	0.75
1:C:1545:LYS:HB3	1:C:1571:PHE:CZ	2.22	0.75
1:R:1585:LEU:HA	1:R:1588:ARG:HG2	1.69	0.75
1:B:1556:TRP:O	1:B:1559:GLN:HG3	1.85	0.75
1:E:1554:LEU:HD21	1:E:1571:PHE:HB3	1.69	0.75
1:L:1558:LEU:HD13	1:L:1565:CYS:CB	2.16	0.74
1:S:1578:ARG:HB2	1:S:1578:ARG:HH11	1.51	0.74
1:H:1550:ALA:HB1	1:H:1571:PHE:CE2	2.22	0.74
1:Q:1578:ARG:NH2	1:Q:1580:ASP:HB2	2.02	0.74
1:Q:1550:ALA:HB1	1:Q:1571:PHE:CE2	2.22	0.74
1:Q:1591:ILE:C	1:Q:1592:MET:SD	2.66	0.74
1:E:1592:MET:HE2	1:E:1592:MET:N	2.02	0.74
1:F:1561:GLU:HB3	1:F:1564:GLU:HB2	1.69	0.74
1:A:1509:HIS:O	1:A:1510:SER:CB	2.36	0.74
1:C:1547:THR:HG22	1:C:1548:GLU:H	1.52	0.74
1:K:1546:ASP:H	1:K:1550:ALA:CB	1.93	0.74
1:T:1604:LYS:NZ	1:U:1613:LEU:HG	2.03	0.74
1:W:1554:LEU:HD21	1:W:1571:PHE:HB3	1.68	0.74
1:K:1554:LEU:HD21	1:K:1571:PHE:HB3	1.68	0.74
1:S:1587:TRP:HZ2	1:T:1592:MET:H	1.34	0.73
1:G:1546:ASP:HB2	1:G:1550:ALA:HB2	1.69	0.73
1:I:1585:LEU:HA	1:I:1588:ARG:HG2	1.70	0.73
1:O:1591:ILE:HG22	1:O:1592:MET:N	2.03	0.73
1:S:1601:GLN:O	1:S:1605:GLU:HG3	1.89	0.73
1:M:1602:VAL:HA	1:M:1605:GLU:CD	2.08	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:1563:ARG:HA	1:K:1566:PHE:CD1	2.23	0.73
1:Q:1554:LEU:HD21	1:Q:1571:PHE:HB3	1.70	0.73
1:Q:1563:ARG:HA	1:Q:1566:PHE:CD1	2.23	0.73
1:T:1604:LYS:NZ	1:U:1612:LYS:HE2	2.03	0.73
1:A:1593:ASP:HA	1:C:1587:TRP:CZ3	2.23	0.73
1:B:1591:ILE:O	1:B:1592:MET:SD	2.45	0.73
1:C:1545:LYS:HB3	1:C:1571:PHE:HZ	1.52	0.73
1:E:1588:ARG:HA	1:E:1588:ARG:HE	1.54	0.73
1:P:1508:HIS:CG	1:P:1509:HIS:H	2.07	0.73
1:W:1563:ARG:HA	1:W:1566:PHE:CD1	2.24	0.73
1:M:1601:GLN:O	1:M:1605:GLU:HG3	1.89	0.73
1:T:1604:LYS:HZ1	1:U:1613:LEU:HG	1.53	0.73
1:Q:1588:ARG:HA	1:Q:1588:ARG:HE	1.51	0.72
1:B:1554:LEU:HD21	1:B:1571:PHE:HB3	1.70	0.72
1:D:1560:GLU:HG3	1:D:1561:GLU:N	2.03	0.72
1:E:1577:LEU:HB3	1:F:1603:MET:CE	2.19	0.72
1:T:1601:GLN:HA	1:U:1609:LYS:HE3	1.70	0.72
1:L:1602:VAL:O	1:L:1602:VAL:HG12	1.88	0.72
1:Q:1546:ASP:HB2	1:Q:1549:LEU:HB2	1.69	0.72
1:V:1509:HIS:O	1:V:1510:SER:HB3	1.88	0.72
1:W:1604:LYS:CG	1:X:1609:LYS:HE3	2.20	0.72
1:J:1572:THR:CA	1:J:1578:ARG:HH22	2.03	0.72
1:L:1533:LEU:CD2	1:L:1534:TYR:H	2.02	0.72
1:O:1572:THR:O	1:O:1575:ASP:HB3	1.88	0.72
1:F:1581:VAL:C	1:F:1583:LEU:H	1.92	0.72
1:O:1554:LEU:CD1	1:O:1568:ALA:HB1	2.19	0.72
1:F:1581:VAL:O	1:F:1583:LEU:N	2.23	0.72
1:K:1566:PHE:O	1:K:1570:LEU:HD12	1.88	0.72
1:V:1572:THR:CA	1:V:1578:ARG:NH2	2.47	0.72
1:X:1547:THR:HG22	1:X:1548:GLU:H	1.54	0.72
1:X:1572:THR:HG21	1:X:1578:ARG:HB3	1.72	0.72
1:K:1604:LYS:HZ1	1:L:1613:LEU:CG	2.02	0.72
1:E:1586:ALA:HA	1:E:1592:MET:HG2	1.72	0.71
1:J:1593:ASP:HA	1:L:1587:TRP:CZ3	2.25	0.71
1:K:1587:TRP:CH2	1:L:1594:PHE:N	2.57	0.71
1:T:1578:ARG:NH2	1:T:1580:ASP:HB2	2.04	0.71
1:X:1591:ILE:HG22	1:X:1592:MET:N	2.03	0.71
1:F:1591:ILE:HG22	1:F:1592:MET:N	2.03	0.71
1:N:1579:PRO:CG	1:O:1599:PHE:HB3	2.19	0.71
1:O:1561:GLU:HB3	1:O:1564:GLU:HB2	1.73	0.71
1:V:1554:LEU:HD22	1:V:1568:ALA:HB1	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1533:LEU:CD2	1:U:1534:TYR:H	2.03	0.71
1:A:1521:TRP:O	1:A:1522:LYS:HB2	1.88	0.71
1:H:1581:VAL:O	1:H:1585:LEU:HD23	1.89	0.71
1:L:1591:ILE:HG22	1:L:1592:MET:N	2.04	0.71
1:Q:1563:ARG:HD3	1:Q:1563:ARG:H	1.54	0.71
1:T:1604:LYS:HG3	1:U:1609:LYS:CD	2.19	0.71
1:W:1567:GLY:HA2	1:W:1570:LEU:HD13	1.73	0.71
1:W:1578:ARG:NH2	1:W:1580:ASP:HB2	2.05	0.71
1:E:1550:ALA:HB1	1:E:1571:PHE:CE2	2.26	0.71
1:I:1572:THR:HG21	1:I:1578:ARG:HB3	1.71	0.71
1:S:1509:HIS:O	1:S:1510:SER:HB3	1.91	0.71
1:T:1554:LEU:HD21	1:T:1571:PHE:HB3	1.71	0.71
1:L:1616:SER:O	1:L:1620:ARG:HG2	1.91	0.71
1:P:1601:GLN:O	1:P:1605:GLU:HG3	1.91	0.71
1:H:1554:LEU:HD21	1:H:1571:PHE:HB3	1.72	0.71
1:K:1581:VAL:O	1:K:1585:LEU:HD23	1.90	0.71
1:T:1588:ARG:HA	1:T:1588:ARG:HE	1.55	0.71
1:W:1607:LEU:HD23	1:X:1612:LYS:HZ2	1.55	0.71
1:C:1585:LEU:HA	1:C:1588:ARG:HG2	1.72	0.71
1:C:1591:ILE:HG22	1:C:1592:MET:N	2.06	0.71
1:I:1619:LEU:HA	1:I:1622:GLU:OE2	1.91	0.71
1:K:1577:LEU:HB3	1:L:1603:MET:HE2	1.71	0.71
1:T:1549:LEU:O	1:T:1553:LEU:HG	1.91	0.70
1:V:1529:LYS:O	1:V:1530:LYS:HB2	1.90	0.70
1:J:1593:ASP:HA	1:L:1587:TRP:HZ3	1.55	0.70
1:V:1560:GLU:HG3	1:V:1561:GLU:H	1.56	0.70
1:B:1563:ARG:H	1:B:1563:ARG:HD3	1.54	0.70
1:F:1616:SER:O	1:F:1620:ARG:HG2	1.91	0.70
1:O:1616:SER:O	1:O:1620:ARG:HG2	1.91	0.70
1:B:1581:VAL:O	1:B:1581:VAL:HG12	1.90	0.70
1:D:1620:ARG:HA	1:D:1620:ARG:HE	1.57	0.70
1:C:1561:GLU:HB3	1:C:1564:GLU:HB2	1.74	0.70
1:G:1521:TRP:O	1:G:1522:LYS:HB2	1.91	0.70
1:K:1554:LEU:O	1:K:1558:LEU:HD13	1.90	0.70
1:L:1602:VAL:HA	1:L:1605:GLU:OE1	1.91	0.70
1:X:1616:SER:O	1:X:1620:ARG:HG2	1.92	0.70
1:F:1585:LEU:HA	1:F:1588:ARG:HG2	1.74	0.70
1:W:1607:LEU:HD23	1:X:1612:LYS:NZ	2.07	0.70
1:M:1535:LYS:O	1:M:1539:GLN:HG3	1.92	0.70
1:W:1550:ALA:HB1	1:W:1571:PHE:CE2	2.26	0.70
1:A:1554:LEU:HD22	1:A:1568:ALA:HB1	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:1579:PRO:HB2	1:L:1599:PHE:HD1	1.57	0.69
1:P:1620:ARG:HA	1:P:1620:ARG:HE	1.57	0.69
1:R:1619:LEU:HA	1:R:1622:GLU:OE2	1.92	0.69
1:E:1579:PRO:HB2	1:F:1599:PHE:CD1	2.27	0.69
1:H:1563:ARG:HA	1:H:1566:PHE:CD1	2.27	0.69
1:K:1547:THR:O	1:K:1551:GLU:HG3	1.92	0.69
1:L:1547:THR:HG22	1:L:1548:GLU:H	1.56	0.69
1:I:1558:LEU:HD13	1:I:1565:CYS:CB	2.22	0.69
1:R:1561:GLU:HB3	1:R:1564:GLU:HB2	1.73	0.69
1:T:1571:PHE:HA	1:T:1574:TYR:CD2	2.27	0.69
1:U:1547:THR:HG22	1:U:1548:GLU:H	1.56	0.69
1:R:1533:LEU:CD2	1:R:1534:TYR:H	2.05	0.69
1:U:1616:SER:O	1:U:1620:ARG:HG2	1.92	0.69
1:H:1597:PRO:O	1:H:1598:TYR:HB2	1.93	0.69
1:Q:1549:LEU:O	1:Q:1553:LEU:HG	1.92	0.69
1:E:1567:GLY:HA2	1:E:1570:LEU:HD13	1.74	0.69
1:K:1588:ARG:HA	1:K:1588:ARG:HE	1.56	0.69
1:W:1581:VAL:O	1:W:1585:LEU:HD23	1.92	0.69
1:B:1571:PHE:HA	1:B:1574:TYR:CD2	2.27	0.69
1:F:1547:THR:HG22	1:F:1548:GLU:H	1.58	0.69
1:F:1581:VAL:C	1:F:1583:LEU:N	2.46	0.69
1:H:1578:ARG:NH2	1:H:1580:ASP:HB2	2.08	0.69
1:Q:1567:GLY:HA2	1:Q:1570:LEU:HD13	1.74	0.69
1:T:1563:ARG:HA	1:T:1566:PHE:CD1	2.28	0.69
1:X:1558:LEU:HD13	1:X:1565:CYS:CB	2.22	0.69
1:U:1602:VAL:HA	1:U:1605:GLU:OE1	1.92	0.69
1:V:1620:ARG:HA	1:V:1620:ARG:HE	1.58	0.69
1:W:1563:ARG:HD3	1:W:1563:ARG:H	1.57	0.69
1:F:1533:LEU:CD2	1:F:1534:TYR:H	2.06	0.69
1:O:1547:THR:HG22	1:O:1548:GLU:H	1.58	0.69
1:P:1529:LYS:O	1:P:1530:LYS:HB2	1.93	0.68
1:R:1558:LEU:HD13	1:R:1565:CYS:HB3	1.72	0.68
1:U:1591:ILE:HG22	1:U:1592:MET:N	2.08	0.68
1:W:1546:ASP:HB2	1:W:1549:LEU:HB2	1.75	0.68
1:F:1554:LEU:CD1	1:F:1568:ALA:HB1	2.24	0.68
1:F:1572:THR:O	1:F:1575:ASP:HB3	1.92	0.68
1:I:1533:LEU:CD2	1:I:1534:TYR:H	2.06	0.68
1:M:1521:TRP:O	1:M:1522:LYS:HB2	1.94	0.68
1:O:1572:THR:HG21	1:O:1578:ARG:HB3	1.76	0.68
1:U:1558:LEU:HD13	1:U:1565:CYS:HB3	1.75	0.68
1:W:1566:PHE:O	1:W:1570:LEU:HD12	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:1571:PHE:HA	1:Q:1574:TYR:CD2	2.28	0.68
1:T:1591:ILE:C	1:T:1592:MET:SD	2.71	0.68
1:V:1508:HIS:CG	1:V:1509:HIS:H	2.11	0.68
1:B:1549:LEU:O	1:B:1553:LEU:HG	1.94	0.68
1:O:1581:VAL:C	1:O:1583:LEU:H	1.96	0.68
1:A:1572:THR:CA	1:A:1578:ARG:HH22	2.07	0.68
1:I:1551:GLU:HA	1:I:1554:LEU:HD23	1.76	0.68
1:G:1546:ASP:CB	1:G:1550:ALA:HB2	2.24	0.68
1:I:1583:LEU:HD22	1:I:1583:LEU:N	2.09	0.68
1:K:1604:LYS:HG3	1:L:1609:LYS:CD	2.23	0.68
1:B:1546:ASP:H	1:B:1550:ALA:CB	2.06	0.68
1:P:1565:CYS:O	1:P:1569:CYS:SG	2.47	0.68
1:G:1509:HIS:O	1:G:1510:SER:HB3	1.93	0.68
1:G:1602:VAL:HA	1:G:1605:GLU:CD	2.13	0.68
1:O:1533:LEU:CD2	1:O:1534:TYR:H	2.07	0.68
1:A:1508:HIS:CG	1:A:1509:HIS:H	2.12	0.68
1:E:1554:LEU:HD23	1:E:1572:THR:OG1	1.94	0.68
1:K:1604:LYS:HG3	1:L:1609:LYS:HE3	1.77	0.67
1:N:1586:ALA:HA	1:N:1592:MET:HG2	1.76	0.67
1:O:1602:VAL:O	1:O:1602:VAL:HG12	1.93	0.67
1:P:1507:HIS:NE2	1:P:1522:LYS:HG2	2.08	0.67
1:S:1508:HIS:CG	1:S:1509:HIS:H	2.11	0.67
1:W:1597:PRO:O	1:W:1598:TYR:HB2	1.94	0.67
1:J:1602:VAL:HA	1:J:1605:GLU:CD	2.14	0.67
1:A:1546:ASP:HB2	1:A:1550:ALA:HB2	1.77	0.67
1:C:1533:LEU:CD2	1:C:1534:TYR:H	2.07	0.67
1:E:1597:PRO:O	1:E:1598:TYR:HB2	1.94	0.67
1:L:1572:THR:HG21	1:L:1578:ARG:HB3	1.76	0.67
1:N:1588:ARG:HA	1:N:1588:ARG:HE	1.58	0.67
1:R:1547:THR:HG22	1:R:1548:GLU:H	1.59	0.67
1:W:1604:LYS:HE3	1:X:1609:LYS:HD2	1.76	0.67
1:G:1578:ARG:H	1:G:1579:PRO:CD	2.07	0.67
1:L:1533:LEU:CG	1:V:1588:ARG:CZ	2.73	0.67
1:O:1595:ALA:O	1:O:1596:MET:SD	2.53	0.67
1:Q:1546:ASP:H	1:Q:1550:ALA:CB	2.06	0.67
1:R:1537:ALA:HB3	1:R:1538:MET:HE1	1.77	0.67
1:T:1567:GLY:HA2	1:T:1570:LEU:HD13	1.75	0.67
1:J:1620:ARG:HA	1:J:1620:ARG:HE	1.60	0.67
1:K:1549:LEU:O	1:K:1553:LEU:HG	1.95	0.67
1:O:1585:LEU:HA	1:O:1588:ARG:HG2	1.76	0.66
1:S:1594:PHE:CG	1:S:1595:ALA:N	2.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1611:ASP:HB3	1:H:1612:LYS:NZ	2.11	0.66
1:L:1558:LEU:CD1	1:L:1565:CYS:HB3	2.25	0.66
1:P:1509:HIS:O	1:P:1510:SER:HB3	1.94	0.66
1:A:1602:VAL:HA	1:A:1605:GLU:CD	2.16	0.66
1:R:1572:THR:HG21	1:R:1578:ARG:HB3	1.77	0.66
1:X:1533:LEU:CD2	1:X:1534:TYR:H	2.08	0.66
1:L:1594:PHE:O	1:L:1595:ALA:HB2	1.95	0.66
1:S:1575:ASP:HB2	1:S:1578:ARG:CZ	2.26	0.66
1:F:1558:LEU:HA	1:F:1565:CYS:SG	2.35	0.66
1:Q:1597:PRO:O	1:Q:1598:TYR:HB2	1.93	0.66
1:U:1619:LEU:HA	1:U:1622:GLU:OE2	1.96	0.66
1:W:1571:PHE:HA	1:W:1574:TYR:CD2	2.29	0.66
1:O:1596:MET:N	1:O:1597:PRO:HD3	2.11	0.66
1:P:1546:ASP:HB2	1:P:1550:ALA:HB2	1.78	0.66
1:S:1620:ARG:HA	1:S:1620:ARG:HE	1.61	0.66
1:N:1577:LEU:HB3	1:O:1603:MET:HE3	1.78	0.66
1:O:1591:ILE:CG2	1:O:1592:MET:H	2.08	0.66
1:Q:1554:LEU:HD23	1:Q:1572:THR:OG1	1.95	0.66
1:X:1561:GLU:HB3	1:X:1564:GLU:HB2	1.76	0.66
1:E:1554:LEU:O	1:E:1558:LEU:HD13	1.96	0.66
1:E:1563:ARG:HA	1:E:1566:PHE:CD1	2.31	0.66
1:H:1571:PHE:HA	1:H:1574:TYR:CD2	2.30	0.66
1:J:1560:GLU:HG3	1:J:1561:GLU:H	1.61	0.66
1:M:1620:ARG:HA	1:M:1620:ARG:HE	1.61	0.66
1:N:1546:ASP:HB2	1:N:1549:LEU:HB2	1.77	0.66
1:R:1602:VAL:O	1:R:1602:VAL:HG12	1.94	0.66
1:S:1529:LYS:O	1:S:1530:LYS:HB2	1.96	0.66
1:L:1561:GLU:HB3	1:L:1564:GLU:HB2	1.78	0.66
1:U:1558:LEU:HA	1:U:1565:CYS:SG	2.36	0.66
1:B:1597:PRO:O	1:B:1598:TYR:HB2	1.96	0.65
1:L:1572:THR:O	1:L:1575:ASP:HB3	1.95	0.65
1:N:1549:LEU:O	1:N:1553:LEU:HG	1.96	0.65
1:Q:1554:LEU:O	1:Q:1558:LEU:HD13	1.96	0.65
1:T:1554:LEU:HD23	1:T:1572:THR:OG1	1.96	0.65
1:N:1563:ARG:H	1:N:1563:ARG:HD3	1.59	0.65
1:R:1591:ILE:HG22	1:R:1592:MET:N	2.10	0.65
1:T:1546:ASP:N	1:T:1550:ALA:HB2	2.01	0.65
1:U:1596:MET:N	1:U:1597:PRO:HD3	2.11	0.65
1:V:1602:VAL:HA	1:V:1605:GLU:CD	2.17	0.65
1:E:1583:LEU:HD22	1:F:1596:MET:HG2	1.77	0.65
1:G:1577:LEU:HD12	1:G:1577:LEU:H	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1555:GLN:O	1:I:1559:GLN:HG2	1.96	0.65
1:J:1601:GLN:O	1:J:1605:GLU:HG3	1.95	0.65
1:N:1563:ARG:HA	1:N:1566:PHE:CD1	2.31	0.65
1:W:1588:ARG:HE	1:W:1588:ARG:HA	1.60	0.65
1:X:1537:ALA:HB3	1:X:1538:MET:HE1	1.78	0.65
1:D:1602:VAL:HG13	1:F:1577:LEU:HD13	1.78	0.65
1:G:1620:ARG:HA	1:G:1620:ARG:HE	1.62	0.65
1:K:1587:TRP:HH2	1:L:1594:PHE:H	1.44	0.65
1:W:1592:MET:SD	1:W:1592:MET:N	2.70	0.65
1:B:1567:GLY:HA2	1:B:1570:LEU:HD13	1.77	0.65
1:H:1588:ARG:HA	1:H:1588:ARG:HE	1.61	0.65
1:J:1509:HIS:O	1:J:1510:SER:CB	2.45	0.65
1:D:1602:VAL:HA	1:D:1605:GLU:CD	2.17	0.65
1:F:1572:THR:HG21	1:F:1578:ARG:HB3	1.77	0.65
1:I:1547:THR:HG22	1:I:1548:GLU:N	2.12	0.65
1:H:1566:PHE:O	1:H:1570:LEU:HD12	1.97	0.65
1:I:1603:MET:O	1:I:1607:LEU:HD23	1.97	0.65
1:D:1560:GLU:O	1:D:1561:GLU:HB2	1.97	0.65
1:F:1592:MET:SD	1:F:1593:ASP:N	2.70	0.65
1:H:1549:LEU:O	1:H:1553:LEU:HG	1.96	0.65
1:R:1537:ALA:HB3	1:R:1538:MET:CE	2.26	0.65
1:W:1549:LEU:O	1:W:1553:LEU:HG	1.97	0.65
1:J:1507:HIS:O	1:J:1508:HIS:HB2	1.97	0.65
1:O:1572:THR:CG2	1:O:1578:ARG:HB3	2.26	0.65
1:S:1578:ARG:H	1:S:1579:PRO:CD	2.10	0.65
1:E:1593:ASP:CG	1:E:1594:PHE:H	2.00	0.64
1:K:1604:LYS:NZ	1:L:1613:LEU:CG	2.57	0.64
1:V:1545:LYS:HG2	1:V:1546:ASP:N	2.12	0.64
1:O:1621:LYS:O	1:O:1621:LYS:HD3	1.97	0.64
1:A:1535:LYS:O	1:A:1539:GLN:HG3	1.98	0.64
1:B:1554:LEU:O	1:B:1558:LEU:HD13	1.96	0.64
1:C:1603:MET:O	1:C:1607:LEU:HD23	1.97	0.64
1:K:1597:PRO:O	1:K:1598:TYR:HB2	1.96	0.64
1:L:1572:THR:CG2	1:L:1578:ARG:HB3	2.27	0.64
1:U:1554:LEU:CD1	1:U:1568:ALA:HB1	2.27	0.64
1:L:1533:LEU:HD22	1:L:1534:TYR:N	2.11	0.64
1:L:1533:LEU:HD13	1:L:1534:TYR:CE1	2.32	0.64
1:N:1583:LEU:HD22	1:O:1596:MET:HG2	1.80	0.64
1:R:1585:LEU:HD13	1:R:1588:ARG:HG3	1.78	0.64
1:D:1521:TRP:O	1:D:1522:LYS:HB2	1.97	0.64
1:Q:1588:ARG:HA	1:Q:1588:ARG:NE	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:1592:MET:SD	1:Q:1592:MET:N	2.71	0.64
1:S:1535:LYS:O	1:S:1539:GLN:HG3	1.98	0.64
1:V:1545:LYS:CG	1:V:1546:ASP:H	2.09	0.64
1:A:1577:LEU:H	1:A:1577:LEU:HD12	1.63	0.64
1:M:1529:LYS:O	1:M:1530:LYS:HB2	1.97	0.64
1:T:1604:LYS:CD	1:U:1612:LYS:CE	2.75	0.64
1:X:1619:LEU:HA	1:X:1622:GLU:OE2	1.98	0.64
1:J:1546:ASP:HB2	1:J:1550:ALA:HB2	1.79	0.63
1:K:1605:GLU:O	1:K:1609:LYS:HG3	1.97	0.63
1:M:1560:GLU:HG3	1:M:1561:GLU:N	2.13	0.63
1:N:1577:LEU:HB3	1:O:1603:MET:CE	2.28	0.63
1:E:1563:ARG:H	1:E:1563:ARG:HD3	1.62	0.63
1:K:1567:GLY:HA2	1:K:1570:LEU:HD13	1.80	0.63
1:X:1572:THR:HG22	1:X:1572:THR:O	1.98	0.63
1:A:1620:ARG:HA	1:A:1620:ARG:HE	1.62	0.63
1:E:1549:LEU:O	1:E:1553:LEU:HG	1.98	0.63
1:Q:1593:ASP:CG	1:Q:1594:PHE:H	2.00	0.63
1:O:1581:VAL:O	1:O:1583:LEU:N	2.31	0.63
1:V:1546:ASP:HB2	1:V:1550:ALA:HB2	1.80	0.63
1:N:1547:THR:O	1:N:1551:GLU:HG3	1.99	0.63
1:T:1604:LYS:HZ2	1:U:1612:LYS:HE2	1.63	0.63
1:W:1604:LYS:CD	1:X:1609:LYS:HD2	2.29	0.63
1:B:1593:ASP:CG	1:B:1594:PHE:H	2.02	0.63
1:C:1591:ILE:CG2	1:C:1592:MET:H	2.12	0.63
1:D:1535:LYS:O	1:D:1539:GLN:HG3	1.99	0.63
1:F:1619:LEU:HA	1:F:1622:GLU:OE2	1.98	0.63
1:I:1572:THR:CG2	1:I:1578:ARG:HB3	2.29	0.63
1:I:1599:PHE:CD2	1:I:1599:PHE:N	2.65	0.63
1:L:1585:LEU:HA	1:L:1588:ARG:HG2	1.80	0.63
1:U:1544:SER:O	1:U:1545:LYS:HD2	1.98	0.63
1:X:1554:LEU:HD22	1:X:1554:LEU:N	2.13	0.63
1:F:1594:PHE:O	1:F:1595:ALA:HB2	1.99	0.63
1:K:1563:ARG:H	1:K:1563:ARG:HD3	1.64	0.63
1:U:1579:PRO:HD3	1:U:1598:TYR:OH	1.98	0.63
1:C:1554:LEU:O	1:C:1558:LEU:HD23	1.98	0.63
1:H:1567:GLY:HA2	1:H:1570:LEU:HD13	1.79	0.63
1:K:1571:PHE:HA	1:K:1574:TYR:CD2	2.34	0.63
1:Q:1547:THR:O	1:Q:1551:GLU:HG3	1.98	0.63
1:G:1594:PHE:CG	1:G:1595:ALA:N	2.67	0.62
1:L:1603:MET:O	1:L:1607:LEU:HD23	1.99	0.62
1:M:1507:HIS:NE2	1:M:1522:LYS:HG2	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1560:GLU:HG3	1:S:1561:GLU:H	1.64	0.62
1:V:1578:ARG:H	1:V:1579:PRO:CD	2.12	0.62
1:W:1554:LEU:O	1:W:1558:LEU:HD13	1.98	0.62
1:C:1572:THR:O	1:C:1575:ASP:HB3	1.98	0.62
1:D:1546:ASP:HB2	1:D:1550:ALA:HB2	1.82	0.62
1:K:1554:LEU:HD23	1:K:1572:THR:OG1	1.99	0.62
1:T:1546:ASP:HB2	1:T:1549:LEU:HB2	1.80	0.62
1:U:1558:LEU:HD13	1:U:1565:CYS:CB	2.29	0.62
1:X:1572:THR:O	1:X:1575:ASP:HB3	1.99	0.62
1:O:1554:LEU:O	1:O:1558:LEU:HD23	1.99	0.62
1:O:1578:ARG:HH22	1:O:1580:ASP:HB2	1.65	0.62
1:R:1602:VAL:HA	1:R:1605:GLU:OE1	2.00	0.62
1:T:1586:ALA:HA	1:T:1592:MET:HG2	1.80	0.62
1:V:1535:LYS:O	1:V:1539:GLN:HG3	1.98	0.62
1:M:1577:LEU:H	1:M:1577:LEU:HD12	1.65	0.62
1:N:1597:PRO:O	1:N:1598:TYR:HB2	1.99	0.62
1:S:1521:TRP:O	1:S:1522:LYS:HB2	1.99	0.62
1:T:1592:MET:N	1:T:1592:MET:HE2	2.13	0.62
1:V:1601:GLN:O	1:V:1605:GLU:HG3	1.99	0.62
1:E:1571:PHE:HA	1:E:1574:TYR:CD2	2.35	0.62
1:L:1555:GLN:O	1:L:1559:GLN:HG2	1.98	0.62
1:X:1606:TYR:O	1:X:1609:LYS:HB3	1.99	0.62
1:I:1572:THR:O	1:I:1575:ASP:HB3	2.00	0.62
1:J:1507:HIS:NE2	1:J:1522:LYS:HG2	2.15	0.62
1:X:1603:MET:O	1:X:1607:LEU:HD23	1.99	0.62
1:G:1515:PRO:O	1:G:1516:ARG:HB3	2.00	0.62
1:H:1554:LEU:O	1:H:1558:LEU:HD13	2.00	0.62
1:J:1596:MET:N	1:J:1596:MET:SD	2.72	0.62
1:L:1581:VAL:C	1:L:1583:LEU:H	2.02	0.62
1:B:1593:ASP:O	1:B:1594:PHE:HB2	1.98	0.62
1:F:1572:THR:CG2	1:F:1578:ARG:HB3	2.30	0.62
1:J:1575:ASP:HB2	1:J:1578:ARG:CZ	2.30	0.62
1:S:1560:GLU:HG3	1:S:1561:GLU:N	2.15	0.62
1:U:1547:THR:HG22	1:U:1548:GLU:N	2.15	0.62
1:N:1558:LEU:HA	1:N:1565:CYS:SG	2.40	0.62
1:R:1530:LYS:HZ3	1:R:1563:ARG:NE	1.98	0.62
1:W:1554:LEU:HD23	1:W:1572:THR:OG1	1.99	0.62
1:W:1592:MET:N	1:W:1592:MET:HE2	2.15	0.62
1:B:1604:LYS:CE	1:C:1609:LYS:HD2	2.30	0.61
1:E:1577:LEU:HB3	1:F:1603:MET:HE3	1.80	0.61
1:F:1533:LEU:HG	1:G:1588:ARG:NH1	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1535:LYS:O	1:G:1539:GLN:HG3	2.00	0.61
1:U:1554:LEU:O	1:U:1558:LEU:HB2	1.99	0.61
1:I:1599:PHE:HA	1:I:1602:VAL:CG2	2.29	0.61
1:N:1567:GLY:HA2	1:N:1570:LEU:HD13	1.81	0.61
1:Q:1586:ALA:HA	1:Q:1592:MET:HG2	1.81	0.61
1:S:1578:ARG:H	1:S:1579:PRO:HD3	1.65	0.61
1:F:1602:VAL:HA	1:F:1605:GLU:OE1	2.00	0.61
1:H:1546:ASP:N	1:H:1550:ALA:HB2	2.01	0.61
1:H:1606:TYR:HA	1:H:1609:LYS:CE	2.30	0.61
1:T:1597:PRO:O	1:T:1598:TYR:HB2	1.97	0.61
1:L:1581:VAL:O	1:L:1583:LEU:N	2.34	0.61
1:Q:1554:LEU:HD11	1:Q:1571:PHE:HD2	1.65	0.61
1:R:1581:VAL:C	1:R:1583:LEU:H	2.02	0.61
1:U:1595:ALA:C	1:U:1597:PRO:HD3	2.21	0.61
1:A:1546:ASP:CB	1:A:1550:ALA:HB2	2.31	0.61
1:C:1602:VAL:O	1:C:1602:VAL:HG12	1.98	0.61
1:K:1584:GLU:O	1:K:1588:ARG:NH1	2.33	0.61
1:O:1581:VAL:C	1:O:1583:LEU:N	2.49	0.61
1:R:1621:LYS:O	1:R:1621:LYS:HD3	2.00	0.61
1:V:1578:ARG:H	1:V:1579:PRO:HD3	1.64	0.61
1:F:1591:ILE:CG2	1:F:1592:MET:H	2.13	0.61
1:I:1591:ILE:CG2	1:I:1592:MET:H	2.12	0.61
1:P:1572:THR:CA	1:P:1578:ARG:HH22	2.09	0.61
1:I:1599:PHE:N	1:I:1599:PHE:HD2	1.98	0.61
1:M:1546:ASP:HB2	1:M:1550:ALA:HB2	1.82	0.61
1:C:1547:THR:HG22	1:C:1548:GLU:N	2.15	0.61
1:G:1508:HIS:CG	1:G:1509:HIS:H	2.17	0.61
1:K:1558:LEU:HA	1:K:1565:CYS:SG	2.40	0.61
1:M:1558:LEU:HA	1:M:1565:CYS:SG	2.40	0.61
1:R:1558:LEU:HD13	1:R:1565:CYS:CB	2.30	0.61
1:U:1606:TYR:O	1:U:1609:LYS:HB3	1.99	0.61
1:D:1507:HIS:NE2	1:D:1522:LYS:HG2	2.16	0.61
1:P:1535:LYS:O	1:P:1539:GLN:HG3	2.00	0.61
1:W:1593:ASP:O	1:W:1594:PHE:HB2	2.00	0.61
1:B:1546:ASP:HB2	1:B:1549:LEU:HB2	1.82	0.61
1:D:1509:HIS:ND1	1:D:1510:SER:N	2.48	0.61
1:F:1559:GLN:NE2	1:F:1585:LEU:HD11	2.16	0.61
1:T:1583:LEU:O	1:T:1586:ALA:HB3	2.01	0.61
1:F:1601:GLN:O	1:F:1605:GLU:CD	2.40	0.60
1:X:1581:VAL:C	1:X:1583:LEU:H	2.04	0.60
1:H:1606:TYR:HA	1:H:1609:LYS:HE2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:1591:ILE:CG2	1:L:1592:MET:H	2.12	0.60
1:O:1554:LEU:HD12	1:O:1568:ALA:HB1	1.82	0.60
1:U:1594:PHE:O	1:U:1595:ALA:HB2	2.00	0.60
1:U:1602:VAL:HG12	1:U:1602:VAL:O	1.99	0.60
1:X:1537:ALA:HB3	1:X:1538:MET:CE	2.31	0.60
1:X:1547:THR:HG22	1:X:1548:GLU:N	2.16	0.60
1:G:1578:ARG:H	1:G:1579:PRO:HD3	1.63	0.60
1:I:1621:LYS:O	1:I:1621:LYS:HD3	2.00	0.60
1:S:1546:ASP:HB2	1:S:1550:ALA:HB2	1.83	0.60
1:I:1595:ALA:O	1:I:1596:MET:SD	2.59	0.60
1:K:1577:LEU:HB3	1:L:1603:MET:CE	2.30	0.60
1:D:1551:GLU:HB3	1:D:1555:GLN:HE22	1.67	0.60
1:N:1571:PHE:HA	1:N:1574:TYR:CD2	2.36	0.60
1:R:1599:PHE:CD2	1:R:1599:PHE:N	2.68	0.60
1:I:1595:ALA:C	1:I:1597:PRO:HD3	2.22	0.60
1:Q:1580:ASP:HA	1:Q:1583:LEU:HD13	1.84	0.60
1:U:1599:PHE:N	1:U:1599:PHE:CD2	2.67	0.60
1:X:1535:LYS:O	1:X:1536:ASP:HB2	2.02	0.60
1:A:1611:ASP:HB3	1:B:1612:LYS:NZ	2.15	0.60
1:D:1513:LEU:HD13	1:D:1513:LEU:C	2.22	0.60
1:O:1568:ALA:O	1:O:1571:PHE:HB3	2.02	0.60
1:T:1604:LYS:HZ2	1:U:1612:LYS:HB3	1.67	0.60
1:A:1578:ARG:H	1:A:1579:PRO:HD3	1.66	0.60
1:L:1606:TYR:O	1:L:1609:LYS:HB3	2.02	0.60
1:N:1554:LEU:HD23	1:N:1572:THR:OG1	2.01	0.60
1:R:1559:GLN:NE2	1:R:1585:LEU:HD11	2.16	0.60
1:X:1551:GLU:HA	1:X:1554:LEU:HD23	1.82	0.60
1:H:1605:GLU:O	1:H:1609:LYS:HG3	2.01	0.60
1:N:1591:ILE:C	1:N:1592:MET:SD	2.80	0.60
1:S:1509:HIS:O	1:S:1510:SER:CB	2.49	0.60
1:B:1554:LEU:HD23	1:B:1572:THR:OG1	2.02	0.60
1:C:1594:PHE:O	1:C:1595:ALA:HB2	2.02	0.60
1:G:1529:LYS:O	1:G:1530:LYS:HB2	2.02	0.60
1:U:1599:PHE:N	1:U:1599:PHE:HD2	2.00	0.60
1:U:1621:LYS:O	1:U:1621:LYS:HD3	2.02	0.60
1:V:1545:LYS:HG2	1:V:1546:ASP:H	1.66	0.60
1:X:1558:LEU:HD13	1:X:1565:CYS:HB3	1.82	0.60
1:C:1577:LEU:HD22	1:C:1598:TYR:CE2	2.36	0.59
1:E:1558:LEU:HA	1:E:1565:CYS:SG	2.42	0.59
1:H:1554:LEU:HD23	1:H:1572:THR:OG1	2.01	0.59
1:M:1509:HIS:O	1:M:1510:SER:CB	2.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1545:LYS:HG2	1:M:1546:ASP:N	2.17	0.59
1:O:1558:LEU:HD13	1:O:1565:CYS:CB	2.32	0.59
1:S:1572:THR:CA	1:S:1578:ARG:NH2	2.51	0.59
1:U:1607:LEU:C	1:U:1609:LYS:H	2.04	0.59
1:W:1599:PHE:HA	1:W:1602:VAL:HG23	1.82	0.59
1:D:1507:HIS:O	1:D:1508:HIS:HB2	2.02	0.59
1:L:1547:THR:HG22	1:L:1548:GLU:N	2.16	0.59
1:B:1588:ARG:HA	1:B:1588:ARG:HE	1.67	0.59
1:J:1508:HIS:CG	1:J:1509:HIS:H	2.20	0.59
1:Q:1558:LEU:HA	1:Q:1565:CYS:SG	2.41	0.59
1:R:1554:LEU:CD1	1:R:1568:ALA:HB1	2.33	0.59
1:D:1513:LEU:HD13	1:D:1513:LEU:O	2.02	0.59
1:A:1545:LYS:HG2	1:A:1546:ASP:H	1.66	0.59
1:C:1572:THR:HG21	1:C:1578:ARG:HB3	1.84	0.59
1:N:1583:LEU:O	1:N:1586:ALA:HB3	2.03	0.59
1:O:1514:VAL:HG13	1:T:1531:ASP:CG	2.23	0.59
1:P:1508:HIS:CD2	1:P:1509:HIS:H	2.20	0.59
1:G:1513:LEU:HD13	1:G:1513:LEU:C	2.22	0.59
1:X:1579:PRO:HD3	1:X:1598:TYR:OH	2.02	0.59
1:E:1593:ASP:O	1:E:1594:PHE:HB2	2.03	0.59
1:F:1554:LEU:HD12	1:F:1568:ALA:HB1	1.83	0.59
1:G:1560:GLU:HG3	1:G:1561:GLU:N	2.18	0.59
1:P:1508:HIS:CG	1:P:1509:HIS:N	2.69	0.59
1:P:1568:ALA:O	1:P:1571:PHE:HB3	2.01	0.59
1:X:1581:VAL:O	1:X:1583:LEU:N	2.36	0.59
1:F:1579:PRO:HG2	1:F:1580:ASP:OD1	2.02	0.59
1:F:1603:MET:O	1:F:1607:LEU:HD23	2.02	0.59
1:G:1513:LEU:HD13	1:G:1513:LEU:O	2.02	0.59
1:H:1542:SER:HA	1:H:1571:PHE:CE1	2.38	0.59
1:P:1575:ASP:HB2	1:P:1578:ARG:NH1	2.18	0.59
1:P:1578:ARG:H	1:P:1579:PRO:HD3	1.66	0.59
1:M:1508:HIS:CG	1:M:1509:HIS:H	2.20	0.59
1:O:1577:LEU:HD22	1:O:1598:TYR:CE2	2.38	0.59
1:U:1603:MET:O	1:U:1607:LEU:HD23	2.01	0.59
1:X:1554:LEU:CD1	1:X:1568:ALA:HB1	2.33	0.59
1:X:1602:VAL:O	1:X:1602:VAL:HG12	2.03	0.59
1:A:1545:LYS:HG2	1:A:1546:ASP:N	2.18	0.59
1:B:1599:PHE:HA	1:B:1602:VAL:HG23	1.85	0.59
1:G:1604:LYS:CD	1:H:1605:GLU:OE1	2.49	0.59
1:I:1559:GLN:NE2	1:I:1585:LEU:HD11	2.16	0.59
1:I:1585:LEU:HD13	1:I:1588:ARG:HG3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1554:LEU:O	1:J:1557:PHE:N	2.35	0.59
1:O:1585:LEU:HD13	1:O:1588:ARG:HG3	1.85	0.59
1:O:1609:LYS:HA	1:O:1609:LYS:HZ2	1.68	0.59
1:P:1546:ASP:CB	1:P:1550:ALA:HB2	2.33	0.59
1:P:1578:ARG:H	1:P:1579:PRO:CD	2.16	0.59
1:R:1601:GLN:O	1:R:1605:GLU:CD	2.41	0.59
1:S:1545:LYS:HG2	1:S:1546:ASP:N	2.17	0.59
1:F:1540:TYR:HB3	1:H:1563:ARG:HB3	1.85	0.58
1:F:1558:LEU:HD13	1:F:1565:CYS:CB	2.33	0.58
1:F:1585:LEU:HD13	1:F:1588:ARG:HG3	1.85	0.58
1:F:1621:LYS:O	1:F:1621:LYS:HD3	2.03	0.58
1:I:1599:PHE:HA	1:I:1602:VAL:HG21	1.85	0.58
1:J:1578:ARG:H	1:J:1579:PRO:HD3	1.68	0.58
1:R:1603:MET:O	1:R:1607:LEU:HD23	2.02	0.58
1:T:1599:PHE:HA	1:T:1602:VAL:HG23	1.84	0.58
1:C:1578:ARG:HH22	1:C:1580:ASP:HB2	1.69	0.58
1:F:1596:MET:N	1:F:1597:PRO:HD3	2.18	0.58
1:L:1530:LYS:HZ3	1:L:1563:ARG:HD2	1.68	0.58
1:M:1551:GLU:HB3	1:M:1555:GLN:HE22	1.68	0.58
1:N:1577:LEU:HD22	1:O:1602:VAL:O	2.02	0.58
1:P:1520:MET:N	1:P:1520:MET:SD	2.76	0.58
1:R:1599:PHE:N	1:R:1599:PHE:HD2	2.01	0.58
1:S:1513:LEU:C	1:S:1513:LEU:HD13	2.23	0.58
1:S:1572:THR:C	1:S:1578:ARG:HH22	2.06	0.58
1:V:1587:TRP:HA	1:V:1587:TRP:CE3	2.38	0.58
1:B:1580:ASP:HA	1:B:1583:LEU:HD13	1.86	0.58
1:B:1596:MET:H	1:B:1596:MET:HE2	1.68	0.58
1:C:1554:LEU:CD1	1:C:1568:ALA:HB1	2.33	0.58
1:C:1603:MET:O	1:C:1605:GLU:N	2.36	0.58
1:D:1545:LYS:HG2	1:D:1546:ASP:N	2.18	0.58
1:O:1579:PRO:HG2	1:O:1580:ASP:OD1	2.03	0.58
1:Q:1542:SER:HA	1:Q:1571:PHE:CE1	2.39	0.58
1:S:1596:MET:H	1:S:1597:PRO:HD3	1.69	0.58
1:W:1554:LEU:HD11	1:W:1571:PHE:HD2	1.66	0.58
1:G:1580:ASP:O	1:G:1584:GLU:OE2	2.21	0.58
1:Q:1606:TYR:O	1:Q:1610:VAL:HG23	2.03	0.58
1:U:1559:GLN:NE2	1:U:1585:LEU:HD11	2.18	0.58
1:X:1591:ILE:CG2	1:X:1592:MET:H	2.15	0.58
1:C:1578:ARG:NE	1:C:1578:ARG:HA	2.19	0.58
1:C:1613:LEU:O	1:C:1617:GLU:HG3	2.04	0.58
1:M:1545:LYS:CG	1:M:1546:ASP:H	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1551:GLU:HB3	1:P:1555:GLN:HE22	1.68	0.58
1:J:1546:ASP:CB	1:J:1550:ALA:HB2	2.33	0.58
1:O:1547:THR:HG22	1:O:1548:GLU:N	2.18	0.58
1:S:1602:VAL:HA	1:S:1605:GLU:CD	2.23	0.58
1:A:1578:ARG:H	1:A:1579:PRO:CD	2.16	0.58
1:R:1598:TYR:O	1:R:1602:VAL:HG23	2.03	0.58
1:X:1581:VAL:C	1:X:1583:LEU:N	2.54	0.58
1:F:1558:LEU:HD13	1:F:1565:CYS:HB3	1.86	0.58
1:J:1545:LYS:HG2	1:J:1546:ASP:N	2.19	0.58
1:M:1541:ALA:HB3	1:M:1571:PHE:CE2	2.38	0.58
1:P:1558:LEU:HA	1:P:1565:CYS:SG	2.43	0.58
1:R:1581:VAL:O	1:R:1583:LEU:N	2.34	0.58
1:X:1594:PHE:O	1:X:1595:ALA:HB2	2.02	0.58
1:C:1551:GLU:HA	1:C:1554:LEU:HD23	1.85	0.58
1:G:1509:HIS:O	1:G:1510:SER:CB	2.52	0.58
1:S:1577:LEU:H	1:S:1577:LEU:HD12	1.68	0.58
1:T:1599:PHE:O	1:T:1602:VAL:N	2.37	0.58
1:A:1545:LYS:CG	1:A:1546:ASP:H	2.15	0.58
1:L:1579:PRO:HD3	1:L:1598:TYR:OH	2.04	0.58
1:S:1545:LYS:CG	1:S:1546:ASP:H	2.16	0.58
1:E:1547:THR:O	1:E:1551:GLU:HG3	2.04	0.57
1:F:1547:THR:HG22	1:F:1548:GLU:N	2.18	0.57
1:L:1599:PHE:CD2	1:L:1599:PHE:N	2.72	0.57
1:P:1515:PRO:O	1:P:1516:ARG:HB3	2.04	0.57
1:R:1569:CYS:C	1:R:1571:PHE:H	2.07	0.57
1:S:1555:GLN:O	1:S:1559:GLN:N	2.37	0.57
1:W:1607:LEU:CD2	1:X:1612:LYS:NZ	2.67	0.57
1:C:1596:MET:N	1:C:1597:PRO:HD3	2.19	0.57
1:L:1581:VAL:C	1:L:1583:LEU:N	2.57	0.57
1:M:1560:GLU:HG3	1:M:1561:GLU:H	1.69	0.57
1:C:1583:LEU:HD22	1:C:1583:LEU:N	2.20	0.57
1:J:1535:LYS:O	1:J:1539:GLN:HG3	2.04	0.57
1:L:1533:LEU:CG	1:V:1588:ARG:NH1	2.65	0.57
1:O:1609:LYS:HA	1:O:1609:LYS:NZ	2.19	0.57
1:D:1596:MET:N	1:D:1596:MET:SD	2.76	0.57
1:G:1560:GLU:O	1:G:1561:GLU:HB2	2.05	0.57
1:H:1546:ASP:HB2	1:H:1549:LEU:HB2	1.84	0.57
1:H:1586:ALA:HA	1:H:1592:MET:HG2	1.86	0.57
1:I:1558:LEU:CD1	1:I:1565:CYS:HB3	2.32	0.57
1:M:1515:PRO:O	1:M:1516:ARG:HB3	2.03	0.57
1:R:1581:VAL:C	1:R:1583:LEU:N	2.57	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:1585:LEU:HD13	1:R:1588:ARG:CG	2.35	0.57
1:R:1613:LEU:O	1:R:1617:GLU:HG3	2.04	0.57
1:V:1546:ASP:CB	1:V:1550:ALA:HB2	2.34	0.57
1:X:1602:VAL:HA	1:X:1605:GLU:OE1	2.03	0.57
1:H:1554:LEU:HD11	1:H:1571:PHE:HD2	1.67	0.57
1:K:1586:ALA:HA	1:K:1592:MET:HG2	1.85	0.57
1:N:1588:ARG:HA	1:N:1588:ARG:NE	2.19	0.57
1:O:1595:ALA:C	1:O:1597:PRO:HD3	2.25	0.57
1:V:1507:HIS:NE2	1:V:1522:LYS:HG2	2.19	0.57
1:W:1588:ARG:HA	1:W:1588:ARG:NE	2.19	0.57
1:E:1606:TYR:O	1:E:1610:VAL:HG23	2.05	0.57
1:J:1606:TYR:HB2	1:L:1577:LEU:HD11	1.87	0.57
1:K:1529:LYS:C	1:K:1530:LYS:HG2	2.25	0.57
1:K:1554:LEU:HD11	1:K:1571:PHE:HD2	1.70	0.57
1:O:1603:MET:O	1:O:1607:LEU:HD23	2.04	0.57
1:T:1558:LEU:HA	1:T:1565:CYS:SG	2.45	0.57
1:D:1580:ASP:O	1:D:1584:GLU:OE2	2.22	0.57
1:H:1572:THR:HG23	1:H:1578:ARG:HB3	1.87	0.57
1:I:1594:PHE:O	1:I:1595:ALA:HB2	2.04	0.57
1:I:1596:MET:N	1:I:1597:PRO:HD3	2.19	0.57
1:M:1513:LEU:C	1:M:1513:LEU:HD13	2.25	0.57
1:R:1530:LYS:HZ3	1:R:1563:ARG:HD2	1.69	0.57
1:R:1547:THR:HG22	1:R:1548:GLU:N	2.19	0.57
1:R:1599:PHE:HA	1:R:1602:VAL:CG2	2.34	0.57
1:U:1533:LEU:HD13	1:U:1534:TYR:CE1	2.39	0.57
1:V:1575:ASP:HB2	1:V:1578:ARG:CZ	2.35	0.57
1:W:1586:ALA:HA	1:W:1592:MET:HG2	1.86	0.57
1:X:1555:GLN:O	1:X:1559:GLN:HG2	2.05	0.57
1:X:1585:LEU:HD13	1:X:1588:ARG:HG3	1.85	0.57
1:E:1588:ARG:HA	1:E:1588:ARG:NE	2.18	0.57
1:O:1537:ALA:CB	1:T:1566:PHE:CD1	2.87	0.57
1:P:1580:ASP:O	1:P:1584:GLU:OE2	2.22	0.57
1:C:1621:LYS:O	1:C:1621:LYS:HD3	2.05	0.57
1:E:1580:ASP:HA	1:E:1583:LEU:HD13	1.87	0.57
1:J:1568:ALA:O	1:J:1571:PHE:HB3	2.05	0.57
1:K:1587:TRP:HH2	1:L:1594:PHE:N	2.00	0.57
1:O:1537:ALA:HB3	1:O:1538:MET:HE1	1.87	0.57
1:O:1592:MET:SD	1:O:1593:ASP:N	2.78	0.57
1:Q:1605:GLU:O	1:Q:1609:LYS:HG3	2.05	0.57
1:S:1508:HIS:CG	1:S:1509:HIS:N	2.72	0.57
1:E:1604:LYS:HD2	1:F:1612:LYS:HZ3	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1578:ARG:NE	1:F:1578:ARG:HA	2.20	0.57
1:J:1551:GLU:HB3	1:J:1555:GLN:HE22	1.69	0.57
1:K:1604:LYS:HZ1	1:L:1613:LEU:HG	1.63	0.57
1:P:1519:HIS:N	1:P:1520:MET:HE1	2.19	0.57
1:V:1551:GLU:HB3	1:V:1555:GLN:HE22	1.70	0.57
1:C:1606:TYR:O	1:C:1609:LYS:HB3	2.05	0.56
1:P:1575:ASP:HB2	1:P:1578:ARG:CZ	2.34	0.56
1:T:1528:ALA:O	1:T:1529:LYS:HB2	2.05	0.56
1:G:1554:LEU:HA	1:G:1557:PHE:CD2	2.40	0.56
1:J:1578:ARG:H	1:J:1579:PRO:CD	2.18	0.56
1:M:1545:LYS:HG2	1:M:1546:ASP:H	1.71	0.56
1:R:1530:LYS:HZ3	1:R:1563:ARG:CD	2.16	0.56
1:T:1579:PRO:HG3	1:U:1599:PHE:HB3	1.87	0.56
1:A:1509:HIS:ND1	1:A:1510:SER:N	2.54	0.56
1:B:1572:THR:HG23	1:B:1578:ARG:HB3	1.87	0.56
1:B:1606:TYR:HA	1:B:1609:LYS:HE2	1.87	0.56
1:C:1530:LYS:HZ3	1:C:1563:ARG:NE	2.03	0.56
1:C:1535:LYS:O	1:C:1536:ASP:HB2	2.05	0.56
1:D:1545:LYS:CG	1:D:1546:ASP:H	2.17	0.56
1:H:1580:ASP:HA	1:H:1583:LEU:HD13	1.85	0.56
1:K:1588:ARG:HA	1:K:1588:ARG:NE	2.21	0.56
1:O:1594:PHE:O	1:O:1595:ALA:HB2	2.03	0.56
1:R:1572:THR:CG2	1:R:1578:ARG:HB3	2.35	0.56
1:V:1560:GLU:HG3	1:V:1561:GLU:N	2.20	0.56
1:W:1580:ASP:HA	1:W:1583:LEU:HD13	1.87	0.56
1:A:1554:LEU:O	1:A:1558:LEU:HD13	2.06	0.56
1:F:1606:TYR:O	1:F:1609:LYS:HB3	2.06	0.56
1:M:1542:SER:C	1:M:1544:SER:H	2.08	0.56
1:N:1529:LYS:C	1:N:1530:LYS:HG2	2.26	0.56
1:R:1533:LEU:HD22	1:R:1534:TYR:N	2.18	0.56
1:R:1575:ASP:C	1:R:1576:LEU:HD22	2.25	0.56
1:T:1604:LYS:HD3	1:U:1612:LYS:HZ1	1.63	0.56
1:V:1519:HIS:N	1:V:1520:MET:HE1	2.20	0.56
1:B:1606:TYR:HA	1:B:1609:LYS:CE	2.36	0.56
1:C:1558:LEU:HD13	1:C:1565:CYS:HB3	1.87	0.56
1:I:1598:TYR:O	1:I:1602:VAL:HG23	2.04	0.56
1:K:1604:LYS:HG3	1:L:1609:LYS:CE	2.35	0.56
1:P:1509:HIS:O	1:P:1510:SER:CB	2.54	0.56
1:C:1575:ASP:C	1:C:1576:LEU:HD22	2.26	0.56
1:I:1579:PRO:HD3	1:I:1598:TYR:OH	2.06	0.56
1:I:1602:VAL:HA	1:I:1605:GLU:OE1	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:1621:LYS:O	1:L:1621:LYS:HD3	2.06	0.56
1:N:1542:SER:HA	1:N:1571:PHE:CE1	2.40	0.56
1:V:1509:HIS:ND1	1:V:1510:SER:N	2.52	0.56
1:V:1549:LEU:O	1:V:1553:LEU:HD13	2.06	0.56
1:X:1568:ALA:O	1:X:1571:PHE:HB3	2.06	0.56
1:O:1569:CYS:C	1:O:1571:PHE:H	2.09	0.56
1:O:1578:ARG:NE	1:O:1578:ARG:HA	2.21	0.56
1:O:1619:LEU:HD23	1:O:1622:GLU:OE2	2.06	0.56
1:W:1604:LYS:HG3	1:X:1609:LYS:CE	2.33	0.56
1:D:1508:HIS:CG	1:D:1509:HIS:H	2.24	0.56
1:D:1560:GLU:HG3	1:D:1561:GLU:H	1.69	0.56
1:R:1606:TYR:O	1:R:1609:LYS:HB3	2.06	0.56
1:E:1529:LYS:C	1:E:1530:LYS:HG2	2.27	0.56
1:G:1507:HIS:NE2	1:G:1522:LYS:HG2	2.21	0.56
1:J:1572:THR:CA	1:J:1578:ARG:NH2	2.55	0.56
1:T:1588:ARG:HA	1:T:1588:ARG:NE	2.21	0.56
1:D:1568:ALA:O	1:D:1571:PHE:HB3	2.06	0.56
1:L:1542:SER:HB2	1:L:1571:PHE:HD2	1.70	0.56
1:M:1549:LEU:O	1:M:1553:LEU:HD13	2.05	0.56
1:T:1554:LEU:HD11	1:T:1571:PHE:HD2	1.71	0.56
1:V:1507:HIS:O	1:V:1508:HIS:HB2	2.05	0.56
1:X:1572:THR:CG2	1:X:1578:ARG:HB3	2.34	0.56
1:X:1613:LEU:O	1:X:1617:GLU:HG3	2.05	0.56
1:G:1545:LYS:HG2	1:G:1546:ASP:N	2.21	0.55
1:N:1550:ALA:HB1	1:N:1571:PHE:CE2	2.41	0.55
1:N:1554:LEU:O	1:N:1558:LEU:HD13	2.06	0.55
1:N:1572:THR:HG23	1:N:1578:ARG:HB3	1.86	0.55
1:S:1558:LEU:CB	1:S:1585:LEU:HD13	2.35	0.55
1:U:1533:LEU:HD22	1:U:1534:TYR:N	2.17	0.55
1:V:1529:LYS:O	1:V:1530:LYS:CB	2.54	0.55
1:V:1572:THR:C	1:V:1578:ARG:HH22	2.09	0.55
1:C:1599:PHE:N	1:C:1599:PHE:CD2	2.73	0.55
1:K:1542:SER:HA	1:K:1571:PHE:CE1	2.41	0.55
1:L:1609:LYS:HA	1:L:1609:LYS:NZ	2.21	0.55
1:Q:1579:PRO:O	1:Q:1581:VAL:N	2.39	0.55
1:S:1507:HIS:NE2	1:S:1522:LYS:HG2	2.21	0.55
1:W:1548:GLU:HA	1:W:1551:GLU:OE1	2.05	0.55
1:B:1529:LYS:O	1:B:1530:LYS:HG2	2.06	0.55
1:N:1605:GLU:O	1:N:1609:LYS:HG3	2.06	0.55
1:S:1507:HIS:O	1:S:1508:HIS:HB2	2.06	0.55
1:V:1580:ASP:O	1:V:1584:GLU:OE2	2.23	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:1599:PHE:O	1:W:1602:VAL:N	2.40	0.55
1:D:1509:HIS:O	1:D:1510:SER:HB3	2.07	0.55
1:D:1578:ARG:H	1:D:1579:PRO:HD3	1.69	0.55
1:K:1593:ASP:CG	1:K:1594:PHE:H	2.09	0.55
1:B:1590:ASN:O	1:B:1592:MET:SD	2.65	0.55
1:L:1530:LYS:HZ3	1:L:1563:ARG:CD	2.19	0.55
1:L:1585:LEU:HD13	1:L:1588:ARG:HG3	1.88	0.55
1:Q:1584:GLU:O	1:Q:1588:ARG:NH1	2.40	0.55
1:Q:1592:MET:N	1:Q:1592:MET:HE2	2.21	0.55
1:U:1575:ASP:C	1:U:1576:LEU:HD22	2.27	0.55
1:A:1508:HIS:CD2	1:A:1509:HIS:H	2.24	0.55
1:E:1577:LEU:HB3	1:F:1603:MET:HE2	1.87	0.55
1:G:1558:LEU:HD12	1:G:1558:LEU:N	2.22	0.55
1:J:1521:TRP:O	1:J:1522:LYS:HB2	2.05	0.55
1:J:1560:GLU:HG3	1:J:1561:GLU:N	2.22	0.55
1:K:1579:PRO:HB2	1:L:1599:PHE:CD1	2.39	0.55
1:N:1554:LEU:HD11	1:N:1571:PHE:HD2	1.70	0.55
1:N:1581:VAL:O	1:N:1585:LEU:HD23	2.06	0.55
1:N:1583:LEU:HD21	1:O:1599:PHE:CE1	2.42	0.55
1:W:1606:TYR:CA	1:W:1609:LYS:HE2	2.34	0.55
1:B:1599:PHE:O	1:B:1602:VAL:N	2.40	0.55
1:Q:1593:ASP:O	1:Q:1594:PHE:HB2	2.05	0.55
1:B:1588:ARG:HA	1:B:1588:ARG:NE	2.22	0.55
1:F:1613:LEU:O	1:F:1617:GLU:HG3	2.07	0.55
1:J:1545:LYS:CG	1:J:1546:ASP:H	2.18	0.55
1:K:1583:LEU:HD12	1:K:1583:LEU:N	2.21	0.55
1:T:1534:TYR:O	1:T:1538:MET:SD	2.64	0.55
1:T:1577:LEU:HB3	1:U:1603:MET:HE2	1.88	0.55
1:V:1554:LEU:HA	1:V:1557:PHE:CD2	2.42	0.55
1:D:1545:LYS:HG2	1:D:1546:ASP:H	1.72	0.55
1:D:1578:ARG:H	1:D:1579:PRO:CD	2.20	0.55
1:F:1599:PHE:CD2	1:F:1599:PHE:N	2.74	0.55
1:F:1602:VAL:O	1:F:1602:VAL:HG12	2.06	0.55
1:N:1606:TYR:O	1:N:1610:VAL:HG23	2.06	0.55
1:O:1545:LYS:O	1:O:1546:ASP:HB2	2.06	0.55
1:O:1563:ARG:N	1:O:1564:GLU:OE1	2.40	0.55
1:O:1601:GLN:O	1:O:1605:GLU:CD	2.46	0.55
1:Q:1577:LEU:HD11	1:R:1606:TYR:HB3	1.88	0.55
1:A:1594:PHE:CG	1:A:1595:ALA:N	2.75	0.55
1:B:1554:LEU:HD11	1:B:1571:PHE:HD2	1.71	0.55
1:D:1609:LYS:O	1:D:1613:LEU:HG	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1535:LYS:O	1:I:1536:ASP:HB2	2.07	0.55
1:J:1542:SER:C	1:J:1544:SER:H	2.10	0.55
1:M:1560:GLU:OE1	1:M:1560:GLU:HA	2.06	0.55
1:X:1545:LYS:O	1:X:1546:ASP:HB2	2.07	0.55
1:C:1599:PHE:N	1:C:1599:PHE:HD2	2.05	0.54
1:D:1519:HIS:N	1:D:1520:MET:HE1	2.22	0.54
1:F:1533:LEU:HG	1:G:1588:ARG:HH12	1.71	0.54
1:F:1599:PHE:N	1:F:1599:PHE:HD2	2.05	0.54
1:H:1535:LYS:HZ3	1:H:1563:ARG:NH2	2.05	0.54
1:I:1525:VAL:HG12	1:I:1526:GLU:N	2.15	0.54
1:I:1575:ASP:C	1:I:1576:LEU:HD22	2.26	0.54
1:L:1599:PHE:N	1:L:1599:PHE:HD2	2.05	0.54
1:P:1594:PHE:CG	1:P:1595:ALA:N	2.75	0.54
1:Q:1605:GLU:O	1:Q:1609:LYS:HE2	2.07	0.54
1:S:1546:ASP:CB	1:S:1550:ALA:HB2	2.37	0.54
1:S:1560:GLU:O	1:S:1561:GLU:HB2	2.07	0.54
1:S:1575:ASP:HB2	1:S:1578:ARG:NH2	2.22	0.54
1:U:1619:LEU:HD23	1:U:1622:GLU:OE2	2.07	0.54
1:A:1529:LYS:O	1:A:1530:LYS:HB2	2.07	0.54
1:A:1580:ASP:O	1:A:1584:GLU:OE2	2.25	0.54
1:G:1515:PRO:O	1:G:1516:ARG:CB	2.55	0.54
1:I:1554:LEU:CD1	1:I:1568:ALA:HB1	2.37	0.54
1:N:1577:LEU:HD22	1:O:1602:VAL:HG12	1.89	0.54
1:V:1508:HIS:CG	1:V:1509:HIS:N	2.75	0.54
1:B:1548:GLU:HA	1:B:1551:GLU:OE1	2.07	0.54
1:C:1602:VAL:HA	1:C:1605:GLU:OE1	2.07	0.54
1:E:1554:LEU:HD11	1:E:1571:PHE:HD2	1.72	0.54
1:U:1525:VAL:HG12	1:U:1526:GLU:N	2.17	0.54
1:G:1554:LEU:O	1:G:1558:LEU:CD1	2.54	0.54
1:H:1591:ILE:C	1:H:1592:MET:SD	2.86	0.54
1:I:1578:ARG:HA	1:I:1578:ARG:NE	2.22	0.54
1:J:1577:LEU:HD12	1:J:1577:LEU:H	1.73	0.54
1:J:1594:PHE:CG	1:J:1595:ALA:N	2.73	0.54
1:L:1596:MET:N	1:L:1597:PRO:HD3	2.23	0.54
1:N:1584:GLU:O	1:N:1588:ARG:NH1	2.39	0.54
1:P:1529:LYS:O	1:P:1530:LYS:CB	2.55	0.54
1:T:1599:PHE:HA	1:T:1602:VAL:CG2	2.38	0.54
1:C:1585:LEU:HD13	1:C:1588:ARG:HG3	1.89	0.54
1:E:1545:LYS:HA	1:E:1571:PHE:HZ	1.73	0.54
1:G:1545:LYS:CG	1:G:1546:ASP:H	2.20	0.54
1:J:1565:CYS:O	1:J:1569:CYS:SG	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:1604:LYS:CG	1:L:1609:LYS:HD2	2.36	0.54
1:L:1533:LEU:HD13	1:L:1534:TYR:CD1	2.41	0.54
1:N:1579:PRO:HB2	1:O:1599:PHE:CD1	2.42	0.54
1:N:1580:ASP:HA	1:N:1583:LEU:HD13	1.90	0.54
1:O:1535:LYS:O	1:O:1536:ASP:HB2	2.07	0.54
1:P:1529:LYS:NZ	1:P:1529:LYS:HB3	2.23	0.54
1:S:1545:LYS:HG2	1:S:1546:ASP:H	1.72	0.54
1:U:1554:LEU:HD12	1:U:1568:ALA:HB1	1.88	0.54
1:U:1591:ILE:CG2	1:U:1592:MET:H	2.20	0.54
1:B:1584:GLU:O	1:B:1588:ARG:NH1	2.41	0.54
1:H:1558:LEU:HA	1:H:1565:CYS:SG	2.48	0.54
1:I:1561:GLU:HB3	1:I:1564:GLU:HB2	1.89	0.54
1:L:1551:GLU:HA	1:L:1554:LEU:HD23	1.89	0.54
1:L:1586:ALA:CB	1:L:1592:MET:HB2	2.38	0.54
1:T:1585:LEU:HA	1:T:1588:ARG:HD2	1.90	0.54
1:U:1577:LEU:O	1:U:1578:ARG:HB2	2.08	0.54
1:U:1581:VAL:C	1:U:1583:LEU:N	2.61	0.54
1:X:1530:LYS:HZ3	1:X:1563:ARG:HD2	1.71	0.54
1:X:1569:CYS:C	1:X:1571:PHE:H	2.11	0.54
1:X:1575:ASP:C	1:X:1576:LEU:HD22	2.28	0.54
1:X:1595:ALA:C	1:X:1597:PRO:HD3	2.28	0.54
1:A:1513:LEU:HD13	1:A:1513:LEU:C	2.28	0.54
1:B:1604:LYS:HE3	1:C:1609:LYS:HD2	1.90	0.54
1:C:1537:ALA:HB3	1:C:1538:MET:HE1	1.90	0.54
1:D:1580:ASP:O	1:D:1581:VAL:C	2.45	0.54
1:J:1554:LEU:HA	1:J:1557:PHE:CD2	2.42	0.54
1:J:1580:ASP:O	1:J:1584:GLU:OE2	2.24	0.54
1:P:1549:LEU:HD22	1:P:1549:LEU:H	1.71	0.54
1:R:1535:LYS:O	1:R:1536:ASP:HB2	2.07	0.54
1:R:1577:LEU:HD22	1:R:1598:TYR:CE2	2.42	0.54
1:V:1577:LEU:H	1:V:1577:LEU:HD12	1.72	0.54
1:A:1549:LEU:O	1:A:1553:LEU:HD13	2.07	0.54
1:F:1568:ALA:O	1:F:1571:PHE:HB3	2.08	0.54
1:M:1572:THR:CA	1:M:1578:ARG:HH22	2.16	0.54
1:P:1577:LEU:H	1:P:1577:LEU:HD12	1.73	0.54
1:C:1609:LYS:HA	1:C:1609:LYS:NZ	2.23	0.54
1:J:1529:LYS:NZ	1:J:1529:LYS:HB3	2.22	0.54
1:M:1541:ALA:HB3	1:M:1571:PHE:HE2	1.72	0.54
1:N:1579:PRO:HB2	1:O:1599:PHE:HD1	1.73	0.54
1:O:1599:PHE:HA	1:O:1602:VAL:CG2	2.38	0.54
1:J:1575:ASP:HB2	1:J:1578:ARG:NH1	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1507:HIS:O	1:M:1508:HIS:HB2	2.07	0.54
1:N:1574:TYR:C	1:N:1576:LEU:H	2.12	0.54
1:O:1533:LEU:HD13	1:O:1534:TYR:CE1	2.43	0.54
1:S:1542:SER:C	1:S:1544:SER:H	2.11	0.54
1:T:1583:LEU:N	1:T:1583:LEU:HD12	2.23	0.54
1:W:1542:SER:HA	1:W:1571:PHE:CE1	2.43	0.54
1:A:1562:LYS:HD3	1:A:1562:LYS:N	2.22	0.53
1:I:1602:VAL:O	1:I:1602:VAL:CG1	2.56	0.53
1:P:1555:GLN:OE1	1:P:1555:GLN:N	2.40	0.53
1:P:1587:TRP:HA	1:P:1587:TRP:CE3	2.41	0.53
1:S:1549:LEU:O	1:S:1553:LEU:HD13	2.08	0.53
1:U:1581:VAL:C	1:U:1583:LEU:H	2.11	0.53
1:E:1591:ILE:C	1:E:1592:MET:SD	2.87	0.53
1:G:1587:TRP:CE3	1:G:1587:TRP:HA	2.43	0.53
1:O:1599:PHE:CD2	1:O:1599:PHE:N	2.76	0.53
1:T:1531:ASP:HA	1:T:1534:TYR:CD1	2.44	0.53
1:C:1530:LYS:HZ3	1:C:1563:ARG:CD	2.22	0.53
1:F:1533:LEU:HD13	1:F:1534:TYR:CE1	2.43	0.53
1:O:1575:ASP:C	1:O:1576:LEU:HD22	2.29	0.53
1:R:1533:LEU:HD13	1:R:1534:TYR:CE1	2.43	0.53
1:V:1555:GLN:O	1:V:1559:GLN:N	2.41	0.53
1:B:1592:MET:SD	1:B:1592:MET:N	2.79	0.53
1:C:1595:ALA:C	1:C:1597:PRO:HD3	2.28	0.53
1:C:1599:PHE:HA	1:C:1602:VAL:CG2	2.39	0.53
1:F:1591:ILE:CG2	1:F:1592:MET:N	2.71	0.53
1:F:1619:LEU:HD23	1:F:1622:GLU:OE2	2.09	0.53
1:G:1611:ASP:HB3	1:H:1612:LYS:HZ1	1.72	0.53
1:P:1513:LEU:C	1:P:1513:LEU:HD13	2.29	0.53
1:R:1608:THR:O	1:R:1608:THR:HG22	2.08	0.53
1:S:1513:LEU:HD13	1:S:1513:LEU:O	2.08	0.53
1:U:1603:MET:O	1:U:1605:GLU:N	2.41	0.53
1:X:1533:LEU:HD13	1:X:1534:TYR:CE1	2.44	0.53
1:K:1580:ASP:HA	1:K:1583:LEU:HD13	1.90	0.53
1:L:1592:MET:SD	1:L:1593:ASP:N	2.82	0.53
1:M:1546:ASP:CB	1:M:1550:ALA:HB2	2.38	0.53
1:U:1613:LEU:O	1:U:1617:GLU:HG3	2.08	0.53
1:W:1583:LEU:O	1:W:1586:ALA:HB3	2.09	0.53
1:X:1583:LEU:N	1:X:1583:LEU:HD22	2.24	0.53
1:C:1549:LEU:HD13	1:C:1552:GLU:OE2	2.08	0.53
1:C:1614:ASP:HB3	1:P:1624:GLU:OE1	2.09	0.53
1:E:1583:LEU:HD11	1:F:1599:PHE:HE1	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1549:LEU:O	1:G:1553:LEU:HD13	2.08	0.53
1:H:1581:VAL:O	1:H:1581:VAL:HG12	2.08	0.53
1:I:1550:ALA:O	1:I:1553:LEU:HB2	2.08	0.53
1:K:1592:MET:HE2	1:K:1592:MET:N	2.24	0.53
1:N:1556:TRP:HE1	1:X:1513:LEU:HD23	1.74	0.53
1:O:1602:VAL:HA	1:O:1605:GLU:OE1	2.09	0.53
1:P:1532:SER:O	1:P:1533:LEU:HB2	2.09	0.53
1:B:1542:SER:HA	1:B:1571:PHE:CE1	2.44	0.53
1:M:1532:SER:O	1:M:1533:LEU:HB2	2.09	0.53
1:M:1578:ARG:H	1:M:1579:PRO:HD3	1.73	0.53
1:N:1583:LEU:HD12	1:N:1583:LEU:N	2.23	0.53
1:R:1591:ILE:CG2	1:R:1592:MET:H	2.19	0.53
1:U:1519:HIS:HE1	1:U:1540:TYR:OH	1.91	0.53
1:U:1579:PRO:HG2	1:U:1580:ASP:OD1	2.09	0.53
1:D:1516:ARG:HG3	1:D:1516:ARG:O	2.07	0.53
1:E:1542:SER:HA	1:E:1571:PHE:CE1	2.43	0.53
1:F:1533:LEU:HD22	1:F:1534:TYR:N	2.19	0.53
1:G:1601:GLN:NE2	1:G:1601:GLN:H	2.07	0.53
1:K:1572:THR:HG23	1:K:1578:ARG:HB3	1.91	0.53
1:L:1619:LEU:HA	1:L:1622:GLU:OE2	2.09	0.53
1:P:1554:LEU:O	1:P:1555:GLN:C	2.47	0.53
1:R:1578:ARG:NE	1:R:1578:ARG:HA	2.24	0.53
1:R:1596:MET:N	1:R:1597:PRO:HD3	2.24	0.53
1:G:1507:HIS:O	1:G:1508:HIS:HB2	2.08	0.53
1:I:1568:ALA:O	1:I:1571:PHE:HB3	2.08	0.53
1:J:1549:LEU:O	1:J:1553:LEU:HD13	2.09	0.53
1:K:1545:LYS:HA	1:K:1571:PHE:HZ	1.73	0.53
1:K:1592:MET:SD	1:K:1592:MET:N	2.82	0.53
1:B:1558:LEU:HA	1:B:1565:CYS:SG	2.48	0.53
1:D:1577:LEU:H	1:D:1577:LEU:HD12	1.74	0.53
1:G:1529:LYS:NZ	1:G:1529:LYS:HB3	2.23	0.53
1:I:1577:LEU:HD22	1:I:1598:TYR:CE2	2.43	0.53
1:I:1606:TYR:O	1:I:1609:LYS:HB3	2.08	0.53
1:O:1532:SER:HB2	1:S:1588:ARG:CD	2.39	0.53
1:A:1551:GLU:HB3	1:A:1555:GLN:HE22	1.73	0.52
1:Q:1583:LEU:N	1:Q:1583:LEU:HD12	2.25	0.52
1:C:1533:LEU:HD22	1:C:1534:TYR:N	2.21	0.52
1:K:1550:ALA:HB1	1:K:1571:PHE:CE2	2.44	0.52
1:O:1558:LEU:CD1	1:O:1565:CYS:HB3	2.36	0.52
1:Q:1539:GLN:OE1	1:Q:1539:GLN:N	2.42	0.52
1:W:1558:LEU:HA	1:W:1565:CYS:SG	2.49	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1575:ASP:C	1:F:1576:LEU:HD22	2.28	0.52
1:V:1515:PRO:O	1:V:1516:ARG:HB3	2.09	0.52
1:X:1591:ILE:CG2	1:X:1592:MET:N	2.73	0.52
1:D:1549:LEU:O	1:D:1553:LEU:HD13	2.09	0.52
1:D:1554:LEU:HA	1:D:1557:PHE:CD2	2.44	0.52
1:U:1568:ALA:O	1:U:1571:PHE:HB3	2.09	0.52
1:V:1601:GLN:NE2	1:V:1601:GLN:H	2.08	0.52
1:A:1507:HIS:NE2	1:A:1522:LYS:HG2	2.25	0.52
1:A:1611:ASP:HB3	1:B:1612:LYS:HZ3	1.73	0.52
1:C:1555:GLN:O	1:C:1559:GLN:HG2	2.10	0.52
1:F:1598:TYR:O	1:F:1602:VAL:HG23	2.09	0.52
1:G:1593:ASP:HA	1:I:1587:TRP:CZ3	2.45	0.52
1:I:1530:LYS:HZ1	1:I:1563:ARG:CZ	2.21	0.52
1:I:1533:LEU:HD13	1:I:1534:TYR:CE1	2.45	0.52
1:I:1577:LEU:O	1:I:1578:ARG:HB2	2.09	0.52
1:J:1578:ARG:N	1:J:1579:PRO:CD	2.73	0.52
1:O:1533:LEU:HD22	1:O:1534:TYR:N	2.20	0.52
1:U:1585:LEU:HD13	1:U:1588:ARG:HG3	1.90	0.52
1:V:1558:LEU:N	1:V:1558:LEU:HD12	2.24	0.52
1:A:1612:LYS:HE2	1:C:1608:THR:CG2	2.40	0.52
1:D:1602:VAL:CG1	1:F:1577:LEU:HD13	2.39	0.52
1:E:1583:LEU:HD12	1:E:1583:LEU:N	2.25	0.52
1:H:1563:ARG:HG2	1:H:1564:GLU:OE1	2.09	0.52
1:H:1588:ARG:HA	1:H:1588:ARG:NE	2.23	0.52
1:N:1592:MET:HE2	1:N:1592:MET:N	2.24	0.52
1:P:1545:LYS:CG	1:P:1546:ASP:H	2.22	0.52
1:U:1583:LEU:N	1:U:1583:LEU:HD22	2.24	0.52
1:X:1578:ARG:NE	1:X:1578:ARG:HA	2.24	0.52
1:I:1609:LYS:HA	1:I:1609:LYS:NZ	2.24	0.52
1:M:1519:HIS:N	1:M:1520:MET:HE1	2.25	0.52
1:U:1586:ALA:CB	1:U:1592:MET:HB2	2.39	0.52
1:A:1532:SER:O	1:A:1533:LEU:HB2	2.09	0.52
1:F:1530:LYS:HZ3	1:F:1563:ARG:HD2	1.74	0.52
1:S:1515:PRO:O	1:S:1516:ARG:HB3	2.10	0.52
1:U:1577:LEU:HD22	1:U:1598:TYR:CE2	2.45	0.52
1:V:1521:TRP:O	1:V:1522:LYS:HB2	2.08	0.52
1:G:1551:GLU:HB3	1:G:1555:GLN:HE22	1.75	0.52
1:J:1575:ASP:HB2	1:J:1578:ARG:NH2	2.25	0.52
1:L:1623:GLU:HG3	1:L:1624:GLU:H	1.75	0.52
1:O:1599:PHE:N	1:O:1599:PHE:HD2	2.07	0.52
1:P:1509:HIS:ND1	1:P:1510:SER:N	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1545:LYS:HG2	1:P:1546:ASP:N	2.25	0.52
1:S:1551:GLU:HB3	1:S:1555:GLN:HE22	1.75	0.52
1:T:1563:ARG:HG2	1:T:1564:GLU:OE1	2.08	0.52
1:V:1551:GLU:O	1:V:1553:LEU:N	2.42	0.52
1:W:1605:GLU:HG2	1:W:1606:TYR:N	2.23	0.52
1:W:1608:THR:CG2	1:W:1612:LYS:HZ1	2.23	0.52
1:F:1595:ALA:C	1:F:1597:PRO:HD3	2.30	0.52
1:J:1549:LEU:HD22	1:J:1549:LEU:H	1.75	0.52
1:R:1568:ALA:O	1:R:1571:PHE:HB3	2.10	0.52
1:S:1596:MET:N	1:S:1597:PRO:CD	2.73	0.52
1:V:1516:ARG:HG3	1:V:1516:ARG:O	2.08	0.52
1:X:1559:GLN:NE2	1:X:1585:LEU:HD11	2.25	0.52
1:F:1530:LYS:HZ3	1:F:1563:ARG:NE	2.08	0.51
1:G:1508:HIS:CD2	1:G:1509:HIS:H	2.28	0.51
1:K:1548:GLU:HA	1:K:1551:GLU:OE1	2.10	0.51
1:O:1519:HIS:HE1	1:O:1540:TYR:OH	1.93	0.51
1:R:1542:SER:HB2	1:R:1571:PHE:HD2	1.75	0.51
1:M:1568:ALA:O	1:M:1571:PHE:HB3	2.10	0.51
1:S:1529:LYS:NZ	1:S:1529:LYS:HB3	2.24	0.51
1:T:1548:GLU:HA	1:T:1551:GLU:OE1	2.10	0.51
1:U:1592:MET:SD	1:U:1594:PHE:O	2.68	0.51
1:V:1578:ARG:N	1:V:1579:PRO:CD	2.71	0.51
1:A:1515:PRO:O	1:A:1516:ARG:HB3	2.09	0.51
1:C:1579:PRO:HD3	1:C:1598:TYR:OH	2.09	0.51
1:E:1583:LEU:HD22	1:F:1596:MET:CG	2.40	0.51
1:E:1583:LEU:O	1:E:1586:ALA:HB3	2.10	0.51
1:F:1599:PHE:HA	1:F:1602:VAL:CG2	2.40	0.51
1:L:1595:ALA:C	1:L:1597:PRO:HD3	2.31	0.51
1:Q:1534:TYR:O	1:Q:1538:MET:SD	2.68	0.51
1:R:1545:LYS:O	1:R:1546:ASP:HB2	2.10	0.51
1:R:1595:ALA:C	1:R:1597:PRO:HD3	2.31	0.51
1:A:1538:MET:O	1:A:1538:MET:HG2	2.11	0.51
1:C:1581:VAL:C	1:C:1583:LEU:H	2.12	0.51
1:I:1533:LEU:HD22	1:I:1534:TYR:N	2.19	0.51
1:L:1535:LYS:O	1:L:1536:ASP:HB2	2.11	0.51
1:M:1549:LEU:HD22	1:M:1549:LEU:H	1.74	0.51
1:O:1548:GLU:O	1:O:1551:GLU:N	2.43	0.51
1:P:1549:LEU:O	1:P:1553:LEU:HD13	2.10	0.51
1:P:1560:GLU:HG3	1:P:1561:GLU:H	1.75	0.51
1:S:1509:HIS:ND1	1:S:1510:SER:N	2.59	0.51
1:U:1535:LYS:O	1:U:1536:ASP:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1569:CYS:C	1:U:1571:PHE:H	2.14	0.51
1:V:1549:LEU:H	1:V:1549:LEU:HD22	1.75	0.51
1:C:1592:MET:SD	1:C:1593:ASP:N	2.83	0.51
1:F:1535:LYS:O	1:F:1536:ASP:HB2	2.11	0.51
1:F:1542:SER:HB2	1:F:1571:PHE:HD2	1.75	0.51
1:F:1558:LEU:HD13	1:F:1565:CYS:SG	2.51	0.51
1:G:1549:LEU:H	1:G:1549:LEU:HD22	1.75	0.51
1:K:1560:GLU:HG2	1:K:1561:GLU:H	1.76	0.51
1:K:1604:LYS:HZ2	1:L:1609:LYS:HD3	1.76	0.51
1:L:1613:LEU:O	1:L:1617:GLU:HG3	2.10	0.51
1:K:1604:LYS:NZ	1:L:1613:LEU:CD2	2.74	0.51
1:S:1566:PHE:O	1:S:1569:CYS:HB2	2.11	0.51
1:V:1509:HIS:O	1:V:1510:SER:CB	2.58	0.51
1:A:1507:HIS:O	1:A:1508:HIS:HB2	2.10	0.51
1:A:1575:ASP:HB2	1:A:1578:ARG:CZ	2.41	0.51
1:C:1607:LEU:C	1:C:1609:LYS:H	2.13	0.51
1:L:1619:LEU:HD23	1:L:1622:GLU:OE2	2.11	0.51
1:P:1516:ARG:HG3	1:P:1516:ARG:O	2.10	0.51
1:R:1554:LEU:O	1:R:1558:LEU:HD23	2.10	0.51
1:R:1557:PHE:C	1:R:1561:GLU:OE1	2.49	0.51
1:T:1590:ASN:O	1:T:1592:MET:HE1	2.10	0.51
1:U:1607:LEU:C	1:U:1609:LYS:N	2.64	0.51
1:A:1566:PHE:O	1:A:1569:CYS:HB2	2.10	0.51
1:B:1586:ALA:HA	1:B:1592:MET:HG2	1.92	0.51
1:C:1533:LEU:HD13	1:C:1534:TYR:CE1	2.46	0.51
1:F:1530:LYS:HZ3	1:F:1563:ARG:CD	2.24	0.51
1:F:1596:MET:HE2	1:F:1596:MET:O	2.10	0.51
1:G:1508:HIS:CG	1:G:1509:HIS:N	2.78	0.51
1:I:1530:LYS:HZ3	1:I:1563:ARG:HD2	1.76	0.51
1:J:1602:VAL:HG13	1:L:1577:LEU:HD13	1.92	0.51
1:M:1515:PRO:O	1:M:1516:ARG:CB	2.58	0.51
1:M:1601:GLN:NE2	1:M:1601:GLN:H	2.09	0.51
1:O:1607:LEU:C	1:O:1609:LYS:H	2.14	0.51
1:R:1599:PHE:HA	1:R:1602:VAL:HG21	1.92	0.51
1:S:1568:ALA:O	1:S:1571:PHE:HB3	2.09	0.51
1:X:1599:PHE:HA	1:X:1602:VAL:CG2	2.41	0.51
1:F:1525:VAL:HG12	1:F:1526:GLU:N	2.18	0.51
1:I:1582:VAL:C	1:I:1583:LEU:HD13	2.31	0.51
1:M:1516:ARG:HG3	1:M:1516:ARG:O	2.11	0.51
1:N:1605:GLU:HG2	1:N:1606:TYR:CD2	2.45	0.51
1:W:1583:LEU:N	1:W:1583:LEU:HD12	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1619:LEU:HD23	1:C:1622:GLU:OE2	2.11	0.51
1:F:1577:LEU:HD22	1:F:1598:TYR:CE2	2.46	0.51
1:K:1606:TYR:HA	1:K:1609:LYS:HE2	1.92	0.51
1:M:1610:VAL:HA	1:M:1613:LEU:CD1	2.34	0.51
1:N:1539:GLN:OE1	1:N:1539:GLN:N	2.44	0.51
1:N:1606:TYR:HA	1:N:1609:LYS:CE	2.41	0.51
1:O:1537:ALA:HB3	1:O:1538:MET:CE	2.40	0.51
1:R:1609:LYS:NZ	1:R:1609:LYS:HA	2.25	0.51
1:U:1530:LYS:HZ1	1:U:1563:ARG:CZ	2.23	0.51
1:U:1554:LEU:O	1:U:1558:LEU:HD23	2.11	0.51
1:W:1604:LYS:HZ3	1:X:1613:LEU:HD21	1.76	0.51
1:B:1529:LYS:C	1:B:1530:LYS:HG2	2.32	0.50
1:C:1537:ALA:HB3	1:C:1538:MET:CE	2.41	0.50
1:E:1560:GLU:HG2	1:E:1561:GLU:H	1.77	0.50
1:F:1569:CYS:C	1:F:1571:PHE:H	2.14	0.50
1:P:1599:PHE:HB2	1:R:1580:ASP:OD2	2.10	0.50
1:R:1579:PRO:HG2	1:R:1580:ASP:OD1	2.11	0.50
1:S:1578:ARG:N	1:S:1579:PRO:CD	2.74	0.50
1:T:1607:LEU:HD23	1:U:1612:LYS:HD2	1.93	0.50
1:U:1555:GLN:O	1:U:1559:GLN:HG2	2.11	0.50
1:V:1545:LYS:CG	1:V:1546:ASP:N	2.71	0.50
1:W:1607:LEU:CD2	1:X:1612:LYS:HZ1	2.23	0.50
1:X:1585:LEU:O	1:X:1588:ARG:HB2	2.12	0.50
1:X:1599:PHE:N	1:X:1599:PHE:CD2	2.80	0.50
1:D:1572:THR:CA	1:D:1578:ARG:NH2	2.55	0.50
1:H:1593:ASP:O	1:H:1594:PHE:HB2	2.11	0.50
1:K:1593:ASP:O	1:K:1594:PHE:HB2	2.10	0.50
1:L:1530:LYS:HZ3	1:L:1563:ARG:NE	2.09	0.50
1:L:1602:VAL:O	1:L:1602:VAL:CG1	2.57	0.50
1:M:1594:PHE:CG	1:M:1595:ALA:N	2.79	0.50
1:U:1608:THR:O	1:U:1608:THR:HG22	2.11	0.50
1:C:1525:VAL:CG1	1:C:1526:GLU:H	2.17	0.50
1:H:1548:GLU:HA	1:H:1551:GLU:OE1	2.12	0.50
1:L:1530:LYS:HZ1	1:L:1563:ARG:CZ	2.23	0.50
1:N:1546:ASP:N	1:N:1550:ALA:HB2	2.03	0.50
1:N:1560:GLU:HG2	1:N:1561:GLU:H	1.77	0.50
1:T:1580:ASP:HA	1:T:1583:LEU:HD13	1.92	0.50
1:U:1539:GLN:O	1:U:1542:SER:OG	2.19	0.50
1:W:1531:ASP:HA	1:W:1534:TYR:CD1	2.46	0.50
1:A:1578:ARG:N	1:A:1579:PRO:CD	2.74	0.50
1:D:1583:LEU:HD22	1:E:1596:MET:SD	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1608:THR:HG22	1:F:1608:THR:O	2.11	0.50
1:I:1558:LEU:HA	1:I:1565:CYS:SG	2.51	0.50
1:Q:1531:ASP:HA	1:Q:1534:TYR:CD1	2.47	0.50
1:R:1525:VAL:HG12	1:R:1526:GLU:N	2.20	0.50
1:X:1535:LYS:O	1:X:1536:ASP:CB	2.60	0.50
1:C:1530:LYS:HZ3	1:C:1563:ARG:HD2	1.75	0.50
1:L:1586:ALA:HB2	1:L:1592:MET:HB2	1.93	0.50
1:M:1529:LYS:O	1:M:1530:LYS:CB	2.59	0.50
1:U:1598:TYR:O	1:U:1602:VAL:HG23	2.11	0.50
1:X:1572:THR:HA	1:X:1575:ASP:HB2	1.94	0.50
1:A:1612:LYS:O	1:A:1615:ALA:HB3	2.12	0.50
1:G:1560:GLU:HG3	1:G:1561:GLU:H	1.75	0.50
1:H:1534:TYR:O	1:H:1538:MET:SD	2.69	0.50
1:H:1574:TYR:C	1:H:1576:LEU:H	2.15	0.50
1:L:1579:PRO:HA	1:L:1582:VAL:CG2	2.41	0.50
1:L:1602:VAL:CA	1:L:1605:GLU:OE1	2.59	0.50
1:M:1554:LEU:HA	1:M:1557:PHE:CD2	2.46	0.50
1:M:1578:ARG:H	1:M:1579:PRO:CD	2.24	0.50
1:O:1579:PRO:HD3	1:O:1598:TYR:OH	2.12	0.50
1:O:1613:LEU:O	1:O:1617:GLU:HG3	2.12	0.50
1:W:1584:GLU:O	1:W:1588:ARG:NH1	2.45	0.50
1:A:1568:ALA:O	1:A:1571:PHE:HB3	2.11	0.50
1:A:1587:TRP:HA	1:A:1587:TRP:CE3	2.47	0.50
1:B:1539:GLN:N	1:B:1539:GLN:OE1	2.44	0.50
1:B:1574:TYR:C	1:B:1576:LEU:H	2.14	0.50
1:C:1525:VAL:HG12	1:C:1526:GLU:N	2.16	0.50
1:F:1602:VAL:C	1:F:1605:GLU:OE1	2.50	0.50
1:H:1531:ASP:HA	1:H:1534:TYR:CD1	2.47	0.50
1:P:1578:ARG:N	1:P:1579:PRO:CD	2.73	0.50
1:D:1529:LYS:HB3	1:D:1529:LYS:NZ	2.26	0.50
1:I:1547:THR:CG2	1:I:1548:GLU:H	2.22	0.50
1:T:1574:TYR:C	1:T:1576:LEU:H	2.14	0.50
1:T:1608:THR:O	1:T:1608:THR:HG22	2.12	0.50
1:W:1599:PHE:HA	1:W:1602:VAL:CG2	2.41	0.50
1:A:1519:HIS:N	1:A:1520:MET:HE1	2.27	0.50
1:B:1563:ARG:HG2	1:B:1564:GLU:OE1	2.12	0.50
1:D:1546:ASP:CB	1:D:1550:ALA:HB2	2.42	0.50
1:F:1537:ALA:HB3	1:F:1538:MET:CE	2.42	0.50
1:F:1603:MET:O	1:F:1605:GLU:N	2.45	0.50
1:H:1557:PHE:C	1:H:1558:LEU:HD12	2.32	0.50
1:I:1569:CYS:C	1:I:1571:PHE:H	2.15	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1587:TRP:HA	1:M:1587:TRP:CE3	2.46	0.50
1:O:1514:VAL:CG1	1:T:1531:ASP:CG	2.80	0.50
1:O:1599:PHE:HA	1:O:1602:VAL:HG21	1.93	0.50
1:Q:1583:LEU:O	1:Q:1586:ALA:HB3	2.11	0.50
1:S:1529:LYS:O	1:S:1530:LYS:CB	2.59	0.50
1:U:1602:VAL:HA	1:U:1605:GLU:CD	2.32	0.50
1:W:1559:GLN:HE22	1:W:1560:GLU:HB3	1.77	0.50
1:E:1577:LEU:HD22	1:F:1602:VAL:HG12	1.94	0.49
1:F:1537:ALA:HB3	1:F:1538:MET:HE1	1.94	0.49
1:G:1583:LEU:N	1:G:1583:LEU:HD12	2.26	0.49
1:P:1594:PHE:N	1:R:1587:TRP:CZ3	2.71	0.49
1:S:1587:TRP:CZ2	1:T:1591:ILE:HB	2.47	0.49
1:W:1567:GLY:HA2	1:W:1570:LEU:CD1	2.42	0.49
1:X:1621:LYS:O	1:X:1621:LYS:HD3	2.12	0.49
1:C:1579:PRO:HG2	1:C:1580:ASP:OD1	2.11	0.49
1:G:1578:ARG:N	1:G:1579:PRO:CD	2.73	0.49
1:J:1572:THR:C	1:J:1578:ARG:HH22	2.15	0.49
1:P:1554:LEU:HA	1:P:1557:PHE:CD2	2.48	0.49
1:P:1568:ALA:HA	1:P:1571:PHE:HB3	1.93	0.49
1:S:1554:LEU:HA	1:S:1557:PHE:CD2	2.47	0.49
1:X:1585:LEU:HD13	1:X:1588:ARG:CG	2.42	0.49
1:D:1549:LEU:H	1:D:1549:LEU:HD22	1.76	0.49
1:N:1604:LYS:HD2	1:O:1612:LYS:HZ3	1.76	0.49
1:P:1515:PRO:O	1:P:1516:ARG:CB	2.59	0.49
1:Q:1554:LEU:HD11	1:Q:1571:PHE:CD2	2.45	0.49
1:S:1558:LEU:HB2	1:S:1585:LEU:HD13	1.94	0.49
1:T:1539:GLN:OE1	1:T:1539:GLN:N	2.45	0.49
1:T:1560:GLU:HG2	1:T:1561:GLU:H	1.77	0.49
1:T:1606:TYR:HA	1:T:1609:LYS:HE2	1.94	0.49
1:U:1530:LYS:HZ3	1:U:1563:ARG:HD2	1.77	0.49
1:U:1599:PHE:HA	1:U:1602:VAL:CG2	2.43	0.49
1:B:1605:GLU:HG2	1:B:1606:TYR:CD2	2.47	0.49
1:E:1579:PRO:HG2	1:E:1580:ASP:OD1	2.12	0.49
1:M:1583:LEU:HD12	1:M:1583:LEU:N	2.27	0.49
1:P:1566:PHE:O	1:P:1569:CYS:HB2	2.13	0.49
1:S:1532:SER:O	1:S:1533:LEU:HB2	2.12	0.49
1:A:1541:ALA:HB3	1:A:1571:PHE:CE2	2.48	0.49
1:H:1583:LEU:O	1:H:1586:ALA:HB3	2.11	0.49
1:J:1532:SER:O	1:J:1533:LEU:HB2	2.12	0.49
1:L:1575:ASP:C	1:L:1576:LEU:HD22	2.33	0.49
1:N:1558:LEU:HD23	1:N:1585:LEU:HG	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:1606:TYR:O	1:O:1609:LYS:HB3	2.12	0.49
1:Q:1580:ASP:CA	1:Q:1583:LEU:HD13	2.42	0.49
1:R:1558:LEU:CD1	1:R:1565:CYS:HB3	2.42	0.49
1:S:1549:LEU:HD22	1:S:1549:LEU:H	1.78	0.49
1:V:1575:ASP:HB2	1:V:1578:ARG:NH2	2.27	0.49
1:W:1537:ALA:C	1:W:1539:GLN:N	2.65	0.49
1:W:1580:ASP:CA	1:W:1583:LEU:HD13	2.42	0.49
1:X:1530:LYS:HZ1	1:X:1563:ARG:CZ	2.25	0.49
1:X:1579:PRO:HG2	1:X:1580:ASP:OD1	2.13	0.49
1:B:1560:GLU:HG2	1:B:1561:GLU:H	1.78	0.49
1:C:1582:VAL:C	1:C:1583:LEU:HD13	2.33	0.49
1:H:1606:TYR:O	1:H:1610:VAL:HG23	2.12	0.49
1:M:1520:MET:N	1:M:1520:MET:SD	2.85	0.49
1:N:1605:GLU:O	1:N:1609:LYS:HE2	2.13	0.49
1:N:1606:TYR:HA	1:N:1609:LYS:HE2	1.95	0.49
1:R:1551:GLU:HA	1:R:1554:LEU:HD23	1.95	0.49
1:C:1559:GLN:NE2	1:C:1585:LEU:HD11	2.27	0.49
1:G:1568:ALA:O	1:G:1571:PHE:HB3	2.13	0.49
1:J:1519:HIS:N	1:J:1520:MET:HE1	2.27	0.49
1:T:1537:ALA:C	1:T:1539:GLN:N	2.66	0.49
1:T:1604:LYS:CD	1:U:1612:LYS:HE2	2.42	0.49
1:K:1590:ASN:O	1:K:1592:MET:SD	2.70	0.49
1:K:1604:LYS:HE3	1:L:1609:LYS:HD2	1.94	0.49
1:M:1580:ASP:O	1:M:1584:GLU:OE2	2.31	0.49
1:O:1532:SER:HB2	1:S:1588:ARG:CZ	2.41	0.49
1:T:1600:ILE:HG22	1:U:1609:LYS:HD2	1.94	0.49
1:T:1606:TYR:HA	1:T:1609:LYS:CE	2.42	0.49
1:U:1572:THR:CG2	1:U:1578:ARG:HB3	2.43	0.49
1:X:1609:LYS:HA	1:X:1609:LYS:NZ	2.28	0.49
1:X:1623:GLU:HG3	1:X:1624:GLU:H	1.77	0.49
1:B:1534:TYR:O	1:B:1538:MET:SD	2.71	0.49
1:G:1558:LEU:CB	1:G:1585:LEU:HD13	2.41	0.49
1:N:1531:ASP:HA	1:N:1534:TYR:CD1	2.48	0.49
1:N:1563:ARG:HG2	1:N:1564:GLU:OE1	2.13	0.49
1:S:1508:HIS:CD2	1:S:1509:HIS:H	2.30	0.49
1:S:1513:LEU:HD22	1:S:1514:VAL:N	2.28	0.49
1:S:1554:LEU:O	1:S:1558:LEU:HD13	2.13	0.49
1:C:1572:THR:CG2	1:C:1578:ARG:HB3	2.42	0.49
1:E:1558:LEU:HD23	1:E:1585:LEU:HG	1.94	0.49
1:F:1623:GLU:HG3	1:F:1624:GLU:H	1.78	0.49
1:I:1525:VAL:HG21	1:I:1563:ARG:HH12	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1613:LEU:O	1:I:1617:GLU:HG3	2.13	0.49
1:L:1542:SER:HB2	1:L:1571:PHE:CD2	2.47	0.49
1:N:1593:ASP:O	1:N:1594:PHE:HB2	2.11	0.49
1:P:1545:LYS:HG2	1:P:1546:ASP:H	1.77	0.49
1:W:1560:GLU:HG2	1:W:1561:GLU:H	1.77	0.49
1:A:1555:GLN:N	1:A:1555:GLN:OE1	2.46	0.48
1:G:1518:SER:HB2	1:G:1520:MET:HE1	1.95	0.48
1:G:1568:ALA:HA	1:G:1571:PHE:HB3	1.95	0.48
1:G:1575:ASP:HB2	1:G:1578:ARG:CZ	2.43	0.48
1:O:1512:GLY:O	1:O:1514:VAL:N	2.46	0.48
1:V:1508:HIS:CD2	1:V:1509:HIS:H	2.30	0.48
1:W:1539:GLN:N	1:W:1539:GLN:OE1	2.46	0.48
1:X:1538:MET:N	1:X:1538:MET:SD	2.86	0.48
1:C:1569:CYS:C	1:C:1571:PHE:H	2.16	0.48
1:J:1601:GLN:NE2	1:J:1601:GLN:H	2.10	0.48
1:M:1596:MET:H	1:M:1597:PRO:HD3	1.77	0.48
1:O:1545:LYS:O	1:O:1546:ASP:CB	2.61	0.48
1:Q:1554:LEU:N	1:Q:1554:LEU:CD1	2.76	0.48
1:R:1578:ARG:HH22	1:R:1580:ASP:HB2	1.77	0.48
1:T:1537:ALA:O	1:T:1538:MET:C	2.52	0.48
1:T:1572:THR:HG23	1:T:1578:ARG:HB3	1.95	0.48
1:C:1577:LEU:O	1:C:1578:ARG:HB2	2.12	0.48
1:D:1578:ARG:N	1:D:1579:PRO:CD	2.76	0.48
1:G:1534:TYR:O	1:G:1538:MET:HB2	2.14	0.48
1:G:1579:PRO:O	1:G:1581:VAL:N	2.47	0.48
1:H:1556:TRP:CE3	1:H:1559:GLN:HG2	2.48	0.48
1:H:1599:PHE:O	1:H:1602:VAL:N	2.46	0.48
1:L:1512:GLY:O	1:L:1514:VAL:N	2.45	0.48
1:L:1578:ARG:HA	1:L:1578:ARG:NE	2.27	0.48
1:M:1568:ALA:HA	1:M:1571:PHE:HB3	1.93	0.48
1:P:1572:THR:CA	1:P:1578:ARG:NH2	2.63	0.48
1:Q:1556:TRP:CE3	1:Q:1559:GLN:HG2	2.48	0.48
1:R:1530:LYS:NZ	1:R:1563:ARG:CZ	2.77	0.48
1:T:1535:LYS:HZ1	1:T:1563:ARG:HH21	1.61	0.48
1:T:1550:ALA:HB1	1:T:1571:PHE:CE2	2.48	0.48
1:V:1520:MET:SD	1:V:1520:MET:N	2.86	0.48
1:X:1530:LYS:HZ3	1:X:1563:ARG:CD	2.26	0.48
1:X:1559:GLN:HE22	1:X:1588:ARG:NH2	2.11	0.48
1:C:1558:LEU:HD13	1:C:1565:CYS:CB	2.43	0.48
1:D:1579:PRO:O	1:D:1581:VAL:N	2.46	0.48
1:K:1604:LYS:HZ1	1:L:1613:LEU:CD1	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:1529:LYS:O	1:N:1530:LYS:HG2	2.14	0.48
1:N:1590:ASN:O	1:N:1592:MET:SD	2.71	0.48
1:O:1514:VAL:HG13	1:T:1531:ASP:CB	2.43	0.48
1:P:1534:TYR:O	1:P:1538:MET:HB2	2.14	0.48
1:P:1580:ASP:O	1:P:1581:VAL:C	2.51	0.48
1:U:1512:GLY:O	1:U:1514:VAL:N	2.47	0.48
1:U:1572:THR:HG21	1:U:1578:ARG:HB3	1.96	0.48
1:U:1581:VAL:O	1:U:1583:LEU:N	2.47	0.48
1:V:1594:PHE:CG	1:V:1595:ALA:N	2.81	0.48
1:X:1544:SER:O	1:X:1545:LYS:HD2	2.14	0.48
1:X:1603:MET:O	1:X:1605:GLU:N	2.47	0.48
1:X:1607:LEU:C	1:X:1609:LYS:H	2.17	0.48
1:B:1581:VAL:O	1:B:1585:LEU:HD23	2.13	0.48
1:C:1558:LEU:HA	1:C:1565:CYS:SG	2.53	0.48
1:F:1512:GLY:O	1:F:1514:VAL:N	2.46	0.48
1:F:1592:MET:SD	1:F:1592:MET:C	2.92	0.48
1:G:1541:ALA:HB3	1:G:1571:PHE:CE2	2.49	0.48
1:K:1538:MET:HB2	1:K:1539:GLN:OE1	2.14	0.48
1:K:1591:ILE:O	1:K:1592:MET:SD	2.71	0.48
1:L:1533:LEU:CD1	1:V:1588:ARG:CZ	2.90	0.48
1:M:1560:GLU:O	1:M:1561:GLU:HB2	2.13	0.48
1:N:1558:LEU:HD12	1:N:1565:CYS:HA	1.95	0.48
1:R:1579:PRO:HD3	1:R:1598:TYR:OH	2.14	0.48
1:S:1534:TYR:O	1:S:1538:MET:HB2	2.14	0.48
1:S:1555:GLN:OE1	1:S:1555:GLN:N	2.46	0.48
1:S:1558:LEU:N	1:S:1558:LEU:HD12	2.29	0.48
1:W:1561:GLU:HB3	1:W:1564:GLU:HB2	1.95	0.48
1:W:1572:THR:HG23	1:W:1578:ARG:HB3	1.96	0.48
1:A:1508:HIS:CG	1:A:1509:HIS:N	2.75	0.48
1:F:1516:ARG:CD	1:H:1563:ARG:NH2	2.74	0.48
1:O:1537:ALA:HB1	1:T:1566:PHE:CD1	2.49	0.48
1:O:1579:PRO:HA	1:O:1582:VAL:CG2	2.43	0.48
1:Q:1538:MET:HB2	1:Q:1539:GLN:OE1	2.14	0.48
1:Q:1574:TYR:C	1:Q:1576:LEU:H	2.17	0.48
1:T:1604:LYS:CD	1:U:1609:LYS:HD3	2.43	0.48
1:F:1607:LEU:C	1:F:1609:LYS:H	2.15	0.48
1:H:1535:LYS:NZ	1:H:1563:ARG:HH21	2.12	0.48
1:H:1590:ASN:O	1:H:1592:MET:SD	2.72	0.48
1:L:1579:PRO:HG2	1:L:1580:ASP:OD1	2.13	0.48
1:L:1607:LEU:C	1:L:1609:LYS:H	2.16	0.48
1:Q:1561:GLU:HB3	1:Q:1564:GLU:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1583:LEU:O	1:B:1586:ALA:HB3	2.14	0.48
1:H:1538:MET:HB2	1:H:1539:GLN:OE1	2.14	0.48
1:H:1560:GLU:HG2	1:H:1561:GLU:H	1.79	0.48
1:I:1512:GLY:O	1:I:1514:VAL:N	2.47	0.48
1:O:1514:VAL:CB	1:O:1515:PRO:HD3	2.40	0.48
1:R:1572:THR:O	1:R:1575:ASP:HB3	2.13	0.48
1:X:1577:LEU:HD22	1:X:1598:TYR:CE2	2.49	0.48
1:A:1549:LEU:H	1:A:1549:LEU:HD22	1.79	0.48
1:B:1531:ASP:HA	1:B:1534:TYR:CD1	2.49	0.48
1:C:1568:ALA:O	1:C:1571:PHE:HB3	2.14	0.48
1:J:1545:LYS:CG	1:J:1546:ASP:N	2.77	0.48
1:L:1577:LEU:HD22	1:L:1598:TYR:CE2	2.47	0.48
1:M:1508:HIS:CD2	1:M:1509:HIS:H	2.32	0.48
1:P:1507:HIS:O	1:P:1508:HIS:HB2	2.14	0.48
1:T:1591:ILE:O	1:T:1592:MET:SD	2.72	0.48
1:A:1554:LEU:HA	1:A:1557:PHE:CD2	2.48	0.48
1:C:1554:LEU:O	1:C:1558:LEU:HB2	2.13	0.48
1:D:1620:ARG:HA	1:D:1620:ARG:NE	2.27	0.48
1:J:1509:HIS:ND1	1:J:1510:SER:N	2.62	0.48
1:J:1560:GLU:O	1:J:1561:GLU:HB2	2.14	0.48
1:L:1572:THR:HA	1:L:1575:ASP:HB2	1.94	0.48
1:Q:1588:ARG:NE	1:Q:1588:ARG:CA	2.77	0.48
1:S:1545:LYS:CG	1:S:1546:ASP:N	2.75	0.48
1:X:1602:VAL:C	1:X:1605:GLU:OE1	2.52	0.48
1:B:1579:PRO:O	1:B:1581:VAL:N	2.47	0.47
1:D:1578:ARG:NH1	1:D:1578:ARG:CB	2.70	0.47
1:G:1596:MET:H	1:G:1597:PRO:HD3	1.78	0.47
1:M:1598:TYR:O	1:M:1601:GLN:N	2.44	0.47
1:N:1560:GLU:O	1:N:1561:GLU:HB2	2.14	0.47
1:O:1549:LEU:HD13	1:O:1552:GLU:OE2	2.13	0.47
1:R:1542:SER:HA	1:R:1571:PHE:HE2	1.79	0.47
1:T:1542:SER:HA	1:T:1571:PHE:CE1	2.49	0.47
1:U:1585:LEU:C	1:U:1587:TRP:H	2.17	0.47
1:U:1591:ILE:CG2	1:U:1592:MET:N	2.77	0.47
1:W:1554:LEU:HD11	1:W:1571:PHE:CD2	2.47	0.47
1:W:1574:TYR:C	1:W:1576:LEU:H	2.16	0.47
1:B:1583:LEU:HD12	1:B:1583:LEU:N	2.29	0.47
1:B:1606:TYR:O	1:B:1610:VAL:HG23	2.15	0.47
1:I:1607:LEU:C	1:I:1609:LYS:H	2.16	0.47
1:N:1613:LEU:O	1:N:1617:GLU:HG3	2.14	0.47
1:R:1607:LEU:C	1:R:1609:LYS:H	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:1593:ASP:CG	1:T:1594:PHE:H	2.17	0.47
1:X:1533:LEU:HD22	1:X:1534:TYR:N	2.20	0.47
1:D:1594:PHE:CG	1:D:1595:ALA:N	2.81	0.47
1:G:1611:ASP:HB3	1:H:1612:LYS:HZ3	1.79	0.47
1:H:1554:LEU:HD11	1:H:1571:PHE:CD2	2.48	0.47
1:I:1583:LEU:N	1:I:1583:LEU:CD2	2.77	0.47
1:R:1512:GLY:O	1:R:1514:VAL:N	2.48	0.47
1:R:1525:VAL:HG21	1:R:1563:ARG:HH12	1.79	0.47
1:C:1512:GLY:O	1:C:1514:VAL:N	2.46	0.47
1:C:1582:VAL:O	1:C:1583:LEU:HD13	2.14	0.47
1:J:1545:LYS:HG2	1:J:1546:ASP:H	1.75	0.47
1:K:1574:TYR:C	1:K:1576:LEU:H	2.17	0.47
1:M:1541:ALA:O	1:M:1544:SER:OG	2.33	0.47
1:N:1596:MET:H	1:N:1596:MET:HE2	1.79	0.47
1:O:1583:LEU:N	1:O:1583:LEU:HD22	2.29	0.47
1:R:1603:MET:O	1:R:1605:GLU:N	2.48	0.47
1:S:1554:LEU:O	1:S:1555:GLN:C	2.52	0.47
1:U:1578:ARG:HH22	1:U:1580:ASP:HB2	1.79	0.47
1:X:1512:GLY:O	1:X:1514:VAL:N	2.47	0.47
1:X:1596:MET:HB3	1:X:1599:PHE:CE1	2.48	0.47
1:F:1577:LEU:O	1:F:1578:ARG:HB2	2.14	0.47
1:L:1596:MET:HB3	1:L:1599:PHE:CE1	2.49	0.47
1:L:1602:VAL:C	1:L:1605:GLU:OE1	2.52	0.47
1:Q:1560:GLU:HG2	1:Q:1561:GLU:H	1.79	0.47
1:U:1519:HIS:CE1	1:U:1540:TYR:OH	2.67	0.47
1:V:1566:PHE:O	1:V:1569:CYS:HB2	2.15	0.47
1:W:1558:LEU:HD23	1:W:1585:LEU:HG	1.96	0.47
1:A:1516:ARG:O	1:A:1516:ARG:HG3	2.15	0.47
1:F:1547:THR:HG21	1:H:1543:GLU:OE1	2.15	0.47
1:I:1579:PRO:HG2	1:I:1580:ASP:OD1	2.14	0.47
1:J:1529:LYS:O	1:J:1530:LYS:HB2	2.14	0.47
1:L:1569:CYS:C	1:L:1571:PHE:H	2.18	0.47
1:L:1578:ARG:HH22	1:L:1580:ASP:HB2	1.79	0.47
1:N:1579:PRO:O	1:N:1581:VAL:N	2.48	0.47
1:O:1545:LYS:HB2	1:O:1546:ASP:H	1.55	0.47
1:O:1602:VAL:O	1:O:1602:VAL:CG1	2.61	0.47
1:R:1558:LEU:HA	1:R:1565:CYS:SG	2.54	0.47
1:X:1547:THR:CG2	1:X:1548:GLU:H	2.26	0.47
1:C:1547:THR:CG2	1:C:1548:GLU:H	2.25	0.47
1:C:1623:GLU:HG3	1:C:1624:GLU:H	1.79	0.47
1:D:1515:PRO:O	1:D:1516:ARG:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1580:ASP:OD2	1:F:1596:MET:HE1	2.14	0.47
1:E:1583:LEU:HD11	1:F:1599:PHE:CE1	2.48	0.47
1:E:1604:LYS:HD2	1:F:1612:LYS:NZ	2.28	0.47
1:F:1599:PHE:HA	1:F:1602:VAL:HG21	1.95	0.47
1:I:1585:LEU:HD13	1:I:1588:ARG:CG	2.45	0.47
1:K:1579:PRO:CB	1:L:1599:PHE:HD1	2.24	0.47
1:K:1604:LYS:NZ	1:L:1613:LEU:HD21	2.30	0.47
1:L:1568:ALA:O	1:L:1571:PHE:HB3	2.14	0.47
1:N:1556:TRP:CE3	1:N:1559:GLN:HG2	2.49	0.47
1:S:1575:ASP:HB2	1:S:1578:ARG:NH1	2.29	0.47
1:X:1559:GLN:HE22	1:X:1588:ARG:CZ	2.28	0.47
1:A:1513:LEU:HD22	1:A:1514:VAL:N	2.30	0.47
1:D:1601:GLN:NE2	1:D:1601:GLN:H	2.13	0.47
1:E:1592:MET:HE2	1:E:1592:MET:H	1.75	0.47
1:L:1565:CYS:O	1:L:1569:CYS:N	2.48	0.47
1:M:1596:MET:N	1:M:1597:PRO:CD	2.77	0.47
1:Q:1593:ASP:CG	1:Q:1594:PHE:N	2.68	0.47
1:T:1595:ALA:HA	1:T:1596:MET:HE1	1.97	0.47
1:V:1534:TYR:O	1:V:1538:MET:HB2	2.15	0.47
1:C:1545:LYS:O	1:C:1546:ASP:HB2	2.15	0.47
1:C:1596:MET:HB3	1:C:1599:PHE:CE1	2.50	0.47
1:D:1545:LYS:CG	1:D:1546:ASP:N	2.78	0.47
1:D:1571:PHE:C	1:D:1571:PHE:CD1	2.88	0.47
1:E:1538:MET:HB2	1:E:1539:GLN:OE1	2.14	0.47
1:F:1530:LYS:HZ1	1:F:1563:ARG:CZ	2.27	0.47
1:G:1545:LYS:CG	1:G:1546:ASP:N	2.77	0.47
1:G:1555:GLN:O	1:G:1559:GLN:N	2.48	0.47
1:G:1604:LYS:HD3	1:H:1605:GLU:CG	2.45	0.47
1:J:1534:TYR:CE1	1:J:1535:LYS:HG3	2.50	0.47
1:R:1549:LEU:HD13	1:R:1552:GLU:OE2	2.15	0.47
1:T:1561:GLU:HB3	1:T:1564:GLU:HB2	1.96	0.47
1:B:1608:THR:O	1:B:1612:LYS:HG2	2.15	0.47
1:C:1535:LYS:O	1:C:1536:ASP:CB	2.63	0.47
1:C:1581:VAL:C	1:C:1583:LEU:N	2.68	0.47
1:K:1531:ASP:HA	1:K:1534:TYR:CD1	2.50	0.47
1:M:1579:PRO:O	1:M:1581:VAL:N	2.48	0.47
1:Q:1548:GLU:HA	1:Q:1551:GLU:OE1	2.14	0.47
1:Q:1566:PHE:O	1:Q:1570:LEU:CD1	2.55	0.47
1:A:1561:GLU:HB2	1:A:1564:GLU:HB2	1.96	0.46
1:D:1561:GLU:CB	1:D:1564:GLU:HB2	2.46	0.46
1:L:1550:ALA:O	1:L:1553:LEU:HB2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:1592:MET:SD	1:O:1594:PHE:O	2.73	0.46
1:U:1572:THR:HA	1:U:1575:ASP:HB2	1.97	0.46
1:U:1602:VAL:CA	1:U:1605:GLU:OE1	2.63	0.46
1:V:1572:THR:HG23	1:V:1578:ARG:CZ	2.46	0.46
1:D:1554:LEU:O	1:D:1557:PHE:N	2.46	0.46
1:D:1575:ASP:HB2	1:D:1578:ARG:CZ	2.45	0.46
1:G:1580:ASP:O	1:G:1581:VAL:C	2.53	0.46
1:I:1537:ALA:HB3	1:I:1538:MET:CE	2.45	0.46
1:I:1549:LEU:O	1:I:1553:LEU:HG	2.14	0.46
1:J:1515:PRO:O	1:J:1516:ARG:HB3	2.14	0.46
1:L:1551:GLU:C	1:L:1553:LEU:N	2.68	0.46
1:P:1513:LEU:HD13	1:P:1513:LEU:O	2.15	0.46
1:P:1571:PHE:CD1	1:P:1571:PHE:C	2.89	0.46
1:Q:1572:THR:HG23	1:Q:1578:ARG:HB3	1.97	0.46
1:S:1601:GLN:NE2	1:S:1601:GLN:H	2.13	0.46
1:V:1558:LEU:HD11	1:V:1568:ALA:CB	2.45	0.46
1:B:1535:LYS:HZ1	1:B:1563:ARG:HH21	1.63	0.46
1:C:1545:LYS:HB2	1:C:1546:ASP:H	1.55	0.46
1:N:1595:ALA:HA	1:N:1596:MET:HE1	1.96	0.46
1:P:1560:GLU:HG3	1:P:1561:GLU:N	2.30	0.46
1:X:1572:THR:O	1:X:1572:THR:CG2	2.63	0.46
1:A:1515:PRO:O	1:A:1516:ARG:CB	2.64	0.46
1:C:1554:LEU:HD22	1:C:1554:LEU:N	2.31	0.46
1:D:1562:LYS:HD3	1:D:1562:LYS:N	2.30	0.46
1:E:1563:ARG:HG2	1:E:1564:GLU:OE1	2.15	0.46
1:F:1545:LYS:O	1:F:1546:ASP:HB2	2.15	0.46
1:F:1555:GLN:O	1:F:1559:GLN:HG2	2.15	0.46
1:H:1535:LYS:NZ	1:H:1563:ARG:NH2	2.63	0.46
1:H:1558:LEU:HD23	1:H:1585:LEU:HG	1.97	0.46
1:L:1603:MET:O	1:L:1605:GLU:N	2.48	0.46
1:O:1551:GLU:C	1:O:1553:LEU:N	2.64	0.46
1:O:1603:MET:O	1:O:1605:GLU:N	2.48	0.46
1:R:1549:LEU:O	1:R:1553:LEU:HG	2.14	0.46
1:T:1599:PHE:C	1:T:1601:GLN:N	2.68	0.46
1:V:1515:PRO:O	1:V:1516:ARG:CB	2.63	0.46
1:X:1545:LYS:O	1:X:1546:ASP:CB	2.64	0.46
1:E:1531:ASP:HA	1:E:1534:TYR:CD1	2.51	0.46
1:E:1592:MET:N	1:E:1592:MET:CE	2.77	0.46
1:F:1525:VAL:CG1	1:F:1526:GLU:H	2.17	0.46
1:F:1536:ASP:O	1:F:1540:TYR:CD1	2.68	0.46
1:I:1599:PHE:HA	1:I:1602:VAL:HG23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1608:THR:HG22	1:I:1608:THR:O	2.15	0.46
1:P:1620:ARG:HA	1:P:1620:ARG:NE	2.28	0.46
1:R:1602:VAL:CA	1:R:1605:GLU:OE1	2.64	0.46
1:U:1546:ASP:N	1:U:1550:ALA:HB2	2.31	0.46
1:V:1583:LEU:HD12	1:V:1583:LEU:N	2.30	0.46
1:W:1604:LYS:CD	1:X:1609:LYS:CD	2.93	0.46
1:A:1541:ALA:HB3	1:A:1571:PHE:HE2	1.81	0.46
1:B:1599:PHE:C	1:B:1601:GLN:N	2.68	0.46
1:E:1546:ASP:CB	1:E:1549:LEU:HB2	2.41	0.46
1:F:1542:SER:HB2	1:F:1571:PHE:CD2	2.50	0.46
1:I:1530:LYS:NZ	1:I:1563:ARG:CZ	2.78	0.46
1:M:1508:HIS:CG	1:M:1509:HIS:N	2.83	0.46
1:S:1594:PHE:CD2	1:S:1595:ALA:N	2.82	0.46
1:U:1551:GLU:HA	1:U:1554:LEU:HD23	1.97	0.46
1:X:1599:PHE:N	1:X:1599:PHE:HD2	2.13	0.46
1:E:1587:TRP:CH2	1:F:1594:PHE:N	2.83	0.46
1:K:1554:LEU:HD11	1:K:1571:PHE:CD2	2.49	0.46
1:L:1554:LEU:CD1	1:L:1568:ALA:HB1	2.45	0.46
1:N:1583:LEU:HD12	1:N:1583:LEU:H	1.80	0.46
1:Q:1550:ALA:HB1	1:Q:1571:PHE:HE2	1.80	0.46
1:T:1557:PHE:C	1:T:1558:LEU:HD12	2.36	0.46
1:T:1577:LEU:HB3	1:U:1603:MET:CE	2.46	0.46
1:U:1592:MET:SD	1:U:1593:ASP:N	2.89	0.46
1:B:1558:LEU:HD23	1:B:1585:LEU:HG	1.97	0.46
1:B:1581:VAL:O	1:B:1581:VAL:CG1	2.62	0.46
1:F:1581:VAL:O	1:F:1584:GLU:N	2.49	0.46
1:G:1545:LYS:O	1:G:1546:ASP:HB2	2.16	0.46
1:I:1554:LEU:O	1:I:1558:LEU:HB2	2.16	0.46
1:J:1609:LYS:O	1:J:1613:LEU:HG	2.15	0.46
1:K:1596:MET:HA	1:K:1597:PRO:HD3	1.80	0.46
1:L:1557:PHE:C	1:L:1561:GLU:OE1	2.54	0.46
1:O:1559:GLN:NE2	1:O:1585:LEU:HD11	2.30	0.46
1:O:1586:ALA:CB	1:O:1592:MET:HB2	2.46	0.46
1:Q:1558:LEU:HD23	1:Q:1585:LEU:HG	1.97	0.46
1:B:1557:PHE:C	1:B:1558:LEU:HD12	2.36	0.46
1:D:1558:LEU:HD12	1:D:1558:LEU:N	2.30	0.46
1:D:1568:ALA:HA	1:D:1571:PHE:HB3	1.97	0.46
1:F:1601:GLN:O	1:F:1605:GLU:OE2	2.33	0.46
1:R:1602:VAL:C	1:R:1605:GLU:OE1	2.54	0.46
1:U:1533:LEU:HD13	1:U:1534:TYR:CD1	2.51	0.46
1:A:1624:GLU:OXT	1:R:1618:SER:CB	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1579:PRO:O	1:C:1580:ASP:HB2	2.15	0.46
1:E:1556:TRP:CE3	1:E:1559:GLN:HG2	2.51	0.46
1:F:1530:LYS:NZ	1:F:1563:ARG:CZ	2.79	0.46
1:J:1508:HIS:CD2	1:J:1509:HIS:H	2.34	0.46
1:M:1580:ASP:O	1:M:1581:VAL:C	2.53	0.46
1:R:1623:GLU:HG3	1:R:1624:GLU:H	1.81	0.46
1:S:1515:PRO:O	1:S:1516:ARG:CB	2.64	0.46
1:U:1545:LYS:O	1:U:1546:ASP:HB2	2.16	0.46
1:W:1534:TYR:O	1:W:1538:MET:SD	2.73	0.46
1:D:1542:SER:C	1:D:1544:SER:H	2.18	0.45
1:I:1596:MET:HB3	1:I:1599:PHE:CE1	2.51	0.45
1:R:1542:SER:HB2	1:R:1571:PHE:CD2	2.51	0.45
1:T:1592:MET:SD	1:T:1592:MET:N	2.89	0.45
1:V:1554:LEU:O	1:V:1558:LEU:CD1	2.59	0.45
1:B:1604:LYS:HG3	1:C:1609:LYS:HE3	1.97	0.45
1:C:1599:PHE:HA	1:C:1602:VAL:HG23	1.99	0.45
1:E:1606:TYR:HA	1:E:1609:LYS:HE2	1.98	0.45
1:G:1577:LEU:H	1:G:1577:LEU:CD1	2.27	0.45
1:I:1530:LYS:HZ3	1:I:1563:ARG:CD	2.30	0.45
1:K:1579:PRO:HG2	1:K:1580:ASP:OD1	2.15	0.45
1:L:1563:ARG:N	1:L:1564:GLU:OE1	2.49	0.45
1:L:1565:CYS:O	1:L:1568:ALA:HB3	2.16	0.45
1:L:1612:LYS:HB3	1:L:1612:LYS:HE2	1.81	0.45
1:M:1513:LEU:HD13	1:M:1513:LEU:O	2.14	0.45
1:M:1601:GLN:NE2	1:M:1601:GLN:N	2.64	0.45
1:N:1554:LEU:HD11	1:N:1571:PHE:CD2	2.50	0.45
1:O:1530:LYS:HZ1	1:O:1563:ARG:CZ	2.29	0.45
1:O:1608:THR:O	1:O:1608:THR:HG22	2.16	0.45
1:R:1594:PHE:O	1:R:1595:ALA:HB2	2.17	0.45
1:S:1516:ARG:HG3	1:S:1516:ARG:O	2.16	0.45
1:S:1519:HIS:N	1:S:1520:MET:HE1	2.30	0.45
1:T:1535:LYS:HA	1:T:1538:MET:CE	2.46	0.45
1:U:1609:LYS:HA	1:U:1609:LYS:HZ2	1.82	0.45
1:F:1557:PHE:C	1:F:1561:GLU:OE1	2.55	0.45
1:N:1594:PHE:CD1	1:N:1595:ALA:N	2.85	0.45
1:O:1562:LYS:C	1:O:1564:GLU:H	2.20	0.45
1:R:1554:LEU:HD12	1:R:1568:ALA:HB1	1.98	0.45
1:R:1596:MET:HB3	1:R:1599:PHE:CE1	2.52	0.45
1:V:1542:SER:C	1:V:1544:SER:H	2.18	0.45
1:W:1609:LYS:O	1:W:1613:LEU:HG	2.16	0.45
1:E:1572:THR:HG23	1:E:1578:ARG:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1565:CYS:O	1:F:1569:CYS:SG	2.65	0.45
1:L:1579:PRO:HA	1:L:1582:VAL:HG21	1.99	0.45
1:M:1564:GLU:OE1	1:M:1564:GLU:N	2.50	0.45
1:N:1561:GLU:HB3	1:N:1564:GLU:HB2	1.99	0.45
1:Q:1542:SER:HA	1:Q:1571:PHE:CZ	2.52	0.45
1:R:1591:ILE:CG2	1:R:1592:MET:N	2.78	0.45
1:T:1600:ILE:O	1:U:1609:LYS:HD2	2.17	0.45
1:X:1550:ALA:O	1:X:1553:LEU:HB2	2.17	0.45
1:A:1568:ALA:HA	1:A:1571:PHE:HB3	1.98	0.45
1:D:1531:ASP:O	1:D:1532:SER:OG	2.28	0.45
1:I:1603:MET:O	1:I:1605:GLU:N	2.49	0.45
1:J:1518:SER:HB2	1:J:1520:MET:HE1	1.98	0.45
1:Q:1583:LEU:HD12	1:Q:1583:LEU:H	1.82	0.45
1:R:1602:VAL:O	1:R:1602:VAL:CG1	2.63	0.45
1:B:1547:THR:HG22	1:B:1548:GLU:N	2.31	0.45
1:B:1599:PHE:HA	1:B:1602:VAL:CG2	2.45	0.45
1:E:1554:LEU:HD11	1:E:1571:PHE:CD2	2.51	0.45
1:E:1577:LEU:HD22	1:F:1602:VAL:O	2.17	0.45
1:H:1605:GLU:HG2	1:H:1606:TYR:CD2	2.50	0.45
1:J:1508:HIS:CG	1:J:1509:HIS:N	2.84	0.45
1:P:1596:MET:SD	1:P:1596:MET:N	2.89	0.45
1:V:1587:TRP:HA	1:V:1587:TRP:HE3	1.80	0.45
1:W:1592:MET:N	1:W:1592:MET:CE	2.78	0.45
1:E:1561:GLU:HB3	1:E:1564:GLU:HB2	1.98	0.45
1:E:1587:TRP:HH2	1:F:1594:PHE:HA	1.82	0.45
1:F:1536:ASP:O	1:F:1540:TYR:HD1	2.00	0.45
1:I:1535:LYS:O	1:I:1536:ASP:CB	2.65	0.45
1:I:1542:SER:HB2	1:I:1571:PHE:HD2	1.81	0.45
1:K:1606:TYR:O	1:K:1610:VAL:HG23	2.17	0.45
1:M:1583:LEU:N	1:M:1583:LEU:CD1	2.79	0.45
1:S:1596:MET:H	1:S:1597:PRO:CD	2.30	0.45
1:V:1566:PHE:N	1:V:1566:PHE:CD2	2.84	0.45
1:G:1519:HIS:N	1:G:1520:MET:HE1	2.32	0.45
1:L:1601:GLN:O	1:L:1605:GLU:CD	2.55	0.45
1:O:1596:MET:HE2	1:O:1596:MET:O	2.17	0.45
1:T:1601:GLN:HA	1:U:1609:LYS:CE	2.42	0.45
1:V:1579:PRO:O	1:V:1581:VAL:N	2.50	0.45
1:E:1534:TYR:O	1:E:1538:MET:SD	2.74	0.45
1:G:1541:ALA:HB3	1:G:1571:PHE:HE2	1.81	0.45
1:G:1601:GLN:NE2	1:G:1601:GLN:N	2.65	0.45
1:H:1538:MET:HG3	1:H:1557:PHE:CZ	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1545:LYS:O	1:I:1546:ASP:HB2	2.16	0.45
1:I:1549:LEU:HD13	1:I:1552:GLU:OE2	2.17	0.45
1:N:1577:LEU:HD12	1:O:1607:LEU:CD2	2.47	0.45
1:O:1535:LYS:O	1:O:1536:ASP:CB	2.65	0.45
1:R:1580:ASP:O	1:R:1581:VAL:C	2.55	0.45
1:T:1537:ALA:O	1:T:1539:GLN:N	2.50	0.45
1:T:1556:TRP:CE3	1:T:1559:GLN:HG2	2.52	0.45
1:E:1577:LEU:HD11	1:F:1606:TYR:HB3	1.99	0.45
1:E:1596:MET:HA	1:E:1597:PRO:HD3	1.82	0.45
1:I:1578:ARG:HH22	1:I:1580:ASP:HB2	1.82	0.45
1:L:1530:LYS:NZ	1:L:1563:ARG:CZ	2.80	0.45
1:L:1599:PHE:HA	1:L:1602:VAL:CG2	2.47	0.45
1:M:1578:ARG:N	1:M:1579:PRO:CD	2.79	0.45
1:Q:1529:LYS:C	1:Q:1530:LYS:HG2	2.38	0.45
1:A:1561:GLU:CB	1:A:1564:GLU:HB2	2.47	0.44
1:C:1530:LYS:NZ	1:C:1563:ARG:CZ	2.80	0.44
1:H:1580:ASP:CA	1:H:1583:LEU:HD13	2.47	0.44
1:K:1604:LYS:HZ1	1:L:1613:LEU:HD11	1.81	0.44
1:M:1554:LEU:O	1:M:1555:GLN:C	2.56	0.44
1:N:1566:PHE:O	1:N:1570:LEU:CD1	2.60	0.44
1:R:1599:PHE:HA	1:R:1602:VAL:HG23	1.98	0.44
1:U:1537:ALA:HB3	1:U:1538:MET:CE	2.47	0.44
1:U:1572:THR:O	1:U:1575:ASP:CB	2.61	0.44
1:A:1571:PHE:C	1:A:1571:PHE:CD1	2.90	0.44
1:B:1554:LEU:HD11	1:B:1571:PHE:CD2	2.51	0.44
1:H:1537:ALA:C	1:H:1539:GLN:N	2.70	0.44
1:I:1556:TRP:O	1:I:1561:GLU:OE1	2.35	0.44
1:L:1540:TYR:HB3	1:W:1563:ARG:HB3	1.99	0.44
1:L:1577:LEU:O	1:L:1578:ARG:HB2	2.18	0.44
1:O:1519:HIS:CE1	1:O:1540:TYR:OH	2.70	0.44
1:T:1571:PHE:HD1	1:T:1574:TYR:HD2	1.63	0.44
1:W:1547:THR:HG22	1:W:1548:GLU:N	2.32	0.44
1:C:1565:CYS:O	1:C:1569:CYS:SG	2.68	0.44
1:E:1537:ALA:C	1:E:1539:GLN:N	2.70	0.44
1:E:1560:GLU:O	1:E:1561:GLU:HB2	2.17	0.44
1:K:1556:TRP:CE3	1:K:1559:GLN:HG2	2.52	0.44
1:O:1530:LYS:HZ3	1:O:1563:ARG:HD2	1.82	0.44
1:R:1545:LYS:O	1:R:1546:ASP:CB	2.65	0.44
1:R:1609:LYS:HA	1:R:1609:LYS:HZ2	1.82	0.44
1:U:1586:ALA:HB1	1:U:1592:MET:HB2	1.99	0.44
1:V:1620:ARG:HA	1:V:1620:ARG:NE	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1577:LEU:H	1:A:1577:LEU:CD1	2.30	0.44
1:B:1552:GLU:O	1:B:1554:LEU:N	2.51	0.44
1:K:1545:LYS:HB2	1:K:1571:PHE:CZ	2.51	0.44
1:N:1593:ASP:CG	1:N:1594:PHE:H	2.21	0.44
1:P:1564:GLU:OE1	1:P:1564:GLU:N	2.51	0.44
1:Q:1577:LEU:HD11	1:R:1606:TYR:CB	2.48	0.44
1:Q:1579:PRO:HG2	1:Q:1580:ASP:OD1	2.18	0.44
1:S:1520:MET:N	1:S:1520:MET:SD	2.91	0.44
1:U:1623:GLU:HG3	1:U:1624:GLU:H	1.81	0.44
1:A:1513:LEU:HD13	1:A:1513:LEU:O	2.18	0.44
1:F:1549:LEU:HD13	1:F:1552:GLU:OE2	2.18	0.44
1:T:1580:ASP:CA	1:T:1583:LEU:HD13	2.47	0.44
1:T:1600:ILE:HD12	1:U:1606:TYR:OH	2.17	0.44
1:U:1585:LEU:HD13	1:U:1588:ARG:CG	2.48	0.44
1:V:1601:GLN:H	1:V:1601:GLN:HE21	1.65	0.44
1:W:1538:MET:HB2	1:W:1539:GLN:OE1	2.18	0.44
1:A:1558:LEU:CB	1:A:1585:LEU:HD13	2.48	0.44
1:E:1558:LEU:HD12	1:E:1565:CYS:HA	1.98	0.44
1:F:1595:ALA:C	1:F:1596:MET:HG3	2.37	0.44
1:J:1513:LEU:HD13	1:J:1513:LEU:C	2.38	0.44
1:L:1591:ILE:CG2	1:L:1592:MET:N	2.73	0.44
1:T:1548:GLU:HA	1:T:1551:GLU:HB2	1.99	0.44
1:T:1608:THR:O	1:T:1612:LYS:HG2	2.18	0.44
1:W:1559:GLN:NE2	1:W:1560:GLU:HB3	2.32	0.44
1:A:1596:MET:H	1:A:1597:PRO:HD3	1.83	0.44
1:C:1546:ASP:N	1:C:1550:ALA:HB2	2.33	0.44
1:D:1508:HIS:CG	1:D:1509:HIS:N	2.86	0.44
1:E:1588:ARG:NE	1:E:1588:ARG:CA	2.79	0.44
1:I:1545:LYS:HB2	1:I:1546:ASP:H	1.66	0.44
1:J:1541:ALA:HB3	1:J:1571:PHE:CE2	2.52	0.44
1:L:1583:LEU:N	1:L:1583:LEU:HD22	2.32	0.44
1:S:1523:GLN:O	1:S:1524:SER:HB3	2.18	0.44
1:S:1561:GLU:CB	1:S:1564:GLU:HB2	2.48	0.44
1:T:1581:VAL:O	1:T:1585:LEU:HD23	2.18	0.44
1:V:1571:PHE:CD1	1:V:1571:PHE:C	2.90	0.44
1:C:1554:LEU:HD12	1:C:1568:ALA:HB1	2.00	0.44
1:E:1605:GLU:O	1:E:1609:LYS:HG3	2.17	0.44
1:H:1558:LEU:HD12	1:H:1565:CYS:HA	2.00	0.44
1:H:1561:GLU:HB3	1:H:1564:GLU:HB2	2.00	0.44
1:K:1544:SER:O	1:K:1545:LYS:HB3	2.18	0.44
1:K:1595:ALA:HA	1:K:1596:MET:HE1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:1544:SER:O	1:N:1545:LYS:HB3	2.17	0.44
1:R:1582:VAL:O	1:R:1582:VAL:HG12	2.18	0.44
1:R:1583:LEU:N	1:R:1583:LEU:HD22	2.33	0.44
1:T:1545:LYS:HA	1:T:1571:PHE:HZ	1.81	0.44
1:A:1560:GLU:O	1:A:1561:GLU:HB2	2.18	0.44
1:G:1558:LEU:HB2	1:G:1585:LEU:HD13	1.99	0.44
1:I:1523:GLN:O	1:I:1524:SER:HB3	2.18	0.44
1:I:1546:ASP:N	1:I:1550:ALA:HB2	2.32	0.44
1:J:1520:MET:N	1:J:1520:MET:SD	2.91	0.44
1:J:1538:MET:O	1:J:1538:MET:HG2	2.16	0.44
1:K:1547:THR:HG22	1:K:1548:GLU:N	2.33	0.44
1:K:1563:ARG:HG2	1:K:1564:GLU:OE1	2.16	0.44
1:L:1545:LYS:O	1:L:1546:ASP:HB2	2.17	0.44
1:M:1620:ARG:HA	1:M:1620:ARG:NE	2.32	0.44
1:R:1535:LYS:O	1:R:1536:ASP:CB	2.65	0.44
1:R:1563:ARG:N	1:R:1564:GLU:OE1	2.51	0.44
1:R:1601:GLN:O	1:R:1605:GLU:OE2	2.36	0.44
1:T:1558:LEU:HD11	1:T:1568:ALA:HB3	2.00	0.44
1:C:1603:MET:C	1:C:1605:GLU:H	2.22	0.43
1:F:1549:LEU:O	1:F:1553:LEU:HG	2.17	0.43
1:F:1579:PRO:HD3	1:F:1598:TYR:OH	2.17	0.43
1:H:1571:PHE:O	1:H:1574:TYR:HB2	2.18	0.43
1:M:1509:HIS:ND1	1:M:1510:SER:N	2.66	0.43
1:T:1588:ARG:NE	1:T:1588:ARG:CA	2.82	0.43
1:U:1530:LYS:HZ3	1:U:1563:ARG:CD	2.30	0.43
1:U:1585:LEU:C	1:U:1587:TRP:N	2.69	0.43
1:W:1561:GLU:CB	1:W:1564:GLU:HB2	2.48	0.43
1:B:1572:THR:CG2	1:B:1578:ARG:HB3	2.48	0.43
1:C:1599:PHE:HA	1:C:1602:VAL:HG21	2.00	0.43
1:D:1560:GLU:O	1:D:1561:GLU:OE1	2.35	0.43
1:F:1572:THR:HA	1:F:1575:ASP:HB2	2.00	0.43
1:P:1549:LEU:H	1:P:1549:LEU:CD2	2.30	0.43
1:P:1575:ASP:HB2	1:P:1578:ARG:NH2	2.33	0.43
1:P:1579:PRO:O	1:P:1581:VAL:N	2.51	0.43
1:Q:1545:LYS:HB2	1:Q:1571:PHE:CZ	2.53	0.43
1:W:1571:PHE:HD1	1:W:1574:TYR:HD2	1.65	0.43
1:W:1605:GLU:HG2	1:W:1606:TYR:CD2	2.53	0.43
1:X:1554:LEU:N	1:X:1554:LEU:CD2	2.79	0.43
1:X:1602:VAL:HA	1:X:1605:GLU:CD	2.38	0.43
1:A:1538:MET:O	1:A:1538:MET:CG	2.66	0.43
1:B:1595:ALA:HA	1:B:1596:MET:HE1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1598:TYR:O	1:C:1602:VAL:HG23	2.19	0.43
1:E:1529:LYS:O	1:E:1530:LYS:HG2	2.19	0.43
1:F:1550:ALA:O	1:F:1553:LEU:HB2	2.18	0.43
1:F:1583:LEU:N	1:F:1583:LEU:HD22	2.33	0.43
1:G:1532:SER:O	1:G:1533:LEU:HB2	2.19	0.43
1:L:1533:LEU:CD2	1:L:1534:TYR:N	2.76	0.43
1:M:1601:GLN:H	1:M:1601:GLN:HE21	1.66	0.43
1:O:1579:PRO:HA	1:O:1582:VAL:HG21	2.01	0.43
1:R:1523:GLN:O	1:R:1524:SER:HB3	2.18	0.43
1:R:1525:VAL:CG1	1:R:1526:GLU:H	2.20	0.43
1:R:1559:GLN:HB3	1:R:1560:GLU:OE1	2.19	0.43
1:X:1558:LEU:CD1	1:X:1565:CYS:HB3	2.47	0.43
1:C:1542:SER:HB2	1:C:1571:PHE:HD2	1.82	0.43
1:E:1580:ASP:CA	1:E:1583:LEU:HD13	2.49	0.43
1:H:1572:THR:CG2	1:H:1578:ARG:HB3	2.49	0.43
1:K:1542:SER:HA	1:K:1571:PHE:CZ	2.54	0.43
1:L:1546:ASP:O	1:L:1550:ALA:HB2	2.17	0.43
1:L:1547:THR:CG2	1:L:1548:GLU:H	2.28	0.43
1:M:1549:LEU:H	1:M:1549:LEU:CD2	2.32	0.43
1:S:1602:VAL:CG1	1:U:1577:LEU:HD13	2.48	0.43
1:U:1578:ARG:NE	1:U:1578:ARG:HA	2.33	0.43
1:W:1604:LYS:HD2	1:X:1609:LYS:CD	2.48	0.43
1:B:1556:TRP:CE3	1:B:1559:GLN:HG2	2.53	0.43
1:F:1594:PHE:O	1:F:1595:ALA:CB	2.64	0.43
1:H:1537:ALA:O	1:H:1538:MET:C	2.56	0.43
1:H:1599:PHE:HA	1:H:1602:VAL:HG23	2.01	0.43
1:I:1554:LEU:HD22	1:I:1554:LEU:N	2.33	0.43
1:O:1542:SER:HB2	1:O:1571:PHE:HD2	1.83	0.43
1:R:1545:LYS:HB2	1:R:1546:ASP:H	1.60	0.43
1:R:1554:LEU:N	1:R:1554:LEU:HD22	2.34	0.43
1:T:1560:GLU:O	1:T:1561:GLU:HB2	2.17	0.43
1:U:1558:LEU:CD1	1:U:1565:CYS:HB3	2.44	0.43
1:U:1602:VAL:O	1:U:1602:VAL:CG1	2.67	0.43
1:V:1580:ASP:O	1:V:1581:VAL:C	2.56	0.43
1:W:1535:LYS:NZ	1:W:1563:ARG:NH2	2.67	0.43
1:A:1546:ASP:O	1:A:1550:ALA:HB2	2.19	0.43
1:A:1572:THR:CA	1:A:1578:ARG:NH2	2.64	0.43
1:B:1545:LYS:HB2	1:B:1571:PHE:CZ	2.53	0.43
1:C:1523:GLN:O	1:C:1524:SER:HB3	2.18	0.43
1:D:1532:SER:O	1:D:1533:LEU:HB2	2.19	0.43
1:E:1554:LEU:N	1:E:1554:LEU:CD1	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1556:TRP:C	1:E:1559:GLN:HG3	2.37	0.43
1:E:1592:MET:N	1:E:1592:MET:SD	2.91	0.43
1:F:1554:LEU:O	1:F:1558:LEU:HD23	2.19	0.43
1:G:1601:GLN:H	1:G:1601:GLN:HE21	1.67	0.43
1:H:1593:ASP:CG	1:H:1594:PHE:H	2.21	0.43
1:K:1560:GLU:CG	1:K:1561:GLU:H	2.32	0.43
1:Q:1579:PRO:HG3	1:R:1599:PHE:HB3	2.01	0.43
1:R:1530:LYS:HZ1	1:R:1563:ARG:CZ	2.31	0.43
1:V:1558:LEU:N	1:V:1558:LEU:CD1	2.82	0.43
1:A:1545:LYS:CG	1:A:1546:ASP:N	2.78	0.43
1:D:1534:TYR:CE1	1:D:1535:LYS:HG3	2.53	0.43
1:F:1523:GLN:O	1:F:1524:SER:HB3	2.19	0.43
1:F:1554:LEU:HD12	1:F:1558:LEU:HD21	1.99	0.43
1:F:1602:VAL:CA	1:F:1605:GLU:OE1	2.66	0.43
1:G:1583:LEU:N	1:G:1583:LEU:CD1	2.82	0.43
1:J:1568:ALA:HA	1:J:1571:PHE:HB3	2.00	0.43
1:J:1602:VAL:CG1	1:L:1577:LEU:HD13	2.48	0.43
1:K:1604:LYS:HZ1	1:L:1613:LEU:CD2	2.31	0.43
1:N:1534:TYR:O	1:N:1538:MET:SD	2.77	0.43
1:N:1537:ALA:O	1:N:1540:TYR:HD1	2.02	0.43
1:O:1528:ALA:O	1:O:1529:LYS:HG2	2.19	0.43
1:Q:1563:ARG:HG2	1:Q:1564:GLU:OE1	2.19	0.43
1:T:1571:PHE:O	1:T:1574:TYR:HB2	2.19	0.43
1:T:1593:ASP:O	1:T:1594:PHE:HB2	2.18	0.43
1:V:1513:LEU:C	1:V:1513:LEU:HD13	2.38	0.43
1:V:1601:GLN:NE2	1:V:1601:GLN:N	2.66	0.43
1:W:1567:GLY:CA	1:W:1570:LEU:HD13	2.46	0.43
1:X:1542:SER:HB2	1:X:1571:PHE:HD2	1.84	0.43
1:D:1521:TRP:HB3	1:D:1522:LYS:H	1.63	0.43
1:D:1555:GLN:O	1:D:1559:GLN:N	2.51	0.43
1:F:1578:ARG:HH22	1:F:1580:ASP:HB2	1.83	0.43
1:J:1620:ARG:HA	1:J:1620:ARG:NE	2.32	0.43
1:K:1554:LEU:N	1:K:1554:LEU:CD1	2.81	0.43
1:U:1558:LEU:HD13	1:U:1565:CYS:SG	2.58	0.43
1:W:1591:ILE:H	1:W:1591:ILE:HG13	1.64	0.43
1:X:1523:GLN:O	1:X:1524:SER:HB3	2.18	0.43
1:H:1545:LYS:HB2	1:H:1571:PHE:CZ	2.52	0.43
1:I:1558:LEU:HD13	1:I:1565:CYS:SG	2.58	0.43
1:M:1566:PHE:O	1:M:1569:CYS:HB2	2.19	0.43
1:N:1577:LEU:HD11	1:O:1606:TYR:CB	2.45	0.43
1:P:1542:SER:C	1:P:1544:SER:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:1530:LYS:NZ	1:R:1563:ARG:NE	2.66	0.43
1:T:1528:ALA:O	1:T:1529:LYS:CB	2.67	0.43
1:U:1530:LYS:NZ	1:U:1563:ARG:CZ	2.82	0.43
1:B:1545:LYS:HA	1:B:1571:PHE:HZ	1.84	0.43
1:D:1596:MET:H	1:D:1597:PRO:HD3	1.84	0.43
1:H:1542:SER:HA	1:H:1571:PHE:CZ	2.54	0.43
1:I:1554:LEU:O	1:I:1558:LEU:HD23	2.19	0.43
1:I:1591:ILE:CG2	1:I:1592:MET:N	2.70	0.43
1:J:1580:ASP:O	1:J:1583:LEU:HB2	2.18	0.43
1:L:1530:LYS:NZ	1:L:1563:ARG:NE	2.67	0.43
1:N:1596:MET:HE2	1:N:1596:MET:N	2.34	0.43
1:O:1546:ASP:N	1:O:1550:ALA:HB2	2.34	0.43
1:O:1555:GLN:O	1:O:1559:GLN:HG2	2.19	0.43
1:O:1579:PRO:HB2	1:O:1580:ASP:H	1.59	0.43
1:Q:1567:GLY:CA	1:Q:1570:LEU:HD13	2.48	0.43
1:W:1535:LYS:HZ3	1:W:1563:ARG:NH2	2.17	0.43
1:X:1528:ALA:O	1:X:1529:LYS:HG2	2.19	0.43
1:A:1564:GLU:N	1:A:1564:GLU:OE1	2.52	0.42
1:D:1564:GLU:N	1:D:1564:GLU:OE1	2.52	0.42
1:E:1545:LYS:HB2	1:E:1571:PHE:CZ	2.54	0.42
1:F:1609:LYS:HA	1:F:1609:LYS:NZ	2.34	0.42
1:H:1539:GLN:OE1	1:H:1539:GLN:N	2.52	0.42
1:H:1571:PHE:HD1	1:H:1574:TYR:HD2	1.66	0.42
1:R:1528:ALA:O	1:R:1529:LYS:HG2	2.19	0.42
1:R:1585:LEU:HD13	1:R:1588:ARG:HE	1.84	0.42
1:S:1538:MET:O	1:S:1538:MET:HG2	2.18	0.42
1:S:1596:MET:N	1:S:1597:PRO:HD3	2.33	0.42
1:A:1592:MET:O	1:C:1587:TRP:HZ3	2.03	0.42
1:B:1580:ASP:CA	1:B:1583:LEU:HD13	2.49	0.42
1:C:1572:THR:HA	1:C:1575:ASP:HB2	2.00	0.42
1:C:1602:VAL:O	1:C:1602:VAL:CG1	2.67	0.42
1:I:1525:VAL:CG1	1:I:1526:GLU:H	2.15	0.42
1:O:1546:ASP:O	1:O:1550:ALA:HB2	2.18	0.42
1:O:1585:LEU:C	1:O:1587:TRP:N	2.72	0.42
1:P:1598:TYR:O	1:P:1601:GLN:HB2	2.19	0.42
1:R:1556:TRP:O	1:R:1561:GLU:OE1	2.37	0.42
1:V:1596:MET:H	1:V:1597:PRO:HD3	1.84	0.42
1:W:1545:LYS:HA	1:W:1571:PHE:HZ	1.83	0.42
1:W:1608:THR:O	1:W:1612:LYS:HG2	2.19	0.42
1:G:1554:LEU:HD23	1:G:1557:PHE:HD2	1.84	0.42
1:H:1590:ASN:O	1:H:1592:MET:HE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:1563:ARG:HA	1:K:1566:PHE:CG	2.54	0.42
1:K:1588:ARG:NE	1:K:1588:ARG:CA	2.83	0.42
1:K:1606:TYR:HA	1:K:1609:LYS:CE	2.49	0.42
1:M:1580:ASP:O	1:M:1583:LEU:N	2.45	0.42
1:P:1555:GLN:H	1:P:1555:GLN:CD	2.22	0.42
1:U:1523:GLN:O	1:U:1524:SER:HB3	2.19	0.42
1:V:1527:LEU:HA	1:V:1527:LEU:HD13	1.81	0.42
1:V:1532:SER:O	1:V:1533:LEU:HB2	2.19	0.42
1:W:1563:ARG:HG2	1:W:1564:GLU:OE1	2.19	0.42
1:B:1575:ASP:O	1:B:1576:LEU:HB2	2.20	0.42
1:C:1607:LEU:C	1:C:1609:LYS:N	2.72	0.42
1:D:1529:LYS:O	1:D:1530:LYS:HB2	2.20	0.42
1:D:1566:PHE:O	1:D:1569:CYS:HB2	2.19	0.42
1:E:1574:TYR:C	1:E:1576:LEU:H	2.20	0.42
1:F:1563:ARG:N	1:F:1564:GLU:OE1	2.53	0.42
1:G:1529:LYS:O	1:G:1530:LYS:CB	2.65	0.42
1:G:1572:THR:C	1:G:1578:ARG:HH22	2.22	0.42
1:K:1546:ASP:CB	1:K:1549:LEU:HB2	2.40	0.42
1:L:1525:VAL:HG12	1:L:1526:GLU:N	2.25	0.42
1:L:1554:LEU:HD12	1:L:1568:ALA:HB1	2.02	0.42
1:M:1588:ARG:HD3	1:M:1588:ARG:HA	1.83	0.42
1:N:1545:LYS:HB2	1:N:1571:PHE:CZ	2.54	0.42
1:O:1544:SER:O	1:O:1545:LYS:HD2	2.19	0.42
1:Q:1605:GLU:HG2	1:Q:1606:TYR:CD2	2.55	0.42
1:R:1533:LEU:CD2	1:R:1534:TYR:N	2.79	0.42
1:T:1596:MET:HA	1:T:1597:PRO:HD3	1.75	0.42
1:T:1600:ILE:CD1	1:U:1606:TYR:OH	2.67	0.42
1:T:1605:GLU:HG2	1:T:1606:TYR:CD2	2.53	0.42
1:U:1546:ASP:O	1:U:1550:ALA:HB2	2.19	0.42
1:U:1554:LEU:HD22	1:U:1554:LEU:N	2.34	0.42
1:V:1549:LEU:H	1:V:1549:LEU:CD2	2.33	0.42
1:W:1537:ALA:O	1:W:1538:MET:C	2.56	0.42
1:X:1599:PHE:HA	1:X:1602:VAL:HG23	2.01	0.42
1:A:1560:GLU:HG3	1:A:1561:GLU:N	2.33	0.42
1:A:1579:PRO:O	1:A:1581:VAL:N	2.53	0.42
1:E:1567:GLY:HA2	1:E:1570:LEU:CD1	2.44	0.42
1:F:1542:SER:HA	1:F:1571:PHE:HE2	1.85	0.42
1:F:1585:LEU:C	1:F:1587:TRP:N	2.73	0.42
1:K:1561:GLU:HB3	1:K:1564:GLU:HB2	2.01	0.42
1:N:1545:LYS:HA	1:N:1571:PHE:HZ	1.83	0.42
1:O:1549:LEU:O	1:O:1553:LEU:HG	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:1561:GLU:CB	1:Q:1564:GLU:HB2	2.49	0.42
1:S:1545:LYS:O	1:S:1546:ASP:HB2	2.18	0.42
1:S:1546:ASP:O	1:S:1550:ALA:HB2	2.19	0.42
1:S:1596:MET:N	1:S:1596:MET:SD	2.92	0.42
1:D:1560:GLU:CG	1:D:1561:GLU:N	2.79	0.42
1:D:1588:ARG:HG2	1:D:1588:ARG:HH11	1.84	0.42
1:E:1571:PHE:HD1	1:E:1574:TYR:HD2	1.68	0.42
1:H:1599:PHE:C	1:H:1601:GLN:N	2.70	0.42
1:I:1530:LYS:HZ3	1:I:1563:ARG:NE	2.17	0.42
1:J:1579:PRO:O	1:J:1581:VAL:N	2.52	0.42
1:K:1591:ILE:H	1:K:1591:ILE:HG13	1.74	0.42
1:R:1562:LYS:N	1:R:1564:GLU:OE1	2.52	0.42
1:R:1581:VAL:O	1:R:1584:GLU:N	2.53	0.42
1:S:1583:LEU:O	1:S:1584:GLU:C	2.57	0.42
1:U:1547:THR:CG2	1:U:1548:GLU:H	2.27	0.42
1:U:1549:LEU:O	1:U:1553:LEU:HG	2.19	0.42
1:W:1591:ILE:O	1:W:1592:MET:SD	2.78	0.42
1:C:1530:LYS:HZ1	1:C:1563:ARG:CZ	2.33	0.42
1:D:1541:ALA:HB3	1:D:1571:PHE:CE2	2.55	0.42
1:E:1560:GLU:CG	1:E:1561:GLU:H	2.33	0.42
1:G:1516:ARG:O	1:G:1516:ARG:HG3	2.20	0.42
1:G:1596:MET:N	1:G:1597:PRO:CD	2.82	0.42
1:J:1534:TYR:CZ	1:J:1535:LYS:HG3	2.55	0.42
1:K:1604:LYS:CE	1:L:1609:LYS:HD2	2.50	0.42
1:M:1510:SER:OG	1:M:1511:SER:N	2.53	0.42
1:N:1538:MET:HB2	1:N:1539:GLN:OE1	2.20	0.42
1:O:1523:GLN:O	1:O:1524:SER:HB3	2.19	0.42
1:R:1582:VAL:C	1:R:1583:LEU:HD13	2.39	0.42
1:T:1604:LYS:HG3	1:U:1609:LYS:NZ	2.31	0.42
1:U:1530:LYS:HZ3	1:U:1563:ARG:NE	2.18	0.42
1:A:1588:ARG:HD3	1:A:1588:ARG:HA	1.88	0.42
1:C:1594:PHE:O	1:C:1595:ALA:CB	2.67	0.42
1:D:1509:HIS:O	1:D:1510:SER:CB	2.68	0.42
1:F:1585:LEU:HD13	1:F:1588:ARG:CG	2.48	0.42
1:I:1537:ALA:HB3	1:I:1538:MET:HE1	2.02	0.42
1:I:1579:PRO:HA	1:I:1582:VAL:CG2	2.50	0.42
1:J:1551:GLU:O	1:J:1553:LEU:N	2.52	0.42
1:L:1533:LEU:CG	1:V:1588:ARG:NH2	2.83	0.42
1:L:1601:GLN:C	1:L:1603:MET:H	2.22	0.42
1:P:1561:GLU:HB2	1:P:1564:GLU:HB2	2.00	0.42
1:S:1571:PHE:CD1	1:S:1571:PHE:C	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1620:ARG:HA	1:S:1620:ARG:NE	2.33	0.42
1:W:1606:TYR:HA	1:W:1609:LYS:HE3	1.97	0.42
1:C:1528:ALA:O	1:C:1529:LYS:HG2	2.20	0.42
1:I:1528:ALA:O	1:I:1529:LYS:HG2	2.19	0.42
1:K:1599:PHE:O	1:K:1602:VAL:N	2.53	0.42
1:P:1550:ALA:O	1:P:1551:GLU:C	2.59	0.42
1:P:1554:LEU:HD13	1:P:1572:THR:OG1	2.20	0.42
1:R:1555:GLN:O	1:R:1559:GLN:HG2	2.20	0.42
1:W:1593:ASP:CG	1:W:1594:PHE:H	2.22	0.42
1:C:1609:LYS:HA	1:C:1609:LYS:HZ2	1.84	0.42
1:D:1572:THR:C	1:D:1578:ARG:HH22	2.22	0.42
1:D:1575:ASP:HB2	1:D:1578:ARG:NH1	2.35	0.42
1:E:1537:ALA:O	1:E:1540:TYR:HD1	2.03	0.42
1:E:1583:LEU:HD21	1:F:1599:PHE:CE1	2.55	0.42
1:H:1537:ALA:O	1:H:1539:GLN:N	2.53	0.42
1:K:1578:ARG:HD2	1:K:1578:ARG:HA	1.91	0.42
1:K:1579:PRO:CB	1:L:1599:PHE:CD1	3.00	0.42
1:K:1583:LEU:HD12	1:K:1583:LEU:H	1.84	0.42
1:K:1596:MET:H	1:K:1596:MET:HE2	1.84	0.42
1:L:1549:LEU:O	1:L:1553:LEU:HG	2.20	0.42
1:N:1560:GLU:CG	1:N:1561:GLU:H	2.33	0.42
1:R:1519:HIS:HE1	1:R:1540:TYR:OH	2.03	0.42
1:U:1528:ALA:O	1:U:1529:LYS:HG2	2.19	0.42
1:U:1535:LYS:O	1:U:1536:ASP:CB	2.68	0.42
1:V:1551:GLU:C	1:V:1553:LEU:N	2.74	0.42
1:W:1592:MET:HE2	1:W:1592:MET:H	1.83	0.42
1:W:1596:MET:HA	1:W:1597:PRO:HD3	1.77	0.42
1:B:1591:ILE:H	1:B:1591:ILE:HG13	1.60	0.41
1:C:1546:ASP:O	1:C:1550:ALA:HB2	2.20	0.41
1:D:1513:LEU:HD22	1:D:1514:VAL:N	2.35	0.41
1:I:1572:THR:HA	1:I:1575:ASP:HB2	2.01	0.41
1:J:1549:LEU:H	1:J:1549:LEU:CD2	2.32	0.41
1:L:1554:LEU:O	1:L:1558:LEU:HD23	2.20	0.41
1:M:1513:LEU:HD22	1:M:1514:VAL:N	2.35	0.41
1:M:1561:GLU:CB	1:M:1564:GLU:HB2	2.49	0.41
1:N:1542:SER:HA	1:N:1571:PHE:CZ	2.55	0.41
1:N:1574:TYR:C	1:N:1576:LEU:N	2.72	0.41
1:N:1583:LEU:HD22	1:O:1596:MET:CG	2.49	0.41
1:W:1535:LYS:NZ	1:W:1563:ARG:HH21	2.18	0.41
1:W:1560:GLU:O	1:W:1561:GLU:HB2	2.20	0.41
1:D:1554:LEU:O	1:D:1558:LEU:HD13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1562:LYS:C	1:F:1564:GLU:H	2.23	0.41
1:G:1546:ASP:HB3	1:G:1550:ALA:H	1.85	0.41
1:H:1591:ILE:H	1:H:1591:ILE:HG13	1.67	0.41
1:H:1605:GLU:O	1:H:1609:LYS:HE2	2.19	0.41
1:L:1535:LYS:O	1:L:1536:ASP:CB	2.68	0.41
1:P:1554:LEU:O	1:P:1558:LEU:HD13	2.20	0.41
1:P:1596:MET:H	1:P:1597:PRO:HD3	1.85	0.41
1:Q:1548:GLU:HA	1:Q:1551:GLU:HB2	2.03	0.41
1:R:1550:ALA:O	1:R:1553:LEU:HB2	2.20	0.41
1:R:1592:MET:SD	1:R:1593:ASP:N	2.93	0.41
1:S:1518:SER:HB2	1:S:1520:MET:HE1	2.01	0.41
1:X:1598:TYR:O	1:X:1602:VAL:HG23	2.20	0.41
1:B:1537:ALA:O	1:B:1538:MET:C	2.55	0.41
1:B:1552:GLU:O	1:B:1553:LEU:C	2.58	0.41
1:G:1609:LYS:O	1:G:1613:LEU:HG	2.20	0.41
1:H:1592:MET:HE2	1:H:1592:MET:N	2.35	0.41
1:H:1608:THR:O	1:H:1608:THR:HG22	2.20	0.41
1:J:1578:ARG:NH1	1:J:1578:ARG:CB	2.73	0.41
1:M:1618:SER:C	1:M:1620:ARG:H	2.23	0.41
1:O:1554:LEU:O	1:O:1558:LEU:HB2	2.20	0.41
1:U:1547:THR:CG2	1:U:1548:GLU:N	2.83	0.41
1:U:1563:ARG:N	1:U:1564:GLU:OE1	2.52	0.41
1:U:1602:VAL:C	1:U:1605:GLU:OE1	2.58	0.41
1:V:1534:TYR:CE1	1:V:1535:LYS:HG3	2.56	0.41
1:W:1560:GLU:CG	1:W:1561:GLU:H	2.33	0.41
1:W:1604:LYS:NZ	1:X:1609:LYS:HD2	2.35	0.41
1:X:1596:MET:N	1:X:1597:PRO:HD3	2.34	0.41
1:X:1599:PHE:HA	1:X:1602:VAL:HG21	2.02	0.41
1:A:1602:VAL:O	1:A:1602:VAL:HG12	2.20	0.41
1:D:1508:HIS:CD2	1:D:1509:HIS:H	2.38	0.41
1:D:1593:ASP:HA	1:F:1587:TRP:CH2	2.55	0.41
1:E:1583:LEU:HD12	1:E:1583:LEU:H	1.85	0.41
1:F:1528:ALA:O	1:F:1529:LYS:HG2	2.20	0.41
1:G:1604:LYS:HB3	1:H:1605:GLU:HB3	2.03	0.41
1:J:1571:PHE:C	1:J:1571:PHE:CD1	2.94	0.41
1:L:1545:LYS:HB2	1:L:1546:ASP:H	1.54	0.41
1:L:1559:GLN:NE2	1:L:1585:LEU:HD11	2.36	0.41
1:O:1530:LYS:HZ3	1:O:1563:ARG:CD	2.34	0.41
1:S:1521:TRP:HB3	1:S:1522:LYS:H	1.70	0.41
1:V:1554:LEU:O	1:V:1558:LEU:N	2.49	0.41
1:W:1537:ALA:O	1:W:1539:GLN:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1602:VAL:CA	1:X:1605:GLU:OE1	2.68	0.41
1:B:1561:GLU:HB3	1:B:1564:GLU:HB2	2.02	0.41
1:B:1571:PHE:HD1	1:B:1574:TYR:HD2	1.68	0.41
1:E:1581:VAL:O	1:E:1585:LEU:CD2	2.58	0.41
1:H:1606:TYR:HA	1:H:1609:LYS:HE3	2.02	0.41
1:I:1542:SER:HA	1:I:1571:PHE:HE2	1.84	0.41
1:I:1582:VAL:O	1:I:1583:LEU:HD13	2.20	0.41
1:J:1515:PRO:O	1:J:1516:ARG:CB	2.68	0.41
1:J:1521:TRP:HB3	1:J:1522:LYS:H	1.63	0.41
1:L:1528:ALA:O	1:L:1529:LYS:HG2	2.21	0.41
1:O:1525:VAL:HG12	1:O:1526:GLU:N	2.23	0.41
1:P:1561:GLU:CB	1:P:1564:GLU:HB2	2.50	0.41
1:Q:1606:TYR:HA	1:Q:1609:LYS:CE	2.51	0.41
1:R:1588:ARG:O	1:R:1589:HIS:HB2	2.20	0.41
1:S:1531:ASP:O	1:S:1532:SER:OG	2.30	0.41
1:T:1604:LYS:CG	1:U:1609:LYS:CD	2.95	0.41
1:U:1579:PRO:HA	1:U:1582:VAL:CG2	2.51	0.41
1:V:1583:LEU:O	1:V:1584:GLU:C	2.57	0.41
1:X:1554:LEU:HD12	1:X:1568:ALA:HB1	2.01	0.41
1:X:1585:LEU:HD13	1:X:1588:ARG:HE	1.86	0.41
1:A:1575:ASP:HB2	1:A:1578:ARG:NH1	2.34	0.41
1:B:1574:TYR:C	1:B:1576:LEU:N	2.74	0.41
1:D:1520:MET:N	1:D:1520:MET:SD	2.93	0.41
1:F:1547:THR:CG2	1:F:1548:GLU:H	2.31	0.41
1:G:1561:GLU:CB	1:G:1564:GLU:HB2	2.51	0.41
1:I:1554:LEU:HD12	1:I:1568:ALA:HB1	2.01	0.41
1:K:1599:PHE:C	1:K:1601:GLN:N	2.73	0.41
1:N:1580:ASP:CA	1:N:1583:LEU:HD13	2.49	0.41
1:O:1525:VAL:CG1	1:O:1526:GLU:H	2.23	0.41
1:O:1601:GLN:C	1:O:1603:MET:H	2.23	0.41
1:Q:1558:LEU:HD12	1:Q:1565:CYS:HA	2.02	0.41
1:V:1523:GLN:O	1:V:1524:SER:HB3	2.21	0.41
1:V:1558:LEU:HD11	1:V:1568:ALA:HB3	2.02	0.41
1:W:1538:MET:HG3	1:W:1557:PHE:CZ	2.56	0.41
1:W:1579:PRO:O	1:W:1581:VAL:N	2.54	0.41
1:A:1534:TYR:O	1:A:1538:MET:HB2	2.21	0.41
1:A:1542:SER:C	1:A:1544:SER:H	2.23	0.41
1:A:1601:GLN:NE2	1:A:1601:GLN:H	2.18	0.41
1:C:1519:HIS:HE1	1:C:1540:TYR:OH	2.04	0.41
1:D:1515:PRO:O	1:D:1516:ARG:CB	2.69	0.41
1:D:1518:SER:HB2	1:D:1520:MET:HE1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1572:THR:HG23	1:D:1578:ARG:CZ	2.50	0.41
1:D:1593:ASP:HA	1:F:1587:TRP:CZ3	2.56	0.41
1:E:1578:ARG:HD2	1:E:1578:ARG:HA	1.73	0.41
1:E:1593:ASP:CG	1:E:1594:PHE:N	2.69	0.41
1:F:1535:LYS:O	1:F:1536:ASP:CB	2.69	0.41
1:F:1585:LEU:C	1:F:1587:TRP:H	2.24	0.41
1:G:1542:SER:C	1:G:1544:SER:H	2.23	0.41
1:L:1523:GLN:O	1:L:1524:SER:HB3	2.20	0.41
1:M:1554:LEU:O	1:M:1558:LEU:HD13	2.21	0.41
1:M:1575:ASP:HB2	1:M:1578:ARG:CZ	2.51	0.41
1:N:1563:ARG:HA	1:N:1566:PHE:CG	2.55	0.41
1:N:1579:PRO:HG2	1:N:1580:ASP:OD1	2.20	0.41
1:B:1535:LYS:HA	1:B:1538:MET:CE	2.51	0.41
1:C:1601:GLN:O	1:C:1605:GLU:CD	2.59	0.41
1:D:1553:LEU:N	1:D:1553:LEU:CD1	2.84	0.41
1:F:1533:LEU:HD13	1:F:1534:TYR:CD1	2.56	0.41
1:G:1549:LEU:H	1:G:1549:LEU:CD2	2.33	0.41
1:H:1554:LEU:N	1:H:1554:LEU:CD1	2.83	0.41
1:I:1612:LYS:HE2	1:I:1612:LYS:HB3	1.98	0.41
1:K:1534:TYR:O	1:K:1538:MET:SD	2.79	0.41
1:L:1536:ASP:O	1:L:1540:TYR:CD1	2.74	0.41
1:L:1554:LEU:HD22	1:L:1554:LEU:N	2.36	0.41
1:N:1571:PHE:HD1	1:N:1574:TYR:HD2	1.68	0.41
1:P:1580:ASP:O	1:P:1583:LEU:N	2.44	0.41
1:Q:1537:ALA:C	1:Q:1539:GLN:N	2.72	0.41
1:Q:1578:ARG:HH22	1:Q:1580:ASP:CB	2.22	0.41
1:S:1566:PHE:N	1:S:1566:PHE:CD2	2.88	0.41
1:T:1547:THR:HG22	1:T:1548:GLU:N	2.35	0.41
1:T:1561:GLU:CB	1:T:1564:GLU:HB2	2.51	0.41
1:X:1579:PRO:HA	1:X:1582:VAL:CG2	2.50	0.41
1:C:1530:LYS:NZ	1:C:1563:ARG:NE	2.69	0.41
1:C:1572:THR:O	1:C:1572:THR:HG22	2.21	0.41
1:D:1534:TYR:O	1:D:1538:MET:HB2	2.21	0.41
1:D:1560:GLU:O	1:D:1561:GLU:CB	2.65	0.41
1:D:1584:GLU:O	1:D:1586:ALA:N	2.54	0.41
1:E:1563:ARG:HA	1:E:1566:PHE:CG	2.56	0.41
1:F:1554:LEU:HD22	1:F:1554:LEU:N	2.36	0.41
1:G:1546:ASP:HB3	1:G:1550:ALA:N	2.35	0.41
1:G:1555:GLN:O	1:G:1559:GLN:HB2	2.21	0.41
1:H:1570:LEU:HB3	1:H:1574:TYR:CZ	2.56	0.41
1:H:1577:LEU:HD11	1:I:1606:TYR:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1533:LEU:HD13	1:I:1534:TYR:CD1	2.56	0.41
1:I:1585:LEU:C	1:I:1587:TRP:N	2.74	0.41
1:I:1619:LEU:HD23	1:I:1622:GLU:OE2	2.20	0.41
1:J:1558:LEU:N	1:J:1558:LEU:HD12	2.36	0.41
1:J:1561:GLU:CB	1:J:1564:GLU:HB2	2.51	0.41
1:L:1534:TYR:HB3	1:L:1535:LYS:H	1.74	0.41
1:L:1598:TYR:O	1:L:1602:VAL:HG23	2.21	0.41
1:M:1575:ASP:HB2	1:M:1578:ARG:NH1	2.36	0.41
1:N:1548:GLU:HA	1:N:1551:GLU:OE1	2.21	0.41
1:R:1562:LYS:C	1:R:1564:GLU:H	2.24	0.41
1:T:1535:LYS:NZ	1:T:1563:ARG:HH21	2.19	0.41
1:T:1560:GLU:CG	1:T:1561:GLU:H	2.34	0.41
1:T:1570:LEU:HB3	1:T:1574:TYR:CZ	2.56	0.41
1:V:1561:GLU:HB2	1:V:1564:GLU:HB2	2.03	0.41
1:X:1549:LEU:O	1:X:1553:LEU:HG	2.21	0.41
1:H:1547:THR:HG22	1:H:1548:GLU:N	2.36	0.41
1:I:1618:SER:O	1:I:1622:GLU:N	2.54	0.41
1:L:1607:LEU:C	1:L:1609:LYS:N	2.74	0.41
1:N:1572:THR:CG2	1:N:1578:ARG:HB3	2.48	0.41
1:S:1587:TRP:HA	1:S:1587:TRP:CE3	2.56	0.41
1:T:1554:LEU:HD11	1:T:1571:PHE:CD2	2.51	0.41
1:T:1554:LEU:N	1:T:1554:LEU:CD1	2.84	0.41
1:V:1531:ASP:HB2	1:V:1532:SER:H	1.62	0.41
1:X:1519:HIS:HE1	1:X:1540:TYR:OH	2.04	0.41
1:X:1596:MET:SD	1:X:1596:MET:C	2.99	0.41
1:D:1523:GLN:O	1:D:1524:SER:HB3	2.20	0.40
1:D:1541:ALA:HB3	1:D:1571:PHE:HE2	1.87	0.40
1:D:1588:ARG:HG2	1:D:1588:ARG:NH1	2.36	0.40
1:H:1558:LEU:HD11	1:H:1568:ALA:HB3	2.03	0.40
1:M:1523:GLN:O	1:M:1524:SER:HB3	2.22	0.40
1:Q:1596:MET:HA	1:Q:1597:PRO:HD3	1.83	0.40
1:R:1546:ASP:N	1:R:1550:ALA:HB2	2.35	0.40
1:S:1601:GLN:NE2	1:S:1601:GLN:N	2.69	0.40
1:T:1574:TYR:C	1:T:1576:LEU:N	2.75	0.40
1:T:1579:PRO:O	1:T:1581:VAL:N	2.55	0.40
1:T:1583:LEU:HD12	1:T:1583:LEU:H	1.85	0.40
1:V:1621:LYS:HE2	1:V:1621:LYS:HB3	1.93	0.40
1:W:1535:LYS:HZ1	1:W:1563:ARG:HH21	1.68	0.40
1:X:1592:MET:SD	1:X:1593:ASP:N	2.94	0.40
1:F:1596:MET:HB3	1:F:1599:PHE:CE1	2.56	0.40
1:K:1545:LYS:HA	1:K:1571:PHE:CZ	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:1570:LEU:HB3	1:K:1574:TYR:CZ	2.56	0.40
1:P:1596:MET:HG2	1:P:1596:MET:O	2.21	0.40
1:Q:1549:LEU:O	1:Q:1553:LEU:CG	2.66	0.40
1:S:1571:PHE:O	1:S:1575:ASP:OD2	2.39	0.40
1:S:1588:ARG:HD3	1:S:1588:ARG:HA	1.91	0.40
1:V:1596:MET:HG2	1:V:1596:MET:O	2.21	0.40
1:W:1563:ARG:HA	1:W:1566:PHE:CG	2.56	0.40
1:W:1588:ARG:NE	1:W:1588:ARG:CA	2.85	0.40
1:A:1611:ASP:O	1:A:1615:ALA:HB2	2.21	0.40
1:C:1554:LEU:HD12	1:C:1558:LEU:HD21	2.04	0.40
1:D:1509:HIS:CG	1:D:1510:SER:N	2.89	0.40
1:D:1596:MET:N	1:D:1597:PRO:CD	2.85	0.40
1:E:1585:LEU:HA	1:E:1588:ARG:HD2	2.04	0.40
1:H:1529:LYS:C	1:H:1530:LYS:HG2	2.42	0.40
1:H:1574:TYR:C	1:H:1576:LEU:N	2.75	0.40
1:J:1596:MET:H	1:J:1597:PRO:HD3	1.86	0.40
1:O:1603:MET:N	1:O:1603:MET:SD	2.94	0.40
1:Q:1545:LYS:HA	1:Q:1571:PHE:HZ	1.86	0.40
1:Q:1571:PHE:HD1	1:Q:1574:TYR:HD2	1.68	0.40
1:Q:1599:PHE:C	1:Q:1601:GLN:N	2.75	0.40
1:S:1583:LEU:HD12	1:S:1583:LEU:N	2.36	0.40
1:T:1535:LYS:NZ	1:T:1563:ARG:NH2	2.69	0.40
1:T:1551:GLU:O	1:T:1552:GLU:C	2.58	0.40
1:U:1544:SER:O	1:U:1545:LYS:CD	2.69	0.40
1:U:1549:LEU:HD13	1:U:1552:GLU:OE2	2.21	0.40
1:U:1599:PHE:HA	1:U:1602:VAL:HG23	2.02	0.40
1:A:1583:LEU:O	1:A:1584:GLU:C	2.59	0.40
1:A:1592:MET:O	1:C:1587:TRP:CZ3	2.75	0.40
1:A:1618:SER:C	1:A:1620:ARG:H	2.25	0.40
1:G:1571:PHE:C	1:G:1571:PHE:CD1	2.95	0.40
1:H:1596:MET:HA	1:H:1597:PRO:HD3	1.84	0.40
1:K:1579:PRO:O	1:K:1581:VAL:N	2.54	0.40
1:N:1556:TRP:C	1:N:1559:GLN:HG3	2.41	0.40
1:P:1588:ARG:HD3	1:P:1588:ARG:HA	1.88	0.40
1:R:1554:LEU:HD12	1:R:1558:LEU:HD21	2.02	0.40
1:T:1578:ARG:HD2	1:T:1578:ARG:HA	1.82	0.40
1:W:1529:LYS:O	1:W:1530:LYS:HG2	2.21	0.40
1:B:1538:MET:HB2	1:B:1539:GLN:OE1	2.20	0.40
1:E:1542:SER:HA	1:E:1571:PHE:CZ	2.56	0.40
1:K:1558:LEU:HD23	1:K:1585:LEU:HG	2.03	0.40
1:L:1542:SER:HA	1:L:1571:PHE:HE2	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:1547:THR:HG22	1:N:1548:GLU:N	2.36	0.40
1:O:1585:LEU:C	1:O:1587:TRP:H	2.24	0.40
1:O:1607:LEU:C	1:O:1609:LYS:N	2.73	0.40
1:P:1541:ALA:HB3	1:P:1571:PHE:CE2	2.56	0.40
1:P:1558:LEU:HD12	1:P:1558:LEU:N	2.36	0.40
1:S:1534:TYR:H	1:S:1534:TYR:HD1	1.69	0.40
1:S:1603:MET:O	1:S:1607:LEU:HB2	2.22	0.40
1:T:1592:MET:N	1:T:1592:MET:CE	2.83	0.40
1:V:1568:ALA:HA	1:V:1571:PHE:HB3	2.04	0.40
1:W:1558:LEU:HD12	1:W:1565:CYS:HA	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1588:ARG:NH1	1:U:1533:LEU:CG[3_655]	2.17	0.03

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	123/125 (98%)	77 (63%)	29 (24%)	17 (14%)	0 4
1	B	95/125 (76%)	60 (63%)	28 (30%)	7 (7%)	1 16
1	C	123/125 (98%)	78 (63%)	28 (23%)	17 (14%)	0 4
1	D	123/125 (98%)	76 (62%)	29 (24%)	18 (15%)	0 4
1	E	95/125 (76%)	61 (64%)	28 (30%)	6 (6%)	1 19
1	F	123/125 (98%)	78 (63%)	29 (24%)	16 (13%)	0 5
1	G	123/125 (98%)	77 (63%)	29 (24%)	17 (14%)	0 4
1	H	95/125 (76%)	61 (64%)	27 (28%)	7 (7%)	1 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	123/125 (98%)	76 (62%)	31 (25%)	16 (13%)	0	5
1	J	123/125 (98%)	74 (60%)	31 (25%)	18 (15%)	0	4
1	K	95/125 (76%)	59 (62%)	29 (30%)	7 (7%)	1	16
1	L	123/125 (98%)	80 (65%)	26 (21%)	17 (14%)	0	4
1	M	123/125 (98%)	75 (61%)	31 (25%)	17 (14%)	0	4
1	N	95/125 (76%)	62 (65%)	27 (28%)	6 (6%)	1	19
1	O	123/125 (98%)	78 (63%)	28 (23%)	17 (14%)	0	4
1	P	123/125 (98%)	77 (63%)	29 (24%)	17 (14%)	0	4
1	Q	95/125 (76%)	59 (62%)	29 (30%)	7 (7%)	1	16
1	R	123/125 (98%)	79 (64%)	27 (22%)	17 (14%)	0	4
1	S	123/125 (98%)	78 (63%)	27 (22%)	18 (15%)	0	4
1	T	95/125 (76%)	61 (64%)	28 (30%)	6 (6%)	1	19
1	U	123/125 (98%)	77 (63%)	30 (24%)	16 (13%)	0	5
1	V	123/125 (98%)	77 (63%)	27 (22%)	19 (15%)	0	3
1	W	95/125 (76%)	59 (62%)	29 (30%)	7 (7%)	1	16
1	X	123/125 (98%)	78 (63%)	29 (24%)	16 (13%)	0	5
All	All	2728/3000 (91%)	1717 (63%)	685 (25%)	326 (12%)	0	6

All (326) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1508	HIS
1	A	1516	ARG
1	A	1545	LYS
1	A	1578	ARG
1	A	1605	GLU
1	B	1580	ASP
1	C	1513	LEU
1	C	1522	LYS
1	C	1524	SER
1	C	1525	VAL
1	C	1545	LYS
1	C	1589	HIS
1	C	1595	ALA
1	C	1604	LYS
1	D	1508	HIS

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Mol	Chain	Res	Type
1	D	1516	ARG
1	D	1545	LYS
1	D	1577	LEU
1	D	1578	ARG
1	D	1605	GLU
1	E	1530	LYS
1	E	1580	ASP
1	F	1513	LEU
1	F	1522	LYS
1	F	1524	SER
1	F	1525	VAL
1	F	1545	LYS
1	F	1589	HIS
1	F	1595	ALA
1	F	1604	LYS
1	G	1508	HIS
1	G	1516	ARG
1	G	1545	LYS
1	G	1578	ARG
1	G	1605	GLU
1	H	1530	LYS
1	H	1580	ASP
1	I	1513	LEU
1	I	1522	LYS
1	I	1524	SER
1	I	1525	VAL
1	I	1545	LYS
1	I	1589	HIS
1	I	1595	ALA
1	I	1623	GLU
1	J	1508	HIS
1	J	1516	ARG
1	J	1545	LYS
1	J	1577	LEU
1	J	1578	ARG
1	J	1605	GLU
1	K	1530	LYS
1	K	1580	ASP
1	L	1513	LEU
1	L	1522	LYS
1	L	1524	SER
1	L	1525	VAL

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Mol	Chain	Res	Type
1	L	1545	LYS
1	L	1589	HIS
1	L	1595	ALA
1	L	1604	LYS
1	M	1508	HIS
1	M	1516	ARG
1	M	1545	LYS
1	M	1577	LEU
1	M	1605	GLU
1	N	1530	LYS
1	N	1580	ASP
1	O	1513	LEU
1	O	1522	LYS
1	O	1524	SER
1	O	1525	VAL
1	O	1545	LYS
1	O	1589	HIS
1	O	1595	ALA
1	P	1508	HIS
1	P	1516	ARG
1	P	1545	LYS
1	P	1577	LEU
1	P	1578	ARG
1	Q	1580	ASP
1	R	1513	LEU
1	R	1522	LYS
1	R	1524	SER
1	R	1525	VAL
1	R	1545	LYS
1	R	1589	HIS
1	R	1595	ALA
1	S	1508	HIS
1	S	1516	ARG
1	S	1545	LYS
1	S	1578	ARG
1	T	1530	LYS
1	T	1580	ASP
1	U	1513	LEU
1	U	1522	LYS
1	U	1524	SER
1	U	1525	VAL
1	U	1545	LYS

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Mol	Chain	Res	Type
1	U	1589	HIS
1	U	1595	ALA
1	U	1604	LYS
1	V	1508	HIS
1	V	1516	ARG
1	V	1545	LYS
1	V	1577	LEU
1	V	1578	ARG
1	V	1605	GLU
1	W	1580	ASP
1	X	1513	LEU
1	X	1522	LYS
1	X	1524	SER
1	X	1525	VAL
1	X	1545	LYS
1	X	1589	HIS
1	X	1595	ALA
1	X	1604	LYS
1	X	1623	GLU
1	A	1510	SER
1	A	1524	SER
1	A	1577	LEU
1	A	1579	PRO
1	A	1580	ASP
1	B	1530	LYS
1	B	1545	LYS
1	B	1579	PRO
1	B	1597	PRO
1	C	1536	ASP
1	C	1555	GLN
1	C	1575	ASP
1	C	1579	PRO
1	C	1623	GLU
1	D	1524	SER
1	D	1529	LYS
1	D	1579	PRO
1	D	1580	ASP
1	D	1588	ARG
1	E	1545	LYS
1	E	1579	PRO
1	E	1597	PRO
1	F	1536	ASP

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Mol	Chain	Res	Type
1	F	1555	GLN
1	F	1575	ASP
1	F	1579	PRO
1	F	1623	GLU
1	G	1510	SER
1	G	1524	SER
1	G	1577	LEU
1	G	1579	PRO
1	G	1580	ASP
1	H	1545	LYS
1	H	1579	PRO
1	H	1597	PRO
1	I	1536	ASP
1	I	1555	GLN
1	I	1575	ASP
1	I	1579	PRO
1	I	1604	LYS
1	J	1510	SER
1	J	1524	SER
1	J	1529	LYS
1	J	1579	PRO
1	J	1580	ASP
1	K	1545	LYS
1	K	1579	PRO
1	K	1597	PRO
1	L	1536	ASP
1	L	1575	ASP
1	L	1579	PRO
1	L	1623	GLU
1	M	1510	SER
1	M	1524	SER
1	M	1578	ARG
1	M	1579	PRO
1	M	1580	ASP
1	N	1545	LYS
1	N	1579	PRO
1	N	1597	PRO
1	O	1536	ASP
1	O	1575	ASP
1	O	1579	PRO
1	O	1604	LYS
1	O	1623	GLU

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Mol	Chain	Res	Type
1	P	1510	SER
1	P	1524	SER
1	P	1550	ALA
1	P	1579	PRO
1	P	1580	ASP
1	P	1605	GLU
1	Q	1530	LYS
1	Q	1545	LYS
1	Q	1579	PRO
1	Q	1597	PRO
1	R	1536	ASP
1	R	1579	PRO
1	R	1604	LYS
1	R	1623	GLU
1	S	1510	SER
1	S	1524	SER
1	S	1529	LYS
1	S	1577	LEU
1	S	1579	PRO
1	S	1580	ASP
1	S	1588	ARG
1	S	1605	GLU
1	T	1545	LYS
1	T	1579	PRO
1	T	1597	PRO
1	U	1536	ASP
1	U	1555	GLN
1	U	1575	ASP
1	U	1579	PRO
1	U	1623	GLU
1	V	1524	SER
1	V	1529	LYS
1	V	1552	GLU
1	V	1579	PRO
1	V	1580	ASP
1	W	1530	LYS
1	W	1545	LYS
1	W	1579	PRO
1	W	1597	PRO
1	X	1536	ASP
1	X	1575	ASP
1	X	1579	PRO

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Mol	Chain	Res	Type
1	A	1522	LYS
1	A	1550	ALA
1	A	1588	ARG
1	B	1594	PHE
1	C	1514	VAL
1	C	1580	ASP
1	E	1598	TYR
1	F	1514	VAL
1	G	1522	LYS
1	G	1529	LYS
1	G	1550	ALA
1	H	1598	TYR
1	I	1514	VAL
1	J	1552	GLU
1	K	1594	PHE
1	L	1514	VAL
1	L	1555	GLN
1	M	1529	LYS
1	O	1514	VAL
1	O	1555	GLN
1	P	1522	LYS
1	R	1514	VAL
1	R	1555	GLN
1	R	1575	ASP
1	U	1514	VAL
1	V	1510	SER
1	V	1550	ALA
1	W	1594	PHE
1	W	1598	TYR
1	X	1514	VAL
1	A	1546	ASP
1	B	1535	LYS
1	D	1510	SER
1	D	1550	ALA
1	F	1580	ASP
1	G	1552	GLU
1	I	1580	ASP
1	J	1588	ARG
1	K	1598	TYR
1	L	1580	ASP
1	M	1522	LYS
1	M	1550	ALA

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Mol	Chain	Res	Type
1	O	1580	ASP
1	P	1588	ARG
1	Q	1594	PHE
1	R	1580	ASP
1	R	1582	VAL
1	S	1603	MET
1	U	1580	ASP
1	V	1546	ASP
1	V	1588	ARG
1	V	1603	MET
1	X	1580	ASP
1	A	1529	LYS
1	A	1603	MET
1	D	1522	LYS
1	D	1546	ASP
1	D	1585	LEU
1	D	1603	MET
1	F	1582	VAL
1	G	1546	ASP
1	G	1603	MET
1	J	1522	LYS
1	L	1602	VAL
1	M	1530	LYS
1	M	1546	ASP
1	M	1603	MET
1	N	1598	TYR
1	P	1546	ASP
1	P	1603	MET
1	R	1594	PHE
1	S	1522	LYS
1	S	1546	ASP
1	S	1550	ALA
1	T	1598	TYR
1	V	1522	LYS
1	V	1530	LYS
1	X	1555	GLN
1	C	1594	PHE
1	G	1596	MET
1	H	1538	MET
1	J	1521	TRP
1	J	1530	LYS
1	J	1546	ASP

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Mol	Chain	Res	Type
1	L	1582	VAL
1	P	1530	LYS
1	Q	1598	TYR
1	S	1530	LYS
1	S	1596	MET
1	X	1602	VAL
1	D	1596	MET
1	J	1596	MET
1	V	1596	MET
1	I	1602	VAL
1	P	1596	MET
1	A	1596	MET
1	C	1602	VAL
1	M	1596	MET
1	O	1582	VAL
1	O	1602	VAL
1	U	1602	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	113/113 (100%)	103 (91%)	10 (9%)	10	36
1	B	88/113 (78%)	78 (89%)	10 (11%)	5	26
1	C	113/113 (100%)	99 (88%)	14 (12%)	4	24
1	D	113/113 (100%)	102 (90%)	11 (10%)	8	31
1	E	88/113 (78%)	79 (90%)	9 (10%)	7	30
1	F	113/113 (100%)	101 (89%)	12 (11%)	6	29
1	G	113/113 (100%)	101 (89%)	12 (11%)	6	29
1	H	88/113 (78%)	79 (90%)	9 (10%)	7	30
1	I	113/113 (100%)	101 (89%)	12 (11%)	6	29
1	J	113/113 (100%)	102 (90%)	11 (10%)	8	31
1	K	88/113 (78%)	79 (90%)	9 (10%)	7	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	113/113 (100%)	100 (88%)	13 (12%)	5	26
1	M	113/113 (100%)	101 (89%)	12 (11%)	6	29
1	N	88/113 (78%)	80 (91%)	8 (9%)	9	35
1	O	113/113 (100%)	100 (88%)	13 (12%)	5	26
1	P	113/113 (100%)	102 (90%)	11 (10%)	8	31
1	Q	88/113 (78%)	79 (90%)	9 (10%)	7	30
1	R	113/113 (100%)	100 (88%)	13 (12%)	5	26
1	S	113/113 (100%)	102 (90%)	11 (10%)	8	31
1	T	88/113 (78%)	78 (89%)	10 (11%)	5	26
1	U	113/113 (100%)	101 (89%)	12 (11%)	6	29
1	V	113/113 (100%)	101 (89%)	12 (11%)	6	29
1	W	88/113 (78%)	78 (89%)	10 (11%)	5	26
1	X	113/113 (100%)	101 (89%)	12 (11%)	6	29
All	All	2512/2712 (93%)	2247 (90%)	265 (10%)	7	29

All (265) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1520	MET
1	A	1521	TRP
1	A	1526	GLU
1	A	1527	LEU
1	A	1545	LYS
1	A	1555	GLN
1	A	1562	LYS
1	A	1564	GLU
1	A	1578	ARG
1	A	1596	MET
1	B	1530	LYS
1	B	1540	TYR
1	B	1554	LEU
1	B	1563	ARG
1	B	1564	GLU
1	B	1571	PHE
1	B	1588	ARG
1	B	1596	MET
1	B	1603	MET

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Mol	Chain	Res	Type
1	B	1624	GLU
1	C	1516	ARG
1	C	1522	LYS
1	C	1527	LEU
1	C	1533	LEU
1	C	1538	MET
1	C	1545	LYS
1	C	1551	GLU
1	C	1555	GLN
1	C	1556	TRP
1	C	1583	LEU
1	C	1603	MET
1	C	1605	GLU
1	C	1606	TYR
1	C	1609	LYS
1	D	1520	MET
1	D	1521	TRP
1	D	1526	GLU
1	D	1527	LEU
1	D	1534	TYR
1	D	1545	LYS
1	D	1555	GLN
1	D	1562	LYS
1	D	1564	GLU
1	D	1578	ARG
1	D	1596	MET
1	E	1530	LYS
1	E	1540	TYR
1	E	1554	LEU
1	E	1563	ARG
1	E	1564	GLU
1	E	1571	PHE
1	E	1588	ARG
1	E	1596	MET
1	E	1624	GLU
1	F	1516	ARG
1	F	1522	LYS
1	F	1533	LEU
1	F	1538	MET
1	F	1545	LYS
1	F	1551	GLU
1	F	1555	GLN

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Mol	Chain	Res	Type
1	F	1556	TRP
1	F	1603	MET
1	F	1605	GLU
1	F	1606	TYR
1	F	1609	LYS
1	G	1520	MET
1	G	1521	TRP
1	G	1526	GLU
1	G	1527	LEU
1	G	1534	TYR
1	G	1545	LYS
1	G	1555	GLN
1	G	1562	LYS
1	G	1564	GLU
1	G	1571	PHE
1	G	1578	ARG
1	G	1601	GLN
1	H	1530	LYS
1	H	1540	TYR
1	H	1554	LEU
1	H	1563	ARG
1	H	1564	GLU
1	H	1571	PHE
1	H	1588	ARG
1	H	1596	MET
1	H	1624	GLU
1	I	1516	ARG
1	I	1522	LYS
1	I	1533	LEU
1	I	1538	MET
1	I	1545	LYS
1	I	1551	GLU
1	I	1555	GLN
1	I	1556	TRP
1	I	1603	MET
1	I	1605	GLU
1	I	1606	TYR
1	I	1609	LYS
1	J	1520	MET
1	J	1521	TRP
1	J	1526	GLU
1	J	1527	LEU

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Mol	Chain	Res	Type
1	J	1534	TYR
1	J	1545	LYS
1	J	1555	GLN
1	J	1562	LYS
1	J	1564	GLU
1	J	1578	ARG
1	J	1596	MET
1	K	1540	TYR
1	K	1554	LEU
1	K	1563	ARG
1	K	1564	GLU
1	K	1571	PHE
1	K	1588	ARG
1	K	1596	MET
1	K	1603	MET
1	K	1624	GLU
1	L	1516	ARG
1	L	1527	LEU
1	L	1533	LEU
1	L	1538	MET
1	L	1545	LYS
1	L	1551	GLU
1	L	1555	GLN
1	L	1556	TRP
1	L	1583	LEU
1	L	1603	MET
1	L	1605	GLU
1	L	1606	TYR
1	L	1609	LYS
1	M	1520	MET
1	M	1521	TRP
1	M	1526	GLU
1	M	1527	LEU
1	M	1534	TYR
1	M	1545	LYS
1	M	1555	GLN
1	M	1562	LYS
1	M	1564	GLU
1	M	1578	ARG
1	M	1596	MET
1	M	1601	GLN
1	N	1540	TYR

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Mol	Chain	Res	Type
1	N	1554	LEU
1	N	1563	ARG
1	N	1564	GLU
1	N	1571	PHE
1	N	1588	ARG
1	N	1596	MET
1	N	1624	GLU
1	O	1516	ARG
1	O	1522	LYS
1	O	1527	LEU
1	O	1533	LEU
1	O	1538	MET
1	O	1545	LYS
1	O	1551	GLU
1	O	1555	GLN
1	O	1556	TRP
1	O	1603	MET
1	O	1605	GLU
1	O	1606	TYR
1	O	1609	LYS
1	P	1520	MET
1	P	1521	TRP
1	P	1526	GLU
1	P	1527	LEU
1	P	1545	LYS
1	P	1555	GLN
1	P	1562	LYS
1	P	1564	GLU
1	P	1578	ARG
1	P	1596	MET
1	P	1601	GLN
1	Q	1530	LYS
1	Q	1540	TYR
1	Q	1554	LEU
1	Q	1563	ARG
1	Q	1564	GLU
1	Q	1571	PHE
1	Q	1588	ARG
1	Q	1596	MET
1	Q	1624	GLU
1	R	1516	ARG
1	R	1522	LYS

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Mol	Chain	Res	Type
1	R	1527	LEU
1	R	1533	LEU
1	R	1538	MET
1	R	1545	LYS
1	R	1551	GLU
1	R	1555	GLN
1	R	1556	TRP
1	R	1603	MET
1	R	1605	GLU
1	R	1606	TYR
1	R	1609	LYS
1	S	1520	MET
1	S	1521	TRP
1	S	1526	GLU
1	S	1527	LEU
1	S	1534	TYR
1	S	1545	LYS
1	S	1555	GLN
1	S	1562	LYS
1	S	1564	GLU
1	S	1578	ARG
1	S	1601	GLN
1	T	1530	LYS
1	T	1540	TYR
1	T	1554	LEU
1	T	1563	ARG
1	T	1564	GLU
1	T	1571	PHE
1	T	1588	ARG
1	T	1596	MET
1	T	1603	MET
1	T	1624	GLU
1	U	1516	ARG
1	U	1522	LYS
1	U	1527	LEU
1	U	1533	LEU
1	U	1538	MET
1	U	1545	LYS
1	U	1551	GLU
1	U	1555	GLN
1	U	1556	TRP
1	U	1603	MET

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Mol	Chain	Res	Type
1	U	1606	TYR
1	U	1609	LYS
1	V	1520	MET
1	V	1521	TRP
1	V	1526	GLU
1	V	1527	LEU
1	V	1534	TYR
1	V	1545	LYS
1	V	1555	GLN
1	V	1562	LYS
1	V	1564	GLU
1	V	1578	ARG
1	V	1596	MET
1	V	1601	GLN
1	W	1530	LYS
1	W	1540	TYR
1	W	1554	LEU
1	W	1563	ARG
1	W	1564	GLU
1	W	1571	PHE
1	W	1588	ARG
1	W	1596	MET
1	W	1603	MET
1	W	1624	GLU
1	X	1516	ARG
1	X	1522	LYS
1	X	1527	LEU
1	X	1533	LEU
1	X	1538	MET
1	X	1545	LYS
1	X	1551	GLU
1	X	1555	GLN
1	X	1556	TRP
1	X	1603	MET
1	X	1605	GLU
1	X	1606	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1505	HIS
1	A	1601	GLN

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Mol	Chain	Res	Type
1	B	1559	GLN
1	C	1519	HIS
1	C	1523	GLN
1	C	1555	GLN
1	C	1559	GLN
1	C	1590	ASN
1	D	1555	GLN
1	D	1601	GLN
1	E	1559	GLN
1	F	1519	HIS
1	F	1523	GLN
1	F	1539	GLN
1	F	1555	GLN
1	F	1559	GLN
1	F	1590	ASN
1	G	1505	HIS
1	G	1601	GLN
1	H	1559	GLN
1	I	1519	HIS
1	I	1523	GLN
1	I	1539	GLN
1	I	1555	GLN
1	I	1559	GLN
1	I	1590	ASN
1	J	1505	HIS
1	J	1555	GLN
1	J	1601	GLN
1	K	1559	GLN
1	L	1519	HIS
1	L	1523	GLN
1	L	1555	GLN
1	L	1559	GLN
1	L	1590	ASN
1	M	1519	HIS
1	M	1555	GLN
1	M	1601	GLN
1	N	1559	GLN
1	O	1519	HIS
1	O	1523	GLN
1	O	1539	GLN
1	O	1555	GLN
1	O	1559	GLN

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Mol	Chain	Res	Type
1	O	1590	ASN
1	P	1505	HIS
1	P	1509	HIS
1	P	1601	GLN
1	Q	1559	GLN
1	R	1519	HIS
1	R	1523	GLN
1	R	1555	GLN
1	R	1559	GLN
1	R	1590	ASN
1	S	1519	HIS
1	S	1601	GLN
1	T	1559	GLN
1	U	1519	HIS
1	U	1523	GLN
1	U	1539	GLN
1	U	1555	GLN
1	U	1559	GLN
1	U	1590	ASN
1	V	1555	GLN
1	V	1601	GLN
1	W	1559	GLN
1	X	1519	HIS
1	X	1523	GLN
1	X	1539	GLN
1	X	1555	GLN
1	X	1559	GLN
1	X	1590	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	125/125 (100%)	-0.12	5 (4%) 38 31	1, 194, 535, 658	0
1	B	97/125 (77%)	0.58	16 (16%) 1 2	65, 222, 595, 778	0
1	C	125/125 (100%)	0.63	15 (12%) 4 5	30, 257, 615, 873	0
1	D	125/125 (100%)	-0.16	2 (1%) 72 62	1, 195, 535, 658	0
1	E	97/125 (77%)	0.53	15 (15%) 2 2	68, 222, 595, 779	0
1	F	125/125 (100%)	0.40	16 (12%) 3 4	36, 256, 615, 873	0
1	G	125/125 (100%)	-0.14	4 (3%) 47 37	1, 195, 535, 658	0
1	H	97/125 (77%)	0.51	12 (12%) 4 5	69, 222, 595, 778	0
1	I	125/125 (100%)	0.47	16 (12%) 3 4	28, 256, 615, 873	0
1	J	125/125 (100%)	-0.06	9 (7%) 15 12	1, 195, 535, 658	0
1	K	97/125 (77%)	0.25	10 (10%) 6 6	69, 222, 595, 778	0
1	L	125/125 (100%)	0.62	16 (12%) 3 4	30, 257, 615, 873	0
1	M	125/125 (100%)	-0.05	6 (4%) 30 26	7, 195, 535, 658	0
1	N	97/125 (77%)	0.44	12 (12%) 4 5	70, 222, 595, 778	0
1	O	125/125 (100%)	0.37	16 (12%) 3 4	27, 256, 615, 873	0
1	P	125/125 (100%)	0.02	5 (4%) 38 31	14, 194, 536, 658	0
1	Q	97/125 (77%)	0.29	8 (8%) 11 10	68, 221, 595, 778	0
1	R	125/125 (100%)	0.57	16 (12%) 3 4	24, 257, 615, 873	0
1	S	125/125 (100%)	-0.16	5 (4%) 38 31	5, 194, 535, 658	0
1	T	97/125 (77%)	0.49	16 (16%) 1 2	69, 222, 595, 778	0
1	U	125/125 (100%)	0.39	12 (9%) 8 7	37, 256, 615, 873	0
1	V	125/125 (100%)	-0.21	2 (1%) 72 62	1, 194, 535, 658	0
1	W	97/125 (77%)	0.46	13 (13%) 3 3	70, 221, 595, 778	0
1	X	125/125 (100%)	0.40	16 (12%) 3 4	32, 257, 615, 873	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
All	All	2776/3000 (92%)	0.26	263 (9%) 8 7	1, 218, 595, 873	0

All (263) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	1515	PRO	14.5
1	I	1515	PRO	13.6
1	C	1515	PRO	13.3
1	F	1515	PRO	12.3
1	E	1568	ALA	11.7
1	X	1515	PRO	11.6
1	K	1568	ALA	11.4
1	A	1624	GLU	11.3
1	R	1515	PRO	10.8
1	N	1569	CYS	10.0
1	U	1534	TYR	9.8
1	C	1524	SER	9.4
1	O	1534	TYR	9.1
1	C	1517	GLY	9.0
1	U	1515	PRO	9.0
1	R	1517	GLY	9.0
1	N	1568	ALA	8.9
1	T	1568	ALA	8.7
1	E	1569	CYS	8.6
1	C	1534	TYR	8.4
1	B	1624	GLU	8.4
1	L	1529	LYS	8.3
1	P	1536	ASP	8.3
1	I	1534	TYR	8.2
1	P	1624	GLU	8.2
1	U	1529	LYS	8.2
1	B	1568	ALA	8.0
1	Q	1568	ALA	7.9
1	H	1624	GLU	7.8
1	H	1568	ALA	7.6
1	L	1517	GLY	7.6
1	O	1515	PRO	7.5
1	R	1534	TYR	7.5
1	L	1514	VAL	7.3
1	I	1533	LEU	7.2
1	C	1529	LYS	7.2
1	R	1529	LYS	7.1

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Mol	Chain	Res	Type	RSRZ
1	L	1534	TYR	7.1
1	C	1511	SER	6.9
1	O	1533	LEU	6.8
1	W	1568	ALA	6.6
1	F	1534	TYR	6.6
1	T	1624	GLU	6.6
1	Q	1569	CYS	6.5
1	N	1624	GLU	6.4
1	H	1533	LEU	6.4
1	C	1533	LEU	6.4
1	X	1517	GLY	6.4
1	N	1577	LEU	6.3
1	E	1624	GLU	6.3
1	O	1529	LYS	6.2
1	T	1569	CYS	6.2
1	L	1535	LYS	6.2
1	X	1529	LYS	6.2
1	M	1536	ASP	6.2
1	R	1514	VAL	6.1
1	K	1624	GLU	6.0
1	O	1514	VAL	6.0
1	B	1569	CYS	5.7
1	C	1514	VAL	5.6
1	F	1529	LYS	5.6
1	I	1523	GLN	5.6
1	Q	1624	GLU	5.6
1	C	1530	LYS	5.6
1	E	1533	LEU	5.5
1	I	1529	LYS	5.5
1	F	1514	VAL	5.4
1	W	1569	CYS	5.4
1	U	1530	LYS	5.4
1	R	1524	SER	5.3
1	H	1569	CYS	5.3
1	X	1514	VAL	5.3
1	I	1530	LYS	5.2
1	W	1533	LEU	5.2
1	X	1524	SER	5.2
1	I	1624	GLU	5.0
1	Q	1561	GLU	5.0
1	I	1514	VAL	5.0
1	X	1534	TYR	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	1533	LEU	4.9
1	M	1502	SER	4.9
1	B	1561	GLU	4.8
1	L	1524	SER	4.8
1	R	1530	LYS	4.6
1	U	1514	VAL	4.5
1	T	1577	LEU	4.5
1	B	1620	ARG	4.5
1	K	1569	CYS	4.5
1	R	1597	PRO	4.5
1	N	1561	GLU	4.4
1	T	1616	SER	4.4
1	P	1623	GLU	4.4
1	W	1624	GLU	4.4
1	U	1528	ALA	4.2
1	O	1523	GLN	4.2
1	X	1533	LEU	4.1
1	C	1512	GLY	4.1
1	W	1620	ARG	4.1
1	U	1533	LEU	4.1
1	O	1530	LYS	4.1
1	M	1624	GLU	4.0
1	G	1536	ASP	4.0
1	D	1502	SER	4.0
1	E	1572	THR	3.9
1	P	1502	SER	3.9
1	J	1536	ASP	3.9
1	H	1561	GLU	3.9
1	H	1582	VAL	3.8
1	C	1535	LYS	3.8
1	R	1533	LEU	3.8
1	R	1535	LYS	3.8
1	J	1618	SER	3.7
1	K	1561	GLU	3.7
1	G	1624	GLU	3.7
1	X	1535	LYS	3.7
1	N	1533	LEU	3.7
1	D	1536	ASP	3.6
1	S	1536	ASP	3.6
1	L	1530	LYS	3.6
1	R	1523	GLN	3.6
1	W	1561	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	O	1597	PRO	3.6
1	A	1536	ASP	3.6
1	I	1524	SER	3.6
1	C	1523	GLN	3.6
1	L	1533	LEU	3.5
1	J	1624	GLU	3.5
1	F	1524	SER	3.5
1	H	1572	THR	3.5
1	E	1534	TYR	3.4
1	L	1532	SER	3.4
1	U	1511	SER	3.4
1	X	1512	GLY	3.4
1	U	1535	LYS	3.4
1	Q	1572	THR	3.3
1	E	1561	GLU	3.3
1	T	1620	ARG	3.3
1	U	1523	GLN	3.3
1	B	1623	GLU	3.3
1	K	1533	LEU	3.2
1	X	1523	GLN	3.2
1	B	1577	LEU	3.1
1	O	1576	LEU	3.1
1	U	1556	TRP	3.1
1	E	1567	GLY	3.1
1	S	1621	LYS	3.1
1	X	1530	LYS	3.1
1	L	1617	GLU	3.1
1	Q	1616	SER	3.1
1	O	1511	SER	3.0
1	F	1533	LEU	3.0
1	G	1621	LYS	3.0
1	L	1576	LEU	3.0
1	B	1616	SER	3.0
1	S	1502	SER	3.0
1	W	1564	GLU	3.0
1	X	1511	SER	2.9
1	W	1572	THR	2.9
1	S	1624	GLU	2.9
1	J	1620	ARG	2.9
1	K	1623	GLU	2.9
1	V	1502	SER	2.9
1	F	1511	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	T	1533	LEU	2.9
1	K	1567	GLY	2.9
1	J	1502	SER	2.9
1	R	1511	SER	2.9
1	F	1576	LEU	2.9
1	C	1518	SER	2.8
1	C	1624	GLU	2.8
1	V	1536	ASP	2.8
1	C	1603	MET	2.8
1	E	1564	GLU	2.8
1	O	1603	MET	2.8
1	I	1604	LYS	2.8
1	W	1616	SER	2.8
1	B	1564	GLU	2.7
1	F	1556	TRP	2.7
1	R	1624	GLU	2.7
1	K	1564	GLU	2.7
1	L	1523	GLN	2.7
1	O	1524	SER	2.7
1	U	1524	SER	2.7
1	W	1531	ASP	2.7
1	E	1621	LYS	2.6
1	T	1561	GLU	2.6
1	R	1512	GLY	2.6
1	A	1621	LYS	2.6
1	J	1523	GLN	2.6
1	H	1534	TYR	2.6
1	R	1576	LEU	2.6
1	T	1587	TRP	2.6
1	B	1587	TRP	2.5
1	T	1623	GLU	2.5
1	S	1620	ARG	2.5
1	X	1603	MET	2.5
1	M	1573	CYS	2.5
1	I	1517	GLY	2.5
1	F	1603	MET	2.4
1	H	1620	ARG	2.4
1	E	1616	SER	2.4
1	L	1611	ASP	2.4
1	F	1523	GLN	2.4
1	T	1572	THR	2.4
1	B	1585	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	1565	CYS	2.3
1	E	1573	CYS	2.3
1	A	1502	SER	2.3
1	H	1616	SER	2.3
1	H	1531	ASP	2.3
1	L	1603	MET	2.3
1	I	1535	LYS	2.3
1	W	1534	TYR	2.3
1	K	1590	ASN	2.3
1	B	1572	THR	2.2
1	F	1513	LEU	2.2
1	B	1531	ASP	2.2
1	R	1556	TRP	2.2
1	J	1621	LYS	2.2
1	B	1565	CYS	2.2
1	G	1573	CYS	2.2
1	Q	1618	SER	2.2
1	Q	1564	GLU	2.2
1	E	1553	LEU	2.2
1	X	1598	TYR	2.2
1	P	1539	GLN	2.2
1	T	1622	GLU	2.2
1	O	1598	TYR	2.2
1	O	1624	GLU	2.2
1	X	1528	ALA	2.2
1	F	1528	ALA	2.2
1	I	1528	ALA	2.2
1	E	1590	ASN	2.2
1	B	1556	TRP	2.2
1	F	1568	ALA	2.2
1	N	1616	SER	2.2
1	T	1564	GLU	2.2
1	T	1571	PHE	2.2
1	O	1568	ALA	2.2
1	W	1532	SER	2.1
1	I	1512	GLY	2.1
1	X	1556	TRP	2.1
1	F	1512	GLY	2.1
1	J	1619	LEU	2.1
1	F	1530	LYS	2.1
1	M	1599	PHE	2.1
1	H	1557	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	N	1531	ASP	2.1
1	L	1604	LYS	2.1
1	I	1511	SER	2.1
1	T	1540	TYR	2.0
1	N	1565	CYS	2.0
1	A	1573	CYS	2.0
1	O	1566	PHE	2.0
1	N	1587	TRP	2.0
1	T	1565	CYS	2.0
1	N	1564	GLU	2.0
1	E	1556	TRP	2.0
1	J	1617	GLU	2.0
1	N	1623	GLU	2.0
1	M	1574	TYR	2.0
1	I	1597	PRO	2.0
1	W	1557	PHE	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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.