



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:38 PM UTC

PDB ID : 2H1L / pdb_00002h1l
Title : The Structure of the Oncoprotein SV40 Large T Antigen and p53 Tumor Suppressor Complex
Authors : Lilyestrom, W.; Klein, M.G.; Chen, X.S.
Deposited on : 2006-05-16
Resolution : 3.16 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

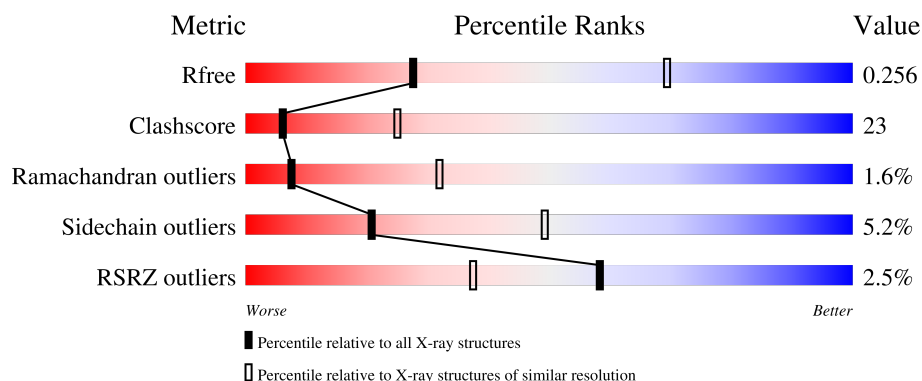
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.16 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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

Mol	Chain	Length	Quality of chain
1	A	370	% 55% 38% 5% •
1	B	370	% 47% 46% 5% •
1	C	370	% 49% 44% 5% •
1	D	370	% 52% 43% • •
1	E	370	% 52% 40% 5% • •

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Mol	Chain	Length	Quality of chain
1	F	370	
1	G	370	
1	H	370	
1	I	370	
1	J	370	
1	K	370	
1	L	370	
2	M	203	
2	N	203	
2	O	203	
2	P	203	
2	Q	203	
2	R	203	
2	S	203	
2	T	203	
2	U	203	
2	V	203	
2	W	203	
2	X	203	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 53920 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 Large T antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	0	0
			2933	1888	493	531	21			
1	B	362	Total	C	N	O	S	0	0	0
			2933	1888	493	531	21			
1	C	363	Total	C	N	O	S	0	0	0
			2940	1892	494	533	21			
1	D	362	Total	C	N	O	S	0	0	0
			2933	1888	493	531	21			
1	E	362	Total	C	N	O	S	0	0	0
			2933	1888	493	531	21			
1	F	363	Total	C	N	O	S	0	0	0
			2940	1892	494	533	21			
1	G	362	Total	C	N	O	S	0	0	0
			2933	1888	493	531	21			
1	H	362	Total	C	N	O	S	0	0	0
			2933	1888	493	531	21			
1	I	363	Total	C	N	O	S	0	0	0
			2940	1892	494	533	21			
1	J	362	Total	C	N	O	S	0	0	0
			2933	1888	493	531	21			
1	K	362	Total	C	N	O	S	0	0	0
			2933	1888	493	531	21			
1	L	363	Total	C	N	O	S	0	0	0
			2940	1892	494	533	21			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	258	GLY	-	cloning artifact	UNP Q9NP68
A	259	SER	-	cloning artifact	UNP Q9NP68
B	258	GLY	-	cloning artifact	UNP Q9NP68
B	259	SER	-	cloning artifact	UNP Q9NP68
C	258	GLY	-	cloning artifact	UNP Q9NP68

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Chain	Residue	Modelled	Actual	Comment	Reference
C	259	SER	-	cloning artifact	UNP Q9NP68
D	258	GLY	-	cloning artifact	UNP Q9NP68
D	259	SER	-	cloning artifact	UNP Q9NP68
E	258	GLY	-	cloning artifact	UNP Q9NP68
E	259	SER	-	cloning artifact	UNP Q9NP68
F	258	GLY	-	cloning artifact	UNP Q9NP68
F	259	SER	-	cloning artifact	UNP Q9NP68
G	258	GLY	-	cloning artifact	UNP Q9NP68
G	259	SER	-	cloning artifact	UNP Q9NP68
H	258	GLY	-	cloning artifact	UNP Q9NP68
H	259	SER	-	cloning artifact	UNP Q9NP68
I	258	GLY	-	cloning artifact	UNP Q9NP68
I	259	SER	-	cloning artifact	UNP Q9NP68
J	258	GLY	-	cloning artifact	UNP Q9NP68
J	259	SER	-	cloning artifact	UNP Q9NP68
K	258	GLY	-	cloning artifact	UNP Q9NP68
K	259	SER	-	cloning artifact	UNP Q9NP68
L	258	GLY	-	cloning artifact	UNP Q9NP68
L	259	SER	-	cloning artifact	UNP Q9NP68

- Molecule 2 is a protein called Cellular tumor antigen p53.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	199	Total	C	N	O	S	0	0	0
			1556	959	286	295	16			
2	N	199	Total	C	N	O	S	0	0	0
			1556	959	286	295	16			
2	O	199	Total	C	N	O	S	0	0	0
			1556	959	286	295	16			
2	P	199	Total	C	N	O	S	0	0	0
			1556	959	286	295	16			
2	Q	199	Total	C	N	O	S	0	0	0
			1556	959	286	295	16			
2	R	199	Total	C	N	O	S	0	0	0
			1556	959	286	295	16			
2	S	199	Total	C	N	O	S	0	0	0
			1556	959	286	295	16			
2	T	199	Total	C	N	O	S	0	0	0
			1556	959	286	295	16			
2	U	199	Total	C	N	O	S	0	0	0
			1556	959	286	295	16			
2	V	199	Total	C	N	O	S	0	0	0
			1556	959	286	295	16			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	W	199	Total	C	N	O	S	0	0	0
			1556	959	286	295	16			
2	X	199	Total	C	N	O	S	0	0	0
			1556	959	286	295	16			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	90	GLY	-	cloning artifact	UNP Q9NP68
M	91	SER	-	cloning artifact	UNP Q9NP68
N	90	GLY	-	cloning artifact	UNP Q9NP68
N	91	SER	-	cloning artifact	UNP Q9NP68
O	90	GLY	-	cloning artifact	UNP Q9NP68
O	91	SER	-	cloning artifact	UNP Q9NP68
P	90	GLY	-	cloning artifact	UNP Q9NP68
P	91	SER	-	cloning artifact	UNP Q9NP68
Q	90	GLY	-	cloning artifact	UNP Q9NP68
Q	91	SER	-	cloning artifact	UNP Q9NP68
R	90	GLY	-	cloning artifact	UNP Q9NP68
R	91	SER	-	cloning artifact	UNP Q9NP68
S	90	GLY	-	cloning artifact	UNP Q9NP68
S	91	SER	-	cloning artifact	UNP Q9NP68
T	90	GLY	-	cloning artifact	UNP Q9NP68
T	91	SER	-	cloning artifact	UNP Q9NP68
U	90	GLY	-	cloning artifact	UNP Q9NP68
U	91	SER	-	cloning artifact	UNP Q9NP68
V	90	GLY	-	cloning artifact	UNP Q9NP68
V	91	SER	-	cloning artifact	UNP Q9NP68
W	90	GLY	-	cloning artifact	UNP Q9NP68
W	91	SER	-	cloning artifact	UNP Q9NP68
X	90	GLY	-	cloning artifact	UNP Q9NP68
X	91	SER	-	cloning artifact	UNP Q9NP68

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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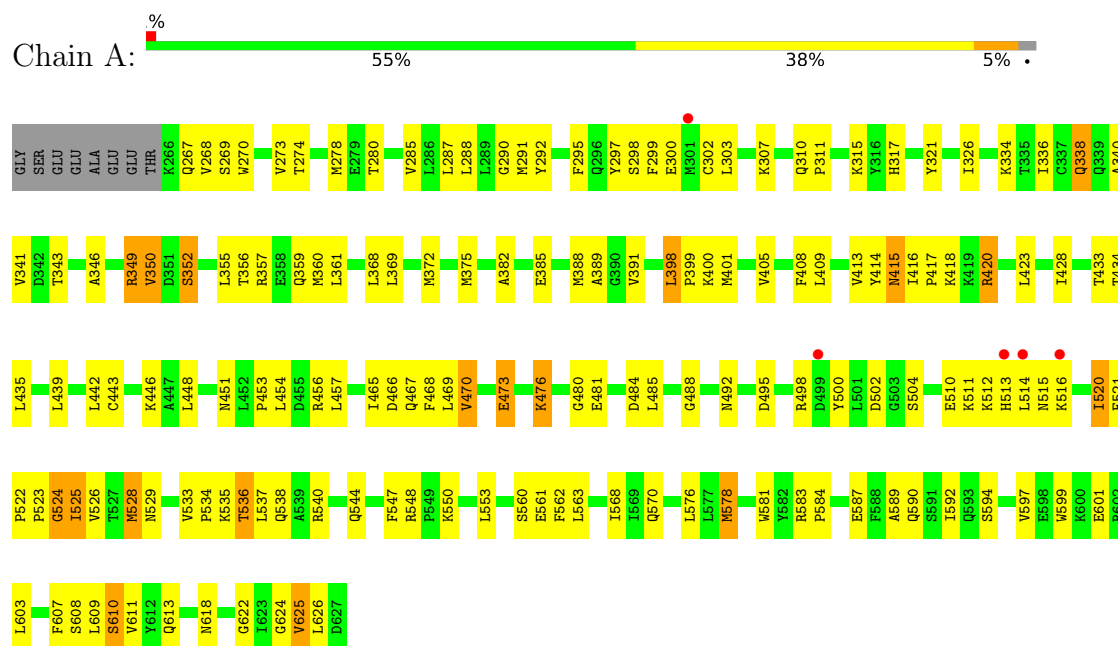
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total 1	Zn 1	0	0
3	E	1	Total 1	Zn 1	0	0
3	F	1	Total 1	Zn 1	0	0
3	G	1	Total 1	Zn 1	0	0
3	H	1	Total 1	Zn 1	0	0
3	I	1	Total 1	Zn 1	0	0
3	J	1	Total 1	Zn 1	0	0
3	K	1	Total 1	Zn 1	0	0
3	L	1	Total 1	Zn 1	0	0
3	M	1	Total 1	Zn 1	0	0
3	N	1	Total 1	Zn 1	0	0
3	O	1	Total 1	Zn 1	0	0
3	P	1	Total 1	Zn 1	0	0
3	Q	1	Total 1	Zn 1	0	0
3	R	1	Total 1	Zn 1	0	0
3	S	1	Total 1	Zn 1	0	0
3	T	1	Total 1	Zn 1	0	0
3	U	1	Total 1	Zn 1	0	0
3	V	1	Total 1	Zn 1	0	0
3	W	1	Total 1	Zn 1	0	0
3	X	1	Total 1	Zn 1	0	0

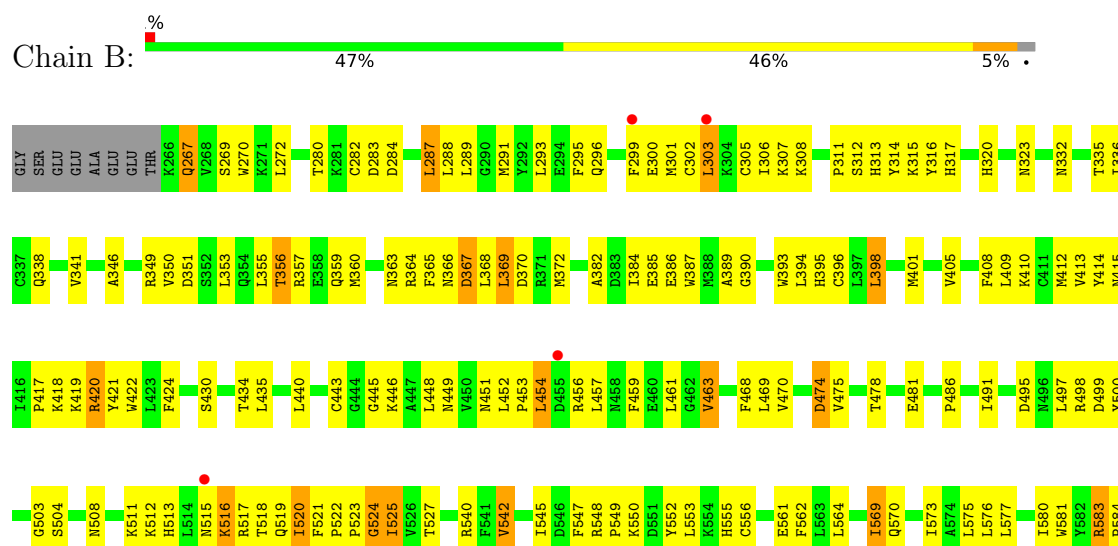
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

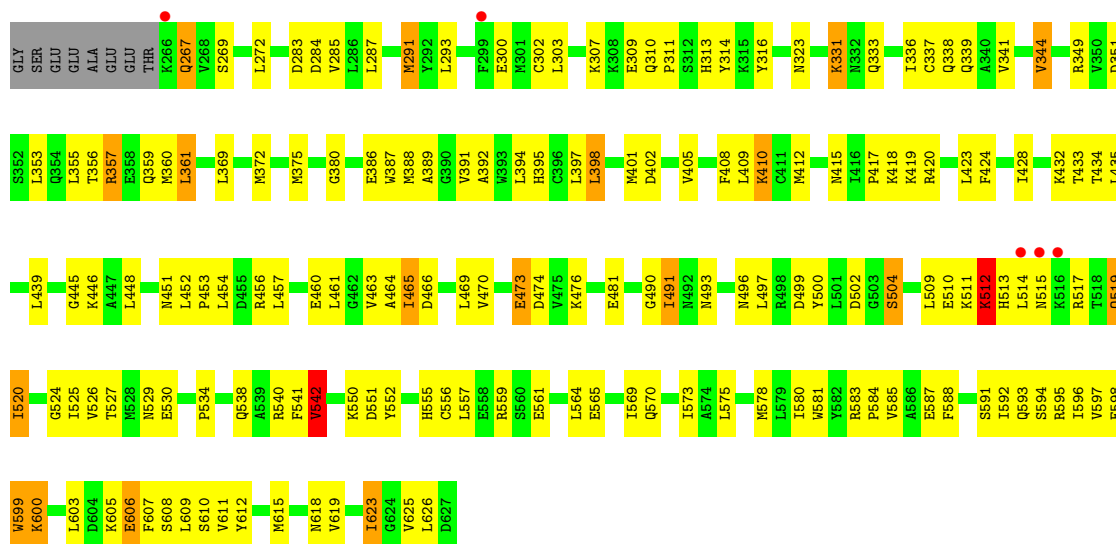
• Molecule 1: Large T antigen



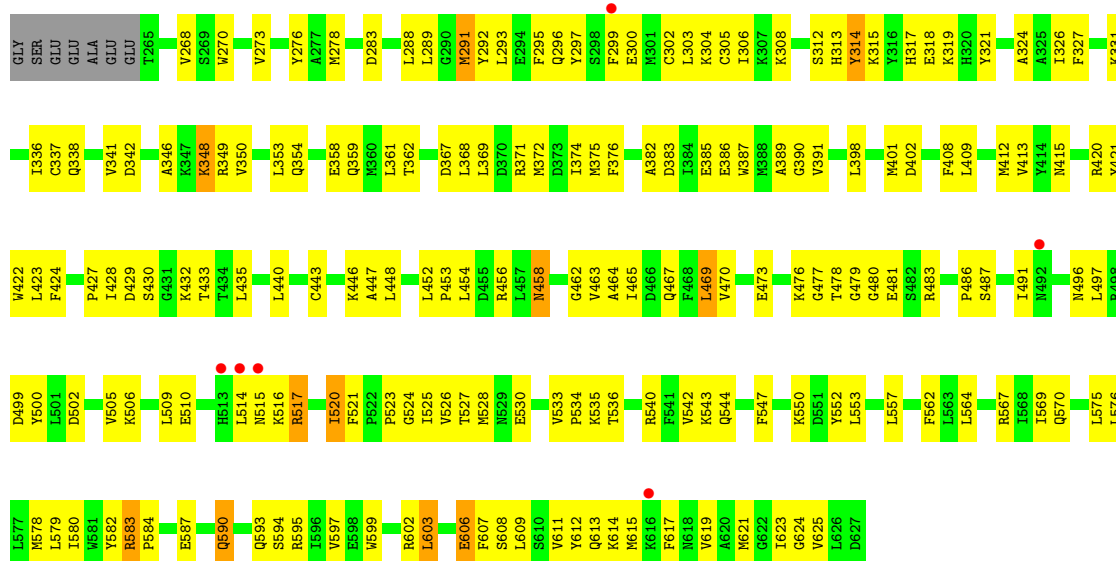
• Molecule 1: Large T antigen



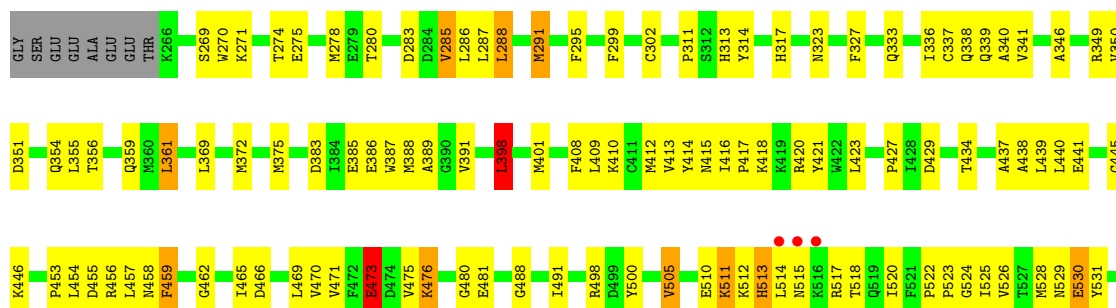




• Molecule 1: Large T antigen

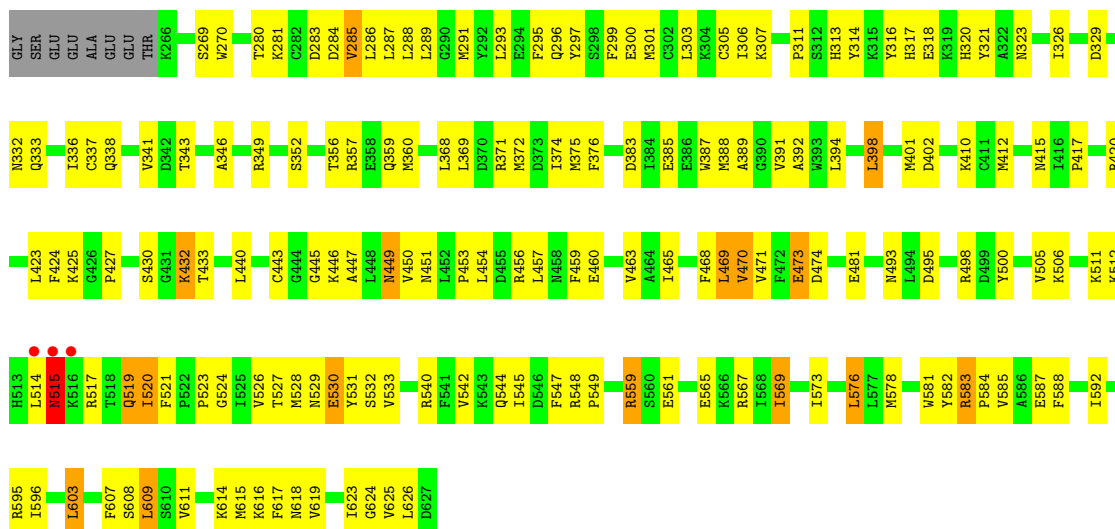


• Molecule 1: Large T antigen

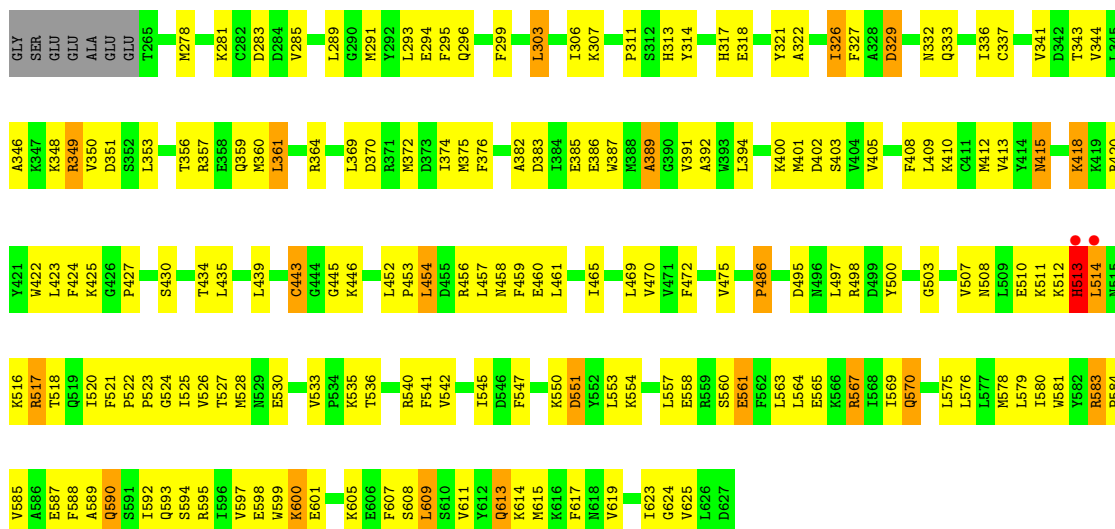




• Molecule 1: Large T antigen

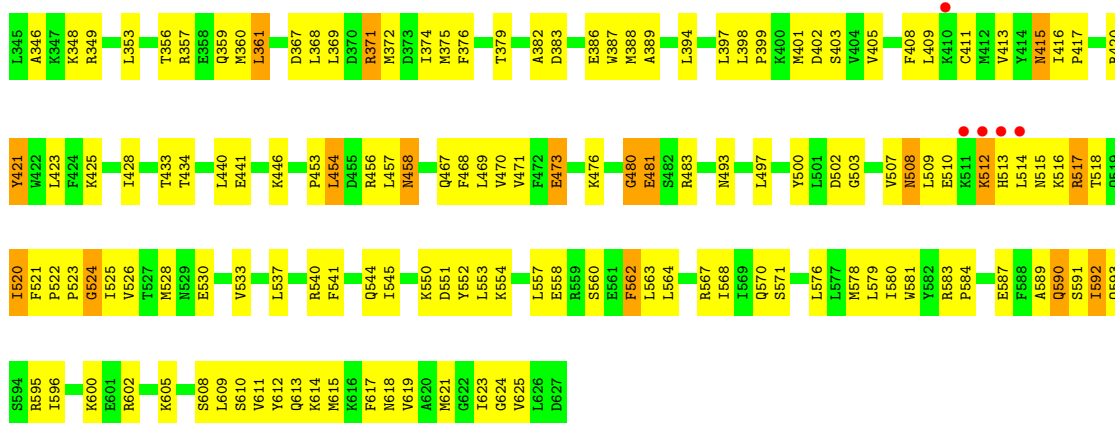


• Molecule 1: Large T antigen

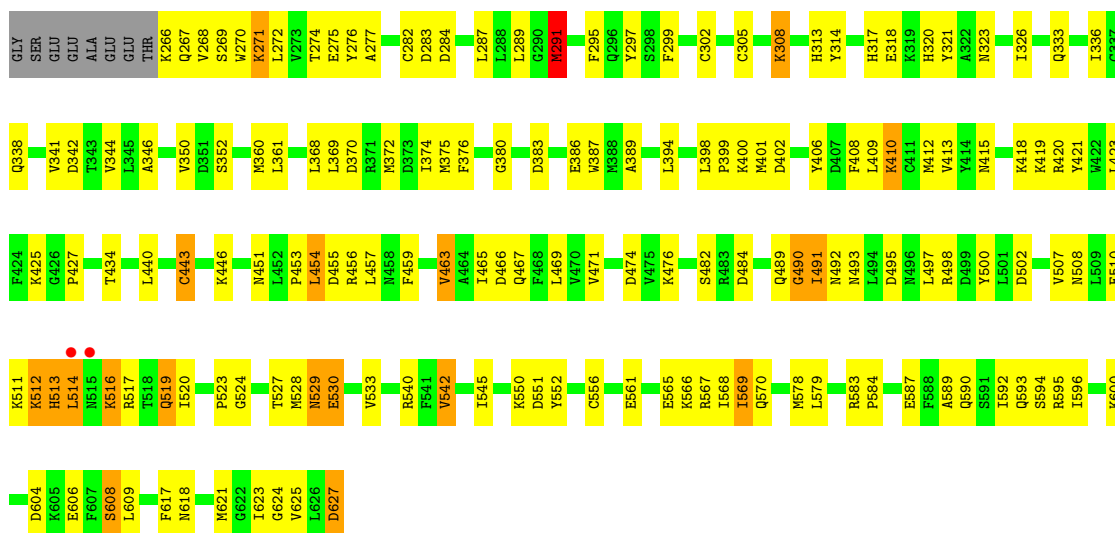


• Molecule 1: Large T antigen

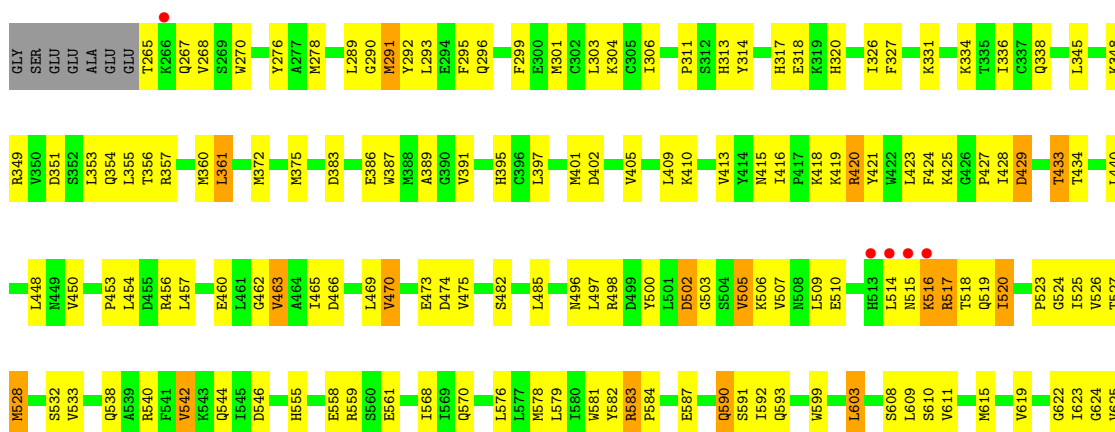




• Molecule 1: Large T antigen



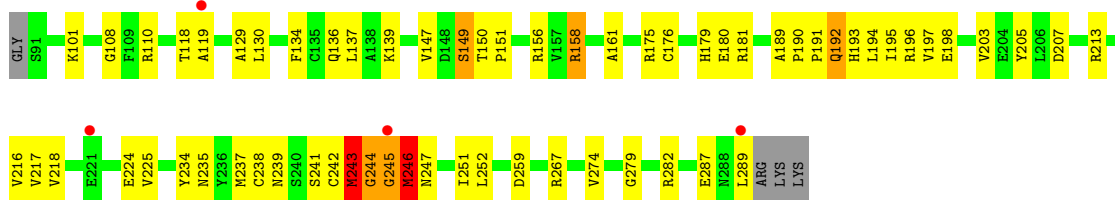
• Molecule 1: Large T antigen



L626
D627

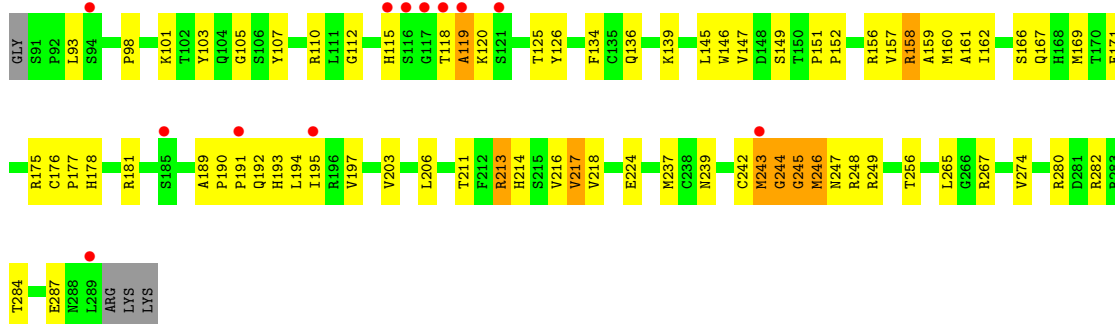
• Molecule 2: Cellular tumor antigen p53

Chain M: 



• Molecule 2: Cellular tumor antigen p53

Chain N: 



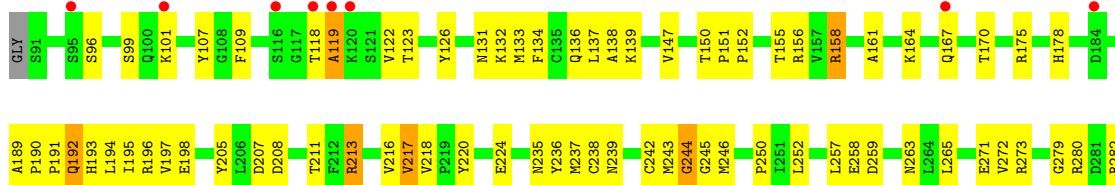
• Molecule 2: Cellular tumor antigen p53

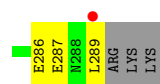
Chain O: 



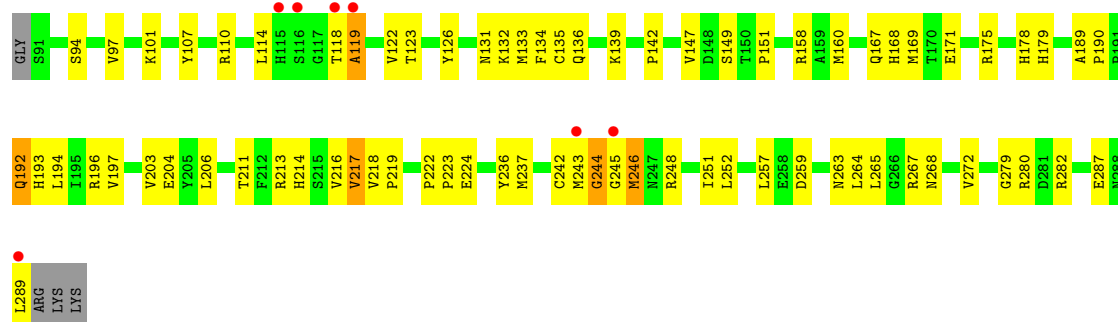
• Molecule 2: Cellular tumor antigen p53

Chain P: 

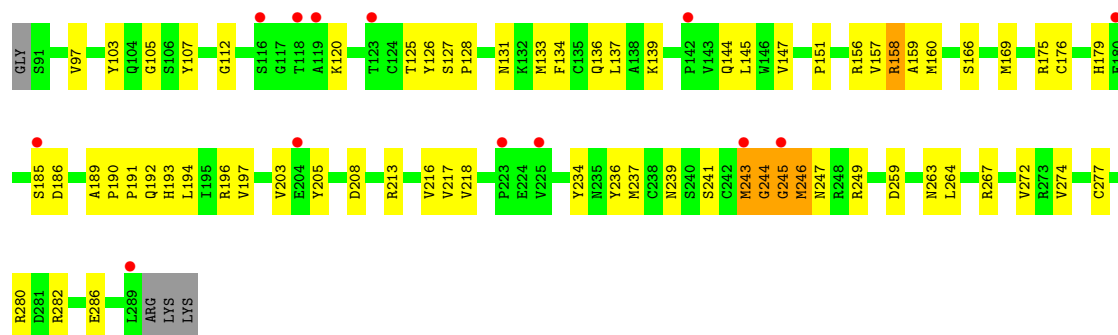




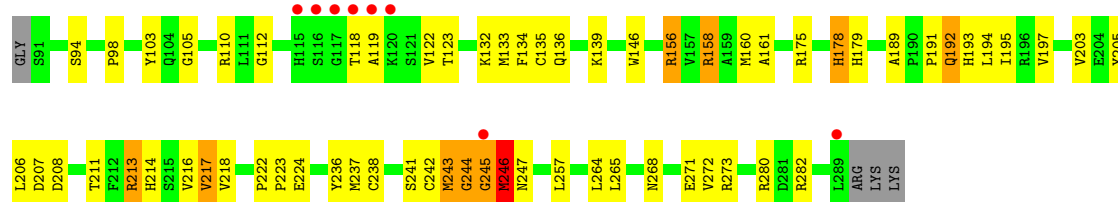
• Molecule 2: Cellular tumor antigen p53



• Molecule 2: Cellular tumor antigen p53



• Molecule 2: Cellular tumor antigen p53

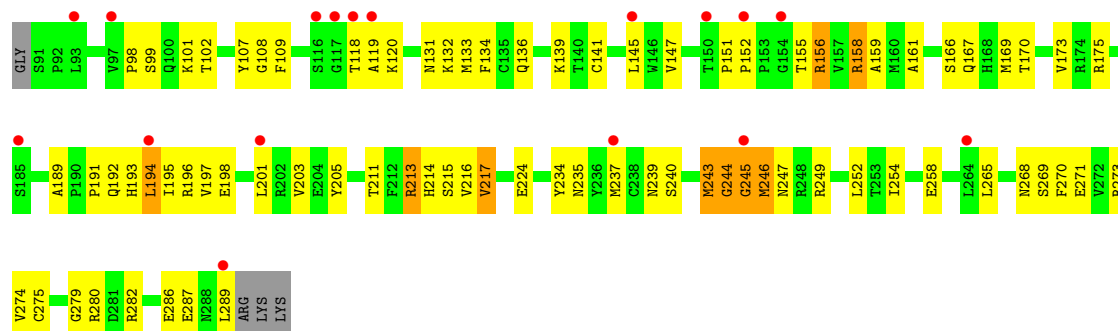


• Molecule 2: Cellular tumor antigen p53

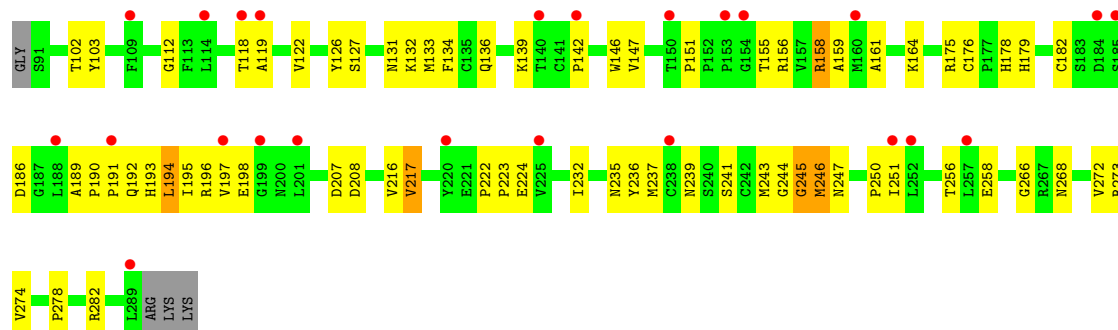




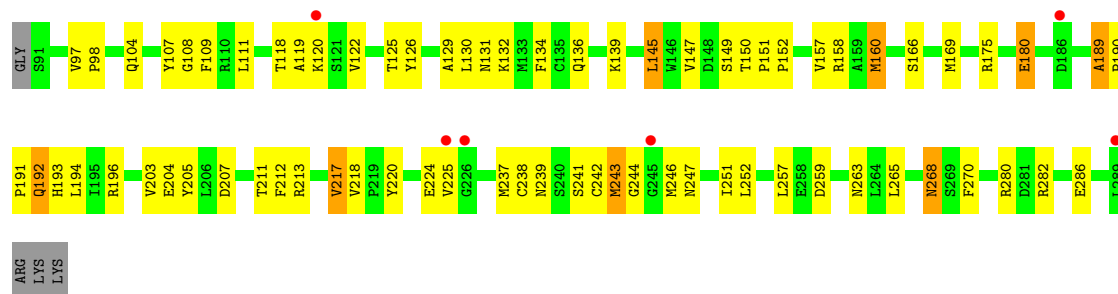
• Molecule 2: Cellular tumor antigen p53



• Molecule 2: Cellular tumor antigen p53

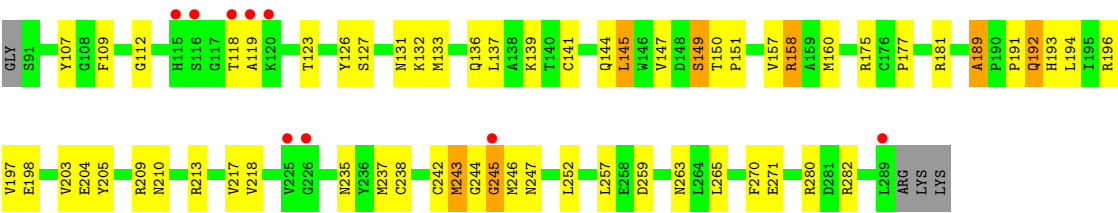


• Molecule 2: Cellular tumor antigen p53



• Molecule 2: Cellular tumor antigen p53





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	127.02Å 182.72Å 262.06Å 90.00° 92.08° 90.00°	Depositor
Resolution (Å)	20.00 – 3.16 20.00 – 3.16	Depositor EDS
% Data completeness (in resolution range)	97.3 (20.00-3.16) 96.7 (20.00-3.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.13 (at 3.15Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.261 , 0.308 0.252 , 0.256	Depositor DCC
R_{free} test set	15212 reflections (7.08%)	wwPDB-VP
Wilson B-factor (Å ²)	81.4	Xtriage
Anisotropy	0.595	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 38.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	53920	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.71	0/2992	0.97	4/4030 (0.1%)
1	B	0.68	0/2992	0.98	6/4030 (0.1%)
1	C	0.67	0/2999	0.91	5/4040 (0.1%)
1	D	0.73	0/2992	0.96	3/4030 (0.1%)
1	E	0.75	2/2992 (0.1%)	0.96	4/4030 (0.1%)
1	F	0.73	0/2999	0.94	1/4040 (0.0%)
1	G	0.82	2/2992 (0.1%)	1.01	6/4030 (0.1%)
1	H	0.77	1/2992 (0.0%)	0.97	4/4030 (0.1%)
1	I	0.68	1/2999 (0.0%)	0.98	9/4040 (0.2%)
1	J	0.64	1/2992 (0.0%)	0.92	6/4030 (0.1%)
1	K	0.77	1/2992 (0.0%)	0.98	3/4030 (0.1%)
1	L	0.85	1/2999 (0.0%)	1.02	8/4040 (0.2%)
2	M	0.78	2/1592 (0.1%)	0.90	0/2160
2	N	0.58	1/1592 (0.1%)	0.84	0/2160
2	O	0.59	1/1592 (0.1%)	0.91	0/2160
2	P	0.66	1/1592 (0.1%)	0.89	0/2160
2	Q	0.62	2/1592 (0.1%)	0.88	0/2160
2	R	0.61	1/1592 (0.1%)	0.86	0/2160
2	S	0.70	2/1592 (0.1%)	0.90	1/2160 (0.0%)
2	T	0.63	1/1592 (0.1%)	0.91	2/2160 (0.1%)
2	U	0.69	1/1592 (0.1%)	0.87	1/2160 (0.0%)
2	V	0.59	1/1592 (0.1%)	0.82	0/2160
2	W	0.80	2/1592 (0.1%)	0.98	7/2160 (0.3%)
2	X	0.84	1/1592 (0.1%)	0.99	5/2160 (0.2%)
All	All	0.72	25/55036 (0.0%)	0.94	75/74320 (0.1%)

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	243	MET	SD-CE	16.35	2.20	1.79
2	U	243	MET	SD-CE	13.41	2.13	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	243	MET	SD-CE	13.14	2.12	1.79
2	W	243	MET	SD-CE	11.98	2.09	1.79
2	S	243	MET	SD-CE	11.69	2.08	1.79
2	R	243	MET	SD-CE	10.68	2.06	1.79
2	T	243	MET	SD-CE	10.00	2.04	1.79
1	G	291	MET	SD-CE	9.76	2.04	1.79
2	N	243	MET	SD-CE	9.62	2.03	1.79
2	V	243	MET	SD-CE	8.71	2.01	1.79
2	P	243	MET	SD-CE	8.37	2.00	1.79
2	O	243	MET	SD-CE	8.01	1.99	1.79
2	Q	243	MET	SD-CE	7.71	1.98	1.79
2	S	246	MET	SD-CE	-6.85	1.62	1.79
2	Q	246	MET	SD-CE	-6.29	1.63	1.79
1	E	542	VAL	CA-CB	-5.78	1.47	1.54
1	K	291	MET	SD-CE	5.61	1.93	1.79
2	W	160	MET	SD-CE	5.58	1.93	1.79
1	L	291	MET	SD-CE	5.54	1.93	1.79
1	G	437	ALA	CA-CB	-5.40	1.44	1.53
1	I	585	VAL	CA-CB	-5.32	1.48	1.54
1	E	291	MET	SD-CE	5.31	1.92	1.79
1	H	285	VAL	CA-CB	-5.10	1.48	1.54
1	J	278	MET	SD-CE	5.01	1.92	1.79
2	M	246	MET	SD-CE	-5.01	1.67	1.79

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	600	LYS	N-CA-C	-9.47	103.82	114.62
1	L	583	ARG	CA-C-N	8.13	128.07	120.03
1	L	583	ARG	C-N-CA	8.13	128.07	120.03
1	H	514	LEU	N-CA-C	7.61	119.21	111.07
1	G	583	ARG	CA-C-N	7.50	127.45	120.03
1	G	583	ARG	C-N-CA	7.50	127.45	120.03
1	G	398	LEU	CA-C-N	6.95	128.04	119.98
1	G	398	LEU	C-N-CA	6.95	128.04	119.98
1	A	578	MET	N-CA-C	-6.73	104.22	113.18
1	J	411	CYS	N-CA-C	-6.70	105.74	114.04
1	J	600	LYS	N-CA-C	-6.57	105.57	113.97
2	T	131	ASN	N-CA-C	-6.47	103.01	111.74
1	B	583	ARG	N-CA-C	6.32	116.87	109.60
1	E	600	LYS	N-CA-C	-6.30	105.56	113.18
1	G	572	GLY	N-CA-C	-6.30	104.71	112.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	512	LYS	CB-CA-C	-6.21	109.42	116.63
1	E	599	TRP	N-CA-C	-6.20	107.56	114.62
1	J	371	ARG	N-CA-C	-6.19	105.38	113.12
2	X	189	ALA	CA-C-N	6.16	124.10	119.66
2	X	189	ALA	C-N-CA	6.16	124.10	119.66
1	I	460	GLU	N-CA-C	-6.13	104.87	112.72
1	A	352	SER	N-CA-C	-6.12	105.10	114.16
1	E	530	GLU	N-CA-C	6.06	118.00	110.91
1	F	517	ARG	N-CA-C	6.04	118.34	108.55
1	C	583	ARG	CA-C-N	5.98	126.48	120.14
1	C	583	ARG	C-N-CA	5.98	126.48	120.14
1	I	326	ILE	N-CA-C	-5.94	105.96	112.80
1	I	461	LEU	N-CA-C	-5.93	105.89	113.01
1	A	524	GLY	N-CA-C	5.85	118.75	110.74
1	H	533	VAL	N-CA-C	5.83	114.93	108.05
1	L	533	VAL	CA-C-N	5.80	125.76	119.78
1	L	533	VAL	C-N-CA	5.80	125.76	119.78
1	L	485	LEU	CA-C-N	5.78	126.07	119.83
1	L	485	LEU	C-N-CA	5.78	126.07	119.83
1	J	524	GLY	N-CA-C	5.78	118.65	110.74
1	J	421	TYR	N-CA-C	5.76	118.30	108.90
1	D	517	ARG	N-CA-C	5.74	117.12	108.46
1	B	583	ARG	CA-C-N	5.72	125.62	119.85
1	B	583	ARG	C-N-CA	5.72	125.62	119.85
1	K	533	VAL	N-CA-C	5.65	114.17	107.73
1	J	517	ARG	N-CA-C	5.61	117.05	108.52
2	U	131	ASN	N-CA-C	-5.61	104.17	111.74
2	W	218	VAL	CA-C-N	5.57	125.50	119.76
2	W	218	VAL	C-N-CA	5.57	125.50	119.76
1	B	367	ASP	N-CA-C	-5.51	107.21	114.04
2	W	189	ALA	CA-C-N	5.50	123.62	119.66
2	W	189	ALA	C-N-CA	5.50	123.62	119.66
1	C	348	LYS	N-CA-C	-5.48	106.64	113.55
1	H	515	ASN	N-CA-C	5.46	117.61	107.99
1	I	533	VAL	CA-C-N	5.46	125.37	119.85
1	I	533	VAL	C-N-CA	5.46	125.37	119.85
1	I	583	ARG	CA-C-N	5.38	125.38	120.21
1	I	583	ARG	C-N-CA	5.38	125.38	120.21
1	L	482	SER	N-CA-C	-5.35	106.43	113.17
1	C	533	VAL	CA-C-N	5.34	125.35	119.90
1	C	533	VAL	C-N-CA	5.34	125.35	119.90
1	I	389	ALA	N-CA-C	-5.33	105.55	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	576	LEU	N-CA-C	-5.28	105.53	111.28
2	W	265	LEU	N-CA-C	-5.27	108.11	114.75
1	B	524	GLY	N-CA-C	5.26	117.95	110.74
2	X	131	ASN	N-CA-C	-5.25	104.65	111.74
2	T	265	LEU	N-CA-C	-5.24	108.14	114.75
2	X	127	SER	CA-C-N	5.24	125.04	119.28
2	X	127	SER	C-N-CA	5.24	125.04	119.28
1	B	369	LEU	N-CA-C	-5.22	105.77	111.82
2	S	178	HIS	N-CA-C	5.20	116.80	111.03
1	D	559	ARG	N-CA-C	-5.20	107.96	114.56
1	A	625	VAL	N-CA-C	5.17	115.31	110.30
1	D	533	VAL	N-CA-C	5.17	114.15	108.05
1	E	496	ASN	N-CA-C	-5.10	106.84	113.16
1	G	473	GLU	N-CA-C	5.10	117.60	109.96
1	K	299	PHE	N-CA-C	-5.09	106.92	113.23
2	W	150	THR	CA-C-N	5.09	125.62	120.38
2	W	150	THR	C-N-CA	5.09	125.62	120.38
1	L	517	ARG	N-CA-C	5.02	116.56	108.32

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	2933	0	2982	141	0
1	B	2933	0	2982	182	0
1	C	2940	0	2989	193	0
1	D	2933	0	2982	159	0
1	E	2933	0	2982	158	0
1	F	2940	0	2989	178	0
1	G	2933	0	2982	137	0
1	H	2933	0	2982	157	0
1	I	2940	0	2989	170	0
1	J	2933	0	2982	170	0
1	K	2933	0	2982	145	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2940	0	2989	147	0
2	M	1556	0	1514	45	0
2	N	1556	0	1515	63	0
2	O	1556	0	1513	71	0
2	P	1556	0	1513	65	0
2	Q	1556	0	1513	50	0
2	R	1556	0	1513	56	0
2	S	1556	0	1513	59	0
2	T	1556	0	1513	60	0
2	U	1556	0	1514	70	0
2	V	1556	0	1515	47	0
2	W	1556	0	1513	46	0
2	X	1556	0	1513	50	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
3	R	1	0	0	0	0
3	S	1	0	0	0	0
3	T	1	0	0	0	0
3	U	1	0	0	0	0
3	V	1	0	0	0	0
3	W	1	0	0	0	0
3	X	1	0	0	0	0
All	All	53920	0	53974	2430	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (2430) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:291:MET:CE	1:G:291:MET:SD	2.04	1.46
2:T:243:MET:SD	2:T:243:MET:CE	2.04	1.46
2:N:243:MET:CE	2:N:243:MET:SD	2.03	1.45
2:R:243:MET:CE	2:R:243:MET:SD	2.06	1.43
2:S:243:MET:CE	2:S:243:MET:SD	2.08	1.41
2:W:243:MET:SD	2:W:243:MET:CE	2.09	1.41
2:X:243:MET:CE	2:X:243:MET:SD	2.12	1.38
2:U:243:MET:CE	2:U:243:MET:SD	2.13	1.37
2:M:243:MET:CE	2:M:243:MET:SD	2.20	1.28
1:G:415:ASN:ND2	1:G:420:ARG:HD2	1.69	1.06
2:O:198:GLU:HB2	2:O:235:ASN:HD21	1.22	1.00
1:J:357:ARG:HA	1:J:360:MET:HE2	1.43	0.99
1:A:446:LYS:HG2	1:A:467:GLN:HE21	1.27	0.98
1:A:415:ASN:HD21	1:A:420:ARG:HH11	1.12	0.96
1:C:520:ILE:HD13	1:C:520:ILE:H	1.30	0.96
2:Q:158:ARG:HG3	2:Q:217:VAL:HG22	1.46	0.95
1:J:520:ILE:HD12	1:J:520:ILE:H	1.30	0.94
1:H:402:ASP:HA	1:H:578:MET:HE3	1.47	0.93
2:M:136:GLN:HB2	2:M:139:LYS:HG3	1.50	0.93
1:E:612:TYR:HA	1:E:615:MET:HE3	1.49	0.92
1:G:361:LEU:HD11	1:G:409:LEU:HD22	1.51	0.90
1:K:267:GLN:HE21	1:K:268:VAL:HG12	1.34	0.90
1:B:269:SER:HB3	1:B:323:ASN:HD21	1.32	0.90
2:O:136:GLN:HB2	2:O:139:LYS:HG3	1.53	0.90
1:G:349:ARG:HH21	1:H:286:LEU:HD12	1.35	0.90
1:B:269:SER:HB3	1:B:323:ASN:ND2	1.86	0.90
1:H:559:ARG:HD2	1:H:624:GLY:H	1.36	0.89
1:L:415:ASN:ND2	1:L:420:ARG:HD2	1.88	0.89
1:G:415:ASN:HD21	1:G:420:ARG:HD2	1.28	0.89
1:G:581:TRP:HE1	2:S:246:MET:HE3	1.38	0.88
1:K:583:ARG:HD3	1:K:587:GLU:OE1	1.73	0.88
2:O:196:ARG:NH1	2:O:237:MET:HE2	1.87	0.88
1:H:401:MET:HG3	1:H:578:MET:HE1	1.55	0.88
1:H:349:ARG:HH22	1:H:515:ASN:HD21	1.20	0.88
2:P:175:ARG:HD3	2:P:191:PRO:O	1.74	0.87
1:B:415:ASN:HD21	1:B:420:ARG:HH11	1.17	0.87
1:H:415:ASN:HD21	1:H:420:ARG:HH11	1.22	0.87
1:B:415:ASN:ND2	1:B:420:ARG:HD2	1.89	0.87
1:I:465:ILE:HD12	1:I:511:LYS:HE3	1.56	0.87
1:E:351:ASP:HB3	1:E:355:LEU:HD12	1.54	0.87
1:E:454:LEU:HB3	1:F:453:PRO:HG2	1.55	0.87
1:I:454:LEU:HA	1:I:457:LEU:HG	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:579:LEU:HD23	1:F:583:ARG:HG3	1.57	0.86
1:J:361:LEU:HD11	1:J:409:LEU:HD22	1.55	0.86
1:F:478:THR:HG22	1:F:487:SER:HB2	1.58	0.86
1:B:449:ASN:HD21	1:B:451:ASN:HB2	1.41	0.85
1:G:514:LEU:HA	1:H:512:LYS:HG3	1.57	0.85
1:E:466:ASP:H	1:E:519:GLN:HE22	1.22	0.85
1:C:284:ASP:HB3	1:C:287:LEU:HB3	1.56	0.85
1:L:423:LEU:HD11	1:L:528:MET:HE3	1.58	0.85
1:E:415:ASN:ND2	1:E:420:ARG:HD2	1.92	0.85
1:G:349:ARG:HH11	1:G:517:ARG:HD2	1.39	0.84
1:A:520:ILE:H	1:A:520:ILE:HD12	1.40	0.84
1:L:357:ARG:HA	1:L:360:MET:HE3	1.59	0.84
1:L:609:LEU:HD22	2:X:246:MET:HE2	1.57	0.84
1:G:454:LEU:HA	1:G:457:LEU:HB2	1.60	0.83
1:F:385:GLU:HA	1:F:607:PHE:HZ	1.41	0.83
1:L:520:ILE:H	1:L:520:ILE:HD12	1.43	0.83
1:K:269:SER:H	1:K:323:ASN:HD21	1.21	0.83
1:E:357:ARG:HA	1:E:360:MET:HE3	1.59	0.83
1:J:408:PHE:CE1	1:J:525:ILE:HD11	2.14	0.83
1:H:608:SER:HB3	1:H:611:VAL:HG23	1.60	0.83
1:D:415:ASN:HD21	1:D:420:ARG:HH11	1.26	0.82
2:S:136:GLN:HB2	2:S:139:LYS:HG3	1.59	0.82
1:B:303:LEU:HD23	1:B:303:LEU:H	1.43	0.82
1:H:581:TRP:HE1	2:T:246:MET:HE3	1.45	0.82
1:J:454:LEU:HB2	1:K:453:PRO:HG2	1.61	0.82
1:F:383:ASP:HB3	1:F:386:GLU:HG3	1.60	0.82
1:F:469:LEU:HD12	1:F:470:VAL:N	1.94	0.82
2:U:258:GLU:HA	2:U:265:LEU:HG	1.61	0.82
2:U:161:ALA:HB2	2:U:195:ILE:HD11	1.61	0.81
1:F:408:PHE:CE1	1:F:525:ILE:HD11	2.16	0.81
1:E:434:THR:HG23	1:E:570:GLN:HB3	1.63	0.81
1:I:517:ARG:HH12	1:J:286:LEU:HD12	1.45	0.80
1:K:415:ASN:HD21	1:K:420:ARG:HH11	1.29	0.80
1:G:349:ARG:NH1	1:G:517:ARG:HD2	1.96	0.80
1:A:428:ILE:HD12	1:A:428:ILE:H	1.46	0.80
1:B:581:TRP:HE1	2:N:246:MET:HE3	1.46	0.80
1:B:302:CYS:O	1:B:306:ILE:HG13	1.80	0.80
1:G:465:ILE:HD12	1:G:511:LYS:HD2	1.64	0.80
2:T:136:GLN:HB2	2:T:139:LYS:HG3	1.63	0.80
2:R:175:ARG:HD3	2:R:191:PRO:O	1.83	0.79
1:A:415:ASN:ND2	1:A:420:ARG:HG2	1.98	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:402:ASP:HA	1:D:578:MET:HE3	1.65	0.79
1:E:451:ASN:HD21	1:E:476:LYS:H	1.31	0.79
1:A:415:ASN:HD21	1:A:420:ARG:NH1	1.80	0.78
1:H:454:LEU:HA	1:H:457:LEU:HB2	1.64	0.78
1:C:454:LEU:HB3	1:C:457:LEU:HD12	1.64	0.78
1:H:369:LEU:HD13	1:H:595:ARG:HD3	1.65	0.78
2:M:161:ALA:HB2	2:M:195:ILE:HD11	1.63	0.78
1:E:361:LEU:HD11	1:E:409:LEU:HD22	1.66	0.78
1:I:415:ASN:ND2	1:I:420:ARG:HD2	1.99	0.77
2:U:158:ARG:HB2	2:U:158:ARG:HH11	1.49	0.77
1:D:401:MET:HG3	1:D:578:MET:HE1	1.66	0.77
2:U:118:THR:HG22	2:U:282:ARG:HD3	1.66	0.77
2:W:136:GLN:HB2	2:W:139:LYS:HG3	1.65	0.77
2:X:175:ARG:HD3	2:X:191:PRO:O	1.83	0.77
1:J:401:MET:HG3	1:J:578:MET:HE1	1.66	0.77
1:E:466:ASP:H	1:E:519:GLN:NE2	1.83	0.77
1:H:559:ARG:HD2	1:H:624:GLY:N	2.00	0.77
1:H:415:ASN:ND2	1:H:420:ARG:HD2	1.99	0.76
1:K:434:THR:HG23	1:K:570:GLN:HB3	1.67	0.76
1:E:428:ILE:H	1:E:428:ILE:HD12	1.48	0.76
1:I:623:ILE:HG22	1:I:624:GLY:H	1.49	0.76
1:K:283:ASP:HA	1:K:341:VAL:HG13	1.66	0.76
1:A:415:ASN:HD22	1:A:420:ARG:HG2	1.50	0.76
1:K:466:ASP:H	1:K:519:GLN:NE2	1.84	0.76
1:E:520:ILE:HD12	1:F:567:ARG:HH12	1.51	0.76
1:D:285:VAL:HG21	1:D:338:GLN:NE2	2.01	0.76
2:O:198:GLU:HB2	2:O:235:ASN:ND2	1.99	0.76
1:A:434:THR:HG23	1:A:570:GLN:HG2	1.68	0.76
1:E:287:LEU:HG	1:E:291:MET:HE2	1.68	0.76
2:U:198:GLU:HB2	2:U:235:ASN:HD21	1.51	0.76
1:H:398:LEU:HD21	1:H:545:ILE:HG21	1.68	0.75
2:P:161:ALA:HB2	2:P:195:ILE:HD11	1.68	0.75
1:E:349:ARG:HH22	1:E:515:ASN:HD21	1.33	0.75
1:I:357:ARG:HA	1:I:360:MET:HE3	1.68	0.75
1:E:424:PHE:HB2	1:E:527:THR:HG22	1.69	0.75
1:H:293:LEU:O	1:H:296:GLN:HG2	1.87	0.75
2:Q:147:VAL:HG21	2:Q:151:PRO:HD3	1.67	0.75
1:G:453:PRO:HG2	1:L:454:LEU:HB2	1.68	0.75
1:G:469:LEU:C	1:G:469:LEU:HD12	2.12	0.75
1:I:418:LYS:HE3	1:I:540:ARG:HH12	1.51	0.75
1:J:584:PRO:HG2	1:J:587:GLU:HG3	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:409:LEU:O	1:C:413:VAL:HG23	1.87	0.74
1:F:349:ARG:CZ	1:F:517:ARG:HD3	2.16	0.74
2:Q:175:ARG:HH21	2:Q:179:HIS:HB3	1.51	0.74
1:I:402:ASP:HA	1:I:578:MET:HE3	1.70	0.74
1:C:451:ASN:HD21	1:C:475:VAL:HA	1.51	0.74
1:J:502:ASP:OD2	1:J:540:ARG:HD2	1.86	0.74
1:G:454:LEU:HB2	1:H:453:PRO:HG2	1.68	0.74
1:J:403:SER:HA	1:J:583:ARG:HH21	1.53	0.74
1:K:454:LEU:H	1:K:454:LEU:HD22	1.53	0.74
1:K:466:ASP:H	1:K:519:GLN:HE22	1.33	0.74
1:L:349:ARG:CZ	1:L:517:ARG:HD3	2.17	0.74
1:L:415:ASN:HD21	1:L:420:ARG:HD2	1.50	0.74
2:V:136:GLN:HB2	2:V:139:LYS:HG3	1.69	0.74
1:A:355:LEU:HD22	1:A:359:GLN:HG2	1.70	0.73
1:C:371:ARG:O	1:C:375:MET:HB2	1.88	0.73
1:J:420:ARG:HB3	1:J:523:PRO:HB3	1.70	0.73
1:C:608:SER:HB2	2:O:280:ARG:HD2	1.70	0.73
1:D:599:TRP:O	1:D:603:LEU:HB2	1.88	0.73
1:L:389:ALA:HB1	1:L:625:VAL:HG21	1.69	0.73
2:P:196:ARG:NH1	2:P:237:MET:HE2	2.03	0.73
1:C:454:LEU:HA	1:C:457:LEU:HB2	1.70	0.73
1:E:331:LYS:N	1:E:331:LYS:HD2	2.04	0.73
1:H:470:VAL:O	1:H:524:GLY:HA3	1.89	0.73
1:J:402:ASP:HA	1:J:578:MET:HE3	1.70	0.73
1:K:446:LYS:HG2	1:K:467:GLN:OE1	1.89	0.73
1:E:401:MET:HE1	1:E:435:LEU:HD22	1.69	0.73
2:R:191:PRO:HG2	2:R:192:GLN:HE21	1.54	0.73
1:C:349:ARG:NH1	1:C:517:ARG:HD2	2.03	0.73
2:T:118:THR:HG22	2:T:282:ARG:HD3	1.70	0.73
1:B:495:ASP:O	1:B:498:ARG:HG3	1.89	0.72
1:H:402:ASP:CA	1:H:578:MET:HE3	2.18	0.72
1:I:372:MET:HA	1:I:375:MET:HG2	1.69	0.72
2:Q:158:ARG:HH21	2:Q:206:LEU:HD22	1.53	0.72
2:R:160:MET:HE2	2:R:213:ARG:HB3	1.72	0.72
1:I:349:ARG:HD2	1:I:517:ARG:CZ	2.20	0.72
1:C:420:ARG:HB3	1:C:523:PRO:HB3	1.70	0.72
1:E:415:ASN:HD21	1:E:420:ARG:HD2	1.54	0.72
2:N:158:ARG:HG3	2:N:217:VAL:HG22	1.72	0.72
2:X:136:GLN:HB2	2:X:139:LYS:HG3	1.70	0.72
1:H:498:ARG:HB3	1:H:540:ARG:HH21	1.55	0.71
1:I:470:VAL:HG23	1:I:522:PRO:HG2	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:454:LEU:HA	1:J:457:LEU:HB2	1.72	0.71
1:L:415:ASN:HD21	1:L:420:ARG:HH11	1.35	0.71
2:Q:136:GLN:HB2	2:Q:139:LYS:HG3	1.72	0.71
1:B:424:PHE:HB2	1:B:527:THR:HG22	1.72	0.71
1:D:550:LYS:HB2	1:D:553:LEU:HD12	1.71	0.71
1:B:417:PRO:HG3	1:C:567:ARG:HH21	1.54	0.71
1:K:412:MET:HE1	1:K:524:GLY:HA2	1.70	0.71
1:A:453:PRO:HG3	1:F:454:LEU:HB3	1.72	0.71
1:C:423:LEU:HD21	1:C:528:MET:HE3	1.71	0.70
1:I:357:ARG:HD3	1:I:413:VAL:O	1.91	0.70
1:C:498:ARG:NH2	1:D:476:LYS:HD3	2.06	0.70
1:B:351:ASP:OD2	1:B:355:LEU:HD11	1.92	0.70
1:L:268:VAL:HG11	1:L:327:PHE:HA	1.72	0.70
1:L:619:VAL:HG22	1:L:625:VAL:HG12	1.73	0.70
1:B:581:TRP:NE1	2:N:246:MET:HE3	2.05	0.70
1:A:415:ASN:ND2	1:A:420:ARG:HH11	1.86	0.70
1:F:590:GLN:HA	1:F:593:GLN:HG3	1.70	0.70
2:W:190:PRO:HB2	2:W:193:HIS:HD2	1.56	0.70
1:C:495:ASP:O	1:C:498:ARG:HG3	1.92	0.70
2:N:190:PRO:HB2	2:N:193:HIS:HD2	1.57	0.70
1:E:491:ILE:O	1:E:491:ILE:HD13	1.92	0.70
1:J:520:ILE:H	1:J:520:ILE:CD1	2.03	0.70
1:B:415:ASN:HD21	1:B:420:ARG:HD2	1.53	0.70
1:G:414:TYR:HB3	1:G:416:ILE:HD11	1.74	0.70
1:H:432:LYS:CE	1:H:433:THR:H	2.05	0.69
1:L:623:ILE:HG22	1:L:624:GLY:H	1.55	0.69
2:V:147:VAL:HG21	2:V:151:PRO:HD3	1.74	0.69
1:F:608:SER:HB3	1:F:611:VAL:HG23	1.73	0.69
1:G:327:PHE:CZ	1:G:333:GLN:HB3	2.27	0.69
2:V:161:ALA:HB2	2:V:195:ILE:HD11	1.74	0.69
2:N:136:GLN:HB2	2:N:139:LYS:HG3	1.73	0.69
1:A:291:MET:HE2	1:F:354:GLN:HE21	1.58	0.69
1:H:443:CYS:HB2	1:H:469:LEU:HD23	1.74	0.69
1:I:550:LYS:HB2	1:I:553:LEU:HD12	1.75	0.69
1:B:608:SER:HB2	2:N:280:ARG:NH1	2.07	0.69
1:L:590:GLN:NE2	1:L:590:GLN:H	1.90	0.69
2:R:196:ARG:NH1	2:R:237:MET:HE2	2.08	0.69
1:C:397:LEU:HB3	1:C:401:MET:HE3	1.75	0.69
1:F:447:ALA:C	1:F:448:LEU:HD23	2.18	0.69
1:K:491:ILE:HG22	1:K:492:ASN:HD22	1.58	0.69
1:G:476:LYS:HE2	1:L:496:ASN:ND2	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:415:ASN:HD21	1:J:420:ARG:HH11	1.41	0.68
1:C:273:VAL:HG22	1:C:292:TYR:CE2	2.28	0.68
1:G:409:LEU:O	1:G:413:VAL:HG23	1.93	0.68
1:D:470:VAL:HG23	1:D:522:PRO:HB2	1.74	0.68
1:C:465:ILE:HG23	1:C:517:ARG:HG2	1.74	0.68
1:G:415:ASN:HD21	1:G:420:ARG:HH11	1.42	0.68
1:J:434:THR:HG23	1:J:570:GLN:HB3	1.74	0.68
1:B:499:ASP:HB3	1:C:473:GLU:HG2	1.75	0.68
1:D:346:ALA:O	1:D:350:VAL:HG23	1.94	0.68
1:K:434:THR:HG21	1:K:569:ILE:HG12	1.75	0.68
1:B:398:LEU:HD21	1:B:545:ILE:HG21	1.75	0.68
1:E:337:CYS:O	1:E:341:VAL:HG23	1.94	0.68
1:F:623:ILE:HG22	1:F:624:GLY:H	1.59	0.68
1:K:512:LYS:HG3	1:K:513:HIS:H	1.57	0.68
1:H:584:PRO:HD2	1:H:587:GLU:HG3	1.75	0.68
1:G:445:GLY:O	1:G:446:LYS:HG2	1.94	0.68
1:G:454:LEU:H	1:G:454:LEU:HD12	1.59	0.68
1:A:285:VAL:HG21	1:A:338:GLN:HE21	1.59	0.67
1:K:346:ALA:HB2	1:L:289:LEU:HD23	1.75	0.67
1:H:420:ARG:HB3	1:H:523:PRO:HB3	1.76	0.67
1:J:557:LEU:HD23	1:J:564:LEU:HD11	1.77	0.67
2:O:175:ARG:HD3	2:O:191:PRO:O	1.94	0.67
1:D:583:ARG:HD3	1:D:587:GLU:OE1	1.95	0.67
1:G:475:VAL:HG12	1:G:491:ILE:HD12	1.75	0.67
1:K:415:ASN:ND2	1:K:420:ARG:HD2	2.10	0.67
1:A:514:LEU:HD23	1:A:515:ASN:H	1.60	0.67
1:H:412:MET:CE	1:H:469:LEU:HB2	2.25	0.67
1:J:337:CYS:O	1:J:341:VAL:HG23	1.94	0.67
1:A:584:PRO:HG2	1:A:587:GLU:HG3	1.77	0.67
1:C:525:ILE:HG22	1:C:526:VAL:N	2.10	0.67
1:I:349:ARG:HD2	1:I:517:ARG:NH1	2.10	0.67
1:K:409:LEU:O	1:K:413:VAL:HG23	1.94	0.67
1:G:420:ARG:HB3	1:G:523:PRO:HB3	1.76	0.67
2:O:147:VAL:HG21	2:O:151:PRO:HD3	1.77	0.67
2:P:119:ALA:O	2:P:279:GLY:HA3	1.95	0.67
2:V:190:PRO:HB2	2:V:193:HIS:HD2	1.60	0.67
1:B:283:ASP:HA	1:B:341:VAL:HG13	1.76	0.66
1:F:520:ILE:H	1:F:520:ILE:HD12	1.59	0.66
1:L:349:ARG:HD3	1:L:517:ARG:NH1	2.10	0.66
2:V:179:HIS:HA	2:V:182:CYS:SG	2.34	0.66
1:J:372:MET:HA	1:J:375:MET:HG2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:481:GLU:CD	1:G:481:GLU:H	2.02	0.66
1:H:440:LEU:HD13	1:H:471:VAL:HG23	1.77	0.66
1:C:375:MET:HE1	1:C:387:TRP:CE2	2.31	0.66
1:I:357:ARG:HG2	1:I:357:ARG:HH11	1.61	0.66
1:I:470:VAL:O	1:I:524:GLY:HA3	1.96	0.66
1:L:454:LEU:HA	1:L:457:LEU:HB2	1.76	0.66
2:R:264:LEU:HD11	2:R:267:ARG:HB2	1.77	0.66
2:S:161:ALA:HB2	2:S:195:ILE:HD11	1.77	0.66
1:B:412:MET:HE1	1:B:524:GLY:N	2.10	0.66
2:X:244:GLY:O	2:X:246:MET:N	2.29	0.66
1:B:369:LEU:HB2	1:B:595:ARG:HH11	1.60	0.66
1:K:383:ASP:HB3	1:K:386:GLU:HG3	1.76	0.66
2:S:243:MET:HB2	2:S:243:MET:HE3	1.77	0.66
1:C:516:LYS:O	1:C:517:ARG:HD3	1.96	0.66
1:F:612:TYR:HA	1:F:615:MET:HE3	1.77	0.66
1:B:520:ILE:CD1	1:C:567:ARG:HH12	2.07	0.66
1:E:481:GLU:H	1:E:481:GLU:CD	2.03	0.66
1:H:281:LYS:HA	1:H:281:LYS:HE2	1.76	0.66
1:H:349:ARG:HH22	1:H:515:ASN:ND2	1.94	0.66
1:L:270:TRP:CE2	1:L:336:ILE:HG12	2.30	0.66
1:B:303:LEU:HA	1:B:306:ILE:HD11	1.77	0.66
1:D:357:ARG:HA	1:D:360:MET:HE3	1.75	0.66
1:F:599:TRP:O	1:F:603:LEU:HD12	1.96	0.66
1:J:579:LEU:C	1:J:581:TRP:H	2.02	0.66
1:L:383:ASP:HB3	1:L:386:GLU:HG3	1.78	0.66
2:T:161:ALA:HB2	2:T:195:ILE:HD11	1.77	0.66
1:A:285:VAL:HG21	1:A:338:GLN:NE2	2.11	0.65
1:D:375:MET:O	1:D:382:ALA:HB3	1.96	0.65
1:A:346:ALA:O	1:A:350:VAL:HG23	1.97	0.65
1:E:395:HIS:HD2	1:E:578:MET:HE3	1.60	0.65
2:R:176:CYS:SG	2:R:179:HIS:HB2	2.37	0.65
1:E:454:LEU:HB3	1:F:453:PRO:CG	2.25	0.65
1:J:576:LEU:O	1:J:580:ILE:HG12	1.96	0.65
1:L:498:ARG:HB3	1:L:540:ARG:HH12	1.61	0.65
2:U:136:GLN:HB2	2:U:139:LYS:HG3	1.79	0.65
1:D:316:TYR:HB3	1:D:320:HIS:HD2	1.62	0.65
1:E:593:GLN:O	1:E:597:VAL:HG23	1.97	0.65
2:R:147:VAL:HG21	2:R:151:PRO:HD3	1.77	0.65
2:T:158:ARG:HB2	2:T:158:ARG:HH11	1.60	0.65
1:I:402:ASP:HA	1:I:578:MET:CE	2.26	0.65
1:B:349:ARG:HG2	1:B:349:ARG:HH11	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:108:GLY:HA3	2:O:148:ASP:OD2	1.97	0.65
2:T:239:ASN:HA	2:T:274:VAL:HB	1.78	0.65
2:U:175:ARG:HD3	2:U:191:PRO:O	1.97	0.65
2:V:158:ARG:HH11	2:V:158:ARG:HB2	1.62	0.65
1:C:454:LEU:HB2	1:D:453:PRO:HG2	1.79	0.65
1:I:581:TRP:NE1	2:U:246:MET:HE3	2.11	0.65
1:B:454:LEU:HB2	1:C:453:PRO:HG2	1.79	0.64
1:E:428:ILE:HD12	1:E:428:ILE:N	2.12	0.64
1:L:454:LEU:H	1:L:454:LEU:HD12	1.61	0.64
1:H:356:THR:HG22	1:H:359:GLN:OE1	1.97	0.64
1:H:498:ARG:HB3	1:H:540:ARG:NH2	2.13	0.64
1:J:408:PHE:HE1	1:J:525:ILE:HD11	1.62	0.64
1:L:583:ARG:NE	1:L:583:ARG:HA	2.12	0.64
2:T:259:ASP:OD2	2:T:263:ASN:HB2	1.98	0.64
1:C:303:LEU:HD23	1:C:303:LEU:H	1.62	0.64
1:D:454:LEU:H	1:D:454:LEU:HD12	1.62	0.64
1:E:451:ASN:ND2	1:E:476:LYS:H	1.95	0.64
1:I:458:ASN:HD22	1:J:456:ARG:NE	1.96	0.64
2:P:137:LEU:O	2:P:139:LYS:HG2	1.98	0.64
1:C:349:ARG:HH11	1:C:517:ARG:HD2	1.62	0.64
1:E:394:LEU:HD21	1:E:569:ILE:O	1.98	0.64
1:H:283:ASP:HA	1:H:341:VAL:HG13	1.80	0.64
1:H:517:ARG:HG3	1:H:519:GLN:HG2	1.79	0.64
1:L:301:MET:O	1:L:303:LEU:HD22	1.97	0.64
1:A:299:PHE:HB3	1:A:317:HIS:CD2	2.33	0.64
1:F:514:LEU:HD23	1:F:516:LYS:HZ2	1.63	0.64
1:K:267:GLN:NE2	1:K:268:VAL:HG12	2.10	0.64
1:A:454:LEU:HA	1:A:457:LEU:HB2	1.79	0.64
1:J:423:LEU:HD23	1:J:544:GLN:HG3	1.79	0.64
1:C:293:LEU:O	1:C:296:GLN:HB3	1.98	0.64
1:J:389:ALA:HB1	1:J:625:VAL:HG21	1.79	0.64
1:K:590:GLN:HA	1:K:593:GLN:HG3	1.80	0.64
2:Q:175:ARG:NH2	2:Q:179:HIS:HB3	2.13	0.64
1:E:349:ARG:HH22	1:E:515:ASN:ND2	1.95	0.64
1:H:608:SER:HB3	1:H:611:VAL:CG2	2.26	0.63
1:I:498:ARG:NH2	1:J:476:LYS:HD3	2.13	0.63
1:B:434:THR:HG23	1:B:570:GLN:HB3	1.79	0.63
1:G:514:LEU:HD23	1:G:515:ASN:N	2.13	0.63
1:J:356:THR:O	1:J:360:MET:HG3	1.99	0.63
1:K:609:LEU:HD11	2:W:247:ASN:HB2	1.80	0.63
2:O:190:PRO:HB2	2:O:193:HIS:HD2	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:156:ARG:HB3	2:S:217:VAL:HG12	1.80	0.63
1:A:446:LYS:HG2	1:A:467:GLN:NE2	2.08	0.63
1:B:608:SER:HB2	2:N:280:ARG:HH11	1.63	0.63
1:D:420:ARG:HG2	1:D:523:PRO:HB3	1.80	0.63
1:I:535:LYS:HE2	1:J:428:ILE:HD12	1.80	0.63
2:P:196:ARG:HH11	2:P:237:MET:HE2	1.62	0.63
2:P:259:ASP:OD2	2:P:263:ASN:HB2	1.98	0.63
1:F:375:MET:HE1	1:F:387:TRP:CZ2	2.34	0.63
1:B:576:LEU:O	1:B:580:ILE:HG12	1.99	0.63
1:B:569:ILE:H	1:B:569:ILE:HD13	1.64	0.63
1:F:303:LEU:HD22	1:F:303:LEU:H	1.64	0.63
1:A:398:LEU:HB2	1:A:401:MET:CE	2.29	0.63
1:B:421:TYR:CE1	1:B:523:PRO:HA	2.34	0.63
2:U:198:GLU:HB2	2:U:235:ASN:ND2	2.13	0.63
2:S:179:HIS:ND1	2:S:238:CYS:HA	2.14	0.63
2:X:197:VAL:HG11	2:X:218:VAL:HG11	1.81	0.62
1:B:272:LEU:HD23	1:B:323:ASN:HD22	1.64	0.62
1:D:405:VAL:HG21	1:D:575:LEU:HD22	1.81	0.62
1:F:401:MET:HG3	1:F:578:MET:HE1	1.81	0.62
2:N:161:ALA:HB2	2:N:195:ILE:HD11	1.81	0.62
1:C:376:PHE:CE1	1:C:384:ILE:HA	2.34	0.62
2:V:236:TYR:CE2	2:V:272:VAL:HG11	2.35	0.62
1:A:372:MET:HA	1:A:375:MET:HG2	1.80	0.62
2:M:243:MET:CE	2:M:243:MET:HB2	2.29	0.62
2:T:132:LYS:HE2	2:T:273:ARG:HB2	1.80	0.62
2:X:243:MET:HB2	2:X:243:MET:HE3	1.80	0.62
1:B:350:VAL:HG21	1:C:290:GLY:HA3	1.81	0.62
1:E:284:ASP:HB3	1:E:287:LEU:HB3	1.82	0.62
1:F:576:LEU:O	1:F:580:ILE:HG12	1.99	0.62
2:S:175:ARG:NE	2:S:237:MET:HB2	2.15	0.62
2:T:244:GLY:O	2:T:246:MET:N	2.33	0.62
2:U:193:HIS:HE1	2:U:215:SER:H	1.48	0.62
1:A:469:LEU:C	1:A:469:LEU:HD12	2.25	0.62
1:E:465:ILE:HD11	1:E:509:LEU:HB2	1.80	0.62
1:I:516:LYS:O	1:I:517:ARG:HD3	2.00	0.62
1:J:386:GLU:O	1:J:389:ALA:HB3	2.00	0.61
2:N:239:ASN:HA	2:N:274:VAL:HB	1.81	0.61
2:X:243:MET:CE	2:X:243:MET:HB2	2.30	0.61
1:B:389:ALA:HB1	1:B:625:VAL:HG21	1.82	0.61
1:C:500:TYR:CZ	1:C:507:VAL:HG11	2.35	0.61
1:J:415:ASN:ND2	1:J:420:ARG:HG2	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:289:LEU:HD11	1:K:333:GLN:HB3	1.82	0.61
1:A:357:ARG:HA	1:A:360:MET:HE3	1.82	0.61
1:C:434:THR:HG23	1:C:570:GLN:HB3	1.82	0.61
1:I:303:LEU:HD23	1:I:303:LEU:H	1.64	0.61
1:B:332:ASN:O	1:B:336:ILE:HG13	2.00	0.61
1:E:283:ASP:HA	1:E:341:VAL:HG13	1.81	0.61
2:S:103:TYR:CZ	2:S:105:GLY:HA2	2.36	0.61
1:B:454:LEU:HD12	1:B:454:LEU:N	2.16	0.61
1:H:425:LYS:HE2	1:H:528:MET:HE2	1.82	0.61
1:I:303:LEU:O	1:I:306:ILE:HG22	2.00	0.61
1:L:361:LEU:HD11	1:L:409:LEU:HD22	1.82	0.61
2:P:198:GLU:HB2	2:P:235:ASN:HD21	1.65	0.61
1:F:463:VAL:O	1:F:463:VAL:HG12	1.99	0.61
1:G:438:ALA:HA	1:G:570:GLN:O	2.00	0.61
1:I:278:MET:HE2	1:I:343:THR:HG22	1.82	0.61
1:J:369:LEU:HB2	1:J:595:ARG:NH1	2.16	0.61
1:B:284:ASP:HB3	1:B:287:LEU:HB2	1.83	0.61
1:B:520:ILE:HD13	1:C:567:ARG:HH12	1.66	0.61
1:E:609:LEU:HA	2:Q:246:MET:HE1	1.83	0.61
1:H:459:PHE:CE2	1:H:512:LYS:HD3	2.35	0.61
2:R:158:ARG:HB2	2:R:158:ARG:HH11	1.66	0.61
1:I:554:LYS:O	1:I:558:GLU:HG3	2.01	0.61
2:U:99:SER:HB2	2:U:101:LYS:HG2	1.83	0.61
1:D:589:ALA:O	1:D:592:ILE:HG22	2.01	0.61
1:I:418:LYS:HE3	1:I:540:ARG:NH1	2.15	0.61
1:L:389:ALA:HB1	1:L:625:VAL:CG2	2.31	0.61
1:L:520:ILE:HD12	1:L:520:ILE:N	2.14	0.61
2:O:191:PRO:HG2	2:O:192:GLN:HE21	1.65	0.61
2:R:137:LEU:O	2:R:139:LYS:HG2	2.01	0.61
1:E:412:MET:HE2	1:E:469:LEU:HD22	1.82	0.61
2:R:244:GLY:O	2:R:246:MET:N	2.33	0.61
2:T:175:ARG:HD3	2:T:191:PRO:O	2.01	0.60
2:U:239:ASN:HA	2:U:274:VAL:HB	1.82	0.60
1:D:415:ASN:HD22	1:D:523:PRO:HG3	1.66	0.60
1:E:349:ARG:NH2	1:E:515:ASN:HD21	1.99	0.60
1:I:420:ARG:NH2	1:I:521:PHE:O	2.31	0.60
1:I:561:GLU:H	1:I:561:GLU:CD	2.09	0.60
1:A:470:VAL:O	1:A:524:GLY:HA3	2.01	0.60
1:H:481:GLU:H	1:H:481:GLU:CD	2.08	0.60
1:J:480:GLY:HA2	1:J:483:ARG:NH2	2.15	0.60
2:P:118:THR:HG22	2:P:282:ARG:HD3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:118:THR:HG22	2:Q:282:ARG:HD3	1.83	0.60
2:Q:133:MET:HE3	2:Q:135:CYS:HB3	1.83	0.60
2:X:107:TYR:O	2:X:147:VAL:HG23	2.01	0.60
1:B:272:LEU:HD23	1:B:323:ASN:ND2	2.16	0.60
1:F:415:ASN:HD21	1:F:420:ARG:HH11	1.48	0.60
1:K:440:LEU:HD22	1:K:471:VAL:HG21	1.83	0.60
2:Q:190:PRO:HB2	2:Q:193:HIS:HD2	1.66	0.60
1:F:303:LEU:HA	1:F:306:ILE:HG22	1.82	0.60
1:J:458:ASN:HB3	1:J:510:GLU:OE2	2.01	0.60
1:J:512:LYS:C	1:J:514:LEU:H	2.09	0.60
1:K:420:ARG:HB3	1:K:523:PRO:HB3	1.83	0.60
2:N:175:ARG:HD3	2:N:191:PRO:O	2.01	0.60
2:V:196:ARG:NH1	2:V:237:MET:HE2	2.15	0.60
1:C:593:GLN:O	1:C:597:VAL:HG23	2.01	0.60
1:D:564:LEU:C	1:D:566:LYS:H	2.08	0.60
1:I:346:ALA:HB2	1:J:289:LEU:HD23	1.84	0.60
1:I:563:LEU:HD11	1:I:625:VAL:HG21	1.84	0.60
1:I:614:LYS:O	1:I:617:PHE:HB3	2.02	0.60
2:P:136:GLN:HB2	2:P:139:LYS:HG3	1.83	0.60
2:Q:132:LYS:HD3	2:Q:134:PHE:CZ	2.36	0.60
2:S:243:MET:CE	2:S:243:MET:HB2	2.31	0.60
1:B:564:LEU:HD23	1:B:569:ILE:HD11	1.82	0.60
1:F:358:GLU:HG2	1:F:413:VAL:HG11	1.84	0.60
1:I:581:TRP:HE1	2:U:246:MET:HE3	1.66	0.60
1:K:398:LEU:HB2	1:K:401:MET:HE2	1.83	0.60
2:Q:107:TYR:O	2:Q:147:VAL:HG23	2.02	0.60
1:C:352:SER:HA	1:C:360:MET:HE2	1.83	0.60
1:C:584:PRO:HB3	2:O:243:MET:HA	1.83	0.60
1:I:425:LYS:HZ3	1:I:530:GLU:HA	1.67	0.60
1:J:583:ARG:HD2	1:J:587:GLU:OE1	2.02	0.60
1:K:529:ASN:O	1:K:530:GLU:HB3	2.02	0.60
2:S:158:ARG:HH11	2:S:158:ARG:HB2	1.67	0.60
1:A:418:LYS:NZ	1:A:540:ARG:HD3	2.16	0.60
1:G:299:PHE:H	1:G:299:PHE:HD2	1.50	0.60
1:K:408:PHE:CZ	1:K:412:MET:HE2	2.37	0.60
1:L:357:ARG:CA	1:L:360:MET:HE3	2.32	0.60
1:J:446:LYS:HG2	1:J:467:GLN:NE2	2.17	0.60
1:K:352:SER:HA	1:K:360:MET:HE2	1.84	0.60
2:Q:244:GLY:HA3	2:Q:248:ARG:HB2	1.83	0.60
1:E:401:MET:O	1:E:405:VAL:HG23	2.02	0.59
1:F:289:LEU:O	1:F:293:LEU:HG	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:285:VAL:HG22	1:I:341:VAL:HG21	1.83	0.59
1:J:550:LYS:HB2	1:J:553:LEU:HD12	1.83	0.59
2:R:145:LEU:HD21	2:R:157:VAL:HG11	1.84	0.59
1:C:470:VAL:O	1:C:524:GLY:HA3	2.02	0.59
1:H:581:TRP:NE1	2:T:246:MET:HE3	2.15	0.59
1:C:454:LEU:C	1:C:456:ARG:H	2.08	0.59
1:G:388:MET:HE2	1:G:391:VAL:HG21	1.84	0.59
1:H:284:ASP:CG	1:H:287:LEU:HB2	2.27	0.59
1:H:285:VAL:HG21	1:H:338:GLN:NE2	2.18	0.59
1:I:391:VAL:HG13	1:I:578:MET:HG3	1.84	0.59
1:J:369:LEU:HB2	1:J:595:ARG:HH11	1.67	0.59
2:R:160:MET:SD	2:R:213:ARG:HG2	2.41	0.59
1:A:420:ARG:HB3	1:A:523:PRO:HB3	1.85	0.59
1:C:520:ILE:H	1:C:520:ILE:CD1	2.05	0.59
1:D:354:GLN:CG	1:E:310:GLN:HE21	2.16	0.59
1:G:356:THR:OG1	1:G:359:GLN:HG3	2.03	0.59
1:G:520:ILE:HD12	1:G:520:ILE:H	1.64	0.59
1:K:410:LYS:HA	1:K:410:LYS:HE3	1.83	0.59
2:M:137:LEU:O	2:M:139:LYS:HG2	2.03	0.59
1:A:291:MET:HE2	1:F:354:GLN:NE2	2.16	0.59
1:G:581:TRP:NE1	2:S:246:MET:HE3	2.13	0.59
2:M:198:GLU:HB2	2:M:235:ASN:ND2	2.18	0.59
1:C:477:GLY:HA3	1:C:491:ILE:HD12	1.83	0.59
1:K:268:VAL:N	1:K:326:ILE:HG21	2.17	0.59
1:A:609:LEU:O	1:A:613:GLN:HB2	2.03	0.59
1:B:287:LEU:HD22	1:B:291:MET:HG3	1.84	0.59
1:C:400:LYS:O	1:C:404:VAL:HG23	2.02	0.59
1:C:447:ALA:C	1:C:448:LEU:HD23	2.28	0.59
1:E:465:ILE:HD12	1:E:517:ARG:HB3	1.84	0.59
1:F:303:LEU:HD22	1:F:303:LEU:N	2.17	0.59
1:H:372:MET:SD	1:H:576:LEU:HD23	2.42	0.59
2:U:147:VAL:HG21	2:U:151:PRO:HD3	1.85	0.59
2:M:147:VAL:HG21	2:M:151:PRO:HD3	1.84	0.59
2:P:224:GLU:H	2:P:224:GLU:CD	2.11	0.59
1:B:495:ASP:HB3	1:C:476:LYS:HZ2	1.68	0.59
1:J:344:VAL:O	1:J:348:LYS:HG2	2.02	0.59
2:S:133:MET:HE2	2:S:272:VAL:HG13	1.83	0.59
1:I:337:CYS:O	1:I:341:VAL:HG23	2.02	0.59
1:B:356:THR:O	1:B:360:MET:HG3	2.03	0.58
1:G:311:PRO:C	1:G:313:HIS:H	2.10	0.58
1:G:354:GLN:HE22	1:H:291:MET:HE3	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:469:LEU:HD12	1:H:470:VAL:N	2.17	0.58
1:L:590:GLN:H	1:L:590:GLN:CD	2.10	0.58
2:X:132:LYS:HE3	2:X:271:GLU:OE2	2.01	0.58
1:A:476:LYS:HB3	1:A:488:GLY:HA3	1.85	0.58
1:C:590:GLN:HA	1:C:593:GLN:HG3	1.85	0.58
1:D:443:CYS:HB3	1:D:468:PHE:CD2	2.38	0.58
1:D:592:ILE:O	1:D:596:ILE:HG12	2.03	0.58
1:E:433:THR:HG23	1:E:473:GLU:CD	2.28	0.58
1:G:414:TYR:HB3	1:G:416:ILE:CD1	2.33	0.58
1:I:608:SER:HB2	2:U:280:ARG:NH1	2.17	0.58
1:K:608:SER:HB2	2:W:280:ARG:HH11	1.69	0.58
1:K:623:ILE:HD11	1:K:627:ASP:OD2	2.02	0.58
2:S:122:VAL:HG12	2:S:123:THR:N	2.18	0.58
2:U:159:ALA:HB2	2:U:234:TYR:OH	2.03	0.58
1:A:273:VAL:HG22	1:A:292:TYR:CZ	2.38	0.58
1:A:274:THR:HG23	1:A:340:ALA:HA	1.84	0.58
1:B:584:PRO:HD2	1:B:587:GLU:HG3	1.85	0.58
1:C:473:GLU:HG3	1:C:474:ASP:H	1.68	0.58
1:E:412:MET:HE1	1:E:524:GLY:HA2	1.85	0.58
1:F:525:ILE:HG22	1:F:526:VAL:N	2.18	0.58
1:F:614:LYS:O	1:F:617:PHE:HB3	2.03	0.58
1:K:454:LEU:H	1:K:454:LEU:CD2	2.16	0.58
1:L:615:MET:O	1:L:619:VAL:HG23	2.02	0.58
1:B:415:ASN:HD21	1:B:420:ARG:NH1	1.95	0.58
1:B:417:PRO:HG3	1:C:567:ARG:NH2	2.17	0.58
1:F:617:PHE:O	1:F:621:MET:HG2	2.02	0.58
1:A:385:GLU:HG2	1:A:626:LEU:HD21	1.86	0.58
1:A:451:ASN:HB3	1:F:496:ASN:ND2	2.19	0.58
1:C:345:LEU:O	1:C:348:LYS:HB2	2.04	0.58
1:I:356:THR:OG1	1:I:359:GLN:HB2	2.03	0.58
1:J:375:MET:HE2	1:J:376:PHE:CZ	2.39	0.58
1:J:552:TYR:HB2	1:J:619:VAL:O	2.04	0.58
2:V:158:ARG:HB3	2:V:256:THR:HB	1.85	0.58
2:V:175:ARG:HD3	2:V:191:PRO:O	2.03	0.58
1:H:432:LYS:CD	1:H:433:THR:H	2.17	0.58
1:L:579:LEU:HD22	1:L:583:ARG:HG3	1.86	0.58
2:O:245:GLY:C	2:O:247:ASN:H	2.10	0.58
1:B:369:LEU:HD23	1:B:372:MET:SD	2.44	0.58
1:B:435:LEU:HD23	1:B:547:PHE:HZ	1.68	0.58
1:C:415:ASN:ND2	1:C:420:ARG:HD2	2.17	0.58
1:G:412:MET:HE1	1:G:524:GLY:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:559:ARG:NH1	1:H:623:ILE:HA	2.18	0.58
1:I:434:THR:HG23	1:I:570:GLN:HB3	1.85	0.58
1:K:402:ASP:HA	1:K:578:MET:HE3	1.85	0.58
2:V:142:PRO:HA	2:V:232:ILE:O	2.04	0.58
1:A:439:LEU:O	1:A:442:LEU:HB3	2.04	0.58
1:I:375:MET:HE1	1:I:387:TRP:CZ2	2.39	0.58
1:K:512:LYS:HG3	1:K:513:HIS:N	2.18	0.58
1:L:583:ARG:HD3	1:L:587:GLU:OE1	2.04	0.58
2:P:158:ARG:HB2	2:P:158:ARG:HH11	1.67	0.58
2:V:224:GLU:CD	2:V:224:GLU:H	2.11	0.58
1:C:473:GLU:HG3	1:C:474:ASP:N	2.19	0.58
1:D:268:VAL:HG11	1:D:327:PHE:HA	1.85	0.58
1:D:466:ASP:H	1:D:519:GLN:HE22	1.52	0.58
1:E:597:VAL:C	1:E:599:TRP:H	2.12	0.58
1:J:615:MET:O	1:J:619:VAL:HG23	2.04	0.58
1:K:454:LEU:CB	1:L:453:PRO:HG2	2.34	0.58
1:J:608:SER:OG	1:J:611:VAL:HG23	2.04	0.57
1:G:349:ARG:NH2	1:H:286:LEU:HD12	2.12	0.57
1:J:579:LEU:C	1:J:581:TRP:N	2.62	0.57
1:K:454:LEU:HD11	1:K:493:ASN:ND2	2.19	0.57
1:L:415:ASN:HD21	1:L:420:ARG:NH1	2.01	0.57
1:C:349:ARG:HD2	1:C:517:ARG:CZ	2.33	0.57
1:K:369:LEU:HB2	1:K:595:ARG:HH11	1.69	0.57
1:K:451:ASN:HD21	1:K:476:LYS:H	1.51	0.57
2:N:118:THR:HG22	2:N:282:ARG:HD3	1.87	0.57
2:R:158:ARG:HG3	2:R:217:VAL:HG22	1.86	0.57
2:S:175:ARG:HD3	2:S:191:PRO:O	2.04	0.57
1:I:608:SER:HB2	2:U:280:ARG:HH11	1.70	0.57
1:J:383:ASP:HB3	1:J:386:GLU:HG3	1.87	0.57
2:M:196:ARG:NH1	2:M:237:MET:HE2	2.20	0.57
2:N:158:ARG:HH21	2:N:206:LEU:CD2	2.18	0.57
2:P:244:GLY:O	2:P:246:MET:N	2.37	0.57
1:C:398:LEU:HB2	1:C:401:MET:HE2	1.84	0.57
1:J:415:ASN:ND2	1:J:420:ARG:HH11	2.02	0.57
1:A:418:LYS:HZ2	1:A:540:ARG:HD3	1.69	0.57
1:I:420:ARG:HB3	1:I:523:PRO:HB3	1.85	0.57
1:L:409:LEU:O	1:L:413:VAL:HG23	2.05	0.57
1:L:514:LEU:HD12	1:L:515:ASN:H	1.69	0.57
1:B:306:ILE:HD12	1:B:307:LYS:N	2.20	0.57
1:C:507:VAL:HG12	1:C:508:ASN:H	1.68	0.57
1:H:412:MET:HE3	1:H:469:LEU:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:497:LEU:O	1:J:500:TYR:HB2	2.04	0.57
1:L:293:LEU:O	1:L:296:GLN:HG2	2.04	0.57
1:L:420:ARG:HB2	1:L:523:PRO:HB3	1.86	0.57
2:N:193:HIS:CE1	2:N:214:HIS:HB3	2.39	0.57
2:S:245:GLY:C	2:S:247:ASN:H	2.11	0.57
1:A:512:LYS:O	1:A:512:LYS:HG2	2.05	0.57
1:B:398:LEU:HB2	1:B:401:MET:HE2	1.86	0.57
1:B:618:ASN:OD1	1:B:623:ILE:HD11	2.05	0.57
1:C:512:LYS:HG3	1:C:512:LYS:O	2.04	0.57
1:I:623:ILE:HG22	1:I:624:GLY:N	2.18	0.57
1:J:340:ALA:O	1:J:344:VAL:HG23	2.05	0.57
1:L:465:ILE:HG12	1:L:509:LEU:HD12	1.87	0.57
1:B:449:ASN:ND2	1:B:451:ASN:H	2.03	0.57
1:G:423:LEU:HD11	1:G:528:MET:HE3	1.86	0.57
1:K:346:ALA:HB1	1:L:290:GLY:H	1.70	0.57
1:K:579:LEU:O	1:K:583:ARG:HB2	2.05	0.57
1:A:270:TRP:CE2	1:A:336:ILE:HG12	2.40	0.56
1:B:419:LYS:HD2	1:B:542:VAL:HG13	1.86	0.56
1:C:383:ASP:HB3	1:C:386:GLU:HG3	1.85	0.56
1:E:423:LEU:HD12	1:E:526:VAL:O	2.05	0.56
1:F:371:ARG:O	1:F:375:MET:HG2	2.05	0.56
1:H:303:LEU:HD23	1:H:306:ILE:HD11	1.87	0.56
1:H:352:SER:HA	1:H:360:MET:HE2	1.87	0.56
1:K:465:ILE:HD12	1:K:511:LYS:HG3	1.85	0.56
2:P:133:MET:HE1	2:P:236:TYR:CE1	2.40	0.56
2:U:196:ARG:NH1	2:U:237:MET:HE2	2.20	0.56
2:M:158:ARG:HB2	2:M:158:ARG:HH11	1.70	0.56
2:S:118:THR:HG22	2:S:282:ARG:HD3	1.87	0.56
1:D:512:LYS:O	1:D:512:LYS:HG2	2.04	0.56
1:H:349:ARG:NH2	1:H:515:ASN:HD21	1.97	0.56
1:I:357:ARG:HG2	1:I:357:ARG:NH1	2.19	0.56
1:K:418:LYS:HG3	1:K:418:LYS:O	2.05	0.56
2:P:282:ARG:O	2:P:286:GLU:HG3	2.05	0.56
2:U:254:ILE:HD13	2:U:269:SER:HB3	1.86	0.56
1:A:398:LEU:HB2	1:A:401:MET:HE2	1.86	0.56
1:B:372:MET:CE	1:B:577:LEU:HG	2.35	0.56
1:B:456:ARG:HH21	1:B:512:LYS:NZ	2.04	0.56
1:B:608:SER:HB3	1:B:611:VAL:HG23	1.87	0.56
1:E:402:ASP:CA	1:E:578:MET:HE2	2.36	0.56
1:F:590:GLN:HA	1:F:593:GLN:CG	2.35	0.56
1:G:417:PRO:HG3	1:H:567:ARG:NH2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:387:TRP:O	1:H:391:VAL:HG23	2.05	0.56
2:R:136:GLN:HB2	2:R:139:LYS:HG3	1.87	0.56
1:A:303:LEU:HD11	1:A:307:LYS:HE3	1.86	0.56
1:A:609:LEU:HD22	2:M:246:MET:HE2	1.87	0.56
1:E:596:ILE:O	1:E:600:LYS:HG3	2.06	0.56
1:F:408:PHE:CE1	1:F:412:MET:HE3	2.39	0.56
2:M:243:MET:HB2	2:M:243:MET:HE3	1.88	0.56
2:P:257:LEU:O	2:P:265:LEU:HB2	2.05	0.56
2:V:132:LYS:HD3	2:V:134:PHE:CZ	2.41	0.56
2:W:118:THR:HG22	2:W:282:ARG:HD3	1.86	0.56
1:J:268:VAL:HG11	1:J:327:PHE:HA	1.88	0.56
1:J:423:LEU:HD11	1:J:528:MET:HE2	1.88	0.56
1:L:433:THR:HG23	1:L:473:GLU:OE2	2.06	0.56
2:R:197:VAL:HG11	2:R:218:VAL:HG11	1.88	0.56
1:G:498:ARG:HB3	1:G:540:ARG:NH2	2.21	0.56
1:L:474:ASP:H	1:L:527:THR:HG1	1.54	0.56
1:B:581:TRP:HZ3	1:B:603:LEU:HB3	1.70	0.56
1:D:343:THR:HG23	1:E:293:LEU:HD13	1.88	0.56
1:E:395:HIS:CD2	1:E:578:MET:HE3	2.41	0.56
1:H:559:ARG:HH11	1:H:623:ILE:HA	1.71	0.56
1:F:480:GLY:HA2	1:F:483:ARG:NH2	2.20	0.56
1:H:460:GLU:O	1:H:463:VAL:HG22	2.06	0.56
1:J:500:TYR:CZ	1:J:507:VAL:HG11	2.41	0.56
1:C:451:ASN:ND2	1:C:475:VAL:HA	2.20	0.55
1:D:416:ILE:HD12	1:E:565:GLU:HA	1.89	0.55
1:D:507:VAL:HG12	1:D:509:LEU:HD22	1.87	0.55
1:E:581:TRP:CZ2	2:Q:246:MET:HE3	2.41	0.55
1:F:382:ALA:HB1	1:F:387:TRP:HE1	1.71	0.55
1:I:311:PRO:C	1:I:313:HIS:H	2.13	0.55
1:K:369:LEU:HB2	1:K:595:ARG:NH1	2.21	0.55
1:L:497:LEU:O	1:L:500:TYR:HB2	2.07	0.55
2:Q:190:PRO:HB3	2:Q:192:GLN:HE22	1.72	0.55
1:A:514:LEU:HD23	1:A:515:ASN:N	2.21	0.55
1:A:576:LEU:C	1:A:578:MET:H	2.15	0.55
2:O:175:ARG:NH2	2:O:237:MET:HB3	2.19	0.55
1:F:283:ASP:HA	1:F:341:VAL:HG13	1.89	0.55
1:I:576:LEU:O	1:I:580:ILE:HG12	2.05	0.55
1:L:416:ILE:O	1:L:420:ARG:HG2	2.07	0.55
2:M:239:ASN:HA	2:M:274:VAL:HB	1.87	0.55
2:N:110:ARG:NH2	2:N:146:TRP:HB3	2.21	0.55
2:O:245:GLY:O	2:O:247:ASN:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:107:TYR:O	2:U:147:VAL:HG23	2.06	0.55
1:C:368:LEU:O	1:C:372:MET:HG3	2.06	0.55
1:C:369:LEU:HD13	1:C:595:ARG:HG2	1.88	0.55
1:D:349:ARG:HH11	1:D:349:ARG:HB2	1.72	0.55
1:D:354:GLN:HE21	1:E:310:GLN:NE2	2.05	0.55
1:G:421:TYR:CE1	1:G:523:PRO:HA	2.42	0.55
1:I:514:LEU:HD23	1:I:516:LYS:HE3	1.88	0.55
1:J:289:LEU:HD11	1:J:333:GLN:HE21	1.72	0.55
1:K:489:GLN:O	1:K:491:ILE:N	2.39	0.55
1:L:356:THR:O	1:L:360:MET:HG3	2.06	0.55
2:P:107:TYR:O	2:P:147:VAL:HG23	2.06	0.55
2:R:245:GLY:C	2:R:247:ASN:H	2.15	0.55
1:A:473:GLU:HG3	1:F:505:VAL:HG21	1.88	0.55
1:C:451:ASN:HD21	1:C:476:LYS:H	1.53	0.55
1:D:354:GLN:NE2	1:E:310:GLN:HE21	2.05	0.55
1:E:386:GLU:O	1:E:389:ALA:HB3	2.05	0.55
1:G:602:ARG:HD3	1:G:602:ARG:C	2.31	0.55
1:I:424:PHE:HB2	1:I:527:THR:HG22	1.87	0.55
2:W:224:GLU:CD	2:W:224:GLU:H	2.14	0.55
1:B:454:LEU:HD12	1:B:454:LEU:H	1.71	0.55
1:F:477:GLY:HA3	1:F:491:ILE:HD12	1.89	0.55
1:G:454:LEU:HA	1:G:457:LEU:CB	2.36	0.55
1:H:581:TRP:HZ3	1:H:603:LEU:HB3	1.71	0.55
1:I:412:MET:HE1	1:I:420:ARG:O	2.07	0.55
1:J:618:ASN:HB3	1:J:624:GLY:O	2.06	0.55
1:K:419:LYS:HA	1:K:542:VAL:HG22	1.88	0.55
1:L:475:VAL:HG22	1:L:528:MET:HB3	1.88	0.55
2:Q:160:MET:HG3	2:Q:214:HIS:O	2.07	0.55
1:A:456:ARG:HG3	1:F:458:ASN:HB2	1.87	0.55
1:C:520:ILE:HD13	1:C:520:ILE:N	2.12	0.55
1:C:568:ILE:C	1:C:570:GLN:H	2.13	0.55
1:G:427:PRO:HG3	1:G:530:GLU:OE1	2.06	0.55
1:J:375:MET:HE3	1:J:382:ALA:CB	2.37	0.55
1:J:433:THR:HG23	1:J:473:GLU:CD	2.31	0.55
1:C:465:ILE:HG21	1:C:517:ARG:HE	1.72	0.55
1:E:502:ASP:OD1	1:E:540:ARG:HD2	2.07	0.55
1:L:450:VAL:HG12	1:L:457:LEU:HD11	1.89	0.55
2:M:190:PRO:HB3	2:M:192:GLN:HE22	1.72	0.55
2:O:119:ALA:O	2:O:279:GLY:HA3	2.07	0.55
2:P:191:PRO:HG2	2:P:192:GLN:HE21	1.71	0.55
2:X:196:ARG:NH1	2:X:237:MET:HE2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:475:VAL:HG12	1:B:491:ILE:HD12	1.88	0.55
1:B:609:LEU:O	1:B:613:GLN:HG3	2.07	0.55
1:G:270:TRP:CE2	1:G:336:ILE:HG12	2.42	0.55
1:K:361:LEU:CD2	1:K:443:CYS:HB3	2.37	0.55
1:L:425:LYS:O	1:L:546:ASP:HA	2.07	0.55
2:T:190:PRO:HB3	2:T:192:GLN:HE22	1.72	0.55
2:V:198:GLU:HB2	2:V:235:ASN:HD21	1.71	0.55
1:B:372:MET:HE3	1:B:573:ILE:HG23	1.88	0.55
1:F:506:LYS:HG2	1:F:520:ILE:HG13	1.89	0.55
1:J:481:GLU:H	1:J:481:GLU:CD	2.15	0.55
2:P:273:ARG:HG3	2:P:273:ARG:HH11	1.72	0.55
2:T:147:VAL:HG21	2:T:151:PRO:HD3	1.89	0.55
1:A:408:PHE:CD2	1:A:439:LEU:HD22	2.41	0.54
1:I:500:TYR:CZ	1:I:507:VAL:HG11	2.41	0.54
1:I:583:ARG:HB3	1:I:587:GLU:OE1	2.06	0.54
2:V:118:THR:HG22	2:V:282:ARG:HD3	1.88	0.54
1:B:270:TRP:CD1	1:B:270:TRP:H	2.24	0.54
1:B:299:PHE:H	1:B:299:PHE:HD2	1.55	0.54
1:C:395:HIS:HD2	1:C:616:LYS:NZ	2.04	0.54
1:D:349:ARG:NE	1:D:517:ARG:HD2	2.21	0.54
1:F:443:CYS:HB2	1:F:469:LEU:HD23	1.90	0.54
1:K:269:SER:N	1:K:323:ASN:HD21	2.00	0.54
2:O:244:GLY:HA3	2:O:248:ARG:HB2	1.89	0.54
1:B:475:VAL:CG1	1:B:491:ILE:HD12	2.37	0.54
1:B:602:ARG:HE	1:B:606:GLU:HG3	1.72	0.54
1:C:375:MET:HE2	1:C:382:ALA:HB1	1.88	0.54
1:C:454:LEU:CA	1:C:457:LEU:HB2	2.35	0.54
1:E:269:SER:OG	1:E:272:LEU:HB2	2.08	0.54
1:F:465:ILE:HG23	1:F:517:ARG:HD2	1.87	0.54
1:G:291:MET:CE	1:G:291:MET:CG	2.86	0.54
1:I:364:ARG:HG2	1:I:443:CYS:O	2.07	0.54
1:L:265:THR:C	1:L:267:GLN:H	2.15	0.54
2:N:193:HIS:ND1	2:N:214:HIS:HB3	2.23	0.54
2:R:196:ARG:O	2:R:234:TYR:HA	2.08	0.54
1:C:419:LYS:HA	1:C:542:VAL:HG22	1.89	0.54
1:G:383:ASP:OD1	1:G:385:GLU:HB3	2.08	0.54
1:I:389:ALA:O	1:I:392:ALA:HB3	2.08	0.54
1:J:415:ASN:HD22	1:J:420:ARG:HG2	1.71	0.54
1:J:589:ALA:C	1:J:591:SER:H	2.16	0.54
2:S:243:MET:CE	2:S:243:MET:CG	2.84	0.54
2:T:189:ALA:HB2	2:T:205:TYR:CZ	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:243:MET:CE	2:X:243:MET:CG	2.85	0.54
1:B:593:GLN:HE22	2:N:181:ARG:HH12	1.55	0.54
1:C:267:GLN:O	1:C:326:ILE:HG21	2.07	0.54
1:C:545:ILE:N	1:C:545:ILE:HD12	2.22	0.54
1:E:625:VAL:HG23	1:E:626:LEU:HG	1.89	0.54
1:G:372:MET:HA	1:G:375:MET:HG2	1.88	0.54
1:G:398:LEU:HB2	1:G:401:MET:CE	2.37	0.54
1:H:300:GLU:O	1:H:301:MET:HE2	2.06	0.54
1:J:357:ARG:HB3	1:J:413:VAL:HG13	1.89	0.54
2:M:287:GLU:C	2:M:289:LEU:H	2.15	0.54
1:C:346:ALA:C	1:C:348:LYS:H	2.15	0.54
1:C:398:LEU:HD12	1:C:401:MET:HE1	1.90	0.54
1:C:581:TRP:HE1	2:O:246:MET:HE3	1.71	0.54
1:E:556:CYS:SG	1:E:619:VAL:HA	2.48	0.54
1:E:585:VAL:HG23	2:Q:242:CYS:HA	1.89	0.54
1:F:497:LEU:O	1:F:500:TYR:HB2	2.08	0.54
1:H:581:TRP:HE3	1:H:603:LEU:HD23	1.73	0.54
1:J:528:MET:HE1	1:J:533:VAL:CG2	2.38	0.54
1:K:561:GLU:O	1:K:565:GLU:HG3	2.07	0.54
2:M:175:ARG:HD3	2:M:191:PRO:O	2.08	0.54
2:P:158:ARG:HG3	2:P:217:VAL:HG22	1.89	0.54
2:X:242:CYS:O	2:X:243:MET:HG3	2.07	0.54
1:B:385:GLU:HA	1:B:607:PHE:CZ	2.43	0.54
1:E:556:CYS:SG	1:E:619:VAL:HG22	2.48	0.54
1:H:454:LEU:HD21	1:H:493:ASN:ND2	2.23	0.54
1:L:470:VAL:O	1:L:524:GLY:HA3	2.08	0.54
2:O:158:ARG:CA	2:O:217:VAL:HG13	2.38	0.54
2:U:155:THR:HG23	2:U:258:GLU:O	2.08	0.54
1:G:469:LEU:C	1:G:469:LEU:CD1	2.81	0.54
1:I:332:ASN:O	1:I:336:ILE:HG13	2.07	0.54
1:L:590:GLN:CD	1:L:590:GLN:N	2.66	0.54
2:S:197:VAL:HG23	2:S:216:VAL:HG21	1.89	0.54
2:X:189:ALA:HB2	2:X:205:TYR:CZ	2.43	0.54
2:X:259:ASP:OD2	2:X:263:ASN:HB2	2.08	0.54
1:I:405:VAL:HG12	1:I:579:LEU:HD21	1.89	0.54
1:J:454:LEU:HD22	1:K:453:PRO:HG3	1.90	0.54
1:K:508:ASN:ND2	1:L:463:VAL:HG11	2.22	0.54
2:M:197:VAL:HG23	2:M:216:VAL:HG21	1.90	0.54
2:R:156:ARG:HB3	2:R:217:VAL:CG1	2.38	0.54
1:A:485:LEU:CD2	1:A:529:ASN:HD22	2.21	0.54
1:B:589:ALA:O	1:B:592:ILE:HG22	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:410:LYS:HE2	1:C:410:LYS:HA	1.89	0.54
1:D:564:LEU:C	1:D:566:LYS:N	2.66	0.54
1:D:584:PRO:HG2	1:D:587:GLU:HG3	1.89	0.54
1:I:495:ASP:O	1:I:498:ARG:HG3	2.07	0.54
1:K:342:ASP:OD2	1:L:334:LYS:HD2	2.08	0.54
2:W:120:LYS:N	2:W:120:LYS:HD2	2.23	0.54
1:A:454:LEU:HB3	1:B:453:PRO:HG2	1.90	0.53
1:E:397:LEU:O	1:E:397:LEU:HG	2.07	0.53
1:F:349:ARG:CZ	1:F:517:ARG:CD	2.86	0.53
1:H:402:ASP:HA	1:H:578:MET:CE	2.31	0.53
1:H:454:LEU:HD12	1:H:454:LEU:H	1.73	0.53
1:K:398:LEU:HB2	1:K:401:MET:CE	2.38	0.53
2:P:122:VAL:HG12	2:P:123:THR:N	2.23	0.53
2:R:196:ARG:CZ	2:R:237:MET:HE2	2.38	0.53
2:X:191:PRO:HG2	2:X:192:GLN:HE21	1.72	0.53
1:D:285:VAL:HG22	1:D:341:VAL:HG21	1.91	0.53
1:D:300:GLU:HB2	1:D:301:MET:SD	2.48	0.53
1:E:465:ILE:O	1:E:466:ASP:HB2	2.07	0.53
1:G:614:LYS:O	1:G:617:PHE:HB3	2.07	0.53
2:W:109:PHE:CD1	2:W:257:LEU:HD22	2.44	0.53
1:C:608:SER:HA	2:O:280:ARG:NH1	2.23	0.53
1:F:408:PHE:HE1	1:F:525:ILE:HD11	1.66	0.53
1:J:311:PRO:C	1:J:313:HIS:H	2.17	0.53
1:L:372:MET:HA	1:L:375:MET:HG2	1.89	0.53
2:W:175:ARG:HD3	2:W:191:PRO:O	2.08	0.53
1:A:443:CYS:HB3	1:A:468:PHE:CD2	2.42	0.53
1:B:618:ASN:HB3	1:B:623:ILE:HG13	1.91	0.53
1:G:594:SER:O	1:G:597:VAL:HG12	2.07	0.53
1:H:506:LYS:HG2	1:H:519:GLN:HA	1.90	0.53
1:I:611:VAL:O	1:I:614:LYS:HB3	2.08	0.53
1:J:417:PRO:HG3	1:K:567:ARG:NH1	2.24	0.53
1:K:454:LEU:HB3	1:L:453:PRO:HG2	1.88	0.53
1:L:460:GLU:O	1:L:463:VAL:HB	2.09	0.53
2:M:176:CYS:SG	2:M:179:HIS:HB2	2.48	0.53
2:N:244:GLY:HA3	2:N:248:ARG:HB2	1.90	0.53
2:O:158:ARG:CZ	2:O:217:VAL:HG21	2.38	0.53
1:C:475:VAL:O	1:C:475:VAL:HG23	2.09	0.53
1:D:295:PHE:HB3	1:D:320:HIS:O	2.09	0.53
1:E:353:LEU:HD21	1:E:517:ARG:HH22	1.74	0.53
1:E:369:LEU:HD12	1:E:592:ILE:HD11	1.90	0.53
1:E:557:LEU:HD13	1:E:564:LEU:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:581:TRP:HZ3	1:E:603:LEU:HB3	1.73	0.53
1:F:452:LEU:HB3	1:F:453:PRO:CD	2.39	0.53
1:G:410:LYS:HA	1:G:410:LYS:HE2	1.91	0.53
1:J:441:GLU:OE1	1:J:571:SER:HA	2.09	0.53
1:J:621:MET:HB2	1:J:623:ILE:HG12	1.90	0.53
2:N:101:LYS:HE2	2:N:101:LYS:N	2.24	0.53
2:R:277:CYS:HB2	2:R:280:ARG:NH2	2.22	0.53
2:W:180:GLU:HG3	2:W:180:GLU:O	2.08	0.53
1:D:402:ASP:CA	1:D:578:MET:HE3	2.38	0.53
1:E:397:LEU:O	1:E:398:LEU:HD13	2.09	0.53
1:E:510:GLU:HG3	1:E:510:GLU:O	2.09	0.53
1:F:608:SER:HB3	1:F:611:VAL:CG2	2.39	0.53
1:H:454:LEU:HB2	1:I:453:PRO:HG2	1.90	0.53
1:I:525:ILE:HG22	1:I:526:VAL:N	2.23	0.53
1:A:285:VAL:HG22	1:A:341:VAL:HG21	1.89	0.53
1:A:511:LYS:HB3	1:A:516:LYS:HG3	1.90	0.53
1:C:389:ALA:HB1	1:C:625:VAL:HG11	1.89	0.53
1:D:296:GLN:HG3	1:D:297:TYR:N	2.24	0.53
1:F:421:TYR:CE1	1:F:523:PRO:HA	2.43	0.53
1:G:567:ARG:NH2	1:L:503:GLY:O	2.42	0.53
1:G:580:ILE:HD13	1:G:596:ILE:HG23	1.89	0.53
1:H:609:LEU:HD22	2:T:246:MET:HE2	1.91	0.53
2:T:107:TYR:CE1	2:T:151:PRO:HA	2.43	0.53
2:U:173:VAL:CG1	2:U:194:LEU:HD12	2.38	0.53
1:C:386:GLU:O	1:C:389:ALA:HB3	2.09	0.53
1:F:389:ALA:HB1	1:F:625:VAL:HG21	1.89	0.53
1:G:351:ASP:O	1:G:355:LEU:HB2	2.08	0.53
1:I:458:ASN:HB2	1:J:456:ARG:HH21	1.74	0.53
1:H:559:ARG:HH11	1:H:559:ARG:HG3	1.74	0.53
1:J:403:SER:HA	1:J:583:ARG:NH2	2.22	0.53
2:Q:224:GLU:CD	2:Q:224:GLU:H	2.16	0.53
2:T:179:HIS:HA	2:T:182:CYS:SG	2.48	0.53
2:V:251:ILE:H	2:V:251:ILE:HD12	1.73	0.53
1:A:520:ILE:H	1:A:520:ILE:CD1	2.18	0.53
1:I:472:PHE:HD2	1:I:526:VAL:HG22	1.74	0.53
1:K:408:PHE:O	1:K:412:MET:HG2	2.08	0.53
2:N:112:GLY:HA3	2:N:146:TRP:HE1	1.74	0.53
2:N:245:GLY:C	2:N:247:ASN:H	2.16	0.53
2:O:176:CYS:SG	2:O:179:HIS:HB2	2.49	0.53
2:U:245:GLY:C	2:U:247:ASN:H	2.17	0.53
2:V:245:GLY:C	2:V:247:ASN:H	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:481:GLU:CD	1:D:481:GLU:H	2.17	0.52
1:E:287:LEU:O	1:E:291:MET:HG3	2.10	0.52
1:H:423:LEU:HD12	1:H:526:VAL:O	2.09	0.52
1:I:594:SER:O	1:I:598:GLU:HG3	2.09	0.52
1:K:276:TYR:OH	1:K:291:MET:HE3	2.09	0.52
1:K:454:LEU:HD22	1:K:454:LEU:N	2.22	0.52
2:R:175:ARG:HG3	2:R:192:GLN:O	2.09	0.52
1:B:614:LYS:O	1:B:617:PHE:HB3	2.09	0.52
2:Q:114:LEU:HD22	2:Q:142:PRO:HG3	1.91	0.52
2:U:196:ARG:HB2	2:U:235:ASN:HB2	1.89	0.52
2:V:159:ALA:HB3	2:V:216:VAL:HG13	1.90	0.52
1:C:538:GLN:HE22	1:C:544:GLN:NE2	2.06	0.52
1:D:314:TYR:CE1	1:D:315:LYS:HG2	2.44	0.52
1:D:336:ILE:O	1:D:337:CYS:C	2.50	0.52
1:E:424:PHE:O	1:E:527:THR:HA	2.09	0.52
1:F:361:LEU:HD13	1:F:361:LEU:O	2.08	0.52
1:F:462:GLY:C	1:F:464:ALA:H	2.18	0.52
1:I:424:PHE:CE1	1:I:545:ILE:HD12	2.44	0.52
1:L:514:LEU:HG	1:L:516:LYS:N	2.24	0.52
2:M:189:ALA:HB2	2:M:205:TYR:CZ	2.44	0.52
1:B:346:ALA:O	1:B:350:VAL:HG23	2.09	0.52
1:G:388:MET:HG3	1:G:607:PHE:CE1	2.44	0.52
1:G:517:ARG:HG2	1:G:518:THR:N	2.24	0.52
1:I:327:PHE:C	1:I:329:ASP:H	2.15	0.52
1:L:469:LEU:C	1:L:469:LEU:HD12	2.34	0.52
2:Q:196:ARG:NH1	2:Q:237:MET:HE2	2.24	0.52
2:U:132:LYS:HE2	2:U:273:ARG:HB2	1.91	0.52
1:B:408:PHE:O	1:B:412:MET:HG2	2.09	0.52
1:C:317:HIS:O	1:C:321:TYR:N	2.41	0.52
1:E:580:ILE:HG21	1:E:599:TRP:HB3	1.91	0.52
1:F:268:VAL:HG11	1:F:327:PHE:HA	1.91	0.52
1:L:299:PHE:CZ	1:L:318:GLU:HB2	2.44	0.52
2:O:244:GLY:O	2:O:246:MET:N	2.43	0.52
2:T:264:LEU:HD11	2:T:267:ARG:HB2	1.91	0.52
1:C:349:ARG:HD2	1:C:517:ARG:NH1	2.25	0.52
1:C:507:VAL:HG12	1:C:508:ASN:N	2.25	0.52
1:C:568:ILE:O	1:C:570:GLN:N	2.43	0.52
1:E:307:LYS:HD2	1:E:309:GLU:HB3	1.92	0.52
1:J:420:ARG:CZ	1:J:503:GLY:HA3	2.40	0.52
1:J:421:TYR:CE1	1:J:523:PRO:HA	2.44	0.52
1:K:346:ALA:O	1:K:350:VAL:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:126:TYR:OH	2:P:131:ASN:ND2	2.42	0.52
1:A:512:LYS:HB2	1:F:514:LEU:HD13	1.92	0.52
1:B:289:LEU:O	1:B:293:LEU:HD12	2.09	0.52
1:C:498:ARG:CZ	1:D:476:LYS:HD3	2.40	0.52
1:I:512:LYS:HG3	1:I:512:LYS:O	2.09	0.52
1:J:415:ASN:HD21	1:J:420:ARG:NH1	2.05	0.52
2:N:147:VAL:HG21	2:N:151:PRO:HD3	1.91	0.52
2:O:189:ALA:HB2	2:O:205:TYR:CZ	2.44	0.52
2:Q:257:LEU:O	2:Q:265:LEU:HB2	2.09	0.52
1:A:520:ILE:HD12	1:A:520:ILE:N	2.16	0.52
1:B:459:PHE:C	1:B:461:LEU:H	2.17	0.52
1:C:454:LEU:HD22	1:D:453:PRO:HG3	1.90	0.52
1:C:560:SER:OG	1:C:625:VAL:HG23	2.09	0.52
1:C:585:VAL:HG13	2:O:242:CYS:HA	1.91	0.52
1:E:314:TYR:C	1:E:314:TYR:CD1	2.88	0.52
1:I:445:GLY:O	1:I:446:LYS:HG2	2.10	0.52
1:I:454:LEU:HB2	1:J:453:PRO:CG	2.40	0.52
1:I:512:LYS:HD3	1:I:516:LYS:NZ	2.25	0.52
1:J:353:LEU:HD21	1:J:517:ARG:NH1	2.24	0.52
2:N:105:GLY:HA3	2:N:265:LEU:O	2.10	0.52
2:V:159:ALA:HB3	2:V:216:VAL:CG1	2.40	0.52
1:G:470:VAL:O	1:G:524:GLY:HA3	2.08	0.52
1:G:589:ALA:O	1:G:593:GLN:HG3	2.10	0.52
1:K:287:LEU:O	1:K:291:MET:HG2	2.10	0.52
2:M:108:GLY:O	2:M:110:ARG:NH1	2.43	0.52
2:Q:158:ARG:CZ	2:Q:217:VAL:HG21	2.40	0.52
2:U:189:ALA:HB2	2:U:205:TYR:CZ	2.45	0.52
1:A:597:VAL:O	1:A:601:GLU:HG3	2.09	0.52
1:C:584:PRO:C	1:C:586:ALA:H	2.18	0.52
1:F:579:LEU:CD2	1:F:583:ARG:HG3	2.37	0.52
1:I:561:GLU:O	1:I:565:GLU:HG3	2.09	0.52
1:C:529:ASN:O	1:C:531:TYR:N	2.41	0.51
1:G:274:THR:HA	1:G:340:ALA:HB1	1.92	0.51
1:H:288:LEU:O	1:H:289:LEU:C	2.53	0.51
1:H:529:ASN:O	1:H:530:GLU:C	2.53	0.51
1:J:356:THR:OG1	1:J:359:GLN:HG3	2.09	0.51
1:J:560:SER:OG	1:J:624:GLY:HA2	2.09	0.51
2:N:203:VAL:HA	2:N:218:VAL:HG12	1.92	0.51
2:T:264:LEU:O	2:T:265:LEU:HD23	2.09	0.51
2:W:158:ARG:HB2	2:W:217:VAL:HG13	1.93	0.51
1:A:357:ARG:HA	1:A:360:MET:CE	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:LEU:HD21	1:B:569:ILE:O	2.11	0.51
1:D:405:VAL:O	1:D:409:LEU:HG	2.09	0.51
1:F:550:LYS:HD3	1:F:552:TYR:OH	2.11	0.51
1:I:405:VAL:CG1	1:I:579:LEU:HD21	2.40	0.51
1:J:581:TRP:NE1	2:V:246:MET:HE3	2.26	0.51
2:T:132:LYS:HE3	2:T:271:GLU:OE2	2.10	0.51
1:C:401:MET:HG3	1:C:578:MET:HE1	1.92	0.51
1:E:451:ASN:HD22	1:E:490:GLY:HA3	1.76	0.51
1:F:510:GLU:HG3	1:F:514:LEU:O	2.10	0.51
1:F:584:PRO:HB3	2:R:243:MET:HA	1.92	0.51
1:I:385:GLU:HA	1:I:607:PHE:CZ	2.45	0.51
1:I:425:LYS:NZ	1:I:530:GLU:HA	2.24	0.51
1:K:368:LEU:O	1:K:372:MET:HG3	2.11	0.51
1:L:351:ASP:O	1:L:355:LEU:HB2	2.11	0.51
1:L:583:ARG:HA	1:L:583:ARG:HE	1.75	0.51
2:U:249:ARG:HG3	2:U:249:ARG:HH11	1.76	0.51
2:W:132:LYS:HD3	2:W:134:PHE:CZ	2.46	0.51
2:W:251:ILE:HG22	2:W:252:LEU:N	2.25	0.51
1:C:454:LEU:H	1:C:454:LEU:HD12	1.75	0.51
1:D:585:VAL:HG23	2:P:242:CYS:HA	1.93	0.51
1:F:349:ARG:NH1	1:F:517:ARG:HD3	2.25	0.51
1:F:550:LYS:HB2	1:F:553:LEU:HD12	1.91	0.51
1:G:456:ARG:HG2	1:G:456:ARG:HH11	1.75	0.51
1:G:458:ASN:OD1	1:G:510:GLU:HG2	2.10	0.51
1:H:454:LEU:HD11	1:H:493:ASN:HD21	1.76	0.51
1:L:581:TRP:CZ2	2:X:246:MET:HE3	2.46	0.51
2:T:163:TYR:CZ	2:T:173:VAL:HG22	2.45	0.51
2:V:155:THR:HG23	2:V:258:GLU:O	2.10	0.51
1:A:389:ALA:HB1	1:A:625:VAL:HG21	1.91	0.51
1:D:343:THR:HG23	1:E:293:LEU:CD1	2.40	0.51
1:D:354:GLN:NE2	1:E:310:GLN:NE2	2.59	0.51
1:E:401:MET:HG3	1:E:578:MET:HE1	1.92	0.51
1:L:454:LEU:HA	1:L:457:LEU:CB	2.38	0.51
2:V:241:SER:HA	2:V:245:GLY:H	1.76	0.51
1:B:335:THR:O	1:B:338:GLN:HB2	2.11	0.51
1:B:385:GLU:HA	1:B:607:PHE:HZ	1.74	0.51
1:C:597:VAL:HG21	2:O:178:HIS:ND1	2.25	0.51
1:D:608:SER:HB3	2:P:280:ARG:HH11	1.75	0.51
1:F:349:ARG:HD3	1:F:517:ARG:NH1	2.25	0.51
1:F:514:LEU:HD23	1:F:516:LYS:HD3	1.92	0.51
1:G:415:ASN:ND2	1:G:420:ARG:CD	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:580:ILE:HG22	1:I:600:LYS:HG3	1.92	0.51
1:L:599:TRP:O	1:L:603:LEU:HB2	2.10	0.51
2:M:118:THR:HG22	2:M:282:ARG:HD3	1.93	0.51
2:M:242:CYS:O	2:M:243:MET:HG3	2.11	0.51
2:T:224:GLU:CD	2:T:224:GLU:H	2.19	0.51
2:V:126:TYR:OH	2:V:131:ASN:HA	2.11	0.51
1:A:295:PHE:HA	1:A:317:HIS:CE1	2.44	0.51
1:A:298:SER:HA	1:A:321:TYR:CE1	2.45	0.51
1:B:386:GLU:O	1:B:389:ALA:HB3	2.11	0.51
1:D:609:LEU:HD22	2:P:246:MET:HE2	1.92	0.51
2:N:158:ARG:HH11	2:N:158:ARG:HB2	1.76	0.51
2:P:175:ARG:HG3	2:P:192:GLN:O	2.11	0.51
2:R:203:VAL:HG23	2:R:218:VAL:CG1	2.41	0.51
2:S:244:GLY:O	2:S:246:MET:N	2.44	0.51
1:E:428:ILE:H	1:E:428:ILE:CD1	2.19	0.51
1:G:476:LYS:HE2	1:L:496:ASN:HD22	1.73	0.51
1:G:592:ILE:O	1:G:596:ILE:HG12	2.11	0.51
1:I:386:GLU:O	1:I:389:ALA:HB3	2.10	0.51
1:I:458:ASN:HB2	1:J:456:ARG:NH2	2.26	0.51
1:I:580:ILE:HG21	1:I:599:TRP:O	2.10	0.51
1:J:398:LEU:HB2	1:J:401:MET:HE2	1.93	0.51
2:P:197:VAL:HG23	2:P:216:VAL:HG21	1.91	0.51
1:A:435:LEU:HD23	1:A:547:PHE:HZ	1.76	0.51
1:B:517:ARG:CZ	1:B:519:GLN:HB3	2.41	0.51
1:D:387:TRP:CZ3	1:D:573:ILE:HB	2.45	0.51
1:E:311:PRO:C	1:E:313:HIS:H	2.19	0.51
1:F:446:LYS:HG3	1:F:463:VAL:HG12	1.92	0.51
1:G:579:LEU:O	1:G:583:ARG:HB2	2.11	0.51
1:K:589:ALA:O	1:K:592:ILE:HG22	2.11	0.51
1:A:428:ILE:H	1:A:428:ILE:CD1	2.21	0.51
1:A:583:ARG:HD3	1:A:587:GLU:OE1	2.10	0.51
1:B:456:ARG:HH21	1:B:512:LYS:HZ3	1.59	0.51
1:G:608:SER:HB2	2:S:280:ARG:HH11	1.76	0.51
1:H:415:ASN:ND2	1:H:420:ARG:HH11	2.01	0.51
1:I:430:SER:HB3	1:I:547:PHE:HB3	1.93	0.51
2:O:114:LEU:N	2:O:114:LEU:HD12	2.26	0.51
1:D:398:LEU:HD21	1:D:545:ILE:HG21	1.93	0.50
1:I:374:ILE:HD12	1:I:374:ILE:N	2.26	0.50
1:I:589:ALA:H	1:I:592:ILE:HD11	1.74	0.50
1:A:287:LEU:O	1:A:291:MET:HB2	2.11	0.50
1:J:375:MET:HE1	1:J:387:TRP:CZ2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:196:ARG:NH1	2:O:237:MET:CE	2.70	0.50
1:A:428:ILE:HD12	1:A:428:ILE:N	2.22	0.50
1:G:459:PHE:HZ	1:G:513:HIS:H	1.58	0.50
1:J:293:LEU:O	1:J:296:GLN:HB3	2.10	0.50
1:J:320:HIS:O	1:J:321:TYR:C	2.54	0.50
1:J:617:PHE:O	1:J:621:MET:HG2	2.11	0.50
1:K:346:ALA:HB1	1:L:290:GLY:N	2.25	0.50
2:P:132:LYS:HE2	2:P:273:ARG:HB2	1.94	0.50
2:U:287:GLU:C	2:U:289:LEU:H	2.19	0.50
1:A:349:ARG:HH11	1:A:349:ARG:HB2	1.76	0.50
1:A:469:LEU:HD12	1:A:470:VAL:N	2.27	0.50
1:D:368:LEU:HD22	1:D:573:ILE:HD13	1.93	0.50
1:D:585:VAL:HG12	1:D:585:VAL:O	2.12	0.50
1:E:412:MET:HE1	1:E:524:GLY:CA	2.42	0.50
1:E:470:VAL:O	1:E:524:GLY:HA3	2.10	0.50
1:I:383:ASP:HB3	1:I:386:GLU:HG3	1.94	0.50
1:L:502:ASP:OD1	1:L:540:ARG:HD2	2.12	0.50
2:S:257:LEU:O	2:S:265:LEU:HB2	2.12	0.50
1:D:424:PHE:HB2	1:D:527:THR:HG22	1.93	0.50
1:E:454:LEU:HD13	1:E:457:LEU:HD22	1.92	0.50
1:J:483:ARG:HG3	1:J:483:ARG:HH11	1.77	0.50
1:L:421:TYR:CE1	1:L:523:PRO:HA	2.47	0.50
2:T:197:VAL:HG23	2:T:216:VAL:HG21	1.94	0.50
1:D:384:ILE:HG23	1:D:385:GLU:N	2.25	0.50
1:F:314:TYR:CD1	1:F:315:LYS:HG3	2.47	0.50
1:G:299:PHE:HA	1:G:302:CYS:HB2	1.93	0.50
1:G:311:PRO:HA	1:G:314:TYR:CE2	2.47	0.50
1:G:423:LEU:CD1	1:G:528:MET:HE3	2.41	0.50
1:J:584:PRO:CG	1:J:587:GLU:HG3	2.41	0.50
1:J:589:ALA:O	1:J:591:SER:N	2.45	0.50
2:O:137:LEU:O	2:O:139:LYS:HG2	2.11	0.50
2:O:203:VAL:HA	2:O:218:VAL:HG12	1.93	0.50
1:D:597:VAL:HG21	2:P:178:HIS:ND1	2.27	0.50
1:E:341:VAL:O	1:E:344:VAL:N	2.45	0.50
1:I:422:TRP:HB2	1:I:525:ILE:HD13	1.94	0.50
1:I:458:ASN:HD22	1:J:456:ARG:HE	1.59	0.50
2:M:197:VAL:HG11	2:M:218:VAL:HG11	1.93	0.50
2:S:224:GLU:H	2:S:224:GLU:CD	2.19	0.50
2:U:108:GLY:O	2:U:147:VAL:HA	2.11	0.50
2:W:166:SER:HA	2:W:169:MET:HE3	1.94	0.50
1:C:300:GLU:CD	1:C:300:GLU:H	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:299:PHE:O	1:G:302:CYS:HB3	2.11	0.50
1:H:375:MET:HE1	1:H:573:ILE:HG21	1.93	0.50
2:W:129:ALA:C	2:W:130:LEU:HD12	2.37	0.50
1:A:609:LEU:HA	2:M:246:MET:HE1	1.93	0.50
1:E:575:LEU:O	1:E:578:MET:HB3	2.12	0.50
1:F:422:TRP:CE2	1:F:543:LYS:HD2	2.47	0.50
1:F:465:ILE:HD12	1:F:517:ARG:HB3	1.92	0.50
1:G:417:PRO:HG3	1:H:567:ARG:CZ	2.42	0.50
1:I:299:PHE:CZ	1:I:318:GLU:HB2	2.47	0.50
1:K:387:TRP:CE3	1:K:568:ILE:HG23	2.47	0.50
2:S:132:LYS:HE2	2:S:273:ARG:HB2	1.93	0.50
2:U:102:THR:HG23	2:U:268:ASN:OD1	2.12	0.50
2:U:119:ALA:O	2:U:279:GLY:HA3	2.11	0.50
1:B:369:LEU:CB	1:B:595:ARG:HH11	2.24	0.49
1:D:375:MET:HE2	1:D:376:PHE:CZ	2.48	0.49
1:F:383:ASP:HB3	1:F:386:GLU:CG	2.37	0.49
1:F:430:SER:OG	1:F:432:LYS:HG3	2.12	0.49
1:G:346:ALA:O	1:G:350:VAL:HG23	2.12	0.49
1:L:622:GLY:C	1:L:623:ILE:HD13	2.37	0.49
2:M:119:ALA:O	2:M:279:GLY:HA3	2.12	0.49
2:Q:101:LYS:HB2	2:Q:267:ARG:HH21	1.76	0.49
2:U:101:LYS:N	2:U:101:LYS:HE2	2.26	0.49
1:E:356:THR:OG1	1:E:359:GLN:HG3	2.11	0.49
1:E:605:LYS:O	1:E:606:GLU:HG2	2.12	0.49
1:G:576:LEU:O	1:G:580:ILE:HG12	2.12	0.49
1:I:424:PHE:HE1	1:I:545:ILE:HD12	1.77	0.49
1:J:375:MET:HE2	1:J:376:PHE:CE2	2.47	0.49
2:W:191:PRO:HG2	2:W:192:GLN:HE21	1.76	0.49
1:B:384:ILE:HG21	1:B:606:GLU:OE2	2.12	0.49
1:E:469:LEU:C	1:E:469:LEU:HD12	2.37	0.49
1:F:433:THR:HG23	1:F:473:GLU:CD	2.37	0.49
1:G:470:VAL:HG23	1:G:522:PRO:HB2	1.94	0.49
1:G:608:SER:HB2	2:S:280:ARG:NH1	2.27	0.49
1:K:517:ARG:HG2	1:K:519:GLN:HG2	1.93	0.49
2:P:287:GLU:C	2:P:289:LEU:H	2.20	0.49
1:C:272:LEU:HD13	1:C:323:ASN:HB2	1.94	0.49
1:D:400:LYS:O	1:D:404:VAL:HG23	2.12	0.49
1:I:357:ARG:HA	1:I:360:MET:CE	2.41	0.49
1:K:440:LEU:HD22	1:K:471:VAL:CG2	2.42	0.49
1:K:502:ASP:CG	1:K:540:ARG:HH11	2.21	0.49
1:K:511:LYS:HB2	1:K:514:LEU:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:618:ASN:ND2	1:K:627:ASP:HB2	2.27	0.49
1:L:423:LEU:CD1	1:L:528:MET:HE3	2.35	0.49
2:O:158:ARG:HA	2:O:217:VAL:HG13	1.93	0.49
2:O:252:LEU:HD12	2:O:271:GLU:HA	1.93	0.49
2:O:257:LEU:O	2:O:265:LEU:HB2	2.12	0.49
2:P:175:ARG:HD2	2:P:193:HIS:O	2.12	0.49
2:Q:197:VAL:HG11	2:Q:218:VAL:HG11	1.93	0.49
1:A:625:VAL:HG23	1:A:626:LEU:H	1.77	0.49
1:L:520:ILE:H	1:L:520:ILE:CD1	2.18	0.49
2:N:160:MET:HE2	2:N:213:ARG:HB3	1.94	0.49
2:U:193:HIS:CE1	2:U:214:HIS:HB3	2.47	0.49
2:W:147:VAL:HG21	2:W:151:PRO:HD3	1.94	0.49
2:W:252:LEU:HD12	2:W:270:PHE:O	2.12	0.49
1:B:282:CYS:SG	1:B:288:LEU:HB2	2.53	0.49
1:B:581:TRP:CZ3	1:B:603:LEU:HB3	2.47	0.49
1:B:583:ARG:HD2	1:B:587:GLU:OE1	2.13	0.49
1:D:425:LYS:HE2	1:D:530:GLU:HA	1.94	0.49
1:E:372:MET:HG3	1:E:573:ILE:HD12	1.94	0.49
1:H:443:CYS:HB3	1:H:468:PHE:CD2	2.47	0.49
1:I:353:LEU:HD12	1:J:287:LEU:HD13	1.94	0.49
1:L:608:SER:O	1:L:609:LEU:C	2.55	0.49
2:S:158:ARG:HH21	2:S:206:LEU:HD23	1.77	0.49
2:U:132:LYS:HG3	2:U:271:GLU:HB3	1.95	0.49
1:B:382:ALA:HB1	1:B:387:TRP:HE1	1.76	0.49
1:C:458:ASN:CG	1:D:456:ARG:HD3	2.38	0.49
1:E:408:PHE:CD2	1:E:439:LEU:HD22	2.48	0.49
1:F:446:LYS:HG2	1:F:467:GLN:OE1	2.13	0.49
1:H:311:PRO:C	1:H:313:HIS:H	2.21	0.49
1:I:469:LEU:HB2	1:I:523:PRO:O	2.12	0.49
1:L:506:LYS:HG2	1:L:520:ILE:HG13	1.95	0.49
2:M:251:ILE:HG22	2:M:252:LEU:N	2.28	0.49
2:Q:280:ARG:HG2	2:Q:280:ARG:HH11	1.77	0.49
2:T:107:TYR:O	2:T:147:VAL:HG23	2.12	0.49
1:B:295:PHE:HA	1:B:317:HIS:CD2	2.48	0.49
1:B:394:LEU:C	1:B:396:CYS:H	2.21	0.49
1:D:608:SER:HB3	2:P:280:ARG:HD2	1.95	0.49
1:F:454:LEU:N	1:F:454:LEU:HD12	2.28	0.49
1:F:470:VAL:O	1:F:524:GLY:HA3	2.13	0.49
1:H:615:MET:O	1:H:616:LYS:C	2.55	0.49
1:J:507:VAL:O	1:J:518:THR:HA	2.12	0.49
1:L:349:ARG:CZ	1:L:517:ARG:CD	2.90	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:211:THR:C	2:N:213:ARG:H	2.20	0.49
2:X:109:PHE:HE1	2:X:145:LEU:HG	1.76	0.49
1:E:410:LYS:HA	1:E:410:LYS:HE3	1.93	0.49
1:F:424:PHE:HB2	1:F:527:THR:HG22	1.93	0.49
1:K:361:LEU:HD23	1:K:443:CYS:HB3	1.95	0.49
1:A:451:ASN:HB3	1:F:496:ASN:HD22	1.78	0.49
1:C:397:LEU:HG	1:C:398:LEU:HG	1.94	0.49
1:C:454:LEU:C	1:C:456:ARG:N	2.68	0.49
1:C:525:ILE:CG2	1:C:526:VAL:N	2.75	0.49
1:D:415:ASN:ND2	1:D:420:ARG:HH11	2.02	0.49
1:D:606:GLU:HB3	1:D:607:PHE:CE1	2.48	0.49
1:F:268:VAL:HG13	1:F:326:ILE:HG22	1.94	0.49
1:F:409:LEU:O	1:F:413:VAL:HG23	2.13	0.49
1:I:557:LEU:HD22	1:I:564:LEU:HG	1.94	0.49
2:R:126:TYR:CE2	2:R:128:PRO:HG3	2.47	0.49
2:S:160:MET:SD	2:S:213:ARG:HG2	2.53	0.49
2:W:122:VAL:HG11	2:W:125:THR:HB	1.95	0.49
2:X:147:VAL:HG21	2:X:151:PRO:HD3	1.95	0.49
1:C:401:MET:HG3	1:C:578:MET:CE	2.43	0.48
1:C:581:TRP:CZ3	1:C:603:LEU:HB3	2.48	0.48
1:D:283:ASP:HA	1:D:341:VAL:HG13	1.95	0.48
1:I:385:GLU:HA	1:I:607:PHE:HZ	1.76	0.48
1:I:608:SER:CB	2:U:280:ARG:NH1	2.76	0.48
1:L:440:LEU:C	1:L:440:LEU:HD23	2.38	0.48
2:M:175:ARG:NH2	2:M:237:MET:HB3	2.28	0.48
2:Q:287:GLU:C	2:Q:289:LEU:H	2.22	0.48
2:R:158:ARG:HH11	2:R:158:ARG:CB	2.26	0.48
2:S:245:GLY:O	2:S:247:ASN:N	2.44	0.48
1:A:391:VAL:HG13	1:A:578:MET:HB2	1.95	0.48
1:A:511:LYS:HB3	1:A:516:LYS:CG	2.43	0.48
1:I:408:PHE:HB2	1:I:422:TRP:CH2	2.49	0.48
1:K:510:GLU:HA	1:K:516:LYS:HA	1.96	0.48
1:K:556:CYS:SG	1:K:625:VAL:HG13	2.54	0.48
2:R:189:ALA:HB2	2:R:205:TYR:CZ	2.49	0.48
1:F:623:ILE:HG22	1:F:624:GLY:N	2.26	0.48
1:H:383:ASP:OD1	1:H:385:GLU:HB3	2.13	0.48
1:J:537:LEU:HG	1:J:541:PHE:CE1	2.48	0.48
1:K:456:ARG:HH11	1:K:456:ARG:HG3	1.77	0.48
2:P:133:MET:HE1	2:P:236:TYR:HE1	1.78	0.48
2:Q:94:SER:HB3	2:Q:211:THR:O	2.14	0.48
2:Q:259:ASP:OD2	2:Q:263:ASN:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:MET:O	1:A:382:ALA:HB3	2.13	0.48
1:A:453:PRO:HG2	1:F:454:LEU:O	2.13	0.48
1:A:608:SER:OG	1:A:611:VAL:HG23	2.12	0.48
1:C:497:LEU:O	1:C:500:TYR:HB2	2.13	0.48
1:D:469:LEU:HD12	1:D:469:LEU:C	2.39	0.48
1:F:359:GLN:O	1:F:362:THR:HB	2.12	0.48
1:G:520:ILE:HD12	1:G:520:ILE:N	2.28	0.48
1:H:410:LYS:HE2	1:H:410:LYS:HA	1.94	0.48
1:H:581:TRP:HD1	1:H:582:TYR:CE1	2.32	0.48
1:J:469:LEU:C	1:J:469:LEU:HD12	2.38	0.48
1:J:525:ILE:HG22	1:J:526:VAL:N	2.28	0.48
1:K:317:HIS:O	1:K:318:GLU:C	2.55	0.48
1:K:592:ILE:O	1:K:596:ILE:HG12	2.12	0.48
1:K:617:PHE:O	1:K:621:MET:HG2	2.14	0.48
2:Q:126:TYR:OH	2:Q:131:ASN:HA	2.12	0.48
2:Q:175:ARG:HD2	2:Q:193:HIS:O	2.13	0.48
2:Q:216:VAL:O	2:Q:216:VAL:HG13	2.13	0.48
2:S:132:LYS:HD3	2:S:134:PHE:CZ	2.49	0.48
2:S:133:MET:HE3	2:S:135:CYS:SG	2.53	0.48
2:S:175:ARG:NH2	2:S:237:MET:HB3	2.28	0.48
2:T:108:GLY:O	2:T:110:ARG:NH1	2.46	0.48
2:T:280:ARG:HH11	2:T:280:ARG:HG2	1.78	0.48
1:C:412:MET:HE1	1:C:420:ARG:O	2.14	0.48
1:C:568:ILE:C	1:C:570:GLN:N	2.69	0.48
1:C:593:GLN:HE22	2:O:177:PRO:HB2	1.79	0.48
1:G:445:GLY:HA3	1:G:469:LEU:O	2.13	0.48
1:I:322:ALA:O	1:I:326:ILE:HG12	2.12	0.48
1:I:592:ILE:O	1:I:595:ARG:N	2.43	0.48
1:K:425:LYS:HE2	1:K:530:GLU:HA	1.95	0.48
1:L:428:ILE:O	1:L:429:ASP:HB2	2.13	0.48
2:O:176:CYS:SG	2:O:179:HIS:N	2.73	0.48
2:W:160:MET:HE2	2:W:213:ARG:HB3	1.95	0.48
1:G:505:VAL:HG11	1:H:447:ALA:HB2	1.96	0.48
1:I:351:ASP:C	1:I:353:LEU:H	2.21	0.48
1:J:592:ILE:HG23	1:J:596:ILE:HD13	1.94	0.48
2:O:197:VAL:HG22	2:O:234:TYR:CE1	2.48	0.48
2:P:155:THR:HG23	2:P:258:GLU:O	2.13	0.48
2:S:132:LYS:HE3	2:S:271:GLU:OE2	2.13	0.48
2:U:244:GLY:O	2:U:246:MET:N	2.47	0.48
1:B:349:ARG:HG2	1:B:349:ARG:NH1	2.28	0.48
1:B:356:THR:HG23	1:B:359:GLN:CD	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:372:MET:HE3	1:C:573:ILE:HG23	1.96	0.48
1:D:269:SER:H	1:D:323:ASN:HD21	1.61	0.48
1:E:293:LEU:HD21	1:E:333:GLN:NE2	2.29	0.48
1:F:583:ARG:HD3	1:F:587:GLU:OE1	2.12	0.48
1:L:295:PHE:CD1	1:L:295:PHE:N	2.79	0.48
2:R:259:ASP:OD2	2:R:263:ASN:HB2	2.14	0.48
2:S:197:VAL:HG11	2:S:218:VAL:HG11	1.96	0.48
1:A:538:GLN:HE22	1:A:544:GLN:NE2	2.12	0.48
1:A:568:ILE:C	1:A:570:GLN:H	2.21	0.48
1:B:419:LYS:HA	1:B:542:VAL:HG22	1.96	0.48
1:B:469:LEU:C	1:B:469:LEU:HD12	2.38	0.48
1:C:532:SER:O	1:C:534:PRO:HD3	2.13	0.48
1:E:581:TRP:CZ3	1:E:603:LEU:HB3	2.49	0.48
1:E:583:ARG:HD3	1:E:587:GLU:OE1	2.13	0.48
1:F:313:HIS:C	1:F:315:LYS:H	2.22	0.48
1:F:440:LEU:HD23	1:F:440:LEU:O	2.14	0.48
1:H:320:HIS:O	1:H:321:TYR:C	2.54	0.48
1:K:421:TYR:O	1:K:542:VAL:HG23	2.14	0.48
1:L:311:PRO:C	1:L:313:HIS:H	2.22	0.48
2:Q:244:GLY:O	2:Q:246:MET:N	2.46	0.48
2:R:203:VAL:HG23	2:R:218:VAL:HG12	1.96	0.48
2:V:132:LYS:HE2	2:V:273:ARG:HB2	1.96	0.48
2:X:158:ARG:HB2	2:X:158:ARG:HH11	1.79	0.48
1:C:278:MET:C	1:C:280:THR:H	2.21	0.48
1:C:451:ASN:HD21	1:C:476:LYS:N	2.12	0.48
1:D:415:ASN:HD21	1:D:420:ARG:NH1	2.03	0.48
1:E:357:ARG:HA	1:E:360:MET:CE	2.37	0.48
1:F:270:TRP:CE2	1:F:336:ILE:HG12	2.48	0.48
1:F:550:LYS:HD3	1:F:552:TYR:CZ	2.49	0.48
1:K:511:LYS:HB3	1:K:514:LEU:HD12	1.94	0.48
1:L:465:ILE:O	1:L:466:ASP:HB2	2.12	0.48
2:O:211:THR:C	2:O:213:ARG:H	2.22	0.48
2:P:197:VAL:HG11	2:P:218:VAL:HG11	1.96	0.48
2:R:125:THR:O	2:R:133:MET:HG3	2.14	0.48
2:W:259:ASP:OD2	2:W:263:ASN:HB2	2.12	0.48
1:B:445:GLY:O	1:B:446:LYS:HG2	2.14	0.48
1:C:387:TRP:CE3	1:C:568:ILE:HG23	2.48	0.48
1:D:308:LYS:HA	1:D:314:TYR:CD2	2.49	0.48
1:D:349:ARG:HE	1:D:517:ARG:HD2	1.79	0.48
1:F:391:VAL:HG13	1:F:578:MET:HB2	1.96	0.48
1:F:448:LEU:HD23	1:F:448:LEU:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:364:ARG:HG2	1:I:443:CYS:C	2.39	0.48
1:I:369:LEU:HD13	1:I:595:ARG:HD3	1.96	0.48
1:J:528:MET:HE1	1:J:533:VAL:HG21	1.96	0.48
1:K:270:TRP:CD1	1:L:331:LYS:HZ2	2.32	0.48
1:K:584:PRO:HD2	1:K:587:GLU:OE1	2.14	0.48
1:L:295:PHE:HA	1:L:317:HIS:CD2	2.49	0.48
2:R:197:VAL:HG23	2:R:216:VAL:HG21	1.94	0.48
2:T:211:THR:C	2:T:213:ARG:H	2.21	0.48
2:U:249:ARG:HG3	2:U:249:ARG:NH1	2.28	0.48
2:X:242:CYS:C	2:X:243:MET:HG3	2.39	0.48
1:B:311:PRO:C	1:B:313:HIS:H	2.22	0.47
1:B:365:PHE:C	1:B:367:ASP:H	2.22	0.47
1:F:435:LEU:HD23	1:F:547:PHE:HZ	1.79	0.47
1:G:291:MET:HE3	1:L:354:GLN:NE2	2.29	0.47
1:I:588:PHE:HB3	1:I:592:ILE:CD1	2.43	0.47
1:J:372:MET:C	1:J:374:ILE:H	2.21	0.47
1:J:554:LYS:O	1:J:558:GLU:HG3	2.14	0.47
1:K:596:ILE:HG22	1:K:600:LYS:HD2	1.95	0.47
1:L:423:LEU:HD12	1:L:526:VAL:O	2.13	0.47
2:P:198:GLU:HB2	2:P:235:ASN:ND2	2.29	0.47
1:E:464:ALA:HB2	1:E:470:VAL:HG11	1.95	0.47
1:H:500:TYR:O	1:H:521:PHE:HB3	2.14	0.47
1:I:415:ASN:HD21	1:I:420:ARG:HD2	1.76	0.47
1:J:268:VAL:HG12	1:J:326:ILE:HB	1.96	0.47
1:K:344:VAL:O	1:K:344:VAL:HG12	2.13	0.47
2:P:164:LYS:HB3	2:P:250:PRO:HG2	1.96	0.47
2:R:186:ASP:OD1	2:R:189:ALA:HB3	2.14	0.47
1:B:269:SER:OG	1:B:272:LEU:HB2	2.13	0.47
1:B:445:GLY:C	1:B:446:LYS:HG2	2.39	0.47
1:C:270:TRP:CE2	1:C:336:ILE:HG12	2.50	0.47
1:C:445:GLY:HA3	1:C:469:LEU:HD23	1.97	0.47
1:E:267:GLN:CA	1:E:267:GLN:HE21	2.26	0.47
1:F:452:LEU:HB3	1:F:453:PRO:HD2	1.95	0.47
1:H:588:PHE:CD2	1:H:596:ILE:HG12	2.49	0.47
1:I:497:LEU:O	1:I:500:TYR:HB2	2.14	0.47
1:J:502:ASP:CG	1:J:540:ARG:HD2	2.39	0.47
1:K:270:TRP:CE2	1:L:331:LYS:HD3	2.49	0.47
1:K:317:HIS:O	1:K:320:HIS:N	2.46	0.47
2:T:132:LYS:HD3	2:T:134:PHE:CZ	2.49	0.47
2:U:107:TYR:CE1	2:U:151:PRO:HA	2.50	0.47
1:A:453:PRO:CG	1:F:454:LEU:HB3	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:500:TYR:O	1:C:521:PHE:HB3	2.14	0.47
1:C:609:LEU:HD22	2:O:246:MET:HE2	1.95	0.47
1:D:322:ALA:C	1:D:324:ALA:H	2.21	0.47
1:E:550:LYS:HD3	1:E:552:TYR:CE2	2.49	0.47
1:F:479:GLY:C	1:F:481:GLU:H	2.23	0.47
1:L:583:ARG:NE	1:L:583:ARG:CA	2.75	0.47
2:U:173:VAL:HG11	2:U:194:LEU:HD12	1.97	0.47
2:X:175:ARG:HD2	2:X:193:HIS:O	2.14	0.47
1:B:497:LEU:O	1:B:500:TYR:HB2	2.14	0.47
1:C:451:ASN:ND2	1:C:476:LYS:H	2.12	0.47
1:D:538:GLN:C	1:D:540:ARG:H	2.22	0.47
1:F:590:GLN:HA	1:F:593:GLN:CD	2.40	0.47
1:G:385:GLU:HA	1:G:607:PHE:CE2	2.49	0.47
1:H:581:TRP:CZ3	1:H:603:LEU:HB3	2.49	0.47
1:K:529:ASN:O	1:K:530:GLU:CB	2.62	0.47
1:L:514:LEU:HD23	1:L:516:LYS:HG2	1.96	0.47
2:O:136:GLN:CB	2:O:139:LYS:HG3	2.36	0.47
2:R:133:MET:HE1	2:R:236:TYR:CE1	2.49	0.47
1:D:317:HIS:HD2	1:D:317:HIS:O	1.97	0.47
1:F:582:TYR:O	1:F:583:ARG:C	2.58	0.47
1:G:462:GLY:HA3	1:G:510:GLU:O	2.14	0.47
1:L:608:SER:HB3	2:X:280:ARG:NH1	2.30	0.47
2:Q:107:TYR:CE1	2:Q:151:PRO:HA	2.50	0.47
2:X:252:LEU:HD12	2:X:270:PHE:O	2.14	0.47
1:A:311:PRO:O	1:A:315:LYS:HB2	2.14	0.47
1:A:502:ASP:CG	1:A:540:ARG:HE	2.23	0.47
1:A:561:GLU:O	1:A:563:LEU:N	2.47	0.47
1:A:581:TRP:HE1	2:M:246:MET:HE3	1.79	0.47
1:B:270:TRP:H	1:B:270:TRP:HD1	1.60	0.47
1:B:272:LEU:HD23	1:B:323:ASN:HB2	1.97	0.47
1:B:356:THR:HG23	1:B:359:GLN:OE1	2.15	0.47
1:B:596:ILE:O	1:B:600:LYS:HG3	2.15	0.47
1:C:299:PHE:CE1	1:C:318:GLU:HB2	2.49	0.47
1:C:391:VAL:HG22	1:C:574:ALA:O	2.15	0.47
1:D:372:MET:HE3	1:D:577:LEU:HD21	1.96	0.47
1:D:383:ASP:OD1	1:D:385:GLU:HB3	2.14	0.47
1:D:513:HIS:ND1	1:E:512:LYS:HE2	2.30	0.47
1:F:291:MET:HE3	1:F:312:SER:HB2	1.97	0.47
1:F:590:GLN:H	1:F:590:GLN:CD	2.22	0.47
1:F:594:SER:O	1:F:597:VAL:HB	2.13	0.47
1:G:469:LEU:HD12	1:G:469:LEU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:525:ILE:HG22	1:G:526:VAL:N	2.29	0.47
1:G:583:ARG:HD3	1:G:587:GLU:OE1	2.15	0.47
1:H:389:ALA:O	1:H:392:ALA:HB3	2.15	0.47
1:I:401:MET:O	1:I:405:VAL:HG23	2.15	0.47
1:K:308:LYS:HA	1:K:314:TYR:CD2	2.50	0.47
2:N:156:ARG:HB3	2:N:217:VAL:HG12	1.97	0.47
2:N:244:GLY:O	2:N:246:MET:N	2.47	0.47
2:R:156:ARG:HB3	2:R:217:VAL:HG12	1.96	0.47
2:S:98:PRO:HD2	2:S:213:ARG:NH1	2.30	0.47
2:S:112:GLY:HA3	2:S:146:TRP:HE1	1.80	0.47
1:E:504:SER:OG	1:F:570:GLN:NE2	2.47	0.47
1:G:408:PHE:CD2	1:G:439:LEU:HD22	2.50	0.47
1:G:412:MET:HE1	1:G:524:GLY:HA2	1.96	0.47
1:H:415:ASN:HD21	1:H:420:ARG:HD2	1.79	0.47
1:H:450:VAL:HG23	1:H:457:LEU:HD11	1.96	0.47
1:H:582:TYR:HD2	2:T:248:ARG:HH21	1.63	0.47
1:I:507:VAL:HG12	1:I:508:ASN:N	2.29	0.47
1:K:270:TRP:CE2	1:K:336:ILE:HG12	2.50	0.47
1:L:418:LYS:HE2	1:L:502:ASP:OD2	2.14	0.47
2:Q:107:TYR:HD1	2:Q:149:SER:O	1.97	0.47
1:A:408:PHE:CZ	1:A:525:ILE:HD11	2.50	0.47
1:B:508:ASN:OD1	1:B:518:THR:HG23	2.15	0.47
1:D:517:ARG:HH11	1:D:517:ARG:HG3	1.79	0.47
1:D:609:LEU:N	1:D:609:LEU:HD23	2.29	0.47
1:F:602:ARG:HE	1:F:606:GLU:HG3	1.80	0.47
1:I:311:PRO:C	1:I:313:HIS:N	2.73	0.47
1:J:308:LYS:HA	1:J:314:TYR:CD2	2.50	0.47
1:J:589:ALA:C	1:J:591:SER:N	2.72	0.47
1:L:345:LEU:O	1:L:348:LYS:HB3	2.15	0.47
2:U:120:LYS:N	2:U:120:LYS:HD2	2.30	0.47
2:V:175:ARG:NH2	2:V:237:MET:HB3	2.30	0.47
2:V:176:CYS:SG	2:V:178:HIS:HB3	2.55	0.47
2:W:189:ALA:HB2	2:W:205:TYR:CZ	2.50	0.47
1:A:528:MET:HE1	1:A:533:VAL:HG22	1.96	0.47
1:A:535:LYS:HG3	1:A:536:THR:N	2.30	0.47
1:A:560:SER:OG	1:A:624:GLY:HA2	2.15	0.47
1:E:448:LEU:HD22	1:E:460:GLU:O	2.14	0.47
1:F:324:ALA:O	1:F:327:PHE:HB3	2.15	0.47
1:G:287:LEU:O	1:G:291:MET:HG3	2.14	0.47
1:G:440:LEU:HD12	1:G:471:VAL:CG2	2.45	0.47
1:G:476:LYS:CE	1:L:496:ASN:ND2	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:289:LEU:O	1:H:293:LEU:HG	2.15	0.47
1:K:282:CYS:SG	1:K:287:LEU:HD23	2.55	0.47
1:L:270:TRP:CZ2	1:L:336:ILE:HG12	2.50	0.47
2:S:158:ARG:NH1	2:S:217:VAL:HG21	2.30	0.47
2:T:243:MET:CE	2:T:243:MET:CG	2.91	0.47
2:U:134:PHE:N	2:U:134:PHE:CD1	2.83	0.47
2:U:224:GLU:H	2:U:224:GLU:CD	2.23	0.47
1:A:608:SER:C	1:A:610:SER:N	2.72	0.46
1:B:393:TRP:CE2	1:B:553:LEU:HD22	2.50	0.46
1:B:405:VAL:HG21	1:B:575:LEU:HD22	1.95	0.46
1:C:614:LYS:O	1:C:617:PHE:HB3	2.14	0.46
1:E:402:ASP:HA	1:E:578:MET:HE2	1.97	0.46
1:H:445:GLY:O	1:H:446:LYS:HG2	2.15	0.46
1:H:495:ASP:OD1	1:I:486:PRO:HG2	2.15	0.46
1:I:278:MET:HE2	1:I:343:THR:CG2	2.45	0.46
1:I:503:GLY:HA2	1:I:520:ILE:HG23	1.96	0.46
1:J:513:HIS:O	1:K:512:LYS:HG2	2.15	0.46
1:K:386:GLU:OE1	1:K:566:LYS:HE3	2.15	0.46
1:K:456:ARG:HG3	1:K:456:ARG:NH1	2.30	0.46
2:O:276:ALA:C	2:O:278:PRO:HD3	2.40	0.46
2:R:175:ARG:HG3	2:R:192:GLN:C	2.40	0.46
1:A:372:MET:SD	1:A:576:LEU:HD23	2.55	0.46
1:C:356:THR:OG1	1:C:359:GLN:HG3	2.15	0.46
1:D:502:ASP:OD2	1:D:540:ARG:HD2	2.15	0.46
1:G:475:VAL:CG1	1:G:491:ILE:HD12	2.45	0.46
1:H:528:MET:HE1	1:H:531:TYR:HB2	1.97	0.46
1:I:581:TRP:O	2:U:245:GLY:HA3	2.16	0.46
1:B:418:LYS:HE3	1:B:540:ARG:HE	1.81	0.46
1:C:443:CYS:HB3	1:C:468:PHE:CD2	2.50	0.46
1:D:270:TRP:CE2	1:D:336:ILE:HG12	2.51	0.46
1:E:333:GLN:HA	1:E:336:ILE:HD12	1.96	0.46
1:E:493:ASN:HD22	1:E:493:ASN:N	2.13	0.46
1:G:280:THR:O	1:G:280:THR:HG22	2.15	0.46
1:G:608:SER:CB	2:S:280:ARG:NH1	2.79	0.46
1:H:280:THR:HG22	1:H:280:THR:O	2.16	0.46
1:I:361:LEU:HD11	1:I:409:LEU:HD22	1.98	0.46
1:L:538:GLN:HE22	1:L:544:GLN:NE2	2.12	0.46
2:N:98:PRO:HG2	2:N:162:ILE:HG21	1.96	0.46
2:T:191:PRO:HG2	2:T:192:GLN:HE21	1.80	0.46
2:U:109:PHE:CE1	2:U:145:LEU:HG	2.51	0.46
2:X:203:VAL:HG22	2:X:204:GLU:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:LYS:HB2	1:A:553:LEU:HD12	1.98	0.46
1:B:430:SER:HB3	1:B:549:PRO:HG3	1.96	0.46
1:B:449:ASN:HD21	1:B:451:ASN:CB	2.22	0.46
1:B:508:ASN:ND2	1:C:463:VAL:HG11	2.30	0.46
1:B:590:GLN:HA	1:B:593:GLN:NE2	2.31	0.46
1:C:375:MET:O	1:C:382:ALA:HB3	2.15	0.46
1:D:557:LEU:C	1:D:559:ARG:H	2.23	0.46
1:F:420:ARG:HD2	1:F:523:PRO:HB3	1.96	0.46
1:G:412:MET:HE1	1:G:524:GLY:CA	2.46	0.46
1:I:454:LEU:C	1:I:456:ARG:H	2.23	0.46
1:J:375:MET:O	1:J:382:ALA:HB3	2.15	0.46
1:J:581:TRP:HE1	2:V:246:MET:HE3	1.80	0.46
1:K:266:LYS:O	1:K:326:ILE:HD12	2.15	0.46
1:L:356:THR:O	1:L:357:ARG:C	2.59	0.46
2:O:236:TYR:CE2	2:O:272:VAL:HG11	2.51	0.46
1:A:280:THR:O	1:A:280:THR:HG22	2.14	0.46
1:B:590:GLN:C	1:B:592:ILE:H	2.23	0.46
1:F:469:LEU:HD12	1:F:469:LEU:C	2.40	0.46
1:H:295:PHE:HA	1:H:317:HIS:CD2	2.51	0.46
1:H:303:LEU:C	1:H:305:CYS:H	2.23	0.46
1:H:420:ARG:NH1	1:H:521:PHE:O	2.49	0.46
1:L:276:TYR:OH	1:L:291:MET:HE3	2.16	0.46
2:N:158:ARG:HH21	2:N:206:LEU:HD23	1.79	0.46
2:O:133:MET:HE3	2:O:135:CYS:HB3	1.96	0.46
2:O:285:GLU:HA	2:O:288:ASN:HD22	1.81	0.46
2:P:109:PHE:CD1	2:P:257:LEU:HD22	2.50	0.46
2:Q:97:VAL:CG1	2:Q:169:MET:HG2	2.45	0.46
2:U:156:ARG:HG2	2:U:156:ARG:HH11	1.80	0.46
2:V:134:PHE:O	2:V:278:PRO:HB3	2.16	0.46
1:D:470:VAL:HG12	1:D:471:VAL:N	2.30	0.46
1:D:589:ALA:O	1:D:590:GLN:C	2.58	0.46
1:E:269:SER:H	1:E:323:ASN:HD21	1.63	0.46
1:F:295:PHE:HE1	1:F:313:HIS:ND1	2.13	0.46
1:F:349:ARG:HD3	1:F:517:ARG:CZ	2.46	0.46
1:J:298:SER:O	1:J:302:CYS:HB2	2.16	0.46
1:J:405:VAL:O	1:J:405:VAL:HG12	2.15	0.46
1:J:590:GLN:HA	1:J:593:GLN:CD	2.40	0.46
1:L:434:THR:HG23	1:L:570:GLN:HG2	1.97	0.46
2:U:197:VAL:HG23	2:U:216:VAL:HG21	1.98	0.46
2:X:203:VAL:HA	2:X:218:VAL:HG12	1.98	0.46
1:A:334:LYS:HD2	1:F:342:ASP:OD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:465:ILE:CG2	1:C:517:ARG:HE	2.28	0.46
1:D:520:ILE:O	1:D:521:PHE:C	2.58	0.46
1:H:450:VAL:O	1:H:450:VAL:HG13	2.16	0.46
1:H:559:ARG:NH1	1:H:559:ARG:HG3	2.31	0.46
1:J:299:PHE:CE1	1:J:318:GLU:HG3	2.50	0.46
1:K:489:GLN:O	1:K:490:GLY:C	2.58	0.46
1:K:497:LEU:O	1:K:500:TYR:HB2	2.14	0.46
1:L:609:LEU:HD22	2:X:246:MET:CE	2.38	0.46
2:M:190:PRO:HB2	2:M:193:HIS:HD2	1.80	0.46
2:N:134:PHE:N	2:N:134:PHE:CD1	2.84	0.46
2:V:198:GLU:HB2	2:V:235:ASN:ND2	2.30	0.46
2:X:132:LYS:HG3	2:X:271:GLU:HB3	1.97	0.46
1:B:311:PRO:C	1:B:313:HIS:N	2.73	0.46
1:B:412:MET:HE3	1:B:523:PRO:HG2	1.98	0.46
1:B:417:PRO:CG	1:C:567:ARG:HE	2.29	0.46
1:C:584:PRO:C	1:C:586:ALA:N	2.71	0.46
1:D:497:LEU:O	1:D:500:TYR:HB2	2.15	0.46
1:F:296:GLN:HG3	1:F:297:TYR:CD1	2.51	0.46
1:F:308:LYS:HA	1:F:314:TYR:CD2	2.51	0.46
1:F:423:LEU:HD11	1:F:528:MET:HE3	1.96	0.46
1:H:316:TYR:HB3	1:H:320:HIS:HD2	1.80	0.46
1:H:356:THR:O	1:H:357:ARG:C	2.59	0.46
1:H:465:ILE:HD12	1:H:511:LYS:HB2	1.98	0.46
1:I:475:VAL:HG23	1:I:475:VAL:O	2.15	0.46
1:J:356:THR:HG23	1:J:359:GLN:OE1	2.16	0.46
2:O:259:ASP:OD1	2:O:261:SER:N	2.47	0.46
2:S:191:PRO:HG2	2:S:192:GLN:HE21	1.79	0.46
2:T:186:ASP:OD1	2:T:189:ALA:HB3	2.16	0.46
2:V:134:PHE:N	2:V:134:PHE:CD1	2.84	0.46
2:X:209:ARG:NH1	2:X:210:ASN:HD21	2.13	0.46
2:X:243:MET:CE	2:X:243:MET:CB	2.94	0.46
1:B:597:VAL:C	1:B:599:TRP:N	2.74	0.46
1:D:414:TYR:HB3	1:D:416:ILE:HD11	1.97	0.46
1:D:461:LEU:HD13	1:D:500:TYR:CE2	2.51	0.46
1:G:476:LYS:HB3	1:G:488:GLY:HA3	1.98	0.46
1:G:583:ARG:HA	1:G:584:PRO:HD3	1.79	0.46
1:H:608:SER:HA	2:T:280:ARG:NH1	2.30	0.46
1:J:401:MET:HG3	1:J:578:MET:CE	2.41	0.46
1:J:425:LYS:HG3	1:J:528:MET:HE3	1.97	0.46
1:J:609:LEU:O	1:J:613:GLN:HB2	2.16	0.46
1:K:283:ASP:CA	1:K:341:VAL:HG13	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:454:LEU:HA	1:K:457:LEU:HB2	1.98	0.46
2:U:282:ARG:O	2:U:286:GLU:HG3	2.16	0.46
2:X:133:MET:HE3	2:X:141:CYS:SG	2.55	0.46
1:B:306:ILE:HD12	1:B:306:ILE:C	2.41	0.46
1:B:368:LEU:O	1:B:372:MET:HG3	2.15	0.46
1:B:405:VAL:O	1:B:409:LEU:HG	2.16	0.46
1:C:349:ARG:CD	1:C:517:ARG:HD2	2.46	0.46
1:C:349:ARG:O	1:C:353:LEU:HB2	2.15	0.46
1:C:608:SER:HB3	1:C:611:VAL:HG23	1.98	0.46
1:F:372:MET:C	1:F:374:ILE:H	2.23	0.46
1:G:269:SER:HB3	1:G:323:ASN:OD1	2.16	0.46
1:I:344:VAL:O	1:I:348:LYS:HG3	2.15	0.46
1:K:369:LEU:O	1:K:370:ASP:C	2.58	0.46
1:L:276:TYR:HB2	1:L:320:HIS:CE1	2.51	0.46
1:L:372:MET:SD	1:L:576:LEU:HD23	2.56	0.46
1:L:555:HIS:O	1:L:559:ARG:HD2	2.16	0.46
2:T:180:GLU:O	2:T:180:GLU:HG3	2.14	0.46
2:U:136:GLN:HA	2:U:275:CYS:O	2.16	0.46
2:V:207:ASP:O	2:V:208:ASP:C	2.59	0.46
2:W:97:VAL:HG13	2:W:169:MET:HG2	1.98	0.46
1:A:267:GLN:HG2	1:A:268:VAL:H	1.81	0.45
1:B:413:VAL:HG13	1:B:414:TYR:N	2.31	0.45
1:C:349:ARG:CD	1:C:517:ARG:NH1	2.80	0.45
1:C:525:ILE:HG22	1:C:526:VAL:H	1.81	0.45
1:D:349:ARG:NH1	1:D:466:ASP:OD2	2.49	0.45
1:D:609:LEU:HD22	2:P:246:MET:CE	2.46	0.45
1:E:461:LEU:C	1:E:463:VAL:H	2.24	0.45
1:E:497:LEU:HB3	1:E:500:TYR:HB2	1.97	0.45
1:G:311:PRO:C	1:G:313:HIS:N	2.71	0.45
1:H:311:PRO:HA	1:H:314:TYR:CE2	2.51	0.45
1:H:520:ILE:HD13	1:H:520:ILE:C	2.41	0.45
1:I:423:LEU:HD21	1:I:528:MET:HE3	1.98	0.45
1:J:581:TRP:CZ2	2:V:246:MET:HE3	2.51	0.45
1:L:311:PRO:HA	1:L:314:TYR:CE2	2.51	0.45
2:N:147:VAL:HG22	2:N:149:SER:H	1.80	0.45
2:R:97:VAL:HG13	2:R:169:MET:HG2	1.98	0.45
2:S:242:CYS:C	2:S:243:MET:HG3	2.41	0.45
2:U:158:ARG:HH12	2:U:217:VAL:HG11	1.80	0.45
2:V:112:GLY:HA3	2:V:146:TRP:HE1	1.81	0.45
2:W:282:ARG:HE	2:W:286:GLU:CD	2.24	0.45
2:X:112:GLY:HA3	2:X:144:GLN:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:LEU:N	1:A:454:LEU:HD12	2.32	0.45
1:B:353:LEU:HD12	1:C:287:LEU:HD13	1.97	0.45
1:D:614:LYS:O	1:D:617:PHE:HB3	2.15	0.45
1:E:432:LYS:HG3	1:E:433:THR:N	2.30	0.45
1:H:430:SER:HB3	1:H:549:PRO:HG3	1.98	0.45
1:H:584:PRO:HD2	1:H:587:GLU:CG	2.44	0.45
1:H:585:VAL:HG23	2:T:242:CYS:HA	1.98	0.45
1:I:570:GLN:HB3	1:I:570:GLN:HE21	1.62	0.45
1:L:510:GLU:HG3	1:L:514:LEU:O	2.16	0.45
2:O:245:GLY:C	2:O:247:ASN:N	2.74	0.45
2:Q:189:ALA:HA	2:Q:190:PRO:HD3	1.86	0.45
2:R:112:GLY:HA3	2:R:144:GLN:HB2	1.98	0.45
2:T:119:ALA:O	2:T:279:GLY:HA3	2.16	0.45
2:T:145:LEU:HD21	2:T:157:VAL:HG21	1.97	0.45
2:W:107:TYR:O	2:W:147:VAL:HG23	2.16	0.45
1:A:268:VAL:HG12	1:A:269:SER:N	2.32	0.45
1:A:584:PRO:HB3	2:M:243:MET:HA	1.97	0.45
1:C:473:GLU:CG	1:C:474:ASP:N	2.78	0.45
1:D:608:SER:CB	2:P:280:ARG:HH11	2.29	0.45
1:F:374:ILE:C	1:F:376:PHE:N	2.75	0.45
1:G:295:PHE:CD1	1:G:317:HIS:HA	2.51	0.45
1:G:386:GLU:O	1:G:389:ALA:HB3	2.15	0.45
1:G:537:LEU:HG	1:G:541:PHE:HE1	1.81	0.45
1:J:353:LEU:HD12	1:K:287:LEU:HD13	1.98	0.45
1:K:274:THR:O	1:K:277:ALA:HB3	2.17	0.45
1:B:474:ASP:HA	1:B:527:THR:O	2.17	0.45
1:B:585:VAL:HG12	1:B:593:GLN:HG2	1.97	0.45
1:D:602:ARG:HD3	1:D:602:ARG:C	2.42	0.45
1:E:351:ASP:HB3	1:E:355:LEU:CD1	2.38	0.45
1:E:351:ASP:OD1	1:E:355:LEU:HD11	2.17	0.45
1:F:372:MET:O	1:F:376:PHE:HB2	2.17	0.45
1:F:520:ILE:HD12	1:F:520:ILE:N	2.29	0.45
1:H:432:LYS:HE3	1:H:433:THR:H	1.78	0.45
1:I:498:ARG:NH2	1:I:536:THR:HG21	2.32	0.45
1:K:469:LEU:C	1:K:469:LEU:HD12	2.42	0.45
2:N:249:ARG:HH11	2:N:249:ARG:HG3	1.81	0.45
2:V:133:MET:HE1	2:V:236:TYR:CE1	2.51	0.45
2:X:217:VAL:HG12	2:X:218:VAL:N	2.30	0.45
1:C:315:LYS:HB3	1:C:316:TYR:CE1	2.52	0.45
1:C:497:LEU:HB3	1:C:500:TYR:HB2	1.99	0.45
1:E:418:LYS:HG2	1:E:502:ASP:OD1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:419:LYS:HA	1:E:542:VAL:HG22	1.96	0.45
1:E:454:LEU:HD11	1:E:493:ASN:ND2	2.32	0.45
1:E:538:GLN:HG3	1:E:538:GLN:O	2.17	0.45
1:G:589:ALA:C	1:G:591:SER:H	2.24	0.45
1:J:346:ALA:O	1:J:349:ARG:HB3	2.15	0.45
1:J:369:LEU:CB	1:J:595:ARG:HH11	2.28	0.45
1:J:590:GLN:HA	1:J:593:GLN:OE1	2.16	0.45
2:N:107:TYR:O	2:N:147:VAL:HG23	2.17	0.45
2:O:136:GLN:OE1	2:O:139:LYS:HE3	2.17	0.45
2:P:252:LEU:HD12	2:P:271:GLU:HA	1.99	0.45
2:X:137:LEU:O	2:X:139:LYS:HG2	2.16	0.45
1:A:446:LYS:CG	1:A:467:GLN:HE21	2.14	0.45
1:A:547:PHE:C	1:A:548:ARG:HD3	2.42	0.45
1:D:418:LYS:HE2	1:D:502:ASP:OD1	2.17	0.45
1:D:550:LYS:HD3	1:D:552:TYR:OH	2.16	0.45
1:E:618:ASN:HA	1:E:623:ILE:HD11	1.98	0.45
1:F:288:LEU:HD23	1:F:337:CYS:HB3	1.98	0.45
1:F:368:LEU:O	1:F:372:MET:HG3	2.17	0.45
1:H:425:LYS:HE2	1:H:528:MET:CE	2.47	0.45
2:P:151:PRO:HB3	2:P:152:PRO:HD2	1.99	0.45
2:W:211:THR:O	2:W:212:PHE:HB2	2.15	0.45
1:A:433:THR:O	1:A:434:THR:C	2.60	0.45
1:E:454:LEU:HD21	1:E:493:ASN:HD21	1.81	0.45
1:F:583:ARG:HA	1:F:584:PRO:HD3	1.80	0.45
1:G:285:VAL:O	1:G:286:LEU:C	2.58	0.45
1:G:441:GLU:HG2	1:G:572:GLY:H	1.82	0.45
1:H:423:LEU:HD23	1:H:544:GLN:HG3	1.99	0.45
1:J:289:LEU:HD11	1:J:333:GLN:NE2	2.32	0.45
1:J:608:SER:C	1:J:610:SER:N	2.70	0.45
1:K:295:PHE:HE1	1:K:313:HIS:ND1	2.15	0.45
2:M:203:VAL:HA	2:M:218:VAL:HG12	1.98	0.45
2:N:166:SER:HA	2:N:169:MET:HB2	1.97	0.45
2:P:132:LYS:HG3	2:P:271:GLU:HB3	1.99	0.45
2:P:246:MET:HE2	2:P:246:MET:HA	1.98	0.45
2:T:193:HIS:CE1	2:T:214:HIS:HB3	2.51	0.45
1:B:412:MET:HE1	1:B:524:GLY:CA	2.47	0.45
1:C:466:ASP:H	1:C:519:GLN:HE22	1.63	0.45
1:F:497:LEU:HB3	1:F:500:TYR:HB2	1.99	0.45
1:G:440:LEU:C	1:G:440:LEU:HD23	2.42	0.45
1:I:283:ASP:HA	1:I:341:VAL:HG13	1.98	0.45
1:J:470:VAL:O	1:J:524:GLY:HA3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:608:SER:C	1:J:610:SER:H	2.24	0.45
1:A:368:LEU:O	1:A:372:MET:HG3	2.17	0.45
1:C:381:SER:O	1:C:382:ALA:HB2	2.17	0.45
1:F:367:ASP:C	1:F:369:LEU:N	2.74	0.45
1:G:271:LYS:HD2	1:H:329:ASP:OD1	2.16	0.45
1:H:432:LYS:HD2	1:H:433:THR:H	1.81	0.45
1:I:375:MET:O	1:I:382:ALA:HB3	2.17	0.45
1:I:410:LYS:HA	1:I:410:LYS:HD3	1.86	0.45
1:L:515:ASN:O	1:L:517:ARG:N	2.50	0.45
1:L:555:HIS:HA	1:L:558:GLU:OE1	2.17	0.45
2:M:245:GLY:C	2:M:247:ASN:H	2.24	0.45
2:O:196:ARG:O	2:O:234:TYR:HA	2.17	0.45
2:S:175:ARG:HD2	2:S:193:HIS:O	2.16	0.45
2:W:98:PRO:HD2	2:W:213:ARG:NH1	2.32	0.45
2:X:126:TYR:O	2:X:282:ARG:CZ	2.65	0.45
1:A:465:ILE:O	1:A:466:ASP:HB2	2.17	0.45
1:A:533:VAL:HG13	1:A:537:LEU:HD23	1.98	0.45
1:B:302:CYS:SG	1:B:305:CYS:N	2.90	0.45
1:B:420:ARG:O	1:B:421:TYR:CD1	2.69	0.45
1:C:581:TRP:HZ3	1:C:603:LEU:HB3	1.81	0.45
1:D:470:VAL:O	1:D:524:GLY:HA3	2.17	0.45
1:D:498:ARG:NH2	1:E:476:LYS:HD3	2.32	0.45
1:F:409:LEU:HD11	1:F:579:LEU:HD11	1.99	0.45
1:G:412:MET:CE	1:G:524:GLY:HA2	2.47	0.45
1:I:590:GLN:CD	1:I:590:GLN:N	2.75	0.45
1:J:398:LEU:HD21	1:J:545:ILE:HG21	1.99	0.45
1:L:402:ASP:HA	1:L:578:MET:HE3	1.99	0.45
2:O:259:ASP:OD2	2:O:263:ASN:HB2	2.17	0.45
2:S:110:ARG:HA	2:S:268:ASN:HD21	1.82	0.45
1:A:388:MET:HA	1:A:391:VAL:HG23	1.98	0.44
1:B:412:MET:HE1	1:B:523:PRO:C	2.42	0.44
1:B:443:CYS:HB3	1:B:468:PHE:CD2	2.51	0.44
1:B:470:VAL:O	1:B:524:GLY:HA3	2.17	0.44
1:F:348:LYS:HB2	1:F:348:LYS:NZ	2.33	0.44
1:I:435:LEU:HD23	1:I:547:PHE:HZ	1.82	0.44
1:J:562:PHE:CD2	1:J:562:PHE:N	2.86	0.44
2:R:282:ARG:O	2:R:286:GLU:HG3	2.17	0.44
2:U:151:PRO:HB3	2:U:152:PRO:HD2	1.99	0.44
1:A:288:LEU:HD23	1:A:288:LEU:O	2.16	0.44
1:C:270:TRP:CD2	1:C:336:ILE:HG12	2.52	0.44
1:C:580:ILE:HG21	1:C:599:TRP:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:435:LEU:HD12	1:E:435:LEU:O	2.17	0.44
1:E:493:ASN:N	1:E:493:ASN:ND2	2.64	0.44
1:I:526:VAL:HG21	1:I:541:PHE:HE2	1.82	0.44
2:M:224:GLU:O	2:M:225:VAL:C	2.59	0.44
2:N:125:THR:OG1	2:N:126:TYR:N	2.49	0.44
2:O:196:ARG:HH12	2:O:237:MET:HE2	1.76	0.44
2:P:190:PRO:HB2	2:P:193:HIS:CD2	2.53	0.44
2:W:119:ALA:HB3	2:W:122:VAL:HG23	1.99	0.44
1:A:512:LYS:O	1:A:513:HIS:C	2.61	0.44
1:D:270:TRP:HE3	1:D:339:GLN:HG2	1.82	0.44
1:F:314:TYR:CD1	1:F:314:TYR:C	2.94	0.44
1:F:338:GLN:HE21	1:F:338:GLN:HA	1.83	0.44
1:G:512:LYS:O	1:G:512:LYS:HD3	2.17	0.44
1:H:288:LEU:HD23	1:H:337:CYS:HB3	1.99	0.44
1:H:609:LEU:HD21	2:T:246:MET:HA	2.00	0.44
1:K:609:LEU:HG	2:W:246:MET:CE	2.47	0.44
1:L:268:VAL:HG12	1:L:326:ILE:HB	2.00	0.44
1:L:303:LEU:HD13	1:L:306:ILE:HD12	1.98	0.44
2:M:244:GLY:O	2:M:246:MET:N	2.50	0.44
2:N:98:PRO:HD2	2:N:213:ARG:NH1	2.32	0.44
2:N:160:MET:SD	2:N:213:ARG:HG2	2.57	0.44
2:S:280:ARG:HH11	2:S:280:ARG:HG2	1.81	0.44
2:T:190:PRO:HB2	2:T:193:HIS:HD2	1.82	0.44
1:A:274:THR:HA	1:A:340:ALA:CB	2.47	0.44
1:A:278:MET:HE2	1:A:343:THR:HG22	1.99	0.44
1:A:495:ASP:CG	1:A:498:ARG:HH21	2.25	0.44
1:B:283:ASP:CA	1:B:341:VAL:HG13	2.45	0.44
1:C:327:PHE:C	1:C:329:ASP:H	2.25	0.44
1:C:474:ASP:O	1:C:475:VAL:C	2.61	0.44
1:F:456:ARG:N	1:F:456:ARG:HD2	2.32	0.44
1:F:510:GLU:HG3	1:F:514:LEU:C	2.41	0.44
1:J:415:ASN:HD22	1:J:415:ASN:HA	1.59	0.44
1:J:521:PHE:HA	1:J:522:PRO:HD3	1.89	0.44
1:J:612:TYR:C	1:J:614:LYS:N	2.75	0.44
1:L:498:ARG:HB3	1:L:540:ARG:NH1	2.30	0.44
2:Q:251:ILE:HG22	2:Q:252:LEU:N	2.32	0.44
1:A:454:LEU:HD12	1:A:454:LEU:H	1.83	0.44
1:B:270:TRP:CD1	1:B:270:TRP:N	2.85	0.44
1:C:421:TYR:CE1	1:C:523:PRO:HA	2.52	0.44
1:C:576:LEU:O	1:C:580:ILE:HG12	2.18	0.44
1:E:388:MET:HG3	1:E:607:PHE:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:540:ARG:HH11	1:F:540:ARG:HG3	1.82	0.44
1:F:557:LEU:HD13	1:F:564:LEU:HD11	1.99	0.44
1:I:469:LEU:HA	1:I:523:PRO:O	2.18	0.44
1:I:551:ASP:O	1:I:554:LYS:HB3	2.17	0.44
1:I:590:GLN:HA	1:I:593:GLN:CD	2.42	0.44
1:I:601:GLU:O	1:I:605:LYS:HB2	2.18	0.44
1:K:376:PHE:HE1	1:K:387:TRP:CD1	2.35	0.44
1:L:514:LEU:CG	1:L:516:LYS:HG2	2.47	0.44
2:M:101:LYS:HB2	2:M:267:ARG:HH21	1.82	0.44
2:O:158:ARG:HB3	2:O:256:THR:HB	1.99	0.44
2:V:156:ARG:HB3	2:V:217:VAL:HG12	2.00	0.44
1:D:314:TYR:CD1	1:D:315:LYS:HG2	2.53	0.44
1:D:372:MET:HA	1:D:375:MET:HG2	1.99	0.44
1:E:555:HIS:O	1:E:559:ARG:HD2	2.17	0.44
1:G:550:LYS:HD3	1:G:552:TYR:OH	2.18	0.44
1:H:356:THR:HG22	1:H:359:GLN:CD	2.43	0.44
1:J:314:TYR:CD1	1:J:315:LYS:N	2.86	0.44
2:N:103:TYR:CZ	2:N:105:GLY:HA2	2.52	0.44
2:P:158:ARG:CZ	2:P:217:VAL:HG21	2.47	0.44
2:R:190:PRO:HB2	2:R:193:HIS:HD2	1.82	0.44
2:U:252:LEU:HD12	2:U:270:PHE:C	2.42	0.44
2:W:107:TYR:OH	2:W:152:PRO:HD3	2.18	0.44
2:W:243:MET:CE	2:W:243:MET:CG	2.93	0.44
1:D:619:VAL:HG22	1:D:625:VAL:HG22	1.99	0.44
1:E:511:LYS:O	1:E:512:LYS:HB3	2.18	0.44
1:J:508:ASN:ND2	1:K:463:VAL:HG11	2.33	0.44
1:K:406:TYR:CE1	1:K:587:GLU:HB3	2.53	0.44
2:T:145:LEU:O	2:T:229:CYS:HB2	2.18	0.44
2:U:161:ALA:HB2	2:U:195:ILE:CD1	2.41	0.44
2:V:197:VAL:HG23	2:V:216:VAL:HG21	1.99	0.44
2:V:239:ASN:HA	2:V:274:VAL:HB	2.00	0.44
2:W:134:PHE:N	2:W:134:PHE:CD1	2.85	0.44
1:A:356:THR:O	1:A:357:ARG:C	2.58	0.44
1:B:440:LEU:HD12	1:B:440:LEU:O	2.17	0.44
1:C:455:ASP:O	1:D:456:ARG:NH2	2.51	0.44
1:C:517:ARG:HH22	1:D:286:LEU:HD13	1.83	0.44
1:D:317:HIS:C	1:D:317:HIS:CD2	2.96	0.44
1:D:593:GLN:O	1:D:596:ILE:HB	2.18	0.44
1:E:451:ASN:HD21	1:E:476:LYS:N	2.09	0.44
1:F:303:LEU:O	1:F:306:ILE:HG22	2.17	0.44
1:F:535:LYS:HG3	1:F:536:THR:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:453:PRO:HD3	1:L:454:LEU:HD22	1.98	0.44
1:J:360:MET:HE3	1:J:468:PHE:CD1	2.53	0.44
1:K:512:LYS:CG	1:K:513:HIS:H	2.21	0.44
1:K:566:LYS:HB2	1:K:568:ILE:HG13	1.98	0.44
2:U:98:PRO:HD2	2:U:213:ARG:NH1	2.33	0.44
1:A:581:TRP:O	1:A:581:TRP:CG	2.71	0.44
1:B:316:TYR:HB3	1:B:320:HIS:CD2	2.53	0.44
1:B:585:VAL:HG23	2:N:242:CYS:HA	2.00	0.44
1:B:597:VAL:C	1:B:599:TRP:H	2.25	0.44
1:D:269:SER:N	1:D:323:ASN:HD21	2.16	0.44
1:D:608:SER:OG	1:D:611:VAL:HG23	2.18	0.44
1:G:299:PHE:HA	1:G:317:HIS:CE1	2.53	0.44
1:H:581:TRP:CE3	1:H:603:LEU:HD23	2.53	0.44
1:I:560:SER:OG	1:I:625:VAL:HG23	2.18	0.44
1:J:394:LEU:O	1:J:397:LEU:HB3	2.17	0.44
1:J:398:LEU:HB2	1:J:401:MET:CE	2.48	0.44
1:J:420:ARG:HB3	1:J:523:PRO:CB	2.45	0.44
1:J:602:ARG:O	1:J:602:ARG:HD3	2.17	0.44
1:K:583:ARG:HA	1:K:584:PRO:HD3	1.83	0.44
1:L:583:ARG:HA	1:L:584:PRO:HD3	1.75	0.44
2:N:93:LEU:HD22	2:N:171:GLU:HA	1.99	0.44
2:N:177:PRO:O	2:N:181:ARG:HG3	2.18	0.44
2:Q:158:ARG:NH1	2:Q:217:VAL:HG21	2.33	0.44
2:U:175:ARG:NH2	2:U:237:MET:HB3	2.33	0.44
2:X:149:SER:O	2:X:150:THR:C	2.61	0.44
1:C:295:PHE:HE1	1:C:313:HIS:ND1	2.15	0.43
1:J:434:THR:HG23	1:J:570:GLN:CB	2.47	0.43
1:K:284:ASP:HB3	1:K:287:LEU:HB3	2.00	0.43
1:L:405:VAL:HG21	1:L:578:MET:HE1	1.99	0.43
2:O:282:ARG:O	2:O:286:GLU:HG3	2.18	0.43
1:B:495:ASP:HB3	1:C:476:LYS:NZ	2.33	0.43
1:C:431:GLY:O	1:C:432:LYS:C	2.61	0.43
1:D:375:MET:HE1	1:D:387:TRP:CZ2	2.53	0.43
1:F:302:CYS:SG	1:F:304:LYS:HB2	2.58	0.43
1:F:303:LEU:H	1:F:303:LEU:CD2	2.29	0.43
1:G:288:LEU:HD13	1:G:337:CYS:SG	2.58	0.43
1:H:583:ARG:HA	1:H:584:PRO:HD3	1.81	0.43
1:L:623:ILE:HG22	1:L:624:GLY:N	2.28	0.43
2:N:136:GLN:HB2	2:N:139:LYS:CG	2.45	0.43
2:S:156:ARG:HG2	2:S:156:ARG:HH11	1.83	0.43
2:T:252:LEU:HD12	2:T:271:GLU:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:LEU:HD23	1:A:372:MET:SD	2.57	0.43
1:B:386:GLU:HG2	1:B:562:PHE:CE1	2.53	0.43
1:C:375:MET:HE1	1:C:387:TRP:NE1	2.33	0.43
1:C:424:PHE:O	1:C:527:THR:HA	2.18	0.43
1:C:557:LEU:HD23	1:C:563:LEU:HD12	2.00	0.43
1:D:588:PHE:N	1:D:588:PHE:CD1	2.86	0.43
1:E:517:ARG:HG2	1:E:519:GLN:HG2	2.00	0.43
1:E:581:TRP:CE3	1:E:603:LEU:HD23	2.53	0.43
1:E:612:TYR:HA	1:E:615:MET:CE	2.34	0.43
1:F:412:MET:SD	1:F:523:PRO:HB2	2.59	0.43
1:H:520:ILE:HD13	1:H:521:PHE:O	2.18	0.43
1:I:400:LYS:O	1:I:403:SER:N	2.50	0.43
1:I:581:TRP:CE2	2:U:246:MET:HE3	2.53	0.43
1:J:398:LEU:HA	1:J:399:PRO:HD3	1.90	0.43
1:L:295:PHE:N	1:L:295:PHE:HD1	2.17	0.43
2:Q:110:ARG:HA	2:Q:268:ASN:ND2	2.32	0.43
2:S:222:PRO:HA	2:S:223:PRO:HD3	1.95	0.43
1:A:521:PHE:HA	1:A:522:PRO:HD3	1.92	0.43
1:B:550:LYS:HD3	1:B:552:TYR:OH	2.18	0.43
1:D:529:ASN:O	1:D:530:GLU:C	2.62	0.43
1:E:412:MET:HE1	1:E:524:GLY:N	2.34	0.43
1:E:588:PHE:CD2	1:E:596:ILE:HG12	2.53	0.43
1:E:615:MET:O	1:E:619:VAL:HG23	2.18	0.43
1:F:514:LEU:HD12	1:F:515:ASN:H	1.84	0.43
1:G:513:HIS:O	1:G:514:LEU:HB2	2.16	0.43
1:H:371:ARG:O	1:H:374:ILE:HG22	2.18	0.43
1:I:500:TYR:CE1	1:I:507:VAL:HG11	2.53	0.43
1:K:398:LEU:HD21	1:K:545:ILE:HG21	2.00	0.43
1:L:349:ARG:NE	1:L:517:ARG:HD3	2.33	0.43
2:T:134:PHE:N	2:T:134:PHE:CD1	2.86	0.43
2:U:133:MET:HE3	2:U:141:CYS:SG	2.58	0.43
2:W:98:PRO:HD2	2:W:213:ARG:HH12	1.82	0.43
1:A:454:LEU:CB	1:B:453:PRO:HG2	2.49	0.43
1:A:485:LEU:HD21	1:A:529:ASN:HD22	1.82	0.43
1:B:300:GLU:O	1:B:301:MET:HE2	2.18	0.43
1:B:452:LEU:HB3	1:B:453:PRO:CD	2.49	0.43
1:C:278:MET:C	1:C:280:THR:N	2.77	0.43
1:C:346:ALA:C	1:C:348:LYS:N	2.76	0.43
1:C:511:LYS:O	1:C:512:LYS:HG2	2.18	0.43
1:F:300:GLU:CD	1:F:300:GLU:H	2.27	0.43
1:F:423:LEU:HD23	1:F:544:GLN:NE2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:483:ARG:HH11	1:F:483:ARG:HG3	1.83	0.43
1:G:595:ARG:O	1:G:598:GLU:HB3	2.19	0.43
1:H:269:SER:HB3	1:H:323:ASN:OD1	2.18	0.43
1:K:401:MET:HG3	1:K:578:MET:HE1	2.00	0.43
1:L:525:ILE:HG22	1:L:526:VAL:N	2.32	0.43
2:R:158:ARG:HG2	2:R:159:ALA:N	2.32	0.43
2:S:241:SER:C	2:S:243:MET:H	2.26	0.43
2:T:132:LYS:HA	2:T:271:GLU:O	2.17	0.43
2:X:118:THR:HG22	2:X:282:ARG:HD3	2.00	0.43
1:A:510:GLU:HB2	1:A:514:LEU:O	2.18	0.43
1:B:452:LEU:HB3	1:B:453:PRO:HD2	2.00	0.43
1:B:583:ARG:HA	1:B:584:PRO:HD3	1.78	0.43
1:C:346:ALA:HA	1:D:286:LEU:HD22	2.00	0.43
1:C:420:ARG:HH21	1:C:501:LEU:C	2.27	0.43
1:C:424:PHE:CZ	1:C:525:ILE:HD13	2.53	0.43
1:E:339:GLN:HE22	1:F:331:LYS:HA	1.84	0.43
1:E:408:PHE:O	1:E:412:MET:HG2	2.18	0.43
1:E:499:ASP:OD1	1:E:499:ASP:N	2.49	0.43
1:F:398:LEU:HB2	1:F:401:MET:CE	2.48	0.43
1:G:285:VAL:O	1:G:288:LEU:N	2.52	0.43
1:I:459:PHE:HZ	1:I:513:HIS:H	1.65	0.43
1:L:420:ARG:CB	1:L:523:PRO:HB3	2.49	0.43
2:U:252:LEU:HD12	2:U:270:PHE:O	2.19	0.43
2:W:196:ARG:NH1	2:W:237:MET:HE2	2.34	0.43
1:A:609:LEU:HD22	2:M:246:MET:CE	2.49	0.43
1:D:433:THR:O	1:D:434:THR:C	2.62	0.43
1:E:512:LYS:HG3	1:E:513:HIS:N	2.34	0.43
1:G:275:GLU:O	1:G:278:MET:HB2	2.18	0.43
1:H:375:MET:HE2	1:H:376:PHE:CE2	2.54	0.43
1:K:451:ASN:ND2	1:K:476:LYS:H	2.15	0.43
1:K:492:ASN:HD22	1:K:492:ASN:N	2.16	0.43
1:K:510:GLU:HB3	1:K:516:LYS:HB3	1.99	0.43
1:L:391:VAL:HG13	1:L:578:MET:HB2	2.00	0.43
2:O:157:VAL:O	2:O:217:VAL:HA	2.19	0.43
2:P:156:ARG:HB3	2:P:217:VAL:HG12	1.99	0.43
2:R:249:ARG:HG3	2:R:249:ARG:HH11	1.84	0.43
2:T:192:GLN:NE2	2:T:192:GLN:H	2.16	0.43
2:U:109:PHE:HE1	2:U:145:LEU:HG	1.83	0.43
1:A:388:MET:HE1	1:A:603:LEU:HD21	2.00	0.43
1:A:405:VAL:O	1:A:409:LEU:HG	2.19	0.43
1:B:293:LEU:O	1:B:296:GLN:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:517:ARG:HG2	1:B:517:ARG:HH11	1.83	0.43
1:D:350:VAL:O	1:D:354:GLN:HG3	2.18	0.43
1:D:435:LEU:HD23	1:D:547:PHE:HZ	1.84	0.43
1:E:595:ARG:O	1:E:596:ILE:C	2.58	0.43
1:F:317:HIS:O	1:F:321:TYR:N	2.51	0.43
1:F:374:ILE:C	1:F:376:PHE:H	2.26	0.43
1:F:402:ASP:HA	1:F:578:MET:HE3	2.00	0.43
1:F:525:ILE:CG2	1:F:526:VAL:N	2.82	0.43
1:H:270:TRP:CE2	1:H:336:ILE:HG12	2.54	0.43
1:H:303:LEU:O	1:H:307:LYS:HG3	2.18	0.43
1:I:314:TYR:CD1	1:I:314:TYR:C	2.96	0.43
1:I:327:PHE:C	1:I:329:ASP:N	2.76	0.43
1:J:454:LEU:HD22	1:K:453:PRO:CG	2.49	0.43
1:J:568:ILE:C	1:J:570:GLN:H	2.27	0.43
1:L:423:LEU:HD23	1:L:544:GLN:NE2	2.34	0.43
1:L:608:SER:CB	2:X:280:ARG:NH1	2.82	0.43
2:N:103:TYR:O	2:N:267:ARG:N	2.49	0.43
2:N:175:ARG:NH2	2:N:237:MET:HB3	2.33	0.43
2:N:243:MET:CE	2:N:243:MET:CG	2.92	0.43
2:P:216:VAL:O	2:P:216:VAL:HG13	2.19	0.43
2:W:203:VAL:HG22	2:W:204:GLU:N	2.33	0.43
1:C:278:MET:O	1:C:280:THR:N	2.51	0.43
1:C:357:ARG:NH1	1:C:357:ARG:HG2	2.34	0.43
1:D:393:TRP:NE1	1:D:557:LEU:HD13	2.33	0.43
1:E:311:PRO:C	1:E:313:HIS:N	2.76	0.43
1:H:424:PHE:O	1:H:527:THR:HA	2.18	0.43
1:I:409:LEU:O	1:I:413:VAL:HG23	2.18	0.43
1:I:409:LEU:HD23	1:I:409:LEU:HA	1.80	0.43
1:L:419:LYS:HA	1:L:542:VAL:HG13	2.00	0.43
2:N:189:ALA:HA	2:N:190:PRO:HD3	1.91	0.43
2:N:224:GLU:CD	2:N:224:GLU:H	2.27	0.43
2:P:99:SER:HB2	2:P:101:LYS:HG2	2.01	0.43
2:P:207:ASP:O	2:P:208:ASP:C	2.61	0.43
2:S:243:MET:CE	2:S:243:MET:CB	2.95	0.43
2:T:127:SER:O	2:T:131:ASN:N	2.49	0.43
2:T:258:GLU:HA	2:T:263:ASN:O	2.19	0.43
1:B:280:THR:O	1:B:280:THR:HG22	2.19	0.43
1:C:608:SER:HB2	2:O:280:ARG:HH11	1.84	0.43
1:D:354:GLN:CD	1:E:310:GLN:HE21	2.27	0.43
1:D:533:VAL:HA	1:D:534:PRO:HD3	1.92	0.43
1:D:559:ARG:HD3	1:D:623:ILE:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:606:GLU:HB3	1:D:607:PHE:CD1	2.54	0.43
1:E:456:ARG:HH11	1:E:456:ARG:HG3	1.84	0.43
1:F:456:ARG:HG3	1:F:456:ARG:HH11	1.84	0.43
1:F:477:GLY:O	1:F:487:SER:HA	2.18	0.43
1:G:354:GLN:NE2	1:H:291:MET:HE3	2.33	0.43
1:G:473:GLU:HG3	1:L:505:VAL:HG21	2.00	0.43
1:H:424:PHE:HB2	1:H:527:THR:HG22	2.01	0.43
1:H:547:PHE:CD1	1:H:547:PHE:N	2.87	0.43
1:I:317:HIS:CD2	1:I:317:HIS:C	2.97	0.43
1:I:497:LEU:HB3	1:I:500:TYR:HB2	2.01	0.43
2:M:129:ALA:C	2:M:130:LEU:HD12	2.44	0.43
2:N:158:ARG:HB3	2:N:256:THR:HB	2.01	0.43
2:V:102:THR:HG23	2:V:268:ASN:OD1	2.19	0.43
1:A:589:ALA:O	1:A:590:GLN:C	2.62	0.42
1:B:272:LEU:HD12	1:B:272:LEU:HA	1.90	0.42
1:B:356:THR:OG1	1:B:359:GLN:HG3	2.19	0.42
1:B:410:LYS:HA	1:B:413:VAL:HG12	2.00	0.42
1:C:591:SER:O	1:C:592:ILE:HG23	2.19	0.42
1:E:461:LEU:C	1:E:463:VAL:N	2.77	0.42
1:H:343:THR:O	1:H:346:ALA:HB3	2.19	0.42
1:H:581:TRP:O	2:T:245:GLY:HA3	2.19	0.42
1:I:512:LYS:HD3	1:I:516:LYS:HZ1	1.84	0.42
1:K:274:THR:O	1:K:275:GLU:C	2.62	0.42
1:K:374:ILE:O	1:K:375:MET:C	2.61	0.42
1:K:482:SER:C	1:K:484:ASP:H	2.25	0.42
1:K:550:LYS:HD3	1:K:552:TYR:OH	2.18	0.42
1:K:604:ASP:C	1:K:606:GLU:H	2.27	0.42
1:L:395:HIS:CD2	1:L:582:TYR:OH	2.72	0.42
1:L:592:ILE:O	1:L:593:GLN:C	2.58	0.42
2:M:241:SER:HA	2:M:245:GLY:H	1.83	0.42
2:N:175:ARG:HD2	2:N:193:HIS:O	2.19	0.42
2:O:109:PHE:CD1	2:O:257:LEU:HD22	2.54	0.42
2:P:137:LEU:O	2:P:138:ALA:C	2.62	0.42
2:P:282:ARG:HE	2:P:286:GLU:CD	2.26	0.42
2:R:241:SER:HA	2:R:245:GLY:H	1.83	0.42
2:T:103:TYR:CZ	2:T:105:GLY:HA2	2.54	0.42
1:A:484:ASP:O	1:F:535:LYS:HE2	2.20	0.42
1:B:599:TRP:C	1:B:601:GLU:N	2.76	0.42
1:C:454:LEU:HB2	1:D:453:PRO:CG	2.47	0.42
1:C:499:ASP:OD2	1:C:499:ASP:N	2.49	0.42
1:C:529:ASN:HB2	1:C:531:TYR:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:555:HIS:HB3	1:C:559:ARG:NH1	2.34	0.42
1:D:564:LEU:O	1:D:566:LYS:N	2.52	0.42
1:F:583:ARG:H	1:F:583:ARG:HG2	1.62	0.42
1:G:351:ASP:HB3	1:G:355:LEU:HD12	2.00	0.42
1:G:387:TRP:CE3	1:G:568:ILE:HG23	2.53	0.42
1:G:455:ASP:O	1:H:456:ARG:HD2	2.19	0.42
1:I:289:LEU:HG	1:I:293:LEU:HD12	2.00	0.42
1:I:609:LEU:O	1:I:613:GLN:HB2	2.18	0.42
1:J:454:LEU:C	1:J:456:ARG:H	2.27	0.42
1:K:440:LEU:HD13	1:K:471:VAL:HG23	2.01	0.42
1:L:608:SER:C	1:L:610:SER:N	2.76	0.42
2:N:151:PRO:HB3	2:N:152:PRO:HD2	2.01	0.42
2:O:175:ARG:CZ	2:O:237:MET:HB3	2.49	0.42
2:Q:119:ALA:O	2:Q:279:GLY:HA3	2.19	0.42
2:Q:222:PRO:HA	2:Q:223:PRO:HD3	1.95	0.42
2:S:133:MET:HE1	2:S:236:TYR:CE1	2.54	0.42
2:U:166:SER:HA	2:U:169:MET:HB2	2.02	0.42
2:V:103:TYR:O	2:V:266:GLY:HA2	2.19	0.42
2:X:177:PRO:O	2:X:181:ARG:HG3	2.19	0.42
1:B:311:PRO:HB3	1:B:315:LYS:HE2	2.01	0.42
1:D:371:ARG:O	1:D:375:MET:HG2	2.18	0.42
1:D:399:PRO:O	1:D:400:LYS:HB2	2.19	0.42
1:D:537:LEU:HG	1:D:541:PHE:CE1	2.54	0.42
1:D:568:ILE:C	1:D:570:GLN:N	2.74	0.42
1:E:534:PRO:HB3	1:F:486:PRO:CG	2.48	0.42
1:F:542:VAL:HG22	1:F:542:VAL:O	2.19	0.42
1:G:505:VAL:HG21	1:H:473:GLU:HG3	2.01	0.42
1:G:529:ASN:HB2	1:G:531:TYR:CE1	2.54	0.42
1:H:511:LYS:HB3	1:H:515:ASN:HB3	2.02	0.42
1:J:299:PHE:CD1	1:J:318:GLU:HG3	2.55	0.42
1:K:394:LEU:HD21	1:K:569:ILE:O	2.19	0.42
1:K:502:ASP:CG	1:K:540:ARG:NH1	2.77	0.42
1:L:424:PHE:O	1:L:527:THR:HA	2.18	0.42
2:N:158:ARG:HH21	2:N:206:LEU:HD22	1.84	0.42
2:O:158:ARG:NH1	2:O:258:GLU:OE1	2.52	0.42
2:R:103:TYR:CZ	2:R:105:GLY:HA2	2.54	0.42
2:T:134:PHE:CD2	2:T:273:ARG:HD3	2.53	0.42
2:X:133:MET:CE	2:X:141:CYS:SG	3.07	0.42
1:D:298:SER:HA	1:D:321:TYR:CE1	2.54	0.42
1:D:305:CYS:SG	1:D:313:HIS:NE2	2.92	0.42
1:E:372:MET:CG	1:E:573:ILE:HD12	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:385:GLU:HA	1:H:607:PHE:CZ	2.54	0.42
1:I:510:GLU:HG2	1:I:511:LYS:N	2.35	0.42
1:I:525:ILE:CG2	1:I:526:VAL:N	2.83	0.42
1:J:283:ASP:HA	1:J:341:VAL:HG13	2.02	0.42
1:J:420:ARG:NE	1:J:503:GLY:HA3	2.35	0.42
1:J:581:TRP:CE2	2:V:246:MET:HE3	2.54	0.42
1:L:349:ARG:NH2	1:L:517:ARG:HG3	2.34	0.42
1:L:514:LEU:C	1:L:516:LYS:H	2.27	0.42
2:N:176:CYS:SG	2:N:178:HIS:HB3	2.59	0.42
2:O:249:ARG:O	2:O:251:ILE:HD12	2.20	0.42
2:P:239:ASN:HB2	2:P:242:CYS:SG	2.59	0.42
2:R:134:PHE:CD1	2:R:134:PHE:N	2.87	0.42
2:R:185:SER:HA	2:R:196:ARG:HH22	1.84	0.42
2:R:216:VAL:HG13	2:R:216:VAL:O	2.19	0.42
1:A:451:ASN:OD1	1:A:476:LYS:HB2	2.19	0.42
1:B:364:ARG:O	1:B:367:ASP:HB2	2.18	0.42
1:B:448:LEU:HG	1:B:470:VAL:HG13	2.01	0.42
1:B:459:PHE:C	1:B:461:LEU:N	2.77	0.42
1:B:602:ARG:HD2	1:B:602:ARG:O	2.18	0.42
1:C:458:ASN:OD1	1:D:456:ARG:HD3	2.20	0.42
1:C:507:VAL:N	1:C:519:GLN:O	2.51	0.42
1:C:535:LYS:HD2	1:D:484:ASP:HB2	2.01	0.42
1:C:592:ILE:O	1:C:596:ILE:HG12	2.19	0.42
1:D:322:ALA:O	1:D:326:ILE:HG13	2.18	0.42
1:E:520:ILE:HD12	1:F:567:ARG:NH1	2.28	0.42
1:F:428:ILE:O	1:F:429:ASP:HB2	2.19	0.42
1:G:618:ASN:OD1	1:G:623:ILE:HD11	2.19	0.42
1:H:456:ARG:HG2	1:H:456:ARG:HH11	1.85	0.42
1:I:317:HIS:O	1:I:321:TYR:N	2.52	0.42
1:I:590:GLN:HA	1:I:593:GLN:HG3	2.01	0.42
1:J:562:PHE:CE2	1:J:563:LEU:HG	2.55	0.42
1:K:465:ILE:HD12	1:K:511:LYS:CG	2.49	0.42
1:L:268:VAL:HG21	1:L:336:ILE:HD13	2.01	0.42
1:L:514:LEU:HD12	1:L:515:ASN:N	2.31	0.42
2:O:145:LEU:HD21	2:O:157:VAL:HG21	2.00	0.42
2:P:107:TYR:CE1	2:P:151:PRO:HA	2.54	0.42
2:Q:236:TYR:CE2	2:Q:272:VAL:HG11	2.54	0.42
1:B:448:LEU:HD22	1:B:463:VAL:HG23	2.01	0.42
1:D:354:GLN:CB	1:E:310:GLN:HE21	2.31	0.42
1:E:423:LEU:HD22	1:E:541:PHE:CD1	2.55	0.42
1:F:302:CYS:SG	1:F:305:CYS:N	2.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:386:GLU:HB3	1:F:562:PHE:HE1	1.85	0.42
1:F:609:LEU:O	1:F:613:GLN:HG3	2.19	0.42
1:J:270:TRP:CE2	1:J:336:ILE:HG12	2.55	0.42
1:J:389:ALA:HB1	1:J:625:VAL:CG2	2.45	0.42
1:K:584:PRO:HD2	1:K:587:GLU:CD	2.44	0.42
1:L:507:VAL:N	1:L:519:GLN:O	2.52	0.42
2:O:107:TYR:O	2:O:147:VAL:HG23	2.19	0.42
2:P:151:PRO:HD2	2:P:220:TYR:CE2	2.54	0.42
2:Q:168:HIS:O	2:Q:171:GLU:N	2.46	0.42
2:S:122:VAL:CG1	2:S:123:THR:N	2.83	0.42
2:S:158:ARG:HH21	2:S:206:LEU:CD2	2.32	0.42
2:S:203:VAL:HA	2:S:218:VAL:HG12	2.01	0.42
2:T:173:VAL:CG1	2:T:194:LEU:HD12	2.49	0.42
1:B:420:ARG:NH2	1:B:521:PHE:O	2.49	0.42
1:B:422:TRP:O	1:B:525:ILE:HA	2.20	0.42
1:C:390:GLY:O	1:C:391:VAL:C	2.59	0.42
1:F:276:TYR:C	1:F:278:MET:N	2.78	0.42
1:F:608:SER:O	1:F:611:VAL:HB	2.20	0.42
1:G:398:LEU:HB2	1:G:401:MET:HE1	2.01	0.42
1:H:412:MET:HE1	1:H:524:GLY:HA2	2.02	0.42
1:I:374:ILE:C	1:I:376:PHE:H	2.27	0.42
1:I:394:LEU:HD21	1:I:569:ILE:O	2.20	0.42
1:K:386:GLU:O	1:K:389:ALA:HB3	2.20	0.42
2:U:201:LEU:C	2:U:203:VAL:H	2.28	0.42
2:W:251:ILE:CG2	2:W:252:LEU:N	2.83	0.42
1:B:353:LEU:HD21	1:B:517:ARG:NH2	2.35	0.42
1:B:625:VAL:HG23	1:B:626:LEU:N	2.34	0.42
1:C:584:PRO:HG3	2:O:243:MET:O	2.20	0.42
1:D:597:VAL:O	1:D:598:GLU:C	2.63	0.42
1:F:590:GLN:CD	1:F:590:GLN:N	2.78	0.42
1:F:590:GLN:N	1:F:590:GLN:OE1	2.53	0.42
1:H:517:ARG:CG	1:H:519:GLN:HG2	2.48	0.42
1:H:615:MET:HE2	1:H:626:LEU:CD2	2.50	0.42
1:H:618:ASN:O	1:H:619:VAL:C	2.63	0.42
1:I:295:PHE:HA	1:I:317:HIS:CD2	2.55	0.42
1:I:402:ASP:CA	1:I:578:MET:HE3	2.46	0.42
1:I:609:LEU:HD13	2:U:246:MET:SD	2.60	0.42
1:J:353:LEU:HD21	1:J:517:ARG:HH12	1.83	0.42
1:L:469:LEU:C	1:L:469:LEU:CD1	2.92	0.42
2:N:158:ARG:NH1	2:N:217:VAL:HG21	2.34	0.42
2:O:175:ARG:NE	2:O:237:MET:HB2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:245:GLY:C	2:T:247:ASN:H	2.28	0.42
1:B:267:GLN:H	1:B:267:GLN:HG2	1.64	0.42
1:B:481:GLU:H	1:B:481:GLU:CD	2.27	0.42
1:B:521:PHE:HA	1:B:522:PRO:HD3	1.86	0.42
1:D:398:LEU:HA	1:D:399:PRO:HD3	1.94	0.42
1:D:580:ILE:CD1	1:D:596:ILE:HG23	2.50	0.42
1:G:608:SER:CB	2:S:280:ARG:HH11	2.32	0.42
1:I:346:ALA:O	1:I:350:VAL:HG23	2.20	0.42
1:I:372:MET:SD	1:I:576:LEU:HD23	2.60	0.42
1:I:615:MET:O	1:I:619:VAL:HG23	2.19	0.42
1:K:507:VAL:N	1:K:519:GLN:O	2.53	0.42
2:Q:264:LEU:HD11	2:Q:267:ARG:HB2	2.02	0.42
2:W:242:CYS:C	2:W:243:MET:HG3	2.44	0.42
1:A:599:TRP:O	1:A:603:LEU:HB2	2.20	0.42
1:B:561:GLU:CD	1:B:561:GLU:H	2.28	0.42
1:C:500:TYR:CE2	1:C:507:VAL:HG11	2.54	0.42
1:D:386:GLU:O	1:D:389:ALA:HB3	2.20	0.42
1:E:561:GLU:O	1:E:565:GLU:HG3	2.20	0.42
1:F:295:PHE:HA	1:F:317:HIS:CE1	2.55	0.42
1:I:299:PHE:CE1	1:I:318:GLU:HB2	2.55	0.42
1:I:592:ILE:C	1:I:594:SER:N	2.77	0.42
1:I:609:LEU:HD13	2:U:246:MET:CE	2.50	0.42
1:J:371:ARG:O	1:J:375:MET:HG2	2.20	0.42
1:J:605:LYS:O	1:J:605:LYS:HG2	2.20	0.42
1:K:495:ASP:O	1:K:498:ARG:HG3	2.20	0.42
2:R:107:TYR:O	2:R:147:VAL:HG23	2.19	0.42
2:T:160:MET:HG3	2:T:214:HIS:O	2.20	0.42
2:T:216:VAL:HG13	2:T:216:VAL:O	2.20	0.42
2:W:104:GLN:HB3	2:W:108:GLY:HA2	2.02	0.42
1:A:385:GLU:HA	1:A:607:PHE:HZ	1.85	0.41
1:A:409:LEU:O	1:A:413:VAL:HG23	2.19	0.41
1:C:389:ALA:HA	1:C:615:MET:SD	2.60	0.41
1:C:449:ASN:ND2	1:C:452:LEU:HG	2.35	0.41
1:C:520:ILE:CD1	1:C:520:ILE:N	2.79	0.41
1:D:454:LEU:HA	1:D:457:LEU:HB2	2.01	0.41
1:D:608:SER:HB3	2:P:280:ARG:NH1	2.35	0.41
1:F:462:GLY:C	1:F:464:ALA:N	2.78	0.41
1:J:562:PHE:N	1:J:562:PHE:HD2	2.18	0.41
1:K:604:ASP:C	1:K:606:GLU:N	2.74	0.41
1:L:424:PHE:HB2	1:L:527:THR:HG22	2.02	0.41
2:M:251:ILE:N	2:M:251:ILE:HD12	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:145:LEU:HD21	2:N:157:VAL:HG21	2.02	0.41
2:O:114:LEU:N	2:O:114:LEU:CD1	2.83	0.41
2:R:120:LYS:N	2:R:120:LYS:HD2	2.35	0.41
2:V:236:TYR:CZ	2:V:272:VAL:HG11	2.55	0.41
2:W:126:TYR:OH	2:W:131:ASN:HA	2.20	0.41
1:B:569:ILE:HD13	1:B:570:GLN:OE1	2.20	0.41
1:C:288:LEU:HG	1:C:337:CYS:SG	2.61	0.41
1:C:394:LEU:HD21	1:C:569:ILE:O	2.21	0.41
1:C:395:HIS:HD2	1:C:616:LYS:HZ2	1.66	0.41
1:C:408:PHE:HA	1:C:422:TRP:CZ2	2.55	0.41
1:C:439:LEU:HD13	1:C:525:ILE:HD11	2.02	0.41
1:C:517:ARG:HH22	1:D:286:LEU:CD1	2.32	0.41
1:C:590:GLN:HA	1:C:593:GLN:CG	2.50	0.41
1:E:303:LEU:O	1:E:307:LYS:HB2	2.20	0.41
1:G:594:SER:HA	2:S:178:HIS:CD2	2.55	0.41
1:H:368:LEU:HD22	1:H:573:ILE:HD13	2.02	0.41
1:H:394:LEU:HD21	1:H:569:ILE:O	2.20	0.41
1:I:508:ASN:OD1	1:I:518:THR:HG23	2.20	0.41
1:J:507:VAL:HG12	1:J:508:ASN:N	2.35	0.41
1:J:579:LEU:O	1:J:581:TRP:N	2.53	0.41
2:N:120:LYS:HD2	2:N:120:LYS:N	2.35	0.41
2:Q:97:VAL:HG13	2:Q:169:MET:HG2	2.02	0.41
2:U:211:THR:OG1	2:U:213:ARG:HB2	2.19	0.41
2:V:127:SER:O	2:V:131:ASN:N	2.52	0.41
2:X:112:GLY:CA	2:X:144:GLN:HB2	2.50	0.41
1:A:625:VAL:HG23	1:A:626:LEU:N	2.35	0.41
1:D:512:LYS:HD3	1:D:514:LEU:HD21	2.02	0.41
1:E:349:ARG:HH11	1:E:349:ARG:HG2	1.85	0.41
1:E:415:ASN:HD22	1:E:420:ARG:HD2	1.80	0.41
1:F:382:ALA:HB1	1:F:387:TRP:NE1	2.35	0.41
1:G:283:ASP:HA	1:G:341:VAL:HG13	2.02	0.41
1:G:510:GLU:O	1:G:511:LYS:HB3	2.21	0.41
1:H:299:PHE:CZ	1:H:318:GLU:HG3	2.55	0.41
1:H:614:LYS:O	1:H:617:PHE:HB3	2.20	0.41
1:I:592:ILE:O	1:I:593:GLN:C	2.60	0.41
1:I:597:VAL:O	1:I:600:LYS:HB2	2.20	0.41
1:J:372:MET:C	1:J:374:ILE:N	2.79	0.41
1:J:568:ILE:C	1:J:570:GLN:N	2.73	0.41
1:L:265:THR:C	1:L:267:GLN:N	2.77	0.41
1:L:387:TRP:CE3	1:L:568:ILE:HG23	2.55	0.41
2:Q:218:VAL:HA	2:Q:219:PRO:HD3	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:MET:HE1	1:B:524:GLY:HA2	2.02	0.41
1:B:612:TYR:O	1:B:613:GLN:C	2.64	0.41
1:D:303:LEU:C	1:D:305:CYS:N	2.77	0.41
1:F:390:GLY:O	1:F:391:VAL:C	2.64	0.41
1:F:465:ILE:HD11	1:F:509:LEU:HB2	2.03	0.41
1:H:356:THR:O	1:H:359:GLN:N	2.51	0.41
1:J:568:ILE:O	1:J:570:GLN:N	2.54	0.41
1:K:291:MET:HG2	1:K:291:MET:H	1.65	0.41
1:K:502:ASP:OD1	1:K:540:ARG:NH1	2.52	0.41
1:L:498:ARG:O	1:L:502:ASP:HB2	2.20	0.41
2:M:110:ARG:HG3	2:M:110:ARG:HH11	1.86	0.41
2:O:151:PRO:HB3	2:O:152:PRO:HD2	2.02	0.41
2:P:189:ALA:HB2	2:P:205:TYR:CZ	2.56	0.41
2:P:211:THR:OG1	2:P:213:ARG:HB2	2.21	0.41
2:S:192:GLN:HB2	2:S:214:HIS:HE1	1.86	0.41
2:U:132:LYS:HB3	2:U:134:PHE:HE1	1.85	0.41
2:X:160:MET:HE3	2:X:160:MET:HB2	1.96	0.41
1:B:369:LEU:HB2	1:B:595:ARG:NH1	2.32	0.41
1:C:369:LEU:O	1:C:372:MET:HB2	2.19	0.41
1:D:295:PHE:HE1	1:D:313:HIS:ND1	2.18	0.41
1:D:521:PHE:HA	1:D:522:PRO:HD3	1.94	0.41
1:E:391:VAL:O	1:E:392:ALA:C	2.63	0.41
1:E:417:PRO:HG3	1:F:567:ARG:CZ	2.50	0.41
1:F:349:ARG:NE	1:F:517:ARG:NE	2.69	0.41
1:I:567:ARG:HG2	1:I:567:ARG:HH11	1.85	0.41
1:J:369:LEU:HD23	1:J:372:MET:SD	2.60	0.41
1:J:493:ASN:O	1:J:497:LEU:HG	2.20	0.41
1:K:623:ILE:HG12	1:K:624:GLY:N	2.34	0.41
1:L:311:PRO:C	1:L:313:HIS:N	2.77	0.41
1:L:540:ARG:HA	1:L:540:ARG:HD3	1.89	0.41
2:M:149:SER:O	2:M:150:THR:C	2.63	0.41
2:S:242:CYS:O	2:S:243:MET:HG3	2.20	0.41
2:V:194:LEU:C	2:V:194:LEU:CD2	2.93	0.41
2:X:280:ARG:HG2	2:X:280:ARG:HH11	1.85	0.41
1:A:485:LEU:HD22	1:A:529:ASN:HD22	1.84	0.41
1:A:500:TYR:O	1:A:521:PHE:HB3	2.20	0.41
1:B:593:GLN:HE21	2:N:181:ARG:HH22	1.69	0.41
1:D:285:VAL:HG21	1:D:338:GLN:HE21	1.82	0.41
1:D:568:ILE:C	1:D:570:GLN:H	2.28	0.41
1:E:623:ILE:HD13	1:E:623:ILE:H	1.85	0.41
1:F:420:ARG:NH1	1:F:521:PHE:O	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:296:GLN:HG3	1:H:297:TYR:N	2.36	0.41
1:H:528:MET:HE3	1:H:528:MET:HB2	1.92	0.41
1:J:557:LEU:HD21	1:J:564:LEU:HD21	2.01	0.41
1:J:612:TYR:C	1:J:614:LYS:H	2.27	0.41
1:K:271:LYS:O	1:K:274:THR:HB	2.21	0.41
1:L:584:PRO:HD2	1:L:587:GLU:CD	2.46	0.41
2:M:134:PHE:CD1	2:M:134:PHE:N	2.88	0.41
2:N:245:GLY:O	2:N:247:ASN:N	2.50	0.41
2:R:236:TYR:CE2	2:R:272:VAL:HG11	2.55	0.41
2:R:239:ASN:HA	2:R:274:VAL:HB	2.02	0.41
2:S:105:GLY:HA3	2:S:265:LEU:O	2.20	0.41
2:T:192:GLN:H	2:T:192:GLN:CD	2.28	0.41
2:U:158:ARG:NH1	2:U:217:VAL:HG11	2.35	0.41
2:W:111:LEU:CD1	2:W:268:ASN:HB3	2.51	0.41
2:W:145:LEU:HD21	2:W:157:VAL:HG11	2.01	0.41
1:A:290:GLY:CA	1:F:346:ALA:HB1	2.51	0.41
1:A:448:LEU:HG	1:A:470:VAL:HG22	2.00	0.41
1:B:503:GLY:O	1:C:567:ARG:NH2	2.53	0.41
1:C:448:LEU:HD23	1:C:448:LEU:N	2.33	0.41
1:G:465:ILE:O	1:G:466:ASP:HB2	2.20	0.41
1:H:311:PRO:C	1:H:313:HIS:N	2.79	0.41
1:J:425:LYS:HE2	1:J:530:GLU:HA	2.03	0.41
1:K:297:TYR:O	1:K:321:TYR:CD1	2.74	0.41
1:K:399:PRO:O	1:K:400:LYS:HB2	2.21	0.41
2:R:277:CYS:HB3	2:R:280:ARG:HB3	2.03	0.41
2:S:189:ALA:HB2	2:S:205:TYR:CZ	2.56	0.41
2:S:207:ASP:O	2:S:208:ASP:C	2.63	0.41
2:S:264:LEU:O	2:S:265:LEU:HD23	2.21	0.41
1:A:399:PRO:O	1:A:400:LYS:HB2	2.21	0.41
1:A:417:PRO:O	1:A:418:LYS:HB3	2.20	0.41
1:A:618:ASN:O	1:A:622:GLY:N	2.53	0.41
1:B:305:CYS:C	1:B:307:LYS:N	2.79	0.41
1:B:311:PRO:O	1:B:315:LYS:HB2	2.21	0.41
1:C:332:ASN:ND2	1:C:332:ASN:N	2.68	0.41
1:C:383:ASP:HB3	1:C:386:GLU:CG	2.48	0.41
1:C:465:ILE:HD13	1:C:517:ARG:HB2	2.02	0.41
1:C:583:ARG:HA	1:C:584:PRO:HD3	1.77	0.41
1:E:375:MET:O	1:E:380:GLY:HA3	2.20	0.41
1:E:401:MET:CG	1:E:578:MET:HE1	2.51	0.41
1:E:452:LEU:HB3	1:E:453:PRO:CD	2.51	0.41
1:F:375:MET:HE2	1:F:376:PHE:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:369:LEU:HB3	1:G:595:ARG:HH21	1.86	0.41
1:H:449:ASN:HD22	1:H:451:ASN:H	1.68	0.41
1:L:397:LEU:HB3	1:L:401:MET:CE	2.51	0.41
1:L:520:ILE:N	1:L:520:ILE:CD1	2.80	0.41
2:M:197:VAL:HB	2:M:203:VAL:HG21	2.02	0.41
2:P:224:GLU:CD	2:P:224:GLU:N	2.78	0.41
2:U:156:ARG:HG2	2:U:156:ARG:NH1	2.36	0.41
1:A:423:LEU:HD11	1:A:528:MET:HE3	2.03	0.41
1:B:305:CYS:HA	1:B:314:TYR:HB3	2.01	0.41
1:B:311:PRO:HA	1:B:314:TYR:CE2	2.56	0.41
1:B:335:THR:O	1:B:336:ILE:C	2.64	0.41
1:B:495:ASP:C	1:B:497:LEU:H	2.28	0.41
1:C:455:ASP:HA	1:D:456:ARG:NH1	2.35	0.41
1:D:289:LEU:HD11	1:D:333:GLN:HE21	1.86	0.41
1:E:387:TRP:C	1:E:389:ALA:N	2.76	0.41
1:E:525:ILE:HG22	1:E:526:VAL:N	2.36	0.41
1:E:583:ARG:HA	1:E:584:PRO:HD3	1.87	0.41
1:E:608:SER:OG	1:E:611:VAL:HG23	2.21	0.41
1:E:625:VAL:HG23	1:E:626:LEU:N	2.35	0.41
1:G:286:LEU:HB2	1:L:517:ARG:HH22	1.86	0.41
1:G:434:THR:HG22	1:G:569:ILE:O	2.21	0.41
1:H:332:ASN:O	1:H:333:GLN:C	2.64	0.41
1:H:385:GLU:HA	1:H:607:PHE:HZ	1.85	0.41
1:H:528:MET:CE	1:H:531:TYR:H	2.34	0.41
1:H:592:ILE:HD12	1:H:592:ILE:HA	1.84	0.41
1:I:306:ILE:HG23	1:I:307:LYS:N	2.34	0.41
1:I:583:ARG:HA	1:I:584:PRO:HD3	1.78	0.41
1:I:589:ALA:O	1:I:593:GLN:HG3	2.21	0.41
1:J:349:ARG:NH2	1:J:516:LYS:HE3	2.36	0.41
1:J:375:MET:HG3	1:J:376:PHE:CD2	2.56	0.41
1:J:416:ILE:CD1	1:K:565:GLU:HA	2.51	0.41
1:J:458:ASN:HD22	1:J:458:ASN:HA	1.61	0.41
1:K:267:GLN:C	1:K:326:ILE:HG21	2.45	0.41
1:K:375:MET:O	1:K:380:GLY:HA3	2.21	0.41
1:K:412:MET:HE2	1:K:469:LEU:HD22	2.02	0.41
1:L:462:GLY:HA3	1:L:510:GLU:O	2.21	0.41
1:L:496:ASN:HD22	1:L:496:ASN:N	2.19	0.41
2:N:119:ALA:C	2:N:120:LYS:HD2	2.45	0.41
2:N:284:THR:O	2:N:287:GLU:HB3	2.21	0.41
2:O:145:LEU:N	2:O:145:LEU:HD12	2.36	0.41
2:O:190:PRO:HD2	2:O:193:HIS:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:133:MET:HE1	2:R:236:TYR:HE1	1.85	0.41
2:R:166:SER:HA	2:R:169:MET:HB2	2.02	0.41
2:X:198:GLU:HB2	2:X:235:ASN:ND2	2.36	0.41
1:A:350:VAL:C	1:A:352:SER:H	2.29	0.41
1:C:423:LEU:HB3	1:C:544:GLN:HG3	2.03	0.41
1:C:593:GLN:NE2	2:O:177:PRO:HB2	2.36	0.41
1:D:387:TRP:HZ3	1:D:573:ILE:HB	1.86	0.41
1:D:615:MET:O	1:D:619:VAL:HG23	2.20	0.41
1:E:445:GLY:O	1:E:446:LYS:HG2	2.21	0.41
1:E:465:ILE:HD13	1:E:509:LEU:HD12	2.03	0.41
1:E:608:SER:CB	2:Q:280:ARG:NH1	2.84	0.41
1:F:533:VAL:HA	1:F:534:PRO:HD3	1.91	0.41
1:H:388:MET:O	1:H:391:VAL:HB	2.21	0.41
1:H:427:PRO:HG3	1:H:530:GLU:OE1	2.21	0.41
1:H:506:LYS:HG2	1:H:519:GLN:CA	2.51	0.41
1:H:548:ARG:HA	1:H:549:PRO:HD3	1.96	0.41
1:I:332:ASN:O	1:I:333:GLN:C	2.64	0.41
1:L:292:TYR:HE1	1:L:320:HIS:ND1	2.19	0.41
1:L:304:LYS:HB3	1:L:313:HIS:CD2	2.56	0.41
2:M:197:VAL:HG22	2:M:234:TYR:CE1	2.56	0.41
2:N:197:VAL:HG23	2:N:216:VAL:HG21	2.03	0.41
2:P:126:TYR:OH	2:P:131:ASN:HA	2.21	0.41
2:R:112:GLY:CA	2:R:144:GLN:HB2	2.50	0.41
2:S:94:SER:HB3	2:S:211:THR:O	2.21	0.41
2:X:107:TYR:CE1	2:X:151:PRO:HA	2.56	0.41
2:X:145:LEU:HD21	2:X:157:VAL:HG11	2.03	0.41
2:X:147:VAL:HG22	2:X:149:SER:H	1.86	0.41
2:X:245:GLY:C	2:X:247:ASN:H	2.29	0.41
1:D:443:CYS:HB3	1:D:468:PHE:HD2	1.84	0.40
1:E:592:ILE:O	1:E:596:ILE:HD13	2.20	0.40
1:E:594:SER:HA	2:Q:178:HIS:CD2	2.56	0.40
1:F:408:PHE:HE1	1:F:525:ILE:CD1	2.32	0.40
1:F:619:VAL:HG22	1:F:625:VAL:HG12	2.03	0.40
1:G:441:GLU:OE1	1:G:571:SER:HA	2.21	0.40
1:I:294:GLU:C	1:I:296:GLN:H	2.28	0.40
1:I:294:GLU:C	1:I:296:GLN:N	2.77	0.40
1:J:368:LEU:HD23	1:J:368:LEU:HA	1.91	0.40
1:J:402:ASP:CA	1:J:578:MET:HE3	2.47	0.40
1:K:459:PHE:CZ	1:K:512:LYS:HD3	2.56	0.40
2:O:115:HIS:C	2:O:117:GLY:H	2.29	0.40
2:P:134:PHE:CD1	2:P:134:PHE:N	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:119:ALA:C	2:T:120:LYS:HD2	2.46	0.40
2:T:175:ARG:NH2	2:T:237:MET:HB3	2.36	0.40
2:V:119:ALA:O	2:V:122:VAL:HG23	2.21	0.40
2:W:239:ASN:C	2:W:241:SER:H	2.29	0.40
2:X:257:LEU:O	2:X:265:LEU:HB2	2.21	0.40
1:A:423:LEU:HD12	1:A:526:VAL:O	2.21	0.40
1:A:534:PRO:HB3	1:B:486:PRO:HG2	2.02	0.40
1:A:608:SER:C	1:A:610:SER:H	2.29	0.40
1:C:357:ARG:HG2	1:C:357:ARG:HH11	1.86	0.40
1:D:387:TRP:CE3	1:D:568:ILE:HG23	2.56	0.40
1:D:506:LYS:HB3	1:D:518:THR:HG22	2.03	0.40
1:F:469:LEU:HD13	1:F:524:GLY:HA2	2.03	0.40
1:F:575:LEU:O	1:F:576:LEU:C	2.64	0.40
1:H:432:LYS:HE2	1:H:432:LYS:N	2.36	0.40
1:H:561:GLU:O	1:H:565:GLU:HG3	2.21	0.40
1:I:356:THR:O	1:I:360:MET:HG3	2.21	0.40
1:I:408:PHE:HB2	1:I:422:TRP:CZ3	2.56	0.40
1:J:440:LEU:HD12	1:J:471:VAL:CG2	2.51	0.40
1:K:305:CYS:O	1:K:308:LYS:HG3	2.21	0.40
2:O:103:TYR:O	2:O:266:GLY:HA2	2.21	0.40
2:O:159:ALA:HB3	2:O:216:VAL:CG1	2.52	0.40
2:O:160:MET:HE2	2:O:213:ARG:HB3	2.04	0.40
2:O:180:GLU:O	2:O:180:GLU:HG3	2.16	0.40
2:P:96:SER:OG	2:P:211:THR:HB	2.20	0.40
2:T:190:PRO:HD2	2:T:193:HIS:CD2	2.56	0.40
2:U:158:ARG:HA	2:U:217:VAL:HG13	2.03	0.40
2:V:164:LYS:HB3	2:V:250:PRO:HG2	2.04	0.40
2:X:259:ASP:C	2:X:259:ASP:OD1	2.64	0.40
1:A:268:VAL:HG22	1:A:326:ILE:HG22	2.02	0.40
1:A:287:LEU:HD12	1:F:350:VAL:HG22	2.02	0.40
1:A:548:ARG:HD3	1:A:548:ARG:N	2.36	0.40
1:B:511:LYS:O	1:B:512:LYS:C	2.64	0.40
1:B:555:HIS:O	1:B:556:CYS:C	2.64	0.40
1:D:369:LEU:HD23	1:D:372:MET:SD	2.61	0.40
1:D:393:TRP:CZ2	1:D:553:LEU:HD22	2.56	0.40
1:D:441:GLU:HG2	1:D:572:GLY:HA3	2.03	0.40
1:D:609:LEU:HA	2:P:246:MET:HE1	2.03	0.40
1:F:273:VAL:HG22	1:F:292:TYR:CE2	2.57	0.40
1:I:439:LEU:HD23	1:I:575:LEU:CD1	2.52	0.40
1:I:512:LYS:HE3	1:I:512:LYS:HB2	1.89	0.40
1:J:296:GLN:NE2	1:J:328:ALA:HB1	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:189:ALA:HA	2:O:205:TYR:CD2	2.56	0.40
2:P:272:VAL:HG12	2:P:273:ARG:N	2.35	0.40
2:Q:122:VAL:HG12	2:Q:123:THR:N	2.35	0.40
2:R:196:ARG:HD2	2:R:237:MET:SD	2.61	0.40
2:T:109:PHE:CE2	2:T:257:LEU:HB2	2.57	0.40
2:U:246:MET:O	2:U:247:ASN:HB3	2.22	0.40
1:A:414:TYR:HB3	1:A:416:ILE:HG13	2.03	0.40
1:B:291:MET:HE1	1:B:312:SER:OG	2.21	0.40
1:D:322:ALA:C	1:D:324:ALA:N	2.79	0.40
1:D:424:PHE:O	1:D:527:THR:HA	2.21	0.40
1:D:439:LEU:HD23	1:D:575:LEU:HD13	2.03	0.40
1:F:349:ARG:CD	1:F:517:ARG:CZ	2.99	0.40
1:F:594:SER:OG	1:F:595:ARG:N	2.53	0.40
1:G:327:PHE:CE2	1:G:333:GLN:HB3	2.56	0.40
1:I:452:LEU:HB3	1:I:453:PRO:CD	2.51	0.40
1:J:270:TRP:CD1	1:J:270:TRP:H	2.39	0.40
1:J:583:ARG:HD3	1:J:583:ARG:HA	1.92	0.40
1:K:289:LEU:CD1	1:K:333:GLN:HB3	2.49	0.40
2:P:150:THR:HA	2:P:151:PRO:HD3	1.91	0.40
2:R:127:SER:O	2:R:131:ASN:N	2.55	0.40
2:U:193:HIS:ND1	2:U:214:HIS:HB3	2.36	0.40
1:A:590:GLN:HG3	2:M:181:ARG:NH1	2.36	0.40
1:B:366:ASN:HD21	1:B:592:ILE:HD13	1.87	0.40
1:B:387:TRP:O	1:B:390:GLY:N	2.54	0.40
1:B:516:LYS:N	1:B:516:LYS:HD3	2.36	0.40
1:B:548:ARG:O	1:B:548:ARG:HG3	2.21	0.40
1:C:394:LEU:C	1:C:396:CYS:H	2.30	0.40
1:C:397:LEU:HB3	1:C:401:MET:CE	2.49	0.40
1:C:440:LEU:HD13	1:C:471:VAL:HG23	2.04	0.40
1:C:583:ARG:HB3	1:C:587:GLU:OE1	2.21	0.40
1:C:617:PHE:C	1:C:617:PHE:CD1	2.99	0.40
1:D:327:PHE:C	1:D:329:ASP:H	2.29	0.40
1:F:299:PHE:CZ	1:F:318:GLU:HB2	2.57	0.40
1:F:375:MET:HE2	1:F:376:PHE:CE2	2.57	0.40
1:G:354:GLN:HE22	1:H:291:MET:CE	2.34	0.40
1:H:311:PRO:HA	1:H:314:TYR:CZ	2.57	0.40
1:H:454:LEU:HD12	1:H:454:LEU:N	2.36	0.40
1:H:506:LYS:HG2	1:H:519:GLN:C	2.47	0.40
1:I:405:VAL:HG21	1:I:578:MET:HE1	2.04	0.40
1:I:415:ASN:HB3	1:J:567:ARG:NH2	2.36	0.40
1:J:356:THR:HG23	1:J:359:GLN:CD	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:423:LEU:HD11	1:K:528:MET:SD	2.62	0.40
1:L:456:ARG:HH11	1:L:456:ARG:HG3	1.86	0.40
2:M:156:ARG:HG2	2:M:156:ARG:HH11	1.87	0.40
2:N:159:ALA:HB3	2:N:216:VAL:HG13	2.02	0.40
2:Q:203:VAL:HG22	2:Q:204:GLU:N	2.36	0.40
2:V:186:ASP:OD1	2:V:189:ALA:HB3	2.22	0.40
2:V:222:PRO:HA	2:V:223:PRO:HD3	1.97	0.40
2:W:151:PRO:HD2	2:W:220:TYR:CE2	2.56	0.40
2:W:224:GLU:O	2:W:225:VAL:C	2.63	0.40
2:W:237:MET:N	2:W:237:MET:SD	2.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	360/370 (97%)	320 (89%)	35 (10%)	5 (1%)	9	34
1	B	360/370 (97%)	310 (86%)	44 (12%)	6 (2%)	7	30
1	C	361/370 (98%)	306 (85%)	44 (12%)	11 (3%)	3	19
1	D	360/370 (97%)	312 (87%)	43 (12%)	5 (1%)	9	34
1	E	360/370 (97%)	316 (88%)	38 (11%)	6 (2%)	7	30
1	F	361/370 (98%)	309 (86%)	46 (13%)	6 (2%)	7	30
1	G	360/370 (97%)	326 (91%)	29 (8%)	5 (1%)	9	34
1	H	360/370 (97%)	317 (88%)	39 (11%)	4 (1%)	11	39
1	I	361/370 (98%)	321 (89%)	36 (10%)	4 (1%)	11	39
1	J	360/370 (97%)	319 (89%)	37 (10%)	4 (1%)	11	39
1	K	360/370 (97%)	329 (91%)	26 (7%)	5 (1%)	9	34
1	L	361/370 (98%)	330 (91%)	29 (8%)	2 (1%)	21	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	M	197/203 (97%)	174 (88%)	19 (10%)	4 (2%)	6	27
2	N	197/203 (97%)	175 (89%)	17 (9%)	5 (2%)	4	22
2	O	197/203 (97%)	177 (90%)	15 (8%)	5 (2%)	4	22
2	P	197/203 (97%)	174 (88%)	20 (10%)	3 (2%)	8	33
2	Q	197/203 (97%)	172 (87%)	22 (11%)	3 (2%)	8	33
2	R	197/203 (97%)	172 (87%)	21 (11%)	4 (2%)	6	27
2	S	197/203 (97%)	173 (88%)	20 (10%)	4 (2%)	6	27
2	T	197/203 (97%)	178 (90%)	15 (8%)	4 (2%)	6	27
2	U	197/203 (97%)	172 (87%)	22 (11%)	3 (2%)	8	33
2	V	197/203 (97%)	180 (91%)	14 (7%)	3 (2%)	8	33
2	W	197/203 (97%)	180 (91%)	16 (8%)	1 (0%)	24	55
2	X	197/203 (97%)	176 (89%)	19 (10%)	2 (1%)	12	41
All	All	6688/6876 (97%)	5918 (88%)	666 (10%)	104 (2%)	7	32

All (104) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	473	GLU
1	C	475	VAL
1	D	530	GLU
1	E	514	LEU
1	H	530	GLU
1	J	512	LYS
1	K	490	GLY
1	K	514	LEU
2	T	245	GLY
2	X	119	ALA
1	A	297	TYR
1	A	562	PHE
1	B	474	ASP
1	C	530	GLU
1	C	625	VAL
1	L	516	LYS
2	M	245	GLY
2	N	115	HIS
2	N	119	ALA
2	N	246	MET
2	O	245	GLY

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Mol	Chain	Res	Type
2	O	246	MET
2	P	245	GLY
2	R	245	GLY
2	S	245	GLY
2	S	246	MET
2	T	119	ALA
2	U	245	GLY
2	V	245	GLY
2	X	245	GLY
1	A	480	GLY
1	B	308	LYS
1	B	513	HIS
1	C	382	ALA
1	C	569	ILE
1	E	300	GLU
1	E	598	GLU
1	F	530	GLU
1	I	486	PRO
1	I	513	HIS
1	I	514	LEU
1	J	312	SER
1	J	590	GLN
1	K	427	PRO
1	K	530	GLU
2	N	245	GLY
2	O	244	GLY
2	Q	244	GLY
2	R	244	GLY
2	R	246	MET
2	U	244	GLY
2	U	246	MET
2	V	244	GLY
2	V	246	MET
2	W	244	GLY
1	A	310	GLN
1	B	395	HIS
1	C	266	LYS
1	C	279	GLU
1	C	592	ILE
1	D	515	ASN
1	E	512	LYS
1	F	314	TYR

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Mol	Chain	Res	Type
1	G	285	VAL
1	G	561	GLU
1	K	308	LYS
2	M	246	MET
2	N	244	GLY
2	O	119	ALA
2	O	194	LEU
2	P	119	ALA
2	P	244	GLY
2	Q	119	ALA
2	S	119	ALA
2	T	244	GLY
2	T	259	ASP
1	A	300	GLU
1	B	515	ASN
1	B	591	SER
1	C	308	LYS
1	D	330	SER
1	E	606	GLU
1	F	427	PRO
1	F	583	ARG
1	G	511	LYS
1	H	505	VAL
1	H	583	ARG
1	I	427	PRO
2	M	244	GLY
1	D	427	PRO
1	F	502	ASP
1	J	480	GLY
2	M	259	ASP
2	R	208	ASP
1	D	268	VAL
1	H	569	ILE
2	S	244	GLY
1	C	490	GLY
1	E	465	ILE
1	L	427	PRO
2	Q	245	GLY
1	F	569	ILE
1	G	592	ILE
1	G	480	GLY

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	323/329 (98%)	302 (94%)	21 (6%)	15	42
1	B	323/329 (98%)	302 (94%)	21 (6%)	15	42
1	C	324/329 (98%)	308 (95%)	16 (5%)	22	51
1	D	323/329 (98%)	309 (96%)	14 (4%)	26	54
1	E	323/329 (98%)	299 (93%)	24 (7%)	13	38
1	F	324/329 (98%)	312 (96%)	12 (4%)	30	58
1	G	323/329 (98%)	304 (94%)	19 (6%)	18	45
1	H	323/329 (98%)	305 (94%)	18 (6%)	19	47
1	I	324/329 (98%)	303 (94%)	21 (6%)	15	42
1	J	323/329 (98%)	304 (94%)	19 (6%)	18	45
1	K	323/329 (98%)	299 (93%)	24 (7%)	13	38
1	L	324/329 (98%)	301 (93%)	23 (7%)	13	40
2	M	179/182 (98%)	169 (94%)	10 (6%)	19	47
2	N	179/182 (98%)	173 (97%)	6 (3%)	32	60
2	O	179/182 (98%)	173 (97%)	6 (3%)	32	60
2	P	179/182 (98%)	171 (96%)	8 (4%)	24	53
2	Q	179/182 (98%)	174 (97%)	5 (3%)	38	63
2	R	179/182 (98%)	177 (99%)	2 (1%)	65	75
2	S	179/182 (98%)	173 (97%)	6 (3%)	32	60
2	T	179/182 (98%)	171 (96%)	8 (4%)	24	53
2	U	179/182 (98%)	170 (95%)	9 (5%)	22	50
2	V	179/182 (98%)	175 (98%)	4 (2%)	45	67
2	W	179/182 (98%)	170 (95%)	9 (5%)	22	50
2	X	179/182 (98%)	171 (96%)	8 (4%)	24	53
All	All	6028/6132 (98%)	5715 (95%)	313 (5%)	21	49

All (313) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	302	CYS
1	A	338	GLN
1	A	349	ARG
1	A	350	VAL
1	A	361	LEU
1	A	398	LEU
1	A	415	ASN
1	A	420	ARG
1	A	470	VAL
1	A	473	GLU
1	A	476	LYS
1	A	481	GLU
1	A	492	ASN
1	A	504	SER
1	A	520	ILE
1	A	525	ILE
1	A	528	MET
1	A	536	THR
1	A	592	ILE
1	A	594	SER
1	A	610	SER
1	B	267	GLN
1	B	287	LEU
1	B	303	LEU
1	B	356	THR
1	B	357	ARG
1	B	363	ASN
1	B	370	ASP
1	B	398	LEU
1	B	420	ARG
1	B	454	LEU
1	B	457	LEU
1	B	463	VAL
1	B	478	THR
1	B	504	SER
1	B	516	LYS
1	B	520	ILE
1	B	525	ILE
1	B	542	VAL
1	B	569	ILE
1	B	587	GLU
1	B	610	SER
1	C	307	LYS

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Mol	Chain	Res	Type
1	C	326	ILE
1	C	332	ASN
1	C	349	ARG
1	C	353	LEU
1	C	361	LEU
1	C	368	LEU
1	C	375	MET
1	C	415	ASN
1	C	417	PRO
1	C	454	LEU
1	C	457	LEU
1	C	460	GLU
1	C	474	ASP
1	C	507	VAL
1	C	520	ILE
1	D	286	LEU
1	D	302	CYS
1	D	309	GLU
1	D	349	ARG
1	D	361	LEU
1	D	388	MET
1	D	473	GLU
1	D	478	THR
1	D	492	ASN
1	D	506	LYS
1	D	513	HIS
1	D	557	LEU
1	D	570	GLN
1	D	609	LEU
1	E	267	GLN
1	E	285	VAL
1	E	302	CYS
1	E	316	TYR
1	E	331	LYS
1	E	338	GLN
1	E	344	VAL
1	E	357	ARG
1	E	361	LEU
1	E	398	LEU
1	E	410	LYS
1	E	473	GLU
1	E	474	ASP

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Mol	Chain	Res	Type
1	E	491	ILE
1	E	504	SER
1	E	512	LYS
1	E	519	GLN
1	E	520	ILE
1	E	529	ASN
1	E	542	VAL
1	E	551	ASP
1	E	591	SER
1	E	610	SER
1	E	623	ILE
1	F	291	MET
1	F	319	LYS
1	F	348	LYS
1	F	353	LEU
1	F	458	ASN
1	F	469	LEU
1	F	476	LYS
1	F	499	ASP
1	F	520	ILE
1	F	590	GLN
1	F	603	LEU
1	F	606	GLU
1	G	288	LEU
1	G	338	GLN
1	G	339	GLN
1	G	361	LEU
1	G	398	LEU
1	G	418	LYS
1	G	429	ASP
1	G	459	PHE
1	G	473	GLU
1	G	476	LYS
1	G	500	TYR
1	G	505	VAL
1	G	513	HIS
1	G	530	GLU
1	G	591	SER
1	G	598	GLU
1	G	603	LEU
1	G	621	MET
1	G	625	VAL

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Mol	Chain	Res	Type
1	H	326	ILE
1	H	398	LEU
1	H	417	PRO
1	H	432	LYS
1	H	449	ASN
1	H	469	LEU
1	H	470	VAL
1	H	473	GLU
1	H	474	ASP
1	H	515	ASN
1	H	519	GLN
1	H	520	ILE
1	H	532	SER
1	H	542	VAL
1	H	559	ARG
1	H	603	LEU
1	H	609	LEU
1	H	625	VAL
1	I	281	LYS
1	I	291	MET
1	I	303	LEU
1	I	329	ASP
1	I	349	ARG
1	I	361	LEU
1	I	370	ASP
1	I	415	ASN
1	I	418	LYS
1	I	443	CYS
1	I	454	LEU
1	I	513	HIS
1	I	517	ARG
1	I	542	VAL
1	I	551	ASP
1	I	561	GLU
1	I	567	ARG
1	I	570	GLN
1	I	590	GLN
1	I	609	LEU
1	I	613	GLN
1	J	271	LYS
1	J	309	GLU
1	J	315	LYS

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Mol	Chain	Res	Type
1	J	361	LEU
1	J	367	ASP
1	J	379	THR
1	J	388	MET
1	J	415	ASN
1	J	454	LEU
1	J	458	ASN
1	J	473	GLU
1	J	481	GLU
1	J	508	ASN
1	J	509	LEU
1	J	515	ASN
1	J	520	ILE
1	J	551	ASP
1	J	562	PHE
1	J	592	ILE
1	K	271	LYS
1	K	272	LEU
1	K	291	MET
1	K	302	CYS
1	K	338	GLN
1	K	410	LYS
1	K	443	CYS
1	K	454	LEU
1	K	455	ASP
1	K	463	VAL
1	K	474	ASP
1	K	491	ILE
1	K	513	HIS
1	K	516	LYS
1	K	519	GLN
1	K	520	ILE
1	K	527	THR
1	K	529	ASN
1	K	542	VAL
1	K	551	ASP
1	K	569	ILE
1	K	594	SER
1	K	608	SER
1	K	627	ASP
1	L	278	MET
1	L	338	GLN

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Mol	Chain	Res	Type
1	L	353	LEU
1	L	361	LEU
1	L	410	LYS
1	L	420	ARG
1	L	429	ASP
1	L	433	THR
1	L	448	LEU
1	L	463	VAL
1	L	470	VAL
1	L	502	ASP
1	L	505	VAL
1	L	518	THR
1	L	520	ILE
1	L	528	MET
1	L	532	SER
1	L	542	VAL
1	L	561	GLU
1	L	590	GLN
1	L	591	SER
1	L	603	LEU
1	L	611	VAL
2	M	149	SER
2	M	158	ARG
2	M	180	GLU
2	M	192	GLN
2	M	194	LEU
2	M	207	ASP
2	M	213	ARG
2	M	217	VAL
2	M	238	CYS
2	M	243	MET
2	N	158	ARG
2	N	167	GLN
2	N	192	GLN
2	N	194	LEU
2	N	213	ARG
2	N	217	VAL
2	O	101	LYS
2	O	180	GLU
2	O	192	GLN
2	O	194	LEU
2	O	213	ARG

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Mol	Chain	Res	Type
2	O	217	VAL
2	P	158	ARG
2	P	167	GLN
2	P	170	THR
2	P	192	GLN
2	P	194	LEU
2	P	213	ARG
2	P	217	VAL
2	P	238	CYS
2	Q	167	GLN
2	Q	192	GLN
2	Q	194	LEU
2	Q	213	ARG
2	Q	217	VAL
2	R	158	ARG
2	R	194	LEU
2	S	156	ARG
2	S	158	ARG
2	S	192	GLN
2	S	194	LEU
2	S	213	ARG
2	S	217	VAL
2	T	158	ARG
2	T	180	GLU
2	T	192	GLN
2	T	194	LEU
2	T	213	ARG
2	T	217	VAL
2	T	274	VAL
2	T	289	LEU
2	U	156	ARG
2	U	158	ARG
2	U	167	GLN
2	U	170	THR
2	U	192	GLN
2	U	194	LEU
2	U	213	ARG
2	U	217	VAL
2	U	240	SER
2	V	158	ARG
2	V	192	GLN
2	V	194	LEU

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Mol	Chain	Res	Type
2	V	217	VAL
2	W	145	LEU
2	W	149	SER
2	W	180	GLU
2	W	192	GLN
2	W	194	LEU
2	W	207	ASP
2	W	217	VAL
2	W	238	CYS
2	W	268	ASN
2	X	123	THR
2	X	145	LEU
2	X	149	SER
2	X	158	ARG
2	X	192	GLN
2	X	194	LEU
2	X	213	ARG
2	X	238	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (248) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	333	GLN
1	A	338	GLN
1	A	415	ASN
1	A	467	GLN
1	A	508	ASN
1	A	513	HIS
1	A	529	ASN
1	A	538	GLN
1	A	544	GLN
1	A	570	GLN
1	B	267	GLN
1	B	320	HIS
1	B	323	ASN
1	B	332	ASN
1	B	333	GLN
1	B	415	ASN
1	B	449	ASN
1	B	458	ASN
1	B	492	ASN
1	B	493	ASN

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Mol	Chain	Res	Type
1	B	529	ASN
1	B	538	GLN
1	B	593	GLN
1	C	310	GLN
1	C	320	HIS
1	C	332	ASN
1	C	333	GLN
1	C	339	GLN
1	C	395	HIS
1	C	415	ASN
1	C	451	ASN
1	C	458	ASN
1	C	513	HIS
1	C	529	ASN
1	C	544	GLN
1	C	613	GLN
1	D	320	HIS
1	D	333	GLN
1	D	338	GLN
1	D	415	ASN
1	D	458	ASN
1	D	467	GLN
1	D	508	ASN
1	D	519	GLN
1	D	529	ASN
1	D	538	GLN
1	D	544	GLN
1	D	570	GLN
1	E	267	GLN
1	E	310	GLN
1	E	313	HIS
1	E	338	GLN
1	E	339	GLN
1	E	354	GLN
1	E	415	ASN
1	E	451	ASN
1	E	467	GLN
1	E	492	ASN
1	E	493	ASN
1	E	515	ASN
1	E	519	GLN
1	E	529	ASN

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Mol	Chain	Res	Type
1	F	310	GLN
1	F	333	GLN
1	F	338	GLN
1	F	354	GLN
1	F	395	HIS
1	F	415	ASN
1	F	489	GLN
1	F	496	ASN
1	F	529	ASN
1	F	544	GLN
1	F	570	GLN
1	F	613	GLN
1	G	296	GLN
1	G	339	GLN
1	G	354	GLN
1	G	415	ASN
1	G	529	ASN
1	G	538	GLN
1	G	544	GLN
1	G	570	GLN
1	G	613	GLN
1	H	296	GLN
1	H	320	HIS
1	H	323	ASN
1	H	333	GLN
1	H	338	GLN
1	H	415	ASN
1	H	449	ASN
1	H	467	GLN
1	H	493	ASN
1	H	515	ASN
1	H	519	GLN
1	H	529	ASN
1	H	538	GLN
1	H	544	GLN
1	H	590	GLN
1	I	310	GLN
1	I	320	HIS
1	I	333	GLN
1	I	339	GLN
1	I	395	HIS
1	I	415	ASN

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Mol	Chain	Res	Type
1	I	449	ASN
1	I	458	ASN
1	I	492	ASN
1	I	529	ASN
1	I	570	GLN
1	I	613	GLN
1	J	296	GLN
1	J	320	HIS
1	J	333	GLN
1	J	338	GLN
1	J	415	ASN
1	J	458	ASN
1	J	492	ASN
1	J	508	ASN
1	J	529	ASN
1	J	544	GLN
1	J	570	GLN
1	J	618	ASN
1	K	267	GLN
1	K	323	ASN
1	K	332	ASN
1	K	333	GLN
1	K	339	GLN
1	K	354	GLN
1	K	415	ASN
1	K	451	ASN
1	K	492	ASN
1	K	493	ASN
1	K	519	GLN
1	K	529	ASN
1	K	538	GLN
1	K	544	GLN
1	K	590	GLN
1	L	310	GLN
1	L	332	ASN
1	L	333	GLN
1	L	354	GLN
1	L	395	HIS
1	L	415	ASN
1	L	458	ASN
1	L	496	ASN
1	L	538	GLN

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Mol	Chain	Res	Type
1	L	544	GLN
1	L	570	GLN
1	L	590	GLN
1	L	613	GLN
2	M	131	ASN
2	M	144	GLN
2	M	168	HIS
2	M	178	HIS
2	M	192	GLN
2	M	193	HIS
2	M	210	ASN
2	M	214	HIS
2	M	235	ASN
2	N	131	ASN
2	N	136	GLN
2	N	179	HIS
2	N	192	GLN
2	N	193	HIS
2	N	200	ASN
2	N	210	ASN
2	O	165	GLN
2	O	192	GLN
2	O	193	HIS
2	O	210	ASN
2	O	235	ASN
2	O	239	ASN
2	O	288	ASN
2	P	100	GLN
2	P	104	GLN
2	P	131	ASN
2	P	192	GLN
2	P	193	HIS
2	P	210	ASN
2	P	235	ASN
2	Q	100	GLN
2	Q	104	GLN
2	Q	131	ASN
2	Q	144	GLN
2	Q	165	GLN
2	Q	179	HIS
2	Q	192	GLN
2	Q	193	HIS

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Mol	Chain	Res	Type
2	Q	210	ASN
2	Q	239	ASN
2	Q	268	ASN
2	R	100	GLN
2	R	131	ASN
2	R	165	GLN
2	R	192	GLN
2	R	193	HIS
2	R	200	ASN
2	R	210	ASN
2	R	214	HIS
2	R	288	ASN
2	S	100	GLN
2	S	131	ASN
2	S	192	GLN
2	S	210	ASN
2	S	214	HIS
2	S	233	HIS
2	T	104	GLN
2	T	131	ASN
2	T	144	GLN
2	T	165	GLN
2	T	178	HIS
2	T	179	HIS
2	T	192	GLN
2	T	193	HIS
2	T	200	ASN
2	T	210	ASN
2	T	233	HIS
2	U	104	GLN
2	U	131	ASN
2	U	144	GLN
2	U	193	HIS
2	U	210	ASN
2	U	214	HIS
2	U	235	ASN
2	V	104	GLN
2	V	131	ASN
2	V	165	GLN
2	V	179	HIS
2	V	193	HIS
2	V	200	ASN

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Mol	Chain	Res	Type
2	V	210	ASN
2	V	235	ASN
2	W	100	GLN
2	W	104	GLN
2	W	131	ASN
2	W	165	GLN
2	W	168	HIS
2	W	192	GLN
2	W	193	HIS
2	W	210	ASN
2	W	235	ASN
2	X	100	GLN
2	X	131	ASN
2	X	192	GLN
2	X	210	ASN
2	X	235	ASN
2	X	247	ASN
2	X	288	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 24 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	362/370 (97%)	-0.29	5 (1%) 73 53	38, 60, 99, 131	0
1	B	362/370 (97%)	-0.19	4 (1%) 78 60	43, 70, 103, 139	0
1	C	363/370 (98%)	-0.03	4 (1%) 78 60	40, 74, 110, 136	0
1	D	362/370 (97%)	-0.24	5 (1%) 73 53	39, 62, 102, 148	0
1	E	362/370 (97%)	-0.29	5 (1%) 73 53	35, 61, 97, 124	0
1	F	363/370 (98%)	-0.14	6 (1%) 69 48	36, 66, 110, 133	0
1	G	362/370 (97%)	-0.52	3 (0%) 82 66	28, 52, 91, 129	0
1	H	362/370 (97%)	-0.38	3 (0%) 82 66	33, 57, 98, 133	0
1	I	363/370 (98%)	-0.21	2 (0%) 85 72	41, 68, 103, 135	0
1	J	362/370 (97%)	-0.17	5 (1%) 73 53	44, 74, 106, 123	0
1	K	362/370 (97%)	-0.48	2 (0%) 85 72	32, 56, 91, 127	0
1	L	363/370 (98%)	-0.51	5 (1%) 73 53	28, 48, 97, 134	0
2	M	199/203 (98%)	0.25	4 (2%) 65 44	50, 75, 120, 137	0
2	N	199/203 (98%)	0.69	12 (6%) 27 16	80, 110, 144, 151	0
2	O	199/203 (98%)	0.64	8 (4%) 42 24	67, 96, 134, 146	0
2	P	199/203 (98%)	0.34	9 (4%) 38 22	55, 87, 131, 144	0
2	Q	199/203 (98%)	0.30	7 (3%) 47 28	64, 94, 126, 137	0
2	R	199/203 (98%)	0.71	13 (6%) 25 14	69, 104, 142, 152	0
2	S	199/203 (98%)	0.37	8 (4%) 42 24	53, 88, 129, 143	0
2	T	199/203 (98%)	0.41	4 (2%) 65 44	60, 91, 128, 138	0
2	U	199/203 (98%)	0.78	17 (8%) 16 9	72, 103, 138, 147	0
2	V	199/203 (98%)	0.94	24 (12%) 8 5	85, 123, 147, 154	0
2	W	199/203 (98%)	0.03	6 (3%) 52 32	41, 70, 109, 123	0
2	X	199/203 (98%)	0.03	9 (4%) 38 22	35, 65, 112, 136	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
All	All	6736/6876 (97%)	-0.02	170 (2%)	58	37	28, 71, 126, 154	0

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	S	118	THR	7.1
2	N	118	THR	5.8
2	S	115	HIS	5.4
2	S	119	ALA	5.3
2	X	119	ALA	5.2
2	N	119	ALA	5.1
2	W	245	GLY	4.9
2	M	119	ALA	4.9
2	W	225	VAL	4.7
2	R	225	VAL	4.7
2	N	117	GLY	4.7
1	L	514	LEU	4.6
1	D	514	LEU	4.5
2	V	289	LEU	4.5
2	O	289	LEU	4.3
2	N	289	LEU	4.3
2	S	116	SER	4.3
1	C	513	HIS	4.2
2	P	119	ALA	4.1
2	P	289	LEU	4.1
2	R	289	LEU	4.1
1	A	514	LEU	4.0
1	F	514	LEU	4.0
1	J	514	LEU	4.0
1	I	514	LEU	3.9
1	E	516	LYS	3.9
2	X	118	THR	3.8
2	Q	243	MET	3.7
2	N	115	HIS	3.7
1	F	513	HIS	3.7
2	S	117	GLY	3.6
2	T	118	THR	3.6
2	Q	116	SER	3.6
2	P	95	SER	3.6
2	U	117	GLY	3.5
1	G	515	ASN	3.4
1	J	410	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	514	LEU	3.4
2	U	289	LEU	3.4
2	U	118	THR	3.4
1	H	514	LEU	3.3
2	R	123	THR	3.3
2	Q	289	LEU	3.3
2	W	289	LEU	3.3
1	B	515	ASN	3.2
1	L	515	ASN	3.2
1	G	514	LEU	3.2
1	D	513	HIS	3.2
2	X	116	SER	3.2
2	T	289	LEU	3.1
2	N	116	SER	3.1
2	T	119	ALA	3.1
2	P	118	THR	3.1
2	Q	118	THR	3.1
2	M	289	LEU	3.1
2	V	251	ILE	3.1
2	V	188	LEU	3.0
2	U	150	THR	3.0
1	E	515	ASN	3.0
2	R	245	GLY	2.9
2	R	119	ALA	2.9
1	A	513	HIS	2.9
1	A	516	LYS	2.9
2	R	118	THR	2.9
2	M	245	GLY	2.9
1	D	515	ASN	2.8
2	P	120	LYS	2.8
1	G	516	LYS	2.8
1	L	513	HIS	2.8
2	S	289	LEU	2.8
2	V	114	LEU	2.7
2	U	245	GLY	2.7
2	V	119	ALA	2.7
2	V	185	SER	2.6
1	I	513	HIS	2.6
2	S	120	LYS	2.6
2	V	142	PRO	2.6
1	H	515	ASN	2.6
1	E	514	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
2	U	97	VAL	2.6
2	V	153	PRO	2.6
1	E	299	PHE	2.5
2	X	245	GLY	2.5
1	D	299	PHE	2.5
2	V	238	CYS	2.5
2	U	185	SER	2.5
1	F	299	PHE	2.5
1	D	511	LYS	2.5
1	J	513	HIS	2.5
2	O	245	GLY	2.5
2	U	119	ALA	2.4
2	O	118	THR	2.4
2	O	243	MET	2.4
1	B	299	PHE	2.4
2	N	121	SER	2.4
2	P	101	LYS	2.4
1	K	514	LEU	2.4
2	R	116	SER	2.4
2	R	185	SER	2.4
2	V	150	THR	2.4
2	R	142	PRO	2.4
2	X	225	VAL	2.4
2	V	118	THR	2.3
2	O	273	ARG	2.3
2	U	152	PRO	2.3
1	F	616	LYS	2.3
1	B	303	LEU	2.3
2	V	197	VAL	2.3
1	A	301	MET	2.3
2	Q	115	HIS	2.3
2	V	160	MET	2.3
2	P	184	ASP	2.3
2	O	203	VAL	2.3
2	O	116	SER	2.3
2	V	225	VAL	2.3
2	V	154	GLY	2.3
2	U	145	LEU	2.3
2	U	201	LEU	2.3
2	U	264	LEU	2.2
1	C	516	LYS	2.2
1	L	516	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	N	94	SER	2.2
2	P	116	SER	2.2
1	F	515	ASN	2.2
2	R	223	PRO	2.2
2	V	199	GLY	2.2
2	W	226	GLY	2.2
1	C	299	PHE	2.2
2	T	122	VAL	2.1
2	X	289	LEU	2.1
2	R	243	MET	2.1
2	U	116	SER	2.1
2	V	109	PHE	2.1
2	U	93	LEU	2.1
2	N	191	PRO	2.1
1	B	455	ASP	2.1
2	V	201	LEU	2.1
2	U	237	MET	2.1
2	M	221	GLU	2.1
2	Q	245	GLY	2.1
1	K	515	ASN	2.1
1	A	499	ASP	2.1
2	V	184	ASP	2.1
2	W	120	LYS	2.1
2	V	220	TYR	2.1
2	Q	119	ALA	2.1
2	S	245	GLY	2.1
2	U	154	GLY	2.1
1	L	266	LYS	2.1
2	X	120	LYS	2.1
2	V	252	LEU	2.1
2	N	243	MET	2.1
2	R	204	GLU	2.1
2	V	191	PRO	2.1
1	J	511	LYS	2.0
1	J	512	LYS	2.0
1	F	492	ASN	2.0
2	N	195	ILE	2.0
2	W	186	ASP	2.0
2	X	226	GLY	2.0
1	E	266	LYS	2.0
1	H	516	LYS	2.0
2	R	180	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
2	V	257	LEU	2.0
2	N	185	SER	2.0
2	X	115	HIS	2.0
2	O	119	ALA	2.0
2	V	140	THR	2.0
2	P	167	GLN	2.0
2	U	194	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	ZN	D	3	1/1	0.92	0.06	84,84,84,84	0
3	ZN	E	4	1/1	0.96	0.05	57,57,57,57	0
3	ZN	A	1	1/1	0.98	0.03	66,66,66,66	0
3	ZN	C	6	1/1	0.98	0.04	79,79,79,79	0
3	ZN	I	8	1/1	0.98	0.03	60,60,60,60	0
3	ZN	J	10	1/1	0.98	0.03	76,76,76,76	0
3	ZN	K	11	1/1	0.98	0.03	59,59,59,59	0
3	ZN	V	22	1/1	0.98	0.03	85,85,85,85	0
3	ZN	B	2	1/1	0.99	0.02	71,71,71,71	0
3	ZN	F	5	1/1	0.99	0.04	68,68,68,68	0
3	ZN	G	7	1/1	0.99	0.02	66,66,66,66	0
3	ZN	L	12	1/1	0.99	0.03	57,57,57,57	0
3	ZN	M	13	1/1	0.99	0.04	55,55,55,55	0
3	ZN	N	14	1/1	0.99	0.05	81,81,81,81	0
3	ZN	O	15	1/1	0.99	0.02	61,61,61,61	0
3	ZN	P	16	1/1	0.99	0.04	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	Q	17	1/1	0.99	0.02	44,44,44,44	0
3	ZN	R	18	1/1	0.99	0.03	74,74,74,74	0
3	ZN	S	19	1/1	0.99	0.02	45,45,45,45	0
3	ZN	T	20	1/1	0.99	0.02	51,51,51,51	0
3	ZN	U	21	1/1	0.99	0.03	78,78,78,78	0
3	ZN	H	9	1/1	0.99	0.03	60,60,60,60	0
3	ZN	W	23	1/1	0.99	0.02	45,45,45,45	0
3	ZN	X	24	1/1	0.99	0.03	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.