



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 06:50 am BST

PDB ID : 3RWR
Title : Crystal structure of the human XRCC4-XLF complex
Authors : Andres, S.N.; Junop, M.S.
Deposited on : 2011-05-09
Resolution : 3.94 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
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) : 2.11

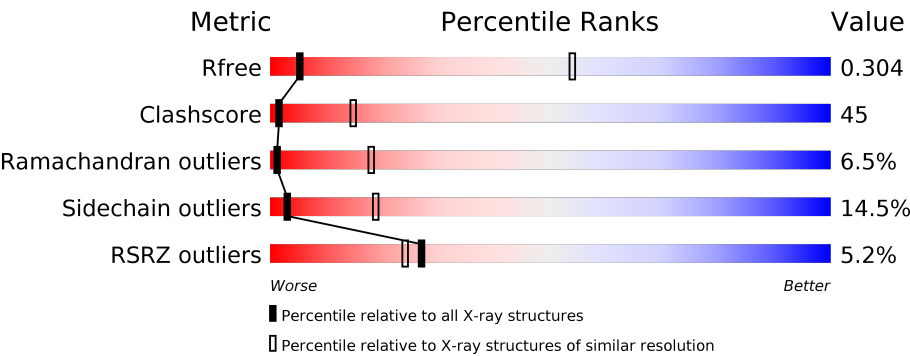
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.94 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	1036 (4.20-3.68)
Clashscore	141614	1009 (4.18-3.70)
Ramachandran outliers	138981	1057 (4.20-3.68)
Sidechain outliers	138945	1049 (4.20-3.68)
RSRZ outliers	127900	1007 (4.24-3.64)

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

Mol	Chain	Length	Quality of chain
1	A	163	<div><div>13%</div><div>26%</div><div>52%</div><div>10%</div><div>10%</div></div>
1	B	163	<div><div>12%</div><div>33%</div><div>45%</div><div>13%</div><div>7%</div></div>
1	F	163	<div><div>10%</div><div>35%</div><div>49%</div><div>12%</div><div></div></div>
1	G	163	<div><div>7%</div><div>36%</div><div>50%</div><div>10%</div><div></div></div>
1	J	163	<div><div>12%</div><div>39%</div><div>45%</div><div>12%</div><div></div></div>
1	K	163	<div><div>13%</div><div>34%</div><div>50%</div><div>11%</div><div></div></div>

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Mol	Chain	Length	Quality of chain
1	N	163	
1	P	163	
1	R	163	
1	U	163	
1	V	163	
1	Y	163	
2	D	230	
2	E	230	
2	H	230	
2	I	230	
2	L	230	
2	M	230	
2	O	230	
2	Q	230	
2	S	230	
2	T	230	
2	W	230	
2	X	230	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	TBR	D	231	-	-	-	X
3	TBR	J	164	-	-	X	X
3	TBR	M	164	-	-	-	X
3	TBR	P	2	-	-	X	-
3	TBR	X	5	-	-	X	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 36833 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 DNA repair protein XRCC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	147	Total	C	N	O	S	0	0	0
			1171	741	193	231	6			
1	B	152	Total	C	N	O	S	0	0	0
			1239	782	207	244	6			
1	F	157	Total	C	N	O	S	0	0	0
			1264	797	212	249	6			
1	G	157	Total	C	N	O	S	0	0	0
			1264	797	212	249	6			
1	J	157	Total	C	N	O	S	0	0	0
			1264	797	212	249	6			
1	K	157	Total	C	N	O	S	0	0	0
			1264	797	212	249	6			
1	N	157	Total	C	N	O	S	0	0	0
			1264	797	212	249	6			
1	P	157	Total	C	N	O	S	0	0	0
			1264	797	212	249	6			
1	R	157	Total	C	N	O	S	0	0	0
			1264	797	212	249	6			
1	V	157	Total	C	N	O	S	0	0	0
			1264	797	212	249	6			
1	U	157	Total	C	N	O	S	0	0	0
			1264	797	212	249	6			
1	Y	157	Total	C	N	O	S	0	0	0
			1264	797	212	249	6			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	158	HIS	-	EXPRESSION TAG	UNP Q13426
A	159	HIS	-	EXPRESSION TAG	UNP Q13426
A	160	HIS	-	EXPRESSION TAG	UNP Q13426
A	161	HIS	-	EXPRESSION TAG	UNP Q13426
A	162	HIS	-	EXPRESSION TAG	UNP Q13426

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Chain	Residue	Modelled	Actual	Comment	Reference
A	163	HIS	-	EXPRESSION TAG	UNP Q13426
B	658	HIS	-	EXPRESSION TAG	UNP Q13426
B	659	HIS	-	EXPRESSION TAG	UNP Q13426
B	660	HIS	-	EXPRESSION TAG	UNP Q13426
B	661	HIS	-	EXPRESSION TAG	UNP Q13426
B	662	HIS	-	EXPRESSION TAG	UNP Q13426
B	663	HIS	-	EXPRESSION TAG	UNP Q13426
F	158	HIS	-	EXPRESSION TAG	UNP Q13426
F	159	HIS	-	EXPRESSION TAG	UNP Q13426
F	160	HIS	-	EXPRESSION TAG	UNP Q13426
F	161	HIS	-	EXPRESSION TAG	UNP Q13426
F	162	HIS	-	EXPRESSION TAG	UNP Q13426
F	163	HIS	-	EXPRESSION TAG	UNP Q13426
G	658	HIS	-	EXPRESSION TAG	UNP Q13426
G	659	HIS	-	EXPRESSION TAG	UNP Q13426
G	660	HIS	-	EXPRESSION TAG	UNP Q13426
G	661	HIS	-	EXPRESSION TAG	UNP Q13426
G	662	HIS	-	EXPRESSION TAG	UNP Q13426
G	663	HIS	-	EXPRESSION TAG	UNP Q13426
J	158	HIS	-	EXPRESSION TAG	UNP Q13426
J	159	HIS	-	EXPRESSION TAG	UNP Q13426
J	160	HIS	-	EXPRESSION TAG	UNP Q13426
J	161	HIS	-	EXPRESSION TAG	UNP Q13426
J	162	HIS	-	EXPRESSION TAG	UNP Q13426
J	163	HIS	-	EXPRESSION TAG	UNP Q13426
K	658	HIS	-	EXPRESSION TAG	UNP Q13426
K	659	HIS	-	EXPRESSION TAG	UNP Q13426
K	660	HIS	-	EXPRESSION TAG	UNP Q13426
K	661	HIS	-	EXPRESSION TAG	UNP Q13426
K	662	HIS	-	EXPRESSION TAG	UNP Q13426
K	663	HIS	-	EXPRESSION TAG	UNP Q13426
N	158	HIS	-	EXPRESSION TAG	UNP Q13426
N	159	HIS	-	EXPRESSION TAG	UNP Q13426
N	160	HIS	-	EXPRESSION TAG	UNP Q13426
N	161	HIS	-	EXPRESSION TAG	UNP Q13426
N	162	HIS	-	EXPRESSION TAG	UNP Q13426
N	163	HIS	-	EXPRESSION TAG	UNP Q13426
P	658	HIS	-	EXPRESSION TAG	UNP Q13426
P	659	HIS	-	EXPRESSION TAG	UNP Q13426
P	660	HIS	-	EXPRESSION TAG	UNP Q13426
P	661	HIS	-	EXPRESSION TAG	UNP Q13426
P	662	HIS	-	EXPRESSION TAG	UNP Q13426

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Chain	Residue	Modelled	Actual	Comment	Reference
P	663	HIS	-	EXPRESSION TAG	UNP Q13426
R	158	HIS	-	EXPRESSION TAG	UNP Q13426
R	159	HIS	-	EXPRESSION TAG	UNP Q13426
R	160	HIS	-	EXPRESSION TAG	UNP Q13426
R	161	HIS	-	EXPRESSION TAG	UNP Q13426
R	162	HIS	-	EXPRESSION TAG	UNP Q13426
R	163	HIS	-	EXPRESSION TAG	UNP Q13426
V	658	HIS	-	EXPRESSION TAG	UNP Q13426
V	659	HIS	-	EXPRESSION TAG	UNP Q13426
V	660	HIS	-	EXPRESSION TAG	UNP Q13426
V	661	HIS	-	EXPRESSION TAG	UNP Q13426
V	662	HIS	-	EXPRESSION TAG	UNP Q13426
V	663	HIS	-	EXPRESSION TAG	UNP Q13426
U	158	HIS	-	EXPRESSION TAG	UNP Q13426
U	159	HIS	-	EXPRESSION TAG	UNP Q13426
U	160	HIS	-	EXPRESSION TAG	UNP Q13426
U	161	HIS	-	EXPRESSION TAG	UNP Q13426
U	162	HIS	-	EXPRESSION TAG	UNP Q13426
U	163	HIS	-	EXPRESSION TAG	UNP Q13426
Y	658	HIS	-	EXPRESSION TAG	UNP Q13426
Y	659	HIS	-	EXPRESSION TAG	UNP Q13426
Y	660	HIS	-	EXPRESSION TAG	UNP Q13426
Y	661	HIS	-	EXPRESSION TAG	UNP Q13426
Y	662	HIS	-	EXPRESSION TAG	UNP Q13426
Y	663	HIS	-	EXPRESSION TAG	UNP Q13426

- Molecule 2 is a protein called Non-homologous end-joining factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	227	Total	C	N	O	S	0	0	0
			1811	1156	307	333	15			
2	E	227	Total	C	N	O	S	0	0	0
			1811	1156	307	333	15			
2	H	227	Total	C	N	O	S	0	0	0
			1811	1156	307	333	15			
2	I	227	Total	C	N	O	S	0	0	0
			1811	1156	307	333	15			
2	L	227	Total	C	N	O	S	0	0	0
			1811	1156	307	333	15			
2	M	227	Total	C	N	O	S	0	0	0
			1811	1156	307	333	15			
2	O	227	Total	C	N	O	S	0	0	0
			1807	1153	306	333	15			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Q	227	Total	C	N	O	S	0	0	0
			1811	1156	307	333	15			
2	S	218	Total	C	N	O	S	0	0	0
			1744	1115	295	319	15			
2	W	227	Total	C	N	O	S	0	0	0
			1811	1156	307	333	15			
2	T	224	Total	C	N	O	S	0	0	0
			1789	1142	302	330	15			
2	X	227	Total	C	N	O	S	0	0	0
			1811	1156	307	333	15			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	225	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
D	226	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
D	227	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
D	228	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
D	229	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
D	230	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
E	725	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
E	726	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
E	727	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
E	728	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
E	729	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
E	730	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
H	225	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
H	226	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
H	227	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
H	228	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
H	229	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
H	230	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
I	725	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
I	726	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
I	727	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
I	728	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
I	729	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
I	730	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
L	225	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
L	226	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
L	227	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
L	228	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
L	229	HIS	-	EXPRESSION TAG	UNP Q9H9Q4

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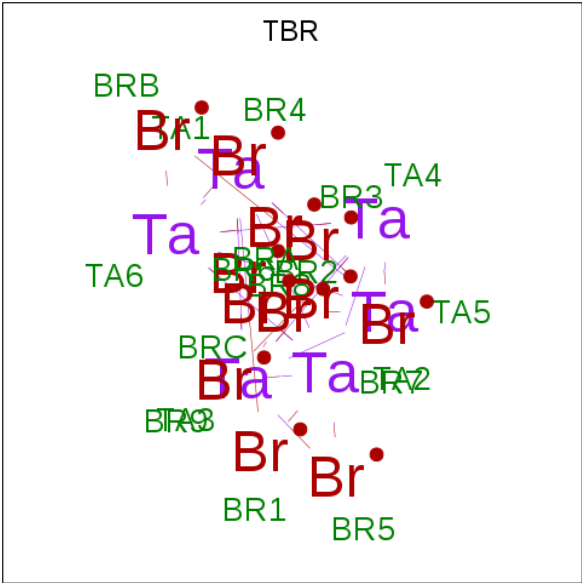
Chain	Residue	Modelled	Actual	Comment	Reference
L	230	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
M	725	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
M	726	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
M	727	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
M	728	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
M	729	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
M	730	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
O	225	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
O	226	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
O	227	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
O	228	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
O	229	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
O	230	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
Q	725	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
Q	726	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
Q	727	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
Q	728	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
Q	729	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
Q	730	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
S	225	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
S	226	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
S	227	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
S	228	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
S	229	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
S	230	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
W	725	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
W	726	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
W	727	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
W	728	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
W	729	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
W	730	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
T	225	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
T	226	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
T	227	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
T	228	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
T	229	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
T	230	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
X	725	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
X	726	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
X	727	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
X	728	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
X	729	HIS	-	EXPRESSION TAG	UNP Q9H9Q4

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Chain	Residue	Modelled	Actual	Comment	Reference
X	730	HIS	-	EXPRESSION TAG	UNP Q9H9Q4

- Molecule 3 is HEXATANTALUM DODECABROMIDE (three-letter code: TBR) (formula: Br₁₂Ta₆).

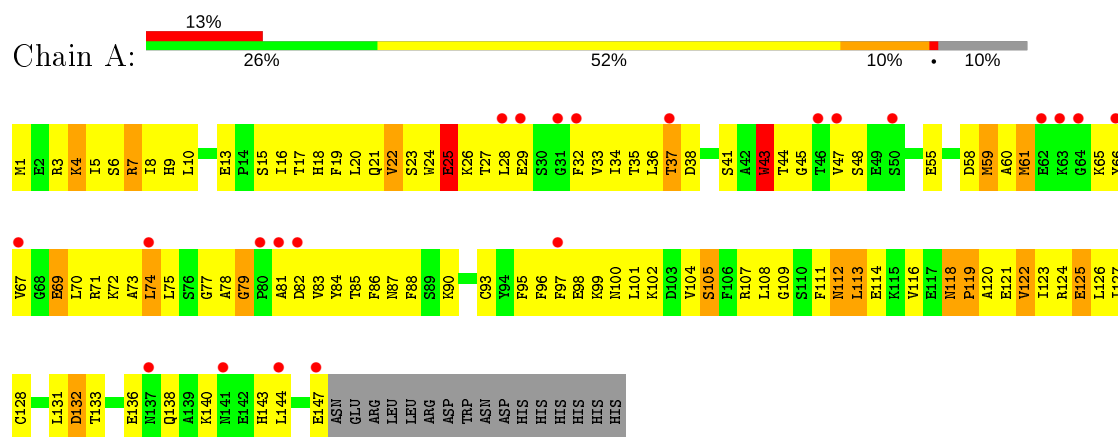


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	Br	Ta	0	0
			18	12	6		
3	H	1	Total	Br	Ta	0	0
			18	12	6		
3	J	1	Total	Br	Ta	0	0
			18	12	6		
3	M	1	Total	Br	Ta	0	0
			18	12	6		
3	P	1	Total	Br	Ta	0	0
			18	12	6		
3	V	1	Total	Br	Ta	0	0
			18	12	6		
3	X	1	Total	Br	Ta	0	0
			18	12	6		
3	Y	1	Total	Br	Ta	0	0
			18	12	6		

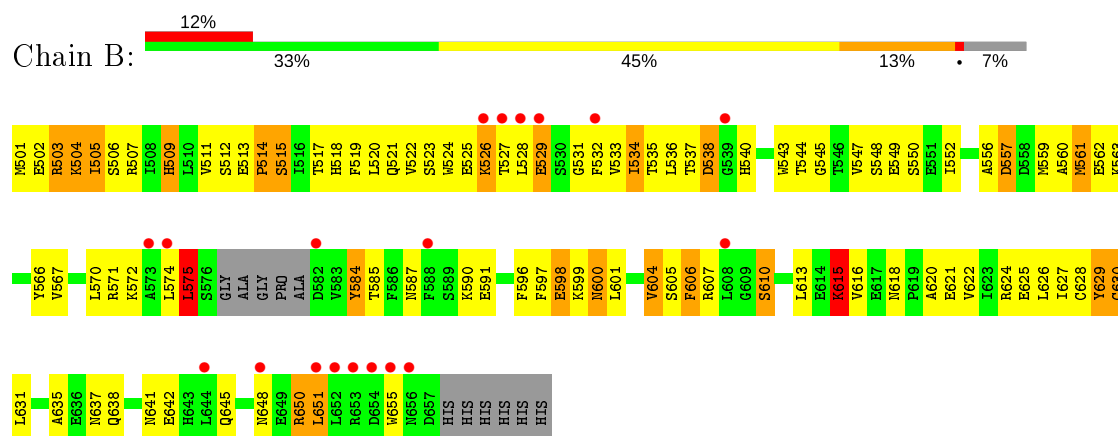
3 Residue-property plots [i](#)

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

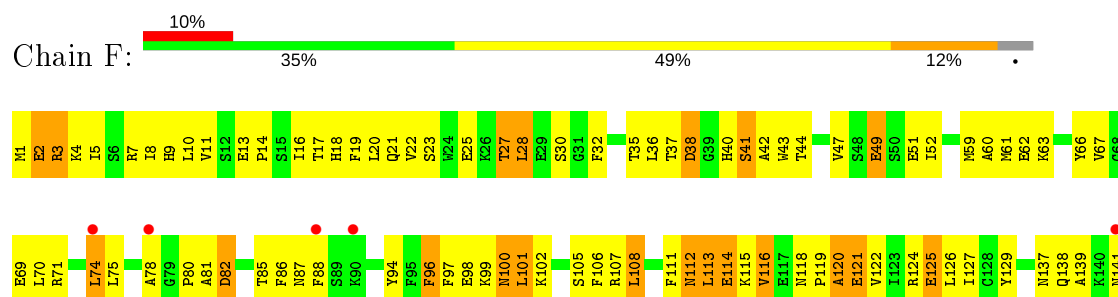
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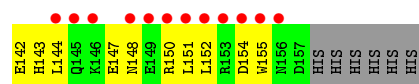


• Molecule 1: DNA repair protein XRCC4

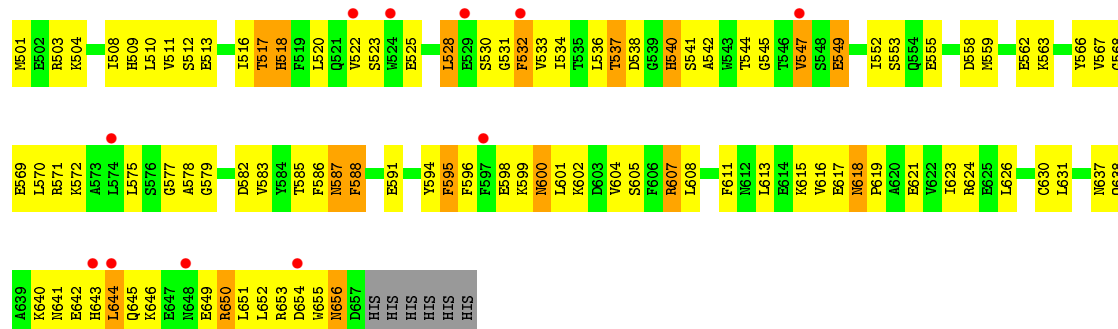


• Molecule 1: DNA repair protein XRCC4

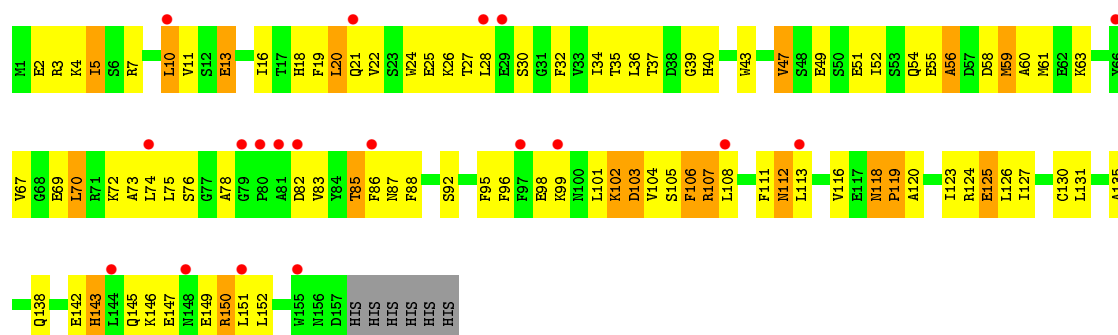




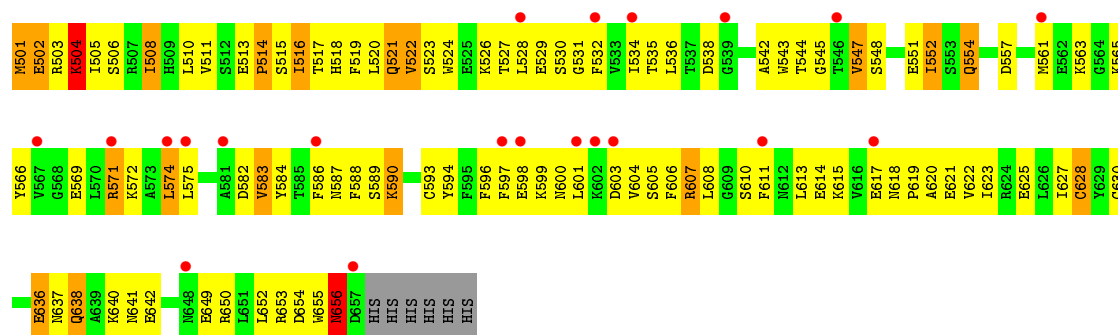
• Molecule 1: DNA repair protein XRCC4



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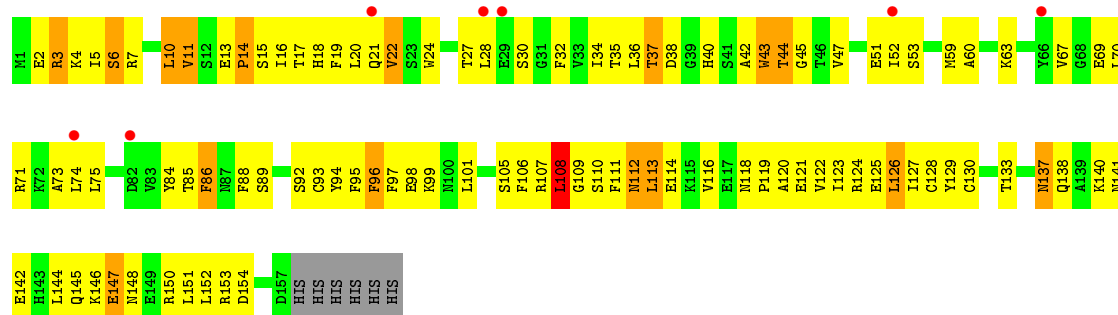


• Molecule 1: DNA repair protein XRCC4

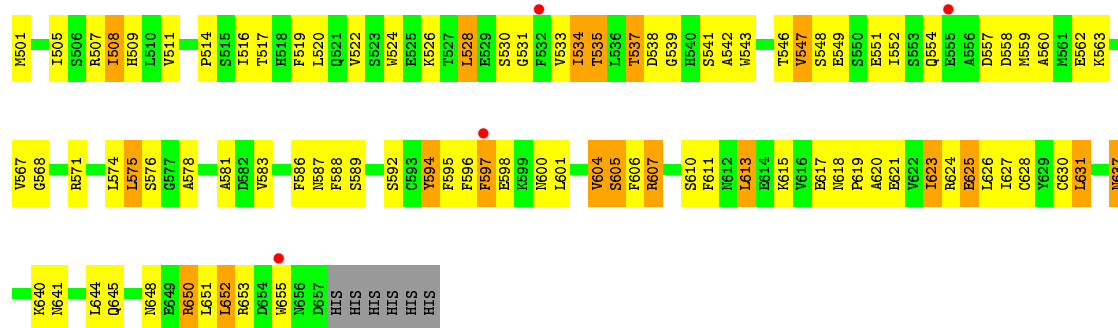


• Molecule 1: DNA repair protein XRCC4

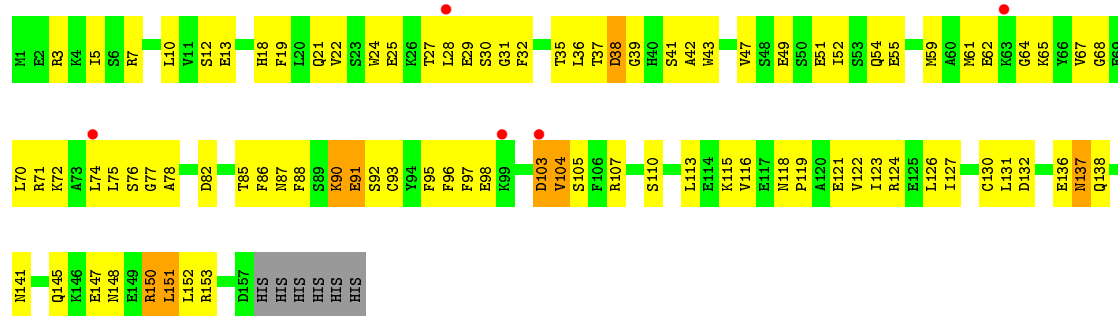




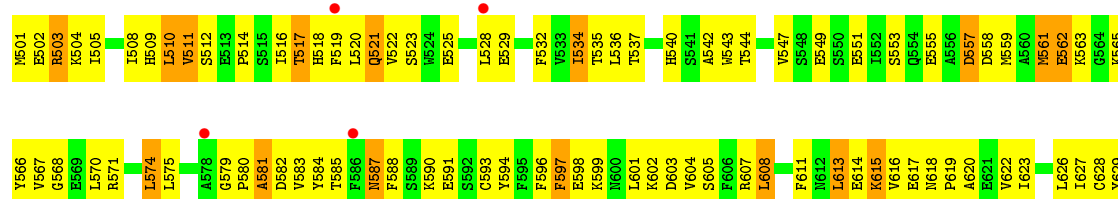
• Molecule 1: DNA repair protein XRCC4



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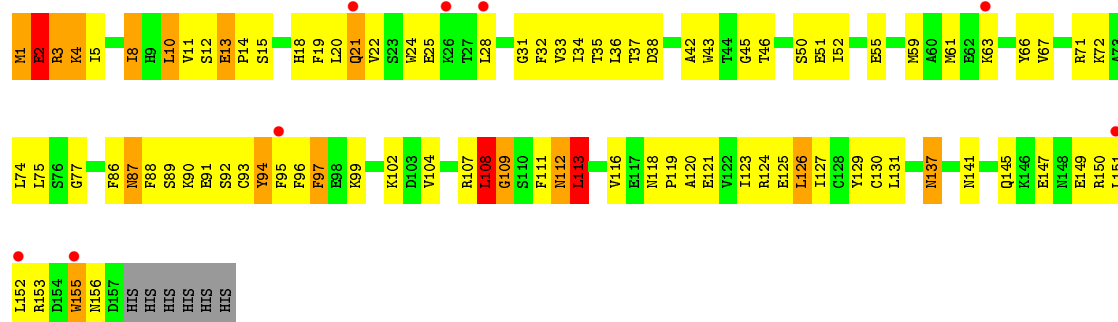


• Molecule 1: DNA repair protein XRCC4

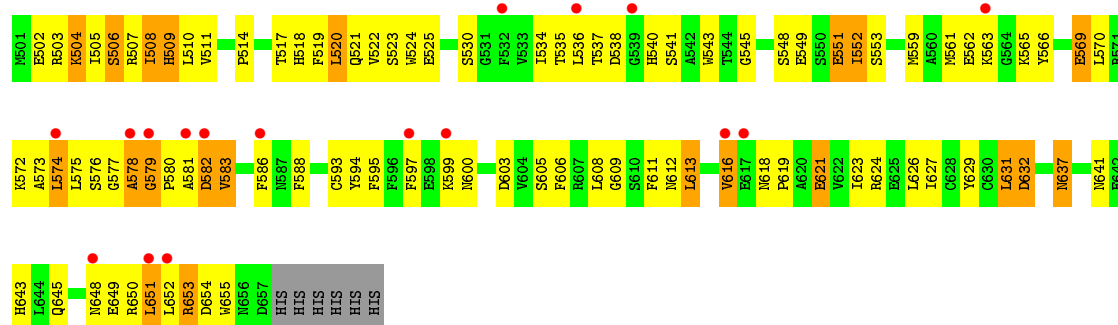




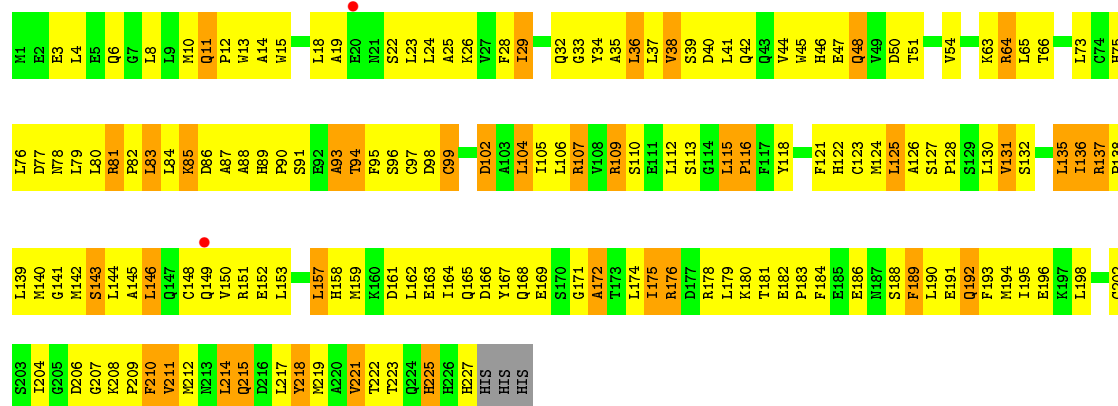
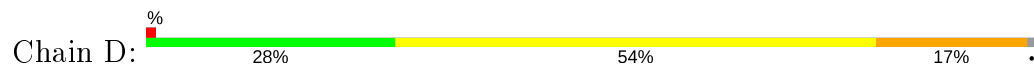
• Molecule 1: DNA repair protein XRCC4



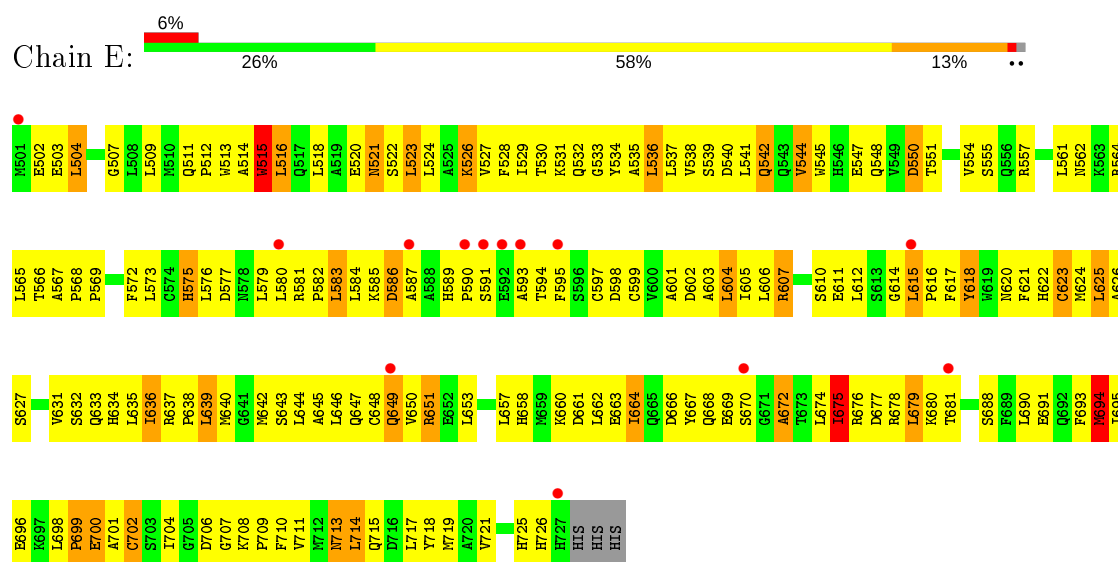
• Molecule 1: DNA repair protein XRCC4



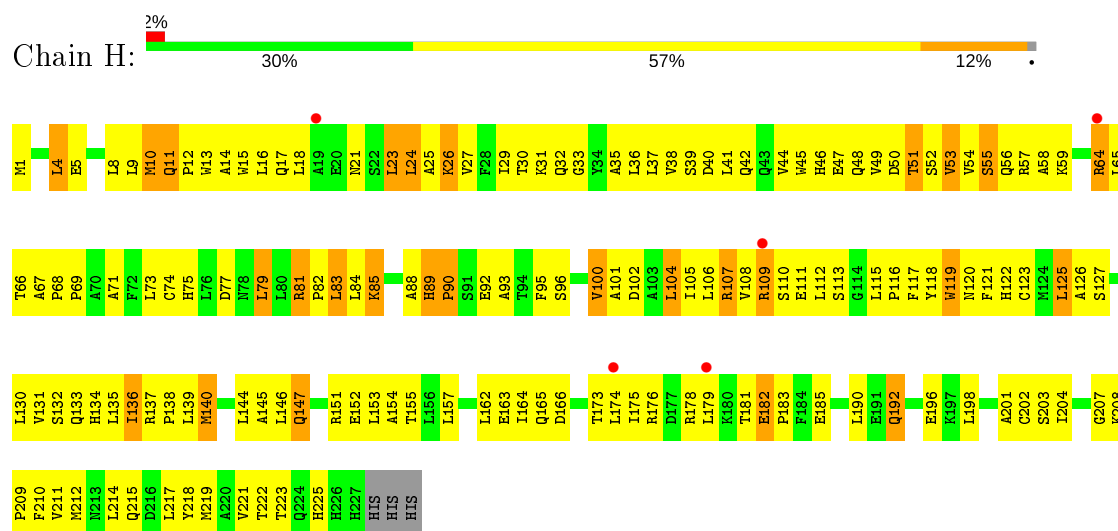
• Molecule 2: Non-homologous end-joining factor 1



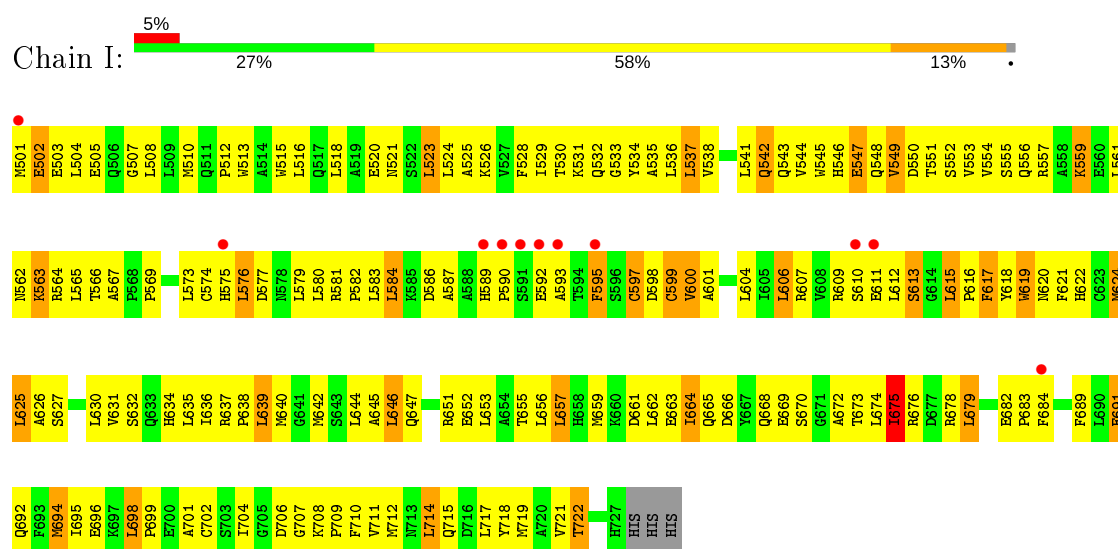
• Molecule 2: Non-homologous end-joining factor 1



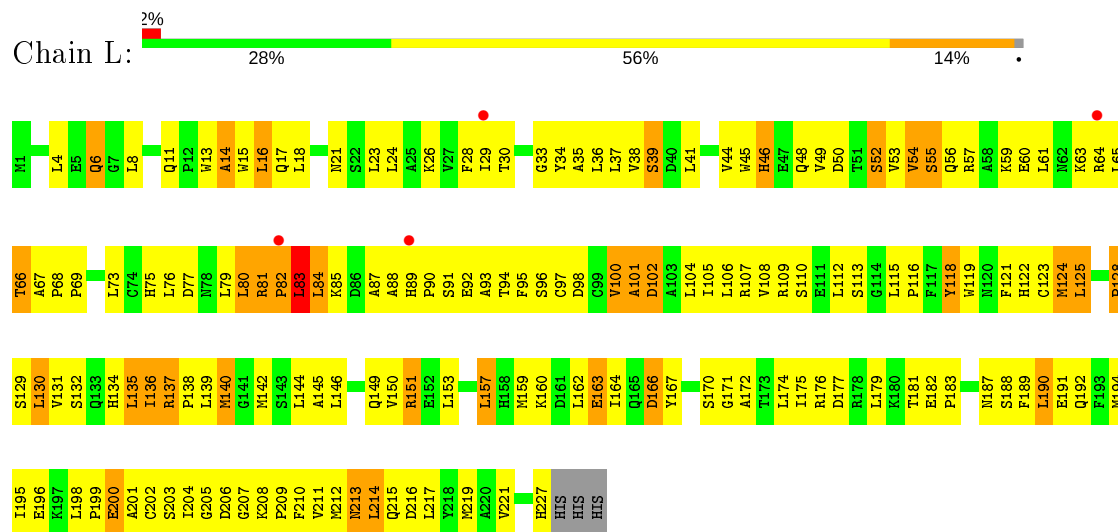
- Molecule 2: Non-homologous end-joining factor 1



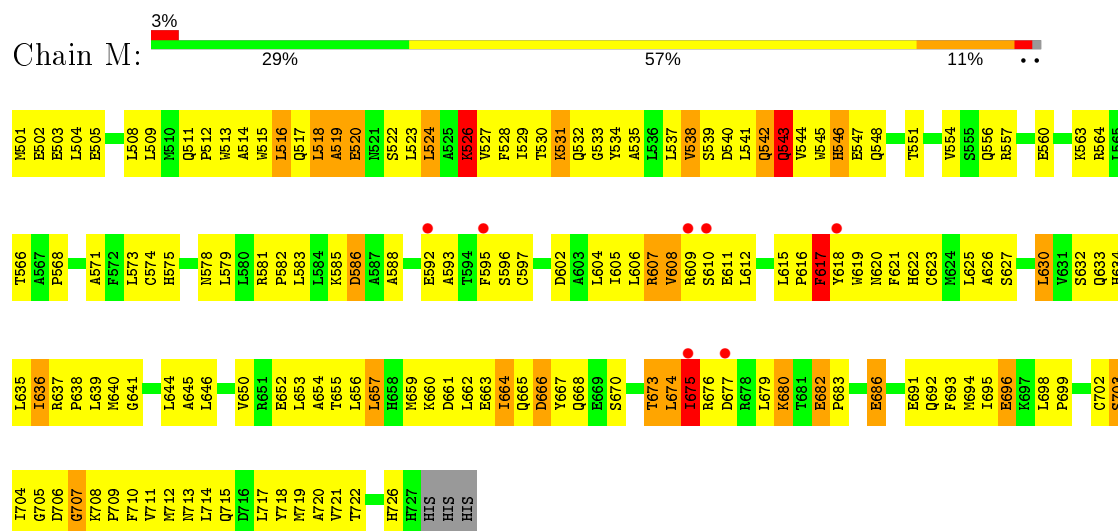
- Molecule 2: Non-homologous end-joining factor 1



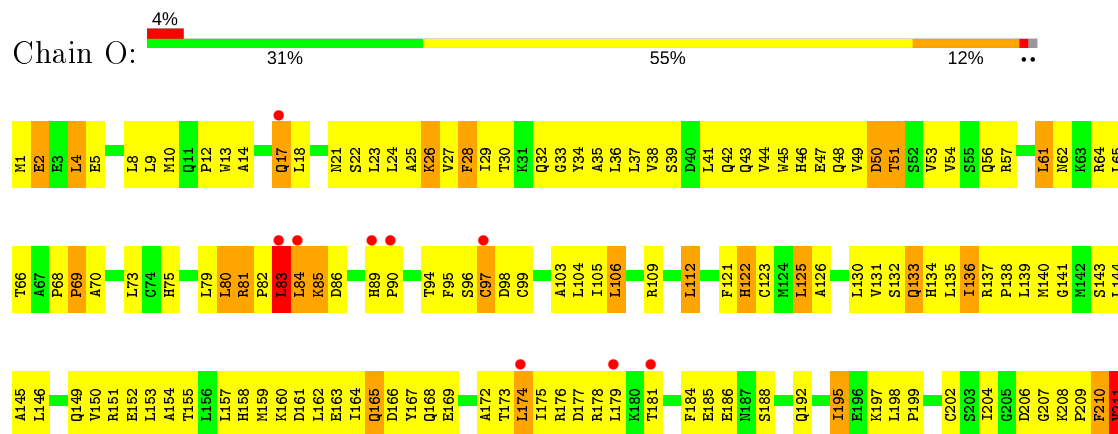
- Molecule 2: Non-homologous end-joining factor 1



- Molecule 2: Non-homologous end-joining factor 1

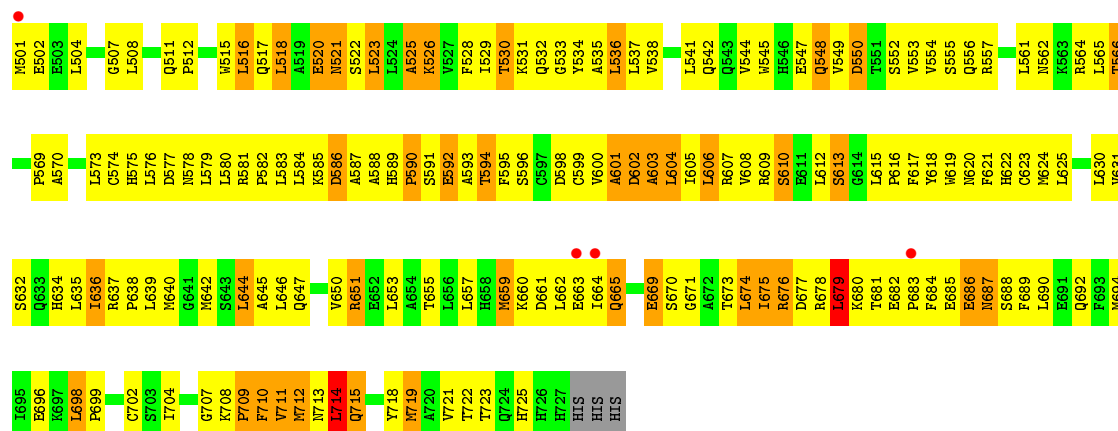


- Molecule 2: Non-homologous end-joining factor 1

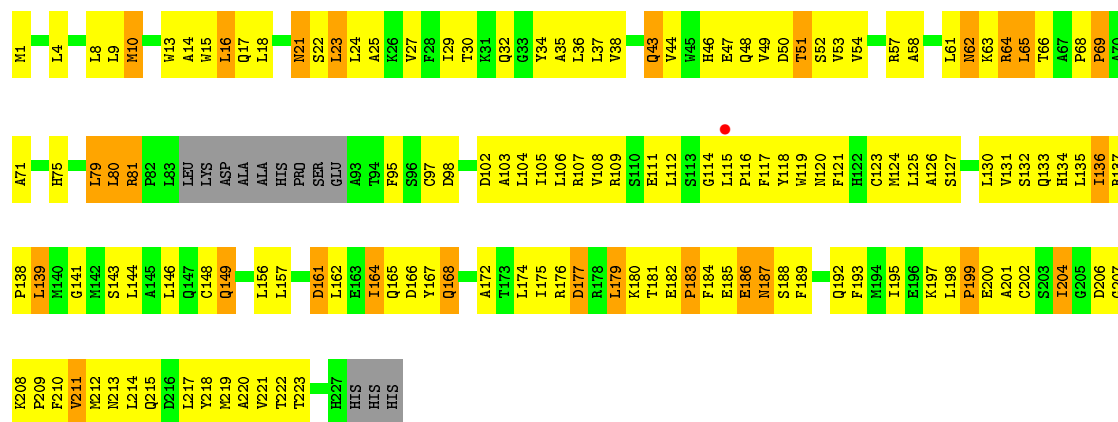




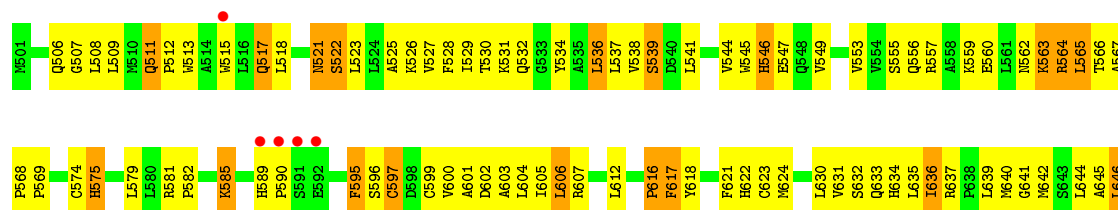
• Molecule 2: Non-homologous end-joining factor 1

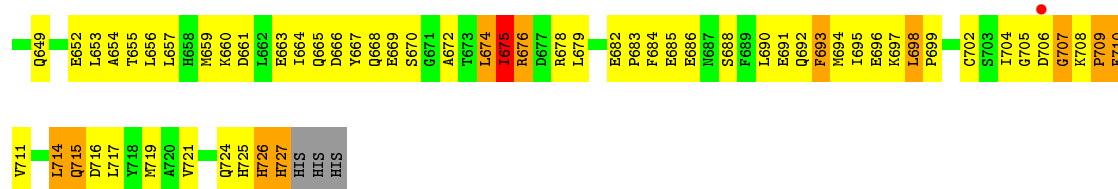


• Molecule 2: Non-homologous end-joining factor 1

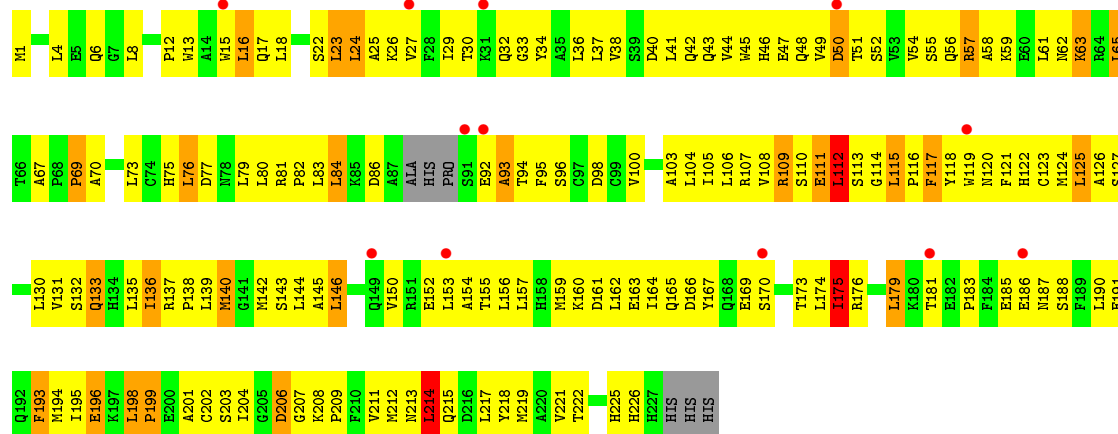


• Molecule 2: Non-homologous end-joining factor 1

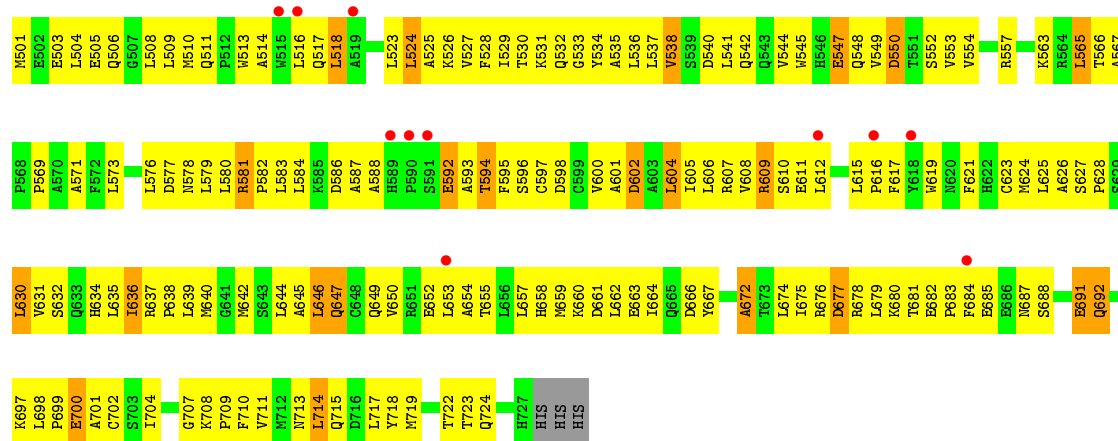




• Molecule 2: Non-homologous end-joining factor 1



• Molecule 2: Non-homologous end-joining factor 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	745.38Å 149.59Å 80.47Å 90.00° 94.72° 90.00°	Depositor
Resolution (Å)	49.03 – 3.94 49.03 – 3.94	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.03-3.94) 99.2 (49.03-3.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 4.00Å)	Xtriage
Refinement program	PHENIX 1.7.2_869, CNS	Depositor
R, R_{free}	0.271 , 0.326 0.241 , 0.304	Depositor DCC
R_{free} test set	3887 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	135.1	Xtriage
Anisotropy	0.618	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 130.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.055 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	36833	wwPDB-VP
Average B, all atoms (Å ²)	176.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.26	0/1194	0.44	0/1608
1	B	0.26	0/1262	0.44	0/1698
1	F	0.26	0/1289	0.44	0/1737
1	G	0.25	0/1289	0.42	0/1737
1	J	0.26	0/1289	0.42	0/1737
1	K	0.26	0/1289	0.43	0/1737
1	N	0.25	0/1289	0.43	0/1737
1	P	0.26	0/1289	0.44	0/1737
1	R	0.25	0/1289	0.42	0/1737
1	U	0.25	0/1289	0.42	0/1737
1	V	0.25	0/1289	0.43	0/1737
1	Y	0.25	0/1289	0.43	0/1737
2	D	0.24	0/1851	0.48	0/2511
2	E	0.24	0/1851	0.46	0/2511
2	H	0.24	0/1851	0.46	0/2511
2	I	0.24	0/1851	0.45	0/2511
2	L	0.24	0/1851	0.49	0/2511
2	M	0.24	0/1851	0.46	0/2511
2	O	0.24	0/1847	0.45	0/2507
2	Q	0.24	0/1851	0.47	0/2511
2	S	0.24	0/1781	0.45	0/2414
2	T	0.24	0/1826	0.45	0/2474
2	W	0.24	0/1851	0.47	0/2511
2	X	0.24	0/1851	0.46	0/2511
All	All	0.25	0/37459	0.45	0/50670

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1171	0	1136	118	0
1	B	1239	0	1193	127	0
1	F	1264	0	1220	118	0
1	G	1264	0	1217	94	0
1	J	1264	0	1220	106	0
1	K	1264	0	1217	125	34
1	N	1264	0	1220	125	0
1	P	1264	0	1217	113	0
1	R	1264	0	1220	105	0
1	U	1264	0	1220	116	0
1	V	1264	0	1217	110	0
1	Y	1264	0	1217	95	0
2	D	1811	0	1811	222	0
2	E	1811	0	1808	250	0
2	H	1811	0	1811	211	0
2	I	1811	0	1808	213	0
2	L	1811	0	1811	219	0
2	M	1811	0	1808	231	0
2	O	1807	0	1800	171	0
2	Q	1811	0	1808	212	0
2	S	1744	0	1747	165	0
2	T	1789	0	1791	220	2
2	W	1811	0	1808	191	0
2	X	1811	0	1808	184	0
3	D	18	0	0	0	0
3	H	18	0	0	0	0
3	J	18	0	0	2	2
3	M	18	0	0	3	0
3	P	18	0	0	1	34
3	V	18	0	0	0	0
3	X	18	0	0	4	0
3	Y	18	0	0	3	0
All	All	36833	0	36133	3315	36

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 45.

All (3315) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:605:ILE:CD1	3:X:5:TBR:BR4	2.35	1.28
2:M:560:GLU:OE2	3:M:164:TBR:BR8	2.13	1.22
2:X:605:ILE:HD13	3:X:5:TBR:BR4	1.99	1.14
1:A:18:HIS:HB3	1:A:36:LEU:HD11	1.29	1.13
2:E:606:LEU:HB2	2:E:621:PHE:HB2	1.31	1.11
1:J:125:GLU:OE2	3:J:164:TBR:BR7	2.24	1.10
2:X:525:ALA:HB2	2:X:538:VAL:HG13	1.36	1.07
1:B:559:MET:HB3	2:H:64:ARG:HE	1.17	1.05
1:Y:632:ASP:OD2	3:Y:10:TBR:BRA	2.30	1.05
2:X:605:ILE:HD12	3:X:5:TBR:BR4	2.11	1.04
2:H:89:HIS:HB3	2:H:90:PRO:HA	1.39	1.02
2:W:547:GLU:HB2	2:W:623:CYS:HB3	1.41	1.02
2:O:146:LEU:HB3	2:Q:646:LEU:HD22	1.42	1.02
2:W:603:ALA:HA	2:W:624:MET:HA	1.42	1.01
1:P:618:ASN:HD22	1:P:621:GLU:HB3	1.26	1.00
2:X:607:ARG:NH2	3:X:5:TBR:BRC	2.51	0.99
2:H:30:THR:HG23	2:H:32:GLN:H	1.26	0.98
2:S:14:ALA:HA	2:S:211:VAL:HG11	1.46	0.98
2:D:204:ILE:HG23	2:E:640:MET:HE1	1.46	0.97
2:L:204:ILE:HD12	2:M:640:MET:HE2	1.44	0.97
2:D:18:LEU:HD13	2:D:96:SER:HA	1.46	0.97
2:T:106:LEU:HB3	2:T:121:PHE:HB2	1.44	0.96
2:T:96:SER:HB2	2:T:107:ARG:H	1.29	0.96
2:S:81:ARG:HH11	2:S:81:ARG:HB2	1.29	0.96
2:E:599:CYS:HB3	2:E:604:LEU:HD12	1.48	0.96
2:D:47:GLU:HB2	2:D:123:CYS:HA	1.47	0.95
1:J:49:GLU:HA	1:J:52:ILE:HG22	1.45	0.95
2:Q:512:PRO:HB3	2:Q:719:MET:HG2	1.47	0.95
2:T:25:ALA:HB2	2:T:38:VAL:HG13	1.48	0.94
1:R:107:ARG:HB3	2:W:564:ARG:HA	1.45	0.94
2:W:512:PRO:HB3	2:W:719:MET:HG2	1.50	0.94
2:X:504:LEU:HB3	2:X:535:ALA:HB2	1.47	0.94
1:U:42:ALA:HB3	1:U:116:VAL:HG21	1.46	0.93
1:U:1:MET:HA	1:U:24:TRP:O	1.67	0.93
2:M:560:GLU:CD	3:M:164:TBR:BR8	2.62	0.93
2:H:25:ALA:HB2	2:H:38:VAL:HG13	1.50	0.92
1:U:2:GLU:HA	1:U:2:GLU:OE1	1.68	0.92
2:O:47:GLU:HB2	2:O:123:CYS:HB3	1.51	0.92
2:D:136:ILE:HD12	2:E:635:LEU:HD23	1.49	0.92
2:S:204:ILE:HD11	2:W:640:MET:HG2	1.50	0.92
2:L:181:THR:HG21	2:M:660:LYS:HG2	1.49	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:106:LEU:HB3	2:S:121:PHE:HB2	1.50	0.91
2:D:164:ILE:HD11	2:E:664:ILE:HG22	1.50	0.90
2:H:112:LEU:HB2	2:H:117:PHE:HB2	1.52	0.90
2:I:665:GLN:HA	2:I:668:GLN:HE21	1.37	0.90
1:F:8:ILE:HG22	1:F:9:HIS:H	1.36	0.89
1:F:10:LEU:HD11	1:F:36:LEU:HD21	1.54	0.89
2:Q:711:VAL:HA	2:Q:715:GLN:HG2	1.53	0.89
2:S:209:PRO:HB2	2:W:644:LEU:HD11	1.52	0.89
2:Q:685:GLU:HG3	2:Q:688:SER:H	1.37	0.89
2:L:211:VAL:HA	2:L:215:GLN:HE21	1.37	0.89
1:A:118:ASN:HD22	1:A:118:ASN:H	1.20	0.89
2:D:42:GLN:HE22	2:E:637:ARG:HD2	1.38	0.88
2:D:139:LEU:HD23	2:E:639:LEU:HD22	1.54	0.88
1:B:604:VAL:HG11	2:H:67:ALA:HA	1.54	0.88
2:D:144:LEU:HD11	2:E:709:PRO:HB2	1.54	0.88
2:H:139:LEU:HD23	2:I:639:LEU:HD12	1.56	0.88
1:A:22:VAL:HG12	1:A:34:ILE:HA	1.55	0.88
1:J:59:MET:HB3	2:M:564:ARG:HD2	1.54	0.88
1:Y:504:LYS:HZ2	1:Y:504:LYS:HA	1.39	0.88
2:L:132:SER:HA	2:L:136:ILE:HB	1.55	0.87
2:L:150:VAL:HG22	2:M:650:VAL:HG23	1.56	0.87
1:Y:521:GLN:HB3	1:Y:535:THR:HB	1.57	0.87
1:G:544:THR:HG22	1:G:545:GLY:H	1.39	0.86
2:M:560:GLU:OE1	3:M:164:TBR:BR8	2.47	0.86
1:V:543:TRP:HA	1:V:615:LYS:HA	1.56	0.86
2:W:515:TRP:HZ3	2:W:522:SER:HB2	1.40	0.86
2:T:135:LEU:HD12	2:X:636:ILE:HD12	1.57	0.86
2:E:537:LEU:HD11	2:E:544:VAL:HG12	1.57	0.86
1:R:98:GLU:HG2	1:R:107:ARG:HA	1.55	0.86
2:S:81:ARG:NH1	2:S:81:ARG:HB2	1.90	0.86
2:T:199:PRO:HG3	2:X:724:GLN:HE21	1.38	0.86
2:D:140:MET:HE2	2:E:704:ILE:HD12	1.57	0.86
2:L:140:MET:HA	2:M:639:LEU:HD22	1.56	0.86
1:F:36:LEU:HD12	1:F:37:THR:H	1.39	0.86
1:G:518:HIS:HB3	1:G:536:LEU:HD11	1.56	0.86
2:H:146:LEU:HB3	2:I:646:LEU:HD23	1.58	0.85
1:N:151:LEU:HD21	1:P:652:LEU:HD23	1.57	0.85
1:Y:632:ASP:CG	3:Y:10:TBR:BRA	2.69	0.85
2:L:15:TRP:HB2	2:L:211:VAL:HG11	1.58	0.85
2:L:139:LEU:HD11	2:M:640:MET:HG3	1.56	0.85
2:D:176:ARG:HB2	2:D:176:ARG:HH11	1.42	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:166:ASP:HB2	2:Q:675:ILE:HG22	1.59	0.84
2:W:693:PHE:HB3	2:W:694:MET:HE3	1.60	0.84
2:L:14:ALA:HB1	2:L:82:PRO:HB3	1.60	0.84
2:S:49:VAL:HG13	2:S:53:VAL:HB	1.57	0.84
2:E:579:LEU:HD11	2:E:612:LEU:HD21	1.58	0.84
2:I:581:ARG:HB3	2:I:582:PRO:HD3	1.59	0.84
2:S:208:LYS:HB3	2:S:209:PRO:HD3	1.60	0.84
1:G:646:LYS:HG3	1:Y:650:ARG:HH22	1.43	0.84
2:S:64:ARG:HD2	2:S:64:ARG:H	1.41	0.84
2:T:140:MET:HG2	2:X:639:LEU:HD11	1.59	0.84
1:B:520:LEU:HD11	1:B:534:ILE:HD11	1.60	0.83
2:T:139:LEU:HD21	2:X:640:MET:HA	1.60	0.83
2:X:637:ARG:HB2	2:X:638:PRO:HD3	1.61	0.83
1:J:18:HIS:HB3	1:J:36:LEU:HD11	1.60	0.83
1:N:32:PHE:HE2	1:N:52:ILE:HD11	1.42	0.83
1:V:520:LEU:HD11	1:V:534:ILE:HG12	1.60	0.83
1:F:42:ALA:HB3	1:F:116:VAL:HG21	1.59	0.83
1:N:5:ILE:HG22	1:N:6:SER:H	1.42	0.82
2:H:83:LEU:H	2:H:83:LEU:HD22	1.41	0.82
2:M:663:GLU:HA	2:M:666:ASP:HB3	1.61	0.82
1:P:600:ASN:HA	1:P:605:SER:HB2	1.61	0.82
2:Q:581:ARG:HB3	2:Q:582:PRO:HD3	1.60	0.82
2:I:534:TYR:H	2:I:549:VAL:HG12	1.42	0.82
2:O:157:LEU:HG	2:Q:657:LEU:HG	1.61	0.82
2:S:135:LEU:O	2:S:139:LEU:HB2	1.80	0.82
2:H:9:LEU:HB3	2:H:10:MET:HE1	1.62	0.81
1:J:69:GLU:HB3	1:J:108:LEU:HD11	1.62	0.81
2:Q:589:HIS:N	2:Q:590:PRO:HD2	1.95	0.81
2:T:41:LEU:HD11	2:T:206:ASP:HA	1.60	0.81
2:H:47:GLU:HB2	2:H:123:CYS:HA	1.62	0.81
2:O:83:LEU:H	2:O:83:LEU:HD12	1.45	0.81
2:X:530:THR:HG23	2:X:532:GLN:H	1.45	0.81
1:J:150:ARG:HB2	1:J:150:ARG:HH11	1.43	0.81
2:T:145:ALA:HA	2:X:701:ALA:HB1	1.63	0.81
1:B:606:PHE:HB3	2:H:65:LEU:HA	1.62	0.81
2:W:565:LEU:HD22	2:W:566:THR:N	1.96	0.81
2:I:513:TRP:HB3	2:I:524:LEU:HD11	1.61	0.80
2:T:47:GLU:HB2	2:T:123:CYS:HA	1.63	0.80
1:B:504:LYS:HB3	1:B:522:VAL:HG23	1.63	0.80
1:J:72:LYS:HB2	1:J:78:ALA:HA	1.63	0.80
2:L:106:LEU:HB3	2:L:121:PHE:HB2	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:111:GLU:HA	2:T:116:PRO:HA	1.64	0.80
1:U:2:GLU:CA	1:U:2:GLU:OE1	2.30	0.80
2:I:682:GLU:HG2	2:I:683:PRO:HD2	1.64	0.80
1:V:561:MET:HB3	1:V:565:LYS:NZ	1.96	0.79
2:W:579:LEU:HD11	2:W:612:LEU:HD13	1.62	0.79
2:X:508:LEU:HD22	2:X:535:ALA:HB1	1.64	0.79
2:H:1:MET:H1	1:R:107:ARG:HH22	1.30	0.79
2:T:57:ARG:HB2	2:T:57:ARG:HH11	1.46	0.79
2:D:146:LEU:HD22	2:E:646:LEU:HB3	1.64	0.79
1:A:22:VAL:HB	1:A:33:VAL:O	1.83	0.79
1:A:47:VAL:HG12	1:A:48:SER:H	1.47	0.79
2:E:524:LEU:HD11	2:E:707:GLY:HA3	1.63	0.79
2:H:137:ARG:HB2	2:H:138:PRO:HD3	1.65	0.79
1:B:559:MET:HB3	2:H:64:ARG:NE	1.96	0.78
2:D:145:ALA:HB2	2:E:702:CYS:HA	1.64	0.78
1:P:541:SER:HA	1:P:619:PRO:HB3	1.65	0.78
2:E:593:ALA:HB2	2:E:610:SER:HB3	1.63	0.78
2:H:14:ALA:HA	2:H:211:VAL:HG21	1.64	0.78
2:O:210:PHE:O	2:O:214:LEU:HB2	1.82	0.78
2:H:89:HIS:HB3	2:H:90:PRO:CA	2.13	0.78
1:N:93:CYS:HB3	1:N:113:LEU:O	1.83	0.78
2:W:538:VAL:HG12	2:W:545:TRP:HB2	1.64	0.78
2:L:128:PRO:O	2:L:131:VAL:HG12	1.83	0.78
2:D:81:ARG:HB2	2:D:82:PRO:HD3	1.66	0.78
2:M:539:SER:HB2	2:M:543:GLN:O	1.83	0.78
2:O:65:LEU:HD12	2:O:66:THR:H	1.48	0.78
2:Q:525:ALA:O	2:Q:526:LYS:HB2	1.81	0.78
2:T:146:LEU:HB3	2:X:646:LEU:HD22	1.66	0.78
2:X:682:GLU:HG3	2:X:683:PRO:HD2	1.64	0.78
2:D:157:LEU:HD12	2:E:653:LEU:HD22	1.65	0.78
2:M:518:LEU:HD23	2:M:518:LEU:H	1.48	0.77
1:Y:504:LYS:HG2	1:Y:575:LEU:HG	1.66	0.77
1:V:561:MET:HB3	1:V:565:LYS:HZ3	1.48	0.77
1:Y:578:ALA:HB1	1:Y:582:ASP:HB2	1.65	0.77
2:L:124:MET:HB2	2:Q:624:MET:HE1	1.66	0.77
1:N:16:ILE:HG22	1:N:17:THR:H	1.49	0.77
1:P:531:GLY:HA3	1:P:548:SER:HA	1.64	0.77
1:F:141:ASN:HD21	1:G:640:LYS:HB3	1.49	0.77
1:G:544:THR:O	1:G:613:LEU:HB2	1.85	0.77
2:Q:607:ARG:HG3	2:Q:620:ASN:ND2	1.99	0.77
1:U:10:LEU:HD11	1:U:88:PHE:N	2.00	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:151:LEU:HD13	1:Y:651:LEU:HD22	1.66	0.77
2:D:140:MET:CE	2:E:710:PHE:HB2	2.14	0.76
2:H:179:LEU:H	2:H:179:LEU:HD12	1.50	0.76
2:L:144:LEU:HD21	2:M:710:PHE:HA	1.65	0.76
1:Y:535:THR:HA	1:Y:543:TRP:O	1.85	0.76
2:L:153:LEU:HD13	2:M:653:LEU:HB2	1.68	0.76
1:U:11:VAL:O	1:U:14:PRO:HD3	1.86	0.76
2:M:547:GLU:HB2	2:M:623:CYS:HB3	1.65	0.76
2:S:214:LEU:HD11	2:W:644:LEU:HA	1.67	0.76
1:A:44:THR:HG22	1:A:116:VAL:HG22	1.67	0.76
2:H:138:PRO:HB3	2:H:222:THR:HG22	1.66	0.76
2:Q:562:ASN:ND2	2:Q:618:TYR:H	1.83	0.76
2:M:513:TRP:HB3	2:M:524:LEU:HD11	1.67	0.76
2:D:46:HIS:HE1	2:D:48:GLN:HB3	1.49	0.76
2:I:565:LEU:HD11	2:I:567:ALA:HB2	1.66	0.76
2:I:652:GLU:O	2:I:655:THR:HG22	1.86	0.76
1:J:95:PHE:H	1:J:112:ASN:HA	1.50	0.76
2:O:175:ILE:HG13	2:Q:670:SER:HB2	1.68	0.76
1:B:503:ARG:HG3	1:B:523:SER:HB3	1.69	0.75
2:Q:603:ALA:HB2	2:Q:624:MET:HG2	1.68	0.75
2:X:708:LYS:HB3	2:X:709:PRO:HD3	1.68	0.75
2:D:174:LEU:HD22	2:D:180:LYS:HD3	1.66	0.75
2:D:84:LEU:HD21	2:D:90:PRO:HB3	1.66	0.75
1:F:70:LEU:HG	1:F:74:LEU:HD22	1.67	0.75
2:D:47:GLU:HG3	2:D:122:HIS:O	1.87	0.75
2:H:24:LEU:HD21	2:H:41:LEU:HD21	1.67	0.75
2:T:16:LEU:HD11	2:T:18:LEU:HG	1.69	0.75
2:W:517:GLN:HA	2:W:517:GLN:HE21	1.52	0.75
2:E:632:SER:HB2	2:E:637:ARG:HG3	1.69	0.75
2:L:208:LYS:HB3	2:L:209:PRO:HD3	1.69	0.75
1:N:144:LEU:HD22	1:P:644:LEU:HB3	1.68	0.75
2:O:224:GLN:NE2	2:Q:699:PRO:HG3	2.02	0.75
1:F:99:LYS:HD2	2:I:615:LEU:HD11	1.68	0.74
2:Q:588:ALA:C	2:Q:590:PRO:HD2	2.07	0.74
1:F:87:ASN:HB2	1:F:96:PHE:CE1	2.23	0.74
2:D:106:LEU:HB3	2:D:121:PHE:HB2	1.69	0.74
2:D:65:LEU:HD22	2:D:66:THR:H	1.51	0.74
2:H:144:LEU:HD23	2:I:714:LEU:HD12	1.69	0.74
2:L:14:ALA:CB	2:L:82:PRO:HB3	2.18	0.74
1:U:11:VAL:HG22	1:U:87:ASN:HA	1.69	0.74
1:B:604:VAL:HG12	1:B:605:SER:H	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:695:ILE:HG23	2:E:696:GLU:HG3	1.70	0.74
1:J:40:HIS:NE2	1:K:619:PRO:HB2	2.01	0.74
1:J:67:VAL:HA	1:J:70:LEU:HD21	1.70	0.74
1:U:1:MET:CA	1:U:24:TRP:O	2.36	0.74
2:D:175:ILE:H	2:D:175:ILE:HD12	1.50	0.73
2:S:75:HIS:NE2	2:S:112:LEU:HB2	2.02	0.73
1:A:8:ILE:HG22	1:A:9:HIS:H	1.53	0.73
2:T:65:LEU:HD12	2:T:67:ALA:H	1.53	0.73
1:U:112:ASN:HD22	1:U:113:LEU:N	1.87	0.73
1:Y:503:ARG:HG2	1:Y:523:SER:HB3	1.71	0.73
2:O:105:ILE:HG22	2:O:122:HIS:HA	1.70	0.73
2:W:538:VAL:HG22	2:W:539:SER:H	1.53	0.73
2:M:711:VAL:HA	2:M:715:GLN:HG2	1.69	0.73
2:S:63:LYS:H	2:S:64:ARG:HH11	1.35	0.73
2:T:103:ALA:HB2	2:T:124:MET:HG2	1.71	0.73
2:H:140:MET:HA	2:I:639:LEU:HD11	1.69	0.73
1:U:99:LYS:HB2	1:U:108:LEU:HD21	1.70	0.73
2:Q:635:LEU:O	2:Q:639:LEU:HB3	1.89	0.73
1:B:504:LYS:HA	1:B:504:LYS:HZ2	1.53	0.73
1:J:5:ILE:HD12	1:J:21:GLN:HE21	1.53	0.73
1:P:530:SER:HA	1:P:549:GLU:HG3	1.70	0.73
2:S:146:LEU:HD12	2:W:646:LEU:HB3	1.71	0.73
1:A:67:VAL:HG12	1:A:71:ARG:HG3	1.68	0.73
2:L:146:LEU:HD22	2:M:646:LEU:HB3	1.70	0.73
1:K:503:ARG:HG2	1:K:504:LYS:N	2.04	0.72
2:L:163:GLU:HG3	2:M:680:LYS:HA	1.70	0.72
1:P:598:GLU:HB3	1:P:607:ARG:HA	1.70	0.72
2:Q:536:LEU:HD12	2:Q:537:LEU:H	1.54	0.72
1:U:112:ASN:C	1:U:112:ASN:HD22	1.92	0.72
2:X:608:VAL:HG12	2:X:609:ARG:H	1.52	0.72
1:A:60:ALA:HB3	2:E:616:PRO:HB2	1.71	0.72
1:K:506:SER:O	1:K:519:PHE:HA	1.90	0.72
2:E:515:TRP:CZ3	2:E:522:SER:HB3	2.25	0.72
1:G:536:LEU:HD12	1:G:537:THR:H	1.54	0.72
1:F:120:ALA:HB1	1:F:124:ARG:HH12	1.54	0.72
2:L:100:VAL:HG11	2:Q:600:VAL:HB	1.72	0.72
2:M:704:ILE:HG22	2:M:707:GLY:HA2	1.71	0.72
1:R:138:GLN:HE21	1:V:637:ASN:ND2	1.87	0.72
2:X:632:SER:HA	2:X:636:ILE:HB	1.71	0.72
2:X:529:ILE:HG22	2:X:534:TYR:HB3	1.70	0.72
1:G:572:LYS:HA	1:G:577:GLY:HA3	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:545:TRP:HD1	2:Q:625:LEU:HA	1.54	0.72
1:R:88:PHE:HD1	1:R:95:PHE:HB2	1.54	0.72
2:W:675:ILE:HD12	2:W:676:ARG:H	1.53	0.72
1:B:604:VAL:HG21	2:H:67:ALA:HB1	1.71	0.72
2:I:634:HIS:O	2:I:635:LEU:HD23	1.90	0.72
1:G:567:VAL:HA	1:G:570:LEU:HD12	1.72	0.72
2:I:665:GLN:HA	2:I:668:GLN:NE2	2.05	0.72
1:A:113:LEU:HD23	1:A:113:LEU:H	1.54	0.71
2:D:157:LEU:HA	2:E:657:LEU:HD21	1.70	0.71
1:F:5:ILE:HD12	1:F:5:ILE:H	1.53	0.71
1:K:593:CYS:HB2	1:K:613:LEU:H	1.55	0.71
2:W:515:TRP:CZ3	2:W:522:SER:HB2	2.24	0.71
2:D:176:ARG:HB2	2:D:176:ARG:NH1	2.03	0.71
2:E:555:SER:HB3	2:E:569:PRO:HG3	1.72	0.71
1:J:19:PHE:HE1	1:K:627:ILE:HB	1.54	0.71
1:R:88:PHE:CD1	1:R:95:PHE:HB2	2.25	0.71
2:D:93:ALA:HA	2:D:109:ARG:NH1	2.05	0.71
2:E:511:GLN:O	2:E:526:LYS:HE3	1.91	0.71
1:G:508:ILE:HD12	1:G:509:HIS:H	1.55	0.71
1:J:130:CYS:HB3	1:K:630:CYS:HB3	1.72	0.71
2:S:30:THR:HG23	2:S:32:GLN:H	1.55	0.71
2:E:547:GLU:HB2	2:E:623:CYS:HA	1.73	0.71
2:Q:523:LEU:HD13	2:Q:538:VAL:HG21	1.73	0.71
1:K:566:TYR:HE1	1:K:608:LEU:HD11	1.56	0.71
2:O:137:ARG:HB2	2:O:138:PRO:HD3	1.72	0.71
2:S:51:THR:HG23	2:S:69:PRO:HB3	1.70	0.71
1:R:70:LEU:HD23	1:R:74:LEU:HD12	1.73	0.71
2:H:145:ALA:HB2	2:I:702:CYS:HB3	1.73	0.71
2:O:208:LYS:HB3	2:O:209:PRO:HD3	1.71	0.71
1:R:151:LEU:HD11	1:V:652:LEU:HD13	1.71	0.71
1:A:7:ARG:HB3	1:A:7:ARG:HH11	1.56	0.71
2:I:606:LEU:HB3	2:I:621:PHE:HB2	1.73	0.71
2:M:518:LEU:HD21	2:M:523:LEU:HB2	1.73	0.71
2:L:139:LEU:HD21	2:M:640:MET:HA	1.72	0.71
2:E:527:VAL:HB	2:E:536:LEU:HB2	1.71	0.70
2:O:150:VAL:HG23	2:Q:650:VAL:HG22	1.71	0.70
2:X:547:GLU:HB3	2:X:623:CYS:HA	1.73	0.70
1:B:561:MET:HE3	2:H:115:LEU:HA	1.73	0.70
2:H:154:ALA:HB2	2:I:653:LEU:HD13	1.72	0.70
1:P:604:VAL:HG23	1:P:605:SER:H	1.55	0.70
2:D:140:MET:HE2	2:E:704:ILE:HG23	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:10:LEU:HA	1:F:86:PHE:O	1.90	0.70
1:F:61:MET:HE1	2:I:615:LEU:HD23	1.73	0.70
1:R:5:ILE:HG13	1:R:21:GLN:HB2	1.73	0.70
2:S:23:LEU:HD13	2:S:38:VAL:HG13	1.72	0.70
2:T:37:LEU:HG	2:T:46:HIS:HB2	1.73	0.70
1:P:618:ASN:ND2	1:P:621:GLU:HB3	2.04	0.70
2:E:524:LEU:HD12	2:E:524:LEU:H	1.56	0.70
2:W:555:SER:HB2	2:W:569:PRO:HG3	1.72	0.70
2:D:146:LEU:HB3	2:E:646:LEU:HD23	1.72	0.70
1:K:534:ILE:O	1:K:544:THR:HG23	1.91	0.70
1:R:59:MET:HB3	2:W:564:ARG:HG3	1.72	0.70
2:H:204:ILE:HD11	2:I:640:MET:SD	2.32	0.70
2:T:61:LEU:HD22	2:T:120:ASN:HD22	1.56	0.70
2:W:565:LEU:HD22	2:W:566:THR:H	1.53	0.70
1:B:523:SER:OG	1:B:533:VAL:HB	1.90	0.70
2:M:654:ALA:HA	2:M:657:LEU:HD12	1.73	0.70
2:T:127:SER:HB3	2:T:130:LEU:HG	1.72	0.70
1:V:616:VAL:HG21	1:V:622:VAL:HG21	1.74	0.70
2:W:665:GLN:HA	2:W:668:GLN:HE21	1.57	0.70
2:D:140:MET:CE	2:E:704:ILE:HG23	2.21	0.70
2:H:30:THR:HG22	2:H:33:GLY:O	1.91	0.70
2:I:599:CYS:HB2	2:I:604:LEU:HA	1.72	0.70
2:W:523:LEU:HD13	2:W:538:VAL:HG21	1.74	0.70
1:J:24:TRP:HB3	1:J:32:PHE:HB3	1.74	0.69
1:N:34:ILE:HD12	1:N:35:THR:H	1.56	0.69
2:T:153:LEU:HD22	2:X:653:LEU:HB3	1.73	0.69
2:D:84:LEU:HD11	2:D:90:PRO:HA	1.73	0.69
2:I:523:LEU:HD22	2:I:538:VAL:HB	1.72	0.69
2:L:176:ARG:HD2	2:L:179:LEU:HD13	1.74	0.69
2:M:534:TYR:HH	2:M:619:TRP:HZ2	1.38	0.69
2:O:62:ASN:HB3	2:O:65:LEU:HB3	1.74	0.69
2:O:12:PRO:HG2	2:O:83:LEU:HD21	1.74	0.69
2:L:38:VAL:HG22	2:L:39:SER:H	1.57	0.69
2:L:162:LEU:HB2	2:M:679:LEU:HD11	1.74	0.69
2:T:23:LEU:HD12	2:T:38:VAL:HG11	1.74	0.69
2:D:116:PRO:HB3	2:D:118:TYR:HE1	1.58	0.69
2:E:573:LEU:HA	2:E:576:LEU:HD23	1.74	0.69
2:D:145:ALA:HB2	2:E:702:CYS:CA	2.22	0.69
1:J:78:ALA:HB1	1:J:82:ASP:HB2	1.74	0.69
2:O:9:LEU:HD12	2:O:10:MET:N	2.07	0.69
1:V:536:LEU:HD13	1:V:537:THR:N	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:607:ARG:HD3	2:M:620:ASN:HD21	1.56	0.69
2:Q:604:LEU:HD22	2:Q:605:ILE:N	2.08	0.69
1:A:67:VAL:HG13	1:A:70:LEU:HD22	1.74	0.69
1:K:597:PHE:HE2	1:K:608:LEU:HD12	1.58	0.69
1:J:127:ILE:HD11	1:K:623:ILE:HD11	1.75	0.69
1:R:51:GLU:HA	1:R:54:GLN:HB3	1.74	0.69
2:L:115:LEU:HD22	2:L:116:PRO:HD2	1.75	0.69
2:D:42:GLN:NE2	2:E:637:ARG:HD2	2.07	0.69
2:S:148:CYS:HB2	2:W:693:PHE:HZ	1.58	0.69
2:T:150:VAL:HG13	2:X:653:LEU:HD11	1.75	0.69
1:U:2:GLU:O	1:U:3:ARG:HB2	1.93	0.69
1:Y:518:HIS:HB3	1:Y:536:LEU:HD11	1.74	0.69
1:A:107:ARG:HG2	2:E:564:ARG:HD3	1.75	0.68
1:G:599:LYS:HE3	1:G:601:LEU:HD21	1.75	0.68
1:K:543:TRP:HB3	1:K:613:LEU:HD22	1.75	0.68
2:L:204:ILE:HD11	2:M:641:GLY:HA2	1.73	0.68
1:P:640:LYS:O	1:P:644:LEU:HB2	1.93	0.68
2:D:4:LEU:HB3	2:D:35:ALA:HB2	1.74	0.68
1:K:544:THR:O	1:K:614:GLU:HG2	1.93	0.68
1:R:72:LYS:HA	1:R:77:GLY:H	1.56	0.68
2:T:92:GLU:HG2	2:T:110:SER:HB2	1.73	0.68
2:W:538:VAL:CG1	2:W:545:TRP:HB2	2.24	0.68
2:D:218:TYR:O	2:D:222:THR:HG23	1.94	0.68
2:E:555:SER:HB3	2:E:569:PRO:CG	2.22	0.68
1:G:572:LYS:HA	1:G:577:GLY:CA	2.23	0.68
2:O:130:LEU:HD12	2:O:133:GLN:HG3	1.73	0.68
1:F:10:LEU:HD13	1:F:88:PHE:HB3	1.76	0.68
1:N:10:LEU:HD21	1:N:88:PHE:HB3	1.76	0.68
1:N:59:MET:O	2:Q:616:PRO:HG2	1.93	0.68
2:S:18:LEU:HD22	2:S:95:PHE:HB2	1.75	0.68
2:S:221:VAL:HG13	2:W:702:CYS:SG	2.33	0.68
1:B:556:ALA:HB3	1:B:563:LYS:HZ3	1.59	0.68
1:K:516:ILE:HD12	1:K:518:HIS:NE2	2.08	0.68
1:J:99:LYS:HE2	1:J:101:LEU:HD21	1.76	0.68
2:T:23:LEU:HD12	2:T:38:VAL:CG1	2.24	0.68
2:T:45:TRP:HA	2:T:125:LEU:HA	1.76	0.68
1:R:104:VAL:HG13	2:W:565:LEU:HD23	1.76	0.68
1:Y:570:LEU:HA	1:Y:573:ALA:HB3	1.74	0.68
2:D:84:LEU:HB3	2:D:87:ALA:HA	1.74	0.68
2:M:544:VAL:HB	2:M:626:ALA:HB3	1.74	0.68
1:N:28:LEU:HD13	1:N:71:ARG:HG2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:24:LEU:HD21	2:S:207:GLY:HA3	1.74	0.68
1:F:87:ASN:HB2	1:F:96:PHE:HE1	1.59	0.68
1:N:42:ALA:O	1:N:43:TRP:HB2	1.93	0.68
1:N:126:LEU:HD21	1:P:627:ILE:HG23	1.76	0.68
2:O:174:LEU:HD21	2:Q:663:GLU:HG3	1.76	0.68
2:D:54:VAL:HG21	2:D:73:LEU:HD21	1.76	0.67
1:B:585:THR:HB	1:B:600:ASN:HD22	1.58	0.67
2:I:639:LEU:HD21	2:I:710:PHE:HE2	1.59	0.67
2:L:30:THR:O	2:L:73:LEU:HD13	1.94	0.67
2:O:153:LEU:HB3	2:Q:653:LEU:CD2	2.24	0.67
1:R:39:GLY:HA2	1:R:123:ILE:HD12	1.76	0.67
2:S:44:VAL:HG21	2:S:131:VAL:HG23	1.76	0.67
2:W:559:LYS:HE3	2:W:567:ALA:H	1.58	0.67
2:D:204:ILE:HD12	2:E:640:MET:CE	2.24	0.67
1:B:600:ASN:HA	1:B:605:SER:OG	1.95	0.67
2:L:82:PRO:HG2	2:L:85:LYS:HG2	1.75	0.67
2:L:8:LEU:HD13	2:L:35:ALA:O	1.95	0.67
1:N:120:ALA:HB1	1:N:124:ARG:NH1	2.09	0.67
2:O:17:GLN:HA	2:O:22:SER:OG	1.94	0.67
1:B:604:VAL:HG11	2:H:67:ALA:CA	2.25	0.67
2:Q:541:LEU:HD11	2:Q:707:GLY:N	2.09	0.67
2:S:132:SER:HA	2:S:136:ILE:HB	1.77	0.67
1:G:588:PHE:HB2	1:G:595:PHE:HA	1.76	0.67
2:H:83:LEU:HD23	2:H:84:LEU:H	1.59	0.67
1:K:510:LEU:HD23	1:K:511:VAL:N	2.09	0.67
1:R:116:VAL:HG22	1:R:118:ASN:H	1.59	0.67
1:Y:503:ARG:HB3	1:Y:521:GLN:HE22	1.59	0.67
2:M:602:ASP:HB3	2:M:625:LEU:HG	1.76	0.67
2:T:117:PHE:HD1	2:T:118:TYR:N	1.91	0.67
2:T:77:ASP:O	2:T:81:ARG:HG2	1.95	0.67
2:W:717:LEU:O	2:W:721:VAL:HG23	1.93	0.67
1:A:20:LEU:HD22	1:A:21:GLN:H	1.59	0.67
1:P:519:PHE:HB2	1:P:537:THR:HG23	1.76	0.67
1:P:637:ASN:O	1:P:641:ASN:HB2	1.95	0.67
1:B:504:LYS:HA	1:B:504:LYS:NZ	2.09	0.67
1:B:531:GLY:HA3	1:B:548:SER:HA	1.75	0.67
2:I:635:LEU:O	2:I:639:LEU:HB2	1.94	0.67
1:J:54:GLN:O	1:J:58:ASP:HB2	1.95	0.67
1:N:88:PHE:HB2	1:N:95:PHE:HD1	1.59	0.67
2:O:164:ILE:HD13	2:Q:663:GLU:OE2	1.94	0.67
2:T:24:LEU:HD12	2:T:24:LEU:H	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:537:LEU:HD12	2:W:545:TRP:O	1.95	0.67
1:K:607:ARG:NH2	2:T:100:VAL:HA	2.10	0.67
2:L:153:LEU:HD11	2:M:650:VAL:HG13	1.77	0.67
2:O:4:LEU:HD21	2:O:35:ALA:HB2	1.77	0.67
2:S:137:ARG:HB2	2:S:138:PRO:HD3	1.76	0.67
2:S:218:TYR:O	2:S:222:THR:HG22	1.95	0.67
2:T:13:TRP:HH2	2:T:37:LEU:HD22	1.60	0.67
2:T:199:PRO:HG3	2:X:724:GLN:NE2	2.09	0.67
2:T:211:VAL:HG12	2:T:215:GLN:NE2	2.10	0.67
2:T:96:SER:HB2	2:T:107:ARG:N	2.07	0.67
2:D:77:ASP:C	2:D:79:LEU:H	1.98	0.66
1:J:126:LEU:HD21	1:K:627:ILE:HG21	1.77	0.66
2:O:44:VAL:HG21	2:O:131:VAL:HG13	1.75	0.66
2:X:547:GLU:HG3	2:X:547:GLU:O	1.94	0.66
2:E:603:ALA:HA	2:E:624:MET:HA	1.77	0.66
2:M:652:GLU:O	2:M:655:THR:HG22	1.95	0.66
2:Q:698:LEU:HB3	2:Q:699:PRO:HD3	1.77	0.66
2:I:632:SER:HB3	2:I:636:ILE:HD12	1.77	0.66
1:J:87:ASN:HB3	1:J:96:PHE:CE1	2.29	0.66
2:L:157:LEU:HG	2:M:657:LEU:HG	1.76	0.66
2:L:174:LEU:HD11	2:L:176:ARG:HB2	1.75	0.66
2:L:24:LEU:HD11	2:L:207:GLY:HA3	1.77	0.66
2:T:18:LEU:HD22	2:T:94:THR:HG23	1.77	0.66
1:U:18:HIS:HB3	1:U:36:LEU:HD11	1.76	0.66
1:U:71:ARG:O	1:U:75:LEU:HB2	1.94	0.66
2:W:525:ALA:HB2	2:W:538:VAL:HG23	1.77	0.66
1:B:501:MET:HG2	1:B:523:SER:HB2	1.78	0.66
1:J:125:GLU:CD	3:J:164:TBR:BR7	2.89	0.66
2:L:129:SER:HB2	2:M:542:GLN:HE22	1.60	0.66
2:Q:589:HIS:N	2:Q:590:PRO:CD	2.58	0.66
2:W:536:LEU:HD12	2:W:537:LEU:N	2.10	0.66
2:D:149:GLN:NE2	2:E:690:LEU:HD22	2.10	0.66
2:D:39:SER:HB2	2:D:44:VAL:HA	1.78	0.66
2:E:642:MET:HG2	2:E:721:VAL:HG21	1.77	0.66
2:E:715:GLN:NE2	2:E:718:TYR:HD2	1.93	0.66
2:I:606:LEU:CB	2:I:621:PHE:HB2	2.26	0.66
2:L:209:PRO:HB2	2:M:644:LEU:HD11	1.78	0.66
1:G:587:ASN:HB3	1:G:596:PHE:CZ	2.31	0.66
2:H:81:ARG:N	2:H:82:PRO:CD	2.58	0.66
2:D:75:HIS:NE2	2:D:112:LEU:HD11	2.10	0.66
2:L:33:GLY:HA2	2:L:73:LEU:HD11	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:214:LEU:HD11	2:Q:644:LEU:HA	1.76	0.66
1:R:119:PRO:O	1:R:123:ILE:HG22	1.96	0.66
2:T:127:SER:O	2:T:131:VAL:HG23	1.95	0.66
2:S:139:LEU:HB3	2:W:639:LEU:HD12	1.78	0.66
2:D:44:VAL:HG23	2:D:126:ALA:HB3	1.78	0.66
2:D:140:MET:CE	2:E:704:ILE:HD12	2.25	0.66
2:E:627:SER:O	2:E:631:VAL:HG23	1.95	0.66
1:K:510:LEU:HD12	1:K:518:HIS:NE2	2.09	0.66
2:L:34:TYR:CZ	2:L:49:VAL:HG21	2.31	0.66
2:M:509:LEU:HA	2:M:634:HIS:HE1	1.61	0.66
1:P:601:LEU:HB2	1:P:604:VAL:HG23	1.78	0.66
1:V:645:GLN:O	1:V:649:GLU:HG2	1.96	0.66
1:Y:645:GLN:O	1:Y:649:GLU:HG2	1.95	0.66
1:K:569:GLU:HB3	1:K:599:LYS:NZ	2.11	0.66
1:J:130:CYS:HB3	1:K:630:CYS:CB	2.25	0.66
2:L:29:ILE:HG23	2:L:73:LEU:HD22	1.78	0.66
2:M:581:ARG:HB3	2:M:582:PRO:HD3	1.78	0.66
2:Q:529:ILE:HG22	2:Q:530:THR:N	2.10	0.66
1:U:72:LYS:HA	1:U:77:GLY:HA3	1.78	0.66
2:X:581:ARG:NH2	2:X:582:PRO:HG3	2.11	0.66
2:D:47:GLU:CB	2:D:123:CYS:HA	2.26	0.66
1:P:559:MET:O	1:P:559:MET:HG2	1.96	0.66
2:D:142:MET:O	2:D:146:LEU:HB2	1.95	0.65
2:O:65:LEU:HD12	2:O:66:THR:N	2.11	0.65
1:R:124:ARG:NH2	1:V:516:ILE:HD11	2.11	0.65
2:D:37:LEU:HD23	2:D:38:VAL:N	2.11	0.65
2:E:606:LEU:HB2	2:E:621:PHE:CB	2.19	0.65
2:D:210:PHE:HB2	2:E:640:MET:CE	2.26	0.65
2:M:596:SER:HB3	2:M:607:ARG:HB2	1.77	0.65
1:N:36:LEU:HG	1:N:37:THR:H	1.61	0.65
2:Q:575:HIS:ND1	2:Q:612:LEU:HD11	2.12	0.65
2:L:16:LEU:HA	2:L:84:LEU:HD11	1.76	0.65
2:O:106:LEU:HG	2:O:121:PHE:HB2	1.78	0.65
2:Q:598:ASP:O	2:Q:605:ILE:HG22	1.96	0.65
1:A:21:GLN:O	1:A:22:VAL:HG22	1.96	0.65
2:H:105:ILE:HD11	2:H:120:ASN:HB3	1.77	0.65
1:Y:536:LEU:HD12	1:Y:537:THR:H	1.61	0.65
1:F:116:VAL:CG2	1:F:122:VAL:HG21	2.27	0.65
2:T:51:THR:O	2:T:54:VAL:HG12	1.97	0.65
1:U:127:ILE:HD11	1:Y:627:ILE:HG12	1.77	0.65
2:X:563:LYS:H	2:X:563:LYS:HD2	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:529:ILE:HG12	2:Q:576:LEU:HD12	1.77	0.65
2:Q:562:ASN:HD21	2:Q:618:TYR:H	1.42	0.65
1:J:19:PHE:CE1	1:K:627:ILE:HB	2.31	0.65
1:N:140:LYS:HD2	1:P:641:ASN:HD21	1.62	0.65
2:S:14:ALA:CA	2:S:211:VAL:HG11	2.22	0.65
2:T:1:MET:N	2:T:4:LEU:HD12	2.12	0.65
1:J:131:LEU:HD23	1:K:630:CYS:SG	2.36	0.65
2:M:509:LEU:HA	2:M:634:HIS:CE1	2.31	0.65
1:V:503:ARG:HB3	1:V:523:SER:HB3	1.79	0.65
1:A:59:MET:SD	1:A:61:MET:HB2	2.37	0.65
2:D:132:SER:O	2:D:137:ARG:HB2	1.96	0.65
1:N:94:TYR:HA	1:N:112:ASN:ND2	2.11	0.65
2:E:611:GLU:HA	2:E:617:PHE:H	1.61	0.64
1:P:554:GLN:O	1:P:558:ASP:HB2	1.97	0.64
1:V:519:PHE:O	1:V:536:LEU:HD22	1.96	0.64
2:S:204:ILE:HD12	2:W:644:LEU:HD13	1.79	0.64
1:F:49:GLU:O	1:F:52:ILE:HG22	1.96	0.64
2:M:531:LYS:NZ	2:M:531:LYS:HA	2.12	0.64
1:N:5:ILE:HG22	1:N:6:SER:N	2.12	0.64
2:O:132:SER:HA	2:O:136:ILE:HB	1.79	0.64
2:Q:545:TRP:CD1	2:Q:625:LEU:HA	2.32	0.64
2:T:201:ALA:HB1	2:X:645:ALA:HA	1.78	0.64
1:F:8:ILE:HD11	1:F:20:LEU:HB2	1.79	0.64
2:L:191:GLU:O	2:L:195:ILE:HD13	1.97	0.64
2:X:604:LEU:HD23	2:X:623:CYS:HB3	1.78	0.64
2:H:137:ARG:HH21	2:I:704:ILE:HD12	1.62	0.64
2:L:38:VAL:HG22	2:L:39:SER:N	2.13	0.64
2:D:211:VAL:O	2:D:215:GLN:HG2	1.98	0.64
2:W:665:GLN:HA	2:W:668:GLN:HG2	1.80	0.64
1:Y:629:TYR:HB2	3:Y:10:TBR:BR6	2.53	0.64
1:B:503:ARG:HA	1:B:523:SER:HA	1.78	0.64
2:H:225:HIS:CE1	2:I:704:ILE:HD11	2.33	0.64
2:H:27:VAL:HG23	2:H:36:LEU:HB2	1.80	0.64
2:I:717:LEU:O	2:I:721:VAL:HG23	1.97	0.64
1:P:604:VAL:O	1:P:605:SER:HB3	1.97	0.64
1:R:49:GLU:HA	1:R:52:ILE:HD12	1.80	0.64
2:T:106:LEU:CB	2:T:121:PHE:HB2	2.23	0.64
1:B:620:ALA:HB1	1:B:624:ARG:NH1	2.12	0.64
2:D:132:SER:HA	2:D:136:ILE:HB	1.80	0.64
2:L:204:ILE:HG23	2:M:640:MET:CE	2.28	0.64
2:H:179:LEU:HD22	2:I:666:ASP:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:137:ARG:HB3	2:I:704:ILE:HD13	1.79	0.64
2:T:162:LEU:HB2	2:X:679:LEU:HD11	1.79	0.64
2:X:501:MET:HG2	2:X:548:GLN:HE22	1.62	0.64
2:D:96:SER:HB3	2:D:107:ARG:HG2	1.78	0.64
2:H:140:MET:SD	2:I:704:ILE:HG23	2.37	0.64
2:L:50:ASP:OD2	2:L:52:SER:HB3	1.98	0.64
2:M:704:ILE:CG2	2:M:707:GLY:HA2	2.27	0.64
1:P:650:ARG:HH11	1:P:650:ARG:HB3	1.63	0.64
2:T:15:TRP:HA	2:T:24:LEU:HA	1.79	0.64
2:D:204:ILE:HD12	2:E:640:MET:HE1	1.80	0.64
1:F:5:ILE:HG12	1:F:126:LEU:HD11	1.80	0.64
2:I:676:ARG:HE	2:I:678:ARG:HD2	1.61	0.64
1:K:510:LEU:HD22	1:K:513:GLU:H	1.63	0.64
2:Q:639:LEU:HD12	2:Q:710:PHE:HE2	1.63	0.64
2:S:107:ARG:HA	2:S:120:ASN:OD1	1.97	0.64
2:X:587:ALA:HB3	2:X:592:GLU:HA	1.80	0.64
2:X:638:PRO:HB3	2:X:722:THR:HG22	1.80	0.64
2:E:544:VAL:HB	2:E:626:ALA:CB	2.28	0.63
2:O:153:LEU:HB3	2:Q:653:LEU:HD22	1.78	0.63
2:T:30:THR:HG23	2:T:32:GLN:H	1.64	0.63
1:U:38:ASP:O	1:Y:624:ARG:HD3	1.98	0.63
1:A:128:CYS:O	1:A:132:ASP:HB2	1.98	0.63
2:H:175:ILE:HB	2:H:176:ARG:HD2	1.80	0.63
2:L:17:GLN:HG2	2:L:84:LEU:HD13	1.79	0.63
2:X:549:VAL:CG1	2:X:553:VAL:HB	2.28	0.63
2:X:708:LYS:O	2:X:711:VAL:HG12	1.98	0.63
2:E:717:LEU:O	2:E:721:VAL:HG23	1.99	0.63
1:F:152:LEU:HD22	1:G:650:ARG:HH21	1.62	0.63
2:S:44:VAL:HB	2:S:126:ALA:HB3	1.79	0.63
2:T:211:VAL:O	2:T:215:GLN:HB2	1.99	0.63
1:V:512:SER:H	1:V:587:ASN:HD21	1.46	0.63
2:X:510:MET:SD	2:X:723:THR:HG22	2.39	0.63
2:H:81:ARG:HH12	2:H:84:LEU:HB3	1.62	0.63
1:U:43:TRP:HB3	1:U:113:LEU:HD13	1.79	0.63
1:A:27:THR:HB	1:A:29:GLU:HG2	1.81	0.63
1:K:516:ILE:HD13	1:K:517:THR:N	2.14	0.63
2:O:27:VAL:HB	2:O:36:LEU:HD13	1.80	0.63
1:P:623:ILE:O	1:P:623:ILE:HD13	1.99	0.63
1:V:587:ASN:HB3	1:V:596:PHE:CE2	2.34	0.63
1:Y:588:PHE:HB2	1:Y:595:PHE:HD2	1.63	0.63
2:D:140:MET:HE3	2:E:710:PHE:HB2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:99:LYS:HB2	1:N:108:LEU:HD21	1.79	0.63
1:R:150:ARG:NH1	1:R:151:LEU:HG	2.14	0.63
2:T:44:VAL:HG22	2:T:126:ALA:HB3	1.81	0.63
1:G:572:LYS:HA	1:G:577:GLY:H	1.64	0.63
2:I:557:ARG:NH1	2:I:622:HIS:H	1.95	0.63
2:W:698:LEU:HB3	2:W:699:PRO:HD3	1.81	0.63
2:O:10:MET:SD	2:O:223:THR:HG23	2.39	0.63
1:R:121:GLU:HG3	1:R:124:ARG:HH22	1.62	0.63
1:V:565:LYS:HE2	1:V:566:TYR:N	2.14	0.63
2:X:526:LYS:HG3	2:X:537:LEU:HB3	1.81	0.63
2:O:135:LEU:HD12	2:Q:636:ILE:HG23	1.80	0.62
1:Y:510:LEU:HD11	1:Y:536:LEU:HD21	1.81	0.62
1:A:69:GLU:HB2	1:A:99:LYS:HD2	1.81	0.62
1:J:131:LEU:HD22	1:K:505:ILE:HG21	1.82	0.62
1:K:503:ARG:HG2	1:K:504:LYS:H	1.64	0.62
2:T:152:GLU:O	2:T:155:THR:HG22	1.98	0.62
1:Y:543:TRP:HB3	1:Y:613:LEU:HD13	1.80	0.62
1:F:62:GLU:HG2	1:F:63:LYS:H	1.64	0.62
2:L:194:MET:HA	2:L:198:LEU:HB2	1.80	0.62
2:M:519:ALA:O	2:M:520:GLU:HB2	2.00	0.62
2:M:637:ARG:HG2	2:M:637:ARG:HH11	1.62	0.62
2:Q:554:VAL:HG13	2:Q:555:SER:N	2.14	0.62
1:R:150:ARG:HD3	1:R:151:LEU:N	2.13	0.62
2:X:719:MET:O	2:X:723:THR:HG23	1.98	0.62
2:D:153:LEU:HD13	2:E:653:LEU:HB2	1.80	0.62
1:F:8:ILE:HG22	1:F:9:HIS:N	2.12	0.62
2:I:502:GLU:HG3	2:I:503:GLU:N	2.14	0.62
2:L:201:ALA:HB1	2:M:645:ALA:HA	1.80	0.62
2:X:513:TRP:NE1	2:X:526:LYS:HE3	2.14	0.62
1:G:559:MET:HE1	1:G:566:TYR:HA	1.81	0.62
2:H:102:ASP:HA	2:H:125:LEU:HD23	1.80	0.62
2:I:557:ARG:HH12	2:I:622:HIS:H	1.45	0.62
2:L:37:LEU:HG	2:L:45:TRP:O	1.98	0.62
2:T:195:ILE:O	2:T:196:GLU:HB2	1.98	0.62
1:V:616:VAL:HG22	1:V:618:ASN:H	1.64	0.62
2:W:616:PRO:HB3	2:W:618:TYR:HE1	1.64	0.62
1:F:43:TRP:CD1	1:F:115:LYS:HA	2.34	0.62
1:F:36:LEU:CD1	1:F:37:THR:H	2.09	0.62
2:H:4:LEU:HD12	2:H:35:ALA:HB3	1.81	0.62
2:Q:659:MET:HA	2:Q:662:LEU:HD12	1.80	0.62
2:S:193:PHE:HD1	2:S:197:LYS:HE2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:547:VAL:HG23	1:V:551:GLU:HG3	1.79	0.62
1:A:87:ASN:HB2	1:A:96:PHE:CZ	2.35	0.62
1:F:18:HIS:HB3	1:F:36:LEU:HD11	1.80	0.62
2:M:547:GLU:HG3	2:M:622:HIS:O	1.98	0.62
2:L:149:GLN:OE1	2:M:650:VAL:HG21	2.00	0.62
2:T:218:TYR:CZ	2:T:222:THR:HG21	2.34	0.62
1:R:104:VAL:HG13	2:W:565:LEU:CD2	2.30	0.62
1:B:519:PHE:HB2	1:B:537:THR:HG23	1.82	0.62
2:D:137:ARG:HG2	2:D:137:ARG:HH11	1.65	0.62
1:G:595:PHE:HB3	1:G:611:PHE:HB2	1.82	0.62
1:G:615:LYS:HD2	1:G:616:VAL:H	1.64	0.62
2:H:179:LEU:O	2:H:181:THR:HG23	2.00	0.62
2:Q:536:LEU:HD12	2:Q:537:LEU:N	2.15	0.62
2:Q:604:LEU:HD22	2:Q:605:ILE:H	1.64	0.62
1:G:572:LYS:HA	1:G:577:GLY:N	2.14	0.62
2:D:159:MET:HA	2:D:162:LEU:HD12	1.82	0.62
2:E:632:SER:O	2:E:638:PRO:HD2	2.00	0.62
2:L:142:MET:O	2:L:146:LEU:HB2	2.00	0.62
2:S:202:CYS:CA	2:W:645:ALA:HB2	2.29	0.62
2:T:54:VAL:HA	2:T:57:ARG:HH12	1.65	0.62
2:W:562:ASN:HB2	2:W:565:LEU:HD12	1.81	0.62
2:D:214:LEU:H	2:D:214:LEU:HD12	1.65	0.61
2:H:12:PRO:HD3	2:H:219:MET:SD	2.40	0.61
2:I:642:MET:O	2:I:646:LEU:HB2	1.99	0.61
1:N:118:ASN:OD1	1:N:121:GLU:HB2	1.99	0.61
2:H:166:ASP:HB3	2:I:675:ILE:HG22	1.82	0.61
2:I:674:LEU:HG	2:I:675:ILE:H	1.63	0.61
2:M:504:LEU:HD21	2:M:535:ALA:HB2	1.82	0.61
1:N:88:PHE:HD1	1:N:95:PHE:HB2	1.65	0.61
2:O:18:LEU:HB2	2:O:21:ASN:O	2.00	0.61
1:P:597:PHE:H	1:P:597:PHE:HD2	1.46	0.61
2:T:76:LEU:HD23	2:T:79:LEU:HD23	1.82	0.61
2:E:635:LEU:O	2:E:639:LEU:HB2	2.00	0.61
2:H:202:CYS:HA	2:I:645:ALA:HB2	1.83	0.61
2:M:504:LEU:CD2	2:M:535:ALA:HB2	2.31	0.61
2:Q:521:ASN:H	2:Q:521:ASN:HD22	1.48	0.61
1:G:532:PHE:CB	1:G:547:VAL:HG23	2.31	0.61
2:I:508:LEU:HD22	2:I:535:ALA:HB1	1.80	0.61
1:J:70:LEU:HA	1:J:73:ALA:HB3	1.83	0.61
2:T:98:ASP:HB3	2:T:104:LEU:HA	1.80	0.61
2:X:536:LEU:HD11	2:X:538:VAL:HG22	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:539:SER:HB2	2:E:544:VAL:HG13	1.82	0.61
1:J:22:VAL:HG22	1:J:34:ILE:HD13	1.82	0.61
2:O:141:GLY:N	2:Q:704:ILE:HD11	2.15	0.61
2:O:14:ALA:HB1	2:O:83:LEU:HA	1.83	0.61
1:V:620:ALA:HA	1:V:623:ILE:HD11	1.81	0.61
2:W:605:ILE:HG21	2:W:607:ARG:NE	2.15	0.61
2:W:657:LEU:HD22	2:W:684:PHE:HB2	1.82	0.61
2:E:544:VAL:HB	2:E:626:ALA:HB3	1.83	0.61
2:M:530:THR:HG23	2:M:532:GLN:H	1.66	0.61
1:U:108:LEU:H	1:U:108:LEU:HD12	1.66	0.61
2:E:583:LEU:HD23	2:E:587:ALA:HA	1.82	0.61
1:N:53:SER:HB2	1:N:63:LYS:NZ	2.15	0.61
2:O:5:GLU:HB2	2:O:48:GLN:HE22	1.66	0.61
2:O:159:MET:HB3	2:Q:681:THR:HG21	1.82	0.61
2:T:176:ARG:HB2	2:X:666:ASP:OD2	2.01	0.61
1:U:141:ASN:O	1:U:145:GLN:HB2	1.98	0.61
1:A:8:ILE:HG22	1:A:9:HIS:N	2.16	0.61
2:D:171:GLY:O	2:D:172:ALA:HB2	2.01	0.61
2:H:54:VAL:HG11	2:H:73:LEU:HG	1.80	0.61
2:O:152:GLU:O	2:O:155:THR:HG22	2.01	0.61
2:X:642:MET:O	2:X:646:LEU:HB2	2.00	0.61
2:E:675:ILE:N	2:E:675:ILE:HD13	2.16	0.61
2:D:140:MET:HE1	2:E:710:PHE:HB2	1.82	0.61
2:D:149:GLN:OE1	2:E:650:VAL:HG11	2.00	0.61
2:D:93:ALA:HA	2:D:109:ARG:HH11	1.64	0.61
1:F:16:ILE:HG13	1:G:624:ARG:CZ	2.31	0.61
1:K:542:ALA:O	1:K:615:LYS:HA	2.00	0.61
1:N:146:LYS:O	1:N:150:ARG:HG2	2.01	0.61
2:O:29:ILE:HG23	2:O:73:LEU:HD22	1.83	0.61
2:S:29:ILE:HG23	2:S:34:TYR:HB3	1.83	0.61
2:S:175:ILE:HG12	2:W:666:ASP:HB3	1.83	0.61
1:B:527:THR:HG22	1:B:529:GLU:H	1.66	0.60
2:I:515:TRP:HB3	2:I:708:LYS:NZ	2.16	0.60
2:I:711:VAL:HG12	2:I:715:GLN:HB2	1.81	0.60
1:J:32:PHE:O	1:J:47:VAL:HG23	2.01	0.60
2:M:571:ALA:HA	2:M:574:CYS:SG	2.41	0.60
1:N:11:VAL:HA	1:N:14:PRO:HG3	1.83	0.60
1:P:511:VAL:HB	1:P:587:ASN:HD21	1.66	0.60
2:S:51:THR:HG23	2:S:69:PRO:CB	2.31	0.60
2:X:548:GLN:HG3	2:X:548:GLN:O	2.01	0.60
2:X:698:LEU:HB3	2:X:699:PRO:HD3	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:4:LEU:HA	2:L:28:PHE:HE2	1.66	0.60
2:M:575:HIS:ND1	2:M:612:LEU:HD11	2.16	0.60
1:V:570:LEU:O	1:V:574:LEU:HG	2.00	0.60
2:W:575:HIS:CE1	2:W:612:LEU:HD11	2.36	0.60
2:W:660:LYS:O	2:W:664:ILE:HG23	2.01	0.60
1:F:102:LYS:HE2	2:I:574:CYS:HB3	1.83	0.60
2:M:515:TRP:HB3	2:M:708:LYS:NZ	2.16	0.60
2:O:198:LEU:HB3	2:O:199:PRO:HD3	1.83	0.60
2:S:57:ARG:HD2	2:S:61:LEU:HD11	1.82	0.60
2:T:13:TRP:HB2	2:T:215:GLN:HE22	1.65	0.60
1:U:10:LEU:HD11	1:U:88:PHE:H	1.64	0.60
1:B:536:LEU:HD12	1:B:537:THR:H	1.65	0.60
1:A:61:MET:HG2	2:E:616:PRO:HG2	1.83	0.60
2:E:688:SER:HA	2:E:691:GLU:HG2	1.84	0.60
1:F:17:THR:HG22	1:F:18:HIS:H	1.66	0.60
2:Q:603:ALA:HA	2:Q:624:MET:HA	1.84	0.60
2:W:639:LEU:HD22	2:W:642:MET:HE2	1.82	0.60
1:A:47:VAL:HG12	1:A:48:SER:N	2.16	0.60
1:R:36:LEU:HD12	1:R:37:THR:H	1.67	0.60
2:T:15:TRP:HE1	2:T:22:SER:HB3	1.67	0.60
1:U:32:PHE:HE2	1:U:52:ILE:HD11	1.66	0.60
1:V:627:ILE:HD12	1:V:627:ILE:H	1.66	0.60
2:D:148:CYS:HB2	2:E:693:PHE:HZ	1.66	0.60
2:D:208:LYS:O	2:D:211:VAL:HG23	2.00	0.60
2:D:36:LEU:HG	2:D:37:LEU:N	2.16	0.60
1:F:120:ALA:HB1	1:F:124:ARG:NH1	2.17	0.60
1:F:141:ASN:ND2	1:G:640:LYS:HB3	2.16	0.60
2:L:76:LEU:HA	2:L:79:LEU:HD12	1.83	0.60
2:Q:544:VAL:HG21	2:Q:631:VAL:HG13	1.84	0.60
1:V:518:HIS:HD2	1:V:536:LEU:HD11	1.67	0.60
1:B:529:GLU:HA	1:B:552:ILE:HD13	1.82	0.60
1:B:519:PHE:HB2	1:B:537:THR:CG2	2.31	0.60
1:B:545:GLY:N	1:B:613:LEU:HD13	2.17	0.60
2:E:536:LEU:HD12	2:E:537:LEU:N	2.16	0.60
2:I:714:LEU:HD23	2:I:714:LEU:O	2.02	0.60
1:K:503:ARG:HG3	1:K:521:GLN:HG3	1.84	0.60
1:N:145:GLN:HA	1:P:644:LEU:HD21	1.82	0.60
2:O:1:MET:SD	2:O:48:GLN:HG3	2.42	0.60
1:B:504:LYS:HZ2	1:B:505:ILE:H	1.48	0.60
2:L:199:PRO:HB2	2:L:200:GLU:OE2	2.01	0.60
2:L:210:PHE:HB2	2:M:640:MET:CE	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:204:ILE:HG22	2:O:206:ASP:O	2.02	0.60
1:P:511:VAL:O	1:P:514:PRO:HD3	2.02	0.60
1:P:524:TRP:CH2	1:P:575:LEU:HD13	2.36	0.60
2:T:96:SER:O	2:T:106:LEU:HA	2.02	0.60
2:T:139:LEU:HD22	2:X:639:LEU:HD22	1.84	0.60
1:V:511:VAL:O	1:V:514:PRO:HD3	2.02	0.60
2:S:180:LYS:HA	2:W:663:GLU:CD	2.22	0.60
2:D:182:GLU:HG3	2:D:183:PRO:HD2	1.83	0.60
1:K:511:VAL:HB	1:K:587:ASN:HA	1.84	0.60
1:R:41:SER:HA	1:R:119:PRO:HB3	1.82	0.60
1:U:131:LEU:HD11	1:Y:505:ILE:HG22	1.84	0.60
1:B:520:LEU:HA	1:B:535:THR:O	2.02	0.60
1:G:511:VAL:HG23	1:G:586:PHE:O	2.02	0.60
1:K:561:MET:HE1	1:K:565:LYS:HB3	1.84	0.60
2:S:1:MET:SD	2:S:4:LEU:HD12	2.42	0.60
2:T:34:TYR:CE2	2:T:49:VAL:HB	2.37	0.60
2:D:163:GLU:OE1	2:E:664:ILE:HD12	2.01	0.59
1:F:98:GLU:HB3	1:F:105:SER:HB3	1.84	0.59
1:N:98:GLU:HG2	1:N:107:ARG:HA	1.84	0.59
1:R:68:GLY:HA2	1:R:71:ARG:HD2	1.84	0.59
1:U:2:GLU:HB2	1:U:24:TRP:CE2	2.37	0.59
1:B:567:VAL:HA	1:B:570:LEU:HD12	1.84	0.59
2:H:26:LYS:HD3	2:H:37:LEU:HD23	1.85	0.59
2:Q:534:TYR:HE2	2:Q:619:TRP:HZ2	1.49	0.59
2:Q:708:LYS:N	2:Q:709:PRO:HD2	2.17	0.59
1:R:107:ARG:O	2:W:564:ARG:HB3	2.01	0.59
2:T:198:LEU:HB3	2:T:199:PRO:HD3	1.85	0.59
1:A:101:LEU:HB3	2:E:615:LEU:HD11	1.84	0.59
2:E:509:LEU:HD12	2:E:634:HIS:CD2	2.36	0.59
2:E:535:ALA:HB2	2:E:548:GLN:HG3	1.83	0.59
1:F:151:LEU:O	1:G:651:LEU:HD13	2.02	0.59
2:H:42:GLN:HA	2:H:42:GLN:HE21	1.65	0.59
2:H:81:ARG:H	2:H:82:PRO:CD	2.16	0.59
2:L:50:ASP:O	2:L:54:VAL:HG23	2.02	0.59
1:R:32:PHE:H	1:R:47:VAL:HB	1.67	0.59
1:B:521:GLN:HG2	1:B:535:THR:HB	1.84	0.59
2:I:515:TRP:CE2	2:I:524:LEU:HB2	2.37	0.59
1:R:29:GLU:HB3	1:R:67:VAL:HG21	1.84	0.59
2:T:181:THR:HG21	2:X:660:LYS:HA	1.84	0.59
1:G:508:ILE:HD12	1:G:509:HIS:N	2.17	0.59
2:L:36:LEU:HG	2:L:37:LEU:N	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:135:LEU:HD12	2:W:636:ILE:HG23	1.84	0.59
2:T:98:ASP:OD1	2:T:100:VAL:HG22	2.02	0.59
1:U:20:LEU:HD23	1:U:34:ILE:HD11	1.85	0.59
1:F:138:GLN:HA	1:F:138:GLN:OE1	2.02	0.59
1:G:532:PHE:HB2	1:G:547:VAL:HG23	1.83	0.59
2:M:660:LYS:O	2:M:663:GLU:HG2	2.01	0.59
2:S:13:TRP:HB2	2:S:211:VAL:HG22	1.85	0.59
1:V:626:LEU:O	1:V:630:CYS:HB2	2.03	0.59
1:Y:641:ASN:O	1:Y:645:GLN:HB2	2.02	0.59
1:J:119:PRO:HG2	1:J:120:ALA:H	1.68	0.59
2:M:542:GLN:O	2:M:543:GLN:HB2	2.02	0.59
2:X:635:LEU:O	2:X:639:LEU:HB2	2.02	0.59
2:D:25:ALA:HB2	2:D:38:VAL:HB	1.83	0.59
2:E:632:SER:HA	2:E:636:ILE:HB	1.85	0.59
1:G:528:LEU:HD21	1:G:571:ARG:HH22	1.67	0.59
2:T:106:LEU:HD13	2:T:121:PHE:HD2	1.65	0.59
2:W:692:GLN:O	2:W:696:GLU:HG2	2.02	0.59
2:X:718:TYR:O	2:X:722:THR:HG23	2.02	0.59
1:A:4:LYS:HE3	1:A:75:LEU:HD11	1.84	0.59
2:D:22:SER:O	2:D:23:LEU:HD23	2.03	0.59
2:M:717:LEU:O	2:M:721:VAL:HG23	2.03	0.59
2:S:202:CYS:HA	2:W:645:ALA:HB2	1.85	0.59
2:X:544:VAL:HG21	2:X:631:VAL:HG22	1.84	0.59
1:F:113:LEU:N	1:F:113:LEU:HD23	2.18	0.59
1:J:120:ALA:O	1:J:124:ARG:HG3	2.03	0.59
2:O:30:THR:O	2:O:73:LEU:HD13	2.03	0.59
2:S:164:ILE:HG13	2:W:664:ILE:HG22	1.85	0.59
2:S:181:THR:OG1	2:W:660:LYS:HG2	2.03	0.59
2:T:209:PRO:HB2	2:X:644:LEU:HD11	1.85	0.59
1:B:529:GLU:OE1	1:B:549:GLU:HG3	2.03	0.58
1:B:627:ILE:O	1:B:631:LEU:HG	2.02	0.58
2:I:515:TRP:HB3	2:I:708:LYS:HZ2	1.68	0.58
2:Q:639:LEU:HD12	2:Q:710:PHE:CE2	2.37	0.58
1:Y:507:ARG:HG2	1:Y:508:ILE:H	1.67	0.58
1:Y:616:VAL:HG12	1:Y:618:ASN:H	1.66	0.58
1:Y:649:GLU:O	1:Y:653:ARG:HB2	2.02	0.58
2:D:163:GLU:HA	2:E:679:LEU:HD13	1.86	0.58
1:G:569:GLU:OE1	1:G:599:LYS:HD2	2.04	0.58
2:H:102:ASP:HB3	2:H:125:LEU:HB2	1.85	0.58
2:L:146:LEU:HD22	2:M:646:LEU:CB	2.33	0.58
2:O:98:ASP:HB3	2:O:105:ILE:HG13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:552:SER:HB3	2:S:124:MET:HB3	1.85	0.58
2:D:164:ILE:CD1	2:E:664:ILE:HG22	2.28	0.58
1:B:561:MET:N	2:H:116:PRO:HG3	2.19	0.58
2:H:12:PRO:HB2	2:H:215:GLN:HE21	1.67	0.58
1:J:16:ILE:HD12	1:J:16:ILE:H	1.67	0.58
2:L:153:LEU:O	2:L:157:LEU:HB2	2.03	0.58
2:O:4:LEU:CD2	2:O:35:ALA:HB2	2.33	0.58
2:T:45:TRP:HA	2:T:126:ALA:H	1.68	0.58
1:V:553:SER:O	1:V:557:ASP:HB3	2.03	0.58
1:F:28:LEU:HD22	1:F:71:ARG:HG2	1.86	0.58
2:I:512:PRO:HB3	2:I:719:MET:HG3	1.84	0.58
1:J:49:GLU:HA	1:J:52:ILE:CG2	2.27	0.58
2:O:12:PRO:HB3	2:O:219:MET:HB2	1.85	0.58
2:Q:688:SER:O	2:Q:692:GLN:HB2	2.03	0.58
2:W:637:ARG:HD3	2:W:726:HIS:NE2	2.18	0.58
2:E:579:LEU:HD22	2:E:610:SER:HB2	1.86	0.58
1:J:70:LEU:H	1:J:70:LEU:HD23	1.66	0.58
2:M:513:TRP:CE3	2:M:524:LEU:HG	2.38	0.58
2:L:181:THR:CG2	2:M:660:LYS:HG2	2.27	0.58
2:Q:504:LEU:HD11	2:Q:533:GLY:O	2.03	0.58
1:R:49:GLU:HA	1:R:52:ILE:CD1	2.33	0.58
1:R:78:ALA:HB1	1:R:82:ASP:HB2	1.85	0.58
1:V:547:VAL:HB	1:V:611:PHE:CE2	2.38	0.58
2:D:202:CYS:HB3	2:E:645:ALA:HB2	1.86	0.58
2:H:210:PHE:O	2:H:214:LEU:HB2	2.04	0.58
2:I:607:ARG:HA	2:I:620:ASN:ND2	2.19	0.58
1:J:11:VAL:HG21	1:J:85:THR:HB	1.86	0.58
2:L:170:SER:HB2	2:M:673:THR:HG21	1.84	0.58
2:L:34:TYR:CE1	2:L:121:PHE:HE1	2.22	0.58
2:M:515:TRP:HB3	2:M:708:LYS:HZ1	1.67	0.58
2:O:175:ILE:HG13	2:Q:670:SER:CB	2.34	0.58
1:R:62:GLU:HG2	1:R:64:GLY:H	1.68	0.58
1:V:512:SER:N	1:V:587:ASN:HD21	2.01	0.58
1:J:21:GLN:O	1:J:34:ILE:HD12	2.04	0.58
2:L:16:LEU:H	2:L:16:LEU:HD23	1.69	0.58
2:T:142:MET:HE2	2:T:214:LEU:HD22	1.84	0.58
1:G:638:GLN:O	1:G:642:GLU:HG3	2.04	0.58
2:I:695:ILE:O	2:I:695:ILE:HG22	2.03	0.58
2:M:543:GLN:HB3	2:M:545:TRP:CZ3	2.38	0.58
2:L:140:MET:HE2	2:M:710:PHE:CG	2.39	0.58
1:N:74:LEU:O	1:N:75:LEU:HD23	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:568:GLY:O	1:P:571:ARG:HG2	2.03	0.58
2:Q:507:GLY:HA3	2:Q:528:PHE:CD2	2.38	0.58
1:F:11:VAL:O	1:F:14:PRO:HD3	2.04	0.58
2:I:708:LYS:N	2:I:709:PRO:HD2	2.18	0.58
2:M:518:LEU:O	2:M:520:GLU:N	2.37	0.58
1:P:604:VAL:HG23	1:P:605:SER:N	2.19	0.58
2:Q:619:TRP:C	2:Q:620:ASN:HD22	2.07	0.58
2:S:131:VAL:HG13	2:S:136:ILE:HD12	1.86	0.58
2:W:642:MET:O	2:W:646:LEU:HB2	2.04	0.58
1:Y:511:VAL:O	1:Y:514:PRO:HD3	2.04	0.58
1:Y:541:SER:HA	1:Y:619:PRO:HB3	1.85	0.58
1:A:120:ALA:HB2	1:B:540:HIS:HB2	1.85	0.58
2:D:175:ILE:HD12	2:D:175:ILE:N	2.17	0.58
1:F:63:LYS:O	1:F:67:VAL:HG23	2.03	0.58
2:H:210:PHE:HD2	2:H:214:LEU:HD12	1.69	0.58
2:I:549:VAL:HG22	2:I:550:ASP:H	1.69	0.58
2:I:550:ASP:O	2:I:554:VAL:HG23	2.04	0.58
1:K:569:GLU:HB3	1:K:599:LYS:HZ1	1.67	0.58
2:L:217:LEU:O	2:L:221:VAL:HG23	2.04	0.58
2:M:537:LEU:HD12	2:M:546:HIS:HB2	1.86	0.58
1:J:105:SER:HB2	2:M:566:THR:HB	1.86	0.58
1:P:508:ILE:HD12	1:P:520:LEU:HB2	1.86	0.58
2:Q:565:LEU:HD12	2:Q:566:THR:H	1.69	0.58
2:O:139:LEU:HD11	2:Q:640:MET:HE3	1.84	0.58
2:W:581:ARG:HG2	2:W:585:LYS:NZ	2.19	0.58
1:B:606:PHE:HD1	2:H:65:LEU:HB2	1.69	0.57
1:G:583:VAL:HG23	1:G:600:ASN:HB3	1.86	0.57
2:H:136:ILE:HG23	2:I:635:LEU:HD13	1.86	0.57
1:P:549:GLU:HA	1:P:552:ILE:HG22	1.86	0.57
2:Q:580:LEU:HA	2:Q:583:LEU:HD11	1.84	0.57
2:O:136:ILE:HD11	2:Q:631:VAL:HG12	1.86	0.57
2:T:195:ILE:HG22	2:T:195:ILE:O	2.04	0.57
2:T:4:LEU:HD22	2:T:34:TYR:O	2.04	0.57
1:U:126:LEU:HD21	1:Y:627:ILE:HG23	1.85	0.57
2:D:93:ALA:HB1	2:D:109:ARG:HD3	1.86	0.57
2:E:511:GLN:HG3	2:E:528:PHE:HB2	1.85	0.57
2:E:516:LEU:H	2:E:516:LEU:CD2	2.15	0.57
2:E:612:LEU:HD23	2:E:617:PHE:HB2	1.85	0.57
2:E:666:ASP:O	2:E:670:SER:HB2	2.05	0.57
2:H:163:GLU:HA	2:I:679:LEU:HD22	1.84	0.57
2:L:82:PRO:CG	2:L:85:LYS:HG2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:104:VAL:HG21	2:M:575:HIS:NE2	2.20	0.57
2:L:164:ILE:HG21	2:M:663:GLU:OE2	2.04	0.57
2:Q:530:THR:O	2:Q:573:LEU:HD13	2.03	0.57
2:T:107:ARG:HG2	2:T:120:ASN:OD1	2.03	0.57
2:X:606:LEU:HB3	2:X:621:PHE:HB2	1.84	0.57
1:Y:505:ILE:HA	1:Y:520:LEU:O	2.05	0.57
2:M:529:ILE:HG22	2:M:530:THR:H	1.70	0.57
2:O:94:THR:HG22	2:O:109:ARG:HB3	1.87	0.57
2:Q:547:GLU:HG2	2:Q:548:GLN:H	1.69	0.57
2:T:208:LYS:N	2:T:209:PRO:HD2	2.20	0.57
2:W:661:ASP:O	2:W:664:ILE:HG12	2.03	0.57
2:X:501:MET:HG2	2:X:548:GLN:NE2	2.20	0.57
1:U:5:ILE:HD11	1:Y:631:LEU:HG	1.86	0.57
2:D:166:ASP:OD1	2:E:675:ILE:HB	2.03	0.57
2:E:523:LEU:HD22	2:E:540:ASP:HB3	1.84	0.57
2:E:573:LEU:HA	2:E:576:LEU:CD2	2.33	0.57
1:B:560:ALA:C	2:H:116:PRO:HG3	2.25	0.57
2:H:13:TRP:CE3	2:H:24:LEU:HD12	2.40	0.57
2:H:218:TYR:O	2:H:222:THR:HG23	2.03	0.57
2:H:35:ALA:HB2	2:H:48:GLN:HE22	1.69	0.57
2:H:65:LEU:HD12	2:H:66:THR:N	2.19	0.57
2:I:515:TRP:CZ2	2:I:524:LEU:HB2	2.39	0.57
2:T:194:MET:HB2	2:T:195:ILE:HD12	1.85	0.57
1:U:1:MET:HA	1:U:25:GLU:HA	1.86	0.57
2:W:546:HIS:ND1	2:W:547:GLU:N	2.52	0.57
1:Y:562:GLU:HG3	1:Y:565:LYS:H	1.69	0.57
1:A:140:LYS:HA	1:A:143:HIS:HB3	1.85	0.57
2:E:597:CYS:HB2	2:E:606:LEU:HD23	1.85	0.57
2:E:708:LYS:N	2:E:709:PRO:HD2	2.19	0.57
2:H:146:LEU:HD13	2:I:646:LEU:HB3	1.87	0.57
2:M:515:TRP:CZ2	2:M:707:GLY:HA3	2.39	0.57
2:M:711:VAL:CA	2:M:715:GLN:HG2	2.34	0.57
1:N:4:LYS:HG3	1:N:24:TRP:CH2	2.40	0.57
2:I:600:VAL:HG23	2:W:600:VAL:HG21	1.87	0.57
2:E:573:LEU:O	2:E:576:LEU:HG	2.04	0.57
2:I:664:ILE:HG13	2:I:665:GLN:N	2.19	0.57
1:J:36:LEU:HD12	1:J:37:THR:H	1.70	0.57
2:L:29:ILE:CG2	2:L:73:LEU:HD22	2.34	0.57
1:V:547:VAL:HA	1:V:551:GLU:OE2	2.03	0.57
2:E:557:ARG:HG2	2:E:561:LEU:HD11	1.87	0.57
2:H:32:GLN:HA	2:H:51:THR:HG23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:510:LEU:HD21	1:K:588:PHE:HB3	1.86	0.57
1:K:607:ARG:HG3	1:K:608:LEU:N	2.18	0.57
2:M:529:ILE:HG22	2:M:530:THR:N	2.20	0.57
1:U:127:ILE:HD11	1:Y:627:ILE:CG1	2.34	0.57
2:E:675:ILE:HD13	2:E:675:ILE:H	1.70	0.57
1:B:561:MET:HA	2:H:116:PRO:HD3	1.86	0.57
2:I:599:CYS:O	2:I:600:VAL:HG13	2.04	0.57
1:K:534:ILE:HB	1:K:545:GLY:H	1.69	0.57
1:N:88:PHE:CD1	1:N:95:PHE:HB2	2.40	0.57
2:O:218:TYR:O	2:O:222:THR:HG23	2.05	0.57
2:Q:661:ASP:HA	2:Q:664:ILE:HG12	1.87	0.57
2:T:105:ILE:HA	2:T:121:PHE:O	2.04	0.57
2:W:530:THR:HG23	2:W:532:GLN:HB3	1.87	0.57
2:E:639:LEU:HA	2:E:642:MET:CE	2.35	0.57
2:H:152:GLU:O	2:H:155:THR:HG22	2.04	0.57
2:M:538:VAL:O	2:M:545:TRP:HB2	2.04	0.57
2:O:163:GLU:HA	2:Q:679:LEU:HD12	1.87	0.57
2:T:18:LEU:HD13	2:T:95:PHE:HB2	1.87	0.57
1:U:36:LEU:HD12	1:U:37:THR:H	1.70	0.57
2:W:531:LYS:NZ	2:W:574:CYS:HA	2.20	0.57
1:A:123:ILE:O	1:A:127:ILE:HG12	2.05	0.57
1:G:571:ARG:HA	1:G:575:LEU:HB2	1.86	0.57
1:G:591:GLU:H	1:G:591:GLU:CD	2.09	0.57
1:K:599:LYS:HG2	1:K:600:ASN:N	2.20	0.57
2:L:84:LEU:HB3	2:L:91:SER:OG	2.04	0.57
2:M:675:ILE:HD11	2:M:680:LYS:HE3	1.86	0.57
2:M:698:LEU:HB3	2:M:699:PRO:HD3	1.87	0.57
2:M:718:TYR:O	2:M:722:THR:HG23	2.05	0.57
2:Q:531:LYS:HE3	2:Q:574:CYS:SG	2.45	0.57
1:V:519:PHE:HB2	1:V:537:THR:HG23	1.87	0.57
2:W:693:PHE:CD1	2:W:697:LYS:HB3	2.40	0.57
2:T:166:ASP:O	2:X:675:ILE:HD13	2.05	0.57
2:H:17:GLN:H	2:H:17:GLN:CD	2.08	0.56
2:I:711:VAL:HA	2:I:715:GLN:HB2	1.87	0.56
1:K:501:MET:HG3	1:K:523:SER:OG	2.05	0.56
1:P:508:ILE:H	1:P:508:ILE:HD13	1.69	0.56
2:Q:632:SER:HA	2:Q:636:ILE:HB	1.87	0.56
2:X:659:MET:HA	2:X:662:LEU:HD12	1.87	0.56
2:H:49:VAL:HG13	2:H:53:VAL:HG23	1.87	0.56
2:H:54:VAL:HG21	2:H:73:LEU:HD11	1.87	0.56
1:J:61:MET:HE1	2:M:615:LEU:HD23	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:145:ALA:HB2	2:M:702:CYS:CA	2.35	0.56
1:N:13:GLU:C	1:N:15:SER:H	2.09	0.56
1:P:511:VAL:HB	1:P:587:ASN:ND2	2.19	0.56
1:R:87:ASN:HB3	1:R:96:PHE:CE1	2.40	0.56
1:U:94:TYR:CD2	1:U:112:ASN:HB2	2.41	0.56
2:X:581:ARG:HH11	2:X:581:ARG:HB3	1.68	0.56
1:F:116:VAL:HG13	1:F:118:ASN:H	1.69	0.56
1:P:563:LYS:O	1:P:567:VAL:HG23	2.05	0.56
2:D:208:LYS:HE2	2:D:212:MET:SD	2.46	0.56
2:E:544:VAL:HG21	2:E:631:VAL:HG13	1.86	0.56
2:E:694:MET:HA	2:E:698:LEU:HB2	1.87	0.56
2:L:29:ILE:HG23	2:L:34:TYR:HB3	1.87	0.56
2:L:41:LEU:HB3	2:M:637:ARG:NH1	2.20	0.56
2:M:692:GLN:O	2:M:696:GLU:HG3	2.04	0.56
1:N:16:ILE:HG22	1:N:17:THR:N	2.20	0.56
1:P:624:ARG:HA	1:P:627:ILE:HD12	1.87	0.56
2:Q:659:MET:HG3	2:Q:662:LEU:HD12	1.86	0.56
2:T:190:LEU:O	2:T:194:MET:HG2	2.04	0.56
2:T:136:ILE:HG23	2:X:635:LEU:HD12	1.88	0.56
1:Y:583:VAL:O	1:Y:583:VAL:HG13	2.05	0.56
1:A:28:LEU:HD23	1:A:67:VAL:HG11	1.85	0.56
1:A:98:GLU:HG2	1:A:107:ARG:HA	1.87	0.56
2:H:30:THR:HG23	2:H:32:GLN:N	2.09	0.56
2:I:537:LEU:HD22	2:I:545:TRP:O	2.04	0.56
2:Q:637:ARG:HH11	2:Q:637:ARG:HG3	1.71	0.56
2:T:13:TRP:CZ2	2:T:26:LYS:HE3	2.40	0.56
2:X:513:TRP:HA	2:X:525:ALA:O	2.05	0.56
2:T:135:LEU:HD12	2:X:636:ILE:HG23	1.87	0.56
1:Y:583:VAL:HG22	1:Y:600:ASN:HB2	1.88	0.56
2:E:534:TYR:HH	2:E:621:PHE:HD1	1.52	0.56
1:F:116:VAL:HG22	1:F:122:VAL:HG21	1.87	0.56
2:L:211:VAL:HA	2:L:215:GLN:NE2	2.15	0.56
1:N:113:LEU:HD22	1:N:113:LEU:N	2.20	0.56
2:H:1:MET:N	1:R:107:ARG:HH22	2.02	0.56
2:T:6:GLN:HE22	2:T:226:HIS:CE1	2.23	0.56
1:A:79:GLY:H	1:A:82:ASP:HB2	1.70	0.56
1:F:147:GLU:OE2	1:F:150:ARG:HD3	2.06	0.56
2:H:37:LEU:HD12	2:H:45:TRP:O	2.06	0.56
2:H:81:ARG:NH1	2:H:81:ARG:HA	2.21	0.56
2:L:140:MET:HE3	2:M:541:LEU:HD11	1.88	0.56
2:O:185:GLU:HB2	2:O:188:SER:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:89:HIS:HB3	2:O:90:PRO:HD3	1.88	0.56
1:U:10:LEU:HD13	1:U:11:VAL:N	2.21	0.56
1:A:118:ASN:H	1:A:118:ASN:ND2	1.97	0.56
1:F:152:LEU:HD13	1:G:651:LEU:HD22	1.88	0.56
1:B:606:PHE:CB	2:H:65:LEU:HA	2.34	0.56
2:O:45:TRP:HA	2:O:126:ALA:H	1.70	0.56
2:Q:603:ALA:CB	2:Q:624:MET:HG2	2.36	0.56
1:R:42:ALA:CB	1:R:122:VAL:HG11	2.36	0.56
1:U:43:TRP:HB3	1:U:113:LEU:HD22	1.88	0.56
1:U:3:ARG:HG2	1:U:4:LYS:N	2.20	0.56
2:W:589:HIS:HB3	2:W:590:PRO:HD2	1.88	0.56
1:A:118:ASN:N	1:A:118:ASN:HD22	1.90	0.56
2:D:165:GLN:HA	2:D:168:GLN:HG2	1.86	0.56
2:D:79:LEU:HD21	2:D:95:PHE:HZ	1.70	0.56
1:F:78:ALA:HB1	1:F:82:ASP:OD1	2.05	0.56
2:H:182:GLU:HG3	2:H:183:PRO:HD2	1.88	0.56
2:I:518:LEU:HD22	2:I:595:PHE:O	2.05	0.56
1:K:617:GLU:C	1:K:619:PRO:HD3	2.27	0.56
2:M:547:GLU:HB2	2:M:623:CYS:CB	2.34	0.56
2:Q:541:LEU:HD11	2:Q:707:GLY:CA	2.36	0.56
1:R:118:ASN:HB2	1:R:121:GLU:OE2	2.06	0.56
2:S:111:GLU:HA	2:S:117:PHE:H	1.71	0.56
2:W:675:ILE:CD1	2:W:676:ARG:H	2.19	0.56
1:A:112:ASN:HD22	1:A:112:ASN:H	1.53	0.56
1:F:61:MET:CE	2:I:615:LEU:HD23	2.34	0.56
2:I:642:MET:HE3	2:I:718:TYR:HA	1.87	0.56
1:K:584:TYR:CE1	1:K:599:LYS:HG3	2.41	0.56
2:Q:511:GLN:HG3	2:Q:512:PRO:HD2	1.86	0.56
1:Y:521:GLN:OE1	1:Y:626:LEU:HD12	2.06	0.56
1:A:34:ILE:HG21	1:A:113:LEU:HD22	1.86	0.56
2:D:96:SER:HB3	2:D:107:ARG:HB3	1.88	0.56
2:D:157:LEU:HB3	2:D:184:PHE:CD2	2.41	0.56
2:E:579:LEU:HD21	2:E:612:LEU:HD21	1.86	0.56
2:H:92:GLU:OE2	2:H:111:GLU:HB2	2.05	0.56
2:L:41:LEU:HD13	2:L:204:ILE:HG22	1.88	0.56
2:M:579:LEU:O	2:M:582:PRO:HD2	2.06	0.56
2:T:185:GLU:HG3	2:T:188:SER:H	1.71	0.56
2:T:47:GLU:OE2	2:T:49:VAL:HG23	2.06	0.56
1:B:501:MET:HA	1:B:525:GLU:OE2	2.06	0.55
2:D:175:ILE:HB	2:E:666:ASP:OD2	2.07	0.55
2:E:513:TRP:N	2:E:715:GLN:NE2	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:593:ALA:HA	2:I:609:ARG:O	2.06	0.55
1:K:505:ILE:HG22	1:K:506:SER:H	1.70	0.55
1:K:531:GLY:HA3	1:K:548:SER:HA	1.88	0.55
2:M:518:LEU:HD12	2:M:597:CYS:HB2	1.87	0.55
2:L:105:ILE:HB	2:Q:601:ALA:CB	2.36	0.55
1:R:141:ASN:O	1:R:145:GLN:HB2	2.06	0.55
2:S:105:ILE:HG23	2:S:105:ILE:O	2.06	0.55
2:S:131:VAL:HG13	2:S:132:SER:N	2.21	0.55
2:S:204:ILE:HD13	2:W:641:GLY:HA2	1.87	0.55
1:V:504:LYS:HB3	1:V:575:LEU:HD22	1.87	0.55
1:A:34:ILE:HG22	1:A:113:LEU:HD13	1.87	0.55
2:E:502:GLU:HG2	2:E:503:GLU:H	1.70	0.55
1:G:544:THR:HG22	1:G:545:GLY:N	2.17	0.55
2:H:140:MET:HE2	2:I:710:PHE:CD2	2.41	0.55
2:H:81:ARG:CZ	2:H:81:ARG:HA	2.37	0.55
1:N:141:ASN:O	1:N:145:GLN:HB2	2.07	0.55
1:R:21:GLN:HG2	1:R:22:VAL:N	2.21	0.55
2:W:512:PRO:HB2	2:W:715:GLN:HE21	1.70	0.55
2:W:606:LEU:CB	2:W:621:PHE:HB2	2.36	0.55
2:X:537:LEU:HD12	2:X:545:TRP:O	2.06	0.55
1:B:642:GLU:HA	1:B:645:GLN:HB3	1.87	0.55
2:D:210:PHE:HB2	2:E:640:MET:HE3	1.86	0.55
2:H:27:VAL:HB	2:H:36:LEU:HD13	1.88	0.55
2:H:65:LEU:HD12	2:H:66:THR:H	1.72	0.55
2:L:159:MET:HA	2:L:162:LEU:HD12	1.89	0.55
2:O:75:HIS:NE2	2:O:112:LEU:HB2	2.22	0.55
2:Q:676:ARG:HG3	2:Q:677:ASP:OD2	2.06	0.55
2:T:75:HIS:NE2	2:T:112:LEU:HD21	2.22	0.55
2:E:516:LEU:H	2:E:516:LEU:HD23	1.71	0.55
2:H:157:LEU:HG	2:I:657:LEU:HA	1.88	0.55
2:Q:570:ALA:HA	2:Q:573:LEU:HD12	1.88	0.55
2:S:146:LEU:HD21	2:S:217:LEU:HD22	1.87	0.55
1:B:504:LYS:O	1:B:521:GLN:HA	2.07	0.55
1:B:536:LEU:HD12	1:B:537:THR:N	2.22	0.55
2:H:89:HIS:CB	2:H:90:PRO:HA	2.22	0.55
1:N:147:GLU:HB3	1:P:648:ASN:ND2	2.22	0.55
2:Q:516:LEU:HD11	2:Q:595:PHE:CD2	2.42	0.55
2:Q:630:LEU:O	2:Q:634:HIS:HB2	2.07	0.55
2:T:32:GLN:HB3	2:T:51:THR:HG22	1.88	0.55
2:T:36:LEU:HD12	2:T:37:LEU:H	1.72	0.55
1:Y:549:GLU:HA	1:Y:552:ILE:HD11	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:523:LEU:HB2	2:E:538:VAL:CG2	2.37	0.55
1:F:3:ARG:HD3	1:F:129:TYR:CE1	2.41	0.55
2:H:217:LEU:O	2:H:221:VAL:HG23	2.06	0.55
1:J:150:ARG:HG3	1:J:151:LEU:H	1.72	0.55
1:P:650:ARG:HA	1:P:653:ARG:HE	1.72	0.55
2:Q:537:LEU:HG	2:Q:545:TRP:O	2.06	0.55
2:T:25:ALA:HB2	2:T:38:VAL:CG1	2.31	0.55
2:W:517:GLN:HE21	2:W:517:GLN:CA	2.20	0.55
2:W:529:ILE:HG22	2:W:531:LYS:H	1.71	0.55
1:B:616:VAL:HG12	1:B:618:ASN:H	1.71	0.55
2:E:581:ARG:HB3	2:E:582:PRO:HD3	1.89	0.55
2:E:675:ILE:HG12	2:E:677:ASP:H	1.72	0.55
1:F:100:ASN:O	1:F:101:LEU:HD22	2.06	0.55
1:G:501:MET:HG3	1:G:523:SER:HB2	1.89	0.55
2:I:534:TYR:H	2:I:549:VAL:CG1	2.16	0.55
1:N:36:LEU:HG	1:N:37:THR:N	2.21	0.55
1:P:534:ILE:HD13	1:P:535:THR:N	2.22	0.55
1:P:587:ASN:HB2	1:P:596:PHE:CE1	2.42	0.55
1:R:49:GLU:CD	1:R:52:ILE:HD12	2.26	0.55
2:S:10:MET:HG3	2:S:223:THR:HG22	1.87	0.55
2:W:596:SER:HB2	2:W:607:ARG:HB2	1.89	0.55
2:X:514:ALA:HA	2:X:711:VAL:HG21	1.88	0.55
1:A:32:PHE:H	1:A:47:VAL:HB	1.71	0.55
2:D:193:PHE:C	2:D:195:ILE:H	2.09	0.55
1:A:105:SER:HB2	2:E:566:THR:HB	1.89	0.55
2:D:179:LEU:HD21	2:E:662:LEU:HB2	1.88	0.55
1:F:5:ILE:HB	1:G:631:LEU:HD11	1.89	0.55
2:H:105:ILE:HG13	2:H:107:ARG:HG3	1.89	0.55
1:K:520:LEU:HG	1:K:522:VAL:HG22	1.89	0.55
1:K:589:SER:OG	1:K:594:TYR:HB2	2.06	0.55
2:S:211:VAL:HA	2:S:215:GLN:HG2	1.89	0.55
1:U:5:ILE:HA	1:U:20:LEU:O	2.07	0.55
1:B:511:VAL:HB	1:B:587:ASN:OD1	2.07	0.55
1:B:532:PHE:HE1	1:B:534:ILE:HB	1.72	0.55
2:D:143:SER:HB2	2:E:643:SER:OG	2.06	0.55
1:F:16:ILE:HG23	1:G:624:ARG:NE	2.21	0.55
2:H:115:LEU:HB3	2:H:116:PRO:HD2	1.89	0.55
2:H:14:ALA:HA	2:H:211:VAL:CG2	2.35	0.55
2:H:83:LEU:HD22	2:H:83:LEU:N	2.18	0.55
2:L:179:LEU:HD23	2:L:179:LEU:O	2.07	0.55
2:M:518:LEU:HD23	2:M:518:LEU:N	2.18	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:534:TYR:OH	2:M:619:TRP:HZ2	1.89	0.55
2:L:140:MET:CE	2:M:541:LEU:HD11	2.37	0.55
1:U:87:ASN:HB2	1:U:96:PHE:CE2	2.42	0.55
1:A:118:ASN:HB2	1:A:121:GLU:HG3	1.89	0.55
1:A:73:ALA:HB2	1:A:84:TYR:CG	2.42	0.55
1:B:618:ASN:O	1:B:622:VAL:HG23	2.07	0.55
2:H:109:ARG:HH21	2:H:116:PRO:HA	1.72	0.55
2:H:112:LEU:HB2	2:H:117:PHE:CB	2.31	0.55
1:J:5:ILE:HD12	1:J:21:GLN:NE2	2.20	0.55
1:K:510:LEU:HD22	1:K:513:GLU:N	2.21	0.55
1:K:534:ILE:HD12	1:K:545:GLY:HA3	1.88	0.55
2:L:18:LEU:HD23	2:L:97:CYS:HB3	1.89	0.55
1:N:89:SER:OG	1:N:92:SER:HB3	2.06	0.55
2:O:49:VAL:HG13	2:O:53:VAL:HB	1.88	0.55
2:X:581:ARG:NH1	2:X:581:ARG:HB3	2.22	0.55
2:X:608:VAL:HG12	2:X:609:ARG:N	2.20	0.55
1:Y:575:LEU:C	1:Y:577:GLY:H	2.09	0.55
2:D:109:ARG:HG2	2:D:110:SER:N	2.21	0.54
2:D:193:PHE:HZ	2:E:648:CYS:HB2	1.72	0.54
2:E:515:TRP:HB2	2:E:524:LEU:HA	1.90	0.54
1:F:8:ILE:HD11	1:F:20:LEU:CB	2.37	0.54
2:H:57:ARG:HD2	2:H:119:TRP:CZ3	2.42	0.54
2:M:617:PHE:HD2	2:M:618:TYR:N	2.05	0.54
1:N:67:VAL:O	1:N:71:ARG:HG3	2.07	0.54
1:P:557:ASP:HB3	3:P:2:TBR:BR2	2.62	0.54
1:U:99:LYS:N	1:U:108:LEU:HD11	2.22	0.54
1:U:126:LEU:HD23	1:U:127:ILE:N	2.21	0.54
2:S:197:LYS:HE3	2:W:652:GLU:OE1	2.06	0.54
2:W:708:LYS:N	2:W:709:PRO:HD2	2.22	0.54
1:B:549:GLU:O	1:B:550:SER:HB3	2.05	0.54
2:D:45:TRP:HD1	2:D:125:LEU:HA	1.73	0.54
2:D:138:PRO:HA	2:D:225:HIS:CE1	2.43	0.54
2:E:545:TRP:CZ3	2:E:604:LEU:HD13	2.42	0.54
2:H:105:ILE:HG21	2:H:107:ARG:HH21	1.73	0.54
1:J:7:ARG:HH22	1:K:628:CYS:HA	1.71	0.54
2:S:79:LEU:O	2:S:81:ARG:HG3	2.07	0.54
2:T:69:PRO:HG2	2:T:70:ALA:H	1.72	0.54
1:A:138:GLN:HG2	1:B:637:ASN:HD21	1.71	0.54
1:A:85:THR:OG1	1:A:100:ASN:HB2	2.07	0.54
2:D:80:LEU:HB3	2:D:81:ARG:NH2	2.23	0.54
2:E:605:ILE:HD12	2:E:607:ARG:CZ	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:639:LEU:HA	2:E:642:MET:HE3	1.90	0.54
2:I:694:MET:HG3	2:I:698:LEU:HD13	1.90	0.54
2:L:170:SER:HB2	2:M:673:THR:CG2	2.37	0.54
2:L:18:LEU:N	2:L:18:LEU:HD12	2.23	0.54
2:M:503:GLU:HG3	2:M:504:LEU:H	1.73	0.54
2:L:204:ILE:HD11	2:M:641:GLY:CA	2.37	0.54
2:T:24:LEU:HD21	2:T:207:GLY:HA3	1.88	0.54
2:T:47:GLU:HG3	2:T:122:HIS:O	2.07	0.54
1:V:555:GLU:HG3	1:V:566:TYR:OH	2.07	0.54
1:A:119:PRO:HG2	1:A:120:ALA:H	1.72	0.54
2:D:46:HIS:CE1	2:D:48:GLN:HB3	2.36	0.54
2:E:607:ARG:NH1	2:E:607:ARG:HB2	2.23	0.54
1:F:1:MET:HG3	1:F:23:SER:HB3	1.90	0.54
2:O:17:GLN:NE2	2:O:17:GLN:H	2.03	0.54
2:Q:690:LEU:O	2:Q:694:MET:HG2	2.08	0.54
2:T:136:ILE:HG13	2:X:636:ILE:HD11	1.89	0.54
2:T:140:MET:HA	2:X:639:LEU:HD21	1.90	0.54
2:E:593:ALA:CB	2:E:610:SER:HB3	2.34	0.54
1:G:568:GLY:O	1:G:571:ARG:HG2	2.07	0.54
2:H:9:LEU:HA	2:H:134:HIS:HE1	1.73	0.54
2:O:149:GLN:O	2:O:153:LEU:HB2	2.08	0.54
1:P:597:PHE:N	1:P:597:PHE:CD2	2.76	0.54
2:E:664:ILE:O	2:E:668:GLN:HG2	2.07	0.54
1:F:112:ASN:HD22	1:F:113:LEU:H	1.55	0.54
1:P:567:VAL:HG12	1:P:571:ARG:NH2	2.22	0.54
2:Q:534:TYR:HE2	2:Q:619:TRP:CZ2	2.25	0.54
2:S:198:LEU:N	2:S:199:PRO:CD	2.70	0.54
2:S:25:ALA:HB2	2:S:38:VAL:HG22	1.89	0.54
2:T:115:LEU:HD22	2:T:115:LEU:N	2.23	0.54
2:T:103:ALA:HA	2:T:124:MET:HA	1.88	0.54
2:T:196:GLU:O	2:T:199:PRO:HD2	2.08	0.54
2:T:76:LEU:HD23	2:T:79:LEU:HB3	1.89	0.54
2:W:606:LEU:HB3	2:W:621:PHE:HB2	1.89	0.54
2:X:526:LYS:HD2	2:X:537:LEU:HD23	1.89	0.54
1:B:561:MET:HE2	1:B:562:GLU:H	1.71	0.54
2:D:192:GLN:HA	2:D:195:ILE:HD12	1.89	0.54
2:E:561:LEU:HD22	2:E:620:ASN:HD22	1.72	0.54
1:B:561:MET:HG3	2:H:64:ARG:NH2	2.23	0.54
1:K:524:TRP:HZ3	1:K:575:LEU:HD21	1.72	0.54
1:K:518:HIS:CE1	1:K:538:ASP:HB3	2.42	0.54
1:K:524:TRP:CZ3	1:K:575:LEU:HD21	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:20:LEU:HD12	1:N:34:ILE:HD11	1.89	0.54
1:P:576:SER:C	1:P:578:ALA:H	2.10	0.54
1:V:627:ILE:O	1:V:631:LEU:HG	2.07	0.54
2:X:549:VAL:HG12	2:X:550:ASP:N	2.22	0.54
2:D:176:ARG:HH11	2:D:179:LEU:HD12	1.71	0.54
1:F:21:GLN:OE1	1:F:126:LEU:HD12	2.08	0.54
2:H:81:ARG:N	2:H:82:PRO:HD2	2.23	0.54
2:O:57:ARG:O	2:O:61:LEU:HD12	2.06	0.54
2:Q:607:ARG:HG3	2:Q:620:ASN:HD21	1.71	0.54
2:T:98:ASP:OD2	2:T:105:ILE:HB	2.08	0.54
2:T:135:LEU:O	2:T:139:LEU:HB2	2.07	0.54
2:X:531:LYS:O	2:X:532:GLN:HG3	2.08	0.54
2:X:533:GLY:H	2:X:573:LEU:HD11	1.71	0.54
1:Y:504:LYS:HB3	1:Y:522:VAL:HG23	1.90	0.54
2:D:65:LEU:HD22	2:D:66:THR:N	2.21	0.54
2:H:132:SER:O	2:H:137:ARG:HB2	2.08	0.54
2:I:692:GLN:O	2:I:696:GLU:HB2	2.07	0.54
2:L:105:ILE:HA	2:L:121:PHE:O	2.08	0.54
2:M:523:LEU:HG	2:M:538:VAL:CG2	2.38	0.54
2:O:139:LEU:HB3	2:Q:639:LEU:CD2	2.38	0.54
2:S:104:LEU:HB3	2:S:123:CYS:SG	2.48	0.54
2:D:128:PRO:C	2:D:130:LEU:H	2.11	0.54
2:D:165:GLN:NE2	2:D:168:GLN:HG3	2.23	0.54
1:F:139:ALA:HA	1:F:142:GLU:HG2	1.90	0.54
1:N:21:GLN:OE1	1:N:126:LEU:HD12	2.08	0.54
2:Q:525:ALA:O	2:Q:526:LYS:CB	2.54	0.54
1:R:29:GLU:O	1:R:52:ILE:HG21	2.07	0.54
2:S:79:LEU:HD23	2:S:80:LEU:N	2.23	0.54
2:T:195:ILE:N	2:T:195:ILE:HD12	2.22	0.54
2:S:146:LEU:HB3	2:W:646:LEU:HD22	1.89	0.54
1:A:104:VAL:HG12	1:A:105:SER:N	2.23	0.53
1:A:112:ASN:ND2	1:A:112:ASN:H	2.06	0.53
2:E:565:LEU:HD23	2:E:566:THR:N	2.23	0.53
1:G:646:LYS:HG3	1:Y:650:ARG:NH2	2.19	0.53
2:H:166:ASP:HB3	2:I:675:ILE:CG2	2.38	0.53
1:K:607:ARG:HH22	2:T:100:VAL:HA	1.72	0.53
1:K:638:GLN:O	1:K:642:GLU:HG2	2.07	0.53
2:L:108:VAL:CG2	2:L:119:TRP:HB3	2.37	0.53
2:M:537:LEU:HD22	2:M:634:HIS:CD2	2.43	0.53
1:N:126:LEU:O	1:N:130:CYS:HB2	2.07	0.53
2:X:615:LEU:HD22	2:X:616:PRO:HD2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:549:GLU:HG2	1:B:550:SER:H	1.73	0.53
2:D:36:LEU:HG	2:D:37:LEU:H	1.71	0.53
2:I:698:LEU:HB3	2:I:699:PRO:HD3	1.91	0.53
1:K:563:LYS:HA	1:K:566:TYR:HB3	1.90	0.53
2:O:192:GLN:HA	2:O:195:ILE:HD11	1.90	0.53
2:X:611:GLU:HA	2:X:615:LEU:O	2.08	0.53
1:Y:559:MET:HB3	1:Y:561:MET:HE3	1.90	0.53
1:A:104:VAL:HG12	1:A:105:SER:H	1.74	0.53
1:G:616:VAL:HG22	1:G:618:ASN:OD1	2.08	0.53
2:I:515:TRP:CD1	2:I:524:LEU:HD13	2.43	0.53
2:H:146:LEU:CB	2:I:646:LEU:HD23	2.35	0.53
1:N:3:ARG:HH22	1:N:21:GLN:NE2	2.05	0.53
2:O:202:CYS:SG	2:Q:721:VAL:HG13	2.49	0.53
1:P:597:PHE:N	1:P:597:PHE:HD2	2.05	0.53
2:Q:692:GLN:HG3	2:Q:696:GLU:OE2	2.09	0.53
1:R:124:ARG:CZ	1:V:516:ILE:HD11	2.38	0.53
2:T:146:LEU:HD21	2:X:647:GLN:NE2	2.23	0.53
2:T:150:VAL:HG13	2:X:653:LEU:CD1	2.38	0.53
1:V:534:ILE:HD13	1:V:535:THR:N	2.23	0.53
2:D:12:PRO:HD3	2:D:219:MET:SD	2.49	0.53
2:E:524:LEU:HD12	2:E:524:LEU:N	2.24	0.53
2:E:557:ARG:NH1	2:E:622:HIS:H	2.06	0.53
1:F:152:LEU:CD2	1:G:650:ARG:HH21	2.22	0.53
2:H:12:PRO:CB	2:H:215:GLN:HE21	2.22	0.53
2:H:204:ILE:HD12	2:I:640:MET:HB3	1.90	0.53
2:M:607:ARG:HD3	2:M:620:ASN:ND2	2.22	0.53
2:Q:554:VAL:HG13	2:Q:555:SER:H	1.71	0.53
2:Q:657:LEU:O	2:Q:660:LYS:HB3	2.09	0.53
2:T:165:GLN:O	2:T:169:GLU:HG2	2.08	0.53
1:V:547:VAL:HB	1:V:611:PHE:HE2	1.73	0.53
1:A:127:ILE:CD1	1:B:627:ILE:HG12	2.39	0.53
1:B:621:GLU:HG2	1:B:624:ARG:NH2	2.23	0.53
2:H:140:MET:HA	2:I:639:LEU:CD1	2.38	0.53
2:H:29:ILE:HB	2:H:77:ASP:OD2	2.09	0.53
2:O:80:LEU:O	2:O:81:ARG:CB	2.56	0.53
2:Q:687:ASN:C	2:Q:689:PHE:H	2.11	0.53
2:S:63:LYS:H	2:S:64:ARG:NH1	2.03	0.53
2:T:13:TRP:CH2	2:T:37:LEU:HD22	2.43	0.53
2:X:544:VAL:HB	2:X:626:ALA:HB3	1.90	0.53
1:Y:502:GLU:HB3	1:Y:524:TRP:CE2	2.43	0.53
2:E:715:GLN:HE22	2:E:718:TYR:HD2	1.54	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:176:ARG:HB2	2:H:179:LEU:CD1	2.38	0.53
2:H:209:PRO:HB2	2:I:644:LEU:CD1	2.38	0.53
2:I:710:PHE:HD1	2:I:711:VAL:HG13	1.73	0.53
1:K:601:LEU:HD22	1:K:606:PHE:HE2	1.73	0.53
2:L:159:MET:HA	2:L:162:LEU:CD1	2.38	0.53
1:J:61:MET:CE	2:M:615:LEU:HD23	2.39	0.53
2:O:37:LEU:HD12	2:O:45:TRP:O	2.08	0.53
2:O:39:SER:HB2	2:O:44:VAL:HG13	1.91	0.53
2:O:202:CYS:HB3	2:Q:645:ALA:HB2	1.91	0.53
2:Q:646:LEU:O	2:Q:650:VAL:HG23	2.08	0.53
2:E:562:ASN:HD22	2:E:565:LEU:HD22	1.73	0.53
2:E:617:PHE:HD2	2:E:618:TYR:H	1.56	0.53
1:F:118:ASN:O	1:F:122:VAL:HG23	2.08	0.53
1:G:537:THR:OG1	1:G:538:ASP:N	2.41	0.53
1:G:649:GLU:O	1:G:652:LEU:HD13	2.09	0.53
1:J:99:LYS:HB2	1:J:108:LEU:HD12	1.90	0.53
2:O:103:ALA:HB1	2:O:123:CYS:O	2.08	0.53
2:O:144:LEU:HD11	2:Q:709:PRO:HG3	1.90	0.53
2:S:127:SER:H	2:S:130:LEU:HD12	1.73	0.53
2:T:173:THR:HG22	2:T:174:LEU:H	1.74	0.53
2:T:63:LYS:HA	2:T:63:LYS:HE3	1.91	0.53
2:W:512:PRO:HD3	2:W:719:MET:SD	2.49	0.53
1:Y:572:LYS:O	1:Y:578:ALA:HB3	2.09	0.53
1:G:595:PHE:HB2	1:G:613:LEU:HD22	1.90	0.53
1:K:571:ARG:O	1:K:575:LEU:HB2	2.08	0.53
2:M:609:ARG:HH11	2:M:618:TYR:HE1	1.56	0.53
1:N:10:LEU:HD23	1:N:86:PHE:O	2.08	0.53
2:T:131:VAL:O	2:T:135:LEU:HB2	2.08	0.53
2:W:690:LEU:O	2:W:694:MET:HG2	2.08	0.53
2:E:711:VAL:HA	2:E:715:GLN:OE1	2.08	0.53
2:I:530:THR:O	2:I:531:LYS:HD2	2.08	0.53
2:I:579:LEU:HD21	2:I:612:LEU:HD21	1.90	0.53
2:L:55:SER:HB2	2:L:69:PRO:HG3	1.90	0.53
2:M:518:LEU:CD2	2:M:523:LEU:HB2	2.39	0.53
2:Q:529:ILE:CG2	2:Q:530:THR:N	2.71	0.53
2:T:16:LEU:HD12	2:T:17:GLN:N	2.24	0.53
2:T:173:THR:HG21	2:X:672:ALA:HB2	1.90	0.53
2:E:545:TRP:HD1	2:E:625:LEU:HA	1.73	0.53
2:H:57:ARG:NH2	2:H:122:HIS:HB2	2.24	0.53
2:M:583:LEU:N	2:M:583:LEU:HD23	2.23	0.53
1:P:650:ARG:HA	1:P:653:ARG:NE	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:676:ARG:NH1	2:Q:676:ARG:HB2	2.24	0.53
2:T:154:ALA:HA	2:T:157:LEU:HD12	1.91	0.53
1:U:61:MET:HB2	1:U:66:TYR:HB2	1.90	0.53
2:W:605:ILE:HG21	2:W:607:ARG:HE	1.74	0.53
1:B:604:VAL:HG21	2:H:67:ALA:CB	2.37	0.52
2:E:537:LEU:HD12	2:E:545:TRP:O	2.09	0.52
2:E:557:ARG:O	2:E:561:LEU:HG	2.08	0.52
2:E:698:LEU:HB3	2:E:699:PRO:HD3	1.91	0.52
1:F:32:PHE:HE2	1:F:52:ILE:HD12	1.73	0.52
1:J:61:MET:HE3	2:M:616:PRO:HD3	1.91	0.52
1:P:620:ALA:O	1:P:623:ILE:HG22	2.08	0.52
1:N:105:SER:O	2:Q:565:LEU:HD12	2.09	0.52
1:B:524:TRP:HZ3	1:B:575:LEU:HD22	1.73	0.52
2:E:515:TRP:HZ2	2:E:708:LYS:HZ3	1.57	0.52
1:F:36:LEU:O	1:F:42:ALA:HB1	2.08	0.52
2:I:546:HIS:CG	2:I:547:GLU:H	2.27	0.52
2:M:706:ASP:C	2:M:708:LYS:H	2.12	0.52
2:O:46:HIS:ND1	2:O:47:GLU:N	2.57	0.52
1:R:10:LEU:HD21	1:R:88:PHE:HB3	1.90	0.52
2:T:76:LEU:O	2:T:79:LEU:HB3	2.09	0.52
1:U:126:LEU:HD21	1:Y:627:ILE:CG2	2.39	0.52
1:U:150:ARG:HA	1:U:153:ARG:NH1	2.24	0.52
2:E:668:GLN:O	2:E:672:ALA:HA	2.10	0.52
1:F:11:VAL:HG11	2:S:69:PRO:HD3	1.91	0.52
1:F:5:ILE:HG12	1:F:126:LEU:CD1	2.39	0.52
2:Q:686:GLU:O	2:Q:690:LEU:HG	2.09	0.52
2:T:194:MET:O	2:T:198:LEU:HB3	2.09	0.52
1:B:513:GLU:N	1:B:514:PRO:HD3	2.25	0.52
1:B:572:LYS:HD3	1:B:584:TYR:HE1	1.73	0.52
1:K:571:ARG:HG3	1:K:572:LYS:H	1.75	0.52
2:L:167:TYR:CD1	2:M:667:TYR:HB2	2.45	0.52
2:L:80:LEU:HA	2:L:83:LEU:HD12	1.90	0.52
1:N:126:LEU:HD21	1:P:627:ILE:CG2	2.39	0.52
1:P:520:LEU:HD21	1:P:534:ILE:HG12	1.91	0.52
2:Q:608:VAL:HG12	2:Q:619:TRP:O	2.10	0.52
1:V:536:LEU:O	1:V:542:ALA:HB1	2.08	0.52
1:V:512:SER:H	1:V:587:ASN:ND2	2.06	0.52
2:W:507:GLY:HA3	2:W:528:PHE:CE2	2.44	0.52
1:Y:549:GLU:HG3	1:Y:552:ILE:HD11	1.91	0.52
1:F:116:VAL:HG21	1:F:122:VAL:HG21	1.91	0.52
1:F:43:TRP:HB3	1:F:113:LEU:HG	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:559:MET:CE	1:G:566:TYR:HA	2.40	0.52
1:J:20:LEU:HD23	1:J:34:ILE:HD11	1.92	0.52
1:N:36:LEU:O	1:N:37:THR:HB	2.09	0.52
2:O:175:ILE:HD11	2:Q:671:GLY:HA2	1.91	0.52
1:P:537:THR:HB	1:P:542:ALA:HB2	1.91	0.52
2:L:101:ALA:HB1	2:Q:622:HIS:CG	2.44	0.52
2:T:154:ALA:O	2:T:157:LEU:HB2	2.10	0.52
1:V:536:LEU:HD22	1:V:537:THR:H	1.74	0.52
1:V:567:VAL:HG23	1:V:568:GLY:N	2.25	0.52
2:W:599:CYS:HB2	2:W:604:LEU:HD13	1.91	0.52
2:W:513:TRP:H	2:W:715:GLN:NE2	2.08	0.52
1:A:126:LEU:HD22	1:B:627:ILE:HD13	1.92	0.52
2:D:175:ILE:H	2:D:175:ILE:CD1	2.20	0.52
1:K:596:PHE:HA	1:K:610:SER:CB	2.40	0.52
1:K:617:GLU:O	1:K:619:PRO:HD3	2.09	0.52
1:R:151:LEU:HD11	1:V:652:LEU:CD1	2.40	0.52
2:T:142:MET:O	2:T:146:LEU:HB2	2.09	0.52
2:W:553:VAL:HA	2:W:556:GLN:HG2	1.90	0.52
1:U:137:ASN:HB3	1:Y:637:ASN:HD22	1.73	0.52
1:A:102:LYS:O	1:A:104:VAL:HG23	2.09	0.52
2:I:512:PRO:HB2	2:I:715:GLN:CD	2.30	0.52
2:I:526:LYS:HG3	2:I:526:LYS:O	2.10	0.52
2:I:718:TYR:O	2:I:722:THR:HG23	2.09	0.52
1:J:138:GLN:O	1:J:142:GLU:HG3	2.10	0.52
1:J:7:ARG:NH2	1:K:628:CYS:HA	2.25	0.52
1:K:590:LYS:HA	1:K:590:LYS:NZ	2.23	0.52
2:O:8:LEU:HD22	2:O:35:ALA:HB1	1.92	0.52
1:R:104:VAL:HA	2:W:567:ALA:HB2	1.91	0.52
1:U:8:ILE:H	1:U:8:ILE:HD13	1.75	0.52
1:V:547:VAL:HA	1:V:551:GLU:CD	2.31	0.52
2:T:140:MET:HB3	2:X:704:ILE:HD11	1.91	0.52
2:D:4:LEU:HD12	2:D:35:ALA:N	2.25	0.52
2:I:530:THR:C	2:I:531:LYS:HD2	2.30	0.52
1:N:20:LEU:CD1	1:N:34:ILE:HD11	2.39	0.52
2:O:164:ILE:HG22	2:O:168:GLN:CD	2.30	0.52
2:O:18:LEU:HD22	2:O:95:PHE:HB3	1.91	0.52
1:P:594:TYR:CE1	1:P:610:SER:HB2	2.44	0.52
2:S:189:PHE:O	2:S:192:GLN:HG3	2.10	0.52
2:S:49:VAL:HG22	2:S:53:VAL:HG11	1.92	0.52
1:U:21:GLN:HB3	1:U:35:THR:HB	1.91	0.52
1:V:528:LEU:HD12	1:V:571:ARG:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:598:ASP:O	2:X:604:LEU:HA	2.09	0.52
1:A:28:LEU:HD23	1:A:71:ARG:HE	1.75	0.52
1:F:11:VAL:HB	1:F:87:ASN:ND2	2.25	0.52
1:F:42:ALA:HB3	1:F:122:VAL:HG11	1.92	0.52
2:H:208:LYS:HB3	2:H:209:PRO:HD3	1.91	0.52
2:I:612:LEU:HG	2:I:617:PHE:HD2	1.74	0.52
1:K:514:PRO:HG2	1:K:515:SER:H	1.74	0.52
1:K:534:ILE:HB	1:K:545:GLY:N	2.25	0.52
2:O:211:VAL:O	2:O:212:MET:C	2.48	0.52
2:Q:515:TRP:CZ2	2:Q:708:LYS:HD3	2.45	0.52
1:V:604:VAL:HG22	1:V:605:SER:N	2.25	0.52
1:B:503:ARG:HH21	1:B:629:TYR:HB3	1.74	0.52
2:H:81:ARG:NH1	2:H:84:LEU:HB3	2.24	0.52
2:I:581:ARG:C	2:I:583:LEU:H	2.14	0.52
2:L:135:LEU:HD12	2:M:636:ILE:HG23	1.92	0.52
2:L:84:LEU:HD23	2:L:84:LEU:H	1.75	0.52
2:Q:592:GLU:HG2	2:Q:593:ALA:H	1.75	0.52
2:S:68:PRO:HG2	2:S:71:ALA:HB3	1.92	0.52
1:U:34:ILE:HD12	1:U:35:THR:H	1.74	0.52
2:W:632:SER:HA	2:W:636:ILE:HB	1.91	0.52
1:U:120:ALA:HB2	1:Y:540:HIS:HD2	1.75	0.52
2:D:85:LYS:HB2	2:D:85:LYS:NZ	2.25	0.51
2:I:557:ARG:HG2	2:I:561:LEU:HD12	1.91	0.51
1:F:105:SER:HB2	2:I:566:THR:HB	1.92	0.51
2:I:709:PRO:HA	2:I:712:MET:HG2	1.91	0.51
2:L:176:ARG:CZ	2:M:666:ASP:HB2	2.40	0.51
1:P:522:VAL:HA	1:P:533:VAL:O	2.11	0.51
2:W:661:ASP:OD1	2:W:683:PRO:HA	2.10	0.51
2:X:594:THR:OG1	2:X:609:ARG:HD3	2.10	0.51
2:T:170:SER:OG	2:X:675:ILE:HG12	2.10	0.51
1:Y:593:CYS:HB3	1:Y:613:LEU:O	2.10	0.51
1:A:44:THR:CG2	1:A:116:VAL:HG22	2.40	0.51
2:D:98:ASP:HB2	2:D:105:ILE:CG2	2.41	0.51
2:E:579:LEU:HD21	2:E:612:LEU:CD2	2.40	0.51
1:F:144:LEU:HB3	1:G:644:LEU:HD22	1.92	0.51
2:H:82:PRO:HB3	2:H:90:PRO:HB3	1.92	0.51
2:I:624:MET:O	2:I:625:LEU:C	2.48	0.51
2:I:691:GLU:HG3	2:I:692:GLN:N	2.25	0.51
2:L:29:ILE:HD13	2:L:77:ASP:HA	1.92	0.51
2:M:512:PRO:HB3	2:M:719:MET:SD	2.50	0.51
2:O:75:HIS:CD2	2:O:112:LEU:HD22	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:159:MET:HA	2:T:162:LEU:HD12	1.91	0.51
1:U:51:GLU:O	1:U:55:GLU:HG2	2.10	0.51
1:V:601:LEU:HB2	1:V:604:VAL:HG13	1.91	0.51
1:A:69:GLU:HG3	1:A:108:LEU:HD11	1.92	0.51
2:D:157:LEU:HA	2:E:657:LEU:CD2	2.39	0.51
1:B:559:MET:CB	2:H:64:ARG:HH21	2.23	0.51
2:I:546:HIS:CD2	2:I:547:GLU:H	2.28	0.51
2:M:518:LEU:HD11	2:M:523:LEU:HD22	1.91	0.51
2:M:710:PHE:O	2:M:714:LEU:HB2	2.10	0.51
1:B:549:GLU:HG2	1:B:550:SER:N	2.25	0.51
1:J:138:GLN:HA	1:K:637:ASN:HD21	1.74	0.51
1:K:518:HIS:HB3	1:K:536:LEU:HD11	1.91	0.51
1:N:13:GLU:O	1:N:15:SER:N	2.44	0.51
1:N:3:ARG:CZ	1:N:3:ARG:HB3	2.40	0.51
2:Q:676:ARG:HB3	2:Q:679:LEU:HB2	1.92	0.51
2:X:573:LEU:O	2:X:576:LEU:HB3	2.09	0.51
2:X:608:VAL:HG23	2:X:619:TRP:O	2.10	0.51
1:B:621:GLU:HG2	1:B:624:ARG:HH21	1.75	0.51
2:E:524:LEU:CD1	2:E:524:LEU:H	2.21	0.51
2:E:545:TRP:CD1	2:E:625:LEU:HA	2.45	0.51
2:E:611:GLU:HG2	2:E:616:PRO:HA	1.92	0.51
2:I:536:LEU:HD12	2:I:537:LEU:H	1.73	0.51
1:J:88:PHE:HB2	1:J:95:PHE:CD1	2.46	0.51
2:L:109:ARG:HG2	2:L:118:TYR:HD2	1.75	0.51
2:L:139:LEU:HD21	2:M:640:MET:CA	2.40	0.51
2:O:37:LEU:HD11	2:O:44:VAL:HG12	1.91	0.51
2:Q:593:ALA:O	2:Q:594:THR:C	2.49	0.51
2:Q:579:LEU:HD21	2:Q:610:SER:HB2	1.92	0.51
1:R:24:TRP:HB3	1:R:32:PHE:HB3	1.92	0.51
1:V:598:GLU:HA	1:V:607:ARG:HA	1.93	0.51
2:W:655:THR:O	2:W:659:MET:HG3	2.10	0.51
2:W:698:LEU:H	2:W:699:PRO:CD	2.24	0.51
2:X:545:TRP:CE3	2:X:604:LEU:HD13	2.46	0.51
2:D:116:PRO:HB3	2:D:118:TYR:CE1	2.44	0.51
2:H:105:ILE:CG1	2:H:107:ARG:HG3	2.41	0.51
2:L:108:VAL:HG23	2:L:119:TRP:HB3	1.93	0.51
2:L:96:SER:OG	2:L:107:ARG:HD2	2.11	0.51
2:M:694:MET:HA	2:M:698:LEU:HD22	1.92	0.51
1:N:47:VAL:HA	1:N:51:GLU:OE1	2.10	0.51
1:N:89:SER:CB	1:N:92:SER:HB3	2.40	0.51
2:O:62:ASN:CB	2:O:65:LEU:HB3	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:27:VAL:HG21	2:T:80:LEU:HD13	1.93	0.51
2:W:529:ILE:HG12	2:W:534:TYR:HB2	1.93	0.51
2:W:606:LEU:HB3	2:W:621:PHE:HD2	1.74	0.51
2:W:709:PRO:HG2	2:W:710:PHE:H	1.76	0.51
2:X:514:ALA:CA	2:X:711:VAL:HG21	2.41	0.51
2:D:109:ARG:HG2	2:D:110:SER:H	1.75	0.51
1:J:151:LEU:HD22	1:K:652:LEU:HD13	1.91	0.51
2:M:606:LEU:HG	2:M:621:PHE:HB2	1.93	0.51
1:N:130:CYS:SG	1:P:631:LEU:HD22	2.50	0.51
2:O:12:PRO:CG	2:O:83:LEU:HD21	2.38	0.51
1:P:528:LEU:HD11	1:P:575:LEU:HD21	1.92	0.51
2:Q:515:TRP:CH2	2:Q:522:SER:HB2	2.46	0.51
2:Q:599:CYS:HB2	2:Q:604:LEU:HD23	1.92	0.51
2:S:50:ASP:O	2:S:52:SER:N	2.44	0.51
2:T:167:TYR:OH	2:X:680:LYS:HE2	2.10	0.51
1:G:653:ARG:HH21	1:Y:643:HIS:HD2	1.57	0.51
1:B:596:PHE:HA	1:B:610:SER:OG	2.11	0.51
2:D:142:MET:HG2	2:D:221:VAL:HG21	1.92	0.51
2:D:85:LYS:HD3	2:D:86:ASP:N	2.26	0.51
2:D:139:LEU:CD2	2:E:639:LEU:HD22	2.33	0.51
1:G:640:LYS:O	1:G:644:LEU:HB2	2.10	0.51
2:H:96:SER:HB2	2:H:107:ARG:HB2	1.91	0.51
2:I:611:GLU:HG2	2:I:616:PRO:HA	1.92	0.51
2:I:632:SER:HB2	2:I:636:ILE:HB	1.92	0.51
2:L:94:THR:HG21	2:L:109:ARG:HB2	1.93	0.51
2:M:517:GLN:HE22	2:M:708:LYS:HZ1	1.58	0.51
1:P:501:MET:HA	1:P:524:TRP:O	2.10	0.51
1:N:140:LYS:HD2	1:P:641:ASN:ND2	2.25	0.51
2:S:30:THR:HG23	2:S:32:GLN:N	2.24	0.51
2:W:603:ALA:HA	2:W:624:MET:CA	2.29	0.51
2:X:652:GLU:O	2:X:655:THR:HG22	2.11	0.51
1:Y:506:SER:HB3	1:Y:576:SER:HB2	1.93	0.51
1:Y:618:ASN:OD1	1:Y:621:GLU:HB3	2.10	0.51
1:B:503:ARG:HH22	1:B:625:GLU:HG2	1.75	0.51
2:E:537:LEU:HD12	2:E:538:VAL:N	2.26	0.51
2:H:164:ILE:CG1	2:I:664:ILE:HG22	2.41	0.51
2:H:175:ILE:HG13	2:I:670:SER:HB2	1.91	0.51
1:J:56:ALA:HB1	1:J:63:LYS:HA	1.91	0.51
2:L:129:SER:CB	2:M:542:GLN:HE22	2.24	0.51
1:N:124:ARG:CZ	1:P:516:ILE:HG21	2.41	0.51
1:N:153:ARG:HG3	1:N:154:ASP:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:202:CYS:CA	2:Q:645:ALA:HB2	2.40	0.51
1:P:589:SER:CB	1:P:592:SER:HB3	2.41	0.51
1:R:39:GLY:C	1:V:623:ILE:HD12	2.31	0.51
2:X:549:VAL:HG11	2:X:553:VAL:HB	1.93	0.51
2:X:545:TRP:CA	2:X:626:ALA:HB2	2.41	0.51
2:X:688:SER:HA	2:X:691:GLU:CG	2.41	0.51
1:Y:648:ASN:O	1:Y:652:LEU:HB2	2.11	0.51
1:A:5:ILE:HA	1:A:20:LEU:O	2.11	0.51
2:D:146:LEU:CD2	2:E:646:LEU:HD23	2.41	0.51
2:E:541:LEU:HD11	2:E:707:GLY:N	2.26	0.51
2:H:175:ILE:HG13	2:I:670:SER:CB	2.40	0.51
2:H:10:MET:CE	2:H:223:THR:HG22	2.41	0.51
2:I:507:GLY:HA3	2:I:528:PHE:CE2	2.46	0.51
2:I:525:ALA:HB2	2:I:538:VAL:HG12	1.93	0.51
1:K:504:LYS:HB3	1:K:575:LEU:HD22	1.93	0.51
2:M:664:ILE:HG13	2:M:665:GLN:HG3	1.92	0.51
1:R:150:ARG:HH11	1:R:151:LEU:HG	1.75	0.51
1:U:1:MET:HG2	1:U:25:GLU:HA	1.91	0.51
2:E:699:PRO:C	2:E:701:ALA:H	2.14	0.50
1:F:37:THR:OG1	1:F:38:ASP:N	2.44	0.50
2:H:106:LEU:HB3	2:H:121:PHE:HB2	1.93	0.50
2:H:71:ALA:HA	2:H:74:CYS:SG	2.51	0.50
2:M:540:ASP:C	2:M:542:GLN:H	2.15	0.50
2:L:132:SER:HB2	2:M:541:LEU:O	2.11	0.50
2:M:547:GLU:HB2	2:M:623:CYS:HA	1.92	0.50
2:L:157:LEU:HD11	2:M:656:LEU:HD23	1.93	0.50
1:F:107:ARG:HD2	2:S:50:ASP:OD2	2.11	0.50
1:U:59:MET:HB2	1:U:61:MET:HG3	1.93	0.50
2:X:530:THR:HG23	2:X:532:GLN:N	2.20	0.50
2:X:606:LEU:O	2:X:621:PHE:HB2	2.11	0.50
2:D:157:LEU:HG	2:E:657:LEU:HG	1.92	0.50
1:G:530:SER:HA	1:G:549:GLU:HB2	1.93	0.50
1:G:579:GLY:HA3	1:G:582:ASP:HB2	1.93	0.50
2:I:717:LEU:HG	2:I:721:VAL:CG2	2.42	0.50
2:L:182:GLU:OE1	2:L:183:PRO:HD2	2.11	0.50
2:M:532:GLN:NE2	1:N:89:SER:HB3	2.26	0.50
2:M:630:LEU:HD22	2:M:634:HIS:CD2	2.46	0.50
1:N:123:ILE:O	1:N:127:ILE:HG13	2.12	0.50
2:O:68:PRO:HB3	2:O:69:PRO:HD2	1.93	0.50
1:P:589:SER:HB3	1:P:592:SER:HB3	1.93	0.50
2:L:100:VAL:CG1	2:Q:600:VAL:HB	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:146:LEU:HA	2:S:149:GLN:HB2	1.93	0.50
1:U:137:ASN:CB	1:Y:637:ASN:HD22	2.24	0.50
1:U:20:LEU:HA	1:U:35:THR:O	2.11	0.50
1:U:22:VAL:HG22	1:U:34:ILE:HD13	1.93	0.50
2:W:657:LEU:HD22	2:W:684:PHE:CB	2.41	0.50
2:X:503:GLU:HA	2:X:506:GLN:OE1	2.11	0.50
2:D:79:LEU:C	2:D:82:PRO:HD2	2.32	0.50
2:I:627:SER:O	2:I:631:VAL:HG23	2.11	0.50
1:J:98:GLU:HA	1:J:108:LEU:H	1.75	0.50
2:M:546:HIS:HE1	2:M:548:GLN:HB2	1.76	0.50
2:T:16:LEU:HD11	2:T:18:LEU:CG	2.39	0.50
1:V:503:ARG:HH21	1:V:521:GLN:HG3	1.76	0.50
2:W:532:GLN:O	2:W:532:GLN:HG3	2.11	0.50
2:E:516:LEU:HD23	2:E:522:SER:OG	2.11	0.50
2:H:24:LEU:CD2	2:H:207:GLY:HA3	2.41	0.50
2:I:653:LEU:O	2:I:657:LEU:HB2	2.12	0.50
2:I:512:PRO:HB2	2:I:715:GLN:CG	2.42	0.50
1:K:516:ILE:HD13	1:K:517:THR:H	1.76	0.50
2:L:17:GLN:HE21	2:L:92:GLU:HB2	1.77	0.50
2:L:56:GLN:O	2:L:60:GLU:HG3	2.11	0.50
2:O:27:VAL:HG22	2:O:28:PHE:N	2.27	0.50
2:T:115:LEU:H	2:T:115:LEU:HD22	1.76	0.50
2:T:160:LYS:HE3	2:X:664:ILE:HD12	1.94	0.50
2:W:518:LEU:HB2	2:W:521:ASN:O	2.11	0.50
1:A:107:ARG:HH11	2:E:564:ARG:NH1	2.10	0.50
2:I:551:THR:O	2:I:554:VAL:HB	2.10	0.50
2:L:209:PRO:CB	2:M:644:LEU:HD11	2.40	0.50
2:O:158:HIS:O	2:O:162:LEU:HG	2.10	0.50
1:R:39:GLY:O	1:V:623:ILE:HD12	2.12	0.50
2:T:175:ILE:HG12	2:X:667:TYR:OH	2.11	0.50
1:U:45:GLY:HA3	1:U:113:LEU:HA	1.92	0.50
1:U:127:ILE:CD1	1:Y:627:ILE:HG12	2.41	0.50
1:V:574:LEU:HD21	1:V:597:PHE:CE2	2.46	0.50
2:X:550:ASP:O	2:X:554:VAL:HG23	2.12	0.50
2:D:136:ILE:HD12	2:E:635:LEU:CD2	2.34	0.50
2:D:13:TRP:H	2:D:215:GLN:HE21	1.57	0.50
2:D:167:TYR:CD1	2:E:675:ILE:HG21	2.46	0.50
2:D:214:LEU:HD11	2:E:644:LEU:HD12	1.93	0.50
2:E:579:LEU:HD13	2:E:610:SER:OG	2.11	0.50
1:G:641:ASN:O	1:G:645:GLN:HB2	2.11	0.50
2:H:147:GLN:HA	2:H:147:GLN:HE21	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:55:SER:OG	2:H:69:PRO:HG3	2.11	0.50
1:J:13:GLU:OE2	1:J:16:ILE:HD13	2.11	0.50
2:M:665:GLN:HA	2:M:668:GLN:CD	2.31	0.50
1:N:5:ILE:O	1:N:6:SER:HB2	2.11	0.50
2:S:137:ARG:CB	2:S:138:PRO:HD3	2.42	0.50
1:U:21:GLN:OE1	1:U:126:LEU:HB2	2.12	0.50
1:V:565:LYS:HE2	1:V:565:LYS:C	2.32	0.50
1:Y:569:GLU:OE2	1:Y:599:LYS:HD2	2.11	0.50
2:D:132:SER:OG	2:E:542:GLN:HA	2.12	0.50
1:F:17:THR:HG22	1:F:18:HIS:N	2.26	0.50
2:I:533:GLY:HA2	2:I:573:LEU:HD11	1.93	0.50
2:I:579:LEU:HD22	2:I:610:SER:OG	2.12	0.50
2:L:132:SER:HA	2:L:136:ILE:CB	2.35	0.50
2:O:134:HIS:O	2:O:135:LEU:HD22	2.12	0.50
2:O:154:ALA:HB1	2:O:184:PHE:HE2	1.77	0.50
2:Q:520:GLU:CD	2:Q:520:GLU:H	2.15	0.50
1:R:72:LYS:HA	1:R:77:GLY:N	2.24	0.50
2:T:159:MET:SD	2:X:681:THR:HG22	2.52	0.50
2:T:29:ILE:HD13	2:T:77:ASP:OD1	2.11	0.50
2:H:57:ARG:HH22	2:H:122:HIS:HB2	1.76	0.50
2:I:637:ARG:HB3	2:I:637:ARG:CZ	2.42	0.50
1:K:521:GLN:H	1:K:535:THR:HB	1.77	0.50
2:T:93:ALA:HB3	2:T:109:ARG:O	2.12	0.50
2:D:136:ILE:CD1	2:E:635:LEU:HB3	2.41	0.50
2:H:115:LEU:N	2:H:115:LEU:HD22	2.27	0.50
2:H:164:ILE:HD13	2:I:663:GLU:OE1	2.12	0.50
2:I:545:TRP:CD2	2:I:604:LEU:HD13	2.46	0.50
2:I:552:SER:OG	2:S:103:ALA:HB2	2.12	0.50
1:J:88:PHE:HB2	1:J:95:PHE:HD1	1.76	0.50
1:K:598:GLU:HG2	1:K:607:ARG:HD3	1.93	0.50
2:L:202:CYS:SG	2:M:721:VAL:HG13	2.52	0.50
2:Q:547:GLU:HB2	2:Q:623:CYS:SG	2.52	0.50
1:R:59:MET:CE	2:W:564:ARG:HE	2.25	0.50
2:S:161:ASP:OD2	2:W:660:LYS:HE2	2.12	0.50
2:T:117:PHE:HD1	2:T:118:TYR:H	1.58	0.50
2:W:575:HIS:O	2:W:579:LEU:HG	2.12	0.50
1:A:23:SER:O	1:A:32:PHE:HB2	2.12	0.49
1:A:19:PHE:O	1:A:36:LEU:HD12	2.12	0.49
2:E:504:LEU:HG	2:E:535:ALA:HB2	1.94	0.49
1:J:127:ILE:O	1:J:131:LEU:HG	2.12	0.49
1:J:25:GLU:HG3	1:J:26:LYS:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:561:MET:CE	1:K:565:LYS:HB3	2.42	0.49
1:K:510:LEU:HD11	1:K:588:PHE:CD2	2.47	0.49
1:K:584:TYR:HE1	1:K:599:LYS:HG3	1.77	0.49
2:M:515:TRP:CZ2	2:M:524:LEU:HB2	2.47	0.49
1:N:124:ARG:NE	1:P:516:ILE:HG12	2.27	0.49
2:Q:511:GLN:O	2:Q:526:LYS:HE3	2.12	0.49
1:N:107:ARG:HB3	2:Q:564:ARG:O	2.12	0.49
2:S:164:ILE:HG22	2:S:165:GLN:N	2.26	0.49
2:S:63:LYS:N	2:S:64:ARG:HH11	2.06	0.49
2:T:185:GLU:C	2:T:187:ASN:H	2.15	0.49
1:V:602:LYS:O	1:V:603:ASP:HB2	2.12	0.49
2:W:711:VAL:O	2:W:715:GLN:HG2	2.12	0.49
1:Y:581:ALA:C	1:Y:583:VAL:H	2.15	0.49
2:E:676:ARG:CZ	2:E:678:ARG:HG3	2.42	0.49
1:F:152:LEU:HB2	1:G:651:LEU:HD22	1.95	0.49
1:F:59:MET:O	1:F:60:ALA:HB3	2.10	0.49
1:F:86:PHE:CD2	1:F:97:PHE:HB3	2.47	0.49
1:J:88:PHE:CD1	1:J:95:PHE:HB2	2.47	0.49
1:K:503:ARG:HA	1:K:522:VAL:O	2.12	0.49
2:T:23:LEU:N	2:T:23:LEU:HD23	2.27	0.49
2:W:676:ARG:CB	2:W:676:ARG:HH11	2.25	0.49
2:W:704:ILE:HG22	2:W:705:GLY:O	2.12	0.49
2:X:540:ASP:O	2:X:542:GLN:HG2	2.12	0.49
1:B:604:VAL:HG12	1:B:605:SER:N	2.26	0.49
2:D:137:ARG:HD3	2:E:541:LEU:O	2.11	0.49
2:D:80:LEU:HB3	2:D:81:ARG:NE	2.28	0.49
1:F:108:LEU:H	1:F:108:LEU:HD12	1.77	0.49
1:F:13:GLU:HB2	1:F:18:HIS:NE2	2.28	0.49
1:F:35:THR:HA	1:F:43:TRP:O	2.12	0.49
1:G:563:LYS:O	1:G:567:VAL:HG12	2.12	0.49
1:G:650:ARG:HE	1:G:651:LEU:HD23	1.77	0.49
1:K:566:TYR:CE1	1:K:608:LEU:HD11	2.43	0.49
1:N:89:SER:HB2	1:N:92:SER:HB3	1.94	0.49
2:S:34:TYR:OH	2:S:119:TRP:HZ2	1.95	0.49
1:U:66:TYR:OH	1:U:109:GLY:HA3	2.12	0.49
1:V:561:MET:HB3	1:V:565:LYS:HZ2	1.76	0.49
2:W:633:GLN:HE21	2:W:726:HIS:CD2	2.29	0.49
2:X:602:ASP:HB2	2:X:625:LEU:HB2	1.93	0.49
2:X:653:LEU:O	2:X:657:LEU:HB2	2.13	0.49
2:D:77:ASP:O	2:D:79:LEU:N	2.44	0.49
2:D:96:SER:HB3	2:D:107:ARG:CG	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:163:GLU:OE1	2:E:680:LYS:HD2	2.12	0.49
2:E:513:TRP:H	2:E:715:GLN:NE2	2.11	0.49
1:P:530:SER:HA	1:P:549:GLU:CG	2.38	0.49
2:Q:675:ILE:HD11	2:Q:680:LYS:HB2	1.93	0.49
2:S:64:ARG:H	2:S:64:ARG:CD	2.19	0.49
2:T:98:ASP:HB2	2:T:105:ILE:N	2.27	0.49
2:T:132:SER:O	2:T:138:PRO:HD2	2.11	0.49
2:T:32:GLN:HB3	2:T:51:THR:CG2	2.42	0.49
2:T:50:ASP:O	2:T:54:VAL:HB	2.12	0.49
1:U:112:ASN:ND2	1:U:112:ASN:C	2.64	0.49
1:U:3:ARG:HD2	1:U:129:TYR:CD2	2.47	0.49
1:U:20:LEU:HD21	1:U:95:PHE:CZ	2.48	0.49
2:W:589:HIS:CB	2:W:590:PRO:HD2	2.42	0.49
2:D:3:GLU:HG2	2:D:32:GLN:HE22	1.77	0.49
1:F:3:ARG:HH11	1:F:3:ARG:HG2	1.77	0.49
1:F:74:LEU:O	1:F:75:LEU:HD12	2.11	0.49
1:F:8:ILE:HG21	1:F:86:PHE:HB2	1.95	0.49
2:H:112:LEU:HD13	2:H:117:PHE:CD2	2.47	0.49
2:L:18:LEU:HB2	2:L:21:ASN:O	2.13	0.49
2:M:606:LEU:O	2:M:608:VAL:N	2.46	0.49
1:U:2:GLU:N	1:U:24:TRP:O	2.46	0.49
1:U:92:SER:O	1:U:93:CYS:HB2	2.12	0.49
2:W:538:VAL:HG22	2:W:539:SER:N	2.24	0.49
2:W:604:LEU:N	2:W:623:CYS:O	2.43	0.49
2:X:527:VAL:HG22	2:X:536:LEU:HD12	1.94	0.49
2:X:711:VAL:O	2:X:715:GLN:HG2	2.12	0.49
2:D:44:VAL:HG21	2:D:131:VAL:HG23	1.95	0.49
2:E:529:ILE:HG13	2:E:534:TYR:HB3	1.93	0.49
2:E:676:ARG:O	2:E:677:ASP:HB2	2.12	0.49
2:D:140:MET:HG3	2:E:710:PHE:HD2	1.78	0.49
2:H:139:LEU:HD21	2:I:640:MET:HA	1.95	0.49
2:I:637:ARG:HB2	2:I:638:PRO:CD	2.43	0.49
1:K:503:ARG:HD3	1:K:521:GLN:OE1	2.12	0.49
1:K:543:TRP:CD1	1:K:615:LYS:HB2	2.48	0.49
1:R:91:GLU:C	1:R:93:CYS:H	2.16	0.49
2:T:160:LYS:O	2:T:164:ILE:HG23	2.13	0.49
2:T:217:LEU:O	2:T:221:VAL:HG23	2.12	0.49
2:D:169:GLU:C	2:D:171:GLY:H	2.16	0.49
2:D:45:TRP:CD1	2:D:125:LEU:HA	2.48	0.49
2:E:530:THR:O	2:E:573:LEU:HD13	2.12	0.49
2:H:127:SER:O	2:H:130:LEU:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:675:ILE:N	2:I:675:ILE:HD13	2.28	0.49
2:L:36:LEU:HD12	2:L:37:LEU:H	1.78	0.49
2:M:641:GLY:O	2:M:645:ALA:HB2	2.13	0.49
2:L:179:LEU:HD21	2:M:662:LEU:HB2	1.94	0.49
2:M:708:LYS:N	2:M:709:PRO:HD2	2.28	0.49
1:N:112:ASN:O	1:N:113:LEU:HD13	2.12	0.49
2:O:204:ILE:O	2:O:209:PRO:HG2	2.13	0.49
2:W:527:VAL:HG22	2:W:528:PHE:N	2.28	0.49
2:T:204:ILE:HD12	2:X:640:MET:SD	2.53	0.49
1:Y:507:ARG:HG2	1:Y:508:ILE:N	2.28	0.49
1:A:7:ARG:HB3	1:A:7:ARG:NH1	2.25	0.49
2:D:4:LEU:HD11	2:D:33:GLY:O	2.13	0.49
1:F:42:ALA:HB3	1:F:116:VAL:CG2	2.38	0.49
1:F:80:PRO:HG2	1:F:81:ALA:H	1.78	0.49
2:H:32:GLN:HA	2:H:51:THR:CG2	2.43	0.49
1:B:604:VAL:HG22	2:H:68:PRO:HD2	1.95	0.49
1:K:571:ARG:HG3	1:K:572:LYS:N	2.28	0.49
2:M:547:GLU:HB2	2:M:623:CYS:CA	2.43	0.49
2:M:612:LEU:HB2	2:M:617:PHE:HD1	1.77	0.49
2:O:163:GLU:OE1	2:Q:680:LYS:HA	2.13	0.49
1:P:607:ARG:HG2	1:P:607:ARG:HH11	1.77	0.49
1:R:105:SER:O	2:W:565:LEU:HA	2.13	0.49
2:T:26:LYS:O	2:T:26:LYS:HG3	2.13	0.49
1:U:2:GLU:O	1:U:3:ARG:CB	2.60	0.49
2:W:523:LEU:HD11	2:W:597:CYS:SG	2.53	0.49
2:T:139:LEU:HD11	2:X:640:MET:HB2	1.95	0.49
2:X:697:LYS:O	2:X:700:GLU:HG3	2.13	0.49
2:X:510:MET:O	2:X:719:MET:HB3	2.12	0.49
1:Y:503:ARG:HB3	1:Y:521:GLN:NE2	2.27	0.49
1:Y:504:LYS:HZ1	1:Y:505:ILE:H	1.60	0.49
1:Y:505:ILE:HD12	1:Y:626:LEU:HD11	1.93	0.49
2:E:614:GLY:O	2:E:616:PRO:HD3	2.11	0.49
1:J:35:THR:HA	1:J:43:TRP:O	2.12	0.49
1:K:518:HIS:HB3	1:K:536:LEU:CD1	2.43	0.49
2:L:151:ARG:HB2	2:L:151:ARG:HH11	1.76	0.49
2:M:503:GLU:HG3	2:M:504:LEU:N	2.28	0.49
2:M:617:PHE:CD2	2:M:617:PHE:C	2.86	0.49
2:O:207:GLY:O	2:O:210:PHE:HB3	2.13	0.49
2:Q:632:SER:HA	2:Q:636:ILE:CG1	2.43	0.49
2:S:62:ASN:ND2	2:S:64:ARG:HD3	2.28	0.49
1:U:19:PHE:O	1:U:36:LEU:HA	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:107:ARG:HG2	2:W:563:LYS:HE2	1.94	0.49
1:A:125:GLU:O	1:A:128:CYS:HB2	2.13	0.49
1:B:556:ALA:HB2	1:B:566:TYR:CD2	2.48	0.49
2:D:73:LEU:O	2:D:76:LEU:HB3	2.13	0.49
2:E:651:ARG:HH11	2:E:651:ARG:HG2	1.77	0.49
2:H:93:ALA:HB2	2:H:110:SER:HB2	1.94	0.49
2:H:17:GLN:HG2	2:H:17:GLN:O	2.13	0.49
2:L:145:ALA:HB2	2:M:702:CYS:HA	1.95	0.49
2:L:189:PHE:O	2:L:192:GLN:HG3	2.13	0.49
2:M:705:GLY:C	2:M:707:GLY:H	2.15	0.49
2:O:69:PRO:HG2	2:O:70:ALA:H	1.78	0.49
2:Q:549:VAL:HB	2:Q:553:VAL:HB	1.95	0.49
1:R:35:THR:HA	1:R:43:TRP:O	2.13	0.49
1:R:51:GLU:O	1:R:55:GLU:HG2	2.13	0.49
2:T:161:ASP:O	2:T:164:ILE:HG12	2.13	0.49
2:T:161:ASP:OD1	2:T:183:PRO:HA	2.13	0.49
1:U:107:ARG:O	1:U:109:GLY:N	2.46	0.49
1:R:141:ASN:HD22	1:V:640:LYS:HB3	1.78	0.49
2:S:175:ILE:HG13	2:W:670:SER:HB2	1.95	0.49
1:A:20:LEU:HD13	1:A:21:GLN:N	2.28	0.48
2:E:676:ARG:NH2	2:E:678:ARG:HG3	2.27	0.48
2:H:25:ALA:CB	2:H:38:VAL:HG22	2.43	0.48
1:K:508:ILE:N	1:K:508:ILE:HD13	2.28	0.48
2:M:635:LEU:O	2:M:638:PRO:HG2	2.13	0.48
1:N:42:ALA:O	1:N:43:TRP:CB	2.61	0.48
2:Q:557:ARG:HG2	2:Q:561:LEU:HD23	1.95	0.48
2:Q:685:GLU:HB3	2:Q:688:SER:OG	2.12	0.48
2:S:132:SER:O	2:S:137:ARG:HD3	2.13	0.48
2:T:143:SER:OG	2:X:639:LEU:HD23	2.13	0.48
2:T:1:MET:H2	2:T:4:LEU:HD12	1.76	0.48
1:A:20:LEU:HD22	1:A:21:GLN:N	2.27	0.48
1:A:36:LEU:HD12	1:A:37:THR:H	1.78	0.48
2:D:193:PHE:CG	2:E:649:GLN:NE2	2.81	0.48
2:H:8:LEU:HD13	2:H:35:ALA:O	2.12	0.48
1:J:86:PHE:HD2	1:J:95:PHE:HZ	1.60	0.48
1:N:22:VAL:HG22	1:N:34:ILE:HD13	1.95	0.48
1:N:84:TYR:CE1	1:N:99:LYS:HG3	2.49	0.48
1:P:581:ALA:C	1:P:583:VAL:H	2.17	0.48
2:T:191:GLU:O	2:T:195:ILE:HD13	2.13	0.48
2:X:563:LYS:HD2	2:X:563:LYS:N	2.27	0.48
2:X:658:HIS:O	2:X:662:LEU:HG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:553:SER:OG	1:Y:563:LYS:HE2	2.13	0.48
1:A:5:ILE:HG22	1:A:6:SER:N	2.27	0.48
1:G:528:LEU:CD2	1:G:571:ARG:HH22	2.25	0.48
1:K:552:ILE:O	1:K:552:ILE:HD13	2.13	0.48
1:K:510:LEU:HD11	1:K:588:PHE:HD2	1.77	0.48
2:L:171:GLY:O	2:L:172:ALA:HB3	2.13	0.48
2:L:211:VAL:HG23	2:L:212:MET:N	2.28	0.48
1:N:69:GLU:OE1	1:N:99:LYS:HD2	2.13	0.48
2:T:46:HIS:HB3	2:T:126:ALA:HB2	1.94	0.48
1:A:83:VAL:HG12	1:A:84:TYR:H	1.78	0.48
1:A:88:PHE:CZ	1:A:93:CYS:HA	2.48	0.48
2:D:141:GLY:HA2	2:E:704:ILE:HD11	1.94	0.48
1:G:587:ASN:HB3	1:G:596:PHE:CE2	2.48	0.48
2:I:524:LEU:O	2:I:538:VAL:HA	2.14	0.48
2:I:617:PHE:HD1	2:I:618:TYR:N	2.12	0.48
1:J:135:ALA:O	1:J:138:GLN:HB2	2.14	0.48
1:K:536:LEU:HB3	1:K:543:TRP:HB2	1.95	0.48
2:L:16:LEU:HD23	2:L:16:LEU:N	2.29	0.48
2:L:194:MET:C	2:L:195:ILE:HD12	2.33	0.48
2:L:36:LEU:CG	2:L:37:LEU:N	2.76	0.48
2:O:195:ILE:N	2:O:195:ILE:HD13	2.29	0.48
2:S:176:ARG:HB2	2:S:179:LEU:HB2	1.95	0.48
2:E:581:ARG:HG2	2:E:585:LYS:HE3	1.96	0.48
1:F:42:ALA:O	1:F:116:VAL:HB	2.13	0.48
1:F:19:PHE:O	1:F:36:LEU:HD12	2.13	0.48
1:G:553:SER:HA	1:G:563:LYS:HE2	1.96	0.48
2:H:209:PRO:HB2	2:I:644:LEU:HD13	1.94	0.48
2:H:174:LEU:HD11	2:I:666:ASP:HB3	1.96	0.48
2:M:501:MET:HG3	2:M:502:GLU:N	2.28	0.48
2:M:513:TRP:HB2	2:M:711:VAL:HG12	1.95	0.48
2:S:157:LEU:HG	2:W:657:LEU:HG	1.95	0.48
2:W:676:ARG:O	2:W:678:ARG:HG3	2.13	0.48
2:W:678:ARG:O	2:W:679:LEU:HD23	2.13	0.48
1:Y:543:TRP:O	1:Y:613:LEU:HD22	2.14	0.48
1:A:20:LEU:HD22	1:A:35:THR:O	2.13	0.48
1:B:511:VAL:O	1:B:514:PRO:HD3	2.14	0.48
1:B:585:THR:HG22	1:B:598:GLU:HG2	1.96	0.48
2:H:126:ALA:HB1	2:H:130:LEU:HD23	1.94	0.48
2:H:154:ALA:HB2	2:I:653:LEU:CD1	2.43	0.48
2:H:82:PRO:HG2	2:H:83:LEU:HD13	1.94	0.48
2:O:165:GLN:O	2:O:169:GLU:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:1:MET:HA	2:S:4:LEU:HG	1.94	0.48
2:S:57:ARG:O	2:S:61:LEU:HG	2.13	0.48
2:T:202:CYS:CA	2:X:645:ALA:HB2	2.43	0.48
2:T:175:ILE:HG22	2:X:666:ASP:CG	2.34	0.48
1:A:72:LYS:HB3	1:A:84:TYR:CZ	2.49	0.48
1:A:8:ILE:HG21	1:A:86:PHE:CD1	2.48	0.48
1:B:631:LEU:O	1:B:635:ALA:HB3	2.13	0.48
2:D:181:THR:OG1	2:E:660:LYS:HE2	2.12	0.48
1:G:583:VAL:CG2	1:G:600:ASN:HB3	2.43	0.48
1:B:601:LEU:HD22	2:H:113:SER:HB2	1.95	0.48
2:I:512:PRO:HD3	2:I:719:MET:SD	2.53	0.48
1:J:47:VAL:HA	1:J:51:GLU:OE1	2.13	0.48
1:K:510:LEU:CD2	1:K:588:PHE:HB3	2.43	0.48
2:Q:508:LEU:HD13	2:Q:535:ALA:O	2.14	0.48
1:R:31:GLY:N	1:R:52:ILE:HD11	2.28	0.48
2:S:10:MET:CE	2:S:223:THR:HG22	2.44	0.48
2:X:569:PRO:O	2:X:571:ALA:N	2.38	0.48
1:B:518:HIS:HD2	1:B:536:LEU:HD11	1.78	0.48
1:B:537:THR:OG1	1:B:538:ASP:N	2.46	0.48
1:B:638:GLN:HA	1:B:641:ASN:HB3	1.96	0.48
2:D:189:PHE:O	2:D:192:GLN:HG3	2.13	0.48
2:D:80:LEU:HD23	2:D:85:LYS:HB3	1.96	0.48
2:E:688:SER:HA	2:E:691:GLU:OE2	2.13	0.48
1:F:62:GLU:HG2	1:F:63:LYS:N	2.28	0.48
2:H:192:GLN:HB2	2:H:196:GLU:OE2	2.14	0.48
2:I:545:TRP:NE1	2:I:625:LEU:HD12	2.28	0.48
1:K:519:PHE:O	1:K:536:LEU:HA	2.14	0.48
2:L:181:THR:HG22	2:M:663:GLU:OE1	2.13	0.48
2:L:188:SER:HA	2:L:191:GLU:OE1	2.14	0.48
2:L:210:PHE:HB2	2:M:640:MET:HE3	1.96	0.48
1:N:36:LEU:CG	1:N:37:THR:H	2.26	0.48
2:Q:526:LYS:NZ	2:Q:718:TYR:OH	2.47	0.48
1:V:579:GLY:HA3	1:V:581:ALA:H	1.78	0.48
1:V:583:VAL:HG12	1:V:584:TYR:H	1.79	0.48
1:Y:507:ARG:O	1:Y:508:ILE:HG23	2.14	0.48
1:A:99:LYS:HG3	1:A:108:LEU:HD12	1.96	0.48
1:B:650:ARG:NH1	1:B:651:LEU:HA	2.29	0.48
2:D:153:LEU:HD13	2:E:653:LEU:CB	2.43	0.48
2:E:688:SER:O	2:E:691:GLU:HG2	2.14	0.48
2:E:514:ALA:C	2:E:711:VAL:HG11	2.34	0.48
2:L:214:LEU:C	2:L:214:LEU:HD23	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:80:LEU:CB	2:L:83:LEU:HB2	2.44	0.48
2:M:504:LEU:HD11	2:M:534:TYR:N	2.29	0.48
2:M:518:LEU:CD1	2:M:523:LEU:HD22	2.43	0.48
2:M:527:VAL:HG22	2:M:528:PHE:H	1.78	0.48
2:O:144:LEU:HD23	2:O:144:LEU:O	2.14	0.48
1:R:126:LEU:HD23	1:V:627:ILE:HG12	1.96	0.48
2:T:1:MET:H1	2:T:4:LEU:HD12	1.77	0.48
1:V:563:LYS:HB3	1:V:563:LYS:NZ	2.27	0.48
1:V:619:PRO:O	1:V:623:ILE:HG12	2.14	0.48
2:D:4:LEU:HB3	2:D:35:ALA:CB	2.41	0.48
2:D:167:TYR:HB3	2:E:667:TYR:HD2	1.79	0.48
1:G:621:GLU:HA	1:G:624:ARG:NH1	2.28	0.48
2:H:9:LEU:HD21	2:H:133:GLN:O	2.14	0.48
2:H:163:GLU:OE1	2:I:664:ILE:HD13	2.14	0.48
2:I:600:VAL:O	2:I:601:ALA:HB3	2.14	0.48
1:N:127:ILE:HD11	1:P:623:ILE:HD11	1.96	0.48
2:Q:602:ASP:HB3	2:Q:603:ALA:H	1.43	0.48
2:Q:674:LEU:N	2:Q:674:LEU:HD12	2.28	0.48
2:S:57:ARG:CD	2:S:61:LEU:HD11	2.44	0.48
2:S:139:LEU:HD22	2:W:639:LEU:HD12	1.96	0.48
2:X:583:LEU:HD23	2:X:583:LEU:O	2.14	0.48
2:T:145:ALA:HB2	2:X:702:CYS:N	2.28	0.48
1:F:41:SER:HA	1:F:119:PRO:HB3	1.94	0.47
2:H:153:LEU:HD12	2:I:689:PHE:CE2	2.49	0.47
2:I:695:ILE:N	2:I:695:ILE:HD12	2.28	0.47
2:L:198:LEU:HD21	2:M:720:ALA:O	2.13	0.47
2:L:38:VAL:O	2:L:39:SER:CB	2.60	0.47
2:M:635:LEU:O	2:M:639:LEU:HB2	2.14	0.47
2:M:656:LEU:HD12	2:M:659:MET:HE3	1.95	0.47
2:W:665:GLN:HG2	2:W:668:GLN:HE21	1.79	0.47
2:S:175:ILE:HG13	2:W:670:SER:CB	2.44	0.47
2:T:145:ALA:HB2	2:X:702:CYS:CA	2.44	0.47
2:D:15:TRP:HE1	2:D:22:SER:HG	1.60	0.47
2:D:217:LEU:O	2:D:218:TYR:C	2.52	0.47
1:F:3:ARG:O	1:F:4:LYS:HG2	2.13	0.47
1:J:145:GLN:O	1:J:149:GLU:HG3	2.14	0.47
1:J:34:ILE:HD12	1:J:35:THR:H	1.79	0.47
2:S:62:ASN:HD22	2:S:64:ARG:HD3	1.78	0.47
2:S:68:PRO:HG2	2:S:71:ALA:CB	2.43	0.47
2:W:634:HIS:O	2:W:635:LEU:HD12	2.14	0.47
2:X:605:ILE:HA	2:X:621:PHE:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:534:ILE:HD13	1:B:613:LEU:HD11	1.97	0.47
2:D:149:GLN:O	2:D:153:LEU:HG	2.15	0.47
2:D:65:LEU:HD13	2:D:66:THR:N	2.30	0.47
1:F:144:LEU:O	1:F:148:ASN:HB2	2.15	0.47
2:I:504:LEU:HD21	2:I:534:TYR:O	2.15	0.47
1:J:43:TRP:HB3	1:J:113:LEU:HG	1.96	0.47
1:K:508:ILE:H	1:K:508:ILE:HD13	1.78	0.47
2:L:6:GLN:HE21	2:L:6:GLN:HA	1.79	0.47
2:L:29:ILE:HB	2:L:77:ASP:HB2	1.96	0.47
2:M:509:LEU:HD11	2:M:633:GLN:O	2.14	0.47
1:N:107:ARG:HG2	1:N:108:LEU:N	2.29	0.47
1:N:120:ALA:HB1	1:N:124:ARG:CZ	2.44	0.47
1:N:144:LEU:HD22	1:P:644:LEU:HD23	1.96	0.47
2:T:24:LEU:HD21	2:T:207:GLY:CA	2.44	0.47
2:T:36:LEU:HG	2:T:37:LEU:N	2.28	0.47
1:V:562:GLU:HB2	1:V:565:LYS:HB3	1.96	0.47
2:X:675:ILE:HD12	2:X:675:ILE:N	2.29	0.47
2:X:707:GLY:O	2:X:710:PHE:HB3	2.14	0.47
1:Y:502:GLU:HB3	1:Y:524:TRP:CZ2	2.49	0.47
1:Y:588:PHE:CD1	1:Y:595:PHE:HB2	2.49	0.47
2:D:214:LEU:CD1	2:E:644:LEU:HD12	2.44	0.47
2:E:651:ARG:HG2	2:E:651:ARG:NH1	2.29	0.47
2:I:544:VAL:HB	2:I:626:ALA:HB3	1.95	0.47
2:I:651:ARG:NH1	2:I:651:ARG:HB3	2.30	0.47
2:L:18:LEU:CD2	2:L:97:CYS:HB3	2.44	0.47
2:M:661:ASP:OD1	2:M:683:PRO:HA	2.14	0.47
2:L:179:LEU:HD11	2:M:662:LEU:HB3	1.96	0.47
2:L:140:MET:HE2	2:M:710:PHE:CD1	2.49	0.47
1:N:32:PHE:CE2	1:N:52:ILE:HD11	2.33	0.47
1:N:28:LEU:HD22	1:N:70:LEU:HD23	1.96	0.47
2:O:80:LEU:O	2:O:81:ARG:HB3	2.13	0.47
1:P:537:THR:OG1	1:P:538:ASP:N	2.47	0.47
2:Q:698:LEU:H	2:Q:699:PRO:CD	2.27	0.47
2:T:146:LEU:HD23	2:X:646:LEU:HD22	1.96	0.47
2:T:156:LEU:O	2:T:160:LYS:HB2	2.14	0.47
2:W:682:GLU:CD	2:W:683:PRO:HD2	2.35	0.47
2:X:609:ARG:C	2:X:609:ARG:HE	2.17	0.47
1:A:84:TYR:HB3	1:A:97:PHE:HE1	1.79	0.47
2:D:135:LEU:O	2:D:139:LEU:HB3	2.15	0.47
2:E:579:LEU:HD22	2:E:610:SER:CB	2.44	0.47
2:E:694:MET:HG2	2:E:694:MET:H	1.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:534:TYR:CE1	2:I:549:VAL:HB	2.49	0.47
2:I:632:SER:CB	2:I:636:ILE:HB	2.44	0.47
1:R:96:PHE:HB3	1:R:110:SER:OG	2.15	0.47
1:R:59:MET:CB	2:W:564:ARG:HG3	2.43	0.47
1:A:70:LEU:HD21	1:A:74:LEU:HD11	1.97	0.47
1:B:606:PHE:CD2	1:B:606:PHE:N	2.80	0.47
2:D:79:LEU:HD21	2:D:95:PHE:CZ	2.50	0.47
1:G:513:GLU:HB3	1:G:516:ILE:HD12	1.95	0.47
2:I:512:PRO:HB2	2:I:715:GLN:NE2	2.30	0.47
1:J:124:ARG:HE	1:K:516:ILE:HD11	1.80	0.47
2:L:138:PRO:O	2:L:142:MET:HG3	2.15	0.47
2:L:17:GLN:C	2:L:18:LEU:HD12	2.35	0.47
2:M:597:CYS:HA	2:M:605:ILE:O	2.15	0.47
1:P:601:LEU:HB2	1:P:604:VAL:CG2	2.43	0.47
2:T:142:MET:CE	2:T:214:LEU:HD22	2.44	0.47
2:T:42:GLN:HG3	2:T:43:GLN:N	2.30	0.47
1:V:567:VAL:O	1:V:571:ARG:HG2	2.14	0.47
2:W:508:LEU:HD11	2:W:526:LYS:O	2.15	0.47
2:W:526:LYS:HG3	2:W:526:LYS:O	2.14	0.47
2:W:537:LEU:HD22	2:W:634:HIS:ND1	2.30	0.47
2:W:639:LEU:HD22	2:W:642:MET:CE	2.44	0.47
2:X:533:GLY:H	2:X:573:LEU:CD1	2.28	0.47
2:X:652:GLU:HA	2:X:655:THR:HG22	1.96	0.47
1:B:535:THR:OG1	1:B:544:THR:HG23	2.14	0.47
2:D:11:GLN:O	2:D:26:LYS:HE2	2.15	0.47
2:E:605:ILE:HG22	2:E:622:HIS:HD2	1.80	0.47
1:F:20:LEU:C	1:F:20:LEU:HD23	2.34	0.47
2:H:44:VAL:HG21	2:H:131:VAL:HG22	1.97	0.47
2:I:552:SER:HB2	2:S:102:ASP:HB3	1.96	0.47
2:I:559:LYS:HA	2:I:559:LYS:NZ	2.29	0.47
1:J:3:ARG:HA	1:J:22:VAL:O	2.14	0.47
1:J:60:ALA:HB1	2:M:618:TYR:OH	2.14	0.47
2:L:59:LYS:O	2:L:63:LYS:HG2	2.14	0.47
2:M:556:GLN:HG3	2:M:557:ARG:N	2.29	0.47
2:M:578:ASN:O	2:M:582:PRO:HG2	2.15	0.47
2:O:29:ILE:HG12	2:O:34:TYR:CB	2.45	0.47
2:O:62:ASN:HB3	2:O:65:LEU:CB	2.43	0.47
1:P:509:HIS:O	1:P:586:PHE:HB2	2.15	0.47
2:S:137:ARG:HH12	2:W:541:LEU:HD13	1.79	0.47
1:U:28:LEU:HD12	1:U:71:ARG:HG2	1.95	0.47
1:V:518:HIS:CD2	1:V:536:LEU:HD11	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:652:LEU:HG	1:V:656:ASN:HD22	1.79	0.47
2:X:661:ASP:OD1	2:X:683:PRO:HA	2.14	0.47
1:B:616:VAL:HG11	1:B:622:VAL:HG21	1.96	0.47
2:D:165:GLN:HE21	2:D:168:GLN:HG3	1.78	0.47
1:F:13:GLU:HB3	1:F:16:ILE:HB	1.97	0.47
1:K:503:ARG:HD3	1:K:521:GLN:CD	2.35	0.47
2:O:13:TRP:O	2:O:83:LEU:HD23	2.14	0.47
2:O:36:LEU:HD11	2:O:38:VAL:HG23	1.95	0.47
2:Q:606:LEU:HB3	2:Q:621:PHE:HD2	1.78	0.47
1:U:127:ILE:HD12	1:Y:626:LEU:HD23	1.97	0.47
1:U:147:GLU:HG2	1:Y:648:ASN:OD1	2.15	0.47
1:A:22:VAL:CG1	1:A:34:ILE:HA	2.37	0.47
1:B:521:GLN:O	1:B:534:ILE:HA	2.14	0.47
2:D:79:LEU:O	2:D:79:LEU:HD22	2.15	0.47
1:F:143:HIS:CE1	1:F:147:GLU:HG3	2.50	0.47
2:H:25:ALA:HB1	2:H:38:VAL:HG22	1.96	0.47
1:J:147:GLU:O	1:J:150:ARG:HG3	2.15	0.47
1:K:574:LEU:HG	1:K:586:PHE:CZ	2.50	0.47
2:M:518:LEU:O	2:M:519:ALA:C	2.53	0.47
2:M:545:TRP:CG	2:M:604:LEU:HD22	2.50	0.47
1:J:107:ARG:O	2:M:564:ARG:HB3	2.14	0.47
2:M:661:ASP:HA	2:M:664:ILE:HG23	1.96	0.47
2:O:176:ARG:O	2:O:178:ARG:N	2.45	0.47
1:P:507:ARG:CZ	1:P:507:ARG:HB3	2.45	0.47
2:Q:511:GLN:C	2:Q:719:MET:HE3	2.35	0.47
2:S:105:ILE:HG12	2:S:107:ARG:NE	2.29	0.47
1:U:119:PRO:O	1:U:123:ILE:HG12	2.15	0.47
1:U:150:ARG:HG3	1:U:153:ARG:HH12	1.80	0.47
2:X:524:LEU:HD23	2:X:524:LEU:N	2.30	0.47
2:X:604:LEU:O	2:X:604:LEU:HD23	2.13	0.47
2:X:508:LEU:HG	2:X:634:HIS:CE1	2.49	0.47
2:D:36:LEU:CG	2:D:37:LEU:N	2.77	0.47
2:D:80:LEU:HB3	2:D:81:ARG:HH21	1.79	0.47
2:E:586:ASP:O	2:E:589:HIS:HB2	2.15	0.47
2:E:579:LEU:CD1	2:E:612:LEU:HD21	2.38	0.47
2:E:711:VAL:C	2:E:715:GLN:HB2	2.34	0.47
2:H:44:VAL:HG12	2:H:45:TRP:N	2.29	0.47
1:B:561:MET:HG3	2:H:64:ARG:HH22	1.80	0.47
2:I:557:ARG:CZ	2:I:622:HIS:ND1	2.78	0.47
2:I:577:ASP:HA	2:I:580:LEU:HB2	1.96	0.47
1:J:150:ARG:NH1	1:J:150:ARG:HB2	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:49:GLU:C	1:J:51:GLU:H	2.18	0.47
1:J:131:LEU:HD11	1:K:519:PHE:CE1	2.50	0.47
2:M:512:PRO:HB3	2:M:719:MET:CG	2.45	0.47
1:N:112:ASN:C	1:N:113:LEU:HD13	2.36	0.47
1:N:34:ILE:CD1	1:N:35:THR:H	2.23	0.47
2:O:1:MET:HB2	2:O:50:ASP:OD1	2.15	0.47
2:O:140:MET:HB3	2:Q:704:ILE:CD1	2.45	0.47
1:V:587:ASN:HD22	1:V:587:ASN:HA	1.56	0.47
1:A:131:LEU:HD11	1:B:505:ILE:HB	1.97	0.47
2:E:537:LEU:HD23	2:E:634:HIS:ND1	2.30	0.47
2:D:167:TYR:CD2	2:E:667:TYR:HB3	2.50	0.47
2:E:668:GLN:HG3	2:E:669:GLU:H	1.80	0.47
2:H:153:LEU:HD21	2:I:653:LEU:HB3	1.96	0.47
2:H:174:LEU:HD21	2:H:179:LEU:HB2	1.97	0.47
2:I:637:ARG:HB2	2:I:638:PRO:HD3	1.96	0.47
2:M:637:ARG:HG2	2:M:637:ARG:NH1	2.30	0.47
2:O:32:GLN:HA	2:O:51:THR:HG23	1.97	0.47
2:S:8:LEU:HD11	2:S:35:ALA:HB3	1.96	0.47
2:T:104:LEU:HB3	2:T:123:CYS:HB2	1.97	0.47
2:T:58:ALA:HA	2:T:62:ASN:ND2	2.30	0.47
1:V:585:THR:O	1:V:585:THR:HG23	2.14	0.47
2:W:675:ILE:O	2:W:676:ARG:HG3	2.15	0.47
2:W:686:GLU:O	2:W:690:LEU:HD23	2.14	0.47
2:W:642:MET:HG2	2:W:721:VAL:HG21	1.97	0.47
2:X:579:LEU:O	2:X:580:LEU:HB2	2.15	0.47
2:X:597:CYS:HB2	2:X:606:LEU:HD12	1.97	0.47
2:E:527:VAL:HG13	2:E:584:LEU:HD21	1.97	0.46
2:E:507:GLY:HA3	2:E:528:PHE:CE2	2.50	0.46
1:F:8:ILE:CG2	1:F:86:PHE:HB2	2.45	0.46
2:H:79:LEU:HD23	2:H:79:LEU:C	2.36	0.46
2:I:529:ILE:HG12	2:I:534:TYR:CB	2.45	0.46
2:I:619:TRP:C	2:I:620:ASN:HD22	2.18	0.46
2:I:657:LEU:HD13	2:I:684:PHE:CD1	2.50	0.46
1:K:619:PRO:O	1:K:623:ILE:HG22	2.15	0.46
2:L:38:VAL:O	2:L:39:SER:HB2	2.15	0.46
2:M:504:LEU:HD11	2:M:534:TYR:CA	2.45	0.46
2:M:579:LEU:C	2:M:582:PRO:HD2	2.34	0.46
2:Q:508:LEU:HD11	2:Q:537:LEU:CB	2.45	0.46
1:R:87:ASN:HB3	1:R:96:PHE:HE1	1.80	0.46
1:V:522:VAL:HB	1:V:575:LEU:CD2	2.45	0.46
2:D:102:ASP:O	2:D:125:LEU:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:210:PHE:HB2	2:E:640:MET:HE2	1.94	0.46
1:F:3:ARG:HD3	1:F:129:TYR:CZ	2.50	0.46
1:K:504:LYS:HB3	1:K:575:LEU:CD2	2.44	0.46
1:K:636:GLU:O	1:K:640:LYS:HG3	2.15	0.46
2:M:545:TRP:CE2	2:M:604:LEU:HD13	2.51	0.46
1:N:59:MET:HB3	2:Q:564:ARG:NH2	2.30	0.46
2:O:9:LEU:HD12	2:O:9:LEU:C	2.36	0.46
2:Q:586:ASP:C	2:Q:588:ALA:H	2.18	0.46
2:Q:637:ARG:N	2:Q:638:PRO:HD2	2.30	0.46
2:T:193:PHE:HD2	2:T:194:MET:SD	2.39	0.46
2:T:76:LEU:CD2	2:T:79:LEU:HD23	2.44	0.46
1:V:505:ILE:HD13	1:V:626:LEU:CD1	2.45	0.46
1:B:556:ALA:HB1	1:B:561:MET:O	2.16	0.46
1:G:508:ILE:HD11	1:G:586:PHE:HB2	1.97	0.46
2:H:83:LEU:CD2	2:H:84:LEU:H	2.28	0.46
2:M:674:LEU:HD23	2:M:675:ILE:HD12	1.97	0.46
1:N:127:ILE:HB	1:P:519:PHE:CE2	2.50	0.46
2:O:17:GLN:CD	2:O:17:GLN:H	2.18	0.46
2:O:30:THR:HG22	2:O:33:GLY:O	2.15	0.46
1:R:151:LEU:HB3	1:V:651:LEU:HD22	1.97	0.46
2:T:13:TRP:CZ3	2:T:26:LYS:HG2	2.51	0.46
1:U:59:MET:HB2	1:U:61:MET:SD	2.55	0.46
2:W:595:PHE:HA	2:W:607:ARG:O	2.15	0.46
1:Y:511:VAL:HG23	1:Y:586:PHE:O	2.16	0.46
1:B:557:ASP:N	1:B:557:ASP:OD2	2.48	0.46
1:B:626:LEU:O	1:B:630:CYS:HB3	2.15	0.46
2:E:668:GLN:HG3	2:E:669:GLU:N	2.31	0.46
1:F:144:LEU:CB	1:G:644:LEU:HD22	2.45	0.46
1:G:588:PHE:HB2	1:G:594:TYR:O	2.15	0.46
1:J:116:VAL:C	1:J:118:ASN:H	2.18	0.46
2:M:512:PRO:HD3	2:M:719:MET:SD	2.54	0.46
1:P:520:LEU:HD22	1:P:522:VAL:HG23	1.97	0.46
1:P:543:TRP:CZ2	1:P:615:LYS:HE2	2.50	0.46
1:V:588:PHE:CZ	1:V:593:CYS:HA	2.51	0.46
1:V:593:CYS:HB3	1:V:613:LEU:O	2.14	0.46
1:Y:521:GLN:O	1:Y:521:GLN:HG3	2.15	0.46
1:B:584:TYR:CE2	1:B:599:LYS:HD2	2.51	0.46
2:D:148:CYS:HA	2:D:151:ARG:HB3	1.97	0.46
2:D:157:LEU:HD13	2:D:184:PHE:CG	2.50	0.46
2:D:77:ASP:C	2:D:79:LEU:N	2.67	0.46
2:D:136:ILE:HD12	2:E:635:LEU:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:713:ASN:O	2:E:714:LEU:HB2	2.15	0.46
1:F:121:GLU:O	1:F:125:GLU:HB2	2.15	0.46
2:H:137:ARG:HB3	2:H:137:ARG:HE	1.51	0.46
2:L:79:LEU:HD22	2:L:110:SER:OG	2.15	0.46
2:O:136:ILE:HD11	2:Q:631:VAL:CG1	2.45	0.46
2:O:157:LEU:HD23	2:O:157:LEU:O	2.16	0.46
2:O:13:TRP:CE3	2:O:24:LEU:HB3	2.51	0.46
2:Q:508:LEU:HD11	2:Q:537:LEU:HB3	1.97	0.46
2:Q:565:LEU:HG	2:Q:566:THR:N	2.31	0.46
2:Q:579:LEU:O	2:Q:579:LEU:HD23	2.16	0.46
2:W:547:GLU:HG2	2:W:549:VAL:HG13	1.96	0.46
1:A:112:ASN:ND2	1:A:112:ASN:N	2.64	0.46
2:D:104:LEU:HD22	2:D:105:ILE:N	2.30	0.46
2:D:137:ARG:N	2:D:138:PRO:HD2	2.31	0.46
2:D:141:GLY:CA	2:E:704:ILE:HD11	2.46	0.46
2:E:707:GLY:C	2:E:709:PRO:HD2	2.36	0.46
2:H:133:GLN:O	2:H:138:PRO:HG2	2.16	0.46
2:H:175:ILE:HB	2:H:176:ARG:NH1	2.30	0.46
2:I:598:ASP:HB3	2:I:607:ARG:NH2	2.31	0.46
2:L:94:THR:CG2	2:L:109:ARG:HB2	2.44	0.46
2:O:181:THR:HG21	2:Q:660:LYS:HA	1.97	0.46
1:U:10:LEU:HD13	1:U:11:VAL:H	1.80	0.46
1:U:36:LEU:HB3	1:U:43:TRP:HB2	1.97	0.46
2:W:547:GLU:HB2	2:W:623:CYS:CB	2.27	0.46
2:W:674:LEU:H	2:W:674:LEU:HD12	1.80	0.46
2:X:516:LEU:HD13	2:X:595:PHE:CE2	2.50	0.46
2:X:524:LEU:HD11	2:X:541:LEU:HD21	1.96	0.46
1:U:124:ARG:HD3	1:Y:538:ASP:C	2.36	0.46
1:B:512:SER:O	1:B:513:GLU:HG3	2.15	0.46
2:E:550:ASP:O	2:E:554:VAL:HG23	2.16	0.46
2:I:673:THR:HG22	2:I:674:LEU:H	1.80	0.46
2:I:691:GLU:HG3	2:I:692:GLN:H	1.78	0.46
1:J:59:MET:HB3	2:M:564:ARG:CD	2.36	0.46
2:L:198:LEU:HG	2:L:202:CYS:SG	2.56	0.46
2:L:39:SER:HB2	2:L:44:VAL:HA	1.98	0.46
2:M:531:LYS:HZ3	2:M:531:LYS:HA	1.81	0.46
2:O:157:LEU:HD22	2:O:184:PHE:CD2	2.50	0.46
2:Q:517:GLN:HE21	2:Q:518:LEU:H	1.63	0.46
1:V:601:LEU:HB2	1:V:604:VAL:CG1	2.45	0.46
2:W:537:LEU:HD22	2:W:630:LEU:HD21	1.97	0.46
2:T:135:LEU:HB3	2:X:636:ILE:CD1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:685:GLU:CD	2:X:688:SER:HB3	2.35	0.46
1:Y:579:GLY:C	1:Y:581:ALA:H	2.18	0.46
1:A:133:THR:HA	1:A:136:GLU:HG2	1.96	0.46
2:D:14:ALA:O	2:D:24:LEU:HA	2.16	0.46
2:E:555:SER:HB3	2:E:569:PRO:HG2	1.98	0.46
2:E:674:LEU:HD12	2:E:674:LEU:N	2.31	0.46
1:F:36:LEU:HD12	1:F:37:THR:N	2.20	0.46
1:F:66:TYR:O	1:F:69:GLU:HB3	2.15	0.46
1:G:619:PRO:O	1:G:623:ILE:HG12	2.16	0.46
2:H:106:LEU:CB	2:H:121:PHE:HB2	2.46	0.46
2:M:554:VAL:HG21	2:M:573:LEU:HD21	1.97	0.46
2:O:24:LEU:O	2:O:38:VAL:HG13	2.16	0.46
2:O:29:ILE:CG2	2:O:73:LEU:HD22	2.46	0.46
2:Q:516:LEU:O	2:Q:518:LEU:HD22	2.15	0.46
1:R:137:ASN:HB3	1:V:637:ASN:ND2	2.31	0.46
2:S:10:MET:HE2	2:S:223:THR:HG22	1.97	0.46
2:T:137:ARG:HB3	2:T:138:PRO:HD3	1.97	0.46
2:T:81:ARG:N	2:T:82:PRO:CD	2.79	0.46
1:R:19:PHE:CE2	1:V:627:ILE:HB	2.50	0.46
2:W:530:THR:HG23	2:W:532:GLN:H	1.80	0.46
1:Y:519:PHE:O	1:Y:536:LEU:HD12	2.16	0.46
1:Y:645:GLN:OE1	1:Y:645:GLN:HA	2.16	0.46
1:A:55:GLU:OE2	1:A:109:GLY:HA2	2.15	0.46
1:A:74:LEU:C	1:A:75:LEU:HD22	2.37	0.46
2:D:10:MET:SD	2:D:223:THR:HG22	2.56	0.46
2:D:140:MET:HA	2:E:639:LEU:CD2	2.46	0.46
1:F:127:ILE:HD13	1:G:626:LEU:HD22	1.98	0.46
2:H:75:HIS:CE1	2:H:112:LEU:HD11	2.51	0.46
1:J:47:VAL:HG22	1:J:111:PHE:CE2	2.50	0.46
1:K:547:VAL:HG21	1:K:611:PHE:CZ	2.51	0.46
1:J:40:HIS:NE2	1:K:620:ALA:N	2.64	0.46
2:L:105:ILE:HD12	2:Q:601:ALA:HB2	1.98	0.46
2:M:634:HIS:C	2:M:638:PRO:HG3	2.36	0.46
2:O:34:TYR:HE1	2:O:47:GLU:HG2	1.81	0.46
1:P:594:TYR:HE1	1:P:611:PHE:N	2.14	0.46
2:O:135:LEU:CD1	2:Q:636:ILE:HG23	2.45	0.46
2:T:95:PHE:CE2	2:T:108:VAL:HG13	2.50	0.46
1:V:616:VAL:HG21	1:V:622:VAL:CG2	2.44	0.46
1:V:652:LEU:HG	1:V:656:ASN:ND2	2.30	0.46
2:W:698:LEU:H	2:W:699:PRO:HD2	1.80	0.46
2:D:24:LEU:HD21	2:D:206:ASP:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:36:LEU:CG	1:F:37:THR:N	2.79	0.46
2:H:65:LEU:HD11	2:H:67:ALA:HB2	1.98	0.46
2:I:586:ASP:CG	2:I:587:ALA:H	2.19	0.46
2:I:592:GLU:O	2:I:610:SER:HA	2.16	0.46
2:I:665:GLN:O	2:I:669:GLU:HG2	2.16	0.46
2:L:153:LEU:CD1	2:M:650:VAL:HA	2.46	0.46
2:M:711:VAL:CB	2:M:715:GLN:HG2	2.46	0.46
1:N:138:GLN:O	1:N:142:GLU:HG3	2.16	0.46
1:N:74:LEU:HD21	1:N:97:PHE:CE2	2.50	0.46
2:O:167:TYR:O	2:O:172:ALA:HB3	2.16	0.46
1:R:141:ASN:ND2	1:V:640:LYS:HB3	2.30	0.46
2:S:24:LEU:HD13	2:S:210:PHE:HD1	1.81	0.46
1:U:37:THR:CG2	1:U:123:ILE:HD13	2.46	0.46
1:U:97:PHE:N	1:U:97:PHE:CD1	2.84	0.46
2:W:511:GLN:HB2	2:W:511:GLN:HE21	1.55	0.46
2:W:515:TRP:NE1	2:W:707:GLY:HA3	2.30	0.46
2:T:153:LEU:CD1	2:X:650:VAL:HG13	2.46	0.46
2:T:162:LEU:C	2:X:679:LEU:HD21	2.37	0.46
2:E:530:THR:HG23	2:E:532:GLN:H	1.81	0.45
2:E:634:HIS:O	2:E:635:LEU:HD12	2.16	0.45
2:H:18:LEU:HD23	2:H:95:PHE:HB3	1.97	0.45
2:H:44:VAL:HG12	2:H:45:TRP:H	1.81	0.45
1:B:604:VAL:CG1	2:H:67:ALA:HA	2.36	0.45
2:H:68:PRO:HA	2:H:69:PRO:HD3	1.89	0.45
2:L:105:ILE:HB	2:Q:601:ALA:HB2	1.97	0.45
2:L:145:ALA:HB2	2:M:702:CYS:CB	2.46	0.45
2:L:37:LEU:HG	2:L:46:HIS:HB2	1.98	0.45
2:O:27:VAL:HG23	2:O:36:LEU:HB2	1.97	0.45
2:Q:687:ASN:C	2:Q:689:PHE:N	2.68	0.45
1:V:561:MET:O	1:V:565:LYS:HD3	2.17	0.45
1:V:562:GLU:O	1:V:565:LYS:N	2.47	0.45
2:W:630:LEU:HD21	2:W:634:HIS:ND1	2.30	0.45
1:A:119:PRO:O	1:A:122:VAL:HG23	2.16	0.45
1:A:61:MET:HG2	2:E:616:PRO:CG	2.47	0.45
1:A:8:ILE:HD13	1:A:86:PHE:CZ	2.51	0.45
2:H:11:GLN:HB3	2:H:11:GLN:HE21	1.50	0.45
2:H:29:ILE:HD12	2:H:77:ASP:HA	1.98	0.45
2:I:606:LEU:HB2	2:I:621:PHE:HB2	1.99	0.45
1:J:27:THR:HB	1:J:30:SER:OG	2.17	0.45
1:K:502:GLU:O	1:K:503:ARG:HB3	2.16	0.45
1:K:532:PHE:HZ	1:K:611:PHE:CE2	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:598:GLU:CG	1:K:607:ARG:HD3	2.47	0.45
2:M:630:LEU:HD22	2:M:634:HIS:HD2	1.80	0.45
2:M:693:PHE:C	2:M:695:ILE:H	2.18	0.45
1:N:144:LEU:O	1:N:144:LEU:HD23	2.17	0.45
2:O:33:GLY:HA2	2:O:73:LEU:HD11	1.97	0.45
1:U:126:LEU:HD23	1:U:127:ILE:HG12	1.98	0.45
2:W:581:ARG:O	2:W:585:LYS:HG3	2.16	0.45
2:X:516:LEU:HD21	2:X:582:PRO:HG2	1.99	0.45
2:X:685:GLU:HB3	2:X:688:SER:OG	2.16	0.45
1:B:534:ILE:CD1	1:B:613:LEU:HD11	2.46	0.45
2:D:211:VAL:HA	2:D:215:GLN:HG2	1.98	0.45
2:D:81:ARG:HB2	2:D:82:PRO:CD	2.43	0.45
2:I:545:TRP:CD1	2:I:604:LEU:HB3	2.52	0.45
1:J:20:LEU:C	1:J:20:LEU:HD22	2.37	0.45
2:O:13:TRP:HD1	2:O:218:TYR:CE2	2.35	0.45
2:Q:531:LYS:HB2	2:Q:532:GLN:HE21	1.81	0.45
1:R:127:ILE:HD11	1:V:627:ILE:CD1	2.47	0.45
1:R:49:GLU:OE1	1:R:52:ILE:HD12	2.17	0.45
1:R:88:PHE:HB2	1:R:95:PHE:HD1	1.82	0.45
2:S:62:ASN:ND2	2:S:118:TYR:HB2	2.30	0.45
2:T:13:TRP:H	2:T:215:GLN:NE2	2.14	0.45
1:U:32:PHE:CE2	1:U:52:ILE:HD11	2.49	0.45
1:U:74:LEU:HD12	1:U:74:LEU:N	2.30	0.45
1:V:598:GLU:HB3	1:V:607:ARG:HA	1.98	0.45
2:W:665:GLN:O	2:W:669:GLU:HG2	2.16	0.45
2:X:504:LEU:HD11	2:X:530:THR:HG22	1.97	0.45
1:B:517:THR:HG22	1:B:518:HIS:N	2.32	0.45
2:D:194:MET:SD	2:D:198:LEU:HD22	2.56	0.45
2:E:520:GLU:O	2:E:521:ASN:C	2.54	0.45
1:B:559:MET:HB2	2:H:64:ARG:HH21	1.80	0.45
1:J:13:GLU:HG2	1:J:16:ILE:HD13	1.99	0.45
1:J:5:ILE:HG23	1:J:21:GLN:HB3	1.98	0.45
1:J:131:LEU:CD2	1:K:505:ILE:HG21	2.45	0.45
2:L:198:LEU:N	2:L:199:PRO:CD	2.79	0.45
2:L:213:ASN:O	2:L:214:LEU:HB3	2.14	0.45
2:M:547:GLU:CB	2:M:623:CYS:HB3	2.42	0.45
2:O:153:LEU:HD23	2:O:153:LEU:HA	1.86	0.45
2:S:202:CYS:N	2:W:645:ALA:HB2	2.31	0.45
2:S:47:GLU:HB2	2:S:123:CYS:HA	1.97	0.45
2:T:24:LEU:HD23	2:T:211:VAL:HG13	1.98	0.45
1:U:63:LYS:O	1:U:67:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:685:GLU:HG3	2:W:688:SER:H	1.80	0.45
1:Y:561:MET:HG2	1:Y:565:LYS:HG2	1.99	0.45
1:A:72:LYS:HA	1:A:77:GLY:HA3	1.99	0.45
2:D:208:LYS:HB3	2:D:209:PRO:HD3	1.98	0.45
1:J:51:GLU:O	1:J:55:GLU:HG2	2.17	0.45
2:L:166:ASP:HB3	2:M:675:ILE:HG22	1.98	0.45
2:L:57:ARG:CZ	2:L:122:HIS:ND1	2.80	0.45
2:L:80:LEU:HB3	2:L:83:LEU:HB2	1.97	0.45
2:M:513:TRP:CZ2	2:M:635:LEU:HD21	2.52	0.45
2:M:637:ARG:N	2:M:638:PRO:HD2	2.31	0.45
1:N:18:HIS:HB3	1:N:37:THR:O	2.16	0.45
2:Q:508:LEU:O	2:Q:526:LYS:HE2	2.16	0.45
2:Q:545:TRP:HZ2	2:Q:599:CYS:HG	1.64	0.45
2:O:135:LEU:HB3	2:Q:636:ILE:CD1	2.47	0.45
2:T:106:LEU:HD13	2:T:121:PHE:CD2	2.49	0.45
1:U:11:VAL:HG23	1:U:12:SER:N	2.32	0.45
1:U:88:PHE:CE1	1:U:113:LEU:HD11	2.52	0.45
2:W:581:ARG:HB3	2:W:582:PRO:HD3	1.98	0.45
2:W:654:ALA:HB1	2:W:684:PHE:HE2	1.82	0.45
2:D:124:MET:O	2:D:125:LEU:C	2.54	0.45
2:E:568:PRO:HA	2:E:569:PRO:HD3	1.86	0.45
2:E:711:VAL:O	2:E:715:GLN:HB2	2.16	0.45
2:H:215:GLN:HA	2:H:218:TYR:HB3	1.97	0.45
2:I:661:ASP:O	2:I:665:GLN:HG3	2.17	0.45
2:L:190:LEU:O	2:L:194:MET:HG2	2.17	0.45
2:L:213:ASN:C	2:L:215:GLN:H	2.20	0.45
2:L:80:LEU:HA	2:L:83:LEU:CB	2.47	0.45
2:M:508:LEU:HD13	2:M:535:ALA:O	2.17	0.45
2:M:630:LEU:HD23	2:M:630:LEU:HA	1.81	0.45
1:N:34:ILE:HD12	1:N:35:THR:N	2.28	0.45
1:P:586:PHE:HB3	1:P:595:PHE:HE2	1.82	0.45
1:P:607:ARG:HG2	1:P:607:ARG:NH1	2.31	0.45
1:P:652:LEU:O	1:P:652:LEU:HD13	2.16	0.45
2:Q:657:LEU:HD23	2:Q:657:LEU:O	2.17	0.45
2:T:40:ASP:C	2:T:42:GLN:H	2.20	0.45
1:V:565:LYS:HE2	1:V:566:TYR:HA	1.99	0.45
2:W:556:GLN:O	2:W:560:GLU:HB2	2.16	0.45
1:A:88:PHE:HB2	1:A:95:PHE:CD1	2.51	0.45
2:E:512:PRO:HB2	2:E:715:GLN:HE21	1.81	0.45
1:F:11:VAL:HB	1:F:87:ASN:CG	2.37	0.45
1:K:600:ASN:HA	1:K:605:SER:CB	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:547:VAL:HG11	1:K:611:PHE:CE1	2.52	0.45
2:L:95:PHE:O	2:L:96:SER:C	2.54	0.45
1:J:61:MET:SD	2:M:615:LEU:HD23	2.57	0.45
2:O:131:VAL:O	2:O:135:LEU:HB2	2.16	0.45
2:O:160:LYS:HG2	2:Q:681:THR:OG1	2.16	0.45
2:O:179:LEU:CD2	2:Q:662:LEU:HB3	2.47	0.45
2:S:98:ASP:O	2:S:105:ILE:HG22	2.16	0.45
2:T:137:ARG:HB3	2:T:138:PRO:CD	2.47	0.45
2:T:36:LEU:CD1	2:T:37:LEU:H	2.29	0.45
2:W:617:PHE:CD1	2:W:617:PHE:C	2.90	0.45
2:X:676:ARG:HB3	2:X:679:LEU:HB3	1.98	0.45
1:A:24:TRP:HB3	1:A:32:PHE:HB3	1.99	0.45
2:D:146:LEU:HD11	2:E:647:GLN:OE1	2.17	0.45
2:D:161:ASP:OD1	2:D:183:PRO:HA	2.16	0.45
1:F:3:ARG:HA	1:F:22:VAL:O	2.15	0.45
1:G:523:SER:OG	1:G:533:VAL:HB	2.16	0.45
2:H:208:LYS:O	2:H:211:VAL:HG13	2.16	0.45
2:I:505:GLU:OE2	2:I:508:LEU:HD23	2.16	0.45
2:I:589:HIS:CG	2:I:590:PRO:HD2	2.52	0.45
1:K:535:THR:HG22	1:K:536:LEU:N	2.32	0.45
1:K:649:GLU:O	1:K:653:ARG:HB2	2.17	0.45
2:O:106:LEU:N	2:O:106:LEU:HD23	2.32	0.45
1:R:152:LEU:HA	1:V:651:LEU:HD11	1.98	0.45
1:R:7:ARG:NH2	1:V:628:CYS:SG	2.90	0.45
2:T:29:ILE:HD12	2:T:29:ILE:N	2.32	0.45
1:A:74:LEU:O	1:A:75:LEU:HD22	2.17	0.45
2:D:8:LEU:HA	2:D:28:PHE:HB2	1.99	0.45
1:F:106:PHE:CD2	2:I:615:LEU:HD22	2.50	0.45
1:J:74:LEU:C	1:J:76:SER:H	2.19	0.45
1:N:44:THR:C	1:N:113:LEU:HD12	2.37	0.45
1:P:516:ILE:HG13	1:P:517:THR:N	2.32	0.45
1:P:604:VAL:CG2	1:P:605:SER:H	2.21	0.45
1:R:29:GLU:O	1:R:52:ILE:HD13	2.17	0.45
2:T:110:SER:O	2:T:116:PRO:HA	2.17	0.45
2:T:218:TYR:CE2	2:T:222:THR:HG21	2.52	0.45
1:V:517:THR:HG22	1:V:518:HIS:H	1.81	0.45
1:B:518:HIS:CD2	1:B:536:LEU:HD11	2.52	0.45
2:D:179:LEU:HD22	2:E:663:GLU:HA	1.99	0.45
2:E:583:LEU:HD11	2:E:591:SER:HA	1.99	0.45
1:F:101:LEU:HD11	2:I:613:SER:OG	2.17	0.45
2:I:513:TRP:CE3	2:I:524:LEU:HG	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:715:GLN:O	2:I:718:TYR:HB3	2.16	0.45
2:L:216:ASP:HA	2:L:219:MET:CE	2.47	0.45
2:L:6:GLN:HE21	2:L:6:GLN:CA	2.30	0.45
2:O:202:CYS:N	2:Q:645:ALA:HB2	2.32	0.45
2:O:28:PHE:O	2:O:34:TYR:HA	2.17	0.45
1:R:97:PHE:N	1:R:97:PHE:CD2	2.85	0.45
2:T:114:GLY:O	2:T:116:PRO:HD3	2.16	0.45
2:T:65:LEU:CD1	2:T:67:ALA:H	2.25	0.45
2:T:96:SER:OG	2:T:107:ARG:HB2	2.17	0.45
1:U:149:GLU:C	1:U:151:LEU:H	2.20	0.45
2:T:163:GLU:HA	2:X:679:LEU:HG	1.98	0.45
1:A:7:ARG:H	1:A:7:ARG:HG2	1.39	0.44
1:B:505:ILE:CD1	1:B:630:CYS:HB2	2.47	0.44
2:D:153:LEU:O	2:D:157:LEU:HB2	2.16	0.44
2:D:193:PHE:CE1	2:E:649:GLN:HG2	2.52	0.44
1:F:47:VAL:HA	1:F:51:GLU:OE1	2.17	0.44
2:H:81:ARG:H	2:H:82:PRO:HD3	1.81	0.44
1:K:590:LYS:HZ3	1:K:590:LYS:HA	1.82	0.44
2:L:41:LEU:HD11	2:L:206:ASP:HA	1.99	0.44
2:M:702:CYS:O	2:M:703:SER:C	2.55	0.44
2:M:706:ASP:O	2:M:708:LYS:N	2.50	0.44
1:N:73:ALA:HB2	1:N:84:TYR:CZ	2.52	0.44
2:O:140:MET:HG3	2:Q:710:PHE:HD2	1.81	0.44
1:R:123:ILE:HD11	1:V:623:ILE:HB	1.99	0.44
2:S:186:GLU:HG3	2:S:187:ASN:N	2.31	0.44
2:S:207:GLY:O	2:S:208:LYS:C	2.56	0.44
2:S:27:VAL:HG13	2:S:27:VAL:O	2.17	0.44
2:W:575:HIS:ND1	2:W:612:LEU:HD11	2.32	0.44
2:X:610:SER:O	2:X:611:GLU:HG3	2.17	0.44
2:E:504:LEU:HD22	2:E:530:THR:CG2	2.47	0.44
1:B:606:PHE:CZ	2:H:115:LEU:HG	2.52	0.44
2:H:157:LEU:O	2:H:157:LEU:HD23	2.18	0.44
2:I:534:TYR:HE1	2:I:547:GLU:CG	2.29	0.44
2:I:579:LEU:HD21	2:I:612:LEU:CD2	2.46	0.44
2:L:118:TYR:N	2:L:118:TYR:CD1	2.85	0.44
2:L:167:TYR:HD1	2:M:667:TYR:HB2	1.81	0.44
2:L:80:LEU:O	2:L:81:ARG:HG3	2.17	0.44
2:M:656:LEU:HA	2:M:659:MET:HE3	1.98	0.44
2:L:174:LEU:HD13	2:M:667:TYR:CZ	2.51	0.44
1:N:22:VAL:HG21	1:N:74:LEU:O	2.17	0.44
2:O:137:ARG:HG2	2:O:137:ARG:HH11	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:518:LEU:HD23	2:Q:518:LEU:N	2.32	0.44
2:Q:682:GLU:HG2	2:Q:683:PRO:HD2	1.99	0.44
2:O:143:SER:HB3	2:Q:714:LEU:CD1	2.48	0.44
2:O:143:SER:HB3	2:Q:714:LEU:HD13	1.99	0.44
2:S:131:VAL:CG1	2:S:132:SER:N	2.80	0.44
2:S:23:LEU:HD13	2:S:38:VAL:CG1	2.44	0.44
2:T:173:THR:HG22	2:T:174:LEU:N	2.31	0.44
2:X:557:ARG:HD2	2:X:619:TRP:CH2	2.52	0.44
1:Y:549:GLU:O	1:Y:552:ILE:HG13	2.17	0.44
1:G:643:HIS:NE2	1:Y:651:LEU:HG	2.32	0.44
2:D:140:MET:HA	2:E:639:LEU:HD21	1.97	0.44
1:R:61:MET:HG2	1:R:65:LYS:HD3	1.99	0.44
2:S:50:ASP:O	2:S:51:THR:C	2.56	0.44
2:S:8:LEU:HD11	2:S:35:ALA:O	2.17	0.44
1:V:532:PHE:CZ	1:V:547:VAL:HG11	2.52	0.44
2:X:679:LEU:HD12	2:X:679:LEU:O	2.18	0.44
2:E:509:LEU:C	2:E:511:GLN:H	2.20	0.44
2:E:537:LEU:CD1	2:E:545:TRP:O	2.66	0.44
2:H:207:GLY:O	2:H:210:PHE:HB3	2.18	0.44
2:I:583:LEU:HG	2:I:589:HIS:CB	2.48	0.44
1:J:28:LEU:C	1:J:30:SER:H	2.21	0.44
1:J:39:GLY:O	1:K:623:ILE:HD13	2.17	0.44
2:L:105:ILE:HG12	2:L:106:LEU:N	2.32	0.44
1:N:126:LEU:HD23	1:N:127:ILE:N	2.31	0.44
2:O:132:SER:CA	2:O:136:ILE:HB	2.47	0.44
1:R:98:GLU:OE1	1:R:105:SER:HB3	2.18	0.44
1:R:27:THR:HG21	1:R:29:GLU:OE2	2.18	0.44
2:S:105:ILE:HG12	2:S:107:ARG:CZ	2.47	0.44
2:T:79:LEU:HD11	2:T:110:SER:HB3	2.00	0.44
1:U:5:ILE:HG22	1:U:21:GLN:HA	1.99	0.44
1:U:88:PHE:HD1	1:U:95:PHE:HA	1.83	0.44
2:W:506:GLN:HB3	2:W:727:HIS:NE2	2.33	0.44
1:Y:575:LEU:O	1:Y:575:LEU:HD23	2.18	0.44
1:Y:593:CYS:O	1:Y:612:ASN:HA	2.18	0.44
1:B:502:GLU:O	1:B:523:SER:HA	2.18	0.44
1:B:556:ALA:CB	1:B:563:LYS:HZ3	2.27	0.44
1:B:571:ARG:O	1:B:575:LEU:HG	2.18	0.44
2:D:128:PRO:C	2:D:130:LEU:N	2.70	0.44
2:D:80:LEU:HB3	2:D:81:ARG:CZ	2.47	0.44
2:E:580:LEU:O	2:E:584:LEU:HD13	2.17	0.44
2:I:590:PRO:C	2:I:592:GLU:H	2.19	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:199:PRO:C	2:L:201:ALA:H	2.21	0.44
2:L:41:LEU:HD13	2:L:204:ILE:CG2	2.47	0.44
2:M:568:PRO:HD2	2:M:571:ALA:HB3	1.99	0.44
1:N:44:THR:O	1:N:113:LEU:HB3	2.18	0.44
2:O:5:GLU:HB2	2:O:48:GLN:NE2	2.32	0.44
1:R:24:TRP:HB2	1:R:27:THR:O	2.18	0.44
1:R:39:GLY:O	1:R:123:ILE:HD12	2.18	0.44
1:U:94:TYR:CE2	1:U:112:ASN:HB2	2.53	0.44
1:U:87:ASN:HB2	1:U:96:PHE:CZ	2.51	0.44
2:S:137:ARG:HH11	2:W:541:LEU:HB3	1.82	0.44
2:X:677:ASP:OD1	2:X:678:ARG:HG2	2.18	0.44
2:D:188:SER:HA	2:D:191:GLU:OE2	2.18	0.44
2:D:193:PHE:C	2:D:195:ILE:N	2.71	0.44
2:E:523:LEU:HD12	2:E:538:VAL:HG21	2.00	0.44
2:E:530:THR:HG23	2:E:532:GLN:N	2.33	0.44
1:G:541:SER:O	1:G:542:ALA:HB2	2.17	0.44
2:H:9:LEU:HA	2:H:134:HIS:CE1	2.53	0.44
1:J:126:LEU:HD21	1:K:627:ILE:CG2	2.46	0.44
1:J:34:ILE:HG13	1:J:35:THR:N	2.32	0.44
1:N:44:THR:HG22	1:N:116:VAL:HG22	1.98	0.44
2:O:12:PRO:HD3	2:O:219:MET:HG3	1.99	0.44
2:O:179:LEU:HD23	2:Q:662:LEU:HB3	2.00	0.44
1:R:28:LEU:HD22	1:R:75:LEU:CD1	2.48	0.44
1:R:91:GLU:HG3	1:R:92:SER:H	1.83	0.44
2:S:168:GLN:NE2	2:S:180:LYS:NZ	2.65	0.44
2:T:16:LEU:HD12	2:T:17:GLN:H	1.83	0.44
2:T:41:LEU:HB3	2:X:637:ARG:HH11	1.83	0.44
2:T:45:TRP:HB3	2:T:123:CYS:CB	2.47	0.44
2:T:16:LEU:HD13	2:T:83:LEU:HG	2.00	0.44
2:X:630:LEU:HD12	2:X:634:HIS:HD2	1.82	0.44
1:B:503:ARG:HA	1:B:523:SER:CA	2.44	0.44
2:D:54:VAL:HG11	2:D:73:LEU:HD22	2.00	0.44
2:E:690:LEU:O	2:E:694:MET:HG2	2.18	0.44
1:F:8:ILE:CD1	1:F:20:LEU:HB2	2.46	0.44
2:I:638:PRO:O	2:I:642:MET:HG3	2.17	0.44
2:L:90:PRO:HG2	2:L:91:SER:H	1.83	0.44
2:M:691:GLU:O	2:M:695:ILE:HG13	2.17	0.44
1:N:3:ARG:NH1	1:N:3:ARG:HB3	2.32	0.44
2:O:99:CYS:SG	2:O:104:LEU:HD12	2.58	0.44
2:Q:605:ILE:HG21	2:Q:607:ARG:HH21	1.83	0.44
2:Q:718:TYR:O	2:Q:722:THR:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:24:LEU:HD22	2:S:211:VAL:CG2	2.47	0.44
2:S:79:LEU:O	2:S:81:ARG:NE	2.50	0.44
2:S:9:LEU:HD23	2:S:9:LEU:HA	1.85	0.44
1:U:102:LYS:C	1:U:104:VAL:H	2.19	0.44
1:U:33:VAL:HG22	1:U:46:THR:HA	1.99	0.44
1:U:22:VAL:HG21	1:U:74:LEU:O	2.18	0.44
2:W:706:ASP:C	2:W:708:LYS:H	2.20	0.44
2:X:646:LEU:O	2:X:649:GLN:HB2	2.17	0.44
2:X:715:GLN:C	2:X:717:LEU:N	2.71	0.44
2:D:35:ALA:HA	2:D:48:GLN:HA	1.99	0.44
2:E:564:ARG:O	2:E:565:LEU:HB2	2.18	0.44
2:H:110:SER:OG	2:H:111:GLU:N	2.51	0.44
2:H:41:LEU:HD11	2:H:207:GLY:CA	2.47	0.44
2:H:31:LYS:HB2	2:H:32:GLN:NE2	2.32	0.44
1:B:606:PHE:HB2	2:H:64:ARG:O	2.17	0.44
2:I:566:THR:HG23	2:S:53:VAL:HG22	2.00	0.44
1:K:520:LEU:HD23	1:K:574:LEU:HD22	2.00	0.44
2:M:585:LYS:O	2:M:586:ASP:HB2	2.18	0.44
1:N:124:ARG:CZ	1:P:516:ILE:HG12	2.47	0.44
2:O:179:LEU:HD23	2:Q:662:LEU:O	2.18	0.44
2:Q:517:GLN:HE21	2:Q:518:LEU:N	2.15	0.44
2:X:517:GLN:C	2:X:518:LEU:HD23	2.38	0.44
2:X:600:VAL:HG12	2:X:600:VAL:O	2.18	0.44
2:X:676:ARG:HB3	2:X:679:LEU:CB	2.48	0.44
1:A:47:VAL:HG13	1:A:111:PHE:CZ	2.52	0.44
2:D:99:CYS:HA	2:D:104:LEU:HD23	2.00	0.44
2:E:575:HIS:CE1	2:E:612:LEU:HB3	2.53	0.44
2:I:682:GLU:CG	2:I:683:PRO:HD2	2.40	0.44
1:J:143:HIS:O	1:J:147:GLU:HG2	2.18	0.44
2:M:612:LEU:HD22	2:M:617:PHE:CD1	2.53	0.44
1:N:151:LEU:HD23	1:P:651:LEU:O	2.18	0.44
1:N:96:PHE:HB2	1:N:109:GLY:O	2.17	0.44
2:O:57:ARG:NH2	2:O:122:HIS:HB2	2.33	0.44
2:O:198:LEU:C	2:O:198:LEU:HD23	2.39	0.44
2:O:64:ARG:NE	2:O:64:ARG:HA	2.32	0.44
2:Q:504:LEU:HD22	2:Q:535:ALA:CB	2.48	0.44
2:Q:582:PRO:C	2:Q:584:LEU:H	2.21	0.44
2:Q:709:PRO:HG2	2:Q:710:PHE:H	1.83	0.44
1:R:10:LEU:HD12	1:R:18:HIS:ND1	2.33	0.44
2:S:108:VAL:HB	2:S:119:TRP:O	2.18	0.44
1:U:59:MET:CE	1:U:108:LEU:HA	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:676:ARG:HB2	2:W:676:ARG:HH11	1.82	0.44
1:B:505:ILE:HD11	1:B:630:CYS:HB2	2.00	0.43
2:D:109:ARG:CG	2:D:110:SER:N	2.81	0.43
1:F:74:LEU:O	1:F:74:LEU:HG	2.18	0.43
1:G:626:LEU:O	1:G:630:CYS:HB2	2.18	0.43
2:H:198:LEU:HA	2:H:201:ALA:HB3	2.00	0.43
2:H:38:VAL:HG12	2:H:39:SER:N	2.33	0.43
2:I:709:PRO:HA	2:I:712:MET:CG	2.48	0.43
2:M:504:LEU:HD12	2:M:530:THR:CG2	2.48	0.43
2:M:617:PHE:HD2	2:M:617:PHE:C	2.21	0.43
2:Q:644:LEU:O	2:Q:647:GLN:HB3	2.17	0.43
2:S:182:GLU:OE2	2:S:183:PRO:HD2	2.18	0.43
1:A:140:LYS:HE2	1:A:144:LEU:HD11	2.00	0.43
1:B:626:LEU:HD23	1:B:627:ILE:N	2.33	0.43
2:E:569:PRO:O	2:E:572:PHE:HB3	2.18	0.43
1:F:16:ILE:HG13	1:G:624:ARG:NH2	2.33	0.43
1:F:16:ILE:HG22	1:F:17:THR:O	2.18	0.43
2:I:676:ARG:C	2:I:678:ARG:H	2.21	0.43
2:I:710:PHE:C	2:I:710:PHE:CD1	2.91	0.43
1:J:4:LYS:HG2	1:J:75:LEU:HB3	2.00	0.43
2:L:84:LEU:O	2:L:85:LYS:C	2.56	0.43
2:M:513:TRP:HA	2:M:526:LYS:HB3	1.99	0.43
2:M:627:SER:HB3	2:Q:556:GLN:HG3	1.99	0.43
2:M:711:VAL:HG23	2:M:712:MET:N	2.33	0.43
1:N:2:GLU:HB3	1:N:24:TRP:NE1	2.34	0.43
1:N:128:CYS:SG	1:P:507:ARG:HD3	2.58	0.43
1:P:625:GLU:HG3	1:P:626:LEU:N	2.32	0.43
2:Q:537:LEU:HD23	2:Q:537:LEU:O	2.18	0.43
1:R:85:THR:HG22	1:R:86:PHE:N	2.33	0.43
1:V:505:ILE:HG23	1:V:521:GLN:HA	2.00	0.43
2:W:513:TRP:N	2:W:715:GLN:NE2	2.66	0.43
2:W:617:PHE:HD1	2:W:617:PHE:C	2.21	0.43
1:Y:508:ILE:HB	1:Y:509:HIS:H	1.54	0.43
1:A:38:ASP:O	1:B:624:ARG:HD3	2.17	0.43
2:D:13:TRP:H	2:D:215:GLN:NE2	2.15	0.43
2:D:166:ASP:CG	2:E:675:ILE:HB	2.38	0.43
2:D:93:ALA:HB1	2:D:109:ARG:O	2.18	0.43
2:H:221:VAL:HG13	2:I:702:CYS:SG	2.58	0.43
2:I:520:GLU:O	2:I:521:ASN:HB2	2.18	0.43
2:I:534:TYR:CD1	2:I:534:TYR:C	2.92	0.43
2:I:565:LEU:HG	2:I:567:ALA:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:98:GLU:HB3	1:J:107:ARG:HA	1.99	0.43
1:K:638:GLN:HA	1:K:641:ASN:ND2	2.32	0.43
2:L:198:LEU:HB3	2:L:199:PRO:HD3	2.01	0.43
2:M:606:LEU:O	2:M:608:VAL:HG23	2.18	0.43
2:M:665:GLN:HA	2:M:668:GLN:NE2	2.33	0.43
1:N:144:LEU:CD2	1:P:644:LEU:HD23	2.49	0.43
2:Q:669:GLU:HG3	2:Q:670:SER:N	2.32	0.43
2:Q:708:LYS:N	2:Q:709:PRO:CD	2.81	0.43
2:S:46:HIS:ND1	2:S:47:GLU:N	2.66	0.43
2:W:568:PRO:HA	2:W:569:PRO:HD3	1.90	0.43
1:U:151:LEU:CD1	1:Y:651:LEU:HD22	2.43	0.43
1:A:127:ILE:HG22	1:A:131:LEU:HD23	1.99	0.43
1:B:509:HIS:CE1	1:B:517:THR:HA	2.53	0.43
2:D:80:LEU:HB3	2:D:81:ARG:HE	1.83	0.43
1:F:30:SER:HA	1:F:49:GLU:HG2	2.00	0.43
2:H:18:LEU:HD23	2:H:95:PHE:CB	2.49	0.43
2:I:525:ALA:CB	2:I:538:VAL:HG12	2.48	0.43
2:H:136:ILE:HD12	2:I:635:LEU:HD12	2.01	0.43
2:L:157:LEU:HG	2:M:657:LEU:CG	2.44	0.43
2:L:87:ALA:HB3	2:L:91:SER:OG	2.18	0.43
1:N:101:LEU:HD13	2:Q:613:SER:OG	2.19	0.43
2:Q:529:ILE:C	2:Q:530:THR:HG22	2.38	0.43
2:Q:712:MET:C	2:Q:713:ASN:HD22	2.22	0.43
1:R:88:PHE:CE1	1:R:113:LEU:HD12	2.53	0.43
2:S:18:LEU:HB2	2:S:21:ASN:O	2.18	0.43
2:S:29:ILE:HG23	2:S:34:TYR:CB	2.48	0.43
2:T:130:LEU:HA	2:T:133:GLN:HG3	2.01	0.43
2:T:137:ARG:O	2:T:140:MET:HB2	2.18	0.43
2:T:57:ARG:C	2:T:59:LYS:H	2.21	0.43
1:U:97:PHE:CD2	1:U:108:LEU:HD13	2.54	0.43
1:U:10:LEU:HD12	1:U:12:SER:H	1.83	0.43
2:W:544:VAL:HG21	2:W:631:VAL:HG23	2.01	0.43
1:Y:534:ILE:HG23	1:Y:613:LEU:HD23	1.99	0.43
1:A:47:VAL:HG22	1:A:111:PHE:CZ	2.53	0.43
2:D:118:TYR:CD1	2:D:118:TYR:N	2.86	0.43
2:D:195:ILE:HG22	2:D:196:GLU:HG3	1.99	0.43
2:D:38:VAL:HG23	2:D:39:SER:N	2.33	0.43
2:E:579:LEU:HD11	2:E:612:LEU:CD2	2.41	0.43
1:F:20:LEU:CD2	1:F:22:VAL:HG22	2.49	0.43
2:H:14:ALA:O	2:H:24:LEU:CB	2.66	0.43
2:H:4:LEU:HD12	2:H:35:ALA:CB	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:597:CYS:HB2	2:I:606:LEU:HD22	1.99	0.43
2:I:637:ARG:HG2	2:I:637:ARG:HH11	1.83	0.43
1:J:20:LEU:O	1:J:20:LEU:HD22	2.19	0.43
2:L:201:ALA:HB1	2:M:645:ALA:CA	2.48	0.43
2:L:216:ASP:HA	2:L:219:MET:HE3	2.01	0.43
2:M:509:LEU:HD21	2:M:726:HIS:CE1	2.54	0.43
1:N:53:SER:HB2	1:N:63:LYS:HZ1	1.83	0.43
2:O:82:PRO:HB2	2:O:85:LYS:CB	2.48	0.43
1:N:137:ASN:HB3	1:P:637:ASN:OD1	2.19	0.43
1:R:132:ASP:O	1:R:136:GLU:HG3	2.18	0.43
2:T:30:THR:HG23	2:T:32:GLN:N	2.30	0.43
1:V:535:THR:OG1	1:V:544:THR:HG23	2.18	0.43
2:X:545:TRP:HA	2:X:626:ALA:H	1.82	0.43
1:A:44:THR:HG1	1:A:45:GLY:H	1.66	0.43
1:B:517:THR:HG22	1:B:518:HIS:H	1.82	0.43
2:E:637:ARG:HB2	2:E:638:PRO:CD	2.49	0.43
1:J:20:LEU:HB3	1:J:36:LEU:HD13	1.99	0.43
1:K:597:PHE:CE1	1:K:610:SER:HA	2.53	0.43
2:L:80:LEU:HA	2:L:83:LEU:HB2	2.00	0.43
2:M:515:TRP:HZ2	2:M:707:GLY:HA3	1.81	0.43
2:O:125:LEU:O	2:O:126:ALA:C	2.56	0.43
2:O:157:LEU:HD22	2:O:184:PHE:CG	2.53	0.43
2:O:37:LEU:HD11	2:O:44:VAL:CG1	2.48	0.43
2:O:75:HIS:HD2	2:O:112:LEU:HD22	1.83	0.43
1:P:505:ILE:HD12	1:P:505:ILE:N	2.32	0.43
2:S:185:GLU:O	2:S:186:GLU:C	2.57	0.43
2:T:61:LEU:HD12	2:T:119:TRP:HA	2.01	0.43
2:W:596:SER:HB2	2:W:607:ARG:HG3	2.01	0.43
2:X:584:LEU:C	2:X:586:ASP:H	2.22	0.43
2:X:654:ALA:HA	2:X:684:PHE:HE2	1.84	0.43
2:T:153:LEU:HD23	2:X:657:LEU:HD12	2.01	0.43
2:T:160:LYS:HG3	2:X:664:ILE:HD11	2.00	0.43
1:Y:510:LEU:HD12	1:Y:518:HIS:CD2	2.52	0.43
1:B:504:LYS:CA	1:B:504:LYS:HZ2	2.27	0.43
1:B:504:LYS:HZ2	1:B:505:ILE:N	2.13	0.43
2:D:113:SER:C	2:D:115:LEU:H	2.21	0.43
2:D:150:VAL:HG23	2:E:650:VAL:HG22	2.00	0.43
2:D:182:GLU:CG	2:D:183:PRO:HD2	2.49	0.43
2:D:24:LEU:HD21	2:D:207:GLY:HA3	2.00	0.43
2:D:29:ILE:HD12	2:D:77:ASP:CG	2.39	0.43
2:E:516:LEU:HD12	2:E:595:PHE:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:583:LEU:O	2:I:583:LEU:HD23	2.18	0.43
1:K:543:TRP:HB3	1:K:613:LEU:HB3	2.00	0.43
1:K:543:TRP:CG	1:K:613:LEU:HD13	2.54	0.43
2:M:523:LEU:HD12	2:M:523:LEU:HA	1.90	0.43
2:M:682:GLU:HB2	2:M:683:PRO:HD2	2.01	0.43
1:N:45:GLY:CA	1:N:113:LEU:HD12	2.49	0.43
1:P:549:GLU:HA	1:P:552:ILE:CG2	2.47	0.43
2:O:140:MET:HE3	2:Q:710:PHE:HB2	2.01	0.43
1:R:67:VAL:O	1:R:71:ARG:HG3	2.18	0.43
1:U:74:LEU:O	1:U:75:LEU:HD23	2.18	0.43
1:V:549:GLU:O	1:V:549:GLU:HG2	2.19	0.43
2:W:513:TRP:CZ3	2:W:526:LYS:HG2	2.54	0.43
2:W:529:ILE:HG12	2:W:534:TYR:CB	2.48	0.43
2:W:544:VAL:HG21	2:W:631:VAL:CG2	2.48	0.43
1:Y:575:LEU:C	1:Y:577:GLY:N	2.72	0.43
1:A:33:VAL:HG12	1:A:34:ILE:H	1.82	0.43
2:D:176:ARG:HH12	2:E:666:ASP:CG	2.22	0.43
2:E:667:TYR:N	2:E:667:TYR:CD1	2.87	0.43
1:F:3:ARG:NH1	1:F:3:ARG:HG2	2.34	0.43
2:I:546:HIS:CG	2:I:547:GLU:N	2.87	0.43
2:I:576:LEU:HD22	2:I:580:LEU:CD1	2.48	0.43
2:H:164:ILE:HG12	2:I:664:ILE:HG22	2.00	0.43
1:J:150:ARG:HG3	1:J:151:LEU:N	2.34	0.43
1:K:583:VAL:O	1:K:600:ASN:HB2	2.19	0.43
2:L:109:ARG:HG2	2:L:118:TYR:CD2	2.53	0.43
2:L:139:LEU:HD22	2:M:639:LEU:HB3	2.01	0.43
2:L:79:LEU:C	2:L:80:LEU:HG	2.39	0.43
2:M:641:GLY:O	2:M:645:ALA:CB	2.67	0.43
1:P:551:GLU:O	1:P:554:GLN:HB3	2.19	0.43
2:Q:565:LEU:CD1	2:Q:566:THR:H	2.30	0.43
1:R:70:LEU:C	1:R:72:LYS:H	2.22	0.43
1:R:71:ARG:HA	1:R:75:LEU:HB2	2.00	0.43
2:S:27:VAL:HB	2:S:36:LEU:HD13	2.01	0.43
1:V:627:ILE:N	1:V:627:ILE:HD12	2.31	0.43
2:W:653:LEU:HD23	2:W:653:LEU:HA	1.82	0.43
2:X:527:VAL:HG13	2:X:536:LEU:CA	2.49	0.43
1:G:501:MET:HB2	1:G:525:GLU:OE2	2.19	0.43
1:G:532:PHE:HB3	1:G:547:VAL:HG23	2.00	0.43
1:G:604:VAL:O	1:G:605:SER:HB3	2.19	0.43
2:L:45:TRP:NE1	2:L:125:LEU:HD23	2.33	0.43
2:M:515:TRP:CD1	2:M:708:LYS:HA	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:626:LEU:O	1:P:630:CYS:HB2	2.18	0.43
2:Q:557:ARG:NH1	2:Q:622:HIS:H	2.17	0.43
2:Q:638:PRO:HG2	2:Q:639:LEU:H	1.84	0.43
2:T:58:ALA:O	2:T:59:LYS:HD3	2.19	0.43
1:Y:608:LEU:HB3	1:Y:609:GLY:H	1.70	0.43
1:B:511:VAL:O	1:B:511:VAL:HG12	2.19	0.43
2:D:171:GLY:O	2:D:172:ALA:CB	2.66	0.43
2:D:157:LEU:HD13	2:D:184:PHE:CD1	2.54	0.43
2:D:97:CYS:HA	2:D:105:ILE:O	2.18	0.43
2:E:706:ASP:C	2:E:708:LYS:H	2.23	0.43
1:G:553:SER:HA	1:G:563:LYS:CE	2.49	0.43
2:H:90:PRO:HG2	2:H:93:ALA:HB3	2.01	0.43
2:I:516:LEU:HD21	2:I:595:PHE:CD2	2.54	0.43
2:L:144:LEU:HD21	2:M:710:PHE:CA	2.41	0.43
2:L:17:GLN:HG2	2:L:84:LEU:CD1	2.47	0.43
2:L:195:ILE:CG2	2:L:195:ILE:O	2.67	0.43
2:L:53:VAL:O	2:L:54:VAL:C	2.57	0.43
2:M:534:TYR:C	2:M:534:TYR:CD1	2.92	0.43
2:M:666:ASP:O	2:M:670:SER:HB2	2.19	0.43
1:N:145:GLN:OE1	1:P:644:LEU:HD11	2.19	0.43
2:O:162:LEU:O	2:O:165:GLN:HB2	2.19	0.43
2:O:197:LYS:HA	2:O:197:LYS:NZ	2.34	0.43
2:O:14:ALA:HA	2:O:211:VAL:HG11	2.01	0.43
2:Q:550:ASP:OD2	2:Q:552:SER:HB3	2.18	0.43
2:Q:533:GLY:HA2	2:Q:573:LEU:HD21	2.01	0.43
2:S:157:LEU:HD22	2:S:184:PHE:CB	2.49	0.43
2:S:157:LEU:HD22	2:S:184:PHE:HB3	2.01	0.43
2:S:219:MET:HA	2:S:222:THR:CG2	2.49	0.43
2:S:219:MET:HA	2:S:222:THR:HG22	2.00	0.43
2:T:106:LEU:HD22	2:T:121:PHE:CD2	2.54	0.43
1:V:509:HIS:NE2	1:V:517:THR:HG23	2.33	0.43
2:S:139:LEU:HD22	2:W:639:LEU:CD1	2.48	0.43
2:D:4:LEU:HD12	2:D:35:ALA:CB	2.49	0.42
2:D:37:LEU:HD23	2:D:37:LEU:C	2.39	0.42
2:D:39:SER:CB	2:D:44:VAL:HA	2.47	0.42
1:F:137:ASN:HB3	1:G:637:ASN:HD22	1.83	0.42
1:B:601:LEU:CD2	2:H:113:SER:HB2	2.49	0.42
2:H:173:THR:HG22	2:H:174:LEU:O	2.19	0.42
2:H:37:LEU:HD22	2:H:134:HIS:CD2	2.54	0.42
2:H:46:HIS:ND1	2:H:47:GLU:N	2.67	0.42
2:I:651:ARG:HH11	2:I:651:ARG:HB3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:41:LEU:CD1	2:L:204:ILE:HG22	2.49	0.42
2:L:204:ILE:HG23	2:M:640:MET:SD	2.59	0.42
1:N:11:VAL:O	1:N:14:PRO:HD3	2.19	0.42
2:O:145:ALA:HB2	2:Q:702:CYS:CB	2.49	0.42
1:P:520:LEU:HA	1:P:535:THR:O	2.19	0.42
2:S:167:TYR:HB3	2:W:667:TYR:CD1	2.54	0.42
2:S:195:ILE:HD12	2:S:195:ILE:N	2.34	0.42
2:X:627:SER:HA	2:X:628:PRO:HD3	1.94	0.42
1:Y:599:LYS:O	1:Y:605:SER:HA	2.18	0.42
1:A:32:PHE:HD1	1:A:33:VAL:O	2.02	0.42
1:A:71:ARG:O	1:A:75:LEU:HB2	2.20	0.42
1:B:543:TRP:O	1:B:613:LEU:HD12	2.19	0.42
2:E:632:SER:O	2:E:634:HIS:N	2.52	0.42
1:F:112:ASN:HD22	1:F:113:LEU:N	2.17	0.42
1:K:516:ILE:HG23	1:K:518:HIS:CD2	2.54	0.42
1:K:552:ILE:HG23	1:K:563:LYS:NZ	2.33	0.42
1:K:599:LYS:CG	1:K:600:ASN:N	2.81	0.42
1:P:604:VAL:O	1:P:605:SER:CB	2.67	0.42
1:N:19:PHE:HE1	1:P:624:ARG:HG3	1.84	0.42
2:Q:521:ASN:N	2:Q:521:ASN:HD22	2.10	0.42
2:T:166:ASP:HB3	2:X:674:LEU:HD11	2.01	0.42
1:V:520:LEU:HD12	1:V:521:GLN:N	2.34	0.42
1:V:565:LYS:HE2	1:V:566:TYR:CA	2.48	0.42
2:X:511:GLN:OE1	2:X:528:PHE:HA	2.19	0.42
2:X:604:LEU:CD2	2:X:623:CYS:HB3	2.48	0.42
2:T:202:CYS:N	2:X:645:ALA:HB2	2.34	0.42
1:Y:559:MET:HE1	1:Y:566:TYR:HE1	1.84	0.42
1:A:72:LYS:HB3	1:A:84:TYR:CE1	2.54	0.42
1:G:534:ILE:HG22	1:G:545:GLY:O	2.18	0.42
2:H:153:LEU:HB2	2:I:689:PHE:CE2	2.54	0.42
2:I:541:LEU:HD11	2:I:707:GLY:CA	2.49	0.42
2:L:157:LEU:O	2:L:160:LYS:HB2	2.19	0.42
2:L:48:GLN:HG3	2:L:48:GLN:O	2.19	0.42
1:N:13:GLU:C	1:N:15:SER:N	2.73	0.42
2:O:57:ARG:HH22	2:O:122:HIS:HB2	1.85	0.42
1:P:600:ASN:HA	1:P:605:SER:CB	2.42	0.42
2:Q:713:ASN:HD22	2:Q:713:ASN:N	2.17	0.42
2:S:133:GLN:O	2:S:138:PRO:HG2	2.19	0.42
2:S:148:CYS:HB2	2:W:693:PHE:CZ	2.46	0.42
2:S:27:VAL:HG23	2:S:36:LEU:HB2	2.02	0.42
2:T:215:GLN:OE1	2:T:215:GLN:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:89:SER:C	1:U:91:GLU:H	2.22	0.42
2:W:531:LYS:HZ2	2:W:574:CYS:HA	1.83	0.42
1:R:104:VAL:CG1	2:W:565:LEU:HD23	2.49	0.42
2:X:606:LEU:HB3	2:X:621:PHE:CB	2.48	0.42
2:X:692:GLN:HB2	2:X:692:GLN:HE21	1.50	0.42
1:A:84:TYR:HB3	1:A:97:PHE:CE1	2.54	0.42
1:B:599:LYS:O	1:B:605:SER:HB3	2.20	0.42
2:D:54:VAL:HG11	2:D:73:LEU:CD2	2.49	0.42
1:F:138:GLN:O	1:F:142:GLU:HG2	2.20	0.42
2:H:176:ARG:C	2:H:178:ARG:H	2.23	0.42
2:I:656:LEU:HA	2:I:659:MET:HB2	2.00	0.42
2:I:682:GLU:HG2	2:I:683:PRO:CD	2.41	0.42
2:L:104:LEU:C	2:L:104:LEU:HD23	2.40	0.42
2:L:187:ASN:O	2:L:190:LEU:HG	2.19	0.42
2:L:38:VAL:CG2	2:L:39:SER:N	2.82	0.42
2:M:632:SER:HA	2:M:636:ILE:HB	2.01	0.42
1:N:140:LYS:O	1:N:144:LEU:HB2	2.19	0.42
1:N:27:THR:HG22	1:N:71:ARG:HH12	1.84	0.42
1:P:516:ILE:HG13	1:P:517:THR:H	1.84	0.42
1:P:537:THR:HB	1:P:542:ALA:CB	2.50	0.42
2:Q:529:ILE:CG2	2:Q:530:THR:H	2.33	0.42
2:Q:664:ILE:HG13	2:Q:665:GLN:N	2.34	0.42
2:O:221:VAL:HG13	2:Q:702:CYS:SG	2.59	0.42
1:R:59:MET:HE3	2:W:564:ARG:HE	1.84	0.42
2:S:16:LEU:O	2:S:18:LEU:HG	2.18	0.42
2:T:146:LEU:CD2	2:X:646:LEU:HB3	2.49	0.42
2:T:166:ASP:OD1	2:X:675:ILE:HB	2.19	0.42
2:T:79:LEU:O	2:T:79:LEU:HD12	2.18	0.42
2:W:574:CYS:SG	2:W:575:HIS:N	2.93	0.42
1:Y:545:GLY:CA	1:Y:613:LEU:HB3	2.50	0.42
1:A:144:LEU:HD13	1:B:645:GLN:HA	2.01	0.42
1:B:514:PRO:O	1:B:515:SER:HB2	2.19	0.42
1:B:526:LYS:HB2	1:B:527:THR:H	1.66	0.42
1:B:620:ALA:O	1:B:624:ARG:HB2	2.19	0.42
2:D:93:ALA:HB1	2:D:110:SER:HA	2.02	0.42
2:D:136:ILE:HG22	2:D:137:ARG:N	2.34	0.42
2:H:50:ASP:O	2:H:51:THR:C	2.58	0.42
2:I:691:GLU:CG	2:I:692:GLN:N	2.82	0.42
1:J:152:LEU:O	1:J:152:LEU:HG	2.19	0.42
1:K:582:ASP:O	1:K:583:VAL:HB	2.19	0.42
2:L:176:ARG:CD	2:L:179:LEU:HD13	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:13:TRP:HZ3	2:L:24:LEU:O	2.03	0.42
2:L:80:LEU:O	2:L:81:ARG:NH1	2.53	0.42
1:N:19:PHE:CE1	1:P:624:ARG:HG3	2.54	0.42
2:Q:547:GLU:HG2	2:Q:548:GLN:N	2.33	0.42
2:Q:554:VAL:CG1	2:Q:555:SER:N	2.81	0.42
2:Q:565:LEU:CG	2:Q:566:THR:N	2.83	0.42
1:N:106:PHE:CE2	2:Q:615:LEU:HD22	2.54	0.42
2:Q:651:ARG:O	2:Q:655:THR:HG23	2.19	0.42
1:R:70:LEU:C	1:R:72:LYS:N	2.72	0.42
2:S:182:GLU:CD	2:S:183:PRO:HD2	2.38	0.42
2:S:25:ALA:CB	2:S:38:VAL:HG22	2.49	0.42
2:T:41:LEU:HD11	2:T:206:ASP:CA	2.41	0.42
1:U:55:GLU:HB3	1:U:109:GLY:HA3	2.00	0.42
1:R:59:MET:HE3	2:W:564:ARG:HH21	1.85	0.42
2:W:622:HIS:N	2:W:622:HIS:CD2	2.86	0.42
2:X:708:LYS:CB	2:X:709:PRO:HD3	2.46	0.42
1:A:1:MET:HA	1:A:24:TRP:O	2.19	0.42
2:H:18:LEU:HB2	2:H:21:ASN:O	2.19	0.42
1:J:58:ASP:C	1:J:60:ALA:H	2.22	0.42
2:L:181:THR:HG21	2:M:660:LYS:CG	2.35	0.42
2:M:533:GLY:O	2:M:534:TYR:HB3	2.19	0.42
1:N:94:TYR:HA	1:N:112:ASN:HD21	1.82	0.42
2:O:211:VAL:O	2:O:213:ASN:N	2.53	0.42
2:O:14:ALA:CB	2:O:83:LEU:HA	2.47	0.42
1:R:103:ASP:N	1:R:103:ASP:OD2	2.51	0.42
1:R:39:GLY:CA	1:R:123:ILE:HD12	2.47	0.42
2:T:36:LEU:CG	2:T:37:LEU:N	2.81	0.42
1:U:1:MET:HG2	1:U:25:GLU:CA	2.50	0.42
1:U:123:ILE:HG21	1:Y:623:ILE:HG21	2.02	0.42
1:A:16:ILE:HG22	1:A:18:HIS:CD2	2.55	0.42
2:D:29:ILE:HG23	2:D:34:TYR:CB	2.50	0.42
2:E:509:LEU:HD12	2:E:634:HIS:HD2	1.84	0.42
2:E:566:THR:O	2:E:567:ALA:HB2	2.20	0.42
2:L:102:ASP:N	2:L:102:ASP:OD2	2.52	0.42
2:Q:504:LEU:HD23	2:Q:528:PHE:HD2	1.84	0.42
2:Q:642:MET:O	2:Q:646:LEU:HB2	2.20	0.42
2:Q:682:GLU:CG	2:Q:683:PRO:HD2	2.49	0.42
2:S:127:SER:HB3	2:S:130:LEU:HD12	2.02	0.42
2:S:214:LEU:HD11	2:W:644:LEU:CA	2.44	0.42
2:S:36:LEU:HD12	2:S:37:LEU:H	1.84	0.42
1:R:152:LEU:HD23	1:V:651:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:509:LEU:HD23	2:W:727:HIS:HD2	1.84	0.42
1:A:25:GLU:HB3	1:A:26:LYS:H	1.65	0.42
1:A:3:ARG:HB3	1:A:23:SER:HA	2.00	0.42
2:E:607:ARG:HD3	2:E:620:ASN:OD1	2.20	0.42
2:E:675:ILE:N	2:E:675:ILE:CD1	2.83	0.42
1:F:100:ASN:C	1:F:101:LEU:HD22	2.39	0.42
1:F:101:LEU:HB3	1:F:102:LYS:H	1.62	0.42
2:H:151:ARG:HH22	2:H:190:LEU:HD13	1.84	0.42
1:K:510:LEU:HD13	1:K:513:GLU:HB2	2.00	0.42
1:K:627:ILE:HG13	1:K:627:ILE:H	1.57	0.42
2:L:112:LEU:HD23	2:L:113:SER:OG	2.20	0.42
2:L:26:LYS:HZ3	2:L:134:HIS:HB3	1.84	0.42
1:N:151:LEU:HG	1:P:655:TRP:CE3	2.54	0.42
1:N:148:ASN:O	1:N:152:LEU:HB2	2.20	0.42
1:N:5:ILE:HA	1:N:20:LEU:O	2.20	0.42
2:O:26:LYS:HG3	2:O:26:LYS:O	2.19	0.42
2:O:29:ILE:HG12	2:O:34:TYR:HB3	2.01	0.42
1:P:598:GLU:CB	1:P:607:ARG:HA	2.44	0.42
1:P:618:ASN:N	1:P:619:PRO:HD3	2.35	0.42
2:Q:609:ARG:O	2:Q:610:SER:HB3	2.20	0.42
2:I:555:SER:HB3	2:S:124:MET:SD	2.60	0.42
2:S:166:ASP:OD2	2:W:676:ARG:HD3	2.20	0.42
1:V:559:MET:C	1:V:561:MET:N	2.72	0.42
2:W:642:MET:HB3	2:W:717:LEU:CD2	2.50	0.42
2:D:118:TYR:N	2:D:118:TYR:HD1	2.17	0.42
2:E:612:LEU:HD23	2:E:617:PHE:CB	2.50	0.42
2:E:509:LEU:HA	2:E:634:HIS:NE2	2.34	0.42
2:E:637:ARG:CZ	2:E:637:ARG:HB3	2.49	0.42
2:I:581:ARG:CB	2:I:582:PRO:HD3	2.36	0.42
1:J:102:LYS:O	1:J:104:VAL:HG23	2.20	0.42
2:L:175:ILE:O	2:L:175:ILE:HG22	2.20	0.42
2:M:638:PRO:HG2	2:M:639:LEU:H	1.85	0.42
1:N:142:GLU:O	1:N:145:GLN:HB3	2.20	0.42
1:N:3:ARG:HD3	1:N:129:TYR:CG	2.54	0.42
1:P:547:VAL:HG12	1:P:551:GLU:OE1	2.20	0.42
1:P:588:PHE:HA	1:P:594:TYR:O	2.20	0.42
2:Q:596:SER:O	2:Q:607:ARG:N	2.51	0.42
2:S:139:LEU:HB3	2:W:639:LEU:CD1	2.49	0.42
1:V:505:ILE:HG12	1:V:521:GLN:CG	2.50	0.42
2:W:706:ASP:O	2:W:708:LYS:N	2.53	0.42
2:W:708:LYS:N	2:W:709:PRO:CD	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:221:VAL:HG13	2:X:702:CYS:HB2	2.01	0.42
1:A:61:MET:SD	1:A:65:LYS:HD2	2.60	0.42
2:D:186:GLU:O	2:D:190:LEU:HD12	2.19	0.42
1:G:531:GLY:O	1:G:532:PHE:HD1	2.02	0.42
2:I:695:ILE:O	2:I:695:ILE:CG2	2.67	0.42
1:K:571:ARG:CG	1:K:572:LYS:N	2.83	0.42
1:K:620:ALA:C	1:K:622:VAL:H	2.23	0.42
2:L:105:ILE:HD13	2:L:107:ARG:NH1	2.35	0.42
2:M:545:TRP:CD2	2:M:604:LEU:HD22	2.55	0.42
2:M:610:SER:OG	2:M:611:GLU:N	2.53	0.42
2:O:13:TRP:CD1	2:O:218:TYR:CE2	3.08	0.42
2:O:152:GLU:HA	2:O:155:THR:HG22	2.02	0.42
1:N:144:LEU:HD21	1:P:645:GLN:HA	2.01	0.42
2:O:164:ILE:HG21	2:Q:663:GLU:OE2	2.19	0.42
1:R:29:GLU:HB3	1:R:67:VAL:CG2	2.50	0.42
2:T:18:LEU:CD2	2:T:94:THR:HG23	2.47	0.42
1:U:3:ARG:HD2	1:U:129:TYR:CE2	2.54	0.42
1:V:543:TRP:HH2	1:V:590:LYS:HE3	1.85	0.42
1:R:127:ILE:CD1	1:V:626:LEU:HB3	2.50	0.42
1:R:138:GLN:NE2	1:V:637:ASN:ND2	2.63	0.42
2:W:581:ARG:HH11	2:W:581:ARG:HG3	1.84	0.42
2:W:685:GLU:HB3	2:W:688:SER:HB3	2.01	0.42
2:X:545:TRP:CD1	2:X:604:LEU:HB3	2.54	0.42
2:T:144:LEU:HD22	2:X:704:ILE:HD13	2.02	0.42
1:A:85:THR:HB	1:A:98:GLU:O	2.20	0.41
1:B:563:LYS:HD3	1:B:566:TYR:HD2	1.85	0.41
2:D:149:GLN:HB3	2:E:650:VAL:CG1	2.50	0.41
2:D:39:SER:HB2	2:D:44:VAL:HG12	2.01	0.41
2:E:534:TYR:C	2:E:534:TYR:CD1	2.93	0.41
2:E:509:LEU:HA	2:E:634:HIS:HE2	1.84	0.41
1:G:509:HIS:NE2	1:G:517:THR:HG22	2.34	0.41
1:G:555:GLU:OE1	1:G:555:GLU:HA	2.19	0.41
2:H:18:LEU:HB2	2:H:21:ASN:C	2.39	0.41
2:H:1:MET:H1	1:R:107:ARG:NH2	2.08	0.41
2:H:55:SER:O	2:H:58:ALA:HB3	2.20	0.41
2:I:710:PHE:O	2:I:714:LEU:HB3	2.20	0.41
1:J:142:GLU:O	1:J:146:LYS:HD3	2.20	0.41
1:J:30:SER:HB2	1:J:49:GLU:OE2	2.20	0.41
2:L:4:LEU:HA	2:L:28:PHE:CE2	2.51	0.41
2:L:67:ALA:HA	2:L:68:PRO:HD3	1.96	0.41
2:Q:529:ILE:CG2	2:Q:577:ASP:HB2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:37:THR:OG1	1:R:38:ASP:N	2.53	0.41
2:S:157:LEU:HD13	2:S:184:PHE:CG	2.55	0.41
1:V:510:LEU:HD11	1:V:518:HIS:CE1	2.55	0.41
1:R:130:CYS:HB2	1:V:630:CYS:SG	2.60	0.41
2:X:527:VAL:HG13	2:X:536:LEU:HA	2.01	0.41
2:D:79:LEU:CD2	2:D:95:PHE:HZ	2.33	0.41
2:E:695:ILE:C	2:E:696:GLU:HG3	2.40	0.41
2:H:40:ASP:O	2:H:41:LEU:HB2	2.20	0.41
2:I:505:GLU:O	2:I:508:LEU:HB3	2.19	0.41
2:I:542:GLN:O	2:I:543:GLN:HG3	2.20	0.41
2:I:577:ASP:O	2:I:581:ARG:N	2.53	0.41
2:I:676:ARG:HB3	2:I:679:LEU:HD11	2.02	0.41
2:I:708:LYS:O	2:I:712:MET:HG2	2.20	0.41
2:L:137:ARG:HD2	2:M:541:LEU:HB3	2.02	0.41
2:M:526:LYS:CD	2:M:537:LEU:HB3	2.50	0.41
1:N:95:PHE:HB3	1:N:111:PHE:O	2.20	0.41
2:O:44:VAL:O	2:O:125:LEU:HD13	2.20	0.41
2:O:41:LEU:HB3	2:Q:637:ARG:CD	2.50	0.41
1:P:562:GLU:HG2	1:P:563:LYS:N	2.35	0.41
1:P:606:PHE:N	1:P:606:PHE:CD2	2.88	0.41
2:S:157:LEU:HD13	2:S:184:PHE:CD2	2.55	0.41
2:S:64:ARG:N	2:S:64:ARG:HD2	2.20	0.41
2:T:92:GLU:HB3	2:T:110:SER:HA	2.02	0.41
2:X:533:GLY:HA3	2:X:549:VAL:O	2.20	0.41
2:X:536:LEU:HD11	2:X:538:VAL:CG2	2.49	0.41
2:X:602:ASP:CB	2:X:625:LEU:HB2	2.49	0.41
1:A:112:ASN:HD22	1:A:112:ASN:N	2.13	0.41
2:E:504:LEU:HD22	2:E:530:THR:HG22	2.02	0.41
1:F:152:LEU:HD22	1:G:651:LEU:HD21	2.01	0.41
1:F:36:LEU:HG	1:F:37:THR:N	2.35	0.41
2:H:104:LEU:HD22	2:H:104:LEU:HA	1.85	0.41
2:M:586:ASP:C	2:M:588:ALA:H	2.23	0.41
2:M:593:ALA:HB3	2:M:595:PHE:HE1	1.85	0.41
1:N:5:ILE:CG2	1:N:6:SER:H	2.22	0.41
1:P:613:LEU:HD23	1:P:613:LEU:N	2.35	0.41
1:P:650:ARG:HH12	1:P:651:LEU:HB2	1.85	0.41
2:S:174:LEU:HD12	2:S:175:ILE:H	1.84	0.41
2:S:174:LEU:HD21	2:S:179:LEU:HB3	2.01	0.41
2:S:63:LYS:C	2:S:65:LEU:H	2.23	0.41
1:U:37:THR:HG21	1:U:123:ILE:HD13	2.02	0.41
2:X:602:ASP:HB3	2:X:625:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:664:ILE:CG2	2:X:680:LYS:HZ1	2.32	0.41
2:T:162:LEU:O	2:X:679:LEU:HD21	2.20	0.41
1:Y:548:SER:O	1:Y:551:GLU:HB2	2.21	0.41
1:A:107:ARG:NH1	2:E:564:ARG:HD3	2.36	0.41
1:A:120:ALA:O	1:A:124:ARG:HG3	2.20	0.41
1:A:20:LEU:HD11	1:A:22:VAL:HG13	2.02	0.41
1:A:5:ILE:HG23	1:A:20:LEU:O	2.20	0.41
2:D:84:LEU:HA	2:D:88:ALA:H	1.85	0.41
2:D:214:LEU:HD11	2:E:644:LEU:HA	2.02	0.41
2:D:149:GLN:HE22	2:E:690:LEU:HD22	1.81	0.41
1:G:567:VAL:O	1:G:570:LEU:HB2	2.20	0.41
2:H:14:ALA:O	2:H:24:LEU:HA	2.20	0.41
1:J:123:ILE:O	1:J:127:ILE:HG13	2.20	0.41
1:K:510:LEU:HD23	1:K:511:VAL:H	1.81	0.41
1:K:528:LEU:HD12	1:K:531:GLY:O	2.21	0.41
2:L:190:LEU:HD23	2:L:190:LEU:N	2.36	0.41
2:M:602:ASP:HB3	2:M:625:LEU:CG	2.47	0.41
1:N:5:ILE:HG21	1:P:631:LEU:HD21	2.01	0.41
2:Q:562:ASN:HD21	2:Q:618:TYR:N	2.13	0.41
1:R:27:THR:HG22	1:R:30:SER:OG	2.20	0.41
2:T:211:VAL:HG12	2:T:215:GLN:HE21	1.85	0.41
2:T:46:HIS:HB3	2:T:126:ALA:CB	2.51	0.41
1:U:152:LEU:O	1:U:155:TRP:HB2	2.19	0.41
1:U:20:LEU:HD23	1:U:34:ILE:CD1	2.51	0.41
1:V:543:TRP:CH2	1:V:590:LYS:HE3	2.55	0.41
1:R:148:ASN:ND2	1:V:647:GLU:HG2	2.36	0.41
2:X:595:PHE:O	2:X:607:ARG:HB2	2.19	0.41
1:Y:574:LEU:HD23	1:Y:574:LEU:N	2.35	0.41
1:A:45:GLY:HA3	1:A:113:LEU:HB3	2.02	0.41
1:B:534:ILE:C	1:B:534:ILE:HD13	2.41	0.41
2:D:80:LEU:O	2:D:83:LEU:HD22	2.20	0.41
2:E:547:GLU:HB2	2:E:623:CYS:SG	2.60	0.41
2:E:545:TRP:CE3	2:E:604:LEU:HD13	2.55	0.41
1:F:59:MET:CE	1:F:108:LEU:HA	2.50	0.41
1:G:618:ASN:N	1:G:619:PRO:HD3	2.35	0.41
1:G:626:LEU:HD23	1:G:626:LEU:C	2.40	0.41
1:K:528:LEU:C	1:K:530:SER:H	2.24	0.41
1:K:596:PHE:HA	1:K:610:SER:HB3	2.02	0.41
2:L:24:LEU:HD12	2:L:24:LEU:N	2.34	0.41
2:L:75:HIS:CD2	2:L:112:LEU:HD12	2.55	0.41
2:M:707:GLY:C	2:M:709:PRO:HD2	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:124:ARG:NH1	1:P:516:ILE:HG21	2.35	0.41
2:Q:534:TYR:C	2:Q:534:TYR:CD1	2.94	0.41
2:S:199:PRO:O	2:S:201:ALA:N	2.53	0.41
1:U:18:HIS:HB3	1:U:36:LEU:CD1	2.46	0.41
1:U:35:THR:HA	1:U:43:TRP:O	2.20	0.41
1:U:86:PHE:CD2	1:U:97:PHE:HB3	2.55	0.41
1:V:635:ALA:O	1:V:638:GLN:HB2	2.20	0.41
2:X:536:LEU:HD22	2:X:621:PHE:CD1	2.55	0.41
2:X:549:VAL:HG13	2:X:553:VAL:HB	2.02	0.41
2:D:167:TYR:HD2	2:E:667:TYR:HB3	1.85	0.41
2:D:204:ILE:HD13	2:E:644:LEU:HD22	2.02	0.41
1:F:27:THR:HG23	1:F:30:SER:OG	2.21	0.41
1:G:615:LYS:HG3	1:G:616:VAL:N	2.35	0.41
2:H:18:LEU:HD11	2:H:23:LEU:HG	2.02	0.41
2:H:42:GLN:HA	2:H:42:GLN:NE2	2.32	0.41
1:K:597:PHE:CE2	1:K:608:LEU:HD12	2.45	0.41
2:L:208:LYS:O	2:L:212:MET:HG2	2.19	0.41
2:L:57:ARG:O	2:L:61:LEU:HD23	2.21	0.41
1:J:61:MET:CE	2:M:616:PRO:HD3	2.49	0.41
1:N:63:LYS:O	1:N:67:VAL:HG23	2.20	0.41
1:P:511:VAL:HB	1:P:587:ASN:OD1	2.20	0.41
2:Q:673:THR:HG22	2:Q:674:LEU:N	2.35	0.41
2:S:13:TRP:HZ2	2:S:134:HIS:O	2.03	0.41
2:S:176:ARG:O	2:S:177:ASP:C	2.59	0.41
2:S:22:SER:C	2:S:23:LEU:HG	2.41	0.41
2:T:179:LEU:HD22	2:X:663:GLU:HA	2.03	0.41
2:T:8:LEU:HG	2:T:26:LYS:CD	2.50	0.41
1:U:8:ILE:CD1	1:U:8:ILE:H	2.33	0.41
2:W:649:GLN:O	2:W:653:LEU:HB2	2.20	0.41
2:W:653:LEU:O	2:W:657:LEU:HB2	2.20	0.41
2:E:617:PHE:CD2	2:E:618:TYR:N	2.81	0.41
2:E:545:TRP:NE1	2:E:625:LEU:HD22	2.35	0.41
1:G:553:SER:O	1:G:563:LYS:HE2	2.20	0.41
1:G:540:HIS:O	1:G:619:PRO:HB3	2.21	0.41
2:H:37:LEU:HD13	2:H:130:LEU:HD21	2.03	0.41
2:H:25:ALA:HB2	2:H:38:VAL:CG1	2.36	0.41
1:J:102:LYS:HG3	1:J:103:ASP:OD1	2.20	0.41
1:K:588:PHE:HD1	1:K:594:TYR:O	2.04	0.41
2:L:45:TRP:CD2	2:L:104:LEU:HD13	2.56	0.41
2:L:98:ASP:O	2:L:105:ILE:HG22	2.20	0.41
2:O:25:ALA:CB	2:O:38:VAL:HG22	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:534:TYR:CE2	2:Q:619:TRP:HZ2	2.33	0.41
2:O:204:ILE:HG13	2:Q:725:HIS:HE1	1.86	0.41
1:R:12:SER:O	1:R:13:GLU:HG3	2.21	0.41
2:T:81:ARG:HH21	2:T:84:LEU:CD2	2.33	0.41
1:V:501:MET:HG2	1:V:502:GLU:N	2.36	0.41
1:V:528:LEU:HD11	1:V:575:LEU:HD12	2.02	0.41
1:V:532:PHE:CE2	1:V:547:VAL:HG11	2.55	0.41
2:W:557:ARG:HA	2:W:560:GLU:HB2	2.02	0.41
1:A:74:LEU:H	1:A:74:LEU:HD23	1.86	0.41
1:B:504:LYS:HB3	1:B:522:VAL:CG2	2.43	0.41
2:E:541:LEU:HD22	2:E:704:ILE:HG21	2.03	0.41
1:G:601:LEU:HB2	1:G:604:VAL:HG23	2.02	0.41
2:H:174:LEU:HD23	2:H:176:ARG:O	2.21	0.41
2:H:210:PHE:CD2	2:H:214:LEU:HD12	2.54	0.41
2:I:550:ASP:OD1	2:I:553:VAL:HG23	2.20	0.41
2:I:562:ASN:O	2:I:563:LYS:C	2.59	0.41
1:K:552:ILE:C	1:K:552:ILE:HD13	2.41	0.41
2:L:215:GLN:HA	2:L:215:GLN:OE1	2.20	0.41
2:O:154:ALA:HB1	2:O:184:PHE:CE2	2.55	0.41
2:O:83:LEU:HB2	2:O:84:LEU:H	1.64	0.41
1:P:501:MET:HE2	1:P:501:MET:HA	2.02	0.41
2:Q:534:TYR:HD1	2:Q:535:ALA:N	2.19	0.41
2:S:217:LEU:O	2:S:220:ALA:HB3	2.21	0.41
2:S:51:THR:HG22	2:S:52:SER:N	2.34	0.41
2:T:76:LEU:HD21	2:T:108:VAL:HG11	2.02	0.41
2:T:16:LEU:HD13	2:T:83:LEU:CD1	2.51	0.41
1:V:503:ARG:HD2	1:V:629:TYR:CE1	2.55	0.41
1:B:522:VAL:HG12	1:B:534:ILE:HB	2.03	0.41
2:D:139:LEU:CD2	2:E:639:LEU:HB3	2.50	0.41
2:E:533:GLY:H	2:E:573:LEU:HD11	1.86	0.41
1:G:512:SER:OG	1:G:587:ASN:ND2	2.53	0.41
2:I:630:LEU:O	2:I:632:SER:N	2.54	0.41
2:I:647:GLN:O	2:I:651:ARG:HG2	2.21	0.41
2:L:95:PHE:HA	2:L:107:ARG:O	2.21	0.41
2:L:34:TYR:CE2	2:L:49:VAL:HG21	2.56	0.41
2:M:516:LEU:C	2:M:516:LEU:HD12	2.41	0.41
2:M:596:SER:HB3	2:M:607:ARG:CB	2.46	0.41
2:M:665:GLN:HG2	2:M:668:GLN:NE2	2.35	0.41
2:M:676:ARG:NH1	2:M:676:ARG:HG3	2.36	0.41
2:O:4:LEU:HD11	2:O:34:TYR:CA	2.51	0.41
2:Q:604:LEU:HD13	2:Q:604:LEU:C	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:584:TYR:CE1	1:V:599:LYS:HD3	2.55	0.41
2:W:563:LYS:C	2:W:563:LYS:HD3	2.41	0.41
2:T:135:LEU:HB3	2:X:636:ILE:HD12	2.03	0.41
1:A:20:LEU:HD21	1:A:22:VAL:CG1	2.51	0.41
1:A:35:THR:HA	1:A:43:TRP:O	2.20	0.41
1:B:563:LYS:HA	1:B:566:TYR:HB3	2.03	0.41
2:E:599:CYS:HB3	2:E:604:LEU:CD1	2.35	0.41
2:D:193:PHE:CZ	2:E:648:CYS:HB2	2.53	0.41
2:H:140:MET:CE	2:I:710:PHE:HB2	2.51	0.41
2:I:537:LEU:HD22	2:I:546:HIS:HA	2.02	0.41
2:L:21:ASN:ND2	2:L:23:LEU:HD21	2.36	0.41
2:M:505:GLU:OE2	2:M:630:LEU:HD11	2.21	0.41
2:M:514:ALA:N	2:M:711:VAL:HG11	2.35	0.41
2:O:39:SER:CB	2:O:44:VAL:HA	2.51	0.41
2:Q:675:ILE:HB	2:Q:676:ARG:H	1.50	0.41
2:Q:515:TRP:CE2	2:Q:708:LYS:HD3	2.56	0.41
2:S:174:LEU:HG	2:S:176:ARG:H	1.86	0.41
2:S:185:GLU:OE1	2:S:187:ASN:HB3	2.21	0.41
2:S:9:LEU:O	2:S:222:THR:HG23	2.21	0.41
2:T:62:ASN:HB3	2:T:65:LEU:HB2	2.03	0.41
1:U:124:ARG:HD3	1:Y:538:ASP:CA	2.51	0.41
1:U:3:ARG:HG2	1:U:4:LYS:H	1.86	0.41
1:U:2:GLU:HB3	1:U:3:ARG:H	1.54	0.41
1:V:620:ALA:HA	1:V:623:ILE:CD1	2.50	0.41
2:X:545:TRP:CD2	2:X:604:LEU:HD13	2.56	0.41
1:G:547:VAL:HG21	1:G:611:PHE:CE1	2.55	0.41
1:G:621:GLU:HA	1:G:624:ARG:HH11	1.85	0.41
1:G:654:ASP:C	1:G:656:ASN:H	2.24	0.41
2:I:510:MET:O	2:I:719:MET:HG2	2.21	0.41
2:I:599:CYS:C	2:I:600:VAL:HG22	2.41	0.41
2:L:34:TYR:CE1	2:L:121:PHE:CE1	3.07	0.41
2:L:65:LEU:HD23	2:L:66:THR:N	2.36	0.41
2:Q:665:GLN:HB3	2:Q:665:GLN:HE21	1.65	0.41
1:R:138:GLN:HE21	1:V:637:ASN:HD21	1.65	0.41
2:T:198:LEU:H	2:T:199:PRO:CD	2.34	0.41
2:W:530:THR:C	2:W:532:GLN:H	2.24	0.41
1:A:33:VAL:HG12	1:A:34:ILE:N	2.37	0.40
1:B:574:LEU:C	1:B:575:LEU:HD23	2.42	0.40
2:D:40:ASP:O	2:D:41:LEU:HB2	2.21	0.40
2:E:597:CYS:SG	2:E:604:LEU:HD11	2.61	0.40
2:E:708:LYS:N	2:E:709:PRO:CD	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:16:ILE:HD12	1:J:16:ILE:N	2.34	0.40
2:L:208:LYS:O	2:L:211:VAL:HG22	2.20	0.40
1:N:59:MET:O	1:N:60:ALA:HB3	2.20	0.40
2:O:208:LYS:O	2:O:212:MET:HG2	2.21	0.40
2:Q:632:SER:HA	2:Q:636:ILE:CB	2.51	0.40
2:O:140:MET:HB2	2:Q:639:LEU:HD11	2.03	0.40
2:S:149:GLN:HG3	2:W:693:PHE:CD2	2.56	0.40
2:S:65:LEU:HD22	2:S:66:THR:N	2.36	0.40
2:T:45:TRP:HB3	2:T:123:CYS:HB2	2.02	0.40
1:U:74:LEU:HD11	1:U:97:PHE:CZ	2.56	0.40
2:W:567:ALA:HA	2:W:568:PRO:HD3	1.95	0.40
2:W:664:ILE:HG13	2:W:665:GLN:N	2.35	0.40
2:W:674:LEU:O	2:W:675:ILE:HG23	2.21	0.40
1:A:58:ASP:O	2:E:564:ARG:HG3	2.22	0.40
1:B:528:LEU:HD13	1:B:528:LEU:O	2.21	0.40
1:B:615:LYS:HB2	1:B:615:LYS:HE3	1.91	0.40
2:H:176:ARG:C	2:H:178:ARG:N	2.74	0.40
2:I:556:GLN:HE22	2:S:125:LEU:HB3	1.87	0.40
2:I:580:LEU:O	2:I:584:LEU:N	2.53	0.40
2:H:202:CYS:CA	2:I:645:ALA:HB2	2.50	0.40
2:I:653:LEU:HA	2:I:653:LEU:HD23	1.97	0.40
2:I:699:PRO:C	2:I:701:ALA:H	2.23	0.40
2:L:144:LEU:HD23	2:M:714:LEU:HD12	2.03	0.40
2:L:82:PRO:HB2	2:L:85:LYS:HG2	2.04	0.40
2:M:665:GLN:HA	2:M:668:GLN:CG	2.51	0.40
2:O:130:LEU:C	2:O:132:SER:N	2.73	0.40
2:Q:547:GLU:O	2:Q:548:GLN:HB2	2.21	0.40
1:R:92:SER:O	1:R:93:CYS:HB2	2.21	0.40
2:S:174:LEU:HD22	2:S:180:LYS:HB2	2.03	0.40
2:S:50:ASP:O	2:S:53:VAL:HG23	2.21	0.40
2:S:141:GLY:N	2:W:704:ILE:HD11	2.36	0.40
2:T:167:TYR:CE2	2:X:674:LEU:HD13	2.56	0.40
1:A:55:GLU:O	1:A:59:MET:HG2	2.21	0.40
1:B:513:GLU:O	1:B:515:SER:N	2.54	0.40
2:E:545:TRP:HE1	2:E:625:LEU:HD22	1.86	0.40
2:E:603:ALA:HB2	2:E:624:MET:SD	2.61	0.40
1:G:585:THR:HG23	1:G:600:ASN:HD22	1.85	0.40
2:H:118:TYR:O	2:H:119:TRP:HB2	2.21	0.40
2:I:529:ILE:HG12	2:I:534:TYR:HB2	2.03	0.40
2:I:695:ILE:H	2:I:695:ILE:HD12	1.85	0.40
1:J:67:VAL:HA	1:J:70:LEU:CD2	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:554:GLN:HB2	1:K:554:GLN:HE21	1.58	0.40
2:L:130:LEU:HA	2:L:130:LEU:HD22	1.93	0.40
2:L:45:TRP:HB3	2:L:123:CYS:HB3	2.02	0.40
2:L:167:TYR:HE2	2:M:675:ILE:HG13	1.86	0.40
1:N:13:GLU:N	1:N:14:PRO:HD3	2.36	0.40
1:N:123:ILE:HG21	1:P:539:GLY:HA2	2.03	0.40
1:P:548:SER:H	1:P:551:GLU:CG	2.35	0.40
1:N:144:LEU:CD2	1:P:644:LEU:HB3	2.46	0.40
2:Q:518:LEU:CD2	2:Q:518:LEU:N	2.84	0.40
1:R:27:THR:CG2	1:R:29:GLU:HG3	2.52	0.40
2:S:144:LEU:HG	2:W:714:LEU:HD12	2.04	0.40
2:S:80:LEU:C	2:S:81:ARG:HG3	2.41	0.40
1:U:13:GLU:C	1:U:15:SER:H	2.24	0.40
1:U:11:VAL:HG11	1:U:87:ASN:OD1	2.21	0.40
2:S:137:ARG:NH1	2:W:541:LEU:HD13	2.36	0.40
1:Y:530:SER:HA	1:Y:549:GLU:HB2	2.03	0.40
1:Y:586:PHE:CD2	1:Y:597:PHE:HB3	2.56	0.40
1:B:511:VAL:HA	1:B:514:PRO:HG3	2.03	0.40
2:E:699:PRO:O	2:E:701:ALA:N	2.48	0.40
2:D:144:LEU:CD1	2:E:709:PRO:HB2	2.39	0.40
1:F:114:GLU:HG3	1:F:114:GLU:H	1.59	0.40
1:F:40:HIS:O	1:F:41:SER:HB2	2.22	0.40
2:H:48:GLN:HA	2:H:48:GLN:HE21	1.86	0.40
2:I:501:MET:HE1	2:I:532:GLN:HB3	2.03	0.40
2:L:100:VAL:HG13	2:L:100:VAL:O	2.20	0.40
2:L:115:LEU:HD22	2:L:116:PRO:CD	2.49	0.40
2:L:102:ASP:O	2:L:124:MET:HA	2.21	0.40
2:L:164:ILE:HG12	2:M:664:ILE:HG22	2.04	0.40
1:N:101:LEU:HD11	2:Q:615:LEU:HD12	2.03	0.40
2:O:153:LEU:HG	2:Q:689:PHE:CZ	2.55	0.40
2:O:2:GLU:H	2:O:2:GLU:HG2	1.49	0.40
1:P:623:ILE:CD1	1:P:627:ILE:HD11	2.52	0.40
2:Q:529:ILE:HD12	2:Q:529:ILE:H	1.87	0.40
2:Q:657:LEU:HD22	2:Q:684:PHE:CG	2.57	0.40
2:T:122:HIS:ND1	2:T:122:HIS:N	2.70	0.40
2:T:55:SER:O	2:T:58:ALA:HB3	2.21	0.40
2:W:668:GLN:O	2:W:672:ALA:HA	2.21	0.40
2:W:678:ARG:HG2	2:W:678:ARG:HH11	1.86	0.40
2:X:509:LEU:HA	2:X:634:HIS:CE1	2.57	0.40
2:X:508:LEU:HD13	2:X:535:ALA:O	2.22	0.40
2:X:577:ASP:CG	2:X:577:ASP:O	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:717:LEU:O	2:X:718:TYR:C	2.58	0.40
1:Y:536:LEU:HD23	1:Y:588:PHE:CD2	2.57	0.40
1:Y:597:PHE:CZ	1:Y:609:GLY:HA3	2.57	0.40
1:A:126:LEU:HD21	1:B:627:ILE:CG2	2.52	0.40
1:A:34:ILE:HD12	1:A:34:ILE:N	2.36	0.40
1:A:86:PHE:CZ	1:A:95:PHE:HZ	2.39	0.40
1:A:10:LEU:CD1	1:A:88:PHE:H	2.34	0.40
1:B:559:MET:HE3	1:B:607:ARG:C	2.41	0.40
2:D:135:LEU:HB3	2:E:636:ILE:CD1	2.52	0.40
2:D:157:LEU:CD1	2:E:653:LEU:HD22	2.44	0.40
1:F:2:GLU:OE1	1:F:2:GLU:N	2.55	0.40
1:G:520:LEU:CD2	1:G:522:VAL:HG23	2.52	0.40
1:G:598:GLU:HB3	1:G:607:ARG:HA	2.03	0.40
2:H:179:LEU:HD23	2:I:662:LEU:CB	2.52	0.40
2:I:694:MET:HA	2:I:698:LEU:CB	2.50	0.40
1:J:49:GLU:C	1:J:51:GLU:N	2.75	0.40
1:K:511:VAL:CB	1:K:587:ASN:HA	2.51	0.40
1:N:27:THR:HB	1:N:30:SER:OG	2.22	0.40
1:N:88:PHE:HA	1:N:94:TYR:O	2.21	0.40
2:O:131:VAL:O	2:O:131:VAL:HG12	2.22	0.40
2:O:94:THR:HG22	2:O:109:ARG:CB	2.51	0.40
1:P:586:PHE:CD2	1:P:597:PHE:HB3	2.57	0.40
2:S:47:GLU:HB2	2:S:123:CYS:HB3	2.04	0.40
2:S:54:VAL:O	2:S:58:ALA:N	2.42	0.40
2:T:45:TRP:HD1	2:T:125:LEU:H	1.70	0.40
2:T:208:LYS:N	2:T:209:PRO:CD	2.84	0.40
2:T:217:LEU:HD13	2:T:221:VAL:HG21	2.04	0.40
2:T:33:GLY:H	2:T:73:LEU:HD13	1.85	0.40
1:U:102:LYS:HG3	1:U:102:LYS:O	2.22	0.40
1:U:150:ARG:HA	1:U:153:ARG:HH11	1.85	0.40
1:U:22:VAL:HG22	1:U:34:ILE:CD1	2.51	0.40
1:V:522:VAL:HB	1:V:575:LEU:HD23	2.03	0.40
2:W:518:LEU:N	2:W:518:LEU:HD12	2.36	0.40
2:W:531:LYS:HZ3	2:W:574:CYS:HA	1.85	0.40
2:W:606:LEU:HB3	2:W:621:PHE:CD2	2.55	0.40

All (36) 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:K:655:TRP:CB	3:P:2:TBR:BR9[1_554]	0.28	1.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:654:ASP:CA	3:P:2:TBR:TA6[1_554]	0.64	1.56
2:T:176:ARG:NH1	3:J:164:TBR:BR5[1_556]	0.77	1.43
1:K:654:ASP:CB	3:P:2:TBR:BRB[1_554]	1.19	1.01
1:K:654:ASP:C	3:P:2:TBR:TA6[1_554]	1.24	0.96
1:K:654:ASP:N	3:P:2:TBR:TA6[1_554]	1.27	0.93
1:K:656:ASN:N	3:P:2:TBR:BR5[1_554]	1.29	0.91
1:K:653:ARG:O	3:P:2:TBR:BR4[1_554]	1.29	0.91
1:K:655:TRP:N	3:P:2:TBR:TA2[1_554]	1.30	0.90
1:K:654:ASP:O	3:P:2:TBR:TA4[1_554]	1.31	0.89
1:K:652:LEU:O	3:P:2:TBR:BRC[1_554]	1.31	0.89
1:K:655:TRP:C	3:P:2:TBR:BR5[1_554]	1.33	0.87
1:K:655:TRP:CD1	3:P:2:TBR:BR8[1_554]	1.36	0.84
1:K:655:TRP:CA	3:P:2:TBR:TA2[1_554]	1.40	0.80
1:K:655:TRP:C	3:P:2:TBR:TA2[1_554]	1.44	0.76
1:K:655:TRP:CA	3:P:2:TBR:BR9[1_554]	1.48	0.72
1:K:655:TRP:O	3:P:2:TBR:TA2[1_554]	1.48	0.72
1:K:655:TRP:CG	3:P:2:TBR:BR9[1_554]	1.50	0.70
1:K:654:ASP:CG	3:P:2:TBR:BRB[1_554]	1.55	0.65
1:K:653:ARG:C	3:P:2:TBR:BR4[1_554]	1.55	0.65
1:K:655:TRP:O	3:P:2:TBR:BR5[1_554]	1.59	0.61
2:T:176:ARG:CZ	3:J:164:TBR:BR5[1_556]	1.65	0.55
1:K:656:ASN:CA	3:P:2:TBR:BR5[1_554]	1.65	0.55
1:K:654:ASP:O	3:P:2:TBR:TA5[1_554]	1.66	0.54
1:K:654:ASP:C	3:P:2:TBR:TA4[1_554]	1.81	0.39
1:K:652:LEU:C	3:P:2:TBR:BRC[1_554]	1.81	0.39
1:K:655:TRP:N	3:P:2:TBR:TA6[1_554]	1.88	0.32
1:K:655:TRP:NE1	3:P:2:TBR:BR8[1_554]	1.90	0.30
1:K:654:ASP:CB	3:P:2:TBR:TA6[1_554]	1.92	0.28
1:K:654:ASP:OD2	3:P:2:TBR:BRB[1_554]	1.96	0.24
1:K:655:TRP:CA	3:P:2:TBR:TA4[1_554]	1.96	0.24
1:K:654:ASP:CA	3:P:2:TBR:BRB[1_554]	2.04	0.16
1:K:654:ASP:N	3:P:2:TBR:BR4[1_554]	2.05	0.15
1:K:655:TRP:N	3:P:2:TBR:TA4[1_554]	2.07	0.13
1:K:655:TRP:O	3:P:2:TBR:BR1[1_554]	2.09	0.11
1:K:654:ASP:O	3:P:2:TBR:BR7[1_554]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	145/163 (89%)	108 (74%)	27 (19%)	10 (7%)	1	16
1	B	148/163 (91%)	116 (78%)	21 (14%)	11 (7%)	1	15
1	F	155/163 (95%)	120 (77%)	31 (20%)	4 (3%)	5	34
1	G	155/163 (95%)	114 (74%)	35 (23%)	6 (4%)	3	26
1	J	155/163 (95%)	114 (74%)	30 (19%)	11 (7%)	1	16
1	K	155/163 (95%)	110 (71%)	34 (22%)	11 (7%)	1	16
1	N	155/163 (95%)	121 (78%)	26 (17%)	8 (5%)	2	21
1	P	155/163 (95%)	126 (81%)	23 (15%)	6 (4%)	3	26
1	R	155/163 (95%)	125 (81%)	22 (14%)	8 (5%)	2	21
1	U	155/163 (95%)	130 (84%)	17 (11%)	8 (5%)	2	21
1	V	155/163 (95%)	126 (81%)	21 (14%)	8 (5%)	2	21
1	Y	155/163 (95%)	125 (81%)	20 (13%)	10 (6%)	1	18
2	D	225/230 (98%)	160 (71%)	51 (23%)	14 (6%)	1	18
2	E	225/230 (98%)	157 (70%)	50 (22%)	18 (8%)	1	14
2	H	225/230 (98%)	166 (74%)	45 (20%)	14 (6%)	1	18
2	I	225/230 (98%)	164 (73%)	52 (23%)	9 (4%)	3	26
2	L	225/230 (98%)	153 (68%)	56 (25%)	16 (7%)	1	16
2	M	225/230 (98%)	156 (69%)	51 (23%)	18 (8%)	1	14
2	O	225/230 (98%)	156 (69%)	51 (23%)	18 (8%)	1	14
2	Q	225/230 (98%)	156 (69%)	48 (21%)	21 (9%)	0	11
2	S	214/230 (93%)	151 (71%)	46 (22%)	17 (8%)	1	14
2	T	220/230 (96%)	161 (73%)	39 (18%)	20 (9%)	1	12
2	W	225/230 (98%)	169 (75%)	41 (18%)	15 (7%)	1	17
2	X	225/230 (98%)	156 (69%)	54 (24%)	15 (7%)	1	17
All	All	4527/4716 (96%)	3340 (74%)	891 (20%)	296 (6%)	1	18

All (296) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	GLU
2	D	94	THR
2	D	136	ILE
2	D	172	ALA
2	E	521	ASN
2	E	636	ILE
2	E	714	LEU
2	H	108	VAL
2	H	136	ILE
1	K	583	VAL
1	K	603	ASP
1	K	656	ASN
2	L	52	SER
2	L	54	VAL
2	L	81	ARG
2	L	82	PRO
2	L	100	VAL
2	L	177	ASP
2	M	519	ALA
2	M	520	GLU
1	N	40	HIS
1	P	617	GLU
2	O	81	ARG
2	O	85	LYS
2	O	136	ILE
2	O	211	VAL
2	O	212	MET
2	Q	525	ALA
2	Q	526	LYS
2	Q	569	PRO
2	Q	603	ALA
1	V	540	HIS
2	S	51	THR
2	W	725	HIS
2	T	52	SER
2	T	125	LEU
2	T	175	ILE
2	T	196	GLU
2	T	212	MET
2	T	214	LEU
2	X	552	SER
2	X	581	ARG

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Mol	Chain	Res	Type
2	X	636	ILE
2	X	713	ASN
1	U	108	LEU
1	Y	508	ILE
1	Y	583	VAL
1	A	22	VAL
1	A	43	TRP
1	A	59	MET
1	A	66	TYR
1	A	81	ALA
1	B	515	SER
1	B	590	LYS
2	D	19	ALA
2	D	93	ALA
2	D	175	ILE
2	E	542	GLN
2	E	633	GLN
2	E	700	GLU
2	E	713	ASN
2	E	725	HIS
2	E	726	HIS
1	F	38	ASP
1	G	517	THR
1	G	540	HIS
2	H	85	LYS
2	I	547	GLU
2	I	563	LYS
2	I	564	ARG
2	I	675	ILE
1	J	2	GLU
1	J	10	LEU
1	J	83	VAL
1	J	102	LYS
2	L	39	SER
2	L	101	ALA
2	M	636	ILE
2	M	675	ILE
2	M	713	ASN
1	N	6	SER
2	O	83	LEU
2	O	97	CYS
2	O	177	ASP

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Mol	Chain	Res	Type
2	Q	542	GLN
2	Q	548	GLN
2	Q	586	ASP
2	Q	594	THR
2	Q	601	ALA
2	Q	675	ILE
1	R	104	VAL
1	R	115	LYS
2	S	17	GLN
2	S	114	GLY
2	S	136	ILE
2	W	585	LYS
2	W	636	ILE
2	W	675	ILE
2	W	698	LEU
2	T	93	ALA
2	T	112	LEU
2	T	113	SER
2	T	186	GLU
2	X	565	LEU
2	X	672	ALA
1	U	3	ARG
1	U	4	LYS
1	U	90	LYS
1	U	109	GLY
1	A	78	ALA
1	B	506	SER
1	B	575	LEU
1	B	610	SER
2	D	78	ASN
2	D	99	CYS
2	D	214	LEU
2	E	515	TRP
2	E	590	PRO
2	E	672	ALA
2	E	681	THR
2	E	694	MET
1	F	41	SER
1	F	120	ALA
2	H	51	THR
2	H	52	SER
2	H	88	ALA

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Mol	Chain	Res	Type
2	H	89	HIS
2	H	101	ALA
2	H	107	ARG
2	I	672	ALA
2	I	714	LEU
1	J	56	ALA
1	J	107	ARG
1	K	514	PRO
1	K	529	GLU
1	K	604	VAL
2	L	83	LEU
2	L	88	ALA
2	L	128	PRO
2	L	203	SER
2	M	543	GLN
2	M	563	LYS
2	M	703	SER
2	M	707	GLY
1	N	14	PRO
1	N	38	ASP
1	N	119	PRO
1	P	574	LEU
2	O	96	SER
2	O	122	HIS
2	O	210	PHE
1	R	76	SER
1	R	91	GLU
1	R	103	ASP
1	V	581	ALA
1	V	608	LEU
2	S	21	ASN
2	S	80	LEU
2	S	187	ASN
2	S	199	PRO
2	S	200	GLU
2	S	212	MET
2	W	595	PHE
2	W	710	PHE
2	X	596	SER
2	X	601	ALA
2	X	612	LEU
1	U	2	GLU

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Mol	Chain	Res	Type
1	U	31	GLY
1	U	113	LEU
1	Y	578	ALA
1	A	79	GLY
1	B	505	ILE
1	B	584	TYR
1	B	615	LYS
2	D	63	LYS
2	D	116	PRO
2	E	601	ALA
1	F	25	GLU
1	G	602	LYS
1	G	656	ASN
2	H	119	TRP
2	I	625	LEU
1	J	103	ASP
1	J	112	ASN
1	K	502	GLU
1	K	527	THR
2	L	14	ALA
2	M	607	ARG
2	M	686	GLU
2	M	696	GLU
1	N	37	THR
1	N	108	LEU
2	O	86	ASP
2	O	186	GLU
2	Q	585	LYS
2	Q	587	ALA
2	Q	636	ILE
2	Q	679	LEU
2	Q	710	PHE
2	Q	714	LEU
1	R	25	GLU
1	R	38	ASP
2	S	172	ALA
2	S	183	PRO
2	S	186	GLU
2	W	616	PRO
2	W	674	LEU
2	W	707	GLY
2	W	714	LEU

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Mol	Chain	Res	Type
2	T	136	ILE
2	T	203	SER
2	X	588	ALA
2	X	593	ALA
2	X	602	ASP
2	X	714	LEU
1	Y	525	GLU
1	Y	582	ASP
1	A	90	LYS
1	A	119	PRO
1	B	514	PRO
1	B	526	LYS
1	B	538	ASP
2	D	64	ARG
2	D	189	PHE
2	D	218	TYR
2	E	551	THR
2	E	699	PRO
1	G	504	LYS
1	G	578	ALA
2	H	81	ARG
2	I	619	TRP
1	J	92	SER
1	J	106	PHE
1	K	504	LYS
1	K	526	LYS
2	L	93	ALA
2	L	136	ILE
2	M	526	LYS
2	M	592	GLU
2	M	617	PHE
1	N	43	TRP
1	P	526	LYS
1	P	560	ALA
1	P	604	VAL
1	P	605	SER
2	O	26	LYS
2	O	69	PRO
2	O	80	LEU
2	Q	590	PRO
1	V	525	GLU
1	V	561	MET

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Mol	Chain	Res	Type
1	V	562	GLU
2	S	43	GLN
2	S	69	PRO
2	W	539	SER
2	W	709	PRO
2	T	69	PRO
2	T	84	LEU
2	T	193	PHE
2	T	198	LEU
2	T	206	ASP
2	T	219	MET
2	X	592	GLU
1	Y	509	HIS
1	Y	603	ASP
2	H	203	SER
2	L	205	GLY
2	M	586	ASP
2	M	680	LYS
2	O	174	LEU
2	Q	591	SER
2	Q	610	SER
2	Q	698	LEU
1	R	90	LYS
1	V	511	VAL
2	W	601	ALA
1	Y	579	GLY
2	I	569	PRO
2	M	608	VAL
2	Q	709	PRO
2	W	695	ILE
2	T	199	PRO
2	E	675	ILE
2	H	100	VAL
2	S	116	PRO
2	S	211	VAL
1	J	119	PRO
1	Y	616	VAL
2	O	54	VAL
2	T	12	PRO
2	X	567	ALA
1	Y	580	PRO
1	K	522	VAL

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Mol	Chain	Res	Type
2	H	90	PRO
1	V	580	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	129/146 (88%)	108 (84%)	21 (16%)	2	15
1	B	138/146 (94%)	114 (83%)	24 (17%)	2	13
1	F	139/146 (95%)	115 (83%)	24 (17%)	2	13
1	G	139/146 (95%)	117 (84%)	22 (16%)	2	16
1	J	139/146 (95%)	126 (91%)	13 (9%)	8	31
1	K	139/146 (95%)	117 (84%)	22 (16%)	2	16
1	N	139/146 (95%)	119 (86%)	20 (14%)	3	19
1	P	139/146 (95%)	120 (86%)	19 (14%)	3	21
1	R	139/146 (95%)	131 (94%)	8 (6%)	20	48
1	U	139/146 (95%)	117 (84%)	22 (16%)	2	16
1	V	139/146 (95%)	117 (84%)	22 (16%)	2	16
1	Y	139/146 (95%)	119 (86%)	20 (14%)	3	19
2	D	201/204 (98%)	162 (81%)	39 (19%)	1	9
2	E	201/204 (98%)	166 (83%)	35 (17%)	2	13
2	H	201/204 (98%)	171 (85%)	30 (15%)	3	18
2	I	201/204 (98%)	171 (85%)	30 (15%)	3	18
2	L	201/204 (98%)	172 (86%)	29 (14%)	3	19
2	M	201/204 (98%)	178 (89%)	23 (11%)	5	25
2	O	200/204 (98%)	171 (86%)	29 (14%)	3	19
2	Q	201/204 (98%)	166 (83%)	35 (17%)	2	13
2	S	194/204 (95%)	166 (86%)	28 (14%)	3	19
2	T	199/204 (98%)	175 (88%)	24 (12%)	5	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	W	201/204 (98%)	176 (88%)	25 (12%)	4	23
2	X	201/204 (98%)	177 (88%)	24 (12%)	5	24
All	All	4059/4200 (97%)	3471 (86%)	588 (14%)	3	19

All (588) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	7	ARG
1	A	13	GLU
1	A	15	SER
1	A	17	THR
1	A	25	GLU
1	A	37	THR
1	A	41	SER
1	A	43	TRP
1	A	61	MET
1	A	69	GLU
1	A	74	LEU
1	A	105	SER
1	A	112	ASN
1	A	113	LEU
1	A	114	GLU
1	A	118	ASN
1	A	122	VAL
1	A	125	GLU
1	A	132	ASP
1	A	147	GLU
1	B	503	ARG
1	B	504	LYS
1	B	507	ARG
1	B	509	HIS
1	B	529	GLU
1	B	534	ILE
1	B	547	VAL
1	B	557	ASP
1	B	561	MET
1	B	575	LEU
1	B	591	GLU
1	B	597	PHE
1	B	598	GLU

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Mol	Chain	Res	Type
1	B	600	ASN
1	B	604	VAL
1	B	606	PHE
1	B	615	LYS
1	B	628	CYS
1	B	629	TYR
1	B	630	CYS
1	B	648	ASN
1	B	650	ARG
1	B	651	LEU
1	B	655	TRP
2	D	6	GLN
2	D	11	GLN
2	D	29	ILE
2	D	36	LEU
2	D	38	VAL
2	D	48	GLN
2	D	50	ASP
2	D	51	THR
2	D	64	ARG
2	D	81	ARG
2	D	83	LEU
2	D	85	LYS
2	D	89	HIS
2	D	91	SER
2	D	94	THR
2	D	102	ASP
2	D	104	LEU
2	D	107	ARG
2	D	109	ARG
2	D	115	LEU
2	D	125	LEU
2	D	127	SER
2	D	131	VAL
2	D	135	LEU
2	D	137	ARG
2	D	143	SER
2	D	146	LEU
2	D	152	GLU
2	D	157	LEU
2	D	158	HIS
2	D	176	ARG

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Mol	Chain	Res	Type
2	D	178	ARG
2	D	192	GLN
2	D	210	PHE
2	D	211	VAL
2	D	215	GLN
2	D	221	VAL
2	D	225	HIS
2	D	227	HIS
2	E	504	LEU
2	E	515	TRP
2	E	516	LEU
2	E	518	LEU
2	E	523	LEU
2	E	526	LYS
2	E	531	LYS
2	E	536	LEU
2	E	544	VAL
2	E	550	ASP
2	E	575	HIS
2	E	577	ASP
2	E	583	LEU
2	E	586	ASP
2	E	594	THR
2	E	598	ASP
2	E	602	ASP
2	E	604	LEU
2	E	607	ARG
2	E	615	LEU
2	E	618	TYR
2	E	623	CYS
2	E	625	LEU
2	E	639	LEU
2	E	649	GLN
2	E	651	ARG
2	E	658	HIS
2	E	661	ASP
2	E	664	ILE
2	E	675	ILE
2	E	679	LEU
2	E	694	MET
2	E	700	GLU
2	E	702	CYS

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Mol	Chain	Res	Type
2	E	719	MET
1	F	2	GLU
1	F	3	ARG
1	F	7	ARG
1	F	27	THR
1	F	28	LEU
1	F	44	THR
1	F	49	GLU
1	F	74	LEU
1	F	82	ASP
1	F	85	THR
1	F	94	TYR
1	F	96	PHE
1	F	100	ASN
1	F	101	LEU
1	F	108	LEU
1	F	111	PHE
1	F	112	ASN
1	F	113	LEU
1	F	114	GLU
1	F	116	VAL
1	F	121	GLU
1	F	125	GLU
1	F	154	ASP
1	F	155	TRP
1	G	503	ARG
1	G	510	LEU
1	G	518	HIS
1	G	528	LEU
1	G	532	PHE
1	G	537	THR
1	G	547	VAL
1	G	549	GLU
1	G	552	ILE
1	G	558	ASP
1	G	562	GLU
1	G	587	ASN
1	G	588	PHE
1	G	595	PHE
1	G	600	ASN
1	G	607	ARG
1	G	608	LEU

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Mol	Chain	Res	Type
1	G	617	GLU
1	G	618	ASN
1	G	644	LEU
1	G	650	ARG
1	G	655	TRP
2	H	4	LEU
2	H	5	GLU
2	H	10	MET
2	H	11	GLN
2	H	15	TRP
2	H	16	LEU
2	H	23	LEU
2	H	24	LEU
2	H	26	LYS
2	H	53	VAL
2	H	55	SER
2	H	56	GLN
2	H	59	LYS
2	H	64	ARG
2	H	79	LEU
2	H	83	LEU
2	H	85	LYS
2	H	100	VAL
2	H	104	LEU
2	H	109	ARG
2	H	125	LEU
2	H	135	LEU
2	H	140	MET
2	H	147	GLN
2	H	162	LEU
2	H	165	GLN
2	H	182	GLU
2	H	185	GLU
2	H	192	GLN
2	H	212	MET
2	I	502	GLU
2	I	523	LEU
2	I	537	LEU
2	I	542	GLN
2	I	548	GLN
2	I	549	VAL
2	I	559	LYS

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Mol	Chain	Res	Type
2	I	575	HIS
2	I	576	LEU
2	I	584	LEU
2	I	595	PHE
2	I	597	CYS
2	I	599	CYS
2	I	600	VAL
2	I	606	LEU
2	I	613	SER
2	I	615	LEU
2	I	617	PHE
2	I	624	MET
2	I	639	LEU
2	I	646	LEU
2	I	657	LEU
2	I	664	ILE
2	I	675	ILE
2	I	679	LEU
2	I	691	GLU
2	I	694	MET
2	I	698	LEU
2	I	706	ASP
2	I	722	THR
1	J	5	ILE
1	J	10	LEU
1	J	13	GLU
1	J	20	LEU
1	J	47	VAL
1	J	59	MET
1	J	70	LEU
1	J	85	THR
1	J	106	PHE
1	J	118	ASN
1	J	125	GLU
1	J	143	HIS
1	J	150	ARG
1	K	501	MET
1	K	504	LYS
1	K	508	ILE
1	K	516	ILE
1	K	521	GLN
1	K	547	VAL

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Mol	Chain	Res	Type
1	K	551	GLU
1	K	552	ILE
1	K	554	GLN
1	K	557	ASP
1	K	571	ARG
1	K	574	LEU
1	K	590	LYS
1	K	607	ARG
1	K	618	ASN
1	K	621	GLU
1	K	625	GLU
1	K	628	CYS
1	K	636	GLU
1	K	638	GLN
1	K	650	ARG
1	K	656	ASN
2	L	6	GLN
2	L	11	GLN
2	L	16	LEU
2	L	46	HIS
2	L	55	SER
2	L	64	ARG
2	L	66	THR
2	L	80	LEU
2	L	83	LEU
2	L	84	LEU
2	L	89	HIS
2	L	102	ASP
2	L	118	TYR
2	L	124	MET
2	L	125	LEU
2	L	130	LEU
2	L	135	LEU
2	L	137	ARG
2	L	140	MET
2	L	151	ARG
2	L	157	LEU
2	L	163	GLU
2	L	166	ASP
2	L	190	LEU
2	L	196	GLU
2	L	200	GLU

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Mol	Chain	Res	Type
2	L	213	ASN
2	L	214	LEU
2	L	227	HIS
2	M	511	GLN
2	M	516	LEU
2	M	518	LEU
2	M	522	SER
2	M	524	LEU
2	M	526	LYS
2	M	531	LYS
2	M	538	VAL
2	M	542	GLN
2	M	543	GLN
2	M	546	HIS
2	M	551	THR
2	M	617	PHE
2	M	630	LEU
2	M	657	LEU
2	M	664	ILE
2	M	666	ASP
2	M	673	THR
2	M	674	LEU
2	M	675	ILE
2	M	677	ASP
2	M	682	GLU
2	M	686	GLU
1	N	3	ARG
1	N	7	ARG
1	N	10	LEU
1	N	11	VAL
1	N	22	VAL
1	N	44	THR
1	N	85	THR
1	N	86	PHE
1	N	96	PHE
1	N	108	LEU
1	N	110	SER
1	N	112	ASN
1	N	113	LEU
1	N	114	GLU
1	N	122	VAL
1	N	125	GLU

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Mol	Chain	Res	Type
1	N	126	LEU
1	N	133	THR
1	N	137	ASN
1	N	147	GLU
1	P	508	ILE
1	P	528	LEU
1	P	534	ILE
1	P	535	THR
1	P	537	THR
1	P	546	THR
1	P	547	VAL
1	P	575	LEU
1	P	594	TYR
1	P	597	PHE
1	P	607	ARG
1	P	613	LEU
1	P	623	ILE
1	P	625	GLU
1	P	628	CYS
1	P	631	LEU
1	P	637	ASN
1	P	650	ARG
1	P	652	LEU
2	O	2	GLU
2	O	4	LEU
2	O	17	GLN
2	O	23	LEU
2	O	28	PHE
2	O	42	GLN
2	O	43	GLN
2	O	50	ASP
2	O	51	THR
2	O	56	GLN
2	O	61	LEU
2	O	79	LEU
2	O	83	LEU
2	O	84	LEU
2	O	97	CYS
2	O	106	LEU
2	O	112	LEU
2	O	125	LEU
2	O	133	GLN

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Mol	Chain	Res	Type
2	O	151	ARG
2	O	161	ASP
2	O	165	GLN
2	O	173	THR
2	O	195	ILE
2	O	211	VAL
2	O	215	GLN
2	O	216	ASP
2	O	219	MET
2	O	223	THR
2	Q	501	MET
2	Q	502	GLU
2	Q	516	LEU
2	Q	518	LEU
2	Q	520	GLU
2	Q	521	ASN
2	Q	523	LEU
2	Q	530	THR
2	Q	536	LEU
2	Q	550	ASP
2	Q	566	THR
2	Q	578	ASN
2	Q	592	GLU
2	Q	602	ASP
2	Q	604	LEU
2	Q	606	LEU
2	Q	613	SER
2	Q	617	PHE
2	Q	644	LEU
2	Q	651	ARG
2	Q	659	MET
2	Q	665	GLN
2	Q	669	GLU
2	Q	674	LEU
2	Q	676	ARG
2	Q	678	ARG
2	Q	679	LEU
2	Q	686	GLU
2	Q	687	ASN
2	Q	711	VAL
2	Q	712	MET
2	Q	714	LEU

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Mol	Chain	Res	Type
2	Q	715	GLN
2	Q	719	MET
2	Q	723	THR
1	R	3	ARG
1	R	90	LYS
1	R	131	LEU
1	R	137	ASN
1	R	147	GLU
1	R	150	ARG
1	R	151	LEU
1	R	153	ARG
1	V	503	ARG
1	V	508	ILE
1	V	510	LEU
1	V	517	THR
1	V	521	GLN
1	V	529	GLU
1	V	534	ILE
1	V	557	ASP
1	V	558	ASP
1	V	574	LEU
1	V	582	ASP
1	V	587	ASN
1	V	591	GLU
1	V	594	TYR
1	V	597	PHE
1	V	608	LEU
1	V	613	LEU
1	V	614	GLU
1	V	615	LYS
1	V	617	GLU
1	V	630	CYS
1	V	650	ARG
2	S	10	MET
2	S	15	TRP
2	S	16	LEU
2	S	23	LEU
2	S	43	GLN
2	S	48	GLN
2	S	62	ASN
2	S	64	ARG
2	S	65	LEU

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Mol	Chain	Res	Type
2	S	79	LEU
2	S	81	ARG
2	S	97	CYS
2	S	109	ARG
2	S	115	LEU
2	S	139	LEU
2	S	143	SER
2	S	149	GLN
2	S	156	LEU
2	S	161	ASP
2	S	162	LEU
2	S	164	ILE
2	S	168	GLN
2	S	177	ASP
2	S	179	LEU
2	S	188	SER
2	S	204	ILE
2	S	206	ASP
2	S	213	ASN
2	W	511	GLN
2	W	517	GLN
2	W	521	ASN
2	W	522	SER
2	W	536	LEU
2	W	546	HIS
2	W	563	LYS
2	W	564	ARG
2	W	565	LEU
2	W	575	HIS
2	W	597	CYS
2	W	602	ASP
2	W	606	LEU
2	W	617	PHE
2	W	646	LEU
2	W	656	LEU
2	W	675	ILE
2	W	676	ARG
2	W	691	GLU
2	W	693	PHE
2	W	715	GLN
2	W	716	ASP
2	W	724	GLN

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Mol	Chain	Res	Type
2	W	726	HIS
2	W	727	HIS
2	T	16	LEU
2	T	23	LEU
2	T	24	LEU
2	T	48	GLN
2	T	50	ASP
2	T	56	GLN
2	T	57	ARG
2	T	63	LYS
2	T	65	LEU
2	T	76	LEU
2	T	86	ASP
2	T	109	ARG
2	T	111	GLU
2	T	112	LEU
2	T	115	LEU
2	T	117	PHE
2	T	133	GLN
2	T	140	MET
2	T	146	LEU
2	T	175	ILE
2	T	179	LEU
2	T	213	ASN
2	T	214	LEU
2	T	225	HIS
2	X	505	GLU
2	X	518	LEU
2	X	523	LEU
2	X	524	LEU
2	X	538	VAL
2	X	547	GLU
2	X	550	ASP
2	X	565	LEU
2	X	566	THR
2	X	578	ASN
2	X	594	THR
2	X	604	LEU
2	X	609	ARG
2	X	617	PHE
2	X	624	MET
2	X	630	LEU

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Mol	Chain	Res	Type
2	X	646	LEU
2	X	647	GLN
2	X	677	ASP
2	X	687	ASN
2	X	691	GLU
2	X	692	GLN
2	X	700	GLU
2	X	714	LEU
1	U	1	MET
1	U	2	GLU
1	U	8	ILE
1	U	10	LEU
1	U	13	GLU
1	U	21	GLN
1	U	50	SER
1	U	87	ASN
1	U	94	TYR
1	U	97	PHE
1	U	108	LEU
1	U	111	PHE
1	U	112	ASN
1	U	113	LEU
1	U	118	ASN
1	U	121	GLU
1	U	125	GLU
1	U	126	LEU
1	U	130	CYS
1	U	137	ASN
1	U	155	TRP
1	U	156	ASN
1	Y	504	LYS
1	Y	506	SER
1	Y	517	THR
1	Y	520	LEU
1	Y	551	GLU
1	Y	552	ILE
1	Y	569	GLU
1	Y	574	LEU
1	Y	594	TYR
1	Y	606	PHE
1	Y	611	PHE
1	Y	613	LEU

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Mol	Chain	Res	Type
1	Y	621	GLU
1	Y	631	LEU
1	Y	632	ASP
1	Y	637	ASN
1	Y	651	LEU
1	Y	653	ARG
1	Y	654	ASP
1	Y	655	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (165) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
1	A	112	ASN
1	A	118	ASN
1	A	138	GLN
1	A	145	GLN
1	B	600	ASN
1	B	637	ASN
2	D	17	GLN
2	D	32	GLN
2	D	42	GLN
2	D	46	HIS
2	D	48	GLN
2	D	78	ASN
2	D	120	ASN
2	D	165	GLN
2	D	215	GLN
2	D	226	HIS
2	E	511	GLN
2	E	575	HIS
2	E	633	GLN
2	E	668	GLN
2	E	692	GLN
2	E	724	GLN
1	F	87	ASN
1	F	100	ASN
1	F	112	ASN
1	F	118	ASN
1	F	141	ASN
1	F	143	HIS
1	G	554	GLN

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Mol	Chain	Res	Type
1	G	587	ASN
1	G	600	ASN
1	G	656	ASN
2	H	6	GLN
2	H	11	GLN
2	H	21	ASN
2	H	42	GLN
2	H	48	GLN
2	H	75	HIS
2	H	134	HIS
2	H	147	GLN
2	H	192	GLN
2	H	213	ASN
2	H	215	GLN
2	H	224	GLN
2	H	225	HIS
2	I	542	GLN
2	I	546	HIS
2	I	556	GLN
2	I	647	GLN
2	I	668	GLN
2	I	724	GLN
1	J	21	GLN
1	J	137	ASN
1	J	138	GLN
1	J	156	ASN
1	K	554	GLN
1	K	612	ASN
1	K	618	ASN
1	K	637	ASN
1	K	641	ASN
1	K	656	ASN
2	L	6	GLN
2	L	17	GLN
2	L	48	GLN
2	L	78	ASN
2	L	120	ASN
2	L	168	GLN
2	L	215	GLN
2	L	224	GLN
2	L	226	HIS
2	M	517	GLN

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Mol	Chain	Res	Type
2	M	542	GLN
2	M	543	GLN
2	M	556	GLN
2	M	620	ASN
2	M	622	HIS
2	M	633	GLN
2	M	634	HIS
2	M	665	GLN
2	M	668	GLN
2	M	687	ASN
2	M	724	GLN
2	M	725	HIS
1	N	112	ASN
1	N	137	ASN
1	N	141	ASN
1	P	612	ASN
1	P	618	ASN
1	P	641	ASN
1	P	656	ASN
2	O	17	GLN
2	O	32	GLN
2	O	43	GLN
2	O	48	GLN
2	O	56	GLN
2	O	120	ASN
2	O	133	GLN
2	O	165	GLN
2	O	215	GLN
2	O	224	GLN
2	Q	517	GLN
2	Q	521	ASN
2	Q	532	GLN
2	Q	542	GLN
2	Q	562	ASN
2	Q	578	ASN
2	Q	620	ASN
2	Q	665	GLN
2	Q	668	GLN
2	Q	687	ASN
2	Q	713	ASN
1	R	18	HIS
1	R	21	GLN

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Mol	Chain	Res	Type
1	R	137	ASN
1	R	141	ASN
1	R	148	ASN
1	V	518	HIS
1	V	554	GLN
1	V	587	ASN
1	V	612	ASN
1	V	637	ASN
1	V	656	ASN
2	S	6	GLN
2	S	43	GLN
2	S	48	GLN
2	S	62	ASN
2	S	168	GLN
2	S	192	GLN
2	S	225	HIS
2	S	226	HIS
2	W	511	GLN
2	W	517	GLN
2	W	521	ASN
2	W	633	GLN
2	W	668	GLN
2	W	715	GLN
2	W	724	GLN
2	T	6	GLN
2	T	17	GLN
2	T	21	ASN
2	T	48	GLN
2	T	62	ASN
2	T	133	GLN
2	T	165	GLN
2	T	215	GLN
2	T	225	HIS
2	X	548	GLN
2	X	575	HIS
2	X	634	HIS
2	X	647	GLN
2	X	649	GLN
2	X	665	GLN
2	X	668	GLN
2	X	692	GLN
2	X	725	HIS

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Mol	Chain	Res	Type
1	U	40	HIS
1	U	112	ASN
1	U	118	ASN
1	U	156	ASN
1	Y	540	HIS
1	Y	612	ASN
1	Y	637	ASN
1	Y	643	HIS
1	Y	656	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	TBR	X	5	-	0,36,36	0.00	-	-		
3	TBR	P	2	-	0,36,36	0.00	-	-		
3	TBR	D	231	-	0,36,36	0.00	-	-		
3	TBR	V	1	-	0,36,36	0.00	-	-		
3	TBR	M	164	-	0,36,36	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	TBR	J	164	-	0,36,36	0.00	-	-		
3	TBR	Y	10	-	0,36,36	0.00	-	-		
3	TBR	H	231	-	0,36,36	0.00	-	-		

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

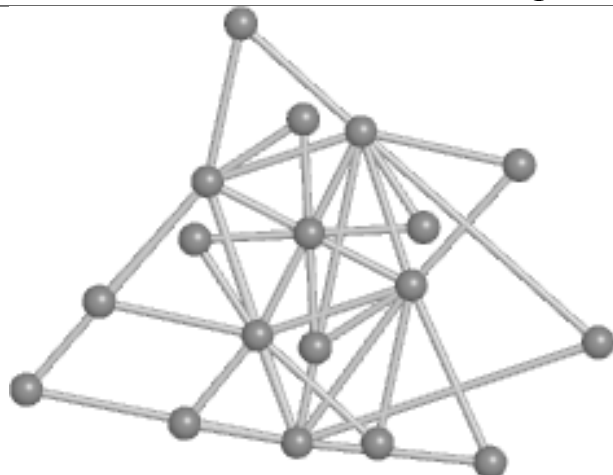
There are no ring outliers.

5 monomers are involved in 49 short contacts:

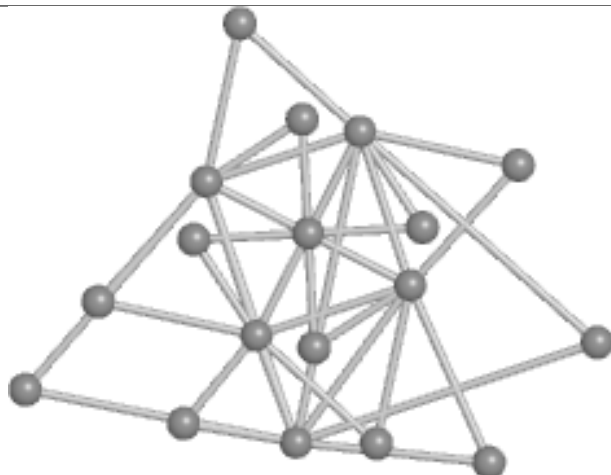
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	X	5	TBR	4	0
3	P	2	TBR	1	34
3	M	164	TBR	3	0
3	J	164	TBR	2	2
3	Y	10	TBR	3	0

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

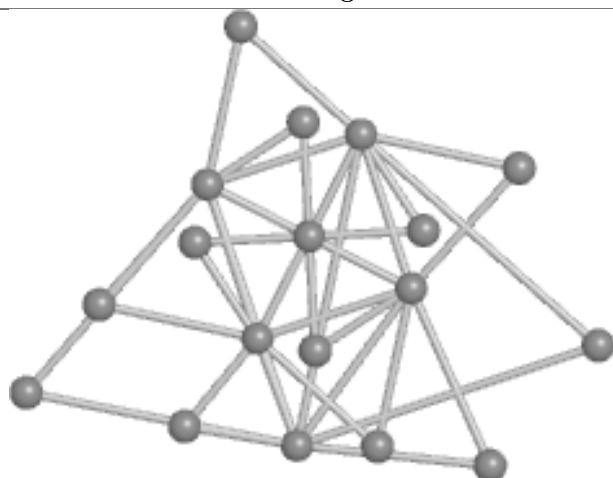
Ligand TBR X 5



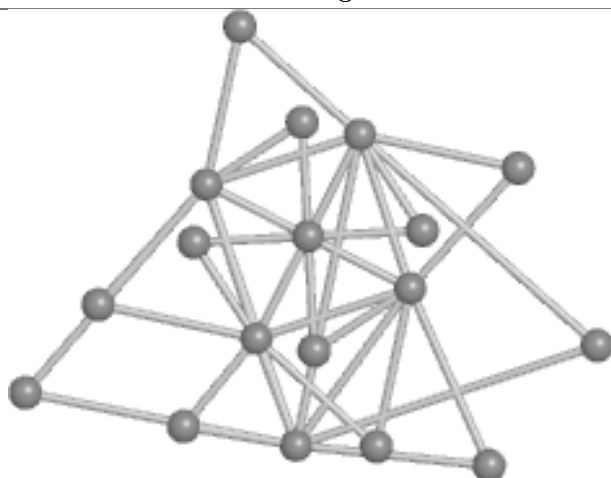
Bond lengths



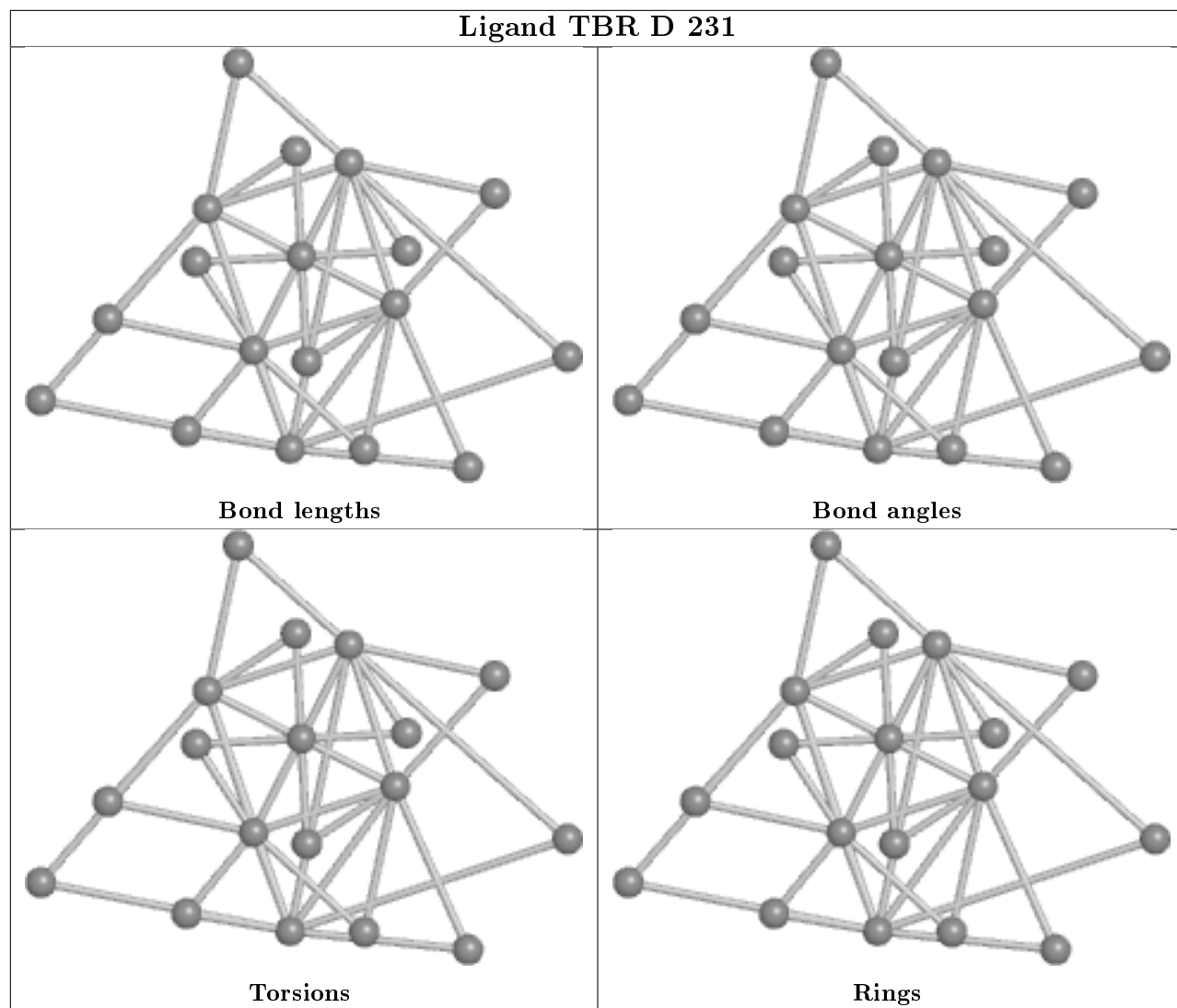
Bond angles

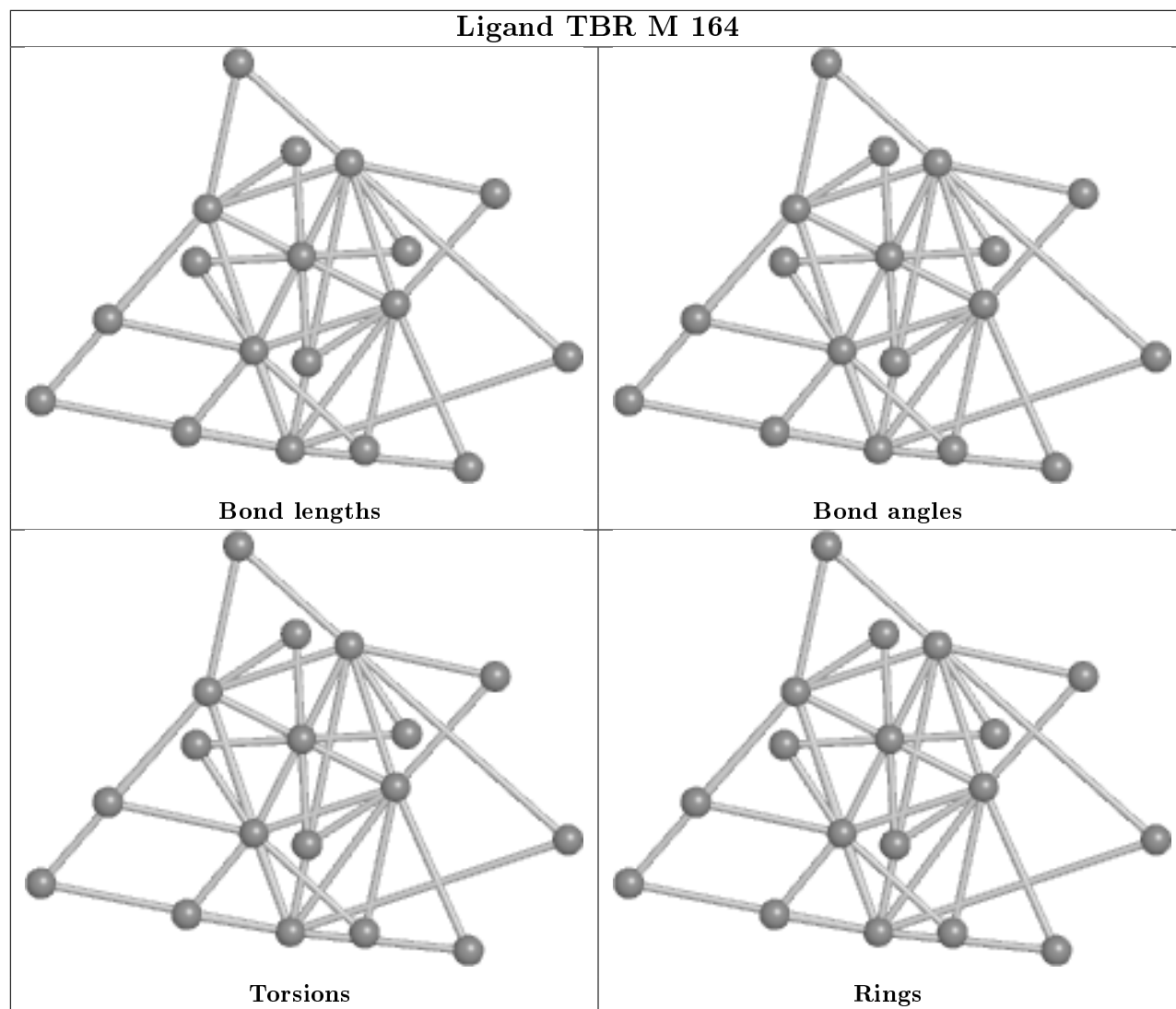


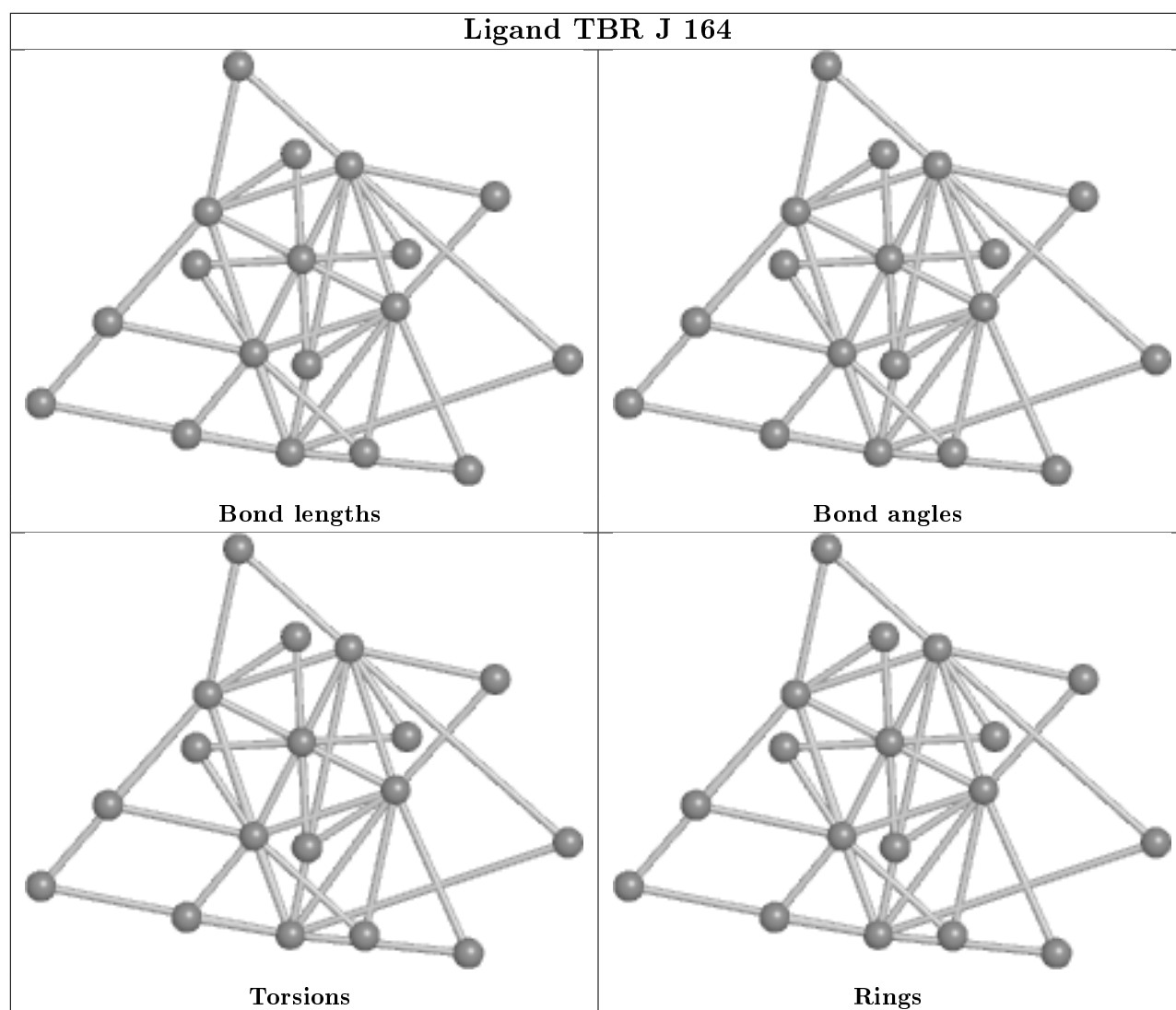
Torsions



Rings







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	147/163 (90%)	0.80	22 (14%)	2 2	143, 217, 261, 290	0
1	B	152/163 (93%)	0.60	19 (12%)	3 5	130, 199, 240, 289	0
1	F	157/163 (96%)	0.35	17 (10%)	5 5	121, 173, 263, 314	0
1	G	157/163 (96%)	0.30	11 (7%)	16 13	119, 173, 217, 265	0
1	J	157/163 (96%)	0.48	19 (12%)	4 5	168, 209, 241, 255	0
1	K	157/163 (96%)	0.66	21 (13%)	3 3	175, 216, 268, 312	0
1	N	157/163 (96%)	0.14	7 (4%)	33 28	115, 159, 206, 250	0
1	P	157/163 (96%)	0.31	4 (2%)	57 47	109, 169, 230, 262	0
1	R	157/163 (96%)	0.19	5 (3%)	47 37	145, 184, 217, 234	0
1	U	157/163 (96%)	0.22	8 (5%)	28 24	147, 184, 233, 291	0
1	V	157/163 (96%)	0.19	4 (2%)	57 47	123, 184, 219, 273	0
1	Y	157/163 (96%)	0.51	17 (10%)	5 5	148, 202, 251, 276	0
2	D	227/230 (98%)	0.06	2 (0%)	84 77	87, 144, 202, 244	0
2	E	227/230 (98%)	0.23	13 (5%)	23 20	99, 156, 233, 269	0
2	H	227/230 (98%)	0.12	5 (2%)	62 52	107, 152, 210, 256	0
2	I	227/230 (98%)	0.25	11 (4%)	30 26	113, 156, 213, 277	0
2	L	227/230 (98%)	0.12	4 (1%)	68 60	98, 152, 218, 251	0
2	M	227/230 (98%)	0.13	7 (3%)	49 38	106, 167, 210, 244	0
2	O	227/230 (98%)	0.19	9 (3%)	38 31	109, 165, 225, 311	0
2	Q	227/230 (98%)	0.20	4 (1%)	68 60	99, 150, 211, 239	0
2	S	218/230 (94%)	-0.02	1 (0%)	91 85	111, 167, 216, 241	0
2	T	224/230 (97%)	0.24	12 (5%)	25 22	146, 199, 243, 267	0
2	W	227/230 (98%)	0.18	6 (2%)	56 46	107, 160, 206, 242	0
2	X	227/230 (98%)	0.17	11 (4%)	30 26	140, 189, 233, 303	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
All	All	4581/4716 (97%)	0.25	239 (5%)	27	24	87, 175, 238, 314	0

All (239) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	151	LEU	6.6
2	E	591	SER	6.4
1	G	529	GLU	5.7
1	J	81	ALA	5.7
2	O	89	HIS	5.6
1	K	597	PHE	5.6
1	F	152	LEU	5.6
1	B	644	LEU	5.6
2	E	501	MET	5.2
1	F	153	ARG	5.1
1	J	82	ASP	5.0
1	B	648	ASN	4.8
2	I	501	MET	4.7
2	X	590	PRO	4.6
1	B	527	THR	4.3
1	F	154	ASP	4.3
1	J	80	PRO	4.2
1	P	655	TRP	3.9
2	X	589	HIS	3.9
1	J	108	LEU	3.9
1	K	603	ASP	3.8
2	I	593	ALA	3.8
1	B	528	LEU	3.8
1	Y	582	ASP	3.8
1	B	652	LEU	3.7
2	T	181	THR	3.7
2	I	610	SER	3.7
1	N	28	LEU	3.6
2	E	592	GLU	3.6
1	A	31	GLY	3.5
2	W	515	TRP	3.5
2	E	593	ALA	3.4
1	R	74	LEU	3.4
2	H	179	LEU	3.4
2	Q	664	ILE	3.4
2	O	174	LEU	3.4
1	G	532	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	J	74	LEU	3.4
2	T	170	SER	3.3
2	O	179	LEU	3.3
1	B	654	ASP	3.3
1	J	79	GLY	3.3
2	M	610	SER	3.3
1	A	141	ASN	3.3
2	I	592	GLU	3.3
2	H	174	LEU	3.3
1	B	574	LEU	3.2
1	A	32	PHE	3.2
1	A	64	GLY	3.2
1	Y	578	ALA	3.2
1	B	532	PHE	3.2
1	F	155	TRP	3.2
1	Y	574	LEU	3.2
1	A	62	GLU	3.1
1	Y	617	GLU	3.1
2	L	89	HIS	3.1
1	J	99	LYS	3.1
2	T	153	LEU	3.1
1	K	598	GLU	3.1
1	A	47	VAL	3.1
1	A	147	GLU	3.0
2	X	519	ALA	3.0
2	T	91	SER	3.0
1	U	151	LEU	3.0
1	A	137	ASN	3.0
2	O	83	LEU	3.0
1	B	651	LEU	3.0
1	J	148	ASN	3.0
2	E	727	HIS	3.0
2	T	119	TRP	3.0
1	U	63	LYS	2.9
1	K	601	LEU	2.9
2	D	149	GLN	2.9
2	W	592	GLU	2.9
1	A	28	LEU	2.9
1	N	29	GLU	2.9
2	E	587	ALA	2.9
2	O	181	THR	2.9
1	Y	563	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	J	28	LEU	2.9
1	J	144	LEU	2.9
1	U	152	LEU	2.9
1	K	648	ASN	2.9
2	H	19	ALA	2.9
1	Y	651	LEU	2.9
1	A	46	THR	2.8
2	X	616	PRO	2.8
2	I	589	HIS	2.8
2	Q	663	GLU	2.8
2	X	591	SER	2.8
1	A	144	LEU	2.8
1	K	574	LEU	2.8
1	B	655	TRP	2.7
1	F	141	ASN	2.7
2	X	515	TRP	2.7
1	G	648	ASN	2.7
1	B	539	GLY	2.7
1	K	586	PHE	2.7
1	A	97	PHE	2.7
2	X	684	PHE	2.7
1	Y	579	GLY	2.7
1	Y	652	LEU	2.6
1	F	90	LYS	2.6
2	H	64	ARG	2.6
2	X	653	LEU	2.6
1	B	656	ASN	2.6
1	K	571	ARG	2.6
1	A	80	PRO	2.6
2	T	15	TRP	2.6
2	I	591	SER	2.6
1	F	74	LEU	2.6
1	K	575	LEU	2.6
1	R	28	LEU	2.6
2	D	20	GLU	2.6
2	M	618	TYR	2.6
1	K	611	PHE	2.6
1	U	21	GLN	2.6
1	K	539	GLY	2.6
1	A	37	THR	2.6
1	Y	536	LEU	2.5
2	I	595	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	573	ALA	2.5
1	V	578	ALA	2.5
1	R	63	LYS	2.5
1	Y	586	PHE	2.5
1	Y	597	PHE	2.5
2	O	97	CYS	2.5
1	P	555	GLU	2.5
1	B	653	ARG	2.5
1	Y	581	ALA	2.5
1	J	151	LEU	2.5
2	H	109	ARG	2.5
1	A	67	VAL	2.5
1	F	145	GLN	2.5
2	T	92	GLU	2.5
1	G	547	VAL	2.5
1	J	29	GLU	2.5
2	I	684	PHE	2.5
1	N	21	GLN	2.5
1	P	532	PHE	2.5
2	W	589	HIS	2.5
2	M	609	ARG	2.5
1	Y	648	ASN	2.5
1	J	97	PHE	2.5
1	A	66	TYR	2.4
2	X	612	LEU	2.4
1	K	602	LYS	2.4
2	O	90	PRO	2.4
1	V	528	LEU	2.4
2	Q	501	MET	2.4
1	G	643	HIS	2.4
1	F	149	GLU	2.4
2	T	50	ASP	2.4
1	V	519	PHE	2.4
1	K	561	MET	2.4
2	M	675	ILE	2.4
1	F	148	ASN	2.4
1	G	574	LEU	2.4
2	M	592	GLU	2.3
1	J	66	TYR	2.3
1	K	534	ILE	2.3
1	A	29	GLU	2.3
1	V	586	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
2	T	27	VAL	2.3
1	J	86	PHE	2.3
2	E	595	PHE	2.3
1	F	150	ARG	2.3
1	K	532	PHE	2.3
2	E	615	LEU	2.3
2	T	31	LYS	2.3
2	L	82	PRO	2.3
1	G	654	ASP	2.3
1	A	82	ASP	2.3
2	M	677	ASP	2.3
1	K	657	ASP	2.3
1	A	81	ALA	2.3
2	L	29	ILE	2.3
1	J	113	LEU	2.3
2	W	591	SER	2.3
2	W	706	ASP	2.3
2	X	516	LEU	2.3
1	F	88	PHE	2.3
1	F	156	ASN	2.3
1	Y	539	GLY	2.3
1	N	52	ILE	2.3
2	E	681	THR	2.3
2	I	611	GLU	2.2
2	E	670	SER	2.2
1	G	522	VAL	2.2
1	U	28	LEU	2.2
1	N	66	TYR	2.2
1	B	526	LYS	2.2
1	A	50	SER	2.2
1	F	146	LYS	2.2
1	P	597	PHE	2.2
2	I	575	HIS	2.2
1	B	582	ASP	2.2
1	B	529	GLU	2.2
1	G	524	TRP	2.2
1	B	588	PHE	2.2
1	A	63	LYS	2.2
1	K	546	THR	2.2
2	T	186	GLU	2.2
1	G	597	PHE	2.1
1	J	155	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	R	99	LYS	2.1
2	E	580	LEU	2.1
2	L	64	ARG	2.1
1	K	528	LEU	2.1
1	N	74	LEU	2.1
2	W	590	PRO	2.1
1	K	617	GLU	2.1
2	T	149	GLN	2.1
1	J	21	GLN	2.1
1	R	103	ASP	2.1
2	E	590	PRO	2.1
2	Q	683	PRO	2.1
1	U	26	LYS	2.1
1	A	74	LEU	2.1
1	Y	616	VAL	2.1
1	F	144	LEU	2.1
1	U	95	PHE	2.1
2	S	115	LEU	2.1
2	E	649	GLN	2.1
2	O	84	LEU	2.1
1	G	644	LEU	2.0
1	K	567	VAL	2.0
1	N	82	ASP	2.0
1	K	581	ALA	2.0
1	U	155	TRP	2.0
1	Y	532	PHE	2.0
1	F	78	ALA	2.0
1	Y	599	LYS	2.0
2	O	17	GLN	2.0
1	B	608	LEU	2.0
2	M	595	PHE	2.0
1	J	10	LEU	2.0
2	X	618	TYR	2.0
2	I	590	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

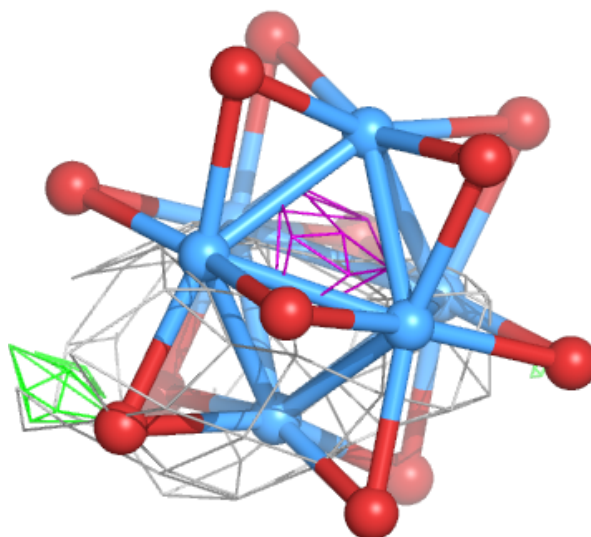
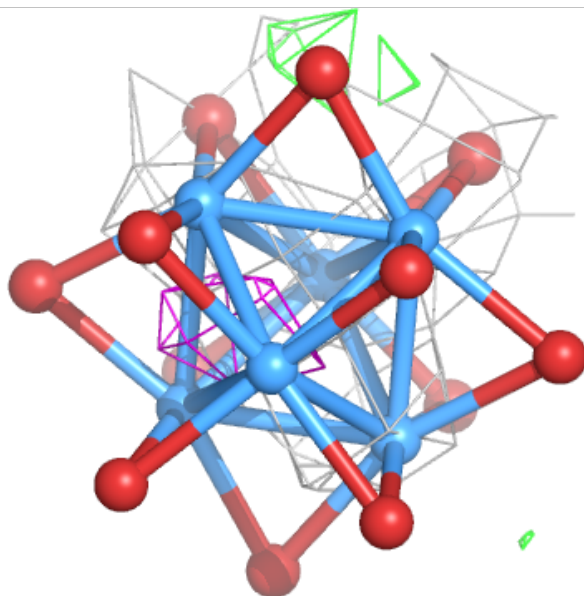
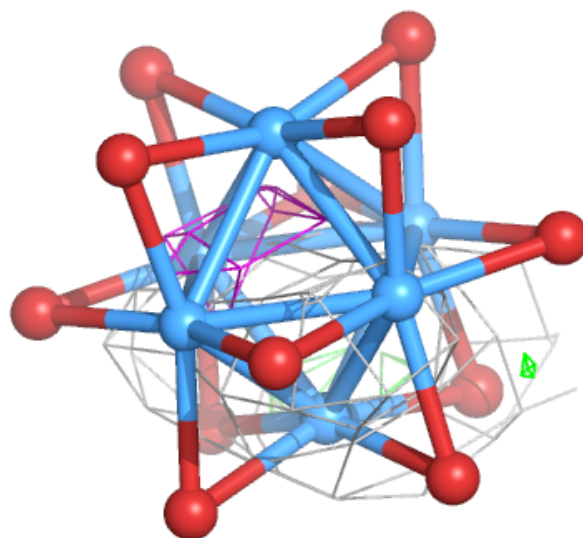
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	TBR	J	164	18/18	0.55	0.56	162,195,258,266	18
3	TBR	D	231	18/18	0.63	0.45	126,168,199,206	18
3	TBR	X	5	18/18	0.72	0.41	134,172,195,230	18
3	TBR	M	164	18/18	0.73	0.42	151,181,255,301	18
3	TBR	H	231	18/18	0.79	0.38	128,160,180,224	18
3	TBR	P	2	18/18	0.83	0.17	210,281,466,490	18
3	TBR	V	1	18/18	0.87	0.26	103,151,191,204	18
3	TBR	Y	10	18/18	0.89	0.20	130,168,192,193	18

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

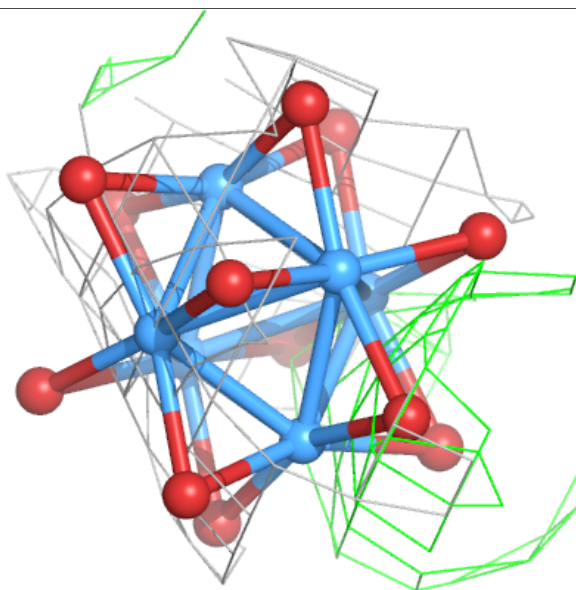
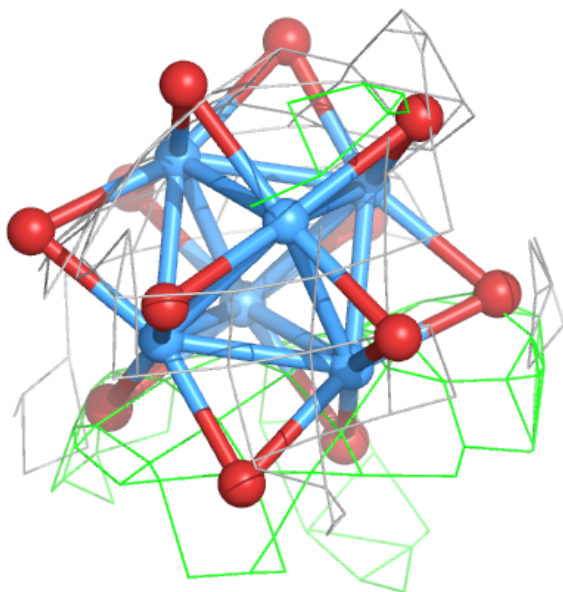
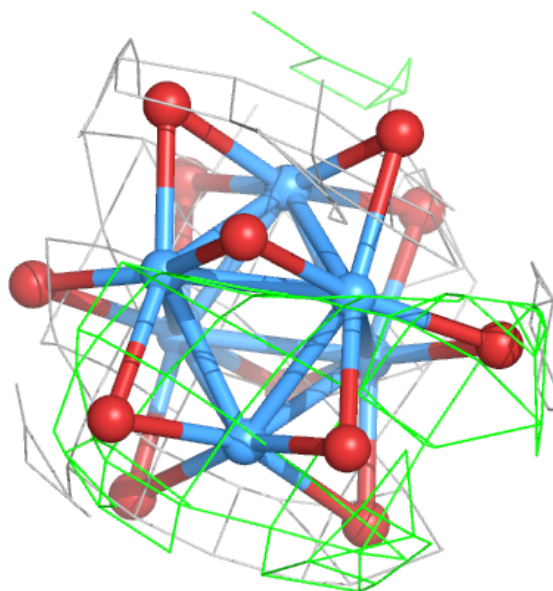
Electron density around TBR J 164:

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



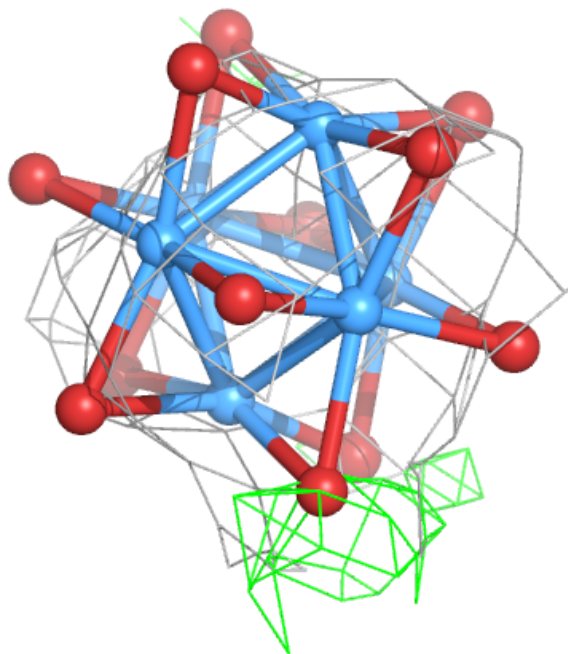
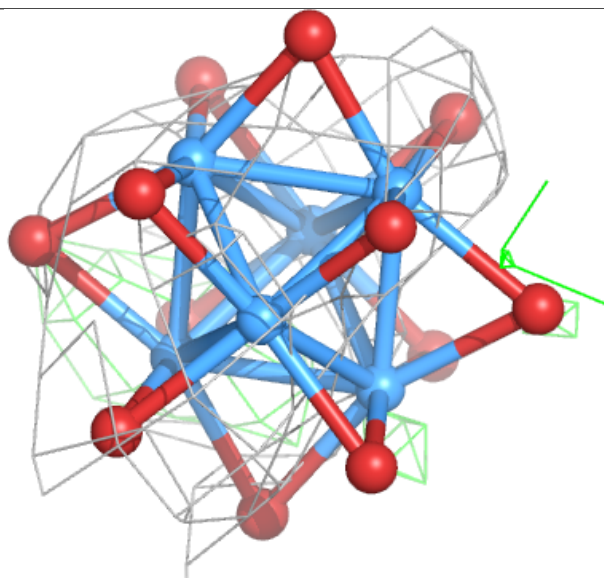
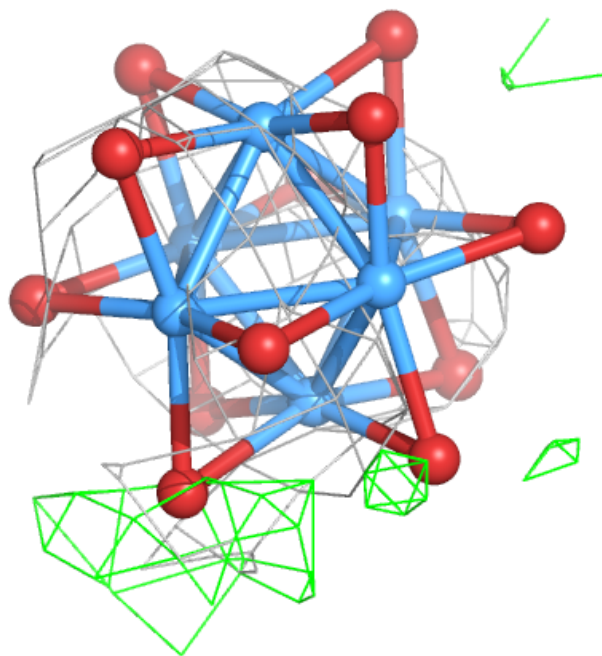
Electron density around TBR D 231:

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



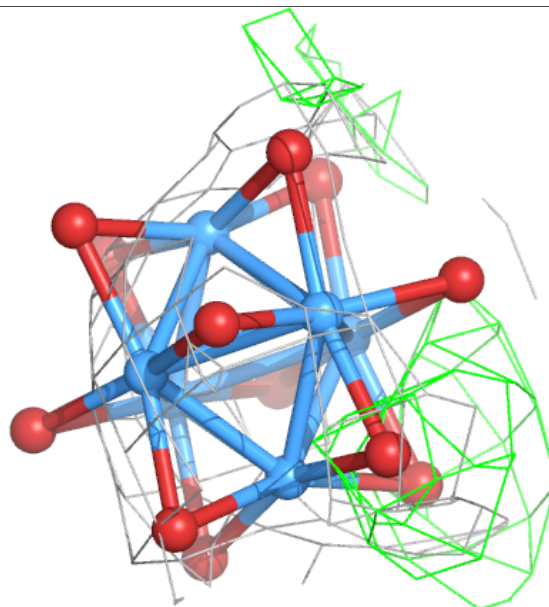
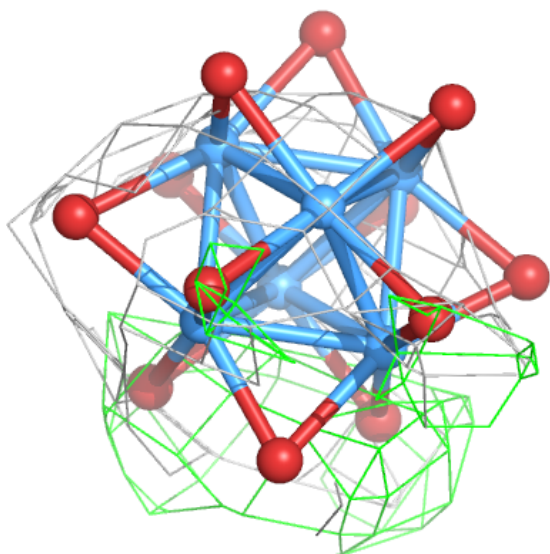
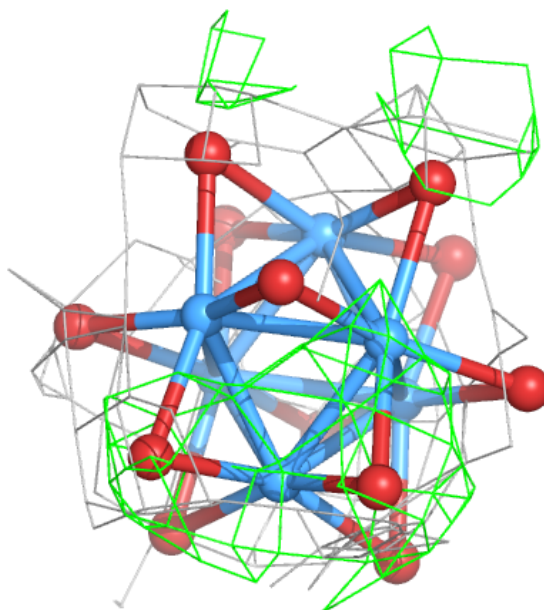
Electron density around TBR X 5:

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



Electron density around TBR M 164:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.