



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:23 PM UTC

PDB ID : 5AEK / pdb_00005aek
Title : Crystal structure of the human SENP2 C548S in complex with the human SUMO1 K48M F66W
Authors : Gallego, P.; Grana-Montes, R.; Espargaro, A.; Castillo, V.; Torrent, J.; Lange, R.; Papaleo, E.; Lindorff-Larsen, K.; Ventura, S.; Reverter, D.
Deposited on : 2014-12-23
Resolution : 3.00 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

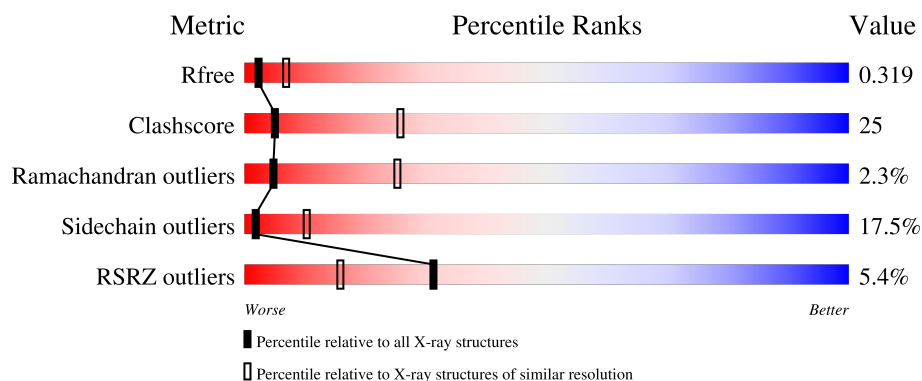
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.



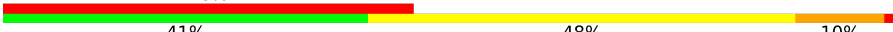
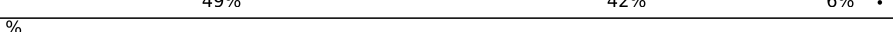
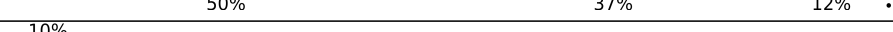
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	224	
1	C	224	
1	E	224	
1	G	224	
1	I	224	

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Mol	Chain	Length	Quality of chain
1	K	224	
1	M	224	
1	O	224	
1	Q	224	
1	S	224	
1	U	224	
1	W	224	
2	B	78	
2	D	78	
2	F	78	
2	H	78	
2	J	78	
2	L	78	
2	N	78	
2	P	78	
2	R	78	
2	T	78	
2	V	78	
2	X	78	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 29972 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 SENTRIN-SPECIFIC PROTEASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1860	1195	325	330	10			
1	C	224	Total	C	N	O	S	0	0	0
			1865	1198	326	331	10			
1	E	224	Total	C	N	O	S	0	0	0
			1865	1198	326	331	10			
1	G	223	Total	C	N	O	S	0	0	0
			1860	1195	325	330	10			
1	I	223	Total	C	N	O	S	0	0	0
			1860	1195	325	330	10			
1	K	223	Total	C	N	O	S	0	0	0
			1860	1195	325	330	10			
1	M	222	Total	C	N	O	S	0	0	0
			1851	1190	324	327	10			
1	O	223	Total	C	N	O	S	0	0	0
			1860	1195	325	330	10			
1	Q	224	Total	C	N	O	S	0	0	0
			1865	1198	326	331	10			
1	S	224	Total	C	N	O	S	0	0	0
			1865	1198	326	331	10			
1	U	223	Total	C	N	O	S	0	0	0
			1860	1195	325	330	10			
1	W	222	Total	C	N	O	S	0	0	0
			1851	1190	324	327	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	548	SER	CYS	engineered mutation	UNP Q9HC62
C	548	SER	CYS	engineered mutation	UNP Q9HC62
E	548	SER	CYS	engineered mutation	UNP Q9HC62
G	548	SER	CYS	engineered mutation	UNP Q9HC62
I	548	SER	CYS	engineered mutation	UNP Q9HC62

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Chain	Residue	Modelled	Actual	Comment	Reference
K	548	SER	CYS	engineered mutation	UNP Q9HC62
M	548	SER	CYS	engineered mutation	UNP Q9HC62
O	548	SER	CYS	engineered mutation	UNP Q9HC62
Q	548	SER	CYS	engineered mutation	UNP Q9HC62
S	548	SER	CYS	engineered mutation	UNP Q9HC62
U	548	SER	CYS	engineered mutation	UNP Q9HC62
W	548	SER	CYS	engineered mutation	UNP Q9HC62

- Molecule 2 is a protein called SMALL UBIQUITIN-RELATED MODIFIER 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	78	Total 639	C 401	N 109	O 124	S 5	0	0	0
2	D	78	Total 639	C 401	N 109	O 124	S 5	0	0	0
2	F	78	Total 639	C 401	N 109	O 124	S 5	0	0	0
2	H	77	Total 630	C 396	N 108	O 121	S 5	0	0	0
2	J	78	Total 639	C 401	N 109	O 124	S 5	0	0	0
2	L	77	Total 630	C 396	N 108	O 121	S 5	0	0	0
2	N	78	Total 639	C 401	N 109	O 124	S 5	0	0	0
2	P	78	Total 639	C 401	N 109	O 124	S 5	0	0	0
2	R	78	Total 639	C 401	N 109	O 124	S 5	0	0	0
2	T	78	Total 639	C 401	N 109	O 124	S 5	0	0	0
2	V	78	Total 639	C 401	N 109	O 124	S 5	0	0	0
2	X	78	Total 639	C 401	N 109	O 124	S 5	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	48	MET	LYS	engineered mutation	UNP P63165
B	66	TRP	PHE	engineered mutation	UNP P63165
D	48	MET	LYS	engineered mutation	UNP P63165

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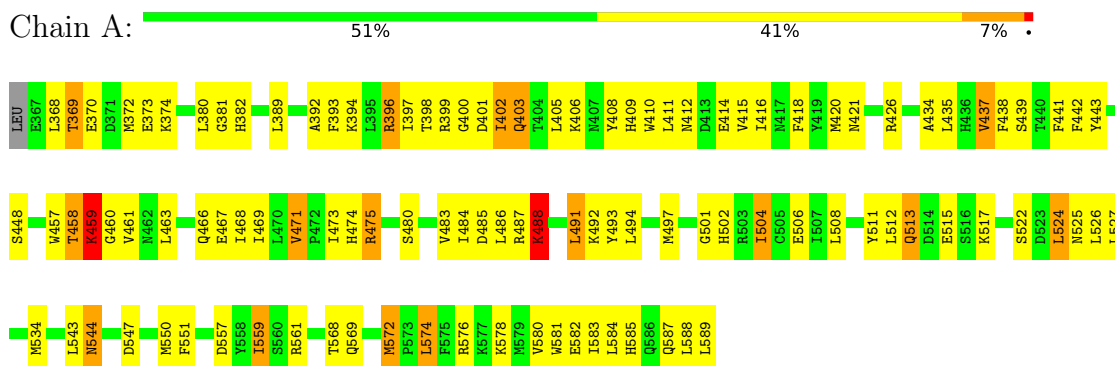
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Chain	Residue	Modelled	Actual	Comment	Reference
D	66	TRP	PHE	engineered mutation	UNP P63165
F	48	MET	LYS	engineered mutation	UNP P63165
F	66	TRP	PHE	engineered mutation	UNP P63165
H	48	MET	LYS	engineered mutation	UNP P63165
H	66	TRP	PHE	engineered mutation	UNP P63165
J	48	MET	LYS	engineered mutation	UNP P63165
J	66	TRP	PHE	engineered mutation	UNP P63165
L	48	MET	LYS	engineered mutation	UNP P63165
L	66	TRP	PHE	engineered mutation	UNP P63165
N	48	MET	LYS	engineered mutation	UNP P63165
N	66	TRP	PHE	engineered mutation	UNP P63165
P	48	MET	LYS	engineered mutation	UNP P63165
P	66	TRP	PHE	engineered mutation	UNP P63165
R	48	MET	LYS	engineered mutation	UNP P63165
R	66	TRP	PHE	engineered mutation	UNP P63165
T	48	MET	LYS	engineered mutation	UNP P63165
T	66	TRP	PHE	engineered mutation	UNP P63165
V	48	MET	LYS	engineered mutation	UNP P63165
V	66	TRP	PHE	engineered mutation	UNP P63165
X	48	MET	LYS	engineered mutation	UNP P63165
X	66	TRP	PHE	engineered mutation	UNP P63165

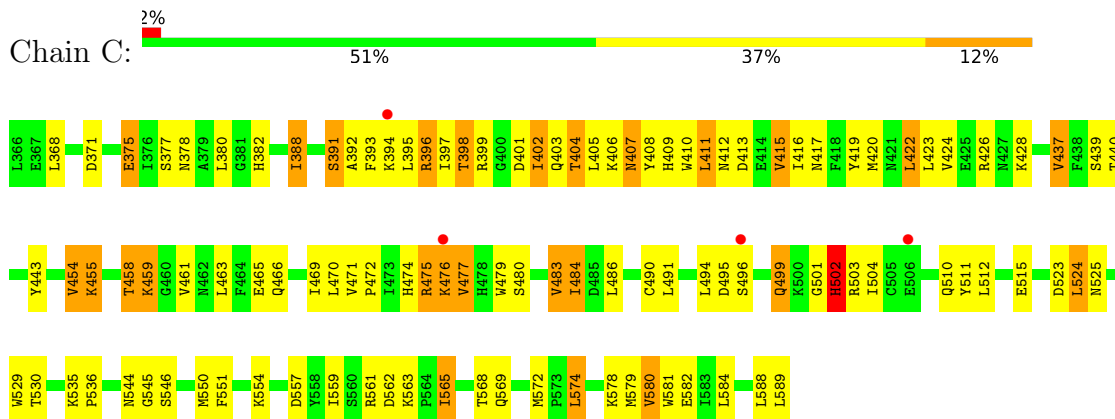
3 Residue-property plots

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.

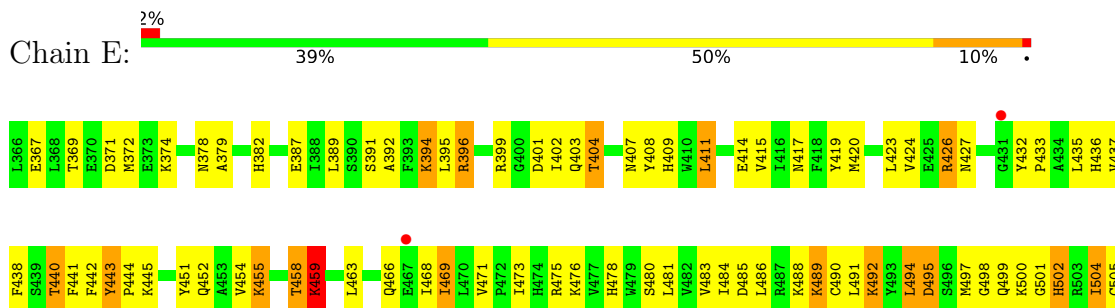
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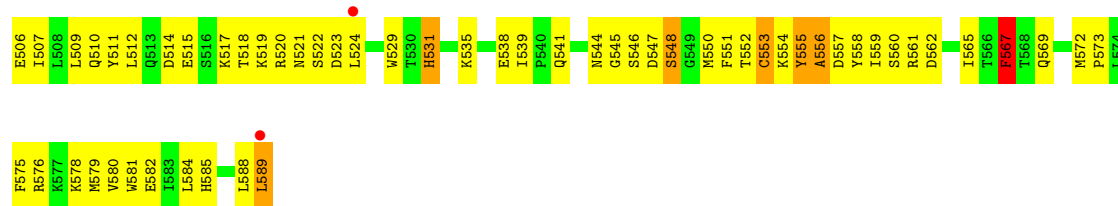


• Molecule 1: SENTRIN-SPECIFIC PROTEASE 2



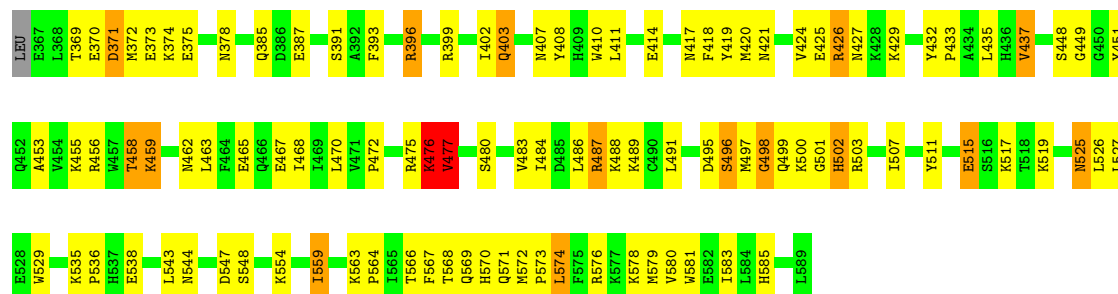
• Molecule 1: SENTRIN-SPECIFIC PROTEASE 2





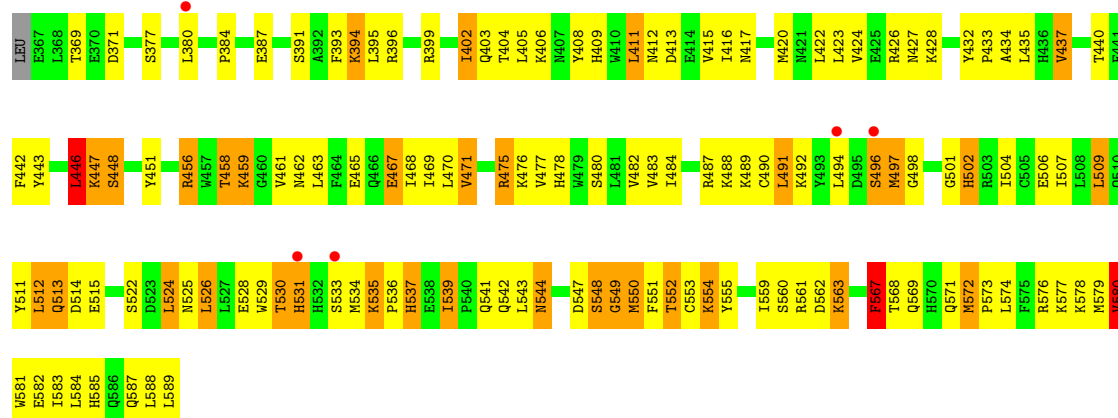
• Molecule 1: SENTRIN-SPECIFIC PROTEASE 2

Chain G: 52% 40% 7% .



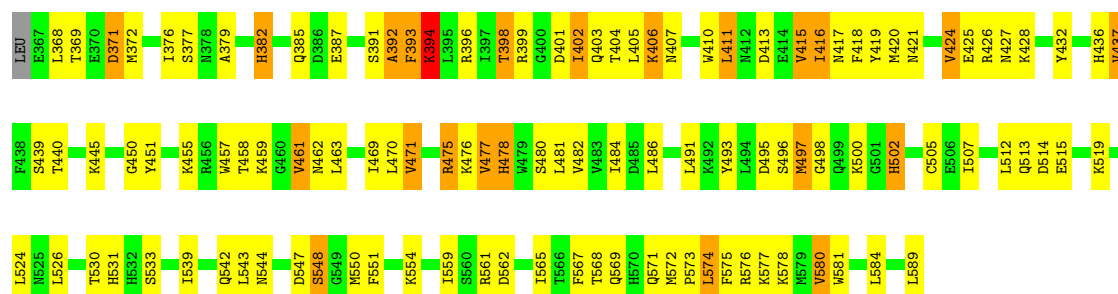
• Molecule 1: SENTRIN-SPECIFIC PROTEASE 2

Chain I: 2% 38% 45% 15% .



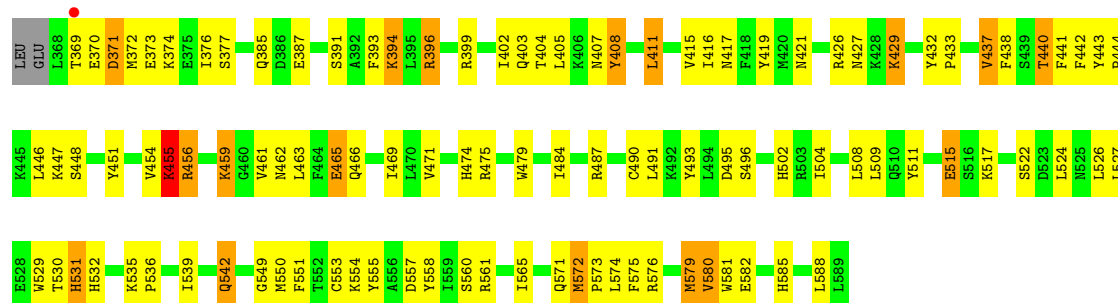
• Molecule 1: SENTRIN-SPECIFIC PROTEASE 2

Chain K: 49% 41% 10%

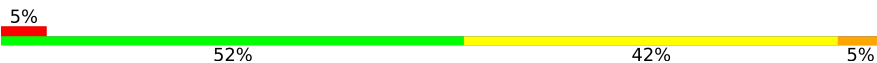


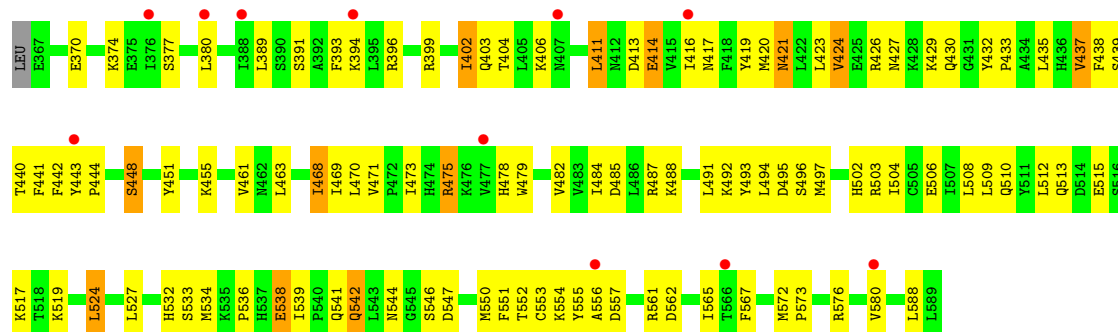
• Molecule 1: SENTRIN-SPECIFIC PROTEASE 2

Chain M: 



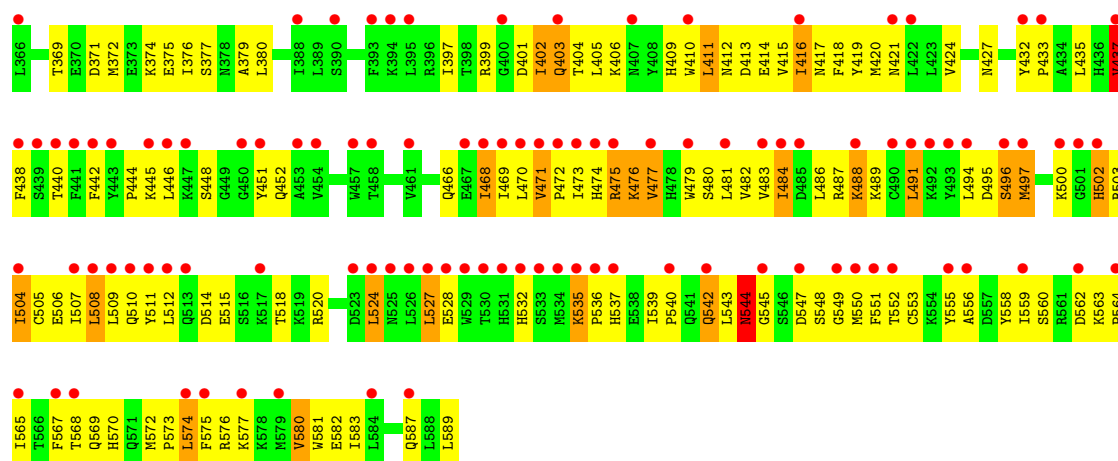
• Molecule 1: SENTRIN-SPECIFIC PROTEASE 2

Chain O: 



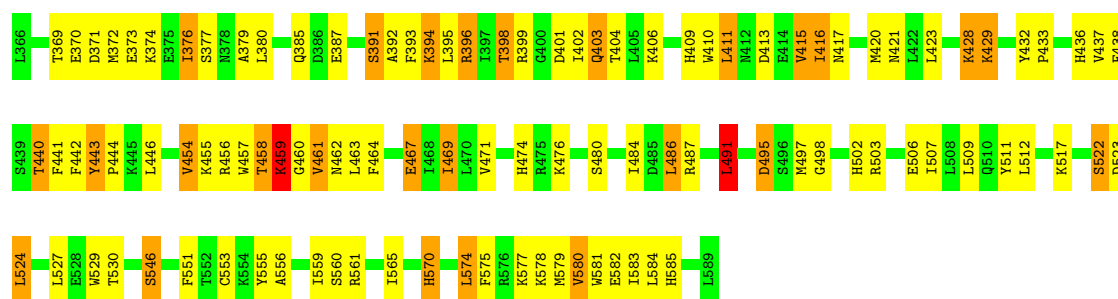
• Molecule 1: SENTRIN-SPECIFIC PROTEASE 2

Chain Q: 

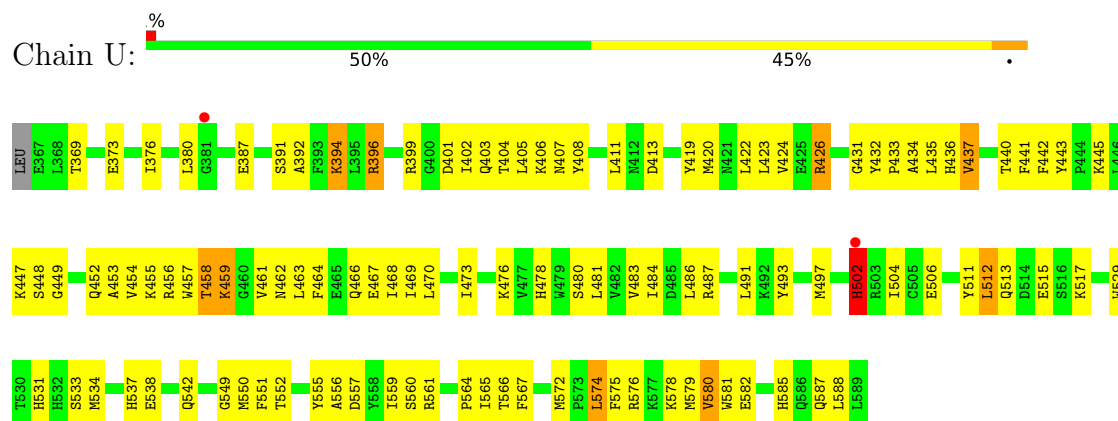


• Molecule 1: SENTRIN-SPECIFIC PROTEASE 2

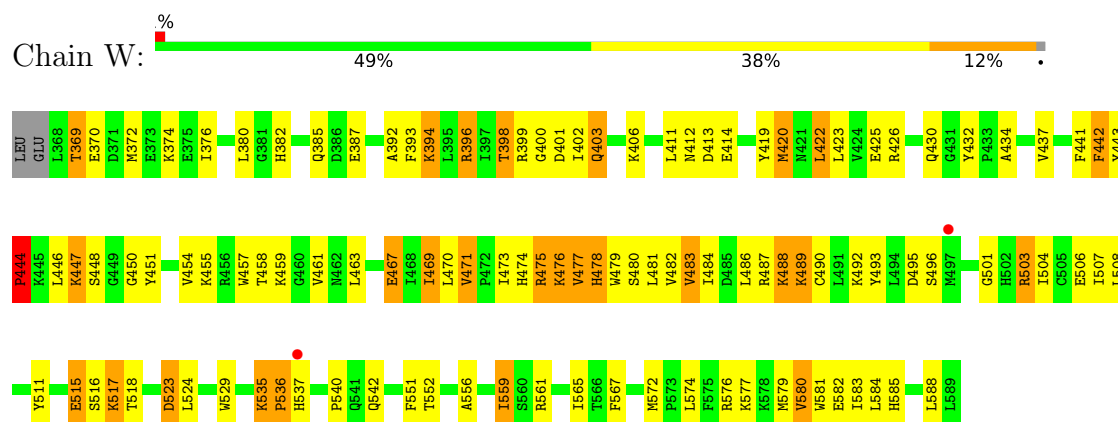
Chain S: 



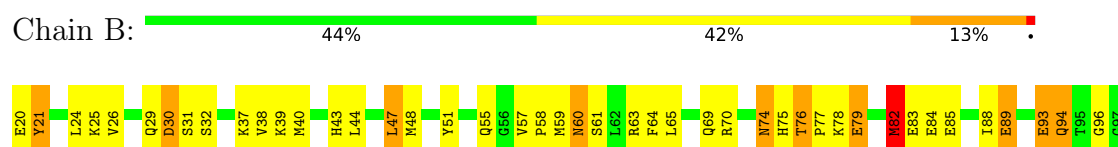
• Molecule 1: SENTRIN-SPECIFIC PROTEASE 2



• Molecule 1: SENTRIN-SPECIFIC PROTEASE 2

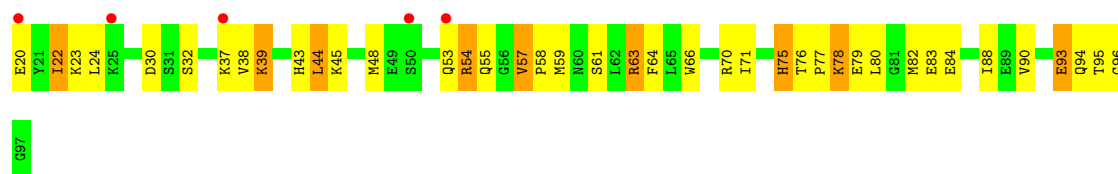


• Molecule 2: SMALL UBIQUITIN-RELATED MODIFIER 1

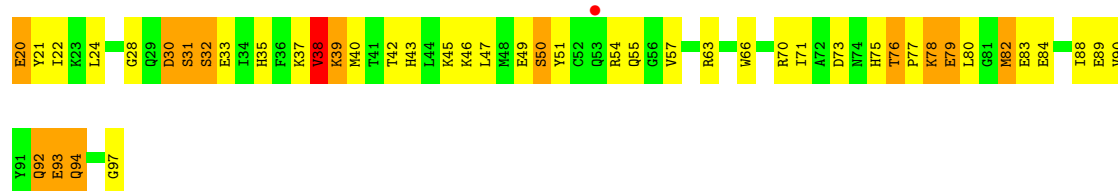


• Molecule 2: SMALL UBIQUITIN-RELATED MODIFIER 1





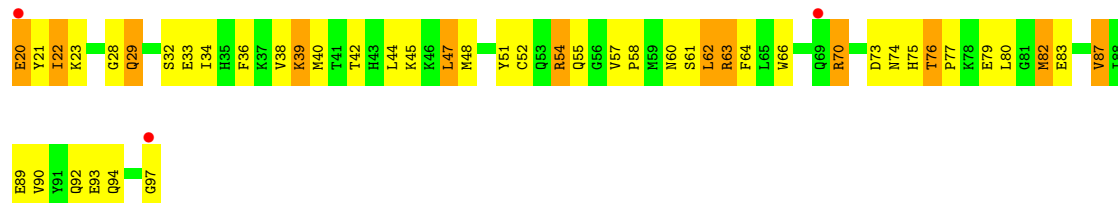
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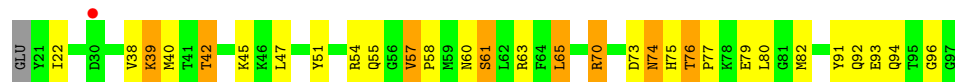
• Molecule 2: SMALL UBIQUITIN-RELATED MODIFIER 1



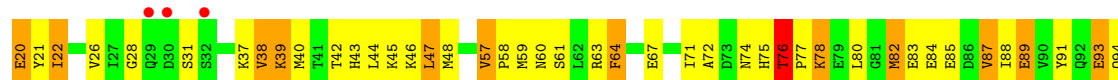
• Molecule 2: SMALL UBIQUITIN-RELATED MODIFIER 1



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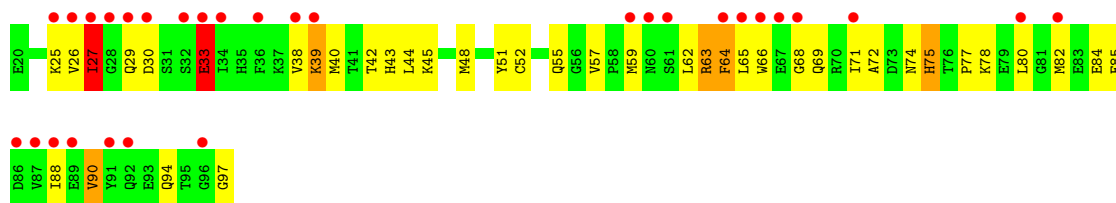
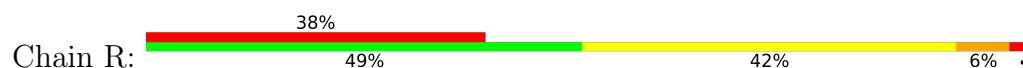




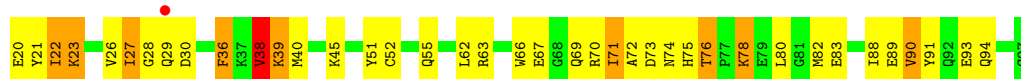
• Molecule 2: SMALL UBIQUITIN-RELATED MODIFIER 1



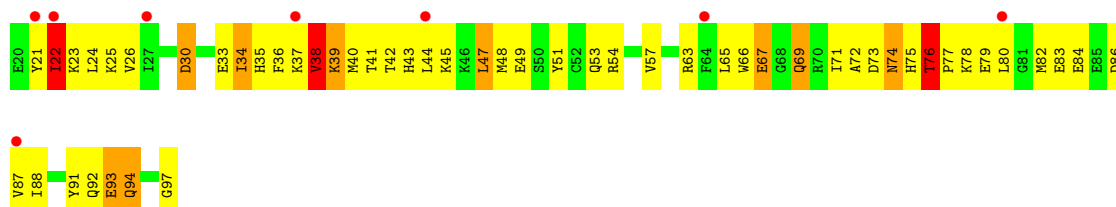
• Molecule 2: SMALL UBIQUITIN-RELATED MODIFIER 1



• Molecule 2: SMALL UBIQUITIN-RELATED MODIFIER 1



• Molecule 2: SMALL UBIQUITIN-RELATED MODIFIER 1



• Molecule 2: SMALL UBIQUITIN-RELATED MODIFIER 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	113.72Å 119.32Å 199.84Å 90.00° 89.67° 90.00°	Depositor
Resolution (Å)	47.00 – 3.00 47.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.7 (47.00-3.00) 94.1 (47.00-3.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.257 , 0.326 0.255 , 0.319	Depositor DCC
R_{free} test set	3167 reflections (3.14%)	wwPDB-VP
Wilson B-factor (Å ²)	65.2	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l 0.000 for -k,-h,-l 0.023 for h,-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	29972	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.03 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4011e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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](#)

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	0.87	1/1906 (0.1%)	1.12	4/2567 (0.2%)
1	C	0.70	0/1911	0.99	0/2574
1	E	0.74	0/1911	1.04	3/2574 (0.1%)
1	G	0.83	0/1906	1.05	1/2567 (0.0%)
1	I	0.78	0/1906	1.13	9/2567 (0.4%)
1	K	0.86	0/1906	1.12	8/2567 (0.3%)
1	M	0.87	0/1897	1.12	2/2555 (0.1%)
1	O	0.74	0/1906	1.01	1/2567 (0.0%)
1	Q	0.81	2/1911 (0.1%)	1.17	14/2574 (0.5%)
1	S	0.82	0/1911	1.12	6/2574 (0.2%)
1	U	0.81	0/1906	1.07	2/2567 (0.1%)
1	W	0.70	0/1897	1.02	4/2555 (0.2%)
2	B	0.83	0/650	1.14	4/869 (0.5%)
2	D	0.74	0/650	1.06	1/869 (0.1%)
2	F	0.90	0/650	1.09	1/869 (0.1%)
2	H	0.76	0/641	1.05	1/857 (0.1%)
2	J	0.77	0/650	1.10	2/869 (0.2%)
2	L	0.78	0/641	1.14	2/857 (0.2%)
2	N	0.88	0/650	1.11	3/869 (0.3%)
2	P	0.69	0/650	1.06	3/869 (0.3%)
2	R	0.89	1/650 (0.2%)	1.03	2/869 (0.2%)
2	T	0.85	0/650	1.16	5/869 (0.6%)
2	V	0.77	0/650	1.15	4/869 (0.5%)
2	X	0.85	0/650	1.17	5/869 (0.6%)
All	All	0.80	4/30656 (0.0%)	1.09	87/41212 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	P	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	471	VAL	CA-CB	6.70	1.60	1.54
1	Q	484	ILE	CA-CB	5.86	1.59	1.53
2	R	27	ILE	CA-CB	5.35	1.61	1.54
1	Q	471	VAL	CA-CB	5.20	1.58	1.54

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	452	GLN	OE1-CD-NE2	-15.77	106.83	122.60
1	W	535	LYS	CA-C-N	10.93	133.50	119.84
1	W	535	LYS	C-N-CA	10.93	133.50	119.84
2	X	38	VAL	N-CA-C	10.04	122.86	109.21
1	Q	452	GLN	CG-CD-NE2	9.65	130.87	116.40
1	S	443	TYR	CA-C-N	-9.65	108.33	118.85
1	S	443	TYR	C-N-CA	-9.65	108.33	118.85
1	Q	535	LYS	CA-C-N	8.79	130.83	119.84
1	Q	535	LYS	C-N-CA	8.79	130.83	119.84
2	J	38	VAL	N-CA-C	8.60	121.24	109.80
1	Q	437	VAL	N-CA-C	8.09	118.64	106.42
2	T	38	VAL	N-CA-C	7.38	124.69	109.34
1	I	539	ILE	CA-C-N	7.33	127.38	119.90
1	I	539	ILE	C-N-CA	7.33	127.38	119.90
1	Q	497	MET	N-CA-C	-7.25	104.59	113.50
2	V	38	VAL	N-CA-C	7.15	119.11	108.96
2	P	31	SER	N-CA-C	7.07	121.73	108.65
1	A	504	ILE	N-CA-C	-6.97	103.51	110.62
2	L	38	VAL	N-CA-C	6.96	119.76	108.97
1	I	550	MET	N-CA-C	-6.83	104.20	112.54
2	F	38	VAL	N-CA-C	6.80	118.38	108.58
2	D	38	VAL	N-CA-C	6.73	118.23	107.73
1	K	471	VAL	N-CA-C	6.65	114.73	108.15
1	I	535	LYS	CA-C-N	6.57	128.05	119.84
1	I	535	LYS	C-N-CA	6.57	128.05	119.84
2	P	36	PHE	N-CA-C	6.51	120.14	109.72
1	K	547	ASP	N-CA-C	6.49	120.94	112.89
1	I	467	GLU	N-CA-C	6.46	118.87	111.11
2	V	76	THR	CA-C-N	6.45	126.14	119.56
2	V	76	THR	C-N-CA	6.45	126.14	119.56
1	Q	496	SER	N-CA-C	6.42	121.16	112.88
1	E	443	TYR	CA-C-N	-6.40	113.10	119.56
1	E	443	TYR	C-N-CA	-6.40	113.10	119.56
2	J	36	PHE	N-CA-C	6.35	120.05	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	22	ILE	N-CA-C	6.21	117.24	108.36
1	U	512	LEU	N-CA-C	-6.20	103.83	111.33
2	T	36	PHE	CA-C-N	6.18	129.71	120.31
2	T	36	PHE	C-N-CA	6.18	129.71	120.31
2	X	36	PHE	N-CA-C	6.17	119.59	110.46
2	R	38	VAL	N-CA-C	6.10	117.10	110.21
1	I	567	PHE	N-CA-C	6.07	118.14	110.24
2	B	82	MET	N-CA-C	-6.01	102.56	110.43
1	W	422	LEU	N-CA-C	-5.98	104.67	111.07
2	R	33	GLU	N-CA-C	5.96	118.64	110.24
1	W	483	VAL	N-CA-C	5.91	116.12	107.37
1	G	468	ILE	N-CA-C	5.78	116.40	107.78
1	S	416	ILE	N-CA-C	5.76	115.89	110.30
2	B	21	TYR	N-CA-C	5.76	120.59	113.50
1	O	555	TYR	N-CA-C	-5.76	104.91	111.07
1	S	461	VAL	N-CA-C	5.74	118.41	108.95
2	X	79	GLU	N-CA-C	5.67	117.46	111.28
1	Q	502	HIS	CA-C-N	5.64	127.83	120.28
1	Q	502	HIS	C-N-CA	5.64	127.83	120.28
2	T	22	ILE	N-CA-C	5.64	115.27	108.06
2	V	22	ILE	N-CA-C	5.53	117.53	108.97
2	B	75	HIS	N-CA-C	5.52	118.03	110.24
1	K	471	VAL	CB-CA-C	-5.47	105.88	111.08
2	X	37	LYS	N-CA-CB	-5.46	103.63	111.54
1	E	567	PHE	N-CA-C	5.31	117.67	110.35
2	T	75	HIS	N-CA-C	5.29	117.90	110.23
2	N	76	THR	CB-CA-C	5.25	116.47	109.65
1	A	572	MET	CA-C-N	-5.24	113.63	119.19
1	A	572	MET	C-N-CA	-5.24	113.63	119.19
1	I	471	VAL	CA-C-N	5.21	125.46	119.83
1	I	471	VAL	C-N-CA	5.21	125.46	119.83
1	K	393	PHE	N-CA-C	-5.19	106.53	112.86
1	Q	528	GLU	N-CA-C	-5.19	106.95	113.28
1	U	459	LYS	N-CA-C	5.19	117.33	111.11
1	Q	574	LEU	N-CA-C	-5.18	105.71	111.36
2	X	29	GLN	N-CA-C	-5.16	105.34	110.97
1	S	491	LEU	N-CA-C	5.16	117.04	107.60
2	H	38	VAL	N-CA-C	5.14	116.04	109.30
1	K	416	ILE	CB-CA-C	-5.14	105.30	111.88
1	K	539	ILE	CA-C-N	-5.14	114.66	119.85
1	K	539	ILE	C-N-CA	-5.14	114.66	119.85
1	A	488	LYS	N-CA-C	-5.13	107.05	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	65	LEU	N-CA-C	5.13	117.00	108.02
1	Q	418	PHE	N-CA-C	-5.11	105.40	110.97
1	M	437	VAL	CB-CA-C	5.10	118.35	110.50
1	Q	532	HIS	N-CA-C	5.10	116.94	108.02
1	K	394	LYS	CB-CA-C	5.09	118.96	111.73
2	N	38	VAL	N-CA-C	5.09	116.61	108.87
1	S	522	SER	N-CA-C	5.08	116.65	108.32
2	N	87	VAL	CB-CA-C	-5.05	103.97	110.84
1	M	404	THR	N-CA-C	-5.03	107.09	113.18
2	B	79	GLU	N-CA-C	5.02	118.17	111.75
1	Q	442	PHE	N-CA-C	5.02	116.44	110.97

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	P	30	ASP	Peptide

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	1860	0	1870	90	0
1	C	1865	0	1872	82	0
1	E	1865	0	1872	160	0
1	G	1860	0	1870	84	0
1	I	1860	0	1870	127	0
1	K	1860	0	1870	87	0
1	M	1851	0	1864	75	1
1	O	1860	0	1870	68	0
1	Q	1865	0	1872	110	0
1	S	1865	0	1872	83	1
1	U	1860	0	1870	89	0
1	W	1851	0	1864	90	0
2	B	639	0	629	35	0
2	D	639	0	629	43	0
2	F	639	0	629	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	630	0	623	19	0
2	J	639	0	629	36	0
2	L	630	0	623	21	0
2	N	639	0	629	31	0
2	P	639	0	629	24	0
2	R	639	0	629	34	0
2	T	639	0	629	30	0
2	V	639	0	629	52	0
2	X	639	0	629	48	0
All	All	29972	0	29972	1490	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (1490) 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:I:496:SER:HA	1:I:555:TYR:OH	1.45	1.16
1:U:550:MET:HE1	1:U:579:MET:HE3	1.23	1.10
1:Q:520:ARG:HH21	1:Q:524:LEU:HD21	1.12	1.09
1:E:420:MET:HB3	1:E:437:VAL:HG21	1.31	1.09
1:E:426:ARG:HH11	1:E:426:ARG:HG3	1.18	1.05
1:G:375:GLU:HA	1:G:378:ASN:HD22	1.24	1.03
2:F:63:ARG:HB3	2:F:70:ARG:HH21	1.22	1.01
2:V:77:PRO:HA	2:V:80:LEU:HD12	1.43	1.01
1:C:477:VAL:O	2:D:96:GLY:HA2	1.61	1.00
1:E:387:GLU:OE1	1:E:399:ARG:NH1	1.95	1.00
2:V:21:TYR:HB2	2:V:40:MET:HG3	1.43	0.99
1:S:420:MET:HB3	1:S:437:VAL:HG11	1.46	0.98
2:T:39:LYS:H	2:T:39:LYS:HD2	1.30	0.96
1:I:420:MET:HB3	1:I:437:VAL:HG21	1.48	0.95
1:E:550:MET:SD	1:E:579:MET:HE1	2.06	0.95
1:E:548:SER:HB3	2:F:97:GLY:C	1.91	0.95
1:M:438:PHE:HD2	1:M:471:VAL:HG22	1.32	0.95
1:E:426:ARG:HD2	1:E:427:ASN:N	1.82	0.94
1:K:417:ASN:OD1	1:K:440:THR:HG23	1.66	0.94
1:S:484:ILE:HG12	1:S:491:LEU:HD11	1.48	0.93
2:T:39:LYS:H	2:T:39:LYS:CD	1.80	0.93
1:Q:520:ARG:NH2	1:Q:524:LEU:HD21	1.84	0.93
1:Q:496:SER:HB3	1:Q:555:TYR:OH	1.69	0.92
1:K:463:LEU:HD22	1:K:469:ILE:HD11	1.52	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:417:ASN:HD21	1:S:440:THR:CG2	1.82	0.91
1:O:536:PRO:HA	1:O:541:GLN:HE21	1.31	0.91
2:T:63:ARG:NH2	2:T:93:GLU:HB2	1.85	0.91
1:E:391:SER:HB2	1:E:396:ARG:HD3	1.52	0.90
2:T:63:ARG:HH21	2:T:93:GLU:HB2	1.37	0.90
1:E:548:SER:HB3	2:F:97:GLY:O	1.72	0.89
1:E:554:LYS:HG3	1:E:572:MET:HE1	1.55	0.89
1:I:417:ASN:HD21	1:I:440:THR:HG22	1.35	0.88
1:C:399:ARG:O	1:C:403:GLN:HG2	1.74	0.88
2:F:39:LYS:H	2:F:39:LYS:HD2	1.38	0.88
1:I:498:GLY:H	1:I:541:GLN:NE2	1.72	0.88
1:G:419:TYR:OH	1:G:554:LYS:NZ	2.06	0.88
2:F:76:THR:HG22	2:F:79:GLU:H	1.38	0.88
1:Q:411:LEU:HD23	1:Q:411:LEU:H	1.36	0.88
1:C:404:THR:HG22	1:C:411:LEU:HA	1.54	0.88
1:G:375:GLU:HA	1:G:378:ASN:ND2	1.89	0.87
1:S:387:GLU:OE1	1:S:399:ARG:NH1	2.07	0.87
2:V:23:LYS:HZ1	2:V:35:HIS:HB3	1.39	0.87
1:I:498:GLY:H	1:I:541:GLN:HE22	1.21	0.87
1:I:544:ASN:HD21	1:I:547:ASP:HB2	1.38	0.86
1:W:414:GLU:OE2	2:X:70:ARG:NH2	2.07	0.86
1:A:466:GLN:O	1:A:486:LEU:HD12	1.75	0.86
1:S:417:ASN:ND2	1:S:440:THR:HG22	1.91	0.85
2:R:51:TYR:HD2	2:R:64:PHE:CE2	1.94	0.85
2:B:48:MET:HE3	2:B:64:PHE:HB2	1.59	0.84
1:E:535:LYS:HG3	1:E:538:GLU:HG3	1.59	0.84
1:I:498:GLY:N	1:I:541:GLN:HE22	1.76	0.84
1:G:420:MET:HB3	1:G:437:VAL:HG21	1.58	0.84
2:N:77:PRO:HA	2:N:82:MET:HG3	1.60	0.84
2:L:75:HIS:HB3	2:L:80:LEU:HD11	1.59	0.84
1:E:483:VAL:HG23	1:E:494:LEU:HD11	1.60	0.83
1:M:455:LYS:HG2	1:M:456:ARG:HG2	1.60	0.83
2:J:70:ARG:HH11	2:J:70:ARG:CG	1.92	0.83
1:E:423:LEU:HD21	1:E:557:ASP:HA	1.60	0.82
1:Q:487:ARG:NH2	1:Q:562:ASP:OD1	2.11	0.82
1:E:548:SER:HB3	2:F:97:GLY:OXT	1.79	0.82
1:M:440:THR:OG1	2:N:94:GLN:OE1	1.97	0.82
1:O:494:LEU:HG	1:O:534:MET:HG3	1.63	0.81
1:S:417:ASN:ND2	1:S:440:THR:CG2	2.41	0.81
1:U:394:LYS:H	1:U:394:LYS:HE2	1.44	0.81
2:R:51:TYR:HD2	2:R:64:PHE:HE2	1.26	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:572:MET:HA	1:Q:575:PHE:HB2	1.63	0.81
1:M:405:LEU:HD23	1:M:411:LEU:HD22	1.62	0.80
1:Q:401:ASP:HA	1:Q:412:ASN:HD21	1.46	0.80
1:E:483:VAL:HB	1:E:492:LYS:HG3	1.63	0.80
1:W:482:VAL:HG11	1:W:508:LEU:HD12	1.61	0.80
1:A:434:ALA:HB3	1:A:467:GLU:HG3	1.64	0.80
1:C:404:THR:HG21	1:C:412:ASN:H	1.45	0.80
2:N:57:VAL:HG12	2:N:58:PRO:HD2	1.64	0.80
1:E:423:LEU:CD2	1:E:557:ASP:HA	2.12	0.80
1:G:467:GLU:HB3	1:G:487:ARG:HD3	1.63	0.80
2:J:39:LYS:HG2	2:J:42:THR:OG1	1.82	0.80
1:M:394:LYS:HE2	1:M:394:LYS:H	1.47	0.80
1:U:550:MET:CE	1:U:579:MET:HE3	2.09	0.80
2:D:48:MET:HG2	2:D:64:PHE:CD2	2.17	0.79
1:K:505:CYS:HB3	1:K:531:HIS:HD2	1.46	0.79
2:X:63:ARG:NH2	2:X:93:GLU:HG3	1.96	0.79
2:P:45:LYS:HB3	2:P:73:ASP:HB3	1.65	0.79
1:C:404:THR:CG2	1:C:411:LEU:HA	2.12	0.79
1:E:548:SER:CB	2:F:97:GLY:O	2.30	0.79
1:I:496:SER:CA	1:I:555:TYR:OH	2.30	0.79
1:I:413:ASP:HB2	1:I:440:THR:HG21	1.63	0.79
2:B:76:THR:HG22	2:B:79:GLU:H	1.48	0.79
1:I:547:ASP:O	1:I:549:GLY:N	2.15	0.78
1:E:558:TYR:HE2	1:E:567:PHE:CD2	2.01	0.78
1:Q:510:GLN:NE2	1:Q:514:ASP:OD1	2.16	0.78
1:E:558:TYR:CE2	1:E:567:PHE:CD2	2.72	0.78
1:U:550:MET:HE1	1:U:579:MET:CE	2.11	0.78
2:F:75:HIS:HB3	2:F:80:LEU:HD11	1.66	0.77
1:I:394:LYS:HD2	1:I:394:LYS:N	1.97	0.77
1:M:582:GLU:HG2	1:M:588:LEU:HA	1.65	0.77
1:E:440:THR:OG1	2:F:94:GLN:OE1	2.02	0.77
2:R:64:PHE:HD1	2:R:64:PHE:H	1.27	0.77
2:R:85:GLU:OE1	2:R:85:GLU:HA	1.85	0.77
1:U:483:VAL:HG11	1:U:559:ILE:HG21	1.65	0.77
1:E:417:ASN:HD21	1:E:440:THR:HG23	1.50	0.77
1:G:503:ARG:O	1:G:507:ILE:HG12	1.84	0.77
1:U:399:ARG:O	1:U:403:GLN:HG2	1.84	0.77
1:W:503:ARG:O	1:W:507:ILE:HG12	1.85	0.76
2:F:63:ARG:HD2	2:F:70:ARG:HH22	1.50	0.76
1:I:548:SER:HB3	2:J:97:GLY:O	1.85	0.76
2:V:26:VAL:HG22	2:V:88:ILE:HD12	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:70:ARG:HH11	2:J:70:ARG:HG2	1.50	0.76
1:E:420:MET:CB	1:E:437:VAL:HG21	2.14	0.76
1:Q:520:ARG:HH21	1:Q:524:LEU:CD2	1.96	0.76
2:V:23:LYS:NZ	2:V:35:HIS:HB3	1.99	0.76
1:A:394:LYS:HD3	1:A:396:ARG:HH22	1.51	0.75
1:E:498:GLY:N	1:E:541:GLN:HE22	1.83	0.75
2:V:44:LEU:HD12	2:V:75:HIS:O	1.85	0.75
1:E:531:HIS:CG	1:E:531:HIS:O	2.38	0.75
1:O:469:ILE:HB	1:O:484:ILE:HB	1.66	0.75
1:K:543:LEU:HB2	1:K:569:GLN:HG2	1.68	0.75
2:B:77:PRO:HA	2:B:82:MET:HG3	1.67	0.75
1:A:513:GLN:CA	1:A:513:GLN:HE21	1.99	0.75
1:I:548:SER:CB	2:J:97:GLY:O	2.35	0.75
2:J:77:PRO:HA	2:J:82:MET:HG3	1.65	0.75
1:S:484:ILE:HG12	1:S:491:LEU:CD1	2.17	0.75
2:H:39:LYS:HG2	2:H:42:THR:HB	1.70	0.74
1:I:552:THR:HG22	1:I:553:CYS:N	2.02	0.74
1:E:426:ARG:HG3	1:E:426:ARG:NH1	1.95	0.74
1:A:508:LEU:O	1:A:511:TYR:HB3	1.87	0.74
1:S:380:LEU:HD22	1:S:406:LYS:HG3	1.69	0.74
1:I:417:ASN:ND2	1:I:440:THR:HG22	2.03	0.74
1:E:494:LEU:HD12	1:E:494:LEU:N	2.03	0.74
2:F:63:ARG:NH2	2:F:93:GLU:HB2	2.03	0.73
2:V:80:LEU:HD13	2:V:82:MET:HE3	1.70	0.73
1:A:426:ARG:NH2	1:A:557:ASP:OD1	2.19	0.73
1:E:471:VAL:HG12	1:E:473:ILE:HD12	1.71	0.73
2:T:39:LYS:HD2	2:T:39:LYS:N	2.03	0.73
1:C:474:HIS:HB2	1:C:479:TRP:CZ3	2.22	0.73
1:S:394:LYS:HA	1:S:396:ARG:NH2	2.04	0.73
1:U:449:GLY:O	1:U:453:ALA:HB2	1.88	0.73
1:C:394:LYS:HE2	1:C:394:LYS:H	1.53	0.73
2:R:64:PHE:CD1	2:R:64:PHE:N	2.54	0.73
2:P:31:SER:OG	2:P:32:SER:N	2.22	0.72
2:D:22:ILE:HG13	2:D:84:GLU:HA	1.70	0.72
2:R:51:TYR:CD2	2:R:64:PHE:HE2	2.06	0.72
2:X:20:GLU:C	2:X:21:TYR:HD1	1.98	0.72
2:F:76:THR:HG22	2:F:79:GLU:HB2	1.72	0.72
1:Q:438:PHE:HD2	1:Q:471:VAL:HG22	1.55	0.72
1:C:406:LYS:HB2	1:C:409:HIS:ND1	2.03	0.72
1:C:495:ASP:OD2	1:C:499:GLN:HB2	1.88	0.72
1:U:420:MET:HB3	1:U:437:VAL:HG21	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:401:ASP:O	1:C:404:THR:OG1	2.08	0.72
1:O:417:ASN:HD21	1:O:440:THR:HG22	1.54	0.72
2:X:20:GLU:O	2:X:21:TYR:HD1	1.71	0.72
1:Q:551:PHE:CE1	1:Q:572:MET:HE3	2.26	0.71
1:E:550:MET:SD	1:E:579:MET:CE	2.78	0.71
1:K:463:LEU:HD22	1:K:469:ILE:CD1	2.19	0.71
1:A:543:LEU:HD12	1:A:569:GLN:HG2	1.73	0.71
1:E:466:GLN:O	1:E:486:LEU:HD12	1.90	0.71
1:E:581:TRP:CZ3	1:E:589:LEU:HD21	2.25	0.71
1:G:375:GLU:CA	1:G:378:ASN:HD22	2.02	0.71
1:I:497:MET:O	1:I:497:MET:HG2	1.89	0.71
2:R:51:TYR:CD2	2:R:64:PHE:CE2	2.78	0.71
1:C:469:ILE:HB	1:C:484:ILE:HB	1.72	0.70
1:E:417:ASN:ND2	1:E:440:THR:HG23	2.05	0.70
2:F:76:THR:CG2	2:F:79:GLU:H	2.03	0.70
1:E:426:ARG:CZ	1:E:561:ARG:HD2	2.20	0.70
2:J:62:LEU:HD13	2:J:64:PHE:HE1	1.55	0.70
2:X:76:THR:HG23	2:X:79:GLU:H	1.56	0.70
1:U:387:GLU:OE1	1:U:399:ARG:NH1	2.15	0.70
1:E:399:ARG:O	1:E:403:GLN:HG3	1.91	0.70
1:Q:558:TYR:HD2	1:Q:565:ILE:HA	1.57	0.70
1:A:513:GLN:HE21	1:A:513:GLN:C	1.99	0.70
1:E:419:TYR:HD2	1:E:553:CYS:HG	1.38	0.70
1:C:420:MET:HB3	1:C:437:VAL:HG21	1.73	0.69
1:G:483:VAL:HG21	1:G:559:ILE:HG21	1.74	0.69
2:J:75:HIS:HB3	2:J:80:LEU:HD11	1.73	0.69
1:K:427:ASN:HA	1:K:432:TYR:HB2	1.73	0.69
1:Q:470:LEU:HD22	1:Q:481:LEU:HD21	1.75	0.69
1:E:544:ASN:ND2	1:E:547:ASP:OD2	2.22	0.69
1:O:493:TYR:O	1:O:534:MET:HG2	1.92	0.69
1:Q:411:LEU:HD21	1:Q:549:GLY:HA3	1.74	0.69
1:C:535:LYS:HB3	1:C:536:PRO:HD2	1.74	0.69
2:V:40:MET:O	2:V:41:THR:HG22	1.93	0.69
1:S:420:MET:HB3	1:S:437:VAL:CG1	2.22	0.69
1:K:513:GLN:HE22	1:K:524:LEU:H	1.39	0.69
2:N:63:ARG:NH2	2:N:93:GLU:HB2	2.08	0.69
1:E:459:LYS:HD3	1:E:459:LYS:C	2.18	0.68
2:F:31:SER:HB3	2:N:84:GLU:OE2	1.93	0.68
1:I:396:ARG:NH1	2:J:74:ASN:OD1	2.26	0.68
2:T:63:ARG:HH21	2:T:93:GLU:CB	2.04	0.68
1:W:399:ARG:O	1:W:403:GLN:HG2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:551:PHE:CD1	1:Q:572:MET:HE3	2.29	0.68
1:Q:445:LYS:HD2	2:R:29:GLN:NE2	2.09	0.68
2:P:76:THR:O	2:P:80:LEU:HD13	1.92	0.68
1:S:420:MET:HA	1:S:423:LEU:HD12	1.75	0.68
1:S:417:ASN:CG	1:S:440:THR:HG22	2.19	0.68
2:V:26:VAL:HG22	2:V:88:ILE:CD1	2.24	0.68
1:M:451:TYR:HE1	1:M:515:GLU:HG2	1.59	0.68
1:C:408:TYR:OH	1:W:432:TYR:O	2.11	0.67
2:D:53:GLN:C	2:D:55:GLN:H	2.03	0.67
1:I:542:GLN:NE2	1:I:548:SER:HB3	2.09	0.67
1:K:371:ASP:OD1	1:K:371:ASP:N	2.24	0.67
2:F:77:PRO:HA	2:F:82:MET:HG3	1.75	0.67
1:Q:417:ASN:HD21	1:Q:440:THR:H	1.42	0.67
2:H:39:LYS:CG	2:H:42:THR:HB	2.25	0.67
1:K:426:ARG:CZ	1:K:561:ARG:HD2	2.24	0.67
2:D:48:MET:HA	2:D:64:PHE:HE2	1.60	0.67
1:K:420:MET:HB3	1:K:437:VAL:HG21	1.75	0.67
2:R:25:LYS:HD2	2:R:33:GLU:OE2	1.95	0.67
1:S:417:ASN:HD21	1:S:440:THR:HG22	1.49	0.67
1:A:544:ASN:ND2	1:A:544:ASN:H	1.92	0.67
2:L:76:THR:HG22	2:L:79:GLU:H	1.60	0.67
1:E:438:PHE:HZ	1:E:463:LEU:HD11	1.60	0.66
1:I:567:PHE:CD1	1:I:567:PHE:C	2.73	0.66
1:E:578:LYS:O	1:E:582:GLU:HG3	1.95	0.66
2:F:42:THR:HG22	2:F:43:HIS:O	1.95	0.66
1:I:550:MET:O	1:I:554:LYS:HB2	1.95	0.66
1:C:486:LEU:HD23	1:C:529:TRP:HH2	1.61	0.66
1:G:515:GLU:OE2	1:G:519:LYS:HD2	1.95	0.66
1:E:486:LEU:O	1:E:489:LYS:HD2	1.95	0.66
1:K:436:HIS:NE2	1:K:461:VAL:HG11	2.10	0.66
1:U:404:THR:HB	1:U:411:LEU:HA	1.78	0.66
1:E:394:LYS:HA	1:E:396:ARG:HH21	1.60	0.66
1:M:376:ILE:HG12	1:M:580:VAL:HG22	1.77	0.66
1:M:411:LEU:HG	1:M:549:GLY:HA3	1.78	0.66
1:U:463:LEU:HB3	1:U:469:ILE:HD11	1.77	0.65
2:N:39:LYS:HG2	2:N:42:THR:OG1	1.96	0.65
2:F:63:ARG:HB3	2:F:70:ARG:NH2	2.03	0.65
1:S:393:PHE:CD2	1:S:421:ASN:HB3	2.32	0.65
1:E:426:ARG:HH11	1:E:426:ARG:CG	2.02	0.65
1:G:543:LEU:N	1:G:569:GLN:OE1	2.29	0.65
1:S:574:LEU:HD13	1:S:578:LYS:HE3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:451:TYR:OH	1:E:515:GLU:OE2	2.14	0.65
1:W:493:TYR:CE2	1:W:495:ASP:HB2	2.32	0.65
1:E:481:LEU:HB2	1:E:552:THR:HG23	1.79	0.65
2:P:77:PRO:HA	2:P:82:MET:HG3	1.78	0.65
1:Q:484:ILE:HG21	1:Q:512:LEU:HD11	1.79	0.65
1:A:394:LYS:HA	1:A:396:ARG:NH2	2.13	0.64
2:T:39:LYS:CD	2:T:39:LYS:N	2.58	0.64
1:I:547:ASP:C	1:I:549:GLY:H	2.05	0.64
1:W:501:GLY:HA2	1:W:504:ILE:HD12	1.80	0.64
1:U:436:HIS:HB2	1:U:466:GLN:HG3	1.79	0.64
1:W:442:PHE:HA	1:W:457:TRP:CZ3	2.32	0.64
1:A:408:TYR:CD1	1:U:434:ALA:HB2	2.33	0.64
1:I:437:VAL:HG23	1:I:470:LEU:HB2	1.79	0.64
1:M:419:TYR:CD2	1:M:553:CYS:HB3	2.32	0.64
1:U:481:LEU:HB2	1:U:552:THR:HG23	1.79	0.64
1:E:471:VAL:HG12	1:E:473:ILE:CD1	2.27	0.64
1:O:394:LYS:HE2	1:O:394:LYS:H	1.61	0.64
2:D:39:LYS:HD3	2:D:39:LYS:H	1.61	0.64
1:G:393:PHE:CD2	1:G:421:ASN:HB2	2.33	0.64
1:I:404:THR:HB	1:I:411:LEU:HA	1.78	0.64
1:K:568:THR:N	1:K:571:GLN:OE1	2.26	0.64
2:F:30:ASP:OD1	2:F:30:ASP:C	2.40	0.64
2:P:80:LEU:HD22	2:P:82:MET:HE2	1.79	0.64
1:Q:475:ARG:NH1	1:Q:476:LYS:HG3	2.12	0.64
2:D:77:PRO:HA	2:D:82:MET:HG3	1.80	0.63
2:V:33:GLU:O	2:V:34:ILE:HG13	1.98	0.63
1:S:440:THR:OG1	2:T:94:GLN:OE1	2.16	0.63
1:E:391:SER:CB	1:E:396:ARG:HD3	2.28	0.63
1:E:426:ARG:HD2	1:E:426:ARG:C	2.23	0.63
2:F:63:ARG:HD2	2:F:70:ARG:NH2	2.13	0.63
2:V:22:ILE:HD12	2:V:84:GLU:HB2	1.79	0.63
1:Q:543:LEU:HD12	1:Q:569:GLN:HG2	1.81	0.63
1:C:406:LYS:O	1:C:409:HIS:HB2	1.98	0.63
1:I:417:ASN:HD21	1:I:440:THR:CG2	2.09	0.63
1:K:405:LEU:O	1:K:576:ARG:HD3	1.98	0.63
1:W:482:VAL:HG11	1:W:508:LEU:CD1	2.29	0.63
1:W:535:LYS:O	1:W:537:HIS:N	2.32	0.63
1:A:484:ILE:HG12	1:A:491:LEU:CD1	2.29	0.63
1:E:419:TYR:HD2	1:E:553:CYS:SG	2.21	0.63
1:G:371:ASP:N	1:G:371:ASP:OD1	2.32	0.63
1:Q:438:PHE:CD2	1:Q:471:VAL:HG22	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:506:GLU:HA	1:E:509:LEU:HB3	1.81	0.62
1:U:441:PHE:CZ	2:V:63:ARG:HG3	2.34	0.62
1:A:513:GLN:HG2	1:A:526:LEU:HD21	1.80	0.62
2:B:76:THR:CG2	2:B:79:GLU:H	2.12	0.62
1:I:435:LEU:HD21	1:I:470:LEU:HD12	1.80	0.62
1:W:463:LEU:HD22	1:W:469:ILE:HD12	1.81	0.62
1:W:508:LEU:O	1:W:511:TYR:HB3	1.99	0.62
1:K:578:LYS:HG2	1:K:589:LEU:HD12	1.80	0.62
1:O:504:ILE:HG22	1:O:508:LEU:HD12	1.82	0.62
2:P:45:LYS:HE3	2:P:46:LYS:HG2	1.82	0.62
1:S:581:TRP:CE2	1:S:585:HIS:CD2	2.87	0.62
1:U:463:LEU:HD22	1:U:469:ILE:HD13	1.81	0.62
1:A:406:LYS:O	1:A:576:ARG:NH1	2.32	0.62
1:O:399:ARG:HA	1:O:402:ILE:HG22	1.81	0.62
1:A:581:TRP:CZ3	1:A:589:LEU:HD21	2.34	0.62
1:W:475:ARG:O	1:W:476:LYS:C	2.43	0.62
1:C:474:HIS:HB2	1:C:479:TRP:HZ3	1.63	0.61
1:I:497:MET:HE3	1:I:542:GLN:OE1	2.00	0.61
1:I:513:GLN:HA	1:I:524:LEU:HD22	1.82	0.61
2:L:39:LYS:HG2	2:L:42:THR:OG1	2.00	0.61
1:Q:548:SER:OG	2:R:97:GLY:C	2.44	0.61
2:R:48:MET:HE3	2:R:64:PHE:CD1	2.35	0.61
1:U:435:LEU:HD22	1:U:560:SER:HB2	1.82	0.61
1:C:475:ARG:HE	1:C:475:ARG:HA	1.65	0.61
1:A:581:TRP:CE2	1:A:585:HIS:CD2	2.88	0.61
1:K:505:CYS:HB3	1:K:531:HIS:CD2	2.31	0.61
1:E:554:LYS:CG	1:E:572:MET:HE1	2.29	0.61
1:E:567:PHE:C	1:E:567:PHE:CD1	2.79	0.61
1:E:569:GLN:O	1:E:572:MET:HB2	2.00	0.61
1:K:551:PHE:CD1	1:K:572:MET:HE3	2.35	0.61
2:P:52:CYS:SG	2:P:62:LEU:HD11	2.39	0.61
1:Q:491:LEU:CD2	1:Q:505:CYS:O	2.48	0.61
2:N:40:MET:HE1	2:N:82:MET:O	1.99	0.61
1:O:444:PRO:O	1:O:448:SER:HB3	2.01	0.61
1:Q:471:VAL:HG12	1:Q:472:PRO:O	2.01	0.61
1:E:407:ASN:O	1:E:408:TYR:HB2	2.00	0.61
1:W:426:ARG:O	1:W:430:GLN:HG2	2.00	0.61
1:C:412:ASN:HA	2:D:94:GLN:O	2.01	0.61
1:E:475:ARG:HD3	1:E:476:LYS:H	1.66	0.61
2:L:58:PRO:O	2:L:61:SER:HB3	2.00	0.61
2:D:44:LEU:O	2:D:48:MET:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:582:GLU:HA	1:Q:587:GLN:O	2.01	0.61
1:S:404:THR:HB	1:S:411:LEU:HA	1.83	0.61
1:W:473:ILE:HB	1:W:480:SER:O	2.01	0.60
1:W:422:LEU:O	1:W:423:LEU:C	2.44	0.60
1:G:564:PRO:O	1:G:566:THR:HG23	2.01	0.60
1:I:469:ILE:HB	1:I:484:ILE:HB	1.82	0.60
1:Q:542:GLN:OE1	1:Q:548:SER:HB3	2.02	0.60
2:B:51:TYR:O	2:B:55:GLN:HG2	2.02	0.60
1:I:369:THR:HG22	1:I:371:ASP:H	1.67	0.60
1:S:432:TYR:HB3	1:S:433:PRO:HD2	1.83	0.60
1:E:420:MET:HA	1:E:423:LEU:HD12	1.84	0.60
1:A:443:TYR:OH	1:A:504:ILE:HA	2.01	0.60
1:Q:411:LEU:H	1:Q:411:LEU:CD2	2.13	0.60
1:W:471:VAL:HG21	1:W:508:LEU:HD13	1.83	0.60
1:S:399:ARG:O	1:S:403:GLN:HG2	2.00	0.60
1:S:438:PHE:HD2	1:S:471:VAL:HG22	1.66	0.60
1:M:432:TYR:HB3	1:M:433:PRO:CD	2.31	0.60
1:Q:558:TYR:CD2	1:Q:565:ILE:HA	2.35	0.60
1:C:371:ASP:O	1:C:375:GLU:HB2	2.02	0.60
1:O:491:LEU:O	1:O:492:LYS:HG3	2.01	0.60
2:R:27:ILE:HG22	2:R:33:GLU:HB2	1.84	0.60
1:K:417:ASN:CG	1:K:440:THR:HG23	2.26	0.59
1:M:438:PHE:CD2	1:M:471:VAL:HG22	2.24	0.59
1:S:380:LEU:HD22	1:S:406:LYS:CG	2.30	0.59
1:E:554:LYS:HE3	1:E:575:PHE:CD1	2.36	0.59
1:W:394:LYS:HA	1:W:396:ARG:NH2	2.17	0.59
1:E:548:SER:OG	2:F:97:GLY:O	2.18	0.59
2:N:20:GLU:C	2:N:21:TYR:CD1	2.80	0.59
1:O:441:PHE:HZ	2:P:63:ARG:HG3	1.68	0.59
1:U:478:HIS:CE1	1:U:497:MET:HE2	2.37	0.59
1:I:456:ARG:O	1:I:459:LYS:HB2	2.02	0.59
2:V:66:TRP:CE2	2:V:67:GLU:HG3	2.37	0.59
2:P:40:MET:O	2:P:77:PRO:HD2	2.03	0.59
1:C:405:LEU:HD13	1:C:580:VAL:HG12	1.84	0.59
1:E:483:VAL:CG2	1:E:494:LEU:HD11	2.33	0.59
2:H:45:LYS:HB2	2:H:73:ASP:HB3	1.83	0.59
1:I:544:ASN:HD21	1:I:547:ASP:CB	2.15	0.59
1:M:399:ARG:O	1:M:403:GLN:HG3	2.03	0.59
1:O:496:SER:O	1:O:542:GLN:HB3	2.02	0.59
2:R:40:MET:HE1	2:R:82:MET:O	2.02	0.59
2:R:44:LEU:HG	2:R:77:PRO:HD3	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:410:TRP:HZ3	1:C:477:VAL:HB	1.67	0.59
1:K:398:THR:O	1:K:401:ASP:N	2.36	0.59
2:L:77:PRO:HA	2:L:82:MET:HG3	1.85	0.58
1:M:387:GLU:OE1	1:M:399:ARG:NH1	2.35	0.58
1:A:426:ARG:CZ	1:A:561:ARG:HD2	2.33	0.58
1:I:443:TYR:CE2	1:I:504:ILE:HG23	2.38	0.58
1:K:368:LEU:HD22	1:K:372:MET:HE2	1.84	0.58
1:K:379:ALA:HB2	1:K:584:LEU:HD11	1.85	0.58
1:M:539:ILE:HD12	1:M:555:TYR:CZ	2.37	0.58
1:S:524:LEU:HD12	1:S:529:TRP:HE1	1.68	0.58
1:U:486:LEU:HD23	1:U:529:TRP:HH2	1.67	0.58
2:V:24:LEU:HD13	2:V:88:ILE:HD11	1.84	0.58
2:D:44:LEU:HD11	2:D:82:MET:HE3	1.86	0.58
1:E:436:HIS:HE1	1:E:438:PHE:CE1	2.21	0.58
1:M:531:HIS:ND1	1:M:531:HIS:C	2.61	0.58
2:N:28:GLY:H	2:N:31:SER:HB3	1.67	0.58
1:U:574:LEU:HD22	1:U:578:LYS:HG3	1.85	0.58
2:V:26:VAL:HG13	2:V:88:ILE:HB	1.85	0.58
2:X:21:TYR:HB2	2:X:40:MET:HB2	1.83	0.58
1:C:426:ARG:C	1:C:426:ARG:HD2	2.29	0.58
2:F:30:ASP:O	2:F:32:SER:N	2.36	0.58
2:H:48:MET:SD	2:H:64:PHE:CD1	2.96	0.58
1:M:426:ARG:NH1	1:M:561:ARG:HD3	2.18	0.58
1:Q:466:GLN:O	1:Q:486:LEU:HD12	2.03	0.58
1:U:445:LYS:HD3	2:V:91:TYR:OH	2.03	0.58
2:N:80:LEU:HD13	2:N:82:MET:HE3	1.85	0.58
2:P:84:GLU:HG3	2:P:85:GLU:HG2	1.86	0.58
1:A:492:LYS:HD3	1:A:534:MET:HE2	1.84	0.58
1:E:495:ASP:OD1	1:E:497:MET:N	2.33	0.58
2:R:65:LEU:HD23	2:R:68:GLY:O	2.04	0.58
1:S:484:ILE:CG1	1:S:491:LEU:HD11	2.27	0.58
1:W:385:GLN:O	1:W:398:THR:OG1	2.21	0.58
1:C:413:ASP:OD2	2:D:63:ARG:NH2	2.29	0.58
2:X:52:CYS:SG	2:X:62:LEU:HD12	2.44	0.58
1:A:398:THR:O	1:A:401:ASP:HB2	2.03	0.58
1:K:394:LYS:NZ	1:K:396:ARG:HH22	2.01	0.58
2:P:51:TYR:O	2:P:55:GLN:HG2	2.01	0.58
2:R:66:TRP:CZ3	2:R:80:LEU:O	2.57	0.58
1:W:426:ARG:HG3	1:W:588:LEU:HD12	1.86	0.58
1:W:443:TYR:O	1:W:446:LEU:HB3	2.04	0.58
1:S:517:LYS:HD2	1:S:523:ASP:OD1	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:393:PHE:HZ	1:C:422:LEU:HD23	1.69	0.58
1:I:475:ARG:HE	1:I:475:ARG:HA	1.68	0.58
1:I:497:MET:HB3	1:I:542:GLN:OE1	2.03	0.58
1:K:420:MET:HB3	1:K:437:VAL:CG2	2.34	0.58
1:O:370:GLU:O	1:O:374:LYS:HB2	2.03	0.58
1:Q:473:ILE:N	1:Q:480:SER:O	2.37	0.58
1:K:478:HIS:NE2	1:K:495:ASP:OD1	2.37	0.57
1:O:478:HIS:HE2	1:O:495:ASP:CG	2.11	0.57
1:S:517:LYS:HA	1:S:522:SER:H	1.69	0.57
1:U:376:ILE:HG12	1:U:580:VAL:HG22	1.86	0.57
2:V:22:ILE:O	2:V:38:VAL:HG22	2.04	0.57
1:E:391:SER:HB2	1:E:396:ARG:CD	2.32	0.57
1:E:483:VAL:HG23	1:E:494:LEU:CD1	2.33	0.57
2:F:39:LYS:H	2:F:39:LYS:CD	2.12	0.57
1:S:369:THR:HG22	1:S:371:ASP:H	1.69	0.57
1:A:467:GLU:HB3	1:A:487:ARG:HD3	1.87	0.57
1:C:416:ILE:O	1:C:417:ASN:C	2.46	0.57
1:I:451:TYR:CD2	1:I:514:ASP:HB2	2.39	0.57
1:M:524:LEU:HD11	1:M:529:TRP:HE1	1.69	0.57
1:S:393:PHE:CD2	1:S:421:ASN:CB	2.87	0.57
1:S:411:LEU:HD13	1:S:415:VAL:HG11	1.86	0.57
1:U:443:TYR:CE1	1:U:504:ILE:HG23	2.40	0.57
1:I:579:MET:O	1:I:582:GLU:N	2.37	0.57
1:Q:476:LYS:NZ	1:Q:476:LYS:HB3	2.19	0.57
1:C:510:GLN:O	1:C:511:TYR:C	2.48	0.57
1:U:426:ARG:HB2	1:U:588:LEU:HD12	1.86	0.57
2:X:76:THR:O	2:X:80:LEU:HD12	2.03	0.57
2:B:48:MET:HE3	2:B:64:PHE:CB	2.32	0.57
1:E:473:ILE:N	1:E:480:SER:O	2.25	0.57
1:C:398:THR:HG23	1:C:401:ASP:OD2	2.05	0.57
1:A:381:GLY:O	1:A:382:HIS:HB2	2.05	0.57
1:A:513:GLN:CA	1:A:513:GLN:NE2	2.68	0.57
2:V:38:VAL:HG12	2:V:47:LEU:HD11	1.87	0.57
1:W:425:GLU:O	1:W:426:ARG:C	2.47	0.57
1:E:567:PHE:C	1:E:567:PHE:HD1	2.13	0.57
1:G:495:ASP:OD2	1:G:499:GLN:HB2	2.04	0.57
1:O:399:ARG:O	1:O:403:GLN:HG3	2.05	0.57
1:W:517:LYS:HD3	1:W:523:ASP:OD1	2.05	0.57
1:E:432:TYR:HB3	1:E:433:PRO:HD2	1.87	0.56
2:N:43:HIS:HA	2:N:75:HIS:O	2.05	0.56
1:O:494:LEU:HG	1:O:534:MET:CG	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:441:PHE:CZ	2:X:63:ARG:HG3	2.40	0.56
1:A:420:MET:HB3	1:A:437:VAL:HG21	1.87	0.56
1:C:483:VAL:HG21	1:C:559:ILE:HG21	1.87	0.56
1:G:483:VAL:CG2	1:G:559:ILE:HG21	2.35	0.56
1:A:544:ASN:ND2	1:A:544:ASN:N	2.51	0.56
1:C:501:GLY:O	1:C:502:HIS:C	2.49	0.56
1:E:394:LYS:HA	1:E:396:ARG:NH2	2.21	0.56
1:E:551:PHE:O	1:E:552:THR:C	2.47	0.56
1:E:551:PHE:O	1:E:554:LYS:N	2.37	0.56
2:F:43:HIS:HB3	2:F:73:ASP:O	2.05	0.56
1:G:425:GLU:O	1:G:429:LYS:HG3	2.05	0.56
2:J:76:THR:HG22	2:J:79:GLU:H	1.70	0.56
1:M:394:LYS:HE2	1:M:394:LYS:N	2.18	0.56
1:M:417:ASN:OD1	1:M:440:THR:HG22	2.05	0.56
1:S:495:ASP:OD1	1:S:497:MET:N	2.38	0.56
1:G:385:GLN:HA	1:G:385:GLN:OE1	2.05	0.56
1:K:404:THR:HB	1:K:411:LEU:HA	1.86	0.56
2:R:39:LYS:HG2	2:R:42:THR:OG1	2.04	0.56
1:C:398:THR:O	1:C:401:ASP:HB2	2.05	0.56
1:O:484:ILE:HG21	1:O:512:LEU:HD11	1.87	0.56
1:M:441:PHE:O	1:M:444:PRO:HG2	2.06	0.56
2:P:66:TRP:CZ3	2:P:80:LEU:HB3	2.41	0.56
1:Q:475:ARG:HH12	1:Q:476:LYS:HG3	1.70	0.56
2:D:43:HIS:C	2:D:45:LYS:H	2.14	0.56
2:H:44:LEU:HD12	2:H:71:ILE:HG21	1.87	0.56
1:U:442:PHE:HA	1:U:457:TRP:CZ3	2.41	0.56
2:B:30:ASP:N	2:B:30:ASP:OD1	2.39	0.56
1:Q:403:GLN:O	1:Q:406:LYS:HG3	2.06	0.56
1:G:370:GLU:HA	1:G:373:GLU:HB2	1.88	0.56
2:H:44:LEU:HD22	2:H:47:LEU:HD12	1.87	0.56
2:J:70:ARG:HG2	2:J:70:ARG:NH1	2.17	0.56
1:Q:508:LEU:O	1:Q:511:TYR:HB3	2.06	0.56
2:X:45:LYS:HB2	2:X:73:ASP:HB3	1.87	0.56
1:A:426:ARG:NH1	1:A:561:ARG:HD2	2.21	0.55
1:I:394:LYS:HD2	1:I:394:LYS:H	1.71	0.55
1:S:417:ASN:HD21	1:S:440:THR:HG23	1.68	0.55
1:U:483:VAL:HG11	1:U:559:ILE:CG2	2.36	0.55
1:A:544:ASN:N	1:A:544:ASN:HD22	2.04	0.55
1:E:423:LEU:O	1:E:424:VAL:C	2.48	0.55
2:T:66:TRP:CZ3	2:T:80:LEU:HB3	2.41	0.55
1:U:407:ASN:O	1:U:408:TYR:HB2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:60:ASN:OD1	2:B:60:ASN:N	2.38	0.55
2:F:21:TYR:HB3	2:F:40:MET:HE2	1.89	0.55
1:K:394:LYS:HZ3	1:K:396:ARG:HH22	1.54	0.55
1:K:572:MET:HB2	1:K:573:PRO:HD3	1.89	0.55
1:U:463:LEU:HD22	1:U:469:ILE:CD1	2.35	0.55
2:J:63:ARG:NH2	2:J:93:GLU:HB2	2.22	0.55
2:P:76:THR:HG23	2:P:79:GLU:H	1.71	0.55
1:U:413:ASP:HB3	2:V:94:GLN:HG3	1.87	0.55
1:W:434:ALA:H	1:W:467:GLU:HG3	1.72	0.55
1:U:426:ARG:CZ	1:U:561:ARG:HD2	2.36	0.55
2:X:34:ILE:HD12	2:X:51:TYR:CE1	2.42	0.55
1:E:517:LYS:O	1:E:521:ASN:HA	2.07	0.55
2:F:70:ARG:HG3	2:F:71:ILE:N	2.22	0.55
2:P:63:ARG:HH21	2:P:93:GLU:HB2	1.72	0.55
1:Q:505:CYS:HB2	1:Q:506:GLU:HG3	1.87	0.55
1:Q:563:LYS:HG2	1:Q:564:PRO:HD2	1.89	0.55
1:O:404:THR:HB	1:O:411:LEU:HA	1.88	0.55
1:O:424:VAL:HG13	1:O:435:LEU:HB3	1.89	0.55
1:O:432:TYR:CZ	1:O:561:ARG:HG2	2.41	0.55
1:S:461:VAL:HG22	1:S:462:ASN:N	2.22	0.55
2:V:39:LYS:HG3	2:V:42:THR:CB	2.37	0.55
1:W:414:GLU:CD	2:X:70:ARG:HH22	2.13	0.55
1:W:457:TRP:HA	2:X:67:GLU:O	2.07	0.55
2:X:39:LYS:H	2:X:39:LYS:HD3	1.71	0.55
1:G:420:MET:O	1:G:424:VAL:HG23	2.06	0.55
1:I:548:SER:OG	2:J:97:GLY:C	2.50	0.55
1:K:505:CYS:CB	1:K:531:HIS:HD2	2.19	0.55
1:Q:401:ASP:HA	1:Q:412:ASN:ND2	2.19	0.55
1:W:419:TYR:O	1:W:420:MET:C	2.50	0.55
2:F:63:ARG:CB	2:F:70:ARG:HH21	2.09	0.55
1:I:494:LEU:HD23	1:I:539:ILE:HG21	1.88	0.55
1:W:504:ILE:O	1:W:507:ILE:HB	2.06	0.55
2:F:28:GLY:O	2:F:31:SER:HB2	2.07	0.55
1:K:391:SER:O	1:K:392:ALA:HB2	2.07	0.55
1:A:405:LEU:C	1:A:576:ARG:HH11	2.16	0.54
1:G:476:LYS:C	1:G:477:VAL:HG23	2.32	0.54
1:K:482:VAL:HG23	1:K:493:TYR:HD1	1.71	0.54
1:W:580:VAL:O	1:W:584:LEU:HG	2.07	0.54
1:C:568:THR:O	1:C:569:GLN:C	2.48	0.54
2:L:47:LEU:C	2:L:47:LEU:HD23	2.32	0.54
1:Q:540:PRO:O	1:Q:551:PHE:HE2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:48:MET:HE1	2:V:71:ILE:O	2.08	0.54
1:W:511:TYR:CZ	1:W:515:GLU:HG2	2.42	0.54
2:X:80:LEU:HD12	2:X:80:LEU:H	1.72	0.54
1:G:568:THR:N	1:G:571:GLN:OE1	2.22	0.54
1:E:458:THR:O	1:E:458:THR:OG1	2.25	0.54
1:E:495:ASP:OD1	1:E:495:ASP:C	2.50	0.54
2:F:51:TYR:O	2:F:55:GLN:HG2	2.07	0.54
1:I:435:LEU:HD12	1:I:468:ILE:HB	1.90	0.54
1:M:576:ARG:O	1:M:579:MET:N	2.41	0.54
1:O:541:GLN:HA	1:O:541:GLN:OE1	2.08	0.54
1:S:442:PHE:CD1	1:S:442:PHE:C	2.86	0.54
1:A:426:ARG:HG3	1:A:588:LEU:HD12	1.89	0.54
1:G:451:TYR:OH	1:G:515:GLU:HA	2.08	0.54
1:I:402:ILE:O	1:I:403:GLN:C	2.49	0.54
1:K:410:TRP:HB3	2:L:96:GLY:O	2.07	0.54
2:P:39:LYS:HG2	2:P:42:THR:OG1	2.07	0.54
2:V:39:LYS:HG3	2:V:42:THR:HG21	1.89	0.54
2:X:31:SER:HB2	2:X:51:TYR:OH	2.07	0.54
1:A:435:LEU:HD12	1:A:468:ILE:HB	1.89	0.54
1:E:423:LEU:HD21	1:E:557:ASP:CA	2.34	0.54
1:E:550:MET:SD	1:E:576:ARG:HG2	2.48	0.54
1:O:402:ILE:HG12	1:O:402:ILE:O	2.07	0.54
1:U:484:ILE:HG12	1:U:491:LEU:HD23	1.90	0.54
1:E:495:ASP:OD1	1:E:498:GLY:N	2.41	0.54
1:G:375:GLU:CA	1:G:378:ASN:ND2	2.67	0.54
1:I:461:VAL:HG22	1:I:462:ASN:H	1.73	0.54
1:I:576:ARG:O	1:I:577:LYS:C	2.51	0.54
1:W:393:PHE:HZ	1:W:422:LEU:HD23	1.73	0.54
1:W:515:GLU:HA	1:W:515:GLU:OE1	2.07	0.54
2:X:26:VAL:HG13	2:X:88:ILE:HB	1.90	0.54
2:F:76:THR:O	2:F:80:LEU:HD12	2.08	0.54
2:F:80:LEU:HD13	2:F:82:MET:HE2	1.89	0.54
1:Q:470:LEU:HB3	1:Q:481:LEU:HD11	1.89	0.54
1:W:413:ASP:HB3	2:X:94:GLN:HB2	1.90	0.54
1:Q:497:MET:HE3	1:Q:545:GLY:HA2	1.89	0.54
1:M:558:TYR:HD2	1:M:565:ILE:HA	1.74	0.53
1:Q:374:LYS:HD3	1:Q:377:SER:HB2	1.89	0.53
1:Q:471:VAL:O	1:Q:482:VAL:N	2.38	0.53
1:Q:577:LYS:O	1:Q:580:VAL:HG13	2.08	0.53
1:A:420:MET:HB3	1:A:437:VAL:CG2	2.38	0.53
1:A:469:ILE:HB	1:A:484:ILE:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:414:GLU:OE1	1:E:414:GLU:HA	2.07	0.53
1:E:499:GLN:OE1	1:E:499:GLN:HA	2.08	0.53
2:J:20:GLU:O	2:J:21:TYR:CD1	2.61	0.53
1:M:462:ASN:HB3	1:M:465:GLU:CG	2.37	0.53
1:W:581:TRP:CE2	1:W:585:HIS:CD2	2.96	0.53
1:Q:581:TRP:C	1:Q:583:ILE:H	2.16	0.53
2:X:48:MET:HG2	2:X:64:PHE:CD2	2.43	0.53
1:G:387:GLU:OE1	1:G:399:ARG:NH1	2.42	0.53
1:W:474:HIS:HB2	1:W:479:TRP:CZ3	2.44	0.53
1:G:408:TYR:OH	1:K:432:TYR:O	2.22	0.53
2:N:76:THR:O	2:N:80:LEU:HD12	2.08	0.53
2:T:89:GLU:HB2	2:T:91:TYR:HE1	1.74	0.53
1:W:551:PHE:CD1	1:W:572:MET:HE3	2.44	0.53
1:M:474:HIS:CE1	2:N:94:GLN:HB3	2.44	0.53
2:X:64:PHE:CD1	2:X:64:PHE:N	2.77	0.53
1:C:454:VAL:O	1:C:455:LYS:C	2.51	0.53
2:D:22:ILE:HG12	2:D:23:LYS:N	2.23	0.53
1:I:572:MET:O	1:I:573:PRO:C	2.52	0.53
2:J:63:ARG:N	2:J:63:ARG:CD	2.71	0.53
2:L:40:MET:O	2:L:76:THR:HG23	2.09	0.53
1:Q:468:ILE:HD13	1:Q:559:ILE:O	2.09	0.53
1:Q:537:HIS:C	1:Q:537:HIS:CD2	2.87	0.53
1:S:577:LYS:O	1:S:580:VAL:HG13	2.09	0.53
1:C:484:ILE:HG13	1:C:491:LEU:CD1	2.38	0.53
1:K:462:ASN:OD1	1:K:462:ASN:C	2.52	0.52
1:Q:419:TYR:CD2	1:Q:553:CYS:HB3	2.43	0.52
1:E:469:ILE:HB	1:E:484:ILE:HB	1.91	0.52
1:O:417:ASN:ND2	1:O:440:THR:HG22	2.23	0.52
1:U:470:LEU:HD13	1:U:556:ALA:HB1	1.91	0.52
1:G:500:LYS:HB3	1:G:502:HIS:CD2	2.44	0.52
2:L:40:MET:O	2:L:77:PRO:HD2	2.10	0.52
1:A:410:TRP:HB3	2:B:96:GLY:O	2.10	0.52
1:E:427:ASN:HA	1:E:432:TYR:HB2	1.91	0.52
1:M:416:ILE:HD12	1:M:479:TRP:CE2	2.44	0.52
1:O:417:ASN:HD21	1:O:440:THR:CG2	2.23	0.52
2:V:77:PRO:HA	2:V:80:LEU:CD1	2.30	0.52
1:C:420:MET:HB3	1:C:437:VAL:CG2	2.40	0.52
1:I:446:LEU:C	1:I:446:LEU:HD12	2.35	0.52
1:M:496:SER:HB2	1:M:542:GLN:HB3	1.92	0.52
1:O:380:LEU:HD13	1:O:406:LYS:HG2	1.92	0.52
1:Q:468:ILE:HD12	1:Q:560:SER:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:62:LEU:HD22	2:T:90:VAL:HG13	1.92	0.52
2:V:38:VAL:CG1	2:V:47:LEU:HD11	2.39	0.52
1:A:513:GLN:HE21	1:A:513:GLN:HA	1.75	0.52
1:E:520:ARG:C	1:E:522:SER:H	2.17	0.52
1:Q:481:LEU:HG	1:Q:482:VAL:N	2.24	0.52
2:X:20:GLU:C	2:X:21:TYR:CD1	2.83	0.52
2:B:76:THR:HG22	2:B:79:GLU:HB2	1.91	0.52
2:B:84:GLU:HG3	2:B:85:GLU:HG2	1.91	0.52
1:E:485:ASP:HB3	1:E:488:LYS:HB2	1.92	0.52
1:G:525:ASN:C	1:G:527:LEU:H	2.17	0.52
1:O:441:PHE:CZ	2:P:63:ARG:HG3	2.44	0.52
2:V:76:THR:HG23	2:V:79:GLU:CB	2.40	0.52
2:X:66:TRP:C	2:X:68:GLY:N	2.68	0.52
1:U:493:TYR:O	1:U:534:MET:HB2	2.09	0.52
2:D:48:MET:HE3	2:D:64:PHE:CG	2.45	0.52
1:E:572:MET:O	1:E:573:PRO:C	2.52	0.52
2:D:48:MET:HG2	2:D:64:PHE:HD2	1.70	0.51
1:E:547:ASP:HB3	1:E:550:MET:HB2	1.91	0.51
1:E:417:ASN:CG	1:E:440:THR:HG23	2.34	0.51
1:I:462:ASN:HB3	1:I:465:GLU:CG	2.41	0.51
1:K:403:GLN:C	1:K:405:LEU:N	2.68	0.51
2:T:23:LYS:HA	2:T:36:PHE:O	2.10	0.51
1:W:369:THR:HG22	1:W:372:MET:H	1.74	0.51
1:A:544:ASN:HD21	1:A:569:GLN:CD	2.18	0.51
2:B:26:VAL:HG22	2:B:88:ILE:HB	1.92	0.51
1:E:438:PHE:HD2	1:E:471:VAL:HG22	1.76	0.51
1:G:581:TRP:CE2	1:G:585:HIS:CD2	2.98	0.51
1:Q:437:VAL:O	1:Q:437:VAL:CG1	2.59	0.51
1:S:551:PHE:O	1:S:555:TYR:CG	2.62	0.51
1:W:392:ALA:C	1:W:394:LYS:N	2.66	0.51
1:A:412:ASN:HA	2:B:94:GLN:O	2.10	0.51
1:C:474:HIS:CD2	2:D:94:GLN:HB3	2.46	0.51
1:E:572:MET:O	1:E:575:PHE:HB2	2.11	0.51
1:G:399:ARG:O	1:G:403:GLN:HG2	2.10	0.51
1:G:426:ARG:O	1:G:427:ASN:C	2.52	0.51
1:O:420:MET:HA	1:O:423:LEU:HD12	1.93	0.51
1:Q:437:VAL:O	1:Q:437:VAL:HG12	2.09	0.51
2:X:65:LEU:HD12	2:X:70:ARG:HA	1.92	0.51
1:E:486:LEU:O	1:E:489:LYS:CD	2.58	0.51
1:W:493:TYR:HE2	1:W:495:ASP:HB2	1.75	0.51
1:A:493:TYR:CD2	1:A:501:GLY:HA3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:548:SER:OG	2:J:97:GLY:O	2.28	0.51
2:N:48:MET:HE3	2:N:64:PHE:HB2	1.92	0.51
1:S:410:TRP:CD1	1:S:546:SER:HB3	2.46	0.51
2:V:30:ASP:HB2	2:V:92:GLN:HG3	1.92	0.51
1:G:547:ASP:OD1	1:G:576:ARG:NH2	2.40	0.51
2:J:47:LEU:HD23	2:J:47:LEU:C	2.36	0.51
2:P:52:CYS:SG	2:P:59:MET:HG2	2.50	0.51
2:F:33:GLU:OE2	2:F:35:HIS:NE2	2.43	0.51
2:F:45:LYS:HB2	2:F:73:ASP:HB3	1.92	0.51
1:G:437:VAL:HG23	1:G:470:LEU:HB2	1.92	0.51
2:H:63:ARG:NH2	2:H:93:GLU:HB2	2.26	0.51
2:J:22:ILE:HG12	2:J:23:LYS:N	2.26	0.51
1:K:451:TYR:CD1	1:K:514:ASP:HB2	2.46	0.51
1:S:376:ILE:HD11	1:S:581:TRP:HB2	1.92	0.51
2:V:63:ARG:NH2	2:V:93:GLU:HB2	2.26	0.51
1:O:414:GLU:OE1	1:O:414:GLU:HA	2.09	0.51
1:U:537:HIS:CD2	1:U:538:GLU:HG2	2.46	0.51
1:E:469:ILE:HG22	1:E:469:ILE:O	2.10	0.51
1:I:471:VAL:HB	1:I:482:VAL:HB	1.92	0.51
1:I:542:GLN:HE22	1:I:548:SER:HB3	1.75	0.51
1:A:513:GLN:NE2	1:A:513:GLN:HA	2.26	0.50
2:B:48:MET:HA	2:B:64:PHE:CE2	2.46	0.50
2:D:53:GLN:C	2:D:55:GLN:N	2.66	0.50
1:S:391:SER:O	1:S:392:ALA:HB2	2.10	0.50
1:S:495:ASP:OD1	1:S:495:ASP:C	2.54	0.50
1:U:419:TYR:O	1:U:422:LEU:N	2.43	0.50
2:X:63:ARG:HH21	2:X:93:GLU:HG3	1.72	0.50
2:D:24:LEU:HD13	2:D:88:ILE:HD11	1.93	0.50
1:I:427:ASN:O	1:I:428:LYS:C	2.54	0.50
1:I:561:ARG:C	1:I:563:LYS:H	2.19	0.50
1:Q:411:LEU:HD21	1:Q:549:GLY:CA	2.42	0.50
1:A:405:LEU:HD21	1:A:415:VAL:HG11	1.93	0.50
1:G:396:ARG:HH12	2:H:74:ASN:HD21	1.59	0.50
1:K:415:VAL:HG12	1:K:416:ILE:N	2.25	0.50
1:Q:420:MET:HE1	1:Q:481:LEU:HD13	1.93	0.50
2:T:20:GLU:O	2:T:21:TYR:CD1	2.63	0.50
1:U:420:MET:HB3	1:U:437:VAL:CG2	2.40	0.50
1:U:426:ARG:NH1	1:U:557:ASP:OD1	2.37	0.50
1:U:542:GLN:NE2	2:V:97:GLY:O	2.44	0.50
1:U:550:MET:CE	1:U:579:MET:CE	2.81	0.50
1:U:551:PHE:CE1	1:U:572:MET:HE3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:HIS:C	1:A:475:ARG:O	2.48	0.50
1:C:544:ASN:HD21	1:C:569:GLN:NE2	2.09	0.50
2:N:89:GLU:OE1	2:N:91:TYR:OH	2.28	0.50
1:O:482:VAL:HG11	1:O:508:LEU:HD13	1.92	0.50
1:O:550:MET:HB3	1:O:572:MET:SD	2.52	0.50
2:X:66:TRP:O	2:X:68:GLY:N	2.44	0.50
1:E:435:LEU:HD12	1:E:468:ILE:HB	1.93	0.50
1:E:510:GLN:HA	1:E:510:GLN:OE1	2.10	0.50
1:O:419:TYR:CE2	1:O:423:LEU:HD21	2.46	0.50
1:W:406:LYS:O	1:W:576:ARG:NH1	2.44	0.50
1:A:394:LYS:HD3	1:A:396:ARG:NH2	2.23	0.50
1:A:544:ASN:H	1:A:544:ASN:HD22	1.60	0.50
2:D:48:MET:HG2	2:D:64:PHE:CE2	2.46	0.50
1:E:404:THR:O	1:E:409:HIS:HB2	2.11	0.50
1:E:581:TRP:NE1	1:E:585:HIS:CD2	2.80	0.50
1:I:416:ILE:HG22	1:I:417:ASN:N	2.27	0.50
2:J:48:MET:HG2	2:J:64:PHE:CD2	2.47	0.50
2:L:51:TYR:O	2:L:55:GLN:HG2	2.12	0.50
1:O:451:TYR:CD1	1:O:451:TYR:C	2.90	0.50
2:R:40:MET:HG3	2:R:78:LYS:HB2	1.93	0.50
1:A:408:TYR:CE1	1:U:434:ALA:HB2	2.47	0.50
1:C:411:LEU:O	2:D:95:THR:HA	2.12	0.50
2:F:47:LEU:C	2:F:47:LEU:HD23	2.36	0.50
1:I:567:PHE:HA	1:I:571:GLN:HE22	1.77	0.50
1:Q:547:ASP:OD1	1:Q:576:ARG:NE	2.41	0.50
1:W:469:ILE:HB	1:W:484:ILE:HB	1.94	0.50
2:D:63:ARG:NH2	2:D:93:GLU:HB2	2.27	0.50
2:F:20:GLU:C	2:F:21:TYR:CD1	2.90	0.50
1:I:435:LEU:HD21	1:I:470:LEU:CD1	2.42	0.50
1:K:561:ARG:O	1:K:562:ASP:HB2	2.11	0.50
2:N:47:LEU:O	2:N:47:LEU:HD23	2.10	0.50
1:Q:399:ARG:O	1:Q:403:GLN:HG2	2.12	0.50
2:X:22:ILE:HG12	2:X:40:MET:SD	2.51	0.50
2:X:52:CYS:SG	2:X:64:PHE:HZ	2.35	0.50
2:B:43:HIS:CD2	2:B:74:ASN:HA	2.47	0.50
1:K:515:GLU:O	1:K:519:LYS:N	2.44	0.50
2:P:76:THR:CG2	2:P:79:GLU:H	2.24	0.50
1:W:394:LYS:HD3	1:W:396:ARG:HH22	1.77	0.50
1:E:432:TYR:HB3	1:E:433:PRO:CD	2.42	0.49
1:K:551:PHE:CE1	1:K:572:MET:HE3	2.47	0.49
1:Q:372:MET:HG2	1:Q:581:TRP:CD1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:470:LEU:HD23	1:Q:483:VAL:HA	1.94	0.49
2:B:47:LEU:C	2:B:47:LEU:HD23	2.37	0.49
1:E:379:ALA:HB1	1:E:389:LEU:HD13	1.93	0.49
1:E:483:VAL:O	1:E:484:ILE:HG13	2.12	0.49
1:I:552:THR:O	1:I:553:CYS:C	2.55	0.49
1:M:474:HIS:ND1	2:N:94:GLN:HB3	2.26	0.49
1:M:571:GLN:HB3	1:M:575:PHE:CE2	2.47	0.49
1:Q:410:TRP:N	1:Q:410:TRP:CD1	2.80	0.49
2:F:24:LEU:HD12	2:F:38:VAL:HG11	1.94	0.49
1:G:410:TRP:N	1:G:410:TRP:CD1	2.77	0.49
2:L:77:PRO:HA	2:L:82:MET:CG	2.41	0.49
1:M:419:TYR:CE2	1:M:553:CYS:HB3	2.47	0.49
1:M:551:PHE:CE1	1:M:572:MET:HE2	2.47	0.49
1:O:393:PHE:CD2	1:O:421:ASN:HB3	2.47	0.49
1:O:567:PHE:CD1	1:O:567:PHE:C	2.90	0.49
1:Q:500:LYS:HB3	1:Q:502:HIS:ND1	2.27	0.49
1:S:559:ILE:C	1:S:561:ARG:H	2.18	0.49
1:I:484:ILE:HG23	1:I:491:LEU:HD11	1.95	0.49
1:S:417:ASN:OD1	1:S:440:THR:HG22	2.11	0.49
1:W:470:LEU:HD22	1:W:481:LEU:HD21	1.95	0.49
2:D:48:MET:HE3	2:D:64:PHE:CD2	2.47	0.49
1:E:572:MET:O	1:E:575:PHE:N	2.45	0.49
1:K:394:LYS:H	1:K:394:LYS:HE2	1.77	0.49
1:A:416:ILE:O	1:A:420:MET:HG2	2.13	0.49
1:C:551:PHE:CD1	1:C:572:MET:HE3	2.48	0.49
1:G:497:MET:O	1:G:498:GLY:C	2.54	0.49
1:G:498:GLY:HA3	1:G:536:PRO:HG3	1.94	0.49
1:I:513:GLN:HA	1:I:524:LEU:CD2	2.43	0.49
2:J:63:ARG:N	2:J:63:ARG:HD3	2.28	0.49
1:M:484:ILE:HG12	1:M:491:LEU:HG	1.95	0.49
1:A:438:PHE:HD2	1:A:471:VAL:HG22	1.78	0.49
1:A:459:LYS:O	1:A:461:VAL:N	2.40	0.49
1:G:579:MET:O	1:G:583:ILE:HG13	2.13	0.49
1:O:536:PRO:HA	1:O:541:GLN:NE2	2.14	0.49
1:A:441:PHE:CZ	2:B:63:ARG:HG3	2.47	0.49
2:D:83:GLU:O	2:D:84:GLU:C	2.55	0.49
1:A:393:PHE:CD2	1:A:421:ASN:HB3	2.47	0.49
2:N:47:LEU:HD23	2:N:47:LEU:C	2.37	0.49
1:Q:582:GLU:HG2	1:Q:589:LEU:H	1.77	0.49
1:S:372:MET:O	1:S:376:ILE:HD12	2.13	0.49
1:U:550:MET:HE2	1:U:576:ARG:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:420:MET:HE1	1:W:556:ALA:CB	2.43	0.49
1:W:488:LYS:O	1:W:489:LYS:C	2.56	0.49
1:A:409:HIS:O	1:A:576:ARG:NH2	2.28	0.48
1:A:442:PHE:HE2	1:A:508:LEU:HD21	1.78	0.48
2:D:48:MET:HE3	2:D:64:PHE:HB2	1.93	0.48
1:I:525:ASN:HB3	1:I:528:GLU:OE2	2.13	0.48
1:M:558:TYR:CD2	1:M:565:ILE:HA	2.48	0.48
2:N:20:GLU:O	2:N:21:TYR:CD1	2.66	0.48
1:Q:409:HIS:O	1:Q:576:ARG:NH2	2.42	0.48
1:U:484:ILE:HG23	1:U:491:LEU:HG	1.94	0.48
2:V:34:ILE:HD13	2:V:54:ARG:HD2	1.94	0.48
1:C:581:TRP:O	1:C:582:GLU:C	2.57	0.48
1:E:501:GLY:O	1:E:505:CYS:SG	2.54	0.48
1:K:544:ASN:C	1:K:544:ASN:OD1	2.55	0.48
1:M:511:TYR:CZ	1:M:515:GLU:HG3	2.47	0.48
1:U:567:PHE:CD1	1:U:567:PHE:C	2.91	0.48
2:V:43:HIS:C	2:V:45:LYS:H	2.20	0.48
2:X:76:THR:CG2	2:X:79:GLU:HB2	2.43	0.48
1:E:401:ASP:O	1:E:404:THR:OG1	2.28	0.48
1:I:581:TRP:CE2	1:I:585:HIS:CD2	3.01	0.48
1:K:542:GLN:OE1	1:K:548:SER:HB3	2.14	0.48
1:M:572:MET:SD	1:M:575:PHE:HD2	2.36	0.48
1:Q:540:PRO:O	1:Q:551:PHE:CE2	2.67	0.48
2:D:76:THR:HG22	2:D:79:GLU:CD	2.38	0.48
1:I:576:ARG:O	1:I:578:LYS:N	2.47	0.48
1:K:410:TRP:CG	2:L:96:GLY:O	2.66	0.48
1:Q:550:MET:CE	1:Q:575:PHE:HB3	2.43	0.48
2:T:66:TRP:HB2	2:T:71:ILE:HD11	1.94	0.48
2:B:26:VAL:HG21	2:B:47:LEU:HD21	1.94	0.48
1:G:458:THR:HG21	1:G:511:TYR:OH	2.13	0.48
1:G:484:ILE:HG12	1:G:491:LEU:HG	1.95	0.48
2:B:63:ARG:NH2	2:B:93:GLU:HB2	2.28	0.48
1:C:404:THR:HG21	1:C:412:ASN:N	2.21	0.48
2:D:64:PHE:CD1	2:D:90:VAL:HG22	2.48	0.48
1:G:574:LEU:O	1:G:574:LEU:HD23	2.13	0.48
1:I:404:THR:OG1	1:I:415:VAL:HG21	2.14	0.48
1:Q:376:ILE:HD11	1:Q:581:TRP:HB2	1.94	0.48
1:Q:402:ILE:HG13	1:Q:405:LEU:HD12	1.95	0.48
2:T:28:GLY:O	2:T:30:ASP:N	2.46	0.48
1:W:446:LEU:O	1:W:450:GLY:N	2.46	0.48
2:D:58:PRO:HG2	2:D:61:SER:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:27:ILE:CG2	2:H:28:GLY:N	2.76	0.48
1:Q:397:ILE:HG23	1:Q:401:ASP:HB2	1.96	0.48
2:R:43:HIS:C	2:R:45:LYS:H	2.21	0.48
1:W:481:LEU:HD21	1:W:556:ALA:HB2	1.96	0.48
2:X:76:THR:HG23	2:X:79:GLU:N	2.28	0.48
1:C:428:LYS:HB2	1:I:408:TYR:HE2	1.79	0.48
1:G:449:GLY:O	1:G:453:ALA:HB2	2.14	0.48
1:G:574:LEU:HD22	1:G:578:LYS:HD2	1.95	0.48
2:J:39:LYS:CG	2:J:42:THR:OG1	2.56	0.48
1:K:484:ILE:HG23	1:K:491:LEU:HG	1.96	0.48
1:M:407:ASN:O	1:M:408:TYR:HB2	2.14	0.48
2:B:21:TYR:HB2	2:B:40:MET:HB2	1.94	0.48
1:C:419:TYR:HE1	1:C:582:GLU:OE1	1.96	0.48
1:C:459:LYS:HE3	1:C:459:LYS:O	2.14	0.48
1:M:394:LYS:H	1:M:394:LYS:CE	2.22	0.48
1:C:581:TRP:CZ3	1:C:589:LEU:HD21	2.49	0.48
1:E:454:VAL:O	1:E:455:LYS:C	2.56	0.48
1:E:473:ILE:HB	1:E:480:SER:HB2	1.95	0.48
1:I:432:TYR:HB3	1:I:433:PRO:HD2	1.96	0.48
1:K:581:TRP:CZ3	1:K:589:LEU:HD21	2.49	0.48
1:Q:380:LEU:HD11	1:Q:580:VAL:HG11	1.95	0.48
2:V:22:ILE:HG13	2:V:83:GLU:HA	1.96	0.48
1:W:481:LEU:CD2	1:W:556:ALA:HB2	2.43	0.48
2:H:49:GLU:HA	2:H:52:CYS:HB2	1.95	0.47
1:I:477:VAL:O	1:I:478:HIS:HB2	2.14	0.47
1:M:438:PHE:HD2	1:M:471:VAL:CG2	2.17	0.47
1:M:557:ASP:O	1:M:560:SER:OG	2.27	0.47
2:N:64:PHE:N	2:N:64:PHE:CD1	2.82	0.47
1:A:473:ILE:HB	1:A:480:SER:HB2	1.95	0.47
1:E:555:TYR:O	1:E:558:TYR:N	2.44	0.47
2:N:26:VAL:HG22	2:N:88:ILE:HB	1.96	0.47
1:S:399:ARG:O	1:S:403:GLN:CG	2.61	0.47
1:U:426:ARG:NH1	1:U:561:ARG:HD2	2.29	0.47
1:U:581:TRP:CE2	1:U:585:HIS:CD2	3.02	0.47
1:W:501:GLY:HA2	1:W:504:ILE:CD1	2.43	0.47
2:B:48:MET:HE3	2:B:64:PHE:CG	2.49	0.47
1:E:426:ARG:CZ	1:E:561:ARG:CD	2.91	0.47
1:E:555:TYR:O	1:E:556:ALA:C	2.56	0.47
2:J:66:TRP:HD1	2:J:87:VAL:O	1.96	0.47
1:Q:375:GLU:O	1:Q:379:ALA:HB2	2.14	0.47
2:R:85:GLU:OE1	2:R:85:GLU:CA	2.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:394:LYS:HD3	1:S:396:ARG:HH22	1.79	0.47
1:S:581:TRP:CE2	1:S:585:HIS:HD2	2.32	0.47
1:U:380:LEU:HD22	1:U:406:LYS:HG3	1.97	0.47
2:V:76:THR:HG23	2:V:79:GLU:HB2	1.96	0.47
1:W:396:ARG:NH1	2:X:74:ASN:ND2	2.62	0.47
2:X:22:ILE:HG22	2:X:24:LEU:HG	1.97	0.47
1:A:414:GLU:OE2	2:B:70:ARG:NH2	2.42	0.47
1:E:491:LEU:CD2	1:E:505:CYS:HB3	2.44	0.47
1:M:462:ASN:HB3	1:M:465:GLU:HG3	1.96	0.47
1:O:492:LYS:HA	1:O:532:HIS:O	2.14	0.47
1:Q:401:ASP:HB3	1:Q:415:VAL:HG23	1.95	0.47
1:Q:567:PHE:CE1	1:Q:572:MET:HE1	2.49	0.47
1:S:395:LEU:HD23	2:T:70:ARG:HH11	1.79	0.47
1:U:432:TYR:CZ	1:U:561:ARG:HG2	2.50	0.47
1:E:550:MET:CE	1:E:579:MET:HE1	2.45	0.47
1:E:554:LYS:O	1:E:555:TYR:C	2.57	0.47
1:M:432:TYR:HB3	1:M:433:PRO:HD2	1.95	0.47
1:O:510:GLN:O	1:O:513:GLN:HB3	2.14	0.47
2:R:72:ALA:O	2:R:75:HIS:HB2	2.15	0.47
1:S:495:ASP:OD1	1:S:498:GLY:N	2.48	0.47
1:A:581:TRP:NE1	1:A:585:HIS:CD2	2.82	0.47
1:C:463:LEU:O	1:C:466:GLN:HB2	2.15	0.47
1:E:414:GLU:OE2	2:F:70:ARG:NH1	2.48	0.47
1:E:417:ASN:OD1	1:E:440:THR:HG23	2.14	0.47
1:I:551:PHE:CE1	1:I:567:PHE:HE1	2.32	0.47
1:K:451:TYR:CE2	1:K:455:LYS:HB2	2.49	0.47
2:N:58:PRO:O	2:N:61:SER:HB3	2.15	0.47
1:C:411:LEU:HD13	1:C:415:VAL:HG11	1.96	0.47
2:F:76:THR:O	2:F:77:PRO:C	2.56	0.47
1:I:526:LEU:HA	1:I:529:TRP:CD1	2.50	0.47
1:K:403:GLN:O	1:K:405:LEU:N	2.48	0.47
1:M:394:LYS:HD3	1:M:396:ARG:HH22	1.79	0.47
1:Q:572:MET:N	1:Q:573:PRO:HD2	2.29	0.47
1:S:579:MET:HA	1:S:582:GLU:HB2	1.95	0.47
2:V:36:PHE:HB3	2:V:38:VAL:CG1	2.45	0.47
1:W:398:THR:OG1	1:W:399:ARG:N	2.45	0.47
1:A:484:ILE:HG12	1:A:491:LEU:HD11	1.96	0.47
1:A:524:LEU:HD12	1:A:525:ASN:H	1.80	0.47
1:C:469:ILE:HB	1:C:484:ILE:CB	2.43	0.47
1:E:550:MET:HE1	1:E:579:MET:CE	2.45	0.47
1:G:393:PHE:CE2	1:G:421:ASN:HB2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:502:HIS:O	1:U:506:GLU:CG	2.63	0.47
1:W:475:ARG:O	1:W:478:HIS:N	2.45	0.47
1:W:577:LYS:O	1:W:580:VAL:HG13	2.15	0.47
1:E:494:LEU:N	1:E:494:LEU:CD1	2.76	0.47
1:O:468:ILE:HD11	1:O:487:ARG:CZ	2.45	0.47
1:Q:470:LEU:HD13	1:Q:556:ALA:HB1	1.96	0.47
1:Q:488:LYS:O	1:Q:489:LYS:C	2.58	0.47
2:F:93:GLU:HG3	2:F:94:GLN:N	2.29	0.47
1:I:394:LYS:HG3	2:J:75:HIS:CE1	2.50	0.47
1:I:469:ILE:HD12	1:I:484:ILE:HG21	1.96	0.47
1:K:445:LYS:HD3	2:L:91:TYR:OH	2.15	0.47
1:K:554:LYS:HA	1:K:554:LYS:HD3	1.71	0.47
2:N:64:PHE:HB3	2:N:71:ILE:HD12	1.96	0.47
1:O:573:PRO:O	1:O:576:ARG:HB2	2.15	0.47
2:V:74:ASN:OD1	2:V:74:ASN:N	2.43	0.47
1:E:558:TYR:CE2	1:E:567:PHE:CE2	3.04	0.46
1:K:402:ILE:O	1:K:403:GLN:C	2.58	0.46
1:Q:402:ILE:C	1:Q:404:THR:H	2.23	0.46
1:U:550:MET:SD	1:U:579:MET:CE	3.04	0.46
1:A:393:PHE:CD2	1:A:421:ASN:CB	2.97	0.46
1:C:544:ASN:O	1:C:546:SER:N	2.37	0.46
2:D:63:ARG:HD2	2:D:70:ARG:NH2	2.30	0.46
2:J:52:CYS:SG	2:J:62:LEU:HD11	2.55	0.46
1:M:443:TYR:OH	1:M:504:ILE:HG12	2.16	0.46
1:Q:495:ASP:C	1:Q:495:ASP:OD1	2.58	0.46
1:U:433:PRO:HB2	1:U:468:ILE:HD12	1.98	0.46
2:V:33:GLU:C	2:V:34:ILE:HG13	2.40	0.46
1:E:489:LYS:HG3	1:E:529:TRP:CE2	2.50	0.46
1:I:458:THR:HG21	1:I:511:TYR:OH	2.15	0.46
1:I:459:LYS:HD2	1:I:459:LYS:HA	1.57	0.46
2:J:54:ARG:HE	2:J:54:ARG:HA	1.81	0.46
1:K:436:HIS:HB3	1:K:469:ILE:HG12	1.97	0.46
1:W:426:ARG:NH1	1:W:561:ARG:HD2	2.30	0.46
1:A:442:PHE:HA	1:A:457:TRP:CZ3	2.50	0.46
1:C:550:MET:HE1	1:C:579:MET:HE3	1.97	0.46
2:D:45:LYS:O	2:D:48:MET:N	2.48	0.46
1:G:407:ASN:ND2	1:K:428:LYS:HE3	2.30	0.46
1:G:410:TRP:CZ3	1:G:477:VAL:HG12	2.50	0.46
2:H:74:ASN:OD1	2:H:74:ASN:N	2.45	0.46
1:Q:542:GLN:OE1	1:Q:548:SER:CB	2.64	0.46
1:G:417:ASN:O	1:G:418:PHE:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:420:MET:HB3	1:G:437:VAL:CG2	2.40	0.46
1:I:543:LEU:HB2	1:I:569:GLN:HG2	1.96	0.46
1:K:426:ARG:NH1	1:K:561:ARG:HD2	2.30	0.46
2:N:44:LEU:HD21	2:N:77:PRO:HG3	1.98	0.46
1:E:372:MET:HE3	1:E:581:TRP:CD2	2.51	0.46
1:E:545:GLY:N	1:I:467:GLU:OE2	2.49	0.46
2:F:20:GLU:C	2:F:21:TYR:HD1	2.23	0.46
1:I:475:ARG:O	1:I:476:LYS:C	2.59	0.46
1:K:572:MET:O	1:K:573:PRO:C	2.58	0.46
1:M:407:ASN:OD1	1:M:407:ASN:N	2.48	0.46
2:R:64:PHE:HB3	2:R:88:ILE:CG2	2.46	0.46
1:O:438:PHE:HZ	1:O:463:LEU:HD11	1.80	0.46
2:R:51:TYR:CE2	2:R:90:VAL:HG11	2.51	0.46
1:W:483:VAL:HG21	1:W:559:ILE:HG21	1.98	0.46
2:B:58:PRO:O	2:B:61:SER:HB3	2.16	0.46
1:C:554:LYS:HA	1:C:554:LYS:HD2	1.82	0.46
1:G:455:LYS:O	1:G:519:LYS:NZ	2.49	0.46
1:Q:552:THR:HA	1:Q:555:TYR:CD2	2.51	0.46
1:S:464:PHE:HA	1:S:486:LEU:CD1	2.45	0.46
1:U:435:LEU:HD11	1:U:470:LEU:HG	1.97	0.46
2:V:66:TRP:O	2:V:69:GLN:HB2	2.16	0.46
2:X:84:GLU:HG3	2:X:85:GLU:HG3	1.97	0.46
1:E:427:ASN:ND2	1:E:560:SER:O	2.47	0.46
1:K:403:GLN:C	1:K:405:LEU:H	2.23	0.46
1:Q:444:PRO:O	1:Q:448:SER:HB2	2.16	0.46
1:U:502:HIS:O	1:U:506:GLU:HG2	2.15	0.46
1:A:380:LEU:HD23	1:A:402:ILE:HG23	1.98	0.46
1:C:484:ILE:HG12	1:C:512:LEU:HD11	1.98	0.46
2:J:58:PRO:O	2:J:61:SER:HB3	2.15	0.46
2:J:70:ARG:HH11	2:J:70:ARG:HG3	1.76	0.46
1:Q:491:LEU:HD21	1:Q:505:CYS:O	2.16	0.46
1:Q:535:LYS:O	1:Q:537:HIS:N	2.47	0.46
1:W:476:LYS:C	1:W:477:VAL:HG23	2.41	0.46
2:X:39:LYS:HG3	2:X:42:THR:OG1	2.16	0.46
1:I:420:MET:O	1:I:423:LEU:HB2	2.17	0.45
1:Q:548:SER:HG	2:R:97:GLY:C	2.24	0.45
1:S:391:SER:HB3	1:S:396:ARG:NE	2.31	0.45
1:S:416:ILE:O	1:S:417:ASN:C	2.59	0.45
1:S:556:ALA:O	1:S:560:SER:HB3	2.16	0.45
1:S:574:LEU:O	1:S:575:PHE:C	2.59	0.45
1:A:405:LEU:C	1:A:576:ARG:NH1	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:LEU:HD13	2:B:88:ILE:HD11	1.98	0.45
1:C:458:THR:HG21	1:C:511:TYR:OH	2.16	0.45
2:H:55:GLN:HE21	2:H:55:GLN:C	2.24	0.45
1:K:475:ARG:HE	1:K:475:ARG:HA	1.81	0.45
1:Q:427:ASN:ND2	1:Q:560:SER:O	2.49	0.45
2:T:63:ARG:HB3	2:T:70:ARG:HE	1.81	0.45
1:W:451:TYR:O	1:W:454:VAL:HG22	2.16	0.45
1:A:368:LEU:HD23	1:A:372:MET:HE2	1.98	0.45
1:A:544:ASN:HD21	1:A:569:GLN:NE2	2.14	0.45
1:C:420:MET:O	1:C:423:LEU:HB2	2.15	0.45
1:C:440:THR:HA	1:C:472:PRO:HG2	1.96	0.45
1:E:387:GLU:CD	1:E:399:ARG:HH12	2.17	0.45
1:E:426:ARG:NH1	1:E:426:ARG:CG	2.66	0.45
1:E:490:CYS:SG	1:E:491:LEU:N	2.90	0.45
1:I:512:LEU:HD23	1:I:512:LEU:HA	1.84	0.45
2:J:34:ILE:HD12	2:J:51:TYR:CD1	2.52	0.45
1:K:406:LYS:O	1:K:407:ASN:C	2.60	0.45
1:O:493:TYR:CE1	1:O:495:ASP:HB2	2.52	0.45
1:Q:502:HIS:ND1	1:Q:502:HIS:N	2.63	0.45
1:W:426:ARG:HD2	1:W:430:GLN:HG3	1.98	0.45
1:W:579:MET:O	1:W:583:ILE:HG13	2.15	0.45
1:A:493:TYR:C	1:A:494:LEU:HD12	2.42	0.45
1:E:394:LYS:HD3	1:E:396:ARG:NH2	2.32	0.45
1:E:407:ASN:HB2	1:I:428:LYS:HE3	1.97	0.45
2:F:46:LYS:O	2:F:50:SER:OG	2.33	0.45
1:G:407:ASN:O	1:G:408:TYR:HB2	2.15	0.45
1:G:495:ASP:OD1	1:G:497:MET:N	2.48	0.45
1:K:496:SER:HB2	1:K:542:GLN:HB3	1.98	0.45
2:L:74:ASN:OD1	2:L:74:ASN:N	2.47	0.45
1:O:475:ARG:HE	1:O:475:ARG:HA	1.82	0.45
1:Q:472:PRO:HA	1:Q:481:LEU:HA	1.98	0.45
1:W:467:GLU:HB3	1:W:487:ARG:HD3	1.99	0.45
1:I:475:ARG:HE	1:I:475:ARG:CA	2.30	0.45
1:I:498:GLY:HA3	1:I:536:PRO:HG3	1.98	0.45
2:J:40:MET:HE1	2:J:82:MET:O	2.16	0.45
1:O:524:LEU:HD13	1:O:524:LEU:HA	1.82	0.45
1:S:442:PHE:CD1	1:S:443:TYR:N	2.84	0.45
1:E:451:TYR:HE1	1:E:515:GLU:HG2	1.82	0.45
2:J:44:LEU:HG	2:J:77:PRO:HD3	1.98	0.45
2:P:85:GLU:OE1	2:P:85:GLU:HA	2.15	0.45
2:V:72:ALA:O	2:V:73:ASP:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:454:VAL:O	1:W:457:TRP:HB2	2.17	0.45
1:C:407:ASN:O	1:C:408:TYR:HB2	2.16	0.45
1:G:432:TYR:O	1:G:433:PRO:C	2.56	0.45
2:H:44:LEU:HD21	2:H:77:PRO:HG3	1.97	0.45
1:I:412:ASN:ND2	2:J:93:GLU:OE1	2.45	0.45
1:K:576:ARG:O	1:K:577:LYS:C	2.60	0.45
1:M:469:ILE:HB	1:M:484:ILE:HB	1.99	0.45
1:M:581:TRP:CE2	1:M:585:HIS:CD2	3.05	0.45
2:R:62:LEU:HB3	2:R:90:VAL:CG2	2.47	0.45
2:T:51:TYR:O	2:T:55:GLN:HG2	2.16	0.45
1:U:424:VAL:HG22	1:U:435:LEU:HB3	1.99	0.45
1:U:457:TRP:CD1	2:V:67:GLU:C	2.95	0.45
1:A:574:LEU:O	1:A:578:LYS:N	2.39	0.45
1:E:558:TYR:CE2	1:E:567:PHE:HD2	2.31	0.45
1:I:426:ARG:HG3	1:I:588:LEU:HD12	1.98	0.45
1:I:443:TYR:OH	1:I:504:ILE:HD13	2.16	0.45
1:I:583:ILE:O	1:I:584:LEU:C	2.60	0.45
1:K:368:LEU:CD2	1:K:372:MET:HE2	2.46	0.45
1:K:424:VAL:HG12	1:K:425:GLU:N	2.31	0.45
1:O:554:LYS:HA	1:O:557:ASP:HB3	1.99	0.45
2:R:48:MET:HG2	2:R:64:PHE:CD2	2.52	0.45
2:T:27:ILE:HG22	2:T:28:GLY:N	2.31	0.45
2:X:66:TRP:O	2:X:67:GLU:C	2.60	0.45
1:A:584:LEU:HD23	1:A:584:LEU:HA	1.81	0.45
2:B:32:SER:HB2	2:F:21:TYR:O	2.17	0.45
1:M:385:GLN:O	1:M:385:GLN:HG3	2.17	0.45
1:M:417:ASN:OD1	1:M:440:THR:CG2	2.65	0.45
1:O:419:TYR:HE2	1:O:553:CYS:O	2.00	0.45
2:B:57:VAL:HA	2:B:58:PRO:HD3	1.87	0.45
1:C:393:PHE:CZ	1:C:422:LEU:HD23	2.50	0.45
2:D:64:PHE:HB3	2:D:71:ILE:HD12	1.98	0.45
1:I:394:LYS:HZ2	1:I:396:ARG:HH22	1.64	0.45
1:K:500:LYS:HG2	1:K:533:SER:OG	2.17	0.45
1:M:451:TYR:CE1	1:M:515:GLU:HG2	2.47	0.45
1:M:535:LYS:HB3	1:M:536:PRO:HD2	1.98	0.45
2:N:77:PRO:CA	2:N:82:MET:HG3	2.40	0.45
1:W:394:LYS:HE2	1:W:394:LYS:H	1.82	0.45
2:B:65:LEU:HB3	2:B:89:GLU:OE1	2.17	0.44
1:C:391:SER:O	1:C:392:ALA:HB2	2.16	0.44
2:F:55:GLN:HA	2:F:55:GLN:NE2	2.31	0.44
1:Q:451:TYR:OH	1:Q:515:GLU:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:HIS:O	1:A:474:HIS:ND1	2.50	0.44
1:C:388:ILE:HD11	1:C:396:ARG:HB3	1.99	0.44
1:E:484:ILE:O	1:E:484:ILE:HG22	2.16	0.44
2:F:76:THR:HG22	2:F:79:GLU:N	2.19	0.44
1:G:567:PHE:CD1	1:G:567:PHE:C	2.95	0.44
1:O:494:LEU:HD23	1:O:539:ILE:HG21	1.99	0.44
1:O:538:GLU:H	1:O:538:GLU:HG2	1.59	0.44
1:Q:432:TYR:HB3	1:Q:433:PRO:CD	2.47	0.44
2:R:51:TYR:HE2	2:R:90:VAL:HG11	1.82	0.44
1:U:484:ILE:HG21	1:U:512:LEU:HD11	1.99	0.44
2:X:59:MET:C	2:X:61:SER:H	2.25	0.44
1:A:392:ALA:C	1:A:394:LYS:N	2.74	0.44
1:E:517:LYS:NZ	1:U:517:LYS:HD2	2.33	0.44
1:M:572:MET:O	1:M:573:PRO:C	2.61	0.44
1:Q:413:ASP:HB2	1:Q:440:THR:OG1	2.17	0.44
1:S:456:ARG:HD2	2:T:67:GLU:OE2	2.17	0.44
2:T:20:GLU:C	2:T:21:TYR:CD1	2.95	0.44
2:T:40:MET:HE1	2:T:82:MET:O	2.18	0.44
1:U:458:THR:HG21	1:U:511:TYR:OH	2.16	0.44
1:A:459:LYS:HD2	1:A:459:LYS:HA	1.61	0.44
1:G:501:GLY:O	1:G:502:HIS:C	2.60	0.44
1:I:443:TYR:CD1	1:I:443:TYR:C	2.95	0.44
1:I:506:GLU:O	1:I:509:LEU:N	2.49	0.44
1:K:470:LEU:HD22	1:K:481:LEU:HD21	2.00	0.44
2:L:76:THR:O	2:L:77:PRO:C	2.60	0.44
1:O:413:ASP:OD1	1:O:413:ASP:N	2.50	0.44
2:P:62:LEU:HD13	2:P:64:PHE:CE1	2.53	0.44
1:U:473:ILE:HB	1:U:480:SER:HB2	1.99	0.44
1:U:511:TYR:O	1:U:512:LEU:C	2.60	0.44
1:I:582:GLU:HG2	1:I:587:GLN:O	2.17	0.44
1:W:481:LEU:HD13	1:W:552:THR:HG23	1.99	0.44
1:A:544:ASN:ND2	1:U:431:GLY:O	2.50	0.44
1:E:395:LEU:HD23	2:F:70:ARG:HD2	1.98	0.44
1:E:494:LEU:HD12	1:E:494:LEU:H	1.80	0.44
1:I:384:PRO:HB2	1:I:387:GLU:HB2	1.99	0.44
1:I:492:LYS:HD3	1:I:534:MET:HE2	1.99	0.44
1:M:426:ARG:NH2	1:M:557:ASP:OD1	2.48	0.44
1:Q:416:ILE:HG22	1:Q:417:ASN:N	2.31	0.44
1:A:463:LEU:O	1:A:486:LEU:HD11	2.17	0.44
1:C:469:ILE:HD12	1:C:484:ILE:HG21	1.99	0.44
1:C:477:VAL:O	2:D:96:GLY:CA	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:30:ASP:OD1	2:F:30:ASP:O	2.36	0.44
2:F:83:GLU:O	2:F:84:GLU:C	2.60	0.44
1:G:572:MET:O	1:G:573:PRO:C	2.61	0.44
2:H:45:LYS:HG2	2:H:49:GLU:OE2	2.18	0.44
2:H:76:THR:HG22	2:H:79:GLU:H	1.82	0.44
2:N:76:THR:HG23	2:N:78:LYS:HB3	2.00	0.44
1:O:427:ASN:HA	1:O:432:TYR:HB2	1.99	0.44
2:X:39:LYS:CG	2:X:42:THR:OG1	2.66	0.44
1:E:392:ALA:O	1:E:395:LEU:HB2	2.17	0.44
2:J:76:THR:O	2:J:77:PRO:C	2.61	0.44
1:M:426:ARG:C	1:M:426:ARG:HD2	2.42	0.44
1:Q:476:LYS:NZ	1:Q:476:LYS:CB	2.80	0.44
1:U:411:LEU:HG	1:U:549:GLY:HA3	2.00	0.44
1:U:512:LEU:O	1:U:515:GLU:HB3	2.18	0.44
1:W:567:PHE:CD1	1:W:567:PHE:C	2.96	0.44
1:W:579:MET:HA	1:W:582:GLU:HB2	2.00	0.44
1:E:555:TYR:O	1:E:557:ASP:N	2.51	0.44
1:E:557:ASP:O	1:E:560:SER:OG	2.32	0.44
1:I:461:VAL:HG22	1:I:462:ASN:N	2.33	0.44
1:I:488:LYS:O	1:I:489:LYS:C	2.61	0.44
1:Q:397:ILE:HD12	1:Q:414:GLU:O	2.17	0.44
1:Q:544:ASN:OD1	1:Q:544:ASN:N	2.42	0.44
1:S:503:ARG:O	1:S:507:ILE:HG12	2.17	0.44
1:W:447:LYS:O	1:W:448:SER:C	2.61	0.44
1:C:561:ARG:C	1:C:563:LYS:H	2.26	0.43
1:I:577:LYS:O	1:I:580:VAL:HG13	2.18	0.43
2:N:60:ASN:OD1	2:N:61:SER:N	2.51	0.43
1:S:415:VAL:HG22	1:S:583:ILE:CD1	2.48	0.43
1:S:446:LEU:HB2	1:S:454:VAL:HG11	2.00	0.43
1:U:515:GLU:HA	1:U:515:GLU:OE1	2.16	0.43
2:V:39:LYS:HG3	2:V:42:THR:CG2	2.48	0.43
1:W:444:PRO:C	1:W:446:LEU:N	2.76	0.43
1:W:488:LYS:O	1:W:490:CYS:HB2	2.18	0.43
2:D:20:GLU:HA	2:D:39:LYS:HA	2.00	0.43
1:G:451:TYR:HE1	1:G:515:GLU:HG2	1.82	0.43
1:G:487:ARG:HE	1:G:487:ARG:HB2	1.69	0.43
2:H:34:ILE:HG13	2:H:51:TYR:CD2	2.53	0.43
1:I:402:ILE:C	1:I:404:THR:N	2.75	0.43
1:I:416:ILE:HG12	1:I:553:CYS:SG	2.58	0.43
1:K:405:LEU:HD23	1:K:405:LEU:HA	1.72	0.43
1:K:484:ILE:HG21	1:K:512:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:454:VAL:O	1:M:455:LYS:C	2.61	0.43
1:O:389:LEU:HD12	1:O:402:ILE:HG21	1.99	0.43
1:Q:509:LEU:C	1:Q:511:TYR:H	2.26	0.43
2:X:83:GLU:O	2:X:84:GLU:C	2.60	0.43
2:D:57:VAL:HG13	2:D:58:PRO:HD2	2.01	0.43
1:E:394:LYS:HD3	1:E:396:ARG:HH22	1.82	0.43
1:E:426:ARG:O	1:E:427:ASN:C	2.61	0.43
2:F:45:LYS:O	2:F:49:GLU:HG3	2.17	0.43
1:G:544:ASN:OD1	1:G:544:ASN:C	2.61	0.43
1:M:443:TYR:O	1:M:444:PRO:C	2.60	0.43
1:Q:405:LEU:HD21	1:Q:415:VAL:HG11	2.00	0.43
1:U:405:LEU:HD23	1:U:411:LEU:HD22	2.00	0.43
1:A:483:VAL:HG21	1:A:559:ILE:HD13	2.00	0.43
1:C:388:ILE:HD13	1:C:388:ILE:HA	1.66	0.43
1:C:437:VAL:HG23	1:C:470:LEU:HB2	1.99	0.43
1:E:443:TYR:OH	1:E:504:ILE:HG12	2.18	0.43
1:E:504:ILE:HA	1:E:507:ILE:HD12	1.99	0.43
1:E:559:ILE:H	1:E:559:ILE:HG12	1.57	0.43
1:G:486:LEU:CD2	1:G:529:TRP:HH2	2.32	0.43
1:G:511:TYR:CZ	1:G:515:GLU:HG3	2.53	0.43
1:K:392:ALA:C	1:K:394:LYS:N	2.74	0.43
1:K:495:ASP:OD2	1:K:498:GLY:N	2.50	0.43
1:O:492:LYS:HB3	1:O:534:MET:HE2	2.00	0.43
2:R:26:VAL:HG22	2:R:88:ILE:HB	1.99	0.43
2:V:82:MET:HA	2:V:86:ASP:OD2	2.17	0.43
1:W:412:ASN:HA	2:X:94:GLN:O	2.18	0.43
2:X:76:THR:HG23	2:X:79:GLU:HB2	2.00	0.43
1:A:406:LYS:O	1:A:409:HIS:HB2	2.18	0.43
1:G:535:LYS:O	1:G:538:GLU:N	2.36	0.43
1:O:424:VAL:CG1	1:O:435:LEU:HB3	2.48	0.43
1:A:484:ILE:HG12	1:A:491:LEU:HD12	1.98	0.43
1:A:502:HIS:O	1:A:506:GLU:HG3	2.19	0.43
1:E:442:PHE:O	1:E:445:LYS:HB3	2.19	0.43
1:E:514:ASP:O	1:E:517:LYS:HB2	2.18	0.43
1:G:467:GLU:HB3	1:G:487:ARG:CD	2.40	0.43
1:O:470:LEU:HD13	1:O:556:ALA:HB1	2.00	0.43
2:R:63:ARG:O	2:R:90:VAL:HA	2.18	0.43
1:S:474:HIS:CD2	2:T:94:GLN:HB3	2.54	0.43
2:T:52:CYS:SG	2:T:62:LEU:HD12	2.59	0.43
1:W:463:LEU:CD2	1:W:469:ILE:HD12	2.47	0.43
1:A:473:ILE:HG21	1:A:504:ILE:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:388:ILE:HD11	1:C:396:ARG:CB	2.48	0.43
1:G:451:TYR:CE1	1:G:515:GLU:HG2	2.54	0.43
1:G:458:THR:CG2	1:G:511:TYR:OH	2.66	0.43
1:I:535:LYS:HB3	1:I:537:HIS:CE1	2.54	0.43
1:I:567:PHE:HA	1:I:571:GLN:NE2	2.34	0.43
2:J:28:GLY:O	2:J:29:GLN:C	2.61	0.43
1:M:371:ASP:OD1	1:M:371:ASP:N	2.51	0.43
1:O:443:TYR:CE1	1:O:504:ILE:HG23	2.53	0.43
1:O:544:ASN:HD21	1:O:547:ASP:CG	2.27	0.43
1:S:486:LEU:HD23	1:S:486:LEU:HA	1.75	0.43
1:U:401:ASP:O	1:U:404:THR:OG1	2.36	0.43
1:U:462:ASN:OD1	1:U:464:PHE:N	2.49	0.43
1:E:403:GLN:O	1:E:409:HIS:ND1	2.52	0.43
1:I:469:ILE:HD12	1:I:484:ILE:CG2	2.48	0.43
1:K:376:ILE:HG23	1:K:580:VAL:HG21	2.01	0.43
1:M:429:LYS:HB3	1:M:429:LYS:HE3	1.22	0.43
1:Q:468:ILE:H	1:Q:468:ILE:HG13	1.59	0.43
2:X:84:GLU:OE1	2:X:84:GLU:HA	2.18	0.43
2:F:66:TRP:HB2	2:F:71:ILE:HD11	2.01	0.43
1:G:372:MET:O	1:G:373:GLU:C	2.62	0.43
2:L:65:LEU:HD12	2:L:70:ARG:HD3	2.01	0.43
1:M:446:LEU:HD21	1:M:511:TYR:HB2	2.00	0.43
1:M:487:ARG:HE	1:M:487:ARG:HB2	1.57	0.43
2:P:72:ALA:O	2:P:75:HIS:HB2	2.19	0.43
2:R:66:TRP:HZ3	2:R:80:LEU:O	1.99	0.43
1:S:396:ARG:HH12	2:T:72:ALA:HB1	1.84	0.43
1:S:428:LYS:HE2	1:S:428:LYS:HB3	1.63	0.43
1:W:489:LYS:HB3	1:W:529:TRP:CD2	2.53	0.43
2:X:38:VAL:HG11	2:X:47:LEU:HD12	2.01	0.43
1:A:524:LEU:HD13	1:A:524:LEU:HA	1.87	0.43
1:C:474:HIS:NE2	2:D:94:GLN:HB3	2.34	0.43
1:C:476:LYS:O	1:C:476:LYS:HG3	2.19	0.43
2:F:24:LEU:HD13	2:F:88:ILE:HD11	2.01	0.43
1:G:374:LYS:O	1:G:378:ASN:ND2	2.51	0.43
2:T:27:ILE:CG2	2:T:28:GLY:N	2.82	0.43
1:C:377:SER:O	1:C:378:ASN:C	2.62	0.42
1:E:471:VAL:O	1:E:481:LEU:HA	2.19	0.42
1:G:462:ASN:O	1:G:463:LEU:C	2.63	0.42
1:I:380:LEU:HD23	1:I:402:ILE:HG23	2.01	0.42
1:K:382:HIS:CD2	1:K:382:HIS:C	2.96	0.42
2:R:62:LEU:HB3	2:R:90:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:559:ILE:C	1:S:561:ARG:N	2.77	0.42
1:S:578:LYS:O	1:S:581:TRP:HB3	2.19	0.42
2:D:32:SER:HB3	2:D:55:GLN:OE1	2.18	0.42
1:E:558:TYR:HD2	1:E:565:ILE:HG13	1.84	0.42
1:I:511:TYR:CD2	1:I:511:TYR:C	2.94	0.42
1:I:582:GLU:HG2	1:I:588:LEU:HA	2.02	0.42
2:N:72:ALA:O	2:N:75:HIS:HB2	2.19	0.42
1:Q:397:ILE:CD1	1:Q:414:GLU:O	2.67	0.42
1:Q:503:ARG:HG3	1:Q:504:ILE:N	2.34	0.42
1:S:398:THR:O	1:S:401:ASP:N	2.52	0.42
1:U:487:ARG:HE	1:U:487:ARG:HB2	1.65	0.42
1:U:513:GLN:C	1:U:513:GLN:HE21	2.27	0.42
2:V:49:GLU:H	2:V:49:GLU:HG2	1.62	0.42
2:X:63:ARG:HH22	2:X:93:GLU:HG3	1.82	0.42
1:C:524:LEU:HD13	1:C:524:LEU:HA	1.92	0.42
1:I:456:ARG:H	1:I:456:ARG:HG2	1.41	0.42
1:K:392:ALA:C	1:K:393:PHE:CD2	2.98	0.42
1:O:542:GLN:HB2	1:O:551:PHE:CE2	2.54	0.42
2:X:40:MET:HE1	2:X:82:MET:O	2.19	0.42
1:E:417:ASN:OD1	1:E:440:THR:CG2	2.68	0.42
2:F:70:ARG:CG	2:F:71:ILE:N	2.80	0.42
1:G:399:ARG:O	1:G:403:GLN:CG	2.68	0.42
1:G:421:ASN:O	1:G:425:GLU:HG2	2.19	0.42
1:I:462:ASN:O	1:I:463:LEU:C	2.62	0.42
2:J:76:THR:O	2:J:79:GLU:N	2.52	0.42
1:M:462:ASN:HB3	1:M:465:GLU:HG2	2.01	0.42
1:Q:399:ARG:O	1:Q:403:GLN:CG	2.67	0.42
1:S:379:ALA:HB2	1:S:584:LEU:HD11	2.01	0.42
1:U:537:HIS:NE2	1:U:538:GLU:HG2	2.34	0.42
1:E:517:LYS:O	1:E:521:ASN:N	2.53	0.42
1:G:495:ASP:CG	1:G:497:MET:H	2.27	0.42
1:I:542:GLN:HG2	1:I:544:ASN:O	2.19	0.42
1:O:440:THR:OG1	1:O:479:TRP:HH2	2.02	0.42
1:S:413:ASP:HB2	1:S:440:THR:HG21	2.01	0.42
1:S:441:PHE:O	1:S:444:PRO:HD2	2.19	0.42
1:S:457:TRP:C	1:S:459:LYS:H	2.27	0.42
2:T:26:VAL:HG22	2:T:88:ILE:HB	2.00	0.42
1:U:550:MET:SD	1:U:579:MET:HE1	2.59	0.42
1:U:555:TYR:O	1:U:559:ILE:HG12	2.19	0.42
1:E:478:HIS:CE1	1:E:497:MET:HB2	2.55	0.42
1:G:418:PHE:CE1	1:G:583:ILE:HG23	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:37:LYS:H	2:H:37:LYS:HD2	1.83	0.42
1:I:579:MET:O	1:I:580:VAL:C	2.62	0.42
2:J:70:ARG:CG	2:J:70:ARG:NH1	2.62	0.42
1:Q:419:TYR:CE2	1:Q:553:CYS:HB3	2.55	0.42
1:S:393:PHE:CE2	1:S:421:ASN:HB3	2.54	0.42
1:C:398:THR:O	1:C:401:ASP:N	2.52	0.42
2:D:53:GLN:O	2:D:55:GLN:N	2.53	0.42
1:E:475:ARG:O	1:E:476:LYS:C	2.62	0.42
2:F:76:THR:HG23	2:F:78:LYS:HB3	2.02	0.42
1:G:475:ARG:O	1:G:476:LYS:C	2.62	0.42
1:K:410:TRP:CZ3	1:K:477:VAL:HG12	2.55	0.42
1:Q:411:LEU:O	1:Q:479:TRP:NE1	2.35	0.42
1:Q:411:LEU:HD11	1:Q:549:GLY:C	2.45	0.42
1:Q:469:ILE:HD11	1:Q:486:LEU:HD11	2.02	0.42
2:T:45:LYS:HB3	2:T:73:ASP:HB3	2.00	0.42
1:U:581:TRP:O	1:U:582:GLU:C	2.63	0.42
1:W:540:PRO:HG3	1:W:567:PHE:O	2.20	0.42
1:I:393:PHE:C	1:I:395:LEU:H	2.26	0.42
1:I:403:GLN:O	1:I:405:LEU:N	2.53	0.42
1:I:582:GLU:OE2	1:I:589:LEU:N	2.43	0.42
2:J:63:ARG:CZ	2:J:93:GLU:HB2	2.50	0.42
1:K:486:LEU:HD23	1:K:486:LEU:HA	1.81	0.42
1:M:474:HIS:HB2	1:M:479:TRP:CZ3	2.54	0.42
1:O:420:MET:HB3	1:O:437:VAL:HG21	2.01	0.42
2:P:84:GLU:O	2:P:85:GLU:HB2	2.19	0.42
1:S:393:PHE:CD2	1:S:421:ASN:HB2	2.54	0.42
1:S:574:LEU:HD13	1:S:578:LYS:CE	2.47	0.42
1:W:444:PRO:C	1:W:446:LEU:H	2.27	0.42
1:C:410:TRP:CZ3	1:C:477:VAL:HB	2.51	0.42
2:D:54:ARG:NH2	2:H:40:MET:HE2	2.33	0.42
1:E:426:ARG:HD2	1:E:427:ASN:H	1.79	0.42
1:E:438:PHE:CZ	1:E:463:LEU:HD11	2.48	0.42
1:I:399:ARG:O	1:I:403:GLN:HG2	2.20	0.42
1:I:501:GLY:O	1:I:502:HIS:C	2.62	0.42
1:M:491:LEU:O	1:M:531:HIS:HA	2.19	0.42
1:M:550:MET:SD	1:M:579:MET:HE3	2.59	0.42
1:A:400:GLY:HA2	1:A:403:GLN:HG3	2.02	0.42
2:B:44:LEU:O	2:B:48:MET:HG3	2.20	0.42
1:E:554:LYS:HB3	1:E:567:PHE:CE2	2.55	0.42
1:G:414:GLU:HA	1:G:414:GLU:OE1	2.20	0.42
1:G:459:LYS:HD2	1:G:459:LYS:HA	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:490:CYS:O	1:I:491:LEU:HD12	2.20	0.42
1:I:542:GLN:HA	1:I:551:PHE:HE2	1.85	0.42
2:R:51:TYR:O	2:R:55:GLN:HG2	2.19	0.42
1:S:581:TRP:CZ2	1:S:585:HIS:CD2	3.07	0.42
2:V:76:THR:O	2:V:79:GLU:N	2.53	0.42
1:W:486:LEU:HA	1:W:486:LEU:HD23	1.68	0.42
1:E:452:GLN:OE1	1:E:452:GLN:HA	2.20	0.41
1:G:489:LYS:HB3	1:G:529:TRP:CD2	2.55	0.41
1:I:462:ASN:HB3	1:I:465:GLU:HG3	2.00	0.41
1:K:495:ASP:OD2	1:K:497:MET:C	2.63	0.41
1:K:550:MET:HE3	1:K:550:MET:HB3	1.94	0.41
2:N:22:ILE:HD11	2:N:83:GLU:C	2.45	0.41
1:O:473:ILE:HD11	1:O:482:VAL:HG23	2.02	0.41
1:Q:474:HIS:CD2	2:R:94:GLN:HB3	2.55	0.41
1:S:454:VAL:O	1:S:455:LYS:C	2.62	0.41
1:W:387:GLU:O	1:W:398:THR:HA	2.20	0.41
1:W:454:VAL:O	1:W:455:LYS:C	2.63	0.41
1:A:485:ASP:CG	1:A:488:LYS:HG3	2.45	0.41
2:F:92:GLN:H	2:F:92:GLN:HG2	1.42	0.41
1:I:501:GLY:O	1:I:504:ILE:N	2.44	0.41
1:Q:476:LYS:HB3	1:Q:476:LYS:HZ3	1.84	0.41
1:Q:550:MET:HE2	1:Q:575:PHE:HB3	2.02	0.41
1:Q:569:GLN:HG3	1:Q:569:GLN:O	2.21	0.41
1:S:391:SER:HB3	1:S:396:ARG:HE	1.84	0.41
2:X:29:GLN:HG2	2:X:92:GLN:HG2	2.02	0.41
1:A:426:ARG:C	1:A:426:ARG:HD2	2.45	0.41
1:A:484:ILE:HD13	1:A:512:LEU:HD11	2.02	0.41
1:C:423:LEU:O	1:C:424:VAL:C	2.63	0.41
1:C:501:GLY:O	1:C:504:ILE:N	2.54	0.41
2:D:64:PHE:CE1	2:D:90:VAL:HG22	2.55	0.41
1:Q:487:ARG:NH2	1:Q:562:ASP:CG	2.78	0.41
1:S:436:HIS:O	1:S:469:ILE:HA	2.20	0.41
1:U:424:VAL:O	1:U:424:VAL:CG1	2.68	0.41
2:V:25:LYS:HG2	2:V:35:HIS:ND1	2.34	0.41
1:W:398:THR:OG1	1:W:400:GLY:N	2.51	0.41
1:W:474:HIS:NE2	2:X:95:THR:O	2.53	0.41
1:A:389:LEU:HD23	1:A:389:LEU:HA	1.92	0.41
2:B:21:TYR:CD1	2:B:21:TYR:N	2.88	0.41
1:E:489:LYS:HG3	1:E:529:TRP:NE1	2.35	0.41
1:I:403:GLN:C	1:I:405:LEU:H	2.28	0.41
1:K:567:PHE:CD1	1:K:567:PHE:C	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:39:LYS:O	2:L:42:THR:HB	2.20	0.41
1:M:371:ASP:O	1:M:374:LYS:HE2	2.20	0.41
1:M:455:LYS:HE2	1:M:456:ARG:HH21	1.85	0.41
1:O:439:SER:O	1:O:442:PHE:HB3	2.20	0.41
2:P:44:LEU:HD21	2:P:77:PRO:HD3	2.01	0.41
2:R:27:ILE:HG22	2:R:33:GLU:CB	2.50	0.41
1:S:403:GLN:O	1:S:409:HIS:CD2	2.74	0.41
1:U:376:ILE:HG12	1:U:580:VAL:CG2	2.49	0.41
1:U:391:SER:O	1:U:392:ALA:HB2	2.20	0.41
1:W:376:ILE:HG12	1:W:580:VAL:HG22	2.01	0.41
1:A:458:THR:HG21	1:A:511:TYR:OH	2.21	0.41
1:E:433:PRO:HB2	1:E:468:ILE:CD1	2.50	0.41
1:E:581:TRP:CE2	1:E:585:HIS:CD2	3.09	0.41
1:G:427:ASN:HD22	1:G:435:LEU:HB2	1.84	0.41
1:K:457:TRP:CD1	1:K:457:TRP:N	2.89	0.41
1:O:393:PHE:CE2	1:O:421:ASN:HB3	2.55	0.41
1:O:403:GLN:O	1:O:406:LYS:HB2	2.20	0.41
1:Q:488:LYS:HB2	1:Q:488:LYS:HE3	1.88	0.41
1:S:442:PHE:HD1	1:S:443:TYR:N	2.18	0.41
1:S:511:TYR:CD2	1:S:511:TYR:C	2.94	0.41
1:U:441:PHE:HZ	2:V:63:ARG:HG3	1.81	0.41
2:V:43:HIS:CD2	2:V:43:HIS:H	2.38	0.41
1:W:442:PHE:HA	1:W:457:TRP:HZ3	1.84	0.41
1:A:369:THR:HG22	1:A:370:GLU:H	1.85	0.41
2:B:65:LEU:O	2:B:89:GLU:N	2.50	0.41
1:C:394:LYS:HE2	1:C:394:LYS:N	2.28	0.41
2:D:39:LYS:H	2:D:39:LYS:CD	2.31	0.41
1:E:441:PHE:O	1:E:444:PRO:HD2	2.20	0.41
1:E:558:TYR:CD2	1:E:565:ILE:HG13	2.56	0.41
1:G:495:ASP:OD1	1:G:496:SER:N	2.54	0.41
1:M:372:MET:HG2	1:M:581:TRP:NE1	2.35	0.41
1:M:394:LYS:HD3	1:M:396:ARG:NH2	2.35	0.41
1:O:416:ILE:O	1:O:420:MET:HG2	2.21	0.41
1:U:394:LYS:HA	1:U:396:ARG:HH21	1.85	0.41
1:U:572:MET:O	1:U:575:PHE:HB2	2.20	0.41
1:W:398:THR:HG23	1:W:401:ASP:CG	2.46	0.41
1:W:551:PHE:CE1	1:W:572:MET:HE3	2.56	0.41
2:B:47:LEU:C	2:B:47:LEU:CD2	2.94	0.41
2:D:22:ILE:CG1	2:D:23:LYS:N	2.83	0.41
2:D:63:ARG:HD2	2:D:70:ARG:HH21	1.85	0.41
2:F:46:LYS:O	2:F:47:LEU:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:369:THR:HG22	1:G:372:MET:HB2	2.03	0.41
1:G:548:SER:HB3	2:H:97:GLY:O	2.19	0.41
1:I:483:VAL:HG21	1:I:559:ILE:HG21	2.03	0.41
1:M:456:ARG:HB2	2:N:67:GLU:HG2	2.02	0.41
1:S:415:VAL:HG12	1:S:416:ILE:N	2.36	0.41
1:U:454:VAL:O	1:U:457:TRP:HB2	2.20	0.41
2:V:36:PHE:HB3	2:V:38:VAL:HG13	2.02	0.41
1:W:473:ILE:HD13	1:W:473:ILE:HA	1.91	0.41
2:X:76:THR:O	2:X:79:GLU:N	2.53	0.41
1:C:423:LEU:HD23	1:C:588:LEU:HD11	2.02	0.41
1:C:428:LYS:HB2	1:I:408:TYR:CE2	2.56	0.41
1:C:474:HIS:ND1	1:C:474:HIS:O	2.53	0.41
1:E:485:ASP:HB3	1:E:488:LYS:CB	2.51	0.41
1:G:420:MET:HE3	1:G:472:PRO:HG3	2.02	0.41
1:K:392:ALA:C	1:K:394:LYS:H	2.28	0.41
1:K:418:PHE:O	1:K:419:TYR:C	2.63	0.41
1:O:485:ASP:OD1	1:O:485:ASP:C	2.64	0.41
1:O:572:MET:HB3	1:O:573:PRO:HD3	2.01	0.41
1:Q:411:LEU:HD11	1:Q:549:GLY:O	2.21	0.41
2:T:76:THR:HG23	2:T:78:LYS:HB3	2.02	0.41
1:U:452:GLN:OE1	1:U:455:LYS:HD3	2.21	0.41
1:U:564:PRO:O	1:U:566:THR:HG23	2.20	0.41
1:W:535:LYS:HA	1:W:536:PRO:HD2	1.62	0.41
1:A:547:ASP:O	1:A:550:MET:N	2.49	0.41
1:A:551:PHE:CD1	1:A:572:MET:HE3	2.55	0.41
1:A:588:LEU:O	1:A:589:LEU:HD23	2.21	0.41
1:C:443:TYR:CE1	1:C:504:ILE:HG23	2.56	0.41
1:C:443:TYR:OH	1:C:504:ILE:HG12	2.21	0.41
1:E:433:PRO:HB2	1:E:468:ILE:HD12	2.03	0.41
1:E:550:MET:CE	1:E:579:MET:CE	2.99	0.41
1:G:407:ASN:HD22	1:K:428:LYS:HE3	1.84	0.41
1:G:456:ARG:O	1:G:459:LYS:HB2	2.21	0.41
1:G:525:ASN:C	1:G:527:LEU:N	2.79	0.41
1:I:403:GLN:C	1:I:405:LEU:N	2.78	0.41
1:I:446:LEU:O	1:I:448:SER:N	2.54	0.41
1:K:376:ILE:HG12	1:K:580:VAL:HG22	2.03	0.41
1:K:391:SER:O	1:K:392:ALA:CB	2.69	0.41
1:M:459:LYS:HA	1:M:459:LYS:HD2	1.80	0.41
1:M:493:TYR:CE2	1:M:495:ASP:HB2	2.56	0.41
1:O:413:ASP:HB3	2:P:94:GLN:OE1	2.20	0.41
1:S:484:ILE:HG21	1:S:512:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:419:TYR:O	1:U:420:MET:C	2.63	0.41
2:V:91:TYR:CD1	2:V:91:TYR:N	2.89	0.41
1:W:396:ARG:NH1	2:X:74:ASN:HD22	2.18	0.41
2:B:57:VAL:HG12	2:B:61:SER:HB3	2.02	0.41
1:C:565:ILE:H	1:C:565:ILE:HG12	1.37	0.41
1:E:369:THR:HG22	1:E:371:ASP:H	1.85	0.41
1:E:408:TYR:CE1	1:I:434:ALA:HB2	2.56	0.41
1:E:443:TYR:CD1	1:E:443:TYR:C	2.99	0.41
1:K:410:TRP:CB	2:L:96:GLY:O	2.68	0.41
1:K:413:ASP:HB3	2:L:94:GLN:HG3	2.02	0.41
1:K:493:TYR:HB3	1:K:533:SER:HA	2.03	0.41
2:N:47:LEU:C	2:N:47:LEU:CD2	2.94	0.41
1:O:416:ILE:HD12	1:O:479:TRP:CZ2	2.56	0.41
1:S:467:GLU:OE1	1:S:487:ARG:HD3	2.21	0.41
1:W:486:LEU:HD22	1:W:529:TRP:HH2	1.86	0.41
1:A:394:LYS:HD3	1:A:394:LYS:HA	1.91	0.40
2:B:20:GLU:C	2:B:21:TYR:HD1	2.29	0.40
2:D:43:HIS:HA	2:D:75:HIS:O	2.21	0.40
2:D:66:TRP:CH2	2:D:80:LEU:O	2.74	0.40
1:G:427:ASN:ND2	1:G:435:LEU:HB2	2.36	0.40
1:I:406:LYS:HB2	1:I:409:HIS:ND1	2.36	0.40
1:I:530:THR:O	1:I:531:HIS:HB3	2.21	0.40
1:I:561:ARG:O	1:I:562:ASP:HB2	2.22	0.40
1:K:394:LYS:HE2	1:K:394:LYS:N	2.36	0.40
1:M:369:THR:HG22	1:M:370:GLU:N	2.36	0.40
1:Q:581:TRP:C	1:Q:583:ILE:N	2.76	0.40
1:U:394:LYS:HE2	1:U:394:LYS:N	2.25	0.40
1:U:424:VAL:O	1:U:424:VAL:HG12	2.20	0.40
2:V:34:ILE:HD12	2:V:51:TYR:CE1	2.57	0.40
2:V:45:LYS:O	2:V:49:GLU:HG2	2.21	0.40
1:W:392:ALA:C	1:W:394:LYS:H	2.29	0.40
1:A:494:LEU:HD12	1:A:494:LEU:N	2.36	0.40
2:B:31:SER:HB3	2:B:51:TYR:OH	2.21	0.40
1:C:574:LEU:HD22	1:C:578:LYS:HE3	2.04	0.40
1:E:411:LEU:HD13	1:E:415:VAL:HG11	2.04	0.40
1:I:387:GLU:OE1	1:I:399:ARG:NH1	2.54	0.40
2:L:45:LYS:HB2	2:L:73:ASP:HB3	2.03	0.40
1:M:393:PHE:CD2	1:M:421:ASN:HB3	2.55	0.40
1:S:570:HIS:ND1	1:S:570:HIS:N	2.68	0.40
1:U:440:THR:HB	2:V:94:GLN:OE1	2.21	0.40
1:W:458:THR:HG21	1:W:463:LEU:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:ILE:HG13	1:A:418:PHE:CD2	2.56	0.40
1:A:582:GLU:HA	1:A:587:GLN:O	2.22	0.40
1:E:404:THR:HB	1:E:411:LEU:HA	2.03	0.40
1:I:417:ASN:ND2	1:I:440:THR:CG2	2.76	0.40
1:I:509:LEU:HD12	1:I:509:LEU:O	2.21	0.40
1:K:502:HIS:ND1	1:K:502:HIS:N	2.68	0.40
1:M:426:ARG:O	1:M:427:ASN:C	2.63	0.40
2:T:66:TRP:CB	2:T:71:ILE:HD11	2.52	0.40
1:U:419:TYR:CE2	1:U:423:LEU:HD21	2.56	0.40
2:V:77:PRO:CA	2:V:80:LEU:HD12	2.31	0.40
1:E:561:ARG:O	1:E:562:ASP:HB2	2.21	0.40
1:K:463:LEU:HD23	1:K:463:LEU:HA	1.66	0.40
1:M:496:SER:HA	1:M:555:TYR:OH	2.21	0.40
1:O:515:GLU:OE2	1:O:519:LYS:NZ	2.55	0.40
1:U:442:PHE:HA	1:U:457:TRP:HZ3	1.85	0.40
1:W:482:VAL:HA	1:W:492:LYS:O	2.21	0.40
2:X:40:MET:O	2:X:77:PRO:HG2	2.20	0.40
1:A:405:LEU:O	1:A:576:ARG:HD3	2.22	0.40
2:B:64:PHE:N	2:B:64:PHE:CD1	2.90	0.40
1:C:380:LEU:HD23	1:C:402:ILE:HG23	2.04	0.40
1:E:511:TYR:CD1	1:E:511:TYR:C	3.00	0.40
1:G:385:GLN:OE1	1:G:385:GLN:CA	2.69	0.40
1:I:487:ARG:HE	1:I:487:ARG:HB2	1.58	0.40
1:I:501:GLY:O	1:I:504:ILE:HG12	2.22	0.40
1:I:550:MET:HB3	1:I:550:MET:HE3	1.67	0.40
1:K:574:LEU:O	1:K:575:PHE:C	2.65	0.40
2:L:57:VAL:HG12	2:L:58:PRO:CD	2.51	0.40
1:M:405:LEU:CD2	1:M:411:LEU:HD22	2.43	0.40
1:Q:401:ASP:CA	1:Q:412:ASN:HD21	2.26	0.40
1:U:467:GLU:HB3	1:U:487:ARG:HD3	2.02	0.40
2:V:37:LYS:HD2	2:V:37:LYS:H	1.87	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:377:SER:OG	1:S:429:LYS:O[1_544]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	221/224 (99%)	199 (90%)	19 (9%)	3 (1%)	9	36
1	C	222/224 (99%)	187 (84%)	30 (14%)	5 (2%)	5	25
1	E	222/224 (99%)	185 (83%)	31 (14%)	6 (3%)	4	22
1	G	221/224 (99%)	192 (87%)	21 (10%)	8 (4%)	2	16
1	I	221/224 (99%)	172 (78%)	38 (17%)	11 (5%)	1	10
1	K	221/224 (99%)	183 (83%)	30 (14%)	8 (4%)	2	16
1	M	220/224 (98%)	189 (86%)	27 (12%)	4 (2%)	6	31
1	O	221/224 (99%)	198 (90%)	20 (9%)	3 (1%)	9	36
1	Q	222/224 (99%)	188 (85%)	29 (13%)	5 (2%)	5	25
1	S	222/224 (99%)	195 (88%)	23 (10%)	4 (2%)	6	31
1	U	221/224 (99%)	194 (88%)	26 (12%)	1 (0%)	24	60
1	W	220/224 (98%)	189 (86%)	24 (11%)	7 (3%)	3	18
2	B	76/78 (97%)	68 (90%)	7 (9%)	1 (1%)	9	38
2	D	76/78 (97%)	61 (80%)	11 (14%)	4 (5%)	1	9
2	F	76/78 (97%)	65 (86%)	10 (13%)	1 (1%)	9	38
2	H	75/78 (96%)	69 (92%)	6 (8%)	0	100	100
2	J	76/78 (97%)	70 (92%)	5 (7%)	1 (1%)	9	38
2	L	75/78 (96%)	69 (92%)	5 (7%)	1 (1%)	9	38
2	N	76/78 (97%)	69 (91%)	5 (7%)	2 (3%)	4	23
2	P	76/78 (97%)	68 (90%)	8 (10%)	0	100	100
2	R	76/78 (97%)	63 (83%)	12 (16%)	1 (1%)	9	38
2	T	76/78 (97%)	71 (93%)	3 (4%)	2 (3%)	4	23
2	V	76/78 (97%)	66 (87%)	9 (12%)	1 (1%)	9	38
2	X	76/78 (97%)	67 (88%)	6 (8%)	3 (4%)	2	14
All	All	3564/3624 (98%)	3077 (86%)	405 (11%)	82 (2%)	5	25

All (82) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	459	LYS
2	F	31	SER
1	G	502	HIS
1	G	570	HIS
1	I	502	HIS
1	I	548	SER
1	Q	536	PRO
2	T	29	GLN
1	W	477	VAL
1	W	536	PRO
1	C	455	LYS
1	C	477	VAL
1	C	502	HIS
2	D	75	HIS
2	D	78	LYS
1	E	455	LYS
1	E	502	HIS
1	E	504	ILE
1	G	498	GLY
1	G	526	LEU
1	I	446	LEU
1	I	447	LYS
1	I	552	THR
1	K	548	SER
2	N	46	LYS
1	Q	527	LEU
1	S	458	THR
1	S	459	LYS
1	S	460	GLY
1	S	565	ILE
1	A	459	LYS
1	A	475	ARG
2	B	29	GLN
1	C	545	GLY
1	C	562	ASP
2	D	54	ARG
1	E	556	ALA
1	G	448	SER
2	J	73	ASP
1	K	385	GLN
1	K	406	LYS
1	K	526	LEU

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Mol	Chain	Res	Type
1	M	455	LYS
1	O	433	PRO
1	O	455	LYS
2	X	67	GLU
2	D	44	LEU
1	I	442	PHE
1	K	478	HIS
1	Q	544	ASN
2	R	27	ILE
1	U	502	HIS
1	W	489	LYS
1	E	555	TYR
1	G	476	LYS
1	G	559	ILE
1	I	531	HIS
1	I	580	VAL
1	K	392	ALA
1	K	399	ARG
1	M	448	SER
1	M	466	GLN
2	N	45	LYS
1	O	552	THR
1	Q	403	GLN
1	W	442	PHE
1	I	424	VAL
1	I	496	SER
2	L	93	GLU
1	M	442	PHE
1	W	447	LYS
1	W	476	LYS
2	X	60	ASN
1	A	460	GLY
2	T	38	VAL
1	W	444	PRO
1	I	549	GLY
1	K	450	GLY
2	X	58	PRO
1	G	477	VAL
1	Q	477	VAL
2	V	34	ILE

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	207/208 (100%)	179 (86%)	28 (14%)	4	18
1	C	207/208 (100%)	163 (79%)	44 (21%)	1	6
1	E	207/208 (100%)	172 (83%)	35 (17%)	2	11
1	G	207/208 (100%)	184 (89%)	23 (11%)	6	25
1	I	207/208 (100%)	170 (82%)	37 (18%)	2	10
1	K	207/208 (100%)	177 (86%)	30 (14%)	3	15
1	M	206/208 (99%)	168 (82%)	38 (18%)	1	9
1	O	207/208 (100%)	173 (84%)	34 (16%)	2	12
1	Q	207/208 (100%)	177 (86%)	30 (14%)	3	15
1	S	207/208 (100%)	168 (81%)	39 (19%)	1	9
1	U	207/208 (100%)	186 (90%)	21 (10%)	7	29
1	W	206/208 (99%)	170 (82%)	36 (18%)	2	10
2	B	71/71 (100%)	54 (76%)	17 (24%)	1	4
2	D	71/71 (100%)	62 (87%)	9 (13%)	4	20
2	F	71/71 (100%)	52 (73%)	19 (27%)	0	2
2	H	70/71 (99%)	51 (73%)	19 (27%)	0	2
2	J	71/71 (100%)	48 (68%)	23 (32%)	0	1
2	L	70/71 (99%)	58 (83%)	12 (17%)	2	11
2	N	71/71 (100%)	54 (76%)	17 (24%)	1	4
2	P	71/71 (100%)	57 (80%)	14 (20%)	1	8
2	R	71/71 (100%)	57 (80%)	14 (20%)	1	8
2	T	71/71 (100%)	59 (83%)	12 (17%)	2	11
2	V	71/71 (100%)	55 (78%)	16 (22%)	1	5
2	X	71/71 (100%)	54 (76%)	17 (24%)	1	4
All	All	3332/3348 (100%)	2748 (82%)	584 (18%)	2	10

All (584) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	369	THR
1	A	373	GLU
1	A	374	LYS
1	A	396	ARG
1	A	399	ARG
1	A	402	ILE
1	A	403	GLN
1	A	411	LEU
1	A	437	VAL
1	A	439	SER
1	A	448	SER
1	A	458	THR
1	A	459	LYS
1	A	488	LYS
1	A	491	LEU
1	A	497	MET
1	A	513	GLN
1	A	515	GLU
1	A	517	LYS
1	A	522	SER
1	A	524	LEU
1	A	527	LEU
1	A	544	ASN
1	A	559	ILE
1	A	568	THR
1	A	574	LEU
1	A	580	VAL
1	A	583	ILE
2	B	25	LYS
2	B	30	ASP
2	B	37	LYS
2	B	38	VAL
2	B	39	LYS
2	B	47	LEU
2	B	59	MET
2	B	60	ASN
2	B	69	GLN
2	B	74	ASN
2	B	76	THR
2	B	78	LYS
2	B	82	MET
2	B	83	GLU
2	B	89	GLU

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Mol	Chain	Res	Type
2	B	93	GLU
2	B	94	GLN
1	C	368	LEU
1	C	375	GLU
1	C	382	HIS
1	C	388	ILE
1	C	391	SER
1	C	395	LEU
1	C	396	ARG
1	C	397	ILE
1	C	398	THR
1	C	402	ILE
1	C	404	THR
1	C	407	ASN
1	C	411	LEU
1	C	415	VAL
1	C	422	LEU
1	C	437	VAL
1	C	439	SER
1	C	454	VAL
1	C	458	THR
1	C	459	LYS
1	C	461	VAL
1	C	465	GLU
1	C	471	VAL
1	C	475	ARG
1	C	476	LYS
1	C	480	SER
1	C	483	VAL
1	C	484	ILE
1	C	490	CYS
1	C	494	LEU
1	C	496	SER
1	C	499	GLN
1	C	502	HIS
1	C	503	ARG
1	C	515	GLU
1	C	523	ASP
1	C	524	LEU
1	C	525	ASN
1	C	530	THR
1	C	557	ASP

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Mol	Chain	Res	Type
1	C	565	ILE
1	C	574	LEU
1	C	580	VAL
1	C	584	LEU
2	D	22	ILE
2	D	30	ASP
2	D	37	LYS
2	D	39	LYS
2	D	57	VAL
2	D	59	MET
2	D	63	ARG
2	D	78	LYS
2	D	93	GLU
1	E	367	GLU
1	E	374	LYS
1	E	378	ASN
1	E	382	HIS
1	E	394	LYS
1	E	396	ARG
1	E	402	ILE
1	E	404	THR
1	E	411	LEU
1	E	426	ARG
1	E	440	THR
1	E	458	THR
1	E	459	LYS
1	E	469	ILE
1	E	489	LYS
1	E	492	LYS
1	E	494	LEU
1	E	495	ASP
1	E	500	LYS
1	E	502	HIS
1	E	512	LEU
1	E	518	THR
1	E	519	LYS
1	E	523	ASP
1	E	524	LEU
1	E	531	HIS
1	E	539	ILE
1	E	546	SER
1	E	548	SER

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Mol	Chain	Res	Type
1	E	553	CYS
1	E	567	PHE
1	E	580	VAL
1	E	584	LEU
1	E	588	LEU
1	E	589	LEU
2	F	20	GLU
2	F	22	ILE
2	F	30	ASP
2	F	32	SER
2	F	37	LYS
2	F	38	VAL
2	F	39	LYS
2	F	50	SER
2	F	54	ARG
2	F	57	VAL
2	F	76	THR
2	F	78	LYS
2	F	79	GLU
2	F	82	MET
2	F	89	GLU
2	F	90	VAL
2	F	92	GLN
2	F	93	GLU
2	F	94	GLN
1	G	371	ASP
1	G	391	SER
1	G	396	ARG
1	G	402	ILE
1	G	403	GLN
1	G	411	LEU
1	G	426	ARG
1	G	437	VAL
1	G	458	THR
1	G	459	LYS
1	G	465	GLU
1	G	476	LYS
1	G	477	VAL
1	G	480	SER
1	G	487	ARG
1	G	488	LYS
1	G	496	SER

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Mol	Chain	Res	Type
1	G	515	GLU
1	G	517	LYS
1	G	525	ASN
1	G	563	LYS
1	G	574	LEU
1	G	580	VAL
2	H	22	ILE
2	H	24	LEU
2	H	27	ILE
2	H	38	VAL
2	H	39	LYS
2	H	42	THR
2	H	44	LEU
2	H	47	LEU
2	H	49	GLU
2	H	55	GLN
2	H	57	VAL
2	H	63	ARG
2	H	74	ASN
2	H	76	THR
2	H	78	LYS
2	H	80	LEU
2	H	85	GLU
2	H	86	ASP
2	H	90	VAL
1	I	377	SER
1	I	391	SER
1	I	394	LYS
1	I	402	ILE
1	I	411	LEU
1	I	422	LEU
1	I	437	VAL
1	I	446	LEU
1	I	447	LYS
1	I	448	SER
1	I	456	ARG
1	I	458	THR
1	I	459	LYS
1	I	475	ARG
1	I	480	SER
1	I	491	LEU
1	I	497	MET

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Mol	Chain	Res	Type
1	I	507	ILE
1	I	509	LEU
1	I	512	LEU
1	I	513	GLN
1	I	515	GLU
1	I	522	SER
1	I	524	LEU
1	I	526	LEU
1	I	530	THR
1	I	533	SER
1	I	537	HIS
1	I	544	ASN
1	I	554	LYS
1	I	560	SER
1	I	563	LYS
1	I	567	PHE
1	I	568	THR
1	I	572	MET
1	I	574	LEU
1	I	580	VAL
2	J	20	GLU
2	J	22	ILE
2	J	29	GLN
2	J	32	SER
2	J	33	GLU
2	J	39	LYS
2	J	45	LYS
2	J	47	LEU
2	J	54	ARG
2	J	55	GLN
2	J	57	VAL
2	J	60	ASN
2	J	62	LEU
2	J	63	ARG
2	J	70	ARG
2	J	76	THR
2	J	82	MET
2	J	83	GLU
2	J	87	VAL
2	J	89	GLU
2	J	90	VAL
2	J	92	GLN

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Mol	Chain	Res	Type
2	J	94	GLN
1	K	369	THR
1	K	371	ASP
1	K	377	SER
1	K	382	HIS
1	K	387	GLU
1	K	394	LYS
1	K	398	THR
1	K	402	ILE
1	K	411	LEU
1	K	415	VAL
1	K	421	ASN
1	K	424	VAL
1	K	437	VAL
1	K	439	SER
1	K	458	THR
1	K	459	LYS
1	K	461	VAL
1	K	471	VAL
1	K	475	ARG
1	K	476	LYS
1	K	477	VAL
1	K	480	SER
1	K	497	MET
1	K	502	HIS
1	K	507	ILE
1	K	530	THR
1	K	559	ILE
1	K	565	ILE
1	K	574	LEU
1	K	580	VAL
2	L	22	ILE
2	L	39	LYS
2	L	42	THR
2	L	54	ARG
2	L	57	VAL
2	L	60	ASN
2	L	61	SER
2	L	63	ARG
2	L	70	ARG
2	L	74	ASN
2	L	76	THR

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Mol	Chain	Res	Type
2	L	92	GLN
1	M	371	ASP
1	M	373	GLU
1	M	391	SER
1	M	394	LYS
1	M	396	ARG
1	M	402	ILE
1	M	408	TYR
1	M	411	LEU
1	M	415	VAL
1	M	429	LYS
1	M	437	VAL
1	M	440	THR
1	M	447	LYS
1	M	455	LYS
1	M	456	ARG
1	M	459	LYS
1	M	461	VAL
1	M	463	LEU
1	M	465	GLU
1	M	475	ARG
1	M	490	CYS
1	M	502	HIS
1	M	508	LEU
1	M	509	LEU
1	M	515	GLU
1	M	517	LYS
1	M	522	SER
1	M	526	LEU
1	M	527	LEU
1	M	530	THR
1	M	531	HIS
1	M	532	HIS
1	M	542	GLN
1	M	554	LYS
1	M	572	MET
1	M	574	LEU
1	M	579	MET
1	M	580	VAL
2	N	20	GLU
2	N	22	ILE
2	N	37	LYS

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Mol	Chain	Res	Type
2	N	38	VAL
2	N	39	LYS
2	N	47	LEU
2	N	57	VAL
2	N	59	MET
2	N	64	PHE
2	N	74	ASN
2	N	76	THR
2	N	78	LYS
2	N	82	MET
2	N	85	GLU
2	N	87	VAL
2	N	89	GLU
2	N	93	GLU
1	O	377	SER
1	O	391	SER
1	O	396	ARG
1	O	402	ILE
1	O	411	LEU
1	O	414	GLU
1	O	421	ASN
1	O	424	VAL
1	O	426	ARG
1	O	429	LYS
1	O	430	GLN
1	O	437	VAL
1	O	448	SER
1	O	461	VAL
1	O	468	ILE
1	O	471	VAL
1	O	475	ARG
1	O	488	LYS
1	O	497	MET
1	O	502	HIS
1	O	503	ARG
1	O	506	GLU
1	O	509	LEU
1	O	517	LYS
1	O	524	LEU
1	O	527	LEU
1	O	533	SER
1	O	538	GLU

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Mol	Chain	Res	Type
1	O	542	GLN
1	O	546	SER
1	O	562	ASP
1	O	565	ILE
1	O	580	VAL
1	O	588	LEU
2	P	20	GLU
2	P	27	ILE
2	P	32	SER
2	P	38	VAL
2	P	39	LYS
2	P	42	THR
2	P	45	LYS
2	P	57	VAL
2	P	60	ASN
2	P	62	LEU
2	P	69	GLN
2	P	74	ASN
2	P	92	GLN
2	P	94	GLN
1	Q	369	THR
1	Q	371	ASP
1	Q	402	ILE
1	Q	411	LEU
1	Q	416	ILE
1	Q	421	ASN
1	Q	424	VAL
1	Q	435	LEU
1	Q	437	VAL
1	Q	446	LEU
1	Q	468	ILE
1	Q	475	ARG
1	Q	476	LYS
1	Q	477	VAL
1	Q	488	LYS
1	Q	491	LEU
1	Q	494	LEU
1	Q	504	ILE
1	Q	507	ILE
1	Q	508	LEU
1	Q	518	THR
1	Q	524	LEU

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Mol	Chain	Res	Type
1	Q	527	LEU
1	Q	539	ILE
1	Q	542	GLN
1	Q	544	ASN
1	Q	568	THR
1	Q	570	HIS
1	Q	574	LEU
1	Q	580	VAL
2	R	30	ASP
2	R	33	GLU
2	R	39	LYS
2	R	52	CYS
2	R	57	VAL
2	R	59	MET
2	R	63	ARG
2	R	64	PHE
2	R	69	GLN
2	R	71	ILE
2	R	74	ASN
2	R	75	HIS
2	R	84	GLU
2	R	90	VAL
1	S	370	GLU
1	S	373	GLU
1	S	374	LYS
1	S	376	ILE
1	S	377	SER
1	S	385	GLN
1	S	391	SER
1	S	394	LYS
1	S	396	ARG
1	S	398	THR
1	S	402	ILE
1	S	403	GLN
1	S	411	LEU
1	S	415	VAL
1	S	428	LYS
1	S	429	LYS
1	S	440	THR
1	S	454	VAL
1	S	458	THR
1	S	459	LYS

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Mol	Chain	Res	Type
1	S	463	LEU
1	S	467	GLU
1	S	469	ILE
1	S	476	LYS
1	S	480	SER
1	S	486	LEU
1	S	491	LEU
1	S	495	ASP
1	S	502	HIS
1	S	506	GLU
1	S	509	LEU
1	S	524	LEU
1	S	527	LEU
1	S	530	THR
1	S	546	SER
1	S	553	CYS
1	S	570	HIS
1	S	574	LEU
1	S	580	VAL
2	T	22	ILE
2	T	23	LYS
2	T	27	ILE
2	T	38	VAL
2	T	39	LYS
2	T	69	GLN
2	T	71	ILE
2	T	74	ASN
2	T	76	THR
2	T	78	LYS
2	T	83	GLU
2	T	90	VAL
1	U	369	THR
1	U	373	GLU
1	U	394	LYS
1	U	396	ARG
1	U	402	ILE
1	U	426	ARG
1	U	437	VAL
1	U	447	LYS
1	U	448	SER
1	U	456	ARG
1	U	458	THR

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Mol	Chain	Res	Type
1	U	459	LYS
1	U	461	VAL
1	U	476	LYS
1	U	502	HIS
1	U	531	HIS
1	U	533	SER
1	U	565	ILE
1	U	574	LEU
1	U	580	VAL
1	U	587	GLN
2	V	22	ILE
2	V	30	ASP
2	V	38	VAL
2	V	39	LYS
2	V	47	LEU
2	V	53	GLN
2	V	57	VAL
2	V	65	LEU
2	V	67	GLU
2	V	69	GLN
2	V	74	ASN
2	V	76	THR
2	V	78	LYS
2	V	87	VAL
2	V	93	GLU
2	V	94	GLN
1	W	369	THR
1	W	370	GLU
1	W	374	LYS
1	W	380	LEU
1	W	382	HIS
1	W	394	LYS
1	W	396	ARG
1	W	398	THR
1	W	402	ILE
1	W	403	GLN
1	W	411	LEU
1	W	420	MET
1	W	437	VAL
1	W	444	PRO
1	W	459	LYS
1	W	461	VAL

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Mol	Chain	Res	Type
1	W	467	GLU
1	W	469	ILE
1	W	471	VAL
1	W	475	ARG
1	W	478	HIS
1	W	488	LYS
1	W	496	SER
1	W	503	ARG
1	W	506	GLU
1	W	515	GLU
1	W	516	SER
1	W	517	LYS
1	W	518	THR
1	W	523	ASP
1	W	524	LEU
1	W	542	GLN
1	W	559	ILE
1	W	565	ILE
1	W	574	LEU
1	W	580	VAL
2	X	22	ILE
2	X	23	LYS
2	X	26	VAL
2	X	27	ILE
2	X	31	SER
2	X	32	SER
2	X	37	LYS
2	X	39	LYS
2	X	53	GLN
2	X	55	GLN
2	X	59	MET
2	X	64	PHE
2	X	69	GLN
2	X	80	LEU
2	X	83	GLU
2	X	84	GLU
2	X	95	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	407	ASN

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Mol	Chain	Res	Type
1	A	452	GLN
1	A	513	GLN
1	A	544	ASN
2	B	43	HIS
2	B	55	GLN
1	C	403	GLN
1	C	430	GLN
1	C	544	ASN
1	C	570	HIS
2	D	35	HIS
2	D	92	GLN
1	E	403	GLN
1	E	436	HIS
1	E	521	ASN
1	E	537	HIS
1	E	541	GLN
1	E	570	HIS
2	F	53	GLN
2	F	55	GLN
1	G	378	ASN
1	G	403	GLN
1	G	407	ASN
1	G	427	ASN
2	H	29	GLN
2	H	43	HIS
1	I	513	GLN
1	I	541	GLN
1	I	544	ASN
1	K	382	HIS
1	K	452	GLN
1	K	513	GLN
1	K	531	HIS
2	L	29	GLN
2	L	92	GLN
1	M	403	GLN
1	M	513	GLN
1	O	403	GLN
1	O	499	GLN
1	O	531	HIS
1	O	537	HIS
1	O	541	GLN
1	Q	407	ASN

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Mol	Chain	Res	Type
1	Q	412	ASN
1	Q	417	ASN
1	Q	452	GLN
1	Q	513	GLN
1	Q	537	HIS
2	R	29	GLN
2	R	55	GLN
2	R	94	GLN
1	S	385	GLN
1	S	403	GLN
1	S	409	HIS
1	S	525	ASN
1	S	585	HIS
1	U	403	GLN
1	U	436	HIS
1	U	513	GLN
1	U	521	ASN
1	U	532	HIS
1	U	585	HIS
2	V	43	HIS
2	V	69	GLN
1	W	385	GLN
1	W	403	GLN
1	W	521	ASN
1	W	537	HIS
2	X	74	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 [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	223/224 (99%)	-0.08	0 100 100	26, 40, 65, 77	0
1	C	224/224 (100%)	0.43	4 (1%) 67 44	42, 60, 84, 88	0
1	E	224/224 (100%)	0.51	4 (1%) 67 44	35, 58, 88, 98	0
1	G	223/224 (99%)	-0.09	0 100 100	23, 43, 72, 85	0
1	I	223/224 (99%)	0.42	5 (2%) 62 39	25, 56, 84, 89	0
1	K	223/224 (99%)	-0.09	0 100 100	22, 42, 69, 73	0
1	M	222/224 (99%)	0.04	1 (0%) 87 72	25, 43, 67, 95	0
1	O	223/224 (99%)	0.85	11 (4%) 35 18	57, 74, 92, 101	0
1	Q	224/224 (100%)	2.09	104 (46%) 0 0	71, 94, 110, 114	0
1	S	224/224 (100%)	-0.00	0 100 100	24, 44, 67, 74	0
1	U	223/224 (99%)	0.02	2 (0%) 81 61	24, 45, 69, 77	0
1	W	222/224 (99%)	0.47	2 (0%) 81 61	40, 63, 89, 94	0
2	B	78/78 (100%)	0.09	0 100 100	37, 47, 60, 64	0
2	D	78/78 (100%)	0.73	5 (6%) 25 13	51, 66, 76, 77	0
2	F	78/78 (100%)	0.24	1 (1%) 75 53	35, 50, 64, 69	0
2	H	77/78 (98%)	0.67	3 (3%) 43 24	32, 66, 83, 85	0
2	J	78/78 (100%)	0.49	3 (3%) 44 24	54, 60, 72, 74	0
2	L	77/78 (98%)	0.15	1 (1%) 75 53	35, 46, 61, 65	0
2	N	78/78 (100%)	0.32	3 (3%) 44 24	39, 48, 70, 72	0
2	P	78/78 (100%)	1.02	6 (7%) 19 10	69, 87, 101, 103	0
2	R	78/78 (100%)	1.83	30 (38%) 1 1	88, 99, 113, 117	0
2	T	78/78 (100%)	0.22	1 (1%) 75 53	29, 50, 64, 65	0
2	V	78/78 (100%)	0.93	8 (10%) 12 6	35, 77, 89, 89	0
2	X	78/78 (100%)	0.34	1 (1%) 75 53	46, 57, 70, 72	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
All	All	3612/3624 (99%)	0.43	195 (5%)	31	16	22, 56, 96, 117	0

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	529	TRP	5.9
1	Q	530	THR	5.1
1	Q	512	LEU	5.0
1	Q	525	ASN	5.0
1	Q	490	CYS	4.7
2	R	87	VAL	4.7
1	Q	484	ILE	4.6
1	Q	555	TYR	4.6
2	R	27	ILE	4.5
1	Q	453	ALA	4.5
1	Q	556	ALA	4.5
1	Q	483	VAL	4.4
1	E	431	GLY	4.4
1	Q	454	VAL	4.3
2	R	66	TRP	4.2
1	O	477	VAL	4.2
1	Q	536	PRO	4.2
1	Q	535	LYS	4.2
1	Q	526	LEU	4.1
1	Q	437	VAL	4.1
1	Q	511	TYR	4.1
2	R	88	ILE	4.1
1	Q	440	THR	4.1
1	Q	510	GLN	4.0
1	Q	532	HIS	4.0
1	Q	450	GLY	3.9
1	Q	467	GLU	3.9
2	R	34	ILE	3.9
2	R	67	GLU	3.8
1	Q	468	ILE	3.8
1	Q	527	LEU	3.8
1	E	524	LEU	3.8
1	Q	494	LEU	3.7
1	Q	509	LEU	3.6
1	Q	552	THR	3.6
1	Q	400	GLY	3.6
1	Q	507	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	Q	457	TRP	3.6
1	Q	395	LEU	3.6
1	Q	491	LEU	3.6
1	Q	492	LYS	3.5
1	Q	508	LEU	3.5
1	Q	445	LYS	3.5
1	Q	479	TRP	3.4
1	Q	559	ILE	3.4
2	R	96	GLY	3.4
1	Q	550	MET	3.3
1	Q	472	PRO	3.3
1	Q	446	LEU	3.3
1	O	556	ALA	3.3
2	R	91	TYR	3.3
1	Q	547	ASP	3.3
1	Q	531	HIS	3.3
2	R	38	VAL	3.2
1	Q	524	LEU	3.2
2	R	71	ILE	3.2
2	H	41	THR	3.2
1	Q	447	LYS	3.1
2	R	29	GLN	3.0
2	R	30	ASP	3.0
2	N	29	GLN	3.0
2	H	37	LYS	3.0
1	Q	451	TYR	3.0
1	Q	513	GLN	3.0
1	Q	534	MET	2.9
1	Q	477	VAL	2.9
2	V	64	PHE	2.9
2	V	80	LEU	2.9
1	Q	488	LYS	2.9
1	Q	533	SER	2.9
2	R	65	LEU	2.9
1	O	394	LYS	2.8
1	Q	496	SER	2.8
1	Q	474	HIS	2.8
2	N	30	ASP	2.8
2	P	57	VAL	2.8
1	Q	481	LEU	2.7
1	Q	523	ASP	2.7
1	Q	469	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	Q	502	HIS	2.7
1	Q	517	LYS	2.7
2	R	68	GLY	2.6
1	Q	485	ASP	2.6
2	R	86	ASP	2.6
1	Q	433	PRO	2.6
2	P	74	ASN	2.6
2	R	36	PHE	2.6
1	Q	458	THR	2.6
1	Q	438	PHE	2.6
1	O	407	ASN	2.6
2	R	28	GLY	2.6
2	N	32	SER	2.6
2	R	80	LEU	2.6
1	E	467	GLU	2.5
1	Q	461	VAL	2.5
1	O	388	ILE	2.5
1	Q	497	MET	2.5
1	Q	441	PHE	2.5
1	Q	540	PRO	2.5
1	Q	422	LEU	2.5
2	R	26	VAL	2.5
1	Q	410	TRP	2.5
2	V	37	LYS	2.5
2	X	37	LYS	2.5
1	Q	473	ILE	2.5
1	Q	407	ASN	2.4
1	Q	470	LEU	2.4
1	Q	587	GLN	2.4
2	R	92	GLN	2.4
1	Q	439	SER	2.4
1	Q	471	VAL	2.4
1	I	531	HIS	2.4
1	Q	388	ILE	2.4
1	Q	565	ILE	2.4
2	R	82	MET	2.4
2	J	20	GLU	2.4
1	I	533	SER	2.4
2	V	87	VAL	2.4
1	Q	500	LYS	2.3
1	O	380	LEU	2.3
2	D	20	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	Q	564	PRO	2.3
1	Q	493	TYR	2.3
1	Q	542	GLN	2.3
1	C	476	LYS	2.3
2	D	25	LYS	2.3
1	C	496	SER	2.3
1	Q	501	GLY	2.3
1	I	380	LEU	2.3
2	R	64	PHE	2.3
1	Q	504	ILE	2.3
1	Q	549	GLY	2.3
2	R	59	MET	2.3
1	Q	390	SER	2.3
1	O	416	ILE	2.3
1	Q	579	MET	2.3
1	Q	537	HIS	2.3
1	Q	442	PHE	2.3
2	V	21	TYR	2.3
1	Q	577	LYS	2.3
2	R	33	GLU	2.2
1	M	369	THR	2.2
1	Q	551	PHE	2.2
1	Q	575	PHE	2.2
2	D	50	SER	2.2
2	L	30	ASP	2.2
1	W	497	MET	2.2
1	Q	443	TYR	2.2
1	O	580	VAL	2.2
2	D	53	GLN	2.2
1	Q	475	ARG	2.2
1	O	443	TYR	2.2
2	J	69	GLN	2.2
2	H	59	MET	2.2
1	Q	567	PHE	2.2
1	O	376	ILE	2.2
2	R	32	SER	2.2
1	E	589	LEU	2.2
1	Q	366	LEU	2.2
1	Q	528	GLU	2.2
2	V	27	ILE	2.1
1	Q	584	LEU	2.1
2	T	29	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	Q	393	PHE	2.1
1	U	502	HIS	2.1
1	W	537	HIS	2.1
1	C	506	GLU	2.1
1	Q	421	ASN	2.1
1	I	494	LEU	2.1
1	Q	394	LYS	2.1
1	Q	432	TYR	2.1
2	P	21	TYR	2.1
2	J	97	GLY	2.1
1	C	394	LYS	2.1
2	R	39	LYS	2.1
1	Q	574	LEU	2.1
1	Q	403	GLN	2.1
1	Q	545	GLY	2.1
1	U	381	GLY	2.1
2	P	97	GLY	2.1
1	I	496	SER	2.1
2	R	61	SER	2.1
2	P	60	ASN	2.1
2	V	44	LEU	2.1
1	O	566	THR	2.1
2	D	37	LYS	2.0
2	R	60	ASN	2.0
2	V	22	ILE	2.0
2	F	53	GLN	2.0
2	R	25	LYS	2.0
2	R	89	GLU	2.0
2	P	27	ILE	2.0
1	Q	568	THR	2.0
1	Q	562	ASP	2.0
1	Q	416	ILE	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.