



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 07:11 PM GMT

PDB ID : 1PMA  
Title : PROTEASOME FROM THERMOPLASMA ACIDOPHILUM  
Authors : Loewe, J.; Stock, D.; Jap, B.; Zwickl, P.; Baumeister, W.; Huber, R.  
Deposited on : 1994-12-19  
Resolution : 3.40 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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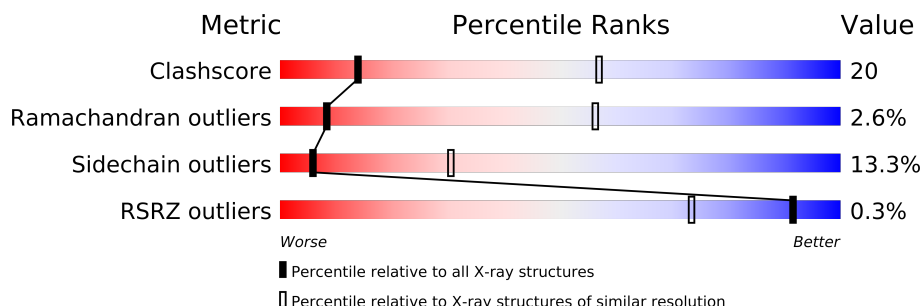
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.40 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.











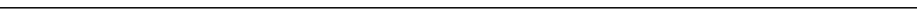



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1214 (3.50-3.30)
Ramachandran outliers	78287	1177 (3.50-3.30)
Sidechain outliers	78261	1177 (3.50-3.30)
RSRZ outliers	66119	1017 (3.52-3.28)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	233	
1	C	233	
1	D	233	
1	E	233	
1	F	233	
1	G	233	
1	H	233	
1	I	233	
1	J	233	
1	K	233	
1	L	233	
1	M	233	
1	N	233	
1	O	233	
2	1	211	
2	2	211	

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Mol	Chain	Length	Quality of chain
2	B	211	
2	P	211	
2	Q	211	
2	R	211	
2	S	211	
2	T	211	
2	U	211	
2	V	211	
2	W	211	
2	X	211	
2	Y	211	
2	Z	211	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 56294 atoms, of which 10402 are hydrogens and 0 are deuterium.

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 PROTEASOME.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	C	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	D	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	E	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	F	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	G	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	H	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	I	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	J	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	K	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	L	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	M	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	N	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	O	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			

- Molecule 2 is a protein called PROTEASOME.

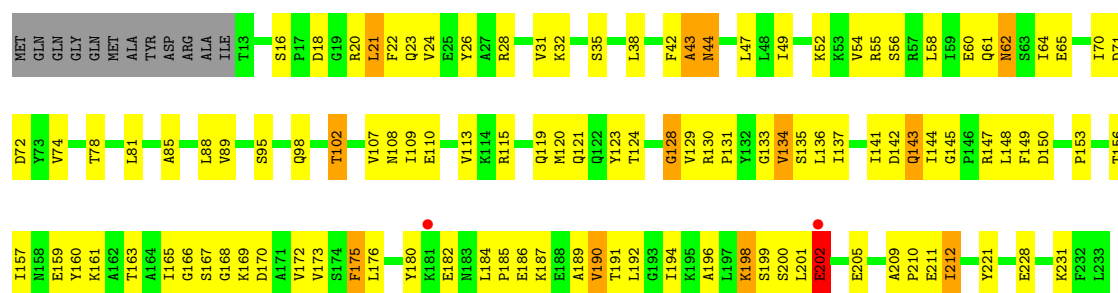
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	203	Total 1908	C 985	H 350	N 264	O 298	S 11	0	0	0
2	P	203	Total 1908	C 985	H 350	N 264	O 298	S 11	0	0	0
2	Q	203	Total 1908	C 985	H 350	N 264	O 298	S 11	0	0	0
2	R	203	Total 1908	C 985	H 350	N 264	O 298	S 11	0	0	0
2	S	203	Total 1908	C 985	H 350	N 264	O 298	S 11	0	0	0
2	T	203	Total 1908	C 985	H 350	N 264	O 298	S 11	0	0	0
2	U	203	Total 1908	C 985	H 350	N 264	O 298	S 11	0	0	0
2	V	203	Total 1908	C 985	H 350	N 264	O 298	S 11	0	0	0
2	W	203	Total 1908	C 985	H 350	N 264	O 298	S 11	0	0	0
2	X	203	Total 1908	C 985	H 350	N 264	O 298	S 11	0	0	0
2	Y	203	Total 1908	C 985	H 350	N 264	O 298	S 11	0	0	0
2	Z	203	Total 1908	C 985	H 350	N 264	O 298	S 11	0	0	0
2	1	203	Total 1908	C 985	H 350	N 264	O 298	S 11	0	0	0
2	2	203	Total 1908	C 985	H 350	N 264	O 298	S 11	0	0	0

### 3 Residue-property plots

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

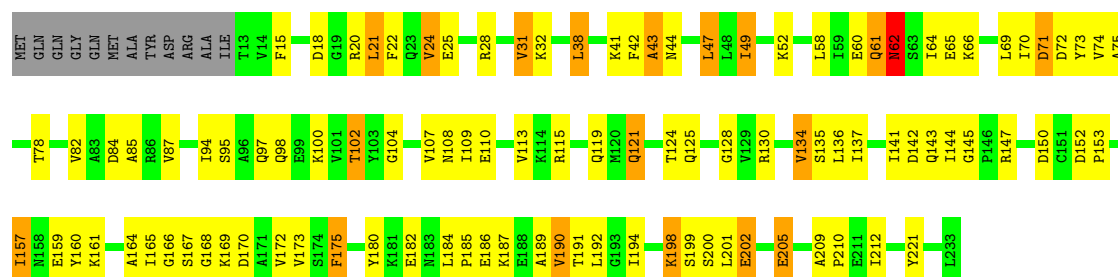
#### • Molecule 1: PROTEASOME

Chain A: 



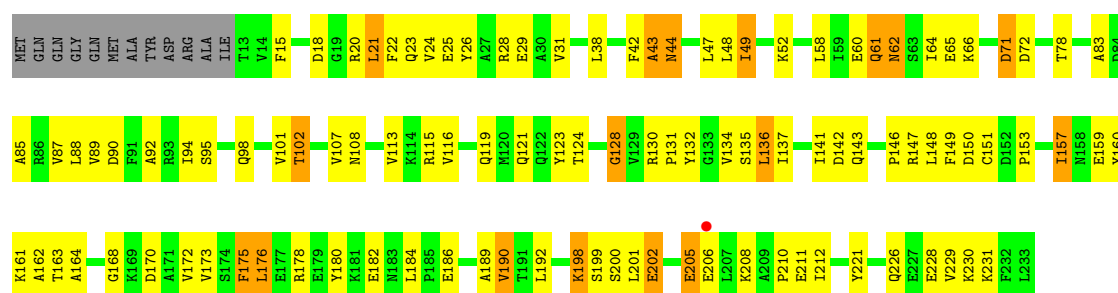
#### • Molecule 1: PROTEASOME

Chain C: 



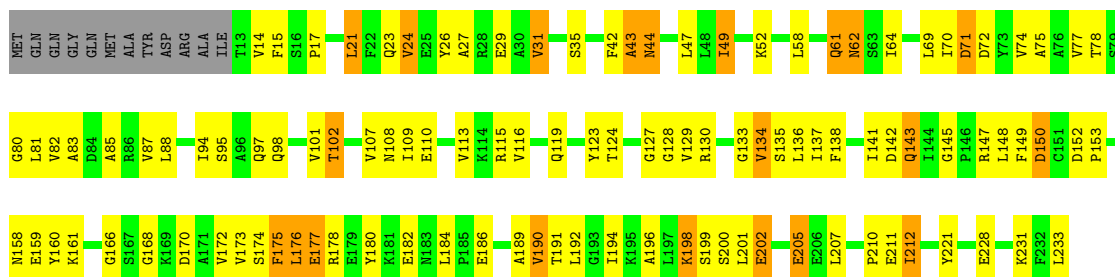
#### • Molecule 1: PROTEASOME

Chain D: 



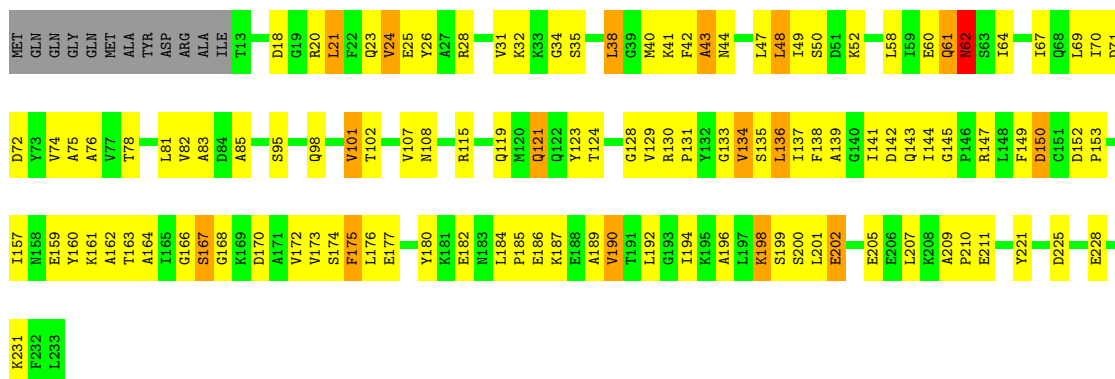
#### • Molecule 1: PROTEASOME

## Chain E:



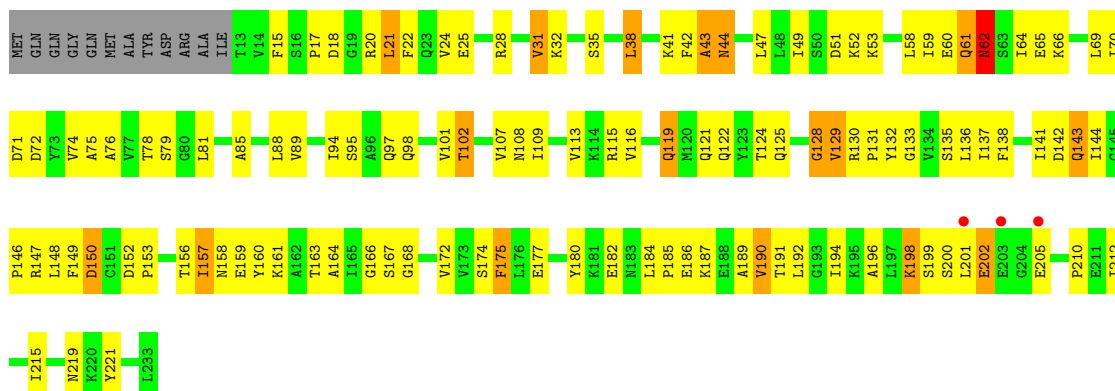
- Molecule 1: PROTEASOME

## Chain F:



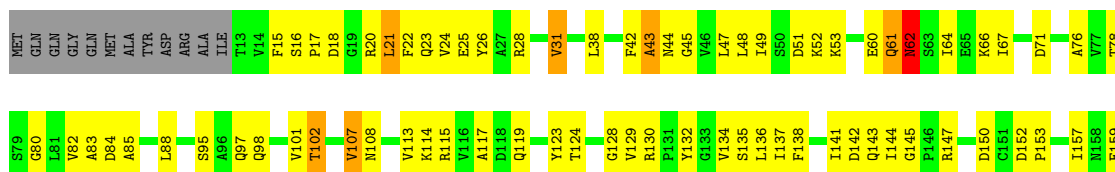
- Molecule 1: PROTEASOME

Chain G:



- Molecule 1: PROTEASOME

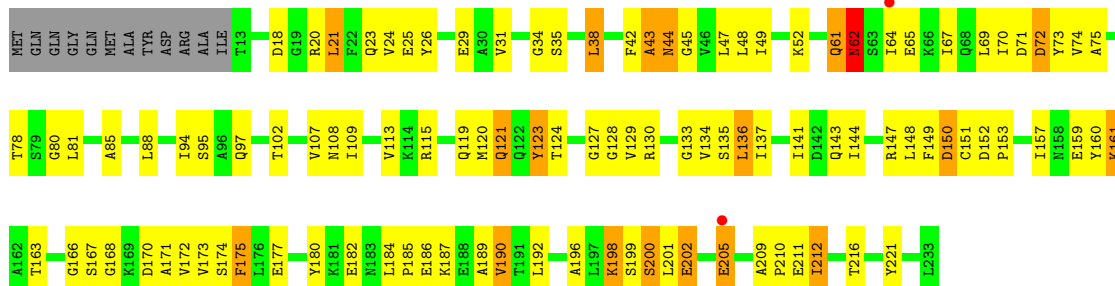
## Chain H:





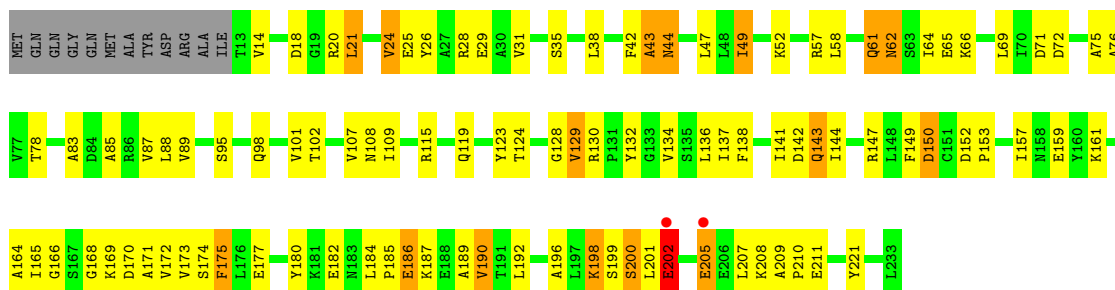
- Molecule 1: PROTEASOME

Chain I:



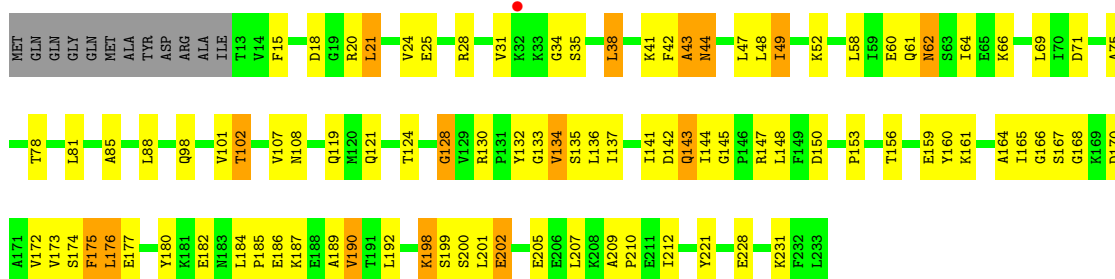
- Molecule 1: PROTEASOME

Chain J:



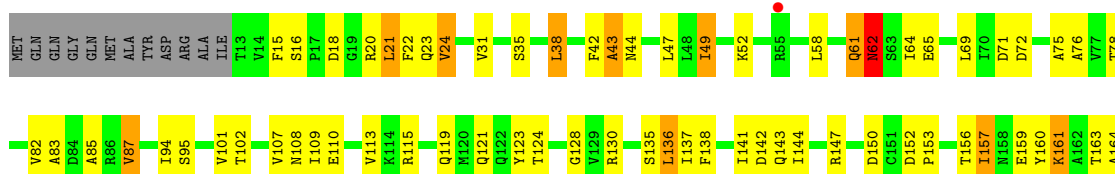
- Molecule 1: PROTEASOME

Chain K:

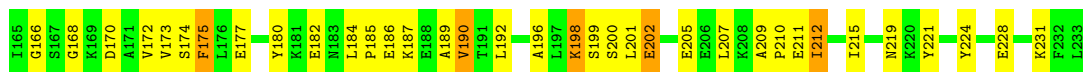


- Molecule 1: PROTEASOME

Chain L:







- Molecule 1: PROTEASOME

Chain M:



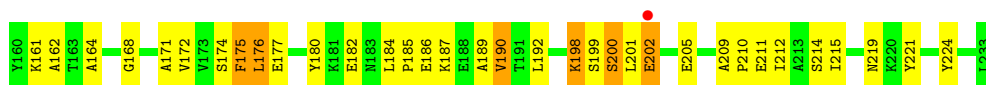
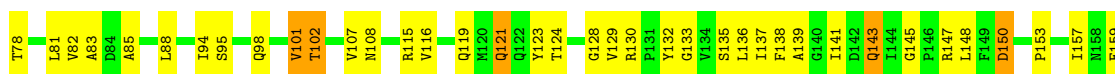
- Molecule 1: PROTEASOME

Chain N:



- Molecule 1: PROTEASOME

Chain O:



- Molecule 2: PROTEASOME

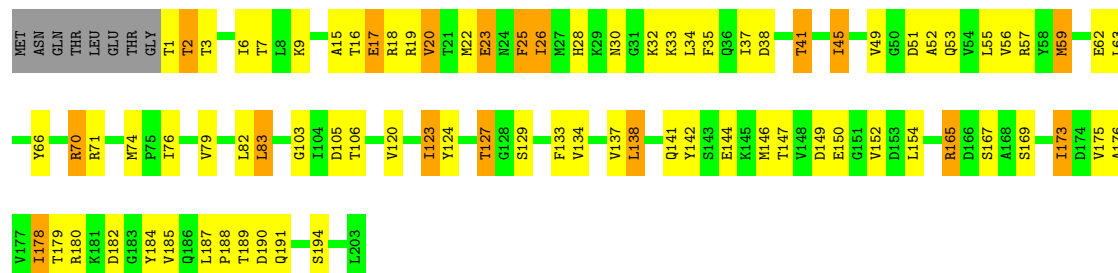
Chain B:





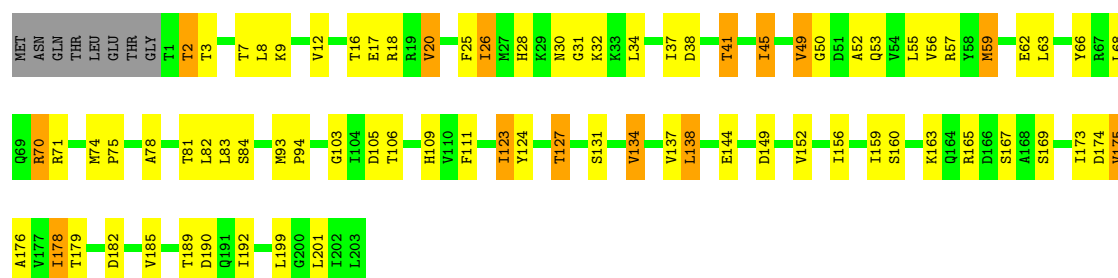
- Molecule 2: PROTEASOME

Chain P:



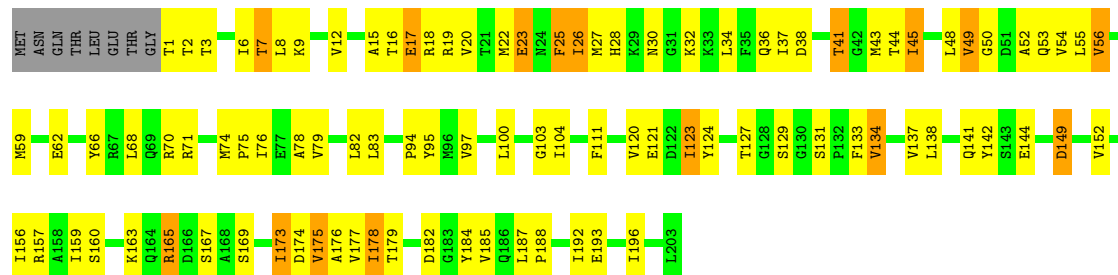
- Molecule 2: PROTEASOME

Chain Q:



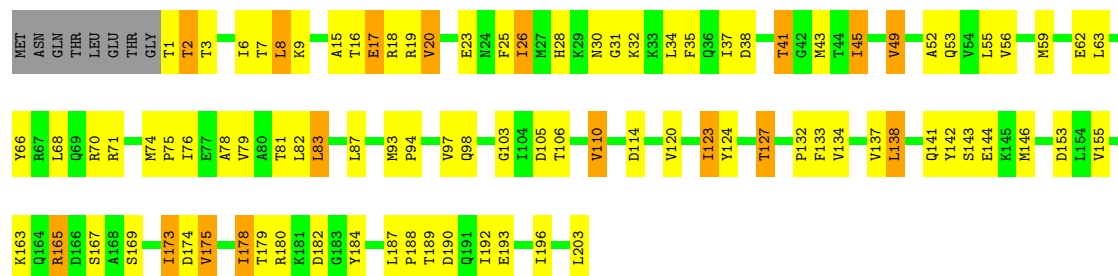
- Molecule 2: PROTEASOME

Chain R:



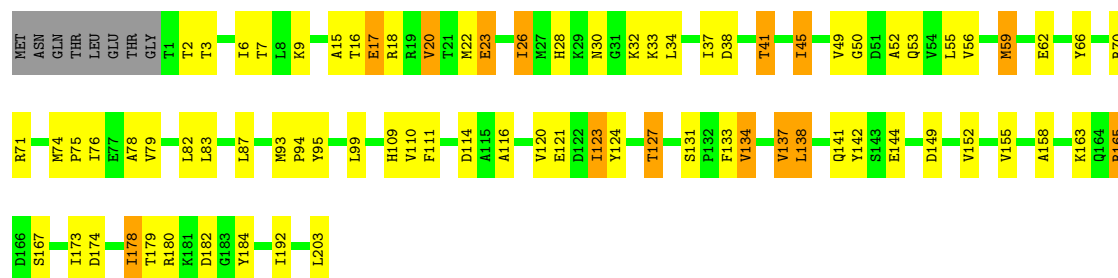
- Molecule 2: PROTEASOME

Chain S:



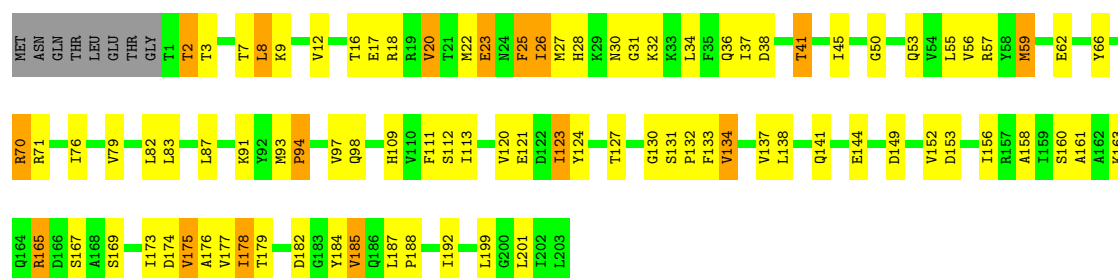
- Molecule 2: PROTEASOME

Chain T:



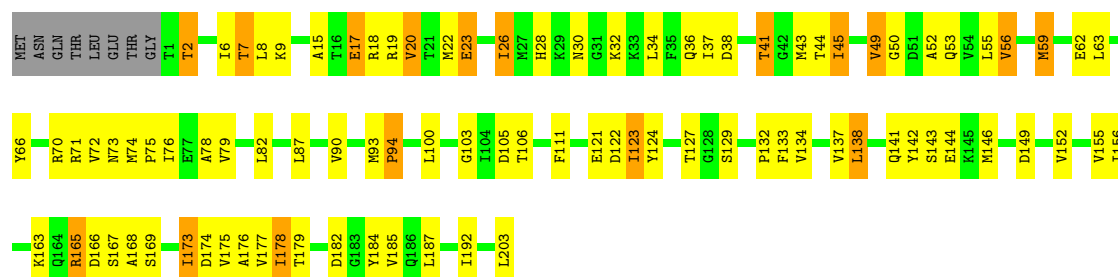
- Molecule 2: PROTEASOME

Chain U:



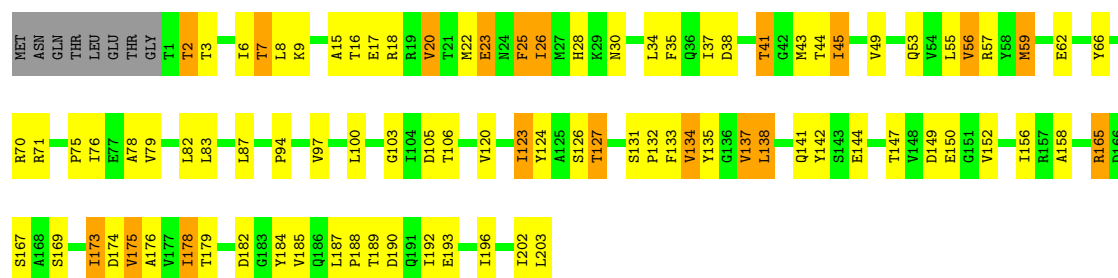
- Molecule 2: PROTEASOME

Chain V:



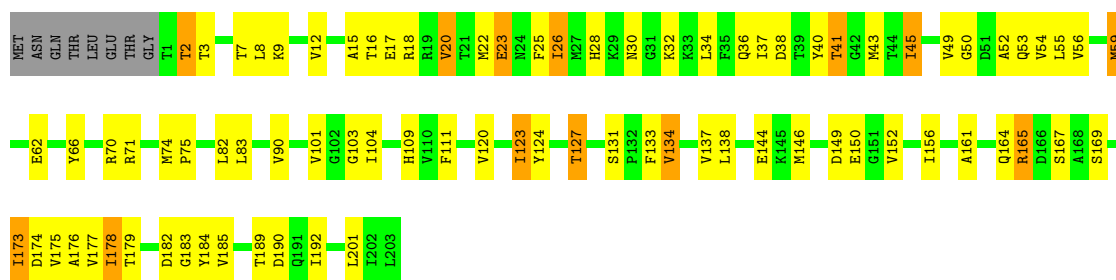
- Molecule 2: PROTEASOME

Chain W:



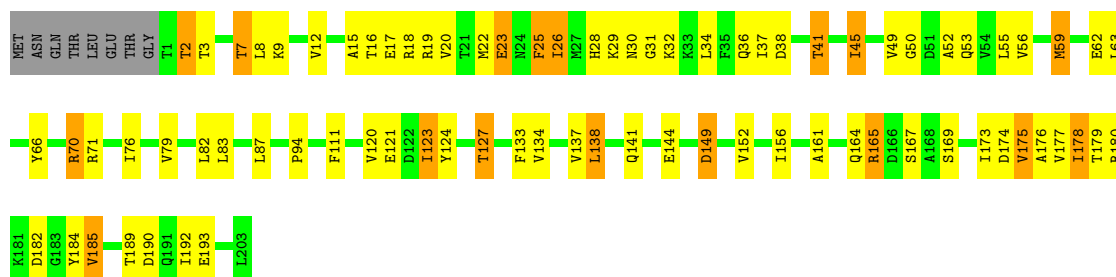
- Molecule 2: PROTEASOME

Chain X:



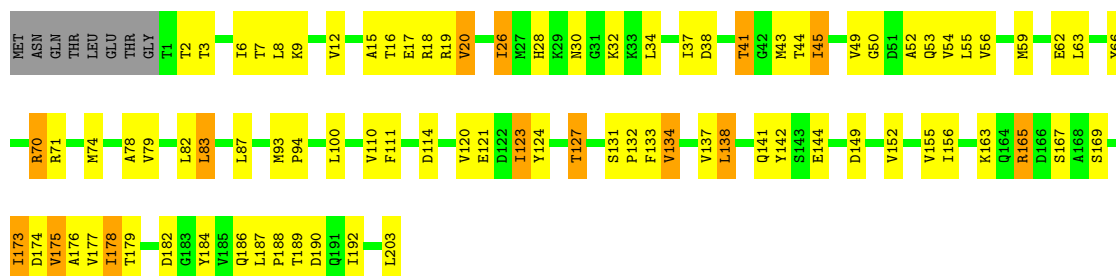
- Molecule 2: PROTEASOME

Chain Y:



- Molecule 2: PROTEASOME

Chain Z:



- Molecule 2: PROTEASOME

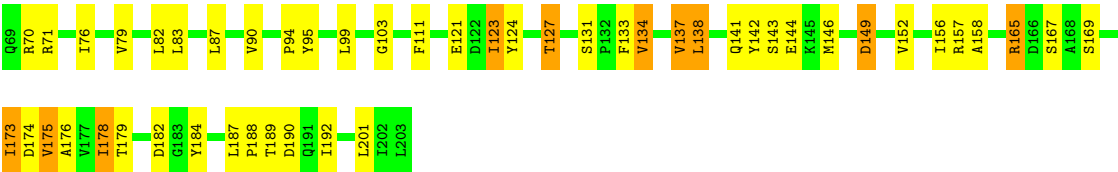
Chain 1:



- Molecule 2: PROTEASOME

Chain 2:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	311.90Å 209.70Å 117.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.40 20.97 – 3.40	Depositor EDS
% Data completeness (in resolution range)	85.7 (10.00-3.40) 85.0 (20.97-3.40)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.72 (at 3.37Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.221 , (Not available) 0.208 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	80.4	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 88.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 90045 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	56294	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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	0.52	0/1743	0.71	1/2348 (0.0%)
1	C	0.51	0/1743	0.71	0/2348
1	D	0.52	0/1743	0.70	1/2348 (0.0%)
1	E	0.55	0/1743	0.72	0/2348
1	F	0.52	0/1743	0.70	0/2348
1	G	0.54	0/1743	0.69	0/2348
1	H	0.53	0/1743	0.70	0/2348
1	I	0.50	0/1743	0.70	0/2348
1	J	0.51	0/1743	0.69	0/2348
1	K	0.51	0/1743	0.69	1/2348 (0.0%)
1	L	0.53	0/1743	0.70	0/2348
1	M	0.51	0/1743	0.70	0/2348
1	N	0.54	0/1743	0.70	0/2348
1	O	0.52	0/1743	0.71	0/2348
2	1	0.55	0/1577	0.74	1/2129 (0.0%)
2	2	0.53	0/1577	0.75	1/2129 (0.0%)
2	B	0.56	0/1577	0.76	0/2129
2	P	0.57	0/1577	0.76	0/2129
2	Q	0.54	0/1577	0.75	0/2129
2	R	0.55	0/1577	0.77	2/2129 (0.1%)
2	S	0.57	0/1577	0.77	0/2129
2	T	0.55	0/1577	0.75	1/2129 (0.0%)
2	U	0.54	0/1577	0.74	0/2129
2	V	0.56	0/1577	0.77	0/2129
2	W	0.57	0/1577	0.75	1/2129 (0.0%)
2	X	0.54	0/1577	0.73	0/2129
2	Y	0.52	0/1577	0.74	0/2129
2	Z	0.54	0/1577	0.75	0/2129
All	All	0.53	0/46480	0.72	9/62678 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	95	TYR	N-CA-C	-5.91	95.06	111.00
2	1	8	LEU	CA-CB-CG	5.55	128.06	115.30
1	D	128	GLY	N-CA-C	5.36	126.49	113.10
2	W	8	LEU	CA-CB-CG	5.32	127.54	115.30
1	K	128	GLY	N-CA-C	5.31	126.39	113.10
1	A	128	GLY	N-CA-C	5.07	125.78	113.10
2	2	95	TYR	N-CA-C	-5.05	97.37	111.00
2	T	95	TYR	N-CA-C	-5.03	97.41	111.00
2	R	8	LEU	CA-CB-CG	5.03	126.87	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1720	393	1361	77	0
1	C	1720	393	1361	73	0
1	D	1720	393	1361	77	0
1	E	1720	393	1361	81	0
1	F	1720	393	1361	81	0
1	G	1720	393	1361	98	0
1	H	1720	393	1361	81	0
1	I	1720	393	1361	80	0
1	J	1720	393	1361	72	0
1	K	1720	393	1361	69	0
1	L	1720	393	1361	77	0
1	M	1720	393	1361	72	0
1	N	1720	393	1361	66	0
1	O	1720	393	1361	75	0
2	1	1558	350	1259	74	0
2	2	1558	350	1259	59	0
2	B	1558	350	1259	82	0
2	P	1558	350	1259	64	0
2	Q	1558	350	1259	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	1558	350	1259	69	0
2	S	1558	350	1259	78	0
2	T	1558	350	1259	59	0
2	U	1558	350	1259	65	0
2	V	1558	350	1259	74	0
2	W	1558	350	1259	69	0
2	X	1558	350	1259	61	0
2	Y	1558	350	1259	66	0
2	Z	1558	350	1259	67	0
All	All	45892	10402	36680	1849	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 20.

All (1849) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:38:ASP:HB3	2:B:41:THR:HG23	1.38	1.03
2:T:38:ASP:HB3	2:T:41:THR:HG23	1.44	1.00
2:Q:45:ILE:HG12	2:Q:52:ALA:HB1	1.44	0.99
2:Q:38:ASP:HB3	2:Q:41:THR:HG23	1.46	0.98
2:R:38:ASP:HB3	2:R:41:THR:HG23	1.45	0.98
2:B:66:TYR:OH	1:H:107:VAL:HG11	1.62	0.97
2:T:45:ILE:HG12	2:T:52:ALA:HB1	1.46	0.96
1:M:107:VAL:HG11	2:1:66:TYR:OH	1.65	0.96
2:U:38:ASP:HB3	2:U:41:THR:HG23	1.47	0.95
2:2:38:ASP:HB3	2:2:41:THR:HG23	1.47	0.95
2:Y:38:ASP:HB3	2:Y:41:THR:HG23	1.48	0.95
2:W:38:ASP:HB3	2:W:41:THR:HG23	1.45	0.95
2:P:38:ASP:HB3	2:P:41:THR:HG23	1.49	0.94
1:K:107:VAL:HG11	2:Y:66:TYR:OH	1.68	0.94
1:I:107:VAL:HG11	2:W:66:TYR:OH	1.68	0.93
2:1:38:ASP:HB3	2:1:41:THR:HG23	1.50	0.93
2:Z:38:ASP:HB3	2:Z:41:THR:HG23	1.50	0.93
1:A:107:VAL:HG11	2:P:66:TYR:OH	1.69	0.93
1:L:107:VAL:HG11	2:Z:66:TYR:OH	1.69	0.92
1:D:107:VAL:HG11	2:R:66:TYR:OH	1.70	0.91
1:N:107:VAL:HG11	2:2:66:TYR:OH	1.69	0.91
2:X:45:ILE:HG12	2:X:52:ALA:HB1	1.53	0.91
1:F:107:VAL:HG11	2:T:66:TYR:OH	1.71	0.90
2:1:37:ILE:HD11	2:1:59:MET:HB3	1.54	0.90
2:X:38:ASP:HB3	2:X:41:THR:HG23	1.54	0.89
1:E:107:VAL:HG11	2:S:66:TYR:OH	1.73	0.89

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:X:53:GLN:O	2:X:56:VAL:HG12	1.73	0.88
2:Z:59:MET:HE2	2:Z:79:VAL:HG23	1.54	0.88
2:T:37:ILE:HD11	2:T:59:MET:HB3	1.56	0.87
1:J:107:VAL:HG11	2:X:66:TYR:OH	1.75	0.85
1:D:108:ASN:HB3	2:R:70:ARG:HG2	1.57	0.85
2:S:38:ASP:HB3	2:S:41:THR:HG23	1.59	0.85
1:L:124:THR:HG22	1:M:130:ARG:HH21	1.42	0.84
2:V:38:ASP:HB3	2:V:41:THR:HG23	1.57	0.84
1:O:107:VAL:HG11	2:V:66:TYR:OH	1.78	0.84
1:M:168:GLY:O	1:M:172:VAL:HG12	1.77	0.83
2:U:53:GLN:O	2:U:56:VAL:HG12	1.78	0.83
1:I:130:ARG:HH21	1:O:124:THR:HG22	1.43	0.83
1:G:124:THR:HG22	1:H:130:ARG:HH21	1.41	0.83
2:P:123:ILE:HG12	2:P:124:TYR:HD1	1.44	0.83
2:Q:37:ILE:HD11	2:Q:59:MET:HB3	1.61	0.82
1:C:107:VAL:HG11	2:Q:66:TYR:OH	1.79	0.81
2:Z:123:ILE:HG12	2:Z:124:TYR:HD1	1.44	0.81
2:T:20:VAL:HG13	2:T:28:HIS:HB2	1.62	0.81
1:A:52:LYS:NZ	1:A:62:ASN:HA	1.96	0.81
2:W:123:ILE:HG12	2:W:124:TYR:HD1	1.46	0.80
1:I:108:ASN:HB3	2:W:70:ARG:HG2	1.62	0.80
1:K:124:THR:HG22	1:L:130:ARG:HH21	1.47	0.80
1:G:107:VAL:HG11	2:U:66:TYR:OH	1.83	0.79
2:R:123:ILE:HG12	2:R:124:TYR:HD1	1.48	0.78
2:B:123:ILE:HG12	2:B:124:TYR:HD1	1.48	0.78
1:F:124:THR:HG22	1:G:130:ARG:HH21	1.46	0.78
2:B:70:ARG:HG2	1:H:108:ASN:HB3	1.65	0.78
2:P:53:GLN:O	2:P:56:VAL:HG12	1.83	0.78
1:A:186:GLU:O	1:A:190:VAL:HG12	1.84	0.78
1:K:52:LYS:NZ	1:K:62:ASN:HA	2.00	0.77
1:M:107:VAL:HG11	2:1:66:TYR:HH	1.49	0.76
2:W:53:GLN:O	2:W:56:VAL:HG12	1.86	0.76
2:2:53:GLN:O	2:2:56:VAL:HG12	1.86	0.76
1:H:168:GLY:O	1:H:172:VAL:HG12	1.85	0.76
1:C:18:ASP:OD2	1:C:20:ARG:HD3	1.85	0.76
1:K:108:ASN:HB3	2:Y:70:ARG:HG2	1.66	0.76
1:I:198:LYS:O	1:I:202:GLU:HB2	1.85	0.76
2:V:123:ILE:HG12	2:V:124:TYR:HD1	1.49	0.76
1:A:124:THR:HG22	1:C:130:ARG:HH21	1.51	0.75
2:U:32:LYS:HE2	2:U:34:LEU:O	1.85	0.75
1:K:78:THR:HG21	1:K:85:ALA:HB1	1.67	0.75
1:F:21:LEU:HD11	1:G:130:ARG:HD2	1.68	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:S:53:GLN:O	2:S:56:VAL:HG12	1.87	0.75
2:1:13:THR:OG1	2:1:127:THR:HG22	1.86	0.75
2:1:53:GLN:O	2:1:56:VAL:HG12	1.86	0.74
2:Y:53:GLN:O	2:Y:56:VAL:HG12	1.87	0.74
1:G:21:LEU:O	1:G:24:VAL:HG12	1.87	0.73
2:S:2:THR:HG22	2:S:169:SER:OG	1.89	0.73
1:E:135:SER:OG	1:E:153:PRO:HD3	1.88	0.73
1:M:78:THR:HG21	1:M:85:ALA:HB1	1.71	0.73
2:1:123:ILE:HD13	2:1:123:ILE:H	1.52	0.73
2:2:37:ILE:HD11	2:2:59:MET:HB3	1.71	0.73
1:A:78:THR:HG21	1:A:85:ALA:HB1	1.70	0.73
1:I:130:ARG:HD2	1:O:21:LEU:HD11	1.69	0.73
2:P:38:ASP:HB3	2:P:41:THR:CG2	2.19	0.73
2:P:103:GLY:HA2	2:P:178:ILE:HD11	1.71	0.73
2:U:62:GLU:HG2	2:U:82:LEU:HD21	1.70	0.72
1:M:198:LYS:O	1:M:202:GLU:HB2	1.89	0.72
1:L:198:LYS:O	1:L:202:GLU:HB2	1.90	0.72
1:I:78:THR:HG21	1:I:85:ALA:HB1	1.71	0.72
1:D:52:LYS:NZ	1:D:62:ASN:HA	2.04	0.72
2:X:123:ILE:HG12	2:X:124:TYR:HD1	1.54	0.72
1:A:168:GLY:O	1:A:172:VAL:HG12	1.89	0.72
1:J:184:LEU:HD23	1:J:189:ALA:HA	1.71	0.72
1:J:78:THR:HG21	1:J:85:ALA:HB1	1.70	0.72
2:B:53:GLN:O	2:B:56:VAL:HG12	1.89	0.72
2:T:123:ILE:HG12	2:T:124:TYR:HD1	1.53	0.72
1:J:198:LYS:O	1:J:202:GLU:HB2	1.89	0.71
2:B:32:LYS:HE2	2:B:34:LEU:O	1.89	0.71
1:K:168:GLY:O	1:K:172:VAL:HG12	1.89	0.71
2:S:7:THR:HB	2:S:123:ILE:O	1.90	0.71
2:2:18:ARG:HB2	2:2:31:GLY:O	1.91	0.71
2:B:43:MET:HE1	2:B:56:VAL:HG23	1.72	0.71
2:S:20:VAL:HG13	2:S:28:HIS:HB2	1.71	0.71
2:R:167:SER:HB2	2:V:167:SER:HB2	1.73	0.71
1:K:184:LEU:HD23	1:K:189:ALA:HA	1.73	0.71
1:F:52:LYS:NZ	1:F:62:ASN:HA	2.06	0.71
1:K:21:LEU:O	1:K:24:VAL:HG12	1.90	0.70
1:M:186:GLU:O	1:M:190:VAL:HG12	1.90	0.70
2:B:59:MET:HE2	2:B:79:VAL:HG23	1.73	0.70
1:D:98:GLN:O	1:D:102:THR:HG22	1.91	0.70
2:V:149:ASP:O	2:V:152:VAL:HG12	1.91	0.70
2:U:37:ILE:HD11	2:U:59:MET:HB3	1.73	0.70
2:P:103:GLY:HA2	2:P:178:ILE:CD1	2.22	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:2:55:LEU:HD23	2:2:99:LEU:HD11	1.74	0.70
2:X:3:THR:OG1	2:X:127:THR:HG22	1.92	0.70
2:Q:123:ILE:H	2:Q:123:ILE:HD13	1.56	0.70
2:1:62:GLU:HG2	2:1:82:LEU:HD21	1.73	0.69
1:H:21:LEU:O	1:H:24:VAL:HG12	1.92	0.69
2:Z:53:GLN:O	2:Z:56:VAL:HG12	1.92	0.69
2:Q:45:ILE:CG1	2:Q:52:ALA:HB1	2.22	0.69
1:J:42:PHE:HB2	1:J:184:LEU:O	1.91	0.69
2:B:45:ILE:HG12	2:B:52:ALA:HB1	1.74	0.69
2:W:38:ASP:HB3	2:W:41:THR:CG2	2.19	0.69
1:G:198:LYS:O	1:G:202:GLU:HB2	1.92	0.69
2:V:124:TYR:CD2	2:V:138:LEU:HD23	2.28	0.69
2:P:62:GLU:HG2	2:P:82:LEU:HD21	1.74	0.69
1:G:52:LYS:NZ	1:G:62:ASN:HA	2.06	0.69
2:Y:45:ILE:HG12	2:Y:52:ALA:HB1	1.74	0.69
2:S:193:GLU:HA	2:S:196:ILE:HD12	1.74	0.69
1:K:52:LYS:HZ2	1:K:62:ASN:HA	1.56	0.69
1:A:184:LEU:HD23	1:A:189:ALA:HA	1.75	0.69
2:X:32:LYS:HE2	2:X:34:LEU:O	1.92	0.69
2:B:167:SER:HB2	2:Y:167:SER:HB2	1.75	0.69
2:R:12:VAL:HG13	2:R:178:ILE:HG23	1.74	0.69
1:C:42:PHE:HB2	1:C:184:LEU:O	1.92	0.69
2:Q:53:GLN:O	2:Q:56:VAL:HG12	1.91	0.69
1:D:135:SER:OG	1:D:153:PRO:HD3	1.92	0.69
2:Z:15:ALA:HB2	2:Z:175:VAL:HB	1.74	0.68
2:V:123:ILE:H	2:V:123:ILE:HD13	1.58	0.68
2:Y:32:LYS:HE2	2:Y:34:LEU:O	1.93	0.68
2:1:32:LYS:HE2	2:1:34:LEU:O	1.93	0.68
2:T:53:GLN:O	2:T:56:VAL:HG12	1.93	0.68
2:W:43:MET:HE1	2:W:56:VAL:HG23	1.74	0.68
2:T:3:THR:OG1	2:T:127:THR:HG22	1.93	0.68
2:X:37:ILE:HD11	2:X:59:MET:HB3	1.75	0.68
1:G:52:LYS:HE3	1:G:64:ILE:HG23	1.75	0.68
1:D:198:LYS:O	1:D:202:GLU:HB2	1.94	0.68
1:O:198:LYS:O	1:O:202:GLU:HB2	1.93	0.68
2:Q:149:ASP:O	2:Q:152:VAL:HG12	1.94	0.68
2:W:18:ARG:HE	2:W:30:ASN:HD22	1.41	0.68
1:C:78:THR:HG21	1:C:85:ALA:HB1	1.74	0.68
1:O:52:LYS:NZ	1:O:62:ASN:HA	2.09	0.68
1:M:109:ILE:CG2	1:M:147:ARG:HD3	2.24	0.68
1:M:184:LEU:HD23	1:M:189:ALA:HA	1.76	0.68
1:J:186:GLU:O	1:J:190:VAL:HG12	1.94	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:52:LYS:NZ	1:I:62:ASN:HA	2.08	0.68
2:U:38:ASP:HB3	2:U:41:THR:CG2	2.21	0.67
1:L:168:GLY:O	1:L:172:VAL:HG12	1.94	0.67
2:R:7:THR:HB	2:R:123:ILE:O	1.93	0.67
1:N:78:THR:HG21	1:N:85:ALA:HB1	1.75	0.67
1:H:95:SER:OG	1:H:115:ARG:HD3	1.94	0.67
2:V:53:GLN:O	2:V:56:VAL:HG12	1.95	0.67
1:E:198:LYS:O	1:E:202:GLU:HB2	1.95	0.67
2:P:133:PHE:CZ	2:P:165:ARG:HB3	2.30	0.67
1:H:198:LYS:O	1:H:202:GLU:HB2	1.95	0.67
2:B:59:MET:SD	2:B:83:LEU:HD13	2.35	0.67
1:E:78:THR:HG21	1:E:85:ALA:HB1	1.75	0.67
1:K:198:LYS:O	1:K:202:GLU:HB2	1.95	0.67
1:C:168:GLY:O	1:C:172:VAL:HG12	1.95	0.67
1:I:23:GLN:OE1	1:O:14:VAL:HB	1.95	0.67
1:M:69:LEU:HD23	1:M:75:ALA:HB2	1.75	0.67
2:T:18:ARG:HE	2:T:30:ASN:HD22	1.42	0.66
1:G:21:LEU:HD11	1:H:130:ARG:HD2	1.76	0.66
2:Z:111:PHE:CE2	2:Z:121:GLU:HB2	2.29	0.66
1:G:184:LEU:HD23	1:G:189:ALA:HA	1.77	0.66
2:V:6:ILE:HD11	2:V:142:TYR:CD1	2.31	0.66
1:G:186:GLU:O	1:G:190:VAL:HG12	1.95	0.66
2:W:124:TYR:CD2	2:W:138:LEU:HD23	2.31	0.66
2:R:28:HIS:CD2	2:S:120:VAL:HG11	2.31	0.66
1:C:108:ASN:HB3	2:Q:70:ARG:HG2	1.78	0.66
1:D:21:LEU:O	1:D:25:GLU:HG2	1.95	0.66
2:P:7:THR:HB	2:P:123:ILE:O	1.96	0.66
2:Q:2:THR:HG22	2:Q:169:SER:OG	1.96	0.66
2:Z:18:ARG:HE	2:Z:30:ASN:HD22	1.42	0.66
1:D:108:ASN:CB	2:R:70:ARG:HG2	2.25	0.66
2:R:123:ILE:HG12	2:R:124:TYR:CD1	2.31	0.66
1:G:78:THR:HG21	1:G:85:ALA:HB1	1.76	0.66
2:Q:75:PRO:O	2:Q:78:ALA:HB3	1.96	0.66
1:F:168:GLY:O	1:F:172:VAL:HG12	1.96	0.66
2:2:45:ILE:HG12	2:2:52:ALA:HB1	1.77	0.66
1:A:198:LYS:O	1:A:202:GLU:HB2	1.96	0.66
2:V:7:THR:HB	2:V:123:ILE:O	1.96	0.65
1:L:49:ILE:HD11	1:L:210:PRO:HB3	1.78	0.65
2:V:45:ILE:HG12	2:V:52:ALA:HB1	1.78	0.65
2:U:123:ILE:H	2:U:123:ILE:HD13	1.59	0.65
1:F:69:LEU:HD23	1:F:75:ALA:HB2	1.79	0.65
1:I:43:ALA:HB2	1:I:185:PRO:HA	1.79	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:98:GLN:O	1:O:102:THR:HG22	1.96	0.65
1:F:186:GLU:O	1:F:190:VAL:HG12	1.96	0.65
2:S:37:ILE:HD11	2:S:59:MET:HB3	1.79	0.65
2:S:59:MET:SD	2:S:83:LEU:HD13	2.36	0.65
1:E:124:THR:HG22	1:F:130:ARG:HH21	1.62	0.65
1:I:21:LEU:HD11	1:J:130:ARG:HD2	1.79	0.65
2:2:32:LYS:HE2	2:2:34:LEU:O	1.97	0.65
1:A:159:GLU:HG2	1:C:60:GLU:HG3	1.79	0.65
1:E:52:LYS:NZ	1:E:62:ASN:HA	2.10	0.65
1:L:52:LYS:NZ	1:L:62:ASN:HA	2.11	0.65
2:B:38:ASP:HB3	2:B:41:THR:CG2	2.20	0.65
2:T:45:ILE:CG1	2:T:52:ALA:HB1	2.26	0.65
1:L:170:ASP:O	1:L:173:VAL:HG12	1.96	0.65
1:N:98:GLN:O	1:N:102:THR:HG22	1.97	0.65
1:A:52:LYS:HZ2	1:A:62:ASN:HA	1.60	0.65
2:S:123:ILE:HG12	2:S:124:TYR:HD1	1.61	0.65
1:F:198:LYS:O	1:F:202:GLU:HB2	1.97	0.65
1:M:21:LEU:O	1:M:24:VAL:HG12	1.97	0.65
1:N:198:LYS:O	1:N:202:GLU:HB2	1.96	0.65
1:F:21:LEU:O	1:F:24:VAL:HG12	1.98	0.64
2:P:45:ILE:HG12	2:P:52:ALA:HB1	1.79	0.64
1:H:61:GLN:O	1:H:64:ILE:HG22	1.96	0.64
2:1:59:MET:SD	2:1:83:LEU:HD13	2.37	0.64
1:A:61:GLN:O	1:A:64:ILE:HG22	1.95	0.64
1:A:21:LEU:HD11	1:C:130:ARG:HD2	1.79	0.64
2:T:124:TYR:CD2	2:T:138:LEU:HD23	2.31	0.64
1:N:21:LEU:O	1:N:24:VAL:HG12	1.97	0.64
2:Y:37:ILE:HD11	2:Y:59:MET:HB3	1.79	0.64
2:P:20:VAL:HG13	2:P:28:HIS:HB2	1.79	0.64
2:U:123:ILE:HG12	2:U:124:TYR:HD2	1.61	0.64
2:X:20:VAL:HG13	2:X:28:HIS:HB2	1.80	0.64
1:G:121:GLN:O	1:G:124:THR:HB	1.96	0.64
2:Z:149:ASP:O	2:Z:152:VAL:HG12	1.97	0.64
2:Y:124:TYR:CD1	2:Y:138:LEU:HD23	2.32	0.64
1:L:108:ASN:HB3	2:Z:70:ARG:HG2	1.80	0.64
2:P:124:TYR:CD2	2:P:138:LEU:HD23	2.32	0.64
1:N:52:LYS:NZ	1:N:62:ASN:HA	2.13	0.64
2:T:49:VAL:HG23	2:T:50:GLY:H	1.61	0.64
1:L:144:ILE:HD12	1:L:147:ARG:NH1	2.13	0.64
2:W:3:THR:OG1	2:W:127:THR:HG22	1.97	0.64
1:M:109:ILE:HG22	1:M:142:ASP:OD1	1.98	0.64
2:Q:18:ARG:HE	2:Q:30:ASN:HD22	1.45	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:137:ILE:HG22	1:G:150:ASP:HB2	1.78	0.64
2:V:103:GLY:HA2	2:V:178:ILE:CD1	2.28	0.64
2:S:124:TYR:CD2	2:S:138:LEU:HD23	2.33	0.63
1:G:135:SER:OG	1:G:153:PRO:HD3	1.98	0.63
2:S:18:ARG:HB2	2:S:31:GLY:O	1.98	0.63
2:Y:7:THR:HB	2:Y:123:ILE:O	1.98	0.63
2:V:76:ILE:O	2:V:79:VAL:HG12	1.98	0.63
1:J:21:LEU:O	1:J:24:VAL:HG12	1.98	0.63
1:H:52:LYS:NZ	1:H:62:ASN:HA	2.14	0.63
1:J:108:ASN:HB3	2:X:70:ARG:HG2	1.79	0.63
1:M:52:LYS:NZ	1:M:62:ASN:HA	2.12	0.63
2:1:123:ILE:HG12	2:1:124:TYR:CD1	2.34	0.63
2:1:123:ILE:HG12	2:1:124:TYR:HD1	1.63	0.63
2:Y:59:MET:HE2	2:Y:79:VAL:HG23	1.79	0.63
2:2:2:THR:HG22	2:2:169:SER:OG	1.98	0.63
2:V:32:LYS:HE2	2:V:34:LEU:O	1.98	0.63
1:F:180:TYR:HA	1:F:192:LEU:HD21	1.80	0.63
1:F:108:ASN:HB3	2:T:70:ARG:HG2	1.78	0.63
2:W:3:THR:HB	2:W:16:THR:HG22	1.80	0.63
1:J:52:LYS:NZ	1:J:62:ASN:HA	2.14	0.63
2:Q:103:GLY:HA2	2:Q:178:ILE:HD13	1.81	0.63
1:C:52:LYS:HE3	1:C:64:ILE:HG23	1.81	0.63
1:I:137:ILE:HG22	1:I:150:ASP:HB2	1.81	0.63
1:G:168:GLY:O	1:G:172:VAL:HG12	1.99	0.63
1:N:168:GLY:O	1:N:172:VAL:HG12	1.97	0.63
1:J:168:GLY:O	1:J:172:VAL:HG12	1.99	0.63
2:B:124:TYR:CD2	2:B:138:LEU:HD23	2.33	0.63
2:B:123:ILE:HG12	2:B:124:TYR:CD1	2.33	0.63
1:D:49:ILE:HD11	1:D:210:PRO:HB3	1.80	0.63
2:R:59:MET:HE3	2:R:82:LEU:HD23	1.81	0.63
2:R:193:GLU:HA	2:R:196:ILE:HD12	1.81	0.63
1:D:61:GLN:O	1:D:64:ILE:HG22	1.98	0.62
2:P:167:SER:HB2	2:X:167:SER:HB2	1.81	0.62
2:U:167:SER:HB2	2:Z:167:SER:HB2	1.81	0.62
1:E:108:ASN:HB3	2:S:70:ARG:HG2	1.81	0.62
2:S:15:ALA:HB2	2:S:175:VAL:HB	1.81	0.62
1:C:94:ILE:HG13	1:C:95:SER:N	2.14	0.62
1:N:184:LEU:HD23	1:N:189:ALA:HA	1.82	0.62
2:R:3:THR:HB	2:R:16:THR:HG22	1.80	0.62
2:V:124:TYR:HD2	2:V:138:LEU:HD23	1.61	0.62
2:U:133:PHE:CZ	2:U:165:ARG:HB3	2.34	0.62
2:B:55:LEU:HD21	2:B:87:LEU:HD11	1.80	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:21:LEU:O	1:D:24:VAL:HG12	2.00	0.62
1:O:108:ASN:HB3	2:V:70:ARG:HG2	1.81	0.62
2:P:76:ILE:O	2:P:79:VAL:HG12	2.00	0.62
2:Z:38:ASP:HB3	2:Z:41:THR:CG2	2.27	0.62
2:Q:103:GLY:HA2	2:Q:178:ILE:CD1	2.29	0.62
2:Z:19:ARG:NE	2:Z:26:ILE:HG13	2.15	0.62
2:1:18:ARG:HB2	2:1:31:GLY:O	2.00	0.62
1:H:78:THR:HG21	1:H:85:ALA:HB1	1.82	0.62
1:I:168:GLY:O	1:I:172:VAL:HG12	1.99	0.62
2:P:37:ILE:HD11	2:P:59:MET:HB3	1.82	0.62
1:O:61:GLN:O	1:O:64:ILE:HG22	2.00	0.62
1:L:52:LYS:HZ2	1:L:62:ASN:HA	1.64	0.62
2:X:124:TYR:CD2	2:X:138:LEU:HD23	2.35	0.62
1:F:52:LYS:HE3	1:F:64:ILE:HG23	1.82	0.62
1:M:21:LEU:O	1:M:25:GLU:HG2	1.99	0.62
2:Y:62:GLU:HG2	2:Y:82:LEU:HD21	1.82	0.62
1:N:70:ILE:HD12	1:N:74:VAL:HG22	1.81	0.62
1:G:18:ASP:OD2	1:G:20:ARG:HD3	2.00	0.62
2:T:123:ILE:HG12	2:T:124:TYR:CD1	2.33	0.61
2:T:123:ILE:H	2:T:123:ILE:HD13	1.65	0.61
2:T:149:ASP:O	2:T:152:VAL:HG12	1.99	0.61
1:C:186:GLU:O	1:C:190:VAL:HG12	1.99	0.61
1:F:70:ILE:HD12	1:F:74:VAL:HG22	1.82	0.61
1:F:78:THR:HG21	1:F:85:ALA:HB1	1.81	0.61
1:F:170:ASP:O	1:F:173:VAL:HG12	1.99	0.61
2:X:18:ARG:HE	2:X:30:ASN:HD22	1.47	0.61
2:Y:174:ASP:HA	2:Y:192:ILE:HD13	1.83	0.61
1:M:175:PHE:CD2	1:M:196:ALA:HA	2.36	0.61
2:B:2:THR:HG22	2:B:169:SER:OG	2.00	0.61
2:R:141:GLN:NE2	2:W:141:GLN:NE2	2.48	0.61
1:J:170:ASP:O	1:J:173:VAL:HG12	2.01	0.61
2:B:43:MET:CE	2:B:56:VAL:HG23	2.29	0.61
1:J:124:THR:HG22	1:K:130:ARG:HH21	1.65	0.61
2:U:179:THR:HG23	2:U:182:ASP:H	1.66	0.61
2:B:37:ILE:HD11	2:B:59:MET:HB3	1.82	0.61
2:U:76:ILE:O	2:U:79:VAL:HG12	2.00	0.61
2:Z:44:THR:OG1	2:Z:100:LEU:HB3	2.00	0.61
1:L:124:THR:HG22	1:M:130:ARG:NH2	2.13	0.61
1:L:184:LEU:HD23	1:L:189:ALA:HA	1.82	0.61
1:A:61:GLN:OE1	1:A:62:ASN:HB3	2.01	0.61
1:K:21:LEU:O	1:K:25:GLU:HG2	2.01	0.61
2:Y:123:ILE:HG12	2:Y:124:TYR:HD2	1.66	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:137:ILE:HG22	1:O:150:ASP:HB2	1.83	0.61
1:A:121:GLN:O	1:A:124:THR:HB	2.00	0.60
1:E:61:GLN:O	1:E:64:ILE:HG22	2.00	0.60
1:A:88:LEU:HD21	1:A:120:MET:SD	2.41	0.60
1:K:18:ASP:OD2	1:K:20:ARG:HD3	2.01	0.60
1:D:186:GLU:O	1:D:190:VAL:HG12	2.01	0.60
1:L:21:LEU:O	1:L:24:VAL:HG12	2.02	0.60
1:K:52:LYS:HE3	1:K:64:ILE:HG23	1.83	0.60
1:L:43:ALA:HB2	1:L:185:PRO:HA	1.84	0.60
1:L:156:THR:HG23	1:M:82:VAL:HG11	1.82	0.60
2:S:38:ASP:HB3	2:S:41:THR:CG2	2.32	0.60
2:X:62:GLU:HG2	2:X:82:LEU:HD21	1.82	0.60
1:H:170:ASP:O	1:H:173:VAL:HG12	2.01	0.60
1:K:21:LEU:HD11	1:L:130:ARG:HD2	1.83	0.60
1:C:43:ALA:HB2	1:C:185:PRO:HA	1.82	0.60
2:W:178:ILE:HB	2:W:184:TYR:HA	1.83	0.60
1:D:168:GLY:O	1:D:172:VAL:HG12	2.02	0.60
1:I:135:SER:OG	1:I:153:PRO:HD3	2.01	0.60
1:J:18:ASP:OD2	1:J:20:ARG:HD3	2.00	0.60
2:1:38:ASP:HB3	2:1:41:THR:CG2	2.29	0.60
1:E:24:VAL:O	1:E:27:ALA:HB3	2.02	0.60
1:C:198:LYS:O	1:C:202:GLU:HB2	2.01	0.60
1:H:98:GLN:O	1:H:102:THR:HG22	2.01	0.60
1:N:135:SER:OG	1:N:153:PRO:HD3	2.01	0.60
1:A:49:ILE:HD12	1:A:211:GLU:O	2.01	0.60
2:V:111:PHE:CE2	2:V:121:GLU:HB2	2.37	0.60
1:G:61:GLN:O	1:G:64:ILE:HG22	2.01	0.60
2:Q:38:ASP:HB2	2:Q:63:LEU:HD23	1.84	0.60
1:A:28:ARG:O	1:A:31:VAL:HG22	2.02	0.60
1:A:42:PHE:HD1	1:A:43:ALA:N	2.00	0.60
1:C:198:LYS:HG2	1:C:202:GLU:HG2	1.82	0.60
1:K:88:LEU:HD13	1:K:132:TYR:CD2	2.36	0.60
1:I:49:ILE:HD12	1:I:211:GLU:O	2.01	0.60
2:S:3:THR:HB	2:S:16:THR:HG22	1.83	0.60
1:O:98:GLN:O	1:O:101:VAL:HG12	2.02	0.60
1:N:52:LYS:HB3	1:N:209:ALA:O	2.01	0.60
1:N:61:GLN:O	1:N:64:ILE:HG22	2.02	0.60
1:C:84:ASP:O	1:C:87:VAL:HG12	2.02	0.60
2:S:32:LYS:HE2	2:S:34:LEU:O	2.01	0.60
2:X:43:MET:HE1	2:X:56:VAL:HA	1.83	0.60
1:D:52:LYS:HA	1:D:66:LYS:NZ	2.17	0.60
1:O:52:LYS:HE3	1:O:64:ILE:HG23	1.83	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:X:2:THR:HG22	2:X:169:SER:OG	2.02	0.60
1:K:186:GLU:O	1:K:190:VAL:HG12	2.01	0.59
2:V:62:GLU:HG2	2:V:82:LEU:HD21	1.82	0.59
2:Y:133:PHE:CZ	2:Y:165:ARG:HB3	2.37	0.59
2:Y:18:ARG:HE	2:Y:30:ASN:HD22	1.49	0.59
1:N:170:ASP:O	1:N:173:VAL:HG12	2.02	0.59
2:1:20:VAL:HG13	2:1:28:HIS:HB2	1.83	0.59
1:I:186:GLU:O	1:I:190:VAL:HG12	2.03	0.59
2:T:133:PHE:CZ	2:T:165:ARG:HB3	2.36	0.59
2:U:178:ILE:HB	2:U:184:TYR:HA	1.84	0.59
2:Z:12:VAL:HG13	2:Z:178:ILE:HG23	1.82	0.59
2:Y:111:PHE:CE2	2:Y:121:GLU:HB2	2.37	0.59
2:R:152:VAL:O	2:R:156:ILE:HG13	2.03	0.59
2:Z:37:ILE:HD11	2:Z:59:MET:HB3	1.84	0.59
1:A:52:LYS:HZ3	1:A:62:ASN:HA	1.66	0.59
2:W:124:TYR:HD2	2:W:138:LEU:HD23	1.67	0.59
1:M:52:LYS:HB3	1:M:209:ALA:O	2.01	0.59
1:J:61:GLN:O	1:J:64:ILE:HG22	2.00	0.59
1:A:142:ASP:HD2	1:A:145:GLY:H	1.49	0.59
1:O:49:ILE:HD12	1:O:211:GLU:O	2.01	0.59
2:Y:2:THR:HG22	2:Y:169:SER:OG	2.02	0.59
1:K:98:GLN:O	1:K:102:THR:HG22	2.03	0.59
2:T:38:ASP:HB3	2:T:41:THR:CG2	2.27	0.59
2:1:66:TYR:CZ	2:1:70:ARG:HD2	2.37	0.59
1:O:49:ILE:HD11	1:O:210:PRO:HB3	1.83	0.59
1:M:94:ILE:HG13	1:M:95:SER:N	2.17	0.59
2:R:38:ASP:HB3	2:R:41:THR:CG2	2.26	0.59
1:A:49:ILE:HD11	1:A:210:PRO:HB3	1.85	0.59
2:R:159:ILE:O	2:R:163:LYS:HG3	2.02	0.59
2:R:32:LYS:HE2	2:R:34:LEU:O	2.02	0.59
2:U:3:THR:HB	2:U:16:THR:HG22	1.83	0.59
1:F:121:GLN:O	1:F:124:THR:HB	2.03	0.59
2:R:124:TYR:CD2	2:R:138:LEU:HD23	2.37	0.59
1:G:95:SER:OG	1:G:115:ARG:HD3	2.03	0.59
2:2:36:GLN:HB2	2:2:184:TYR:CE1	2.37	0.59
1:G:148:LEU:O	1:G:159:GLU:HG3	2.03	0.59
2:B:8:LEU:O	2:B:8:LEU:HD12	2.03	0.59
1:M:136:LEU:HD13	1:M:138:PHE:CE2	2.37	0.59
1:F:95:SER:OG	1:F:115:ARG:HD3	2.03	0.59
2:P:123:ILE:HD13	2:P:123:ILE:H	1.68	0.58
2:Q:7:THR:HB	2:Q:123:ILE:O	2.03	0.58
1:N:124:THR:HG22	1:O:130:ARG:HH21	1.68	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:42:PHE:HB2	1:I:184:LEU:O	2.03	0.58
1:E:176:LEU:HB3	1:F:58:LEU:HD21	1.85	0.58
1:I:34:GLY:O	1:I:167:SER:HB2	2.03	0.58
1:E:21:LEU:HD11	1:F:130:ARG:HD2	1.85	0.58
2:2:3:THR:OG1	2:2:127:THR:HG22	2.02	0.58
1:L:18:ASP:OD2	1:L:20:ARG:HD3	2.03	0.58
2:P:123:ILE:HG12	2:P:124:TYR:CD1	2.32	0.58
1:I:184:LEU:HD23	1:I:189:ALA:HA	1.86	0.58
1:L:61:GLN:O	1:L:64:ILE:HG22	2.04	0.58
1:K:121:GLN:O	1:K:124:THR:HB	2.04	0.58
1:O:81:LEU:HD23	1:O:133:GLY:HA3	1.84	0.58
2:B:123:ILE:HD13	2:B:123:ILE:H	1.68	0.58
2:P:149:ASP:O	2:P:152:VAL:HG12	2.03	0.58
2:R:123:ILE:H	2:R:123:ILE:HD13	1.68	0.58
2:2:76:ILE:HG22	2:2:111:PHE:CE2	2.38	0.58
1:G:42:PHE:HB2	1:G:184:LEU:O	2.03	0.58
1:I:124:THR:HG22	1:J:130:ARG:HH21	1.69	0.58
1:G:49:ILE:HD11	1:G:210:PRO:HB3	1.86	0.58
2:W:133:PHE:CZ	2:W:165:ARG:HB3	2.39	0.58
1:D:78:THR:HG21	1:D:85:ALA:HB1	1.85	0.58
2:R:131:SER:O	2:R:134:VAL:HG13	2.04	0.58
1:G:108:ASN:HB3	2:U:70:ARG:HG2	1.86	0.58
2:S:28:HIS:CD2	2:T:120:VAL:HG11	2.39	0.58
1:F:124:THR:HG22	1:G:130:ARG:NH2	2.18	0.58
1:N:21:LEU:O	1:N:25:GLU:HG2	2.03	0.58
2:2:179:THR:HG23	2:2:182:ASP:H	1.69	0.58
2:Z:133:PHE:CZ	2:Z:165:ARG:HB3	2.39	0.58
2:V:28:HIS:CD2	2:W:120:VAL:HG11	2.39	0.58
1:M:42:PHE:HB2	1:M:184:LEU:O	2.03	0.57
1:D:101:VAL:HG23	2:Q:57:ARG:HB3	1.85	0.57
2:B:152:VAL:O	2:B:156:ILE:HG13	2.04	0.57
2:2:149:ASP:O	2:2:152:VAL:HG12	2.04	0.57
1:L:121:GLN:O	1:L:124:THR:HB	2.04	0.57
2:R:20:VAL:HG22	2:R:28:HIS:HB2	1.86	0.57
2:X:179:THR:HG23	2:X:182:ASP:H	1.69	0.57
1:L:186:GLU:O	1:L:190:VAL:HG12	2.05	0.57
1:I:95:SER:OG	1:I:115:ARG:HD3	2.04	0.57
2:Z:59:MET:CE	2:Z:82:LEU:HD23	2.34	0.57
1:O:70:ILE:HD12	1:O:74:VAL:HG22	1.86	0.57
2:Y:12:VAL:HG13	2:Y:178:ILE:HG23	1.85	0.57
1:G:98:GLN:O	1:G:102:THR:HG22	2.04	0.57
1:F:61:GLN:O	1:F:64:ILE:HG22	2.05	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:P:51:ASP:O	2:P:55:LEU:HB2	2.04	0.57
1:A:135:SER:OG	1:A:153:PRO:HD3	2.04	0.57
1:J:42:PHE:HD1	1:J:43:ALA:N	2.02	0.57
1:I:49:ILE:HD11	1:I:210:PRO:HB3	1.86	0.57
1:J:49:ILE:HD11	1:J:210:PRO:HB3	1.85	0.57
2:1:49:VAL:HG23	2:1:50:GLY:H	1.68	0.57
1:O:135:SER:OG	1:O:153:PRO:HD3	2.04	0.57
1:A:23:GLN:HE21	1:H:15:PHE:HB2	1.70	0.57
1:H:180:TYR:HA	1:H:192:LEU:HD21	1.85	0.57
1:L:78:THR:HG21	1:L:85:ALA:HB1	1.86	0.57
2:T:75:PRO:O	2:T:78:ALA:HB3	2.04	0.57
1:G:124:THR:HG22	1:H:130:ARG:NH2	2.16	0.57
2:V:20:VAL:HG13	2:V:28:HIS:HB2	1.85	0.57
1:C:159:GLU:HG2	1:D:60:GLU:HG3	1.85	0.57
1:F:144:ILE:HD12	1:F:147:ARG:NH1	2.19	0.57
2:W:55:LEU:HD21	2:W:87:LEU:HD11	1.87	0.57
2:Q:199:LEU:HB3	2:Q:201:LEU:HD13	1.85	0.57
1:K:81:LEU:HD23	1:K:133:GLY:HA3	1.85	0.57
2:W:20:VAL:HG13	2:W:28:HIS:HB2	1.87	0.57
2:T:28:HIS:CD2	2:U:120:VAL:HG11	2.39	0.57
2:Q:160:SER:O	2:Q:163:LYS:HB2	2.04	0.57
1:L:35:SER:O	1:L:166:GLY:HA3	2.05	0.57
1:E:49:ILE:HD13	1:E:212:ILE:HB	1.87	0.57
2:W:43:MET:CE	2:W:56:VAL:HG23	2.33	0.57
1:H:76:ALA:HB2	1:H:138:PHE:CD1	2.40	0.57
2:2:7:THR:HB	2:2:123:ILE:O	2.05	0.57
1:A:35:SER:O	1:A:166:GLY:HA3	2.03	0.57
2:R:45:ILE:HG12	2:R:52:ALA:HB1	1.87	0.57
1:D:15:PHE:HD2	1:E:23:GLN:HE21	1.53	0.57
1:G:42:PHE:HD1	1:G:43:ALA:N	2.03	0.57
1:E:52:LYS:HZ2	1:E:62:ASN:HA	1.69	0.57
1:I:69:LEU:HD23	1:I:75:ALA:HB2	1.87	0.57
1:E:94:ILE:HG13	1:E:95:SER:N	2.20	0.57
2:S:43:MET:CE	2:S:56:VAL:HG23	2.35	0.56
2:B:37:ILE:HD11	2:B:59:MET:CG	2.35	0.56
2:Z:178:ILE:HB	2:Z:184:TYR:HA	1.86	0.56
2:Q:3:THR:OG1	2:Q:127:THR:HG22	2.05	0.56
2:U:174:ASP:HA	2:U:192:ILE:HD13	1.87	0.56
1:I:21:LEU:O	1:I:24:VAL:HG12	2.05	0.56
2:Z:152:VAL:O	2:Z:156:ILE:HG13	2.05	0.56
2:V:6:ILE:HD11	2:V:142:TYR:HD1	1.68	0.56
2:U:124:TYR:CD1	2:U:138:LEU:HD23	2.39	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:R:59:MET:HE2	2:R:79:VAL:HG23	1.88	0.56
2:R:18:ARG:HE	2:R:30:ASN:HD22	1.52	0.56
1:J:88:LEU:HD13	1:J:132:TYR:CD2	2.39	0.56
2:X:133:PHE:CZ	2:X:165:ARG:HB3	2.40	0.56
2:U:152:VAL:O	2:U:156:ILE:HG13	2.05	0.56
2:1:75:PRO:O	2:1:78:ALA:HB3	2.06	0.56
1:F:175:PHE:CD2	1:F:196:ALA:HA	2.39	0.56
2:S:179:THR:HG23	2:S:182:ASP:H	1.71	0.56
2:T:178:ILE:HB	2:T:184:TYR:HA	1.87	0.56
1:O:184:LEU:HD23	1:O:189:ALA:HA	1.87	0.56
2:2:62:GLU:HG2	2:2:82:LEU:HD21	1.86	0.56
1:A:43:ALA:HB2	1:A:185:PRO:HA	1.88	0.56
1:E:81:LEU:HD23	1:E:133:GLY:HA3	1.85	0.56
1:L:76:ALA:HB2	1:L:138:PHE:CD2	2.41	0.56
1:I:108:ASN:CB	2:W:70:ARG:HG2	2.33	0.56
1:H:52:LYS:HB3	1:H:209:ALA:O	2.05	0.56
2:2:123:ILE:HD13	2:2:123:ILE:H	1.70	0.56
2:X:26:ILE:HD13	2:X:26:ILE:C	2.26	0.56
2:Q:123:ILE:HG12	2:Q:124:TYR:HD1	1.69	0.56
1:I:38:LEU:HG	1:I:49:ILE:HG23	1.86	0.56
2:B:174:ASP:HA	2:B:192:ILE:HD13	1.88	0.56
2:T:32:LYS:HE2	2:T:34:LEU:O	2.06	0.56
2:B:120:VAL:HG11	2:U:28:HIS:CD2	2.41	0.56
2:B:70:ARG:HG2	1:H:108:ASN:CB	2.36	0.56
1:E:49:ILE:HD12	1:E:211:GLU:O	2.05	0.56
1:I:198:LYS:HG2	1:I:202:GLU:HG2	1.88	0.56
2:Q:167:SER:HB2	2:W:167:SER:HB2	1.88	0.56
2:1:174:ASP:HA	2:1:192:ILE:HD13	1.87	0.56
1:K:61:GLN:O	1:K:64:ILE:HG22	2.06	0.56
1:O:52:LYS:HZ1	1:O:62:ASN:HA	1.71	0.56
1:H:137:ILE:HG22	1:H:150:ASP:HB2	1.86	0.56
2:X:149:ASP:O	2:X:152:VAL:HG12	2.06	0.56
2:B:66:TYR:HH	1:H:107:VAL:HG11	1.69	0.55
2:V:152:VAL:O	2:V:156:ILE:HG13	2.06	0.55
1:L:49:ILE:HD12	1:L:211:GLU:O	2.06	0.55
1:J:21:LEU:HD11	1:K:130:ARG:HD2	1.88	0.55
1:I:61:GLN:O	1:I:64:ILE:HG22	2.06	0.55
1:N:108:ASN:HB3	2:2:70:ARG:HG2	1.88	0.55
1:L:38:LEU:HA	1:L:164:ALA:HA	1.87	0.55
2:U:26:ILE:HD13	2:U:26:ILE:C	2.27	0.55
2:Z:123:ILE:HD13	2:Z:123:ILE:H	1.71	0.55
1:G:85:ALA:O	1:G:89:VAL:HG23	2.06	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:42:PHE:HD1	1:H:43:ALA:N	2.04	0.55
1:H:186:GLU:O	1:H:190:VAL:HG12	2.06	0.55
2:Z:6:ILE:HD11	2:Z:142:TYR:CD1	2.41	0.55
1:G:70:ILE:HD12	1:G:74:VAL:HG22	1.88	0.55
2:X:37:ILE:HD11	2:X:59:MET:CG	2.36	0.55
1:L:175:PHE:CD2	1:L:196:ALA:HA	2.41	0.55
1:O:186:GLU:O	1:O:190:VAL:HG12	2.06	0.55
2:Z:59:MET:HE3	2:Z:82:LEU:HD23	1.88	0.55
1:D:52:LYS:HZ3	1:D:62:ASN:HA	1.71	0.55
2:2:18:ARG:HE	2:2:30:ASN:HD22	1.54	0.55
2:T:76:ILE:HG21	2:T:109:HIS:HB2	1.87	0.55
2:P:17:GLU:O	2:P:33:LYS:HD2	2.07	0.55
2:T:37:ILE:HD11	2:T:59:MET:CB	2.35	0.55
2:Z:124:TYR:CD2	2:Z:138:LEU:HD23	2.41	0.55
1:K:108:ASN:CB	2:Y:70:ARG:HG2	2.37	0.55
2:X:28:HIS:CD2	2:Y:120:VAL:HG11	2.42	0.55
1:I:130:ARG:NH2	1:O:124:THR:HG22	2.15	0.55
1:H:42:PHE:HB2	1:H:184:LEU:O	2.06	0.55
1:E:170:ASP:O	1:E:173:VAL:HG12	2.07	0.55
1:G:156:THR:HG23	1:H:82:VAL:HG11	1.88	0.55
1:N:15:PHE:HB2	1:O:23:GLN:HE21	1.72	0.55
2:U:66:TYR:CZ	2:U:70:ARG:HD2	2.41	0.55
1:M:52:LYS:HZ2	1:M:62:ASN:HA	1.71	0.55
1:O:48:LEU:HD13	1:O:139:ALA:HB3	1.89	0.55
1:F:38:LEU:HG	1:F:49:ILE:HG23	1.89	0.55
2:1:131:SER:O	2:1:134:VAL:HG13	2.07	0.55
1:C:121:GLN:O	1:C:124:THR:HB	2.06	0.55
1:G:175:PHE:CD2	1:G:196:ALA:HA	2.41	0.55
1:L:137:ILE:HG22	1:L:150:ASP:HB2	1.89	0.55
1:A:70:ILE:HD12	1:A:74:VAL:HG22	1.88	0.55
1:D:26:TYR:O	1:D:29:GLU:HB2	2.06	0.55
1:A:95:SER:OG	1:A:115:ARG:HD3	2.07	0.55
1:E:184:LEU:HD23	1:E:189:ALA:HA	1.87	0.54
1:F:52:LYS:HZ2	1:F:62:ASN:HA	1.72	0.54
1:M:49:ILE:HD11	1:M:210:PRO:HB3	1.88	0.54
2:S:123:ILE:H	2:S:123:ILE:HD13	1.72	0.54
1:H:21:LEU:O	1:H:25:GLU:HG2	2.08	0.54
1:I:42:PHE:HD1	1:I:43:ALA:N	2.05	0.54
1:C:165:ILE:HG13	1:C:166:GLY:H	1.73	0.54
1:K:52:LYS:HA	1:K:66:LYS:NZ	2.23	0.54
1:D:52:LYS:HZ2	1:D:62:ASN:HA	1.70	0.54
2:B:62:GLU:HG2	2:B:82:LEU:HD21	1.87	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:78:THR:HG21	1:O:85:ALA:HB1	1.88	0.54
2:2:26:ILE:C	2:2:26:ILE:HD13	2.27	0.54
1:C:38:LEU:HA	1:C:164:ALA:HA	1.89	0.54
2:Z:124:TYR:HD2	2:Z:138:LEU:HD23	1.73	0.54
2:1:7:THR:HB	2:1:123:ILE:O	2.08	0.54
1:K:198:LYS:HG2	1:K:202:GLU:HG2	1.89	0.54
2:B:159:ILE:O	2:B:163:LYS:HG3	2.08	0.54
2:S:132:PRO:HA	2:V:133:PHE:HE1	1.72	0.54
2:B:179:THR:HG23	2:B:182:ASP:H	1.73	0.54
1:A:124:THR:HG22	1:C:130:ARG:NH2	2.23	0.54
1:C:109:ILE:CG2	1:C:147:ARG:HD3	2.37	0.54
1:C:61:GLN:O	1:C:64:ILE:HG22	2.08	0.54
1:I:109:ILE:CG2	1:I:147:ARG:HD3	2.37	0.54
1:H:174:SER:O	1:H:177:GLU:HB3	2.08	0.54
2:Z:45:ILE:HG12	2:Z:52:ALA:HB1	1.90	0.54
1:D:38:LEU:HA	1:D:164:ALA:HA	1.89	0.54
1:M:61:GLN:OE1	1:M:62:ASN:HB3	2.07	0.54
2:R:62:GLU:HG2	2:R:82:LEU:HD21	1.90	0.54
2:W:193:GLU:O	2:W:196:ILE:HB	2.08	0.54
1:J:69:LEU:HD23	1:J:75:ALA:HB2	1.89	0.54
1:L:94:ILE:HG13	1:L:95:SER:N	2.23	0.54
1:A:143:GLN:HE22	1:A:143:GLN:HA	1.73	0.54
2:Z:62:GLU:HG2	2:Z:82:LEU:HD21	1.89	0.54
1:F:187:LYS:O	1:F:190:VAL:HG13	2.08	0.54
2:Y:49:VAL:HG23	2:Y:50:GLY:H	1.73	0.54
2:Q:131:SER:O	2:Q:134:VAL:HG13	2.08	0.54
2:W:59:MET:SD	2:W:83:LEU:HD13	2.48	0.54
1:K:137:ILE:HG22	1:K:150:ASP:HB2	1.89	0.54
2:V:15:ALA:HB2	2:V:175:VAL:HB	1.89	0.54
1:A:42:PHE:HB2	1:A:184:LEU:O	2.08	0.54
1:A:198:LYS:HG2	1:A:202:GLU:HG2	1.88	0.54
2:B:6:ILE:HD11	2:B:142:TYR:CD1	2.42	0.54
1:I:174:SER:O	1:I:177:GLU:HB3	2.08	0.54
1:O:51:ASP:HB3	1:O:53:LYS:NZ	2.23	0.54
2:X:131:SER:O	2:X:134:VAL:HG13	2.08	0.54
1:I:31:VAL:HA	1:I:80:GLY:HA2	1.90	0.54
1:E:107:VAL:HG11	2:S:66:TYR:HH	1.73	0.53
1:C:95:SER:OG	1:C:115:ARG:HD3	2.08	0.53
1:I:144:ILE:HD12	1:I:147:ARG:NH1	2.22	0.53
2:U:199:LEU:HB3	2:U:201:LEU:HD13	1.90	0.53
2:S:45:ILE:HG12	2:S:52:ALA:HB1	1.90	0.53
1:O:168:GLY:O	1:O:172:VAL:HG12	2.09	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:174:SER:O	1:K:177:GLU:HB3	2.08	0.53
1:E:71:ASP:OD2	1:E:74:VAL:HG12	2.08	0.53
2:V:55:LEU:HD21	2:V:87:LEU:HD11	1.90	0.53
1:N:88:LEU:HD13	1:N:132:TYR:CD2	2.42	0.53
1:H:97:GLN:OE1	1:H:97:GLN:HA	2.07	0.53
1:L:52:LYS:HE3	1:L:64:ILE:HG23	1.89	0.53
1:E:180:TYR:HA	1:E:192:LEU:HD21	1.90	0.53
1:D:88:LEU:HD13	1:D:132:TYR:CD2	2.44	0.53
2:S:62:GLU:HG2	2:S:82:LEU:HD21	1.91	0.53
1:G:61:GLN:OE1	1:G:62:ASN:HB3	2.09	0.53
2:Z:19:ARG:HE	2:Z:26:ILE:HG13	1.74	0.53
2:U:149:ASP:O	2:U:152:VAL:HG12	2.08	0.53
1:A:49:ILE:HD13	1:A:212:ILE:HB	1.89	0.53
2:B:26:ILE:HD13	2:B:26:ILE:C	2.28	0.53
2:Q:3:THR:HB	2:Q:16:THR:HG22	1.90	0.53
2:W:26:ILE:HD13	2:W:26:ILE:O	2.08	0.53
1:K:124:THR:HG22	1:L:130:ARG:NH2	2.20	0.53
2:R:141:GLN:NE2	2:W:141:GLN:HE22	2.07	0.53
2:W:37:ILE:HD11	2:W:59:MET:CG	2.39	0.53
2:W:35:PHE:CE2	2:W:45:ILE:HD12	2.43	0.53
2:Y:26:ILE:HD13	2:Y:26:ILE:C	2.29	0.53
1:N:113:VAL:HG22	1:N:157:ILE:HD12	1.91	0.53
2:P:3:THR:HB	2:P:16:THR:HG22	1.90	0.53
2:1:124:TYR:CD2	2:1:138:LEU:HD23	2.44	0.53
1:J:202:GLU:HG3	1:J:205:GLU:O	2.08	0.53
2:B:133:PHE:CZ	2:B:165:ARG:HB3	2.43	0.53
2:Q:32:LYS:HE2	2:Q:34:LEU:O	2.08	0.53
2:Z:174:ASP:HA	2:Z:192:ILE:HD13	1.91	0.53
1:K:15:PHE:HB2	1:L:23:GLN:HE21	1.74	0.53
1:E:109:ILE:CG2	1:E:147:ARG:HD3	2.38	0.53
2:2:103:GLY:HA2	2:2:178:ILE:HD13	1.90	0.53
1:J:43:ALA:HB2	1:J:185:PRO:HA	1.91	0.53
1:C:144:ILE:HD12	1:C:147:ARG:NH1	2.24	0.53
2:1:111:PHE:CE2	2:1:121:GLU:HB2	2.44	0.53
2:S:26:ILE:HD13	2:S:26:ILE:O	2.09	0.53
2:Q:26:ILE:C	2:Q:26:ILE:HD13	2.29	0.53
1:J:42:PHE:CD1	1:J:43:ALA:N	2.76	0.53
1:J:198:LYS:HG3	1:J:207:LEU:HD22	1.91	0.53
1:C:165:ILE:HG13	1:C:166:GLY:N	2.24	0.53
2:S:35:PHE:CE2	2:S:45:ILE:HD12	2.43	0.53
1:E:175:PHE:CD2	1:E:196:ALA:HA	2.44	0.53
1:J:95:SER:OG	1:J:115:ARG:HD3	2.09	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:X:50:GLY:O	2:X:54:VAL:HG12	2.08	0.53
1:F:41:LYS:HE3	1:F:160:TYR:O	2.09	0.53
1:G:52:LYS:HZ2	1:G:62:ASN:HA	1.70	0.52
1:H:184:LEU:HD23	1:H:189:ALA:HA	1.92	0.52
2:S:133:PHE:HE1	2:V:132:PRO:HA	1.74	0.52
2:R:26:ILE:C	2:R:26:ILE:HD13	2.29	0.52
2:V:133:PHE:CZ	2:V:165:ARG:HB3	2.43	0.52
1:F:159:GLU:HG2	1:G:60:GLU:HG3	1.91	0.52
1:K:170:ASP:O	1:K:173:VAL:HG12	2.09	0.52
2:T:6:ILE:HD11	2:T:142:TYR:CD1	2.44	0.52
1:J:52:LYS:HB3	1:J:209:ALA:O	2.10	0.52
2:W:59:MET:HE3	2:W:82:LEU:HD23	1.91	0.52
1:M:35:SER:O	1:M:166:GLY:HA3	2.10	0.52
2:U:131:SER:O	2:U:134:VAL:HG13	2.09	0.52
2:T:55:LEU:HD23	2:T:99:LEU:HD11	1.91	0.52
2:Q:37:ILE:HD11	2:Q:59:MET:CB	2.38	0.52
2:2:76:ILE:HG22	2:2:111:PHE:HE2	1.74	0.52
1:F:198:LYS:HG3	1:F:207:LEU:HD22	1.90	0.52
1:J:24:VAL:O	1:J:28:ARG:HG3	2.09	0.52
2:R:37:ILE:HD11	2:R:59:MET:HB3	1.90	0.52
1:A:130:ARG:HH21	1:H:124:THR:HG22	1.74	0.52
2:R:173:ILE:C	2:R:173:ILE:HD13	2.30	0.52
1:A:144:ILE:HD12	1:A:147:ARG:NH1	2.24	0.52
2:Q:28:HIS:CD2	2:R:120:VAL:HG11	2.44	0.52
1:C:180:TYR:HA	1:C:192:LEU:HD21	1.91	0.52
1:L:21:LEU:HD11	1:M:130:ARG:HD2	1.91	0.52
1:A:42:PHE:CD1	1:A:43:ALA:N	2.78	0.52
1:M:42:PHE:HD1	1:M:43:ALA:N	2.08	0.52
1:L:95:SER:OG	1:L:115:ARG:HD3	2.09	0.52
2:B:3:THR:HB	2:B:16:THR:HG22	1.90	0.52
2:P:18:ARG:HE	2:P:30:ASN:HD22	1.57	0.52
1:F:21:LEU:O	1:F:25:GLU:HG2	2.09	0.52
2:R:103:GLY:HA2	2:R:178:ILE:HD13	1.91	0.52
1:G:43:ALA:HB2	1:G:185:PRO:HA	1.91	0.52
1:D:24:VAL:O	1:D:28:ARG:HG3	2.09	0.52
2:P:45:ILE:CG1	2:P:52:ALA:HB1	2.39	0.52
1:G:94:ILE:HG13	1:G:95:SER:N	2.24	0.52
1:G:144:ILE:HD12	1:G:147:ARG:NH1	2.24	0.52
2:1:3:THR:HB	2:1:16:THR:HG22	1.91	0.52
1:L:109:ILE:CG2	1:L:147:ARG:HD3	2.39	0.52
1:J:61:GLN:OE1	1:J:62:ASN:HB3	2.07	0.52
1:L:42:PHE:HB2	1:L:184:LEU:O	2.09	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:R:15:ALA:HB2	2:R:175:VAL:HB	1.92	0.52
2:S:55:LEU:HD21	2:S:87:LEU:HD11	1.92	0.52
2:U:18:ARG:HE	2:U:30:ASN:HD22	1.58	0.52
1:M:108:ASN:HB3	2:1:70:ARG:HG2	1.91	0.52
1:H:61:GLN:OE1	1:H:62:ASN:HB3	2.09	0.52
1:A:70:ILE:HB	1:A:74:VAL:HG13	1.92	0.52
1:A:160:TYR:CD2	1:A:163:THR:HB	2.45	0.52
1:H:160:TYR:CD2	1:H:163:THR:HB	2.44	0.52
1:G:21:LEU:O	1:G:25:GLU:HG2	2.09	0.52
1:H:135:SER:OG	1:H:153:PRO:HD3	2.10	0.52
2:P:63:LEU:HD11	2:P:74:MET:SD	2.48	0.52
2:Y:179:THR:HG23	2:Y:182:ASP:H	1.75	0.52
1:G:160:TYR:CD2	1:G:163:THR:HB	2.45	0.52
2:W:137:VAL:HG21	2:W:158:ALA:HA	1.90	0.52
2:R:165:ARG:HA	2:V:26:ILE:HG23	1.92	0.52
2:1:59:MET:HE2	2:1:79:VAL:HG23	1.91	0.52
1:E:175:PHE:C	1:E:175:PHE:HD1	2.14	0.52
2:R:36:GLN:HB2	2:R:184:TYR:CE1	2.43	0.52
2:Q:124:TYR:CD2	2:Q:138:LEU:HD23	2.45	0.52
2:V:103:GLY:HA2	2:V:178:ILE:HD11	1.91	0.52
2:W:59:MET:CE	2:W:82:LEU:HD23	2.40	0.52
1:H:214:SER:HG	1:H:224:TYR:HE1	1.56	0.52
2:Q:189:THR:HG23	2:Q:190:ASP:N	2.25	0.52
2:S:103:GLY:HA2	2:S:178:ILE:CD1	2.39	0.52
2:R:53:GLN:O	2:R:56:VAL:HG12	2.10	0.52
1:H:49:ILE:HD11	1:H:210:PRO:HB3	1.92	0.52
1:F:108:ASN:CB	2:T:70:ARG:HG2	2.41	0.51
1:M:109:ILE:HG22	1:M:147:ARG:HD3	1.92	0.51
2:W:131:SER:O	2:W:134:VAL:HG13	2.10	0.51
1:M:113:VAL:HG22	1:M:157:ILE:HD12	1.91	0.51
2:U:2:THR:HG22	2:U:169:SER:OG	2.10	0.51
1:J:137:ILE:HG22	1:J:150:ASP:HA	1.91	0.51
2:1:19:ARG:NE	2:1:26:ILE:HG13	2.25	0.51
2:T:20:VAL:CG1	2:T:28:HIS:HB2	2.36	0.51
2:2:111:PHE:CE1	2:2:121:GLU:HB2	2.46	0.51
1:J:21:LEU:O	1:J:25:GLU:HG2	2.10	0.51
1:D:15:PHE:HD2	1:E:23:GLN:NE2	2.09	0.51
2:Y:152:VAL:O	2:Y:156:ILE:HG13	2.10	0.51
1:J:26:TYR:O	1:J:29:GLU:HB2	2.09	0.51
2:1:37:ILE:HD11	2:1:59:MET:CB	2.35	0.51
1:A:85:ALA:O	1:A:89:VAL:HG23	2.11	0.51
1:N:52:LYS:HZ2	1:N:62:ASN:HA	1.75	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:175:PHE:CD1	1:E:175:PHE:C	2.83	0.51
2:Y:28:HIS:CD2	2:Z:120:VAL:HG11	2.45	0.51
1:J:38:LEU:HA	1:J:164:ALA:HA	1.92	0.51
2:W:173:ILE:C	2:W:173:ILE:HD13	2.30	0.51
1:A:21:LEU:O	1:A:24:VAL:HG12	2.10	0.51
1:I:70:ILE:HB	1:I:74:VAL:HG13	1.91	0.51
2:X:174:ASP:HA	2:X:192:ILE:HD13	1.91	0.51
1:L:69:LEU:HD23	1:L:75:ALA:HB2	1.93	0.51
1:I:175:PHE:CD1	1:I:175:PHE:C	2.83	0.51
1:K:143:GLN:HA	1:K:143:GLN:HE22	1.76	0.51
1:L:135:SER:OG	1:L:153:PRO:HD3	2.11	0.51
1:K:165:ILE:HG13	1:K:166:GLY:N	2.25	0.51
1:H:18:ASP:OD2	1:H:20:ARG:HD3	2.11	0.51
1:E:14:VAL:HB	1:F:23:GLN:OE1	2.10	0.51
2:B:116:ALA:O	2:U:50:GLY:HA3	2.11	0.51
2:V:123:ILE:HG12	2:V:124:TYR:CD1	2.37	0.51
2:S:124:TYR:HD2	2:S:138:LEU:HD23	1.76	0.51
1:G:198:LYS:HG2	1:G:202:GLU:HG2	1.91	0.51
1:J:187:LYS:O	1:J:190:VAL:HG13	2.10	0.51
1:J:109:ILE:CG2	1:J:147:ARG:HD3	2.40	0.51
1:F:34:GLY:O	1:F:167:SER:HB2	2.11	0.51
1:J:174:SER:O	1:J:177:GLU:HB3	2.10	0.51
2:B:173:ILE:C	2:B:173:ILE:HD13	2.31	0.51
1:H:24:VAL:O	1:H:28:ARG:HG3	2.09	0.51
2:B:45:ILE:CG1	2:B:52:ALA:HB1	2.39	0.51
1:I:52:LYS:HB3	1:I:209:ALA:O	2.11	0.51
1:C:113:VAL:HG22	1:C:157:ILE:HD12	1.92	0.51
2:R:174:ASP:HA	2:R:192:ILE:HD13	1.92	0.51
2:S:167:SER:HB2	2:2:167:SER:HB2	1.92	0.51
1:G:35:SER:O	1:G:166:GLY:HA3	2.11	0.51
2:R:25:PHE:C	2:R:25:PHE:CD1	2.80	0.51
2:X:123:ILE:HG12	2:X:124:TYR:CD1	2.39	0.51
1:D:198:LYS:HG2	1:D:202:GLU:HG2	1.93	0.51
1:M:159:GLU:HG2	1:N:60:GLU:HG3	1.92	0.51
1:A:156:THR:HG23	1:C:82:VAL:HG11	1.92	0.51
1:F:184:LEU:HD23	1:F:189:ALA:HA	1.92	0.51
1:K:49:ILE:HD11	1:K:210:PRO:HB3	1.92	0.51
2:V:174:ASP:HA	2:V:192:ILE:HD13	1.93	0.51
2:T:49:VAL:HG23	2:T:50:GLY:N	2.25	0.51
1:G:137:ILE:HG22	1:G:150:ASP:CB	2.40	0.51
1:C:52:LYS:NZ	1:C:62:ASN:HA	2.26	0.51
2:2:124:TYR:CD1	2:2:138:LEU:HD23	2.46	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:110:GLU:O	1:E:113:VAL:HG13	2.10	0.51
2:1:6:ILE:HD11	2:1:142:TYR:CD1	2.45	0.51
1:A:191:THR:O	1:A:194:ILE:HG22	2.11	0.51
2:Z:123:ILE:HG12	2:Z:124:TYR:CD1	2.35	0.51
2:Q:160:SER:HA	2:Q:163:LYS:HD3	1.93	0.51
1:N:49:ILE:HD11	1:N:210:PRO:HB3	1.93	0.51
1:F:40:MET:HA	1:F:162:ALA:HA	1.93	0.51
1:E:143:GLN:HE22	1:E:143:GLN:HA	1.76	0.51
1:F:24:VAL:O	1:F:28:ARG:HG3	2.11	0.50
1:G:52:LYS:HZ1	1:G:62:ASN:HA	1.74	0.50
1:J:52:LYS:HE3	1:J:64:ILE:HG23	1.93	0.50
1:M:49:ILE:HD12	1:M:211:GLU:O	2.11	0.50
1:H:212:ILE:HG23	1:H:224:TYR:HB2	1.93	0.50
2:Y:3:THR:OG1	2:Y:127:THR:HG22	2.11	0.50
2:Z:28:HIS:CD2	2:1:120:VAL:HG11	2.46	0.50
1:F:123:TYR:CD1	1:F:123:TYR:N	2.78	0.50
2:P:66:TYR:CZ	2:P:70:ARG:HD2	2.46	0.50
2:1:3:THR:CB	2:1:16:THR:HG22	2.42	0.50
1:O:52:LYS:HB3	1:O:209:ALA:O	2.11	0.50
1:I:175:PHE:HD1	1:I:175:PHE:C	2.15	0.50
1:K:38:LEU:HG	1:K:49:ILE:HG23	1.92	0.50
2:2:50:GLY:O	2:2:54:VAL:HG12	2.10	0.50
1:F:43:ALA:HB2	1:F:185:PRO:HA	1.92	0.50
1:K:69:LEU:HD23	1:K:75:ALA:HB2	1.92	0.50
1:O:180:TYR:HA	1:O:192:LEU:HD21	1.91	0.50
1:M:21:LEU:HD11	1:N:130:ARG:HD2	1.93	0.50
1:H:43:ALA:HB2	1:H:185:PRO:HA	1.94	0.50
2:T:131:SER:O	2:T:134:VAL:HG13	2.10	0.50
1:D:95:SER:OG	1:D:115:ARG:HD3	2.10	0.50
2:B:178:ILE:HB	2:B:184:TYR:HA	1.93	0.50
1:M:98:GLN:O	1:M:102:THR:HG22	2.12	0.50
1:M:180:TYR:HB3	1:N:57:ARG:NH2	2.24	0.50
2:X:37:ILE:HD11	2:X:59:MET:CB	2.39	0.50
1:I:62:ASN:O	1:I:65:GLU:HG2	2.11	0.50
2:R:141:GLN:HE22	2:W:141:GLN:NE2	2.10	0.50
2:U:36:GLN:HB2	2:U:184:TYR:CE1	2.46	0.50
1:E:95:SER:OG	1:E:115:ARG:HD3	2.11	0.50
2:X:12:VAL:HG13	2:X:178:ILE:HG23	1.93	0.50
1:A:180:TYR:HA	1:A:192:LEU:HD21	1.93	0.50
2:B:176:ALA:HA	2:B:186:GLN:HA	1.92	0.50
2:X:59:MET:CE	2:X:82:LEU:HD23	2.42	0.50
1:I:52:LYS:HZ3	1:I:62:ASN:HA	1.74	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:S:133:PHE:CZ	2:S:165:ARG:HB3	2.47	0.50
1:O:172:VAL:O	1:O:176:LEU:HD22	2.11	0.50
1:F:137:ILE:HG22	1:F:150:ASP:HB2	1.92	0.50
2:T:62:GLU:HG2	2:T:82:LEU:HD21	1.93	0.50
1:E:98:GLN:O	1:E:102:THR:HG22	2.11	0.50
2:Q:62:GLU:HG2	2:Q:82:LEU:HD21	1.94	0.50
2:W:152:VAL:O	2:W:156:ILE:HG13	2.11	0.50
2:T:26:ILE:HD13	2:T:26:ILE:O	2.11	0.50
1:A:149:PHE:CE1	1:A:159:GLU:HB2	2.46	0.50
2:U:20:VAL:HG13	2:U:28:HIS:HB2	1.93	0.50
2:X:15:ALA:HB2	2:X:175:VAL:HB	1.94	0.50
2:Z:3:THR:HB	2:Z:16:THR:HG22	1.94	0.50
2:P:59:MET:CE	2:P:82:LEU:HD23	2.41	0.50
1:M:43:ALA:HB2	1:M:185:PRO:HA	1.94	0.50
2:S:173:ILE:HD13	2:S:173:ILE:C	2.32	0.50
1:D:137:ILE:HG22	1:D:150:ASP:HB2	1.93	0.50
1:G:17:PRO:HA	1:H:26:TYR:CD1	2.46	0.50
2:2:133:PHE:CZ	2:2:165:ARG:HB3	2.47	0.50
1:I:52:LYS:HZ2	1:I:62:ASN:HA	1.75	0.50
2:V:43:MET:CE	2:V:56:VAL:HG23	2.41	0.50
2:V:43:MET:HE2	2:V:56:VAL:HG23	1.93	0.50
1:E:61:GLN:OE1	1:E:62:ASN:HB3	2.12	0.50
1:C:70:ILE:HD12	1:C:74:VAL:HG22	1.92	0.50
1:N:121:GLN:O	1:N:124:THR:HB	2.11	0.50
1:M:62:ASN:O	1:M:65:GLU:HG2	2.12	0.50
1:C:198:LYS:CG	1:C:202:GLU:HG2	2.42	0.50
2:W:28:HIS:CD2	2:X:120:VAL:HG11	2.47	0.50
1:E:49:ILE:HD11	1:E:210:PRO:HB3	1.94	0.50
1:O:51:ASP:HB3	1:O:53:LYS:HZ2	1.76	0.50
2:U:112:SER:O	2:U:113:ILE:HD13	2.12	0.50
1:A:26:TYR:CD1	1:H:17:PRO:HA	2.45	0.50
2:1:152:VAL:O	2:1:156:ILE:HG13	2.11	0.50
1:D:175:PHE:C	1:D:175:PHE:CD1	2.85	0.50
1:F:52:LYS:HB3	1:F:209:ALA:O	2.12	0.49
2:U:123:ILE:HG12	2:U:124:TYR:CD2	2.44	0.49
2:1:18:ARG:HE	2:1:30:ASN:HD22	1.59	0.49
1:K:38:LEU:HA	1:K:164:ALA:HA	1.93	0.49
2:X:161:ALA:O	2:X:164:GLN:HB2	2.12	0.49
1:D:113:VAL:HG22	1:D:157:ILE:HD12	1.94	0.49
1:O:174:SER:O	1:O:177:GLU:HB3	2.11	0.49
1:C:170:ASP:O	1:C:173:VAL:HG12	2.10	0.49
1:O:28:ARG:O	1:O:31:VAL:HG22	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:S:43:MET:HE1	2:S:56:VAL:HG23	1.94	0.49
2:2:3:THR:HB	2:2:16:THR:HG22	1.93	0.49
1:A:175:PHE:HD1	1:A:175:PHE:C	2.15	0.49
2:X:38:ASP:HB3	2:X:41:THR:CG2	2.36	0.49
1:O:21:LEU:O	1:O:24:VAL:HG12	2.12	0.49
1:D:62:ASN:O	1:D:65:GLU:HG2	2.11	0.49
1:D:22:PHE:O	1:D:25:GLU:HB2	2.12	0.49
1:A:175:PHE:CD1	1:A:175:PHE:C	2.84	0.49
2:V:75:PRO:O	2:V:78:ALA:HB3	2.12	0.49
2:Y:189:THR:HG23	2:Y:190:ASP:N	2.27	0.49
1:O:38:LEU:HA	1:O:164:ALA:HA	1.94	0.49
2:2:174:ASP:HA	2:2:192:ILE:HD13	1.93	0.49
1:I:107:VAL:HG11	2:W:66:TYR:HH	1.76	0.49
1:H:52:LYS:HZ1	1:H:62:ASN:HA	1.76	0.49
2:Y:76:ILE:O	2:Y:79:VAL:HG12	2.13	0.49
1:I:94:ILE:HG13	1:I:95:SER:N	2.27	0.49
2:W:149:ASP:O	2:W:152:VAL:HG12	2.11	0.49
1:A:137:ILE:HG22	1:A:150:ASP:HB2	1.95	0.49
1:H:84:ASP:O	1:H:88:LEU:HB2	2.13	0.49
1:O:95:SER:OG	1:O:115:ARG:HD3	2.12	0.49
1:A:170:ASP:O	1:A:173:VAL:HG12	2.13	0.49
1:G:116:VAL:HG11	1:G:138:PHE:CZ	2.46	0.49
2:W:123:ILE:HG12	2:W:124:TYR:CD1	2.36	0.49
2:T:124:TYR:HD2	2:T:138:LEU:HD23	1.76	0.49
2:S:189:THR:HG23	2:S:190:ASP:N	2.28	0.49
2:Y:123:ILE:HD13	2:Y:123:ILE:H	1.76	0.49
1:E:42:PHE:HB2	1:E:184:LEU:O	2.13	0.49
2:P:3:THR:OG1	2:P:127:THR:HG22	2.12	0.49
2:1:12:VAL:HG13	2:1:178:ILE:HG23	1.95	0.49
1:A:110:GLU:O	1:A:113:VAL:HG12	2.13	0.49
1:I:49:ILE:HD13	1:I:212:ILE:HB	1.95	0.49
1:F:134:VAL:CG2	1:F:135:SER:N	2.76	0.49
1:J:175:PHE:HD2	1:J:199:SER:HG	1.61	0.49
1:E:17:PRO:HA	1:F:26:TYR:CD1	2.48	0.49
1:G:128:GLY:O	1:G:129:VAL:HB	2.13	0.49
2:W:25:PHE:CD1	2:W:25:PHE:C	2.84	0.49
1:E:135:SER:OG	1:E:152:ASP:HA	2.12	0.49
2:R:175:VAL:CG2	2:R:176:ALA:N	2.75	0.49
2:V:15:ALA:HB3	2:V:155:VAL:HG11	1.95	0.49
1:A:137:ILE:HG22	1:A:150:ASP:CB	2.43	0.49
1:G:174:SER:O	1:G:177:GLU:HB3	2.12	0.49
1:N:175:PHE:C	1:N:175:PHE:CD1	2.86	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:2:157:ARG:HA	2:2:201:LEU:HD21	1.95	0.49
1:C:184:LEU:HD23	1:C:189:ALA:HA	1.95	0.49
2:1:149:ASP:O	2:1:152:VAL:HG12	2.12	0.49
1:H:88:LEU:HD13	1:H:132:TYR:CD2	2.47	0.49
2:Q:174:ASP:HA	2:Q:192:ILE:HD13	1.94	0.49
1:L:110:GLU:O	1:L:113:VAL:HG13	2.13	0.49
2:Z:173:ILE:C	2:Z:173:ILE:HD13	2.34	0.49
1:L:42:PHE:HD1	1:L:43:ALA:N	2.11	0.49
1:D:38:LEU:HB3	1:D:164:ALA:HB2	1.94	0.49
2:Y:25:PHE:CD1	2:Y:25:PHE:C	2.83	0.49
2:V:38:ASP:HB3	2:V:41:THR:CG2	2.38	0.48
1:L:187:LYS:O	1:L:190:VAL:HG13	2.14	0.48
1:H:42:PHE:CD1	1:H:43:ALA:N	2.81	0.48
1:C:124:THR:HG22	1:D:130:ARG:HH21	1.78	0.48
2:R:133:PHE:CZ	2:R:165:ARG:HB3	2.48	0.48
1:K:52:LYS:HZ1	1:K:62:ASN:HA	1.75	0.48
1:N:21:LEU:HD11	1:O:130:ARG:HD2	1.94	0.48
2:Q:18:ARG:HB2	2:Q:31:GLY:O	2.13	0.48
2:X:152:VAL:O	2:X:156:ILE:HG13	2.13	0.48
1:O:187:LYS:O	1:O:190:VAL:HG13	2.13	0.48
1:F:32:LYS:O	1:F:167:SER:HA	2.14	0.48
1:L:15:PHE:HB2	1:M:23:GLN:HE21	1.78	0.48
1:E:69:LEU:HD23	1:E:75:ALA:HB2	1.96	0.48
1:N:186:GLU:O	1:N:190:VAL:HG12	2.13	0.48
2:P:179:THR:HG23	2:P:182:ASP:H	1.78	0.48
1:I:97:GLN:OE1	1:I:97:GLN:HA	2.13	0.48
1:C:187:LYS:O	1:C:190:VAL:HG13	2.14	0.48
1:M:136:LEU:HD12	1:M:151:CYS:HB3	1.94	0.48
1:G:70:ILE:HB	1:G:74:VAL:HG13	1.95	0.48
2:T:76:ILE:O	2:T:79:VAL:HG12	2.14	0.48
2:R:43:MET:HE1	2:R:56:VAL:HG23	1.95	0.48
1:D:148:LEU:O	1:D:159:GLU:HG3	2.13	0.48
2:P:15:ALA:HB2	2:P:175:VAL:HB	1.93	0.48
2:1:189:THR:HG23	2:1:190:ASP:N	2.29	0.48
2:Y:38:ASP:HB3	2:Y:41:THR:CG2	2.32	0.48
2:W:123:ILE:H	2:W:123:ILE:HD13	1.79	0.48
1:L:198:LYS:HG2	1:L:202:GLU:HG2	1.95	0.48
2:V:45:ILE:CG1	2:V:52:ALA:HB1	2.42	0.48
1:N:98:GLN:O	1:N:101:VAL:HG12	2.13	0.48
2:B:12:VAL:HG13	2:B:178:ILE:HG23	1.96	0.48
2:T:26:ILE:C	2:T:26:ILE:HD13	2.34	0.48
1:A:228:GLU:O	1:A:231:LYS:HB3	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:35:SER:O	1:E:166:GLY:HA3	2.13	0.48
1:K:34:GLY:O	1:K:167:SER:HB2	2.13	0.48
2:2:131:SER:O	2:2:134:VAL:HG13	2.13	0.48
1:D:180:TYR:HA	1:D:192:LEU:HD21	1.95	0.48
2:B:124:TYR:HD2	2:B:138:LEU:HD23	1.76	0.48
1:G:152:ASP:HB2	1:G:153:PRO:CD	2.43	0.48
1:G:175:PHE:C	1:G:175:PHE:CD1	2.87	0.48
2:B:36:GLN:HB2	2:B:184:TYR:CE1	2.48	0.48
2:X:104:ILE:HG22	2:X:178:ILE:HD11	1.94	0.48
1:O:215:ILE:HD11	1:O:219:ASN:O	2.13	0.48
1:J:123:TYR:CE2	1:J:129:VAL:HG21	2.48	0.48
1:C:28:ARG:O	1:C:31:VAL:HG22	2.13	0.48
1:G:69:LEU:HD23	1:G:75:ALA:HB2	1.94	0.48
1:O:175:PHE:C	1:O:175:PHE:CD1	2.87	0.48
1:A:62:ASN:O	1:A:65:GLU:HG2	2.13	0.48
1:F:49:ILE:HD11	1:F:210:PRO:HB3	1.94	0.48
1:J:144:ILE:HD12	1:J:147:ARG:NH1	2.28	0.48
2:Q:109:HIS:HB3	2:Q:111:PHE:HE1	1.79	0.48
1:A:148:LEU:O	1:A:159:GLU:HG3	2.14	0.48
1:E:168:GLY:O	1:E:172:VAL:HG12	2.12	0.48
2:X:123:ILE:H	2:X:123:ILE:HD13	1.77	0.48
1:D:121:GLN:O	1:D:124:THR:HB	2.13	0.48
1:N:24:VAL:O	1:N:28:ARG:HG3	2.14	0.48
2:V:111:PHE:CD2	2:V:121:GLU:HB2	2.49	0.48
1:K:98:GLN:O	1:K:101:VAL:HG12	2.14	0.48
1:D:85:ALA:O	1:D:89:VAL:HG23	2.14	0.48
2:B:17:GLU:HB2	2:B:170:GLY:O	2.14	0.48
2:X:36:GLN:HB2	2:X:184:TYR:CE1	2.48	0.48
2:B:141:GLN:NE2	2:Z:141:GLN:NE2	2.61	0.48
2:W:202:ILE:HG12	2:W:203:LEU:N	2.28	0.48
2:1:137:VAL:HG21	2:1:158:ALA:HA	1.95	0.48
1:E:127:GLY:O	1:E:129:VAL:N	2.47	0.48
1:F:76:ALA:HB2	1:F:138:PHE:CD1	2.48	0.48
2:2:55:LEU:HD21	2:2:87:LEU:HD11	1.96	0.48
1:M:42:PHE:CD1	1:M:43:ALA:N	2.81	0.48
1:H:52:LYS:HA	1:H:66:LYS:NZ	2.29	0.48
1:C:125:GLN:HB3	1:D:130:ARG:NH2	2.28	0.48
2:Z:3:THR:OG1	2:Z:127:THR:HG22	2.14	0.48
1:D:147:ARG:HB3	1:D:149:PHE:HE1	1.79	0.48
2:T:167:SER:HB2	2:1:167:SER:HB2	1.95	0.48
2:Q:66:TYR:CD2	2:Q:74:MET:HE2	2.48	0.48
2:Y:34:LEU:HD21	2:Y:176:ALA:HB3	1.95	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:X:37:ILE:HD11	2:X:59:MET:HG3	1.96	0.48
1:O:52:LYS:HZ2	1:O:62:ASN:HA	1.78	0.48
1:M:61:GLN:O	1:M:64:ILE:HG22	2.12	0.48
1:J:49:ILE:HD12	1:J:211:GLU:O	2.13	0.48
2:1:19:ARG:HE	2:1:26:ILE:HG13	1.79	0.48
2:R:179:THR:HG23	2:R:182:ASP:H	1.79	0.48
2:Y:55:LEU:HD21	2:Y:87:LEU:HD11	1.94	0.48
1:C:175:PHE:C	1:C:175:PHE:CD1	2.88	0.48
2:V:26:ILE:O	2:V:26:ILE:HD13	2.13	0.47
1:F:42:PHE:HB2	1:F:184:LEU:O	2.14	0.47
2:Y:189:THR:HG23	2:Y:190:ASP:H	1.78	0.47
1:O:94:ILE:HG13	1:O:95:SER:N	2.29	0.47
1:C:24:VAL:O	1:C:28:ARG:HG3	2.14	0.47
1:I:113:VAL:HG22	1:I:157:ILE:HD12	1.96	0.47
1:H:48:LEU:HB3	1:H:67:ILE:HD13	1.96	0.47
2:P:22:MET:O	2:P:23:GLU:HB2	2.14	0.47
2:B:66:TYR:CZ	2:B:70:ARG:HD2	2.49	0.47
1:A:108:ASN:HB3	2:P:70:ARG:HG2	1.95	0.47
2:1:15:ALA:HB2	2:1:175:VAL:HB	1.95	0.47
1:G:42:PHE:CD1	1:G:43:ALA:N	2.81	0.47
2:Q:159:ILE:O	2:Q:163:LYS:HG3	2.14	0.47
1:D:90:ASP:O	1:D:94:ILE:HG23	2.14	0.47
2:V:44:THR:OG1	2:V:100:LEU:HB3	2.14	0.47
2:B:126:SER:HB3	2:B:135:TYR:CE2	2.49	0.47
1:E:191:THR:O	1:E:194:ILE:HG22	2.13	0.47
2:2:6:ILE:HD11	2:2:142:TYR:CD1	2.49	0.47
2:R:44:THR:OG1	2:R:100:LEU:HB3	2.14	0.47
2:1:133:PHE:CZ	2:1:165:ARG:HB3	2.49	0.47
1:E:134:VAL:CG2	1:E:135:SER:N	2.76	0.47
1:G:198:LYS:CG	1:G:202:GLU:HG2	2.44	0.47
2:U:123:ILE:N	2:U:123:ILE:HD13	2.26	0.47
2:T:74:MET:HG2	2:T:78:ALA:HB3	1.95	0.47
2:2:123:ILE:HG12	2:2:124:TYR:CD2	2.49	0.47
1:F:38:LEU:CD2	1:F:49:ILE:HG23	2.44	0.47
1:N:187:LYS:O	1:N:190:VAL:HG13	2.14	0.47
2:P:189:THR:HG23	2:P:190:ASP:N	2.28	0.47
2:P:32:LYS:HE2	2:P:34:LEU:O	2.14	0.47
1:C:137:ILE:HG22	1:C:150:ASP:HB2	1.96	0.47
2:R:103:GLY:HA2	2:R:178:ILE:CD1	2.44	0.47
1:E:202:GLU:HG3	1:E:205:GLU:O	2.14	0.47
2:V:103:GLY:HA2	2:V:178:ILE:HD13	1.95	0.47
1:F:49:ILE:HD12	1:F:211:GLU:O	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:W:62:GLU:HG2	2:W:82:LEU:HD21	1.96	0.47
1:D:175:PHE:HD1	1:D:175:PHE:C	2.18	0.47
1:L:113:VAL:HG22	1:L:157:ILE:HD12	1.96	0.47
1:I:81:LEU:HD23	1:I:133:GLY:HA3	1.97	0.47
1:N:26:TYR:O	1:N:29:GLU:HB2	2.15	0.47
1:N:95:SER:OG	1:N:115:ARG:HD3	2.14	0.47
2:U:175:VAL:CG2	2:U:176:ALA:N	2.78	0.47
2:Y:123:ILE:HG12	2:Y:124:TYR:CD2	2.49	0.47
1:N:61:GLN:OE1	1:N:62:ASN:HB3	2.13	0.47
1:M:94:ILE:CG1	1:M:95:SER:N	2.77	0.47
1:L:175:PHE:CD1	1:L:175:PHE:C	2.88	0.47
2:S:132:PRO:HA	2:V:133:PHE:CE1	2.49	0.47
2:U:18:ARG:HB2	2:U:31:GLY:O	2.14	0.47
2:Y:22:MET:O	2:Y:23:GLU:HB2	2.14	0.47
2:U:91:LYS:O	2:U:94:PRO:HD3	2.15	0.47
2:V:143:SER:O	2:V:146:MET:HG3	2.14	0.47
1:I:160:TYR:CD2	1:I:163:THR:HB	2.49	0.47
2:V:17:GLU:HA	2:V:173:ILE:HA	1.96	0.47
2:P:26:ILE:C	2:P:26:ILE:HD13	2.35	0.47
2:T:7:THR:HB	2:T:123:ILE:O	2.14	0.47
2:Z:15:ALA:HB3	2:Z:155:VAL:CG1	2.44	0.47
1:J:62:ASN:O	1:J:65:GLU:HG2	2.14	0.47
1:C:94:ILE:CG1	1:C:95:SER:N	2.78	0.47
2:1:103:GLY:HA2	2:1:178:ILE:HD13	1.97	0.47
1:C:98:GLN:O	1:C:102:THR:HG23	2.15	0.47
1:N:82:VAL:HG13	1:N:83:ALA:N	2.29	0.47
2:1:45:ILE:HG12	2:1:52:ALA:HB1	1.95	0.47
1:M:34:GLY:O	1:M:167:SER:HB2	2.14	0.47
2:1:2:THR:HG22	2:1:169:SER:OG	2.14	0.47
2:U:25:PHE:CD1	2:U:25:PHE:C	2.84	0.47
2:Q:45:ILE:HD11	2:Q:52:ALA:O	2.14	0.47
2:1:59:MET:HE3	2:1:82:LEU:HD23	1.95	0.47
1:K:42:PHE:HB2	1:K:184:LEU:O	2.15	0.47
2:B:83:LEU:HA	2:B:83:LEU:HD12	1.69	0.47
2:X:59:MET:HE3	2:X:82:LEU:HD23	1.97	0.47
2:Q:152:VAL:O	2:Q:156:ILE:HG13	2.14	0.47
1:E:52:LYS:HE3	1:E:64:ILE:HG23	1.96	0.47
2:P:35:PHE:CE2	2:P:45:ILE:HD12	2.50	0.47
1:A:134:VAL:O	1:A:153:PRO:HG3	2.14	0.47
2:Y:19:ARG:HE	2:Y:26:ILE:HG13	1.79	0.47
2:B:103:GLY:HA2	2:B:178:ILE:CD1	2.44	0.47
2:1:104:ILE:HG22	2:1:178:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:Q:179:THR:HG23	2:Q:182:ASP:H	1.79	0.47
1:D:229:VAL:HG13	1:D:230:LYS:N	2.30	0.47
2:S:174:ASP:HA	2:S:192:ILE:HD13	1.96	0.47
1:H:45:GLY:HA3	1:H:216:THR:HA	1.96	0.47
1:J:159:GLU:HG2	1:K:60:GLU:HG3	1.96	0.47
2:T:22:MET:O	2:T:23:GLU:HB2	2.15	0.47
2:U:27:MET:HG2	2:U:27:MET:O	2.15	0.47
1:H:16:SER:HB3	1:H:22:PHE:CE2	2.50	0.47
1:L:109:ILE:HG22	1:L:147:ARG:HD3	1.97	0.47
2:R:59:MET:CE	2:R:82:LEU:HD23	2.43	0.47
1:G:38:LEU:HA	1:G:164:ALA:HA	1.95	0.47
1:C:21:LEU:HD11	1:D:130:ARG:HD2	1.97	0.47
2:B:6:ILE:HD11	2:B:142:TYR:HD1	1.80	0.47
2:Q:175:VAL:CG2	2:Q:176:ALA:N	2.78	0.47
1:I:180:TYR:HB3	1:J:57:ARG:NH2	2.30	0.47
1:O:116:VAL:HG11	1:O:138:PHE:CZ	2.50	0.47
1:N:18:ASP:OD2	1:N:20:ARG:HD3	2.15	0.47
2:B:20:VAL:HG22	2:B:28:HIS:HB2	1.96	0.47
1:L:108:ASN:HA	1:L:142:ASP:OD1	2.15	0.47
2:B:37:ILE:HD11	2:B:59:MET:CB	2.45	0.47
1:O:130:ARG:HG2	1:O:130:ARG:NH1	2.30	0.47
1:N:52:LYS:HE3	1:N:64:ILE:HG23	1.97	0.47
2:W:37:ILE:HD11	2:W:59:MET:HG3	1.97	0.47
2:2:189:THR:HG23	2:2:190:ASP:N	2.30	0.47
1:E:159:GLU:HG2	1:F:60:GLU:HG3	1.96	0.47
1:I:35:SER:O	1:I:166:GLY:HA3	2.15	0.47
1:H:114:LYS:O	1:H:117:ALA:HB3	2.15	0.47
1:C:58:LEU:CD1	1:C:58:LEU:N	2.78	0.47
2:Y:59:MET:CE	2:Y:82:LEU:HD23	2.45	0.47
1:G:152:ASP:HB2	1:G:153:PRO:HD2	1.96	0.47
1:I:135:SER:OG	1:I:152:ASP:HA	2.15	0.47
1:I:187:LYS:O	1:I:190:VAL:HG13	2.14	0.47
1:F:38:LEU:HA	1:F:164:ALA:HA	1.97	0.47
2:V:175:VAL:CG2	2:V:176:ALA:N	2.78	0.47
1:C:110:GLU:O	1:C:113:VAL:HG13	2.15	0.47
1:N:142:ASP:OD2	1:N:147:ARG:HD2	2.16	0.47
2:Q:81:THR:O	2:Q:84:SER:HB3	2.15	0.47
2:V:177:VAL:HG12	2:V:187:LEU:HD11	1.96	0.47
1:E:134:VAL:O	1:E:153:PRO:HG3	2.15	0.46
2:X:124:TYR:HD2	2:X:138:LEU:HD23	1.80	0.46
2:Q:123:ILE:N	2:Q:123:ILE:HD13	2.28	0.46
2:Y:175:VAL:CG2	2:Y:176:ALA:N	2.78	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:2:123:ILE:HG12	2:2:124:TYR:HD2	1.80	0.46
1:F:135:SER:OG	1:F:153:PRO:HD3	2.15	0.46
2:X:22:MET:O	2:X:23:GLU:HB2	2.16	0.46
2:R:74:MET:HG2	2:R:78:ALA:HB3	1.97	0.46
2:U:59:MET:HE2	2:U:79:VAL:HG23	1.97	0.46
2:Y:59:MET:HE2	2:Y:79:VAL:CG2	2.44	0.46
1:O:108:ASN:CB	2:V:70:ARG:HG2	2.44	0.46
2:W:131:SER:HB2	2:W:132:PRO:HD3	1.97	0.46
1:L:152:ASP:HB2	1:L:153:PRO:HD2	1.97	0.46
1:A:98:GLN:O	1:A:102:THR:HG23	2.15	0.46
1:F:98:GLN:O	1:F:101:VAL:HG12	2.16	0.46
2:Z:177:VAL:HG12	2:Z:187:LEU:HD11	1.97	0.46
2:W:138:LEU:HD12	2:W:138:LEU:HA	1.73	0.46
1:I:121:GLN:O	1:I:124:THR:HB	2.14	0.46
2:Y:36:GLN:HB2	2:Y:184:TYR:CE1	2.50	0.46
1:I:48:LEU:HB3	1:I:67:ILE:HD13	1.97	0.46
1:I:72:ASP:HB2	1:I:73:TYR:CD1	2.51	0.46
2:W:76:ILE:HA	2:W:79:VAL:HG12	1.96	0.46
1:H:175:PHE:CD1	1:H:175:PHE:C	2.88	0.46
2:B:177:VAL:HG12	2:B:187:LEU:CD1	2.46	0.46
1:K:172:VAL:O	1:K:176:LEU:HD22	2.16	0.46
2:B:59:MET:HE2	2:B:79:VAL:CG2	2.44	0.46
2:Y:34:LEU:HD21	2:Y:176:ALA:CB	2.46	0.46
2:1:15:ALA:HB3	2:1:155:VAL:HG11	1.98	0.46
1:D:21:LEU:HD11	1:E:130:ARG:HD2	1.97	0.46
2:P:20:VAL:CG1	2:P:28:HIS:HB2	2.44	0.46
1:M:175:PHE:C	1:M:175:PHE:CD1	2.89	0.46
1:D:172:VAL:O	1:D:176:LEU:HD22	2.16	0.46
2:Y:178:ILE:HB	2:Y:184:TYR:HA	1.96	0.46
1:J:88:LEU:HD13	1:J:132:TYR:CE2	2.51	0.46
2:B:165:ARG:HA	2:Y:26:ILE:HG23	1.98	0.46
1:L:180:TYR:HA	1:L:192:LEU:HD21	1.97	0.46
1:A:60:GLU:HG3	1:H:159:GLU:HG2	1.96	0.46
2:R:50:GLY:O	2:R:54:VAL:HG12	2.14	0.46
1:I:18:ASP:OD2	1:I:20:ARG:HD3	2.16	0.46
1:F:107:VAL:HG13	1:F:108:ASN:H	1.80	0.46
1:D:198:LYS:O	1:D:199:SER:C	2.54	0.46
1:A:175:PHE:CD2	1:A:196:ALA:HA	2.50	0.46
2:U:132:PRO:HA	2:1:133:PHE:HE1	1.81	0.46
2:Z:50:GLY:O	2:Z:54:VAL:HG12	2.16	0.46
1:J:165:ILE:HD12	1:J:169:LYS:HD2	1.97	0.46
1:G:142:ASP:HD2	1:G:142:ASP:H	1.62	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:Z:8:LEU:HD12	2:Z:8:LEU:O	2.16	0.46
2:S:43:MET:HE2	2:S:56:VAL:HG23	1.98	0.46
1:L:174:SER:O	1:L:177:GLU:HB3	2.15	0.46
2:S:178:ILE:O	2:S:178:ILE:HG12	2.14	0.46
2:R:48:LEU:HD12	2:R:49:VAL:N	2.31	0.46
2:W:15:ALA:HB2	2:W:175:VAL:HB	1.96	0.46
1:F:228:GLU:O	1:F:231:LYS:HB3	2.15	0.46
1:H:31:VAL:HA	1:H:80:GLY:HA2	1.98	0.46
1:L:161:LYS:HD2	1:M:60:GLU:OE2	2.16	0.46
1:F:81:LEU:HD23	1:F:133:GLY:HA3	1.97	0.46
2:2:25:PHE:C	2:2:25:PHE:CD1	2.89	0.46
1:F:52:LYS:HZ3	1:F:62:ASN:HA	1.79	0.46
2:U:76:ILE:HG21	2:U:109:HIS:HB2	1.96	0.46
1:C:42:PHE:HD1	1:C:43:ALA:N	2.14	0.46
1:O:61:GLN:OE1	1:O:62:ASN:HB3	2.16	0.46
2:R:160:SER:HA	2:R:163:LYS:HD3	1.98	0.46
1:E:70:ILE:HB	1:E:74:VAL:HG13	1.98	0.46
1:H:135:SER:OG	1:H:152:ASP:HA	2.16	0.46
2:V:19:ARG:HE	2:V:26:ILE:HG13	1.81	0.46
2:X:40:TYR:O	2:X:178:ILE:HD11	2.15	0.46
1:F:152:ASP:HB2	1:F:153:PRO:CD	2.46	0.46
2:U:55:LEU:HD21	2:U:87:LEU:HD11	1.97	0.46
1:O:88:LEU:HD13	1:O:132:TYR:CD2	2.51	0.46
2:V:37:ILE:HD11	2:V:59:MET:HB3	1.97	0.46
2:T:179:THR:HG23	2:T:182:ASP:H	1.81	0.46
2:1:22:MET:O	2:1:23:GLU:HB2	2.15	0.46
2:S:75:PRO:O	2:S:78:ALA:HB3	2.16	0.46
1:E:108:ASN:CB	2:S:70:ARG:HG2	2.43	0.46
2:2:59:MET:HE2	2:2:79:VAL:HG23	1.98	0.46
1:J:198:LYS:HG2	1:J:202:GLU:HG2	1.96	0.46
2:1:15:ALA:HB3	2:1:155:VAL:CG1	2.46	0.46
2:V:26:ILE:C	2:V:26:ILE:HD13	2.36	0.46
2:S:103:GLY:HA2	2:S:178:ILE:HD11	1.98	0.46
2:B:72:VAL:HG22	2:B:73:ASN:N	2.31	0.46
2:Q:49:VAL:HG23	2:Q:50:GLY:H	1.81	0.46
1:K:228:GLU:O	1:K:231:LYS:HB3	2.16	0.46
1:G:130:ARG:HA	1:G:131:PRO:HD3	1.82	0.46
1:L:38:LEU:HG	1:L:49:ILE:HG23	1.98	0.46
1:E:42:PHE:CD1	1:E:43:ALA:N	2.84	0.46
2:P:175:VAL:CG2	2:P:176:ALA:N	2.78	0.46
2:X:146:MET:HE2	2:X:150:GLU:HB3	1.97	0.46
2:U:109:HIS:HB3	2:U:111:PHE:HE1	1.81	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:52:LYS:HZ2	1:H:62:ASN:HA	1.81	0.46
1:I:137:ILE:HG22	1:I:150:ASP:CB	2.45	0.46
1:H:187:LYS:O	1:H:190:VAL:HG13	2.16	0.46
1:N:88:LEU:HD13	1:N:132:TYR:CE2	2.51	0.46
2:R:17:GLU:HA	2:R:173:ILE:HA	1.98	0.46
1:G:109:ILE:CG2	1:G:147:ARG:HD3	2.46	0.46
2:R:165:ARG:C	2:V:26:ILE:HG22	2.36	0.46
2:1:26:ILE:HD13	2:1:26:ILE:O	2.16	0.46
1:D:94:ILE:HG13	1:D:95:SER:N	2.29	0.46
1:K:43:ALA:HB2	1:K:185:PRO:HA	1.97	0.46
1:E:77:VAL:CG1	1:E:137:ILE:HG12	2.46	0.46
2:T:174:ASP:HA	2:T:192:ILE:HD13	1.98	0.46
2:B:193:GLU:HA	2:B:196:ILE:HD12	1.98	0.46
1:K:175:PHE:C	1:K:175:PHE:CD1	2.89	0.46
2:R:124:TYR:HD2	2:R:138:LEU:HD23	1.80	0.45
1:E:198:LYS:O	1:E:199:SER:C	2.54	0.45
2:Y:18:ARG:HB2	2:Y:31:GLY:O	2.16	0.45
1:H:38:LEU:HG	1:H:49:ILE:HG23	1.98	0.45
2:Z:32:LYS:HE2	2:Z:34:LEU:O	2.16	0.45
2:R:111:PHE:CE2	2:R:121:GLU:HB2	2.51	0.45
2:U:187:LEU:HA	2:U:188:PRO:HD3	1.81	0.45
2:R:27:MET:O	2:R:27:MET:HG2	2.16	0.45
1:G:81:LEU:HD23	1:G:133:GLY:HA3	1.97	0.45
1:K:198:LYS:HG3	1:K:207:LEU:HD22	1.98	0.45
1:F:194:ILE:O	1:F:198:LYS:HB2	2.16	0.45
2:W:103:GLY:HA2	2:W:178:ILE:CD1	2.46	0.45
2:R:43:MET:CE	2:R:56:VAL:HG23	2.45	0.45
2:W:189:THR:HG23	2:W:190:ASP:N	2.31	0.45
2:T:15:ALA:HB3	2:T:155:VAL:HG11	1.98	0.45
1:I:148:LEU:O	1:I:159:GLU:HG3	2.16	0.45
2:1:123:ILE:HD13	2:1:123:ILE:N	2.28	0.45
2:X:59:MET:SD	2:X:83:LEU:HD13	2.56	0.45
2:U:124:TYR:HD1	2:U:138:LEU:HD23	1.81	0.45
1:H:52:LYS:HE3	1:H:64:ILE:HG23	1.99	0.45
2:B:55:LEU:HA	2:B:55:LEU:HD12	1.50	0.45
2:B:132:PRO:HA	2:Z:133:PHE:HE1	1.81	0.45
2:R:75:PRO:O	2:R:78:ALA:HB3	2.16	0.45
1:J:76:ALA:HB2	1:J:138:PHE:CD1	2.52	0.45
2:T:110:VAL:HG13	2:T:110:VAL:O	2.16	0.45
1:N:58:LEU:N	1:N:58:LEU:CD1	2.79	0.45
1:A:52:LYS:HE3	1:A:64:ILE:HG23	1.99	0.45
2:B:7:THR:HB	2:B:123:ILE:O	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:52:LYS:HE3	1:D:64:ILE:HG23	1.98	0.45
1:F:61:GLN:OE1	1:F:62:ASN:HB3	2.16	0.45
2:1:175:VAL:CG2	2:1:176:ALA:N	2.78	0.45
1:M:124:THR:HG22	1:N:130:ARG:HH21	1.82	0.45
1:C:49:ILE:HD11	1:C:210:PRO:HB3	1.98	0.45
2:W:26:ILE:HD13	2:W:26:ILE:C	2.35	0.45
2:P:105:ASP:OD1	2:P:106:THR:N	2.49	0.45
2:B:111:PHE:CE2	2:B:121:GLU:HB2	2.51	0.45
1:I:130:ARG:HH21	1:O:124:THR:CG2	2.22	0.45
2:Z:15:ALA:HB3	2:Z:155:VAL:HG11	1.97	0.45
1:I:42:PHE:CD1	1:I:43:ALA:N	2.83	0.45
2:S:18:ARG:HE	2:S:30:ASN:HD22	1.65	0.45
2:R:149:ASP:O	2:R:152:VAL:HG12	2.17	0.45
1:L:152:ASP:HB2	1:L:153:PRO:CD	2.46	0.45
1:J:175:PHE:C	1:J:175:PHE:CD1	2.90	0.45
2:X:189:THR:HG23	2:X:190:ASP:N	2.31	0.45
2:1:93:MET:N	2:1:94:PRO:CD	2.79	0.45
2:W:147:THR:OG1	2:W:150:GLU:HG3	2.16	0.45
2:2:76:ILE:O	2:2:79:VAL:HG12	2.17	0.45
1:M:198:LYS:HG2	1:M:202:GLU:HG2	1.98	0.45
2:U:130:GLY:O	2:U:134:VAL:HG12	2.17	0.45
2:Q:20:VAL:HG13	2:Q:28:HIS:HB2	1.97	0.45
1:G:51:ASP:HB3	1:G:53:LYS:NZ	2.31	0.45
1:D:18:ASP:OD2	1:D:20:ARG:HD3	2.15	0.45
1:G:143:GLN:HA	1:G:143:GLN:HE22	1.82	0.45
1:E:44:ASN:HD22	1:E:44:ASN:HA	1.63	0.45
2:B:27:MET:HG2	2:B:27:MET:O	2.17	0.45
1:A:44:ASN:HA	1:A:44:ASN:HD22	1.61	0.45
2:2:66:TYR:CZ	2:2:70:ARG:HD2	2.52	0.45
2:Z:59:MET:SD	2:Z:83:LEU:HD13	2.57	0.45
1:K:52:LYS:CE	1:K:64:ILE:HG23	2.46	0.45
2:U:37:ILE:HD11	2:U:59:MET:CG	2.46	0.45
1:O:198:LYS:O	1:O:199:SER:C	2.55	0.45
1:C:198:LYS:O	1:C:199:SER:C	2.55	0.45
2:T:6:ILE:O	2:T:6:ILE:HG23	2.17	0.45
2:X:103:GLY:HA2	2:X:178:ILE:HD13	1.99	0.45
2:Y:190:ASP:HA	2:Y:193:GLU:HG2	1.99	0.45
1:E:148:LEU:O	1:E:159:GLU:HG3	2.17	0.45
1:I:171:ALA:HB3	1:I:200:SER:OG	2.17	0.45
1:C:69:LEU:HD23	1:C:75:ALA:HB2	1.98	0.45
1:G:15:PHE:HB2	1:H:23:GLN:HE21	1.82	0.45
1:M:228:GLU:O	1:M:231:LYS:HB3	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:24:VAL:O	1:A:28:ARG:HG3	2.17	0.45
1:E:21:LEU:O	1:E:24:VAL:HG12	2.16	0.45
1:M:175:PHE:C	1:M:175:PHE:HD1	2.20	0.45
1:C:175:PHE:HD1	1:C:175:PHE:C	2.20	0.45
2:U:93:MET:N	2:U:94:PRO:CD	2.78	0.45
1:M:99:GLU:HG3	1:M:103:TYR:HD2	1.81	0.45
1:N:136:LEU:HD12	1:N:151:CYS:HB3	1.97	0.45
1:H:123:TYR:N	1:H:123:TYR:CD1	2.85	0.45
1:D:44:ASN:HD22	1:D:44:ASN:HA	1.64	0.45
2:P:173:ILE:C	2:P:173:ILE:HD13	2.37	0.45
2:X:45:ILE:CG1	2:X:52:ALA:HB1	2.34	0.45
1:I:198:LYS:O	1:I:199:SER:C	2.55	0.45
1:A:49:ILE:HD11	1:A:210:PRO:CB	2.47	0.45
2:S:19:ARG:NE	2:S:26:ILE:HG13	2.32	0.45
1:F:149:PHE:CE2	1:F:159:GLU:HB2	2.52	0.45
1:C:134:VAL:CG2	1:C:135:SER:N	2.79	0.45
1:D:228:GLU:O	1:D:231:LYS:HB3	2.17	0.45
2:2:143:SER:O	2:2:146:MET:HG3	2.17	0.45
2:1:55:LEU:HD12	2:1:55:LEU:HA	1.85	0.45
1:D:123:TYR:N	1:D:123:TYR:CD1	2.85	0.45
1:O:121:GLN:O	1:O:124:THR:HB	2.17	0.45
2:2:59:MET:CE	2:2:82:LEU:HD23	2.46	0.45
1:H:22:PHE:O	1:H:25:GLU:HB2	2.17	0.45
1:E:176:LEU:O	1:E:178:ARG:N	2.49	0.45
2:B:179:THR:O	2:B:183:GLY:N	2.50	0.45
2:P:189:THR:HG23	2:P:190:ASP:H	1.82	0.45
1:E:186:GLU:O	1:E:190:VAL:HG12	2.17	0.45
2:Q:105:ASP:OD1	2:Q:106:THR:N	2.50	0.45
2:Z:2:THR:HG22	2:Z:169:SER:OG	2.16	0.45
2:P:146:MET:HA	2:P:150:GLU:OE1	2.17	0.45
2:2:22:MET:O	2:2:23:GLU:HB2	2.16	0.45
2:B:180:ARG:HA	2:B:180:ARG:HD2	1.79	0.45
2:Z:111:PHE:CD2	2:Z:121:GLU:HB2	2.53	0.44
1:K:130:ARG:HH11	1:K:130:ARG:HG2	1.83	0.44
1:J:52:LYS:HZ2	1:J:62:ASN:HA	1.80	0.44
2:2:103:GLY:HA2	2:2:178:ILE:CD1	2.47	0.44
1:I:175:PHE:CD2	1:I:196:ALA:HA	2.52	0.44
2:1:189:THR:HG23	2:1:190:ASP:H	1.82	0.44
1:I:161:LYS:HG2	1:I:180:TYR:HE2	1.82	0.44
2:P:6:ILE:HD11	2:P:142:TYR:CD1	2.52	0.44
2:S:6:ILE:HD11	2:S:142:TYR:CD1	2.52	0.44
1:N:180:TYR:HA	1:N:192:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:X:173:ILE:C	2:X:173:ILE:HD13	2.37	0.44
2:P:138:LEU:HD12	2:P:154:LEU:HD11	1.98	0.44
1:K:24:VAL:O	1:K:28:ARG:HG3	2.17	0.44
1:L:198:LYS:O	1:L:199:SER:C	2.56	0.44
1:C:42:PHE:HD2	1:C:47:LEU:HD23	1.83	0.44
1:N:52:LYS:HZ3	1:N:62:ASN:HA	1.81	0.44
1:M:82:VAL:HG13	1:M:83:ALA:N	2.32	0.44
1:E:15:PHE:HD2	1:F:23:GLN:NE2	2.15	0.44
1:N:49:ILE:HD12	1:N:211:GLU:O	2.17	0.44
2:Z:93:MET:N	2:Z:94:PRO:CD	2.79	0.44
2:U:97:VAL:HG22	2:U:98:GLN:N	2.32	0.44
2:U:160:SER:HA	2:U:163:LYS:HD3	2.00	0.44
1:I:170:ASP:O	1:I:173:VAL:HG12	2.16	0.44
1:L:82:VAL:HG13	1:L:83:ALA:N	2.33	0.44
2:S:110:VAL:O	2:S:110:VAL:HG13	2.16	0.44
1:M:198:LYS:O	1:M:199:SER:C	2.56	0.44
1:N:42:PHE:HB2	1:N:184:LEU:O	2.17	0.44
1:M:159:GLU:O	1:N:60:GLU:HB2	2.17	0.44
1:N:82:VAL:HG13	1:N:83:ALA:H	1.81	0.44
2:S:74:MET:HG2	2:S:78:ALA:HB3	2.00	0.44
2:W:75:PRO:O	2:W:78:ALA:HB3	2.18	0.44
2:B:22:MET:O	2:B:23:GLU:HB2	2.17	0.44
1:L:212:ILE:HG23	1:L:224:TYR:HB2	1.99	0.44
1:J:58:LEU:N	1:J:58:LEU:CD1	2.81	0.44
2:2:90:VAL:O	2:2:90:VAL:HG22	2.17	0.44
1:J:107:VAL:HG11	2:X:66:TYR:HH	1.81	0.44
2:U:37:ILE:HD11	2:U:59:MET:CB	2.43	0.44
1:G:187:LYS:O	1:G:190:VAL:HG13	2.17	0.44
1:M:125:GLN:HB3	1:N:130:ARG:NH2	2.32	0.44
1:D:49:ILE:HD12	1:D:211:GLU:O	2.17	0.44
1:G:149:PHE:CE2	1:G:159:GLU:HB2	2.53	0.44
2:S:19:ARG:HE	2:S:26:ILE:HG13	1.83	0.44
1:I:70:ILE:HD12	1:I:74:VAL:HG22	1.99	0.44
2:Z:20:VAL:HG22	2:Z:28:HIS:HB2	1.99	0.44
2:S:17:GLU:HA	2:S:173:ILE:HA	1.99	0.44
2:B:141:GLN:NE2	2:Z:141:GLN:HE22	2.15	0.44
2:S:93:MET:N	2:S:94:PRO:CD	2.80	0.44
2:V:18:ARG:HE	2:V:30:ASN:HD22	1.66	0.44
1:M:170:ASP:O	1:M:173:VAL:HG12	2.17	0.44
1:A:18:ASP:OD2	1:A:20:ARG:HD3	2.17	0.44
1:K:148:LEU:O	1:K:159:GLU:HG3	2.17	0.44
2:P:2:THR:HG22	2:P:169:SER:OG	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:Y:133:PHE:CE2	2:Y:165:ARG:HB3	2.52	0.44
2:Q:189:THR:HG23	2:Q:190:ASP:H	1.82	0.44
1:E:174:SER:O	1:E:177:GLU:HB3	2.18	0.44
2:B:29:LYS:NZ	2:Y:164:GLN:NE2	2.64	0.44
1:J:180:TYR:HA	1:J:192:LEU:HD21	1.99	0.44
1:D:124:THR:HG22	1:E:130:ARG:HH21	1.83	0.44
1:L:62:ASN:O	1:L:65:GLU:HG2	2.18	0.44
2:Z:26:ILE:C	2:Z:26:ILE:HD13	2.38	0.44
1:K:165:ILE:HG13	1:K:166:GLY:H	1.82	0.44
2:R:49:VAL:HG23	2:R:50:GLY:H	1.83	0.44
1:L:83:ALA:O	1:L:87:VAL:HG12	2.18	0.44
1:A:81:LEU:HD23	1:A:133:GLY:HA3	2.00	0.44
1:K:180:TYR:HA	1:K:192:LEU:HD21	2.00	0.44
1:O:123:TYR:CE2	1:O:129:VAL:HG21	2.53	0.44
1:G:28:ARG:O	1:G:31:VAL:HG13	2.18	0.44
1:N:165:ILE:HD12	1:N:169:LYS:HD2	2.00	0.44
1:G:180:TYR:HA	1:G:192:LEU:HD21	2.00	0.44
1:K:135:SER:OG	1:K:153:PRO:HD3	2.17	0.44
1:E:123:TYR:CD1	1:E:123:TYR:N	2.84	0.44
1:A:78:THR:CG2	1:A:85:ALA:HB1	2.45	0.44
1:G:52:LYS:HA	1:G:66:LYS:NZ	2.32	0.44
2:U:7:THR:HB	2:U:123:ILE:O	2.18	0.44
1:J:52:LYS:HZ3	1:J:62:ASN:HA	1.80	0.44
2:Y:161:ALA:O	2:Y:164:GLN:HB2	2.17	0.44
1:A:32:LYS:O	1:A:167:SER:HA	2.18	0.44
2:Z:74:MET:HG2	2:Z:78:ALA:HB3	2.00	0.44
2:Z:55:LEU:HD21	2:Z:87:LEU:HD11	1.99	0.44
2:R:55:LEU:HD12	2:R:55:LEU:HA	1.79	0.44
2:B:25:PHE:CD1	2:B:25:PHE:C	2.90	0.44
1:C:20:ARG:CZ	1:C:22:PHE:CE1	3.01	0.44
1:I:202:GLU:HG3	1:I:205:GLU:O	2.18	0.44
2:B:165:ARG:CZ	2:Y:29:LYS:HE3	2.48	0.44
1:O:38:LEU:HB3	1:O:164:ALA:HB2	1.99	0.44
1:L:228:GLU:O	1:L:231:LYS:HB3	2.17	0.44
1:N:191:THR:O	1:N:194:ILE:HG22	2.18	0.44
2:U:8:LEU:HD12	2:U:8:LEU:O	2.17	0.44
1:M:107:VAL:HG13	1:M:108:ASN:N	2.32	0.44
2:B:59:MET:HE3	2:B:82:LEU:HD23	1.98	0.44
2:Q:123:ILE:HG12	2:Q:124:TYR:CD1	2.51	0.44
1:M:52:LYS:HZ3	1:M:62:ASN:HA	1.81	0.44
1:J:52:LYS:HA	1:J:66:LYS:NZ	2.33	0.44
2:R:76:ILE:O	2:R:79:VAL:HG12	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:133:PHE:HE1	2:Z:132:PRO:HA	1.83	0.44
1:J:83:ALA:O	1:J:87:VAL:HG12	2.18	0.44
1:D:136:LEU:HD12	1:D:151:CYS:HB3	1.99	0.44
1:D:184:LEU:HD23	1:D:189:ALA:HA	1.99	0.44
2:X:101:VAL:O	2:X:101:VAL:HG13	2.18	0.44
2:Y:59:MET:HE1	2:Y:82:LEU:HD23	2.00	0.43
1:H:175:PHE:HD1	1:H:175:PHE:C	2.22	0.43
1:F:225:ASP:OD1	1:F:228:GLU:HB2	2.18	0.43
1:O:145:GLY:O	1:O:147:ARG:HG3	2.18	0.43
2:S:180:ARG:HA	2:S:180:ARG:HD2	1.71	0.43
2:S:8:LEU:O	2:S:8:LEU:HD12	2.17	0.43
2:P:25:PHE:C	2:P:25:PHE:CD1	2.91	0.43
2:Z:7:THR:HB	2:Z:123:ILE:O	2.19	0.43
1:O:98:GLN:O	1:O:102:THR:CG2	2.66	0.43
1:D:130:ARG:HA	1:D:131:PRO:HD3	1.86	0.43
1:E:137:ILE:HG22	1:E:150:ASP:HB2	2.00	0.43
1:L:16:SER:HB3	1:L:22:PHE:CE2	2.52	0.43
2:T:141:GLN:NE2	2:2:141:GLN:NE2	2.67	0.43
2:W:6:ILE:HD11	2:W:142:TYR:CD1	2.53	0.43
1:A:16:SER:HB3	1:A:22:PHE:CE2	2.53	0.43
1:F:82:VAL:HG13	1:F:83:ALA:H	1.83	0.43
1:F:107:VAL:HG13	1:F:108:ASN:N	2.33	0.43
2:W:7:THR:HB	2:W:123:ILE:O	2.18	0.43
2:S:20:VAL:CG1	2:S:28:HIS:HB2	2.45	0.43
1:L:52:LYS:HB3	1:L:209:ALA:O	2.18	0.43
1:H:52:LYS:CE	1:H:64:ILE:HG23	2.48	0.43
1:C:52:LYS:HB3	1:C:209:ALA:O	2.18	0.43
1:C:202:GLU:HG3	1:C:205:GLU:O	2.19	0.43
1:J:147:ARG:HB3	1:J:149:PHE:HE1	1.83	0.43
1:M:180:TYR:HB3	1:N:57:ARG:HH22	1.82	0.43
1:M:38:LEU:HA	1:M:164:ALA:HA	1.98	0.43
1:K:145:GLY:O	1:K:147:ARG:HG3	2.19	0.43
1:C:32:LYS:O	1:C:167:SER:HA	2.18	0.43
2:B:202:ILE:HG12	2:B:203:LEU:N	2.34	0.43
1:G:97:GLN:OE1	1:G:97:GLN:HA	2.18	0.43
1:A:109:ILE:CG2	1:A:147:ARG:HD3	2.48	0.43
1:O:175:PHE:HD1	1:O:175:PHE:C	2.21	0.43
1:L:159:GLU:HG2	1:M:60:GLU:HG3	2.00	0.43
2:T:93:MET:N	2:T:94:PRO:CD	2.81	0.43
1:D:205:GLU:HG3	1:D:206:GLU:N	2.34	0.43
1:E:158:ASN:HB2	1:E:160:TYR:CE1	2.53	0.43
2:U:141:GLN:NE2	2:1:141:GLN:NE2	2.66	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:136:LEU:HD12	1:I:151:CYS:HB3	1.99	0.43
2:S:76:ILE:HA	2:S:79:VAL:HG12	2.00	0.43
1:I:44:ASN:HA	1:I:44:ASN:HD22	1.63	0.43
1:G:107:VAL:HG13	1:G:108:ASN:N	2.34	0.43
1:J:14:VAL:O	1:J:21:LEU:HD12	2.18	0.43
2:R:34:LEU:HD21	2:R:176:ALA:HB3	2.00	0.43
1:G:175:PHE:C	1:G:175:PHE:HD1	2.21	0.43
2:S:178:ILE:HB	2:S:184:TYR:HA	2.01	0.43
1:G:113:VAL:HA	1:G:116:VAL:HG12	2.01	0.43
2:W:187:LEU:HA	2:W:188:PRO:HD3	1.67	0.43
2:W:2:THR:HG22	2:W:169:SER:OG	2.18	0.43
2:P:141:GLN:NE2	2:Y:141:GLN:NE2	2.66	0.43
1:O:44:ASN:HA	1:O:44:ASN:HD22	1.62	0.43
2:B:90:VAL:HG22	2:B:90:VAL:O	2.18	0.43
2:Y:180:ARG:HA	2:Y:180:ARG:HD2	1.75	0.43
2:P:124:TYR:HD2	2:P:138:LEU:HD23	1.78	0.43
1:A:52:LYS:HB3	1:A:209:ALA:O	2.19	0.43
2:X:3:THR:HB	2:X:16:THR:HG22	2.01	0.43
2:S:189:THR:HG23	2:S:190:ASP:H	1.84	0.43
2:2:2:THR:HG22	2:2:169:SER:CB	2.49	0.43
2:S:3:THR:OG1	2:S:127:THR:HG22	2.19	0.43
1:A:130:ARG:NH1	1:A:131:PRO:O	2.51	0.43
2:B:17:GLU:HA	2:B:173:ILE:HA	2.01	0.43
2:Z:131:SER:O	2:Z:134:VAL:HG13	2.19	0.43
2:1:97:VAL:HG22	2:1:98:GLN:N	2.34	0.43
1:G:44:ASN:HA	1:G:44:ASN:HD22	1.64	0.43
2:X:90:VAL:O	2:X:90:VAL:HG22	2.19	0.43
1:O:24:VAL:O	1:O:28:ARG:HG3	2.18	0.43
2:2:59:MET:SD	2:2:83:LEU:HD13	2.58	0.43
2:T:138:LEU:HD12	2:T:138:LEU:HA	1.86	0.43
2:Z:43:MET:HE1	2:Z:56:VAL:HA	2.01	0.43
1:N:25:GLU:O	1:N:28:ARG:HB2	2.18	0.43
1:L:175:PHE:C	1:L:175:PHE:HD1	2.21	0.43
1:F:160:TYR:CD2	1:F:163:THR:HB	2.53	0.43
1:G:146:PRO:O	1:G:147:ARG:HG2	2.17	0.43
2:Y:149:ASP:O	2:Y:152:VAL:HG12	2.18	0.43
1:M:26:TYR:O	1:M:29:GLU:HB2	2.18	0.43
2:T:87:LEU:HD23	2:T:114:ASP:O	2.19	0.43
2:R:6:ILE:HD11	2:R:142:TYR:CD1	2.53	0.43
2:B:15:ALA:HB2	2:B:175:VAL:HB	1.99	0.43
1:J:208:LYS:HA	1:J:208:LYS:HD2	1.82	0.43
1:J:143:GLN:HA	1:J:143:GLN:HE22	1.84	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:107:VAL:HG11	2:Y:66:TYR:HH	1.76	0.43
2:U:111:PHE:CE2	2:U:121:GLU:HB2	2.53	0.43
1:H:198:LYS:O	1:H:199:SER:C	2.56	0.43
2:V:19:ARG:NE	2:V:26:ILE:HG13	2.34	0.43
1:J:109:ILE:HG22	1:J:147:ARG:HD3	2.01	0.43
2:B:28:HIS:CD2	2:P:120:VAL:HG11	2.54	0.43
1:K:142:ASP:OD2	1:K:147:ARG:HD2	2.18	0.43
2:2:187:LEU:HA	2:2:188:PRO:HD3	1.81	0.43
2:B:131:SER:O	2:B:134:VAL:HG13	2.19	0.43
1:C:71:ASP:O	1:C:73:TYR:N	2.51	0.43
1:O:148:LEU:O	1:O:159:GLU:HG3	2.19	0.43
1:I:107:VAL:HG13	1:I:108:ASN:H	1.84	0.43
2:Y:15:ALA:HB2	2:Y:175:VAL:HB	2.01	0.43
2:V:76:ILE:HA	2:V:79:VAL:HG12	2.01	0.43
2:W:34:LEU:HD21	2:W:176:ALA:HB3	1.99	0.43
2:V:93:MET:N	2:V:94:PRO:CD	2.82	0.43
1:E:83:ALA:O	1:E:87:VAL:HG12	2.19	0.43
1:G:125:GLN:HB3	1:H:130:ARG:NH2	2.34	0.43
2:S:43:MET:HE1	2:S:56:VAL:HA	2.01	0.43
1:E:52:LYS:HZ3	1:E:62:ASN:HA	1.82	0.43
1:F:198:LYS:HG2	1:F:202:GLU:HG2	2.01	0.43
1:C:21:LEU:O	1:C:25:GLU:HG2	2.19	0.43
2:V:36:GLN:HB2	2:V:184:TYR:CE1	2.53	0.43
1:N:143:GLN:HE22	1:N:143:GLN:HA	1.83	0.43
2:1:66:TYR:C	2:1:66:TYR:CD1	2.92	0.42
1:L:198:LYS:HG3	1:L:207:LEU:HD22	2.01	0.42
2:Z:176:ALA:HB2	2:Z:186:GLN:HG3	2.00	0.42
1:K:198:LYS:O	1:K:199:SER:C	2.57	0.42
1:F:130:ARG:HA	1:F:131:PRO:HD3	1.91	0.42
1:C:62:ASN:O	1:C:65:GLU:HG2	2.18	0.42
2:2:152:VAL:O	2:2:156:ILE:HG13	2.19	0.42
1:C:165:ILE:HD12	1:C:169:LYS:HD2	2.01	0.42
1:D:42:PHE:HB2	1:D:184:LEU:O	2.20	0.42
1:F:35:SER:O	1:F:166:GLY:HA3	2.19	0.42
2:V:22:MET:O	2:V:23:GLU:HB2	2.18	0.42
2:2:173:ILE:HD13	2:2:173:ILE:C	2.39	0.42
1:N:44:ASN:HD22	1:N:44:ASN:HA	1.63	0.42
1:O:24:VAL:O	1:O:27:ALA:HB3	2.19	0.42
2:P:187:LEU:HA	2:P:188:PRO:HD3	1.83	0.42
1:A:58:LEU:CD1	1:A:58:LEU:N	2.83	0.42
1:I:123:TYR:N	1:I:123:TYR:CD1	2.88	0.42
1:L:174:SER:O	1:L:175:PHE:C	2.57	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:T:109:HIS:HB3	2:T:111:PHE:HE1	1.84	0.42
1:F:159:GLU:O	1:G:60:GLU:HB2	2.19	0.42
2:Z:20:VAL:HG13	2:Z:28:HIS:HB2	2.00	0.42
2:B:103:GLY:HA2	2:B:178:ILE:HD13	2.01	0.42
1:I:149:PHE:CE2	1:I:159:GLU:HB2	2.54	0.42
2:P:141:GLN:HE22	2:Y:141:GLN:NE2	2.18	0.42
2:W:174:ASP:HA	2:W:192:ILE:HD13	2.00	0.42
1:M:40:MET:HA	1:M:162:ALA:HA	2.01	0.42
2:S:163:LYS:CE	2:S:203:LEU:HD23	2.50	0.42
1:A:187:LYS:O	1:A:190:VAL:HG13	2.19	0.42
1:G:198:LYS:O	1:G:199:SER:C	2.57	0.42
2:1:34:LEU:HD21	2:1:176:ALA:HB3	2.00	0.42
1:I:21:LEU:O	1:I:25:GLU:HG2	2.18	0.42
2:P:45:ILE:CD1	2:P:52:ALA:HB1	2.49	0.42
2:Y:124:TYR:HD1	2:Y:138:LEU:HD23	1.83	0.42
2:S:15:ALA:HB3	2:S:155:VAL:CG1	2.49	0.42
2:R:157:ARG:O	2:R:160:SER:HB2	2.19	0.42
1:L:136:LEU:HD13	1:L:138:PHE:CE1	2.54	0.42
1:F:49:ILE:HD12	1:F:50:SER:N	2.34	0.42
2:S:165:ARG:HA	2:2:26:ILE:HG23	2.00	0.42
1:D:146:PRO:O	1:D:147:ARG:HG2	2.19	0.42
1:O:88:LEU:HA	1:O:88:LEU:HD12	1.91	0.42
1:K:142:ASP:HD2	1:K:145:GLY:H	1.67	0.42
2:T:114:ASP:OD1	2:T:116:ALA:HB3	2.20	0.42
1:A:56:SER:OG	1:A:58:LEU:HB2	2.20	0.42
1:C:100:LYS:O	1:C:104:GLY:CA	2.68	0.42
1:L:160:TYR:CD2	1:L:163:THR:HB	2.55	0.42
2:V:2:THR:HG22	2:V:169:SER:OG	2.19	0.42
2:V:105:ASP:OD1	2:V:106:THR:N	2.53	0.42
1:M:152:ASP:HB2	1:M:153:PRO:CD	2.49	0.42
2:R:187:LEU:HA	2:R:188:PRO:HD3	1.76	0.42
2:V:72:VAL:HG22	2:V:73:ASN:N	2.34	0.42
2:2:137:VAL:HG21	2:2:158:ALA:HA	2.01	0.42
1:C:41:LYS:HE3	1:C:160:TYR:O	2.19	0.42
2:S:105:ASP:OD1	2:S:106:THR:N	2.52	0.42
2:R:1:THR:H3	2:R:129:SER:HB3	1.83	0.42
1:K:44:ASN:HA	1:K:44:ASN:HD22	1.61	0.42
2:Z:87:LEU:HD23	2:Z:114:ASP:O	2.20	0.42
2:U:141:GLN:HE22	2:1:141:GLN:NE2	2.16	0.42
1:E:82:VAL:HG13	1:E:83:ALA:H	1.84	0.42
2:T:137:VAL:HG21	2:T:158:ALA:HA	2.01	0.42
1:N:139:ALA:HB2	1:N:148:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:Z:179:THR:HG23	2:Z:182:ASP:H	1.84	0.42
2:U:22:MET:O	2:U:23:GLU:HB2	2.20	0.42
1:O:43:ALA:HB2	1:O:185:PRO:HA	2.00	0.42
1:D:160:TYR:CD2	1:D:163:THR:HB	2.54	0.42
1:H:51:ASP:HB3	1:H:53:LYS:NZ	2.35	0.42
1:M:70:ILE:HB	1:M:74:VAL:HG13	2.01	0.42
1:C:97:GLN:HA	1:C:97:GLN:OE1	2.19	0.42
2:1:66:TYR:CE1	2:1:70:ARG:HD2	2.54	0.42
2:Q:123:ILE:CD1	2:Q:123:ILE:H	2.31	0.42
1:C:108:ASN:CB	2:Q:70:ARG:HG2	2.48	0.42
1:C:52:LYS:HA	1:C:66:LYS:NZ	2.34	0.42
1:N:134:VAL:CG2	1:N:135:SER:N	2.83	0.42
1:O:42:PHE:HB2	1:O:184:LEU:O	2.19	0.42
1:H:82:VAL:HG13	1:H:83:ALA:N	2.34	0.42
2:Y:19:ARG:NE	2:Y:26:ILE:HG13	2.35	0.42
2:B:165:ARG:C	2:Y:26:ILE:HG22	2.40	0.42
1:I:161:LYS:HG2	1:I:180:TYR:CE2	2.55	0.42
1:L:180:TYR:HB3	1:M:57:ARG:NH2	2.35	0.42
1:D:162:ALA:O	1:D:163:THR:HB	2.19	0.42
2:1:44:THR:OG1	2:1:100:LEU:HB3	2.19	0.42
1:O:82:VAL:HG13	1:O:83:ALA:H	1.84	0.42
2:V:129:SER:OG	2:V:168:ALA:HB3	2.18	0.42
1:C:191:THR:O	1:C:194:ILE:HG22	2.19	0.42
1:O:40:MET:HA	1:O:162:ALA:HA	2.02	0.42
1:N:71:ASP:O	1:N:73:TYR:N	2.53	0.42
1:G:125:GLN:O	1:H:129:VAL:HG23	2.20	0.42
1:D:61:GLN:OE1	1:D:62:ASN:HB3	2.20	0.42
2:S:190:ASP:HA	2:S:193:GLU:HG2	2.02	0.42
2:1:176:ALA:HA	2:1:186:GLN:HA	2.02	0.42
2:S:15:ALA:HB3	2:S:155:VAL:HG11	2.00	0.42
2:T:184:TYR:C	2:T:184:TYR:CD1	2.93	0.42
2:1:173:ILE:O	2:1:192:ILE:HG21	2.20	0.42
1:E:147:ARG:HB3	1:E:149:PHE:HE1	1.83	0.42
1:G:79:SER:OG	1:G:166:GLY:HA2	2.20	0.42
1:O:214:SER:HG	1:O:224:TYR:HE1	1.68	0.42
2:X:74:MET:HA	2:X:75:PRO:HD3	1.88	0.42
1:E:31:VAL:HA	1:E:80:GLY:HA2	2.01	0.42
1:L:215:ILE:HD11	1:L:219:ASN:O	2.19	0.42
2:V:163:LYS:CE	2:V:203:LEU:HD23	2.49	0.42
1:I:26:TYR:N	1:I:26:TYR:CD1	2.88	0.42
1:M:123:TYR:CD1	1:M:123:TYR:N	2.87	0.42
2:V:90:VAL:O	2:V:90:VAL:HG22	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:1:34:LEU:HD21	2:1:176:ALA:CB	2.50	0.42
1:E:130:ARG:HG2	1:E:130:ARG:NH1	2.34	0.42
1:M:82:VAL:HG13	1:M:83:ALA:H	1.83	0.42
2:S:165:ARG:C	2:2:26:ILE:HG22	2.40	0.42
2:S:55:LEU:HD12	2:S:55:LEU:HA	1.67	0.42
2:Y:20:VAL:HG22	2:Y:28:HIS:HB2	2.02	0.42
2:X:175:VAL:CG2	2:X:176:ALA:N	2.83	0.42
1:H:88:LEU:HD13	1:H:132:TYR:CE2	2.55	0.42
2:1:35:PHE:CE2	2:1:45:ILE:HD12	2.55	0.42
1:G:215:ILE:HD11	1:G:219:ASN:O	2.19	0.42
1:G:191:THR:HA	1:G:194:ILE:HG22	2.02	0.42
2:2:66:TYR:C	2:2:66:TYR:CD1	2.93	0.42
2:P:83:LEU:HA	2:P:83:LEU:HD12	1.88	0.42
2:W:83:LEU:HD12	2:W:83:LEU:HA	1.79	0.42
1:K:144:ILE:HD12	1:K:147:ARG:NH1	2.35	0.42
1:J:98:GLN:O	1:J:101:VAL:HG12	2.20	0.42
1:I:88:LEU:HD21	1:I:120:MET:SD	2.59	0.42
2:T:180:ARG:HA	2:T:180:ARG:HD2	1.77	0.42
2:1:27:MET:HG2	2:1:27:MET:O	2.20	0.42
1:G:22:PHE:O	1:G:25:GLU:HB2	2.20	0.42
1:D:64:ILE:O	1:D:64:ILE:HG23	2.20	0.42
1:J:85:ALA:O	1:J:89:VAL:HG23	2.19	0.42
1:F:198:LYS:O	1:F:199:SER:C	2.58	0.42
1:F:58:LEU:CD1	1:F:58:LEU:N	2.83	0.42
1:G:70:ILE:HD11	1:G:76:ALA:HB2	2.01	0.42
1:O:48:LEU:CD1	1:O:139:ALA:HB3	2.49	0.42
2:Q:109:HIS:HB3	2:Q:111:PHE:CE1	2.54	0.42
2:U:97:VAL:HG22	2:U:98:GLN:H	1.85	0.42
1:K:134:VAL:CG2	1:K:135:SER:N	2.82	0.42
1:A:54:VAL:HG22	1:A:55:ARG:N	2.34	0.42
2:1:17:GLU:O	2:1:33:LYS:HD2	2.20	0.42
1:H:208:LYS:HD2	1:H:208:LYS:HA	1.90	0.42
1:O:58:LEU:CD1	1:O:58:LEU:N	2.82	0.42
2:S:25:PHE:CD1	2:S:25:PHE:C	2.91	0.42
1:G:59:ILE:HD13	1:G:59:ILE:HA	1.92	0.42
2:T:66:TYR:CZ	2:T:70:ARG:HD2	2.54	0.41
1:G:62:ASN:O	1:G:65:GLU:HG2	2.20	0.41
1:C:121:GLN:HG3	1:D:83:ALA:HB1	2.02	0.41
2:Q:34:LEU:HD21	2:Q:176:ALA:CB	2.50	0.41
2:B:3:THR:OG1	2:B:127:THR:HG22	2.19	0.41
1:G:41:LYS:HE3	1:G:160:TYR:O	2.20	0.41
1:J:58:LEU:N	1:J:58:LEU:HD12	2.35	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:42:PHE:O	1:D:43:ALA:C	2.59	0.41
1:D:170:ASP:O	1:D:173:VAL:HG12	2.20	0.41
2:1:163:LYS:CE	2:1:203:LEU:HD23	2.50	0.41
2:U:138:LEU:HA	2:U:138:LEU:HD12	1.71	0.41
1:L:94:ILE:CG1	1:L:95:SER:N	2.83	0.41
1:E:102:THR:O	2:S:81:THR:HG22	2.20	0.41
1:H:175:PHE:CD2	1:H:196:ALA:HA	2.56	0.41
1:K:156:THR:HG23	1:L:82:VAL:HG11	2.02	0.41
1:F:174:SER:O	1:F:177:GLU:HB3	2.20	0.41
2:W:126:SER:HB3	2:W:135:TYR:CE2	2.55	0.41
2:V:124:TYR:CE2	2:V:138:LEU:HB3	2.54	0.41
1:F:160:TYR:C	1:G:60:GLU:HG2	2.40	0.41
1:K:175:PHE:C	1:K:175:PHE:HD1	2.24	0.41
2:W:44:THR:OG1	2:W:100:LEU:HB3	2.19	0.41
1:H:142:ASP:HD2	1:H:145:GLY:H	1.69	0.41
2:P:1:THR:H3	2:P:129:SER:HB3	1.85	0.41
2:T:163:LYS:CE	2:T:203:LEU:HD23	2.50	0.41
2:X:109:HIS:HB3	2:X:111:PHE:HE1	1.84	0.41
1:G:88:LEU:HD13	1:G:132:TYR:CD2	2.54	0.41
1:J:44:ASN:HD22	1:J:44:ASN:HA	1.64	0.41
1:E:97:GLN:OE1	1:E:97:GLN:HA	2.19	0.41
1:O:25:GLU:O	1:O:28:ARG:HB2	2.21	0.41
2:X:7:THR:HB	2:X:123:ILE:O	2.21	0.41
2:U:59:MET:SD	2:U:83:LEU:HD13	2.60	0.41
1:G:52:LYS:CE	1:G:64:ILE:HG23	2.46	0.41
1:I:124:THR:HG22	1:J:130:ARG:NH2	2.35	0.41
1:N:28:ARG:O	1:N:31:VAL:HG22	2.20	0.41
1:G:94:ILE:CG1	1:G:95:SER:N	2.82	0.41
1:G:156:THR:CG2	1:H:82:VAL:HG11	2.50	0.41
2:W:193:GLU:HA	2:W:196:ILE:HD12	2.02	0.41
2:S:97:VAL:HG22	2:S:98:GLN:H	1.85	0.41
2:P:191:GLN:O	2:P:194:SER:HB3	2.20	0.41
2:S:143:SER:O	2:S:146:MET:HG3	2.20	0.41
1:E:26:TYR:O	1:E:29:GLU:HB2	2.20	0.41
1:D:71:ASP:OD1	1:D:72:ASP:N	2.53	0.41
2:Z:189:THR:HG23	2:Z:190:ASP:N	2.35	0.41
2:P:180:ARG:HA	2:P:180:ARG:HD2	1.81	0.41
1:L:123:TYR:CD1	1:L:123:TYR:N	2.88	0.41
1:L:42:PHE:CD1	1:L:43:ALA:N	2.89	0.41
2:T:111:PHE:CE2	2:T:121:GLU:HB2	2.55	0.41
1:K:35:SER:O	1:K:166:GLY:HA3	2.20	0.41
2:P:175:VAL:HG22	2:P:176:ALA:N	2.35	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:P:147:THR:OG1	2:P:150:GLU:HG3	2.21	0.41
1:G:157:ILE:HG12	1:G:158:ASN:N	2.34	0.41
1:M:191:THR:O	1:M:194:ILE:HG22	2.21	0.41
1:H:101:VAL:HG23	2:U:57:ARG:HB3	2.03	0.41
1:O:16:SER:HB3	1:O:22:PHE:CE2	2.56	0.41
1:E:228:GLU:O	1:E:231:LYS:HB3	2.20	0.41
1:M:44:ASN:HD22	1:M:44:ASN:HA	1.62	0.41
2:Z:59:MET:HE1	2:Z:82:LEU:HD23	2.03	0.41
2:W:56:VAL:CG1	2:W:57:ARG:N	2.83	0.41
2:1:138:LEU:HA	2:1:138:LEU:HD12	1.83	0.41
1:O:61:GLN:CD	1:O:62:ASN:H	2.24	0.41
2:Y:59:MET:CE	2:Y:79:VAL:HG23	2.48	0.41
2:X:179:THR:O	2:X:183:GLY:N	2.53	0.41
2:P:55:LEU:HD12	2:P:55:LEU:HA	1.90	0.41
2:S:87:LEU:HD23	2:S:114:ASP:O	2.20	0.41
2:V:37:ILE:HD11	2:V:59:MET:CG	2.50	0.41
1:L:16:SER:HB3	1:L:22:PHE:CD2	2.56	0.41
1:I:45:GLY:HA3	1:I:216:THR:HA	2.02	0.41
1:H:144:ILE:HD12	1:H:147:ARG:NH1	2.36	0.41
2:T:17:GLU:O	2:T:33:LYS:HD2	2.20	0.41
1:O:171:ALA:HB3	1:O:200:SER:OG	2.20	0.41
1:E:130:ARG:HH11	1:E:130:ARG:HG2	1.86	0.41
2:2:45:ILE:CG1	2:2:52:ALA:HB1	2.45	0.41
1:A:198:LYS:O	1:A:199:SER:C	2.59	0.41
1:N:130:ARG:HA	1:N:131:PRO:HD3	1.93	0.41
2:B:26:ILE:HG23	2:Y:165:ARG:HA	2.01	0.41
1:H:113:VAL:HG23	1:H:138:PHE:CE2	2.56	0.41
1:C:38:LEU:HG	1:C:49:ILE:HG23	2.02	0.41
1:D:38:LEU:HB3	1:D:164:ALA:CB	2.51	0.41
2:S:97:VAL:HG22	2:S:98:GLN:N	2.36	0.41
2:W:179:THR:HG23	2:W:182:ASP:H	1.86	0.41
1:F:18:ASP:OD2	1:F:20:ARG:HD3	2.21	0.41
1:K:41:LYS:HE3	1:K:160:TYR:O	2.20	0.41
1:C:142:ASP:HD2	1:C:145:GLY:H	1.66	0.41
2:U:158:ALA:O	2:U:161:ALA:HB3	2.21	0.41
1:M:45:GLY:HA3	1:M:216:THR:HA	2.01	0.41
1:J:152:ASP:HB2	1:J:153:PRO:CD	2.50	0.41
2:V:179:THR:HG23	2:V:182:ASP:H	1.86	0.41
1:G:159:GLU:HG2	1:H:60:GLU:HG3	2.03	0.41
1:J:175:PHE:CD2	1:J:196:ALA:HA	2.56	0.41
2:V:129:SER:HG	2:V:166:ASP:CG	2.23	0.41
2:W:105:ASP:OD1	2:W:106:THR:N	2.54	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:2:175:VAL:CG2	2:2:176:ALA:N	2.83	0.41
2:W:22:MET:O	2:W:23:GLU:HB2	2.21	0.41
2:1:180:ARG:HD2	2:1:180:ARG:HA	1.85	0.41
2:P:59:MET:SD	2:P:83:LEU:HD13	2.61	0.41
1:D:134:VAL:CG2	1:D:135:SER:N	2.83	0.41
1:L:38:LEU:HB3	1:L:164:ALA:HB2	2.02	0.41
2:X:20:VAL:HG22	2:X:20:VAL:O	2.20	0.41
1:K:130:ARG:HG2	1:K:130:ARG:NH1	2.36	0.41
1:D:89:VAL:O	1:D:92:ALA:HB3	2.20	0.41
1:L:137:ILE:HG22	1:L:150:ASP:CB	2.50	0.41
2:1:26:ILE:HD13	2:1:26:ILE:C	2.41	0.41
2:V:74:MET:HG2	2:V:78:ALA:HB3	2.02	0.41
1:N:175:PHE:HD1	1:N:175:PHE:C	2.23	0.41
1:F:136:LEU:HD13	1:F:138:PHE:CE2	2.56	0.41
1:G:142:ASP:N	1:G:142:ASP:HD2	2.18	0.41
1:I:26:TYR:O	1:I:29:GLU:HB2	2.21	0.41
2:R:22:MET:O	2:R:23:GLU:HB2	2.21	0.41
1:F:48:LEU:HD13	1:F:139:ALA:HB3	2.02	0.41
2:U:177:VAL:HG13	2:U:185:VAL:HG13	2.03	0.41
1:O:143:GLN:HA	1:O:143:GLN:HE22	1.86	0.41
2:X:55:LEU:HD12	2:X:55:LEU:HA	1.90	0.41
1:N:107:VAL:HG11	2:2:66:TYR:HH	1.82	0.41
2:Z:37:ILE:HD11	2:Z:59:MET:CG	2.51	0.41
2:P:56:VAL:CG1	2:P:57:ARG:N	2.84	0.41
2:V:138:LEU:HA	2:V:138:LEU:HD12	1.88	0.41
2:2:55:LEU:HA	2:2:55:LEU:HD12	1.74	0.41
2:V:6:ILE:HD11	2:V:142:TYR:CE1	2.56	0.41
2:B:19:ARG:HE	2:B:26:ILE:HG13	1.86	0.41
1:K:98:GLN:O	1:K:102:THR:CG2	2.69	0.41
2:Y:3:THR:HB	2:Y:16:THR:HG22	2.03	0.41
1:E:98:GLN:O	1:E:102:THR:CG2	2.69	0.41
1:J:123:TYR:CD1	1:J:123:TYR:N	2.88	0.41
2:W:189:THR:HG23	2:W:190:ASP:H	1.86	0.41
1:L:82:VAL:HG13	1:L:83:ALA:H	1.86	0.41
1:G:191:THR:O	1:G:194:ILE:HG22	2.20	0.41
2:V:49:VAL:HG23	2:V:50:GLY:H	1.86	0.41
1:I:127:GLY:O	1:I:129:VAL:N	2.53	0.41
1:E:207:LEU:HD23	1:E:233:LEU:HD12	2.02	0.41
1:C:15:PHE:HD2	1:D:23:GLN:HE21	1.68	0.41
1:H:188:GLU:O	1:H:191:THR:HB	2.20	0.41
1:O:69:LEU:HD23	1:O:69:LEU:HA	1.90	0.41
1:E:88:LEU:HD12	1:E:88:LEU:HA	1.84	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:S:66:TYR:CZ	2:S:70:ARG:HD2	2.56	0.40
1:K:52:LYS:HB3	1:K:209:ALA:O	2.21	0.40
2:W:103:GLY:HA2	2:W:178:ILE:HD13	2.03	0.40
1:E:42:PHE:HD1	1:E:43:ALA:N	2.19	0.40
1:M:121:GLN:CG	1:N:83:ALA:HB1	2.51	0.40
1:D:226:GLN:O	1:D:229:VAL:HG12	2.20	0.40
2:U:55:LEU:HD12	2:U:55:LEU:HA	1.96	0.40
2:1:97:VAL:HG22	2:1:98:GLN:H	1.86	0.40
2:Z:163:LYS:HE2	2:Z:203:LEU:HD23	2.01	0.40
1:E:116:VAL:HG11	1:E:138:PHE:CZ	2.56	0.40
1:D:142:ASP:HD2	1:D:142:ASP:H	1.68	0.40
1:M:130:ARG:HA	1:M:131:PRO:HD3	1.95	0.40
2:Z:175:VAL:CG2	2:Z:176:ALA:N	2.84	0.40
1:C:108:ASN:OD1	1:C:147:ARG:NH1	2.54	0.40
1:N:198:LYS:O	1:N:199:SER:C	2.59	0.40
1:K:187:LYS:O	1:K:190:VAL:HG13	2.21	0.40
1:G:38:LEU:HG	1:G:49:ILE:HG23	2.03	0.40
1:H:76:ALA:HA	1:H:137:ILE:O	2.21	0.40
1:J:142:ASP:OD2	1:J:147:ARG:HD2	2.21	0.40
2:S:141:GLN:NE2	2:V:141:GLN:HE22	2.19	0.40
2:B:81:THR:O	2:B:84:SER:HB3	2.21	0.40
2:Y:177:VAL:HG13	2:Y:185:VAL:HG13	2.02	0.40
2:Q:93:MET:N	2:Q:94:PRO:CD	2.84	0.40
1:N:86:ARG:HD3	1:N:86:ARG:HH11	1.76	0.40
2:X:25:PHE:C	2:X:25:PHE:CD1	2.92	0.40
1:D:208:LYS:HD2	1:D:208:LYS:HA	1.93	0.40
2:S:20:VAL:HG13	2:S:28:HIS:CB	2.47	0.40
1:O:52:LYS:HA	1:O:66:LYS:NZ	2.36	0.40
2:X:20:VAL:CG1	2:X:28:HIS:HB2	2.50	0.40
2:W:134:VAL:HG23	2:W:158:ALA:HB1	2.04	0.40
1:G:32:LYS:O	1:G:167:SER:HA	2.22	0.40
1:A:165:ILE:HD12	1:A:169:LYS:HD2	2.03	0.40
1:C:152:ASP:HB2	1:C:153:PRO:CD	2.50	0.40
1:J:171:ALA:HB3	1:J:200:SER:OG	2.22	0.40
1:A:123:TYR:N	1:A:123:TYR:CD1	2.88	0.40
1:G:58:LEU:N	1:G:58:LEU:CD1	2.84	0.40
2:T:3:THR:HB	2:T:16:THR:HG22	2.02	0.40
1:H:61:GLN:CD	1:H:62:ASN:H	2.25	0.40
2:V:15:ALA:HB3	2:V:155:VAL:CG1	2.51	0.40
2:P:19:ARG:NE	2:P:26:ILE:HG13	2.36	0.40
2:P:26:ILE:O	2:P:26:ILE:HD13	2.22	0.40
2:Z:187:LEU:HA	2:Z:188:PRO:HD3	1.87	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:202:ILE:CG1	2:B:203:LEU:N	2.85	0.40
2:S:187:LEU:HA	2:S:188:PRO:HD3	1.76	0.40
1:F:142:ASP:HD2	1:F:145:GLY:H	1.67	0.40
1:J:35:SER:O	1:J:166:GLY:HA3	2.21	0.40
2:Z:66:TYR:CZ	2:Z:70:ARG:HD2	2.57	0.40
2:P:178:ILE:HB	2:P:184:TYR:HA	2.03	0.40
1:O:62:ASN:O	1:O:65:GLU:HG2	2.21	0.40
1:D:176:LEU:C	1:D:178:ARG:N	2.74	0.40
2:R:26:ILE:HG23	2:V:165:ARG:HA	2.03	0.40
1:H:222:ARG:NH2	1:H:224:TYR:CZ	2.89	0.40
1:F:123:TYR:HD1	1:F:123:TYR:N	2.19	0.40
1:N:175:PHE:CD2	1:N:196:ALA:HA	2.57	0.40
1:I:180:TYR:HA	1:I:192:LEU:HD21	2.02	0.40
1:F:48:LEU:HB3	1:F:67:ILE:CD1	2.51	0.40
2:R:19:ARG:NH1	2:R:169:SER:O	2.54	0.40
1:E:142:ASP:HD2	1:E:145:GLY:H	1.68	0.40
1:G:119:GLN:O	1:G:122:GLN:HB2	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	219/233 (94%)	184 (84%)	26 (12%)	9 (4%)	4	42
1	C	219/233 (94%)	185 (84%)	25 (11%)	9 (4%)	4	42
1	D	219/233 (94%)	184 (84%)	28 (13%)	7 (3%)	6	51
1	E	219/233 (94%)	188 (86%)	22 (10%)	9 (4%)	4	42
1	F	219/233 (94%)	183 (84%)	25 (11%)	11 (5%)	3	34
1	G	219/233 (94%)	186 (85%)	23 (10%)	10 (5%)	4	37
1	H	219/233 (94%)	186 (85%)	25 (11%)	8 (4%)	5	46
1	I	219/233 (94%)	188 (86%)	22 (10%)	9 (4%)	4	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	219/233 (94%)	182 (83%)	26 (12%)	11 (5%)	3	34
1	K	219/233 (94%)	187 (85%)	26 (12%)	6 (3%)	8	55
1	L	219/233 (94%)	186 (85%)	24 (11%)	9 (4%)	4	42
1	M	219/233 (94%)	184 (84%)	26 (12%)	9 (4%)	4	42
1	N	219/233 (94%)	187 (85%)	23 (10%)	9 (4%)	4	42
1	O	219/233 (94%)	188 (86%)	23 (10%)	8 (4%)	5	46
2	1	201/211 (95%)	184 (92%)	15 (8%)	2 (1%)	22	78
2	2	201/211 (95%)	181 (90%)	19 (10%)	1 (0%)	38	87
2	B	201/211 (95%)	185 (92%)	14 (7%)	2 (1%)	22	78
2	P	201/211 (95%)	183 (91%)	16 (8%)	2 (1%)	22	78
2	Q	201/211 (95%)	180 (90%)	20 (10%)	1 (0%)	38	87
2	R	201/211 (95%)	184 (92%)	15 (8%)	2 (1%)	22	78
2	S	201/211 (95%)	181 (90%)	16 (8%)	4 (2%)	11	62
2	T	201/211 (95%)	176 (88%)	23 (11%)	2 (1%)	22	78
2	U	201/211 (95%)	184 (92%)	15 (8%)	2 (1%)	22	78
2	V	201/211 (95%)	179 (89%)	20 (10%)	2 (1%)	22	78
2	W	201/211 (95%)	186 (92%)	13 (6%)	2 (1%)	22	78
2	X	201/211 (95%)	181 (90%)	18 (9%)	2 (1%)	22	78
2	Y	201/211 (95%)	183 (91%)	16 (8%)	2 (1%)	22	78
2	Z	201/211 (95%)	185 (92%)	14 (7%)	2 (1%)	22	78
All	All	5880/6216 (95%)	5150 (88%)	578 (10%)	152 (3%)	8	56

All (152) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	GLY
1	A	182	GLU
1	A	200	SER
1	C	128	GLY
1	C	200	SER
1	D	128	GLY
1	D	182	GLU
1	D	200	SER
1	E	128	GLY
1	E	182	GLU

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Mol	Chain	Res	Type
1	E	200	SER
1	F	128	GLY
1	F	182	GLU
1	F	200	SER
1	G	128	GLY
1	G	200	SER
1	H	128	GLY
1	H	182	GLU
1	H	200	SER
1	I	128	GLY
1	I	182	GLU
1	I	200	SER
1	I	205	GLU
1	J	128	GLY
1	J	182	GLU
1	J	200	SER
1	K	128	GLY
1	K	182	GLU
1	K	200	SER
1	L	128	GLY
1	L	182	GLU
1	L	200	SER
1	M	43	ALA
1	M	128	GLY
1	M	182	GLU
1	M	200	SER
1	N	128	GLY
1	N	182	GLU
1	N	200	SER
1	O	182	GLU
1	O	200	SER
2	P	9	LYS
2	S	9	LYS
2	T	9	LYS
2	V	9	LYS
2	Y	9	LYS
1	A	43	ALA
1	A	72	ASP
1	A	205	GLU
2	B	9	LYS
1	C	43	ALA
1	C	72	ASP

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Mol	Chain	Res	Type
1	C	182	GLU
1	C	205	GLU
1	D	43	ALA
1	D	205	GLU
1	E	43	ALA
1	E	205	GLU
1	F	72	ASP
1	G	43	ALA
1	G	129	VAL
1	G	182	GLU
1	G	205	GLU
1	H	43	ALA
1	J	43	ALA
1	J	72	ASP
1	J	205	GLU
1	K	43	ALA
1	K	205	GLU
1	L	43	ALA
1	L	205	GLU
1	M	62	ASN
1	M	72	ASP
1	M	205	GLU
1	N	72	ASP
1	N	205	GLU
1	O	43	ALA
1	O	128	GLY
1	O	205	GLU
2	Q	9	LYS
2	R	9	LYS
2	U	9	LYS
2	W	9	LYS
2	X	9	LYS
2	Z	9	LYS
2	1	9	LYS
2	2	9	LYS
2	B	23	GLU
1	E	72	ASP
1	E	177	GLU
1	F	43	ALA
1	F	61	GLN
1	F	198	LYS
1	F	205	GLU

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Mol	Chain	Res	Type
1	G	61	GLN
1	G	62	ASN
1	H	61	GLN
1	H	62	ASN
1	H	198	LYS
1	H	205	GLU
1	I	43	ALA
1	J	186	GLU
1	L	72	ASP
1	M	61	GLN
1	M	198	LYS
1	N	43	ALA
1	N	202	GLU
1	O	61	GLN
1	O	72	ASP
1	O	198	LYS
2	R	23	GLU
2	Y	23	GLU
1	C	61	GLN
1	D	198	LYS
1	E	61	GLN
1	F	62	ASN
1	I	61	GLN
1	I	62	ASN
1	I	72	ASP
1	I	198	LYS
1	K	198	LYS
1	L	62	ASN
1	N	198	LYS
2	T	23	GLU
2	V	23	GLU
2	X	23	GLU
1	A	198	LYS
1	A	202	GLU
1	C	198	LYS
1	G	72	ASP
1	J	61	GLN
1	J	198	LYS
1	J	202	GLU
1	L	198	LYS
1	N	61	GLN
2	S	23	GLU

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Mol	Chain	Res	Type
2	U	23	GLU
2	W	23	GLU
2	1	23	GLU
1	C	62	ASN
1	D	61	GLN
1	E	198	LYS
1	F	129	VAL
1	F	167	SER
1	G	198	LYS
1	L	61	GLN
2	P	23	GLU
2	S	49	VAL
2	Z	110	VAL
1	J	129	VAL
2	S	110	VAL
1	A	129	VAL

### 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	184/193 (95%)	163 (89%)	21 (11%)	8	38
1	C	184/193 (95%)	160 (87%)	24 (13%)	6	31
1	D	184/193 (95%)	159 (86%)	25 (14%)	5	29
1	E	184/193 (95%)	159 (86%)	25 (14%)	5	29
1	F	184/193 (95%)	158 (86%)	26 (14%)	5	28
1	G	184/193 (95%)	162 (88%)	22 (12%)	7	35
1	H	184/193 (95%)	164 (89%)	20 (11%)	9	42
1	I	184/193 (95%)	162 (88%)	22 (12%)	7	35
1	J	184/193 (95%)	162 (88%)	22 (12%)	7	35
1	K	184/193 (95%)	160 (87%)	24 (13%)	6	31
1	L	184/193 (95%)	159 (86%)	25 (14%)	5	29
1	M	184/193 (95%)	162 (88%)	22 (12%)	7	35
1	N	184/193 (95%)	160 (87%)	24 (13%)	6	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	184/193 (95%)	157 (85%)	27 (15%)	4	26
2	1	170/177 (96%)	148 (87%)	22 (13%)	6	32
2	2	170/177 (96%)	144 (85%)	26 (15%)	4	24
2	B	170/177 (96%)	145 (85%)	25 (15%)	4	26
2	P	170/177 (96%)	148 (87%)	22 (13%)	6	32
2	Q	170/177 (96%)	143 (84%)	27 (16%)	4	22
2	R	170/177 (96%)	143 (84%)	27 (16%)	4	22
2	S	170/177 (96%)	146 (86%)	24 (14%)	5	28
2	T	170/177 (96%)	152 (89%)	18 (11%)	10	43
2	U	170/177 (96%)	146 (86%)	24 (14%)	5	28
2	V	170/177 (96%)	145 (85%)	25 (15%)	4	26
2	W	170/177 (96%)	145 (85%)	25 (15%)	4	26
2	X	170/177 (96%)	149 (88%)	21 (12%)	7	34
2	Y	170/177 (96%)	144 (85%)	26 (15%)	4	24
2	Z	170/177 (96%)	150 (88%)	20 (12%)	8	36
All	All	4956/5180 (96%)	4295 (87%)	661 (13%)	6	30

All (661) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	38	LEU
1	A	44	ASN
1	A	47	LEU
1	A	62	ASN
1	A	71	ASP
1	A	102	THR
1	A	119	GLN
1	A	134	VAL
1	A	136	LEU
1	A	141	ILE
1	A	143	GLN
1	A	157	ILE
1	A	161	LYS
1	A	175	PHE
1	A	176	LEU
1	A	190	VAL

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Mol	Chain	Res	Type
1	A	201	LEU
1	A	202	GLU
1	A	212	ILE
1	A	221	TYR
2	B	2	THR
2	B	7	THR
2	B	17	GLU
2	B	25	PHE
2	B	26	ILE
2	B	41	THR
2	B	45	ILE
2	B	49	VAL
2	B	56	VAL
2	B	63	LEU
2	B	71	ARG
2	B	83	LEU
2	B	94	PRO
2	B	97	VAL
2	B	123	ILE
2	B	127	THR
2	B	134	VAL
2	B	137	VAL
2	B	138	LEU
2	B	144	GLU
2	B	165	ARG
2	B	173	ILE
2	B	175	VAL
2	B	178	ILE
2	B	201	LEU
1	C	21	LEU
1	C	24	VAL
1	C	31	VAL
1	C	38	LEU
1	C	44	ASN
1	C	47	LEU
1	C	49	ILE
1	C	62	ASN
1	C	71	ASP
1	C	102	THR
1	C	119	GLN
1	C	121	GLN
1	C	134	VAL

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Mol	Chain	Res	Type
1	C	136	LEU
1	C	141	ILE
1	C	143	GLN
1	C	157	ILE
1	C	161	LYS
1	C	175	PHE
1	C	190	VAL
1	C	201	LEU
1	C	202	GLU
1	C	212	ILE
1	C	221	TYR
1	D	21	LEU
1	D	31	VAL
1	D	44	ASN
1	D	47	LEU
1	D	48	LEU
1	D	49	ILE
1	D	58	LEU
1	D	62	ASN
1	D	71	ASP
1	D	87	VAL
1	D	102	THR
1	D	116	VAL
1	D	119	GLN
1	D	136	LEU
1	D	141	ILE
1	D	143	GLN
1	D	157	ILE
1	D	161	LYS
1	D	175	PHE
1	D	176	LEU
1	D	190	VAL
1	D	201	LEU
1	D	202	GLU
1	D	212	ILE
1	D	221	TYR
1	E	21	LEU
1	E	24	VAL
1	E	31	VAL
1	E	44	ASN
1	E	47	LEU
1	E	49	ILE

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Mol	Chain	Res	Type
1	E	58	LEU
1	E	62	ASN
1	E	71	ASP
1	E	101	VAL
1	E	102	THR
1	E	119	GLN
1	E	134	VAL
1	E	136	LEU
1	E	141	ILE
1	E	143	GLN
1	E	150	ASP
1	E	161	LYS
1	E	175	PHE
1	E	176	LEU
1	E	190	VAL
1	E	201	LEU
1	E	202	GLU
1	E	212	ILE
1	E	221	TYR
1	F	21	LEU
1	F	24	VAL
1	F	31	VAL
1	F	38	LEU
1	F	44	ASN
1	F	47	LEU
1	F	48	LEU
1	F	62	ASN
1	F	71	ASP
1	F	101	VAL
1	F	102	THR
1	F	119	GLN
1	F	121	GLN
1	F	134	VAL
1	F	136	LEU
1	F	141	ILE
1	F	143	GLN
1	F	150	ASP
1	F	157	ILE
1	F	161	LYS
1	F	175	PHE
1	F	176	LEU
1	F	190	VAL

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Mol	Chain	Res	Type
1	F	201	LEU
1	F	202	GLU
1	F	221	TYR
1	G	21	LEU
1	G	31	VAL
1	G	38	LEU
1	G	44	ASN
1	G	47	LEU
1	G	62	ASN
1	G	71	ASP
1	G	101	VAL
1	G	102	THR
1	G	119	GLN
1	G	136	LEU
1	G	141	ILE
1	G	143	GLN
1	G	150	ASP
1	G	157	ILE
1	G	161	LYS
1	G	175	PHE
1	G	190	VAL
1	G	201	LEU
1	G	202	GLU
1	G	212	ILE
1	G	221	TYR
1	H	21	LEU
1	H	31	VAL
1	H	44	ASN
1	H	47	LEU
1	H	62	ASN
1	H	71	ASP
1	H	102	THR
1	H	107	VAL
1	H	119	GLN
1	H	134	VAL
1	H	136	LEU
1	H	141	ILE
1	H	143	GLN
1	H	157	ILE
1	H	161	LYS
1	H	175	PHE
1	H	190	VAL

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Mol	Chain	Res	Type
1	H	201	LEU
1	H	202	GLU
1	H	221	TYR
1	I	21	LEU
1	I	38	LEU
1	I	44	ASN
1	I	47	LEU
1	I	62	ASN
1	I	71	ASP
1	I	102	THR
1	I	119	GLN
1	I	121	GLN
1	I	123	TYR
1	I	134	VAL
1	I	136	LEU
1	I	141	ILE
1	I	143	GLN
1	I	150	ASP
1	I	161	LYS
1	I	175	PHE
1	I	190	VAL
1	I	201	LEU
1	I	202	GLU
1	I	212	ILE
1	I	221	TYR
1	J	21	LEU
1	J	24	VAL
1	J	31	VAL
1	J	44	ASN
1	J	47	LEU
1	J	49	ILE
1	J	62	ASN
1	J	71	ASP
1	J	102	THR
1	J	119	GLN
1	J	134	VAL
1	J	136	LEU
1	J	141	ILE
1	J	143	GLN
1	J	150	ASP
1	J	157	ILE
1	J	161	LYS

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Mol	Chain	Res	Type
1	J	175	PHE
1	J	190	VAL
1	J	201	LEU
1	J	202	GLU
1	J	221	TYR
1	K	21	LEU
1	K	31	VAL
1	K	38	LEU
1	K	44	ASN
1	K	47	LEU
1	K	48	LEU
1	K	49	ILE
1	K	58	LEU
1	K	62	ASN
1	K	71	ASP
1	K	102	THR
1	K	119	GLN
1	K	134	VAL
1	K	136	LEU
1	K	141	ILE
1	K	143	GLN
1	K	161	LYS
1	K	175	PHE
1	K	176	LEU
1	K	190	VAL
1	K	201	LEU
1	K	202	GLU
1	K	212	ILE
1	K	221	TYR
1	L	21	LEU
1	L	24	VAL
1	L	31	VAL
1	L	38	LEU
1	L	44	ASN
1	L	47	LEU
1	L	49	ILE
1	L	58	LEU
1	L	62	ASN
1	L	71	ASP
1	L	87	VAL
1	L	101	VAL
1	L	102	THR

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Mol	Chain	Res	Type
1	L	119	GLN
1	L	136	LEU
1	L	141	ILE
1	L	143	GLN
1	L	157	ILE
1	L	161	LYS
1	L	175	PHE
1	L	190	VAL
1	L	201	LEU
1	L	202	GLU
1	L	212	ILE
1	L	221	TYR
1	M	21	LEU
1	M	31	VAL
1	M	44	ASN
1	M	47	LEU
1	M	49	ILE
1	M	62	ASN
1	M	71	ASP
1	M	102	THR
1	M	119	GLN
1	M	121	GLN
1	M	134	VAL
1	M	136	LEU
1	M	141	ILE
1	M	143	GLN
1	M	157	ILE
1	M	161	LYS
1	M	175	PHE
1	M	190	VAL
1	M	201	LEU
1	M	202	GLU
1	M	212	ILE
1	M	221	TYR
1	N	21	LEU
1	N	31	VAL
1	N	44	ASN
1	N	47	LEU
1	N	49	ILE
1	N	58	LEU
1	N	62	ASN
1	N	71	ASP

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Mol	Chain	Res	Type
1	N	74	VAL
1	N	102	THR
1	N	119	GLN
1	N	121	GLN
1	N	134	VAL
1	N	136	LEU
1	N	141	ILE
1	N	143	GLN
1	N	157	ILE
1	N	161	LYS
1	N	175	PHE
1	N	190	VAL
1	N	201	LEU
1	N	202	GLU
1	N	212	ILE
1	N	221	TYR
1	O	21	LEU
1	O	24	VAL
1	O	31	VAL
1	O	44	ASN
1	O	47	LEU
1	O	49	ILE
1	O	58	LEU
1	O	62	ASN
1	O	71	ASP
1	O	74	VAL
1	O	101	VAL
1	O	102	THR
1	O	119	GLN
1	O	121	GLN
1	O	136	LEU
1	O	141	ILE
1	O	143	GLN
1	O	150	ASP
1	O	157	ILE
1	O	161	LYS
1	O	175	PHE
1	O	176	LEU
1	O	190	VAL
1	O	201	LEU
1	O	202	GLU
1	O	212	ILE

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Mol	Chain	Res	Type
1	O	221	TYR
2	P	2	THR
2	P	17	GLU
2	P	20	VAL
2	P	25	PHE
2	P	26	ILE
2	P	41	THR
2	P	45	ILE
2	P	49	VAL
2	P	59	MET
2	P	70	ARG
2	P	71	ARG
2	P	83	LEU
2	P	123	ILE
2	P	127	THR
2	P	134	VAL
2	P	137	VAL
2	P	138	LEU
2	P	144	GLU
2	P	165	ARG
2	P	173	ILE
2	P	178	ILE
2	P	185	VAL
2	Q	2	THR
2	Q	8	LEU
2	Q	12	VAL
2	Q	17	GLU
2	Q	20	VAL
2	Q	25	PHE
2	Q	26	ILE
2	Q	41	THR
2	Q	45	ILE
2	Q	49	VAL
2	Q	55	LEU
2	Q	59	MET
2	Q	68	LEU
2	Q	70	ARG
2	Q	71	ARG
2	Q	83	LEU
2	Q	123	ILE
2	Q	127	THR
2	Q	134	VAL

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Mol	Chain	Res	Type
2	Q	137	VAL
2	Q	138	LEU
2	Q	144	GLU
2	Q	165	ARG
2	Q	173	ILE
2	Q	175	VAL
2	Q	178	ILE
2	Q	185	VAL
2	R	2	THR
2	R	7	THR
2	R	17	GLU
2	R	25	PHE
2	R	26	ILE
2	R	41	THR
2	R	45	ILE
2	R	49	VAL
2	R	56	VAL
2	R	68	LEU
2	R	71	ARG
2	R	83	LEU
2	R	94	PRO
2	R	97	VAL
2	R	104	ILE
2	R	123	ILE
2	R	127	THR
2	R	134	VAL
2	R	137	VAL
2	R	144	GLU
2	R	149	ASP
2	R	165	ARG
2	R	173	ILE
2	R	175	VAL
2	R	177	VAL
2	R	178	ILE
2	R	185	VAL
2	S	1	THR
2	S	2	THR
2	S	8	LEU
2	S	17	GLU
2	S	20	VAL
2	S	26	ILE
2	S	41	THR

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Mol	Chain	Res	Type
2	S	45	ILE
2	S	49	VAL
2	S	63	LEU
2	S	68	LEU
2	S	71	ARG
2	S	83	LEU
2	S	123	ILE
2	S	127	THR
2	S	134	VAL
2	S	137	VAL
2	S	138	LEU
2	S	144	GLU
2	S	153	ASP
2	S	165	ARG
2	S	173	ILE
2	S	175	VAL
2	S	178	ILE
2	T	2	THR
2	T	17	GLU
2	T	20	VAL
2	T	26	ILE
2	T	41	THR
2	T	45	ILE
2	T	59	MET
2	T	71	ARG
2	T	83	LEU
2	T	123	ILE
2	T	127	THR
2	T	134	VAL
2	T	137	VAL
2	T	138	LEU
2	T	144	GLU
2	T	165	ARG
2	T	173	ILE
2	T	178	ILE
2	U	2	THR
2	U	8	LEU
2	U	12	VAL
2	U	17	GLU
2	U	20	VAL
2	U	25	PHE
2	U	26	ILE

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Mol	Chain	Res	Type
2	U	41	THR
2	U	45	ILE
2	U	59	MET
2	U	70	ARG
2	U	71	ARG
2	U	94	PRO
2	U	123	ILE
2	U	127	THR
2	U	134	VAL
2	U	137	VAL
2	U	144	GLU
2	U	153	ASP
2	U	165	ARG
2	U	173	ILE
2	U	175	VAL
2	U	178	ILE
2	U	185	VAL
2	V	2	THR
2	V	7	THR
2	V	8	LEU
2	V	17	GLU
2	V	20	VAL
2	V	26	ILE
2	V	41	THR
2	V	45	ILE
2	V	49	VAL
2	V	56	VAL
2	V	59	MET
2	V	63	LEU
2	V	71	ARG
2	V	94	PRO
2	V	122	ASP
2	V	123	ILE
2	V	127	THR
2	V	134	VAL
2	V	137	VAL
2	V	138	LEU
2	V	144	GLU
2	V	165	ARG
2	V	173	ILE
2	V	178	ILE
2	V	185	VAL

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Mol	Chain	Res	Type
2	W	2	THR
2	W	7	THR
2	W	17	GLU
2	W	20	VAL
2	W	25	PHE
2	W	26	ILE
2	W	41	THR
2	W	45	ILE
2	W	49	VAL
2	W	56	VAL
2	W	59	MET
2	W	71	ARG
2	W	94	PRO
2	W	97	VAL
2	W	123	ILE
2	W	127	THR
2	W	134	VAL
2	W	137	VAL
2	W	138	LEU
2	W	144	GLU
2	W	165	ARG
2	W	173	ILE
2	W	175	VAL
2	W	178	ILE
2	W	185	VAL
2	X	2	THR
2	X	8	LEU
2	X	17	GLU
2	X	20	VAL
2	X	26	ILE
2	X	41	THR
2	X	45	ILE
2	X	49	VAL
2	X	59	MET
2	X	71	ARG
2	X	123	ILE
2	X	127	THR
2	X	134	VAL
2	X	137	VAL
2	X	144	GLU
2	X	165	ARG
2	X	173	ILE

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Mol	Chain	Res	Type
2	X	177	VAL
2	X	178	ILE
2	X	185	VAL
2	X	201	LEU
2	Y	2	THR
2	Y	7	THR
2	Y	8	LEU
2	Y	17	GLU
2	Y	25	PHE
2	Y	26	ILE
2	Y	41	THR
2	Y	45	ILE
2	Y	59	MET
2	Y	63	LEU
2	Y	70	ARG
2	Y	71	ARG
2	Y	83	LEU
2	Y	94	PRO
2	Y	123	ILE
2	Y	127	THR
2	Y	134	VAL
2	Y	137	VAL
2	Y	138	LEU
2	Y	144	GLU
2	Y	149	ASP
2	Y	165	ARG
2	Y	173	ILE
2	Y	175	VAL
2	Y	178	ILE
2	Y	185	VAL
2	Z	17	GLU
2	Z	20	VAL
2	Z	26	ILE
2	Z	41	THR
2	Z	45	ILE
2	Z	49	VAL
2	Z	63	LEU
2	Z	70	ARG
2	Z	71	ARG
2	Z	83	LEU
2	Z	123	ILE
2	Z	127	THR

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Mol	Chain	Res	Type
2	Z	134	VAL
2	Z	137	VAL
2	Z	138	LEU
2	Z	144	GLU
2	Z	165	ARG
2	Z	173	ILE
2	Z	175	VAL
2	Z	178	ILE
2	1	2	THR
2	1	8	LEU
2	1	17	GLU
2	1	20	VAL
2	1	26	ILE
2	1	41	THR
2	1	45	ILE
2	1	59	MET
2	1	71	ARG
2	1	123	ILE
2	1	127	THR
2	1	134	VAL
2	1	137	VAL
2	1	138	LEU
2	1	144	GLU
2	1	153	ASP
2	1	165	ARG
2	1	173	ILE
2	1	175	VAL
2	1	178	ILE
2	1	185	VAL
2	1	201	LEU
2	2	1	THR
2	2	2	THR
2	2	8	LEU
2	2	12	VAL
2	2	17	GLU
2	2	25	PHE
2	2	26	ILE
2	2	41	THR
2	2	45	ILE
2	2	49	VAL
2	2	59	MET
2	2	63	LEU

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Mol	Chain	Res	Type
2	2	68	LEU
2	2	71	ARG
2	2	94	PRO
2	2	123	ILE
2	2	127	THR
2	2	134	VAL
2	2	137	VAL
2	2	138	LEU
2	2	144	GLU
2	2	149	ASP
2	2	165	ARG
2	2	173	ILE
2	2	175	VAL
2	2	178	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (120) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	44	ASN
1	A	98	GLN
1	A	121	GLN
1	A	125	GLN
1	A	143	GLN
2	B	30	ASN
2	B	164	GLN
1	C	44	ASN
1	C	98	GLN
1	C	121	GLN
1	C	125	GLN
1	C	143	GLN
1	D	23	GLN
1	D	44	ASN
1	D	98	GLN
1	D	121	GLN
1	D	125	GLN
1	D	143	GLN
1	E	44	ASN
1	E	98	GLN
1	E	121	GLN
1	E	125	GLN
1	E	143	GLN

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Mol	Chain	Res	Type
1	F	44	ASN
1	F	98	GLN
1	F	119	GLN
1	F	121	GLN
1	F	125	GLN
1	F	143	GLN
1	G	44	ASN
1	G	121	GLN
1	G	125	GLN
1	G	143	GLN
1	H	44	ASN
1	H	98	GLN
1	H	121	GLN
1	H	125	GLN
1	H	143	GLN
1	I	44	ASN
1	I	98	GLN
1	I	121	GLN
1	I	125	GLN
1	I	143	GLN
1	J	44	ASN
1	J	98	GLN
1	J	121	GLN
1	J	125	GLN
1	J	143	GLN
1	K	44	ASN
1	K	98	GLN
1	K	121	GLN
1	K	125	GLN
1	K	143	GLN
1	L	23	GLN
1	L	44	ASN
1	L	98	GLN
1	L	121	GLN
1	L	125	GLN
1	L	143	GLN
1	M	44	ASN
1	M	98	GLN
1	M	121	GLN
1	M	125	GLN
1	M	143	GLN
1	N	23	GLN

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Mol	Chain	Res	Type
1	N	44	ASN
1	N	98	GLN
1	N	121	GLN
1	N	125	GLN
1	N	143	GLN
1	O	23	GLN
1	O	44	ASN
1	O	98	GLN
1	O	121	GLN
1	O	125	GLN
1	O	143	GLN
2	P	30	ASN
2	P	36	GLN
2	P	164	GLN
2	Q	30	ASN
2	Q	36	GLN
2	Q	141	GLN
2	Q	164	GLN
2	R	28	HIS
2	R	30	ASN
2	R	85	ASN
2	R	141	GLN
2	R	164	GLN
2	S	30	ASN
2	S	141	GLN
2	S	164	GLN
2	T	30	ASN
2	T	141	GLN
2	T	164	GLN
2	U	30	ASN
2	U	164	GLN
2	V	28	HIS
2	V	30	ASN
2	V	85	ASN
2	V	164	GLN
2	W	30	ASN
2	W	73	ASN
2	W	164	GLN
2	X	28	HIS
2	X	30	ASN
2	X	164	GLN
2	Y	30	ASN

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Mol	Chain	Res	Type
2	Y	141	GLN
2	Y	164	GLN
2	Z	28	HIS
2	Z	30	ASN
2	Z	141	GLN
2	Z	164	GLN
2	1	28	HIS
2	1	30	ASN
2	1	141	GLN
2	1	164	GLN
2	2	30	ASN
2	2	164	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

### 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	221/233 (94%)	-0.12	2 (0%) 81 47	17, 56, 117, 155	0
1	C	221/233 (94%)	-0.18	0 100 100	13, 53, 115, 154	0
1	D	221/233 (94%)	-0.17	1 (0%) 88 61	21, 53, 116, 153	0
1	E	221/233 (94%)	-0.19	0 100 100	17, 52, 115, 155	0
1	F	221/233 (94%)	-0.14	0 100 100	16, 57, 116, 153	0
1	G	221/233 (94%)	-0.08	3 (1%) 72 35	20, 56, 118, 155	0
1	H	221/233 (94%)	-0.12	1 (0%) 88 61	21, 57, 116, 154	0
1	I	221/233 (94%)	-0.12	2 (0%) 81 47	17, 55, 116, 155	0
1	J	221/233 (94%)	-0.12	2 (0%) 81 47	21, 55, 116, 156	0
1	K	221/233 (94%)	-0.17	1 (0%) 88 61	20, 55, 116, 153	0
1	L	221/233 (94%)	-0.19	1 (0%) 88 61	13, 53, 116, 153	0
1	M	221/233 (94%)	-0.16	0 100 100	17, 53, 117, 153	0
1	N	221/233 (94%)	-0.17	1 (0%) 88 61	19, 52, 116, 156	0
1	O	221/233 (94%)	-0.17	1 (0%) 88 61	18, 51, 116, 152	0
2	1	203/211 (96%)	-0.38	0 100 100	9, 33, 69, 85	0
2	2	203/211 (96%)	-0.38	0 100 100	6, 33, 69, 88	0
2	B	203/211 (96%)	-0.36	0 100 100	11, 34, 69, 90	0
2	P	203/211 (96%)	-0.36	0 100 100	8, 35, 69, 89	0
2	Q	203/211 (96%)	-0.41	0 100 100	8, 33, 71, 90	0
2	R	203/211 (96%)	-0.45	0 100 100	6, 32, 68, 86	0
2	S	203/211 (96%)	-0.42	0 100 100	7, 33, 68, 91	0
2	T	203/211 (96%)	-0.40	0 100 100	10, 35, 73, 90	0
2	U	203/211 (96%)	-0.39	0 100 100	14, 34, 70, 92	0
2	V	203/211 (96%)	-0.39	0 100 100	11, 32, 69, 89	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
2	W	203/211 (96%)	-0.41	0	100	100	11, 34, 69, 85	0
2	X	203/211 (96%)	-0.43	0	100	100	8, 32, 70, 90	0
2	Y	203/211 (96%)	-0.44	0	100	100	10, 32, 68, 92	0
2	Z	203/211 (96%)	-0.46	0	100	100	9, 32, 69, 91	0
All	All	5936/6216 (95%)	-0.27	15 (0%)	91	73	6, 43, 107, 156	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	205	GLU	2.8
1	G	205	GLU	2.8
1	G	201	LEU	2.7
1	L	55	ARG	2.4
1	I	205	GLU	2.4
1	I	64	ILE	2.3
1	J	205	GLU	2.3
1	O	202	GLU	2.3
1	A	181	LYS	2.2
1	A	202	GLU	2.2
1	G	203	GLU	2.1
1	K	32	LYS	2.0
1	H	205	GLU	2.0
1	D	206	GLU	2.0
1	J	202	GLU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.



## 6.5 Other polymers ⓘ

There are no such residues in this entry.