



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:46 PM BST

PDB ID : 2CGT  
EMDB ID: : EMD-1202  
Title : GROEL-ADP-gp31 COMPLEX  
Authors : Clare, D.K.; Bakkes, P.J.; van Heerikhuizen, H.; van der Vies, S.M.; Saibil, H.R.  
Deposited on : 2006-03-09  
Resolution : 8.20 Å(reported)  
Based on PDB ID : 1A0N,1G31

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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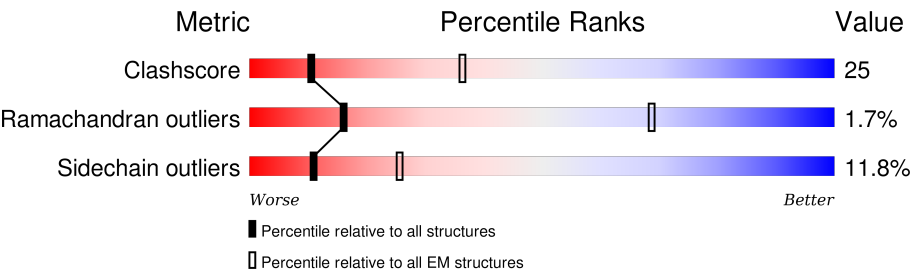
MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 8.20 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.







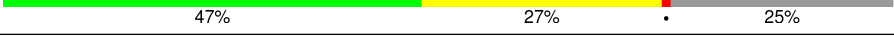
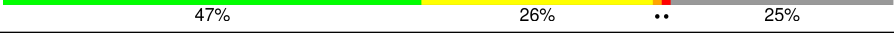

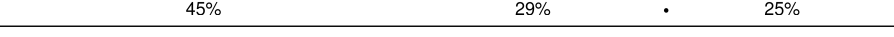

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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

Mol	Chain	Length	Quality of chain
1	A	547	62% 27% 6% .
1	B	547	62% 27% 6% .
1	C	547	62% 27% 6% .
1	D	547	63% 26% 6% .
1	E	547	62% 27% 6% .
1	F	547	63% 27% 6% .
1	G	547	62% 27% 6% .
1	H	547	56% 32% 5% . 6%
1	I	547	55% 33% 5% . 6%

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Mol	Chain	Length	Quality of chain
1	J	547	 55% 33% 5% • 6%
1	K	547	 55% 32% 6% • 6%
1	L	547	 55% 33% 5% • 6%
1	M	547	 55% 33% 6% • 6%
1	N	547	 55% 33% 5% • 6%
2	O	111	 47% 27% • 25%
2	P	111	 47% 26% •• 25%
2	Q	111	 47% 26% •• 25%
2	R	111	 45% 28% •• 25%
2	S	111	 45% 29% • 25%
2	T	111	 45% 29% • 25%
2	U	111	 45% 29% • 25%

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 57953 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 60 KDA GROEL.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	524	Total	C	N	O	S	0	0
			3855	2397	665	773	20		
1	B	524	Total	C	N	O	S	0	0
			3855	2397	665	773	20		
1	C	524	Total	C	N	O	S	0	0
			3855	2397	665	773	20		
1	D	524	Total	C	N	O	S	0	0
			3855	2397	665	773	20		
1	E	524	Total	C	N	O	S	0	0
			3855	2397	665	773	20		
1	F	524	Total	C	N	O	S	0	0
			3855	2397	665	773	20		
1	G	524	Total	C	N	O	S	0	0
			3855	2397	665	773	20		
1	H	515	Total	C	N	O	S	0	0
			3783	2354	656	753	20		
1	I	515	Total	C	N	O	S	0	0
			3783	2354	656	753	20		
1	J	515	Total	C	N	O	S	0	0
			3783	2354	656	753	20		
1	K	515	Total	C	N	O	S	0	0
			3783	2354	656	753	20		
1	L	515	Total	C	N	O	S	0	0
			3783	2354	656	753	20		
1	M	515	Total	C	N	O	S	0	0
			3783	2354	656	753	20		
1	N	515	Total	C	N	O	S	0	0
			3783	2354	656	753	20		

- Molecule 2 is a protein called CAPSID ASSEMBLY PROTEIN GP31.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	O	83	Total	C	N	O	S	0	0
			641	417	106	114	4		

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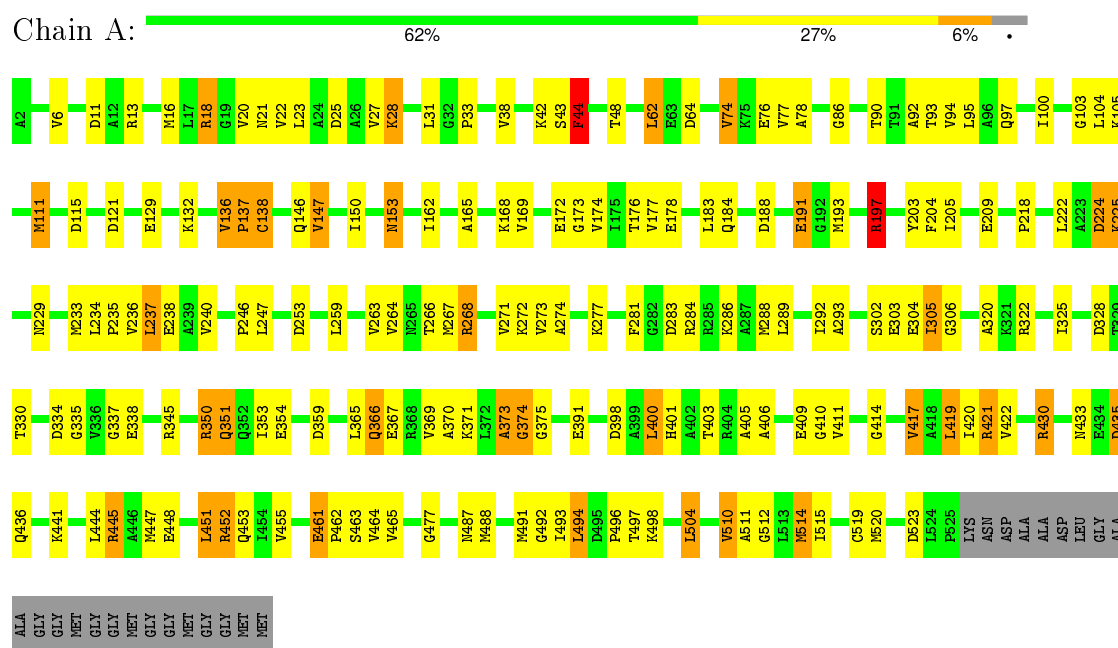
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Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	83	Total 641	C 417	N 106	O 114	S 4	0	0
2	Q	83	Total 641	C 417	N 106	O 114	S 4	0	0
2	R	83	Total 641	C 417	N 106	O 114	S 4	0	0
2	S	83	Total 641	C 417	N 106	O 114	S 4	0	0
2	T	83	Total 641	C 417	N 106	O 114	S 4	0	0
2	U	83	Total 641	C 417	N 106	O 114	S 4	0	0

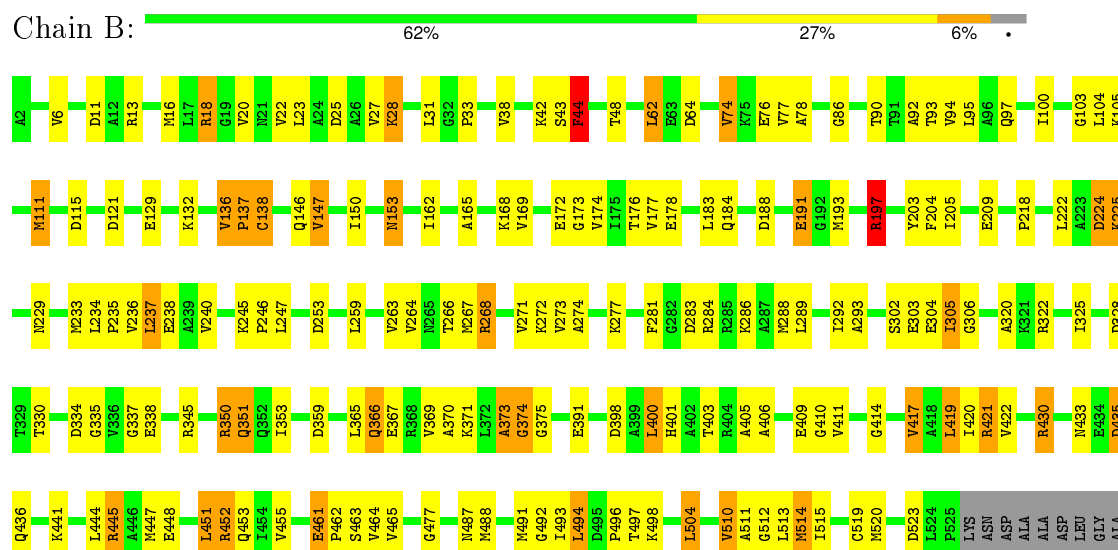
### 3 Residue-property plots

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 60 KDA GROEL



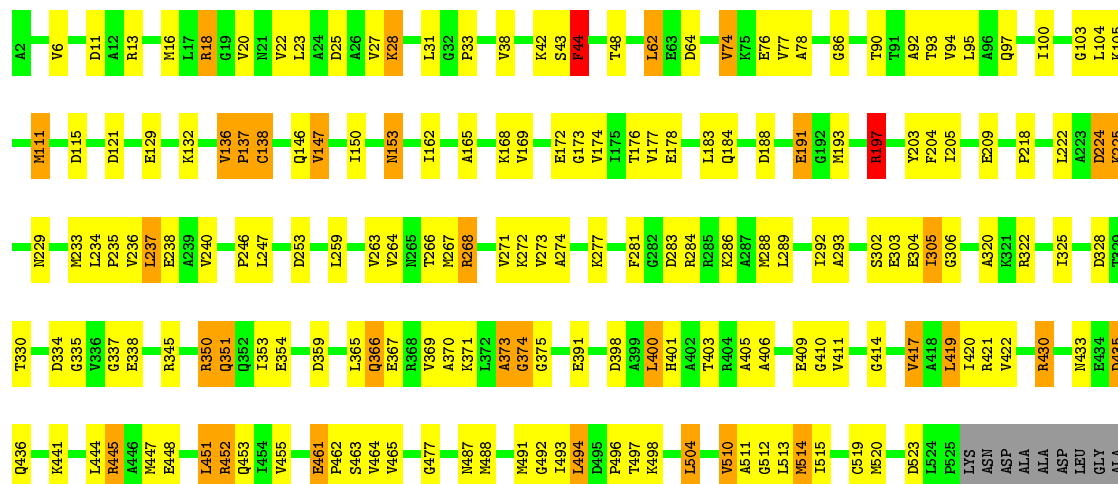
- Molecule 1: 60 KDA GROEL



ALA  
GLY  
GLY  
MET  
GLY  
GLY  
MET  
GLY  
GLY  
MET  
MET

• Molecule 1: 60 KDA GROEL

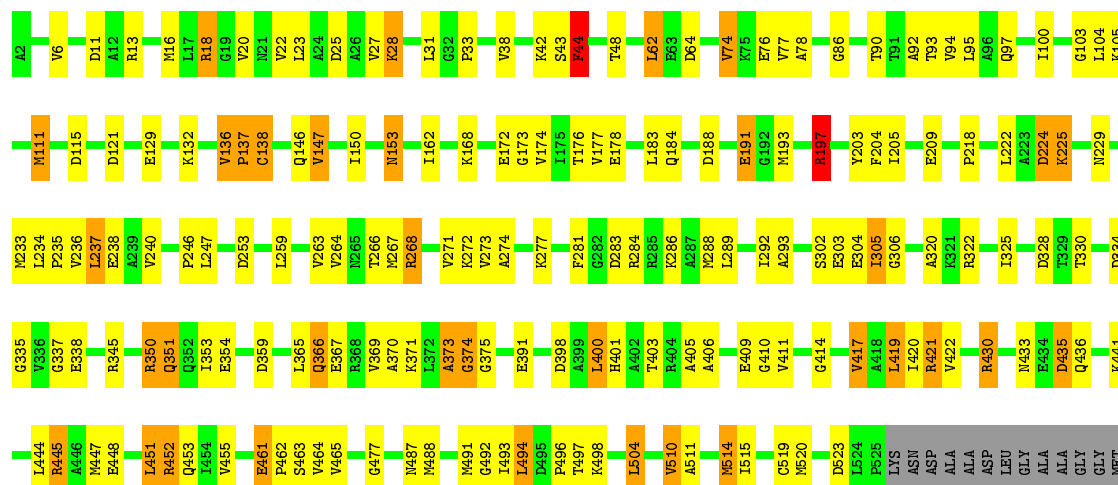
Chain C:  62% 27% 6% •



ALA  
GLY  
GLY  
MET  
GLY  
GLY  
MET  
GLY  
GLY  
MET  
MET

• Molecule 1: 60 KDA GROEL

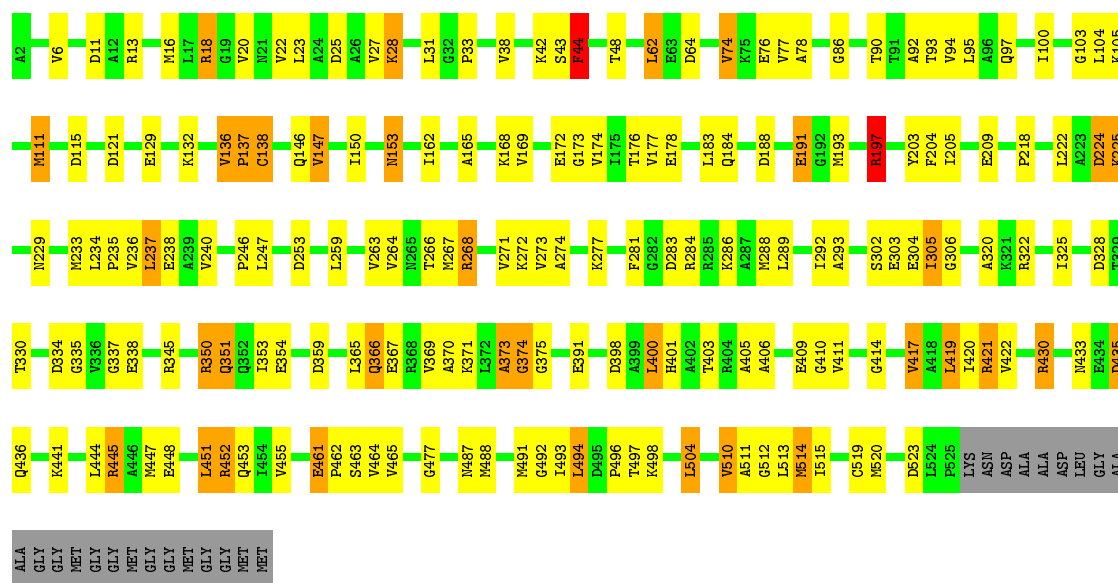
Chain D:  63% 26% 6% •



GLY  
GLY  
MET  
GLY  
GLY  
MET  
GLY  
GLY  
MET  
MET

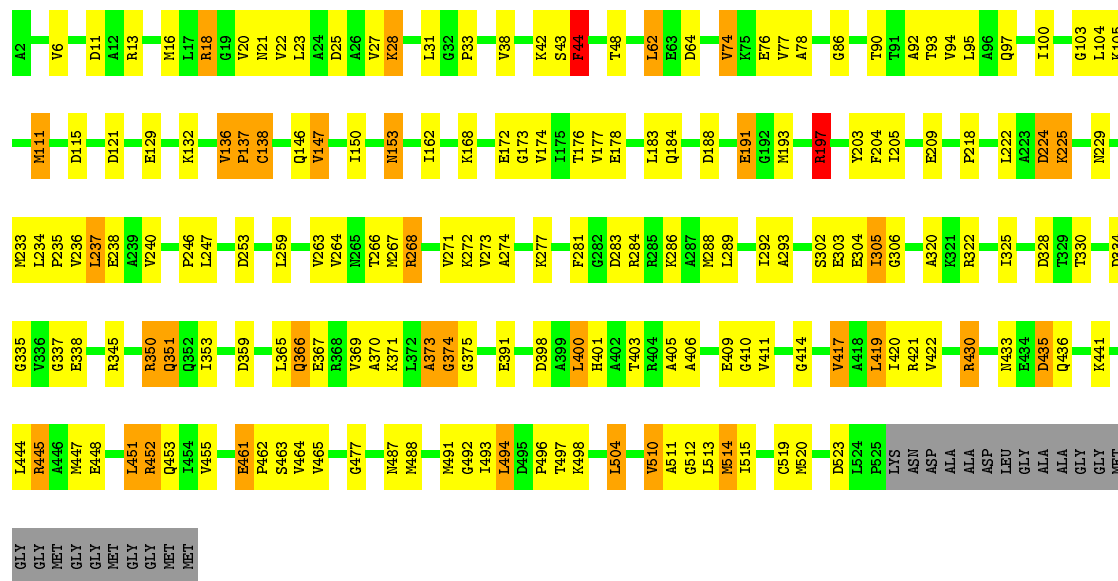
• Molecule 1: 60 KDA GROEL

Chain E:  62% 27% 6% •



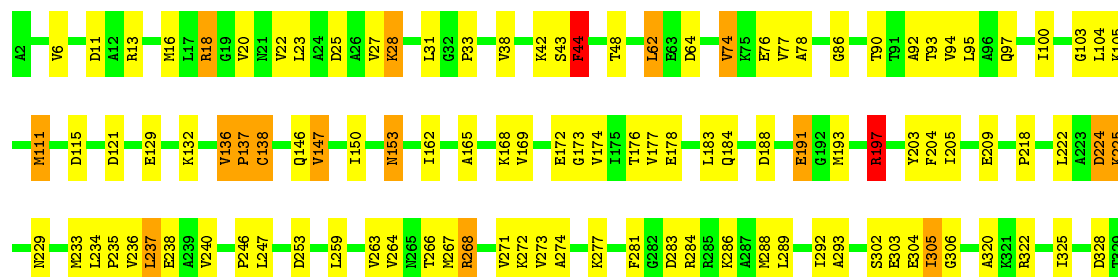
• Molecule 1: 60 KDA GROEL

Chain F:  63% 27% 6%



• Molecule 1: 60 KDA GROEL

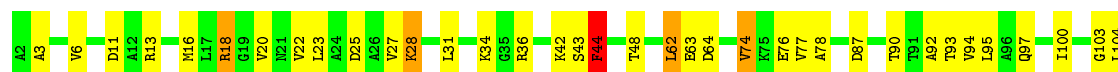
Chain G:  62% 27% 6%

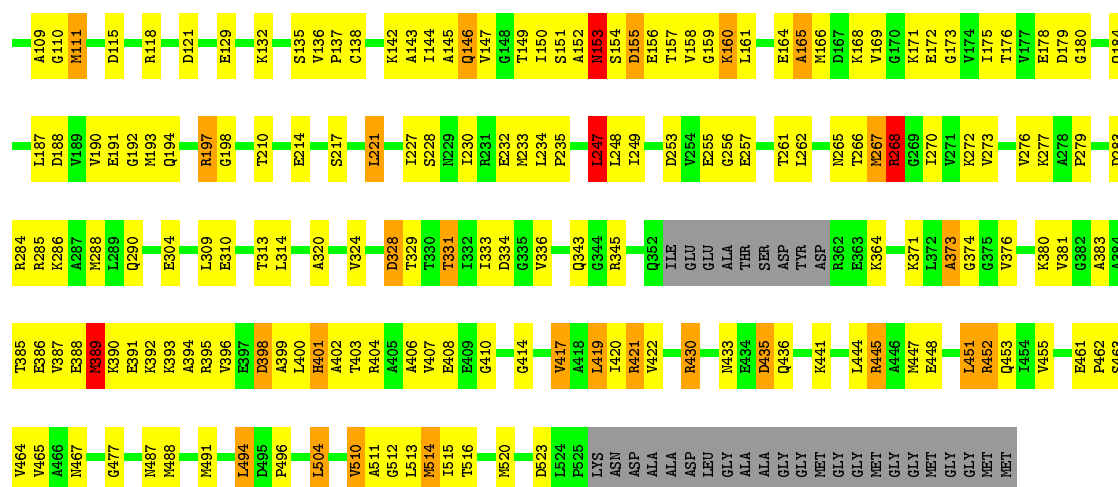






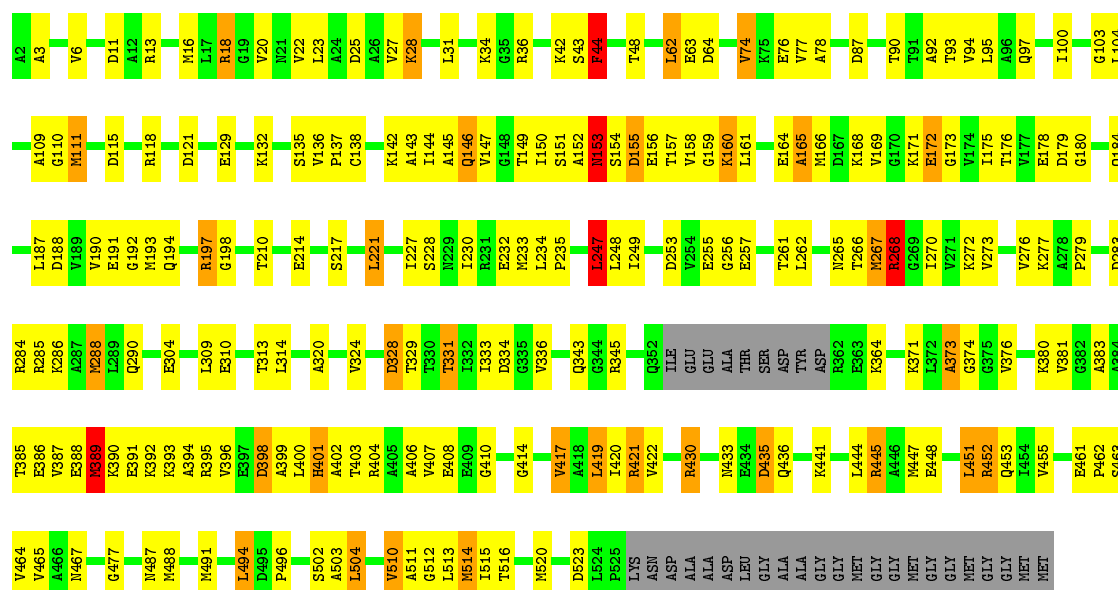
Chain J:  55% 33% 5% • 6%





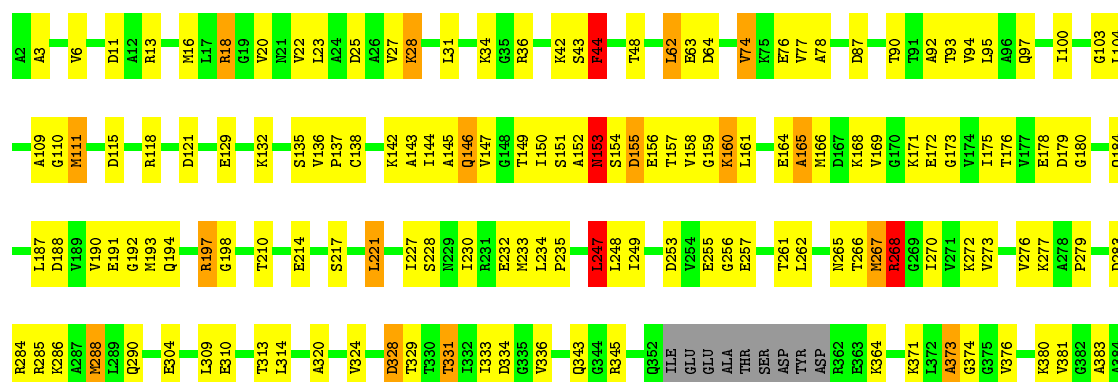
• Molecule 1: 60 KDA GROEL

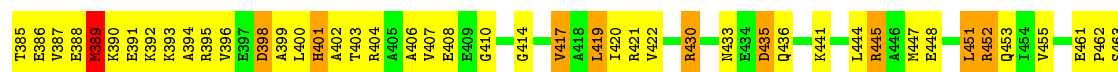
Chain M: 55% 33% 6% • 6%



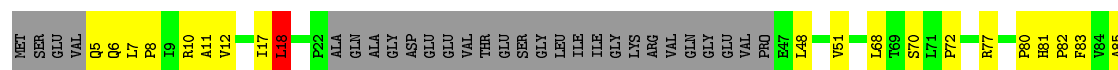
• Molecule 1: 60 KDA GROEL

Chain N: 55% 33% 5% • 6%

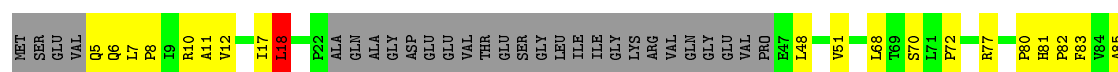




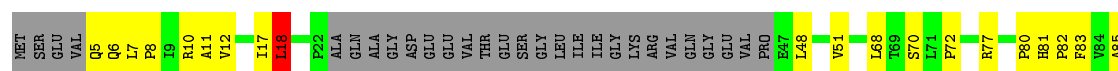
• Molecule 2: CAPSID ASSEMBLY PROTEIN GP31



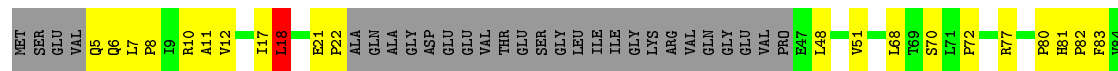
• Molecule 2: CAPSID ASSEMBLY PROTEIN GP31



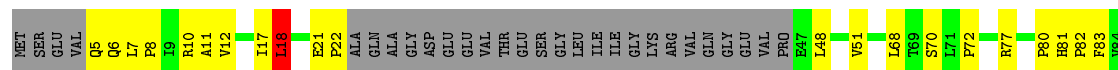
• Molecule 2: CAPSID ASSEMBLY PROTEIN GP31

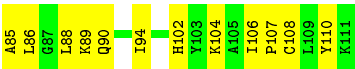


• Molecule 2: CAPSID ASSEMBLY PROTEIN GP31

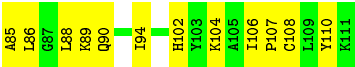
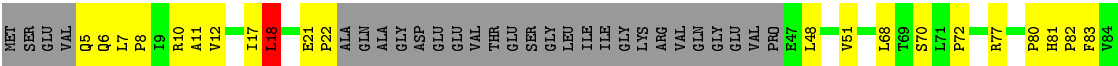


• Molecule 2: CAPSID ASSEMBLY PROTEIN GP31

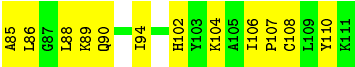
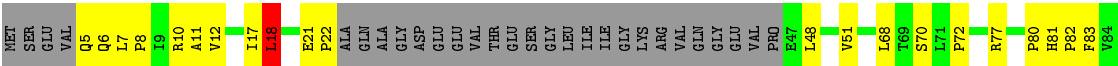




● Molecule 2: CAPSID ASSEMBLY PROTEIN GP31



● Molecule 2: CAPSID ASSEMBLY PROTEIN GP31



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	FULL CORRECTION ON 2D CLASS AVERAGES	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	3300	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO163 FILM	Depositor

## 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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	1.07	3/3882 (0.1%)	1.23	27/5240 (0.5%)
1	B	1.07	3/3882 (0.1%)	1.23	27/5240 (0.5%)
1	C	1.07	3/3882 (0.1%)	1.23	27/5240 (0.5%)
1	D	1.07	3/3882 (0.1%)	1.23	27/5240 (0.5%)
1	E	1.07	3/3882 (0.1%)	1.23	27/5240 (0.5%)
1	F	1.07	3/3882 (0.1%)	1.23	27/5240 (0.5%)
1	G	1.07	3/3882 (0.1%)	1.23	27/5240 (0.5%)
1	H	0.68	1/3806 (0.0%)	1.04	15/5130 (0.3%)
1	I	0.69	1/3806 (0.0%)	1.04	15/5130 (0.3%)
1	J	0.69	1/3806 (0.0%)	1.04	15/5130 (0.3%)
1	K	0.69	1/3806 (0.0%)	1.04	15/5130 (0.3%)
1	L	0.69	1/3806 (0.0%)	1.04	15/5130 (0.3%)
1	M	0.69	1/3806 (0.0%)	1.04	15/5130 (0.3%)
1	N	0.69	1/3806 (0.0%)	1.04	15/5130 (0.3%)
2	O	0.59	0/657	0.79	1/894 (0.1%)
2	P	0.59	0/657	0.79	1/894 (0.1%)
2	Q	0.59	0/657	0.79	1/894 (0.1%)
2	R	0.59	0/657	0.79	1/894 (0.1%)
2	S	0.59	0/657	0.79	1/894 (0.1%)
2	T	0.59	0/657	0.79	1/894 (0.1%)
2	U	0.59	0/657	0.79	1/894 (0.1%)
All	All	0.88	28/58415 (0.0%)	1.12	301/78848 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
1	J	0	1
1	K	0	1
1	L	0	1
1	M	0	1
1	N	0	1
All	All	0	14

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	191	GLU	C-N	-42.62	0.56	1.33
1	A	191	GLU	C-N	-42.60	0.56	1.33
1	C	191	GLU	C-N	-42.60	0.56	1.33
1	E	191	GLU	C-N	-42.60	0.56	1.33
1	D	191	GLU	C-N	-42.59	0.56	1.33
1	G	191	GLU	C-N	-42.59	0.56	1.33
1	B	191	GLU	C-N	-42.57	0.56	1.33
1	G	136	VAL	C-N	26.70	1.84	1.34
1	C	136	VAL	C-N	26.68	1.84	1.34
1	B	136	VAL	C-N	26.68	1.84	1.34
1	A	136	VAL	C-N	26.67	1.84	1.34
1	E	136	VAL	C-N	26.67	1.84	1.34
1	F	136	VAL	C-N	26.66	1.84	1.34
1	D	136	VAL	C-N	26.66	1.84	1.34
1	M	76	GLU	CD-OE1	5.32	1.31	1.25
1	N	76	GLU	CD-OE1	5.30	1.31	1.25
1	K	76	GLU	CD-OE1	5.29	1.31	1.25
1	H	76	GLU	CD-OE1	5.27	1.31	1.25
1	L	76	GLU	CD-OE1	5.26	1.31	1.25
1	I	76	GLU	CD-OE1	5.26	1.31	1.25
1	J	76	GLU	CD-OE1	5.23	1.31	1.25
1	E	76	GLU	CD-OE1	5.16	1.31	1.25
1	C	76	GLU	CD-OE1	5.16	1.31	1.25
1	A	76	GLU	CD-OE1	5.16	1.31	1.25
1	G	76	GLU	CD-OE1	5.15	1.31	1.25
1	D	76	GLU	CD-OE1	5.13	1.31	1.25
1	B	76	GLU	CD-OE1	5.13	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	76	GLU	CD-OE1	5.13	1.31	1.25

All (301) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	373	ALA	O-C-N	-33.61	66.06	123.20
1	H	373	ALA	O-C-N	-33.61	66.06	123.20
1	J	373	ALA	O-C-N	-33.61	66.06	123.20
1	K	373	ALA	O-C-N	-33.60	66.07	123.20
1	L	373	ALA	O-C-N	-33.60	66.07	123.20
1	M	373	ALA	O-C-N	-33.60	66.08	123.20
1	I	373	ALA	O-C-N	-33.58	66.11	123.20
1	D	373	ALA	CA-C-N	-26.40	63.40	116.20
1	G	373	ALA	CA-C-N	-26.40	63.40	116.20
1	F	373	ALA	CA-C-N	-26.39	63.41	116.20
1	A	373	ALA	CA-C-N	-26.39	63.42	116.20
1	C	373	ALA	CA-C-N	-26.39	63.42	116.20
1	E	373	ALA	CA-C-N	-26.39	63.42	116.20
1	B	373	ALA	CA-C-N	-26.38	63.44	116.20
1	G	373	ALA	C-N-CA	-25.57	68.61	122.30
1	C	373	ALA	C-N-CA	-25.57	68.61	122.30
1	D	373	ALA	C-N-CA	-25.57	68.61	122.30
1	A	373	ALA	C-N-CA	-25.56	68.62	122.30
1	F	373	ALA	C-N-CA	-25.56	68.62	122.30
1	E	373	ALA	C-N-CA	-25.55	68.64	122.30
1	B	373	ALA	C-N-CA	-25.55	68.64	122.30
1	E	373	ALA	O-C-N	23.38	162.94	123.20
1	F	373	ALA	O-C-N	23.36	162.91	123.20
1	A	373	ALA	O-C-N	23.36	162.91	123.20
1	G	373	ALA	O-C-N	23.35	162.90	123.20
1	D	373	ALA	O-C-N	23.35	162.90	123.20
1	C	373	ALA	O-C-N	23.35	162.89	123.20
1	B	373	ALA	O-C-N	23.33	162.87	123.20
1	F	191	GLU	C-N-CA	-22.34	75.38	122.30
1	D	191	GLU	C-N-CA	-22.34	75.39	122.30
1	A	191	GLU	C-N-CA	-22.33	75.40	122.30
1	B	191	GLU	C-N-CA	-22.33	75.41	122.30
1	E	191	GLU	C-N-CA	-22.33	75.41	122.30
1	C	191	GLU	C-N-CA	-22.33	75.41	122.30
1	G	191	GLU	C-N-CA	-22.33	75.41	122.30
1	M	373	ALA	C-N-CA	-21.43	77.30	122.30
1	L	373	ALA	C-N-CA	-21.43	77.31	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	373	ALA	C-N-CA	-21.42	77.31	122.30
1	H	373	ALA	C-N-CA	-21.42	77.32	122.30
1	K	373	ALA	C-N-CA	-21.42	77.32	122.30
1	J	373	ALA	C-N-CA	-21.41	77.33	122.30
1	N	373	ALA	C-N-CA	-21.41	77.33	122.30
1	C	191	GLU	CA-C-N	-20.16	75.89	116.20
1	F	191	GLU	CA-C-N	-20.15	75.89	116.20
1	D	191	GLU	CA-C-N	-20.15	75.90	116.20
1	A	191	GLU	CA-C-N	-20.14	75.91	116.20
1	E	191	GLU	CA-C-N	-20.14	75.92	116.20
1	G	191	GLU	CA-C-N	-20.14	75.92	116.20
1	B	191	GLU	CA-C-N	-20.12	75.95	116.20
1	B	191	GLU	O-C-N	-19.28	90.42	123.20
1	D	191	GLU	O-C-N	-19.28	90.43	123.20
1	G	191	GLU	O-C-N	-19.27	90.45	123.20
1	C	191	GLU	O-C-N	-19.26	90.46	123.20
1	E	191	GLU	O-C-N	-19.25	90.47	123.20
1	A	191	GLU	O-C-N	-19.25	90.47	123.20
1	F	191	GLU	O-C-N	-19.22	90.52	123.20
1	D	268	ARG	NE-CZ-NH2	-11.96	114.32	120.30
1	C	268	ARG	NE-CZ-NH2	-11.95	114.33	120.30
1	E	268	ARG	NE-CZ-NH2	-11.94	114.33	120.30
1	F	268	ARG	NE-CZ-NH2	-11.93	114.34	120.30
1	A	268	ARG	NE-CZ-NH2	-11.92	114.34	120.30
1	B	268	ARG	NE-CZ-NH2	-11.91	114.35	120.30
1	G	268	ARG	NE-CZ-NH2	-11.90	114.35	120.30
1	E	268	ARG	NE-CZ-NH1	11.82	126.21	120.30
1	D	268	ARG	NE-CZ-NH1	11.78	126.19	120.30
1	G	268	ARG	NE-CZ-NH1	11.78	126.19	120.30
1	C	268	ARG	NE-CZ-NH1	11.77	126.18	120.30
1	A	268	ARG	NE-CZ-NH1	11.77	126.18	120.30
1	F	268	ARG	NE-CZ-NH1	11.74	126.17	120.30
1	B	268	ARG	NE-CZ-NH1	11.70	126.15	120.30
1	C	136	VAL	CA-C-N	-11.26	85.57	117.10
1	G	136	VAL	CA-C-N	-11.26	85.56	117.10
1	F	136	VAL	CA-C-N	-11.26	85.58	117.10
1	A	136	VAL	CA-C-N	-11.25	85.59	117.10
1	D	136	VAL	CA-C-N	-11.25	85.60	117.10
1	K	373	ALA	CA-C-N	-11.25	93.70	116.20
1	E	136	VAL	CA-C-N	-11.25	85.61	117.10
1	B	136	VAL	CA-C-N	-11.24	85.61	117.10
1	H	373	ALA	CA-C-N	-11.24	93.72	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	373	ALA	CA-C-N	-11.24	93.73	116.20
1	J	373	ALA	CA-C-N	-11.23	93.73	116.20
1	L	373	ALA	CA-C-N	-11.23	93.73	116.20
1	N	373	ALA	CA-C-N	-11.23	93.74	116.20
1	M	373	ALA	CA-C-N	-11.22	93.76	116.20
1	J	523	ASP	CB-CG-OD2	8.99	126.39	118.30
1	K	523	ASP	CB-CG-OD2	8.99	126.39	118.30
1	G	136	VAL	C-N-CA	-8.98	84.28	122.00
1	C	136	VAL	C-N-CA	-8.98	84.30	122.00
1	A	136	VAL	C-N-CA	-8.97	84.31	122.00
1	B	136	VAL	C-N-CA	-8.97	84.31	122.00
1	D	136	VAL	C-N-CA	-8.97	84.31	122.00
1	F	136	VAL	C-N-CA	-8.97	84.31	122.00
1	E	136	VAL	C-N-CA	-8.97	84.32	122.00
1	I	523	ASP	CB-CG-OD2	8.97	126.37	118.30
1	N	523	ASP	CB-CG-OD2	8.95	126.35	118.30
1	H	523	ASP	CB-CG-OD2	8.94	126.35	118.30
1	L	523	ASP	CB-CG-OD2	8.93	126.34	118.30
1	M	523	ASP	CB-CG-OD2	8.92	126.33	118.30
1	F	523	ASP	CB-CG-OD2	8.79	126.21	118.30
1	A	523	ASP	CB-CG-OD2	8.78	126.20	118.30
1	G	523	ASP	CB-CG-OD2	8.77	126.20	118.30
1	D	523	ASP	CB-CG-OD2	8.75	126.18	118.30
1	C	523	ASP	CB-CG-OD2	8.75	126.17	118.30
1	B	523	ASP	CB-CG-OD2	8.74	126.17	118.30
1	E	523	ASP	CB-CG-OD2	8.74	126.16	118.30
1	B	197	ARG	NE-CZ-NH2	-8.72	115.94	120.30
1	G	197	ARG	NE-CZ-NH2	-8.72	115.94	120.30
1	D	197	ARG	NE-CZ-NH2	-8.67	115.97	120.30
1	F	197	ARG	NE-CZ-NH2	-8.64	115.98	120.30
1	A	197	ARG	NE-CZ-NH2	-8.61	116.00	120.30
1	E	197	ARG	NE-CZ-NH2	-8.57	116.01	120.30
1	C	197	ARG	NE-CZ-NH2	-8.55	116.02	120.30
1	G	197	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	B	197	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	D	197	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	A	197	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	F	197	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	E	197	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	C	197	ARG	NE-CZ-NH1	7.49	124.04	120.30
1	M	11	ASP	CB-CG-OD2	7.15	124.74	118.30
1	J	11	ASP	CB-CG-OD2	7.14	124.72	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	11	ASP	CB-CG-OD2	7.13	124.72	118.30
1	H	11	ASP	CB-CG-OD2	7.13	124.72	118.30
1	D	11	ASP	CB-CG-OD2	7.12	124.71	118.30
1	N	11	ASP	CB-CG-OD2	7.12	124.71	118.30
1	F	11	ASP	CB-CG-OD2	7.11	124.70	118.30
1	K	11	ASP	CB-CG-OD2	7.10	124.69	118.30
1	I	11	ASP	CB-CG-OD2	7.10	124.69	118.30
1	B	11	ASP	CB-CG-OD2	7.08	124.67	118.30
1	E	11	ASP	CB-CG-OD2	7.08	124.67	118.30
1	A	11	ASP	CB-CG-OD2	7.07	124.66	118.30
1	C	11	ASP	CB-CG-OD2	7.07	124.66	118.30
1	G	11	ASP	CB-CG-OD2	7.07	124.66	118.30
1	E	115	ASP	CB-CG-OD2	6.85	124.46	118.30
1	C	115	ASP	CB-CG-OD2	6.85	124.46	118.30
1	G	115	ASP	CB-CG-OD2	6.83	124.45	118.30
1	A	115	ASP	CB-CG-OD2	6.83	124.44	118.30
1	B	115	ASP	CB-CG-OD2	6.82	124.44	118.30
1	F	115	ASP	CB-CG-OD2	6.82	124.43	118.30
1	D	115	ASP	CB-CG-OD2	6.81	124.43	118.30
1	I	115	ASP	CB-CG-OD2	6.76	124.38	118.30
1	L	115	ASP	CB-CG-OD2	6.75	124.38	118.30
1	J	115	ASP	CB-CG-OD2	6.74	124.37	118.30
1	K	115	ASP	CB-CG-OD2	6.74	124.37	118.30
1	H	115	ASP	CB-CG-OD2	6.73	124.36	118.30
1	M	115	ASP	CB-CG-OD2	6.71	124.34	118.30
1	N	115	ASP	CB-CG-OD2	6.71	124.34	118.30
1	I	64	ASP	CB-CG-OD2	6.67	124.31	118.30
1	J	64	ASP	CB-CG-OD2	6.66	124.29	118.30
1	L	64	ASP	CB-CG-OD2	6.66	124.29	118.30
1	N	64	ASP	CB-CG-OD2	6.66	124.29	118.30
1	H	64	ASP	CB-CG-OD2	6.65	124.29	118.30
1	M	64	ASP	CB-CG-OD2	6.65	124.29	118.30
1	B	64	ASP	CB-CG-OD2	6.65	124.28	118.30
1	D	64	ASP	CB-CG-OD2	6.64	124.28	118.30
1	E	64	ASP	CB-CG-OD2	6.64	124.28	118.30
1	A	64	ASP	CB-CG-OD2	6.64	124.27	118.30
1	K	64	ASP	CB-CG-OD2	6.64	124.27	118.30
1	F	64	ASP	CB-CG-OD2	6.63	124.27	118.30
1	G	64	ASP	CB-CG-OD2	6.62	124.26	118.30
1	C	64	ASP	CB-CG-OD2	6.61	124.25	118.30
1	E	121	ASP	CB-CG-OD1	6.54	124.19	118.30
1	J	121	ASP	CB-CG-OD1	6.53	124.18	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	435	ASP	CB-CG-OD2	6.51	124.16	118.30
1	N	121	ASP	CB-CG-OD1	6.50	124.15	118.30
1	K	435	ASP	CB-CG-OD2	6.50	124.15	118.30
1	J	435	ASP	CB-CG-OD2	6.50	124.15	118.30
1	I	435	ASP	CB-CG-OD2	6.50	124.15	118.30
1	K	121	ASP	CB-CG-OD1	6.50	124.15	118.30
1	A	435	ASP	CB-CG-OD2	6.49	124.14	118.30
1	E	435	ASP	CB-CG-OD2	6.49	124.14	118.30
1	F	121	ASP	CB-CG-OD1	6.49	124.14	118.30
1	H	435	ASP	CB-CG-OD2	6.49	124.14	118.30
1	L	435	ASP	CB-CG-OD2	6.49	124.14	118.30
1	D	121	ASP	CB-CG-OD1	6.49	124.14	118.30
1	F	435	ASP	CB-CG-OD2	6.49	124.14	118.30
1	D	435	ASP	CB-CG-OD2	6.48	124.13	118.30
1	N	435	ASP	CB-CG-OD2	6.48	124.14	118.30
1	C	435	ASP	CB-CG-OD2	6.48	124.13	118.30
1	G	435	ASP	CB-CG-OD2	6.48	124.13	118.30
1	L	121	ASP	CB-CG-OD1	6.48	124.13	118.30
1	H	121	ASP	CB-CG-OD1	6.48	124.13	118.30
1	G	121	ASP	CB-CG-OD1	6.47	124.12	118.30
1	A	121	ASP	CB-CG-OD1	6.47	124.12	118.30
1	M	435	ASP	CB-CG-OD2	6.47	124.12	118.30
1	B	121	ASP	CB-CG-OD1	6.45	124.10	118.30
1	C	121	ASP	CB-CG-OD1	6.45	124.10	118.30
1	I	268	ARG	NE-CZ-NH1	-6.44	117.08	120.30
1	K	268	ARG	NE-CZ-NH1	-6.44	117.08	120.30
1	M	121	ASP	CB-CG-OD1	6.43	124.09	118.30
1	I	121	ASP	CB-CG-OD1	6.42	124.08	118.30
1	L	268	ARG	NE-CZ-NH1	-6.42	117.09	120.30
1	N	268	ARG	NE-CZ-NH1	-6.38	117.11	120.30
1	J	268	ARG	NE-CZ-NH1	-6.38	117.11	120.30
1	H	268	ARG	NE-CZ-NH1	-6.37	117.11	120.30
1	F	334	ASP	CB-CG-OD2	6.33	124.00	118.30
1	G	334	ASP	CB-CG-OD2	6.33	124.00	118.30
1	N	268	ARG	NE-CZ-NH2	6.33	123.47	120.30
1	M	268	ARG	NE-CZ-NH2	6.33	123.46	120.30
1	E	334	ASP	CB-CG-OD2	6.31	123.98	118.30
1	L	268	ARG	NE-CZ-NH2	6.30	123.45	120.30
1	A	334	ASP	CB-CG-OD2	6.30	123.97	118.30
1	M	268	ARG	NE-CZ-NH1	-6.28	117.16	120.30
1	K	268	ARG	NE-CZ-NH2	6.27	123.44	120.30
1	D	334	ASP	CB-CG-OD2	6.27	123.94	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	334	ASP	CB-CG-OD2	6.27	123.94	118.30
1	H	268	ARG	NE-CZ-NH2	6.27	123.43	120.30
1	I	268	ARG	NE-CZ-NH2	6.26	123.43	120.30
1	B	334	ASP	CB-CG-OD2	6.26	123.93	118.30
1	J	268	ARG	NE-CZ-NH2	6.23	123.41	120.30
1	G	283	ASP	CB-CG-OD2	5.93	123.64	118.30
1	E	283	ASP	CB-CG-OD2	5.92	123.63	118.30
1	D	283	ASP	CB-CG-OD2	5.90	123.61	118.30
1	A	283	ASP	CB-CG-OD2	5.90	123.61	118.30
1	B	283	ASP	CB-CG-OD2	5.89	123.60	118.30
1	C	283	ASP	CB-CG-OD2	5.87	123.59	118.30
1	F	283	ASP	CB-CG-OD2	5.86	123.57	118.30
1	C	136	VAL	O-C-N	-5.55	110.56	121.10
1	E	136	VAL	O-C-N	-5.55	110.56	121.10
1	G	136	VAL	O-C-N	-5.54	110.57	121.10
1	D	136	VAL	O-C-N	-5.54	110.58	121.10
1	A	136	VAL	O-C-N	-5.54	110.58	121.10
1	F	136	VAL	O-C-N	-5.53	110.59	121.10
1	B	136	VAL	O-C-N	-5.53	110.59	121.10
1	F	188	ASP	CB-CG-OD2	5.53	123.28	118.30
1	D	188	ASP	CB-CG-OD2	5.52	123.27	118.30
1	E	188	ASP	CB-CG-OD2	5.52	123.27	118.30
1	F	268	ARG	CD-NE-CZ	5.52	131.32	123.60
1	B	268	ARG	CD-NE-CZ	5.51	131.32	123.60
1	G	268	ARG	CD-NE-CZ	5.51	131.31	123.60
1	C	268	ARG	CD-NE-CZ	5.51	131.31	123.60
1	B	188	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	268	ARG	CD-NE-CZ	5.50	131.29	123.60
1	G	188	ASP	CB-CG-OD2	5.49	123.24	118.30
1	D	268	ARG	CD-NE-CZ	5.49	131.28	123.60
1	A	188	ASP	CB-CG-OD2	5.48	123.23	118.30
1	N	253	ASP	CB-CG-OD2	5.48	123.23	118.30
1	E	268	ARG	CD-NE-CZ	5.47	131.26	123.60
1	C	188	ASP	CB-CG-OD2	5.47	123.22	118.30
1	F	328	ASP	CB-CG-OD2	5.46	123.22	118.30
1	J	253	ASP	CB-CG-OD2	5.46	123.21	118.30
1	M	253	ASP	CB-CG-OD2	5.46	123.21	118.30
1	L	253	ASP	CB-CG-OD2	5.45	123.20	118.30
1	I	253	ASP	CB-CG-OD2	5.44	123.20	118.30
1	H	253	ASP	CB-CG-OD2	5.44	123.19	118.30
1	K	253	ASP	CB-CG-OD2	5.43	123.19	118.30
1	L	247	LEU	CA-CB-CG	5.42	127.76	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	328	ASP	CB-CG-OD2	5.40	123.16	118.30
1	I	247	LEU	CA-CB-CG	5.40	127.72	115.30
1	A	328	ASP	CB-CG-OD2	5.40	123.16	118.30
1	G	328	ASP	CB-CG-OD2	5.40	123.16	118.30
1	K	247	LEU	CA-CB-CG	5.40	127.71	115.30
1	H	247	LEU	CA-CB-CG	5.39	127.70	115.30
1	M	247	LEU	CA-CB-CG	5.39	127.70	115.30
1	N	247	LEU	CA-CB-CG	5.39	127.70	115.30
1	J	247	LEU	CA-CB-CG	5.39	127.70	115.30
1	C	328	ASP	CB-CG-OD2	5.38	123.14	118.30
1	E	328	ASP	CB-CG-OD2	5.38	123.14	118.30
1	B	328	ASP	CB-CG-OD2	5.37	123.13	118.30
1	K	328	ASP	CB-CG-OD2	5.30	123.07	118.30
1	M	328	ASP	CB-CG-OD2	5.30	123.07	118.30
1	N	328	ASP	CB-CG-OD2	5.30	123.07	118.30
1	H	283	ASP	CB-CG-OD2	5.30	123.07	118.30
1	L	328	ASP	CB-CG-OD2	5.30	123.07	118.30
1	D	224	ASP	CB-CG-OD2	5.29	123.06	118.30
1	C	224	ASP	CB-CG-OD2	5.29	123.06	118.30
1	K	283	ASP	CB-CG-OD2	5.28	123.05	118.30
1	L	283	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	224	ASP	CB-CG-OD2	5.28	123.05	118.30
1	J	283	ASP	CB-CG-OD2	5.28	123.05	118.30
1	H	328	ASP	CB-CG-OD2	5.27	123.05	118.30
1	E	224	ASP	CB-CG-OD2	5.27	123.04	118.30
1	M	283	ASP	CB-CG-OD2	5.27	123.04	118.30
1	I	283	ASP	CB-CG-OD2	5.27	123.04	118.30
1	J	328	ASP	CB-CG-OD2	5.26	123.03	118.30
1	N	283	ASP	CB-CG-OD2	5.26	123.03	118.30
1	F	224	ASP	CB-CG-OD2	5.24	123.02	118.30
1	I	328	ASP	CB-CG-OD2	5.24	123.01	118.30
2	R	18	LEU	CA-CB-CG	5.23	127.33	115.30
2	P	18	LEU	CA-CB-CG	5.23	127.33	115.30
2	S	18	LEU	CA-CB-CG	5.23	127.33	115.30
2	Q	18	LEU	CA-CB-CG	5.23	127.32	115.30
2	O	18	LEU	CA-CB-CG	5.22	127.32	115.30
2	T	18	LEU	CA-CB-CG	5.22	127.31	115.30
1	B	224	ASP	CB-CG-OD2	5.22	123.00	118.30
1	G	224	ASP	CB-CG-OD2	5.22	122.99	118.30
2	U	18	LEU	CA-CB-CG	5.22	127.30	115.30
1	B	253	ASP	CB-CG-OD2	5.16	122.94	118.30
1	F	253	ASP	CB-CG-OD2	5.15	122.94	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	253	ASP	CB-CG-OD2	5.14	122.93	118.30
1	C	253	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	253	ASP	CB-CG-OD2	5.12	122.91	118.30
1	G	253	ASP	CB-CG-OD2	5.12	122.90	118.30
1	D	253	ASP	CB-CG-OD2	5.10	122.89	118.30
1	G	359	ASP	CB-CG-OD2	5.10	122.89	118.30
1	B	359	ASP	CB-CG-OD2	5.09	122.88	118.30
1	C	359	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	359	ASP	CB-CG-OD2	5.07	122.86	118.30
1	D	359	ASP	CB-CG-OD2	5.06	122.86	118.30
1	F	359	ASP	CB-CG-OD2	5.05	122.85	118.30
1	E	359	ASP	CB-CG-OD2	5.04	122.83	118.30

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	191	GLU	Mainchain
1	B	191	GLU	Mainchain
1	C	191	GLU	Mainchain
1	D	191	GLU	Mainchain
1	E	191	GLU	Mainchain
1	F	191	GLU	Mainchain
1	G	191	GLU	Mainchain
1	H	373	ALA	Mainchain
1	I	373	ALA	Mainchain
1	J	373	ALA	Mainchain
1	K	373	ALA	Mainchain
1	L	373	ALA	Mainchain
1	M	373	ALA	Mainchain
1	N	373	ALA	Mainchain

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3855	0	3971	193	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3855	0	3971	194	0
1	C	3855	0	3971	197	0
1	D	3855	0	3971	189	0
1	E	3855	0	3971	199	0
1	F	3855	0	3971	196	0
1	G	3855	0	3971	198	0
1	H	3783	0	3916	226	0
1	I	3783	0	3916	233	0
1	J	3783	0	3916	229	0
1	K	3783	0	3916	234	0
1	L	3783	0	3916	228	0
1	M	3783	0	3916	236	0
1	N	3783	0	3916	234	0
2	O	641	0	652	60	0
2	P	641	0	652	61	0
2	Q	641	0	652	61	0
2	R	641	0	652	61	0
2	S	641	0	652	60	0
2	T	641	0	652	60	0
2	U	641	0	652	61	0
All	All	57953	0	59773	2885	0

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

All (2885) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:138:CYS:CB	1:L:410:GLY:HA2	1.38	1.52
1:K:138:CYS:CB	1:K:410:GLY:HA2	1.38	1.51
1:N:138:CYS:CB	1:N:410:GLY:HA2	1.38	1.51
1:M:138:CYS:CB	1:M:410:GLY:HA2	1.38	1.50
1:H:138:CYS:CB	1:H:410:GLY:HA2	1.38	1.49
1:I:138:CYS:CB	1:I:410:GLY:HA2	1.38	1.49
1:L:135:SER:HG	1:L:137:PRO:N	1.11	1.49
1:K:135:SER:HG	1:K:137:PRO:N	1.11	1.48
1:L:138:CYS:HB2	1:L:410:GLY:CA	1.42	1.48
1:E:464:VAL:HG21	1:L:467:ASN:ND2	1.18	1.48
1:N:138:CYS:HB2	1:N:410:GLY:CA	1.42	1.48
1:C:464:VAL:CG2	1:J:467:ASN:HD22	1.27	1.48
1:A:464:VAL:CG2	1:H:467:ASN:HD22	1.27	1.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:138:CYS:CB	1:J:410:GLY:HA2	1.38	1.47
1:F:464:VAL:CG2	1:M:467:ASN:HD22	1.27	1.47
1:D:464:VAL:HG21	1:K:467:ASN:ND2	1.18	1.46
1:G:146:GLN:NE2	1:G:494:LEU:HD11	1.30	1.46
1:H:135:SER:HG	1:H:137:PRO:N	1.13	1.46
1:H:138:CYS:HB2	1:H:410:GLY:CA	1.42	1.46
1:I:138:CYS:HB2	1:I:410:GLY:CA	1.42	1.46
1:A:146:GLN:NE2	1:A:494:LEU:HD11	1.30	1.46
1:M:138:CYS:HB2	1:M:410:GLY:CA	1.42	1.46
1:E:464:VAL:CG2	1:L:467:ASN:HD22	1.27	1.46
1:J:138:CYS:HB2	1:J:410:GLY:CA	1.42	1.46
1:D:464:VAL:CG2	1:K:467:ASN:HD22	1.27	1.45
1:G:464:VAL:CB	1:N:467:ASN:HD22	1.29	1.45
1:I:135:SER:HG	1:I:137:PRO:N	1.12	1.45
1:C:464:VAL:CB	1:J:467:ASN:HD22	1.29	1.45
1:M:135:SER:HG	1:M:137:PRO:N	1.13	1.45
1:C:464:VAL:HG21	1:J:467:ASN:ND2	1.18	1.45
1:A:464:VAL:CB	1:H:467:ASN:HD22	1.29	1.45
1:G:464:VAL:CG2	1:N:467:ASN:ND2	1.80	1.45
1:C:464:VAL:CG2	1:J:467:ASN:ND2	1.80	1.45
1:F:464:VAL:HG21	1:M:467:ASN:ND2	1.18	1.45
1:K:138:CYS:HB2	1:K:410:GLY:CA	1.42	1.44
1:B:146:GLN:NE2	1:B:494:LEU:HD11	1.30	1.44
1:G:464:VAL:CG2	1:N:467:ASN:HD22	1.27	1.44
1:B:464:VAL:CG2	1:I:467:ASN:HD22	1.27	1.44
1:D:464:VAL:CG2	1:K:467:ASN:ND2	1.80	1.43
1:B:464:VAL:CB	1:I:467:ASN:HD22	1.29	1.43
1:F:146:GLN:NE2	1:F:494:LEU:HD11	1.30	1.43
1:E:464:VAL:CB	1:L:467:ASN:HD22	1.29	1.43
1:A:464:VAL:CG2	1:H:467:ASN:ND2	1.80	1.43
1:G:464:VAL:HG21	1:N:467:ASN:ND2	1.18	1.42
1:C:146:GLN:NE2	1:C:494:LEU:HD11	1.30	1.42
1:D:464:VAL:CB	1:K:467:ASN:HD22	1.29	1.42
1:J:135:SER:HG	1:J:137:PRO:N	1.11	1.42
1:A:464:VAL:HG21	1:H:467:ASN:ND2	1.18	1.41
1:F:464:VAL:CB	1:M:467:ASN:HD22	1.29	1.41
1:B:464:VAL:HG21	1:I:467:ASN:ND2	1.18	1.41
1:E:464:VAL:CG2	1:L:467:ASN:ND2	1.80	1.40
1:E:146:GLN:NE2	1:E:494:LEU:HD11	1.30	1.40
1:N:135:SER:HG	1:N:137:PRO:N	1.14	1.40
1:B:464:VAL:CG2	1:I:467:ASN:ND2	1.80	1.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:GLN:NE2	1:D:494:LEU:HD11	1.30	1.39
1:N:150:ILE:CD1	1:N:494:LEU:O	1.71	1.38
1:H:150:ILE:CD1	1:H:494:LEU:O	1.71	1.38
1:M:150:ILE:CD1	1:M:494:LEU:O	1.71	1.37
1:F:464:VAL:CG2	1:M:467:ASN:ND2	1.80	1.37
1:K:150:ILE:CD1	1:K:494:LEU:O	1.71	1.36
1:I:150:ILE:CD1	1:I:494:LEU:O	1.71	1.35
1:J:150:ILE:CD1	1:J:494:LEU:O	1.71	1.35
1:L:150:ILE:CD1	1:L:494:LEU:O	1.71	1.34
1:I:136:VAL:CA	1:I:137:PRO:HD2	1.59	1.32
1:H:136:VAL:CA	1:H:137:PRO:HD2	1.59	1.32
1:E:136:VAL:C	1:E:137:PRO:N	1.84	1.31
1:N:136:VAL:CA	1:N:137:PRO:HD2	1.59	1.30
1:D:136:VAL:C	1:D:137:PRO:N	1.84	1.30
1:F:136:VAL:C	1:F:137:PRO:N	1.84	1.30
1:E:464:VAL:HG21	1:L:467:ASN:CG	1.50	1.30
1:D:464:VAL:HG21	1:K:467:ASN:CG	1.50	1.30
1:C:136:VAL:C	1:C:137:PRO:N	1.84	1.29
1:A:464:VAL:HG21	1:H:467:ASN:CG	1.50	1.28
1:M:136:VAL:CA	1:M:137:PRO:HD2	1.59	1.28
1:F:464:VAL:HG21	1:M:467:ASN:CG	1.50	1.28
1:G:464:VAL:HG21	1:N:467:ASN:CG	1.50	1.28
1:B:464:VAL:HG21	1:I:467:ASN:CG	1.50	1.28
1:G:136:VAL:C	1:G:137:PRO:N	1.85	1.28
1:D:203:TYR:OH	1:E:286:LYS:HD3	1.31	1.27
1:B:203:TYR:OH	1:C:286:LYS:HD3	1.31	1.27
1:L:136:VAL:CA	1:L:137:PRO:HD2	1.59	1.26
1:A:286:LYS:HD3	1:G:203:TYR:OH	1.31	1.26
1:C:464:VAL:HG21	1:J:467:ASN:CG	1.50	1.26
1:F:203:TYR:OH	1:G:286:LYS:HD3	1.31	1.26
1:B:136:VAL:C	1:B:137:PRO:N	1.84	1.25
1:I:191:GLU:O	1:I:334:ASP:HA	1.09	1.25
1:K:136:VAL:CA	1:K:137:PRO:HD2	1.59	1.25
1:A:136:VAL:C	1:A:137:PRO:N	1.84	1.24
1:C:464:VAL:CB	1:J:467:ASN:ND2	1.98	1.24
1:F:464:VAL:CB	1:M:467:ASN:ND2	1.98	1.24
1:A:203:TYR:OH	1:B:286:LYS:HD3	1.31	1.24
1:C:203:TYR:OH	1:D:286:LYS:HD3	1.31	1.24
1:H:191:GLU:O	1:H:334:ASP:HA	1.09	1.24
1:J:191:GLU:O	1:J:334:ASP:HA	1.09	1.23
1:K:136:VAL:HA	1:K:137:PRO:CD	1.68	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:136:VAL:CA	1:J:137:PRO:HD2	1.59	1.22
1:E:203:TYR:OH	1:F:286:LYS:HD3	1.31	1.22
1:L:136:VAL:HA	1:L:137:PRO:CD	1.68	1.22
1:N:191:GLU:O	1:N:334:ASP:HA	1.09	1.22
1:M:191:GLU:O	1:M:334:ASP:HA	1.09	1.22
1:J:136:VAL:HA	1:J:137:PRO:CD	1.68	1.22
1:H:136:VAL:HA	1:H:137:PRO:CD	1.68	1.21
1:I:136:VAL:HA	1:I:137:PRO:CD	1.68	1.21
1:G:464:VAL:CB	1:N:467:ASN:ND2	1.98	1.21
1:M:136:VAL:HA	1:M:137:PRO:CD	1.68	1.21
1:L:191:GLU:O	1:L:334:ASP:HA	1.09	1.21
1:K:191:GLU:O	1:K:334:ASP:HA	1.09	1.21
1:N:136:VAL:HA	1:N:137:PRO:CD	1.68	1.20
1:D:464:VAL:CB	1:K:467:ASN:ND2	1.98	1.20
1:L:18:ARG:CB	1:L:18:ARG:HH11	1.55	1.20
1:E:464:VAL:CB	1:L:467:ASN:ND2	1.98	1.19
1:J:138:CYS:CB	1:J:410:GLY:CA	2.08	1.19
1:N:18:ARG:CB	1:N:18:ARG:HH11	1.55	1.19
1:E:18:ARG:HH11	1:E:18:ARG:CB	1.55	1.19
1:I:147:VAL:HG23	1:I:496:PRO:HG3	1.21	1.19
1:K:18:ARG:CB	1:K:18:ARG:HH11	1.55	1.19
1:J:18:ARG:HH11	1:J:18:ARG:CB	1.55	1.18
1:I:18:ARG:CB	1:I:18:ARG:HH11	1.55	1.18
1:C:18:ARG:CB	1:C:18:ARG:HH11	1.55	1.18
1:H:147:VAL:HG23	1:H:496:PRO:HG3	1.21	1.18
1:E:172:GLU:OE2	1:E:350:ARG:HG3	1.44	1.18
1:H:138:CYS:CB	1:H:410:GLY:CA	2.08	1.18
1:M:18:ARG:CB	1:M:18:ARG:HH11	1.55	1.18
1:B:18:ARG:CB	1:B:18:ARG:HH11	1.55	1.18
1:G:18:ARG:CB	1:G:18:ARG:HH11	1.55	1.18
1:M:138:CYS:CB	1:M:410:GLY:CA	2.08	1.17
1:L:147:VAL:HG23	1:L:496:PRO:HG3	1.21	1.17
1:D:18:ARG:CB	1:D:18:ARG:HH11	1.55	1.17
1:J:516:THR:O	1:K:36:ARG:NH1	1.78	1.17
1:E:464:VAL:CG1	1:L:467:ASN:HD22	1.58	1.17
1:C:464:VAL:CG1	1:J:467:ASN:HD22	1.58	1.17
1:A:464:VAL:CG1	1:H:467:ASN:HD22	1.58	1.17
1:H:36:ARG:NH1	1:N:516:THR:O	1.78	1.17
1:I:516:THR:O	1:J:36:ARG:NH1	1.78	1.17
1:H:516:THR:O	1:I:36:ARG:NH1	1.78	1.17
1:F:18:ARG:HH11	1:F:18:ARG:CB	1.55	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:18:ARG:HH11	1:H:18:ARG:CB	1.55	1.17
1:F:172:GLU:OE2	1:F:350:ARG:HG3	1.44	1.17
1:G:464:VAL:CG1	1:N:467:ASN:HD22	1.58	1.17
1:A:18:ARG:CB	1:A:18:ARG:HH11	1.55	1.17
1:D:464:VAL:CG1	1:K:467:ASN:HD22	1.58	1.16
1:L:138:CYS:CB	1:L:410:GLY:CA	2.08	1.16
1:G:172:GLU:OE2	1:G:350:ARG:HG3	1.44	1.16
1:K:516:THR:O	1:L:36:ARG:NH1	1.78	1.16
1:B:464:VAL:CG1	1:I:467:ASN:HD22	1.58	1.16
1:M:516:THR:O	1:N:36:ARG:NH1	1.78	1.16
1:D:172:GLU:OE2	1:D:350:ARG:HG3	1.44	1.15
1:F:464:VAL:CG1	1:M:467:ASN:HD22	1.58	1.15
1:M:147:VAL:HG23	1:M:496:PRO:HG3	1.21	1.15
1:I:138:CYS:CB	1:I:410:GLY:CA	2.08	1.14
1:I:138:CYS:HB3	1:I:410:GLY:N	1.63	1.14
1:L:138:CYS:HB3	1:L:410:GLY:N	1.63	1.14
1:K:138:CYS:HB3	1:K:410:GLY:N	1.63	1.14
1:J:138:CYS:HB3	1:J:410:GLY:N	1.63	1.14
1:N:147:VAL:HG23	1:N:496:PRO:HG3	1.21	1.14
1:K:138:CYS:CB	1:K:410:GLY:CA	2.08	1.14
1:A:172:GLU:OE2	1:A:350:ARG:HG3	1.44	1.14
1:L:516:THR:O	1:M:36:ARG:NH1	1.78	1.14
1:M:138:CYS:HB3	1:M:410:GLY:N	1.63	1.13
1:K:147:VAL:HG23	1:K:496:PRO:HG3	1.21	1.13
1:H:138:CYS:HB3	1:H:410:GLY:N	1.63	1.13
1:A:464:VAL:CB	1:H:467:ASN:ND2	1.98	1.13
1:C:172:GLU:OE2	1:C:350:ARG:HG3	1.44	1.13
1:N:138:CYS:CB	1:N:410:GLY:CA	2.08	1.13
1:G:197:ARG:HD3	1:G:277:LYS:HB2	1.30	1.13
1:F:197:ARG:HD3	1:F:277:LYS:HB2	1.30	1.13
1:B:172:GLU:OE2	1:B:350:ARG:HG3	1.44	1.13
1:L:191:GLU:O	1:L:334:ASP:CA	1.98	1.12
1:K:191:GLU:O	1:K:334:ASP:CA	1.98	1.12
1:M:191:GLU:O	1:M:334:ASP:CA	1.98	1.12
1:J:191:GLU:O	1:J:334:ASP:CA	1.98	1.11
1:N:138:CYS:HB3	1:N:410:GLY:N	1.63	1.11
1:B:464:VAL:CB	1:I:467:ASN:ND2	1.98	1.11
1:J:147:VAL:HG23	1:J:496:PRO:HG3	1.20	1.11
1:I:191:GLU:O	1:I:334:ASP:CA	1.98	1.11
1:N:191:GLU:O	1:N:334:ASP:CA	1.98	1.11
1:H:191:GLU:O	1:H:334:ASP:CA	1.98	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ARG:HD3	1:A:277:LYS:HB2	1.30	1.10
1:E:197:ARG:HD3	1:E:277:LYS:HB2	1.30	1.10
1:J:136:VAL:CA	1:J:137:PRO:CD	2.28	1.09
1:C:18:ARG:NH1	1:C:18:ARG:HB3	1.68	1.09
1:N:136:VAL:CA	1:N:137:PRO:CD	2.28	1.08
1:E:18:ARG:NH1	1:E:18:ARG:HB3	1.68	1.08
1:F:18:ARG:NH1	1:F:18:ARG:HB3	1.68	1.08
1:N:18:ARG:HB3	1:N:18:ARG:NH1	1.68	1.08
1:M:18:ARG:HB3	1:M:18:ARG:NH1	1.68	1.08
1:A:18:ARG:HB3	1:A:18:ARG:NH1	1.68	1.08
1:G:172:GLU:OE2	1:G:350:ARG:CG	2.03	1.07
1:C:172:GLU:OE2	1:C:350:ARG:CG	2.03	1.07
1:H:18:ARG:HB3	1:H:18:ARG:NH1	1.68	1.07
1:B:197:ARG:HD3	1:B:277:LYS:HB2	1.30	1.07
1:F:464:VAL:HG11	1:M:467:ASN:ND2	1.70	1.07
1:L:18:ARG:HB3	1:L:18:ARG:NH1	1.68	1.07
1:I:18:ARG:HB3	1:I:18:ARG:NH1	1.68	1.07
1:G:18:ARG:NH1	1:G:18:ARG:HB3	1.68	1.07
1:B:204:PHE:HE2	1:B:266:THR:HG21	1.20	1.07
1:L:136:VAL:CA	1:L:137:PRO:CD	2.28	1.07
1:J:18:ARG:HB3	1:J:18:ARG:NH1	1.68	1.07
1:D:18:ARG:HB3	1:D:18:ARG:NH1	1.68	1.07
1:A:172:GLU:OE2	1:A:350:ARG:CG	2.03	1.07
1:D:197:ARG:HD3	1:D:277:LYS:HB2	1.30	1.07
1:C:204:PHE:HE2	1:C:266:THR:HG21	1.20	1.07
1:G:464:VAL:HG11	1:N:467:ASN:ND2	1.70	1.06
1:K:18:ARG:NH1	1:K:18:ARG:HB3	1.68	1.06
1:B:18:ARG:HB3	1:B:18:ARG:NH1	1.68	1.06
1:D:172:GLU:OE2	1:D:350:ARG:CG	2.03	1.06
1:B:172:GLU:OE2	1:B:350:ARG:CG	2.03	1.06
1:I:136:VAL:CA	1:I:137:PRO:CD	2.28	1.06
1:A:464:VAL:HG11	1:H:467:ASN:ND2	1.70	1.06
1:K:147:VAL:HG23	1:K:496:PRO:CG	1.86	1.06
1:F:172:GLU:OE2	1:F:350:ARG:CG	2.03	1.06
1:E:464:VAL:HG11	1:L:467:ASN:ND2	1.70	1.06
1:B:146:GLN:HE21	1:B:494:LEU:CD1	1.69	1.06
1:L:147:VAL:HG23	1:L:496:PRO:CG	1.86	1.06
1:F:204:PHE:HE2	1:F:266:THR:HG21	1.20	1.06
1:K:136:VAL:CA	1:K:137:PRO:CD	2.28	1.06
1:D:464:VAL:HG11	1:K:467:ASN:ND2	1.70	1.06
1:I:147:VAL:HG23	1:I:496:PRO:CG	1.86	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:18:ARG:HB3	1:K:18:ARG:HH11	0.89	1.06
1:G:204:PHE:HE2	1:G:266:THR:HG21	1.20	1.06
1:G:146:GLN:HE21	1:G:494:LEU:CD1	1.69	1.06
1:J:18:ARG:HH11	1:J:18:ARG:HB3	0.89	1.06
1:A:204:PHE:HE2	1:A:266:THR:HG21	1.20	1.06
1:N:147:VAL:HG23	1:N:496:PRO:CG	1.86	1.05
1:H:147:VAL:HG23	1:H:496:PRO:CG	1.86	1.05
1:L:18:ARG:HH11	1:L:18:ARG:HB3	0.89	1.05
1:D:172:GLU:OE2	1:D:350:ARG:CD	2.04	1.05
1:A:172:GLU:OE2	1:A:350:ARG:CD	2.04	1.05
1:C:464:VAL:HG11	1:J:467:ASN:ND2	1.70	1.05
1:F:464:VAL:CG1	1:M:467:ASN:ND2	2.18	1.05
1:D:146:GLN:HE21	1:D:494:LEU:CD1	1.69	1.05
1:G:172:GLU:OE2	1:G:350:ARG:CD	2.04	1.05
1:C:197:ARG:HD3	1:C:277:LYS:HB2	1.30	1.05
1:M:147:VAL:HG23	1:M:496:PRO:CG	1.86	1.05
1:J:147:VAL:HG23	1:J:496:PRO:CG	1.86	1.05
1:E:172:GLU:OE2	1:E:350:ARG:CG	2.03	1.05
1:C:172:GLU:OE2	1:C:350:ARG:CD	2.04	1.05
1:B:464:VAL:HG11	1:I:467:ASN:ND2	1.70	1.05
1:I:18:ARG:HB3	1:I:18:ARG:HH11	0.89	1.05
1:M:18:ARG:HB3	1:M:18:ARG:HH11	0.89	1.05
1:F:172:GLU:OE2	1:F:350:ARG:CD	2.04	1.05
1:A:146:GLN:HE21	1:A:494:LEU:CD1	1.69	1.04
1:A:18:ARG:HB3	1:A:18:ARG:HH11	0.89	1.04
1:E:461:GLU:OE1	1:L:463:SER:HB2	1.57	1.04
1:H:136:VAL:CA	1:H:137:PRO:CD	2.28	1.04
1:G:18:ARG:HH11	1:G:18:ARG:HB3	0.89	1.04
1:F:146:GLN:HE21	1:F:494:LEU:CD1	1.69	1.04
1:D:461:GLU:OE1	1:K:463:SER:HB2	1.57	1.04
1:C:146:GLN:HE21	1:C:494:LEU:CD1	1.69	1.04
1:E:146:GLN:HE21	1:E:494:LEU:CD1	1.69	1.04
1:N:18:ARG:HH11	1:N:18:ARG:HB3	0.89	1.04
1:E:172:GLU:OE2	1:E:350:ARG:CD	2.04	1.04
1:B:172:GLU:OE2	1:B:350:ARG:CD	2.04	1.04
1:G:461:GLU:OE1	1:N:463:SER:HB2	1.57	1.04
1:A:461:GLU:OE1	1:H:463:SER:HB2	1.57	1.04
1:B:18:ARG:HB3	1:B:18:ARG:HH11	0.89	1.03
1:H:18:ARG:HH11	1:H:18:ARG:HB3	0.89	1.03
1:F:461:GLU:OE1	1:M:463:SER:HB2	1.57	1.03
1:D:204:PHE:HE2	1:D:266:THR:HG21	1.20	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:204:PHE:HE2	1:E:266:THR:HG21	1.20	1.03
1:F:172:GLU:OE2	1:F:350:ARG:HD2	1.59	1.03
1:C:172:GLU:OE2	1:C:350:ARG:HD2	1.59	1.03
1:G:464:VAL:CG1	1:N:467:ASN:ND2	2.18	1.03
1:F:18:ARG:HB3	1:F:18:ARG:HH11	0.89	1.03
1:H:135:SER:OG	1:H:137:PRO:N	1.92	1.02
1:C:18:ARG:HB3	1:C:18:ARG:HH11	0.89	1.02
1:E:172:GLU:OE2	1:E:350:ARG:HD2	1.59	1.02
1:N:135:SER:OG	1:N:137:PRO:N	1.92	1.02
1:C:461:GLU:OE1	1:J:463:SER:HB2	1.57	1.02
1:M:135:SER:OG	1:M:137:PRO:N	1.92	1.02
1:G:172:GLU:OE2	1:G:350:ARG:HD2	1.59	1.02
1:B:461:GLU:OE1	1:I:463:SER:HB2	1.57	1.02
1:E:464:VAL:HG21	1:L:467:ASN:CB	1.89	1.02
1:C:464:VAL:HG21	1:J:467:ASN:CB	1.89	1.02
1:J:138:CYS:CA	1:J:410:GLY:HA2	1.90	1.02
1:G:464:VAL:HG21	1:N:467:ASN:CB	1.89	1.02
1:B:464:VAL:HG21	1:I:467:ASN:CB	1.89	1.02
1:B:172:GLU:OE2	1:B:350:ARG:HD2	1.59	1.02
1:K:138:CYS:CA	1:K:410:GLY:HA2	1.90	1.01
1:M:136:VAL:CA	1:M:137:PRO:CD	2.28	1.01
1:I:138:CYS:CA	1:I:410:GLY:HA2	1.90	1.01
1:L:135:SER:OG	1:L:137:PRO:N	1.92	1.01
1:I:135:SER:OG	1:I:137:PRO:N	1.92	1.01
1:F:464:VAL:HG21	1:M:467:ASN:CB	1.89	1.01
1:E:18:ARG:HH11	1:E:18:ARG:HB3	0.89	1.01
1:B:406:ALA:HB2	1:B:496:PRO:HB3	1.40	1.01
1:F:406:ALA:O	1:F:410:GLY:N	1.93	1.01
1:H:138:CYS:CA	1:H:410:GLY:HA2	1.90	1.01
1:A:464:VAL:HG21	1:H:467:ASN:CB	1.89	1.01
1:D:18:ARG:HH11	1:D:18:ARG:HB3	0.89	1.01
1:A:406:ALA:O	1:A:410:GLY:N	1.93	1.01
1:D:406:ALA:O	1:D:410:GLY:N	1.94	1.01
1:F:406:ALA:HB2	1:F:496:PRO:HB3	1.40	1.01
1:J:138:CYS:CB	1:J:410:GLY:N	2.23	1.01
1:D:464:VAL:HG21	1:K:467:ASN:CB	1.89	1.01
1:E:406:ALA:HB2	1:E:496:PRO:HB3	1.40	1.01
1:C:406:ALA:HB2	1:C:496:PRO:HB3	1.40	1.01
1:L:138:CYS:CA	1:L:410:GLY:HA2	1.90	1.00
1:N:138:CYS:CA	1:N:410:GLY:HA2	1.90	1.00
1:E:406:ALA:O	1:E:410:GLY:N	1.94	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:ALA:O	1:B:410:GLY:N	1.94	1.00
1:A:406:ALA:HB2	1:A:496:PRO:HB3	1.40	1.00
1:G:406:ALA:O	1:G:410:GLY:N	1.93	1.00
1:K:138:CYS:CB	1:K:410:GLY:N	2.23	1.00
1:J:135:SER:OG	1:J:137:PRO:N	1.92	1.00
1:D:464:VAL:CG1	1:K:467:ASN:ND2	2.18	1.00
1:B:464:VAL:CG1	1:I:467:ASN:ND2	2.18	1.00
1:A:464:VAL:CG1	1:H:467:ASN:ND2	2.18	1.00
1:B:146:GLN:NE2	1:B:494:LEU:CD1	2.25	1.00
1:E:464:VAL:CG1	1:L:467:ASN:ND2	2.18	1.00
1:C:146:GLN:NE2	1:C:494:LEU:CD1	2.25	1.00
1:A:172:GLU:OE2	1:A:350:ARG:HD2	1.59	1.00
1:G:105:LYS:HG2	1:M:109:ALA:O	1.62	1.00
1:K:135:SER:OG	1:K:137:PRO:N	1.92	1.00
1:M:138:CYS:CA	1:M:410:GLY:HA2	1.90	0.99
1:C:406:ALA:O	1:C:410:GLY:N	1.93	0.99
1:A:105:LYS:HG2	1:N:109:ALA:O	1.62	0.99
1:G:406:ALA:HB2	1:G:496:PRO:HB3	1.40	0.99
1:D:172:GLU:OE2	1:D:350:ARG:HD2	1.59	0.99
1:E:138:CYS:HB3	1:E:410:GLY:HA2	1.45	0.99
1:F:105:LYS:HG2	1:L:109:ALA:O	1.62	0.99
1:D:406:ALA:HB2	1:D:496:PRO:HB3	1.40	0.99
1:A:463:SER:OG	1:H:464:VAL:HG23	1.63	0.99
1:F:138:CYS:HB3	1:F:410:GLY:HA2	1.45	0.99
1:D:463:SER:OG	1:K:464:VAL:HG23	1.63	0.99
1:D:138:CYS:HB3	1:D:410:GLY:HA2	1.45	0.99
1:E:463:SER:OG	1:L:464:VAL:HG23	1.63	0.99
1:G:146:GLN:NE2	1:G:494:LEU:CD1	2.25	0.98
1:C:463:SER:OG	1:J:464:VAL:HG23	1.63	0.98
1:C:138:CYS:HB3	1:C:410:GLY:HA2	1.45	0.98
1:L:138:CYS:CB	1:L:410:GLY:N	2.23	0.98
1:A:146:GLN:NE2	1:A:494:LEU:CD1	2.25	0.98
1:B:105:LYS:HG2	1:H:109:ALA:O	1.62	0.98
1:D:105:LYS:HG2	1:J:109:ALA:O	1.62	0.98
1:B:138:CYS:HB3	1:B:410:GLY:HA2	1.45	0.98
1:G:463:SER:OG	1:N:464:VAL:HG23	1.63	0.98
1:B:203:TYR:HH	1:C:286:LYS:HD3	1.26	0.98
1:D:146:GLN:NE2	1:D:494:LEU:CD1	2.25	0.97
1:C:105:LYS:HG2	1:I:109:ALA:O	1.62	0.97
1:C:464:VAL:CG1	1:J:467:ASN:ND2	2.18	0.97
1:F:146:GLN:NE2	1:F:494:LEU:CD1	2.25	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:138:CYS:CB	1:H:410:GLY:N	2.22	0.97
1:G:138:CYS:HB3	1:G:410:GLY:HA2	1.45	0.97
1:A:138:CYS:HB3	1:A:410:GLY:HA2	1.45	0.97
1:N:138:CYS:CB	1:N:410:GLY:N	2.22	0.97
1:B:463:SER:OG	1:I:464:VAL:HG23	1.63	0.97
1:E:105:LYS:HG2	1:K:109:ALA:O	1.62	0.97
1:E:146:GLN:NE2	1:E:494:LEU:CD1	2.25	0.96
1:F:463:SER:OG	1:M:464:VAL:HG23	1.63	0.96
1:N:150:ILE:HD13	1:N:494:LEU:O	0.78	0.95
1:F:204:PHE:CE2	1:F:266:THR:HG21	2.02	0.95
1:H:150:ILE:HD13	1:H:494:LEU:O	0.78	0.95
1:F:136:VAL:CA	1:F:137:PRO:N	2.30	0.95
1:C:204:PHE:CE2	1:C:266:THR:HG21	2.02	0.95
1:D:204:PHE:CE2	1:D:266:THR:HG21	2.01	0.95
1:E:204:PHE:CE2	1:E:266:THR:HG21	2.02	0.95
1:M:150:ILE:HD13	1:M:494:LEU:O	0.78	0.95
1:I:150:ILE:HD13	1:I:494:LEU:O	0.78	0.95
1:K:150:ILE:HD13	1:K:494:LEU:O	0.78	0.95
1:J:150:ILE:HD13	1:J:494:LEU:O	0.78	0.94
1:N:381:VAL:HG21	1:N:393:LYS:HA	1.48	0.94
1:M:381:VAL:HG21	1:M:393:LYS:HA	1.48	0.94
1:L:150:ILE:HD13	1:L:494:LEU:O	0.78	0.94
1:E:136:VAL:CA	1:E:137:PRO:N	2.30	0.94
1:D:136:VAL:CA	1:D:137:PRO:N	2.30	0.94
1:A:203:TYR:HH	1:B:286:LYS:HD3	1.26	0.94
1:I:138:CYS:CB	1:I:410:GLY:N	2.23	0.94
1:B:204:PHE:CE2	1:B:266:THR:HG21	2.01	0.94
1:L:381:VAL:HG21	1:L:393:LYS:HA	1.48	0.94
1:C:136:VAL:CA	1:C:137:PRO:N	2.30	0.94
1:G:204:PHE:CE2	1:G:266:THR:HG21	2.01	0.94
1:H:381:VAL:HG21	1:H:393:LYS:HA	1.48	0.94
1:A:136:VAL:CA	1:A:137:PRO:N	2.30	0.94
1:A:204:PHE:CE2	1:A:266:THR:HG21	2.01	0.94
1:M:138:CYS:CB	1:M:410:GLY:N	2.22	0.93
1:B:136:VAL:CA	1:B:137:PRO:N	2.30	0.93
1:G:136:VAL:CA	1:G:137:PRO:N	2.30	0.93
2:O:70:SER:OG	2:U:80:PRO:HG2	1.69	0.93
2:P:80:PRO:HG2	2:Q:70:SER:OG	1.69	0.93
2:Q:80:PRO:HG2	2:R:70:SER:OG	1.69	0.93
1:K:381:VAL:HG21	1:K:393:LYS:HA	1.48	0.93
2:R:80:PRO:HG2	2:S:70:SER:OG	1.69	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:381:VAL:HG21	1:I:393:LYS:HA	1.48	0.93
1:F:203:TYR:HH	1:G:286:LYS:HD3	1.20	0.93
1:A:286:LYS:HD3	1:G:203:TYR:HH	1.12	0.93
1:J:381:VAL:HG21	1:J:393:LYS:HA	1.48	0.93
2:O:80:PRO:HG2	2:P:70:SER:OG	1.69	0.92
1:E:463:SER:HB2	1:L:464:VAL:HG21	1.51	0.92
1:G:463:SER:HB2	1:N:464:VAL:HG21	1.51	0.92
2:T:80:PRO:HG2	2:U:70:SER:OG	1.69	0.92
1:A:463:SER:HB2	1:H:464:VAL:HG21	1.51	0.92
1:F:463:SER:HB2	1:M:464:VAL:HG21	1.51	0.92
1:D:463:SER:HB2	1:K:464:VAL:HG21	1.51	0.92
2:S:80:PRO:HG2	2:T:70:SER:OG	1.69	0.92
2:S:17:ILE:HD11	2:T:108:CYS:HB3	1.52	0.91
2:T:17:ILE:HD11	2:U:108:CYS:HB3	1.52	0.91
2:R:17:ILE:HD11	2:S:108:CYS:HB3	1.52	0.91
1:D:203:TYR:HH	1:E:286:LYS:HD3	1.17	0.91
1:E:203:TYR:HH	1:F:286:LYS:HD3	1.09	0.91
2:Q:17:ILE:HD11	2:R:108:CYS:HB3	1.52	0.91
1:J:190:VAL:HG21	1:J:334:ASP:OD2	1.71	0.91
1:C:463:SER:HB2	1:J:464:VAL:HG21	1.51	0.90
1:D:146:GLN:HB3	1:D:494:LEU:HG	1.54	0.90
1:B:463:SER:HB2	1:I:464:VAL:HG21	1.51	0.90
1:H:190:VAL:HG21	1:H:334:ASP:OD2	1.71	0.90
1:I:190:VAL:HG21	1:I:334:ASP:OD2	1.71	0.90
1:E:146:GLN:HB3	1:E:494:LEU:HG	1.54	0.89
1:C:146:GLN:HB3	1:C:494:LEU:HG	1.54	0.89
1:N:190:VAL:HG21	1:N:334:ASP:OD2	1.71	0.89
2:P:17:ILE:HD11	2:Q:108:CYS:HB3	1.52	0.89
1:M:190:VAL:HG21	1:M:334:ASP:OD2	1.71	0.89
2:O:108:CYS:HB3	2:U:17:ILE:HD11	1.52	0.89
1:H:150:ILE:HD13	1:H:494:LEU:C	1.93	0.89
1:J:150:ILE:HD13	1:J:494:LEU:C	1.93	0.89
1:K:190:VAL:HG21	1:K:334:ASP:OD2	1.71	0.89
1:L:190:VAL:HG21	1:L:334:ASP:OD2	1.71	0.89
1:J:143:ALA:O	1:J:146:GLN:HB3	1.73	0.89
2:O:17:ILE:HD11	2:P:108:CYS:HB3	1.52	0.89
1:I:143:ALA:O	1:I:146:GLN:HB3	1.73	0.89
1:M:150:ILE:HD13	1:M:494:LEU:C	1.93	0.88
1:F:146:GLN:HB3	1:F:494:LEU:HG	1.54	0.88
1:N:143:ALA:O	1:N:146:GLN:HB3	1.73	0.88
1:H:143:ALA:O	1:H:146:GLN:HB3	1.73	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:143:ALA:O	1:M:146:GLN:HB3	1.73	0.88
1:K:143:ALA:O	1:K:146:GLN:HB3	1.73	0.88
1:D:463:SER:HB2	1:K:464:VAL:CG2	2.04	0.88
1:B:146:GLN:HB3	1:B:494:LEU:HG	1.54	0.88
1:M:166:MET:HE2	1:M:171:LYS:HA	1.55	0.88
1:C:463:SER:HB2	1:J:464:VAL:CG2	2.04	0.88
2:S:82:PRO:HA	2:T:110:TYR:CE1	2.09	0.88
1:A:463:SER:HB2	1:H:464:VAL:CG2	2.04	0.88
1:E:463:SER:HB2	1:L:464:VAL:CG2	2.04	0.87
2:O:82:PRO:HA	2:P:110:TYR:CE1	2.09	0.87
1:A:146:GLN:HB3	1:A:494:LEU:HG	1.54	0.87
1:G:463:SER:HB2	1:N:464:VAL:CG2	2.04	0.87
1:C:267:MET:SD	1:D:305:ILE:HD12	2.15	0.87
2:O:110:TYR:CE1	2:U:82:PRO:HA	2.09	0.87
2:Q:82:PRO:HA	2:R:110:TYR:CE1	2.09	0.87
1:E:267:MET:SD	1:F:305:ILE:HD12	2.15	0.87
1:N:166:MET:HE2	1:N:171:LYS:HA	1.55	0.87
1:F:267:MET:SD	1:G:305:ILE:HD12	2.15	0.87
1:D:203:TYR:CE2	1:E:304:GLU:OE2	2.28	0.87
1:A:304:GLU:OE2	1:G:203:TYR:CE2	2.28	0.87
1:A:203:TYR:CE2	1:B:304:GLU:OE2	2.28	0.87
2:R:82:PRO:HA	2:S:110:TYR:CE1	2.09	0.87
1:A:267:MET:SD	1:B:305:ILE:HD12	2.15	0.87
1:B:267:MET:SD	1:C:305:ILE:HD12	2.14	0.87
1:F:463:SER:HB2	1:M:464:VAL:CG2	2.04	0.87
1:N:150:ILE:HD13	1:N:494:LEU:C	1.93	0.87
2:T:82:PRO:HA	2:U:110:TYR:CE1	2.09	0.87
1:L:166:MET:HE2	1:L:171:LYS:HA	1.56	0.87
1:I:166:MET:HE2	1:I:171:LYS:HA	1.55	0.87
1:A:305:ILE:HD12	1:G:267:MET:SD	2.15	0.87
1:G:146:GLN:HB3	1:G:494:LEU:HG	1.54	0.87
2:P:82:PRO:HA	2:Q:110:TYR:CE1	2.09	0.87
1:K:150:ILE:HD13	1:K:494:LEU:C	1.93	0.87
1:B:463:SER:HB2	1:I:464:VAL:CG2	2.04	0.86
1:F:203:TYR:CE2	1:G:304:GLU:OE2	2.28	0.86
1:I:150:ILE:HD13	1:I:494:LEU:C	1.93	0.86
1:L:143:ALA:O	1:L:146:GLN:HB3	1.73	0.86
1:B:203:TYR:CE2	1:C:304:GLU:OE2	2.28	0.86
1:C:203:TYR:CE2	1:D:304:GLU:OE2	2.28	0.86
1:E:203:TYR:CE2	1:F:304:GLU:OE2	2.28	0.86
1:A:461:GLU:OE1	1:H:463:SER:CB	2.24	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:461:GLU:OE1	1:J:463:SER:CB	2.24	0.86
1:D:267:MET:SD	1:E:305:ILE:HD12	2.15	0.86
1:G:461:GLU:OE1	1:N:463:SER:CB	2.24	0.86
1:F:461:GLU:OE1	1:M:463:SER:CB	2.24	0.86
1:B:461:GLU:OE1	1:I:463:SER:CB	2.24	0.86
1:L:150:ILE:HD13	1:L:494:LEU:C	1.93	0.86
1:D:461:GLU:OE1	1:K:463:SER:CB	2.24	0.86
1:F:174:VAL:HG21	1:F:367:GLU:HA	1.58	0.85
1:E:174:VAL:HG21	1:E:367:GLU:HA	1.58	0.85
1:J:166:MET:HE2	1:J:171:LYS:HA	1.55	0.85
1:B:90:THR:O	1:B:94:VAL:HG23	1.77	0.85
1:M:90:THR:O	1:M:94:VAL:HG23	1.77	0.85
1:H:166:MET:HE2	1:H:171:LYS:HA	1.55	0.85
1:J:90:THR:O	1:J:94:VAL:HG23	1.77	0.85
1:K:90:THR:O	1:K:94:VAL:HG23	1.77	0.85
1:L:90:THR:O	1:L:94:VAL:HG23	1.77	0.85
1:I:90:THR:O	1:I:94:VAL:HG23	1.77	0.85
1:N:90:THR:O	1:N:94:VAL:HG23	1.77	0.85
1:C:90:THR:O	1:C:94:VAL:HG23	1.77	0.85
1:K:166:MET:HE2	1:K:171:LYS:HA	1.55	0.84
1:E:90:THR:O	1:E:94:VAL:HG23	1.77	0.84
1:A:90:THR:O	1:A:94:VAL:HG23	1.77	0.84
1:E:461:GLU:OE1	1:L:463:SER:CB	2.24	0.84
1:B:174:VAL:HG21	1:B:367:GLU:HA	1.58	0.84
1:G:174:VAL:HG21	1:G:367:GLU:HA	1.58	0.84
1:G:138:CYS:HB2	1:G:411:VAL:HG13	1.59	0.84
1:A:174:VAL:HG21	1:A:367:GLU:HA	1.58	0.84
1:D:90:THR:O	1:D:94:VAL:HG23	1.77	0.84
1:C:174:VAL:HG21	1:C:367:GLU:HA	1.58	0.84
1:F:90:THR:O	1:F:94:VAL:HG23	1.77	0.83
1:D:138:CYS:HB2	1:D:411:VAL:HG13	1.59	0.83
1:A:138:CYS:HB2	1:A:411:VAL:HG13	1.59	0.83
1:D:174:VAL:HG21	1:D:367:GLU:HA	1.58	0.83
1:G:90:THR:O	1:G:94:VAL:HG23	1.77	0.83
1:G:463:SER:CB	1:N:464:VAL:CG2	2.57	0.83
1:F:138:CYS:HB2	1:F:411:VAL:HG13	1.59	0.83
1:D:463:SER:CB	1:K:464:VAL:CG2	2.57	0.83
1:E:138:CYS:HB2	1:E:411:VAL:HG13	1.59	0.83
1:F:463:SER:CB	1:M:464:VAL:CG2	2.57	0.83
1:B:463:SER:CB	1:I:464:VAL:CG2	2.57	0.83
1:E:197:ARG:HD3	1:E:277:LYS:CB	2.09	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:90:THR:O	1:H:94:VAL:HG23	1.77	0.83
1:F:197:ARG:HD3	1:F:277:LYS:CB	2.09	0.82
1:E:463:SER:CB	1:L:464:VAL:CG2	2.57	0.82
1:A:463:SER:CB	1:H:464:VAL:CG2	2.57	0.82
1:N:149:THR:HG23	1:N:159:GLY:HA3	1.61	0.82
1:M:149:THR:HG23	1:M:159:GLY:HA3	1.61	0.82
1:H:149:THR:HG23	1:H:159:GLY:HA3	1.61	0.82
1:A:197:ARG:HD3	1:A:277:LYS:CB	2.09	0.82
1:D:197:ARG:HD3	1:D:277:LYS:CB	2.09	0.82
1:B:197:ARG:HD3	1:B:277:LYS:CB	2.09	0.82
1:C:138:CYS:HB2	1:C:411:VAL:HG13	1.59	0.82
1:C:463:SER:CB	1:J:464:VAL:CG2	2.57	0.82
1:B:138:CYS:HB2	1:B:411:VAL:HG13	1.59	0.82
1:E:172:GLU:CD	1:E:350:ARG:HG3	2.01	0.81
1:L:149:THR:HG23	1:L:159:GLY:HA3	1.61	0.81
1:F:172:GLU:CD	1:F:350:ARG:HG3	2.01	0.81
1:C:197:ARG:HD3	1:C:277:LYS:CB	2.09	0.81
1:C:464:VAL:CG2	1:J:467:ASN:CB	2.59	0.81
1:K:143:ALA:O	1:K:147:VAL:HG12	1.81	0.81
1:J:143:ALA:O	1:J:147:VAL:HG12	1.81	0.81
1:L:406:ALA:O	1:L:410:GLY:N	2.14	0.81
1:J:138:CYS:HB2	1:J:410:GLY:HA2	0.81	0.81
1:J:406:ALA:O	1:J:410:GLY:N	2.14	0.81
1:E:464:VAL:HB	1:L:467:ASN:ND2	1.96	0.81
1:H:143:ALA:O	1:H:147:VAL:HG12	1.81	0.81
1:I:143:ALA:O	1:I:147:VAL:HG12	1.81	0.81
1:L:414:GLY:O	1:L:417:VAL:HG12	1.81	0.81
1:I:149:THR:HG23	1:I:159:GLY:HA3	1.61	0.81
1:K:149:THR:HG23	1:K:159:GLY:HA3	1.61	0.81
1:B:414:GLY:O	1:B:417:VAL:HG12	1.81	0.81
1:M:136:VAL:CA	1:M:137:PRO:N	2.44	0.81
1:M:406:ALA:O	1:M:410:GLY:N	2.14	0.81
1:H:136:VAL:CA	1:H:137:PRO:N	2.44	0.81
1:D:464:VAL:CG2	1:K:467:ASN:CB	2.59	0.81
1:M:143:ALA:O	1:M:147:VAL:HG12	1.81	0.81
1:N:414:GLY:O	1:N:417:VAL:HG12	1.81	0.81
1:K:138:CYS:HB2	1:K:410:GLY:HA2	0.81	0.81
1:N:143:ALA:O	1:N:147:VAL:HG12	1.81	0.81
1:L:143:ALA:O	1:L:147:VAL:HG12	1.81	0.81
1:G:414:GLY:O	1:G:417:VAL:HG12	1.81	0.81
1:K:406:ALA:O	1:K:410:GLY:N	2.14	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:136:VAL:CA	1:N:137:PRO:N	2.44	0.81
1:N:138:CYS:HB2	1:N:410:GLY:HA2	0.81	0.81
1:I:136:VAL:CA	1:I:137:PRO:N	2.44	0.81
1:H:138:CYS:HB2	1:H:410:GLY:HA2	0.81	0.80
1:M:138:CYS:HB2	1:M:410:GLY:HA2	0.81	0.80
1:I:406:ALA:O	1:I:410:GLY:N	2.14	0.80
1:D:172:GLU:CD	1:D:350:ARG:HG3	2.01	0.80
1:B:172:GLU:CD	1:B:350:ARG:HG3	2.01	0.80
1:C:414:GLY:O	1:C:417:VAL:HG12	1.81	0.80
1:K:136:VAL:CA	1:K:137:PRO:N	2.44	0.80
1:J:414:GLY:O	1:J:417:VAL:HG12	1.81	0.80
1:F:414:GLY:O	1:F:417:VAL:HG12	1.81	0.80
1:L:136:VAL:CA	1:L:137:PRO:N	2.44	0.80
1:N:406:ALA:O	1:N:410:GLY:N	2.14	0.80
1:J:149:THR:HG23	1:J:159:GLY:HA3	1.61	0.80
1:E:464:VAL:CG2	1:L:467:ASN:CB	2.59	0.80
1:D:464:VAL:HB	1:K:467:ASN:ND2	1.96	0.80
1:G:172:GLU:CD	1:G:350:ARG:HG3	2.01	0.80
1:G:373:ALA:O	1:G:374:GLY:O	1.85	0.80
1:J:136:VAL:CA	1:J:137:PRO:N	2.44	0.80
1:A:172:GLU:CD	1:A:350:ARG:HG3	2.01	0.80
1:G:464:VAL:CG2	1:N:467:ASN:CB	2.59	0.80
1:K:414:GLY:O	1:K:417:VAL:HG12	1.81	0.80
1:I:414:GLY:O	1:I:417:VAL:HG12	1.81	0.80
1:D:414:GLY:O	1:D:417:VAL:HG12	1.81	0.80
1:H:406:ALA:O	1:H:410:GLY:N	2.14	0.79
1:F:464:VAL:CG2	1:M:467:ASN:CB	2.59	0.79
1:H:414:GLY:O	1:H:417:VAL:HG12	1.81	0.79
1:F:373:ALA:O	1:F:374:GLY:O	1.84	0.79
1:A:414:GLY:O	1:A:417:VAL:HG12	1.81	0.79
1:A:464:VAL:CG2	1:H:467:ASN:CB	2.59	0.79
1:G:197:ARG:HD3	1:G:277:LYS:CB	2.09	0.79
1:A:373:ALA:O	1:A:374:GLY:O	1.84	0.79
1:C:172:GLU:CD	1:C:350:ARG:HG3	2.01	0.79
1:M:414:GLY:O	1:M:417:VAL:HG12	1.81	0.79
1:E:414:GLY:O	1:E:417:VAL:HG12	1.81	0.79
1:I:138:CYS:HB2	1:I:410:GLY:HA2	0.81	0.79
1:C:463:SER:OG	1:J:464:VAL:CG2	2.31	0.79
1:L:169:VAL:HG13	1:L:173:GLY:HA3	1.65	0.79
1:H:63:GLU:HB2	1:N:3:ALA:CB	2.13	0.79
1:B:463:SER:OG	1:I:464:VAL:CG2	2.31	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:3:ALA:CB	1:N:63:GLU:HB2	2.13	0.79
1:M:169:VAL:HG13	1:M:173:GLY:HA3	1.65	0.79
1:A:306:GLY:HA3	1:G:264:VAL:CG1	2.13	0.79
1:J:169:VAL:HG13	1:J:173:GLY:HA3	1.65	0.79
1:B:430:ARG:HG2	1:B:430:ARG:HH11	1.48	0.79
1:F:264:VAL:CG1	1:G:306:GLY:HA3	2.13	0.79
1:A:264:VAL:CG1	1:B:306:GLY:HA3	2.13	0.79
1:K:169:VAL:HG13	1:K:173:GLY:HA3	1.65	0.79
1:A:464:VAL:HB	1:H:467:ASN:ND2	1.96	0.79
1:G:464:VAL:HB	1:N:467:ASN:ND2	1.96	0.79
1:L:3:ALA:CB	1:M:63:GLU:HB2	2.13	0.79
1:I:136:VAL:N	1:I:137:PRO:N	2.25	0.78
1:I:169:VAL:HG13	1:I:173:GLY:HA3	1.65	0.78
1:K:430:ARG:HG2	1:K:430:ARG:HH11	1.48	0.78
1:L:430:ARG:HH11	1:L:430:ARG:HG2	1.48	0.78
1:J:137:PRO:C	1:J:410:GLY:HA3	2.04	0.78
1:D:463:SER:OG	1:K:464:VAL:CG2	2.31	0.78
1:J:3:ALA:CB	1:K:63:GLU:HB2	2.13	0.78
1:B:264:VAL:CG1	1:C:306:GLY:HA3	2.13	0.78
1:H:192:GLY:CA	1:H:376:VAL:HG23	2.14	0.78
1:K:192:GLY:CA	1:K:376:VAL:HG23	2.14	0.78
1:L:192:GLY:CA	1:L:376:VAL:HG23	2.14	0.78
1:F:430:ARG:HH11	1:F:430:ARG:HG2	1.48	0.78
1:A:463:SER:OG	1:H:464:VAL:CG2	2.31	0.78
1:E:264:VAL:CG1	1:F:306:GLY:HA3	2.13	0.78
1:J:192:GLY:CA	1:J:376:VAL:HG23	2.14	0.78
1:H:3:ALA:CB	1:I:63:GLU:HB2	2.13	0.78
1:L:138:CYS:HB2	1:L:410:GLY:HA2	0.81	0.78
1:E:373:ALA:O	1:E:374:GLY:O	1.84	0.78
1:I:3:ALA:CB	1:J:63:GLU:HB2	2.13	0.78
1:G:430:ARG:HG2	1:G:430:ARG:HH11	1.48	0.78
1:A:430:ARG:HG2	1:A:430:ARG:HH11	1.48	0.78
1:B:464:VAL:HB	1:I:467:ASN:ND2	1.96	0.78
1:H:169:VAL:HG13	1:H:173:GLY:HA3	1.65	0.78
1:K:137:PRO:C	1:K:410:GLY:HA3	2.04	0.78
1:H:137:PRO:C	1:H:410:GLY:HA3	2.04	0.78
1:B:464:VAL:CG2	1:I:467:ASN:CB	2.59	0.78
1:N:169:VAL:HG13	1:N:173:GLY:HA3	1.65	0.78
1:N:192:GLY:CA	1:N:376:VAL:HG23	2.14	0.78
1:H:430:ARG:HG2	1:H:430:ARG:HH11	1.48	0.78
1:D:430:ARG:HH11	1:D:430:ARG:HG2	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:137:PRO:C	1:I:410:GLY:HA3	2.04	0.78
1:F:463:SER:OG	1:M:464:VAL:CG2	2.31	0.78
1:K:3:ALA:CB	1:L:63:GLU:HB2	2.13	0.78
1:L:137:PRO:C	1:L:410:GLY:HA3	2.04	0.78
1:E:463:SER:OG	1:L:464:VAL:CG2	2.31	0.78
1:C:373:ALA:O	1:C:374:GLY:O	1.84	0.78
1:M:192:GLY:CA	1:M:376:VAL:HG23	2.14	0.78
1:M:430:ARG:HG2	1:M:430:ARG:HH11	1.48	0.78
1:G:463:SER:OG	1:N:464:VAL:CG2	2.31	0.77
1:A:306:GLY:HA3	1:G:264:VAL:HG11	1.67	0.77
1:F:264:VAL:HG11	1:G:306:GLY:HA3	1.67	0.77
1:A:264:VAL:HG11	1:B:306:GLY:HA3	1.67	0.77
1:I:192:GLY:CA	1:I:376:VAL:HG23	2.14	0.77
1:E:264:VAL:HG11	1:F:306:GLY:HA3	1.67	0.77
1:J:430:ARG:HH11	1:J:430:ARG:HG2	1.48	0.77
1:D:264:VAL:CG1	1:E:306:GLY:HA3	2.13	0.77
1:C:264:VAL:CG1	1:D:306:GLY:HA3	2.13	0.77
1:B:264:VAL:HG11	1:C:306:GLY:HA3	1.67	0.77
1:M:137:PRO:C	1:M:410:GLY:HA3	2.04	0.77
1:L:136:VAL:N	1:L:137:PRO:N	2.25	0.77
1:F:464:VAL:HB	1:M:467:ASN:ND2	1.96	0.77
1:N:137:PRO:C	1:N:410:GLY:HA3	2.04	0.77
1:C:138:CYS:CB	1:C:411:VAL:HG13	2.14	0.77
1:G:138:CYS:CB	1:G:411:VAL:HG13	2.14	0.77
1:B:138:CYS:CB	1:B:411:VAL:HG13	2.14	0.76
1:A:138:CYS:CB	1:A:411:VAL:HG13	2.14	0.76
1:D:264:VAL:HG11	1:E:306:GLY:HA3	1.67	0.76
1:E:430:ARG:HH11	1:E:430:ARG:HG2	1.48	0.76
1:A:138:CYS:CB	1:A:410:GLY:HA2	2.15	0.76
1:C:430:ARG:HG2	1:C:430:ARG:HH11	1.48	0.76
1:C:464:VAL:CG2	1:J:467:ASN:HB2	2.16	0.76
1:A:464:VAL:CG2	1:H:467:ASN:HB2	2.16	0.76
1:D:138:CYS:CB	1:D:411:VAL:HG13	2.14	0.76
1:C:264:VAL:HG11	1:D:306:GLY:HA3	1.67	0.76
1:G:464:VAL:CG2	1:N:467:ASN:HB2	2.16	0.76
1:E:138:CYS:CB	1:E:410:GLY:HA2	2.15	0.76
1:G:138:CYS:CB	1:G:410:GLY:HA2	2.15	0.76
1:C:464:VAL:HB	1:J:467:ASN:ND2	1.96	0.76
1:F:138:CYS:CB	1:F:411:VAL:HG13	2.14	0.76
1:N:430:ARG:HH11	1:N:430:ARG:HG2	1.48	0.76
1:H:136:VAL:N	1:H:137:PRO:N	2.25	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:TYR:OH	1:E:286:LYS:CD	2.25	0.76
1:F:138:CYS:CB	1:F:410:GLY:HA2	2.15	0.76
1:B:172:GLU:O	1:B:369:VAL:HG23	1.86	0.76
1:E:138:CYS:CB	1:E:411:VAL:HG13	2.14	0.76
1:F:463:SER:HG	1:M:464:VAL:HG23	1.48	0.76
1:B:203:TYR:OH	1:C:286:LYS:CD	2.25	0.75
1:B:138:CYS:CB	1:B:410:GLY:HA2	2.15	0.75
1:I:430:ARG:HH11	1:I:430:ARG:HG2	1.48	0.75
1:D:464:VAL:CG2	1:K:467:ASN:HB2	2.16	0.75
1:G:172:GLU:O	1:G:369:VAL:HG23	1.86	0.75
1:D:138:CYS:CB	1:D:410:GLY:HA2	2.15	0.75
1:F:464:VAL:CG2	1:M:467:ASN:HB2	2.16	0.75
1:B:464:VAL:CG2	1:I:467:ASN:HB2	2.16	0.75
1:N:149:THR:CG2	1:N:156:GLU:HA	2.17	0.75
1:B:373:ALA:O	1:B:374:GLY:O	1.84	0.75
1:K:136:VAL:N	1:K:137:PRO:N	2.25	0.75
1:J:149:THR:CG2	1:J:156:GLU:HA	2.17	0.75
1:E:464:VAL:CG2	1:L:467:ASN:HB2	2.16	0.75
1:K:136:VAL:C	1:K:137:PRO:N	2.40	0.75
1:C:203:TYR:OH	1:D:286:LYS:CD	2.26	0.75
1:D:172:GLU:O	1:D:369:VAL:HG23	1.86	0.75
1:C:172:GLU:O	1:C:369:VAL:HG23	1.86	0.75
1:A:172:GLU:O	1:A:369:VAL:HG23	1.86	0.74
1:L:136:VAL:C	1:L:137:PRO:N	2.40	0.74
1:F:172:GLU:O	1:F:369:VAL:HG23	1.86	0.74
1:K:149:THR:CG2	1:K:156:GLU:HA	2.17	0.74
1:H:136:VAL:C	1:H:137:PRO:N	2.40	0.74
1:H:149:THR:CG2	1:H:156:GLU:HA	2.17	0.74
1:L:149:THR:CG2	1:L:156:GLU:HA	2.17	0.74
1:N:136:VAL:N	1:N:137:PRO:N	2.25	0.74
1:D:146:GLN:OE1	1:D:492:GLY:HA2	1.88	0.74
1:I:149:THR:CG2	1:I:156:GLU:HA	2.17	0.74
1:G:146:GLN:OE1	1:G:492:GLY:HA2	1.88	0.74
1:B:105:LYS:HD3	1:H:110:GLY:HA3	1.69	0.74
1:C:105:LYS:HD3	1:I:110:GLY:HA3	1.69	0.74
1:M:149:THR:CG2	1:M:156:GLU:HA	2.17	0.74
1:E:146:GLN:OE1	1:E:492:GLY:HA2	1.88	0.74
1:G:136:VAL:HA	1:G:137:PRO:CD	2.18	0.74
1:B:136:VAL:HA	1:B:137:PRO:CD	2.18	0.74
1:J:136:VAL:HA	1:J:137:PRO:HD2	0.77	0.74
1:J:136:VAL:C	1:J:137:PRO:N	2.40	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:136:VAL:HA	1:F:137:PRO:CD	2.18	0.74
1:C:138:CYS:CB	1:C:410:GLY:HA2	2.15	0.74
1:D:105:LYS:HD3	1:J:110:GLY:HA3	1.69	0.74
1:I:136:VAL:C	1:I:137:PRO:N	2.40	0.74
1:C:146:GLN:OE1	1:C:492:GLY:HA2	1.88	0.74
1:E:136:VAL:HA	1:E:137:PRO:CD	2.18	0.74
1:E:172:GLU:O	1:E:369:VAL:HG23	1.86	0.74
1:N:136:VAL:C	1:N:137:PRO:N	2.40	0.74
1:D:136:VAL:HA	1:D:137:PRO:CD	2.18	0.74
1:A:136:VAL:HA	1:A:137:PRO:CD	2.18	0.74
1:A:105:LYS:HD3	1:N:110:GLY:HA3	1.69	0.74
1:D:138:CYS:SG	1:D:411:VAL:HG13	2.28	0.73
1:B:146:GLN:OE1	1:B:492:GLY:HA2	1.88	0.73
1:C:136:VAL:HA	1:C:137:PRO:CD	2.18	0.73
1:F:138:CYS:SG	1:F:411:VAL:HG13	2.28	0.73
1:G:138:CYS:SG	1:G:411:VAL:HG13	2.28	0.73
1:G:136:VAL:HA	1:G:137:PRO:HD2	1.70	0.73
1:A:146:GLN:OE1	1:A:492:GLY:HA2	1.88	0.73
1:A:136:VAL:HA	1:A:137:PRO:HD2	1.70	0.73
1:A:138:CYS:SG	1:A:411:VAL:HG13	2.28	0.73
1:E:105:LYS:HD3	1:K:110:GLY:HA3	1.69	0.73
1:F:146:GLN:OE1	1:F:492:GLY:HA2	1.88	0.73
1:F:203:TYR:OH	1:G:286:LYS:CD	2.25	0.73
1:D:464:VAL:HG21	1:K:467:ASN:HB2	1.71	0.73
1:B:138:CYS:SG	1:B:411:VAL:HG13	2.28	0.73
1:C:138:CYS:SG	1:C:411:VAL:HG13	2.28	0.73
1:I:136:VAL:HA	1:I:137:PRO:HD2	0.77	0.72
1:M:136:VAL:C	1:M:137:PRO:N	2.40	0.72
1:B:136:VAL:HA	1:B:137:PRO:HD2	1.70	0.72
1:E:138:CYS:SG	1:E:411:VAL:HG13	2.28	0.72
1:A:286:LYS:CD	1:G:203:TYR:OH	2.25	0.72
1:G:173:GLY:HA2	1:G:370:ALA:HB2	1.71	0.72
1:C:464:VAL:HG21	1:J:467:ASN:HB2	1.71	0.72
1:F:173:GLY:HA2	1:F:370:ALA:HB2	1.71	0.72
1:M:136:VAL:N	1:M:137:PRO:N	2.25	0.72
1:E:136:VAL:HA	1:E:137:PRO:HD2	1.70	0.72
1:F:136:VAL:HA	1:F:137:PRO:HD2	1.70	0.72
1:C:136:VAL:HA	1:C:137:PRO:HD2	1.70	0.72
1:C:173:GLY:HA2	1:C:370:ALA:HB2	1.71	0.72
2:O:80:PRO:O	2:P:110:TYR:OH	2.08	0.71
1:G:105:LYS:HD3	1:M:110:GLY:HA3	1.69	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:136:VAL:HA	1:H:137:PRO:HD2	0.77	0.71
1:G:464:VAL:HG21	1:N:467:ASN:HB2	1.71	0.71
1:F:105:LYS:HD3	1:L:110:GLY:HA3	1.69	0.71
1:D:173:GLY:HA2	1:D:370:ALA:HB2	1.71	0.71
2:P:102:HIS:HD2	2:P:104:LYS:H	1.38	0.71
1:A:173:GLY:HA2	1:A:370:ALA:HB2	1.71	0.71
1:B:173:GLY:HA2	1:B:370:ALA:HB2	1.71	0.71
2:S:102:HIS:HD2	2:S:104:LYS:H	1.38	0.71
2:R:102:HIS:HD2	2:R:104:LYS:H	1.38	0.71
1:M:18:ARG:CB	1:M:18:ARG:NH1	2.41	0.71
2:Q:80:PRO:O	2:R:110:TYR:OH	2.08	0.71
2:T:80:PRO:O	2:U:110:TYR:OH	2.08	0.71
1:A:464:VAL:HG21	1:H:467:ASN:HB2	1.71	0.71
1:J:136:VAL:N	1:J:137:PRO:N	2.25	0.71
1:H:18:ARG:CB	1:H:18:ARG:NH1	2.41	0.71
1:D:373:ALA:O	1:D:374:GLY:O	1.84	0.71
2:Q:102:HIS:HD2	2:Q:104:LYS:H	1.38	0.71
1:D:136:VAL:HA	1:D:137:PRO:HD2	1.70	0.71
1:E:203:TYR:OH	1:F:286:LYS:CD	2.26	0.71
2:R:80:PRO:O	2:S:110:TYR:OH	2.08	0.71
1:A:203:TYR:OH	1:B:286:LYS:CD	2.25	0.70
1:F:18:ARG:NH1	1:F:18:ARG:CB	2.41	0.70
2:U:102:HIS:HD2	2:U:104:LYS:H	1.38	0.70
1:K:398:ASP:O	1:K:401:HIS:HB2	1.92	0.70
1:N:136:VAL:HA	1:N:137:PRO:HD2	0.77	0.70
1:N:398:ASP:O	1:N:401:HIS:HB2	1.92	0.70
1:J:398:ASP:O	1:J:401:HIS:HB2	1.92	0.70
2:S:77:ARG:HD3	2:T:72:PRO:CG	2.22	0.70
1:L:398:ASP:O	1:L:401:HIS:HB2	1.92	0.70
1:M:398:ASP:O	1:M:401:HIS:HB2	1.92	0.70
1:D:18:ARG:CB	1:D:18:ARG:NH1	2.41	0.70
1:E:173:GLY:HA2	1:E:370:ALA:HB2	1.71	0.70
1:H:398:ASP:O	1:H:401:HIS:HB2	1.92	0.70
2:S:80:PRO:O	2:T:110:TYR:OH	2.08	0.70
1:F:464:VAL:HG21	1:M:467:ASN:HB2	1.71	0.70
2:R:77:ARG:HD3	2:S:72:PRO:CG	2.22	0.70
1:I:398:ASP:O	1:I:401:HIS:HB2	1.92	0.70
1:L:192:GLY:HA3	1:L:376:VAL:CG2	2.22	0.70
2:T:102:HIS:HD2	2:T:104:LYS:H	1.38	0.69
1:N:192:GLY:HA3	1:N:376:VAL:CG2	2.22	0.69
2:T:77:ARG:HD3	2:U:72:PRO:CG	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:138:CYS:HB2	1:I:410:GLY:C	2.13	0.69
2:O:110:TYR:OH	2:U:80:PRO:O	2.08	0.69
2:P:80:PRO:O	2:Q:110:TYR:OH	2.08	0.69
2:R:80:PRO:CG	2:S:70:SER:OG	2.40	0.69
1:K:136:VAL:HA	1:K:137:PRO:HD2	0.77	0.69
1:K:138:CYS:HB2	1:K:410:GLY:C	2.12	0.69
2:O:72:PRO:CG	2:U:77:ARG:HD3	2.22	0.69
2:O:77:ARG:HD3	2:P:72:PRO:CG	2.22	0.69
2:Q:80:PRO:CG	2:R:70:SER:OG	2.40	0.69
1:L:176:THR:HG21	1:L:333:ILE:HD11	1.75	0.69
1:K:176:THR:HG21	1:K:333:ILE:HD11	1.75	0.69
1:N:176:THR:HG21	1:N:333:ILE:HD11	1.75	0.69
1:L:138:CYS:HB2	1:L:410:GLY:C	2.13	0.69
1:K:192:GLY:HA3	1:K:376:VAL:CG2	2.22	0.69
1:H:176:THR:HG21	1:H:333:ILE:HD11	1.75	0.69
1:M:176:THR:HG21	1:M:333:ILE:HD11	1.75	0.69
1:L:175:ILE:HD12	1:L:175:ILE:N	2.08	0.69
1:M:136:VAL:HA	1:M:137:PRO:HD2	0.77	0.69
1:M:157:THR:O	1:M:160:LYS:HB3	1.93	0.69
1:M:414:GLY:O	1:M:417:VAL:CG1	2.41	0.69
1:J:192:GLY:HA3	1:J:376:VAL:CG2	2.22	0.69
1:N:137:PRO:C	1:N:410:GLY:CA	2.62	0.69
2:P:80:PRO:CG	2:Q:70:SER:OG	2.40	0.69
1:I:192:GLY:HA3	1:I:376:VAL:CG2	2.22	0.69
1:M:137:PRO:C	1:M:410:GLY:CA	2.62	0.68
1:B:18:ARG:CG	1:B:18:ARG:HH11	2.06	0.68
1:H:18:ARG:CG	1:H:18:ARG:HH11	2.06	0.68
1:N:157:THR:O	1:N:160:LYS:HB3	1.93	0.68
1:B:414:GLY:O	1:B:417:VAL:CG1	2.41	0.68
2:O:102:HIS:HD2	2:O:104:LYS:H	1.38	0.68
1:L:157:THR:O	1:L:160:LYS:HB3	1.93	0.68
1:J:176:THR:HG21	1:J:333:ILE:HD11	1.75	0.68
1:L:414:GLY:O	1:L:417:VAL:CG1	2.41	0.68
1:H:192:GLY:HA3	1:H:376:VAL:CG2	2.22	0.68
1:N:192:GLY:C	1:N:376:VAL:HG23	2.14	0.68
1:I:175:ILE:HD12	1:I:175:ILE:N	2.08	0.68
2:Q:77:ARG:HD3	2:R:72:PRO:CG	2.22	0.68
1:K:137:PRO:C	1:K:410:GLY:CA	2.62	0.68
1:E:18:ARG:NH1	1:E:18:ARG:CB	2.41	0.68
1:A:18:ARG:CG	1:A:18:ARG:HH11	2.06	0.68
1:L:381:VAL:HB	1:L:389:MET:HE3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:157:THR:O	1:K:160:LYS:HB3	1.93	0.68
1:N:414:GLY:O	1:N:417:VAL:CG1	2.41	0.68
1:D:414:GLY:O	1:D:417:VAL:CG1	2.41	0.68
1:K:175:ILE:N	1:K:175:ILE:HD12	2.08	0.68
1:C:18:ARG:CG	1:C:18:ARG:HH11	2.07	0.68
1:K:381:VAL:HB	1:K:389:MET:HE3	1.76	0.68
1:F:414:GLY:O	1:F:417:VAL:CG1	2.41	0.68
1:A:414:GLY:O	1:A:417:VAL:CG1	2.41	0.68
1:E:414:GLY:O	1:E:417:VAL:CG1	2.41	0.68
1:I:192:GLY:C	1:I:376:VAL:HG23	2.14	0.68
2:P:77:ARG:HD3	2:Q:72:PRO:CG	2.22	0.68
1:M:175:ILE:HD12	1:M:175:ILE:N	2.08	0.68
1:J:137:PRO:C	1:J:410:GLY:CA	2.62	0.68
1:I:18:ARG:NH1	1:I:18:ARG:CB	2.41	0.68
1:C:18:ARG:NH1	1:C:18:ARG:CB	2.41	0.68
1:G:414:GLY:O	1:G:417:VAL:CG1	2.41	0.68
1:J:18:ARG:HH11	1:J:18:ARG:CG	2.07	0.68
1:G:18:ARG:CG	1:G:18:ARG:HH11	2.06	0.68
1:C:138:CYS:N	1:C:410:GLY:HA2	2.09	0.68
1:N:381:VAL:HB	1:N:389:MET:HE3	1.76	0.68
1:J:192:GLY:C	1:J:376:VAL:HG23	2.14	0.68
1:I:176:THR:HG21	1:I:333:ILE:HD11	1.75	0.68
1:H:137:PRO:C	1:H:410:GLY:CA	2.62	0.68
1:D:18:ARG:CG	1:D:18:ARG:HH11	2.06	0.68
2:O:80:PRO:CG	2:P:70:SER:OG	2.40	0.68
1:H:157:THR:O	1:H:160:LYS:HB3	1.93	0.68
1:J:157:THR:O	1:J:160:LYS:HB3	1.93	0.68
1:M:138:CYS:HB2	1:M:410:GLY:C	2.12	0.68
1:M:18:ARG:CG	1:M:18:ARG:HH11	2.06	0.68
1:F:18:ARG:CG	1:F:18:ARG:HH11	2.06	0.68
1:I:157:THR:O	1:I:160:LYS:HB3	1.93	0.68
1:L:137:PRO:C	1:L:410:GLY:CA	2.62	0.68
1:I:137:PRO:C	1:I:410:GLY:CA	2.62	0.68
1:E:18:ARG:CG	1:E:18:ARG:HH11	2.06	0.68
1:H:175:ILE:N	1:H:175:ILE:HD12	2.08	0.68
1:K:414:GLY:O	1:K:417:VAL:CG1	2.41	0.68
1:L:192:GLY:C	1:L:376:VAL:HG23	2.14	0.68
1:M:192:GLY:HA3	1:M:376:VAL:CG2	2.22	0.68
1:M:192:GLY:C	1:M:376:VAL:HG23	2.14	0.68
2:O:70:SER:OG	2:U:80:PRO:CG	2.40	0.67
2:T:80:PRO:CG	2:U:70:SER:OG	2.40	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:414:GLY:O	1:H:417:VAL:CG1	2.41	0.67
1:I:404:ARG:O	1:I:408:GLU:HG3	1.94	0.67
1:I:381:VAL:HB	1:I:389:MET:HE3	1.76	0.67
1:J:381:VAL:HB	1:J:389:MET:HE3	1.76	0.67
1:C:414:GLY:O	1:C:417:VAL:CG1	2.41	0.67
1:H:404:ARG:O	1:H:408:GLU:HG3	1.94	0.67
1:A:138:CYS:N	1:A:410:GLY:HA2	2.09	0.67
1:E:138:CYS:N	1:E:410:GLY:HA2	2.09	0.67
1:N:18:ARG:HH11	1:N:18:ARG:CG	2.06	0.67
1:I:18:ARG:CG	1:I:18:ARG:HH11	2.07	0.67
1:B:138:CYS:N	1:B:410:GLY:HA2	2.09	0.67
1:H:192:GLY:C	1:H:376:VAL:HG23	2.14	0.67
1:J:192:GLY:HA3	1:J:376:VAL:HG23	1.76	0.67
1:I:192:GLY:HA3	1:I:376:VAL:HG23	1.76	0.67
1:A:304:GLU:OE2	1:G:203:TYR:HE2	1.78	0.67
2:P:82:PRO:CA	2:Q:110:TYR:CE1	2.78	0.67
1:J:414:GLY:O	1:J:417:VAL:CG1	2.41	0.67
1:K:192:GLY:C	1:K:376:VAL:HG23	2.14	0.67
1:C:209:GLU:O	1:D:351:GLN:NE2	2.28	0.67
1:L:136:VAL:HA	1:L:137:PRO:HD2	0.77	0.67
1:J:138:CYS:HB2	1:J:410:GLY:C	2.12	0.67
1:F:138:CYS:N	1:F:410:GLY:HA2	2.09	0.67
1:G:138:CYS:N	1:G:410:GLY:HA2	2.09	0.67
1:L:404:ARG:O	1:L:408:GLU:HG3	1.94	0.67
1:E:209:GLU:O	1:F:351:GLN:NE2	2.28	0.67
1:J:175:ILE:HD12	1:J:175:ILE:N	2.08	0.67
1:A:351:GLN:NE2	1:G:209:GLU:O	2.28	0.67
1:N:138:CYS:HB2	1:N:410:GLY:C	2.12	0.67
1:A:203:TYR:HE2	1:B:304:GLU:OE2	1.78	0.67
1:D:138:CYS:N	1:D:410:GLY:HA2	2.09	0.67
1:I:414:GLY:O	1:I:417:VAL:CG1	2.41	0.67
1:J:404:ARG:O	1:J:408:GLU:HG3	1.94	0.67
1:F:209:GLU:O	1:G:351:GLN:NE2	2.28	0.67
1:N:175:ILE:HD12	1:N:175:ILE:N	2.08	0.67
1:N:404:ARG:O	1:N:408:GLU:HG3	1.94	0.67
1:K:18:ARG:CG	1:K:18:ARG:HH11	2.07	0.67
1:H:381:VAL:HB	1:H:389:MET:HE3	1.76	0.67
1:B:417:VAL:HG11	1:B:488:MET:HG3	1.77	0.67
1:G:13:ARG:HD2	1:G:104:LEU:HD22	1.77	0.67
1:F:203:TYR:HE2	1:G:304:GLU:OE2	1.78	0.67
1:G:138:CYS:HB3	1:G:410:GLY:CA	2.22	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:82:PRO:CA	2:S:110:TYR:CE1	2.78	0.67
2:R:77:ARG:HD3	2:S:72:PRO:HG2	1.77	0.67
2:Q:77:ARG:HD3	2:R:72:PRO:HG2	1.77	0.67
1:L:13:ARG:HD2	1:L:104:LEU:HD22	1.77	0.67
1:C:13:ARG:HD2	1:C:104:LEU:HD22	1.77	0.67
1:A:13:ARG:HD2	1:A:104:LEU:HD22	1.77	0.67
1:D:13:ARG:HD2	1:D:104:LEU:HD22	1.77	0.67
2:S:80:PRO:CG	2:T:70:SER:OG	2.40	0.67
1:K:192:GLY:HA3	1:K:376:VAL:HG23	1.76	0.67
1:J:18:ARG:CB	1:J:18:ARG:NH1	2.41	0.66
1:C:417:VAL:HG11	1:C:488:MET:HG3	1.77	0.66
1:A:417:VAL:HG11	1:A:488:MET:HG3	1.77	0.66
1:F:74:VAL:O	1:F:77:VAL:HG13	1.96	0.66
1:A:74:VAL:O	1:A:77:VAL:HG13	1.95	0.66
1:L:18:ARG:HH11	1:L:18:ARG:CG	2.06	0.66
2:T:82:PRO:CA	2:U:110:TYR:CE1	2.78	0.66
1:H:192:GLY:HA3	1:H:376:VAL:HG23	1.76	0.66
1:H:74:VAL:O	1:H:77:VAL:HG13	1.95	0.66
1:G:74:VAL:O	1:G:77:VAL:HG13	1.96	0.66
1:C:150:ILE:HD11	1:C:493:ILE:HA	1.78	0.66
1:J:13:ARG:HD2	1:J:104:LEU:HD22	1.77	0.66
1:K:13:ARG:HD2	1:K:104:LEU:HD22	1.77	0.66
1:A:209:GLU:O	1:B:351:GLN:NE2	2.28	0.66
1:D:150:ILE:HD11	1:D:493:ILE:HA	1.78	0.66
1:F:138:CYS:HB3	1:F:410:GLY:CA	2.22	0.66
1:A:138:CYS:HB3	1:A:410:GLY:CA	2.22	0.66
1:M:381:VAL:HB	1:M:389:MET:HE3	1.76	0.66
2:Q:82:PRO:CA	2:R:110:TYR:CE1	2.78	0.66
2:S:77:ARG:HD3	2:T:72:PRO:HG2	1.77	0.66
1:K:404:ARG:O	1:K:408:GLU:HG3	1.94	0.66
1:L:74:VAL:O	1:L:77:VAL:HG13	1.95	0.66
1:F:13:ARG:HD2	1:F:104:LEU:HD22	1.77	0.66
1:E:74:VAL:O	1:E:77:VAL:HG13	1.96	0.66
2:S:82:PRO:CA	2:T:110:TYR:CE1	2.78	0.66
1:I:13:ARG:HD2	1:I:104:LEU:HD22	1.78	0.66
1:I:74:VAL:O	1:I:77:VAL:HG13	1.95	0.66
1:E:150:ILE:HD11	1:E:493:ILE:HA	1.78	0.66
1:A:18:ARG:CB	1:A:18:ARG:NH1	2.41	0.66
2:T:77:ARG:HD3	2:U:72:PRO:HG2	1.77	0.66
1:L:452:ARG:HG2	1:L:452:ARG:NH1	2.11	0.66
1:E:13:ARG:HD2	1:E:104:LEU:HD22	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:147:VAL:CG2	1:N:496:PRO:HG3	2.14	0.66
1:D:138:CYS:HB3	1:D:410:GLY:CA	2.22	0.66
1:G:417:VAL:HG11	1:G:488:MET:HG3	1.77	0.66
1:J:417:VAL:HG11	1:J:488:MET:HG3	1.77	0.66
1:D:209:GLU:O	1:E:351:GLN:NE2	2.28	0.66
1:B:13:ARG:HD2	1:B:104:LEU:HD22	1.77	0.66
1:M:13:ARG:HD2	1:M:104:LEU:HD22	1.78	0.66
1:B:209:GLU:O	1:C:351:GLN:NE2	2.28	0.66
1:I:452:ARG:NH1	1:I:452:ARG:HG2	2.11	0.66
1:K:18:ARG:CB	1:K:18:ARG:NH1	2.41	0.66
1:B:138:CYS:HB3	1:B:410:GLY:CA	2.22	0.66
2:O:82:PRO:CA	2:P:110:TYR:CE1	2.78	0.66
2:P:77:ARG:HD3	2:Q:72:PRO:HG2	1.77	0.66
1:B:74:VAL:O	1:B:77:VAL:HG13	1.95	0.66
1:B:452:ARG:HG2	1:B:452:ARG:NH1	2.11	0.66
1:L:417:VAL:HG11	1:L:488:MET:HG3	1.77	0.66
1:M:74:VAL:O	1:M:77:VAL:HG13	1.95	0.66
1:I:138:CYS:N	1:I:410:GLY:HA2	2.11	0.66
1:B:203:TYR:HE2	1:C:304:GLU:OE2	1.78	0.66
1:E:138:CYS:HB3	1:E:410:GLY:CA	2.22	0.66
1:M:417:VAL:HG11	1:M:488:MET:HG3	1.77	0.66
1:L:192:GLY:HA3	1:L:376:VAL:HG23	1.76	0.66
1:B:150:ILE:HD11	1:B:493:ILE:HA	1.78	0.66
1:I:417:VAL:HG11	1:I:488:MET:HG3	1.77	0.66
1:L:3:ALA:HB1	1:M:63:GLU:HB2	1.78	0.66
1:H:13:ARG:HD2	1:H:104:LEU:HD22	1.77	0.66
1:J:74:VAL:O	1:J:77:VAL:HG13	1.95	0.66
1:J:138:CYS:N	1:J:410:GLY:HA2	2.11	0.65
1:C:138:CYS:HB3	1:C:410:GLY:CA	2.22	0.65
1:K:417:VAL:HG11	1:K:488:MET:HG3	1.77	0.65
1:M:404:ARG:O	1:M:408:GLU:HG3	1.94	0.65
1:K:452:ARG:NH1	1:K:452:ARG:HG2	2.11	0.65
1:A:452:ARG:NH1	1:A:452:ARG:HG2	2.11	0.65
1:H:138:CYS:N	1:H:410:GLY:HA2	2.11	0.65
1:D:417:VAL:HG11	1:D:488:MET:HG3	1.77	0.65
1:E:417:VAL:HG11	1:E:488:MET:HG3	1.77	0.65
1:I:155:ASP:OD1	1:I:158:VAL:HG23	1.97	0.65
1:D:74:VAL:O	1:D:77:VAL:HG13	1.96	0.65
1:F:150:ILE:HD11	1:F:493:ILE:HA	1.78	0.65
1:E:464:VAL:HG21	1:L:467:ASN:HB2	1.71	0.65
1:M:155:ASP:OD1	1:M:158:VAL:HG23	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:102:HIS:CD2	2:P:104:LYS:H	2.15	0.65
1:H:138:CYS:HB2	1:H:410:GLY:C	2.12	0.65
1:K:155:ASP:OD1	1:K:158:VAL:HG23	1.97	0.65
2:O:72:PRO:HG2	2:U:77:ARG:HD3	1.77	0.65
2:T:102:HIS:CD2	2:T:104:LYS:H	2.15	0.65
1:K:74:VAL:O	1:K:77:VAL:HG13	1.95	0.65
1:E:452:ARG:NH1	1:E:452:ARG:HG2	2.11	0.65
1:M:452:ARG:HG2	1:M:452:ARG:NH1	2.11	0.65
1:H:452:ARG:NH1	1:H:452:ARG:HG2	2.11	0.65
1:J:452:ARG:HG2	1:J:452:ARG:NH1	2.11	0.65
1:K:138:CYS:N	1:K:410:GLY:HA2	2.11	0.65
1:E:203:TYR:HE2	1:F:304:GLU:OE2	1.78	0.65
2:O:110:TYR:CE1	2:U:82:PRO:CA	2.78	0.65
1:H:63:GLU:HB2	1:N:3:ALA:HB1	1.78	0.65
1:H:3:ALA:HB1	1:I:63:GLU:HB2	1.78	0.65
1:K:448:GLU:HB3	1:K:452:ARG:HD2	1.79	0.65
1:N:13:ARG:HD2	1:N:104:LEU:HD22	1.77	0.65
1:N:417:VAL:HG11	1:N:488:MET:HG3	1.77	0.65
1:F:417:VAL:HG11	1:F:488:MET:HG3	1.77	0.65
2:R:102:HIS:CD2	2:R:104:LYS:H	2.15	0.65
2:U:102:HIS:CD2	2:U:104:LYS:H	2.15	0.65
1:J:155:ASP:OD1	1:J:158:VAL:HG23	1.97	0.65
1:L:448:GLU:HB3	1:L:452:ARG:HD2	1.79	0.65
1:A:150:ILE:HD11	1:A:493:ILE:HA	1.78	0.65
1:C:448:GLU:HB3	1:C:452:ARG:HD2	1.79	0.65
1:N:138:CYS:N	1:N:410:GLY:HA2	2.11	0.65
1:F:146:GLN:HB2	1:F:494:LEU:CD1	2.27	0.65
1:C:203:TYR:HH	1:D:286:LYS:HD3	1.57	0.65
1:N:155:ASP:OD1	1:N:158:VAL:HG23	1.97	0.65
1:H:417:VAL:HG11	1:H:488:MET:HG3	1.77	0.65
1:M:192:GLY:HA3	1:M:376:VAL:HG23	1.76	0.65
1:E:448:GLU:HB3	1:E:452:ARG:HD2	1.79	0.65
1:J:448:GLU:HB3	1:J:452:ARG:HD2	1.79	0.65
1:C:74:VAL:O	1:C:77:VAL:HG13	1.96	0.65
1:D:448:GLU:HB3	1:D:452:ARG:HD2	1.79	0.65
1:G:146:GLN:HB2	1:G:494:LEU:CD1	2.27	0.65
1:L:18:ARG:CB	1:L:18:ARG:NH1	2.41	0.65
2:O:77:ARG:HD3	2:P:72:PRO:HG2	1.77	0.65
1:M:448:GLU:HB3	1:M:452:ARG:HD2	1.79	0.65
1:F:448:GLU:HB3	1:F:452:ARG:HD2	1.79	0.65
1:F:452:ARG:HG2	1:F:452:ARG:NH1	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:74:VAL:O	1:N:77:VAL:HG13	1.95	0.65
1:B:146:GLN:HB2	1:B:494:LEU:CD1	2.27	0.65
1:C:146:GLN:HB2	1:C:494:LEU:CD1	2.27	0.65
1:M:147:VAL:CG2	1:M:496:PRO:HG3	2.14	0.65
1:B:18:ARG:CB	1:B:18:ARG:NH1	2.41	0.65
1:N:192:GLY:HA3	1:N:376:VAL:HG23	1.76	0.65
2:O:102:HIS:CD2	2:O:104:LYS:H	2.15	0.65
1:N:448:GLU:HB3	1:N:452:ARG:HD2	1.79	0.65
1:G:150:ILE:HD11	1:G:493:ILE:HA	1.78	0.65
1:A:146:GLN:HB2	1:A:494:LEU:CD1	2.27	0.64
1:E:146:GLN:HB2	1:E:494:LEU:CD1	2.27	0.64
1:D:146:GLN:HB2	1:D:494:LEU:CD1	2.27	0.64
1:M:3:ALA:HB1	1:N:63:GLU:HB2	1.78	0.64
1:I:448:GLU:HB3	1:I:452:ARG:HD2	1.79	0.64
1:B:448:GLU:HB3	1:B:452:ARG:HD2	1.79	0.64
1:H:448:GLU:HB3	1:H:452:ARG:HD2	1.79	0.64
1:L:138:CYS:N	1:L:410:GLY:HA2	2.11	0.64
1:D:452:ARG:HG2	1:D:452:ARG:NH1	2.11	0.64
1:M:138:CYS:N	1:M:410:GLY:HA2	2.11	0.64
1:I:3:ALA:HB1	1:J:63:GLU:HB2	1.78	0.64
2:S:102:HIS:CD2	2:S:104:LYS:H	2.15	0.64
1:K:171:LYS:HD3	1:K:407:VAL:HG11	1.80	0.64
1:A:448:GLU:HB3	1:A:452:ARG:HD2	1.79	0.64
1:E:452:ARG:HG2	1:E:452:ARG:HH11	1.63	0.64
1:F:452:ARG:HG2	1:F:452:ARG:HH11	1.63	0.64
1:N:452:ARG:NH1	1:N:452:ARG:HG2	2.11	0.64
1:G:452:ARG:NH1	1:G:452:ARG:HG2	2.11	0.64
1:M:87:ASP:OD2	1:M:151:SER:HA	1.98	0.64
1:K:87:ASP:OD2	1:K:151:SER:HA	1.98	0.64
1:N:18:ARG:CB	1:N:18:ARG:NH1	2.41	0.64
1:J:171:LYS:HD3	1:J:407:VAL:HG11	1.80	0.64
1:J:3:ALA:HB1	1:K:63:GLU:HB2	1.78	0.64
2:Q:102:HIS:CD2	2:Q:104:LYS:H	2.15	0.64
1:H:155:ASP:OD1	1:H:158:VAL:HG23	1.97	0.64
1:K:452:ARG:HH11	1:K:452:ARG:HG2	1.63	0.64
1:G:448:GLU:HB3	1:G:452:ARG:HD2	1.79	0.64
1:G:452:ARG:HH11	1:G:452:ARG:HG2	1.63	0.64
1:I:87:ASP:OD2	1:I:151:SER:HA	1.98	0.64
1:L:452:ARG:HG2	1:L:452:ARG:HH11	1.63	0.64
1:J:452:ARG:HG2	1:J:452:ARG:HH11	1.63	0.64
1:C:452:ARG:HG2	1:C:452:ARG:NH1	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:25:ASP:HA	1:K:28:LYS:HE2	1.80	0.64
1:N:87:ASP:OD2	1:N:151:SER:HA	1.98	0.64
1:C:203:TYR:HE2	1:D:304:GLU:OE2	1.78	0.64
1:G:18:ARG:NH1	1:G:18:ARG:CB	2.41	0.64
2:R:10:ARG:O	2:S:108:CYS:HA	1.98	0.64
1:I:452:ARG:HH11	1:I:452:ARG:HG2	1.63	0.64
1:J:25:ASP:HA	1:J:28:LYS:HE2	1.80	0.64
1:I:25:ASP:HA	1:I:28:LYS:HE2	1.80	0.64
1:B:44:PHE:CD1	1:B:44:PHE:N	2.66	0.64
1:G:105:LYS:CG	1:M:109:ALA:O	2.45	0.64
1:A:477:GLY:HA3	1:A:488:MET:SD	2.38	0.64
1:D:452:ARG:HG2	1:D:452:ARG:HH11	1.63	0.64
1:L:155:ASP:OD1	1:L:158:VAL:HG23	1.97	0.64
1:L:25:ASP:HA	1:L:28:LYS:HE2	1.80	0.64
1:C:44:PHE:CD1	1:C:44:PHE:N	2.66	0.64
1:H:25:ASP:HA	1:H:28:LYS:HE2	1.80	0.64
2:P:10:ARG:O	2:Q:108:CYS:HA	1.98	0.64
1:I:171:LYS:HD3	1:I:407:VAL:HG11	1.79	0.64
1:M:477:GLY:HA3	1:M:488:MET:SD	2.38	0.64
1:B:464:VAL:HG21	1:I:467:ASN:HB2	1.71	0.63
1:B:477:GLY:HA3	1:B:488:MET:SD	2.38	0.63
1:G:477:GLY:HA3	1:G:488:MET:SD	2.38	0.63
1:I:477:GLY:HA3	1:I:488:MET:SD	2.38	0.63
1:L:87:ASP:OD2	1:L:151:SER:HA	1.98	0.63
1:H:87:ASP:OD2	1:H:151:SER:HA	1.98	0.63
1:M:157:THR:O	1:M:161:LEU:HD13	1.98	0.63
1:N:477:GLY:HA3	1:N:488:MET:SD	2.38	0.63
1:K:477:GLY:HA3	1:K:488:MET:SD	2.38	0.63
1:A:452:ARG:HH11	1:A:452:ARG:HG2	1.63	0.63
2:Q:10:ARG:O	2:R:108:CYS:HA	1.98	0.63
1:L:477:GLY:HA3	1:L:488:MET:SD	2.39	0.63
1:J:477:GLY:HA3	1:J:488:MET:SD	2.39	0.63
1:A:44:PHE:CD1	1:A:44:PHE:N	2.66	0.63
2:O:108:CYS:HA	2:U:10:ARG:O	1.98	0.63
1:L:171:LYS:HD3	1:L:407:VAL:HG11	1.80	0.63
1:K:3:ALA:HB1	1:L:63:GLU:HB2	1.78	0.63
1:C:452:ARG:HG2	1:C:452:ARG:HH11	1.63	0.63
1:N:452:ARG:HH11	1:N:452:ARG:HG2	1.63	0.63
1:C:477:GLY:HA3	1:C:488:MET:SD	2.38	0.63
1:B:452:ARG:HG2	1:B:452:ARG:HH11	1.63	0.63
1:N:171:LYS:HD3	1:N:407:VAL:HG11	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:PHE:N	1:D:44:PHE:CD1	2.66	0.63
1:M:25:ASP:HA	1:M:28:LYS:HE2	1.80	0.63
1:N:25:ASP:HA	1:N:28:LYS:HE2	1.80	0.63
1:B:25:ASP:HA	1:B:28:LYS:HE2	1.80	0.63
2:T:10:ARG:O	2:U:108:CYS:HA	1.98	0.63
2:O:10:ARG:O	2:P:108:CYS:HA	1.98	0.63
1:N:145:ALA:HA	1:N:159:GLY:O	1.99	0.63
1:F:477:GLY:HA3	1:F:488:MET:SD	2.38	0.63
1:H:452:ARG:HH11	1:H:452:ARG:HG2	1.63	0.63
1:E:44:PHE:N	1:E:44:PHE:CD1	2.66	0.63
1:H:157:THR:O	1:H:161:LEU:HD13	1.98	0.63
1:M:452:ARG:HG2	1:M:452:ARG:HH11	1.63	0.63
1:A:25:ASP:HA	1:A:28:LYS:HE2	1.80	0.63
1:M:138:CYS:N	1:M:410:GLY:CA	2.62	0.63
2:S:10:ARG:O	2:T:108:CYS:HA	1.98	0.63
1:M:171:LYS:HD3	1:M:407:VAL:HG11	1.79	0.63
1:G:44:PHE:N	1:G:44:PHE:CD1	2.66	0.63
1:H:145:ALA:HA	1:H:159:GLY:O	1.99	0.62
1:J:145:ALA:HA	1:J:159:GLY:O	1.99	0.62
1:J:87:ASP:OD2	1:J:151:SER:HA	1.98	0.62
1:C:25:ASP:HA	1:C:28:LYS:HE2	1.80	0.62
1:L:138:CYS:N	1:L:410:GLY:CA	2.62	0.62
1:J:138:CYS:N	1:J:410:GLY:CA	2.62	0.62
1:K:155:ASP:CG	1:K:158:VAL:HG23	2.20	0.62
1:J:155:ASP:CG	1:J:158:VAL:HG23	2.20	0.62
1:I:155:ASP:CG	1:I:158:VAL:HG23	2.20	0.62
1:N:138:CYS:N	1:N:410:GLY:CA	2.62	0.62
2:O:82:PRO:HB3	2:P:110:TYR:CD1	2.35	0.62
2:T:82:PRO:HB3	2:U:110:TYR:CD1	2.35	0.62
1:H:171:LYS:HD3	1:H:407:VAL:HG11	1.80	0.62
1:N:155:ASP:CG	1:N:158:VAL:HG23	2.20	0.62
1:M:145:ALA:HA	1:M:159:GLY:O	1.99	0.62
1:H:477:GLY:HA3	1:H:488:MET:SD	2.38	0.62
1:J:157:THR:O	1:J:161:LEU:HD13	1.98	0.62
2:O:110:TYR:CD1	2:U:82:PRO:HB3	2.35	0.62
1:H:155:ASP:CG	1:H:158:VAL:HG23	2.20	0.62
1:D:25:ASP:HA	1:D:28:LYS:HE2	1.80	0.62
1:N:190:VAL:CG2	1:N:334:ASP:OD2	2.47	0.62
1:E:263:VAL:CG1	1:F:305:ILE:HG22	2.30	0.62
1:N:157:THR:O	1:N:161:LEU:HD13	1.98	0.62
1:K:157:THR:O	1:K:161:LEU:HD13	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:155:ASP:CG	1:L:158:VAL:HG23	2.20	0.62
1:I:138:CYS:N	1:I:410:GLY:CA	2.62	0.62
2:P:82:PRO:HB3	2:Q:110:TYR:CD1	2.35	0.62
1:K:145:ALA:HA	1:K:159:GLY:O	1.99	0.62
1:D:477:GLY:HA3	1:D:488:MET:SD	2.38	0.62
1:J:235:PRO:HG3	1:J:310:GLU:HA	1.82	0.62
1:H:44:PHE:CD1	1:H:44:PHE:N	2.66	0.62
1:H:190:VAL:CG2	1:H:334:ASP:OD2	2.47	0.62
1:F:263:VAL:CG1	1:G:305:ILE:HG22	2.30	0.62
1:L:157:THR:O	1:L:161:LEU:HD13	1.98	0.62
1:I:235:PRO:HG3	1:I:310:GLU:HA	1.82	0.62
1:G:25:ASP:HA	1:G:28:LYS:HE2	1.80	0.62
1:K:138:CYS:N	1:K:410:GLY:CA	2.62	0.62
1:C:263:VAL:CG1	1:D:305:ILE:HG22	2.30	0.62
1:D:263:VAL:CG1	1:E:305:ILE:HG22	2.30	0.62
1:M:155:ASP:CG	1:M:158:VAL:HG23	2.20	0.62
1:E:477:GLY:HA3	1:E:488:MET:SD	2.38	0.62
1:E:25:ASP:HA	1:E:28:LYS:HE2	1.80	0.62
1:I:44:PHE:N	1:I:44:PHE:CD1	2.66	0.62
1:C:146:GLN:HE21	1:C:494:LEU:HD11	0.77	0.62
1:B:263:VAL:CG1	1:C:305:ILE:HG22	2.30	0.62
1:D:203:TYR:HE2	1:E:304:GLU:OE2	1.78	0.61
2:S:82:PRO:HB3	2:T:110:TYR:CD1	2.35	0.61
1:I:157:THR:O	1:I:161:LEU:HD13	1.98	0.61
1:H:235:PRO:HG3	1:H:310:GLU:HA	1.82	0.61
1:L:145:ALA:HA	1:L:159:GLY:O	1.99	0.61
1:H:169:VAL:O	1:H:169:VAL:HG22	2.01	0.61
1:N:235:PRO:HG3	1:N:310:GLU:HA	1.82	0.61
1:A:105:LYS:CG	1:N:109:ALA:O	2.45	0.61
1:I:145:ALA:HA	1:I:159:GLY:O	1.99	0.61
1:K:169:VAL:HG22	1:K:169:VAL:O	2.01	0.61
1:I:169:VAL:O	1:I:169:VAL:HG22	2.01	0.61
1:A:305:ILE:HG22	1:G:263:VAL:CG1	2.30	0.61
1:J:169:VAL:O	1:J:169:VAL:HG22	2.01	0.61
1:F:25:ASP:HA	1:F:28:LYS:HE2	1.80	0.61
1:K:235:PRO:HG3	1:K:310:GLU:HA	1.82	0.61
1:K:190:VAL:CG2	1:K:334:ASP:OD2	2.47	0.61
1:A:325:ILE:HG12	1:A:330:THR:HG23	1.83	0.61
2:R:82:PRO:HB3	2:S:110:TYR:CD1	2.35	0.61
1:A:263:VAL:CG1	1:B:305:ILE:HG22	2.30	0.61
1:F:105:LYS:CG	1:L:109:ALA:O	2.45	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:82:PRO:HB3	2:R:110:TYR:CD1	2.35	0.61
1:J:190:VAL:CG2	1:J:334:ASP:OD2	2.47	0.61
2:P:8:PRO:O	2:Q:110:TYR:HA	2.01	0.61
2:O:8:PRO:O	2:P:110:TYR:HA	2.01	0.61
1:L:169:VAL:HG22	1:L:169:VAL:O	2.01	0.61
1:G:325:ILE:HG12	1:G:330:THR:HG23	1.83	0.61
1:H:138:CYS:N	1:H:410:GLY:CA	2.62	0.61
1:M:190:VAL:CG2	1:M:334:ASP:OD2	2.47	0.61
1:M:235:PRO:HG3	1:M:310:GLU:HA	1.82	0.61
1:M:385:THR:HG23	1:M:388:GLU:HB3	1.83	0.61
2:T:8:PRO:O	2:U:110:TYR:HA	2.01	0.61
1:A:305:ILE:CD1	1:G:267:MET:SD	2.89	0.61
1:B:325:ILE:HG12	1:B:330:THR:HG23	1.83	0.61
1:N:385:THR:HG23	1:N:388:GLU:HB3	1.83	0.60
2:S:8:PRO:O	2:T:110:TYR:HA	2.01	0.60
1:M:44:PHE:CD1	1:M:44:PHE:N	2.66	0.60
1:N:169:VAL:HG22	1:N:169:VAL:O	2.01	0.60
2:O:110:TYR:HA	2:U:8:PRO:O	2.01	0.60
2:Q:8:PRO:O	2:R:110:TYR:HA	2.01	0.60
1:I:190:VAL:CG2	1:I:334:ASP:OD2	2.47	0.60
1:L:385:THR:O	1:L:389:MET:HB2	2.02	0.60
1:K:430:ARG:NH1	1:K:430:ARG:HG2	2.17	0.60
1:F:463:SER:CB	1:M:464:VAL:HG21	2.27	0.60
1:L:385:THR:HG23	1:L:388:GLU:HB3	1.83	0.60
1:K:385:THR:HG23	1:K:388:GLU:HB3	1.83	0.60
1:N:44:PHE:N	1:N:44:PHE:CD1	2.66	0.60
1:L:516:THR:C	1:M:36:ARG:NH1	2.55	0.60
1:E:267:MET:SD	1:F:305:ILE:CD1	2.89	0.60
1:F:267:MET:SD	1:G:305:ILE:CD1	2.89	0.60
1:J:44:PHE:N	1:J:44:PHE:CD1	2.66	0.60
1:I:400:LEU:C	1:I:400:LEU:HD23	2.22	0.60
1:N:400:LEU:HD23	1:N:400:LEU:C	2.22	0.60
1:F:325:ILE:HG12	1:F:330:THR:HG23	1.83	0.60
1:L:235:PRO:HG3	1:L:310:GLU:HA	1.82	0.60
1:K:516:THR:C	1:L:36:ARG:NH1	2.55	0.60
1:N:385:THR:O	1:N:389:MET:HB2	2.02	0.60
2:R:8:PRO:O	2:S:110:TYR:HA	2.01	0.60
1:B:267:MET:SD	1:C:305:ILE:CD1	2.89	0.60
1:N:510:VAL:HG12	1:N:514:MET:CE	2.32	0.60
1:L:147:VAL:CG2	1:L:496:PRO:HB3	2.32	0.60
1:H:385:THR:O	1:H:389:MET:HB2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:430:ARG:HG2	1:M:430:ARG:NH1	2.17	0.60
1:F:146:GLN:HE21	1:F:494:LEU:HD11	0.77	0.60
1:D:146:GLN:HE21	1:D:494:LEU:HD11	0.77	0.60
1:H:385:THR:HG23	1:H:388:GLU:HB3	1.83	0.60
1:M:510:VAL:HG12	1:M:514:MET:CE	2.32	0.60
1:J:400:LEU:HD23	1:J:400:LEU:C	2.22	0.60
1:L:510:VAL:HG12	1:L:514:MET:CE	2.32	0.60
1:K:147:VAL:CG2	1:K:496:PRO:HB3	2.32	0.60
1:M:516:THR:C	1:N:36:ARG:NH1	2.55	0.60
1:K:385:THR:O	1:K:389:MET:HB2	2.02	0.60
1:M:169:VAL:HG22	1:M:169:VAL:O	2.01	0.60
1:H:400:LEU:C	1:H:400:LEU:HD23	2.22	0.60
1:M:385:THR:O	1:M:389:MET:HB2	2.02	0.59
1:J:430:ARG:NH1	1:J:430:ARG:HG2	2.17	0.59
1:G:510:VAL:HG12	1:G:514:MET:CE	2.32	0.59
1:J:385:THR:HG23	1:J:388:GLU:HB3	1.83	0.59
1:F:44:PHE:N	1:F:44:PHE:CD1	2.66	0.59
1:E:510:VAL:HG12	1:E:514:MET:CE	2.32	0.59
1:N:147:VAL:CG2	1:N:496:PRO:HB3	2.32	0.59
1:J:147:VAL:CG2	1:J:496:PRO:HB3	2.32	0.59
1:J:385:THR:O	1:J:389:MET:HB2	2.02	0.59
1:K:400:LEU:C	1:K:400:LEU:HD23	2.22	0.59
1:C:325:ILE:HG12	1:C:330:THR:HG23	1.83	0.59
1:I:147:VAL:CG2	1:I:496:PRO:HB3	2.32	0.59
1:F:406:ALA:CB	1:F:496:PRO:HB3	2.27	0.59
1:F:510:VAL:HG12	1:F:514:MET:CE	2.32	0.59
1:H:147:VAL:CG2	1:H:496:PRO:HB3	2.32	0.59
1:L:430:ARG:NH1	1:L:430:ARG:HG2	2.17	0.59
1:A:510:VAL:HG12	1:A:514:MET:CE	2.32	0.59
1:K:510:VAL:HG12	1:K:514:MET:CE	2.32	0.59
1:M:147:VAL:CG2	1:M:496:PRO:HB3	2.32	0.59
1:J:516:THR:C	1:K:36:ARG:NH1	2.55	0.59
1:I:385:THR:HG23	1:I:388:GLU:HB3	1.83	0.59
1:L:400:LEU:HD23	1:L:400:LEU:C	2.22	0.59
1:D:510:VAL:HG12	1:D:514:MET:CE	2.32	0.59
1:M:400:LEU:C	1:M:400:LEU:HD23	2.22	0.59
1:E:325:ILE:HG12	1:E:330:THR:HG23	1.83	0.59
1:J:385:THR:HG23	1:J:388:GLU:H	1.68	0.59
1:C:510:VAL:HG12	1:C:514:MET:CE	2.32	0.59
1:G:146:GLN:HE21	1:G:494:LEU:HD11	0.77	0.59
1:A:430:ARG:NH1	1:A:430:ARG:HG2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:510:VAL:HG12	1:I:514:MET:CE	2.32	0.59
1:D:325:ILE:HG12	1:D:330:THR:HG23	1.83	0.59
1:F:353:ILE:HG12	1:F:365:LEU:HB3	1.85	0.58
1:I:385:THR:O	1:I:389:MET:HB2	2.02	0.58
1:B:510:VAL:HG12	1:B:514:MET:CE	2.32	0.58
1:J:510:VAL:HG12	1:J:514:MET:CE	2.32	0.58
1:E:353:ILE:HG12	1:E:365:LEU:HB3	1.85	0.58
1:H:36:ARG:NH1	1:N:516:THR:C	2.55	0.58
1:B:353:ILE:HG12	1:B:365:LEU:HB3	1.85	0.58
1:M:385:THR:HG23	1:M:388:GLU:H	1.68	0.58
2:T:11:ALA:HA	2:U:107:PRO:O	2.04	0.58
2:R:81:HIS:HD2	2:R:83:PHE:H	1.52	0.58
1:G:353:ILE:HG12	1:G:365:LEU:HB3	1.85	0.58
2:P:80:PRO:HG2	2:Q:70:SER:HG	1.68	0.58
1:D:224:ASP:HB3	1:D:302:SER:HA	1.86	0.58
2:Q:11:ALA:HA	2:R:107:PRO:O	2.04	0.58
1:D:353:ILE:HG12	1:D:365:LEU:HB3	1.85	0.58
1:C:353:ILE:HG12	1:C:365:LEU:HB3	1.85	0.58
1:B:105:LYS:CG	1:H:109:ALA:O	2.45	0.58
1:L:385:THR:HG23	1:L:388:GLU:H	1.68	0.58
1:H:385:THR:HG23	1:H:388:GLU:H	1.68	0.58
1:H:510:VAL:HG12	1:H:514:MET:CE	2.32	0.58
1:A:353:ILE:HG12	1:A:365:LEU:HB3	1.85	0.58
1:E:105:LYS:CG	1:K:109:ALA:O	2.45	0.58
2:R:11:ALA:HA	2:S:107:PRO:O	2.04	0.58
1:D:409:GLU:CB	1:D:498:LYS:HB2	2.34	0.58
2:P:11:ALA:HA	2:Q:107:PRO:O	2.04	0.58
1:A:409:GLU:CB	1:A:498:LYS:HB2	2.34	0.58
2:O:110:TYR:HD1	2:U:82:PRO:HB3	1.69	0.58
1:C:224:ASP:HB3	1:C:302:SER:HA	1.86	0.58
2:O:11:ALA:HA	2:P:107:PRO:O	2.04	0.58
1:F:409:GLU:CB	1:F:498:LYS:HB2	2.34	0.58
1:L:190:VAL:CG2	1:L:334:ASP:OD2	2.47	0.58
1:B:406:ALA:CB	1:B:496:PRO:HB3	2.27	0.58
2:P:82:PRO:HB3	2:Q:110:TYR:HD1	1.69	0.58
1:C:430:ARG:NH1	1:C:430:ARG:HG2	2.17	0.58
1:K:385:THR:HG23	1:K:388:GLU:H	1.68	0.58
1:D:105:LYS:CG	1:J:109:ALA:O	2.45	0.58
1:I:279:PRO:O	1:I:285:ARG:HB3	2.04	0.58
1:L:44:PHE:N	1:L:44:PHE:CD1	2.66	0.58
1:D:86:GLY:HA3	1:D:401:HIS:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:279:PRO:O	1:M:285:ARG:HB3	2.04	0.58
1:N:279:PRO:O	1:N:285:ARG:HB3	2.04	0.58
1:E:86:GLY:HA3	1:E:401:HIS:HB3	1.86	0.58
1:F:86:GLY:HA3	1:F:401:HIS:HB3	1.86	0.58
1:G:86:GLY:HA3	1:G:401:HIS:HB3	1.86	0.58
2:O:82:PRO:HB3	2:P:110:TYR:HD1	1.69	0.57
1:F:430:ARG:NH1	1:F:430:ARG:HG2	2.17	0.57
1:H:279:PRO:O	1:H:285:ARG:HB3	2.04	0.57
2:S:11:ALA:HA	2:T:107:PRO:O	2.04	0.57
2:Q:82:PRO:HB3	2:R:110:TYR:HD1	1.69	0.57
1:E:224:ASP:HB3	1:E:302:SER:HA	1.86	0.57
1:N:392:LYS:O	1:N:396:VAL:HG23	2.04	0.57
2:T:81:HIS:HD2	2:T:83:PHE:H	1.52	0.57
1:K:44:PHE:CD1	1:K:44:PHE:N	2.66	0.57
2:P:81:HIS:HD2	2:P:83:PHE:H	1.52	0.57
1:L:392:LYS:O	1:L:396:VAL:HG23	2.04	0.57
1:E:146:GLN:HE21	1:E:494:LEU:HD11	0.77	0.57
1:D:147:VAL:HB	1:D:496:PRO:HG3	1.87	0.57
1:H:161:LEU:HD12	1:H:161:LEU:H	1.70	0.57
1:A:86:GLY:HA3	1:A:401:HIS:HB3	1.86	0.57
1:B:409:GLU:CB	1:B:498:LYS:HB2	2.33	0.57
2:S:81:HIS:HD2	2:S:83:PHE:H	1.52	0.57
1:A:146:GLN:HE21	1:A:494:LEU:HD11	0.77	0.57
1:E:147:VAL:HB	1:E:496:PRO:HG3	1.87	0.57
1:N:385:THR:HG23	1:N:388:GLU:H	1.68	0.57
1:I:385:THR:HG23	1:I:388:GLU:H	1.68	0.57
1:D:16:MET:HG3	1:D:520:MET:HE1	1.87	0.57
2:O:48:LEU:CD2	2:U:85:ALA:HA	2.34	0.57
2:O:85:ALA:HA	2:P:48:LEU:CD2	2.34	0.57
1:J:279:PRO:O	1:J:285:ARG:HB3	2.04	0.57
1:H:516:THR:C	1:I:36:ARG:NH1	2.55	0.57
1:F:147:VAL:HB	1:F:496:PRO:HG3	1.87	0.57
2:T:82:PRO:HB3	2:U:110:TYR:HD1	1.69	0.57
1:L:161:LEU:H	1:L:161:LEU:HD12	1.70	0.57
1:F:16:MET:HG3	1:F:520:MET:HE1	1.87	0.57
1:M:16:MET:HG3	1:M:520:MET:HE1	1.87	0.57
2:S:85:ALA:HA	2:T:48:LEU:CD2	2.34	0.57
2:R:82:PRO:HB3	2:S:110:TYR:HD1	1.69	0.57
1:C:409:GLU:CB	1:C:498:LYS:HB2	2.34	0.57
2:U:81:HIS:HD2	2:U:83:PHE:H	1.51	0.57
1:L:279:PRO:O	1:L:285:ARG:HB3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:409:GLU:CB	1:E:498:LYS:HB2	2.34	0.57
2:R:85:ALA:HA	2:S:48:LEU:CD2	2.34	0.57
2:O:107:PRO:O	2:U:11:ALA:HA	2.04	0.57
1:I:516:THR:C	1:J:36:ARG:NH1	2.55	0.57
1:G:147:VAL:HB	1:G:496:PRO:HG3	1.87	0.57
2:S:82:PRO:HB3	2:T:110:TYR:HD1	1.69	0.57
1:B:224:ASP:HB3	1:B:302:SER:HA	1.86	0.57
1:I:16:MET:HG3	1:I:520:MET:HE1	1.87	0.57
1:G:409:GLU:CB	1:G:498:LYS:HB2	2.33	0.57
1:L:138:CYS:SG	1:L:144:ILE:HD13	2.45	0.57
1:K:138:CYS:SG	1:K:144:ILE:HD13	2.45	0.57
2:O:70:SER:HG	2:U:80:PRO:HG2	1.70	0.57
1:D:263:VAL:HG11	1:E:305:ILE:HG22	1.87	0.57
1:G:16:MET:HG3	1:G:520:MET:HE1	1.87	0.57
2:P:85:ALA:HA	2:Q:48:LEU:CD2	2.34	0.57
1:C:147:VAL:HB	1:C:496:PRO:HG3	1.87	0.57
1:I:171:LYS:HD3	1:I:407:VAL:CG1	2.35	0.57
1:H:16:MET:HG3	1:H:520:MET:HE1	1.87	0.57
1:N:16:MET:HG3	1:N:520:MET:HE3	1.87	0.57
1:C:86:GLY:HA3	1:C:401:HIS:HB3	1.86	0.57
1:C:263:VAL:HG11	1:D:305:ILE:HG22	1.87	0.57
1:E:263:VAL:HG11	1:F:305:ILE:HG22	1.87	0.57
1:B:16:MET:HG3	1:B:520:MET:HE1	1.87	0.57
1:I:392:LYS:O	1:I:396:VAL:HG23	2.05	0.57
1:K:392:LYS:O	1:K:396:VAL:HG23	2.04	0.57
2:Q:81:HIS:HD2	2:Q:83:PHE:H	1.52	0.57
1:M:392:LYS:O	1:M:396:VAL:HG23	2.04	0.57
1:M:138:CYS:SG	1:M:144:ILE:HD13	2.45	0.56
1:J:138:CYS:SG	1:J:144:ILE:HD13	2.45	0.56
1:H:171:LYS:HD3	1:H:407:VAL:CG1	2.35	0.56
1:L:16:MET:HG3	1:L:520:MET:HE1	1.87	0.56
1:J:16:MET:HG3	1:J:520:MET:HE1	1.87	0.56
1:K:16:MET:HG3	1:K:520:MET:HE1	1.87	0.56
2:T:85:ALA:HA	2:U:48:LEU:CD2	2.34	0.56
1:K:279:PRO:O	1:K:285:ARG:HB3	2.04	0.56
2:Q:85:ALA:HA	2:R:48:LEU:CD2	2.34	0.56
1:D:406:ALA:CB	1:D:496:PRO:HB3	2.27	0.56
1:J:171:LYS:HD3	1:J:407:VAL:CG1	2.35	0.56
1:K:171:LYS:HD3	1:K:407:VAL:CG1	2.35	0.56
1:A:16:MET:HG3	1:A:520:MET:HE1	1.87	0.56
1:N:138:CYS:SG	1:N:144:ILE:HD13	2.45	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:138:CYS:SG	1:I:144:ILE:HD13	2.45	0.56
1:A:147:VAL:HB	1:A:496:PRO:HG3	1.87	0.56
1:C:105:LYS:CG	1:I:109:ALA:O	2.45	0.56
1:A:267:MET:SD	1:B:305:ILE:CD1	2.89	0.56
1:L:171:LYS:HD3	1:L:407:VAL:CG1	2.35	0.56
1:J:161:LEU:H	1:J:161:LEU:HD12	1.69	0.56
1:E:16:MET:HG3	1:E:520:MET:HE1	1.87	0.56
1:C:16:MET:HG3	1:C:520:MET:HE3	1.87	0.56
1:J:392:LYS:O	1:J:396:VAL:HG23	2.05	0.56
1:H:261:THR:O	1:H:265:ASN:HB2	2.05	0.56
1:I:261:THR:O	1:I:265:ASN:HB2	2.05	0.56
1:J:261:THR:O	1:J:265:ASN:HB2	2.05	0.56
1:G:204:PHE:HE1	1:G:274:ALA:HB2	1.71	0.56
1:B:147:VAL:HB	1:B:496:PRO:HG3	1.87	0.56
1:N:171:LYS:HD3	1:N:407:VAL:CG1	2.35	0.56
1:H:392:LYS:O	1:H:396:VAL:HG23	2.05	0.56
1:B:204:PHE:HE1	1:B:274:ALA:HB2	1.71	0.56
1:F:224:ASP:HB3	1:F:302:SER:HA	1.86	0.56
1:A:263:VAL:HG11	1:B:305:ILE:HG22	1.87	0.56
1:N:16:MET:O	1:N:20:VAL:HG23	2.06	0.56
2:O:81:HIS:HD2	2:O:83:PHE:H	1.52	0.56
1:M:261:THR:O	1:M:265:ASN:HB2	2.05	0.56
1:N:261:THR:O	1:N:265:ASN:HB2	2.05	0.56
1:G:224:ASP:HB3	1:G:302:SER:HA	1.86	0.56
1:J:510:VAL:HG12	1:J:514:MET:HE1	1.88	0.56
1:B:86:GLY:HA3	1:B:401:HIS:HB3	1.86	0.56
1:L:261:THR:O	1:L:265:ASN:HB2	2.05	0.56
1:G:463:SER:CB	1:N:464:VAL:HG21	2.27	0.56
1:F:263:VAL:HG11	1:G:305:ILE:HG22	1.87	0.56
1:M:161:LEU:HD12	1:M:161:LEU:H	1.70	0.56
1:I:161:LEU:HD12	1:I:161:LEU:H	1.69	0.56
1:F:16:MET:O	1:F:20:VAL:HG23	2.06	0.56
1:A:16:MET:O	1:A:20:VAL:HG23	2.06	0.56
1:J:16:MET:O	1:J:20:VAL:HG23	2.06	0.56
1:D:16:MET:O	1:D:20:VAL:HG23	2.06	0.56
1:K:16:MET:O	1:K:20:VAL:HG23	2.06	0.56
1:K:161:LEU:H	1:K:161:LEU:HD12	1.70	0.56
1:B:136:VAL:HA	1:B:137:PRO:N	2.18	0.56
1:E:204:PHE:HE1	1:E:274:ALA:HB2	1.71	0.56
1:A:224:ASP:HB3	1:A:302:SER:HA	1.86	0.56
1:C:16:MET:O	1:C:20:VAL:HG23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:234:LEU:N	1:H:235:PRO:HD2	2.21	0.56
1:H:138:CYS:SG	1:H:144:ILE:HD13	2.45	0.56
1:N:161:LEU:HD12	1:N:161:LEU:H	1.70	0.56
1:G:16:MET:O	1:G:20:VAL:HG23	2.06	0.56
1:B:16:MET:O	1:B:20:VAL:HG23	2.06	0.56
1:C:172:GLU:O	1:C:369:VAL:CG2	2.54	0.55
1:B:172:GLU:O	1:B:369:VAL:CG2	2.54	0.55
1:C:204:PHE:HE1	1:C:274:ALA:HB2	1.71	0.55
1:B:263:VAL:HG11	1:C:305:ILE:HG22	1.87	0.55
1:K:234:LEU:N	1:K:235:PRO:HD2	2.21	0.55
1:N:147:VAL:CG2	1:N:496:PRO:CG	2.75	0.55
1:A:204:PHE:HE1	1:A:274:ALA:HB2	1.71	0.55
1:G:406:ALA:CB	1:G:496:PRO:HB3	2.27	0.55
1:I:16:MET:O	1:I:20:VAL:HG23	2.06	0.55
1:F:204:PHE:HE1	1:F:274:ALA:HB2	1.71	0.55
2:Q:82:PRO:HA	2:R:110:TYR:CD1	2.42	0.55
1:M:171:LYS:HD3	1:M:407:VAL:CG1	2.35	0.55
1:L:16:MET:O	1:L:20:VAL:HG23	2.06	0.55
1:J:419:LEU:HG	1:J:447:MET:HG2	1.89	0.55
1:I:234:LEU:N	1:I:235:PRO:HD2	2.21	0.55
1:A:510:VAL:HG12	1:A:514:MET:HE1	1.89	0.55
1:G:33:PRO:HA	1:G:153:ASN:HD21	1.72	0.55
1:C:33:PRO:HA	1:C:153:ASN:HD21	1.72	0.55
1:E:136:VAL:CA	1:E:137:PRO:CD	2.83	0.55
1:A:77:VAL:HG23	1:A:92:ALA:HB1	1.89	0.55
1:L:419:LEU:HG	1:L:447:MET:HG2	1.89	0.55
1:M:419:LEU:HG	1:M:447:MET:HG2	1.89	0.55
1:K:147:VAL:HG21	1:K:496:PRO:HB3	1.89	0.55
1:D:77:VAL:HG23	1:D:92:ALA:HB1	1.89	0.55
1:M:234:LEU:N	1:M:235:PRO:HD2	2.21	0.55
1:E:510:VAL:HG12	1:E:514:MET:HE1	1.89	0.55
1:K:419:LEU:HG	1:K:447:MET:HG2	1.89	0.55
1:I:419:LEU:HG	1:I:447:MET:HG2	1.89	0.55
2:R:82:PRO:HA	2:S:110:TYR:CD1	2.42	0.55
1:C:77:VAL:HG23	1:C:92:ALA:HB1	1.89	0.55
1:E:419:LEU:HG	1:E:447:MET:HG2	1.89	0.55
1:A:146:GLN:CB	1:A:494:LEU:CD1	2.85	0.55
1:H:147:VAL:CG2	1:H:496:PRO:CG	2.75	0.55
1:A:305:ILE:HG22	1:G:263:VAL:HG11	1.87	0.55
1:E:16:MET:O	1:E:20:VAL:HG23	2.06	0.55
1:B:77:VAL:HG23	1:B:92:ALA:HB1	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:16:MET:O	1:M:20:VAL:HG23	2.06	0.55
1:G:510:VAL:HG12	1:G:514:MET:HE1	1.88	0.55
1:G:146:GLN:CB	1:G:494:LEU:CD1	2.85	0.55
1:L:147:VAL:HG21	1:L:496:PRO:HB3	1.89	0.55
1:E:430:ARG:NH1	1:E:430:ARG:HG2	2.17	0.55
1:L:175:ILE:HD13	1:L:404:ARG:NH2	2.22	0.55
1:N:175:ILE:HD13	1:N:404:ARG:NH2	2.22	0.55
1:G:77:VAL:HG23	1:G:92:ALA:HB1	1.89	0.55
1:M:77:VAL:HG23	1:M:92:ALA:HB1	1.89	0.55
1:C:510:VAL:HG12	1:C:514:MET:HE1	1.89	0.55
1:H:510:VAL:HG12	1:H:514:MET:HE1	1.89	0.55
1:F:33:PRO:HA	1:F:153:ASN:HD21	1.72	0.55
1:D:463:SER:HG	1:K:464:VAL:HG23	1.68	0.55
1:E:146:GLN:CB	1:E:494:LEU:CD1	2.85	0.55
1:D:146:GLN:CB	1:D:494:LEU:CD1	2.85	0.55
1:J:147:VAL:CG2	1:J:496:PRO:HG3	2.14	0.55
1:B:430:ARG:HG2	1:B:430:ARG:NH1	2.17	0.55
1:H:175:ILE:HD13	1:H:404:ARG:NH2	2.22	0.55
1:H:16:MET:O	1:H:20:VAL:HG23	2.06	0.55
1:H:77:VAL:HG23	1:H:92:ALA:HB1	1.89	0.55
1:N:77:VAL:HG23	1:N:92:ALA:HB1	1.89	0.55
1:L:234:LEU:N	1:L:235:PRO:HD2	2.21	0.55
1:B:510:VAL:HG12	1:B:514:MET:HE1	1.89	0.55
1:K:261:THR:O	1:K:265:ASN:HB2	2.05	0.55
1:D:33:PRO:HA	1:D:153:ASN:HD21	1.72	0.55
1:B:146:GLN:CB	1:B:494:LEU:CD1	2.85	0.54
1:G:172:GLU:O	1:G:369:VAL:CG2	2.54	0.54
1:A:172:GLU:O	1:A:369:VAL:CG2	2.54	0.54
1:D:204:PHE:HE1	1:D:274:ALA:HB2	1.71	0.54
2:P:82:PRO:HA	2:Q:110:TYR:CD1	2.42	0.54
1:M:175:ILE:HD13	1:M:404:ARG:NH2	2.22	0.54
1:E:77:VAL:HG23	1:E:92:ALA:HB1	1.89	0.54
1:J:234:LEU:N	1:J:235:PRO:HD2	2.21	0.54
1:L:510:VAL:HG12	1:L:514:MET:HE1	1.90	0.54
1:F:510:VAL:HG12	1:F:514:MET:HE1	1.89	0.54
1:K:510:VAL:HG12	1:K:514:MET:HE1	1.89	0.54
1:A:419:LEU:HG	1:A:447:MET:HG2	1.89	0.54
1:B:33:PRO:HA	1:B:153:ASN:HD21	1.72	0.54
1:K:184:GLN:HA	1:K:184:GLN:OE1	2.07	0.54
1:D:419:LEU:HG	1:D:447:MET:HG2	1.89	0.54
1:M:147:VAL:HG21	1:M:496:PRO:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:172:GLU:O	1:D:369:VAL:CG2	2.54	0.54
2:O:82:PRO:HA	2:P:110:TYR:CD1	2.42	0.54
1:K:175:ILE:HD13	1:K:404:ARG:NH2	2.22	0.54
1:N:234:LEU:N	1:N:235:PRO:HD2	2.21	0.54
1:F:419:LEU:HG	1:F:447:MET:HG2	1.89	0.54
1:J:184:GLN:HA	1:J:184:GLN:OE1	2.07	0.54
1:I:175:ILE:HD13	1:I:404:ARG:NH2	2.22	0.54
1:D:510:VAL:HG12	1:D:514:MET:HE1	1.89	0.54
1:K:441:LYS:HB3	1:K:445:ARG:HH21	1.73	0.54
1:L:441:LYS:HB3	1:L:445:ARG:HH21	1.73	0.54
1:A:33:PRO:HA	1:A:153:ASN:HD21	1.72	0.54
1:N:419:LEU:HG	1:N:447:MET:HG2	1.89	0.54
1:B:146:GLN:HE21	1:B:494:LEU:HD11	0.77	0.54
1:B:146:GLN:CB	1:B:494:LEU:HG	2.34	0.54
1:J:147:VAL:HG21	1:J:496:PRO:HB3	1.89	0.54
2:T:82:PRO:HA	2:U:110:TYR:CD1	2.42	0.54
1:I:510:VAL:HG12	1:I:514:MET:HE1	1.89	0.54
1:L:433:ASN:OD1	1:L:436:GLN:HG3	2.08	0.54
1:I:433:ASN:OD1	1:I:436:GLN:HG3	2.08	0.54
1:C:441:LYS:HB3	1:C:445:ARG:HH21	1.73	0.54
1:E:33:PRO:HA	1:E:153:ASN:HD21	1.72	0.54
1:F:146:GLN:CB	1:F:494:LEU:CD1	2.85	0.54
1:H:147:VAL:HG21	1:H:496:PRO:HB3	1.89	0.54
1:L:77:VAL:HG23	1:L:92:ALA:HB1	1.89	0.54
1:F:433:ASN:OD1	1:F:436:GLN:HG3	2.08	0.54
1:G:433:ASN:OD1	1:G:436:GLN:HG3	2.08	0.54
1:K:433:ASN:OD1	1:K:436:GLN:HG3	2.08	0.54
1:N:441:LYS:HB3	1:N:445:ARG:HH21	1.73	0.54
1:G:111:MET:HG3	1:G:435:ASP:OD1	2.08	0.54
1:F:138:CYS:SG	1:F:411:VAL:CG1	2.96	0.54
2:P:80:PRO:CD	2:Q:70:SER:OG	2.56	0.54
2:O:80:PRO:CD	2:P:70:SER:OG	2.56	0.54
2:T:77:ARG:HD3	2:U:72:PRO:HG3	1.90	0.54
1:J:111:MET:HG3	1:J:435:ASP:OD1	2.08	0.54
1:B:433:ASN:OD1	1:B:436:GLN:HG3	2.08	0.54
1:N:184:GLN:HA	1:N:184:GLN:OE1	2.07	0.54
2:T:80:PRO:CD	2:U:70:SER:OG	2.56	0.54
1:L:149:THR:HG22	1:L:156:GLU:HA	1.90	0.54
1:G:430:ARG:HG2	1:G:430:ARG:NH1	2.17	0.54
2:S:77:ARG:HD3	2:T:72:PRO:HG3	1.90	0.54
1:F:77:VAL:HG23	1:F:92:ALA:HB1	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:ASN:OD1	1:A:436:GLN:HG3	2.08	0.54
1:J:441:LYS:HB3	1:J:445:ARG:HH21	1.73	0.54
1:L:184:GLN:OE1	1:L:184:GLN:HA	2.07	0.54
1:K:18:ARG:CG	1:K:18:ARG:NH1	2.70	0.54
2:S:80:PRO:CD	2:T:70:SER:OG	2.56	0.54
1:M:510:VAL:HG12	1:M:514:MET:HE1	1.89	0.54
1:M:433:ASN:OD1	1:M:436:GLN:HG3	2.08	0.54
1:G:419:LEU:HG	1:G:447:MET:HG2	1.89	0.54
1:H:419:LEU:HG	1:H:447:MET:HG2	1.89	0.54
1:C:146:GLN:CB	1:C:494:LEU:CD1	2.85	0.54
1:C:267:MET:SD	1:D:305:ILE:CD1	2.89	0.54
1:L:149:THR:CG2	1:L:159:GLY:HA3	2.37	0.54
1:K:42:LYS:HG2	1:K:44:PHE:CE2	2.43	0.54
1:E:441:LYS:HB3	1:E:445:ARG:HH21	1.73	0.54
1:I:111:MET:HG3	1:I:435:ASP:OD1	2.08	0.54
1:N:433:ASN:OD1	1:N:436:GLN:HG3	2.08	0.54
1:H:441:LYS:HB3	1:H:445:ARG:HH21	1.73	0.54
1:N:111:MET:HG3	1:N:435:ASP:OD1	2.08	0.54
1:J:433:ASN:OD1	1:J:436:GLN:HG3	2.08	0.54
1:H:111:MET:HG3	1:H:435:ASP:OD1	2.08	0.54
1:I:147:VAL:CG2	1:I:496:PRO:HG3	2.14	0.54
1:C:18:ARG:NH1	1:C:18:ARG:CG	2.70	0.54
1:F:172:GLU:O	1:F:369:VAL:CG2	2.54	0.54
1:D:138:CYS:SG	1:D:411:VAL:CG1	2.96	0.54
2:Q:80:PRO:CD	2:R:70:SER:OG	2.56	0.54
1:J:175:ILE:HD13	1:J:404:ARG:NH2	2.22	0.54
1:I:77:VAL:HG23	1:I:92:ALA:HB1	1.89	0.54
1:K:77:VAL:HG23	1:K:92:ALA:HB1	1.89	0.54
1:J:42:LYS:HG2	1:J:44:PHE:CE2	2.43	0.54
1:H:433:ASN:OD1	1:H:436:GLN:HG3	2.08	0.54
1:B:111:MET:HG3	1:B:435:ASP:OD1	2.08	0.54
1:B:419:LEU:HG	1:B:447:MET:HG2	1.89	0.54
1:C:433:ASN:OD1	1:C:436:GLN:HG3	2.08	0.54
1:J:152:ALA:O	1:J:153:ASN:HB3	2.08	0.54
1:I:184:GLN:OE1	1:I:184:GLN:HA	2.07	0.54
1:B:138:CYS:SG	1:B:411:VAL:CG1	2.96	0.53
1:M:145:ALA:O	1:M:149:THR:HG23	2.08	0.53
1:L:145:ALA:O	1:L:149:THR:HG23	2.08	0.53
1:D:409:GLU:HB3	1:D:498:LYS:HB2	1.90	0.53
1:A:441:LYS:HB3	1:A:445:ARG:HH21	1.73	0.53
1:D:441:LYS:HB3	1:D:445:ARG:HH21	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:111:MET:HG3	1:F:435:ASP:OD1	2.08	0.53
1:K:147:VAL:CG2	1:K:496:PRO:CG	2.75	0.53
1:E:172:GLU:O	1:E:369:VAL:CG2	2.54	0.53
1:M:149:THR:HG22	1:M:156:GLU:HA	1.89	0.53
1:J:77:VAL:HG23	1:J:92:ALA:HB1	1.89	0.53
1:G:42:LYS:HG2	1:G:44:PHE:CE2	2.43	0.53
1:F:42:LYS:HG2	1:F:44:PHE:CE2	2.43	0.53
1:C:111:MET:HG3	1:C:435:ASP:OD1	2.08	0.53
1:F:441:LYS:HB3	1:F:445:ARG:HH21	1.73	0.53
1:K:111:MET:HG3	1:K:435:ASP:OD1	2.08	0.53
1:C:419:LEU:HG	1:C:447:MET:HG2	1.89	0.53
1:J:402:ALA:O	1:J:406:ALA:N	2.32	0.53
1:N:147:VAL:HG21	1:N:496:PRO:HB3	1.89	0.53
2:O:70:SER:OG	2:U:80:PRO:CD	2.56	0.53
1:K:145:ALA:O	1:K:149:THR:HG23	2.08	0.53
1:J:192:GLY:C	1:J:376:VAL:CG2	2.77	0.53
1:M:192:GLY:C	1:M:376:VAL:CG2	2.77	0.53
1:B:42:LYS:HG2	1:B:44:PHE:CE2	2.43	0.53
1:J:386:GLU:HG2	1:J:390:LYS:HE2	1.90	0.53
1:H:152:ALA:O	1:H:153:ASN:HB3	2.08	0.53
1:I:152:ALA:O	1:I:153:ASN:HB3	2.08	0.53
1:I:441:LYS:HB3	1:I:445:ARG:HH21	1.73	0.53
1:E:433:ASN:OD1	1:E:436:GLN:HG3	2.08	0.53
1:M:111:MET:HG3	1:M:435:ASP:OD1	2.08	0.53
1:N:145:ALA:O	1:N:149:THR:HG23	2.08	0.53
1:I:145:ALA:O	1:I:149:THR:HG23	2.08	0.53
1:N:192:GLY:C	1:N:376:VAL:CG2	2.77	0.53
1:N:510:VAL:HG12	1:N:514:MET:HE1	1.89	0.53
1:C:409:GLU:HB3	1:C:498:LYS:HB2	1.90	0.53
1:I:386:GLU:HG2	1:I:390:LYS:HE2	1.90	0.53
1:K:147:VAL:HG23	1:K:496:PRO:CB	2.38	0.53
2:R:77:ARG:HD3	2:S:72:PRO:HG3	1.90	0.53
2:O:72:PRO:HG3	2:U:77:ARG:HD3	1.90	0.53
1:H:42:LYS:HG2	1:H:44:PHE:CE2	2.43	0.53
1:M:42:LYS:HG2	1:M:44:PHE:CE2	2.43	0.53
1:K:386:GLU:HG2	1:K:390:LYS:HE2	1.90	0.53
1:M:441:LYS:HB3	1:M:445:ARG:HH21	1.73	0.53
1:E:111:MET:HG3	1:E:435:ASP:OD1	2.08	0.53
1:M:395:ARG:O	1:M:398:ASP:HB2	2.09	0.53
1:H:395:ARG:O	1:H:398:ASP:HB2	2.09	0.53
1:M:147:VAL:HG23	1:M:496:PRO:CB	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:147:VAL:HG21	1:I:496:PRO:HB3	1.89	0.53
1:G:136:VAL:CA	1:G:137:PRO:CD	2.83	0.53
1:C:138:CYS:SG	1:C:411:VAL:CG1	2.96	0.53
2:S:82:PRO:HA	2:T:110:TYR:CD1	2.42	0.53
1:D:42:LYS:HG2	1:D:44:PHE:CE2	2.43	0.53
1:E:42:LYS:HG2	1:E:44:PHE:CE2	2.43	0.53
1:N:386:GLU:HG2	1:N:390:LYS:HE2	1.90	0.53
1:L:152:ALA:O	1:L:153:ASN:HB3	2.08	0.53
1:H:386:GLU:HG2	1:H:390:LYS:HE2	1.90	0.53
1:A:111:MET:HG3	1:A:435:ASP:OD1	2.08	0.53
1:M:184:GLN:OE1	1:M:184:GLN:HA	2.07	0.53
1:N:395:ARG:O	1:N:398:ASP:HB2	2.09	0.53
2:O:110:TYR:CD1	2:U:82:PRO:HA	2.42	0.53
2:S:17:ILE:CD1	2:T:108:CYS:HB3	2.34	0.53
1:D:267:MET:SD	1:E:305:ILE:CD1	2.89	0.53
1:H:145:ALA:O	1:H:149:THR:HG23	2.08	0.53
1:K:149:THR:HG22	1:K:156:GLU:HA	1.90	0.53
1:I:192:GLY:C	1:I:376:VAL:CG2	2.77	0.53
1:M:152:ALA:O	1:M:153:ASN:HB3	2.08	0.53
1:B:441:LYS:HB3	1:B:445:ARG:HH21	1.73	0.53
1:M:386:GLU:HG2	1:M:390:LYS:HE2	1.90	0.53
1:E:138:CYS:SG	1:E:411:VAL:CG1	2.96	0.53
1:C:42:LYS:HG2	1:C:44:PHE:CE2	2.43	0.53
1:I:42:LYS:HG2	1:I:44:PHE:CE2	2.43	0.53
1:E:409:GLU:HB3	1:E:498:LYS:HB2	1.90	0.53
1:L:267:MET:O	1:L:268:ARG:HB2	2.09	0.53
1:L:386:GLU:HG2	1:L:390:LYS:HE2	1.90	0.53
1:N:147:VAL:HG23	1:N:496:PRO:CB	2.39	0.53
1:I:147:VAL:HG23	1:I:496:PRO:CB	2.39	0.53
2:R:80:PRO:CD	2:S:70:SER:OG	2.56	0.53
1:K:192:GLY:C	1:K:376:VAL:CG2	2.77	0.53
1:D:433:ASN:OD1	1:D:436:GLN:HG3	2.08	0.53
1:D:111:MET:HG3	1:D:435:ASP:OD1	2.08	0.53
1:H:184:GLN:HA	1:H:184:GLN:OE1	2.07	0.53
1:I:395:ARG:O	1:I:398:ASP:HB2	2.09	0.53
1:J:395:ARG:O	1:J:398:ASP:HB2	2.09	0.53
1:K:147:VAL:CG2	1:K:496:PRO:HG3	2.14	0.53
1:I:147:VAL:HA	1:I:150:ILE:HD12	1.91	0.53
1:M:149:THR:CG2	1:M:159:GLY:HA3	2.36	0.53
1:B:409:GLU:HB3	1:B:498:LYS:HB2	1.90	0.53
1:G:409:GLU:HB3	1:G:498:LYS:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:152:ALA:O	1:N:153:ASN:HB3	2.08	0.53
1:C:146:GLN:CB	1:C:494:LEU:HG	2.34	0.52
1:N:147:VAL:HA	1:N:150:ILE:HD12	1.91	0.52
1:C:136:VAL:CA	1:C:137:PRO:CD	2.83	0.52
1:H:192:GLY:C	1:H:376:VAL:CG2	2.77	0.52
1:N:430:ARG:NH1	1:N:430:ARG:HG2	2.17	0.52
1:L:111:MET:HG3	1:L:435:ASP:OD1	2.08	0.52
2:S:5:GLN:HG3	2:S:6:GLN:NE2	2.24	0.52
2:T:5:GLN:HG3	2:T:6:GLN:NE2	2.24	0.52
1:K:395:ARG:O	1:K:398:ASP:HB2	2.09	0.52
1:L:18:ARG:CG	1:L:18:ARG:NH1	2.70	0.52
1:G:138:CYS:SG	1:G:411:VAL:CG1	2.96	0.52
1:N:192:GLY:CA	1:N:376:VAL:CG2	2.83	0.52
1:M:385:THR:CG2	1:M:388:GLU:HB3	2.40	0.52
1:K:403:THR:O	1:K:407:VAL:HG23	2.10	0.52
1:H:44:PHE:HD1	1:H:44:PHE:H	1.55	0.52
1:M:267:MET:O	1:M:268:ARG:HB2	2.09	0.52
1:K:152:ALA:O	1:K:153:ASN:HB3	2.08	0.52
2:O:5:GLN:HG3	2:O:6:GLN:NE2	2.24	0.52
1:L:385:THR:CG2	1:L:388:GLU:HB3	2.40	0.52
1:J:403:THR:O	1:J:407:VAL:HG23	2.10	0.52
2:O:77:ARG:HD3	2:P:72:PRO:HG3	1.90	0.52
1:A:409:GLU:HB3	1:A:498:LYS:HB2	1.90	0.52
1:K:267:MET:O	1:K:268:ARG:HB2	2.09	0.52
1:M:147:VAL:HA	1:M:150:ILE:HD12	1.91	0.52
1:D:18:ARG:CG	1:D:18:ARG:NH1	2.70	0.52
1:I:403:THR:O	1:I:407:VAL:HG23	2.10	0.52
1:H:430:ARG:HG2	1:H:430:ARG:NH1	2.17	0.52
1:D:430:ARG:NH1	1:D:430:ARG:HG2	2.17	0.52
1:L:161:LEU:H	1:L:161:LEU:CD1	2.23	0.52
1:L:42:LYS:HG2	1:L:44:PHE:CE2	2.43	0.52
1:H:147:VAL:HA	1:H:150:ILE:HD12	1.91	0.52
1:N:42:LYS:HG2	1:N:44:PHE:CE2	2.43	0.52
1:G:405:ALA:HB1	1:G:498:LYS:HB3	1.91	0.52
1:C:455:VAL:HG21	1:C:465:VAL:HG11	1.92	0.52
2:Q:5:GLN:HG3	2:Q:6:GLN:NE2	2.24	0.52
1:G:441:LYS:HB3	1:G:445:ARG:HH21	1.73	0.52
2:U:5:GLN:HG3	2:U:6:GLN:NE2	2.24	0.52
1:I:385:THR:CG2	1:I:388:GLU:HB3	2.40	0.52
1:L:403:THR:O	1:L:407:VAL:HG23	2.10	0.52
1:K:161:LEU:H	1:K:161:LEU:CD1	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:145:ALA:O	1:J:149:THR:HG23	2.08	0.52
1:A:405:ALA:HB1	1:A:498:LYS:HB3	1.91	0.52
2:Q:85:ALA:HA	2:R:48:LEU:CD1	2.40	0.52
1:K:455:VAL:HG21	1:K:465:VAL:HG11	1.92	0.52
1:H:267:MET:O	1:H:268:ARG:HB2	2.09	0.52
1:N:161:LEU:CD1	1:N:161:LEU:H	2.23	0.52
1:M:161:LEU:CD1	1:M:161:LEU:H	2.23	0.52
1:F:264:VAL:HG13	1:G:306:GLY:HA3	1.92	0.52
1:L:192:GLY:C	1:L:376:VAL:CG2	2.77	0.52
2:O:48:LEU:CD1	2:U:85:ALA:HA	2.40	0.52
2:O:85:ALA:HA	2:P:48:LEU:CD1	2.40	0.52
1:D:455:VAL:HG21	1:D:465:VAL:HG11	1.92	0.52
2:P:5:GLN:HG3	2:P:6:GLN:NE2	2.24	0.52
2:R:5:GLN:HG3	2:R:6:GLN:NE2	2.24	0.52
1:A:464:VAL:HG22	1:H:467:ASN:HB2	1.92	0.52
1:A:138:CYS:SG	1:A:411:VAL:CG1	2.96	0.52
1:H:403:THR:O	1:H:407:VAL:HG23	2.10	0.52
1:N:149:THR:CG2	1:N:159:GLY:HA3	2.37	0.52
1:C:405:ALA:HB1	1:C:498:LYS:HB3	1.91	0.52
2:P:85:ALA:HA	2:Q:48:LEU:CD1	2.40	0.52
1:L:455:VAL:HG21	1:L:465:VAL:HG11	1.92	0.52
1:M:455:VAL:HG21	1:M:465:VAL:HG11	1.92	0.52
1:N:455:VAL:HG21	1:N:465:VAL:HG11	1.92	0.52
1:H:455:VAL:HG21	1:H:465:VAL:HG11	1.92	0.52
1:J:455:VAL:HG21	1:J:465:VAL:HG11	1.92	0.52
1:C:146:GLN:HB3	1:C:494:LEU:CG	2.35	0.52
1:D:146:GLN:CB	1:D:494:LEU:HG	2.34	0.52
1:B:136:VAL:CA	1:B:137:PRO:CD	2.83	0.52
1:N:149:THR:HG22	1:N:156:GLU:HA	1.90	0.52
2:P:77:ARG:HD3	2:Q:72:PRO:HG3	1.90	0.52
1:A:42:LYS:HG2	1:A:44:PHE:CE2	2.43	0.52
2:R:85:ALA:HA	2:S:48:LEU:CD1	2.40	0.52
2:T:85:ALA:HA	2:U:48:LEU:CD1	2.40	0.52
1:N:267:MET:O	1:N:268:ARG:HB2	2.09	0.52
1:B:464:VAL:HG22	1:I:467:ASN:HB2	1.92	0.51
1:A:136:VAL:CA	1:A:137:PRO:CD	2.83	0.51
1:A:18:ARG:CG	1:A:18:ARG:NH1	2.70	0.51
1:N:385:THR:CG2	1:N:388:GLU:HB3	2.40	0.51
1:J:149:THR:HG22	1:J:156:GLU:HA	1.90	0.51
1:A:306:GLY:HA3	1:G:264:VAL:HG13	1.92	0.51
1:H:192:GLY:CA	1:H:376:VAL:CG2	2.83	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:VAL:HG21	1:B:465:VAL:HG11	1.92	0.51
1:G:487:ASN:O	1:G:491:MET:HG3	2.11	0.51
1:I:455:VAL:HG21	1:I:465:VAL:HG11	1.92	0.51
1:E:146:GLN:HB3	1:E:494:LEU:CG	2.35	0.51
1:H:385:THR:CG2	1:H:388:GLU:HB3	2.40	0.51
1:H:149:THR:HG22	1:H:156:GLU:HA	1.90	0.51
1:D:405:ALA:HB1	1:D:498:LYS:HB3	1.91	0.51
1:F:409:GLU:HB3	1:F:498:LYS:HB2	1.90	0.51
1:E:405:ALA:HB1	1:E:498:LYS:HB3	1.91	0.51
1:I:487:ASN:O	1:I:491:MET:HG3	2.10	0.51
1:J:487:ASN:O	1:J:491:MET:HG3	2.10	0.51
1:I:267:MET:O	1:I:268:ARG:HB2	2.09	0.51
1:L:395:ARG:O	1:L:398:ASP:HB2	2.09	0.51
1:E:146:GLN:CB	1:E:494:LEU:HG	2.34	0.51
1:M:143:ALA:C	1:M:146:GLN:HB3	2.31	0.51
1:K:385:THR:CG2	1:K:388:GLU:HB3	2.40	0.51
1:J:385:THR:CG2	1:J:388:GLU:HB3	2.40	0.51
1:M:403:THR:O	1:M:407:VAL:HG23	2.10	0.51
1:I:161:LEU:CD1	1:I:161:LEU:H	2.23	0.51
1:D:44:PHE:H	1:D:44:PHE:HD1	1.55	0.51
1:N:487:ASN:O	1:N:491:MET:HG3	2.10	0.51
1:H:487:ASN:O	1:H:491:MET:HG3	2.11	0.51
1:K:143:ALA:C	1:K:146:GLN:HB3	2.31	0.51
1:E:18:ARG:CG	1:E:18:ARG:NH1	2.70	0.51
1:N:403:THR:O	1:N:407:VAL:HG23	2.10	0.51
1:H:149:THR:CG2	1:H:159:GLY:HA3	2.37	0.51
1:H:161:LEU:CD1	1:H:161:LEU:H	2.22	0.51
1:H:402:ALA:O	1:H:406:ALA:N	2.32	0.51
1:E:463:SER:HG	1:L:464:VAL:HG23	1.75	0.51
1:J:147:VAL:HA	1:J:150:ILE:HD12	1.91	0.51
2:R:17:ILE:CD1	2:S:108:CYS:HB3	2.34	0.51
1:I:149:THR:HG22	1:I:156:GLU:HA	1.90	0.51
1:E:264:VAL:HG13	1:F:306:GLY:HA3	1.92	0.51
1:B:405:ALA:HB1	1:B:498:LYS:HB3	1.91	0.51
2:O:106:ILE:O	2:U:12:VAL:CG2	2.58	0.51
1:D:464:VAL:HG22	1:K:467:ASN:HB2	1.92	0.51
1:H:147:VAL:HG23	1:H:496:PRO:CB	2.39	0.51
1:F:18:ARG:NH1	1:F:18:ARG:CG	2.70	0.51
1:F:172:GLU:OE1	1:F:350:ARG:HG3	2.11	0.51
2:O:17:ILE:CD1	2:P:108:CYS:HB3	2.34	0.51
1:I:149:THR:CG2	1:I:159:GLY:HA3	2.37	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:85:ALA:HA	2:T:48:LEU:CD1	2.40	0.51
2:O:12:VAL:CG2	2:P:106:ILE:O	2.59	0.51
1:K:487:ASN:O	1:K:491:MET:HG3	2.11	0.51
2:Q:12:VAL:CG2	2:R:106:ILE:O	2.59	0.51
1:A:455:VAL:HG21	1:A:465:VAL:HG11	1.92	0.51
1:J:267:MET:O	1:J:268:ARG:HB2	2.09	0.51
1:B:172:GLU:OE1	1:B:350:ARG:HG3	2.11	0.51
2:T:17:ILE:CD1	2:U:108:CYS:HB3	2.34	0.51
1:I:192:GLY:CA	1:I:376:VAL:CG2	2.83	0.51
1:L:194:GLN:HB2	1:L:331:THR:HB	1.93	0.51
2:P:12:VAL:CG2	2:Q:106:ILE:O	2.58	0.51
1:F:487:ASN:O	1:F:491:MET:HG3	2.11	0.51
1:J:190:VAL:HG22	1:J:191:GLU:N	2.26	0.51
1:A:172:GLU:OE1	1:A:350:ARG:HG3	2.11	0.51
2:Q:77:ARG:HD3	2:R:72:PRO:HG3	1.90	0.51
1:C:44:PHE:HD1	1:C:44:PHE:H	1.55	0.51
1:M:194:GLN:HB2	1:M:331:THR:HB	1.93	0.51
1:F:146:GLN:CB	1:F:494:LEU:HG	2.34	0.51
1:G:18:ARG:NH1	1:G:18:ARG:CG	2.70	0.51
1:G:172:GLU:OE1	1:G:350:ARG:HG3	2.11	0.51
1:E:455:VAL:HG21	1:E:465:VAL:HG11	1.92	0.51
1:I:430:ARG:NH1	1:I:430:ARG:HG2	2.17	0.51
1:J:161:LEU:H	1:J:161:LEU:CD1	2.22	0.51
1:J:44:PHE:H	1:J:44:PHE:HD1	1.55	0.51
1:F:405:ALA:HB1	1:F:498:LYS:HB3	1.91	0.51
2:T:12:VAL:CG2	2:U:106:ILE:O	2.58	0.51
1:E:487:ASN:O	1:E:491:MET:HG3	2.11	0.51
1:A:487:ASN:O	1:A:491:MET:HG3	2.11	0.51
1:I:180:GLY:HA2	1:I:380:LYS:HB3	1.93	0.51
1:L:147:VAL:HA	1:L:150:ILE:HD12	1.91	0.51
1:E:172:GLU:OE1	1:E:350:ARG:HG3	2.11	0.51
1:M:18:ARG:CG	1:M:18:ARG:NH1	2.70	0.51
1:C:172:GLU:OE1	1:C:350:ARG:HG3	2.11	0.51
1:M:381:VAL:HB	1:M:389:MET:CE	2.41	0.51
1:C:487:ASN:O	1:C:491:MET:HG3	2.11	0.51
1:I:190:VAL:HG22	1:I:191:GLU:N	2.26	0.50
1:N:18:ARG:CG	1:N:18:ARG:NH1	2.70	0.50
1:A:406:ALA:CB	1:A:496:PRO:HB3	2.27	0.50
1:N:381:VAL:HB	1:N:389:MET:CE	2.41	0.50
2:O:108:CYS:HB3	2:U:17:ILE:CD1	2.34	0.50
1:E:44:PHE:HD1	1:E:44:PHE:H	1.55	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:147:VAL:CG2	1:L:496:PRO:CG	2.75	0.50
1:M:190:VAL:HG22	1:M:191:GLU:N	2.26	0.50
1:A:264:VAL:HG13	1:B:306:GLY:HA3	1.92	0.50
1:G:455:VAL:HG21	1:G:465:VAL:HG11	1.92	0.50
1:B:487:ASN:O	1:B:491:MET:HG3	2.11	0.50
1:M:487:ASN:O	1:M:491:MET:HG3	2.11	0.50
1:H:147:VAL:CG2	1:H:496:PRO:HG3	2.14	0.50
1:J:147:VAL:CG2	1:J:496:PRO:CG	2.75	0.50
1:M:389:MET:HE1	1:M:389:MET:O	2.12	0.50
2:R:12:VAL:CG2	2:S:106:ILE:O	2.59	0.50
1:I:194:GLN:HB2	1:I:331:THR:HB	1.93	0.50
1:D:487:ASN:O	1:D:491:MET:HG3	2.11	0.50
1:F:455:VAL:HG21	1:F:465:VAL:HG11	1.92	0.50
1:J:180:GLY:HA2	1:J:380:LYS:HB3	1.93	0.50
1:H:180:GLY:HA2	1:H:380:LYS:HB3	1.93	0.50
2:S:12:VAL:CG2	2:T:106:ILE:O	2.58	0.50
1:E:464:VAL:HG22	1:L:467:ASN:HB2	1.92	0.50
1:G:464:VAL:HG22	1:N:467:ASN:HB2	1.92	0.50
1:K:147:VAL:HA	1:K:150:ILE:HD12	1.91	0.50
1:I:143:ALA:C	1:I:146:GLN:HB3	2.31	0.50
1:K:391:GLU:O	1:K:394:ALA:HB3	2.12	0.50
1:L:391:GLU:O	1:L:394:ALA:HB3	2.12	0.50
1:N:194:GLN:HB2	1:N:331:THR:HB	1.93	0.50
1:N:193:MET:HG3	1:N:371:LYS:HB3	1.93	0.50
2:T:18:LEU:HD13	2:T:51:VAL:HA	1.93	0.50
1:H:135:SER:HG	1:H:137:PRO:CA	2.14	0.50
1:A:146:GLN:CB	1:A:494:LEU:HG	2.34	0.50
1:L:147:VAL:HG23	1:L:496:PRO:CB	2.39	0.50
1:D:264:VAL:HG13	1:E:306:GLY:HA3	1.92	0.50
1:H:193:MET:HG3	1:H:371:LYS:HB3	1.93	0.50
1:L:487:ASN:O	1:L:491:MET:HG3	2.11	0.50
2:U:18:LEU:HD13	2:U:51:VAL:HA	1.93	0.50
1:N:402:ALA:O	1:N:406:ALA:N	2.32	0.50
1:H:143:ALA:C	1:H:146:GLN:HB3	2.31	0.50
1:L:44:PHE:HD1	1:L:44:PHE:H	1.55	0.50
1:N:290:GLN:HB3	1:N:345:ARG:HH21	1.77	0.50
1:B:146:GLN:HB3	1:B:494:LEU:CG	2.35	0.50
1:J:147:VAL:HG23	1:J:496:PRO:CB	2.39	0.50
1:L:190:VAL:HG22	1:L:191:GLU:N	2.26	0.50
1:L:381:VAL:HB	1:L:389:MET:CE	2.41	0.50
1:H:381:VAL:HB	1:H:389:MET:CE	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:391:GLU:O	1:N:394:ALA:HB3	2.12	0.50
1:J:391:GLU:O	1:J:394:ALA:HB3	2.12	0.50
1:M:391:GLU:O	1:M:394:ALA:HB3	2.12	0.50
1:K:136:VAL:C	1:K:137:PRO:CB	2.79	0.50
1:F:464:VAL:HG22	1:M:467:ASN:HB2	1.92	0.50
2:Q:17:ILE:CD1	2:R:108:CYS:HB3	2.34	0.50
1:J:149:THR:CG2	1:J:159:GLY:HA3	2.37	0.50
1:J:194:GLN:HB2	1:J:331:THR:HB	1.93	0.50
1:J:136:VAL:C	1:J:137:PRO:CB	2.79	0.50
1:N:190:VAL:HG22	1:N:191:GLU:N	2.26	0.50
1:C:406:ALA:CB	1:C:496:PRO:HB3	2.27	0.50
1:I:193:MET:HG3	1:I:371:LYS:HB3	1.93	0.50
1:H:194:GLN:HB2	1:H:331:THR:HB	1.93	0.50
1:M:193:MET:HG3	1:M:371:LYS:HB3	1.93	0.50
2:S:18:LEU:HD13	2:S:51:VAL:HA	1.94	0.50
1:N:451:LEU:O	1:N:451:LEU:HD22	2.12	0.50
1:I:135:SER:HG	1:I:137:PRO:CA	2.14	0.49
1:I:402:ALA:O	1:I:406:ALA:N	2.32	0.49
1:H:391:GLU:O	1:H:394:ALA:HB3	2.12	0.49
1:K:194:GLN:HB2	1:K:331:THR:HB	1.93	0.49
1:F:451:LEU:O	1:F:451:LEU:HD22	2.12	0.49
1:H:451:LEU:HD22	1:H:451:LEU:O	2.12	0.49
1:N:135:SER:HG	1:N:137:PRO:CA	2.15	0.49
1:J:143:ALA:C	1:J:146:GLN:HB3	2.31	0.49
1:L:143:ALA:C	1:L:146:GLN:HB3	2.31	0.49
1:I:391:GLU:O	1:I:394:ALA:HB3	2.12	0.49
1:L:193:MET:HG3	1:L:371:LYS:HB3	1.93	0.49
1:M:451:LEU:O	1:M:451:LEU:HD22	2.12	0.49
1:H:190:VAL:HG22	1:H:191:GLU:N	2.26	0.49
1:E:406:ALA:CB	1:E:496:PRO:HB3	2.27	0.49
1:M:192:GLY:CA	1:M:376:VAL:CG2	2.83	0.49
1:C:150:ILE:CD1	1:C:493:ILE:HA	2.43	0.49
1:N:214:GLU:HG2	1:N:324:VAL:HG12	1.95	0.49
1:K:180:GLY:HA2	1:K:380:LYS:HB3	1.93	0.49
1:J:193:MET:HG3	1:J:371:LYS:HB3	1.93	0.49
1:L:290:GLN:HB3	1:L:345:ARG:HH21	1.77	0.49
1:K:193:MET:HG3	1:K:371:LYS:HB3	1.93	0.49
1:H:290:GLN:HB3	1:H:345:ARG:HH21	1.77	0.49
1:K:95:LEU:HD13	1:K:504:LEU:HD23	1.95	0.49
1:G:451:LEU:O	1:G:451:LEU:HD22	2.12	0.49
1:I:136:VAL:C	1:I:137:PRO:CB	2.79	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:172:GLU:OE1	1:D:350:ARG:HG3	2.11	0.49
1:F:44:PHE:HD1	1:F:44:PHE:H	1.55	0.49
1:M:214:GLU:HG2	1:M:324:VAL:HG12	1.95	0.49
1:M:290:GLN:HB3	1:M:345:ARG:HH21	1.77	0.49
1:L:180:GLY:HA2	1:L:380:LYS:HB3	1.93	0.49
2:O:18:LEU:HD13	2:O:51:VAL:HA	1.93	0.49
1:M:180:GLY:HA2	1:M:380:LYS:HB3	1.93	0.49
1:E:95:LEU:HD13	1:E:504:LEU:HD23	1.95	0.49
1:L:95:LEU:HD13	1:L:504:LEU:HD23	1.95	0.49
1:K:190:VAL:HG22	1:K:191:GLU:N	2.26	0.49
1:B:264:VAL:HG13	1:C:306:GLY:HA3	1.92	0.49
1:B:44:PHE:HD1	1:B:44:PHE:H	1.55	0.49
1:K:179:ASP:OD2	1:K:390:LYS:HG2	2.13	0.49
1:K:214:GLU:HG2	1:K:324:VAL:HG12	1.94	0.49
1:L:214:GLU:HG2	1:L:324:VAL:HG12	1.95	0.49
1:K:402:ALA:O	1:K:406:ALA:N	2.32	0.49
1:H:136:VAL:C	1:H:137:PRO:CB	2.79	0.49
1:F:146:GLN:HB3	1:F:494:LEU:CG	2.35	0.49
1:N:143:ALA:C	1:N:146:GLN:HB3	2.31	0.49
1:B:18:ARG:CG	1:B:18:ARG:NH1	2.70	0.49
1:I:381:VAL:HB	1:I:389:MET:CE	2.41	0.49
1:E:150:ILE:CD1	1:E:493:ILE:HA	2.43	0.49
1:C:409:GLU:HB2	1:C:498:LYS:HB2	1.94	0.49
1:H:179:ASP:OD2	1:H:390:LYS:HG2	2.13	0.49
1:C:95:LEU:HD13	1:C:504:LEU:HD23	1.95	0.49
1:D:95:LEU:HD13	1:D:504:LEU:HD23	1.95	0.49
1:E:451:LEU:HD22	1:E:451:LEU:O	2.12	0.49
1:D:31:LEU:HD23	1:D:453:GLN:HB3	1.95	0.49
1:L:451:LEU:HD22	1:L:451:LEU:O	2.12	0.49
1:C:451:LEU:O	1:C:451:LEU:HD22	2.12	0.49
1:K:381:VAL:HB	1:K:389:MET:CE	2.41	0.49
1:J:381:VAL:HB	1:J:389:MET:CE	2.41	0.49
1:F:95:LEU:HD13	1:F:504:LEU:HD23	1.95	0.49
1:J:95:LEU:HD13	1:J:504:LEU:HD23	1.95	0.49
1:N:136:VAL:C	1:N:137:PRO:CB	2.79	0.49
1:C:464:VAL:HG22	1:J:467:ASN:HB2	1.92	0.49
1:L:147:VAL:CG2	1:L:496:PRO:HG3	2.14	0.49
1:J:399:ALA:O	1:J:400:LEU:C	2.51	0.49
1:J:179:ASP:OD2	1:J:390:LYS:HG2	2.13	0.49
1:H:214:GLU:HG2	1:H:324:VAL:HG12	1.95	0.49
1:M:221:LEU:HD12	1:M:249:ILE:HG23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:95:LEU:HD13	1:N:504:LEU:HD23	1.95	0.49
1:B:95:LEU:HD13	1:B:504:LEU:HD23	1.95	0.49
2:R:18:LEU:HD13	2:R:51:VAL:HA	1.94	0.49
1:J:214:GLU:HG2	1:J:324:VAL:HG12	1.95	0.49
2:P:18:LEU:HD13	2:P:51:VAL:HA	1.93	0.49
1:N:180:GLY:HA2	1:N:380:LYS:HB3	1.93	0.49
1:I:451:LEU:HD22	1:I:451:LEU:O	2.12	0.49
1:E:203:TYR:HH	1:F:286:LYS:CD	2.01	0.49
1:L:383:ALA:CB	1:L:389:MET:HA	2.43	0.49
1:C:264:VAL:HG13	1:D:306:GLY:HA3	1.92	0.49
1:N:179:ASP:OD2	1:N:390:LYS:HG2	2.13	0.49
1:N:221:LEU:HD12	1:N:249:ILE:HG23	1.95	0.49
1:I:214:GLU:HG2	1:I:324:VAL:HG12	1.95	0.49
1:C:31:LEU:HD23	1:C:453:GLN:HB3	1.95	0.49
1:G:146:GLN:CB	1:G:494:LEU:HG	2.34	0.49
1:H:161:LEU:HD12	1:H:161:LEU:N	2.28	0.49
1:K:399:ALA:O	1:K:400:LEU:C	2.51	0.49
1:L:179:ASP:OD2	1:L:390:LYS:HG2	2.13	0.49
1:M:95:LEU:HD13	1:M:504:LEU:HD23	1.95	0.49
1:B:451:LEU:HD22	1:B:451:LEU:O	2.12	0.49
1:L:137:PRO:C	1:L:410:GLY:HA2	2.34	0.48
1:F:365:LEU:O	1:F:369:VAL:HG13	2.13	0.48
1:G:365:LEU:O	1:G:369:VAL:HG13	2.13	0.48
1:J:161:LEU:HD12	1:J:161:LEU:N	2.28	0.48
1:D:409:GLU:O	1:D:497:THR:HB	2.13	0.48
1:A:409:GLU:O	1:A:497:THR:HB	2.13	0.48
1:E:409:GLU:HB2	1:E:498:LYS:HB2	1.95	0.48
1:G:409:GLU:HB2	1:G:498:LYS:HB2	1.94	0.48
1:G:31:LEU:HD23	1:G:453:GLN:HB3	1.95	0.48
1:L:221:LEU:HD12	1:L:249:ILE:HG23	1.95	0.48
1:M:383:ALA:CB	1:M:389:MET:HA	2.43	0.48
1:H:95:LEU:HD13	1:H:504:LEU:HD23	1.95	0.48
1:N:137:PRO:C	1:N:410:GLY:HA2	2.34	0.48
1:A:365:LEU:O	1:A:369:VAL:HG13	2.13	0.48
1:K:383:ALA:CB	1:K:389:MET:HA	2.43	0.48
1:A:150:ILE:CD1	1:A:493:ILE:HA	2.43	0.48
1:G:44:PHE:H	1:G:44:PHE:HD1	1.55	0.48
1:I:179:ASP:OD2	1:I:390:LYS:HG2	2.13	0.48
1:J:290:GLN:HB3	1:J:345:ARG:HH21	1.77	0.48
1:F:31:LEU:HD23	1:F:453:GLN:HB3	1.95	0.48
1:I:290:GLN:HB3	1:I:345:ARG:HH21	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:GLU:CD	1:A:338:GLU:H	2.17	0.48
1:A:451:LEU:O	1:A:451:LEU:HD22	2.12	0.48
1:D:338:GLU:H	1:D:338:GLU:CD	2.17	0.48
1:M:402:ALA:O	1:M:406:ALA:N	2.32	0.48
1:A:146:GLN:HB3	1:A:494:LEU:CG	2.35	0.48
1:E:365:LEU:O	1:E:369:VAL:HG13	2.13	0.48
1:K:149:THR:CG2	1:K:159:GLY:HA3	2.37	0.48
1:N:399:ALA:O	1:N:400:LEU:C	2.51	0.48
1:A:409:GLU:HB2	1:A:498:LYS:HB2	1.95	0.48
1:H:221:LEU:HD12	1:H:249:ILE:HG23	1.95	0.48
1:N:31:LEU:HD23	1:N:453:GLN:HB3	1.95	0.48
1:B:31:LEU:HD23	1:B:453:GLN:HB3	1.95	0.48
1:J:31:LEU:HD23	1:J:453:GLN:HB3	1.95	0.48
1:D:451:LEU:HD22	1:D:451:LEU:O	2.12	0.48
1:L:402:ALA:O	1:L:406:ALA:N	2.32	0.48
2:P:17:ILE:CD1	2:Q:108:CYS:HB3	2.34	0.48
1:H:399:ALA:O	1:H:400:LEU:C	2.51	0.48
1:E:409:GLU:O	1:E:497:THR:HB	2.14	0.48
1:K:290:GLN:HB3	1:K:345:ARG:HH21	1.77	0.48
1:I:95:LEU:HD13	1:I:504:LEU:HD23	1.95	0.48
1:F:338:GLU:CD	1:F:338:GLU:H	2.17	0.48
1:N:44:PHE:H	1:N:44:PHE:HD1	1.55	0.48
1:M:179:ASP:OD2	1:M:390:LYS:HG2	2.13	0.48
1:A:95:LEU:HD13	1:A:504:LEU:HD23	1.95	0.48
1:K:221:LEU:HD12	1:K:249:ILE:HG23	1.95	0.48
1:E:237:LEU:HD21	1:E:271:VAL:HG21	1.95	0.48
1:J:451:LEU:HD22	1:J:451:LEU:O	2.12	0.48
1:M:135:SER:HG	1:M:137:PRO:CA	2.14	0.48
1:G:146:GLN:HB3	1:G:494:LEU:CG	2.36	0.48
1:M:161:LEU:N	1:M:161:LEU:HD12	2.28	0.48
1:G:150:ILE:CD1	1:G:493:ILE:HA	2.43	0.48
1:A:44:PHE:H	1:A:44:PHE:HD1	1.55	0.48
1:M:399:ALA:O	1:M:400:LEU:C	2.51	0.48
1:B:409:GLU:O	1:B:497:THR:HB	2.13	0.48
1:C:409:GLU:O	1:C:497:THR:HB	2.13	0.48
1:G:409:GLU:O	1:G:497:THR:HB	2.13	0.48
1:G:95:LEU:HD13	1:G:504:LEU:HD23	1.95	0.48
2:Q:18:LEU:HD13	2:Q:51:VAL:HA	1.93	0.48
1:I:221:LEU:HD12	1:I:249:ILE:HG23	1.95	0.48
1:M:31:LEU:HD23	1:M:453:GLN:HB3	1.95	0.48
1:G:338:GLU:H	1:G:338:GLU:CD	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:136:VAL:C	1:K:137:PRO:HB2	2.34	0.48
1:N:136:VAL:C	1:N:137:PRO:HB2	2.34	0.48
1:A:305:ILE:HG22	1:G:263:VAL:HG12	1.96	0.48
1:M:160:LYS:HG2	1:M:164:GLU:OE2	2.14	0.48
1:I:161:LEU:N	1:I:161:LEU:HD12	2.28	0.48
1:F:409:GLU:O	1:F:497:THR:HB	2.13	0.48
1:F:409:GLU:HB2	1:F:498:LYS:HB2	1.95	0.48
1:J:221:LEU:HD12	1:J:249:ILE:HG23	1.95	0.48
1:F:237:LEU:HD21	1:F:271:VAL:HG21	1.95	0.48
1:I:31:LEU:HD23	1:I:453:GLN:HB3	1.95	0.48
1:B:338:GLU:H	1:B:338:GLU:CD	2.17	0.48
1:B:146:GLN:HB2	1:B:494:LEU:HD12	1.96	0.48
1:C:146:GLN:HB2	1:C:494:LEU:HD12	1.96	0.48
1:J:383:ALA:CB	1:J:389:MET:HA	2.43	0.48
1:A:263:VAL:HG12	1:B:305:ILE:HG22	1.96	0.48
1:D:237:LEU:HD21	1:D:271:VAL:HG21	1.95	0.48
1:K:451:LEU:HD22	1:K:451:LEU:O	2.12	0.48
1:N:383:ALA:CB	1:N:389:MET:HA	2.43	0.48
1:K:161:LEU:N	1:K:161:LEU:HD12	2.28	0.48
1:L:161:LEU:N	1:L:161:LEU:HD12	2.28	0.48
1:K:31:LEU:HD23	1:K:453:GLN:HB3	1.95	0.48
1:E:31:LEU:HD23	1:E:453:GLN:HB3	1.95	0.48
1:A:31:LEU:HD23	1:A:453:GLN:HB3	1.95	0.48
1:C:338:GLU:CD	1:C:338:GLU:H	2.17	0.48
1:N:161:LEU:HD12	1:N:161:LEU:N	2.28	0.47
1:L:160:LYS:HG2	1:L:164:GLU:OE2	2.14	0.47
1:B:237:LEU:HD21	1:B:271:VAL:HG21	1.95	0.47
1:E:338:GLU:CD	1:E:338:GLU:H	2.17	0.47
1:M:136:VAL:C	1:M:137:PRO:CB	2.79	0.47
1:I:136:VAL:C	1:I:137:PRO:HB2	2.34	0.47
1:D:365:LEU:O	1:D:369:VAL:HG13	2.13	0.47
1:B:365:LEU:O	1:B:369:VAL:HG13	2.14	0.47
1:B:266:THR:HG23	1:B:272:LYS:HA	1.97	0.47
1:A:266:THR:HG23	1:A:272:LYS:HA	1.96	0.47
1:F:263:VAL:HG12	1:G:305:ILE:HG22	1.96	0.47
1:N:160:LYS:HG2	1:N:164:GLU:OE2	2.14	0.47
1:F:266:THR:HG23	1:F:272:LYS:HA	1.96	0.47
1:H:169:VAL:CG1	1:H:173:GLY:HA3	2.42	0.47
1:N:175:ILE:CD1	1:N:175:ILE:N	2.77	0.47
1:L:399:ALA:O	1:L:400:LEU:C	2.51	0.47
1:B:409:GLU:HB2	1:B:498:LYS:HB2	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:100:ILE:HG13	1:G:511:ALA:HB1	1.97	0.47
1:D:146:GLN:HB2	1:D:494:LEU:HD12	1.96	0.47
1:E:266:THR:HG23	1:E:272:LYS:HA	1.97	0.47
2:R:10:ARG:O	2:S:108:CYS:CA	2.62	0.47
1:K:192:GLY:CA	1:K:376:VAL:CG2	2.83	0.47
1:A:100:ILE:HG13	1:A:511:ALA:HB1	1.97	0.47
1:C:237:LEU:HD21	1:C:271:VAL:HG21	1.95	0.47
1:H:31:LEU:HD23	1:H:453:GLN:HB3	1.95	0.47
1:G:266:THR:HG23	1:G:272:LYS:HA	1.96	0.47
1:H:383:ALA:CB	1:H:389:MET:HA	2.43	0.47
1:J:160:LYS:HG2	1:J:164:GLU:OE2	2.14	0.47
1:I:399:ALA:O	1:I:400:LEU:C	2.51	0.47
1:D:409:GLU:HB2	1:D:498:LYS:HB2	1.94	0.47
1:I:100:ILE:HG13	1:I:511:ALA:HB1	1.97	0.47
1:A:237:LEU:HD21	1:A:271:VAL:HG21	1.95	0.47
1:B:289:LEU:HA	1:B:292:ILE:HD12	1.97	0.47
1:L:136:VAL:C	1:L:137:PRO:HB2	2.34	0.47
1:M:136:VAL:C	1:M:137:PRO:HB2	2.35	0.47
1:C:266:THR:HG23	1:C:272:LYS:HA	1.96	0.47
1:D:266:THR:HG23	1:D:272:LYS:HA	1.96	0.47
1:I:383:ALA:CB	1:I:389:MET:HA	2.43	0.47
1:N:169:VAL:CG1	1:N:173:GLY:HA3	2.42	0.47
1:F:100:ILE:HG13	1:F:511:ALA:HB1	1.97	0.47
1:J:100:ILE:HG13	1:J:511:ALA:HB1	1.97	0.47
1:C:289:LEU:HA	1:C:292:ILE:HD12	1.97	0.47
1:A:218:PRO:HB3	1:A:246:PRO:HB2	1.97	0.47
1:A:289:LEU:HA	1:A:292:ILE:HD12	1.97	0.47
1:M:313:THR:HG22	1:M:314:LEU:H	1.80	0.47
1:F:146:GLN:HB2	1:F:494:LEU:HD12	1.96	0.47
1:I:147:VAL:CG2	1:I:496:PRO:CB	2.93	0.47
1:F:218:PRO:HB3	1:F:246:PRO:HB2	1.97	0.47
1:E:174:VAL:CG2	1:E:367:GLU:HA	2.39	0.47
1:I:169:VAL:CG1	1:I:173:GLY:HA3	2.42	0.47
1:D:150:ILE:CD1	1:D:493:ILE:HA	2.43	0.47
1:B:150:ILE:CD1	1:B:493:ILE:HA	2.43	0.47
1:F:150:ILE:CD1	1:F:493:ILE:HA	2.43	0.47
1:G:237:LEU:HD21	1:G:271:VAL:HG21	1.95	0.47
1:B:218:PRO:HB3	1:B:246:PRO:HB2	1.97	0.47
1:H:100:ILE:HG13	1:H:511:ALA:HB1	1.97	0.47
1:L:31:LEU:HD23	1:L:453:GLN:HB3	1.95	0.47
1:B:100:ILE:HG13	1:B:511:ALA:HB1	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:289:LEU:HA	1:G:292:ILE:HD12	1.97	0.47
1:G:146:GLN:HB2	1:G:494:LEU:HD12	1.96	0.47
1:E:146:GLN:HB2	1:E:494:LEU:HD12	1.96	0.47
1:H:147:VAL:CG2	1:H:496:PRO:CB	2.93	0.47
1:C:365:LEU:O	1:C:369:VAL:HG13	2.14	0.47
1:E:263:VAL:HG12	1:F:305:ILE:HG22	1.96	0.47
1:K:160:LYS:HG2	1:K:164:GLU:OE2	2.14	0.47
1:K:175:ILE:N	1:K:175:ILE:CD1	2.77	0.47
1:I:160:LYS:HG2	1:I:164:GLU:OE2	2.14	0.47
1:F:351:GLN:HG2	1:F:351:GLN:O	2.15	0.47
1:D:289:LEU:HA	1:D:292:ILE:HD12	1.97	0.47
1:L:313:THR:HG22	1:L:314:LEU:H	1.80	0.47
1:M:228:SER:O	1:M:257:GLU:HB3	2.15	0.47
1:H:160:LYS:HG2	1:H:164:GLU:OE2	2.14	0.47
1:M:137:PRO:C	1:M:410:GLY:HA2	2.33	0.47
1:G:218:PRO:HB3	1:G:246:PRO:HB2	1.97	0.47
2:T:7:LEU:HB3	2:T:8:PRO:HD2	1.97	0.47
2:P:83:PHE:HA	2:P:88:LEU:HD12	1.97	0.47
1:N:313:THR:HG22	1:N:314:LEU:H	1.80	0.47
1:N:100:ILE:HG13	1:N:511:ALA:HB1	1.97	0.47
1:N:228:SER:O	1:N:257:GLU:HB3	2.15	0.47
1:I:513:LEU:HA	1:I:513:LEU:HD23	1.72	0.47
1:H:136:VAL:C	1:H:137:PRO:HB2	2.34	0.46
1:N:147:VAL:CG2	1:N:496:PRO:CB	2.93	0.46
1:J:147:VAL:CG2	1:J:496:PRO:CB	2.93	0.46
2:U:7:LEU:HB3	2:U:8:PRO:HD2	1.97	0.46
2:O:10:ARG:O	2:P:108:CYS:CA	2.62	0.46
1:H:157:THR:O	1:H:161:LEU:CD1	2.64	0.46
1:H:175:ILE:N	1:H:175:ILE:CD1	2.77	0.46
1:A:351:GLN:HG2	1:A:351:GLN:O	2.15	0.46
2:O:83:PHE:HA	2:O:88:LEU:HD12	1.97	0.46
1:H:217:SER:HA	1:H:320:ALA:O	2.16	0.46
1:K:313:THR:HG22	1:K:314:LEU:H	1.79	0.46
1:K:217:SER:HA	1:K:320:ALA:O	2.16	0.46
1:J:136:VAL:C	1:J:137:PRO:HB2	2.34	0.46
2:S:7:LEU:HB3	2:S:8:PRO:HD2	1.97	0.46
2:Q:10:ARG:O	2:R:108:CYS:CA	2.62	0.46
1:I:313:THR:HG22	1:I:314:LEU:H	1.79	0.46
1:J:313:THR:HG22	1:J:314:LEU:H	1.80	0.46
1:F:289:LEU:HA	1:F:292:ILE:HD12	1.97	0.46
1:C:218:PRO:HB3	1:C:246:PRO:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:218:PRO:HB3	1:E:246:PRO:HB2	1.97	0.46
1:K:100:ILE:HG13	1:K:511:ALA:HB1	1.97	0.46
1:E:100:ILE:HG13	1:E:511:ALA:HB1	1.97	0.46
1:M:513:LEU:HD23	1:M:513:LEU:HA	1.72	0.46
1:E:461:GLU:OE1	1:L:463:SER:HB3	2.13	0.46
2:P:7:LEU:HB3	2:P:8:PRO:HD2	1.97	0.46
2:Q:7:LEU:HB3	2:Q:8:PRO:HD2	1.98	0.46
2:R:7:LEU:HB3	2:R:8:PRO:HD2	1.97	0.46
1:N:157:THR:O	1:N:161:LEU:CD1	2.64	0.46
1:L:192:GLY:CA	1:L:376:VAL:CG2	2.83	0.46
1:C:351:GLN:O	1:C:351:GLN:HG2	2.15	0.46
1:L:228:SER:O	1:L:257:GLU:HB3	2.15	0.46
1:E:289:LEU:HA	1:E:292:ILE:HD12	1.97	0.46
1:I:228:SER:O	1:I:257:GLU:HB3	2.15	0.46
1:D:464:VAL:HB	1:K:467:ASN:HD21	1.78	0.46
1:D:351:GLN:O	1:D:351:GLN:HG2	2.15	0.46
2:Q:83:PHE:HA	2:Q:88:LEU:HD12	1.97	0.46
1:A:464:VAL:HB	1:H:467:ASN:HD21	1.78	0.46
1:J:137:PRO:C	1:J:410:GLY:HA2	2.33	0.46
2:O:7:LEU:HB3	2:O:8:PRO:HD2	1.97	0.46
1:D:263:VAL:HG12	1:E:305:ILE:HG22	1.96	0.46
1:M:149:THR:HG22	1:M:156:GLU:O	2.16	0.46
1:I:149:THR:HG22	1:I:156:GLU:O	2.16	0.46
1:D:218:PRO:HB3	1:D:246:PRO:HB2	1.97	0.46
1:H:389:MET:HE1	1:H:389:MET:O	2.14	0.46
1:J:149:THR:HG22	1:J:156:GLU:O	2.16	0.46
1:M:169:VAL:CG1	1:M:173:GLY:HA3	2.42	0.46
1:G:351:GLN:HG2	1:G:351:GLN:O	2.15	0.46
1:B:351:GLN:O	1:B:351:GLN:HG2	2.15	0.46
1:H:228:SER:O	1:H:257:GLU:HB3	2.15	0.46
1:C:100:ILE:HG13	1:C:511:ALA:HB1	1.97	0.46
1:K:228:SER:O	1:K:257:GLU:HB3	2.15	0.46
1:L:100:ILE:HG13	1:L:511:ALA:HB1	1.97	0.46
1:B:513:LEU:HD23	1:B:513:LEU:HA	1.73	0.46
2:P:10:ARG:O	2:Q:108:CYS:CA	2.62	0.46
1:N:149:THR:HG22	1:N:156:GLU:O	2.16	0.46
1:H:149:THR:HG22	1:H:156:GLU:O	2.16	0.46
2:U:83:PHE:HA	2:U:88:LEU:HD12	1.97	0.46
1:M:100:ILE:HG13	1:M:511:ALA:HB1	1.97	0.46
1:N:217:SER:HA	1:N:320:ALA:O	2.16	0.46
1:M:227:ILE:HD12	1:M:309:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:227:ILE:HD12	1:K:309:LEU:HD11	1.98	0.46
1:J:217:SER:HA	1:J:320:ALA:O	2.16	0.46
1:H:513:LEU:HA	1:H:513:LEU:HD23	1.72	0.46
1:H:137:PRO:C	1:H:410:GLY:HA2	2.34	0.46
1:C:263:VAL:HG12	1:D:305:ILE:HG22	1.96	0.46
1:J:169:VAL:CG1	1:J:173:GLY:HA3	2.42	0.46
1:D:461:GLU:OE1	1:K:463:SER:HB3	2.13	0.46
2:S:10:ARG:O	2:T:108:CYS:CA	2.62	0.46
1:M:157:THR:O	1:M:161:LEU:CD1	2.64	0.46
1:A:146:GLN:HB2	1:A:494:LEU:HD12	1.96	0.46
1:D:136:VAL:CA	1:D:137:PRO:CD	2.83	0.46
1:H:313:THR:HG22	1:H:314:LEU:H	1.80	0.46
1:J:228:SER:O	1:J:257:GLU:HB3	2.15	0.46
1:F:461:GLU:OE1	1:M:463:SER:HB3	2.13	0.45
1:J:192:GLY:CA	1:J:376:VAL:CG2	2.83	0.45
1:N:227:ILE:HD12	1:N:309:LEU:HD11	1.98	0.45
1:I:217:SER:HA	1:I:320:ALA:O	2.16	0.45
1:D:100:ILE:HG13	1:D:511:ALA:HB1	1.97	0.45
1:L:217:SER:HA	1:L:320:ALA:O	2.16	0.45
1:F:366:GLN:O	1:F:369:VAL:HG22	2.16	0.45
2:R:83:PHE:HA	2:R:88:LEU:HD12	1.97	0.45
2:T:83:PHE:HA	2:T:88:LEU:HD12	1.97	0.45
1:J:227:ILE:HD12	1:J:309:LEU:HD11	1.98	0.45
1:G:366:GLN:O	1:G:369:VAL:HG22	2.16	0.45
2:S:83:PHE:HA	2:S:88:LEU:HD12	1.97	0.45
1:H:227:ILE:HD12	1:H:309:LEU:HD11	1.98	0.45
1:K:147:VAL:CG2	1:K:496:PRO:CB	2.93	0.45
1:L:149:THR:HG22	1:L:156:GLU:O	2.16	0.45
1:L:175:ILE:CD1	1:L:175:ILE:N	2.77	0.45
1:M:175:ILE:CD1	1:M:175:ILE:N	2.77	0.45
1:E:351:GLN:HG2	1:E:351:GLN:O	2.15	0.45
1:C:22:VAL:HG11	1:C:62:LEU:HD11	1.99	0.45
1:I:227:ILE:HD12	1:I:309:LEU:HD11	1.98	0.45
1:K:137:PRO:C	1:K:410:GLY:HA2	2.34	0.45
2:R:80:PRO:HD2	2:S:70:SER:CB	2.47	0.45
1:J:178:GLU:O	1:J:380:LYS:HA	2.17	0.45
1:K:22:VAL:HG11	1:K:62:LEU:HD11	1.99	0.45
1:G:320:ALA:HA	1:G:335:GLY:HA2	1.99	0.45
1:L:22:VAL:HG11	1:L:62:LEU:HD11	1.99	0.45
1:B:22:VAL:HG11	1:B:62:LEU:HD11	1.99	0.45
1:E:366:GLN:O	1:E:369:VAL:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:GLN:O	1:A:369:VAL:HG22	2.16	0.45
1:J:389:MET:O	1:J:389:MET:HE1	2.16	0.45
2:O:80:PRO:HD2	2:P:70:SER:CB	2.47	0.45
1:L:157:THR:O	1:L:161:LEU:CD1	2.64	0.45
1:M:217:SER:HA	1:M:320:ALA:O	2.15	0.45
1:H:187:LEU:HD23	1:H:187:LEU:C	2.37	0.45
1:G:197:ARG:CD	1:G:277:LYS:HB2	2.23	0.45
1:C:197:ARG:CD	1:C:277:LYS:HB2	2.23	0.45
1:C:461:GLU:OE1	1:J:463:SER:HB3	2.13	0.45
2:O:70:SER:CB	2:U:80:PRO:HD2	2.47	0.45
2:O:108:CYS:CA	2:U:10:ARG:O	2.62	0.45
1:K:149:THR:HG22	1:K:156:GLU:O	2.16	0.45
1:K:157:THR:O	1:K:161:LEU:CD1	2.64	0.45
1:L:169:VAL:CG1	1:L:173:GLY:HA3	2.42	0.45
1:K:169:VAL:CG1	1:K:173:GLY:HA3	2.42	0.45
1:D:22:VAL:HG11	1:D:62:LEU:HD11	1.99	0.45
1:N:513:LEU:HD23	1:N:513:LEU:HA	1.72	0.45
1:I:187:LEU:HD23	1:I:187:LEU:C	2.37	0.45
1:G:464:VAL:HB	1:N:467:ASN:HD21	1.78	0.45
1:B:464:VAL:HB	1:I:467:ASN:HD21	1.78	0.45
1:D:366:GLN:O	1:D:369:VAL:HG22	2.16	0.45
2:T:10:ARG:O	2:U:108:CYS:CA	2.62	0.45
1:I:178:GLU:O	1:I:380:LYS:HA	2.17	0.45
1:K:178:GLU:O	1:K:380:LYS:HA	2.17	0.45
1:M:313:THR:HG22	1:M:314:LEU:HD12	1.99	0.45
2:T:21:GLU:HA	2:T:22:PRO:HD3	1.88	0.45
1:L:421:ARG:HA	1:L:421:ARG:HD3	1.78	0.45
1:I:137:PRO:C	1:I:410:GLY:HA2	2.33	0.45
1:M:147:VAL:CG2	1:M:496:PRO:CB	2.93	0.45
1:I:18:ARG:NH1	1:I:18:ARG:CG	2.70	0.45
1:B:263:VAL:HG12	1:C:305:ILE:HG22	1.96	0.45
1:J:157:THR:O	1:J:161:LEU:CD1	2.64	0.45
1:L:313:THR:HG22	1:L:314:LEU:HD12	1.99	0.45
1:F:320:ALA:HA	1:F:335:GLY:HA2	1.99	0.45
1:A:320:ALA:HA	1:A:335:GLY:HA2	1.99	0.45
1:N:187:LEU:HD23	1:N:187:LEU:C	2.37	0.45
1:B:366:GLN:O	1:B:369:VAL:HG22	2.16	0.45
1:B:461:GLU:OE1	1:I:463:SER:HB3	2.13	0.45
1:M:514:MET:HB2	1:M:514:MET:HE3	1.89	0.45
1:C:444:LEU:O	1:C:447:MET:HB2	2.17	0.45
1:I:22:VAL:HG11	1:I:62:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:18:ARG:CG	1:H:18:ARG:NH1	2.70	0.44
1:F:444:LEU:O	1:F:447:MET:HB2	2.17	0.44
1:A:22:VAL:HG11	1:A:62:LEU:HD11	1.99	0.44
1:L:227:ILE:HD12	1:L:309:LEU:HD11	1.98	0.44
1:J:187:LEU:C	1:J:187:LEU:HD23	2.37	0.44
1:I:421:ARG:HD3	1:I:421:ARG:HA	1.78	0.44
1:F:136:VAL:CA	1:F:137:PRO:CD	2.83	0.44
1:C:366:GLN:O	1:C:369:VAL:HG22	2.16	0.44
2:S:80:PRO:HD2	2:T:70:SER:CB	2.47	0.44
1:H:22:VAL:HG11	1:H:62:LEU:HD11	1.99	0.44
1:K:513:LEU:HD23	1:K:513:LEU:HA	1.72	0.44
1:F:174:VAL:CG2	1:F:367:GLU:HA	2.39	0.44
1:H:178:GLU:O	1:H:380:LYS:HA	2.17	0.44
1:N:178:GLU:O	1:N:380:LYS:HA	2.17	0.44
1:K:313:THR:HG22	1:K:314:LEU:HD12	1.99	0.44
1:A:225:LYS:HG2	1:A:303:GLU:HB2	1.99	0.44
1:M:22:VAL:HG11	1:M:62:LEU:HD11	1.99	0.44
1:A:421:ARG:HA	1:A:421:ARG:HD3	1.78	0.44
1:L:135:SER:HG	1:L:137:PRO:CA	2.14	0.44
1:I:44:PHE:HD1	1:I:44:PHE:H	1.55	0.44
2:Q:85:ALA:HA	2:R:48:LEU:HD22	1.99	0.44
1:D:444:LEU:O	1:D:447:MET:HB2	2.17	0.44
1:N:313:THR:HG22	1:N:314:LEU:HD12	1.99	0.44
1:J:313:THR:HG22	1:J:314:LEU:HD12	1.99	0.44
1:B:225:LYS:HG2	1:B:303:GLU:HB2	1.99	0.44
1:L:187:LEU:HD23	1:L:187:LEU:C	2.37	0.44
1:M:187:LEU:HD23	1:M:187:LEU:C	2.37	0.44
2:U:21:GLU:HA	2:U:22:PRO:HD3	1.88	0.44
1:E:320:ALA:HA	1:E:335:GLY:HA2	1.99	0.44
1:A:461:GLU:OE1	1:H:463:SER:HB3	2.13	0.44
2:Q:80:PRO:HD2	2:R:70:SER:CB	2.47	0.44
2:T:80:PRO:HD2	2:U:70:SER:CB	2.47	0.44
1:G:173:GLY:HA2	1:G:370:ALA:CB	2.45	0.44
2:T:85:ALA:HA	2:U:48:LEU:HD22	1.99	0.44
1:B:86:GLY:HA3	1:B:401:HIS:CB	2.48	0.44
1:E:444:LEU:O	1:E:447:MET:HB2	2.17	0.44
1:F:233:MET:HB3	1:F:237:LEU:HD12	1.99	0.44
1:K:187:LEU:C	1:K:187:LEU:HD23	2.37	0.44
1:E:225:LYS:HG2	1:E:303:GLU:HB2	1.99	0.44
1:A:86:GLY:HA3	1:A:401:HIS:CB	2.48	0.44
1:N:444:LEU:O	1:N:447:MET:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:22:VAL:HG11	1:J:62:LEU:HD11	1.99	0.44
1:D:225:LYS:HG2	1:D:303:GLU:HB2	1.99	0.44
1:C:162:ILE:HG12	1:C:400:LEU:HD23	2.00	0.44
1:H:444:LEU:O	1:H:447:MET:HB2	2.17	0.44
1:G:225:LYS:HG2	1:G:303:GLU:HB2	1.99	0.44
1:E:22:VAL:HG11	1:E:62:LEU:HD11	1.99	0.44
1:L:165:ALA:O	1:L:168:LYS:HB2	2.18	0.44
1:F:22:VAL:HG11	1:F:62:LEU:HD11	1.99	0.44
1:B:234:LEU:HB2	1:B:235:PRO:HD3	2.00	0.44
1:N:22:VAL:HG11	1:N:62:LEU:HD11	1.99	0.44
1:A:162:ILE:HG12	1:A:400:LEU:HD23	2.00	0.44
1:C:320:ALA:HA	1:C:335:GLY:HA2	1.99	0.44
1:B:162:ILE:HG12	1:B:400:LEU:HD23	2.00	0.44
1:F:234:LEU:HB2	1:F:235:PRO:HD3	2.00	0.44
1:M:421:ARG:HA	1:M:421:ARG:HD3	1.78	0.44
1:G:513:LEU:HA	1:G:513:LEU:HD23	1.73	0.44
2:T:83:PHE:HD2	2:T:89:LYS:HD2	1.83	0.44
2:R:85:ALA:HA	2:S:48:LEU:HD22	1.99	0.44
2:P:85:ALA:HA	2:Q:48:LEU:HD22	1.99	0.44
1:J:444:LEU:O	1:J:447:MET:HB2	2.17	0.44
1:I:444:LEU:O	1:I:447:MET:HB2	2.17	0.44
1:H:455:VAL:HG11	1:H:462:PRO:HA	2.00	0.44
1:M:178:GLU:O	1:M:380:LYS:HA	2.17	0.44
1:B:320:ALA:HA	1:B:335:GLY:HA2	1.99	0.44
1:D:320:ALA:HA	1:D:335:GLY:HA2	1.99	0.44
1:D:162:ILE:HG12	1:D:400:LEU:HD23	2.00	0.44
2:P:80:PRO:HD2	2:Q:70:SER:CB	2.47	0.44
1:K:158:VAL:C	1:K:160:LYS:N	2.71	0.44
1:K:455:VAL:HG11	1:K:462:PRO:HA	2.00	0.44
1:L:178:GLU:O	1:L:380:LYS:HA	2.17	0.44
1:E:233:MET:HB3	1:E:237:LEU:HD12	1.99	0.44
1:G:233:MET:HB3	1:G:237:LEU:HD12	1.99	0.44
1:I:286:LYS:NZ	1:I:304:GLU:OE1	2.51	0.44
1:G:162:ILE:HG12	1:G:400:LEU:HD23	2.00	0.44
1:K:165:ALA:O	1:K:168:LYS:HB2	2.18	0.44
1:L:513:LEU:HA	1:L:513:LEU:HD23	1.72	0.44
1:J:421:ARG:HA	1:J:421:ARG:HD3	1.78	0.44
1:K:421:ARG:HA	1:K:421:ARG:HD3	1.78	0.44
1:C:464:VAL:HB	1:J:467:ASN:HD21	1.78	0.43
1:L:147:VAL:CG2	1:L:496:PRO:CB	2.93	0.43
2:U:83:PHE:HD2	2:U:89:LYS:HD2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:444:LEU:O	1:M:447:MET:HB2	2.17	0.43
1:B:444:LEU:O	1:B:447:MET:HB2	2.17	0.43
1:J:153:ASN:O	1:J:154:SER:HB2	2.18	0.43
1:I:153:ASN:O	1:I:154:SER:HB2	2.18	0.43
1:N:455:VAL:HG11	1:N:462:PRO:HA	2.00	0.43
1:G:234:LEU:HB2	1:G:235:PRO:HD3	2.00	0.43
1:G:22:VAL:HG11	1:G:62:LEU:HD11	1.99	0.43
1:C:234:LEU:HB2	1:C:235:PRO:HD3	2.00	0.43
1:K:149:THR:HG21	1:K:156:GLU:HA	1.99	0.43
1:M:20:VAL:HG13	1:M:74:VAL:HG11	2.00	0.43
1:G:514:MET:HB2	1:G:514:MET:HE3	1.87	0.43
2:S:83:PHE:HD2	2:S:89:LYS:HD2	1.83	0.43
1:K:153:ASN:O	1:K:154:SER:HB2	2.18	0.43
1:J:455:VAL:HG11	1:J:462:PRO:HA	2.00	0.43
1:D:233:MET:HB3	1:D:237:LEU:HD12	1.99	0.43
1:I:313:THR:HG22	1:I:314:LEU:HD12	1.99	0.43
1:H:313:THR:HG22	1:H:314:LEU:HD12	1.99	0.43
1:J:286:LYS:NZ	1:J:304:GLU:OE1	2.51	0.43
1:A:234:LEU:HB2	1:A:235:PRO:HD3	2.00	0.43
1:N:78:ALA:HB2	1:N:93:THR:OG1	2.18	0.43
1:C:225:LYS:HG2	1:C:303:GLU:HB2	1.99	0.43
1:D:78:ALA:HB2	1:D:93:THR:OG1	2.19	0.43
2:S:86:LEU:HD23	2:T:68:LEU:CD2	2.49	0.43
1:M:286:LYS:NZ	1:M:304:GLU:OE1	2.51	0.43
1:I:389:MET:HE1	1:I:389:MET:O	2.18	0.43
1:I:157:THR:O	1:I:161:LEU:CD1	2.64	0.43
1:N:20:VAL:HG13	1:N:74:VAL:HG11	2.00	0.43
1:I:514:MET:HE3	1:I:514:MET:HB2	1.92	0.43
1:G:86:GLY:HA3	1:G:401:HIS:CB	2.48	0.43
2:P:83:PHE:HD2	2:P:89:LYS:HD2	1.83	0.43
2:O:85:ALA:HA	2:P:48:LEU:HD22	1.99	0.43
1:G:455:VAL:HG11	1:G:462:PRO:HA	2.00	0.43
1:F:455:VAL:HG11	1:F:462:PRO:HA	2.00	0.43
1:A:78:ALA:HB2	1:A:93:THR:OG1	2.18	0.43
2:O:86:LEU:HD23	2:P:68:LEU:CD2	2.49	0.43
1:I:165:ALA:O	1:I:168:LYS:HB2	2.18	0.43
1:E:234:LEU:HB2	1:E:235:PRO:HD3	2.00	0.43
1:J:165:ALA:O	1:J:168:LYS:HB2	2.18	0.43
1:J:18:ARG:NH1	1:J:18:ARG:CG	2.70	0.43
1:G:147:VAL:HG22	1:G:403:THR:HG22	1.99	0.43
1:L:389:MET:HE1	1:L:393:LYS:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:158:VAL:C	1:N:160:LYS:N	2.71	0.43
1:M:149:THR:H	1:M:159:GLY:HA3	1.84	0.43
2:S:85:ALA:HA	2:T:48:LEU:HD22	1.99	0.43
2:Q:83:PHE:HD2	2:Q:89:LYS:HD2	1.83	0.43
1:L:444:LEU:O	1:L:447:MET:HB2	2.17	0.43
1:A:444:LEU:O	1:A:447:MET:HB2	2.17	0.43
1:L:153:ASN:O	1:L:154:SER:HB2	2.18	0.43
2:R:12:VAL:HG23	2:S:106:ILE:O	2.19	0.43
1:D:247:LEU:HB3	1:D:273:VAL:HG12	2.01	0.43
1:N:286:LYS:NZ	1:N:304:GLU:OE1	2.51	0.43
1:B:78:ALA:HB2	1:B:93:THR:OG1	2.18	0.43
1:H:165:ALA:O	1:H:168:LYS:HB2	2.18	0.43
1:B:193:MET:HG3	1:B:371:LYS:HB3	2.01	0.43
1:N:149:THR:H	1:N:159:GLY:HA3	1.84	0.43
1:F:173:GLY:HA2	1:F:370:ALA:CB	2.45	0.43
1:L:20:VAL:HG13	1:L:74:VAL:HG11	2.00	0.43
1:C:20:VAL:HG13	1:C:74:VAL:HG11	2.00	0.43
1:K:44:PHE:H	1:K:44:PHE:HD1	1.55	0.43
1:L:455:VAL:HG11	1:L:462:PRO:HA	2.00	0.43
2:Q:12:VAL:HG23	2:R:106:ILE:O	2.19	0.43
1:K:197:ARG:HG2	1:K:277:LYS:O	2.19	0.43
1:M:165:ALA:O	1:M:168:LYS:HB2	2.18	0.43
1:N:165:ALA:O	1:N:168:LYS:HB2	2.18	0.43
1:C:193:MET:HG3	1:C:371:LYS:HB3	2.00	0.43
1:F:225:LYS:HG2	1:F:303:GLU:HB2	1.99	0.43
1:E:162:ILE:HG12	1:E:400:LEU:HD23	2.00	0.43
1:A:147:VAL:HG22	1:A:403:THR:HG22	1.99	0.43
1:H:153:ASN:O	1:H:154:SER:HB2	2.18	0.43
1:M:153:ASN:O	1:M:154:SER:HB2	2.18	0.43
1:I:455:VAL:HG11	1:I:462:PRO:HA	2.00	0.43
1:H:286:LYS:NZ	1:H:304:GLU:OE1	2.51	0.43
1:F:162:ILE:HG12	1:F:400:LEU:HD23	2.00	0.43
1:C:247:LEU:HB3	1:C:273:VAL:HG12	2.01	0.43
1:D:234:LEU:HB2	1:D:235:PRO:HD3	2.00	0.43
1:E:197:ARG:CD	1:E:277:LYS:HB2	2.23	0.43
1:B:20:VAL:HG13	1:B:74:VAL:HG11	2.00	0.43
1:G:444:LEU:O	1:G:447:MET:HB2	2.17	0.43
1:C:233:MET:HB3	1:C:237:LEU:HD12	1.99	0.43
2:T:86:LEU:HD23	2:U:68:LEU:CD2	2.49	0.43
1:I:78:ALA:HB2	1:I:93:THR:OG1	2.19	0.43
1:F:193:MET:HG3	1:F:371:LYS:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:455:VAL:HG11	1:E:462:PRO:HA	2.00	0.43
1:D:147:VAL:HG22	1:D:403:THR:HG22	1.99	0.43
1:L:389:MET:CE	1:L:389:MET:C	2.87	0.43
1:K:149:THR:H	1:K:159:GLY:HA3	1.83	0.43
1:A:173:GLY:HA2	1:A:370:ALA:CB	2.45	0.43
1:E:514:MET:HB2	1:E:514:MET:HE3	1.92	0.43
1:D:455:VAL:HG11	1:D:462:PRO:HA	2.00	0.43
2:S:12:VAL:HG23	2:T:106:ILE:O	2.19	0.43
1:G:78:ALA:HB2	1:G:93:THR:OG1	2.18	0.43
1:K:286:LYS:NZ	1:K:304:GLU:OE1	2.51	0.43
1:K:78:ALA:HB2	1:K:93:THR:OG1	2.19	0.43
1:G:193:MET:HG3	1:G:371:LYS:HB3	2.00	0.43
1:J:262:LEU:HD22	1:J:273:VAL:HG21	2.01	0.43
1:F:513:LEU:HA	1:F:513:LEU:HD23	1.73	0.43
1:F:464:VAL:HB	1:M:467:ASN:HD21	1.78	0.43
1:B:147:VAL:HG22	1:B:403:THR:HG22	1.99	0.43
1:C:147:VAL:HG22	1:C:403:THR:HG22	1.99	0.43
1:N:389:MET:C	1:N:389:MET:CE	2.87	0.43
1:M:389:MET:C	1:M:389:MET:CE	2.87	0.43
1:K:389:MET:CE	1:K:389:MET:C	2.87	0.43
1:H:149:THR:H	1:H:159:GLY:HA3	1.84	0.43
1:J:149:THR:H	1:J:159:GLY:HA3	1.84	0.43
1:K:20:VAL:HG13	1:K:74:VAL:HG11	2.00	0.43
1:K:444:LEU:O	1:K:447:MET:HB2	2.17	0.43
1:N:153:ASN:O	1:N:154:SER:HB2	2.18	0.43
1:C:455:VAL:HG11	1:C:462:PRO:HA	2.00	0.43
1:A:455:VAL:HG11	1:A:462:PRO:HA	2.00	0.43
1:B:233:MET:HB3	1:B:237:LEU:HD12	1.99	0.43
1:A:233:MET:HB3	1:A:237:LEU:HD12	1.99	0.43
1:D:222:LEU:HD12	1:D:293:ALA:HB2	2.01	0.43
1:C:78:ALA:HB2	1:C:93:THR:OG1	2.19	0.43
1:J:78:ALA:HB2	1:J:93:THR:OG1	2.19	0.43
1:N:197:ARG:HG2	1:N:277:LYS:O	2.19	0.43
1:J:197:ARG:HG2	1:J:277:LYS:O	2.19	0.43
1:C:513:LEU:HA	1:C:513:LEU:HD23	1.73	0.43
1:F:147:VAL:HG22	1:F:403:THR:HG22	1.99	0.43
1:E:147:VAL:HG22	1:E:403:THR:HG22	1.99	0.43
1:J:158:VAL:C	1:J:160:LYS:N	2.71	0.43
1:H:20:VAL:HG13	1:H:74:VAL:HG11	2.00	0.43
1:M:44:PHE:HD1	1:M:44:PHE:H	1.55	0.43
1:M:455:VAL:HG11	1:M:462:PRO:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:106:ILE:O	2:U:12:VAL:HG23	2.19	0.43
2:P:86:LEU:HD23	2:Q:68:LEU:CD2	2.49	0.43
1:B:247:LEU:HB3	1:B:273:VAL:HG12	2.01	0.43
1:L:286:LYS:NZ	1:L:304:GLU:OE1	2.51	0.43
1:K:262:LEU:HD22	1:K:273:VAL:HG21	2.01	0.43
1:M:78:ALA:HB2	1:M:93:THR:OG1	2.19	0.43
1:E:247:LEU:HB3	1:E:273:VAL:HG12	2.01	0.43
1:J:389:MET:CE	1:J:389:MET:C	2.87	0.42
2:R:83:PHE:HD2	2:R:89:LYS:HD2	1.83	0.42
1:F:86:GLY:HA3	1:F:401:HIS:CB	2.48	0.42
2:O:48:LEU:HD22	2:U:85:ALA:HA	1.99	0.42
1:K:198:GLY:O	1:K:276:VAL:HG12	2.19	0.42
2:S:21:GLU:HA	2:S:22:PRO:HD3	1.88	0.42
1:M:147:VAL:CG2	1:M:496:PRO:CG	2.75	0.42
1:G:174:VAL:CG2	1:G:367:GLU:HA	2.40	0.42
1:G:477:GLY:CA	1:G:488:MET:SD	3.07	0.42
1:D:20:VAL:HG13	1:D:74:VAL:HG11	2.00	0.42
2:O:83:PHE:HD2	2:O:89:LYS:HD2	1.83	0.42
1:D:193:MET:HG3	1:D:371:LYS:HB3	2.01	0.42
2:O:68:LEU:CD2	2:U:86:LEU:HD23	2.49	0.42
1:L:262:LEU:HD22	1:L:273:VAL:HG21	2.01	0.42
1:E:193:MET:HG3	1:E:371:LYS:HB3	2.01	0.42
1:N:262:LEU:HD22	1:N:273:VAL:HG21	2.01	0.42
1:E:78:ALA:HB2	1:E:93:THR:OG1	2.18	0.42
1:E:222:LEU:HD12	1:E:293:ALA:HB2	2.01	0.42
1:E:236:VAL:O	1:E:240:VAL:HG23	2.20	0.42
1:E:513:LEU:HA	1:E:513:LEU:HD23	1.73	0.42
1:C:463:SER:CB	1:J:464:VAL:HG21	2.27	0.42
1:G:146:GLN:HB2	1:G:494:LEU:HD11	1.95	0.42
1:H:389:MET:CE	1:H:389:MET:C	2.87	0.42
1:K:389:MET:HE1	1:K:393:LYS:HB2	2.02	0.42
1:I:389:MET:CE	1:I:389:MET:C	2.87	0.42
1:C:259:LEU:O	1:C:263:VAL:HG23	2.19	0.42
1:E:259:LEU:O	1:E:263:VAL:HG23	2.20	0.42
1:D:259:LEU:O	1:D:263:VAL:HG23	2.20	0.42
1:L:149:THR:H	1:L:159:GLY:HA3	1.84	0.42
1:F:20:VAL:HG13	1:F:74:VAL:HG11	2.00	0.42
1:C:405:ALA:HB1	1:C:498:LYS:HD3	2.01	0.42
1:H:78:ALA:HB2	1:H:93:THR:OG1	2.18	0.42
1:F:78:ALA:HB2	1:F:93:THR:OG1	2.18	0.42
1:I:197:ARG:HG2	1:I:277:LYS:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:198:GLY:O	1:I:276:VAL:HG12	2.19	0.42
1:K:118:ARG:HH22	1:L:34:LYS:HE2	1.85	0.42
1:M:197:ARG:HG2	1:M:277:LYS:O	2.19	0.42
2:Q:86:LEU:HD23	2:R:68:LEU:CD2	2.49	0.42
1:L:136:VAL:C	1:L:137:PRO:CB	2.79	0.42
1:A:464:VAL:HG23	1:H:464:VAL:HA	2.01	0.42
1:I:176:THR:HG21	1:I:333:ILE:CD1	2.48	0.42
1:D:405:ALA:HB1	1:D:498:LYS:HD3	2.02	0.42
1:D:86:GLY:HA3	1:D:401:HIS:CB	2.48	0.42
1:B:455:VAL:HG11	1:B:462:PRO:HA	2.00	0.42
1:J:262:LEU:O	1:J:266:THR:HG23	2.19	0.42
1:C:222:LEU:HD12	1:C:293:ALA:HB2	2.01	0.42
1:I:103:GLY:HA3	1:I:515:ILE:HG21	2.02	0.42
1:A:247:LEU:HB3	1:A:273:VAL:HG12	2.01	0.42
1:A:193:MET:HG3	1:A:371:LYS:HB3	2.01	0.42
1:L:78:ALA:HB2	1:L:93:THR:OG1	2.19	0.42
2:R:86:LEU:HD23	2:S:68:LEU:CD2	2.49	0.42
1:G:238:GLU:HA	1:G:238:GLU:OE2	2.20	0.42
1:E:421:ARG:HD3	1:E:421:ARG:HA	1.78	0.42
1:N:136:VAL:C	1:N:137:PRO:CD	2.87	0.42
1:B:464:VAL:HG23	1:I:464:VAL:HA	2.01	0.42
1:M:158:VAL:C	1:M:160:LYS:N	2.71	0.42
1:H:149:THR:N	1:H:159:GLY:HA3	2.35	0.42
1:A:370:ALA:HB1	1:A:375:GLY:O	2.20	0.42
1:G:20:VAL:HG13	1:G:74:VAL:HG11	2.01	0.42
1:J:20:VAL:HG13	1:J:74:VAL:HG11	2.00	0.42
1:E:86:GLY:HA3	1:E:401:HIS:CB	2.48	0.42
1:J:198:GLY:O	1:J:276:VAL:HG12	2.19	0.42
1:B:222:LEU:HD12	1:B:293:ALA:HB2	2.01	0.42
1:H:197:ARG:HG2	1:H:277:LYS:O	2.19	0.42
1:K:103:GLY:HA3	1:K:515:ILE:HG21	2.02	0.42
1:F:146:GLN:HB2	1:F:494:LEU:HD11	1.95	0.42
1:F:259:LEU:O	1:F:263:VAL:HG23	2.20	0.42
1:M:149:THR:N	1:M:159:GLY:HA3	2.35	0.42
1:L:149:THR:N	1:L:159:GLY:HA3	2.35	0.42
1:N:477:GLY:CA	1:N:488:MET:SD	3.07	0.42
1:B:370:ALA:HB1	1:B:375:GLY:O	2.20	0.42
2:P:12:VAL:HG23	2:Q:106:ILE:O	2.19	0.42
1:M:198:GLY:O	1:M:276:VAL:HG12	2.19	0.42
1:J:103:GLY:HA3	1:J:515:ILE:HG21	2.02	0.42
1:N:198:GLY:O	1:N:276:VAL:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:GLU:HA	1:C:238:GLU:OE2	2.20	0.42
1:D:238:GLU:OE2	1:D:238:GLU:HA	2.20	0.42
1:L:103:GLY:HA3	1:L:515:ILE:HG21	2.02	0.42
1:G:259:LEU:O	1:G:263:VAL:HG23	2.20	0.42
1:B:27:VAL:HG12	1:B:90:THR:HG23	2.02	0.42
1:C:174:VAL:CG2	1:C:367:GLU:HA	2.40	0.42
1:L:149:THR:HG21	1:L:156:GLU:HA	1.99	0.42
1:J:477:GLY:CA	1:J:488:MET:SD	3.07	0.42
1:F:477:GLY:CA	1:F:488:MET:SD	3.07	0.42
1:F:405:ALA:HB1	1:F:498:LYS:HD3	2.01	0.42
1:K:262:LEU:O	1:K:266:THR:HG23	2.19	0.42
1:G:236:VAL:O	1:G:240:VAL:HG23	2.19	0.42
1:H:103:GLY:HA3	1:H:515:ILE:HG21	2.02	0.42
1:L:197:ARG:HG2	1:L:277:LYS:O	2.19	0.42
1:H:262:LEU:HD22	1:H:273:VAL:HG21	2.01	0.42
1:I:262:LEU:HD22	1:I:273:VAL:HG21	2.01	0.42
1:H:118:ARG:HH22	1:I:34:LYS:HE2	1.85	0.42
1:F:238:GLU:HA	1:F:238:GLU:OE2	2.20	0.42
1:M:336:VAL:O	1:M:336:VAL:HG12	2.20	0.42
1:C:146:GLN:HE21	1:C:146:GLN:HB2	1.66	0.42
1:J:385:THR:HG23	1:J:388:GLU:CB	2.50	0.42
1:G:302:SER:HB3	1:G:305:ILE:HG12	2.02	0.42
1:B:174:VAL:CG2	1:B:367:GLU:HA	2.40	0.42
1:A:174:VAL:CG2	1:A:367:GLU:HA	2.39	0.42
1:I:20:VAL:HG13	1:I:74:VAL:HG11	2.00	0.42
1:G:405:ALA:HB1	1:G:498:LYS:HD3	2.01	0.42
1:B:245:LYS:HA	1:B:246:PRO:HD3	1.94	0.42
1:I:262:LEU:O	1:I:266:THR:HG23	2.19	0.42
1:M:103:GLY:HA3	1:M:515:ILE:HG21	2.02	0.42
2:Q:90:GLN:H	2:Q:90:GLN:HG3	1.72	0.42
1:G:461:GLU:OE1	1:N:463:SER:HB3	2.13	0.42
1:N:389:MET:HE1	1:N:393:LYS:HB2	2.02	0.42
1:A:302:SER:HB3	1:A:305:ILE:HG12	2.02	0.42
1:J:27:VAL:HG12	1:J:90:THR:HG23	2.02	0.42
1:K:27:VAL:HG12	1:K:90:THR:HG23	2.02	0.42
1:A:27:VAL:HG12	1:A:90:THR:HG23	2.02	0.42
1:D:27:VAL:HG12	1:D:90:THR:HG23	2.02	0.42
1:I:149:THR:H	1:I:159:GLY:HA3	1.84	0.42
1:C:477:GLY:CA	1:C:488:MET:SD	3.07	0.42
1:B:405:ALA:HB1	1:B:498:LYS:HD3	2.01	0.42
2:O:12:VAL:HG23	2:P:106:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:247:LEU:HB3	1:G:273:VAL:HG12	2.01	0.42
1:M:262:LEU:HD22	1:M:273:VAL:HG21	2.01	0.42
1:F:222:LEU:HD12	1:F:293:ALA:HB2	2.01	0.42
1:C:103:GLY:HA3	1:C:515:ILE:HG21	2.02	0.42
1:F:236:VAL:O	1:F:240:VAL:HG23	2.19	0.42
1:M:118:ARG:HH22	1:N:34:LYS:HE2	1.85	0.42
1:A:238:GLU:HA	1:A:238:GLU:OE2	2.20	0.42
1:C:463:SER:HG	1:J:464:VAL:HG23	1.75	0.42
1:J:137:PRO:O	1:J:410:GLY:CA	2.68	0.42
1:G:464:VAL:HG23	1:N:464:VAL:HA	2.01	0.42
1:K:477:GLY:CA	1:K:488:MET:SD	3.07	0.42
1:A:20:VAL:HG13	1:A:74:VAL:HG11	2.00	0.42
1:C:86:GLY:HA3	1:C:401:HIS:CB	2.48	0.42
2:T:12:VAL:HG23	2:U:106:ILE:O	2.19	0.42
1:F:247:LEU:HB3	1:F:273:VAL:HG12	2.01	0.42
1:A:236:VAL:O	1:A:240:VAL:HG23	2.19	0.42
1:L:198:GLY:O	1:L:276:VAL:HG12	2.19	0.42
1:N:336:VAL:HG12	1:N:336:VAL:O	2.20	0.42
1:H:336:VAL:O	1:H:336:VAL:HG12	2.20	0.42
1:E:464:VAL:HG23	1:L:464:VAL:HA	2.01	0.41
1:C:464:VAL:HG23	1:J:464:VAL:HA	2.01	0.41
1:D:463:SER:CB	1:K:464:VAL:HG21	2.27	0.41
1:E:146:GLN:HE21	1:E:146:GLN:HB2	1.66	0.41
1:N:389:MET:HE1	1:N:389:MET:O	2.20	0.41
1:M:389:MET:C	1:M:389:MET:HE1	2.41	0.41
1:C:302:SER:HB3	1:C:305:ILE:HG12	2.02	0.41
1:G:370:ALA:HB1	1:G:375:GLY:O	2.20	0.41
1:C:370:ALA:HB1	1:C:375:GLY:O	2.20	0.41
1:E:370:ALA:HB1	1:E:375:GLY:O	2.20	0.41
1:A:405:ALA:HA	1:A:498:LYS:HD3	2.02	0.41
1:F:103:GLY:HA3	1:F:515:ILE:HG21	2.02	0.41
1:B:103:GLY:HA3	1:B:515:ILE:HG21	2.02	0.41
1:N:137:PRO:O	1:N:410:GLY:CA	2.68	0.41
1:M:385:THR:HG23	1:M:388:GLU:N	2.35	0.41
1:I:385:THR:HG23	1:I:388:GLU:CB	2.49	0.41
1:I:27:VAL:HG12	1:I:90:THR:HG23	2.02	0.41
1:C:27:VAL:HG12	1:C:90:THR:HG23	2.02	0.41
1:N:149:THR:N	1:N:159:GLY:HA3	2.35	0.41
1:J:149:THR:N	1:J:159:GLY:HA3	2.35	0.41
1:A:405:ALA:HB1	1:A:498:LYS:HD3	2.01	0.41
1:B:405:ALA:HA	1:B:498:LYS:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:405:ALA:HA	1:G:498:LYS:HD3	2.02	0.41
1:M:266:THR:HG22	1:M:273:VAL:H	1.85	0.41
1:A:222:LEU:HD12	1:A:293:ALA:HB2	2.01	0.41
1:N:103:GLY:HA3	1:N:515:ILE:HG21	2.02	0.41
1:H:198:GLY:O	1:H:276:VAL:HG12	2.19	0.41
1:L:336:VAL:O	1:L:336:VAL:HG12	2.20	0.41
1:D:464:VAL:HG23	1:K:464:VAL:HA	2.01	0.41
1:E:146:GLN:HB2	1:E:494:LEU:HD11	1.95	0.41
1:K:389:MET:O	1:K:389:MET:HE1	2.20	0.41
1:L:27:VAL:HG12	1:L:90:THR:HG23	2.02	0.41
1:E:27:VAL:HG12	1:E:90:THR:HG23	2.02	0.41
1:B:477:GLY:CA	1:B:488:MET:SD	3.07	0.41
1:D:477:GLY:CA	1:D:488:MET:SD	3.07	0.41
1:E:477:GLY:CA	1:E:488:MET:SD	3.07	0.41
1:E:20:VAL:HG13	1:E:74:VAL:HG11	2.01	0.41
2:R:81:HIS:CG	2:R:94:ILE:HG21	2.56	0.41
1:E:225:LYS:HG3	1:E:225:LYS:H	1.66	0.41
1:C:225:LYS:HG3	1:C:225:LYS:H	1.66	0.41
1:L:262:LEU:O	1:L:266:THR:HG23	2.19	0.41
1:N:266:THR:HG22	1:N:273:VAL:H	1.85	0.41
1:H:262:LEU:O	1:H:266:THR:HG23	2.19	0.41
1:D:236:VAL:O	1:D:240:VAL:HG23	2.19	0.41
1:G:421:ARG:HD3	1:G:421:ARG:HA	1.78	0.41
1:D:421:ARG:HA	1:D:421:ARG:HD3	1.78	0.41
1:H:401:HIS:O	1:H:402:ALA:C	2.59	0.41
1:B:463:SER:CB	1:I:464:VAL:HG21	2.27	0.41
1:I:147:VAL:CG2	1:I:496:PRO:CG	2.75	0.41
1:H:385:THR:HG23	1:H:388:GLU:CB	2.49	0.41
1:F:302:SER:HB3	1:F:305:ILE:HG12	2.02	0.41
1:B:302:SER:HB3	1:B:305:ILE:HG12	2.02	0.41
1:I:149:THR:N	1:I:159:GLY:HA3	2.35	0.41
1:I:477:GLY:CA	1:I:488:MET:SD	3.07	0.41
1:I:158:VAL:C	1:I:160:LYS:N	2.71	0.41
1:C:405:ALA:HA	1:C:498:LYS:HD3	2.02	0.41
1:L:266:THR:HG22	1:L:273:VAL:H	1.85	0.41
1:N:262:LEU:O	1:N:266:THR:HG23	2.19	0.41
1:D:103:GLY:HA3	1:D:515:ILE:HG21	2.02	0.41
1:J:118:ARG:HH22	1:K:34:LYS:HE2	1.85	0.41
1:D:38:VAL:HG22	1:E:519:CYS:HB3	2.03	0.41
1:I:336:VAL:O	1:I:336:VAL:HG12	2.20	0.41
2:P:90:GLN:HG3	2:P:90:GLN:H	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:336:VAL:HG12	1:K:336:VAL:O	2.20	0.41
1:N:401:HIS:O	1:N:402:ALA:C	2.59	0.41
1:F:464:VAL:HG23	1:M:464:VAL:HA	2.01	0.41
1:I:150:ILE:HG21	1:I:494:LEU:O	2.21	0.41
1:D:302:SER:HB3	1:D:305:ILE:HG12	2.02	0.41
1:F:405:ALA:HA	1:F:498:LYS:HD3	2.02	0.41
1:M:262:LEU:O	1:M:266:THR:HG23	2.19	0.41
1:B:512:GLY:O	1:B:515:ILE:HG13	2.21	0.41
1:G:103:GLY:HA3	1:G:515:ILE:HG21	2.02	0.41
1:B:38:VAL:HG22	1:C:519:CYS:HB3	2.03	0.41
1:L:118:ARG:HH22	1:M:34:LYS:HE2	1.85	0.41
1:H:34:LYS:HE2	1:N:118:ARG:HH22	1.85	0.41
1:C:38:VAL:HG22	1:D:519:CYS:HB3	2.03	0.41
1:A:21:ASN:HA	1:A:21:ASN:HD22	1.67	0.41
1:J:136:VAL:C	1:J:137:PRO:CD	2.87	0.41
1:E:461:GLU:HA	1:E:462:PRO:HD3	1.93	0.41
1:B:259:LEU:O	1:B:263:VAL:HG23	2.20	0.41
1:H:166:MET:HE2	1:H:171:LYS:CA	2.40	0.41
1:K:149:THR:N	1:K:159:GLY:HA3	2.35	0.41
1:D:405:ALA:HA	1:D:498:LYS:HD3	2.02	0.41
1:E:405:ALA:HB1	1:E:498:LYS:HD3	2.02	0.41
1:B:236:VAL:O	1:B:240:VAL:HG23	2.20	0.41
1:C:236:VAL:O	1:C:240:VAL:HG23	2.19	0.41
1:A:103:GLY:HA3	1:A:515:ILE:HG21	2.02	0.41
1:E:512:GLY:O	1:E:515:ILE:HG13	2.21	0.41
1:J:336:VAL:HG12	1:J:336:VAL:O	2.20	0.41
1:L:401:HIS:O	1:L:402:ALA:C	2.59	0.41
1:I:137:PRO:O	1:I:410:GLY:CA	2.68	0.41
1:A:146:GLN:HB2	1:A:494:LEU:HD11	1.95	0.41
1:F:197:ARG:CD	1:F:277:LYS:HB2	2.23	0.41
1:L:385:THR:HG23	1:L:388:GLU:CB	2.50	0.41
1:G:27:VAL:HG12	1:G:90:THR:HG23	2.02	0.41
1:H:27:VAL:HG12	1:H:90:THR:HG23	2.02	0.41
1:L:477:GLY:CA	1:L:488:MET:SD	3.07	0.41
1:K:514:MET:HB2	1:K:514:MET:HE3	1.95	0.41
1:J:247:LEU:HB3	1:J:273:VAL:HG12	2.03	0.41
1:H:266:THR:HG22	1:H:273:VAL:H	1.85	0.41
1:I:247:LEU:HB3	1:I:273:VAL:HG12	2.02	0.41
1:I:118:ARG:HH22	1:J:34:LYS:HE2	1.85	0.41
1:G:222:LEU:HD12	1:G:293:ALA:HB2	2.01	0.41
1:B:238:GLU:HA	1:B:238:GLU:OE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:238:GLU:OE2	1:E:238:GLU:HA	2.20	0.41
1:K:137:PRO:O	1:K:410:GLY:CA	2.68	0.41
1:G:224:ASP:CB	1:G:302:SER:HA	2.51	0.41
1:E:302:SER:HB3	1:E:305:ILE:HG12	2.02	0.41
1:M:149:THR:HG21	1:M:156:GLU:HA	1.99	0.41
1:F:370:ALA:HB1	1:F:375:GLY:O	2.20	0.41
1:C:173:GLY:HA2	1:C:370:ALA:CB	2.45	0.41
1:B:173:GLY:HA2	1:B:370:ALA:CB	2.45	0.41
2:T:81:HIS:CG	2:T:94:ILE:HG21	2.56	0.41
2:P:81:HIS:CG	2:P:94:ILE:HG21	2.56	0.41
2:S:81:HIS:CG	2:S:94:ILE:HG21	2.56	0.41
2:U:81:HIS:CG	2:U:94:ILE:HG21	2.56	0.41
2:O:81:HIS:CG	2:O:94:ILE:HG21	2.56	0.41
1:M:512:GLY:O	1:M:515:ILE:HG13	2.20	0.41
1:E:38:VAL:HG22	1:F:519:CYS:HB3	2.03	0.41
1:J:513:LEU:HD23	1:J:513:LEU:HA	1.72	0.41
1:L:137:PRO:O	1:L:410:GLY:CA	2.68	0.41
1:M:401:HIS:O	1:M:402:ALA:C	2.59	0.41
1:M:137:PRO:O	1:M:410:GLY:CA	2.68	0.41
1:I:401:HIS:O	1:I:402:ALA:C	2.59	0.41
1:J:401:HIS:O	1:J:402:ALA:C	2.59	0.41
1:J:150:ILE:HG21	1:J:494:LEU:O	2.21	0.41
1:L:142:LYS:O	1:L:146:GLN:HB2	2.21	0.41
1:N:385:THR:HG23	1:N:388:GLU:CB	2.49	0.41
1:N:385:THR:HG23	1:N:388:GLU:N	2.35	0.41
1:M:385:THR:HG23	1:M:388:GLU:CB	2.49	0.41
1:I:389:MET:HE1	1:I:393:LYS:HB2	2.03	0.41
1:J:385:THR:HG23	1:J:388:GLU:N	2.35	0.41
1:A:259:LEU:O	1:A:263:VAL:HG23	2.20	0.41
1:C:224:ASP:CB	1:C:302:SER:HA	2.51	0.41
1:M:27:VAL:HG12	1:M:90:THR:HG23	2.02	0.41
1:F:27:VAL:HG12	1:F:90:THR:HG23	2.02	0.41
1:D:174:VAL:CG2	1:D:367:GLU:HA	2.40	0.41
1:D:370:ALA:HB1	1:D:375:GLY:O	2.20	0.41
1:K:176:THR:HG21	1:K:333:ILE:CD1	2.48	0.41
1:A:351:GLN:O	1:A:354:GLU:HB2	2.21	0.41
1:N:285:ARG:HA	1:N:288:MET:HB2	2.03	0.41
1:J:285:ARG:HA	1:J:288:MET:HB2	2.03	0.41
1:E:405:ALA:HA	1:E:498:LYS:HD3	2.02	0.41
2:Q:81:HIS:CG	2:Q:94:ILE:HG21	2.56	0.41
1:K:285:ARG:HA	1:K:288:MET:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:187:LEU:HD23	1:M:188:ASP:N	2.36	0.41
1:K:512:GLY:O	1:K:515:ILE:HG13	2.21	0.41
1:J:512:GLY:O	1:J:515:ILE:HG13	2.21	0.41
1:L:512:GLY:O	1:L:515:ILE:HG13	2.21	0.41
1:M:247:LEU:HB3	1:M:273:VAL:HG12	2.02	0.41
1:C:512:GLY:O	1:C:515:ILE:HG13	2.21	0.41
1:N:512:GLY:O	1:N:515:ILE:HG13	2.20	0.41
1:E:103:GLY:HA3	1:E:515:ILE:HG21	2.02	0.41
1:A:38:VAL:HG22	1:B:519:CYS:HB3	2.03	0.41
1:M:502:SER:O	1:M:503:ALA:C	2.60	0.41
1:H:137:PRO:O	1:H:410:GLY:CA	2.68	0.41
1:E:463:SER:CB	1:L:464:VAL:HG21	2.27	0.41
1:J:142:LYS:O	1:J:146:GLN:HB2	2.21	0.41
1:L:389:MET:HE1	1:L:389:MET:O	2.21	0.41
1:K:3:ALA:CB	1:L:63:GLU:CB	2.94	0.41
1:H:158:VAL:C	1:H:160:LYS:N	2.71	0.41
1:N:187:LEU:HD23	1:N:188:ASP:N	2.36	0.41
1:K:187:LEU:HD23	1:K:188:ASP:N	2.36	0.41
1:F:512:GLY:O	1:F:515:ILE:HG13	2.21	0.41
1:A:512:GLY:O	1:A:515:ILE:HG13	2.21	0.41
1:B:421:ARG:HA	1:B:421:ARG:HD3	1.78	0.41
1:H:172:GLU:OE1	1:H:172:GLU:N	2.54	0.41
1:M:142:LYS:O	1:M:146:GLN:HB2	2.21	0.40
1:I:385:THR:HG23	1:I:388:GLU:N	2.35	0.40
1:N:27:VAL:HG12	1:N:90:THR:HG23	2.02	0.40
1:I:3:ALA:CB	1:J:63:GLU:CB	2.94	0.40
1:D:351:GLN:O	1:D:354:GLU:HB2	2.21	0.40
1:E:351:GLN:O	1:E:354:GLU:HB2	2.21	0.40
1:L:187:LEU:HD23	1:L:188:ASP:N	2.36	0.40
1:K:247:LEU:HB3	1:K:273:VAL:HG12	2.02	0.40
1:K:172:GLU:N	1:K:172:GLU:OE1	2.54	0.40
1:K:401:HIS:O	1:K:402:ALA:C	2.59	0.40
1:B:146:GLN:HB2	1:B:494:LEU:HD11	1.95	0.40
1:K:385:THR:HG23	1:K:388:GLU:N	2.35	0.40
1:C:351:GLN:O	1:C:354:GLU:HB2	2.21	0.40
1:A:165:ALA:O	1:A:169:VAL:HG22	2.21	0.40
1:D:146:GLN:HB2	1:D:494:LEU:HD11	1.95	0.40
1:I:142:LYS:O	1:I:146:GLN:HB2	2.21	0.40
1:H:385:THR:HG23	1:H:388:GLU:N	2.35	0.40
1:N:158:VAL:O	1:N:159:GLY:C	2.60	0.40
1:M:158:VAL:O	1:M:159:GLY:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:477:GLY:CA	1:M:488:MET:SD	3.07	0.40
1:N:176:THR:HG21	1:N:333:ILE:CD1	2.48	0.40
1:G:351:GLN:O	1:G:354:GLU:HB2	2.21	0.40
1:H:285:ARG:HA	1:H:288:MET:HB2	2.03	0.40
1:H:193:MET:HG2	1:H:194:GLN:N	2.36	0.40
1:K:266:THR:HG22	1:K:273:VAL:H	1.85	0.40
1:N:247:LEU:HB3	1:N:273:VAL:HG12	2.02	0.40
1:I:266:THR:HG22	1:I:273:VAL:H	1.85	0.40
1:G:512:GLY:O	1:G:515:ILE:HG13	2.21	0.40
2:R:21:GLU:HA	2:R:22:PRO:HD3	1.88	0.40
1:G:165:ALA:O	1:G:169:VAL:HG22	2.21	0.40
1:C:165:ALA:O	1:C:169:VAL:HG22	2.21	0.40
1:E:165:ALA:O	1:E:169:VAL:HG22	2.21	0.40
2:R:90:GLN:H	2:R:90:GLN:HG3	1.73	0.40
1:N:142:LYS:O	1:N:146:GLN:HB2	2.21	0.40
1:H:150:ILE:HG21	1:H:494:LEU:O	2.21	0.40
1:G:246:PRO:HB3	1:G:272:LYS:HB3	2.04	0.40
1:I:193:MET:HG2	1:I:194:GLN:N	2.36	0.40
1:J:178:GLU:HG2	1:J:322:ARG:CZ	2.52	0.40
1:N:193:MET:HG2	1:N:194:GLN:N	2.36	0.40
1:M:165:ALA:O	1:M:168:LYS:N	2.38	0.40
1:L:247:LEU:HB3	1:L:273:VAL:HG12	2.03	0.40
1:I:512:GLY:O	1:I:515:ILE:HG13	2.21	0.40
1:H:247:LEU:HB3	1:H:273:VAL:HG12	2.03	0.40
1:F:38:VAL:HG22	1:G:519:CYS:HB3	2.03	0.40
1:I:172:GLU:OE1	1:I:172:GLU:N	2.54	0.40
1:C:146:GLN:HB2	1:C:494:LEU:HD11	1.95	0.40
1:F:246:PRO:HB3	1:F:272:LYS:HB3	2.04	0.40
1:F:147:VAL:HG11	1:F:411:VAL:HG12	2.04	0.40
1:A:147:VAL:HG11	1:A:411:VAL:HG12	2.04	0.40
1:G:147:VAL:HG11	1:G:411:VAL:HG12	2.04	0.40
1:K:385:THR:HG23	1:K:388:GLU:CB	2.49	0.40
1:N:166:MET:HE2	1:N:171:LYS:CA	2.40	0.40
1:E:224:ASP:CB	1:E:302:SER:HA	2.51	0.40
1:N:149:THR:HG21	1:N:156:GLU:HA	1.99	0.40
1:K:158:VAL:O	1:K:159:GLY:C	2.60	0.40
1:A:477:GLY:CA	1:A:488:MET:SD	3.07	0.40
1:M:285:ARG:HA	1:M:288:MET:HB2	2.03	0.40
1:A:519:CYS:HB3	1:G:38:VAL:HG22	2.03	0.40
1:I:502:SER:O	1:I:503:ALA:C	2.60	0.40
1:B:165:ALA:O	1:B:169:VAL:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:21:ASN:HD22	1:F:21:ASN:HA	1.67	0.40
1:M:172:GLU:N	1:M:172:GLU:OE1	2.54	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	520/547 (95%)	483 (93%)	31 (6%)	6 (1%)	16	61
1	B	520/547 (95%)	483 (93%)	31 (6%)	6 (1%)	16	61
1	C	520/547 (95%)	483 (93%)	31 (6%)	6 (1%)	16	61
1	D	520/547 (95%)	483 (93%)	31 (6%)	6 (1%)	16	61
1	E	520/547 (95%)	483 (93%)	31 (6%)	6 (1%)	16	61
1	F	520/547 (95%)	483 (93%)	31 (6%)	6 (1%)	16	61
1	G	520/547 (95%)	483 (93%)	31 (6%)	6 (1%)	16	61
1	H	505/547 (92%)	447 (88%)	45 (9%)	13 (3%)	7	45
1	I	505/547 (92%)	447 (88%)	45 (9%)	13 (3%)	7	45
1	J	505/547 (92%)	447 (88%)	45 (9%)	13 (3%)	7	45
1	K	505/547 (92%)	447 (88%)	45 (9%)	13 (3%)	7	45
1	L	505/547 (92%)	447 (88%)	45 (9%)	13 (3%)	7	45
1	M	505/547 (92%)	447 (88%)	45 (9%)	13 (3%)	7	45
1	N	505/547 (92%)	447 (88%)	45 (9%)	13 (3%)	7	45
2	O	79/111 (71%)	76 (96%)	3 (4%)	0	100	100
2	P	79/111 (71%)	76 (96%)	3 (4%)	0	100	100
2	Q	79/111 (71%)	76 (96%)	3 (4%)	0	100	100
2	R	79/111 (71%)	76 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	S	79/111 (71%)	76 (96%)	3 (4%)	0	100	100
2	T	79/111 (71%)	76 (96%)	3 (4%)	0	100	100
2	U	79/111 (71%)	76 (96%)	3 (4%)	0	100	100
All	All	7728/8435 (92%)	7042 (91%)	553 (7%)	133 (2%)	16	55

All (133) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	PHE
1	A	137	PRO
1	A	337	GLY
1	B	44	PHE
1	B	137	PRO
1	B	337	GLY
1	C	44	PHE
1	C	137	PRO
1	C	337	GLY
1	D	44	PHE
1	D	137	PRO
1	D	337	GLY
1	E	44	PHE
1	E	137	PRO
1	E	337	GLY
1	F	44	PHE
1	F	137	PRO
1	F	337	GLY
1	G	44	PHE
1	G	137	PRO
1	G	337	GLY
1	H	44	PHE
1	H	146	GLN
1	H	401	HIS
1	I	44	PHE
1	I	146	GLN
1	I	401	HIS
1	J	44	PHE
1	J	146	GLN
1	J	401	HIS
1	K	44	PHE
1	K	146	GLN
1	K	401	HIS

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Mol	Chain	Res	Type
1	L	44	PHE
1	L	146	GLN
1	L	401	HIS
1	M	44	PHE
1	M	146	GLN
1	M	401	HIS
1	N	44	PHE
1	N	146	GLN
1	N	401	HIS
1	A	374	GLY
1	B	374	GLY
1	C	374	GLY
1	D	374	GLY
1	E	374	GLY
1	F	374	GLY
1	G	374	GLY
1	H	270	ILE
1	H	389	MET
1	I	270	ILE
1	I	389	MET
1	J	270	ILE
1	J	389	MET
1	K	270	ILE
1	K	389	MET
1	L	270	ILE
1	L	389	MET
1	M	270	ILE
1	M	389	MET
1	N	270	ILE
1	N	389	MET
1	A	205	ILE
1	B	205	ILE
1	C	205	ILE
1	D	205	ILE
1	E	205	ILE
1	F	205	ILE
1	G	205	ILE
1	H	155	ASP
1	I	155	ASP
1	J	155	ASP
1	K	155	ASP
1	L	155	ASP

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Mol	Chain	Res	Type
1	M	155	ASP
1	N	155	ASP
1	L	398	ASP
1	H	153	ASN
1	H	398	ASP
1	I	153	ASN
1	I	398	ASP
1	J	153	ASN
1	J	398	ASP
1	K	153	ASN
1	K	160	LYS
1	K	398	ASP
1	L	153	ASN
1	L	160	LYS
1	M	153	ASN
1	M	398	ASP
1	N	153	ASN
1	N	398	ASP
1	H	160	LYS
1	H	165	ALA
1	I	160	LYS
1	I	165	ALA
1	J	160	LYS
1	J	165	ALA
1	K	165	ALA
1	L	165	ALA
1	M	160	LYS
1	M	165	ALA
1	N	160	LYS
1	N	165	ALA
1	A	305	ILE
1	B	305	ILE
1	C	305	ILE
1	D	305	ILE
1	E	305	ILE
1	F	305	ILE
1	G	305	ILE
1	H	256	GLY
1	H	374	GLY
1	I	256	GLY
1	I	374	GLY
1	I	387	VAL

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Mol	Chain	Res	Type
1	J	256	GLY
1	J	374	GLY
1	K	256	GLY
1	K	374	GLY
1	L	256	GLY
1	L	374	GLY
1	M	256	GLY
1	M	374	GLY
1	N	256	GLY
1	N	374	GLY
1	H	387	VAL
1	J	387	VAL
1	K	387	VAL
1	L	387	VAL
1	M	387	VAL
1	N	387	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 PDB entries followed by that with respect to all EM entries.

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	404/414 (98%)	352 (87%)	52 (13%)	5	28
1	B	404/414 (98%)	352 (87%)	52 (13%)	5	28
1	C	404/414 (98%)	352 (87%)	52 (13%)	5	28
1	D	404/414 (98%)	352 (87%)	52 (13%)	5	28
1	E	404/414 (98%)	352 (87%)	52 (13%)	5	28
1	F	404/414 (98%)	352 (87%)	52 (13%)	5	28
1	G	404/414 (98%)	352 (87%)	52 (13%)	5	28
1	H	396/414 (96%)	347 (88%)	49 (12%)	6	30
1	I	396/414 (96%)	347 (88%)	49 (12%)	6	30
1	J	396/414 (96%)	347 (88%)	49 (12%)	6	30
1	K	396/414 (96%)	347 (88%)	49 (12%)	6	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	396/414 (96%)	347 (88%)	49 (12%)	6	30
1	M	396/414 (96%)	347 (88%)	49 (12%)	6	30
1	N	396/414 (96%)	347 (88%)	49 (12%)	6	30
2	O	73/96 (76%)	71 (97%)	2 (3%)	52	79
2	P	73/96 (76%)	71 (97%)	2 (3%)	52	79
2	Q	73/96 (76%)	71 (97%)	2 (3%)	52	79
2	R	73/96 (76%)	71 (97%)	2 (3%)	52	79
2	S	73/96 (76%)	71 (97%)	2 (3%)	52	79
2	T	73/96 (76%)	71 (97%)	2 (3%)	52	79
2	U	73/96 (76%)	71 (97%)	2 (3%)	52	79
All	All	6111/6468 (94%)	5390 (88%)	721 (12%)	11	32

All (721) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	VAL
1	A	18	ARG
1	A	23	LEU
1	A	28	LYS
1	A	43	SER
1	A	44	PHE
1	A	48	THR
1	A	62	LEU
1	A	74	VAL
1	A	97	GLN
1	A	111	MET
1	A	129	GLU
1	A	132	LYS
1	A	138	CYS
1	A	147	VAL
1	A	153	ASN
1	A	168	LYS
1	A	176	THR
1	A	177	VAL
1	A	178	GLU
1	A	183	LEU
1	A	184	GLN
1	A	197	ARG

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Mol	Chain	Res	Type
1	A	225	LYS
1	A	229	ASN
1	A	237	LEU
1	A	268	ARG
1	A	281	PHE
1	A	284	ARG
1	A	288	MET
1	A	322	ARG
1	A	345	ARG
1	A	350	ARG
1	A	351	GLN
1	A	366	GLN
1	A	391	GLU
1	A	398	ASP
1	A	400	LEU
1	A	417	VAL
1	A	419	LEU
1	A	420	ILE
1	A	421	ARG
1	A	422	VAL
1	A	430	ARG
1	A	445	ARG
1	A	451	LEU
1	A	452	ARG
1	A	461	GLU
1	A	494	LEU
1	A	504	LEU
1	A	510	VAL
1	A	514	MET
1	B	6	VAL
1	B	18	ARG
1	B	23	LEU
1	B	28	LYS
1	B	43	SER
1	B	44	PHE
1	B	48	THR
1	B	62	LEU
1	B	74	VAL
1	B	97	GLN
1	B	111	MET
1	B	129	GLU
1	B	132	LYS

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Mol	Chain	Res	Type
1	B	138	CYS
1	B	147	VAL
1	B	153	ASN
1	B	168	LYS
1	B	176	THR
1	B	177	VAL
1	B	178	GLU
1	B	183	LEU
1	B	184	GLN
1	B	197	ARG
1	B	225	LYS
1	B	229	ASN
1	B	237	LEU
1	B	268	ARG
1	B	281	PHE
1	B	284	ARG
1	B	288	MET
1	B	322	ARG
1	B	345	ARG
1	B	350	ARG
1	B	351	GLN
1	B	366	GLN
1	B	391	GLU
1	B	398	ASP
1	B	400	LEU
1	B	417	VAL
1	B	419	LEU
1	B	420	ILE
1	B	421	ARG
1	B	422	VAL
1	B	430	ARG
1	B	445	ARG
1	B	451	LEU
1	B	452	ARG
1	B	461	GLU
1	B	494	LEU
1	B	504	LEU
1	B	510	VAL
1	B	514	MET
1	C	6	VAL
1	C	18	ARG
1	C	23	LEU

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Mol	Chain	Res	Type
1	C	28	LYS
1	C	43	SER
1	C	44	PHE
1	C	48	THR
1	C	62	LEU
1	C	74	VAL
1	C	97	GLN
1	C	111	MET
1	C	129	GLU
1	C	132	LYS
1	C	138	CYS
1	C	147	VAL
1	C	153	ASN
1	C	168	LYS
1	C	176	THR
1	C	177	VAL
1	C	178	GLU
1	C	183	LEU
1	C	184	GLN
1	C	197	ARG
1	C	225	LYS
1	C	229	ASN
1	C	237	LEU
1	C	268	ARG
1	C	281	PHE
1	C	284	ARG
1	C	288	MET
1	C	322	ARG
1	C	345	ARG
1	C	350	ARG
1	C	351	GLN
1	C	366	GLN
1	C	391	GLU
1	C	398	ASP
1	C	400	LEU
1	C	417	VAL
1	C	419	LEU
1	C	420	ILE
1	C	421	ARG
1	C	422	VAL
1	C	430	ARG
1	C	445	ARG

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Mol	Chain	Res	Type
1	C	451	LEU
1	C	452	ARG
1	C	461	GLU
1	C	494	LEU
1	C	504	LEU
1	C	510	VAL
1	C	514	MET
1	D	6	VAL
1	D	18	ARG
1	D	23	LEU
1	D	28	LYS
1	D	43	SER
1	D	44	PHE
1	D	48	THR
1	D	62	LEU
1	D	74	VAL
1	D	97	GLN
1	D	111	MET
1	D	129	GLU
1	D	132	LYS
1	D	138	CYS
1	D	147	VAL
1	D	153	ASN
1	D	168	LYS
1	D	176	THR
1	D	177	VAL
1	D	178	GLU
1	D	183	LEU
1	D	184	GLN
1	D	197	ARG
1	D	225	LYS
1	D	229	ASN
1	D	237	LEU
1	D	268	ARG
1	D	281	PHE
1	D	284	ARG
1	D	288	MET
1	D	322	ARG
1	D	345	ARG
1	D	350	ARG
1	D	351	GLN
1	D	366	GLN

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Mol	Chain	Res	Type
1	D	391	GLU
1	D	398	ASP
1	D	400	LEU
1	D	417	VAL
1	D	419	LEU
1	D	420	ILE
1	D	421	ARG
1	D	422	VAL
1	D	430	ARG
1	D	445	ARG
1	D	451	LEU
1	D	452	ARG
1	D	461	GLU
1	D	494	LEU
1	D	504	LEU
1	D	510	VAL
1	D	514	MET
1	E	6	VAL
1	E	18	ARG
1	E	23	LEU
1	E	28	LYS
1	E	43	SER
1	E	44	PHE
1	E	48	THR
1	E	62	LEU
1	E	74	VAL
1	E	97	GLN
1	E	111	MET
1	E	129	GLU
1	E	132	LYS
1	E	138	CYS
1	E	147	VAL
1	E	153	ASN
1	E	168	LYS
1	E	176	THR
1	E	177	VAL
1	E	178	GLU
1	E	183	LEU
1	E	184	GLN
1	E	197	ARG
1	E	225	LYS
1	E	229	ASN

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Mol	Chain	Res	Type
1	E	237	LEU
1	E	268	ARG
1	E	281	PHE
1	E	284	ARG
1	E	288	MET
1	E	322	ARG
1	E	345	ARG
1	E	350	ARG
1	E	351	GLN
1	E	366	GLN
1	E	391	GLU
1	E	398	ASP
1	E	400	LEU
1	E	417	VAL
1	E	419	LEU
1	E	420	ILE
1	E	421	ARG
1	E	422	VAL
1	E	430	ARG
1	E	445	ARG
1	E	451	LEU
1	E	452	ARG
1	E	461	GLU
1	E	494	LEU
1	E	504	LEU
1	E	510	VAL
1	E	514	MET
1	F	6	VAL
1	F	18	ARG
1	F	23	LEU
1	F	28	LYS
1	F	43	SER
1	F	44	PHE
1	F	48	THR
1	F	62	LEU
1	F	74	VAL
1	F	97	GLN
1	F	111	MET
1	F	129	GLU
1	F	132	LYS
1	F	138	CYS
1	F	147	VAL

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Mol	Chain	Res	Type
1	F	153	ASN
1	F	168	LYS
1	F	176	THR
1	F	177	VAL
1	F	178	GLU
1	F	183	LEU
1	F	184	GLN
1	F	197	ARG
1	F	225	LYS
1	F	229	ASN
1	F	237	LEU
1	F	268	ARG
1	F	281	PHE
1	F	284	ARG
1	F	288	MET
1	F	322	ARG
1	F	345	ARG
1	F	350	ARG
1	F	351	GLN
1	F	366	GLN
1	F	391	GLU
1	F	398	ASP
1	F	400	LEU
1	F	417	VAL
1	F	419	LEU
1	F	420	ILE
1	F	421	ARG
1	F	422	VAL
1	F	430	ARG
1	F	445	ARG
1	F	451	LEU
1	F	452	ARG
1	F	461	GLU
1	F	494	LEU
1	F	504	LEU
1	F	510	VAL
1	F	514	MET
1	G	6	VAL
1	G	18	ARG
1	G	23	LEU
1	G	28	LYS
1	G	43	SER

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Mol	Chain	Res	Type
1	G	44	PHE
1	G	48	THR
1	G	62	LEU
1	G	74	VAL
1	G	97	GLN
1	G	111	MET
1	G	129	GLU
1	G	132	LYS
1	G	138	CYS
1	G	147	VAL
1	G	153	ASN
1	G	168	LYS
1	G	176	THR
1	G	177	VAL
1	G	178	GLU
1	G	183	LEU
1	G	184	GLN
1	G	197	ARG
1	G	225	LYS
1	G	229	ASN
1	G	237	LEU
1	G	268	ARG
1	G	281	PHE
1	G	284	ARG
1	G	288	MET
1	G	322	ARG
1	G	345	ARG
1	G	350	ARG
1	G	351	GLN
1	G	366	GLN
1	G	391	GLU
1	G	398	ASP
1	G	400	LEU
1	G	417	VAL
1	G	419	LEU
1	G	420	ILE
1	G	421	ARG
1	G	422	VAL
1	G	430	ARG
1	G	445	ARG
1	G	451	LEU
1	G	452	ARG

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Mol	Chain	Res	Type
1	G	461	GLU
1	G	494	LEU
1	G	504	LEU
1	G	510	VAL
1	G	514	MET
1	H	6	VAL
1	H	18	ARG
1	H	23	LEU
1	H	28	LYS
1	H	43	SER
1	H	44	PHE
1	H	48	THR
1	H	62	LEU
1	H	74	VAL
1	H	97	GLN
1	H	111	MET
1	H	129	GLU
1	H	132	LYS
1	H	153	ASN
1	H	172	GLU
1	H	197	ARG
1	H	210	THR
1	H	221	LEU
1	H	230	ILE
1	H	232	GLU
1	H	233	MET
1	H	247	LEU
1	H	248	LEU
1	H	255	GLU
1	H	267	MET
1	H	268	ARG
1	H	272	LYS
1	H	284	ARG
1	H	288	MET
1	H	328	ASP
1	H	329	THR
1	H	331	THR
1	H	343	GLN
1	H	364	LYS
1	H	389	MET
1	H	417	VAL
1	H	419	LEU

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Mol	Chain	Res	Type
1	H	420	ILE
1	H	421	ARG
1	H	422	VAL
1	H	430	ARG
1	H	445	ARG
1	H	451	LEU
1	H	452	ARG
1	H	461	GLU
1	H	494	LEU
1	H	504	LEU
1	H	510	VAL
1	H	514	MET
1	I	6	VAL
1	I	18	ARG
1	I	23	LEU
1	I	28	LYS
1	I	43	SER
1	I	44	PHE
1	I	48	THR
1	I	62	LEU
1	I	74	VAL
1	I	97	GLN
1	I	111	MET
1	I	129	GLU
1	I	132	LYS
1	I	153	ASN
1	I	172	GLU
1	I	197	ARG
1	I	210	THR
1	I	221	LEU
1	I	230	ILE
1	I	232	GLU
1	I	233	MET
1	I	247	LEU
1	I	248	LEU
1	I	255	GLU
1	I	267	MET
1	I	268	ARG
1	I	272	LYS
1	I	284	ARG
1	I	288	MET
1	I	328	ASP

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Mol	Chain	Res	Type
1	I	329	THR
1	I	331	THR
1	I	343	GLN
1	I	364	LYS
1	I	389	MET
1	I	417	VAL
1	I	419	LEU
1	I	420	ILE
1	I	421	ARG
1	I	422	VAL
1	I	430	ARG
1	I	445	ARG
1	I	451	LEU
1	I	452	ARG
1	I	461	GLU
1	I	494	LEU
1	I	504	LEU
1	I	510	VAL
1	I	514	MET
1	J	6	VAL
1	J	18	ARG
1	J	23	LEU
1	J	28	LYS
1	J	43	SER
1	J	44	PHE
1	J	48	THR
1	J	62	LEU
1	J	74	VAL
1	J	97	GLN
1	J	111	MET
1	J	129	GLU
1	J	132	LYS
1	J	153	ASN
1	J	172	GLU
1	J	197	ARG
1	J	210	THR
1	J	221	LEU
1	J	230	ILE
1	J	232	GLU
1	J	233	MET
1	J	247	LEU
1	J	248	LEU

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Mol	Chain	Res	Type
1	J	255	GLU
1	J	267	MET
1	J	268	ARG
1	J	272	LYS
1	J	284	ARG
1	J	288	MET
1	J	328	ASP
1	J	329	THR
1	J	331	THR
1	J	343	GLN
1	J	364	LYS
1	J	389	MET
1	J	417	VAL
1	J	419	LEU
1	J	420	ILE
1	J	421	ARG
1	J	422	VAL
1	J	430	ARG
1	J	445	ARG
1	J	451	LEU
1	J	452	ARG
1	J	461	GLU
1	J	494	LEU
1	J	504	LEU
1	J	510	VAL
1	J	514	MET
1	K	6	VAL
1	K	18	ARG
1	K	23	LEU
1	K	28	LYS
1	K	43	SER
1	K	44	PHE
1	K	48	THR
1	K	62	LEU
1	K	74	VAL
1	K	97	GLN
1	K	111	MET
1	K	129	GLU
1	K	132	LYS
1	K	153	ASN
1	K	172	GLU
1	K	197	ARG

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Mol	Chain	Res	Type
1	K	210	THR
1	K	221	LEU
1	K	230	ILE
1	K	232	GLU
1	K	233	MET
1	K	247	LEU
1	K	248	LEU
1	K	255	GLU
1	K	267	MET
1	K	268	ARG
1	K	272	LYS
1	K	284	ARG
1	K	288	MET
1	K	328	ASP
1	K	329	THR
1	K	331	THR
1	K	343	GLN
1	K	364	LYS
1	K	389	MET
1	K	417	VAL
1	K	419	LEU
1	K	420	ILE
1	K	421	ARG
1	K	422	VAL
1	K	430	ARG
1	K	445	ARG
1	K	451	LEU
1	K	452	ARG
1	K	461	GLU
1	K	494	LEU
1	K	504	LEU
1	K	510	VAL
1	K	514	MET
1	L	6	VAL
1	L	18	ARG
1	L	23	LEU
1	L	28	LYS
1	L	43	SER
1	L	44	PHE
1	L	48	THR
1	L	62	LEU
1	L	74	VAL

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Mol	Chain	Res	Type
1	L	97	GLN
1	L	111	MET
1	L	129	GLU
1	L	132	LYS
1	L	153	ASN
1	L	172	GLU
1	L	197	ARG
1	L	210	THR
1	L	221	LEU
1	L	230	ILE
1	L	232	GLU
1	L	233	MET
1	L	247	LEU
1	L	248	LEU
1	L	255	GLU
1	L	267	MET
1	L	268	ARG
1	L	272	LYS
1	L	284	ARG
1	L	288	MET
1	L	328	ASP
1	L	329	THR
1	L	331	THR
1	L	343	GLN
1	L	364	LYS
1	L	389	MET
1	L	417	VAL
1	L	419	LEU
1	L	420	ILE
1	L	421	ARG
1	L	422	VAL
1	L	430	ARG
1	L	445	ARG
1	L	451	LEU
1	L	452	ARG
1	L	461	GLU
1	L	494	LEU
1	L	504	LEU
1	L	510	VAL
1	L	514	MET
1	M	6	VAL
1	M	18	ARG

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Mol	Chain	Res	Type
1	M	23	LEU
1	M	28	LYS
1	M	43	SER
1	M	44	PHE
1	M	48	THR
1	M	62	LEU
1	M	74	VAL
1	M	97	GLN
1	M	111	MET
1	M	129	GLU
1	M	132	LYS
1	M	153	ASN
1	M	172	GLU
1	M	197	ARG
1	M	210	THR
1	M	221	LEU
1	M	230	ILE
1	M	232	GLU
1	M	233	MET
1	M	247	LEU
1	M	248	LEU
1	M	255	GLU
1	M	267	MET
1	M	268	ARG
1	M	272	LYS
1	M	284	ARG
1	M	288	MET
1	M	328	ASP
1	M	329	THR
1	M	331	THR
1	M	343	GLN
1	M	364	LYS
1	M	389	MET
1	M	417	VAL
1	M	419	LEU
1	M	420	ILE
1	M	421	ARG
1	M	422	VAL
1	M	430	ARG
1	M	445	ARG
1	M	451	LEU
1	M	452	ARG

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Mol	Chain	Res	Type
1	M	461	GLU
1	M	494	LEU
1	M	504	LEU
1	M	510	VAL
1	M	514	MET
1	N	6	VAL
1	N	18	ARG
1	N	23	LEU
1	N	28	LYS
1	N	43	SER
1	N	44	PHE
1	N	48	THR
1	N	62	LEU
1	N	74	VAL
1	N	97	GLN
1	N	111	MET
1	N	129	GLU
1	N	132	LYS
1	N	153	ASN
1	N	172	GLU
1	N	197	ARG
1	N	210	THR
1	N	221	LEU
1	N	230	ILE
1	N	232	GLU
1	N	233	MET
1	N	247	LEU
1	N	248	LEU
1	N	255	GLU
1	N	267	MET
1	N	268	ARG
1	N	272	LYS
1	N	284	ARG
1	N	288	MET
1	N	328	ASP
1	N	329	THR
1	N	331	THR
1	N	343	GLN
1	N	364	LYS
1	N	389	MET
1	N	417	VAL
1	N	419	LEU

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Mol	Chain	Res	Type
1	N	420	ILE
1	N	421	ARG
1	N	422	VAL
1	N	430	ARG
1	N	445	ARG
1	N	451	LEU
1	N	452	ARG
1	N	461	GLU
1	N	494	LEU
1	N	504	LEU
1	N	510	VAL
1	N	514	MET
2	O	18	LEU
2	O	90	GLN
2	P	18	LEU
2	P	90	GLN
2	Q	18	LEU
2	Q	90	GLN
2	R	18	LEU
2	R	90	GLN
2	S	18	LEU
2	S	90	GLN
2	T	18	LEU
2	T	90	GLN
2	U	18	LEU
2	U	90	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (152) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	97	GLN
1	A	146	GLN
1	A	153	ASN
1	A	348	GLN
1	A	366	GLN
1	A	457	ASN
1	A	475	ASN
1	B	21	ASN
1	B	97	GLN
1	B	146	GLN
1	B	153	ASN

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Mol	Chain	Res	Type
1	B	348	GLN
1	B	351	GLN
1	B	457	ASN
1	B	475	ASN
1	C	21	ASN
1	C	97	GLN
1	C	146	GLN
1	C	153	ASN
1	C	348	GLN
1	C	351	GLN
1	C	457	ASN
1	C	475	ASN
1	D	21	ASN
1	D	97	GLN
1	D	146	GLN
1	D	153	ASN
1	D	348	GLN
1	D	351	GLN
1	D	457	ASN
1	D	475	ASN
1	E	21	ASN
1	E	97	GLN
1	E	146	GLN
1	E	153	ASN
1	E	348	GLN
1	E	351	GLN
1	E	366	GLN
1	E	457	ASN
1	E	475	ASN
1	F	21	ASN
1	F	97	GLN
1	F	146	GLN
1	F	153	ASN
1	F	348	GLN
1	F	351	GLN
1	F	366	GLN
1	F	457	ASN
1	F	475	ASN
1	G	21	ASN
1	G	97	GLN
1	G	146	GLN
1	G	153	ASN

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Mol	Chain	Res	Type
1	G	348	GLN
1	G	366	GLN
1	G	457	ASN
1	G	475	ASN
1	H	21	ASN
1	H	97	GLN
1	H	146	GLN
1	H	153	ASN
1	H	319	GLN
1	H	453	GLN
1	H	457	ASN
1	H	467	ASN
1	H	475	ASN
1	I	21	ASN
1	I	97	GLN
1	I	146	GLN
1	I	153	ASN
1	I	319	GLN
1	I	457	ASN
1	I	467	ASN
1	I	475	ASN
1	J	21	ASN
1	J	97	GLN
1	J	146	GLN
1	J	153	ASN
1	J	319	GLN
1	J	457	ASN
1	J	467	ASN
1	J	475	ASN
1	K	21	ASN
1	K	97	GLN
1	K	146	GLN
1	K	153	ASN
1	K	319	GLN
1	K	457	ASN
1	K	467	ASN
1	K	475	ASN
1	L	21	ASN
1	L	97	GLN
1	L	146	GLN
1	L	153	ASN
1	L	319	GLN

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Mol	Chain	Res	Type
1	L	457	ASN
1	L	467	ASN
1	L	475	ASN
1	M	21	ASN
1	M	97	GLN
1	M	146	GLN
1	M	153	ASN
1	M	319	GLN
1	M	453	GLN
1	M	457	ASN
1	M	467	ASN
1	M	475	ASN
1	N	21	ASN
1	N	97	GLN
1	N	146	GLN
1	N	153	ASN
1	N	319	GLN
1	N	453	GLN
1	N	457	ASN
1	N	467	ASN
1	N	475	ASN
2	O	5	GLN
2	O	6	GLN
2	O	52	HIS
2	O	81	HIS
2	O	102	HIS
2	P	5	GLN
2	P	6	GLN
2	P	52	HIS
2	P	81	HIS
2	P	102	HIS
2	Q	5	GLN
2	Q	6	GLN
2	Q	52	HIS
2	Q	81	HIS
2	Q	102	HIS
2	R	5	GLN
2	R	6	GLN
2	R	52	HIS
2	R	81	HIS
2	R	102	HIS
2	S	5	GLN

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Mol	Chain	Res	Type
2	S	6	GLN
2	S	52	HIS
2	S	81	HIS
2	S	102	HIS
2	T	5	GLN
2	T	6	GLN
2	T	52	HIS
2	T	81	HIS
2	T	102	HIS
2	U	5	GLN
2	U	6	GLN
2	U	52	HIS
2	U	81	HIS
2	U	102	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.