



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:56 PM UTC

PDB ID : 1YG8 / pdb_00001yg8
Title : The structure of a V6A variant of ClpP.
Authors : Bewley, M.C.; Graziano, V.; Griffin, K.; Flanagan, J.M.
Deposited on : 2005-01-04
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

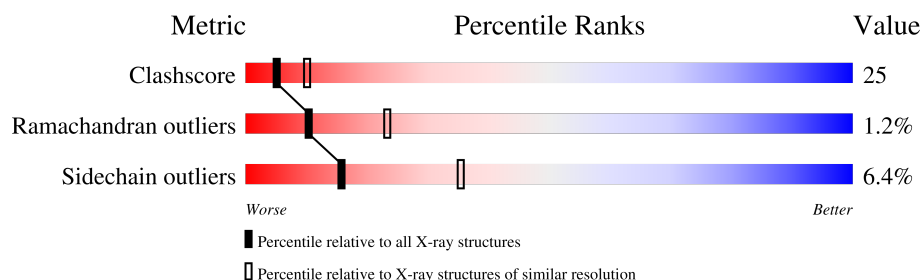
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

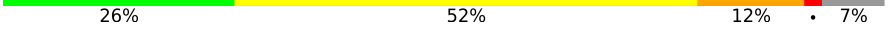
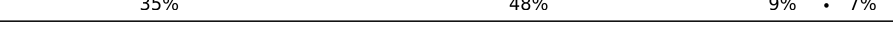
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	193	51% 36% 6% 7%
1	B	193	55% 32% 5% 7%
1	C	193	61% 27% • 7%
1	D	193	54% 32% 7% 7%
1	E	193	45% 42% 6% 7%
1	F	193	49% 39% 5% 7%
1	G	193	56% 31% 6% 7%
1	H	193	61% 28% • 7%

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Mol	Chain	Length	Quality of chain
1	I	193	
1	J	193	
1	K	193	
1	L	193	
1	M	193	
1	N	193	
1	O	193	
1	P	193	
1	Q	193	
1	R	193	
1	S	193	
1	T	193	
1	U	193	
1	V	193	
1	W	193	
1	X	193	
1	Y	193	
1	Z	193	
1	a	193	
1	b	193	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 39312 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 ATP-dependent Clp protease proteolytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	B	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	C	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	D	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	E	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	F	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	G	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	H	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	I	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	J	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	K	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	L	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	M	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	N	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	O	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	P	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	R	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	S	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	T	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	U	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	V	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	W	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	X	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	Y	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	Z	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	a	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	b	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	ALA	VAL	engineered mutation	UNP P19245
B	3	ALA	VAL	engineered mutation	UNP P19245
C	3	ALA	VAL	engineered mutation	UNP P19245
D	3	ALA	VAL	engineered mutation	UNP P19245
E	3	ALA	VAL	engineered mutation	UNP P19245
F	3	ALA	VAL	engineered mutation	UNP P19245
G	3	ALA	VAL	engineered mutation	UNP P19245
H	3	ALA	VAL	engineered mutation	UNP P19245
I	3	ALA	VAL	engineered mutation	UNP P19245
J	3	ALA	VAL	engineered mutation	UNP P19245
K	3	ALA	VAL	engineered mutation	UNP P19245
L	3	ALA	VAL	engineered mutation	UNP P19245
M	3	ALA	VAL	engineered mutation	UNP P19245
N	3	ALA	VAL	engineered mutation	UNP P19245
O	3	ALA	VAL	engineered mutation	UNP P19245

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Chain	Residue	Modelled	Actual	Comment	Reference
P	3	ALA	VAL	engineered mutation	UNP P19245
Q	3	ALA	VAL	engineered mutation	UNP P19245
R	3	ALA	VAL	engineered mutation	UNP P19245
S	3	ALA	VAL	engineered mutation	UNP P19245
T	3	ALA	VAL	engineered mutation	UNP P19245
U	3	ALA	VAL	engineered mutation	UNP P19245
V	3	ALA	VAL	engineered mutation	UNP P19245
W	3	ALA	VAL	engineered mutation	UNP P19245
X	3	ALA	VAL	engineered mutation	UNP P19245
Y	3	ALA	VAL	engineered mutation	UNP P19245
Z	3	ALA	VAL	engineered mutation	UNP P19245
a	3	ALA	VAL	engineered mutation	UNP P19245
b	3	ALA	VAL	engineered mutation	UNP P19245

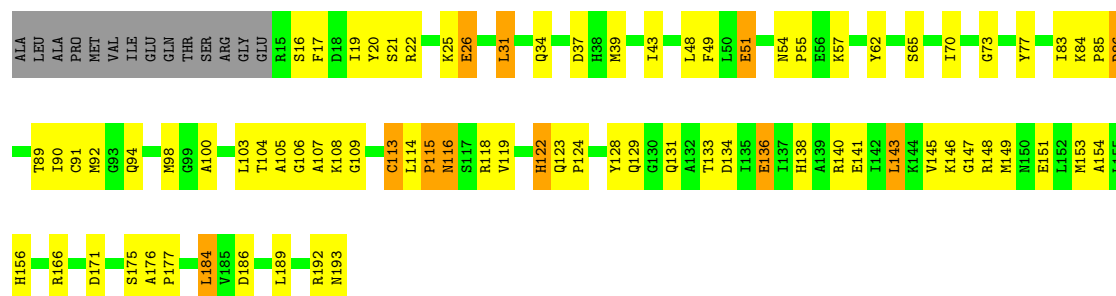
3 Residue-property plots [i](#)

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

Note EDS was not executed.

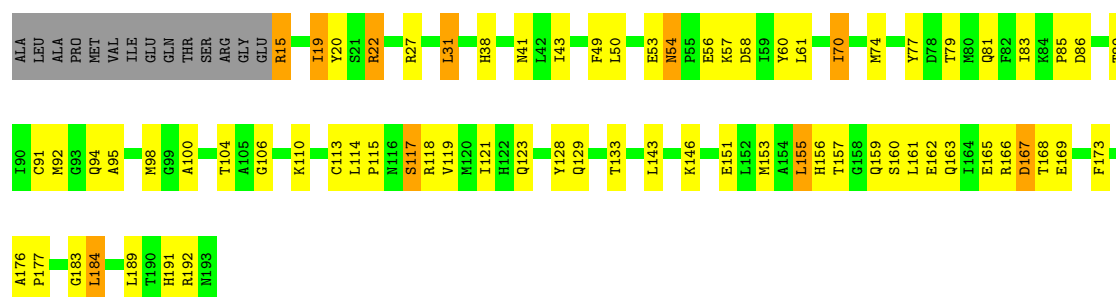
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain A: 



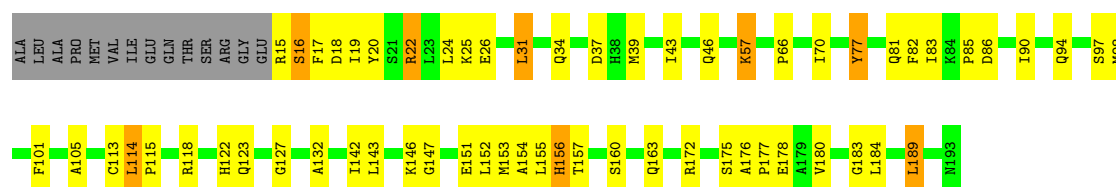
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain B: 



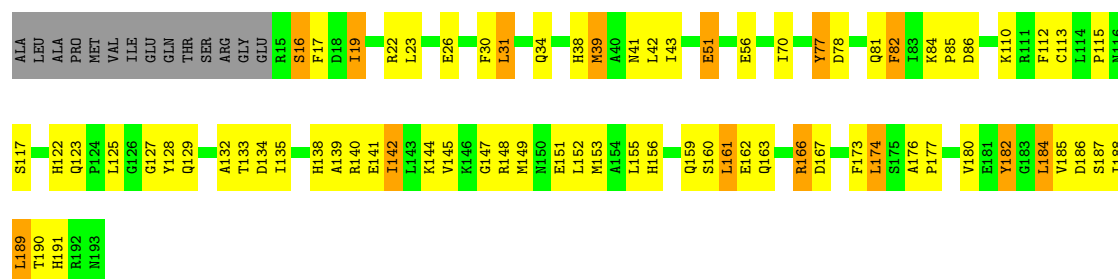
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain C: 



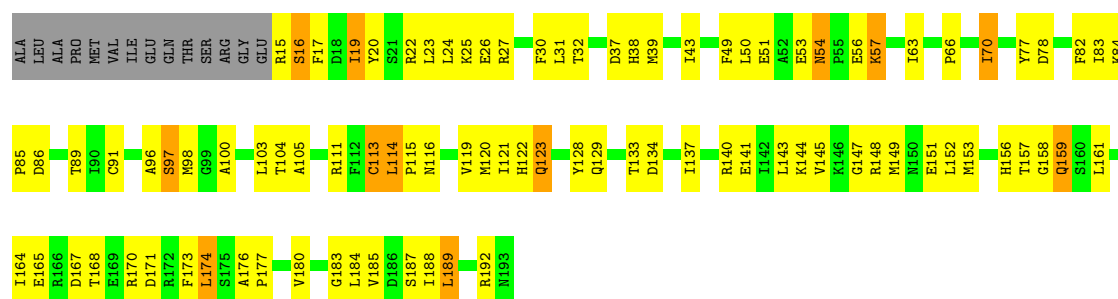
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain D:  54% 32% 7% 7%



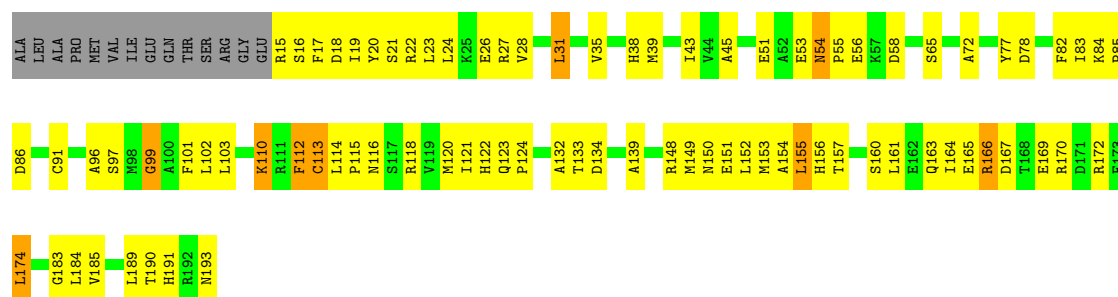
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain E:  45% 42% 6% 7%



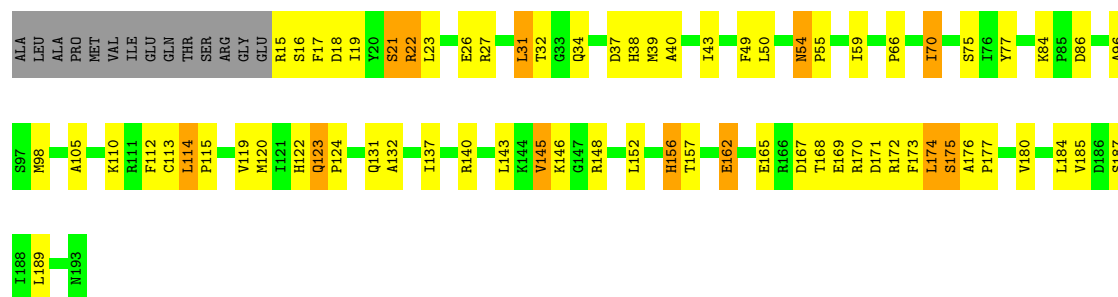
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain F:  49% 39% 5% 7%



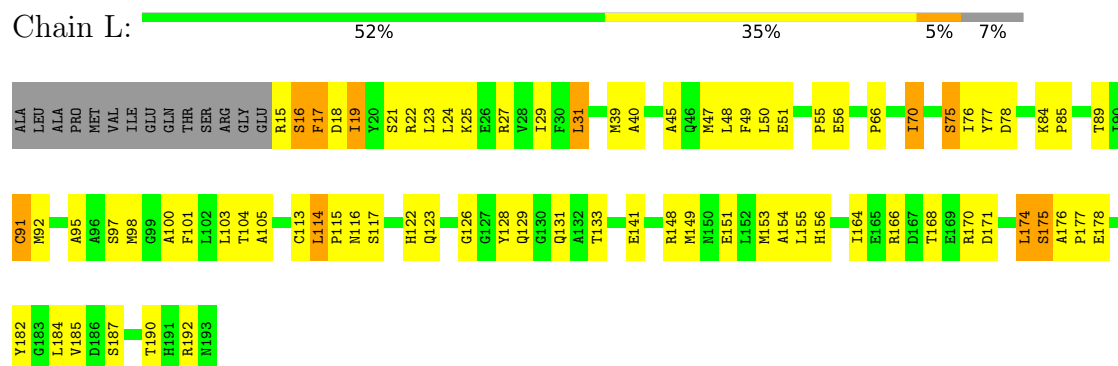
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain G:  56% 31% 6% 7%

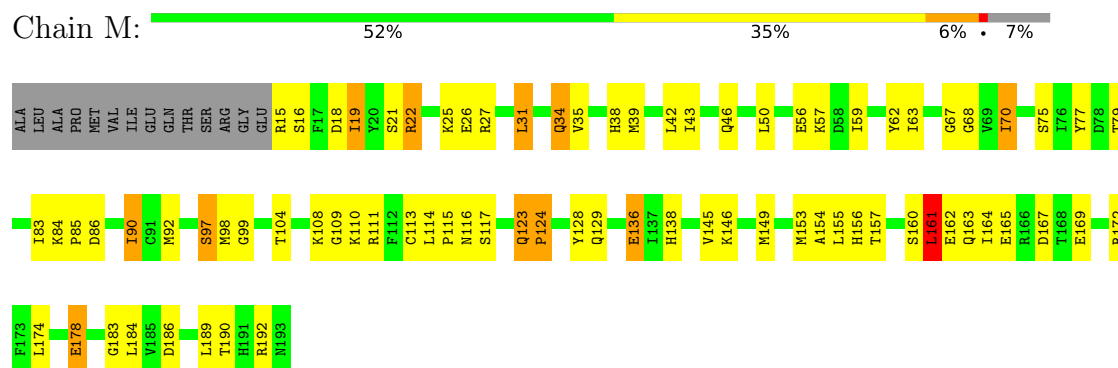


- | | | |
|------|------|-----|
| E165 | T89 | ALA |
| R166 | I90 | LEU |
| D167 | C91 | ALA |
| T168 | A85 | PRO |
| E169 | A86 | MET |
| R170 | S97 | VAL |
| D171 | M98 | ILE |
| R172 | G99 | GLU |
| | A100 | GLN |
| S175 | L103 | THR |
| A176 | T104 | SER |
| P177 | A105 | ARG |
| E178 | G106 | GLY |
| A179 | A107 | GLU |
| V180 | R111 | R15 |
| E181 | F112 | S16 |
| Y182 | C113 | F17 |
| G183 | L114 | D18 |
| L184 | P115 | I19 |
| V185 | N116 | R22 |
| L189 | S117 | L23 |
| T190 | R118 | L24 |
| H191 | M119 | |
| R192 | I121 | R27 |
| N193 | H122 | L31 |
| | Q123 | T32 |
| | Q131 | G33 |
| | A132 | Q34 |
| | E136 | H38 |
| L138 | I137 | M39 |
| H138 | H138 | L42 |
| A139 | A139 | I43 |
| R140 | R140 | V44 |
| E141 | E141 | A45 |
| I142 | I142 | Q46 |
| L143 | L143 | |
| | K146 | F49 |
| | G147 | L50 |
| | R148 | E51 |
| | | I59 |
| | | Y62 |
| | L152 | T70 |
| | M153 | |
| A154 | A154 | S75 |
| H156 | H156 | I76 |
| T157 | T157 | Y77 |
| G158 | G158 | D78 |
| Q159 | Q159 | |
| S160 | S160 | I83 |
| E161 | E161 | K84 |
| E162 | E162 | P85 |
| Q163 | Q163 | |
| L164 | L164 | S88 |

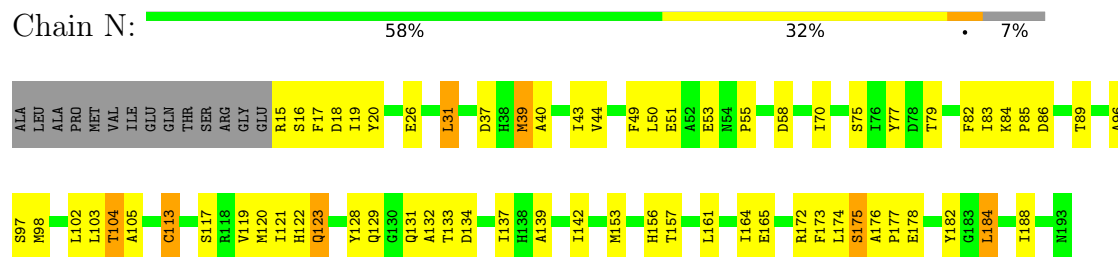
• Molecule 1: ATP-dependent Clp protease proteolytic subunit



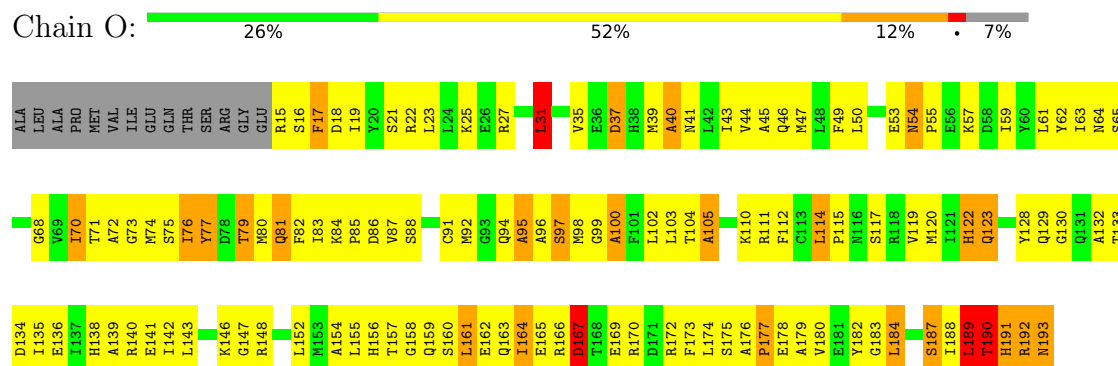
• Molecule 1: ATP-dependent Clp protease proteolytic subunit



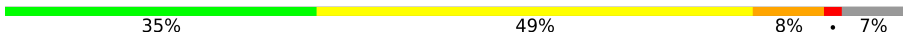
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

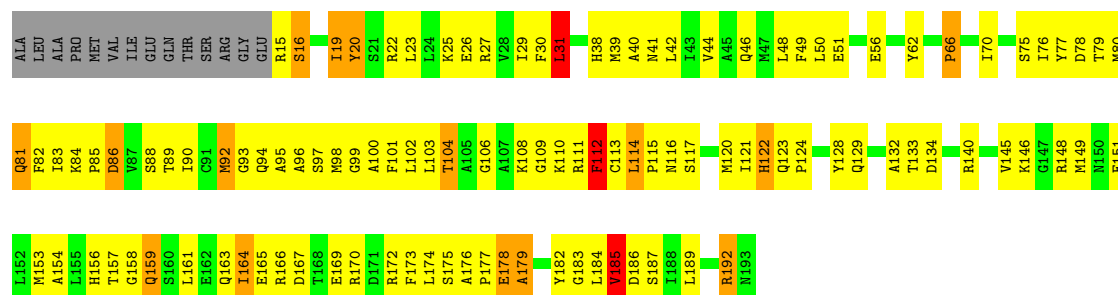


• Molecule 1: ATP-dependent Clp protease proteolytic subunit



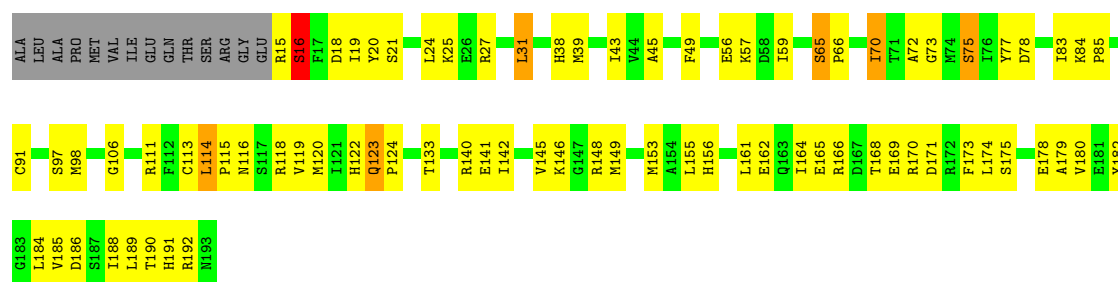
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain P: 



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Q: 



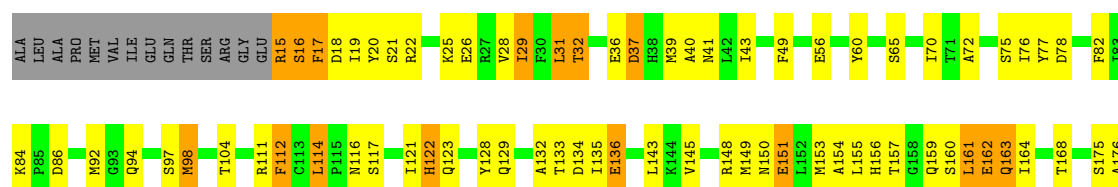
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

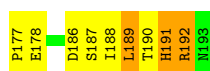
Chain R: 



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

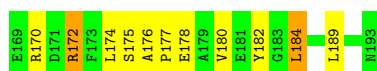
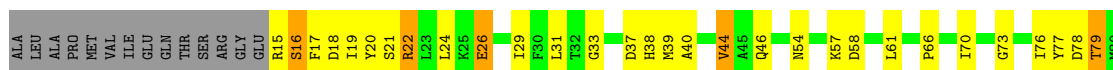
Chain S: 





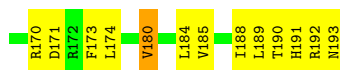
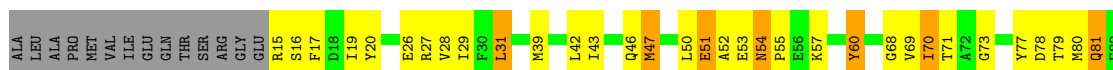
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain T: 50% 37% 6% 7%



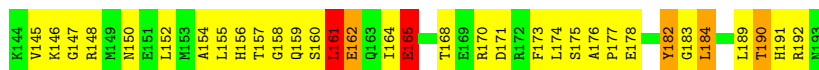
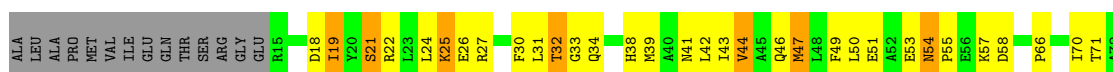
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain U: 49% 36% 8% 7%



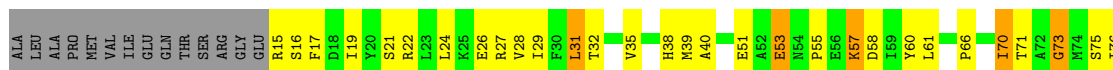
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

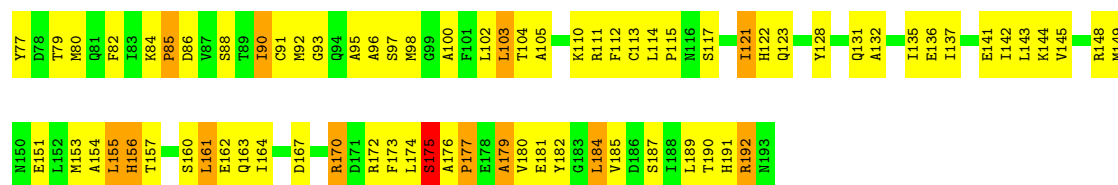
Chain V: 35% 48% 9% 7%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

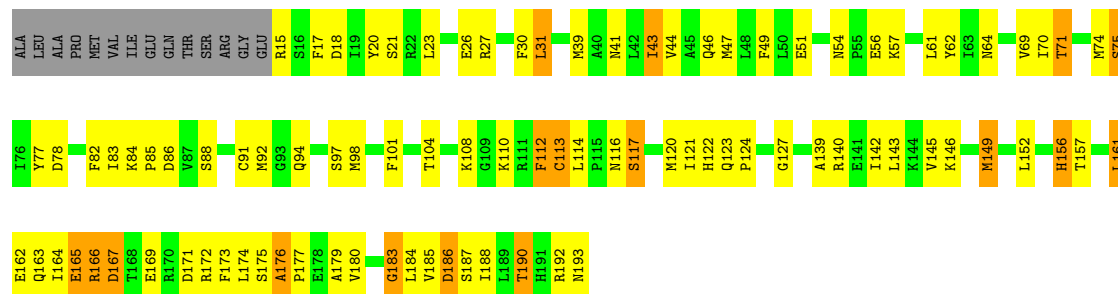
Chain W: 39% 45% 9% 7%





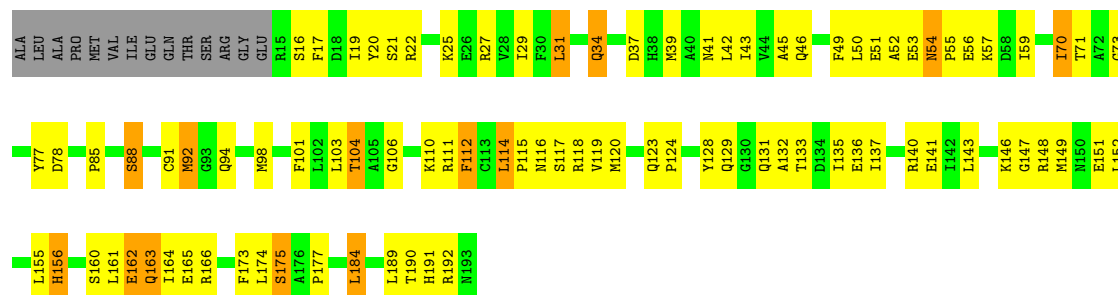
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain X: 45% 39% 9% 7%



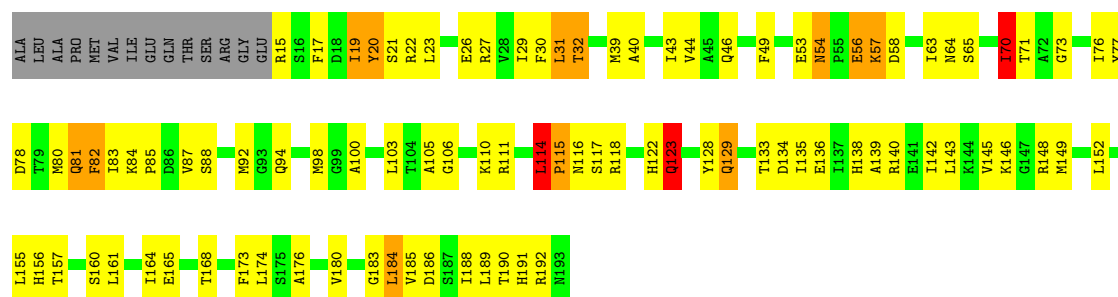
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Y: 46% 39% 7% 7%



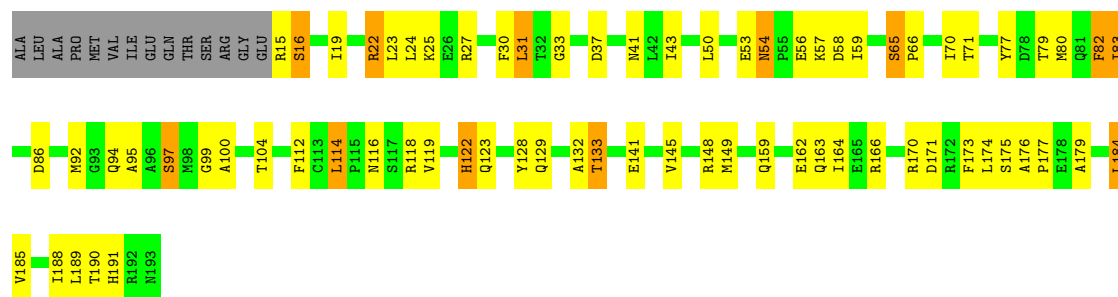
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Z: 44% 41% 6% 7%



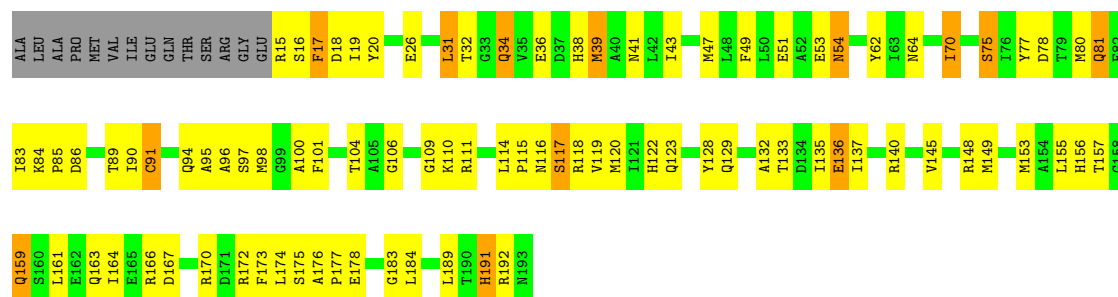
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain a: 55% 31% 6% 7%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain b: 46% 40% 7% 7%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.80Å 161.00Å 186.60Å 90.00° 90.30° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.220 , 0.267	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	39312	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

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	0.80	0/1427	1.23	12/1921 (0.6%)
1	B	0.76	0/1427	1.15	7/1921 (0.4%)
1	C	0.77	0/1427	1.19	12/1921 (0.6%)
1	D	0.76	0/1427	1.15	13/1921 (0.7%)
1	E	0.73	0/1427	1.24	16/1921 (0.8%)
1	F	0.74	0/1427	1.18	9/1921 (0.5%)
1	G	0.73	0/1427	1.20	16/1921 (0.8%)
1	H	0.82	0/1427	1.15	10/1921 (0.5%)
1	I	0.77	0/1427	1.21	15/1921 (0.8%)
1	J	0.77	1/1427 (0.1%)	1.28	13/1921 (0.7%)
1	K	0.77	0/1427	1.25	18/1921 (0.9%)
1	L	0.77	0/1427	1.18	8/1921 (0.4%)
1	M	0.76	1/1427 (0.1%)	1.19	13/1921 (0.7%)
1	N	0.79	1/1427 (0.1%)	1.16	8/1921 (0.4%)
1	O	0.81	1/1427 (0.1%)	1.20	15/1921 (0.8%)
1	P	0.80	2/1427 (0.1%)	1.28	17/1921 (0.9%)
1	Q	0.78	0/1427	1.19	9/1921 (0.5%)
1	R	0.76	1/1427 (0.1%)	1.19	15/1921 (0.8%)
1	S	0.80	0/1427	1.23	18/1921 (0.9%)
1	T	0.77	0/1427	1.19	10/1921 (0.5%)
1	U	0.77	0/1427	1.27	16/1921 (0.8%)
1	V	0.78	0/1427	1.26	17/1921 (0.9%)
1	W	0.75	0/1427	1.26	17/1921 (0.9%)
1	X	0.74	0/1427	1.19	12/1921 (0.6%)
1	Y	0.75	0/1427	1.22	10/1921 (0.5%)
1	Z	0.80	0/1427	1.21	14/1921 (0.7%)
1	a	0.75	0/1427	1.13	6/1921 (0.3%)
1	b	0.74	0/1427	1.20	13/1921 (0.7%)
All	All	0.77	7/39956 (0.0%)	1.21	359/53788 (0.7%)

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
1	B	0	1
1	S	0	1
All	All	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	80	MET	SD-CE	7.56	1.98	1.79
1	N	39	MET	SD-CE	-5.61	1.65	1.79
1	M	70	ILE	CA-CB	5.55	1.60	1.54
1	P	80	MET	SD-CE	5.53	1.93	1.79
1	J	92	MET	SD-CE	5.49	1.93	1.79
1	P	92	MET	SD-CE	5.34	1.93	1.79
1	R	74	MET	SD-CE	-5.29	1.66	1.79

All (359) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	17	PHE	N-CA-C	-12.57	97.21	112.54
1	Y	17	PHE	N-CA-C	-12.13	97.85	112.89
1	J	123	GLN	CA-C-N	10.60	130.69	119.78
1	J	123	GLN	C-N-CA	10.60	130.69	119.78
1	a	37	ASP	N-CA-C	9.54	122.56	111.11
1	N	17	PHE	N-CA-C	-9.40	101.74	113.02
1	E	82	PHE	N-CA-C	9.39	121.12	111.07
1	R	17	PHE	N-CA-C	-9.31	101.08	111.14
1	G	38	HIS	N-CA-C	8.90	121.06	111.36
1	Z	180	VAL	N-CA-C	-8.89	102.17	110.53
1	J	17	PHE	N-CA-C	-8.86	101.71	111.36
1	R	54	ASN	CA-C-N	8.81	128.45	119.82
1	R	54	ASN	C-N-CA	8.81	128.45	119.82
1	P	66	PRO	N-CA-C	-8.80	102.13	114.98
1	U	26	GLU	N-CA-C	-8.80	101.53	112.88
1	Y	163	GLN	N-CA-C	-8.67	101.91	111.36
1	P	153	MET	N-CA-C	-8.52	101.94	111.14
1	A	21	SER	N-CA-C	-8.51	101.94	111.82
1	P	16	SER	N-CA-C	-8.36	101.78	114.16
1	C	180	VAL	N-CA-C	-8.35	102.72	110.82
1	S	17	PHE	N-CA-C	-8.31	98.84	111.56
1	D	82	PHE	N-CA-C	8.26	122.63	112.23
1	C	37	ASP	N-CA-C	8.24	121.30	111.33
1	O	70	ILE	N-CA-C	8.23	118.16	110.42
1	H	38	HIS	N-CA-C	8.20	121.40	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	162	GLU	N-CA-C	8.16	119.86	110.97
1	X	117	SER	N-CA-C	-8.12	100.06	110.53
1	I	37	ASP	N-CA-C	8.06	124.66	111.37
1	K	17	PHE	N-CA-C	-7.99	102.26	110.97
1	U	70	ILE	N-CA-C	7.99	117.93	110.42
1	V	38	HIS	N-CA-C	7.97	119.60	111.07
1	G	26	GLU	N-CA-C	-7.93	103.68	112.72
1	D	39	MET	N-CA-C	-7.92	102.87	112.54
1	W	17	PHE	N-CA-C	-7.90	102.61	111.14
1	W	19	ILE	N-CA-C	7.84	118.62	110.62
1	U	180	VAL	N-CA-C	-7.82	103.18	110.53
1	A	17	PHE	N-CA-C	-7.80	102.77	111.82
1	G	123	GLN	N-CA-C	7.80	119.67	110.31
1	U	112	PHE	N-CA-C	7.74	121.64	109.81
1	W	161	LEU	N-CA-C	-7.72	102.56	110.97
1	Q	65	SER	CA-C-N	7.66	129.42	119.84
1	Q	65	SER	C-N-CA	7.66	129.42	119.84
1	I	117	SER	N-CA-C	-7.64	101.01	110.41
1	M	161	LEU	N-CA-C	-7.64	102.92	111.71
1	C	86	ASP	N-CA-C	-7.57	99.83	110.50
1	K	75	SER	N-CA-C	-7.55	103.06	111.82
1	C	156	HIS	N-CA-C	7.51	120.53	111.82
1	b	135	ILE	N-CA-C	-7.41	103.31	110.42
1	T	38	HIS	N-CA-C	7.41	120.42	111.82
1	D	70	ILE	N-CA-C	7.38	117.47	110.53
1	S	37	ASP	N-CA-C	7.35	123.50	111.37
1	E	57	LYS	N-CA-C	7.32	121.97	110.32
1	J	38	HIS	N-CA-C	7.32	119.05	111.14
1	I	135	ILE	N-CA-C	-7.30	103.66	110.53
1	Z	82	PHE	N-CA-C	7.29	118.87	111.07
1	b	38	HIS	N-CA-C	7.28	119.30	111.36
1	b	117	SER	N-CA-C	-7.22	101.53	110.41
1	R	70	ILE	N-CA-C	7.21	117.19	110.42
1	X	156	HIS	N-CA-C	7.20	121.70	112.34
1	O	31	LEU	N-CA-C	-7.14	96.88	108.52
1	X	161	LEU	N-CA-C	-7.10	103.54	111.28
1	Q	24	LEU	N-CA-C	-7.08	103.90	112.54
1	D	51	GLU	N-CA-C	-7.06	103.19	111.03
1	M	26	GLU	N-CA-C	-7.04	104.57	113.02
1	S	135	ILE	N-CA-C	-7.04	103.67	110.42
1	D	182	TYR	N-CA-C	-7.00	104.72	113.18
1	N	82	PHE	N-CA-C	6.93	118.63	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	117	SER	N-CA-C	-6.91	100.75	110.50
1	S	97	SER	CB-CA-C	-6.90	108.60	116.54
1	R	57	LYS	N-CA-C	6.89	120.48	110.28
1	O	146	LYS	N-CA-C	-6.86	103.81	111.28
1	R	65	SER	CA-C-N	6.86	129.19	120.89
1	R	65	SER	C-N-CA	6.86	129.19	120.89
1	D	38	HIS	N-CA-C	6.85	120.12	111.69
1	B	19	ILE	N-CA-C	6.85	118.43	110.62
1	P	38	HIS	N-CA-C	6.79	119.69	111.40
1	I	46	GLN	N-CA-C	-6.79	103.88	111.28
1	A	113	CYS	N-CA-C	-6.79	98.71	109.23
1	Q	38	HIS	N-CA-C	6.77	118.45	111.14
1	Y	114	LEU	N-CA-C	-6.76	100.25	110.39
1	O	169	GLU	N-CA-C	-6.75	103.85	111.07
1	P	179	ALA	N-CA-C	-6.74	103.73	112.23
1	W	75	SER	N-CA-C	-6.74	104.87	113.23
1	A	100	ALA	N-CA-C	-6.73	104.02	111.36
1	E	97	SER	CB-CA-C	-6.71	108.83	116.54
1	F	26	GLU	N-CA-C	-6.70	105.42	112.93
1	a	114	LEU	N-CA-C	-6.70	100.33	110.39
1	X	39	MET	N-CA-C	-6.70	103.98	111.28
1	T	26	GLU	N-CA-C	-6.69	104.25	112.88
1	U	117	SER	N-CA-C	-6.69	101.70	110.53
1	L	75	SER	N-CA-C	-6.67	104.03	111.71
1	A	138	HIS	N-CA-C	6.67	118.63	111.36
1	W	85	PRO	N-CA-C	6.66	120.86	111.33
1	b	39	MET	N-CA-C	-6.64	104.12	111.36
1	P	187	SER	N-CA-C	6.63	117.33	108.38
1	W	38	HIS	N-CA-C	6.63	118.58	111.36
1	R	26	GLU	N-CA-C	-6.61	105.08	113.02
1	U	123	GLN	N-CA-C	6.60	120.54	110.50
1	F	82	PHE	N-CA-C	6.58	119.43	111.40
1	U	106	GLY	N-CA-C	-6.54	102.50	112.51
1	L	66	PRO	N-CA-C	-6.51	105.47	114.98
1	I	112	PHE	N-CA-C	6.51	119.76	109.81
1	T	114	LEU	N-CA-C	-6.50	100.59	110.01
1	D	117	SER	N-CA-C	-6.47	101.99	110.53
1	G	37	ASP	N-CA-C	6.46	122.04	111.37
1	O	100	ALA	N-CA-C	-6.46	103.47	112.45
1	R	97	SER	CB-CA-C	-6.45	109.15	116.63
1	V	19	ILE	N-CA-C	6.42	117.94	110.62
1	b	26	GLU	N-CA-C	-6.42	104.76	112.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	16	SER	N-CA-C	-6.41	102.72	111.56
1	T	106	GLY	N-CA-C	-6.38	104.01	112.82
1	O	17	PHE	N-CA-C	-6.37	103.63	111.40
1	C	82	PHE	N-CA-C	6.35	119.01	111.33
1	N	175	SER	N-CA-C	-6.33	102.17	110.53
1	X	176	ALA	N-CA-C	-6.33	103.88	112.35
1	O	184	LEU	N-CA-C	-6.31	103.71	111.40
1	B	143	LEU	N-CA-C	-6.27	104.53	111.36
1	X	75	SER	N-CA-C	-6.24	104.47	111.28
1	U	114	LEU	N-CA-C	-6.23	101.14	110.24
1	G	156	HIS	N-CA-C	6.23	119.73	111.75
1	U	17	PHE	N-CA-C	-6.23	104.41	111.07
1	Z	20	TYR	N-CA-C	6.22	117.86	111.14
1	C	114	LEU	CA-C-N	6.22	127.61	119.84
1	C	114	LEU	C-N-CA	6.22	127.61	119.84
1	H	86	ASP	N-CA-C	-6.22	99.52	109.96
1	E	38	HIS	N-CA-C	6.21	118.05	111.28
1	U	185	VAL	N-CA-C	-6.21	98.70	108.95
1	X	112	PHE	N-CA-C	6.21	119.14	109.52
1	P	31	LEU	N-CA-C	-6.20	96.98	108.02
1	K	123	GLN	CA-C-N	6.20	126.14	119.76
1	K	123	GLN	C-N-CA	6.20	126.14	119.76
1	b	159	GLN	N-CA-C	-6.20	100.81	110.42
1	V	75	SER	N-CA-C	-6.20	104.42	112.23
1	Z	63	ILE	N-CA-C	6.20	116.80	107.75
1	Y	175	SER	N-CA-C	-6.19	101.80	110.35
1	G	66	PRO	N-CA-C	-6.19	105.94	114.98
1	E	24	LEU	N-CA-C	-6.18	104.62	111.36
1	E	26	GLU	N-CA-C	-6.18	104.38	112.41
1	T	182	TYR	N-CA-C	-6.18	105.23	112.89
1	K	70	ILE	N-CA-C	6.16	116.33	110.42
1	G	19	ILE	N-CA-C	6.14	116.89	110.62
1	J	66	PRO	N-CA-C	-6.13	106.03	114.98
1	V	115	PRO	N-CA-C	6.13	122.70	113.81
1	Y	156	HIS	N-CA-C	6.12	118.04	111.36
1	O	191	HIS	N-CA-C	6.12	118.66	108.13
1	S	75	SER	N-CA-C	-6.12	104.67	111.71
1	W	79	THR	N-CA-C	-6.11	105.09	112.54
1	H	37	ASP	N-CA-C	6.10	118.43	111.11
1	V	32	THR	N-CA-C	6.09	119.40	109.59
1	I	85	PRO	N-CA-C	6.08	120.88	111.21
1	A	143	LEU	N-CA-C	-6.08	104.73	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	159	GLN	N-CA-C	-6.08	102.34	110.55
1	W	117	SER	N-CA-C	-6.07	102.94	110.41
1	J	158	GLY	N-CA-C	-6.05	107.49	114.69
1	O	40	ALA	N-CA-C	-6.05	104.38	110.97
1	B	167	ASP	N-CA-C	6.04	119.91	112.54
1	Y	37	ASP	N-CA-C	6.03	121.31	111.37
1	V	21	SER	N-CA-C	-6.02	104.80	111.36
1	A	51	GLU	N-CA-C	-6.01	104.81	111.36
1	I	16	SER	N-CA-C	-6.01	104.15	112.03
1	N	37	ASP	N-CA-C	6.01	121.29	111.37
1	P	112	PHE	N-CA-C	6.01	118.54	109.41
1	J	82	PHE	N-CA-C	6.00	118.31	111.11
1	W	73	GLY	N-CA-C	-6.00	105.54	112.50
1	W	53	GLU	N-CA-C	-5.99	106.13	113.50
1	V	182	TYR	N-CA-C	-5.99	105.23	112.54
1	N	75	SER	N-CA-C	-5.99	104.83	111.36
1	C	189	LEU	N-CA-C	-5.99	100.43	109.95
1	S	114	LEU	N-CA-C	-5.98	101.59	110.20
1	T	37	ASP	N-CA-C	5.97	121.23	111.37
1	P	158	GLY	N-CA-C	-5.97	107.08	115.32
1	E	159	GLN	N-CA-C	-5.95	102.81	110.19
1	V	104	THR	N-CA-C	-5.92	105.91	113.01
1	H	17	PHE	N-CA-C	-5.92	104.91	111.36
1	I	114	LEU	N-CA-C	-5.91	101.61	110.24
1	Z	117	SER	N-CA-C	-5.91	103.14	110.41
1	G	21	SER	N-CA-C	-5.90	105.35	112.54
1	H	163	GLN	N-CA-C	-5.90	104.85	111.28
1	V	154	ALA	N-CA-C	-5.89	104.55	110.97
1	S	192	ARG	N-CA-C	-5.87	98.03	108.13
1	C	114	LEU	N-CA-C	-5.87	101.67	110.24
1	J	75	SER	N-CA-C	-5.87	105.38	112.54
1	a	97	SER	CB-CA-C	-5.86	109.80	116.54
1	R	38	HIS	N-CA-C	5.86	117.46	111.14
1	Z	21	SER	N-CA-C	-5.85	104.90	111.28
1	I	154	ALA	N-CA-C	-5.84	104.82	111.07
1	P	186	ASP	N-CA-C	5.84	118.40	111.33
1	R	66	PRO	N-CA-C	-5.84	106.50	114.80
1	Z	114	LEU	N-CA-C	-5.81	102.27	110.29
1	M	38	HIS	N-CA-C	5.81	117.69	111.36
1	M	155	LEU	N-CA-C	5.81	118.36	111.33
1	R	114	LEU	N-CA-C	-5.81	101.84	110.20
1	F	169	GLU	N-CA-C	-5.79	105.31	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	117	SER	N-CA-C	-5.79	101.91	110.48
1	P	75	SER	N-CA-C	-5.79	104.97	111.28
1	O	123	GLN	CA-C-N	5.78	126.68	119.98
1	O	123	GLN	C-N-CA	5.78	126.68	119.98
1	O	37	ASP	N-CA-C	5.77	123.09	110.80
1	E	167	ASP	N-CA-C	5.77	119.42	112.38
1	U	114	LEU	CA-C-N	5.76	127.04	119.84
1	U	114	LEU	C-N-CA	5.76	127.04	119.84
1	Y	117	SER	N-CA-C	-5.73	101.15	110.20
1	K	38	HIS	N-CA-C	5.73	117.60	111.36
1	U	85	PRO	N-CA-C	5.73	120.32	111.21
1	b	137	ILE	N-CA-C	5.72	116.46	110.62
1	T	70	ILE	N-CA-C	5.72	116.37	110.36
1	R	99	GLY	N-CA-C	-5.71	105.30	113.86
1	G	54	ASN	CA-C-N	5.70	126.45	120.12
1	G	54	ASN	C-N-CA	5.70	126.45	120.12
1	A	37	ASP	N-CA-C	5.70	120.77	111.37
1	Q	16	SER	N-CA-C	-5.70	98.67	110.80
1	M	123	GLN	CA-C-N	5.70	125.70	119.89
1	M	123	GLN	C-N-CA	5.70	125.70	119.89
1	X	21	SER	N-CA-C	-5.70	104.99	111.14
1	a	112	PHE	N-CA-C	5.69	118.34	109.52
1	G	70	ILE	N-CA-C	5.68	115.81	110.30
1	E	37	ASP	N-CA-C	5.68	122.90	110.80
1	b	94	GLN	N-CA-C	5.68	117.48	108.79
1	T	79	THR	N-CA-C	-5.67	105.02	111.14
1	X	183	GLY	N-CA-C	-5.67	106.93	115.32
1	X	86	ASP	N-CA-C	-5.66	103.02	110.43
1	K	39	MET	N-CA-C	-5.66	105.88	112.89
1	P	185	VAL	N-CA-C	5.66	116.02	108.27
1	W	90	ILE	CB-CA-C	-5.65	105.03	111.59
1	L	70	ILE	N-CA-C	5.65	116.38	110.62
1	L	187	SER	N-CA-C	5.64	114.98	108.49
1	Z	123	GLN	CA-C-N	5.64	125.57	119.76
1	Z	123	GLN	C-N-CA	5.64	125.57	119.76
1	b	75	SER	N-CA-C	-5.64	105.28	111.82
1	H	70	ILE	N-CA-C	5.64	116.28	110.36
1	a	70	ILE	N-CA-C	5.63	115.82	110.53
1	B	38	HIS	N-CA-C	5.62	118.60	111.69
1	V	140	ARG	N-CA-C	-5.61	104.56	111.40
1	Z	57	LYS	N-CA-C	5.60	118.57	110.28
1	G	175	SER	N-CA-C	-5.59	103.31	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	75	SER	N-CA-C	-5.59	105.34	111.82
1	W	179	ALA	N-CA-C	-5.59	104.88	110.97
1	Y	21	SER	N-CA-C	-5.58	105.28	111.36
1	K	154	ALA	N-CA-C	-5.58	104.89	110.97
1	A	116	ASN	N-CA-C	5.58	119.39	112.59
1	W	93	GLY	N-CA-C	-5.57	99.97	113.18
1	S	65	SER	N-CA-C	5.57	114.71	108.25
1	F	38	HIS	N-CA-C	5.56	117.14	111.14
1	C	77	TYR	N-CA-C	5.55	117.14	111.14
1	Z	65	SER	CA-C-N	5.55	127.76	121.04
1	Z	65	SER	C-N-CA	5.55	127.76	121.04
1	F	139	ALA	N-CA-C	-5.55	104.86	111.69
1	T	19	ILE	N-CA-C	5.55	116.28	110.62
1	W	160	SER	N-CA-C	-5.55	103.37	110.53
1	I	68	GLY	N-CA-C	5.55	117.39	110.29
1	D	26	GLU	N-CA-C	-5.54	106.19	113.17
1	K	140	ARG	N-CA-C	-5.52	104.48	111.11
1	L	16	SER	N-CA-C	-5.50	103.72	110.65
1	K	112	PHE	N-CA-C	5.50	116.98	109.18
1	H	69	VAL	N-CA-C	5.49	116.08	108.84
1	A	86	ASP	N-CA-C	-5.48	102.37	110.48
1	T	112	PHE	N-CA-C	5.47	118.19	109.81
1	H	44	VAL	CB-CA-C	-5.45	104.99	111.97
1	Q	70	ILE	N-CA-C	5.45	115.65	110.42
1	V	53	GLU	N-CA-C	-5.45	107.64	114.56
1	S	112	PHE	N-CA-C	5.45	118.14	109.81
1	J	32	THR	N-CA-C	5.44	117.76	108.90
1	H	39	MET	N-CA-C	-5.42	105.47	111.71
1	J	114	LEU	N-CA-C	-5.42	102.81	110.29
1	L	190	THR	N-CA-C	-5.42	107.32	114.04
1	L	114	LEU	CA-C-N	5.42	126.61	119.84
1	L	114	LEU	C-N-CA	5.42	126.61	119.84
1	P	99	GLY	N-CA-C	-5.41	106.12	113.37
1	Q	75	SER	N-CA-C	-5.39	105.31	111.14
1	U	60	TYR	N-CA-C	5.39	117.31	108.52
1	A	65	SER	N-CA-C	5.38	116.95	108.23
1	M	79	THR	N-CA-C	-5.38	105.49	111.36
1	W	175	SER	N-CA-C	-5.38	102.92	110.35
1	b	114	LEU	N-CA-C	-5.38	102.32	110.39
1	I	51	GLU	N-CA-C	-5.38	105.50	111.36
1	F	99	GLY	N-CA-C	-5.37	105.81	113.86
1	M	169	GLU	N-CA-C	-5.37	105.83	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	165	GLU	N-CA-C	-5.37	104.47	111.02
1	H	57	LYS	N-CA-C	5.35	118.04	110.50
1	S	117	SER	N-CA-C	-5.35	103.63	110.53
1	E	66	PRO	N-CA-C	-5.34	107.22	114.80
1	M	97	SER	CB-CA-C	-5.34	110.44	116.63
1	N	20	TYR	N-CA-C	5.34	117.18	111.36
1	K	99	GLY	N-CA-C	-5.33	106.04	112.49
1	D	159	GLN	N-CA-C	-5.33	103.00	110.35
1	M	154	ALA	N-CA-C	-5.33	105.37	111.07
1	J	117	SER	N-CA-C	-5.32	103.11	110.35
1	V	190	THR	N-CA-C	-5.32	107.34	113.88
1	J	180	VAL	N-CA-C	-5.30	105.68	110.82
1	K	88	SER	N-CA-C	-5.29	102.64	110.48
1	B	70	ILE	N-CA-C	5.29	116.06	110.72
1	Y	70	ILE	N-CA-C	5.28	116.05	110.72
1	Z	70	ILE	N-CA-C	5.27	115.41	110.30
1	E	70	ILE	N-CA-C	5.26	115.89	110.36
1	b	70	ILE	N-CA-C	5.26	115.40	110.30
1	J	24	LEU	N-CA-C	-5.25	105.72	111.82
1	O	190	THR	N-CA-C	5.25	121.99	110.80
1	W	100	ALA	N-CA-C	-5.24	105.24	111.69
1	I	155	LEU	N-CA-C	5.24	117.39	111.11
1	b	155	LEU	N-CA-C	5.24	116.99	111.28
1	N	97	SER	CB-CA-C	-5.23	110.56	116.63
1	X	143	LEU	N-CA-C	-5.23	105.64	112.23
1	D	161	LEU	N-CA-C	-5.21	105.03	111.33
1	X	82	PHE	N-CA-C	5.21	116.77	111.14
1	E	114	LEU	CA-C-N	5.21	126.35	119.84
1	E	114	LEU	C-N-CA	5.21	126.35	119.84
1	F	110	LYS	N-CA-C	5.20	118.94	112.59
1	E	17	PHE	N-CA-C	-5.19	105.80	111.82
1	S	32	THR	N-CA-C	5.19	117.36	108.90
1	K	32	THR	N-CA-C	5.18	117.35	108.90
1	S	82	PHE	N-CA-C	5.18	116.61	111.07
1	a	175	SER	N-CA-C	-5.18	103.85	110.53
1	A	140	ARG	N-CA-C	-5.17	105.72	111.36
1	Z	32	THR	N-CA-C	5.16	117.30	108.90
1	Y	59	ILE	CB-CA-C	-5.15	104.52	110.91
1	I	109	GLY	N-CA-C	-5.15	107.88	114.37
1	U	158	GLY	N-CA-C	-5.15	108.17	115.43
1	D	17	PHE	N-CA-C	-5.15	105.85	111.82
1	S	84	LYS	CA-C-N	-5.15	114.61	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	84	LYS	C-N-CA	-5.15	114.61	119.76
1	M	138	HIS	N-CA-C	5.14	117.79	111.82
1	S	86	ASP	N-CA-C	-5.14	102.77	110.23
1	M	90	ILE	CB-CA-C	-5.14	105.39	111.09
1	V	114	LEU	N-CA-C	-5.14	102.81	110.20
1	K	59	ILE	N-CA-C	-5.13	100.68	108.17
1	R	115	PRO	N-CA-C	5.13	121.39	113.75
1	G	145	VAL	N-CA-C	-5.12	105.50	110.42
1	I	175	SER	N-CA-C	-5.11	103.30	110.35
1	S	26	GLU	N-CA-C	-5.11	107.21	112.93
1	I	17	PHE	N-CA-C	-5.11	105.61	111.07
1	S	151	GLU	N-CA-C	-5.11	104.79	111.02
1	U	51	GLU	N-CA-C	-5.10	105.41	110.97
1	R	37	ASP	N-CA-C	5.10	119.73	111.37
1	K	114	LEU	CA-C-N	5.09	126.20	119.84
1	K	114	LEU	C-N-CA	5.09	126.20	119.84
1	O	105	ALA	N-CA-C	-5.09	106.76	113.17
1	M	75	SER	N-CA-C	-5.09	105.92	111.82
1	D	77	TYR	N-CA-C	5.08	117.21	111.02
1	V	161	LEU	N-CA-C	-5.08	105.25	111.75
1	E	51	GLU	N-CA-C	-5.07	105.40	111.03
1	W	57	LYS	N-CA-C	5.07	116.53	108.67
1	C	57	LYS	N-CA-C	5.05	117.62	110.50
1	N	117	SER	N-CA-C	-5.05	103.74	110.55
1	P	86	ASP	N-CA-C	-5.04	103.01	110.48
1	D	184	LEU	N-CA-C	-5.04	105.86	111.36
1	F	17	PHE	N-CA-C	-5.04	105.70	111.14
1	Q	179	ALA	N-CA-C	-5.03	105.87	111.36
1	E	189	LEU	N-CA-C	-5.03	101.51	109.96
1	b	109	GLY	N-CA-C	-5.03	108.71	114.69
1	F	112	PHE	N-CA-C	5.03	121.51	110.80
1	P	20	TYR	N-CA-C	5.03	118.19	111.75
1	B	155	LEU	N-CA-C	5.02	116.44	111.07
1	G	112	PHE	N-CA-C	5.01	116.61	109.14
1	P	114	LEU	N-CA-C	-5.01	102.87	110.39
1	S	16	SER	N-CA-C	-5.01	107.66	112.97
1	V	94	GLN	N-CA-C	5.01	116.14	108.42
1	O	187	SER	N-CA-C	5.01	116.46	108.79
1	Q	73	GLY	N-CA-C	-5.01	106.36	112.77
1	G	32	THR	N-CA-C	5.00	117.05	108.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	60	TYR	Sidechain
1	S	60	TYR	Sidechain

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	1404	0	1409	71	0
1	B	1404	0	1409	53	0
1	C	1404	0	1409	43	0
1	D	1404	0	1409	66	0
1	E	1404	0	1409	81	0
1	F	1404	0	1409	93	0
1	G	1404	0	1409	70	0
1	H	1404	0	1409	52	0
1	I	1404	0	1409	71	0
1	J	1404	0	1409	92	0
1	K	1404	0	1409	86	0
1	L	1404	0	1409	91	0
1	M	1404	0	1409	69	0
1	N	1404	0	1409	46	0
1	O	1404	0	1409	168	0
1	P	1404	0	1409	125	0
1	Q	1404	0	1409	77	0
1	R	1404	0	1409	66	0
1	S	1404	0	1409	86	0
1	T	1404	0	1409	69	0
1	U	1404	0	1409	74	0
1	V	1404	0	1409	112	0
1	W	1404	0	1409	96	0
1	X	1404	0	1409	80	0
1	Y	1404	0	1409	101	0
1	Z	1404	0	1409	81	0
1	a	1404	0	1409	58	0
1	b	1404	0	1409	86	0
All	All	39312	0	39452	1947	0

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

All (1947) 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:K:163:GLN:HA	1:K:163:GLN:HE21	0.98	1.13
1:D:16:SER:H	1:D:22:ARG:HD2	1.15	1.11
1:W:104:THR:HB	1:W:184:LEU:HD23	1.16	1.10
1:O:40:ALA:HB1	1:O:76:ILE:HD11	1.37	1.06
1:U:124:PRO:HG2	1:U:146:LYS:HA	1.34	1.04
1:D:31:LEU:HD13	1:D:39:MET:HE1	1.33	1.04
1:P:176:ALA:HB3	1:P:177:PRO:HD3	1.38	1.03
1:S:148:ARG:HH11	1:T:116:ASN:ND2	1.57	1.02
1:N:96:ALA:HB1	1:N:120:MET:HE2	1.36	1.02
1:L:15:ARG:HG2	1:L:16:SER:H	1.21	1.01
1:W:15:ARG:HG2	1:W:16:SER:H	1.26	1.01
1:Y:166:ARG:NH1	1:Y:166:ARG:HB2	1.74	1.00
1:E:148:ARG:HH11	1:F:116:ASN:ND2	1.59	1.00
1:E:70:ILE:HA	1:E:98:MET:HE3	1.42	0.99
1:V:104:THR:HB	1:V:184:LEU:HD13	1.42	0.99
1:C:143:LEU:HD11	1:M:136:GLU:HG3	1.45	0.98
1:O:132:ALA:HA	1:O:135:ILE:HD12	1.46	0.97
1:F:31:LEU:HD13	1:F:39:MET:HE1	1.47	0.96
1:O:123:GLN:NE2	1:V:133:THR:H	1.64	0.96
1:O:190:THR:HG22	1:O:191:HIS:N	1.80	0.96
1:K:163:GLN:HA	1:K:163:GLN:NE2	1.77	0.95
1:L:78:ASP:HB3	1:M:114:LEU:HD22	1.49	0.95
1:M:18:ASP:OD1	1:M:21:SER:HB2	1.66	0.95
1:O:133:THR:H	1:V:123:GLN:HE22	1.14	0.94
1:b:153:MET:HE1	1:b:184:LEU:HD21	1.46	0.93
1:J:104:THR:HB	1:J:184:LEU:HD23	1.49	0.93
1:H:31:LEU:HD13	1:H:39:MET:HE1	1.50	0.93
1:E:148:ARG:HH11	1:F:116:ASN:HD21	1.11	0.92
1:O:123:GLN:HE22	1:V:133:THR:N	1.67	0.92
1:A:104:THR:HB	1:A:184:LEU:HD23	1.49	0.92
1:O:133:THR:H	1:V:123:GLN:NE2	1.66	0.91
1:T:22:ARG:HB3	1:T:22:ARG:NH1	1.86	0.90
1:H:176:ALA:HB3	1:H:177:PRO:HD3	1.52	0.90
1:X:74:MET:SD	1:X:149:MET:HE1	2.12	0.89
1:S:123:GLN:HE21	1:Y:132:ALA:HB3	1.36	0.89
1:V:176:ALA:HB3	1:V:177:PRO:HD3	1.55	0.89
1:F:133:THR:H	1:J:123:GLN:HE22	1.15	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:22:ARG:HB3	1:T:22:ARG:HH11	1.37	0.88
1:O:176:ALA:HB3	1:O:177:PRO:HD3	1.54	0.88
1:V:73:GLY:HA3	1:V:98:MET:HE3	1.53	0.88
1:S:121:ILE:HD12	1:S:168:THR:HG22	1.56	0.87
1:P:88:SER:HB2	1:P:110:LYS:O	1.74	0.87
1:L:24:LEU:HD23	1:M:16:SER:HB3	1.58	0.86
1:P:161:LEU:O	1:P:165:GLU:HG3	1.74	0.86
1:L:148:ARG:HH11	1:M:116:ASN:ND2	1.74	0.85
1:W:145:VAL:O	1:W:149:MET:HG2	1.76	0.85
1:P:148:ARG:HH11	1:Q:116:ASN:HD22	1.24	0.84
1:W:31:LEU:HD13	1:W:39:MET:HE1	1.58	0.84
1:Q:18:ASP:OD2	1:Q:21:SER:HB2	1.77	0.84
1:R:136:GLU:HG3	1:Z:143:LEU:HD11	1.59	0.84
1:T:104:THR:HB	1:T:184:LEU:HD23	1.56	0.84
1:W:104:THR:CB	1:W:184:LEU:HD23	2.04	0.84
1:F:155:LEU:HD23	1:F:155:LEU:C	2.03	0.84
1:S:148:ARG:HH11	1:T:116:ASN:HD21	1.25	0.84
1:R:31:LEU:HD13	1:R:39:MET:HE1	1.60	0.83
1:G:31:LEU:HD13	1:G:39:MET:HE1	1.61	0.83
1:I:104:THR:HB	1:I:184:LEU:HD23	1.58	0.83
1:T:92:MET:HB3	1:T:114:LEU:HD12	1.58	0.83
1:Y:166:ARG:HB2	1:Y:166:ARG:HH11	1.42	0.83
1:D:31:LEU:CD1	1:D:39:MET:HE1	2.08	0.83
1:Z:31:LEU:HD13	1:Z:39:MET:HE1	1.59	0.83
1:P:19:ILE:HG23	1:P:20:TYR:H	1.43	0.83
1:W:91:CYS:HB2	1:W:103:LEU:HD13	1.58	0.82
1:F:31:LEU:CD1	1:F:39:MET:HE1	2.10	0.82
1:G:123:GLN:HE21	1:I:132:ALA:HB3	1.43	0.82
1:R:148:ARG:HH11	1:S:116:ASN:HD22	1.26	0.82
1:O:164:ILE:HD13	1:O:182:TYR:OH	1.79	0.81
1:Z:157:THR:HA	1:Z:183:GLY:O	1.80	0.81
1:P:133:THR:H	1:b:123:GLN:HE22	1.27	0.81
1:D:190:THR:HG22	1:D:191:HIS:ND1	1.95	0.81
1:Y:25:LYS:HD2	1:Z:15:ARG:HD3	1.62	0.81
1:J:104:THR:HB	1:J:184:LEU:CD2	2.11	0.81
1:A:116:ASN:ND2	1:G:148:ARG:HH11	1.78	0.81
1:H:104:THR:HB	1:H:184:LEU:HD13	1.60	0.80
1:F:132:ALA:HB3	1:J:123:GLN:HE21	1.46	0.80
1:Q:31:LEU:HD13	1:Q:39:MET:HE1	1.62	0.80
1:E:143:LEU:HD11	1:K:136:GLU:HG2	1.64	0.80
1:D:84:LYS:HG3	1:E:192:ARG:HG2	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:53:GLU:O	1:b:54:ASN:HB2	1.82	0.79
1:A:25:LYS:HE2	1:B:15:ARG:HG3	1.64	0.79
1:L:148:ARG:HH11	1:M:116:ASN:HD22	1.27	0.79
1:P:31:LEU:CD1	1:P:39:MET:HE1	2.11	0.79
1:R:148:ARG:NH1	1:S:116:ASN:HD22	1.80	0.79
1:V:32:THR:OG1	1:b:41:ASN:ND2	2.16	0.79
1:F:15:ARG:HG2	1:F:16:SER:H	1.47	0.78
1:O:176:ALA:O	1:O:179:ALA:HB3	1.81	0.78
1:P:19:ILE:HG23	1:P:20:TYR:N	1.98	0.78
1:U:81:GLN:HE21	1:U:81:GLN:HA	1.47	0.78
1:O:123:GLN:HE21	1:V:132:ALA:N	1.81	0.78
1:I:77:TYR:OH	1:I:156:HIS:HE1	1.67	0.78
1:K:31:LEU:HD12	1:K:39:MET:HE1	1.65	0.77
1:B:53:GLU:O	1:B:54:ASN:HB2	1.83	0.77
1:F:115:PRO:HD3	1:F:189:LEU:O	1.83	0.77
1:K:31:LEU:CD1	1:K:39:MET:HE1	2.14	0.77
1:Q:133:THR:H	1:a:123:GLN:HE22	1.32	0.77
1:D:176:ALA:HB1	1:D:188:ILE:CD1	2.14	0.77
1:S:18:ASP:HB3	1:S:21:SER:HB2	1.65	0.77
1:D:176:ALA:HB1	1:D:188:ILE:HD11	1.67	0.77
1:K:163:GLN:HE21	1:K:163:GLN:CA	1.83	0.77
1:O:40:ALA:HB1	1:O:76:ILE:CD1	2.12	0.77
1:W:173:PHE:C	1:W:174:LEU:HD12	2.10	0.77
1:V:97:SER:HG	1:V:122:HIS:CE1	2.03	0.77
1:O:53:GLU:O	1:O:54:ASN:HB2	1.82	0.77
1:b:176:ALA:HB3	1:b:177:PRO:HD3	1.65	0.77
1:Q:124:PRO:HB2	1:Q:142:ILE:HD11	1.65	0.76
1:E:173:PHE:C	1:E:174:LEU:HD12	2.10	0.76
1:S:190:THR:O	1:S:191:HIS:O	2.03	0.76
1:O:18:ASP:HB3	1:O:21:SER:HB2	1.66	0.76
1:E:141:GLU:OE2	1:F:118:ARG:HD2	1.86	0.76
1:P:121:ILE:O	1:P:122:HIS:HB3	1.85	0.76
1:J:169:GLU:OE1	1:J:169:GLU:HA	1.86	0.76
1:M:161:LEU:O	1:M:165:GLU:HG3	1.86	0.76
1:S:123:GLN:NE2	1:Y:132:ALA:HB3	2.00	0.76
1:P:123:GLN:HE22	1:b:133:THR:H	1.32	0.76
1:V:80:MET:HE3	1:V:87:VAL:HG11	1.67	0.75
1:Y:45:ALA:HB1	1:Z:23:LEU:HD11	1.68	0.75
1:F:133:THR:H	1:J:123:GLN:NE2	1.83	0.75
1:J:35:VAL:HA	1:J:39:MET:HE3	1.68	0.75
1:Z:115:PRO:HD3	1:Z:189:LEU:O	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:98:MET:HE2	1:I:98:MET:HA	1.68	0.75
1:J:41:ASN:ND2	1:K:32:THR:OG1	2.19	0.75
1:R:84:LYS:HG3	1:S:192:ARG:HG2	1.67	0.75
1:R:124:PRO:HD2	1:R:146:LYS:HG3	1.67	0.75
1:S:177:PRO:HG3	1:S:188:ILE:HD11	1.68	0.75
1:Q:175:SER:OG	1:Q:178:GLU:HG3	1.87	0.75
1:D:132:ALA:HB3	1:L:123:GLN:HE21	1.49	0.74
1:J:47:MET:HE1	1:J:80:MET:HG2	1.69	0.74
1:W:113:CYS:SG	1:W:185:VAL:HG11	2.27	0.74
1:O:46:GLN:O	1:O:50:LEU:HG	1.87	0.74
1:H:145:VAL:O	1:H:149:MET:HG2	1.87	0.74
1:P:157:THR:HA	1:P:183:GLY:O	1.88	0.74
1:V:31:LEU:HD12	1:V:39:MET:HE1	1.70	0.74
1:L:148:ARG:NH1	1:M:116:ASN:ND2	2.35	0.74
1:b:153:MET:CE	1:b:184:LEU:HD21	2.18	0.74
1:O:40:ALA:CB	1:O:76:ILE:HD11	2.17	0.74
1:U:81:GLN:HA	1:U:81:GLN:NE2	2.03	0.74
1:Y:115:PRO:HD3	1:Y:189:LEU:O	1.88	0.74
1:E:83:ILE:HB	1:E:85:PRO:HD2	1.69	0.73
1:S:148:ARG:NH1	1:T:116:ASN:ND2	2.35	0.73
1:E:148:ARG:NH1	1:F:116:ASN:ND2	2.33	0.73
1:K:111:ARG:HG2	1:K:111:ARG:HH11	1.53	0.73
1:D:16:SER:H	1:D:22:ARG:CD	1.96	0.73
1:O:49:PHE:CE1	1:P:22:ARG:HG2	2.22	0.73
1:S:136:GLU:HG2	1:Y:143:LEU:HD11	1.70	0.73
1:O:123:GLN:HE22	1:V:133:THR:H	0.82	0.73
1:O:190:THR:HG22	1:O:191:HIS:H	1.53	0.73
1:V:73:GLY:CA	1:V:98:MET:HE3	2.18	0.73
1:V:84:LYS:HG3	1:W:192:ARG:HG2	1.71	0.73
1:X:180:VAL:HA	1:X:185:VAL:O	1.89	0.72
1:H:148:ARG:HH11	1:I:116:ASN:HD22	1.34	0.72
1:L:174:LEU:HD23	1:L:178:GLU:HB3	1.70	0.72
1:L:175:SER:OG	1:L:177:PRO:HD2	1.89	0.72
1:U:81:GLN:HE21	1:U:81:GLN:CA	2.02	0.72
1:b:163:GLN:HA	1:b:166:ARG:HH12	1.53	0.72
1:V:175:SER:OG	1:V:178:GLU:HG3	1.89	0.72
1:Y:25:LYS:HD2	1:Z:15:ARG:CD	2.18	0.72
1:R:24:LEU:HD23	1:S:16:SER:OG	1.89	0.72
1:a:159:GLN:HB2	1:a:164:ILE:CD1	2.19	0.72
1:V:173:PHE:C	1:V:174:LEU:HD12	2.15	0.72
1:L:18:ASP:OD1	1:L:21:SER:HB2	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:147:GLY:O	1:E:151:GLU:HG3	1.90	0.72
1:J:29:ILE:HD13	1:J:46:GLN:HB2	1.70	0.72
1:Y:34:GLN:O	1:Y:39:MET:HE3	1.89	0.72
1:Z:70:ILE:HG22	1:Z:71:THR:N	2.04	0.72
1:U:29:ILE:HG23	1:U:46:GLN:OE1	1.89	0.71
1:O:190:THR:CG2	1:O:191:HIS:N	2.52	0.71
1:U:27:ARG:HG2	1:U:50:LEU:HD22	1.71	0.71
1:J:161:LEU:O	1:J:165:GLU:HG3	1.91	0.71
1:E:123:GLN:HG2	1:E:168:THR:O	1.90	0.71
1:H:70:ILE:HA	1:H:98:MET:HE3	1.72	0.71
1:P:22:ARG:O	1:P:25:LYS:HB2	1.91	0.71
1:W:148:ARG:HA	1:W:151:GLU:OE1	1.90	0.71
1:X:140:ARG:HH11	1:X:140:ARG:HG3	1.52	0.71
1:Q:161:LEU:O	1:Q:165:GLU:HG3	1.91	0.71
1:X:176:ALA:HB3	1:X:177:PRO:HD3	1.72	0.71
1:P:31:LEU:HD13	1:P:39:MET:HE1	1.73	0.71
1:V:164:ILE:HD13	1:V:182:TYR:OH	1.90	0.71
1:b:104:THR:HB	1:b:184:LEU:HD23	1.70	0.71
1:P:113:CYS:HB3	1:P:117:SER:OG	1.90	0.70
1:Y:166:ARG:HH11	1:Y:166:ARG:CB	2.04	0.70
1:C:115:PRO:HD3	1:C:189:LEU:O	1.91	0.70
1:K:77:TYR:OH	1:K:156:HIS:HE1	1.74	0.70
1:M:145:VAL:O	1:M:149:MET:HG2	1.91	0.70
1:O:104:THR:HA	1:O:111:ARG:HD2	1.74	0.70
1:H:115:PRO:HD3	1:H:189:LEU:O	1.90	0.70
1:O:35:VAL:HB	1:O:68:GLY:HA3	1.74	0.70
1:P:77:TYR:OH	1:P:156:HIS:HE1	1.75	0.70
1:F:78:ASP:HB3	1:G:114:LEU:HD12	1.73	0.70
1:a:176:ALA:HB3	1:a:177:PRO:HD3	1.73	0.70
1:R:176:ALA:HB3	1:R:177:PRO:HD3	1.74	0.70
1:Z:100:ALA:O	1:Z:103:LEU:HB3	1.91	0.70
1:N:161:LEU:O	1:N:165:GLU:HG3	1.91	0.70
1:P:176:ALA:HB3	1:P:177:PRO:CD	2.19	0.70
1:V:115:PRO:HD3	1:V:189:LEU:O	1.91	0.70
1:F:15:ARG:HG2	1:F:16:SER:N	2.06	0.70
1:O:76:ILE:O	1:O:79:THR:N	2.25	0.70
1:K:107:ALA:O	1:K:111:ARG:HD3	1.92	0.70
1:L:77:TYR:OH	1:L:156:HIS:HE1	1.75	0.70
1:b:104:THR:HB	1:b:184:LEU:CD2	2.21	0.70
1:T:104:THR:HB	1:T:184:LEU:CD2	2.22	0.69
1:V:51:GLU:CD	1:W:192:ARG:HE	2.00	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ASN:ND2	1:A:57:LYS:HG3	2.07	0.69
1:V:31:LEU:HD13	1:V:43:ILE:CD1	2.22	0.69
1:X:152:LEU:HD11	1:Y:116:ASN:ND2	2.08	0.69
1:D:138:HIS:O	1:D:142:ILE:HG22	1.92	0.69
1:C:175:SER:OG	1:C:178:GLU:HG3	1.93	0.69
1:I:27:ARG:HG2	1:I:50:LEU:HD22	1.75	0.69
1:L:148:ARG:NH1	1:M:116:ASN:HD22	1.91	0.69
1:R:23:LEU:HD12	1:R:30:PHE:HE1	1.58	0.69
1:E:89:THR:HB	1:E:103:LEU:HD12	1.74	0.69
1:J:15:ARG:N	1:J:22:ARG:HD3	2.07	0.69
1:W:170:ARG:HH11	1:W:170:ARG:HG2	1.57	0.69
1:H:148:ARG:HH11	1:H:148:ARG:HG2	1.57	0.69
1:T:115:PRO:HD3	1:T:189:LEU:O	1.93	0.69
1:D:145:VAL:O	1:D:149:MET:HG2	1.93	0.69
1:E:157:THR:HA	1:E:183:GLY:O	1.93	0.69
1:S:40:ALA:HA	1:S:76:ILE:HD11	1.74	0.69
1:B:15:ARG:N	1:B:15:ARG:HH11	1.90	0.68
1:E:31:LEU:CD1	1:E:39:MET:HE1	2.23	0.68
1:P:133:THR:H	1:b:123:GLN:NE2	1.90	0.68
1:M:15:ARG:N	1:M:22:ARG:HD3	2.07	0.68
1:O:176:ALA:HB3	1:O:177:PRO:CD	2.23	0.68
1:Y:55:PRO:HA	1:Y:85:PRO:HG3	1.75	0.68
1:D:153:MET:HE1	1:D:184:LEU:HD21	1.74	0.68
1:O:160:SER:O	1:O:162:GLU:N	2.27	0.68
1:R:31:LEU:CD1	1:R:39:MET:HE1	2.22	0.68
1:R:25:LYS:NZ	1:S:15:ARG:HH22	1.91	0.68
1:V:54:ASN:ND2	1:V:57:LYS:HG3	2.09	0.68
1:I:166:ARG:NH1	1:I:166:ARG:HB2	2.08	0.68
1:K:139:ALA:HA	1:K:142:ILE:HG22	1.75	0.68
1:D:123:GLN:HE22	1:L:133:THR:H	1.42	0.68
1:D:162:GLU:O	1:D:166:ARG:HD3	1.94	0.68
1:P:124:PRO:HD2	1:P:146:LYS:HG3	1.75	0.68
1:C:31:LEU:HD13	1:C:39:MET:HE1	1.76	0.68
1:D:123:GLN:NE2	1:L:133:THR:H	1.91	0.68
1:K:31:LEU:HD13	1:K:43:ILE:CD1	2.24	0.68
1:R:15:ARG:N	1:R:22:ARG:HD3	2.07	0.68
1:V:190:THR:HG22	1:V:191:HIS:CD2	2.28	0.68
1:G:77:TYR:OH	1:G:156:HIS:HE1	1.76	0.68
1:J:158:GLY:CA	1:O:193:ASN:HD21	2.07	0.68
1:R:77:TYR:OH	1:R:156:HIS:HE1	1.77	0.68
1:B:123:GLN:HE22	1:N:133:THR:H	1.39	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:103:LEU:HD12	1:Y:103:LEU:O	1.95	0.67
1:K:115:PRO:HD3	1:K:189:LEU:O	1.94	0.67
1:O:176:ALA:HB1	1:O:188:ILE:HD12	1.76	0.67
1:L:91:CYS:HB2	1:L:103:LEU:HD22	1.77	0.67
1:Y:161:LEU:O	1:Y:165:GLU:HG3	1.94	0.67
1:Z:31:LEU:CD1	1:Z:39:MET:HE1	2.25	0.67
1:S:92:MET:HB3	1:S:114:LEU:HD12	1.75	0.67
1:O:180:VAL:CG2	1:O:187:SER:HA	2.24	0.67
1:F:83:ILE:HB	1:F:85:PRO:HD2	1.77	0.67
1:N:77:TYR:OH	1:N:156:HIS:HE1	1.76	0.67
1:R:49:PHE:CE1	1:S:22:ARG:HD3	2.29	0.67
1:b:104:THR:CB	1:b:184:LEU:HD23	2.24	0.67
1:K:15:ARG:HG2	1:K:16:SER:H	1.59	0.67
1:Y:147:GLY:O	1:Y:151:GLU:HG3	1.95	0.67
1:a:15:ARG:O	1:a:16:SER:HB3	1.93	0.67
1:D:16:SER:N	1:D:22:ARG:HD2	2.01	0.67
1:W:121:ILE:HG21	1:W:153:MET:HE2	1.75	0.67
1:O:132:ALA:HB3	1:V:123:GLN:HE21	1.59	0.66
1:R:15:ARG:O	1:R:22:ARG:HB2	1.94	0.66
1:A:136:GLU:HG2	1:H:143:LEU:HD11	1.76	0.66
1:O:112:PHE:CD2	1:O:189:LEU:HD23	2.30	0.66
1:S:123:GLN:HE22	1:Y:133:THR:H	1.41	0.66
1:H:161:LEU:O	1:H:165:GLU:HG3	1.95	0.66
1:U:53:GLU:O	1:U:54:ASN:HB2	1.95	0.66
1:X:92:MET:HB3	1:X:114:LEU:HD12	1.78	0.66
1:C:123:GLN:NE2	1:C:146:LYS:NZ	2.42	0.66
1:Y:152:LEU:HD11	1:Z:116:ASN:ND2	2.10	0.66
1:R:145:VAL:O	1:R:149:MET:HG2	1.96	0.66
1:I:148:ARG:NH1	1:J:116:ASN:ND2	2.44	0.66
1:O:15:ARG:O	1:O:22:ARG:HD3	1.96	0.66
1:U:77:TYR:OH	1:U:156:HIS:HE1	1.77	0.66
1:X:163:GLN:O	1:X:167:ASP:HB2	1.95	0.66
1:Y:77:TYR:OH	1:Y:156:HIS:HE1	1.78	0.66
1:b:96:ALA:HB1	1:b:120:MET:HB3	1.77	0.66
1:I:176:ALA:HB3	1:I:177:PRO:HD3	1.77	0.66
1:U:146:LYS:HD2	1:W:132:ALA:HB3	1.76	0.66
1:B:31:LEU:HD22	1:B:43:ILE:HD13	1.78	0.66
1:C:31:LEU:CD1	1:C:39:MET:HE1	2.25	0.66
1:J:131:GLN:O	1:J:135:ILE:HG12	1.95	0.66
1:F:132:ALA:HB3	1:J:123:GLN:NE2	2.09	0.66
1:H:77:TYR:OH	1:H:156:HIS:HE1	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:115:PRO:HD3	1:M:189:LEU:O	1.96	0.66
1:U:70:ILE:HG23	1:U:98:MET:HE3	1.78	0.66
1:G:115:PRO:HD3	1:G:189:LEU:O	1.95	0.65
1:V:31:LEU:CD1	1:V:39:MET:HE1	2.25	0.65
1:W:15:ARG:HG2	1:W:16:SER:N	2.01	0.65
1:O:91:CYS:SG	1:O:117:SER:OG	2.53	0.65
1:O:123:GLN:HE21	1:V:132:ALA:H	1.42	0.65
1:O:133:THR:N	1:V:123:GLN:HE22	1.92	0.65
1:L:15:ARG:CG	1:L:16:SER:H	2.00	0.65
1:L:45:ALA:HB1	1:M:19:ILE:HD12	1.78	0.65
1:M:31:LEU:C	1:M:31:LEU:HD12	2.22	0.65
1:W:131:GLN:O	1:W:135:ILE:HG12	1.96	0.65
1:X:77:TYR:OH	1:X:156:HIS:HE1	1.80	0.65
1:Y:91:CYS:HB2	1:Y:103:LEU:HD22	1.78	0.65
1:J:15:ARG:N	1:J:22:ARG:HB2	2.12	0.65
1:T:141:GLU:HG2	1:U:173:PHE:CE1	2.32	0.65
1:Z:128:TYR:HD2	1:Z:135:ILE:HD13	1.61	0.65
1:A:31:LEU:HD13	1:A:39:MET:HE1	1.79	0.65
1:J:128:TYR:HD2	1:J:135:ILE:HD13	1.62	0.65
1:N:104:THR:OG1	1:N:184:LEU:HD23	1.97	0.65
1:Q:120:MET:HE3	1:Q:171:ASP:HB3	1.77	0.65
1:W:167:ASP:CG	1:W:172:ARG:HH21	2.05	0.65
1:A:86:ASP:HB3	1:A:107:ALA:HB2	1.77	0.65
1:O:191:HIS:C	1:O:191:HIS:CD2	2.75	0.65
1:R:82:PHE:CE1	1:S:189:LEU:HD13	2.32	0.65
1:S:148:ARG:NH1	1:T:116:ASN:HD21	1.91	0.65
1:I:121:ILE:HD12	1:I:121:ILE:O	1.97	0.64
1:W:111:ARG:NH1	1:W:156:HIS:O	2.29	0.64
1:a:22:ARG:HE	1:a:25:LYS:HD3	1.62	0.64
1:T:119:VAL:HB	1:T:174:LEU:HB2	1.79	0.64
1:D:113:CYS:HB2	1:D:185:VAL:HG21	1.79	0.64
1:L:24:LEU:HD23	1:M:16:SER:CB	2.27	0.64
1:U:86:ASP:OD2	1:U:110:LYS:HE3	1.97	0.64
1:J:31:LEU:C	1:J:31:LEU:HD12	2.22	0.64
1:V:118:ARG:HG2	1:V:118:ARG:HH11	1.62	0.64
1:X:69:VAL:HG12	1:X:71:THR:HG23	1.80	0.64
1:Y:104:THR:HB	1:Y:184:LEU:HD22	1.80	0.64
1:A:104:THR:HB	1:A:184:LEU:CD2	2.26	0.64
1:O:83:ILE:HD12	1:O:85:PRO:HG2	1.79	0.63
1:V:77:TYR:OH	1:V:156:HIS:HE1	1.81	0.63
1:S:176:ALA:HB3	1:S:177:PRO:HD3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:124:PRO:HG2	1:U:146:LYS:CA	2.20	0.63
1:J:50:LEU:HD12	1:J:59:ILE:HG23	1.81	0.63
1:J:148:ARG:HA	1:J:151:GLU:OE2	1.98	0.63
1:O:31:LEU:HD13	1:O:39:MET:HE1	1.80	0.63
1:T:176:ALA:O	1:T:180:VAL:HG23	1.97	0.63
1:b:70:ILE:HD13	1:b:98:MET:HE2	1.80	0.63
1:b:133:THR:O	1:b:136:GLU:HB3	1.99	0.63
1:A:147:GLY:O	1:A:151:GLU:HG3	1.98	0.63
1:F:91:CYS:HB2	1:F:103:LEU:CD2	2.29	0.63
1:K:78:ASP:OD2	1:L:115:PRO:HD2	1.99	0.63
1:R:25:LYS:HZ1	1:S:15:ARG:HH22	1.44	0.63
1:S:186:ASP:O	1:S:187:SER:HB3	1.97	0.63
1:Q:31:LEU:C	1:Q:31:LEU:HD12	2.24	0.63
1:T:84:LYS:N	1:T:85:PRO:HD2	2.13	0.63
1:V:190:THR:HG22	1:V:191:HIS:NE2	2.13	0.63
1:D:132:ALA:HB3	1:L:123:GLN:NE2	2.13	0.63
1:a:95:ALA:O	1:a:119:VAL:HA	1.99	0.63
1:H:148:ARG:NH1	1:I:116:ASN:ND2	2.47	0.62
1:I:104:THR:HB	1:I:184:LEU:CD2	2.29	0.62
1:W:51:GLU:OE2	1:W:84:LYS:N	2.23	0.62
1:J:104:THR:CB	1:J:184:LEU:HD23	2.27	0.62
1:O:75:SER:OG	1:O:76:ILE:HD12	1.98	0.62
1:P:19:ILE:CG2	1:P:20:TYR:H	2.11	0.62
1:V:84:LYS:HG3	1:W:192:ARG:CG	2.28	0.62
1:Y:41:ASN:ND2	1:Z:32:THR:OG1	2.32	0.62
1:a:94:GLN:HA	1:a:118:ARG:O	1.99	0.62
1:b:115:PRO:HD3	1:b:189:LEU:O	1.98	0.62
1:L:75:SER:HB2	1:M:92:MET:HG3	1.80	0.62
1:T:176:ALA:HB3	1:T:177:PRO:HD3	1.81	0.62
1:V:162:GLU:OE1	1:V:162:GLU:HA	2.00	0.62
1:L:27:ARG:HG2	1:L:27:ARG:HH11	1.64	0.62
1:Q:15:ARG:HG2	1:Q:15:ARG:O	1.98	0.62
1:I:121:ILE:HD12	1:I:121:ILE:C	2.25	0.62
1:A:115:PRO:HD3	1:A:189:LEU:O	1.99	0.62
1:D:162:GLU:HB3	1:D:166:ARG:HH11	1.63	0.62
1:F:45:ALA:HB1	1:G:23:LEU:HD11	1.80	0.62
1:H:148:ARG:HG2	1:H:148:ARG:NH1	2.14	0.62
1:V:161:LEU:HD11	1:V:165:GLU:OE2	1.99	0.62
1:W:153:MET:O	1:W:157:THR:HG23	1.99	0.62
1:H:148:ARG:NH1	1:I:116:ASN:HD22	1.97	0.62
1:P:134:ASP:OD1	1:Q:170:ARG:NH1	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:26:GLU:O	1:Z:27:ARG:HB2	1.97	0.62
1:P:175:SER:O	1:P:176:ALA:C	2.41	0.62
1:Q:175:SER:HG	1:Q:178:GLU:HG3	1.64	0.62
1:b:89:THR:C	1:b:90:ILE:HD13	2.25	0.62
1:H:190:THR:HG22	1:H:191:HIS:ND1	2.15	0.61
1:W:105:ALA:HA	1:W:156:HIS:CD2	2.34	0.61
1:E:57:LYS:O	1:E:85:PRO:HB3	2.00	0.61
1:E:115:PRO:HD3	1:E:189:LEU:O	2.00	0.61
1:G:123:GLN:NE2	1:I:132:ALA:HB3	2.12	0.61
1:N:134:ASP:HA	1:N:137:ILE:HD12	1.82	0.61
1:U:28:VAL:HG22	1:U:60:TYR:HB2	1.82	0.61
1:b:77:TYR:OH	1:b:156:HIS:HE1	1.83	0.61
1:b:118:ARG:HG3	1:b:118:ARG:O	2.00	0.61
1:A:84:LYS:HB2	1:A:85:PRO:HD3	1.82	0.61
1:L:31:LEU:HD13	1:L:39:MET:HE1	1.80	0.61
1:W:58:ASP:OD2	1:W:110:LYS:NZ	2.27	0.61
1:A:83:ILE:HB	1:A:85:PRO:HD2	1.83	0.61
1:D:162:GLU:HB3	1:D:166:ARG:NH1	2.15	0.61
1:J:101:PHE:O	1:J:104:THR:HG22	2.00	0.61
1:M:174:LEU:HD22	1:M:184:LEU:HD12	1.82	0.61
1:W:92:MET:HB2	1:W:114:LEU:HD12	1.83	0.61
1:G:157:THR:HG22	1:G:184:LEU:HD23	1.83	0.61
1:H:22:ARG:HA	1:H:25:LYS:HE2	1.83	0.61
1:J:77:TYR:O	1:J:81:GLN:HG2	2.01	0.61
1:L:25:LYS:HD2	1:M:15:ARG:HH22	1.64	0.61
1:O:95:ALA:HB1	1:O:99:GLY:O	2.01	0.61
1:Z:77:TYR:OH	1:Z:152:LEU:HD22	2.00	0.61
1:b:96:ALA:CB	1:b:120:MET:HB3	2.28	0.61
1:H:167:ASP:OD1	1:H:172:ARG:NH2	2.33	0.61
1:J:121:ILE:H	1:J:121:ILE:HD13	1.63	0.61
1:R:124:PRO:CB	1:R:142:ILE:HD11	2.30	0.61
1:P:96:ALA:HA	1:P:120:MET:O	2.01	0.61
1:S:15:ARG:N	1:S:22:ARG:HB2	2.16	0.61
1:X:175:SER:HB3	1:X:177:PRO:HD2	1.83	0.61
1:b:97:SER:HG	1:b:122:HIS:CE1	2.19	0.61
1:B:123:GLN:NE2	1:N:133:THR:H	1.97	0.61
1:a:163:GLN:NE2	1:a:166:ARG:HH12	1.98	0.61
1:b:106:GLY:O	1:b:111:ARG:HD3	2.01	0.61
1:F:163:GLN:HA	1:F:166:ARG:NH1	2.16	0.60
1:K:95:ALA:O	1:K:100:ALA:HB2	2.00	0.60
1:X:49:PHE:CE1	1:Y:22:ARG:HG2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:31:LEU:C	1:D:31:LEU:HD12	2.25	0.60
1:N:96:ALA:HB1	1:N:120:MET:CE	2.22	0.60
1:P:121:ILE:HG13	1:P:122:HIS:N	2.15	0.60
1:P:175:SER:OG	1:P:178:GLU:HG3	2.01	0.60
1:S:31:LEU:C	1:S:31:LEU:HD12	2.26	0.60
1:W:51:GLU:HG3	1:W:85:PRO:CD	2.31	0.60
1:B:176:ALA:HB3	1:B:177:PRO:HD3	1.82	0.60
1:F:97:SER:HG	1:F:122:HIS:CE1	2.19	0.60
1:J:162:GLU:HB3	1:U:155:LEU:HD22	1.83	0.60
1:K:176:ALA:HB3	1:K:177:PRO:HD3	1.82	0.60
1:O:71:THR:CG2	1:P:94:GLN:HB3	2.30	0.60
1:P:121:ILE:O	1:P:122:HIS:CB	2.48	0.60
1:R:124:PRO:HB2	1:R:142:ILE:HD11	1.82	0.60
1:V:97:SER:OG	1:V:122:HIS:CE1	2.54	0.60
1:Y:31:LEU:HD22	1:Y:43:ILE:CD1	2.30	0.60
1:C:123:GLN:NE2	1:C:146:LYS:HZ1	1.99	0.60
1:F:190:THR:HG22	1:F:191:HIS:ND1	2.16	0.60
1:L:15:ARG:HG2	1:L:16:SER:N	2.04	0.60
1:O:50:LEU:HB2	1:O:59:ILE:HD11	1.82	0.60
1:O:123:GLN:NE2	1:V:132:ALA:N	2.50	0.60
1:H:45:ALA:HB1	1:I:23:LEU:CD1	2.32	0.60
1:N:15:ARG:O	1:N:15:ARG:HG2	2.00	0.60
1:T:92:MET:HB3	1:T:114:LEU:CD1	2.31	0.60
1:G:96:ALA:HB1	1:G:120:MET:HE2	1.83	0.60
1:N:79:THR:O	1:N:83:ILE:HG12	2.01	0.60
1:O:160:SER:C	1:O:162:GLU:N	2.59	0.60
1:R:182:TYR:HD2	1:R:184:LEU:HD23	1.67	0.60
1:O:100:ALA:O	1:O:104:THR:HG23	2.01	0.60
1:O:119:VAL:HG12	1:O:120:MET:H	1.67	0.60
1:S:121:ILE:CD1	1:S:168:THR:HG22	2.30	0.60
1:S:15:ARG:HD3	1:S:16:SER:H	1.66	0.60
1:K:27:ARG:HG2	1:K:50:LEU:HD22	1.83	0.60
1:M:15:ARG:HG3	1:M:16:SER:H	1.65	0.60
1:S:160:SER:O	1:S:161:LEU:C	2.45	0.60
1:T:29:ILE:HG12	1:T:46:GLN:HB3	1.83	0.60
1:Z:123:GLN:NE2	1:Z:146:LYS:HE3	2.17	0.60
1:T:153:MET:HB3	1:T:164:ILE:HG12	1.83	0.59
1:U:146:LYS:O	1:U:150:ASN:ND2	2.35	0.59
1:T:148:ARG:O	1:T:148:ARG:HD3	2.02	0.59
1:F:91:CYS:HB2	1:F:103:LEU:HD22	1.84	0.59
1:K:91:CYS:HB2	1:K:103:LEU:HD13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:70:ILE:HA	1:X:98:MET:HE3	1.84	0.59
1:M:104:THR:HB	1:M:184:LEU:HD23	1.84	0.59
1:P:77:TYR:CE1	1:P:81:GLN:NE2	2.71	0.59
1:T:148:ARG:HD2	1:U:116:ASN:ND2	2.18	0.59
1:G:173:PHE:O	1:G:174:LEU:HD12	2.02	0.59
1:Y:166:ARG:HB2	1:Y:166:ARG:CZ	2.33	0.59
1:O:176:ALA:O	1:O:179:ALA:CB	2.51	0.59
1:P:108:LYS:HD2	1:P:109:GLY:N	2.18	0.59
1:Q:178:GLU:O	1:Q:182:TYR:HB2	2.03	0.59
1:Z:111:ARG:HH21	1:Z:186:ASP:CG	2.11	0.59
1:B:119:VAL:HG11	1:B:184:LEU:CD2	2.32	0.59
1:B:162:GLU:CD	1:B:166:ARG:HH21	2.09	0.59
1:D:174:LEU:HD12	1:D:174:LEU:N	2.18	0.59
1:O:122:HIS:C	1:O:122:HIS:CD2	2.81	0.59
1:R:123:GLN:HE22	1:Z:133:THR:H	1.51	0.59
1:D:140:ARG:HG2	1:D:144:LYS:HE3	1.85	0.59
1:L:40:ALA:HA	1:L:76:ILE:HD11	1.83	0.59
1:S:22:ARG:O	1:S:25:LYS:HB2	2.03	0.59
1:I:98:MET:HE1	1:I:149:MET:HE2	1.85	0.59
1:J:122:HIS:C	1:J:122:HIS:CD2	2.80	0.59
1:O:82:PHE:CE2	1:P:192:ARG:HB2	2.38	0.59
1:S:28:VAL:C	1:S:29:ILE:HD13	2.28	0.59
1:J:42:LEU:O	1:J:46:GLN:HG3	2.03	0.59
1:B:153:MET:O	1:B:157:THR:HG23	2.03	0.58
1:H:86:ASP:OD2	1:H:110:LYS:NZ	2.36	0.58
1:F:155:LEU:HD23	1:F:156:HIS:N	2.18	0.58
1:G:27:ARG:NH2	1:G:54:ASN:O	2.37	0.58
1:I:104:THR:CB	1:I:184:LEU:HD23	2.31	0.58
1:Z:54:ASN:ND2	1:Z:57:LYS:HZ1	2.00	0.58
1:G:172:ARG:HE	1:U:162:GLU:CD	2.12	0.58
1:V:141:GLU:O	1:V:145:VAL:HG23	2.02	0.58
1:W:55:PRO:HB3	1:W:84:LYS:HG2	1.85	0.58
1:X:69:VAL:CG1	1:X:71:THR:HG23	2.33	0.58
1:X:166:ARG:HH11	1:X:166:ARG:CG	2.17	0.58
1:K:122:HIS:C	1:K:122:HIS:CD2	2.80	0.58
1:O:54:ASN:ND2	1:O:57:LYS:HD2	2.19	0.58
1:P:19:ILE:CG2	1:P:20:TYR:N	2.67	0.58
1:P:123:GLN:NE2	1:b:132:ALA:HB3	2.19	0.58
1:W:53:GLU:HA	1:W:53:GLU:OE1	2.02	0.58
1:P:159:GLN:HB2	1:P:164:ILE:HD13	1.86	0.58
1:O:25:LYS:C	1:O:27:ARG:H	2.11	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:86:ASP:OD2	1:P:110:LYS:NZ	2.35	0.58
1:a:23:LEU:HD12	1:a:30:PHE:HE1	1.69	0.58
1:E:111:ARG:O	1:E:185:VAL:HB	2.04	0.58
1:I:19:ILE:HG22	1:I:20:TYR:N	2.19	0.58
1:O:110:LYS:HA	1:O:112:PHE:CE1	2.39	0.58
1:V:73:GLY:C	1:V:98:MET:HE3	2.29	0.58
1:Y:140:ARG:HH11	1:Y:140:ARG:HG3	1.69	0.58
1:b:163:GLN:HA	1:b:166:ARG:NH1	2.19	0.58
1:F:31:LEU:C	1:F:31:LEU:HD12	2.29	0.58
1:F:157:THR:HG22	1:F:183:GLY:O	2.04	0.58
1:N:121:ILE:O	1:N:122:HIS:HB3	2.02	0.58
1:H:19:ILE:HG23	1:H:20:TYR:N	2.19	0.57
1:P:123:GLN:NE2	1:b:133:THR:H	1.99	0.57
1:W:121:ILE:HG21	1:W:153:MET:CE	2.33	0.57
1:O:112:PHE:HB3	1:O:189:LEU:HB2	1.84	0.57
1:P:132:ALA:HB3	1:b:123:GLN:NE2	2.19	0.57
1:V:118:ARG:HG2	1:V:118:ARG:NH1	2.18	0.57
1:F:153:MET:CB	1:F:164:ILE:HD13	2.34	0.57
1:K:34:GLN:O	1:K:39:MET:HE3	2.04	0.57
1:L:97:SER:HG	1:L:122:HIS:CE1	2.22	0.57
1:X:101:PHE:CZ	1:X:149:MET:HE3	2.40	0.57
1:a:104:THR:HB	1:a:184:LEU:HD13	1.85	0.57
1:G:50:LEU:HD13	1:G:59:ILE:HG12	1.86	0.57
1:T:15:ARG:O	1:T:16:SER:OG	2.18	0.57
1:K:121:ILE:HG13	1:K:172:ARG:HB3	1.87	0.57
1:P:112:PHE:N	1:P:112:PHE:CD1	2.72	0.57
1:S:133:THR:H	1:Y:123:GLN:HE22	1.53	0.57
1:a:176:ALA:HB1	1:a:188:ILE:HG12	1.85	0.57
1:D:139:ALA:HA	1:D:142:ILE:CG2	2.35	0.57
1:L:51:GLU:OE1	1:M:192:ARG:NH2	2.38	0.57
1:O:55:PRO:HA	1:O:85:PRO:HD3	1.87	0.57
1:Y:73:GLY:HA3	1:Y:98:MET:SD	2.44	0.57
1:R:23:LEU:HD12	1:R:30:PHE:CE1	2.40	0.57
1:X:166:ARG:HH11	1:X:166:ARG:CB	2.18	0.57
1:I:141:GLU:OE2	1:J:118:ARG:HD2	2.04	0.57
1:P:84:LYS:O	1:P:85:PRO:C	2.47	0.57
1:W:173:PHE:O	1:W:174:LEU:HD12	2.04	0.57
1:X:180:VAL:HG13	1:X:186:ASP:O	2.04	0.57
1:L:166:ARG:NH1	1:L:166:ARG:HB2	2.20	0.57
1:O:37:ASP:OD1	1:O:72:ALA:HB2	2.04	0.57
1:O:130:GLY:O	1:O:135:ILE:HD11	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:140:ARG:HG3	1:X:140:ARG:NH1	2.19	0.57
1:X:184:LEU:HD23	1:X:184:LEU:O	2.05	0.57
1:Z:83:ILE:HB	1:Z:85:PRO:HD2	1.87	0.57
1:H:45:ALA:HB1	1:I:23:LEU:HD13	1.87	0.57
1:O:160:SER:C	1:O:162:GLU:H	2.12	0.57
1:O:180:VAL:HG21	1:O:187:SER:HA	1.87	0.57
1:X:101:PHE:CE1	1:X:149:MET:HE3	2.40	0.57
1:E:31:LEU:HD13	1:E:43:ILE:CD1	2.34	0.56
1:E:161:LEU:O	1:E:165:GLU:HG3	2.05	0.56
1:H:176:ALA:HB1	1:H:188:ILE:HD12	1.86	0.56
1:M:83:ILE:HB	1:M:85:PRO:HD2	1.87	0.56
1:N:139:ALA:O	1:N:142:ILE:HG22	2.04	0.56
1:Q:140:ARG:HG2	1:Q:140:ARG:HH11	1.71	0.56
1:X:31:LEU:HA	1:X:43:ILE:HD11	1.85	0.56
1:Y:88:SER:HB2	1:Y:110:LYS:HB3	1.87	0.56
1:I:115:PRO:HD3	1:I:189:LEU:O	2.05	0.56
1:J:151:GLU:O	1:J:154:ALA:HB3	2.05	0.56
1:K:153:MET:HE1	1:K:184:LEU:HD21	1.86	0.56
1:L:27:ARG:HG2	1:L:50:LEU:HD22	1.87	0.56
1:O:114:LEU:HD22	1:U:78:ASP:HB3	1.86	0.56
1:S:15:ARG:HD3	1:S:16:SER:N	2.20	0.56
1:S:161:LEU:O	1:S:162:GLU:C	2.47	0.56
1:U:81:GLN:NE2	1:U:81:GLN:CA	2.66	0.56
1:b:96:ALA:HA	1:b:120:MET:O	2.05	0.56
1:b:157:THR:HA	1:b:183:GLY:O	2.05	0.56
1:A:141:GLU:HG2	1:B:173:PHE:CD2	2.41	0.56
1:J:29:ILE:CD1	1:J:46:GLN:HB2	2.33	0.56
1:P:132:ALA:HB3	1:b:123:GLN:HE21	1.69	0.56
1:Q:124:PRO:CB	1:Q:142:ILE:HD11	2.35	0.56
1:V:121:ILE:HD12	1:V:168:THR:HG22	1.88	0.56
1:B:91:CYS:SG	1:B:117:SER:HB2	2.46	0.56
1:H:57:LYS:O	1:H:85:PRO:HB3	2.05	0.56
1:L:84:LYS:O	1:L:85:PRO:C	2.48	0.56
1:O:76:ILE:O	1:O:77:TYR:C	2.49	0.56
1:O:141:GLU:HG2	1:P:173:PHE:CE2	2.40	0.56
1:V:76:ILE:O	1:V:80:MET:HG3	2.05	0.56
1:V:78:ASP:N	1:V:78:ASP:OD1	2.38	0.56
1:W:155:LEU:O	1:W:157:THR:N	2.39	0.56
1:J:158:GLY:HA2	1:O:193:ASN:HD21	1.68	0.56
1:O:49:PHE:CD1	1:P:22:ARG:HG2	2.41	0.56
1:Q:31:LEU:CD1	1:Q:39:MET:HE1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:146:LYS:HG2	1:V:150:ASN:HD21	1.71	0.56
1:O:192:ARG:HG2	1:U:51:GLU:OE2	2.05	0.56
1:B:27:ARG:HG2	1:B:50:LEU:HD22	1.87	0.56
1:K:165:GLU:O	1:K:169:GLU:HG2	2.05	0.56
1:Z:40:ALA:O	1:Z:44:VAL:HG23	2.05	0.56
1:a:148:ARG:HH11	1:b:116:ASN:ND2	2.03	0.56
1:E:153:MET:HE1	1:E:184:LEU:HD21	1.88	0.56
1:F:132:ALA:CB	1:J:123:GLN:HE21	2.18	0.56
1:Q:164:ILE:O	1:Q:168:THR:HG23	2.05	0.56
1:I:153:MET:HE3	1:I:164:ILE:HD12	1.87	0.56
1:W:104:THR:HB	1:W:184:LEU:CD2	2.11	0.56
1:D:112:PHE:CD2	1:D:189:LEU:HG	2.41	0.55
1:Q:190:THR:HG22	1:Q:191:HIS:ND1	2.21	0.55
1:S:132:ALA:HB3	1:Y:123:GLN:HE21	1.71	0.55
1:A:91:CYS:HB2	1:A:103:LEU:HD22	1.86	0.55
1:F:153:MET:HB3	1:F:164:ILE:HD13	1.87	0.55
1:G:31:LEU:C	1:G:31:LEU:HD12	2.31	0.55
1:J:31:LEU:CD1	1:J:39:MET:HE1	2.36	0.55
1:K:51:GLU:OE2	1:L:192:ARG:NE	2.40	0.55
1:P:97:SER:OG	1:P:122:HIS:CE1	2.60	0.55
1:X:51:GLU:HG3	1:X:85:PRO:HD3	1.88	0.55
1:X:62:TYR:CD2	1:X:92:MET:HE2	2.41	0.55
1:Z:31:LEU:C	1:Z:31:LEU:HD12	2.32	0.55
1:b:31:LEU:CD1	1:b:39:MET:HE1	2.36	0.55
1:U:51:GLU:O	1:U:55:PRO:N	2.39	0.55
1:a:92:MET:HB3	1:a:114:LEU:HD12	1.88	0.55
1:B:15:ARG:O	1:B:22:ARG:HD3	2.06	0.55
1:C:66:PRO:HB3	1:C:94:GLN:NE2	2.21	0.55
1:D:51:GLU:OE1	1:E:192:ARG:NH2	2.39	0.55
1:O:81:GLN:OE1	1:O:81:GLN:HA	2.05	0.55
1:R:104:THR:HB	1:R:184:LEU:HD13	1.87	0.55
1:W:27:ARG:NE	1:W:57:LYS:HB3	2.22	0.55
1:b:106:GLY:HA3	1:b:111:ARG:HG2	1.89	0.55
1:C:127:GLY:HA3	1:M:129:GLN:HG3	1.88	0.55
1:P:169:GLU:OE1	1:P:169:GLU:HA	2.07	0.55
1:S:15:ARG:O	1:S:22:ARG:HB2	2.06	0.55
1:U:112:PHE:CD2	1:U:189:LEU:HG	2.41	0.55
1:Z:140:ARG:HH11	1:Z:140:ARG:HG3	1.71	0.55
1:M:31:LEU:HG	1:M:63:ILE:HD12	1.89	0.55
1:O:77:TYR:OH	1:O:156:HIS:HE1	1.89	0.55
1:V:192:ARG:NH2	1:b:51:GLU:OE1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:70:ILE:HA	1:E:98:MET:CE	2.28	0.55
1:M:31:LEU:HD13	1:M:39:MET:HE1	1.87	0.55
1:O:15:ARG:HE	1:O:16:SER:H	1.55	0.55
1:V:51:GLU:OE1	1:W:192:ARG:NH2	2.34	0.55
1:a:145:VAL:O	1:a:149:MET:HG2	2.06	0.55
1:E:31:LEU:HD12	1:E:39:MET:HE1	1.87	0.55
1:E:174:LEU:HD12	1:E:174:LEU:N	2.22	0.55
1:N:175:SER:OG	1:N:177:PRO:HD2	2.06	0.55
1:P:148:ARG:HH11	1:P:148:ARG:HG2	1.72	0.55
1:X:146:LYS:NZ	1:X:169:GLU:OE1	2.40	0.55
1:X:161:LEU:O	1:X:165:GLU:HG3	2.07	0.55
1:b:173:PHE:C	1:b:174:LEU:HD12	2.31	0.55
1:H:23:LEU:HD12	1:H:30:PHE:HE1	1.72	0.55
1:Q:84:LYS:N	1:Q:85:PRO:CD	2.70	0.55
1:K:44:VAL:HG11	1:L:92:MET:HE1	1.89	0.55
1:S:136:GLU:CG	1:Y:143:LEU:HD11	2.36	0.55
1:I:98:MET:HE2	1:I:98:MET:CA	2.34	0.54
1:L:27:ARG:HG2	1:L:27:ARG:NH1	2.19	0.54
1:N:119:VAL:HG11	1:N:184:LEU:HD13	1.89	0.54
1:Q:145:VAL:O	1:Q:149:MET:HG2	2.07	0.54
1:W:104:THR:OG1	1:W:184:LEU:HA	2.06	0.54
1:Y:128:TYR:CG	1:Y:129:GLN:N	2.76	0.54
1:b:43:ILE:O	1:b:47:MET:HG3	2.07	0.54
1:b:89:THR:O	1:b:90:ILE:HD13	2.07	0.54
1:G:187:SER:HB3	1:X:162:GLU:OE1	2.07	0.54
1:O:133:THR:N	1:V:123:GLN:NE2	2.47	0.54
1:Q:45:ALA:HB1	1:R:19:ILE:HD12	1.88	0.54
1:Q:140:ARG:HG2	1:Q:140:ARG:NH1	2.21	0.54
1:Z:54:ASN:OD1	1:Z:56:GLU:HB2	2.07	0.54
1:a:24:LEU:HD23	1:b:16:SER:OG	2.06	0.54
1:E:23:LEU:HD12	1:E:30:PHE:HE1	1.72	0.54
1:G:18:ASP:OD1	1:G:21:SER:HB2	2.06	0.54
1:K:152:LEU:HD11	1:L:116:ASN:ND2	2.23	0.54
1:O:72:ALA:O	1:O:76:ILE:HD13	2.07	0.54
1:P:25:LYS:HE3	1:Q:15:ARG:HH21	1.72	0.54
1:B:89:THR:HG23	1:B:106:GLY:HA3	1.88	0.54
1:B:123:GLN:HE21	1:N:132:ALA:HB3	1.72	0.54
1:F:154:ALA:N	1:F:164:ILE:CD1	2.70	0.54
1:F:157:THR:HG22	1:F:183:GLY:C	2.32	0.54
1:G:31:LEU:CD1	1:G:39:MET:HE1	2.36	0.54
1:J:31:LEU:HD13	1:J:39:MET:HE1	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:140:ARG:HG3	1:K:140:ARG:HH11	1.73	0.54
1:U:79:THR:O	1:U:83:ILE:HG23	2.08	0.54
1:V:101:PHE:HZ	1:V:152:LEU:HD12	1.72	0.54
1:b:159:GLN:HG3	1:b:163:GLN:HB3	1.89	0.54
1:A:119:VAL:HG11	1:A:184:LEU:HD13	1.90	0.54
1:C:46:GLN:HA	1:D:19:ILE:HD11	1.90	0.54
1:S:123:GLN:NE2	1:Y:133:THR:H	2.05	0.54
1:U:42:LEU:O	1:U:46:GLN:NE2	2.37	0.54
1:Y:148:ARG:HG2	1:Y:148:ARG:HH11	1.72	0.54
1:Z:31:LEU:HD22	1:Z:43:ILE:HD13	1.88	0.54
1:F:27:ARG:NH1	1:F:27:ARG:HG2	2.23	0.54
1:F:55:PRO:HA	1:F:85:PRO:HG3	1.89	0.54
1:J:51:GLU:OE1	1:K:192:ARG:NH2	2.41	0.54
1:K:119:VAL:HG11	1:K:184:LEU:HD13	1.90	0.54
1:W:137:ILE:HG21	1:X:171:ASP:O	2.07	0.54
1:F:58:ASP:OD2	1:F:110:LYS:HE2	2.08	0.54
1:P:104:THR:HG23	1:P:156:HIS:HB3	1.90	0.54
1:W:51:GLU:HG3	1:W:85:PRO:HD2	1.88	0.54
1:I:166:ARG:HB2	1:I:166:ARG:HH11	1.73	0.54
1:J:54:ASN:OD1	1:J:57:LYS:HG3	2.07	0.54
1:Q:120:MET:HE3	1:Q:171:ASP:CB	2.37	0.54
1:R:101:PHE:O	1:R:104:THR:HG22	2.07	0.54
1:W:91:CYS:SG	1:W:95:ALA:HB2	2.47	0.54
1:Y:25:LYS:HD2	1:Z:15:ARG:NE	2.21	0.54
1:C:176:ALA:HB3	1:C:177:PRO:CD	2.38	0.54
1:E:25:LYS:HB2	1:E:25:LYS:HZ3	1.72	0.54
1:H:22:ARG:HG2	1:N:49:PHE:CE1	2.42	0.54
1:A:116:ASN:HD21	1:G:148:ARG:HD2	1.74	0.53
1:F:84:LYS:N	1:F:85:PRO:CD	2.72	0.53
1:K:170:ARG:O	1:K:171:ASP:C	2.51	0.53
1:O:47:MET:CE	1:O:61:LEU:HD22	2.38	0.53
1:X:46:GLN:HA	1:Y:19:ILE:CD1	2.38	0.53
1:Z:53:GLU:O	1:Z:54:ASN:HB2	2.07	0.53
1:V:107:ALA:HB3	1:V:110:LYS:HB2	1.90	0.53
1:V:123:GLN:O	1:V:124:PRO:O	2.26	0.53
1:W:176:ALA:O	1:W:179:ALA:HB3	2.08	0.53
1:X:46:GLN:HA	1:Y:19:ILE:HD11	1.91	0.53
1:a:188:ILE:HG22	1:a:189:LEU:N	2.24	0.53
1:A:19:ILE:O	1:A:22:ARG:HB3	2.07	0.53
1:A:77:TYR:OH	1:A:156:HIS:HE1	1.92	0.53
1:E:145:VAL:O	1:E:149:MET:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:77:TYR:OH	1:Q:156:HIS:HE1	1.91	0.53
1:U:54:ASN:ND2	1:U:57:LYS:HG3	2.23	0.53
1:A:105:ALA:HA	1:A:156:HIS:CD2	2.43	0.53
1:D:190:THR:HG22	1:D:191:HIS:CE1	2.44	0.53
1:E:22:ARG:O	1:E:25:LYS:HB3	2.08	0.53
1:F:163:GLN:HA	1:F:166:ARG:HH12	1.73	0.53
1:K:89:THR:OG1	1:K:111:ARG:HG3	2.09	0.53
1:L:77:TYR:OH	1:L:156:HIS:CE1	2.60	0.53
1:M:31:LEU:HB2	1:M:43:ILE:CD1	2.39	0.53
1:T:147:GLY:O	1:T:150:ASN:N	2.40	0.53
1:V:170:ARG:O	1:V:171:ASP:C	2.51	0.53
1:P:88:SER:CB	1:P:110:LYS:HB3	2.38	0.53
1:S:98:MET:HE1	1:S:149:MET:HE2	1.91	0.53
1:T:112:PHE:CD2	1:T:189:LEU:HG	2.44	0.53
1:A:98:MET:HE1	1:A:149:MET:CE	2.39	0.53
1:C:147:GLY:O	1:C:151:GLU:HG3	2.09	0.53
1:O:22:ARG:O	1:O:25:LYS:HB2	2.09	0.53
1:O:120:MET:HG3	1:O:173:PHE:CE2	2.44	0.53
1:F:77:TYR:OH	1:F:156:HIS:HE1	1.91	0.53
1:O:138:HIS:O	1:O:142:ILE:HG22	2.08	0.53
1:O:141:GLU:HG2	1:P:173:PHE:CD2	2.44	0.53
1:P:123:GLN:HE21	1:b:132:ALA:HB3	1.71	0.53
1:Q:115:PRO:HD3	1:Q:189:LEU:O	2.08	0.53
1:Y:51:GLU:OE1	1:Z:192:ARG:NH2	2.41	0.53
1:B:77:TYR:O	1:B:81:GLN:HG2	2.08	0.53
1:Q:70:ILE:HA	1:Q:98:MET:HE3	1.91	0.53
1:W:15:ARG:CG	1:W:16:SER:H	2.08	0.53
1:X:83:ILE:HB	1:X:85:PRO:HD2	1.90	0.53
1:X:167:ASP:OD1	1:X:172:ARG:NH1	2.42	0.53
1:A:131:GLN:O	1:A:134:ASP:N	2.42	0.53
1:F:27:ARG:HG2	1:F:27:ARG:HH11	1.74	0.53
1:F:161:LEU:O	1:F:165:GLU:HG3	2.09	0.53
1:F:163:GLN:HA	1:F:163:GLN:NE2	2.24	0.53
1:O:119:VAL:HG12	1:O:120:MET:N	2.24	0.53
1:R:49:PHE:CD1	1:S:22:ARG:HD3	2.44	0.53
1:a:31:LEU:HD22	1:a:43:ILE:HD12	1.90	0.53
1:A:148:ARG:O	1:A:148:ARG:HD3	2.09	0.53
1:H:73:GLY:HA3	1:H:98:MET:HG2	1.91	0.53
1:I:47:MET:HE1	1:I:80:MET:HG3	1.89	0.53
1:V:26:GLU:OE2	1:V:26:GLU:HA	2.09	0.53
1:V:128:TYR:CG	1:V:129:GLN:N	2.77	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:PRO:HB2	1:A:84:LYS:HE3	1.90	0.52
1:B:70:ILE:HA	1:B:98:MET:HE3	1.90	0.52
1:E:49:PHE:CE1	1:F:22:ARG:HG2	2.42	0.52
1:E:176:ALA:HB3	1:E:177:PRO:HD3	1.90	0.52
1:F:21:SER:O	1:F:24:LEU:HB3	2.09	0.52
1:I:31:LEU:HD13	1:I:39:MET:HE1	1.91	0.52
1:I:139:ALA:O	1:I:142:ILE:HG22	2.08	0.52
1:K:167:ASP:OD2	1:K:182:TYR:HE1	1.92	0.52
1:O:45:ALA:HB1	1:P:23:LEU:HD11	1.91	0.52
1:P:148:ARG:HH11	1:Q:116:ASN:ND2	2.02	0.52
1:T:81:GLN:O	1:U:191:HIS:CD2	2.62	0.52
1:E:49:PHE:CZ	1:F:16:SER:HB2	2.45	0.52
1:O:191:HIS:HD2	1:O:192:ARG:N	2.07	0.52
1:P:120:MET:HG2	1:P:121:ILE:N	2.23	0.52
1:P:148:ARG:NH1	1:Q:116:ASN:HD22	2.00	0.52
1:R:124:PRO:CD	1:R:146:LYS:HG3	2.35	0.52
1:X:18:ASP:OD2	1:X:20:TYR:HB2	2.09	0.52
1:b:175:SER:OG	1:b:178:GLU:HG3	2.08	0.52
1:B:157:THR:HA	1:B:183:GLY:O	2.09	0.52
1:E:96:ALA:HB1	1:E:120:MET:HE2	1.91	0.52
1:G:172:ARG:NE	1:U:162:GLU:OE2	2.41	0.52
1:K:42:LEU:HG	1:K:46:GLN:HE21	1.74	0.52
1:N:50:LEU:O	1:N:53:GLU:HB2	2.09	0.52
1:O:177:PRO:C	1:O:179:ALA:N	2.66	0.52
1:P:140:ARG:HH11	1:P:140:ARG:HG3	1.75	0.52
1:Q:119:VAL:HG11	1:Q:184:LEU:HD13	1.92	0.52
1:Q:148:ARG:HG2	1:Q:148:ARG:HH11	1.74	0.52
1:T:91:CYS:SG	1:T:95:ALA:HB2	2.49	0.52
1:W:77:TYR:O	1:W:80:MET:HB2	2.10	0.52
1:C:90:ILE:HD12	1:C:90:ILE:N	2.25	0.52
1:G:15:ARG:HG3	1:G:16:SER:H	1.75	0.52
1:G:105:ALA:HA	1:G:156:HIS:CD2	2.45	0.52
1:J:46:GLN:HA	1:K:19:ILE:HD11	1.92	0.52
1:L:91:CYS:SG	1:L:117:SER:HB2	2.49	0.52
1:O:177:PRO:O	1:O:179:ALA:N	2.42	0.52
1:T:148:ARG:HD3	1:T:152:LEU:HG	1.91	0.52
1:W:90:ILE:O	1:W:90:ILE:HG22	2.09	0.52
1:X:173:PHE:C	1:X:174:LEU:HD12	2.34	0.52
1:Y:173:PHE:O	1:Y:174:LEU:HD23	2.09	0.52
1:Z:58:ASP:OD2	1:Z:110:LYS:NZ	2.41	0.52
1:F:112:PHE:O	1:F:185:VAL:HG11	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:104:THR:HB	1:Y:184:LEU:CD2	2.39	0.52
1:B:115:PRO:HD3	1:B:189:LEU:O	2.09	0.52
1:E:89:THR:CB	1:E:103:LEU:HD12	2.40	0.52
1:W:175:SER:HB2	1:W:177:PRO:HD2	1.90	0.52
1:b:84:LYS:N	1:b:85:PRO:CD	2.72	0.52
1:A:123:GLN:NE2	1:H:133:THR:H	2.07	0.52
1:G:31:LEU:HA	1:G:43:ILE:HD11	1.92	0.52
1:G:162:GLU:H	1:G:162:GLU:CD	2.18	0.52
1:I:122:HIS:C	1:I:122:HIS:CD2	2.88	0.52
1:K:31:LEU:HA	1:K:43:ILE:HD11	1.90	0.52
1:L:164:ILE:HD13	1:L:182:TYR:OH	2.10	0.52
1:O:120:MET:HA	1:O:172:ARG:O	2.10	0.52
1:E:19:ILE:HG23	1:E:20:TYR:N	2.25	0.52
1:A:84:LYS:HG3	1:B:192:ARG:HG2	1.90	0.52
1:D:125:LEU:HD23	1:L:131:GLN:HA	1.91	0.52
1:Y:106:GLY:O	1:Y:111:ARG:HD3	2.10	0.52
1:a:15:ARG:O	1:a:16:SER:CB	2.58	0.52
1:b:32:THR:HA	1:b:64:ASN:O	2.10	0.52
1:A:54:ASN:HD21	1:A:57:LYS:HG3	1.74	0.52
1:J:146:LYS:HG2	1:J:150:ASN:HD21	1.74	0.52
1:O:98:MET:O	1:O:102:LEU:HG	2.10	0.52
1:P:104:THR:OG1	1:P:184:LEU:HA	2.10	0.52
1:b:83:ILE:HB	1:b:85:PRO:HD2	1.91	0.52
1:b:128:TYR:CG	1:b:129:GLN:N	2.78	0.52
1:B:104:THR:O	1:B:156:HIS:HB3	2.10	0.51
1:D:23:LEU:HD13	1:D:30:PHE:HE1	1.75	0.51
1:D:140:ARG:O	1:D:144:LYS:HG3	2.10	0.51
1:F:190:THR:HG22	1:F:191:HIS:CE1	2.45	0.51
1:J:15:ARG:CA	1:J:22:ARG:HD3	2.40	0.51
1:M:128:TYR:CG	1:M:129:GLN:N	2.78	0.51
1:O:152:LEU:HD11	1:P:116:ASN:HD21	1.75	0.51
1:S:133:THR:H	1:Y:123:GLN:NE2	2.08	0.51
1:S:164:ILE:O	1:S:168:THR:HG23	2.10	0.51
1:W:128:TYR:HD2	1:W:135:ILE:HD13	1.74	0.51
1:C:157:THR:HA	1:C:183:GLY:O	2.10	0.51
1:E:113:CYS:O	1:E:188:ILE:HG23	2.10	0.51
1:F:170:ARG:HG2	1:F:170:ARG:HH11	1.76	0.51
1:M:34:GLN:CA	1:M:34:GLN:HE21	2.22	0.51
1:O:180:VAL:HG22	1:O:187:SER:HA	1.91	0.51
1:P:78:ASP:HB3	1:Q:114:LEU:HB3	1.92	0.51
1:S:77:TYR:OH	1:S:156:HIS:HE1	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:161:LEU:O	1:U:165:GLU:HB2	2.10	0.51
1:D:84:LYS:HG3	1:E:192:ARG:CG	2.39	0.51
1:I:81:GLN:OE1	1:I:81:GLN:HA	2.11	0.51
1:L:49:PHE:HE1	1:M:22:ARG:NH1	2.08	0.51
1:Q:141:GLU:OE1	1:Q:141:GLU:HA	2.09	0.51
1:U:153:MET:O	1:U:157:THR:HG23	2.11	0.51
1:E:134:ASP:OD1	1:F:170:ARG:NH1	2.43	0.51
1:F:23:LEU:O	1:F:28:VAL:HB	2.10	0.51
1:F:112:PHE:CD2	1:F:189:LEU:HD21	2.46	0.51
1:Q:91:CYS:HB3	1:Q:113:CYS:HA	1.93	0.51
1:Q:180:VAL:HG21	1:Q:188:ILE:HG13	1.92	0.51
1:W:163:GLN:NE2	1:W:163:GLN:HA	2.24	0.51
1:Z:88:SER:HB2	1:Z:110:LYS:HB3	1.91	0.51
1:O:123:GLN:NE2	1:V:131:GLN:HB3	2.24	0.51
1:W:148:ARG:HD2	1:X:116:ASN:HD21	1.74	0.51
1:A:122:HIS:C	1:A:122:HIS:CD2	2.88	0.51
1:G:123:GLN:NE2	1:I:133:THR:H	2.07	0.51
1:G:175:SER:HB2	1:G:177:PRO:HD2	1.92	0.51
1:L:25:LYS:HD2	1:M:15:ARG:NH2	2.26	0.51
1:O:49:PHE:HE1	1:P:22:ARG:HG2	1.73	0.51
1:O:110:LYS:HA	1:O:112:PHE:HE1	1.76	0.51
1:P:15:ARG:O	1:P:22:ARG:HD3	2.10	0.51
1:T:31:LEU:CD1	1:T:39:MET:HE1	2.40	0.51
1:U:47:MET:CE	1:U:80:MET:HG3	2.41	0.51
1:V:80:MET:HE3	1:V:87:VAL:CG1	2.39	0.51
1:W:21:SER:O	1:W:24:LEU:HB3	2.11	0.51
1:Z:49:PHE:HB2	1:a:23:LEU:HD21	1.92	0.51
1:C:153:MET:O	1:C:157:THR:HG23	2.10	0.51
1:D:78:ASP:CB	1:E:114:LEU:HD13	2.40	0.51
1:K:104:THR:HA	1:K:111:ARG:HH11	1.75	0.51
1:O:64:ASN:HA	1:O:94:GLN:O	2.11	0.51
1:P:163:GLN:HG3	1:P:167:ASP:OD2	2.09	0.51
1:U:84:LYS:HB3	1:U:85:PRO:CD	2.41	0.51
1:V:148:ARG:HG2	1:V:148:ARG:HH11	1.75	0.51
1:W:104:THR:O	1:W:156:HIS:HB3	2.09	0.51
1:W:190:THR:HG22	1:W:191:HIS:ND1	2.26	0.51
1:X:27:ARG:NH2	1:X:57:LYS:O	2.42	0.51
1:D:148:ARG:HH11	1:E:116:ASN:ND2	2.09	0.51
1:L:31:LEU:C	1:L:31:LEU:HD12	2.36	0.51
1:M:163:GLN:HG3	1:M:167:ASP:OD2	2.11	0.51
1:N:153:MET:O	1:N:157:THR:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:176:ALA:O	1:P:179:ALA:HB3	2.10	0.51
1:S:134:ASP:OD1	1:T:170:ARG:NH1	2.44	0.51
1:W:111:ARG:C	1:W:112:PHE:CD2	2.89	0.51
1:Z:164:ILE:O	1:Z:168:THR:HG23	2.10	0.51
1:U:124:PRO:CG	1:U:146:LYS:HA	2.24	0.51
1:W:115:PRO:HD3	1:W:189:LEU:O	2.11	0.51
1:Z:111:ARG:NH2	1:Z:186:ASP:OD1	2.36	0.51
1:Z:161:LEU:O	1:Z:165:GLU:HG3	2.11	0.51
1:b:47:MET:HE1	1:b:80:MET:HG2	1.93	0.51
1:N:164:ILE:HD13	1:N:182:TYR:OH	2.11	0.51
1:Q:15:ARG:O	1:Q:16:SER:HB3	2.11	0.51
1:R:70:ILE:O	1:R:71:THR:C	2.54	0.51
1:U:19:ILE:HG23	1:U:20:TYR:N	2.25	0.51
1:W:112:PHE:CD2	1:W:112:PHE:N	2.75	0.51
1:a:133:THR:HG21	1:b:170:ARG:HD3	1.93	0.51
1:C:77:TYR:OH	1:C:156:HIS:HE1	1.93	0.50
1:D:41:ASN:ND2	1:E:32:THR:OG1	2.44	0.50
1:J:84:LYS:N	1:J:85:PRO:CD	2.73	0.50
1:K:146:LYS:NZ	1:K:169:GLU:OE1	2.44	0.50
1:O:120:MET:HG3	1:O:173:PHE:CD2	2.45	0.50
1:P:167:ASP:OD2	1:P:182:TYR:OH	2.25	0.50
1:Y:31:LEU:HD22	1:Y:43:ILE:HD12	1.94	0.50
1:Z:92:MET:HB3	1:Z:114:LEU:CD1	2.41	0.50
1:Z:94:GLN:HA	1:Z:118:ARG:O	2.11	0.50
1:K:152:LEU:HD11	1:L:116:ASN:HD21	1.76	0.50
1:T:77:TYR:OH	1:T:156:HIS:HE1	1.93	0.50
1:T:84:LYS:NZ	1:U:193:ASN:HA	2.26	0.50
1:V:173:PHE:O	1:V:174:LEU:HD12	2.10	0.50
1:Z:106:GLY:O	1:Z:111:ARG:HD3	2.12	0.50
1:a:31:LEU:CD1	1:a:31:LEU:C	2.84	0.50
1:E:97:SER:HG	1:E:122:HIS:CE1	2.27	0.50
1:H:31:LEU:HB2	1:H:43:ILE:CD1	2.40	0.50
1:I:19:ILE:HG23	1:I:23:LEU:HD12	1.93	0.50
1:K:122:HIS:HD2	1:K:122:HIS:O	1.94	0.50
1:Q:59:ILE:HD12	1:Q:85:PRO:HB2	1.93	0.50
1:S:19:ILE:HG23	1:S:20:TYR:N	2.26	0.50
1:U:128:TYR:CG	1:U:129:GLN:N	2.79	0.50
1:V:84:LYS:N	1:V:85:PRO:HD2	2.26	0.50
1:W:82:PHE:HD1	1:X:190:THR:O	1.94	0.50
1:G:119:VAL:HG11	1:G:184:LEU:CD1	2.42	0.50
1:G:172:ARG:NE	1:U:162:GLU:CD	2.69	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:23:LEU:HD12	1:H:30:PHE:CE1	2.46	0.50
1:Q:15:ARG:O	1:Q:16:SER:CB	2.59	0.50
1:S:132:ALA:CB	1:Y:146:LYS:HD2	2.41	0.50
1:U:70:ILE:HG23	1:U:98:MET:CE	2.42	0.50
1:Y:160:SER:OG	1:Y:163:GLN:HB2	2.12	0.50
1:D:160:SER:O	1:D:161:LEU:C	2.54	0.50
1:F:58:ASP:OD1	1:F:86:ASP:HB2	2.11	0.50
1:J:15:ARG:O	1:J:22:ARG:HG2	2.12	0.50
1:O:163:GLN:O	1:O:164:ILE:C	2.54	0.50
1:Z:54:ASN:ND2	1:Z:57:LYS:NZ	2.58	0.50
1:Z:128:TYR:CG	1:Z:129:GLN:N	2.79	0.50
1:G:123:GLN:NE2	1:G:146:LYS:NZ	2.59	0.50
1:O:84:LYS:N	1:O:85:PRO:HD2	2.26	0.50
1:O:159:GLN:HA	1:O:159:GLN:HE21	1.76	0.50
1:V:160:SER:O	1:V:161:LEU:C	2.55	0.50
1:X:62:TYR:HB3	1:X:92:MET:HE2	1.92	0.50
1:Y:53:GLU:O	1:Y:54:ASN:HB2	2.12	0.50
1:C:83:ILE:HB	1:C:85:PRO:HD2	1.94	0.50
1:F:167:ASP:OD1	1:F:172:ARG:NH1	2.45	0.50
1:G:140:ARG:O	1:G:143:LEU:HB2	2.11	0.50
1:I:166:ARG:HH11	1:I:166:ARG:CB	2.24	0.50
1:J:133:THR:HG21	1:K:170:ARG:NE	2.27	0.50
1:S:122:HIS:C	1:S:122:HIS:CD2	2.89	0.50
1:X:101:PHE:O	1:X:104:THR:HG22	2.11	0.50
1:G:120:MET:HA	1:G:172:ARG:O	2.12	0.50
1:J:41:ASN:HD22	1:K:32:THR:CG2	2.23	0.50
1:O:167:ASP:OD1	1:O:167:ASP:N	2.45	0.50
1:Y:31:LEU:HD13	1:Y:39:MET:HE1	1.93	0.50
1:Z:174:LEU:HD22	1:Z:184:LEU:CD1	2.42	0.50
1:a:122:HIS:C	1:a:122:HIS:CD2	2.90	0.50
1:E:122:HIS:C	1:E:122:HIS:CD2	2.90	0.50
1:O:41:ASN:O	1:O:41:ASN:OD1	2.30	0.50
1:P:40:ALA:O	1:P:44:VAL:HG23	2.11	0.50
1:P:70:ILE:HA	1:P:98:MET:HE3	1.94	0.50
1:P:172:ARG:NH1	1:P:172:ARG:HG2	2.27	0.50
1:R:148:ARG:NH1	1:S:116:ASN:ND2	2.55	0.50
1:V:34:GLN:O	1:V:39:MET:HE3	2.11	0.50
1:X:108:LYS:HD2	1:X:186:ASP:OD1	2.11	0.50
1:Z:128:TYR:HE2	1:Z:134:ASP:HB2	1.76	0.50
1:A:19:ILE:HD11	1:G:49:PHE:CB	2.42	0.49
1:F:45:ALA:HB1	1:G:23:LEU:CD1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:15:ARG:N	1:J:22:ARG:CD	2.74	0.49
1:K:46:GLN:HG2	1:L:19:ILE:CD1	2.42	0.49
1:M:111:ARG:NH1	1:M:156:HIS:O	2.43	0.49
1:O:82:PHE:CD2	1:O:82:PHE:C	2.90	0.49
1:O:132:ALA:CA	1:O:135:ILE:HD12	2.32	0.49
1:W:40:ALA:HA	1:W:76:ILE:HD11	1.94	0.49
1:W:111:ARG:C	1:W:112:PHE:HD2	2.20	0.49
1:C:66:PRO:HB3	1:C:94:GLN:HE22	1.76	0.49
1:D:128:TYR:CG	1:D:129:GLN:N	2.80	0.49
1:E:22:ARG:O	1:E:22:ARG:HD2	2.12	0.49
1:I:175:SER:OG	1:I:177:PRO:HD2	2.12	0.49
1:J:77:TYR:C	1:J:77:TYR:CD2	2.89	0.49
1:R:111:ARG:NH2	1:R:186:ASP:OD1	2.41	0.49
1:D:135:ILE:HD11	1:L:126:GLY:O	2.13	0.49
1:F:154:ALA:N	1:F:164:ILE:HD13	2.28	0.49
1:J:34:GLN:O	1:J:39:MET:HE3	2.11	0.49
1:J:54:ASN:CG	1:J:57:LYS:HG3	2.37	0.49
1:M:22:ARG:HH11	1:M:22:ARG:CG	2.25	0.49
1:O:177:PRO:C	1:O:179:ALA:H	2.19	0.49
1:P:172:ARG:HG2	1:P:172:ARG:HH11	1.77	0.49
1:S:123:GLN:HE21	1:Y:132:ALA:CB	2.15	0.49
1:T:141:GLU:HG2	1:U:173:PHE:CD1	2.46	0.49
1:V:22:ARG:HG2	1:b:49:PHE:CD1	2.47	0.49
1:A:19:ILE:HD11	1:G:49:PHE:HB2	1.93	0.49
1:H:157:THR:HA	1:H:183:GLY:O	2.13	0.49
1:O:157:THR:HA	1:O:183:GLY:O	2.12	0.49
1:O:160:SER:O	1:O:163:GLN:N	2.45	0.49
1:W:92:MET:CB	1:W:114:LEU:HD12	2.41	0.49
1:W:122:HIS:CD2	1:W:123:GLN:O	2.65	0.49
1:B:163:GLN:O	1:B:167:ASP:HB2	2.12	0.49
1:H:31:LEU:C	1:H:31:LEU:HD12	2.38	0.49
1:K:51:GLU:HG3	1:K:85:PRO:HD3	1.93	0.49
1:N:15:ARG:O	1:N:16:SER:HB3	2.13	0.49
1:N:40:ALA:O	1:N:44:VAL:HG23	2.12	0.49
1:Q:120:MET:HE3	1:Q:171:ASP:CG	2.38	0.49
1:S:31:LEU:C	1:S:31:LEU:CD1	2.85	0.49
1:S:36:GLU:O	1:S:39:MET:HG3	2.11	0.49
1:W:167:ASP:CG	1:W:172:ARG:NH2	2.70	0.49
1:Y:25:LYS:HD2	1:Z:15:ARG:HE	1.76	0.49
1:a:128:TYR:CG	1:a:129:GLN:N	2.80	0.49
1:E:53:GLU:O	1:E:54:ASN:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:34:GLN:HE21	1:M:34:GLN:HA	1.77	0.49
1:S:143:LEU:HD11	1:Y:136:GLU:HG3	1.93	0.49
1:Y:70:ILE:HA	1:Y:98:MET:HE3	1.94	0.49
1:I:148:ARG:NH1	1:J:116:ASN:HD21	2.11	0.49
1:K:190:THR:O	1:K:191:HIS:CD2	2.66	0.49
1:P:114:LEU:N	1:P:114:LEU:HD12	2.27	0.49
1:Q:31:LEU:C	1:Q:31:LEU:CD1	2.85	0.49
1:T:119:VAL:O	1:T:174:LEU:N	2.40	0.49
1:W:103:LEU:C	1:W:105:ALA:H	2.19	0.49
1:W:136:GLU:O	1:W:137:ILE:C	2.56	0.49
1:Z:80:MET:HE3	1:Z:87:VAL:HG11	1.94	0.49
1:C:154:ALA:O	1:C:155:LEU:C	2.54	0.49
1:F:121:ILE:O	1:F:122:HIS:HB3	2.12	0.49
1:G:27:ARG:HG2	1:G:50:LEU:HD22	1.94	0.49
1:M:46:GLN:HA	1:N:19:ILE:HD11	1.93	0.49
1:Q:84:LYS:N	1:Q:85:PRO:HD3	2.28	0.49
1:Q:91:CYS:O	1:Q:114:LEU:HD23	2.12	0.49
1:T:97:SER:HG	1:T:122:HIS:CE1	2.30	0.49
1:X:113:CYS:O	1:X:188:ILE:HG23	2.13	0.49
1:a:179:ALA:HB1	1:a:185:VAL:HG22	1.94	0.49
1:b:119:VAL:HG11	1:b:184:LEU:HD13	1.95	0.49
1:A:49:PHE:CE1	1:B:22:ARG:HG2	2.47	0.49
1:A:136:GLU:CG	1:H:143:LEU:HD11	2.41	0.49
1:C:101:PHE:HZ	1:C:152:LEU:HD12	1.78	0.49
1:L:22:ARG:O	1:L:25:LYS:N	2.42	0.49
1:M:31:LEU:HB2	1:M:43:ILE:HD13	1.95	0.49
1:O:128:TYR:CG	1:O:129:GLN:N	2.80	0.49
1:S:148:ARG:C	1:S:148:ARG:HD3	2.38	0.49
1:Y:160:SER:HB2	1:Y:162:GLU:HG3	1.95	0.49
1:D:174:LEU:HD22	1:D:184:LEU:HD12	1.95	0.49
1:E:157:THR:C	1:E:159:GLN:H	2.21	0.49
1:I:140:ARG:HG2	1:I:144:LYS:HZ3	1.77	0.49
1:J:106:GLY:O	1:J:111:ARG:HD3	2.13	0.49
1:N:31:LEU:C	1:N:31:LEU:HD12	2.38	0.49
1:O:45:ALA:HB1	1:P:23:LEU:CD1	2.43	0.49
1:Q:83:ILE:HB	1:Q:85:PRO:HD2	1.94	0.49
1:T:141:GLU:HG2	1:U:173:PHE:CZ	2.47	0.49
1:W:122:HIS:CD2	1:W:122:HIS:C	2.91	0.49
1:Y:42:LEU:O	1:Y:46:GLN:HG3	2.12	0.49
1:Y:119:VAL:CG1	1:Y:120:MET:N	2.76	0.49
1:Z:148:ARG:HH11	1:a:116:ASN:HD22	1.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:119:VAL:HG12	1:E:120:MET:N	2.28	0.48
1:H:148:ARG:HH11	1:I:116:ASN:ND2	2.01	0.48
1:H:192:ARG:NH2	1:N:51:GLU:OE1	2.46	0.48
1:S:70:ILE:HG23	1:S:98:MET:HE3	1.93	0.48
1:H:31:LEU:HB2	1:H:43:ILE:HD13	1.95	0.48
1:I:140:ARG:HH11	1:I:140:ARG:HG3	1.77	0.48
1:K:190:THR:O	1:K:191:HIS:HD2	1.95	0.48
1:L:29:ILE:HD11	1:L:50:LEU:HD12	1.93	0.48
1:O:49:PHE:CZ	1:P:16:SER:HB2	2.48	0.48
1:O:71:THR:HG21	1:P:94:GLN:HB3	1.94	0.48
1:P:122:HIS:CD2	1:P:122:HIS:C	2.91	0.48
1:V:42:LEU:O	1:V:46:GLN:HG3	2.13	0.48
1:W:70:ILE:O	1:W:71:THR:C	2.55	0.48
1:Z:161:LEU:O	1:Z:161:LEU:HD12	2.13	0.48
1:B:92:MET:HB3	1:B:114:LEU:HD12	1.95	0.48
1:I:190:THR:HG22	1:I:191:HIS:ND1	2.28	0.48
1:J:121:ILE:HD13	1:J:121:ILE:N	2.27	0.48
1:L:166:ARG:HB2	1:L:166:ARG:HH11	1.78	0.48
1:U:174:LEU:HD22	1:U:184:LEU:HD12	1.95	0.48
1:X:172:ARG:HG2	1:X:172:ARG:HH11	1.78	0.48
1:a:53:GLU:O	1:a:54:ASN:HB2	2.14	0.48
1:b:15:ARG:HG2	1:b:16:SER:N	2.28	0.48
1:F:148:ARG:HG2	1:F:148:ARG:HH11	1.78	0.48
1:I:174:LEU:CD1	1:I:184:LEU:HD12	2.43	0.48
1:L:92:MET:HB3	1:L:114:LEU:HD12	1.94	0.48
1:L:174:LEU:HD23	1:L:178:GLU:CB	2.41	0.48
1:N:174:LEU:HD22	1:N:184:LEU:HD12	1.94	0.48
1:O:104:THR:HG22	1:O:184:LEU:HB3	1.95	0.48
1:P:25:LYS:HE3	1:Q:15:ARG:NH2	2.28	0.48
1:X:31:LEU:HD22	1:X:43:ILE:HD12	1.95	0.48
1:Z:29:ILE:CD1	1:Z:46:GLN:HB3	2.43	0.48
1:A:123:GLN:NE2	1:A:146:LYS:NZ	2.62	0.48
1:B:79:THR:O	1:B:83:ILE:HG23	2.14	0.48
1:B:161:LEU:O	1:B:165:GLU:HG3	2.12	0.48
1:J:146:LYS:HG2	1:J:150:ASN:ND2	2.28	0.48
1:O:170:ARG:HH11	1:O:170:ARG:HG2	1.79	0.48
1:P:42:LEU:O	1:P:46:GLN:HG3	2.14	0.48
1:P:106:GLY:O	1:P:111:ARG:HD3	2.13	0.48
1:S:104:THR:HA	1:S:111:ARG:HD2	1.94	0.48
1:Y:119:VAL:HG12	1:Y:120:MET:N	2.29	0.48
1:Z:105:ALA:HA	1:Z:156:HIS:CD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:148:ARG:O	1:E:152:LEU:HD12	2.13	0.48
1:F:150:ASN:O	1:F:151:GLU:C	2.54	0.48
1:F:154:ALA:HA	1:F:164:ILE:HD12	1.95	0.48
1:G:180:VAL:O	1:X:166:ARG:NH2	2.46	0.48
1:H:162:GLU:HA	1:H:165:GLU:HG3	1.96	0.48
1:I:148:ARG:HH11	1:J:116:ASN:ND2	2.10	0.48
1:J:115:PRO:HG3	1:J:190:THR:HG22	1.94	0.48
1:T:31:LEU:HD12	1:T:39:MET:HE1	1.94	0.48
1:V:24:LEU:C	1:V:26:GLU:H	2.22	0.48
1:V:112:PHE:CD2	1:V:189:LEU:HG	2.48	0.48
1:Z:82:PHE:HD1	1:a:190:THR:O	1.96	0.48
1:E:105:ALA:HA	1:E:156:HIS:CD2	2.47	0.48
1:L:47:MET:O	1:L:48:LEU:C	2.55	0.48
1:Q:123:GLN:HE22	1:a:133:THR:H	1.60	0.48
1:b:34:GLN:O	1:b:39:MET:HE3	2.14	0.48
1:E:77:TYR:OH	1:E:156:HIS:HE1	1.96	0.48
1:G:55:PRO:HB2	1:G:84:LYS:HD3	1.95	0.48
1:P:78:ASP:HB3	1:Q:114:LEU:HD12	1.96	0.48
1:V:54:ASN:CG	1:V:57:LYS:HG3	2.38	0.48
1:Z:73:GLY:HA3	1:Z:98:MET:SD	2.54	0.48
1:F:122:HIS:C	1:F:122:HIS:CD2	2.92	0.48
1:M:153:MET:O	1:M:157:THR:HG23	2.14	0.48
1:N:31:LEU:HD13	1:N:39:MET:HE1	1.96	0.48
1:N:173:PHE:O	1:N:174:LEU:HD12	2.14	0.48
1:Q:174:LEU:HD12	1:Q:184:LEU:HD12	1.96	0.48
1:X:166:ARG:HG3	1:X:166:ARG:NH1	2.28	0.48
1:Z:176:ALA:HB1	1:Z:188:ILE:HD12	1.95	0.48
1:a:33:GLY:O	1:a:65:SER:HB2	2.14	0.48
1:E:31:LEU:HD23	1:E:63:ILE:HG12	1.95	0.48
1:E:133:THR:O	1:E:137:ILE:HG13	2.14	0.48
1:F:115:PRO:HG3	1:F:190:THR:OG1	2.13	0.48
1:N:16:SER:C	1:N:18:ASP:H	2.20	0.48
1:P:95:ALA:O	1:P:100:ALA:HB2	2.14	0.48
1:P:122:HIS:CD2	1:P:123:GLN:N	2.82	0.48
1:Y:31:LEU:HA	1:Y:43:ILE:HD11	1.95	0.48
1:A:70:ILE:HD11	1:A:124:PRO:HB3	1.96	0.47
1:M:108:LYS:HD2	1:M:186:ASP:OD1	2.14	0.47
1:O:103:LEU:C	1:O:105:ALA:H	2.21	0.47
1:P:49:PHE:HB2	1:Q:19:ILE:HD11	1.96	0.47
1:P:145:VAL:O	1:P:149:MET:HG2	2.14	0.47
1:R:25:LYS:NZ	1:S:15:ARG:NH2	2.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:193:ASN:HD22	1:R:193:ASN:HA	1.49	0.47
1:W:35:VAL:HA	1:W:39:MET:SD	2.54	0.47
1:W:58:ASP:OD1	1:W:86:ASP:HB2	2.14	0.47
1:X:166:ARG:CG	1:X:166:ARG:NH1	2.75	0.47
1:b:70:ILE:HA	1:b:98:MET:HE3	1.94	0.47
1:G:157:THR:CG2	1:G:184:LEU:HD23	2.44	0.47
1:I:132:ALA:O	1:I:133:THR:C	2.57	0.47
1:K:111:ARG:NH1	1:K:184:LEU:O	2.47	0.47
1:U:173:PHE:C	1:U:174:LEU:HD12	2.38	0.47
1:V:54:ASN:ND2	1:V:57:LYS:HE3	2.29	0.47
1:Y:77:TYR:CD1	1:Y:101:PHE:HE2	2.32	0.47
1:A:62:TYR:HA	1:A:90:ILE:O	2.15	0.47
1:D:122:HIS:C	1:D:122:HIS:CD2	2.93	0.47
1:R:41:ASN:ND2	1:S:32:THR:OG1	2.47	0.47
1:T:26:GLU:OE1	1:T:26:GLU:HA	2.14	0.47
1:T:123:GLN:NE2	1:T:146:LYS:HE3	2.29	0.47
1:W:148:ARG:CD	1:X:116:ASN:HD21	2.27	0.47
1:a:27:ARG:NH2	1:a:57:LYS:O	2.38	0.47
1:A:55:PRO:HB2	1:A:84:LYS:CE	2.45	0.47
1:B:53:GLU:O	1:B:54:ASN:CB	2.58	0.47
1:F:155:LEU:C	1:F:155:LEU:CD2	2.77	0.47
1:H:176:ALA:HB3	1:H:177:PRO:CD	2.35	0.47
1:L:18:ASP:CG	1:L:21:SER:HB2	2.39	0.47
1:M:109:GLY:H	1:M:186:ASP:CG	2.23	0.47
1:O:175:SER:O	1:O:176:ALA:C	2.56	0.47
1:P:88:SER:HB2	1:P:110:LYS:HB3	1.96	0.47
1:T:40:ALA:HA	1:T:76:ILE:HD11	1.97	0.47
1:V:91:CYS:SG	1:V:117:SER:OG	2.67	0.47
1:V:146:LYS:HG2	1:V:150:ASN:ND2	2.29	0.47
1:W:51:GLU:HG3	1:W:85:PRO:HD3	1.94	0.47
1:X:57:LYS:O	1:X:85:PRO:HB3	2.13	0.47
1:Y:141:GLU:OE2	1:Z:118:ARG:HD2	2.14	0.47
1:A:104:THR:O	1:A:156:HIS:HB3	2.14	0.47
1:E:113:CYS:HB2	1:E:185:VAL:HG21	1.96	0.47
1:F:133:THR:HG21	1:G:170:ARG:NE	2.30	0.47
1:H:19:ILE:CG2	1:H:20:TYR:N	2.77	0.47
1:M:124:PRO:HD2	1:M:146:LYS:HG3	1.97	0.47
1:Y:119:VAL:HG11	1:Y:184:LEU:CD1	2.45	0.47
1:A:86:ASP:HB3	1:A:107:ALA:CB	2.45	0.47
1:E:121:ILE:HD12	1:E:168:THR:HG22	1.96	0.47
1:M:164:ILE:HG22	1:M:165:GLU:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:86:ASP:OD2	1:O:110:LYS:NZ	2.43	0.47
1:R:136:GLU:HG3	1:Z:143:LEU:CD1	2.37	0.47
1:T:58:ASP:OD1	1:T:86:ASP:HB2	2.15	0.47
1:V:100:ALA:O	1:V:103:LEU:HB3	2.14	0.47
1:Z:139:ALA:O	1:Z:142:ILE:HG22	2.15	0.47
1:A:171:ASP:O	1:G:137:ILE:HG21	2.14	0.47
1:C:16:SER:C	1:C:18:ASP:N	2.66	0.47
1:E:77:TYR:OH	1:E:152:LEU:HD22	2.14	0.47
1:I:77:TYR:C	1:I:77:TYR:CD2	2.92	0.47
1:K:111:ARG:HG2	1:K:111:ARG:NH1	2.25	0.47
1:K:148:ARG:HH11	1:L:116:ASN:ND2	2.13	0.47
1:L:95:ALA:O	1:L:100:ALA:HB2	2.14	0.47
1:L:113:CYS:HB2	1:L:185:VAL:HG11	1.97	0.47
1:M:114:LEU:CD2	1:M:115:PRO:HD2	2.44	0.47
1:O:18:ASP:HB3	1:O:21:SER:CB	2.41	0.47
1:O:31:LEU:HG	1:O:63:ILE:HG23	1.96	0.47
1:O:88:SER:HA	1:O:110:LYS:O	2.15	0.47
1:O:174:LEU:HD22	1:O:184:LEU:HD11	1.95	0.47
1:Q:49:PHE:CZ	1:R:16:SER:HB2	2.49	0.47
1:T:54:ASN:ND2	1:T:57:LYS:HE2	2.30	0.47
1:U:54:ASN:HD21	1:U:57:LYS:HG3	1.78	0.47
1:V:49:PHE:CE1	1:W:22:ARG:HG2	2.50	0.47
1:V:147:GLY:O	1:V:148:ARG:C	2.57	0.47
1:X:174:LEU:HD12	1:X:174:LEU:N	2.28	0.47
1:Z:148:ARG:HH11	1:a:116:ASN:ND2	2.13	0.47
1:b:104:THR:HB	1:b:184:LEU:HD22	1.97	0.47
1:b:163:GLN:HA	1:b:163:GLN:NE2	2.29	0.47
1:A:114:LEU:O	1:A:115:PRO:C	2.58	0.47
1:B:15:ARG:N	1:B:15:ARG:NH1	2.61	0.47
1:D:84:LYS:N	1:D:85:PRO:HD2	2.30	0.47
1:F:133:THR:N	1:J:123:GLN:HE22	1.98	0.47
1:J:133:THR:O	1:J:136:GLU:HB2	2.14	0.47
1:O:44:VAL:HG11	1:P:92:MET:SD	2.54	0.47
1:O:174:LEU:HD22	1:O:184:LEU:CD1	2.45	0.47
1:Q:120:MET:CE	1:Q:171:ASP:CG	2.88	0.47
1:T:148:ARG:HD2	1:U:116:ASN:HD21	1.80	0.47
1:D:77:TYR:OH	1:D:156:HIS:HE1	1.97	0.47
1:I:111:ARG:HH21	1:I:186:ASP:CG	2.22	0.47
1:O:134:ASP:OD1	1:P:170:ARG:NH1	2.38	0.47
1:U:47:MET:HE2	1:U:80:MET:HG3	1.96	0.47
1:A:123:GLN:HB2	1:A:124:PRO:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:THR:H	1:L:123:GLN:HE22	1.63	0.47
1:F:84:LYS:O	1:F:85:PRO:C	2.58	0.47
1:J:121:ILE:HD12	1:J:174:LEU:HD11	1.95	0.47
1:K:106:GLY:O	1:K:111:ARG:HD2	2.15	0.47
1:O:72:ALA:O	1:O:76:ILE:CD1	2.63	0.47
1:S:114:LEU:HD23	1:S:189:LEU:HB3	1.97	0.47
1:b:104:THR:OG1	1:b:184:LEU:HA	2.14	0.47
1:J:162:GLU:HA	1:U:155:LEU:HD21	1.97	0.46
1:N:83:ILE:HB	1:N:85:PRO:HD2	1.96	0.46
1:T:29:ILE:CD1	1:T:46:GLN:HB3	2.45	0.46
1:U:119:VAL:HG12	1:U:120:MET:N	2.29	0.46
1:V:73:GLY:HA3	1:V:98:MET:CE	2.35	0.46
1:V:107:ALA:O	1:V:110:LYS:N	2.41	0.46
1:a:31:LEU:HA	1:a:43:ILE:HD11	1.98	0.46
1:E:91:CYS:HB2	1:E:103:LEU:CD2	2.45	0.46
1:F:96:ALA:CB	1:F:120:MET:HB3	2.45	0.46
1:K:121:ILE:O	1:K:122:HIS:HB3	2.15	0.46
1:M:108:LYS:HD2	1:M:109:GLY:N	2.30	0.46
1:O:164:ILE:HG22	1:O:165:GLU:N	2.29	0.46
1:P:76:ILE:HG22	1:P:102:LEU:HD22	1.97	0.46
1:Q:162:GLU:O	1:Q:166:ARG:HG3	2.15	0.46
1:S:29:ILE:HD13	1:S:29:ILE:N	2.29	0.46
1:T:18:ASP:OD1	1:T:21:SER:OG	2.31	0.46
1:V:119:VAL:HG12	1:V:120:MET:N	2.29	0.46
1:W:161:LEU:O	1:W:164:ILE:HB	2.15	0.46
1:A:89:THR:HG23	1:A:106:GLY:HA3	1.96	0.46
1:C:24:LEU:C	1:C:26:GLU:N	2.74	0.46
1:C:123:GLN:HE22	1:C:146:LYS:NZ	2.13	0.46
1:I:24:LEU:O	1:I:27:ARG:N	2.38	0.46
1:J:159:GLN:N	1:J:159:GLN:HE21	2.12	0.46
1:Q:142:ILE:HD12	1:Q:142:ILE:O	2.15	0.46
1:R:27:ARG:HG2	1:R:50:LEU:HD22	1.96	0.46
1:S:112:PHE:CD1	1:S:112:PHE:N	2.83	0.46
1:S:148:ARG:HH11	1:T:116:ASN:HD22	1.54	0.46
1:S:175:SER:OG	1:S:178:GLU:HG3	2.15	0.46
1:T:106:GLY:O	1:T:111:ARG:HD3	2.15	0.46
1:U:101:PHE:CE2	1:U:149:MET:HE1	2.50	0.46
1:b:96:ALA:O	1:b:97:SER:HB2	2.15	0.46
1:b:153:MET:O	1:b:157:THR:HG23	2.15	0.46
1:B:31:LEU:HB2	1:B:61:LEU:HD11	1.97	0.46
1:H:97:SER:HG	1:H:122:HIS:CE1	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:78:ASP:HB3	1:U:114:LEU:HB3	1.98	0.46
1:V:22:ARG:HG2	1:b:49:PHE:CE1	2.49	0.46
1:C:34:GLN:O	1:C:39:MET:HE3	2.16	0.46
1:E:140:ARG:CG	1:E:144:LYS:HZ2	2.28	0.46
1:G:119:VAL:HG11	1:G:184:LEU:HD12	1.97	0.46
1:I:29:ILE:HG23	1:I:46:GLN:OE1	2.15	0.46
1:O:114:LEU:CD2	1:U:78:ASP:HB3	2.45	0.46
1:P:174:LEU:HA	1:P:178:GLU:OE1	2.15	0.46
1:R:124:PRO:HB3	1:R:142:ILE:HD11	1.98	0.46
1:T:159:GLN:HB2	1:T:164:ILE:HD13	1.96	0.46
1:X:176:ALA:O	1:X:179:ALA:HB3	2.16	0.46
1:B:146:LYS:HD2	1:N:132:ALA:HB3	1.97	0.46
1:D:127:GLY:HA2	1:L:128:TYR:O	2.15	0.46
1:F:53:GLU:O	1:F:54:ASN:HB2	2.14	0.46
1:K:49:PHE:HB2	1:L:23:LEU:HD21	1.97	0.46
1:K:139:ALA:HA	1:K:142:ILE:CG2	2.46	0.46
1:L:123:GLN:HB3	1:L:168:THR:O	2.16	0.46
1:V:58:ASP:OD1	1:V:86:ASP:HB2	2.16	0.46
1:V:112:PHE:HD2	1:V:189:LEU:HG	1.79	0.46
1:X:97:SER:HG	1:X:122:HIS:CE1	2.33	0.46
1:Y:161:LEU:O	1:Y:161:LEU:HG	2.16	0.46
1:b:101:PHE:O	1:b:104:THR:HG22	2.16	0.46
1:B:77:TYR:OH	1:B:156:HIS:HE1	1.99	0.46
1:C:24:LEU:C	1:C:26:GLU:H	2.23	0.46
1:J:88:SER:OG	1:J:112:PHE:HE1	1.99	0.46
1:K:22:ARG:NH1	1:K:22:ARG:HB3	2.30	0.46
1:L:114:LEU:HD23	1:L:115:PRO:HD3	1.97	0.46
1:O:164:ILE:HD13	1:O:164:ILE:HA	1.78	0.46
1:U:92:MET:HB3	1:U:114:LEU:HD12	1.98	0.46
1:V:114:LEU:HD13	1:b:78:ASP:HB3	1.97	0.46
1:Y:54:ASN:C	1:Y:54:ASN:OD1	2.59	0.46
1:Z:40:ALA:HA	1:Z:76:ILE:HD11	1.98	0.46
1:C:77:TYR:O	1:C:81:GLN:HG2	2.16	0.46
1:J:15:ARG:HA	1:J:22:ARG:HD3	1.97	0.46
1:T:93:GLY:O	1:T:117:SER:HA	2.15	0.46
1:U:106:GLY:O	1:U:111:ARG:HD3	2.15	0.46
1:V:30:PHE:HB3	1:b:41:ASN:HD21	1.80	0.46
1:E:78:ASP:HB3	1:F:114:LEU:HB3	1.97	0.46
1:E:141:GLU:HA	1:E:141:GLU:OE1	2.16	0.46
1:F:157:THR:HG22	1:F:184:LEU:HA	1.98	0.46
1:J:115:PRO:HD3	1:J:189:LEU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:148:ARG:HD3	1:J:151:GLU:OE2	2.16	0.46
1:J:153:MET:O	1:J:157:THR:OG1	2.21	0.46
1:O:167:ASP:OD2	1:O:182:TYR:HE1	1.99	0.46
1:S:98:MET:HA	1:S:98:MET:HE2	1.98	0.46
1:V:157:THR:HG22	1:V:183:GLY:O	2.15	0.46
1:V:160:SER:C	1:V:162:GLU:N	2.72	0.46
1:Z:80:MET:HE3	1:Z:87:VAL:CG1	2.46	0.46
1:Z:81:GLN:OE1	1:Z:81:GLN:HA	2.16	0.46
1:I:148:ARG:NH1	1:I:148:ARG:HG2	2.29	0.46
1:M:35:VAL:HG23	1:M:67:GLY:O	2.16	0.46
1:O:27:ARG:NH2	1:O:50:LEU:HB3	2.31	0.46
1:P:164:ILE:HG22	1:P:165:GLU:N	2.30	0.46
1:R:79:THR:O	1:R:83:ILE:HG12	2.15	0.46
1:S:15:ARG:C	1:S:22:ARG:HD2	2.41	0.46
1:U:180:VAL:HG21	1:U:188:ILE:HG13	1.98	0.46
1:V:43:ILE:O	1:V:47:MET:HG3	2.16	0.46
1:V:161:LEU:HD12	1:V:161:LEU:O	2.15	0.46
1:Z:140:ARG:HG3	1:Z:140:ARG:NH1	2.30	0.46
1:a:23:LEU:HD12	1:a:30:PHE:CE1	2.50	0.46
1:b:86:ASP:OD2	1:b:110:LYS:NZ	2.38	0.46
1:A:98:MET:HE1	1:A:149:MET:HE2	1.98	0.45
1:P:111:ARG:HB3	1:P:185:VAL:HG12	1.97	0.45
1:Q:133:THR:H	1:a:123:GLN:NE2	2.06	0.45
1:W:27:ARG:NH2	1:W:57:LYS:O	2.47	0.45
1:W:28:VAL:HG22	1:W:60:TYR:HB2	1.97	0.45
1:b:77:TYR:CE1	1:b:81:GLN:NE2	2.84	0.45
1:A:141:GLU:OE1	1:A:141:GLU:HA	2.16	0.45
1:D:176:ALA:HB1	1:D:188:ILE:HD12	1.94	0.45
1:F:115:PRO:CG	1:F:190:THR:HA	2.46	0.45
1:G:15:ARG:CG	1:G:16:SER:N	2.78	0.45
1:O:148:ARG:HH11	1:P:116:ASN:ND2	2.14	0.45
1:Q:173:PHE:O	1:Q:174:LEU:HD23	2.16	0.45
1:V:96:ALA:O	1:V:99:GLY:N	2.49	0.45
1:X:124:PRO:HG2	1:X:146:LYS:HA	1.97	0.45
1:F:153:MET:HE1	1:F:184:LEU:HD21	1.98	0.45
1:G:22:ARG:HG3	1:G:22:ARG:NH1	2.31	0.45
1:J:41:ASN:HD22	1:K:32:THR:HG21	1.82	0.45
1:J:162:GLU:O	1:J:166:ARG:HB2	2.16	0.45
1:O:176:ALA:CB	1:O:177:PRO:HD3	2.37	0.45
1:U:133:THR:O	1:U:137:ILE:HG12	2.16	0.45
1:Y:112:PHE:N	1:Y:112:PHE:CD1	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:LEU:HD22	1:B:43:ILE:CD1	2.43	0.45
1:B:159:GLN:OE1	1:B:163:GLN:HG2	2.17	0.45
1:E:128:TYR:CG	1:E:129:GLN:N	2.84	0.45
1:S:159:GLN:OE1	1:S:163:GLN:HG2	2.15	0.45
1:T:29:ILE:CG1	1:T:46:GLN:HB3	2.46	0.45
1:W:96:ALA:O	1:W:97:SER:C	2.59	0.45
1:X:139:ALA:O	1:X:142:ILE:HG22	2.17	0.45
1:Y:148:ARG:HG2	1:Y:148:ARG:NH1	2.31	0.45
1:a:66:PRO:HB3	1:a:94:GLN:HE22	1.81	0.45
1:a:79:THR:O	1:a:83:ILE:HG12	2.16	0.45
1:A:26:GLU:OE1	1:A:26:GLU:HA	2.17	0.45
1:E:140:ARG:HG2	1:E:144:LYS:HZ2	1.81	0.45
1:J:121:ILE:HD12	1:J:174:LEU:CD1	2.46	0.45
1:L:176:ALA:HB3	1:L:177:PRO:HD3	1.98	0.45
1:O:41:ASN:OD1	1:O:41:ASN:C	2.59	0.45
1:P:151:GLU:O	1:P:154:ALA:HB3	2.17	0.45
1:R:64:ASN:HA	1:R:94:GLN:O	2.17	0.45
1:U:84:LYS:HB3	1:U:85:PRO:HD3	1.98	0.45
1:Y:98:MET:HE1	1:Y:149:MET:CE	2.47	0.45
1:b:97:SER:OG	1:b:122:HIS:CE1	2.69	0.45
1:A:107:ALA:O	1:A:108:LYS:C	2.59	0.45
1:A:176:ALA:HB3	1:A:177:PRO:CD	2.47	0.45
1:B:114:LEU:HD23	1:B:114:LEU:HA	1.74	0.45
1:G:123:GLN:HE22	1:G:146:LYS:NZ	2.14	0.45
1:I:190:THR:HG22	1:I:191:HIS:CE1	2.51	0.45
1:K:111:ARG:HB3	1:K:185:VAL:HA	1.97	0.45
1:L:55:PRO:HB2	1:L:84:LYS:HD3	1.99	0.45
1:T:120:MET:HA	1:T:172:ARG:O	2.16	0.45
1:V:92:MET:HG3	1:b:75:SER:HB2	1.98	0.45
1:W:29:ILE:O	1:W:61:LEU:HD12	2.16	0.45
1:A:31:LEU:HD22	1:A:43:ILE:CD1	2.47	0.45
1:E:23:LEU:HD12	1:E:30:PHE:CE1	2.52	0.45
1:I:105:ALA:HA	1:I:156:HIS:CD2	2.51	0.45
1:L:170:ARG:O	1:L:171:ASP:C	2.60	0.45
1:M:34:GLN:HE22	1:M:68:GLY:HA2	1.82	0.45
1:N:70:ILE:HA	1:N:98:MET:HE3	1.98	0.45
1:O:164:ILE:O	1:O:165:GLU:C	2.60	0.45
1:O:191:HIS:CD2	1:O:192:ARG:N	2.85	0.45
1:S:145:VAL:O	1:S:149:MET:HG2	2.17	0.45
1:T:128:TYR:O	1:X:127:GLY:HA2	2.16	0.45
1:D:78:ASP:HB3	1:E:114:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:145:VAL:O	1:J:146:LYS:C	2.59	0.45
1:M:70:ILE:HA	1:M:98:MET:HE3	1.99	0.45
1:N:175:SER:OG	1:N:178:GLU:HG3	2.15	0.45
1:O:160:SER:O	1:O:161:LEU:C	2.60	0.45
1:P:148:ARG:HG2	1:P:148:ARG:NH1	2.32	0.45
1:R:123:GLN:NE2	1:Z:133:THR:H	2.15	0.45
1:T:128:TYR:CG	1:T:129:GLN:N	2.85	0.45
1:V:164:ILE:O	1:V:165:GLU:C	2.60	0.45
1:Y:25:LYS:CD	1:Z:15:ARG:HE	2.30	0.45
1:Z:145:VAL:O	1:Z:149:MET:HG2	2.17	0.45
1:B:19:ILE:HG23	1:B:20:TYR:N	2.32	0.45
1:E:27:ARG:HA	1:E:50:LEU:CD1	2.47	0.45
1:F:51:GLU:HA	1:F:85:PRO:HG2	1.98	0.45
1:G:123:GLN:NE2	1:G:146:LYS:HZ1	2.15	0.45
1:H:27:ARG:NE	1:H:57:LYS:HB3	2.32	0.45
1:I:148:ARG:HH11	1:J:116:ASN:HD21	1.64	0.45
1:J:73:GLY:O	1:J:76:ILE:N	2.45	0.45
1:K:121:ILE:HD11	1:K:172:ARG:HG2	1.99	0.45
1:K:161:LEU:O	1:K:165:GLU:HG3	2.17	0.45
1:P:84:LYS:N	1:P:85:PRO:HD2	2.32	0.45
1:T:176:ALA:N	1:T:177:PRO:CD	2.80	0.45
1:V:27:ARG:HA	1:V:50:LEU:HD13	1.98	0.45
1:a:100:ALA:HB2	1:a:119:VAL:HG13	1.98	0.45
1:a:162:GLU:H	1:a:162:GLU:CD	2.25	0.45
1:B:58:ASP:OD2	1:B:110:LYS:NZ	2.45	0.45
1:G:132:ALA:HB3	1:I:123:GLN:NE2	2.31	0.45
1:J:97:SER:HG	1:J:122:HIS:CE1	2.35	0.45
1:L:98:MET:HE1	1:L:149:MET:HE1	1.99	0.45
1:P:19:ILE:O	1:P:22:ARG:HB3	2.17	0.45
1:U:15:ARG:O	1:U:16:SER:C	2.60	0.45
1:Y:77:TYR:CD1	1:Y:101:PHE:CE2	3.05	0.45
1:Z:58:ASP:CG	1:Z:110:LYS:HZ3	2.25	0.45
1:K:77:TYR:OH	1:K:156:HIS:CE1	2.61	0.44
1:K:160:SER:O	1:K:163:GLN:N	2.50	0.44
1:L:89:THR:OG1	1:L:103:LEU:HD12	2.17	0.44
1:O:139:ALA:O	1:O:142:ILE:HG23	2.16	0.44
1:P:89:THR:HG21	1:P:102:LEU:O	2.17	0.44
1:Q:27:ARG:NH2	1:Q:57:LYS:O	2.46	0.44
1:Q:148:ARG:HH11	1:R:116:ASN:HD22	1.66	0.44
1:S:37:ASP:OD1	1:S:72:ALA:HB2	2.16	0.44
1:W:176:ALA:HB3	1:W:177:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:TYR:CG	1:A:129:GLN:N	2.86	0.44
1:F:174:LEU:HD13	1:F:184:LEU:CD1	2.48	0.44
1:H:50:LEU:HD23	1:H:50:LEU:HA	1.88	0.44
1:L:78:ASP:OD2	1:M:116:ASN:N	2.46	0.44
1:O:94:GLN:HG3	1:O:95:ALA:N	2.31	0.44
1:P:123:GLN:HE21	1:b:132:ALA:N	2.14	0.44
1:Q:170:ARG:O	1:Q:171:ASP:C	2.58	0.44
1:W:28:VAL:HA	1:W:60:TYR:O	2.17	0.44
1:X:31:LEU:CD2	1:X:43:ILE:HD12	2.47	0.44
1:X:157:THR:HA	1:X:183:GLY:O	2.18	0.44
1:Y:103:LEU:HD12	1:Y:103:LEU:C	2.42	0.44
1:C:15:ARG:O	1:C:22:ARG:CD	2.66	0.44
1:M:42:LEU:O	1:M:46:GLN:HG3	2.17	0.44
1:O:82:PHE:HE1	1:P:189:LEU:HB3	1.82	0.44
1:Q:78:ASP:HB3	1:R:114:LEU:HB3	2.00	0.44
1:T:44:VAL:HG22	1:T:79:THR:OG1	2.17	0.44
1:W:58:ASP:CG	1:W:110:LYS:HZ3	2.18	0.44
1:X:92:MET:CB	1:X:114:LEU:HD12	2.47	0.44
1:Z:54:ASN:C	1:Z:56:GLU:H	2.25	0.44
1:B:94:GLN:HA	1:B:118:ARG:O	2.18	0.44
1:J:15:ARG:N	1:J:22:ARG:CB	2.80	0.44
1:J:70:ILE:O	1:J:71:THR:C	2.57	0.44
1:K:39:MET:SD	1:K:39:MET:C	3.00	0.44
1:K:175:SER:O	1:K:176:ALA:C	2.60	0.44
1:O:71:THR:O	1:P:93:GLY:HA2	2.17	0.44
1:P:133:THR:N	1:b:123:GLN:HE22	2.06	0.44
1:Q:180:VAL:HA	1:Q:185:VAL:O	2.18	0.44
1:T:24:LEU:HD23	1:U:16:SER:OG	2.16	0.44
1:W:73:GLY:O	1:W:76:ILE:HB	2.17	0.44
1:Y:175:SER:OG	1:Y:177:PRO:HD2	2.18	0.44
1:A:128:TYR:O	1:H:127:GLY:HA2	2.17	0.44
1:E:15:ARG:HG2	1:E:16:SER:H	1.82	0.44
1:J:120:MET:HA	1:J:172:ARG:O	2.17	0.44
1:J:159:GLN:HB3	1:J:163:GLN:HB3	2.00	0.44
1:K:164:ILE:C	1:K:168:THR:HG1	2.23	0.44
1:L:128:TYR:CG	1:L:129:GLN:N	2.85	0.44
1:N:39:MET:O	1:N:43:ILE:HG12	2.17	0.44
1:O:39:MET:O	1:O:43:ILE:HG13	2.18	0.44
1:Q:168:THR:O	1:Q:169:GLU:C	2.59	0.44
1:S:78:ASP:HB3	1:T:114:LEU:HB3	1.99	0.44
1:U:106:GLY:HA3	1:U:111:ARG:HG2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:74:MET:HE1	1:V:77:TYR:CD2	2.53	0.44
1:b:97:SER:O	1:b:100:ALA:N	2.48	0.44
1:C:70:ILE:HA	1:C:98:MET:HE3	1.98	0.44
1:D:152:LEU:HA	1:D:152:LEU:HD23	1.82	0.44
1:E:78:ASP:OD2	1:F:116:ASN:N	2.46	0.44
1:M:114:LEU:HD23	1:M:115:PRO:HD2	1.99	0.44
1:O:65:SER:O	1:O:95:ALA:HA	2.17	0.44
1:T:147:GLY:O	1:T:148:ARG:C	2.59	0.44
1:W:15:ARG:N	1:W:22:ARG:HB2	2.32	0.44
1:X:121:ILE:HG13	1:X:172:ARG:HB3	2.00	0.44
1:Y:27:ARG:HG2	1:Y:50:LEU:HD22	1.99	0.44
1:Y:29:ILE:HD13	1:Y:46:GLN:HB2	1.99	0.44
1:A:143:LEU:HD23	1:A:143:LEU:HA	1.84	0.44
1:D:31:LEU:HB2	1:D:43:ILE:HD13	1.98	0.44
1:D:167:ASP:OD2	1:D:182:TYR:OH	2.30	0.44
1:F:35:VAL:HG12	1:F:72:ALA:HB3	1.99	0.44
1:G:15:ARG:HG3	1:G:16:SER:N	2.32	0.44
1:J:78:ASP:HB3	1:K:114:LEU:HB3	1.99	0.44
1:J:122:HIS:O	1:J:122:HIS:HD2	2.01	0.44
1:L:27:ARG:HH11	1:L:27:ARG:CG	2.30	0.44
1:N:128:TYR:CG	1:N:129:GLN:N	2.85	0.44
1:P:51:GLU:CD	1:Q:192:ARG:HE	2.25	0.44
1:S:18:ASP:CB	1:S:21:SER:HB2	2.41	0.44
1:U:128:TYR:CD2	1:U:129:GLN:N	2.86	0.44
1:X:84:LYS:N	1:X:85:PRO:CD	2.81	0.44
1:b:47:MET:HE1	1:b:80:MET:CG	2.48	0.44
1:B:119:VAL:HG11	1:B:184:LEU:HD22	1.98	0.44
1:B:168:THR:O	1:B:169:GLU:C	2.61	0.44
1:D:177:PRO:O	1:D:180:VAL:HB	2.18	0.44
1:E:91:CYS:HB2	1:E:103:LEU:HD22	2.00	0.44
1:F:58:ASP:OD2	1:F:110:LYS:CE	2.66	0.44
1:G:123:GLN:HE22	1:I:133:THR:H	1.66	0.44
1:G:123:GLN:HB2	1:G:124:PRO:CD	2.47	0.44
1:J:124:PRO:HG2	1:J:146:LYS:HA	1.99	0.44
1:K:131:GLN:O	1:K:132:ALA:C	2.61	0.44
1:L:122:HIS:CD2	1:L:123:GLN:O	2.71	0.44
1:N:58:ASP:OD1	1:N:86:ASP:HB2	2.17	0.44
1:S:190:THR:O	1:S:191:HIS:C	2.59	0.44
1:V:114:LEU:HB3	1:V:115:PRO:HD2	1.99	0.44
1:W:15:ARG:CG	1:W:16:SER:N	2.72	0.44
1:X:176:ALA:N	1:X:177:PRO:CD	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:77:TYR:OH	1:Y:156:HIS:CE1	2.66	0.44
1:Z:98:MET:HE1	1:Z:149:MET:HE1	2.00	0.44
1:a:31:LEU:HD22	1:a:43:ILE:CD1	2.47	0.44
1:C:132:ALA:HB3	1:M:123:GLN:HE21	1.83	0.44
1:D:86:ASP:OD2	1:D:110:LYS:NZ	2.40	0.44
1:F:96:ALA:O	1:F:97:SER:C	2.61	0.44
1:I:70:ILE:HG12	1:I:98:MET:HE3	1.99	0.44
1:I:89:THR:HB	1:I:103:LEU:HD12	1.98	0.44
1:K:31:LEU:HD13	1:K:43:ILE:HD12	2.00	0.44
1:L:70:ILE:HA	1:L:98:MET:HE3	1.99	0.44
1:L:103:LEU:C	1:L:105:ALA:H	2.26	0.44
1:L:176:ALA:N	1:L:177:PRO:CD	2.81	0.44
1:M:116:ASN:C	1:M:117:SER:O	2.56	0.44
1:O:163:GLN:O	1:O:166:ARG:N	2.51	0.44
1:Y:104:THR:C	1:Y:106:GLY:H	2.25	0.44
1:Y:190:THR:HG22	1:Y:191:HIS:ND1	2.33	0.44
1:a:141:GLU:HG2	1:b:173:PHE:CE2	2.53	0.44
1:a:170:ARG:O	1:a:171:ASP:C	2.60	0.44
1:a:188:ILE:CG2	1:a:189:LEU:N	2.81	0.44
1:B:49:PHE:CE1	1:C:22:ARG:HG2	2.53	0.43
1:F:101:PHE:HZ	1:F:152:LEU:HB2	1.82	0.43
1:G:70:ILE:HA	1:G:98:MET:HE3	2.00	0.43
1:G:86:ASP:OD2	1:G:110:LYS:NZ	2.47	0.43
1:G:170:ARG:O	1:G:171:ASP:C	2.61	0.43
1:I:161:LEU:O	1:I:165:GLU:HG3	2.18	0.43
1:J:157:THR:HB	1:J:159:GLN:HG2	2.00	0.43
1:K:123:GLN:NE2	1:K:146:LYS:NZ	2.66	0.43
1:O:155:LEU:HD23	1:O:155:LEU:C	2.44	0.43
1:P:176:ALA:CB	1:P:177:PRO:HD3	2.27	0.43
1:Q:146:LYS:HD2	1:a:132:ALA:HB3	2.00	0.43
1:Q:148:ARG:HG2	1:Q:148:ARG:NH1	2.33	0.43
1:V:70:ILE:O	1:V:71:THR:C	2.60	0.43
1:V:96:ALA:O	1:V:97:SER:C	2.60	0.43
1:W:170:ARG:NH1	1:W:170:ARG:CG	2.81	0.43
1:Z:190:THR:HG22	1:Z:191:HIS:ND1	2.33	0.43
1:b:91:CYS:SG	1:b:117:SER:HB2	2.58	0.43
1:O:104:THR:CG2	1:O:184:LEU:HB3	2.48	0.43
1:P:114:LEU:O	1:P:115:PRO:C	2.59	0.43
1:Q:65:SER:HA	1:Q:66:PRO:HD3	1.61	0.43
1:S:49:PHE:CZ	1:T:16:SER:HB3	2.53	0.43
1:S:132:ALA:HB3	1:Y:123:GLN:NE2	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:123:GLN:O	1:U:124:PRO:C	2.61	0.43
1:V:24:LEU:CD1	1:V:50:LEU:HD11	2.48	0.43
1:W:114:LEU:HD23	1:W:114:LEU:HA	1.75	0.43
1:X:47:MET:CE	1:X:61:LEU:HD22	2.48	0.43
1:A:122:HIS:CD2	1:A:123:GLN:O	2.71	0.43
1:B:86:ASP:OD2	1:B:110:LYS:NZ	2.51	0.43
1:F:123:GLN:HB2	1:F:124:PRO:CD	2.49	0.43
1:H:22:ARG:HD2	1:H:25:LYS:HE3	2.01	0.43
1:L:91:CYS:CB	1:L:103:LEU:HD22	2.48	0.43
1:L:104:THR:HA	1:L:184:LEU:O	2.18	0.43
1:M:160:SER:C	1:M:162:GLU:N	2.74	0.43
1:P:27:ARG:HG2	1:P:50:LEU:HD22	1.99	0.43
1:U:101:PHE:CZ	1:U:149:MET:HE1	2.53	0.43
1:V:112:PHE:CD1	1:V:112:PHE:N	2.87	0.43
1:a:58:ASP:OD1	1:a:86:ASP:HB2	2.18	0.43
1:C:15:ARG:O	1:C:22:ARG:CG	2.66	0.43
1:C:114:LEU:HD23	1:C:189:LEU:HB2	1.99	0.43
1:F:31:LEU:HA	1:F:43:ILE:HD11	1.99	0.43
1:F:134:ASP:CG	1:G:170:ARG:NH1	2.76	0.43
1:F:153:MET:HB3	1:F:164:ILE:CD1	2.49	0.43
1:F:154:ALA:CA	1:F:164:ILE:HD12	2.49	0.43
1:H:175:SER:O	1:H:176:ALA:C	2.60	0.43
1:O:73:GLY:HA3	1:O:98:MET:HE3	1.99	0.43
1:O:76:ILE:O	1:O:79:THR:HB	2.18	0.43
1:O:140:ARG:HH11	1:O:140:ARG:HG3	1.84	0.43
1:Q:106:GLY:O	1:Q:111:ARG:HD3	2.18	0.43
1:V:18:ASP:OD1	1:V:21:SER:HB2	2.19	0.43
1:V:91:CYS:HB2	1:V:103:LEU:CD2	2.48	0.43
1:V:158:GLY:O	1:V:159:GLN:C	2.59	0.43
1:Y:141:GLU:HG2	1:Z:173:PHE:CE2	2.53	0.43
1:I:115:PRO:HG2	1:I:190:THR:HG23	2.00	0.43
1:J:158:GLY:HA3	1:O:193:ASN:HD21	1.81	0.43
1:P:41:ASN:ND2	1:Q:20:TYR:OH	2.52	0.43
1:R:115:PRO:HD3	1:R:189:LEU:O	2.19	0.43
1:T:160:SER:O	1:T:161:LEU:C	2.62	0.43
1:X:91:CYS:SG	1:X:117:SER:HB2	2.58	0.43
1:Y:49:PHE:O	1:Y:52:ALA:N	2.50	0.43
1:Z:76:ILE:O	1:Z:80:MET:HG3	2.18	0.43
1:C:175:SER:O	1:C:176:ALA:C	2.60	0.43
1:F:96:ALA:HA	1:F:120:MET:O	2.19	0.43
1:H:71:THR:O	1:I:93:GLY:HA2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:165:GLU:O	1:O:166:ARG:C	2.62	0.43
1:U:52:ALA:C	1:U:54:ASN:N	2.76	0.43
1:W:55:PRO:CB	1:W:84:LYS:HG2	2.48	0.43
1:Y:141:GLU:HG2	1:Z:173:PHE:CD2	2.54	0.43
1:b:175:SER:N	1:b:178:GLU:OE1	2.39	0.43
1:C:19:ILE:HG23	1:C:20:TYR:N	2.32	0.43
1:G:131:GLN:HG2	1:I:125:LEU:HD23	2.00	0.43
1:K:97:SER:OG	1:K:122:HIS:CE1	2.72	0.43
1:K:164:ILE:HD13	1:K:182:TYR:OH	2.19	0.43
1:N:102:LEU:O	1:N:105:ALA:HB3	2.18	0.43
1:O:191:HIS:O	1:O:192:ARG:C	2.61	0.43
1:P:29:ILE:HG22	1:P:30:PHE:N	2.33	0.43
1:P:88:SER:HB3	1:P:110:LYS:HB3	2.01	0.43
1:Q:31:LEU:HA	1:Q:43:ILE:HD11	2.00	0.43
1:Q:153:MET:HE1	1:Q:184:LEU:HD21	2.00	0.43
1:R:190:THR:HG22	1:R:191:HIS:ND1	2.33	0.43
1:T:84:LYS:N	1:T:85:PRO:CD	2.80	0.43
1:T:145:VAL:O	1:T:149:MET:HG2	2.19	0.43
1:T:148:ARG:HG2	1:T:148:ARG:HH11	1.84	0.43
1:U:104:THR:HB	1:U:184:LEU:HD23	2.00	0.43
1:A:48:LEU:O	1:A:51:GLU:HB3	2.19	0.43
1:A:73:GLY:HA3	1:A:98:MET:SD	2.59	0.43
1:B:95:ALA:O	1:B:100:ALA:HB2	2.18	0.43
1:B:121:ILE:HD12	1:B:168:THR:HG22	2.00	0.43
1:E:180:VAL:CG2	1:E:187:SER:HA	2.49	0.43
1:G:39:MET:SD	1:G:40:ALA:N	2.91	0.43
1:K:70:ILE:HA	1:K:98:MET:HE3	2.01	0.43
1:M:50:LEU:HD13	1:M:59:ILE:HD12	2.00	0.43
1:O:188:ILE:O	1:O:190:THR:N	2.49	0.43
1:P:101:PHE:O	1:P:101:PHE:CG	2.71	0.43
1:P:128:TYR:CG	1:P:129:GLN:N	2.87	0.43
1:S:39:MET:O	1:S:43:ILE:HG12	2.19	0.43
1:W:151:GLU:O	1:W:154:ALA:HB3	2.19	0.43
1:W:155:LEU:HB3	1:W:156:HIS:H	1.63	0.43
1:X:145:VAL:O	1:X:149:MET:HB2	2.18	0.43
1:Y:41:ASN:OD1	1:Y:41:ASN:O	2.37	0.43
1:A:192:ARG:HG3	1:A:193:ASN:N	2.32	0.43
1:C:97:SER:HG	1:C:122:HIS:CE1	2.37	0.43
1:E:70:ILE:HG12	1:E:98:MET:CE	2.49	0.43
1:G:18:ASP:OD2	1:G:18:ASP:C	2.62	0.43
1:H:148:ARG:HD2	1:H:152:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:86:ASP:OD2	1:M:110:LYS:NZ	2.45	0.43
1:Q:45:ALA:CB	1:R:19:ILE:HD12	2.48	0.43
1:R:84:LYS:CG	1:S:192:ARG:HG2	2.43	0.43
1:R:97:SER:OG	1:R:122:HIS:CE1	2.71	0.43
1:S:41:ASN:ND2	1:T:20:TYR:OH	2.47	0.43
1:V:176:ALA:HB3	1:V:177:PRO:CD	2.36	0.43
1:X:84:LYS:HG3	1:Y:192:ARG:HG2	2.01	0.43
1:A:151:GLU:O	1:A:154:ALA:HB3	2.19	0.43
1:D:176:ALA:CB	1:D:188:ILE:HD11	2.42	0.43
1:I:98:MET:HA	1:I:98:MET:CE	2.45	0.43
1:K:15:ARG:CG	1:K:16:SER:H	2.25	0.43
1:K:163:GLN:NE2	1:K:163:GLN:CA	2.55	0.43
1:L:122:HIS:CD2	1:L:122:HIS:C	2.96	0.43
1:O:161:LEU:O	1:O:165:GLU:HB2	2.19	0.43
1:X:64:ASN:HA	1:X:94:GLN:O	2.18	0.43
1:a:50:LEU:HD12	1:a:59:ILE:HG23	1.99	0.43
1:B:41:ASN:ND2	1:C:20:TYR:OH	2.50	0.42
1:C:123:GLN:NE2	1:C:146:LYS:HZ2	2.15	0.42
1:C:132:ALA:CB	1:M:146:LYS:HD2	2.49	0.42
1:D:78:ASP:O	1:D:82:PHE:N	2.49	0.42
1:D:155:LEU:HD23	1:D:155:LEU:C	2.43	0.42
1:I:55:PRO:O	1:I:84:LYS:HB3	2.19	0.42
1:I:123:GLN:HB2	1:I:124:PRO:CD	2.49	0.42
1:L:101:PHE:O	1:L:105:ALA:HB2	2.19	0.42
1:P:26:GLU:O	1:P:27:ARG:HB2	2.17	0.42
1:T:175:SER:OG	1:T:178:GLU:HG3	2.19	0.42
1:U:68:GLY:O	1:U:69:VAL:C	2.62	0.42
1:W:88:SER:OG	1:W:110:LYS:O	2.32	0.42
1:W:141:GLU:O	1:W:142:ILE:C	2.61	0.42
1:Y:131:GLN:O	1:Y:135:ILE:HG13	2.19	0.42
1:b:161:LEU:O	1:b:164:ILE:HB	2.19	0.42
1:A:19:ILE:HG23	1:A:20:TYR:N	2.34	0.42
1:D:123:GLN:CD	1:L:131:GLN:HB3	2.44	0.42
1:I:31:LEU:CD1	1:I:39:MET:HE1	2.49	0.42
1:L:174:LEU:HD23	1:L:178:GLU:C	2.43	0.42
1:N:113:CYS:O	1:N:188:ILE:HA	2.19	0.42
1:S:153:MET:O	1:S:157:THR:OG1	2.27	0.42
1:U:39:MET:SD	1:U:39:MET:C	3.02	0.42
1:V:22:ARG:O	1:V:25:LYS:HG3	2.19	0.42
1:V:80:MET:CE	1:V:87:VAL:HG11	2.45	0.42
1:X:192:ARG:O	1:X:193:ASN:CG	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:133:THR:O	1:Y:137:ILE:HG13	2.19	0.42
1:b:95:ALA:O	1:b:119:VAL:HA	2.19	0.42
1:B:128:TYR:CG	1:B:129:GLN:N	2.86	0.42
1:D:78:ASP:HB2	1:E:114:LEU:HD13	1.99	0.42
1:E:153:MET:HB2	1:E:164:ILE:HG21	2.01	0.42
1:K:84:LYS:O	1:K:85:PRO:C	2.62	0.42
1:K:97:SER:C	1:K:99:GLY:N	2.76	0.42
1:M:174:LEU:HA	1:M:178:GLU:OE1	2.19	0.42
1:P:108:LYS:HD2	1:P:109:GLY:H	1.83	0.42
1:P:110:LYS:C	1:P:112:PHE:CE1	2.97	0.42
1:R:97:SER:HG	1:R:122:HIS:CE1	2.34	0.42
1:W:170:ARG:HG2	1:W:170:ARG:NH1	2.27	0.42
1:X:49:PHE:HE1	1:Y:22:ARG:HG2	1.84	0.42
1:Z:134:ASP:O	1:Z:138:HIS:HD2	2.03	0.42
1:b:163:GLN:NE2	1:b:166:ARG:NH1	2.67	0.42
1:A:133:THR:O	1:A:136:GLU:HB2	2.20	0.42
1:G:31:LEU:HB2	1:G:43:ILE:HD13	2.01	0.42
1:G:122:HIS:CD2	1:G:122:HIS:C	2.97	0.42
1:H:41:ASN:ND2	1:I:20:TYR:CE1	2.87	0.42
1:J:176:ALA:HB3	1:J:177:PRO:CD	2.49	0.42
1:O:25:LYS:C	1:O:27:ARG:N	2.77	0.42
1:R:49:PHE:HE1	1:S:22:ARG:HD3	1.80	0.42
1:S:148:ARG:HD3	1:S:148:ARG:O	2.19	0.42
1:W:97:SER:O	1:W:98:MET:C	2.63	0.42
1:Z:173:PHE:O	1:Z:174:LEU:HD12	2.19	0.42
1:b:17:PHE:HB3	1:b:18:ASP:H	1.73	0.42
1:b:62:TYR:CD2	1:b:90:ILE:HB	2.55	0.42
1:A:98:MET:HE1	1:A:149:MET:HE1	2.01	0.42
1:A:145:VAL:O	1:A:149:MET:HG2	2.19	0.42
1:B:133:THR:H	1:N:123:GLN:HE22	1.67	0.42
1:F:31:LEU:HD21	1:F:102:LEU:CD1	2.49	0.42
1:G:113:CYS:HB2	1:G:176:ALA:HB1	2.02	0.42
1:G:167:ASP:OD1	1:G:172:ARG:NH2	2.53	0.42
1:I:18:ASP:HB3	1:I:21:SER:HB2	2.02	0.42
1:O:122:HIS:C	1:O:122:HIS:HD2	2.27	0.42
1:O:139:ALA:O	1:O:142:ILE:CG2	2.68	0.42
1:O:176:ALA:CB	1:O:177:PRO:CD	2.95	0.42
1:P:114:LEU:HB3	1:P:115:PRO:HD2	2.01	0.42
1:U:70:ILE:O	1:U:71:THR:C	2.62	0.42
1:V:139:ALA:HA	1:V:142:ILE:HG22	2.02	0.42
1:W:141:GLU:O	1:W:144:LYS:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:82:PHE:O	1:a:83:ILE:C	2.62	0.42
1:b:136:GLU:CG	1:b:140:ARG:NH2	2.83	0.42
1:F:101:PHE:CE1	1:F:149:MET:HE3	2.54	0.42
1:J:161:LEU:HG	1:J:165:GLU:OE1	2.20	0.42
1:L:49:PHE:HE1	1:M:22:ARG:HH11	1.68	0.42
1:M:57:LYS:O	1:M:85:PRO:HB3	2.20	0.42
1:M:77:TYR:OH	1:M:156:HIS:CE1	2.73	0.42
1:N:84:LYS:N	1:N:85:PRO:CD	2.83	0.42
1:N:120:MET:HE2	1:N:120:MET:HB3	1.83	0.42
1:P:169:GLU:HG3	1:V:170:ARG:HH21	1.85	0.42
1:R:142:ILE:HD12	1:R:142:ILE:O	2.19	0.42
1:U:170:ARG:O	1:U:171:ASP:C	2.63	0.42
1:V:70:ILE:HA	1:V:98:MET:HE2	2.01	0.42
1:X:23:LEU:HD12	1:X:30:PHE:CE1	2.55	0.42
1:Y:78:ASP:HB3	1:Z:114:LEU:HD22	2.02	0.42
1:C:77:TYR:CE1	1:C:105:ALA:HB1	2.55	0.42
1:C:132:ALA:HB3	1:M:146:LYS:HD2	2.01	0.42
1:J:154:ALA:HA	1:J:164:ILE:CD1	2.50	0.42
1:O:123:GLN:CD	1:V:131:GLN:HB3	2.45	0.42
1:O:132:ALA:O	1:O:133:THR:C	2.62	0.42
1:P:62:TYR:HA	1:P:90:ILE:O	2.19	0.42
1:P:82:PHE:HA	1:Q:191:HIS:HA	2.02	0.42
1:U:70:ILE:O	1:U:73:GLY:N	2.53	0.42
1:W:143:LEU:HD23	1:W:143:LEU:HA	1.88	0.42
1:X:78:ASP:OD2	1:Y:115:PRO:HD2	2.19	0.42
1:X:164:ILE:HD13	1:X:164:ILE:HA	1.92	0.42
1:Y:51:GLU:HG3	1:Y:85:PRO:HD3	2.01	0.42
1:Y:104:THR:CB	1:Y:184:LEU:CD2	2.97	0.42
1:Y:160:SER:C	1:Y:162:GLU:N	2.77	0.42
1:A:123:GLN:HE22	1:H:133:THR:H	1.68	0.42
1:D:141:GLU:HG2	1:E:173:PHE:CD2	2.54	0.42
1:G:168:THR:O	1:G:169:GLU:C	2.62	0.42
1:K:24:LEU:O	1:K:27:ARG:N	2.48	0.42
1:K:157:THR:HA	1:K:183:GLY:O	2.20	0.42
1:M:84:LYS:N	1:M:85:PRO:CD	2.83	0.42
1:O:39:MET:SD	1:O:39:MET:C	3.03	0.42
1:T:153:MET:HE1	1:T:184:LEU:HD11	2.02	0.42
1:V:123:GLN:C	1:V:124:PRO:O	2.62	0.42
1:Y:166:ARG:NH1	1:Y:166:ARG:CB	2.59	0.42
1:F:39:MET:C	1:F:39:MET:SD	3.03	0.42
1:I:145:VAL:O	1:I:146:LYS:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:175:SER:OG	1:K:177:PRO:HD2	2.20	0.42
1:L:98:MET:HE1	1:L:149:MET:CE	2.50	0.42
1:N:89:THR:HB	1:N:103:LEU:HD12	2.02	0.42
1:O:143:LEU:O	1:O:147:GLY:N	2.48	0.42
1:O:148:ARG:NH1	1:O:148:ARG:HG2	2.35	0.42
1:P:48:LEU:HA	1:P:48:LEU:HD23	1.77	0.42
1:Q:19:ILE:HG23	1:Q:20:TYR:N	2.35	0.42
1:R:61:LEU:O	1:R:89:THR:HA	2.18	0.42
1:R:122:HIS:CD2	1:R:122:HIS:C	2.98	0.42
1:R:192:ARG:HG3	1:R:193:ASN:N	2.33	0.42
1:S:15:ARG:C	1:S:17:PHE:H	2.28	0.42
1:W:91:CYS:CB	1:W:103:LEU:HD13	2.40	0.42
1:X:120:MET:SD	1:X:173:PHE:CE2	3.12	0.42
1:Y:54:ASN:OD1	1:Y:56:GLU:N	2.37	0.42
1:Z:70:ILE:O	1:Z:71:THR:C	2.62	0.42
1:A:175:SER:O	1:A:176:ALA:C	2.63	0.42
1:D:115:PRO:HD3	1:D:189:LEU:O	2.20	0.42
1:F:170:ARG:HG2	1:F:170:ARG:NH1	2.34	0.42
1:H:84:LYS:N	1:H:85:PRO:CD	2.82	0.42
1:J:24:LEU:HD11	1:J:46:GLN:HB3	2.01	0.42
1:J:112:PHE:CD1	1:J:112:PHE:N	2.88	0.42
1:M:25:LYS:C	1:M:27:ARG:H	2.27	0.42
1:P:110:LYS:O	1:P:112:PHE:CE1	2.73	0.42
1:Q:31:LEU:HD22	1:Q:43:ILE:CD1	2.50	0.42
1:U:122:HIS:CD2	1:U:122:HIS:C	2.98	0.42
1:U:123:GLN:HB2	1:U:124:PRO:HD2	2.02	0.42
1:V:41:ASN:ND2	1:W:32:THR:OG1	2.53	0.42
1:X:54:ASN:OD1	1:X:54:ASN:C	2.62	0.42
1:X:88:SER:OG	1:X:110:LYS:O	2.36	0.42
1:Y:54:ASN:ND2	1:Y:57:LYS:HE2	2.35	0.42
1:Y:140:ARG:HG3	1:Y:140:ARG:NH1	2.34	0.42
1:C:57:LYS:O	1:C:85:PRO:HB3	2.20	0.41
1:F:18:ASP:HB3	1:F:21:SER:HB2	2.02	0.41
1:F:96:ALA:O	1:F:99:GLY:N	2.44	0.41
1:K:62:TYR:HA	1:K:90:ILE:O	2.20	0.41
1:M:22:ARG:NH1	1:M:22:ARG:CG	2.81	0.41
1:P:104:THR:HG23	1:P:156:HIS:CB	2.50	0.41
1:Q:97:SER:HG	1:Q:122:HIS:CE1	2.37	0.41
1:S:121:ILE:HD12	1:S:168:THR:CG2	2.41	0.41
1:X:41:ASN:ND2	1:Y:20:TYR:OH	2.52	0.41
1:X:123:GLN:NE2	1:X:146:LYS:NZ	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:123:GLN:HB2	1:Y:124:PRO:CD	2.49	0.41
1:a:141:GLU:HG2	1:b:173:PHE:CZ	2.55	0.41
1:A:62:TYR:HB3	1:A:92:MET:HE2	2.02	0.41
1:B:160:SER:O	1:B:161:LEU:C	2.63	0.41
1:D:188:ILE:HA	1:D:188:ILE:HD13	1.75	0.41
1:I:123:GLN:HB2	1:I:124:PRO:HD2	2.02	0.41
1:J:23:LEU:HD23	1:J:23:LEU:HA	1.80	0.41
1:N:176:ALA:N	1:N:177:PRO:CD	2.83	0.41
1:P:44:VAL:HG13	1:P:79:THR:HG21	2.02	0.41
1:S:150:ASN:O	1:S:151:GLU:C	2.63	0.41
1:W:162:GLU:O	1:W:163:GLN:C	2.63	0.41
1:X:112:PHE:HA	1:X:187:SER:O	2.19	0.41
1:Z:84:LYS:N	1:Z:85:PRO:CD	2.83	0.41
1:a:176:ALA:N	1:a:177:PRO:CD	2.83	0.41
1:a:179:ALA:CB	1:a:185:VAL:HG22	2.49	0.41
1:A:31:LEU:HD22	1:A:43:ILE:HD13	2.02	0.41
1:D:160:SER:OG	1:D:163:GLN:N	2.47	0.41
1:E:97:SER:O	1:E:100:ALA:N	2.52	0.41
1:F:86:ASP:OD2	1:F:110:LYS:NZ	2.52	0.41
1:G:167:ASP:CG	1:G:172:ARG:NH2	2.78	0.41
1:H:176:ALA:CB	1:H:177:PRO:HD3	2.36	0.41
1:O:95:ALA:O	1:O:100:ALA:HB2	2.20	0.41
1:O:174:LEU:HD12	1:O:174:LEU:N	2.36	0.41
1:a:31:LEU:C	1:a:31:LEU:HD12	2.45	0.41
1:b:136:GLU:CG	1:b:140:ARG:HH21	2.33	0.41
1:A:116:ASN:ND2	1:G:148:ARG:HD2	2.35	0.41
1:B:70:ILE:O	1:B:74:MET:HG2	2.19	0.41
1:D:147:GLY:O	1:D:151:GLU:HG3	2.20	0.41
1:J:121:ILE:CD1	1:J:172:ARG:HB3	2.51	0.41
1:L:151:GLU:O	1:L:154:ALA:HB3	2.19	0.41
1:P:39:MET:SD	1:P:40:ALA:N	2.93	0.41
1:U:19:ILE:CG2	1:U:20:TYR:N	2.83	0.41
1:V:50:LEU:HD23	1:V:50:LEU:HA	1.69	0.41
1:V:91:CYS:HB2	1:V:103:LEU:HD22	2.03	0.41
1:Y:39:MET:C	1:Y:39:MET:SD	3.04	0.41
1:a:190:THR:HG22	1:a:191:HIS:CE1	2.54	0.41
1:A:91:CYS:HB2	1:A:103:LEU:CD2	2.50	0.41
1:D:127:GLY:CA	1:L:128:TYR:O	2.69	0.41
1:F:134:ASP:OD2	1:G:170:ARG:NH1	2.52	0.41
1:L:141:GLU:OE1	1:L:141:GLU:HA	2.20	0.41
1:O:152:LEU:HD11	1:P:116:ASN:ND2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:127:GLY:CA	1:Z:128:TYR:O	2.68	0.41
1:R:131:GLN:O	1:R:132:ALA:C	2.62	0.41
1:T:33:GLY:C	1:T:66:PRO:HD2	2.46	0.41
1:X:23:LEU:O	1:X:26:GLU:HB2	2.20	0.41
1:b:36:GLU:O	1:b:39:MET:HG3	2.21	0.41
1:E:104:THR:OG1	1:E:184:LEU:HD23	2.21	0.41
1:L:84:LYS:HB3	1:L:85:PRO:HD3	2.02	0.41
1:N:104:THR:HG23	1:N:156:HIS:CB	2.51	0.41
1:O:62:TYR:HB3	1:O:92:MET:HE2	2.03	0.41
1:O:155:LEU:HD23	1:O:155:LEU:O	2.20	0.41
1:O:180:VAL:O	1:O:183:GLY:N	2.36	0.41
1:Y:71:THR:HG21	1:Z:94:GLN:HB3	2.03	0.41
1:Z:19:ILE:HG22	1:Z:20:TYR:N	2.35	0.41
1:A:166:ARG:HG3	1:A:166:ARG:HH11	1.84	0.41
1:B:191:HIS:O	1:B:192:ARG:C	2.61	0.41
1:E:119:VAL:CG1	1:E:120:MET:N	2.83	0.41
1:G:15:ARG:C	1:G:17:PHE:H	2.28	0.41
1:H:22:ARG:HG2	1:N:49:PHE:HE1	1.85	0.41
1:L:17:PHE:HD1	1:L:17:PHE:HA	1.62	0.41
1:M:34:GLN:HA	1:M:34:GLN:NE2	2.36	0.41
1:M:62:TYR:CE1	1:M:90:ILE:HD12	2.56	0.41
1:R:40:ALA:HA	1:R:76:ILE:HD11	2.01	0.41
1:R:50:LEU:HD23	1:R:50:LEU:HA	1.90	0.41
1:U:31:LEU:HD22	1:U:43:ILE:HD12	2.03	0.41
1:V:32:THR:HG22	1:V:33:GLY:N	2.36	0.41
1:X:78:ASP:OD2	1:Y:114:LEU:HB3	2.20	0.41
1:b:145:VAL:O	1:b:149:MET:HG2	2.21	0.41
1:b:163:GLN:NE2	1:b:166:ARG:HH12	2.18	0.41
1:A:116:ASN:ND2	1:G:152:LEU:HD11	2.35	0.41
1:A:118:ARG:HH11	1:G:145:VAL:HG21	1.85	0.41
1:B:57:LYS:O	1:B:85:PRO:HB3	2.20	0.41
1:F:123:GLN:NE2	1:J:133:THR:H	2.19	0.41
1:G:113:CYS:SG	1:G:185:VAL:HG11	2.61	0.41
1:K:140:ARG:O	1:K:143:LEU:HB2	2.20	0.41
1:K:165:GLU:HG3	1:K:165:GLU:H	1.65	0.41
1:O:70:ILE:HA	1:O:98:MET:CE	2.51	0.41
1:O:76:ILE:HD12	1:O:76:ILE:N	2.36	0.41
1:O:82:PHE:CE1	1:P:189:LEU:HB3	2.55	0.41
1:O:84:LYS:CG	1:P:192:ARG:O	2.69	0.41
1:O:136:GLU:HG3	1:V:143:LEU:HD11	2.02	0.41
1:P:178:GLU:O	1:P:182:TYR:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:72:ALA:O	1:Q:75:SER:HB3	2.21	0.41
1:R:42:LEU:O	1:R:46:GLN:HG3	2.21	0.41
1:R:111:ARG:HE	1:R:111:ARG:HB2	1.75	0.41
1:R:153:MET:HB2	1:R:164:ILE:HG21	2.02	0.41
1:S:154:ALA:O	1:S:155:LEU:C	2.63	0.41
1:T:73:GLY:HA3	1:T:98:MET:SD	2.61	0.41
1:V:77:TYR:OH	1:V:156:HIS:CE1	2.67	0.41
1:A:62:TYR:CE1	1:A:90:ILE:HD12	2.56	0.41
1:A:109:GLY:H	1:A:186:ASP:CG	2.29	0.41
1:B:169:GLU:O	1:N:131:GLN:NE2	2.53	0.41
1:C:39:MET:O	1:C:43:ILE:HG12	2.21	0.41
1:E:158:GLY:C	1:E:159:GLN:O	2.61	0.41
1:E:170:ARG:O	1:E:171:ASP:C	2.62	0.41
1:G:162:GLU:HA	1:G:165:GLU:OE1	2.21	0.41
1:I:83:ILE:HD12	1:I:85:PRO:HG2	2.01	0.41
1:I:91:CYS:SG	1:I:95:ALA:HB2	2.61	0.41
1:K:51:GLU:OE1	1:K:83:ILE:HG22	2.21	0.41
1:K:104:THR:HA	1:K:111:ARG:NH1	2.35	0.41
1:K:176:ALA:N	1:K:177:PRO:CD	2.83	0.41
1:L:122:HIS:HB3	1:L:171:ASP:HA	2.02	0.41
1:M:27:ARG:HG2	1:M:50:LEU:HD22	2.03	0.41
1:N:55:PRO:HA	1:N:85:PRO:HG3	2.02	0.41
1:O:81:GLN:OE1	1:O:81:GLN:CA	2.68	0.41
1:P:157:THR:HB	1:P:159:GLN:HG2	2.03	0.41
1:R:127:GLY:HA2	1:Z:128:TYR:O	2.21	0.41
1:W:102:LEU:O	1:W:105:ALA:HB3	2.21	0.41
1:Y:53:GLU:O	1:Y:54:ASN:CB	2.68	0.41
1:a:41:ASN:ND2	1:b:20:TYR:OH	2.54	0.41
1:a:77:TYR:O	1:a:80:MET:HB2	2.20	0.41
1:a:159:GLN:HB2	1:a:164:ILE:HD11	2.01	0.41
1:b:174:LEU:HA	1:b:178:GLU:OE1	2.20	0.41
1:B:27:ARG:NE	1:B:57:LYS:HB2	2.36	0.41
1:F:19:ILE:HG23	1:F:20:TYR:N	2.36	0.41
1:I:60:TYR:CD2	1:I:88:SER:HB3	2.55	0.41
1:J:35:VAL:N	1:J:67:GLY:O	2.51	0.41
1:K:176:ALA:O	1:K:179:ALA:HB3	2.21	0.41
1:P:83:ILE:HD12	1:P:85:PRO:HG2	2.03	0.41
1:P:123:GLN:HE21	1:b:132:ALA:CB	2.34	0.41
1:Q:123:GLN:HE21	1:Q:123:GLN:HB2	1.75	0.41
1:S:128:TYR:CG	1:S:129:GLN:N	2.89	0.41
1:V:44:VAL:HG22	1:V:79:THR:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:64:ASN:HB2	1:Z:92:MET:O	2.20	0.41
1:b:191:HIS:O	1:b:192:ARG:C	2.61	0.41
1:C:160:SER:HG	1:C:163:GLN:H	1.67	0.40
1:D:134:ASP:OD1	1:E:170:ARG:NH1	2.54	0.40
1:E:31:LEU:HD13	1:E:43:ILE:HD13	2.03	0.40
1:F:133:THR:HG21	1:G:170:ARG:CD	2.51	0.40
1:I:100:ALA:O	1:I:103:LEU:HB3	2.21	0.40
1:I:148:ARG:HH11	1:I:148:ARG:HG2	1.86	0.40
1:J:22:ARG:HA	1:J:22:ARG:HD2	1.88	0.40
1:K:122:HIS:C	1:K:122:HIS:HD2	2.26	0.40
1:K:122:HIS:CD2	1:K:123:GLN:O	2.74	0.40
1:L:114:LEU:HB3	1:L:115:PRO:HD2	2.03	0.40
1:M:22:ARG:NH1	1:M:22:ARG:HG3	2.36	0.40
1:Q:140:ARG:HH11	1:Q:140:ARG:CG	2.34	0.40
1:S:175:SER:O	1:S:176:ALA:C	2.62	0.40
1:W:26:GLU:O	1:W:27:ARG:HB2	2.21	0.40
1:W:180:VAL:C	1:W:182:TYR:H	2.30	0.40
1:a:97:SER:C	1:a:99:GLY:N	2.79	0.40
1:a:173:PHE:C	1:a:174:LEU:HD12	2.45	0.40
1:A:176:ALA:N	1:A:177:PRO:HD2	2.36	0.40
1:D:173:PHE:C	1:D:174:LEU:HD12	2.45	0.40
1:H:170:ARG:O	1:H:171:ASP:C	2.64	0.40
1:M:97:SER:C	1:M:99:GLY:N	2.77	0.40
1:O:96:ALA:O	1:O:99:GLY:N	2.44	0.40
1:R:31:LEU:HA	1:R:43:ILE:HD11	2.03	0.40
1:R:83:ILE:HD12	1:R:85:PRO:HG2	2.03	0.40
1:V:157:THR:HA	1:V:183:GLY:O	2.20	0.40
1:W:176:ALA:O	1:W:177:PRO:C	2.64	0.40
1:X:75:SER:OG	1:Y:92:MET:HE3	2.21	0.40
1:a:122:HIS:CD2	1:a:123:GLN:O	2.74	0.40
1:D:151:GLU:HA	1:D:161:LEU:HD13	2.03	0.40
1:E:170:ARG:NH1	1:E:170:ARG:HG2	2.35	0.40
1:F:91:CYS:HB2	1:F:103:LEU:HD21	2.03	0.40
1:L:31:LEU:C	1:L:31:LEU:CD1	2.95	0.40
1:L:103:LEU:C	1:L:105:ALA:N	2.79	0.40
1:L:153:MET:HE1	1:L:184:LEU:HD21	2.03	0.40
1:M:157:THR:HA	1:M:183:GLY:O	2.21	0.40
1:O:154:ALA:O	1:O:158:GLY:N	2.48	0.40
1:S:122:HIS:CD2	1:S:123:GLN:O	2.74	0.40
1:W:112:PHE:HA	1:W:187:SER:O	2.21	0.40
1:X:84:LYS:HG3	1:Y:192:ARG:CG	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:164:ILE:HD13	1:Y:164:ILE:HA	1.90	0.40
1:Z:23:LEU:HD12	1:Z:30:PHE:HE1	1.87	0.40
1:E:27:ARG:HA	1:E:50:LEU:HD11	2.03	0.40
1:J:66:PRO:HB3	1:J:94:GLN:NE2	2.36	0.40
1:O:74:MET:O	1:O:75:SER:C	2.63	0.40
1:O:96:ALA:O	1:O:97:SER:C	2.64	0.40
1:R:141:GLU:OE1	1:R:141:GLU:HA	2.22	0.40
1:T:44:VAL:HG11	1:U:92:MET:SD	2.62	0.40
1:T:61:LEU:HD23	1:T:89:THR:HG22	2.04	0.40
1:U:96:ALA:O	1:U:99:GLY:N	2.49	0.40
1:V:170:ARG:HG2	1:V:170:ARG:HH11	1.86	0.40
1:Y:160:SER:C	1:Y:162:GLU:H	2.29	0.40
1:D:186:ASP:O	1:D:187:SER:HB2	2.22	0.40
1:E:164:ILE:O	1:E:168:THR:HG23	2.22	0.40
1:J:123:GLN:HA	1:J:124:PRO:HD3	1.90	0.40
1:L:77:TYR:O	1:L:78:ASP:C	2.64	0.40
1:O:23:LEU:HD23	1:O:23:LEU:HA	1.85	0.40
1:P:89:THR:HB	1:P:103:LEU:HD12	2.03	0.40
1:Q:141:GLU:HG2	1:R:173:PHE:CG	2.57	0.40
1:S:98:MET:HE1	1:S:149:MET:CE	2.51	0.40
1:V:74:MET:SD	1:V:98:MET:HE1	2.62	0.40
1:X:84:LYS:HB2	1:X:85:PRO:HD3	2.04	0.40
1:Z:54:ASN:HD22	1:Z:57:LYS:HZ1	1.69	0.40
1:Z:78:ASP:HB3	1:a:114:LEU:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	177/193 (92%)	167 (94%)	8 (4%)	2 (1%)	11 25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	177/193 (92%)	166 (94%)	10 (6%)	1 (1%)	21	42
1	C	177/193 (92%)	162 (92%)	14 (8%)	1 (1%)	21	42
1	D	177/193 (92%)	165 (93%)	11 (6%)	1 (1%)	21	42
1	E	177/193 (92%)	165 (93%)	10 (6%)	2 (1%)	11	25
1	F	177/193 (92%)	163 (92%)	12 (7%)	2 (1%)	11	25
1	G	177/193 (92%)	161 (91%)	16 (9%)	0	100	100
1	H	177/193 (92%)	170 (96%)	7 (4%)	0	100	100
1	I	177/193 (92%)	162 (92%)	14 (8%)	1 (1%)	21	42
1	J	177/193 (92%)	162 (92%)	12 (7%)	3 (2%)	7	15
1	K	177/193 (92%)	156 (88%)	18 (10%)	3 (2%)	7	15
1	L	177/193 (92%)	160 (90%)	16 (9%)	1 (1%)	21	42
1	M	177/193 (92%)	167 (94%)	10 (6%)	0	100	100
1	N	177/193 (92%)	163 (92%)	14 (8%)	0	100	100
1	O	177/193 (92%)	144 (81%)	22 (12%)	11 (6%)	1	1
1	P	177/193 (92%)	154 (87%)	20 (11%)	3 (2%)	7	15
1	Q	177/193 (92%)	166 (94%)	10 (6%)	1 (1%)	21	42
1	R	177/193 (92%)	171 (97%)	6 (3%)	0	100	100
1	S	177/193 (92%)	158 (89%)	16 (9%)	3 (2%)	7	15
1	T	177/193 (92%)	162 (92%)	13 (7%)	2 (1%)	11	25
1	U	177/193 (92%)	157 (89%)	18 (10%)	2 (1%)	11	25
1	V	177/193 (92%)	154 (87%)	19 (11%)	4 (2%)	5	9
1	W	177/193 (92%)	157 (89%)	16 (9%)	4 (2%)	5	9
1	X	177/193 (92%)	162 (92%)	14 (8%)	1 (1%)	21	42
1	Y	177/193 (92%)	161 (91%)	14 (8%)	2 (1%)	11	25
1	Z	177/193 (92%)	164 (93%)	10 (6%)	3 (2%)	7	15
1	a	177/193 (92%)	168 (95%)	5 (3%)	4 (2%)	5	9
1	b	177/193 (92%)	161 (91%)	13 (7%)	3 (2%)	7	15
All	All	4956/5404 (92%)	4528 (91%)	368 (7%)	60 (1%)	10	23

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	SER

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Mol	Chain	Res	Type
1	B	54	ASN
1	J	16	SER
1	J	155	LEU
1	O	54	ASN
1	O	189	LEU
1	O	190	THR
1	P	122	HIS
1	Q	16	SER
1	S	191	HIS
1	V	124	PRO
1	W	155	LEU
1	W	156	HIS
1	b	17	PHE
1	b	54	ASN
1	C	16	SER
1	D	16	SER
1	E	19	ILE
1	F	113	CYS
1	J	156	HIS
1	K	155	LEU
1	L	175	SER
1	O	161	LEU
1	O	167	ASP
1	O	192	ARG
1	S	162	GLU
1	T	16	SER
1	T	17	PHE
1	X	17	PHE
1	a	16	SER
1	a	83	ILE
1	K	34	GLN
1	K	159	GLN
1	U	54	ASN
1	Y	54	ASN
1	a	82	PHE
1	b	167	ASP
1	O	77	TYR
1	O	178	GLU
1	P	192	ARG
1	U	192	ARG
1	A	115	PRO
1	E	54	ASN

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Mol	Chain	Res	Type
1	S	98	MET
1	Y	16	SER
1	Z	54	ASN
1	F	54	ASN
1	I	137	ILE
1	O	95	ALA
1	O	97	SER
1	V	54	ASN
1	W	70	ILE
1	Z	122	HIS
1	V	55	PRO
1	Z	115	PRO
1	O	76	ILE
1	V	66	PRO
1	a	54	ASN
1	P	19	ILE
1	W	177	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	151/162 (93%)	142 (94%)	9 (6%)	17	37
1	B	151/162 (93%)	143 (95%)	8 (5%)	20	43
1	C	151/162 (93%)	143 (95%)	8 (5%)	20	43
1	D	151/162 (93%)	141 (93%)	10 (7%)	15	34
1	E	151/162 (93%)	144 (95%)	7 (5%)	24	49
1	F	151/162 (93%)	142 (94%)	9 (6%)	17	37
1	G	151/162 (93%)	145 (96%)	6 (4%)	28	55
1	H	151/162 (93%)	147 (97%)	4 (3%)	40	68
1	I	151/162 (93%)	144 (95%)	7 (5%)	24	49
1	J	151/162 (93%)	134 (89%)	17 (11%)	5	12
1	K	151/162 (93%)	136 (90%)	15 (10%)	7	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	151/162 (93%)	144 (95%)	7 (5%)	24	49
1	M	151/162 (93%)	139 (92%)	12 (8%)	11	26
1	N	151/162 (93%)	144 (95%)	7 (5%)	24	49
1	O	151/162 (93%)	137 (91%)	14 (9%)	8	18
1	P	151/162 (93%)	141 (93%)	10 (7%)	15	34
1	Q	151/162 (93%)	143 (95%)	8 (5%)	20	43
1	R	151/162 (93%)	142 (94%)	9 (6%)	17	37
1	S	151/162 (93%)	141 (93%)	10 (7%)	15	34
1	T	151/162 (93%)	144 (95%)	7 (5%)	24	49
1	U	151/162 (93%)	143 (95%)	8 (5%)	20	43
1	V	151/162 (93%)	139 (92%)	12 (8%)	11	26
1	W	151/162 (93%)	142 (94%)	9 (6%)	17	37
1	X	151/162 (93%)	138 (91%)	13 (9%)	10	22
1	Y	151/162 (93%)	140 (93%)	11 (7%)	13	29
1	Z	151/162 (93%)	136 (90%)	15 (10%)	7	16
1	a	151/162 (93%)	142 (94%)	9 (6%)	17	37
1	b	151/162 (93%)	142 (94%)	9 (6%)	17	37
All	All	4228/4536 (93%)	3958 (94%)	270 (6%)	16	35

All (270) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLU
1	A	31	LEU
1	A	34	GLN
1	A	94	GLN
1	A	113	CYS
1	A	122	HIS
1	A	136	GLU
1	A	153	MET
1	A	184	LEU
1	B	15	ARG
1	B	22	ARG
1	B	31	LEU
1	B	56	GLU
1	B	113	CYS

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Mol	Chain	Res	Type
1	B	151	GLU
1	B	155	LEU
1	B	184	LEU
1	C	22	ARG
1	C	25	LYS
1	C	31	LEU
1	C	113	CYS
1	C	118	ARG
1	C	142	ILE
1	C	172	ARG
1	C	184	LEU
1	D	19	ILE
1	D	31	LEU
1	D	34	GLN
1	D	42	LEU
1	D	56	GLU
1	D	81	GLN
1	D	142	ILE
1	D	166	ARG
1	D	174	LEU
1	D	189	LEU
1	E	16	SER
1	E	56	GLU
1	E	84	LYS
1	E	86	ASP
1	E	113	CYS
1	E	123	GLN
1	E	174	LEU
1	F	31	LEU
1	F	56	GLU
1	F	65	SER
1	F	113	CYS
1	F	155	LEU
1	F	160	SER
1	F	166	ARG
1	F	174	LEU
1	F	193	ASN
1	G	22	ARG
1	G	31	LEU
1	G	34	GLN
1	G	114	LEU
1	G	162	GLU

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Mol	Chain	Res	Type
1	G	174	LEU
1	H	31	LEU
1	H	56	GLU
1	H	174	LEU
1	H	184	LEU
1	I	19	ILE
1	I	21	SER
1	I	23	LEU
1	I	31	LEU
1	I	56	GLU
1	I	113	CYS
1	I	168	THR
1	J	19	ILE
1	J	31	LEU
1	J	39	MET
1	J	42	LEU
1	J	53	GLU
1	J	56	GLU
1	J	108	LYS
1	J	112	PHE
1	J	121	ILE
1	J	133	THR
1	J	136	GLU
1	J	142	ILE
1	J	159	GLN
1	J	162	GLU
1	J	172	ARG
1	J	180	VAL
1	J	184	LEU
1	K	17	PHE
1	K	44	VAL
1	K	111	ARG
1	K	113	CYS
1	K	115	PRO
1	K	122	HIS
1	K	123	GLN
1	K	136	GLU
1	K	137	ILE
1	K	155	LEU
1	K	162	GLU
1	K	163	GLN
1	K	166	ARG

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Mol	Chain	Res	Type
1	K	180	VAL
1	K	181	GLU
1	L	17	PHE
1	L	19	ILE
1	L	31	LEU
1	L	56	GLU
1	L	91	CYS
1	L	155	LEU
1	L	174	LEU
1	M	19	ILE
1	M	22	ARG
1	M	31	LEU
1	M	34	GLN
1	M	56	GLU
1	M	113	CYS
1	M	124	PRO
1	M	136	GLU
1	M	161	LEU
1	M	172	ARG
1	M	178	GLU
1	M	190	THR
1	N	26	GLU
1	N	31	LEU
1	N	104	THR
1	N	113	CYS
1	N	123	GLN
1	N	172	ARG
1	N	184	LEU
1	O	17	PHE
1	O	19	ILE
1	O	31	LEU
1	O	79	THR
1	O	81	GLN
1	O	87	VAL
1	O	114	LEU
1	O	115	PRO
1	O	122	HIS
1	O	164	ILE
1	O	167	ASP
1	O	177	PRO
1	O	189	LEU
1	O	193	ASN

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Mol	Chain	Res	Type
1	P	31	LEU
1	P	56	GLU
1	P	66	PRO
1	P	81	GLN
1	P	104	THR
1	P	112	PHE
1	P	164	ILE
1	P	166	ARG
1	P	178	GLU
1	P	185	VAL
1	Q	25	LYS
1	Q	31	LEU
1	Q	56	GLU
1	Q	114	LEU
1	Q	118	ARG
1	Q	123	GLN
1	Q	155	LEU
1	Q	186	ASP
1	R	19	ILE
1	R	31	LEU
1	R	56	GLU
1	R	113	CYS
1	R	118	ARG
1	R	120	MET
1	R	136	GLU
1	R	184	LEU
1	R	193	ASN
1	S	15	ARG
1	S	29	ILE
1	S	31	LEU
1	S	56	GLU
1	S	94	GLN
1	S	122	HIS
1	S	136	GLU
1	S	161	LEU
1	S	163	GLN
1	S	189	LEU
1	T	22	ARG
1	T	44	VAL
1	T	155	LEU
1	T	164	ILE
1	T	168	THR

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Mol	Chain	Res	Type
1	T	172	ARG
1	T	184	LEU
1	U	31	LEU
1	U	47	MET
1	U	81	GLN
1	U	91	CYS
1	U	108	LYS
1	U	162	GLU
1	U	165	GLU
1	U	190	THR
1	V	19	ILE
1	V	25	LYS
1	V	44	VAL
1	V	47	MET
1	V	81	GLN
1	V	94	GLN
1	V	118	ARG
1	V	142	ILE
1	V	155	LEU
1	V	161	LEU
1	V	165	GLU
1	V	184	LEU
1	W	31	LEU
1	W	66	PRO
1	W	103	LEU
1	W	121	ILE
1	W	170	ARG
1	W	175	SER
1	W	181	GLU
1	W	184	LEU
1	W	192	ARG
1	X	15	ARG
1	X	31	LEU
1	X	43	ILE
1	X	44	VAL
1	X	56	GLU
1	X	71	THR
1	X	113	CYS
1	X	149	MET
1	X	165	GLU
1	X	166	ARG
1	X	167	ASP

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Mol	Chain	Res	Type
1	X	186	ASP
1	X	190	THR
1	Y	31	LEU
1	Y	34	GLN
1	Y	88	SER
1	Y	92	MET
1	Y	94	GLN
1	Y	104	THR
1	Y	112	PHE
1	Y	118	ARG
1	Y	155	LEU
1	Y	162	GLU
1	Y	184	LEU
1	Z	17	PHE
1	Z	19	ILE
1	Z	22	ARG
1	Z	31	LEU
1	Z	56	GLU
1	Z	70	ILE
1	Z	81	GLN
1	Z	114	LEU
1	Z	123	GLN
1	Z	129	GLN
1	Z	136	GLU
1	Z	155	LEU
1	Z	160	SER
1	Z	184	LEU
1	Z	185	VAL
1	a	19	ILE
1	a	22	ARG
1	a	31	LEU
1	a	56	GLU
1	a	65	SER
1	a	71	THR
1	a	122	HIS
1	a	133	THR
1	a	184	LEU
1	b	19	ILE
1	b	31	LEU
1	b	34	GLN
1	b	81	GLN
1	b	91	CYS

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Mol	Chain	Res	Type
1	b	136	GLU
1	b	148	ARG
1	b	172	ARG
1	b	191	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (172) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	116	ASN
1	A	122	HIS
1	A	123	GLN
1	A	156	HIS
1	A	159	GLN
1	B	123	GLN
1	B	156	HIS
1	B	191	HIS
1	C	41	ASN
1	C	116	ASN
1	C	123	GLN
1	C	129	GLN
1	C	156	HIS
1	C	163	GLN
1	D	34	GLN
1	D	41	ASN
1	D	123	GLN
1	D	156	HIS
1	E	34	GLN
1	E	116	ASN
1	E	123	GLN
1	E	156	HIS
1	E	163	GLN
1	E	191	HIS
1	F	116	ASN
1	F	123	GLN
1	F	129	GLN
1	F	156	HIS
1	F	163	GLN
1	G	34	GLN
1	G	116	ASN
1	G	123	GLN
1	G	156	HIS

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Mol	Chain	Res	Type
1	H	38	HIS
1	H	116	ASN
1	H	122	HIS
1	H	123	GLN
1	H	156	HIS
1	I	41	ASN
1	I	46	GLN
1	I	116	ASN
1	I	123	GLN
1	I	156	HIS
1	I	193	ASN
1	J	34	GLN
1	J	41	ASN
1	J	94	GLN
1	J	116	ASN
1	J	123	GLN
1	J	150	ASN
1	J	156	HIS
1	J	159	GLN
1	J	163	GLN
1	K	34	GLN
1	K	41	ASN
1	K	46	GLN
1	K	116	ASN
1	K	123	GLN
1	K	156	HIS
1	K	163	GLN
1	K	191	HIS
1	L	38	HIS
1	L	41	ASN
1	L	46	GLN
1	L	123	GLN
1	L	156	HIS
1	L	163	GLN
1	M	34	GLN
1	M	41	ASN
1	M	116	ASN
1	M	123	GLN
1	M	163	GLN
1	M	191	HIS
1	N	34	GLN
1	N	123	GLN

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Mol	Chain	Res	Type
1	N	129	GLN
1	N	156	HIS
1	O	34	GLN
1	O	41	ASN
1	O	122	HIS
1	O	123	GLN
1	O	129	GLN
1	O	156	HIS
1	O	159	GLN
1	O	163	GLN
1	O	191	HIS
1	O	193	ASN
1	P	41	ASN
1	P	94	GLN
1	P	116	ASN
1	P	122	HIS
1	P	123	GLN
1	P	156	HIS
1	P	163	GLN
1	Q	34	GLN
1	Q	41	ASN
1	Q	116	ASN
1	Q	123	GLN
1	Q	129	GLN
1	Q	156	HIS
1	Q	163	GLN
1	R	41	ASN
1	R	46	GLN
1	R	116	ASN
1	R	123	GLN
1	R	156	HIS
1	R	193	ASN
1	S	34	GLN
1	S	38	HIS
1	S	41	ASN
1	S	116	ASN
1	S	122	HIS
1	S	123	GLN
1	S	129	GLN
1	S	156	HIS
1	T	38	HIS
1	T	116	ASN

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Mol	Chain	Res	Type
1	T	123	GLN
1	T	156	HIS
1	T	163	GLN
1	U	54	ASN
1	U	81	GLN
1	U	123	GLN
1	U	156	HIS
1	V	34	GLN
1	V	41	ASN
1	V	116	ASN
1	V	123	GLN
1	V	138	HIS
1	V	150	ASN
1	V	156	HIS
1	V	163	GLN
1	W	34	GLN
1	W	41	ASN
1	W	129	GLN
1	W	156	HIS
1	W	163	GLN
1	X	34	GLN
1	X	38	HIS
1	X	41	ASN
1	X	94	GLN
1	X	116	ASN
1	X	123	GLN
1	X	129	GLN
1	X	156	HIS
1	X	159	GLN
1	X	163	GLN
1	Y	38	HIS
1	Y	41	ASN
1	Y	123	GLN
1	Y	156	HIS
1	Z	41	ASN
1	Z	123	GLN
1	Z	138	HIS
1	Z	156	HIS
1	Z	163	GLN
1	a	41	ASN
1	a	116	ASN
1	a	122	HIS

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Mol	Chain	Res	Type
1	a	123	GLN
1	a	156	HIS
1	a	163	GLN
1	a	191	HIS
1	b	34	GLN
1	b	38	HIS
1	b	41	ASN
1	b	116	ASN
1	b	123	GLN
1	b	156	HIS
1	b	163	GLN
1	b	191	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.