



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 09:28 pm BST

PDB ID : 5AEK  
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](mailto: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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

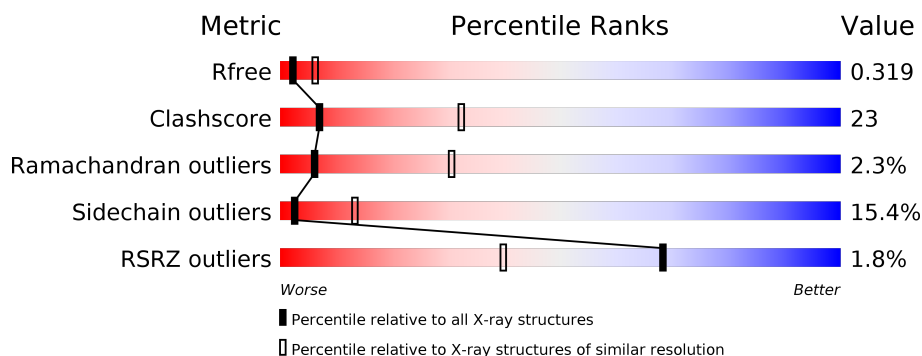
# 1 Overall quality at a glance

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))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	
1	K	224	

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Mol	Chain	Length	Quality of chain
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	C	N	O	S	0	0	0
			639	401	109	124	5			
2	D	78	Total	C	N	O	S	0	0	0
			639	401	109	124	5			
2	F	78	Total	C	N	O	S	0	0	0
			639	401	109	124	5			
2	H	77	Total	C	N	O	S	0	0	0
			630	396	108	121	5			
2	J	78	Total	C	N	O	S	0	0	0
			639	401	109	124	5			
2	L	77	Total	C	N	O	S	0	0	0
			630	396	108	121	5			
2	N	78	Total	C	N	O	S	0	0	0
			639	401	109	124	5			
2	P	78	Total	C	N	O	S	0	0	0
			639	401	109	124	5			
2	R	78	Total	C	N	O	S	0	0	0
			639	401	109	124	5			
2	T	78	Total	C	N	O	S	0	0	0
			639	401	109	124	5			
2	V	78	Total	C	N	O	S	0	0	0
			639	401	109	124	5			
2	X	78	Total	C	N	O	S	0	0	0
			639	401	109	124	5			

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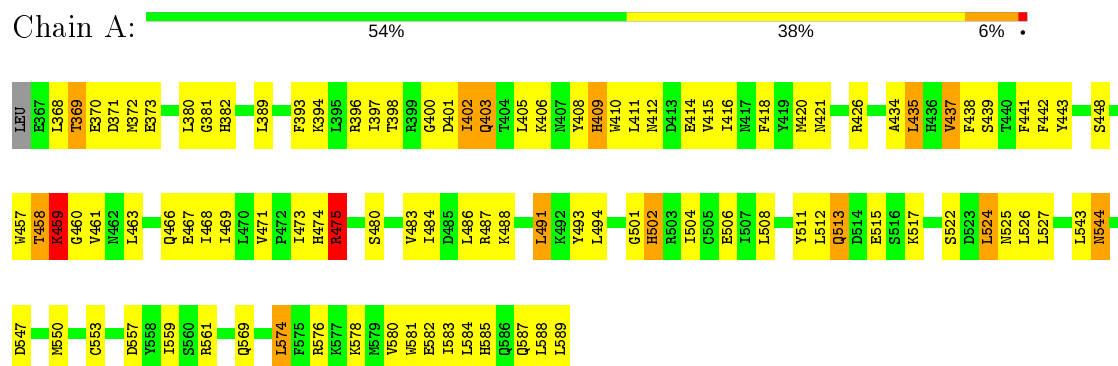
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Chain	Residue	Modelled	Actual	Comment	Reference
D	66	TRP	PHE	engineered mutation	UNP P63165
F	48	MET	LYS	engineered mutation	UNP P63165
F	66	TRP	PHE	engineered mutation	UNP P63165
H	48	MET	LYS	engineered mutation	UNP P63165
H	66	TRP	PHE	engineered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

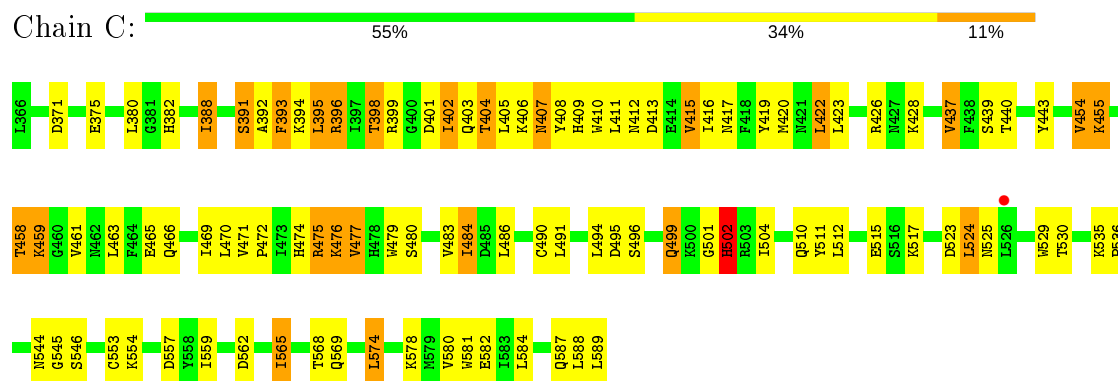
### 3 Residue-property plots [i](#)

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

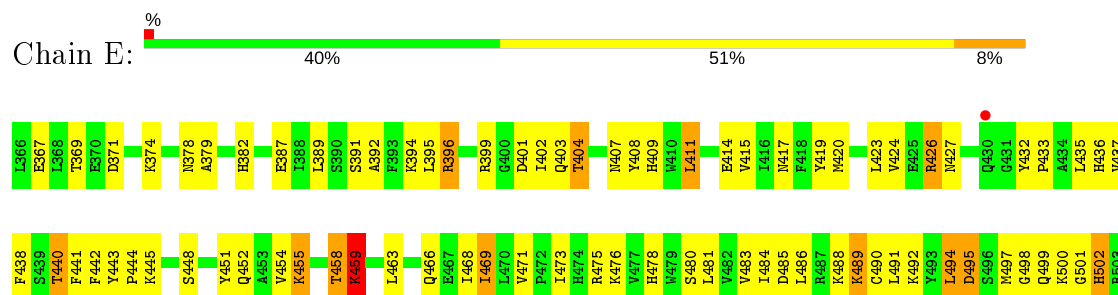
#### • Molecule 1: SENTRIN-SPECIFIC PROTEASE 2



#### • Molecule 1: SENTRIN-SPECIFIC PROTEASE 2



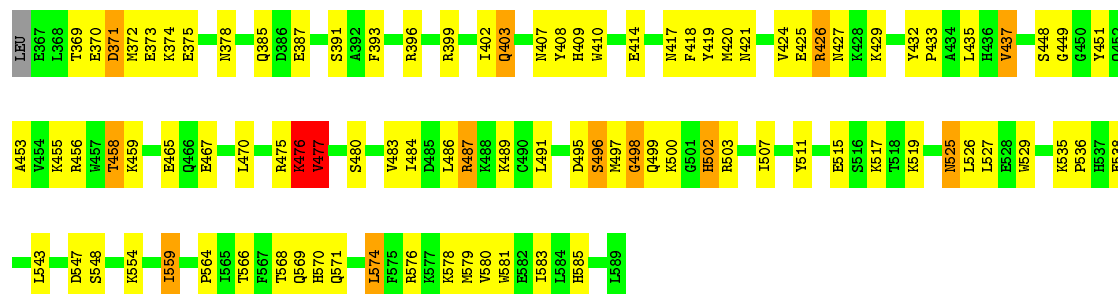
#### • Molecule 1: SENTRIN-SPECIFIC PROTEASE 2





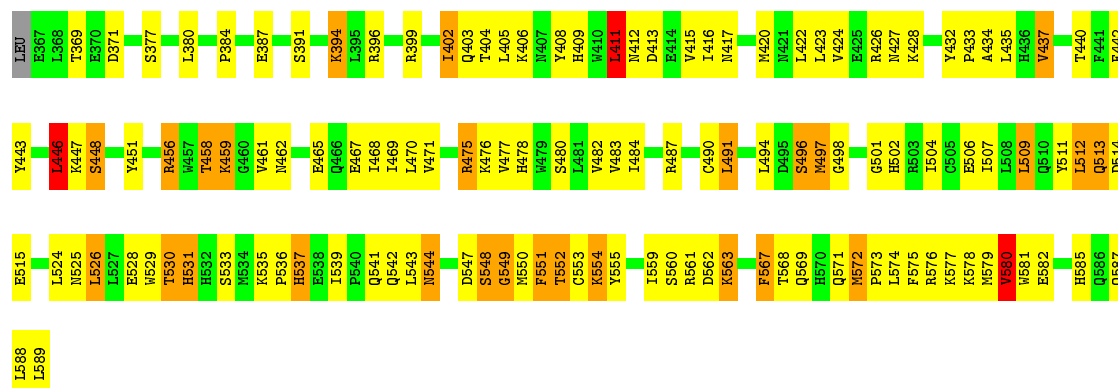
• Molecule 1: SENTRIN-SPECIFIC PROTEASE 2

Chain G: 57% 36% 5% .



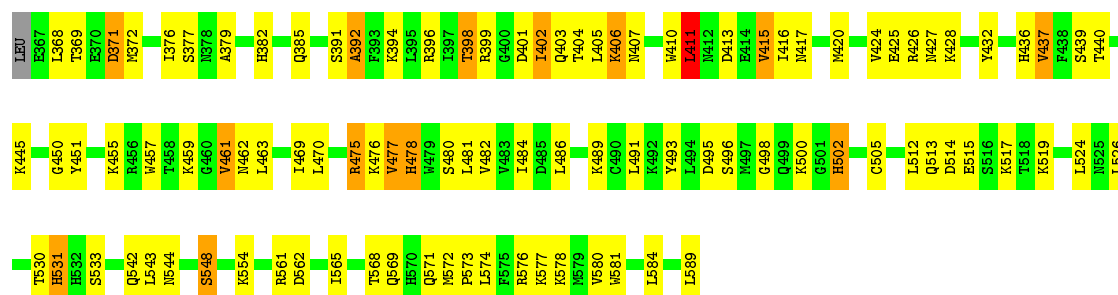
• Molecule 1: SENTRIN-SPECIFIC PROTEASE 2

Chain I: 42% 44% 12% .



• Molecule 1: SENTRIN-SPECIFIC PROTEASE 2

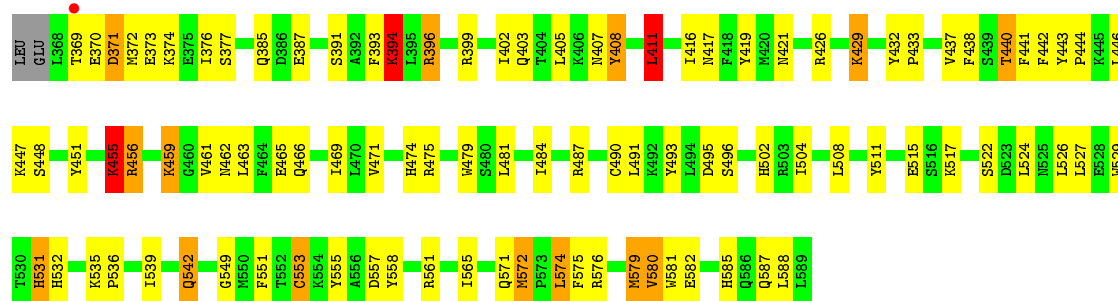
Chain K: 55% 38% 6%



• Molecule 1: SENTRIN-SPECIFIC PROTEASE 2

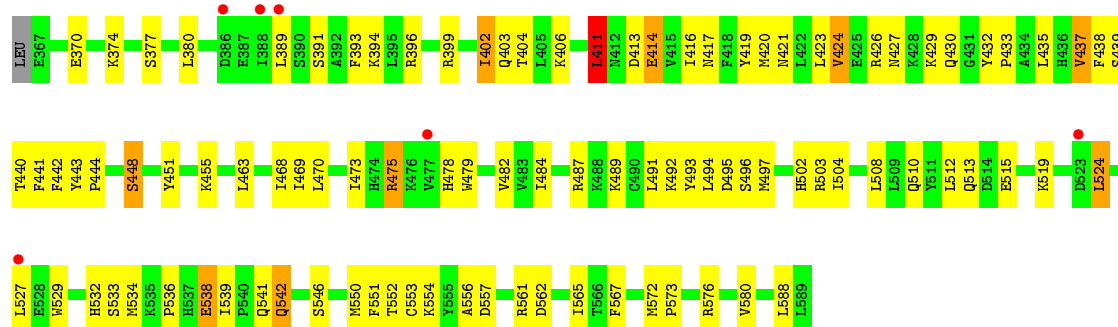


Chain M: 



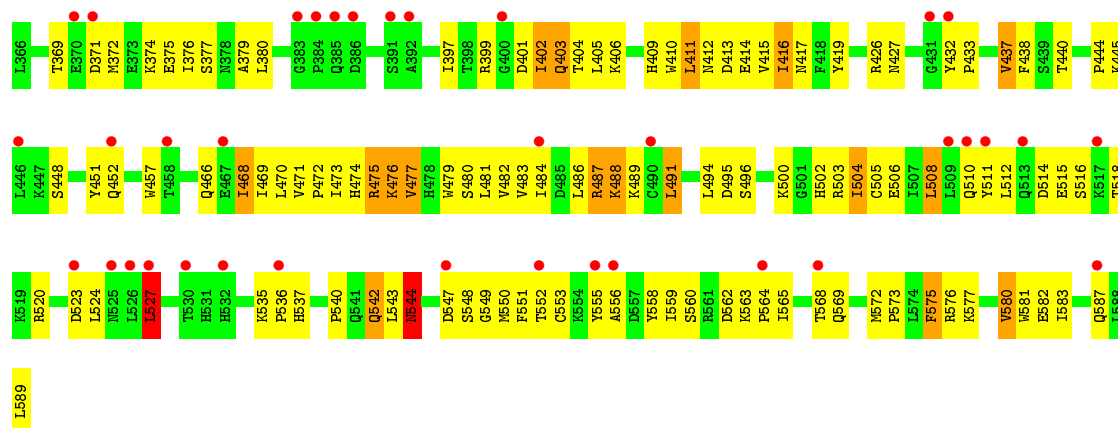
• Molecule 1: SENTRIN-SPECIFIC PROTEASE 2

Chain O: 



• Molecule 1: SENTRIN-SPECIFIC PROTEASE 2

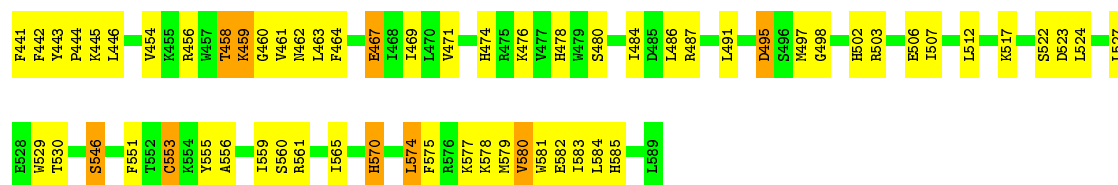
Chain Q: 



• Molecule 1: SENTRIN-SPECIFIC PROTEASE 2

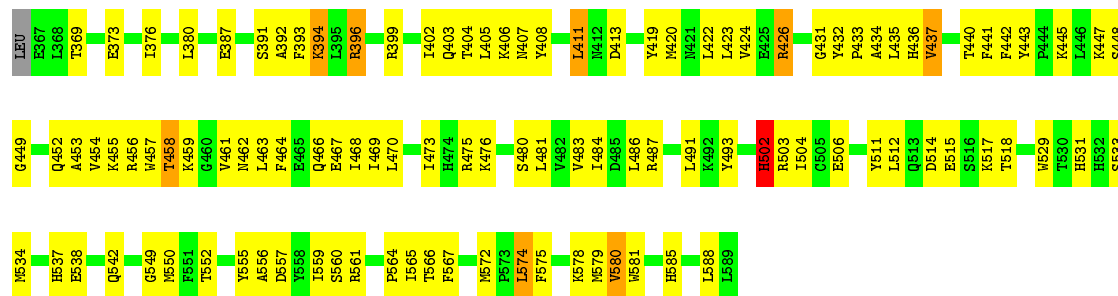
Chain S: 





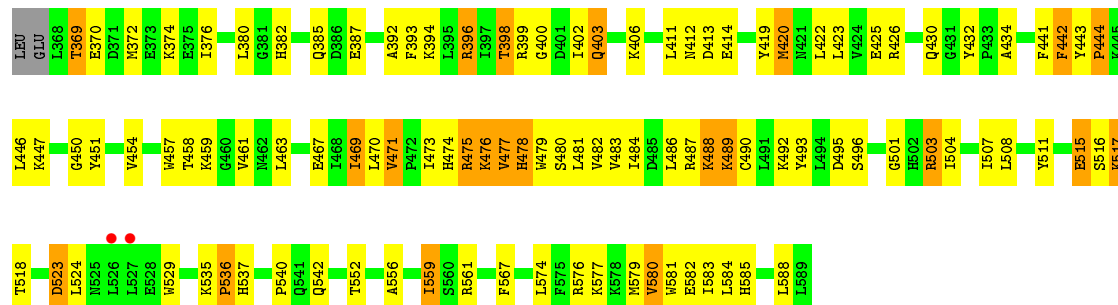
• Molecule 1: SENTRIN-SPECIFIC PROTEASE 2

Chain U: 51% 44%



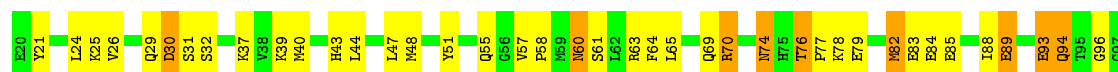
• Molecule 1: SENTRIN-SPECIFIC PROTEASE 2

Chain W: 52% 37% 10%



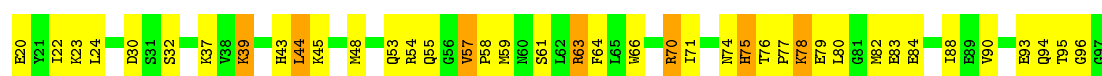
• Molecule 2: SMALL UBIQUITIN-RELATED MODIFIER 1

Chain B: 49% 40% 12%



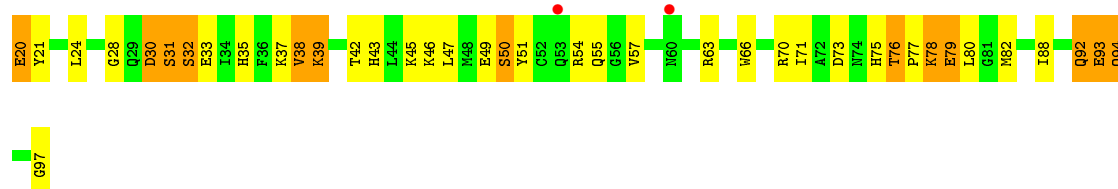
• Molecule 2: SMALL UBIQUITIN-RELATED MODIFIER 1

Chain D: 49% 42% 9%

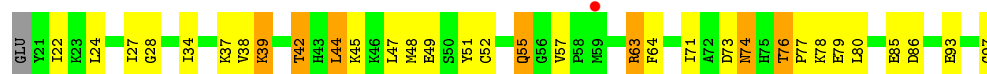


• Molecule 2: SMALL UBIQUITIN-RELATED MODIFIER 1

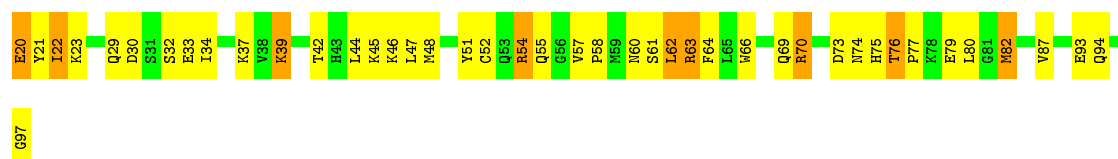
Chain F: 3% 49% 35% 17%



• Molecule 2: SMALL UBIQUITIN-RELATED MODIFIER 1



• Molecule 2: SMALL UBIQUITIN-RELATED MODIFIER 1



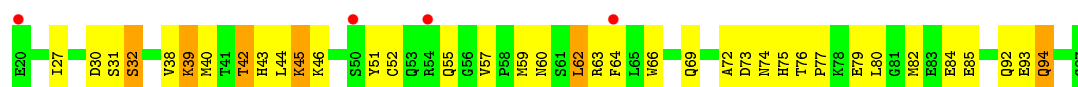
• Molecule 2: SMALL UBIQUITIN-RELATED MODIFIER 1



• Molecule 2: SMALL UBIQUITIN-RELATED MODIFIER 1

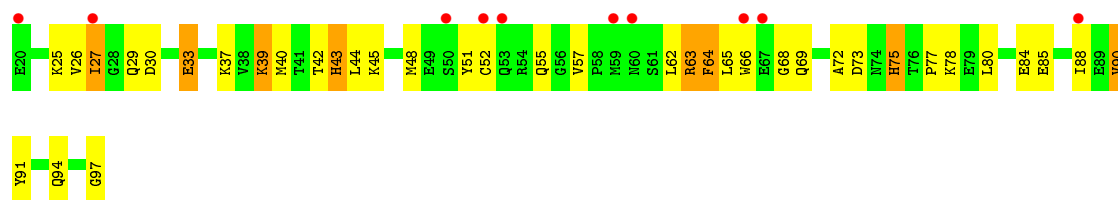


• Molecule 2: SMALL UBIQUITIN-RELATED MODIFIER 1



• Molecule 2: SMALL UBIQUITIN-RELATED MODIFIER 1





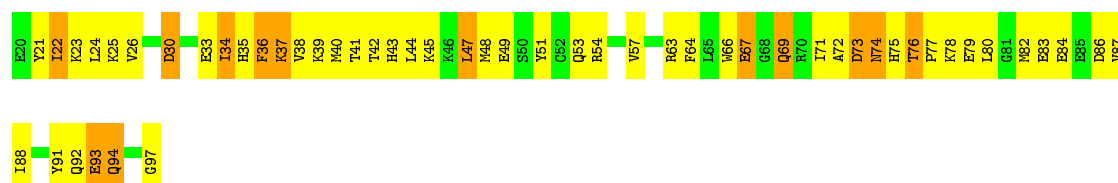
- Molecule 2: SMALL UBIQUITIN-RELATED MODIFIER 1

Chain T: 53% 38% 9%



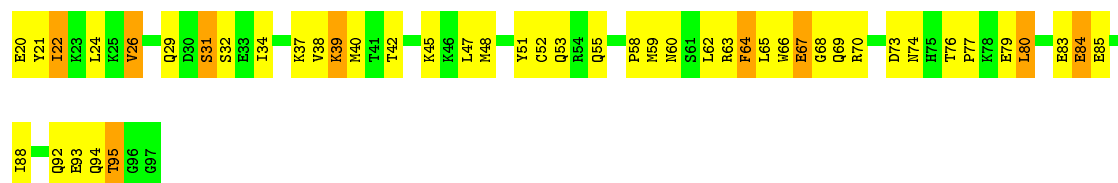
- Molecule 2: SMALL UBIQUITIN-RELATED MODIFIER 1

Chain V: 32% 51% 17%



- Molecule 2: SMALL UBIQUITIN-RELATED MODIFIER 1

Chain X: 40% 49% 12%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.72Å 119.32Å 199.84Å 90.00° 89.67° 90.00°	Depositor
Resolution (Å)	47.00 – 3.00 46.76 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.7 (47.00-3.00) 94.0 (46.76-3.00)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	65.2	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 56.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	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	0.89	EDS
Total number of atoms	29972	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

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	0.72	1/1906 (0.1%)	0.82	1/2567 (0.0%)
1	C	0.60	1/1911 (0.1%)	0.73	1/2574 (0.0%)
1	E	0.63	0/1911	0.74	0/2574
1	G	0.70	0/1906	0.79	0/2567
1	I	0.65	0/1906	0.78	1/2567 (0.0%)
1	K	0.71	0/1906	0.81	1/2567 (0.0%)
1	M	0.73	2/1897 (0.1%)	0.81	3/2555 (0.1%)
1	O	0.57	0/1906	0.73	1/2567 (0.0%)
1	Q	0.61	0/1911	0.77	3/2574 (0.1%)
1	S	0.69	1/1911 (0.1%)	0.80	0/2574
1	U	0.70	0/1906	0.78	1/2567 (0.0%)
1	W	0.58	0/1897	0.69	0/2555
2	B	0.75	0/650	0.84	0/869
2	D	0.62	0/650	0.72	0/869
2	F	0.77	0/650	0.80	0/869
2	H	0.69	0/641	0.76	0/857
2	J	0.65	0/650	0.76	0/869
2	L	0.66	0/641	0.81	0/857
2	N	0.78	0/650	0.82	0/869
2	P	0.57	0/650	0.69	0/869
2	R	0.68	0/650	0.68	0/869
2	T	0.76	0/650	0.81	1/869 (0.1%)
2	V	0.63	0/650	0.73	0/869
2	X	0.71	0/650	0.82	0/869
All	All	0.67	5/30656 (0.0%)	0.77	13/41212 (0.0%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	553	CYS	CB-SG	-6.13	1.71	1.82
1	S	553	CYS	CB-SG	-5.63	1.72	1.81
1	C	553	CYS	CB-SG	-5.21	1.73	1.81
1	M	553	CYS	CB-SG	-5.19	1.73	1.81
1	M	394	LYS	CD-CE	5.01	1.63	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	452	GLN	OE1-CD-NE2	-6.55	106.83	121.90
1	U	411	LEU	CA-CB-CG	6.36	129.93	115.30
1	Q	452	GLN	CG-CD-NE2	5.91	130.87	116.70
1	M	574	LEU	CA-CB-CG	5.83	128.72	115.30
1	O	411	LEU	CA-CB-CG	5.81	128.66	115.30
1	I	411	LEU	CA-CB-CG	5.76	128.54	115.30
1	A	435	LEU	CB-CG-CD2	-5.73	101.26	111.00
1	M	411	LEU	CA-CB-CG	5.70	128.40	115.30
1	K	411	LEU	CA-CB-CG	5.41	127.73	115.30
1	Q	527	LEU	CB-CG-CD2	5.26	119.94	111.00
1	C	395	LEU	CA-CB-CG	5.21	127.27	115.30
1	M	481	LEU	CA-CB-CG	5.21	127.28	115.30
2	T	38	VAL	N-CA-C	5.07	124.69	111.00

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	85	0
1	C	1865	0	1872	77	0
1	E	1865	0	1872	153	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1860	0	1870	73	0
1	I	1860	0	1870	115	0
1	K	1860	0	1870	74	0
1	M	1851	0	1864	68	1
1	O	1860	0	1870	66	0
1	Q	1865	0	1872	101	0
1	S	1865	0	1872	79	1
1	U	1860	0	1870	83	0
1	W	1851	0	1864	82	0
2	B	639	0	629	31	0
2	D	639	0	629	39	0
2	F	639	0	629	49	0
2	H	630	0	623	18	0
2	J	639	0	629	33	0
2	L	630	0	623	20	0
2	N	639	0	629	26	0
2	P	639	0	629	23	0
2	R	639	0	629	33	0
2	T	639	0	629	28	0
2	V	639	0	629	52	0
2	X	639	0	629	44	0
All	All	29972	0	29972	1372	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 23.

All (1372) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:420:MET:HB3	1:I:437:VAL:HG21	1.48	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:CD	2:T:39:LYS:H	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
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
1:E:548:SER:HB3	2:F:97:GLY:C	1.91	0.90
2:T:63:ARG:HH21	2:T:93:GLU:HB2	1.37	0.90
1:G:419:TYR:OH	1:G:554:LYS:NZ	2.06	0.89
1:E:548:SER:HB3	2:F:97:GLY:O	1.72	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:HD2	2:F:39:LYS:H	1.38	0.88
1:I:498:GLY:H	1:I:541:GLN:NE2	1.72	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
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
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:V:23:LYS:HZ1	2:V:35:HIS:HB3	1.42	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:CG	2:J:70:ARG:HH11	1.92	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:548:SER:HB3	2:F:97:GLY:OXT	1.79	0.82
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: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:I:496:SER:HA	1:I:555:TYR:HH	1.43	0.81
1:S:417:ASN:ND2	1:S:440:THR:CG2	2.41	0.81
1:U:394:LYS:HE2	1:U:394:LYS:H	1.44	0.81
2:R:51:TYR:HD2	2:R:64:PHE:HE2	1.26	0.81
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
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
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:H	2:R:64:PHE:HD1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:J:70:ARG:HG2	2:J:70:ARG:HH11	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:HE21	1:A:513:GLN:CA	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:NH1	1:E:426:ARG:HG3	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
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:N	2:T:39:LYS:HD2	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:H	1:C:394:LYS:HE2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:U:550:MET:SD	1:U:579:MET:HE1	2.31	0.71
1:G:375:GLU:CA	1:G:378:ASN:HD22	2.02	0.71
1:I:497:MET:HG2	1:I:497:MET:O	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: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
2:V:40:MET:O	2:V:41:THR:HG22	1.93	0.69
1:C:535:LYS:HB3	1:C:536:PRO:HD2	1.74	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
2:F:31:SER:HB3	2:N:84:GLU:OE2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
2:X:20:GLU:C	2:X:21:TYR:HD1	1.98	0.67
1:I:542:GLN:NE2	1:I:548:SER:HB3	2.09	0.67
1:K:371:ASP:N	1:K:371:ASP:OD1	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
1:E:550:MET:SD	1:E:579:MET:HE1	2.35	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: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:A:513:GLN:C	1:A:513:GLN:HE21	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:574:LEU:HD13	1:S:578:LYS:HE3	1.78	0.65
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: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:E:459:LYS:C	1:E:459:LYS:HD3	2.18	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:A:408:TYR:CD1	1:U:434:ALA:HB2	2.33	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:E:550:MET:SD	1:E:579:MET:HE3	2.38	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
1:Q:475:ARG:NH1	1:Q:476:LYS:HG3	2.12	0.64
2:B:48:MET:HE3	2:B:64:PHE:HB2	1.80	0.63
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
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:S:417:ASN:CG	1:S:440:THR:HG22	2.19	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
2:D:53:GLN:C	2:D:55:GLN:H	2.03	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:I:567:PHE:CD1	1:I:567:PHE:C	2.73	0.62
1:A:581:TRP:CZ3	1:A:589:LEU:HD21	2.34	0.62
1:C:474:HIS:HB2	1:C:479:TRP:HZ3	1.63	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: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:569:GLN:O	1:E:572:MET:HB2	2.00	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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CD2	1:Q:411:LEU:H	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: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
1:O:441:PHE:HZ	2:P:63:ARG:HG3	1.68	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:F:30:ASP:OD1	2:F:30:ASP:C	2.40	0.59
2:R:44:LEU:HG	2:R:77:PRO:HD3	1.82	0.59
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
1:U:550:MET:CE	1:U:579:MET:CE	2.81	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:426:ARG:C	1:E:426:ARG:HD2	2.23	0.58
1:E:436:HIS:HE1	1:E:438:PHE:CE1	2.21	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
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:P:84:GLU:HG3	2:P:85:GLU:HG2	1.86	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
1:C:393:PHE:HZ	1:C:422:LEU:HD23	1.69	0.58
1:E:554:LYS:HG3	1:E:572:MET:HE1	1.85	0.58
1:I:475:ARG:HA	1:I:475:ARG:HE	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:39:LYS:CD	2:F:39:LYS:H	2.12	0.57
1:S:369:THR:HG22	1:S:371:ASP:H	1.69	0.57
1:U:550:MET:HE1	1:U:579:MET:HE3	1.85	0.57
1:A:467:GLU:HB3	1:A:487:ARG:HD3	1.87	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:HB3	1:Q:476:LYS:NZ	2.19	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
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:W:475:ARG:O	1:W:476:LYS:C	2.43	0.57
1:A:381:GLY:O	1:A:382:HIS:HB2	2.05	0.57
1:A:513:GLN:NE2	1:A:513:GLN:CA	2.68	0.57
2:V:38:VAL:HG12	2:V:47:LEU:HD11	1.87	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
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:N	1:A:544:ASN:ND2	2.51	0.56
1:E:567:PHE:C	1:E:567:PHE:CD1	2.79	0.56
1:I:547:ASP:C	1:I:549:GLY:H	2.05	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:E:394:LYS:HA	1:E:396:ARG:NH2	2.21	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:OD1	2:B:30:ASP:N	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:NH1	2:J:70:ARG:HG2	2.17	0.56
1:Q:548:SER:OG	2:R:97:GLY:C	2.44	0.56
1:W:422:LEU:O	1:W:423:LEU:C	2.44	0.56
1:Q:508:LEU:O	1:Q:511:TYR:HB3	2.06	0.56
1:Q:457:TRP:HZ2	2:R:91:TYR:HH	1.54	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
2:F:70:ARG:HG3	2:F:71:ILE:N	2.22	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
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
2:B:60:ASN:N	2:B:60:ASN:OD1	2.38	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:417:ASN:CG	1:K:440:THR:HG23	2.26	0.55
2:N:20:GLU:C	2:N:21:TYR:CD1	2.80	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
2:X:39:LYS:HD3	2:X:39:LYS:H	1.71	0.55
1:W:457:TRP:HA	2:X:67:GLU:O	2.07	0.55
1:G:420:MET:O	1:G:424:VAL:HG23	2.06	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
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:W:515:GLU:HA	1:W:515:GLU:OE1	2.07	0.55
1:K:482:VAL:HG23	1:K:493:TYR:HD1	1.71	0.54
1:U:550:MET:CE	1:U:579:MET:HE3	2.37	0.54
2:V:48:MET:HE1	2:V:71:ILE:O	2.07	0.54
1:W:580:VAL:O	1:W:584:LEU:HG	2.07	0.54
1:Q:540:PRO:O	1:Q:551:PHE:HE2	1.90	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
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: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: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:O	1:O:402:ILE:HG12	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:W:393:PHE:HZ	1:W:422:LEU:HD23	1.73	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
1:M:531:HIS:C	1:M:531:HIS:ND1	2.61	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:C:426:ARG:HD2	1:C:426:ARG:C	2.29	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
1:E:414:GLU:HA	1:E:414:GLU:OE1	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:C:408:TYR:OH	1:W:432:TYR:O	2.11	0.53
1:W:581:TRP:CE2	1:W:585:HIS:CD2	2.96	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
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:M:474:HIS:CE1	2:N:94:GLN:HB3	2.44	0.53
1:O:478:HIS:HE2	1:O:495:ASP:CG	2.11	0.53
2:X:64:PHE:CD1	2:X:64:PHE:N	2.77	0.53
2:D:22:ILE:HG12	2:D:23:LYS:N	2.23	0.53
2:J:63:ARG:CD	2:J:63:ARG:N	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:S:577:LYS:O	1:S:580:VAL:HG13	2.09	0.53
1:C:416:ILE:O	1:C:417:ASN:C	2.46	0.53
1:C:484:ILE:HG13	1:C:491:LEU:CD1	2.38	0.53
1:C:510:GLN:O	1:C:511:TYR:C	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:48:MET:HE3	2:D:64:PHE:HB2	1.92	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:W:425:GLU:O	1:W:426:ARG:C	2.47	0.52
1:C:420:MET:HB3	1:C:437:VAL:CG2	2.40	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
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:567:PHE:HD1	1:E:567:PHE:C	2.13	0.52
1:Q:481:LEU:HG	1:Q:482:VAL:N	2.24	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: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
1:U:493:TYR:O	1:U:534:MET:HB2	2.09	0.52
1:C:501:GLY:O	1:C:502:HIS:C	2.49	0.52
1:E:551:PHE:O	1:E:552:THR:C	2.47	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:510:GLN:OE1	1:E:510:GLN:HA	2.10	0.51
1:I:462:ASN:HB3	1:I:465:GLU:CG	2.41	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:43:HIS:C	2:D:45:LYS:H	2.14	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: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
1:S:391:SER:O	1:S:392:ALA:HB2	2.10	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
1:I:548:SER:OG	2:J:97:GLY:O	2.28	0.51
1:K:561:ARG:O	1:K:562:ASP:HB2	2.11	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: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:E:423:LEU:O	1:E:424:VAL:C	2.48	0.51
1:O:414:GLU:HA	1:O:414:GLU:OE1	2.09	0.51
1:U:537:HIS:CD2	1:U:538:GLU:HG2	2.46	0.51
1:E:469:ILE:O	1:E:469:ILE:HG22	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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:W:414:GLU:CD	2:X:70:ARG:HH22	2.13	0.50
1:E:435:LEU:HD12	1:E:468:ILE:HB	1.93	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:474:HIS:C	1:A:475:ARG:O	2.48	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
2:R:40:MET:HG3	2:R:78:LYS:HB2	1.93	0.50
1:W:419:TYR:O	1:W:420:MET:C	2.50	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
1:I:548:SER:OG	2:J:97:GLY:C	2.50	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:S:417:ASN:OD1	1:S:440:THR:HG22	2.11	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
1:I:435:LEU:HD21	1:I:470:LEU:CD1	2.42	0.50
2:N:47:LEU:HD23	2:N:47:LEU:O	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:C:568:THR:O	1:C:569:GLN:C	2.48	0.50
1:E:550:MET:HE2	1:E:572:MET:SD	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:432:TYR:HB3	1:E:433:PRO:CD	2.42	0.49
1:Q:470:LEU:HD23	1:Q:483:VAL:HA	1.94	0.49
1:Q:372:MET:HG2	1:Q:581:TRP:CD1	2.47	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: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
1:E:495:ASP:C	1:E:495:ASP:OD1	2.50	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
1:G:476:LYS:C	1:G:477:VAL:HG23	2.32	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:O:393:PHE:CD2	1:O:421:ASN:HB3	2.47	0.49
1:Q:500:LYS:HB3	1:Q:502:HIS:ND1	2.27	0.49
1:S:442:PHE:CD1	1:S:442:PHE:C	2.86	0.49
1:I:402:ILE:O	1:I:403:GLN:C	2.49	0.49
1:I:484:ILE:HG23	1:I:491:LEU:HD11	1.95	0.49
2:L:47:LEU:C	2:L:47:LEU:HD23	2.32	0.49
1:W:470:LEU:HD22	1:W:481:LEU:HD21	1.95	0.49
1:E:572:MET:O	1:E:575:PHE:N	2.45	0.49
1:K:394:LYS:HE2	1:K:394:LYS:H	1.77	0.49
1:I:576:ARG:O	1:I:577:LYS:C	2.51	0.49
1:A:416:ILE:O	1:A:420:MET:HG2	2.13	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:HD3	2:J:63:ARG:N	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
1:U:550:MET:CE	1:U:579:MET:HE1	2.42	0.49
1:W:392:ALA:C	1:W:394:LYS:N	2.66	0.49
1:A:393:PHE:CD2	1:A:421:ASN:HB3	2.47	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:Q:581:TRP:C	1:Q:583:ILE:H	2.16	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:A:405:LEU:C	1:A:576:ARG:HH11	2.16	0.48
1:E:501:GLY:O	1:E:505:CYS:SG	2.54	0.48
1:M:511:TYR:CZ	1:M:515:GLU:HG3	2.47	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:H:27:ILE:CG2	2:H:28:GLY:N	2.76	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:484:ILE:HG12	1:G:491:LEU:HG	1.95	0.48
1:G:458:THR:HG21	1:G:511:TYR:OH	2.13	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
1:C:454:VAL:O	1:C:455:LYS:C	2.51	0.48
2:D:53:GLN:C	2:D:55:GLN:N	2.66	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:I:572:MET:O	1:I:573:PRO:C	2.52	0.48
1:Q:402:ILE:HG13	1:Q:405:LEU:HD12	1.95	0.48
1:Q:376:ILE:HD11	1:Q:581:TRP:HB2	1.94	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
1:Q:397:ILE:HG23	1:Q:401:ASP:HB2	1.96	0.48
1:Q:537:HIS:CD2	1:Q:537:HIS:C	2.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:X:20:GLU:C	2:X:21:TYR:CD1	2.83	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:K:462:ASN:C	1:K:462:ASN:OD1	2.52	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: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
2:N:64:PHE:N	2:N:64:PHE:CD1	2.82	0.47
2:X:66:TRP:C	2:X:68:GLY:N	2.68	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:O:489:LYS:HZ3	1:O:529:TRP:HE1	1.62	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
1:E:426:ARG:CZ	1:E:561:ARG:CD	2.91	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:525:ASN:C	1:G:527:LEU:H	2.17	0.47
1:I:446:LEU:C	1:I:446:LEU:HD12	2.35	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: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:520:ARG:C	1:E:522:SER:H	2.17	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:W:420:MET:HE3	1:W:470:LEU:HD13	1.96	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
1:I:526:LEU:HA	1:I:529:TRP:CD1	2.50	0.47
1:M:394:LYS:HD3	1:M:396:ARG:HH22	1.79	0.47
1:E:572:MET:O	1:E:573:PRO:C	2.52	0.47
1:K:403:GLN:O	1:K:405:LEU:N	2.48	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:G:393:PHE:CE2	1:G:421:ASN:HB2	2.50	0.47
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:417:ASN:CG	1:E:440:THR:HG23	2.34	0.47
1:E:494:LEU:CD1	1:E:494:LEU:N	2.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:403:GLN:C	1:K:405:LEU:N	2.68	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:A:544:ASN:HD21	1:A:569:GLN:CD	2.18	0.47
2:F:93:GLU:HG3	2:F:94:GLN:N	2.29	0.47
1:I:469:ILE:HD12	1:I:484:ILE:HG21	1.96	0.47
1:I:394:LYS:HG3	2:J:75:HIS:CE1	2.50	0.47
1:K:554:LYS:HD3	1:K:554:LYS:HA	1.71	0.47
1:K:445:LYS:HD3	2:L:91:TYR:OH	2.15	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:N	2:V:74:ASN:OD1	2.43	0.47
1:E:558:TYR:CE2	1:E:567:PHE:CE2	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
1:E:554:LYS:HG3	1:E:572:MET:CE	2.45	0.46
1:G:426:ARG:O	1:G:427:ASN:C	2.52	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:U:433:PRO:HB2	1:U:468:ILE:HD12	1.98	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
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:I:550:MET:HE1	1:I:575:PHE:HB3	1.97	0.46
1:Q:496:SER:HB3	1:Q:555:TYR:HH	1.76	0.46
1:Q:542:GLN:OE1	1:Q:548:SER:CB	2.64	0.46
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
2:J:47:LEU:C	2:J:47:LEU:HD23	2.36	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:545:GLY:N	1:I:467:GLU:OE2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:407:ASN:N	1:M:407:ASN:OD1	2.48	0.46
2:R:64:PHE:HB3	2:R:88:ILE:CG2	2.46	0.46
1:U:514:ASP:O	1:U:518:THR:OG1	2.30	0.46
1:A:368:LEU:HD23	1:A:372:MET:HE2	1.98	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:HD2	1:C:554:LYS:HA	1.82	0.46
1:G:407:ASN:O	1:G:408:TYR:HB2	2.15	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:I:427:ASN:O	1:I:428:LYS:C	2.54	0.46
1:Q:444:PRO:O	1:Q:448:SER:HB2	2.16	0.46
1:S:495:ASP:C	1:S:495:ASP:OD1	2.54	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:407:ASN:O	1:C:408:TYR:HB2	2.16	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:HG3	2:J:70:ARG:HH11	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
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:S:391:SER:HB3	1:S:396:ARG:NE	2.31	0.45
1:S:556:ALA:O	1:S:560:SER:HB3	2.16	0.45
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:I:561:ARG:C	1:I:563:LYS:H	2.19	0.45
2:J:34:ILE:HD12	2:J:51:TYR:CD1	2.52	0.45
1:K:368:LEU:HD22	1:K:372:MET:HE2	1.98	0.45
1:O:451:TYR:CD1	1:O:451:TYR:C	2.90	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:E:394:LYS:HD3	1:E:396:ARG:NH2	2.32	0.45
2:F:46:LYS:O	2:F:50:SER:OG	2.33	0.45
1:G:495:ASP:OD1	1:G:497:MET:N	2.48	0.45
1:E:407:ASN:HB2	1:I:428:LYS:HE3	1.97	0.45
1:K:496:SER:HB2	1:K:542:GLN:HB3	1.98	0.45
2:L:74:ASN:N	2:L:74:ASN:OD1	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:S:559:ILE:C	1:S:561:ARG:H	2.18	0.45
1:W:467:GLU:HB3	1:W:487:ARG:HD3	1.99	0.45
2:F:20:GLU:C	2:F:21:TYR:CD1	2.90	0.45
1:I:394:LYS:HZ1	1:I:396:ARG:HH22	1.64	0.45
1:I:475:ARG:CA	1:I:475:ARG:HE	2.30	0.45
1:I:498:GLY:HA3	1:I:536:PRO:HG3	1.98	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
2:B:47:LEU:HD23	2:B:47:LEU:C	2.37	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:HA	2:P:85:GLU:OE1	2.15	0.45
1:Q:416:ILE:HG22	1:Q:417:ASN:N	2.31	0.45
1:W:454:VAL:O	1:W:457:TRP:HB2	2.17	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: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:A:574:LEU:O	1:A:578:LYS:N	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:558:TYR:CE2	1:E:567:PHE:HD2	2.31	0.45
2:F:70:ARG:CG	2:F:71:ILE:N	2.80	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:552:THR:O	1:I:553:CYS:C	2.55	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
1:U:550:MET:SD	1:U:579:MET:CE	3.04	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:HG3	1:M:385:GLN:O	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
1:O:567:PHE:CD1	1:O:567:PHE:C	2.90	0.45
2:V:43:HIS:C	2:V:45:LYS:H	2.20	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
2:F:47:LEU:C	2:F:47:LEU:HD23	2.36	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
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:O:538:GLU:H	1:O:538:GLU:HG2	1.59	0.44
1:O:494:LEU:HD23	1:O:539:ILE:HG21	1.99	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
1:G:497:MET:O	1:G:498:GLY:C	2.54	0.44
1:Q:413:ASP:HB2	1:Q:440:THR:OG1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:456:ARG:HD2	2:T:67:GLU:OE2	2.17	0.44
1:U:458:THR:HG21	1:U:511:TYR:OH	2.16	0.44
1:E:517:LYS:NZ	1:U:517:LYS:HD2	2.33	0.44
1:A:459:LYS:HD2	1:A:459:LYS:HA	1.61	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
1:O:413:ASP:N	1:O:413:ASP:OD1	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
2:D:83:GLU:O	2:D:84:GLU:C	2.55	0.44
1:I:582:GLU:HG2	1:I:587:GLN:O	2.17	0.44
2:N:47:LEU:HD23	2:N:47:LEU:C	2.37	0.44
1:W:481:LEU:HD13	1:W:552:THR:HG23	1.99	0.44
1:E:494:LEU:H	1:E:494:LEU:HD12	1.80	0.44
1:E:395:LEU:HD23	2:F:70:ARG:HD2	1.98	0.44
1:I:384:PRO:HB2	1:I:387:GLU:HB2	1.99	0.44
1:M:426:ARG:NH2	1:M:557:ASP:OD1	2.48	0.44
1:A:544:ASN:ND2	1:U:431:GLY:O	2.50	0.44
1:A:463:LEU:O	1:A:486:LEU:HD11	2.17	0.44
1:C:477:VAL:O	2:D:96:GLY:CA	2.50	0.44
1:C:469:ILE:HD12	1:C:484:ILE:HG21	1.99	0.44
2:F:30:ASP:OD1	2:F:30:ASP:O	2.36	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
1:W:488:LYS:O	1:W:489:LYS:C	2.56	0.44
2:X:39:LYS:CG	2:X:42:THR:OG1	2.66	0.44
1:C:581:TRP:O	1:C:582:GLU:C	2.57	0.44
1:E:392:ALA:O	1:E:395:LEU:HB2	2.17	0.44
1:Q:476:LYS:NZ	1:Q:476:LYS:CB	2.80	0.44
1:U:512:LEU:O	1:U:515:GLU:HB3	2.18	0.44
1:U:411:LEU:HG	1:U:549:GLY:HA3	2.00	0.44
1:U:567:PHE:C	1:U:567:PHE:CD1	2.91	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:I:461:VAL:HG22	1:I:462:ASN:N	2.33	0.44
1:K:544:ASN:C	1:K:544:ASN:OD1	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:76:THR:HG22	2:D:79:GLU:CD	2.38	0.43
1:E:555:TYR:O	1:E:556:ALA:C	2.56	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:OE1	1:U:515:GLU:HA	2.16	0.43
2:V:39:LYS:HG3	2:V:42:THR:CG2	2.48	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:487:ARG:HE	1:G:487:ARG:HB2	1.69	0.43
1:G:451:TYR:HE1	1:G:515:GLU:HG2	1.82	0.43
2:H:34:ILE:HG13	2:H:51:TYR:CD2	2.53	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
1:O:389:LEU:HD12	1:O:402:ILE:HG21	1.99	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
2:F:45:LYS:O	2:F:49:GLU:HG3	2.17	0.43
1:M:551:PHE:CE1	1:M:572:MET:HE2	2.53	0.43
1:Q:405:LEU:HD21	1:Q:415:VAL:HG11	2.00	0.43
2:R:43:HIS:C	2:R:45:LYS:H	2.21	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:HA	1:C:388:ILE:HD13	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:454:VAL:O	1:E:455:LYS:C	2.56	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:495:ASP:OD2	1:K:498:GLY:N	2.50	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
2:X:76:THR:HG23	2:X:79:GLU:HB2	2.00	0.43
1:W:412:ASN:HA	2:X:94:GLN:O	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:M:371:ASP:N	1:M:371:ASP:OD1	2.51	0.43
1:O:443:TYR:CE1	1:O:504:ILE:HG23	2.53	0.43
1:S:486:LEU:HA	1:S:486:LEU:HD23	1.75	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:HE3	1:M:429:LYS:HB3	1.22	0.43
1:Q:468:ILE:H	1:Q:468:ILE:HG13	1.59	0.43
2:X:84:GLU:HA	2:X:84:GLU:OE1	2.18	0.43
2:F:66:TRP:HB2	2:F:71:ILE:HD11	2.01	0.43
1:G:432:TYR:O	1:G:433:PRO:C	2.56	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:HB2	1:M:487:ARG:HE	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:HA	1:A:524:LEU:HD13	1.87	0.43
1:C:476:LYS:HG3	1:C:476:LYS:O	2.19	0.43
1:C:474:HIS:NE2	2:D:94:GLN:HB3	2.34	0.43
2:F:24:LEU:HD13	2:F:88:ILE:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:471:VAL:O	1:E:481:LEU:HA	2.19	0.42
1:I:380:LEU:HD23	1:I:402:ILE:HG23	2.01	0.42
2:R:62:LEU:HB3	2:R:90:VAL:HG22	2.01	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: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
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:E:554:LYS:O	1:E:555:TYR:C	2.57	0.42
1:I:456:ARG:H	1:I:456:ARG:HG2	1.41	0.42
1:O:542:GLN:HB2	1:O:551:PHE:CE2	2.54	0.42
1:E:417:ASN:OD1	1:E:440:THR:CG2	2.68	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
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:W:579:MET:HB2	1:W:579:MET:HE3	1.96	0.42
1:E:517:LYS:O	1:E:521:ASN:N	2.53	0.42
2:F:76:THR:O	2:F:77:PRO:C	2.56	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
2:T:26:VAL:HG22	2:T:88:ILE:HB	2.00	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
2:H:37:LYS:HD2	2:H:37:LYS:H	1.83	0.42
2:J:70:ARG:NH1	2:J:70:ARG:CG	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:F:76:THR:HG23	2:F:78:LYS:HB3	2.02	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:469:ILE:HD11	1:Q:486:LEU:HD11	2.02	0.42
1:Q:488:LYS:O	1:Q:489:LYS:C	2.58	0.42
2:T:45:LYS:HB3	2:T:73:ASP:HB3	2.00	0.42
1:W:540:PRO:HG3	1:W:567:PHE:O	2.20	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:HA	1:K:486:LEU:HD23	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:C:410:TRP:CZ3	1:C:477:VAL:HB	2.51	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:K:402:ILE:O	1:K:403:GLN:C	2.58	0.42
1:M:491:LEU:O	1:M:531:HIS:HA	2.19	0.42
1:Q:402:ILE:C	1:Q:404:THR:H	2.23	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:OE1	1:G:414:GLU:HA	2.20	0.42
1:G:459:LYS:HA	1:G:459:LYS:HD2	1.88	0.42
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
1:Q:495:ASP:OD1	1:Q:495:ASP:C	2.58	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:33:GLU:C	2:V:34:ILE:HG13	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:W:387:GLU:O	1:W:398:THR:HA	2.20	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: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:484:ILE:HD13	1:A:512:LEU:HD11	2.02	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:G:417:ASN:O	1:G:418:PHE:C	2.58	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
2:F:20:GLU:C	2:F:21:TYR:HD1	2.23	0.41
1:K:572:MET:O	1:K:573:PRO:C	2.58	0.41
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:I:475:ARG:O	1:I:476:LYS:C	2.59	0.41
1:K:403:GLN:C	1:K:405:LEU:H	2.23	0.41
1:K:457:TRP:N	1:K:457:TRP:CD1	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:403:GLN:O	1:O:406:LYS:HB2	2.20	0.41
1:O:393:PHE:CE2	1:O:421:ASN:HB3	2.55	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
2:V:43:HIS:H	2:V:43:HIS:CD2	2.38	0.41
1:U:441:PHE:HZ	2:V:63:ARG:HG3	1.81	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:N	1:C:394:LYS:HE2	2.28	0.41
2:D:39:LYS:CD	2:D:39:LYS:H	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
2:H:55:GLN:C	2:H:55:GLN:HE21	2.24	0.41
1:M:394:LYS:HD3	1:M:396:ARG:NH2	2.35	0.41
1:M:372:MET:HG2	1:M:581:TRP:NE1	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
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
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
1:U:579:MET:HB2	1:U:579:MET:HE3	1.93	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:476:LYS:C	1:W:477:VAL:HG23	2.41	0.41
1:W:535:LYS:HA	1:W:536:PRO:HD2	1.62	0.41
1:A:405:LEU:C	1:A:576:ARG:NH1	2.74	0.41
1:A:547:ASP:O	1:A:550:MET:N	2.49	0.41
1:C:443:TYR:CE1	1:C:504:ILE:HG23	2.56	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:K:376:ILE:HG12	1:K:580:VAL:HG22	2.03	0.41
1:M:459:LYS:HD2	1:M:459:LYS:HA	1.80	0.41
1:O:413:ASP:HB3	2:P:94:GLN:OE1	2.20	0.41
1:Q:548:SER:HG	2:R:97:GLY:C	2.24	0.41
1:S:484:ILE:HG21	1:S:512:LEU:HD11	2.03	0.41
1:S:574:LEU:O	1:S:575:PHE:C	2.59	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
1:A:588:LEU:O	1:A:589:LEU:HD23	2.21	0.41
1:C:443:TYR:OH	1:C:504:ILE:HG12	2.21	0.41
1:I:446:LEU:O	1:I:448:SER:N	2.54	0.41
1:K:391:SER:O	1:K:392:ALA:CB	2.69	0.41
1:M:493:TYR:CE2	1:M:495:ASP:HB2	2.56	0.41
1:S:416:ILE:O	1:S:417:ASN:C	2.59	0.41
2:B:57:VAL:HG12	2:B:61:SER:HB3	2.02	0.41
1:C:565:ILE:HG12	1:C:565:ILE:H	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:K:406:LYS:O	1:K:407:ASN:C	2.60	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
1:K:410:TRP:CB	2:L:96:GLY:O	2.68	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
1:A:493:TYR:C	1:A:494:LEU:HD12	2.42	0.40
2:D:66:TRP:CH2	2:D:80:LEU:O	2.74	0.40
2:D:43:HIS:HA	2:D:75:HIS:O	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:561:ARG:O	1:I:562:ASP:HB2	2.22	0.40
1:K:394:LYS:N	1:K:394:LYS:HE2	2.36	0.40
1:M:369:THR:HG22	1:M:370:GLU:N	2.36	0.40
1:U:394:LYS:HE2	1:U:394:LYS:N	2.25	0.40
1:U:424:VAL:HG12	1:U:424:VAL:O	2.20	0.40
2:V:45:LYS:O	2:V:49:GLU:HG2	2.21	0.40
2:V:34:ILE:HD12	2:V:51:TYR:CE1	2.57	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:N	1:S:570:HIS:ND1	2.68	0.40
2:V:48:MET:HE3	2:V:64:PHE:HB2	2.03	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
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
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
1:U:457:TRP:CD1	2:V:67:GLU:C	2.95	0.40
2:V:72:ALA:O	2:V:73:ASP:C	2.59	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:HA	1:K:463:LEU:HD23	1.66	0.40
1:K:576:ARG:O	1:K:577:LYS:C	2.60	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:G:385:GLN:CA	1:G:385:GLN:OE1	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	11	43
1	C	222/224 (99%)	187 (84%)	30 (14%)	5 (2%)	6	30
1	E	222/224 (99%)	185 (83%)	31 (14%)	6 (3%)	5	26
1	G	221/224 (99%)	192 (87%)	21 (10%)	8 (4%)	3	19
1	I	221/224 (99%)	172 (78%)	38 (17%)	11 (5%)	2	12
1	K	221/224 (99%)	183 (83%)	30 (14%)	8 (4%)	3	19
1	M	220/224 (98%)	189 (86%)	27 (12%)	4 (2%)	8	37
1	O	221/224 (99%)	198 (90%)	20 (9%)	3 (1%)	11	43
1	Q	222/224 (99%)	188 (85%)	29 (13%)	5 (2%)	6	30
1	S	222/224 (99%)	195 (88%)	23 (10%)	4 (2%)	8	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	U	221/224 (99%)	194 (88%)	26 (12%)	1 (0%)	29	68
1	W	220/224 (98%)	189 (86%)	24 (11%)	7 (3%)	4	22
2	B	76/78 (97%)	68 (90%)	7 (9%)	1 (1%)	12	45
2	D	76/78 (97%)	61 (80%)	11 (14%)	4 (5%)	2	11
2	F	76/78 (97%)	65 (86%)	10 (13%)	1 (1%)	12	45
2	H	75/78 (96%)	69 (92%)	6 (8%)	0	100	100
2	J	76/78 (97%)	70 (92%)	5 (7%)	1 (1%)	12	45
2	L	75/78 (96%)	69 (92%)	5 (7%)	1 (1%)	12	45
2	N	76/78 (97%)	69 (91%)	5 (7%)	2 (3%)	5	27
2	P	76/78 (97%)	68 (90%)	8 (10%)	0	100	100
2	R	76/78 (97%)	63 (83%)	12 (16%)	1 (1%)	12	45
2	T	76/78 (97%)	71 (93%)	3 (4%)	2 (3%)	5	27
2	V	76/78 (97%)	66 (87%)	9 (12%)	1 (1%)	12	45
2	X	76/78 (97%)	67 (88%)	6 (8%)	3 (4%)	3	17
All	All	3564/3624 (98%)	3077 (86%)	405 (11%)	82 (2%)	6	30

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	181 (87%)	26 (13%)	4	20
1	C	207/208 (100%)	167 (81%)	40 (19%)	1	8
1	E	207/208 (100%)	176 (85%)	31 (15%)	3	14
1	G	207/208 (100%)	188 (91%)	19 (9%)	9	34
1	I	207/208 (100%)	172 (83%)	35 (17%)	2	11
1	K	207/208 (100%)	184 (89%)	23 (11%)	6	25
1	M	206/208 (99%)	173 (84%)	33 (16%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	207/208 (100%)	181 (87%)	26 (13%)	4	20
1	Q	207/208 (100%)	181 (87%)	26 (13%)	4	20
1	S	207/208 (100%)	179 (86%)	28 (14%)	4	17
1	U	207/208 (100%)	184 (89%)	23 (11%)	6	25
1	W	206/208 (99%)	175 (85%)	31 (15%)	3	14
2	B	71/71 (100%)	56 (79%)	15 (21%)	1	5
2	D	71/71 (100%)	62 (87%)	9 (13%)	4	19
2	F	71/71 (100%)	56 (79%)	15 (21%)	1	5
2	H	70/71 (99%)	55 (79%)	15 (21%)	1	5
2	J	71/71 (100%)	50 (70%)	21 (30%)	0	1
2	L	70/71 (99%)	60 (86%)	10 (14%)	3	15
2	N	71/71 (100%)	55 (78%)	16 (22%)	1	4
2	P	71/71 (100%)	57 (80%)	14 (20%)	1	7
2	R	71/71 (100%)	57 (80%)	14 (20%)	1	7
2	T	71/71 (100%)	60 (84%)	11 (16%)	2	13
2	V	71/71 (100%)	55 (78%)	16 (22%)	1	4
2	X	71/71 (100%)	56 (79%)	15 (21%)	1	5
All	All	3332/3348 (100%)	2820 (85%)	512 (15%)	2	13

All (512) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	369	THR
1	A	371	ASP
1	A	373	GLU
1	A	402	ILE
1	A	403	GLN
1	A	409	HIS
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	475	ARG
1	A	488	LYS

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Mol	Chain	Res	Type
1	A	491	LEU
1	A	502	HIS
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	574	LEU
1	A	580	VAL
1	A	583	ILE
2	B	25	LYS
2	B	30	ASP
2	B	37	LYS
2	B	39	LYS
2	B	60	ASN
2	B	69	GLN
2	B	70	ARG
2	B	74	ASN
2	B	76	THR
2	B	78	LYS
2	B	82	MET
2	B	83	GLU
2	B	89	GLU
2	B	93	GLU
2	B	94	GLN
1	C	382	HIS
1	C	388	ILE
1	C	391	SER
1	C	393	PHE
1	C	395	LEU
1	C	396	ARG
1	C	398	THR
1	C	402	ILE
1	C	404	THR
1	C	407	ASN
1	C	415	VAL
1	C	422	LEU
1	C	437	VAL
1	C	439	SER
1	C	454	VAL

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Mol	Chain	Res	Type
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	484	ILE
1	C	490	CYS
1	C	494	LEU
1	C	496	SER
1	C	499	GLN
1	C	502	HIS
1	C	515	GLU
1	C	517	LYS
1	C	523	ASP
1	C	524	LEU
1	C	525	ASN
1	C	530	THR
1	C	557	ASP
1	C	565	ILE
1	C	574	LEU
1	C	584	LEU
1	C	587	GLN
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	70	ARG
2	D	74	ASN
2	D	78	LYS
1	E	367	GLU
1	E	374	LYS
1	E	378	ASN
1	E	382	HIS
1	E	396	ARG
1	E	402	ILE
1	E	404	THR
1	E	411	LEU

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Mol	Chain	Res	Type
1	E	426	ARG
1	E	440	THR
1	E	448	SER
1	E	458	THR
1	E	459	LYS
1	E	469	ILE
1	E	489	LYS
1	E	494	LEU
1	E	495	ASP
1	E	500	LYS
1	E	502	HIS
1	E	518	THR
1	E	519	LYS
1	E	523	ASP
1	E	524	LEU
1	E	539	ILE
1	E	546	SER
1	E	548	SER
1	E	553	CYS
1	E	567	PHE
1	E	584	LEU
1	E	588	LEU
1	E	589	LEU
2	F	20	GLU
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	92	GLN
2	F	93	GLU
2	F	94	GLN
1	G	371	ASP
1	G	391	SER
1	G	402	ILE
1	G	403	GLN

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Mol	Chain	Res	Type
1	G	409	HIS
1	G	426	ARG
1	G	437	VAL
1	G	458	THR
1	G	465	GLU
1	G	475	ARG
1	G	476	LYS
1	G	477	VAL
1	G	480	SER
1	G	487	ARG
1	G	496	SER
1	G	517	LYS
1	G	525	ASN
1	G	574	LEU
1	G	580	VAL
2	H	22	ILE
2	H	24	LEU
2	H	38	VAL
2	H	39	LYS
2	H	42	THR
2	H	44	LEU
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
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	448	SER
1	I	456	ARG
1	I	458	THR
1	I	459	LYS

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Mol	Chain	Res	Type
1	I	475	ARG
1	I	480	SER
1	I	491	LEU
1	I	497	MET
1	I	507	ILE
1	I	509	LEU
1	I	512	LEU
1	I	513	GLN
1	I	515	GLU
1	I	526	LEU
1	I	530	THR
1	I	533	SER
1	I	537	HIS
1	I	544	ASN
1	I	551	PHE
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	30	ASP
2	J	32	SER
2	J	33	GLU
2	J	37	LYS
2	J	39	LYS
2	J	45	LYS
2	J	46	LYS
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	69	GLN
2	J	70	ARG
2	J	76	THR

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Mol	Chain	Res	Type
2	J	82	MET
2	J	94	GLN
1	K	369	THR
1	K	371	ASP
1	K	377	SER
1	K	382	HIS
1	K	398	THR
1	K	402	ILE
1	K	411	LEU
1	K	415	VAL
1	K	437	VAL
1	K	439	SER
1	K	459	LYS
1	K	461	VAL
1	K	475	ARG
1	K	476	LYS
1	K	477	VAL
1	K	480	SER
1	K	489	LYS
1	K	502	HIS
1	K	517	LYS
1	K	530	THR
1	K	531	HIS
1	K	565	ILE
1	K	574	LEU
2	L	39	LYS
2	L	40	MET
2	L	42	THR
2	L	54	ARG
2	L	57	VAL
2	L	61	SER
2	L	63	ARG
2	L	70	ARG
2	L	74	ASN
2	L	76	THR
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

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Mol	Chain	Res	Type
1	M	411	LEU
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	475	ARG
1	M	490	CYS
1	M	502	HIS
1	M	508	LEU
1	M	517	LYS
1	M	522	SER
1	M	526	LEU
1	M	527	LEU
1	M	531	HIS
1	M	532	HIS
1	M	542	GLN
1	M	572	MET
1	M	574	LEU
1	M	579	MET
1	M	580	VAL
1	M	587	GLN
2	N	20	GLU
2	N	22	ILE
2	N	30	ASP
2	N	32	SER
2	N	37	LYS
2	N	39	LYS
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	89	GLU
2	N	93	GLU

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Mol	Chain	Res	Type
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	424	VAL
1	O	426	ARG
1	O	429	LYS
1	O	430	GLN
1	O	437	VAL
1	O	448	SER
1	O	475	ARG
1	O	497	MET
1	O	502	HIS
1	O	503	ARG
1	O	524	LEU
1	O	527	LEU
1	O	533	SER
1	O	538	GLU
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	27	ILE
2	P	32	SER
2	P	38	VAL
2	P	39	LYS
2	P	42	THR
2	P	43	HIS
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

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Mol	Chain	Res	Type
1	Q	402	ILE
1	Q	411	LEU
1	Q	416	ILE
1	Q	426	ARG
1	Q	437	VAL
1	Q	468	ILE
1	Q	475	ARG
1	Q	476	LYS
1	Q	477	VAL
1	Q	487	ARG
1	Q	488	LYS
1	Q	491	LEU
1	Q	494	LEU
1	Q	504	ILE
1	Q	508	LEU
1	Q	516	SER
1	Q	518	THR
1	Q	523	ASP
1	Q	527	LEU
1	Q	542	GLN
1	Q	544	ASN
1	Q	568	THR
1	Q	575	PHE
1	Q	580	VAL
2	R	30	ASP
2	R	33	GLU
2	R	37	LYS
2	R	39	LYS
2	R	43	HIS
2	R	52	CYS
2	R	57	VAL
2	R	63	ARG
2	R	64	PHE
2	R	69	GLN
2	R	73	ASP
2	R	75	HIS
2	R	84	GLU
2	R	90	VAL
1	S	373	GLU
1	S	374	LYS
1	S	377	SER
1	S	391	SER

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Mol	Chain	Res	Type
1	S	394	LYS
1	S	396	ARG
1	S	402	ILE
1	S	403	GLN
1	S	415	VAL
1	S	440	THR
1	S	445	LYS
1	S	458	THR
1	S	459	LYS
1	S	463	LEU
1	S	467	GLU
1	S	476	LYS
1	S	478	HIS
1	S	480	SER
1	S	495	ASP
1	S	502	HIS
1	S	506	GLU
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	37	LYS
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	393	PHE
1	U	394	LYS
1	U	396	ARG
1	U	402	ILE
1	U	426	ARG

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Mol	Chain	Res	Type
1	U	437	VAL
1	U	447	LYS
1	U	448	SER
1	U	456	ARG
1	U	458	THR
1	U	459	LYS
1	U	461	VAL
1	U	475	ARG
1	U	476	LYS
1	U	502	HIS
1	U	503	ARG
1	U	531	HIS
1	U	533	SER
1	U	565	ILE
1	U	574	LEU
1	U	580	VAL
2	V	22	ILE
2	V	30	ASP
2	V	36	PHE
2	V	37	LYS
2	V	47	LEU
2	V	53	GLN
2	V	57	VAL
2	V	67	GLU
2	V	69	GLN
2	V	73	ASP
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	396	ARG
1	W	398	THR
1	W	402	ILE
1	W	403	GLN
1	W	411	LEU

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Mol	Chain	Res	Type
1	W	420	MET
1	W	444	PRO
1	W	459	LYS
1	W	461	VAL
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	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	574	LEU
1	W	580	VAL
2	X	22	ILE
2	X	26	VAL
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	513	GLN
1	A	544	ASN

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Mol	Chain	Res	Type
2	B	43	HIS
2	B	55	GLN
1	C	403	GLN
1	C	544	ASN
2	D	35	HIS
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	407	ASN
1	I	541	GLN
1	I	544	ASN
1	K	382	HIS
1	K	513	GLN
1	K	531	HIS
2	L	29	GLN
2	L	92	GLN
1	M	510	GLN
1	O	403	GLN
1	O	417	ASN
1	O	499	GLN
1	O	531	HIS
1	O	541	GLN
1	O	586	GLN
2	P	55	GLN
1	Q	407	ASN
1	Q	412	ASN
1	Q	417	ASN
1	Q	537	HIS
2	R	29	GLN
1	S	409	HIS
1	S	585	HIS
1	U	403	GLN
1	U	513	GLN
1	U	521	ASN
2	V	43	HIS
2	V	69	GLN

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Mol	Chain	Res	Type
1	W	385	GLN
1	W	521	ASN
2	X	55	GLN
2	X	74	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	223/224 (99%)	-0.28	0 <span>100</span> <span>100</span>	26, 40, 65, 77	0
1	C	224/224 (100%)	-0.10	1 (0%) <span>92</span> <span>79</span>	42, 60, 84, 88	0
1	E	224/224 (100%)	-0.10	2 (0%) <span>84</span> <span>63</span>	35, 58, 88, 98	0
1	G	223/224 (99%)	-0.31	0 <span>100</span> <span>100</span>	23, 43, 72, 85	0
1	I	223/224 (99%)	-0.11	0 <span>100</span> <span>100</span>	25, 56, 84, 89	0
1	K	223/224 (99%)	-0.25	0 <span>100</span> <span>100</span>	22, 42, 69, 73	0
1	M	222/224 (99%)	-0.17	1 (0%) <span>91</span> <span>75</span>	25, 43, 67, 95	0
1	O	223/224 (99%)	0.17	6 (2%) <span>54</span> <span>26</span>	57, 74, 92, 101	0
1	Q	224/224 (100%)	1.02	36 (16%) <span>1</span> <span>0</span>	71, 94, 110, 114	0
1	S	224/224 (100%)	-0.27	0 <span>100</span> <span>100</span>	24, 44, 67, 74	0
1	U	223/224 (99%)	-0.21	0 <span>100</span> <span>100</span>	24, 45, 69, 77	0
1	W	222/224 (99%)	-0.01	2 (0%) <span>84</span> <span>63</span>	40, 63, 89, 94	0
2	B	78/78 (100%)	-0.23	0 <span>100</span> <span>100</span>	37, 47, 60, 64	0
2	D	78/78 (100%)	0.03	0 <span>100</span> <span>100</span>	51, 66, 76, 77	0
2	F	78/78 (100%)	-0.05	2 (2%) <span>56</span> <span>27</span>	35, 50, 64, 69	0
2	H	77/78 (98%)	0.05	1 (1%) <span>77</span> <span>51</span>	32, 66, 83, 85	0
2	J	78/78 (100%)	-0.01	0 <span>100</span> <span>100</span>	54, 60, 72, 74	0
2	L	77/78 (98%)	-0.14	0 <span>100</span> <span>100</span>	35, 46, 61, 65	0
2	N	78/78 (100%)	-0.05	0 <span>100</span> <span>100</span>	39, 48, 70, 72	0
2	P	78/78 (100%)	0.48	4 (5%) <span>28</span> <span>10</span>	69, 87, 101, 103	0
2	R	78/78 (100%)	0.95	10 (12%) <span>3</span> <span>1</span>	88, 99, 113, 117	0
2	T	78/78 (100%)	-0.08	0 <span>100</span> <span>100</span>	29, 50, 64, 65	0
2	V	78/78 (100%)	0.15	0 <span>100</span> <span>100</span>	35, 77, 89, 89	0
2	X	78/78 (100%)	-0.08	0 <span>100</span> <span>100</span>	46, 57, 70, 72	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	3612/3624 (99%)	-0.02	65 (1%) 68 40	22, 56, 96, 117	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	530	THR	7.0
1	Q	525	ASN	5.1
1	M	369	THR	4.9
2	R	53	GLN	4.7
1	Q	556	ALA	4.1
1	Q	526	LEU	4.0
1	Q	532	HIS	3.9
1	Q	509	LEU	3.8
1	O	388	ILE	3.7
2	R	59	MET	3.6
1	Q	587	GLN	3.5
1	Q	432	TYR	3.5
1	Q	490	CYS	3.3
2	R	60	ASN	3.2
2	R	20	GLU	3.2
1	Q	385	GLN	3.0
1	Q	564	PRO	3.0
2	R	67	GLU	2.8
2	F	53	GLN	2.8
1	Q	392	ALA	2.8
1	Q	383	GLY	2.7
1	Q	513	GLN	2.7
1	Q	511	TYR	2.7
1	Q	552	THR	2.6
1	O	477	VAL	2.6
1	Q	458	THR	2.6
2	P	54	ARG	2.6
1	Q	568	THR	2.6
1	Q	391	SER	2.5
1	Q	510	GLN	2.5
1	O	523	ASP	2.4
2	F	60	ASN	2.4
1	Q	517	LYS	2.4
1	Q	431	GLY	2.4
1	Q	384	PRO	2.3
2	P	64	PHE	2.3
2	R	52	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	Q	536	PRO	2.3
1	Q	371	ASP	2.3
2	R	66	TRP	2.2
1	Q	386	ASP	2.2
1	Q	484	ILE	2.2
1	Q	370	GLU	2.2
2	R	88	ILE	2.2
1	Q	446	LEU	2.2
1	Q	400	GLY	2.2
1	W	527	LEU	2.2
2	P	20	GLU	2.2
1	O	527	LEU	2.2
2	P	50	SER	2.1
1	Q	527	LEU	2.1
1	O	389	LEU	2.1
1	C	526	LEU	2.1
1	Q	523	ASP	2.1
1	Q	555	TYR	2.1
1	W	526	LEU	2.1
1	Q	467	GLU	2.1
2	R	27	ILE	2.1
1	E	526	LEU	2.1
2	R	50	SER	2.1
1	O	386	ASP	2.0
1	Q	547	ASP	2.0
2	H	59	MET	2.0
1	E	430	GLN	2.0
1	Q	452	GLN	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.