



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2021 – 11:59 AM EDT

PDB ID : 2EU1  
Title : Crystal structure of the chaperonin GroEL-E461K  
Authors : Cabo-Bilbao, A.; Spinelli, S.; Sot, B.; Agirre, J.; Mechaly, A.E.; Muga, A.;  
Guerin, D.M.A.  
Deposited on : 2005-10-28  
Resolution : 3.29 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

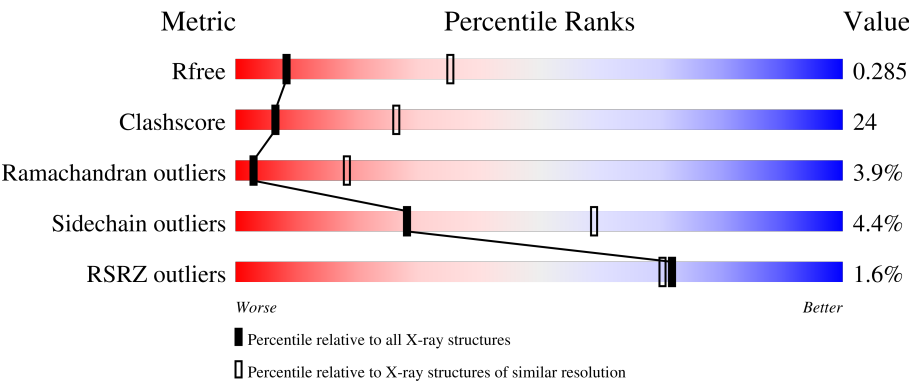
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.29 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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

Mol	Chain	Length	Quality of chain
1	A	548	<div><div>2%</div><div>53%</div><div>38%</div><div>.</div><div>.</div></div>
1	B	548	<div><div>%</div><div>56%</div><div>36%</div><div>.</div><div>.</div></div>
1	C	548	<div><div>%</div><div>57%</div><div>35%</div><div>.</div><div>.</div></div>
1	D	548	<div><div>3%</div><div>53%</div><div>39%</div><div>.</div><div>.</div></div>
1	E	548	<div><div>%</div><div>53%</div><div>39%</div><div>.</div><div>.</div></div>

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Mol	Chain	Length	Quality of chain
1	F	548	<div><div>%</div><div><div></div><div>54%</div><div>38%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div>
1	G	548	<div><div>%</div><div><div></div><div>54%</div><div>38%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div>
1	H	548	<div><div>4%</div><div><div></div><div>55%</div><div>37%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div>
1	I	548	<div><div>%</div><div><div></div><div>57%</div><div>37%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div>
1	J	548	<div><div>2%</div><div><div></div><div>57%</div><div>35%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div>
1	K	548	<div><div>%</div><div><div></div><div>55%</div><div>38%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div>
1	L	548	<div><div>%</div><div><div></div><div>53%</div><div>39%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div>
1	M	548	<div><div>%</div><div><div></div><div>53%</div><div>39%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div>
1	N	548	<div><div>%</div><div><div></div><div>56%</div><div>37%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 53970 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called GROEL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	524	Total	C	N	O	S	0	0	0
			3855	2398	666	771	20			
1	B	524	Total	C	N	O	S	0	0	0
			3855	2398	666	771	20			
1	C	524	Total	C	N	O	S	0	0	0
			3855	2398	666	771	20			
1	D	524	Total	C	N	O	S	0	0	0
			3855	2398	666	771	20			
1	E	524	Total	C	N	O	S	0	0	0
			3855	2398	666	771	20			
1	F	524	Total	C	N	O	S	0	0	0
			3855	2398	666	771	20			
1	G	524	Total	C	N	O	S	0	0	0
			3855	2398	666	771	20			
1	H	524	Total	C	N	O	S	0	0	0
			3855	2398	666	771	20			
1	I	524	Total	C	N	O	S	0	0	0
			3855	2398	666	771	20			
1	J	524	Total	C	N	O	S	0	0	0
			3855	2398	666	771	20			
1	K	524	Total	C	N	O	S	0	0	0
			3855	2398	666	771	20			
1	L	524	Total	C	N	O	S	0	0	0
			3855	2398	666	771	20			
1	M	524	Total	C	N	O	S	0	0	0
			3855	2398	666	771	20			
1	N	524	Total	C	N	O	S	0	0	0
			3855	2398	666	771	20			

There are 14 discrepancies between the modelled and reference sequences:

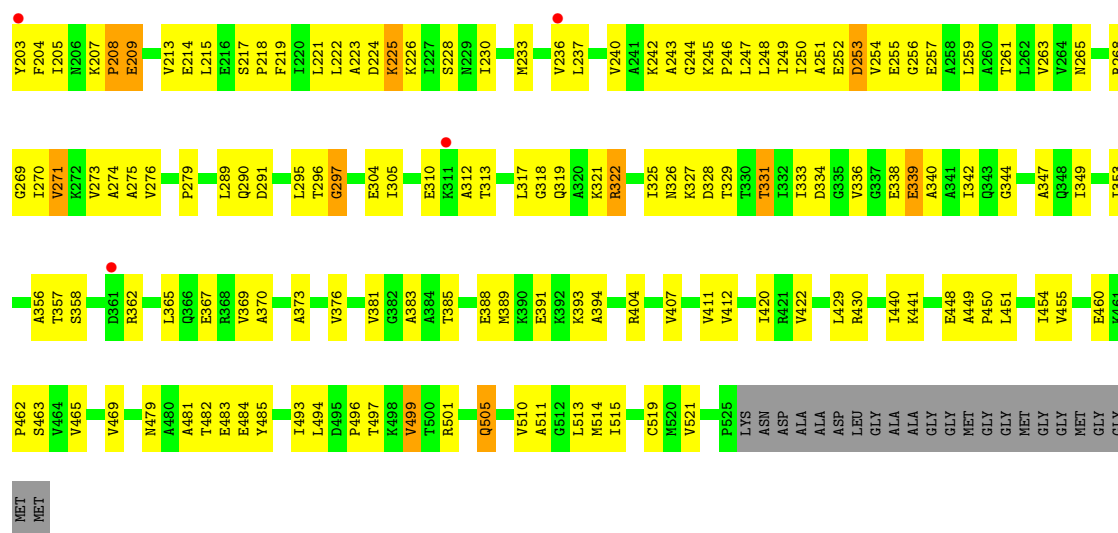
Chain	Residue	Modelled	Actual	Comment	Reference
A	461	LYS	GLU	engineered mutation	UNP P0A6F5

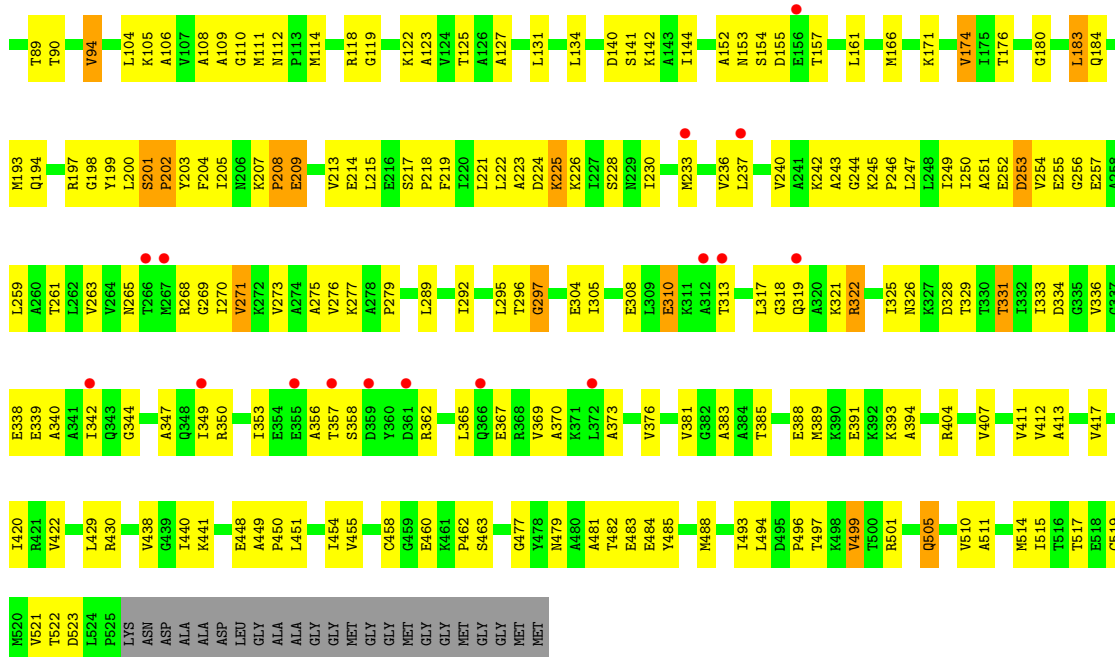
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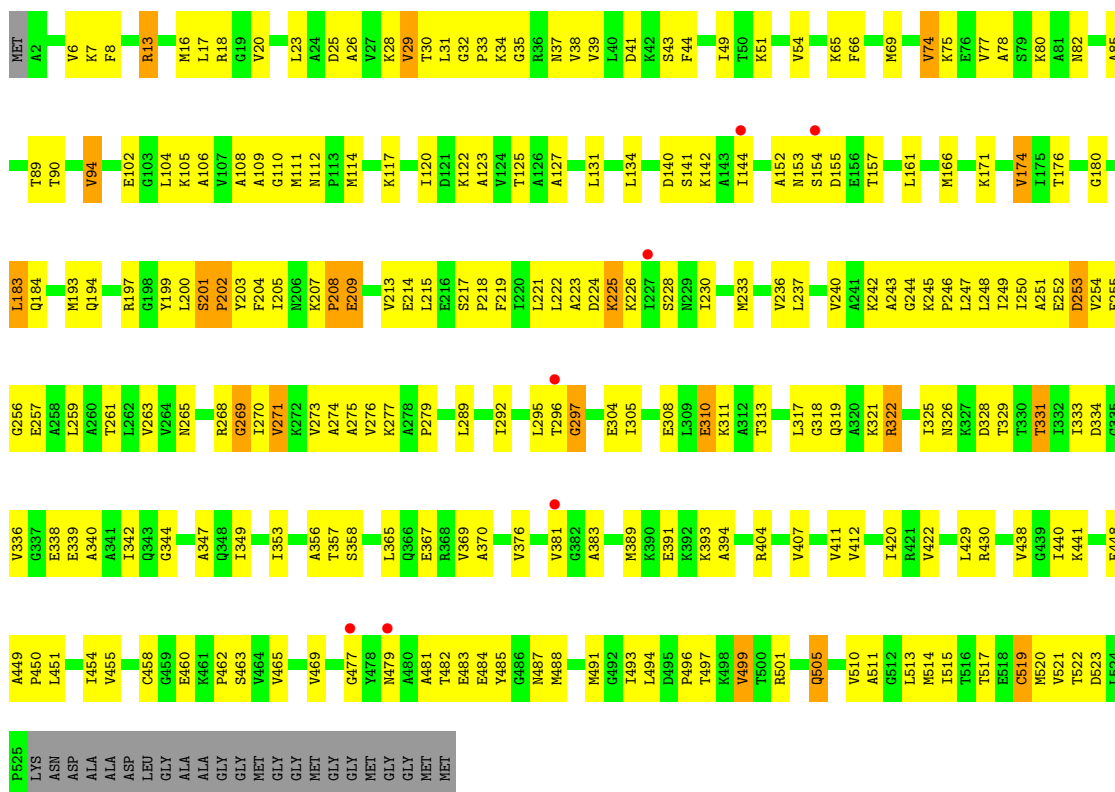
Chain	Residue	Modelled	Actual	Comment	Reference
B	461	LYS	GLU	engineered mutation	UNP P0A6F5
C	461	LYS	GLU	engineered mutation	UNP P0A6F5
D	461	LYS	GLU	engineered mutation	UNP P0A6F5
E	461	LYS	GLU	engineered mutation	UNP P0A6F5
F	461	LYS	GLU	engineered mutation	UNP P0A6F5
G	461	LYS	GLU	engineered mutation	UNP P0A6F5
H	461	LYS	GLU	engineered mutation	UNP P0A6F5
I	461	LYS	GLU	engineered mutation	UNP P0A6F5
J	461	LYS	GLU	engineered mutation	UNP P0A6F5
K	461	LYS	GLU	engineered mutation	UNP P0A6F5
L	461	LYS	GLU	engineered mutation	UNP P0A6F5
M	461	LYS	GLU	engineered mutation	UNP P0A6F5
N	461	LYS	GLU	engineered mutation	UNP P0A6F5







### • Molecule 1: GROEL



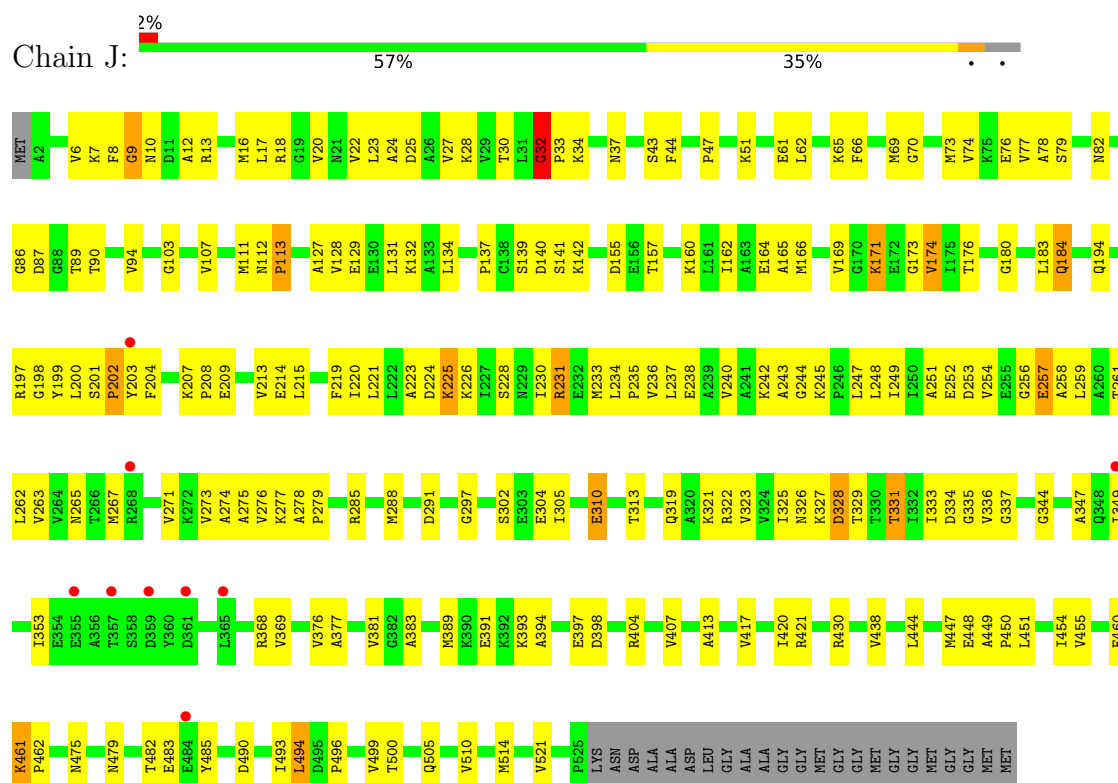
### • Molecule 1: GROEL



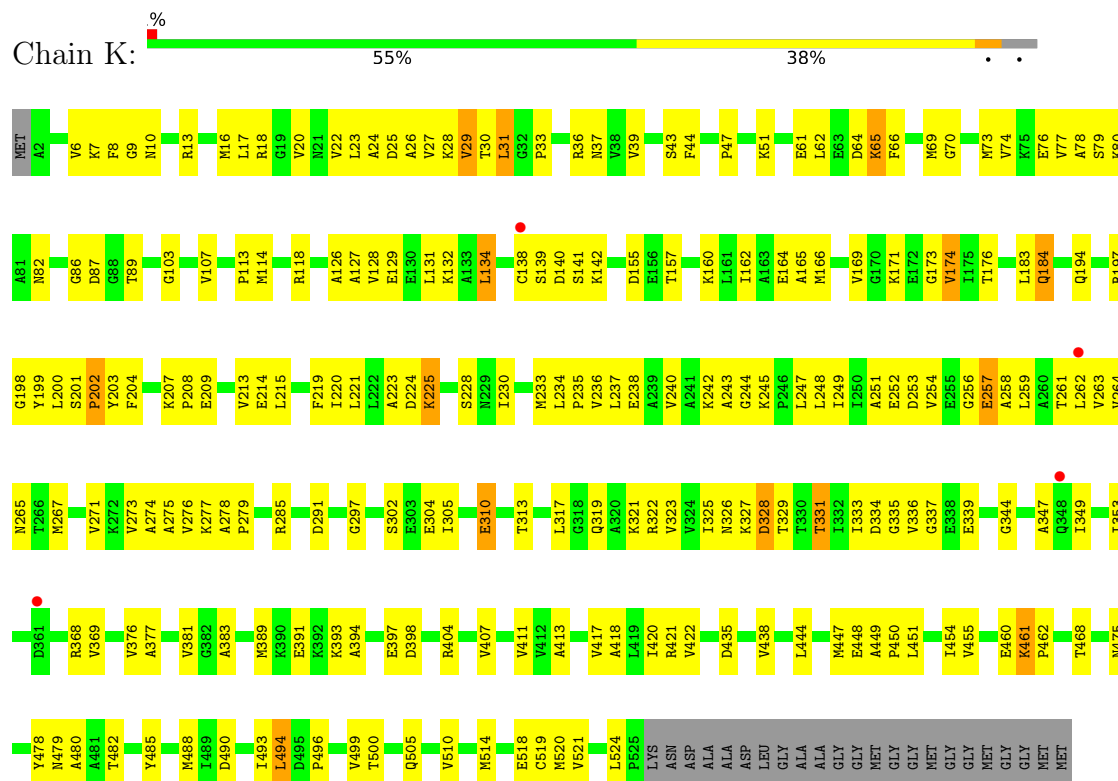






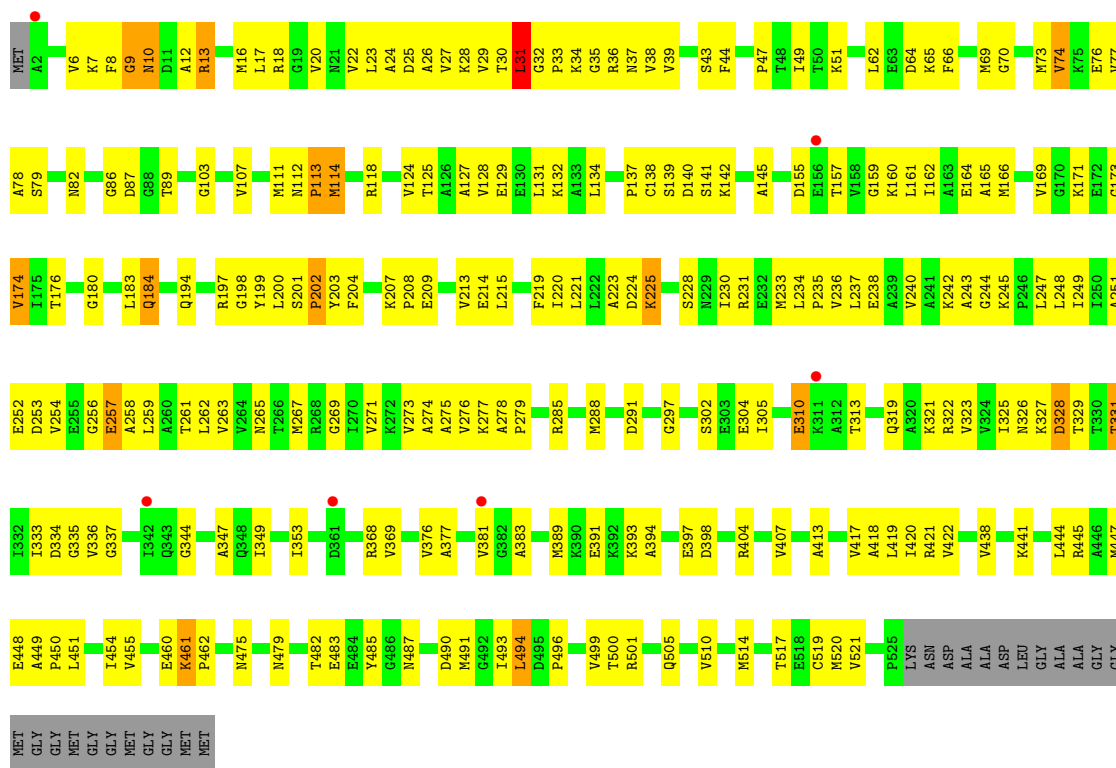


- Molecule 1: GROEL

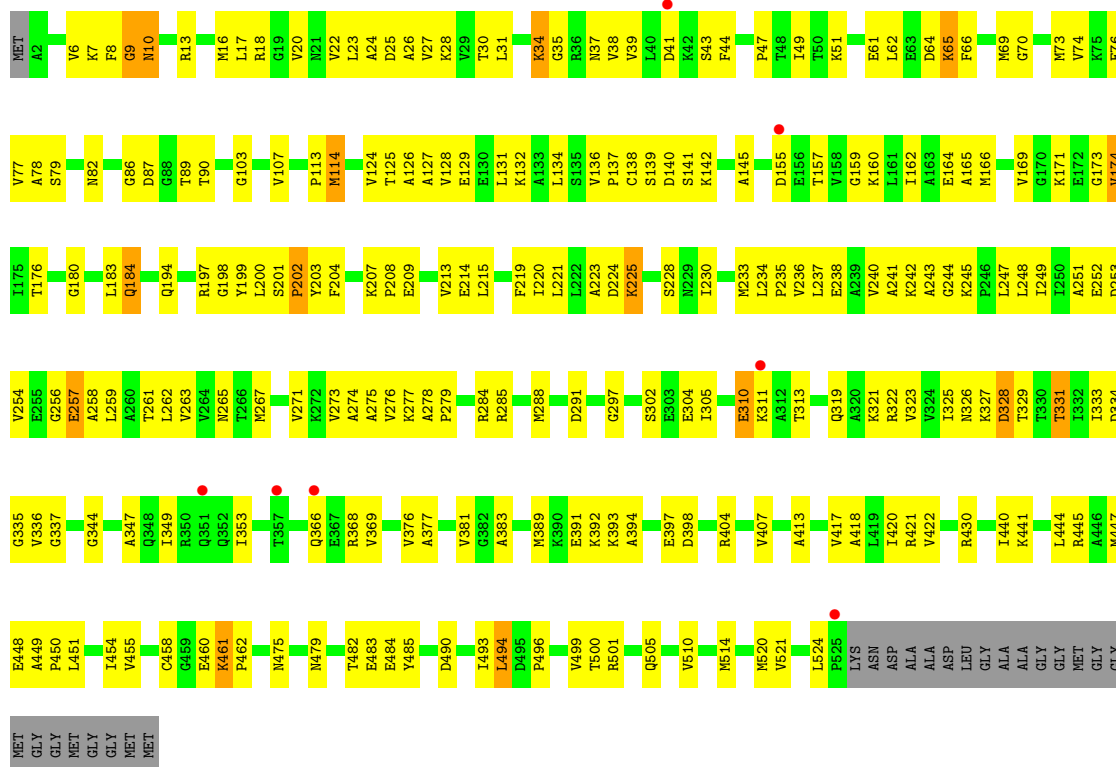


- Molecule 1: GROEL

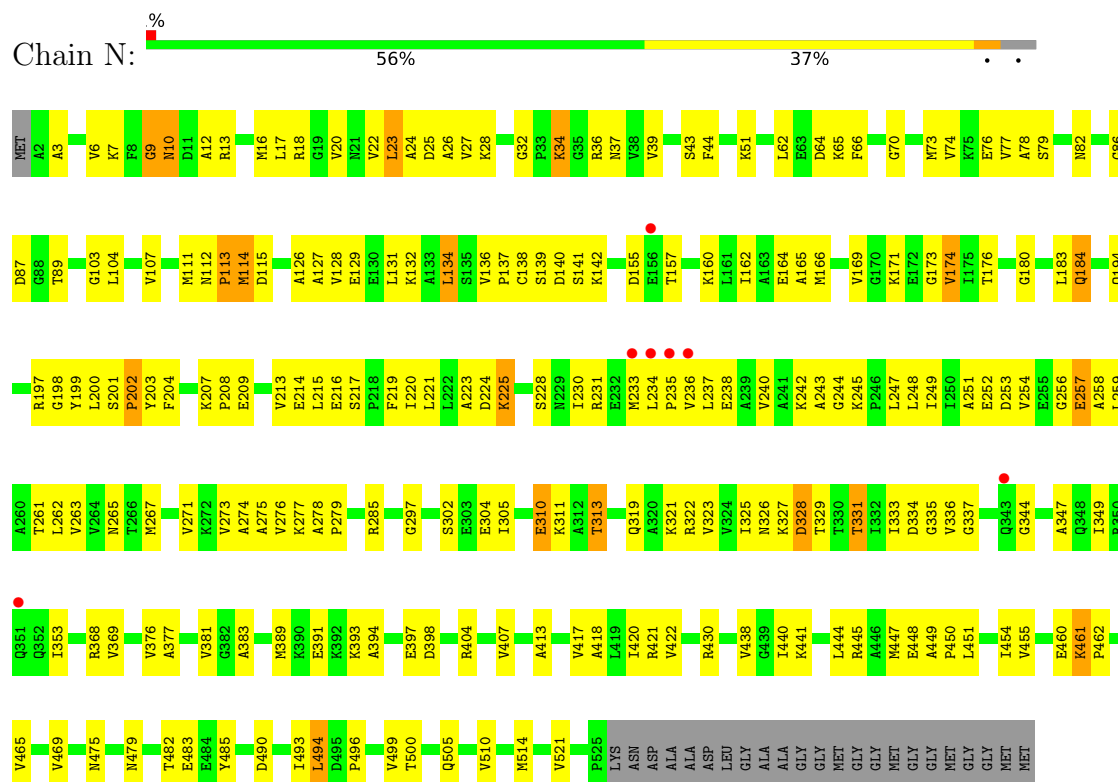




### • Molecule 1: GROEL



- Molecule 1: GROEL



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	267.69Å 290.64Å 247.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.29 39.75 – 3.29	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-3.29) 85.4 (39.75-3.29)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 3.32Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.276 , 0.296 0.266 , 0.285	Depositor DCC
$R_{free}$ test set	6133 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	70.6	Xtriage
Anisotropy	0.555	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 56.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	53970	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.51 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5101e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality

### 5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.56	1/3883 (0.0%)	0.78	3/5242 (0.1%)
1	B	0.59	0/3883	0.66	2/5242 (0.0%)
1	C	0.55	0/3883	0.68	2/5242 (0.0%)
1	D	0.54	0/3883	0.69	2/5242 (0.0%)
1	E	0.53	1/3883 (0.0%)	0.77	3/5242 (0.1%)
1	F	0.54	0/3883	0.68	2/5242 (0.0%)
1	G	0.54	0/3883	0.67	2/5242 (0.0%)
1	H	0.54	0/3883	0.79	3/5242 (0.1%)
1	I	0.57	1/3883 (0.0%)	0.68	2/5242 (0.0%)
1	J	0.53	0/3883	0.82	6/5242 (0.1%)
1	K	0.52	0/3883	0.68	2/5242 (0.0%)
1	L	0.52	0/3883	0.79	3/5242 (0.1%)
1	M	0.54	0/3883	0.83	5/5242 (0.1%)
1	N	0.52	0/3883	0.78	5/5242 (0.1%)
All	All	0.54	3/54362 (0.0%)	0.74	42/73388 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	519	CYS	CB-SG	-5.20	1.73	1.81
1	E	519	CYS	CB-SG	-5.05	1.73	1.81
1	I	519	CYS	CB-SG	-5.05	1.73	1.81

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	284	ARG	NE-CZ-NH1	-24.36	108.12	120.30
1	A	13	ARG	NE-CZ-NH2	-23.32	108.64	120.30
1	H	13	ARG	NE-CZ-NH2	-22.86	108.87	120.30
1	M	284	ARG	NE-CZ-NH2	22.53	131.56	120.30
1	L	13	ARG	NE-CZ-NH2	-22.29	109.15	120.30
1	J	231	ARG	NE-CZ-NH1	-21.84	109.38	120.30
1	E	13	ARG	NE-CZ-NH2	-21.70	109.45	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	231	ARG	NE-CZ-NH2	21.53	131.06	120.30
1	L	13	ARG	NE-CZ-NH1	19.88	130.24	120.30
1	N	368	ARG	NE-CZ-NH1	-19.48	110.56	120.30
1	A	13	ARG	NE-CZ-NH1	19.45	130.02	120.30
1	N	368	ARG	NE-CZ-NH2	19.16	129.88	120.30
1	H	13	ARG	NE-CZ-NH1	18.98	129.79	120.30
1	E	13	ARG	NE-CZ-NH1	17.93	129.27	120.30
1	D	13	ARG	NE-CZ-NH1	-11.62	114.49	120.30
1	M	284	ARG	CD-NE-CZ	11.56	139.79	123.60
1	J	231	ARG	CD-NE-CZ	10.53	138.34	123.60
1	J	13	ARG	NE-CZ-NH1	-9.86	115.37	120.30
1	H	13	ARG	CD-NE-CZ	9.85	137.39	123.60
1	K	13	ARG	NE-CZ-NH1	-9.61	115.50	120.30
1	N	13	ARG	NE-CZ-NH1	-9.55	115.52	120.30
1	E	13	ARG	CD-NE-CZ	9.54	136.96	123.60
1	M	13	ARG	NE-CZ-NH1	-9.52	115.54	120.30
1	F	13	ARG	NE-CZ-NH1	-9.46	115.57	120.30
1	L	13	ARG	CD-NE-CZ	9.40	136.76	123.60
1	A	13	ARG	CD-NE-CZ	9.34	136.68	123.60
1	C	13	ARG	NE-CZ-NH1	-9.27	115.67	120.30
1	G	13	ARG	NE-CZ-NH1	-9.09	115.76	120.30
1	I	13	ARG	NE-CZ-NH1	-8.98	115.81	120.30
1	D	13	ARG	NE-CZ-NH2	8.74	124.67	120.30
1	J	13	ARG	NE-CZ-NH2	8.62	124.61	120.30
1	N	368	ARG	CD-NE-CZ	8.41	135.37	123.60
1	C	13	ARG	NE-CZ-NH2	7.85	124.23	120.30
1	K	13	ARG	NE-CZ-NH2	7.78	124.19	120.30
1	F	13	ARG	NE-CZ-NH2	7.72	124.16	120.30
1	I	13	ARG	NE-CZ-NH2	7.66	124.13	120.30
1	B	13	ARG	NE-CZ-NH1	-7.48	116.56	120.30
1	M	13	ARG	NE-CZ-NH2	7.39	124.00	120.30
1	N	13	ARG	NE-CZ-NH2	7.26	123.93	120.30
1	G	13	ARG	NE-CZ-NH2	6.31	123.45	120.30
1	B	13	ARG	NE-CZ-NH2	6.15	123.38	120.30
1	J	32	GLY	C-N-CD	-6.04	107.32	120.60

There are no chirality outliers.

There are no planarity outliers.



## 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	3983	183	0
1	B	3855	0	3983	168	0
1	C	3855	0	3983	170	0
1	D	3855	0	3983	195	0
1	E	3855	0	3983	198	0
1	F	3855	0	3983	200	1
1	G	3855	0	3983	175	0
1	H	3855	0	3983	205	0
1	I	3855	0	3983	184	0
1	J	3855	0	3983	181	0
1	K	3855	0	3983	208	0
1	L	3855	0	3983	227	0
1	M	3855	0	3983	215	1
1	N	3855	0	3983	206	0
All	All	53970	0	55762	2596	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (2596) 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:F:326:ASN:HD22	1:F:329:THR:HB	1.03	1.12
1:A:326:ASN:HD22	1:A:329:THR:HB	1.05	1.11
1:C:326:ASN:HD22	1:C:329:THR:HB	1.07	1.11
1:E:326:ASN:HD22	1:E:329:THR:HB	1.08	1.09
1:D:326:ASN:HD22	1:D:329:THR:HB	1.04	1.08
1:G:326:ASN:HD22	1:G:329:THR:HB	1.04	1.07
1:B:326:ASN:HD22	1:B:329:THR:HB	1.11	1.05
1:E:519:CYS:HB3	1:F:38:VAL:HG13	1.46	0.98
1:J:169:VAL:HG21	1:J:377:ALA:HB2	1.51	0.91
1:F:326:ASN:ND2	1:F:329:THR:HB	1.87	0.90
1:K:33:PRO:HD2	1:K:454:ILE:HG23	1.54	0.90
1:A:326:ASN:ND2	1:A:329:THR:HB	1.88	0.88
1:G:326:ASN:ND2	1:G:329:THR:HB	1.87	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:169:VAL:HG21	1:L:377:ALA:HB2	1.54	0.88
1:A:455:VAL:HG13	1:A:460:GLU:HB2	1.55	0.88
1:K:169:VAL:HG21	1:K:377:ALA:HB2	1.54	0.88
1:D:326:ASN:ND2	1:D:329:THR:HB	1.88	0.87
1:I:169:VAL:HG21	1:I:377:ALA:HB2	1.56	0.87
1:A:32:GLY:HA3	1:A:454:ILE:HG23	1.55	0.87
1:H:169:VAL:HG21	1:H:377:ALA:HB2	1.57	0.86
1:C:326:ASN:ND2	1:C:329:THR:HB	1.89	0.86
1:K:230:ILE:HD12	1:K:261:THR:HG21	1.58	0.86
1:I:230:ILE:HD12	1:I:261:THR:HG21	1.58	0.86
1:N:169:VAL:HG21	1:N:377:ALA:HB2	1.54	0.85
1:G:455:VAL:HG13	1:G:460:GLU:HB2	1.58	0.84
1:B:455:VAL:HG13	1:B:460:GLU:HB2	1.57	0.84
1:C:455:VAL:HG13	1:C:460:GLU:HB2	1.59	0.84
1:M:169:VAL:HG21	1:M:377:ALA:HB2	1.58	0.83
1:E:326:ASN:ND2	1:E:329:THR:HB	1.92	0.83
1:N:230:ILE:HD12	1:N:261:THR:HG21	1.60	0.83
1:K:33:PRO:HD2	1:K:454:ILE:CG2	2.10	0.82
1:H:230:ILE:HD12	1:H:261:THR:HG21	1.59	0.82
1:J:253:ASP:HB2	1:J:277:LYS:HE3	1.61	0.82
1:H:32:GLY:HA3	1:H:454:ILE:HG23	1.59	0.81
1:H:221:LEU:HD23	1:H:249:ILE:HD12	1.62	0.81
1:K:449:ALA:HB3	1:K:450:PRO:HD3	1.61	0.81
1:M:230:ILE:HD12	1:M:261:THR:HG21	1.62	0.81
1:N:253:ASP:HB2	1:N:277:LYS:HE3	1.62	0.81
1:G:200:LEU:HG	1:G:276:VAL:HA	1.61	0.81
1:J:230:ILE:HD12	1:J:261:THR:HG21	1.63	0.81
1:G:311:LYS:NZ	1:N:313:THR:HG23	1.95	0.81
1:D:200:LEU:HG	1:D:276:VAL:HA	1.64	0.80
1:L:520:MET:HG2	1:M:39:VAL:HB	1.62	0.80
1:N:214:GLU:O	1:N:215:LEU:HD23	1.81	0.80
1:I:449:ALA:HB3	1:I:450:PRO:HD3	1.63	0.80
1:E:517:THR:HG21	1:F:39:VAL:HG23	1.64	0.80
1:E:69:MET:SD	1:F:41:ASP:HB2	2.21	0.80
1:M:449:ALA:HB3	1:M:450:PRO:HD3	1.62	0.80
1:D:455:VAL:HG13	1:D:460:GLU:HB2	1.64	0.79
1:I:253:ASP:HB2	1:I:277:LYS:HE3	1.64	0.79
1:K:27:VAL:O	1:K:30:THR:HG22	1.81	0.79
1:L:230:ILE:HD12	1:L:261:THR:HG21	1.62	0.79
1:L:253:ASP:HB2	1:L:277:LYS:HE3	1.63	0.79
1:C:200:LEU:HG	1:C:276:VAL:HA	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:449:ALA:HB3	1:N:450:PRO:HD3	1.63	0.79
1:F:200:LEU:HG	1:F:276:VAL:HA	1.64	0.79
1:B:200:LEU:HG	1:B:276:VAL:HA	1.64	0.78
1:E:200:LEU:HG	1:E:276:VAL:HA	1.63	0.78
1:L:519:CYS:HB3	1:M:38:VAL:HG13	1.64	0.78
1:K:28:LYS:C	1:K:30:THR:H	1.85	0.78
1:E:8:PHE:HE1	1:F:26:ALA:HA	1.49	0.78
1:J:16:MET:SD	1:J:514:MET:HE2	2.24	0.78
1:K:221:LEU:HD23	1:K:249:ILE:HD12	1.65	0.78
1:E:455:VAL:HG13	1:E:460:GLU:HB2	1.65	0.78
1:J:449:ALA:HB3	1:J:450:PRO:HD3	1.65	0.78
1:M:253:ASP:HB2	1:M:277:LYS:HE3	1.63	0.78
1:N:32:GLY:HA3	1:N:454:ILE:HG23	1.66	0.77
1:J:221:LEU:HD23	1:J:249:ILE:HD12	1.65	0.77
1:L:8:PHE:HZ	1:M:26:ALA:HB2	1.47	0.77
1:I:16:MET:SD	1:I:514:MET:HE2	2.23	0.77
1:L:254:VAL:HG12	1:L:259:LEU:HB2	1.66	0.77
1:M:16:MET:SD	1:M:73:MET:HE1	2.25	0.77
1:L:8:PHE:HE1	1:M:26:ALA:HA	1.48	0.77
1:A:200:LEU:HG	1:A:276:VAL:HA	1.65	0.77
1:G:311:LYS:HZ3	1:N:313:THR:HG23	1.47	0.77
1:N:221:LEU:HD23	1:N:249:ILE:HD12	1.66	0.77
1:J:254:VAL:HG12	1:J:259:LEU:HB2	1.67	0.77
1:H:253:ASP:HB2	1:H:277:LYS:HE3	1.67	0.76
1:I:221:LEU:HD23	1:I:249:ILE:HD12	1.67	0.76
1:K:28:LYS:C	1:K:30:THR:N	2.38	0.76
1:A:34:LYS:HB3	1:G:114:MET:HG3	1.67	0.76
1:M:221:LEU:HD23	1:M:249:ILE:HD12	1.64	0.76
1:N:228:SER:O	1:N:257:GLU:HB3	1.85	0.76
1:L:449:ALA:HB3	1:L:450:PRO:HD3	1.66	0.76
1:K:381:VAL:HG21	1:K:393:LYS:HA	1.67	0.76
1:D:221:LEU:HD23	1:D:249:ILE:HD12	1.68	0.76
1:L:228:SER:O	1:L:257:GLU:HB3	1.85	0.76
1:B:326:ASN:ND2	1:B:329:THR:HB	1.96	0.76
1:H:494:LEU:H	1:H:494:LEU:HD12	1.51	0.76
1:H:449:ALA:HB3	1:H:450:PRO:HD3	1.65	0.76
1:I:381:VAL:HG21	1:I:393:LYS:HA	1.66	0.76
1:N:381:VAL:HG21	1:N:393:LYS:HA	1.68	0.75
1:F:85:ALA:HB1	1:F:499:VAL:HG12	1.69	0.75
1:L:221:LEU:HD23	1:L:249:ILE:HD12	1.67	0.75
1:M:254:VAL:HG12	1:M:259:LEU:HB2	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:494:LEU:H	1:M:494:LEU:HD12	1.51	0.75
1:I:404:ARG:HG2	1:I:404:ARG:HH11	1.51	0.75
1:M:381:VAL:HG21	1:M:393:LYS:HA	1.68	0.75
1:K:254:VAL:HG12	1:K:259:LEU:HB2	1.68	0.75
1:E:311:LYS:HD3	1:I:311:LYS:HB3	1.69	0.75
1:F:221:LEU:HD23	1:F:249:ILE:HD12	1.69	0.75
1:I:254:VAL:HG12	1:I:259:LEU:HB2	1.68	0.75
1:K:16:MET:SD	1:K:73:MET:HE1	2.26	0.75
1:E:311:LYS:HB3	1:I:311:LYS:HD3	1.67	0.75
1:N:16:MET:SD	1:N:514:MET:HE2	2.26	0.75
1:N:494:LEU:H	1:N:494:LEU:HD12	1.51	0.75
1:I:383:ALA:HB3	1:I:389:MET:HB2	1.68	0.74
1:C:85:ALA:HB1	1:C:499:VAL:HG12	1.69	0.74
1:L:381:VAL:HG21	1:L:393:LYS:HA	1.69	0.74
1:L:383:ALA:HB3	1:L:389:MET:HB2	1.67	0.74
1:B:85:ALA:HB1	1:B:499:VAL:HG12	1.69	0.74
1:N:254:VAL:HG12	1:N:259:LEU:HB2	1.70	0.74
1:A:85:ALA:HB1	1:A:499:VAL:HG12	1.69	0.74
1:E:85:ALA:HB1	1:E:499:VAL:HG12	1.70	0.74
1:K:16:MET:HB3	1:K:514:MET:HE1	1.70	0.74
1:K:18:ARG:HG2	1:K:18:ARG:HH11	1.53	0.74
1:A:221:LEU:HD23	1:A:249:ILE:HD12	1.70	0.74
1:H:241:ALA:HB1	1:N:231:ARG:NH1	2.03	0.74
1:I:494:LEU:H	1:I:494:LEU:HD12	1.53	0.74
1:H:461:LYS:HA	1:H:461:LYS:HE3	1.70	0.74
1:J:214:GLU:O	1:J:215:LEU:HD23	1.87	0.73
1:K:228:SER:O	1:K:257:GLU:HB3	1.87	0.73
1:I:461:LYS:HE3	1:I:461:LYS:HA	1.71	0.73
1:F:455:VAL:HG13	1:F:460:GLU:HB2	1.68	0.73
1:M:6:VAL:HG22	1:M:521:VAL:HG22	1.68	0.73
1:F:183:LEU:HD13	1:F:184:GLN:HG3	1.69	0.73
1:H:254:VAL:HG12	1:H:259:LEU:HB2	1.70	0.73
1:N:461:LYS:HA	1:N:461:LYS:HE3	1.71	0.73
1:C:221:LEU:HD23	1:C:249:ILE:HD12	1.69	0.73
1:D:118:ARG:HH22	1:E:34:LYS:HE2	1.53	0.73
1:F:455:VAL:HG11	1:F:462:PRO:HA	1.71	0.73
1:H:228:SER:O	1:H:257:GLU:HB3	1.88	0.73
1:L:461:LYS:HA	1:L:461:LYS:HE3	1.69	0.73
1:J:6:VAL:HG22	1:J:521:VAL:HG22	1.69	0.73
1:J:228:SER:O	1:J:257:GLU:HB3	1.89	0.73
1:K:383:ALA:HB3	1:K:389:MET:HB2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:183:LEU:HD13	1:G:184:GLN:HG3	1.71	0.72
1:I:228:SER:O	1:I:257:GLU:HB3	1.89	0.72
1:J:16:MET:SD	1:J:73:MET:HE1	2.29	0.72
1:K:253:ASP:HB2	1:K:277:LYS:HE3	1.70	0.72
1:L:404:ARG:HG2	1:L:404:ARG:HH11	1.54	0.72
1:M:461:LYS:HA	1:M:461:LYS:HE3	1.71	0.72
1:E:183:LEU:HD13	1:E:184:GLN:HG3	1.72	0.72
1:L:494:LEU:HD12	1:L:494:LEU:H	1.55	0.72
1:G:85:ALA:HB1	1:G:499:VAL:HG12	1.70	0.72
1:J:461:LYS:HA	1:J:461:LYS:HE3	1.70	0.72
1:L:16:MET:HB3	1:L:514:MET:HE1	1.72	0.72
1:L:214:GLU:O	1:L:215:LEU:HD23	1.89	0.72
1:A:252:GLU:O	1:A:253:ASP:HB2	1.90	0.71
1:M:228:SER:O	1:M:257:GLU:HB3	1.89	0.71
1:N:235:PRO:HG3	1:N:310:GLU:HG3	1.72	0.71
1:J:494:LEU:H	1:J:494:LEU:HD12	1.54	0.71
1:C:183:LEU:HD22	1:C:184:GLN:H	1.54	0.71
1:D:183:LEU:HD13	1:D:184:GLN:HG3	1.72	0.71
1:H:214:GLU:O	1:H:215:LEU:HD23	1.89	0.71
1:J:169:VAL:HG12	1:J:173:GLY:HA3	1.72	0.71
1:A:183:LEU:HD13	1:A:184:GLN:HG3	1.72	0.71
1:C:183:LEU:HD13	1:C:184:GLN:HG3	1.71	0.71
1:F:183:LEU:HD22	1:F:184:GLN:H	1.55	0.71
1:M:16:MET:HB3	1:M:514:MET:HE1	1.72	0.71
1:H:381:VAL:HG21	1:H:393:LYS:HA	1.73	0.71
1:H:404:ARG:HG2	1:H:404:ARG:HH11	1.56	0.71
1:I:214:GLU:O	1:I:215:LEU:HD23	1.91	0.71
1:M:214:GLU:O	1:M:215:LEU:HD23	1.90	0.71
1:N:383:ALA:HB3	1:N:389:MET:HB2	1.72	0.71
1:K:169:VAL:HG12	1:K:173:GLY:HA3	1.73	0.71
1:K:404:ARG:HG2	1:K:404:ARG:HH11	1.56	0.71
1:B:183:LEU:HD13	1:B:184:GLN:HG3	1.73	0.71
1:J:235:PRO:HG3	1:J:310:GLU:HG3	1.73	0.71
1:J:383:ALA:HB3	1:J:389:MET:HB2	1.72	0.71
1:B:221:LEU:HD23	1:B:249:ILE:HD12	1.73	0.70
1:D:34:LYS:HD2	1:D:458:CYS:CB	2.21	0.70
1:H:18:ARG:HG2	1:H:18:ARG:HH11	1.56	0.70
1:L:6:VAL:HG22	1:L:521:VAL:HG22	1.71	0.70
1:H:269:GLY:HA3	1:N:257:GLU:HG3	1.72	0.70
1:E:183:LEU:HD22	1:E:184:GLN:H	1.56	0.70
1:K:118:ARG:HH22	1:L:34:LYS:HE2	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:404:ARG:HG2	1:M:404:ARG:HH11	1.57	0.70
1:E:221:LEU:HD23	1:E:249:ILE:HD12	1.74	0.70
1:I:235:PRO:HG3	1:I:310:GLU:HG3	1.74	0.70
1:K:494:LEU:H	1:K:494:LEU:HD12	1.56	0.70
1:M:18:ARG:HG2	1:M:18:ARG:HH11	1.57	0.70
1:N:404:ARG:HG2	1:N:404:ARG:HH11	1.57	0.70
1:L:69:MET:HE2	1:M:39:VAL:HG12	1.73	0.70
1:M:383:ALA:HB3	1:M:389:MET:HB2	1.72	0.70
1:K:235:PRO:HG3	1:K:310:GLU:HG3	1.73	0.70
1:L:235:PRO:HG3	1:L:310:GLU:HG3	1.72	0.70
1:E:252:GLU:O	1:E:253:ASP:HB2	1.91	0.70
1:H:16:MET:HB3	1:H:514:MET:HE1	1.74	0.70
1:G:183:LEU:HD22	1:G:184:GLN:H	1.56	0.69
1:J:404:ARG:HG2	1:J:404:ARG:HH11	1.56	0.69
1:M:22:VAL:HG11	1:M:62:LEU:HD21	1.74	0.69
1:N:6:VAL:HG22	1:N:521:VAL:HG22	1.73	0.69
1:N:16:MET:SD	1:N:73:MET:HE1	2.33	0.69
1:E:8:PHE:HZ	1:F:26:ALA:HB2	1.58	0.69
1:G:221:LEU:HD23	1:G:249:ILE:HD12	1.72	0.69
1:K:461:LYS:HA	1:K:461:LYS:HE3	1.74	0.69
1:A:183:LEU:HD22	1:A:184:GLN:H	1.56	0.69
1:H:383:ALA:HB3	1:H:389:MET:HB2	1.74	0.69
1:N:169:VAL:HG12	1:N:173:GLY:HA3	1.75	0.69
1:H:235:PRO:HG3	1:H:310:GLU:HG3	1.75	0.69
1:F:252:GLU:O	1:F:253:ASP:HB2	1.93	0.69
1:M:31:LEU:HD23	1:M:31:LEU:C	2.13	0.69
1:F:82:ASN:HB2	1:F:89:THR:OG1	1.93	0.69
1:D:85:ALA:HB1	1:D:499:VAL:HG12	1.74	0.68
1:G:252:GLU:O	1:G:253:ASP:HB2	1.93	0.68
1:M:169:VAL:HG12	1:M:173:GLY:HA3	1.75	0.68
1:M:174:VAL:HG23	1:M:376:VAL:HA	1.75	0.68
1:A:455:VAL:HG13	1:A:460:GLU:CB	2.23	0.68
1:J:381:VAL:HG21	1:J:393:LYS:HA	1.74	0.68
1:K:214:GLU:O	1:K:215:LEU:HD23	1.92	0.68
1:N:22:VAL:HG11	1:N:62:LEU:HD21	1.75	0.68
1:F:311:LYS:HB3	1:H:311:LYS:HG2	1.75	0.68
1:L:17:LEU:HA	1:L:20:VAL:HG12	1.73	0.68
1:J:194:GLN:HB2	1:J:331:THR:HB	1.74	0.68
1:L:169:VAL:HG12	1:L:173:GLY:HA3	1.75	0.68
1:M:173:GLY:O	1:M:404:ARG:NH2	2.27	0.68
1:K:194:GLN:HB2	1:K:331:THR:HB	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:194:GLN:HB2	1:L:331:THR:HB	1.76	0.68
1:B:247:LEU:HB3	1:B:273:VAL:HG12	1.73	0.68
1:C:247:LEU:HB3	1:C:273:VAL:HG12	1.74	0.68
1:K:496:PRO:O	1:K:499:VAL:HG13	1.94	0.68
1:H:16:MET:SD	1:H:514:MET:HE2	2.34	0.68
1:H:183:LEU:HD13	1:H:184:GLN:N	2.09	0.68
1:K:183:LEU:HD13	1:K:184:GLN:N	2.09	0.68
1:H:194:GLN:HB2	1:H:331:THR:HB	1.76	0.67
1:L:199:TYR:HA	1:L:276:VAL:HG12	1.76	0.67
1:D:252:GLU:O	1:D:253:ASP:HB2	1.93	0.67
1:L:496:PRO:O	1:L:499:VAL:HG13	1.94	0.67
1:M:199:TYR:HA	1:M:276:VAL:HG12	1.76	0.67
1:D:183:LEU:HD22	1:D:184:GLN:H	1.58	0.67
1:H:420:ILE:HG13	1:H:448:GLU:HG2	1.77	0.67
1:I:17:LEU:HA	1:I:20:VAL:HG12	1.77	0.67
1:D:455:VAL:HG11	1:D:462:PRO:HA	1.77	0.67
1:M:235:PRO:HG3	1:M:310:GLU:HG3	1.74	0.67
1:E:383:ALA:HB3	1:E:389:MET:HB2	1.76	0.67
1:J:496:PRO:O	1:J:499:VAL:HG13	1.95	0.67
1:C:449:ALA:HB3	1:C:450:PRO:HD3	1.77	0.67
1:E:8:PHE:CE1	1:F:26:ALA:HA	2.29	0.67
1:J:199:TYR:HA	1:J:276:VAL:HG12	1.76	0.67
1:M:17:LEU:HA	1:M:20:VAL:HG12	1.76	0.67
1:M:420:ILE:HG13	1:M:448:GLU:HG2	1.76	0.67
1:N:194:GLN:HB2	1:N:331:THR:HB	1.77	0.67
1:F:247:LEU:HB3	1:F:273:VAL:HG12	1.76	0.67
1:H:22:VAL:HG11	1:H:62:LEU:HD21	1.75	0.67
1:H:169:VAL:HG12	1:H:173:GLY:HA3	1.76	0.67
1:B:183:LEU:HD22	1:B:184:GLN:H	1.59	0.67
1:C:252:GLU:O	1:C:253:ASP:HB2	1.93	0.67
1:G:31:LEU:O	1:G:457:ASN:ND2	2.27	0.67
1:E:247:LEU:HB3	1:E:273:VAL:HG12	1.77	0.67
1:H:17:LEU:HA	1:H:20:VAL:HG12	1.77	0.67
1:M:326:ASN:OD1	1:M:329:THR:HB	1.95	0.67
1:J:174:VAL:HG21	1:J:376:VAL:HG22	1.76	0.66
1:L:8:PHE:CZ	1:M:26:ALA:HB2	2.29	0.66
1:B:455:VAL:HG13	1:B:460:GLU:CB	2.25	0.66
1:D:230:ILE:HD12	1:D:261:THR:HG21	1.77	0.66
1:L:22:VAL:HG11	1:L:62:LEU:HD21	1.77	0.66
1:K:237:LEU:O	1:K:237:LEU:HD23	1.96	0.66
1:L:420:ILE:HG13	1:L:448:GLU:HG2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:247:LEU:HB3	1:G:273:VAL:HG12	1.77	0.66
1:H:496:PRO:O	1:H:499:VAL:HG13	1.95	0.66
1:K:219:PHE:O	1:K:247:LEU:HD12	1.95	0.66
1:B:230:ILE:HD12	1:B:261:THR:HG21	1.78	0.66
1:B:252:GLU:O	1:B:253:ASP:HB2	1.94	0.66
1:G:455:VAL:HG13	1:G:460:GLU:CB	2.26	0.66
1:H:16:MET:SD	1:H:73:MET:HE1	2.36	0.66
1:I:22:VAL:HG11	1:I:62:LEU:HD21	1.76	0.66
1:I:169:VAL:HG12	1:I:173:GLY:HA3	1.78	0.66
1:J:18:ARG:HG2	1:J:18:ARG:HH11	1.61	0.66
1:M:194:GLN:HB2	1:M:331:THR:HB	1.77	0.66
1:G:228:SER:O	1:G:257:GLU:HB3	1.95	0.66
1:H:174:VAL:HG23	1:H:376:VAL:HA	1.78	0.66
1:I:199:TYR:HA	1:I:276:VAL:HG12	1.77	0.66
1:M:237:LEU:HD23	1:M:237:LEU:O	1.95	0.66
1:A:230:ILE:HD12	1:A:261:THR:HG21	1.78	0.66
1:A:449:ALA:HB3	1:A:450:PRO:HD3	1.78	0.66
1:G:482:THR:O	1:G:484:GLU:HG3	1.95	0.66
1:H:173:GLY:O	1:H:404:ARG:NH2	2.29	0.66
1:J:174:VAL:HG23	1:J:376:VAL:HA	1.77	0.66
1:L:18:ARG:HG2	1:L:18:ARG:HH11	1.61	0.65
1:L:237:LEU:O	1:L:237:LEU:HD23	1.96	0.65
1:L:519:CYS:O	1:M:39:VAL:N	2.29	0.65
1:A:482:THR:O	1:A:484:GLU:HG3	1.96	0.65
1:B:482:THR:O	1:B:484:GLU:HG3	1.95	0.65
1:J:183:LEU:HD13	1:J:184:GLN:N	2.10	0.65
1:L:69:MET:HE2	1:M:39:VAL:CG1	2.27	0.65
1:M:249:ILE:HB	1:M:275:ALA:HB2	1.77	0.65
1:D:247:LEU:HB3	1:D:273:VAL:HG12	1.76	0.65
1:I:76:GLU:O	1:I:79:SER:HB3	1.97	0.65
1:K:174:VAL:HG23	1:K:376:VAL:HA	1.77	0.65
1:F:230:ILE:HD12	1:F:261:THR:HG21	1.78	0.65
1:G:183:LEU:O	1:G:184:GLN:HB2	1.95	0.65
1:H:199:TYR:HA	1:H:276:VAL:HG12	1.77	0.65
1:N:249:ILE:HB	1:N:275:ALA:HB2	1.78	0.65
1:K:199:TYR:HA	1:K:276:VAL:HG12	1.77	0.65
1:E:482:THR:O	1:E:484:GLU:HG3	1.97	0.65
1:L:174:VAL:HG23	1:L:376:VAL:HA	1.78	0.65
1:B:82:ASN:HB2	1:B:89:THR:OG1	1.97	0.65
1:C:230:ILE:HG22	1:C:257:GLU:OE1	1.97	0.65
1:C:321:LYS:O	1:C:322:ARG:HB2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:183:LEU:O	1:E:184:GLN:HB2	1.97	0.65
1:A:247:LEU:HB3	1:A:273:VAL:HG12	1.79	0.65
1:B:176:THR:HG21	1:B:333:ILE:HD13	1.78	0.65
1:G:230:ILE:HD12	1:G:261:THR:HG21	1.78	0.65
1:I:237:LEU:O	1:I:237:LEU:HD23	1.95	0.65
1:J:326:ASN:OD1	1:J:329:THR:HB	1.97	0.65
1:K:22:VAL:HG11	1:K:62:LEU:HD21	1.79	0.65
1:L:69:MET:SD	1:M:41:ASP:HB2	2.36	0.65
1:B:383:ALA:HB3	1:B:389:MET:HB2	1.79	0.65
1:E:214:GLU:O	1:E:215:LEU:HD23	1.96	0.65
1:F:311:LYS:HD3	1:H:311:LYS:HA	1.77	0.65
1:H:32:GLY:O	1:H:34:LYS:N	2.30	0.65
1:L:520:MET:HA	1:M:39:VAL:O	1.97	0.65
1:N:17:LEU:HA	1:N:20:VAL:HG12	1.79	0.65
1:B:511:ALA:O	1:B:515:ILE:HG13	1.98	0.64
1:C:82:ASN:HB2	1:C:89:THR:OG1	1.97	0.64
1:G:230:ILE:HG22	1:G:257:GLU:OE1	1.96	0.64
1:K:249:ILE:HB	1:K:275:ALA:HB2	1.79	0.64
1:A:214:GLU:O	1:A:215:LEU:HD23	1.98	0.64
1:I:194:GLN:HB2	1:I:331:THR:HB	1.79	0.64
1:J:237:LEU:HD23	1:J:237:LEU:O	1.97	0.64
1:J:249:ILE:HB	1:J:275:ALA:HB2	1.78	0.64
1:N:173:GLY:O	1:N:404:ARG:NH2	2.29	0.64
1:I:18:ARG:HH11	1:I:18:ARG:HG2	1.61	0.64
1:J:22:VAL:HG11	1:J:62:LEU:HD21	1.77	0.64
1:N:420:ILE:HG13	1:N:448:GLU:HG2	1.80	0.64
1:A:183:LEU:O	1:A:184:GLN:HB2	1.98	0.64
1:A:228:SER:O	1:A:257:GLU:HB3	1.96	0.64
1:C:183:LEU:O	1:C:184:GLN:HB2	1.97	0.64
1:C:230:ILE:HD12	1:C:261:THR:HG21	1.77	0.64
1:D:183:LEU:O	1:D:184:GLN:HB2	1.97	0.64
1:E:82:ASN:HB2	1:E:89:THR:OG1	1.98	0.64
1:H:6:VAL:HG22	1:H:521:VAL:HG22	1.78	0.64
1:H:241:ALA:HB1	1:N:231:ARG:HH11	1.63	0.64
1:H:249:ILE:HB	1:H:275:ALA:HB2	1.79	0.64
1:N:183:LEU:HD13	1:N:184:GLN:N	2.13	0.64
1:D:254:VAL:HG12	1:D:259:LEU:HB2	1.80	0.64
1:F:31:LEU:HD23	1:F:94:VAL:HG11	1.78	0.64
1:I:249:ILE:HB	1:I:275:ALA:HB2	1.79	0.64
1:N:237:LEU:O	1:N:237:LEU:HD23	1.97	0.64
1:E:519:CYS:CB	1:F:38:VAL:HG13	2.23	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:18:ARG:HG2	1:N:18:ARG:HH11	1.62	0.64
1:B:202:PRO:HB3	1:B:205:ILE:HD11	1.80	0.64
1:F:7:LYS:HG3	1:F:66:PHE:CZ	2.32	0.64
1:K:8:PHE:HE1	1:L:26:ALA:HA	1.63	0.64
1:G:214:GLU:O	1:G:215:LEU:HD23	1.97	0.64
1:G:254:VAL:HG12	1:G:259:LEU:HB2	1.80	0.64
1:H:174:VAL:HG21	1:H:376:VAL:HG22	1.81	0.64
1:N:37:ASN:HD21	1:N:51:LYS:NZ	1.96	0.64
1:B:183:LEU:O	1:B:184:GLN:HB2	1.96	0.63
1:F:69:MET:SD	1:G:41:ASP:HB2	2.38	0.63
1:F:183:LEU:O	1:F:184:GLN:HB2	1.97	0.63
1:I:496:PRO:O	1:I:499:VAL:HG13	1.96	0.63
1:L:249:ILE:HB	1:L:275:ALA:HB2	1.79	0.63
1:M:166:MET:CE	1:M:171:LYS:HA	2.28	0.63
1:B:230:ILE:HG22	1:B:257:GLU:OE1	1.98	0.63
1:D:202:PRO:HB3	1:D:205:ILE:HD11	1.80	0.63
1:E:228:SER:O	1:E:257:GLU:HB3	1.99	0.63
1:E:230:ILE:HD12	1:E:261:THR:HG21	1.80	0.63
1:G:144:ILE:HD13	1:G:166:MET:SD	2.38	0.63
1:A:222:LEU:HD23	1:A:250:ILE:HB	1.81	0.63
1:E:455:VAL:HG11	1:E:462:PRO:HA	1.79	0.63
1:F:297:GLY:O	1:F:318:GLY:HA2	1.98	0.63
1:L:16:MET:SD	1:L:73:MET:HE1	2.39	0.63
1:A:321:LYS:O	1:A:322:ARG:HB2	1.99	0.63
1:F:90:THR:O	1:F:94:VAL:HG13	1.98	0.63
1:H:237:LEU:O	1:H:237:LEU:HD23	1.98	0.63
1:J:420:ILE:HG13	1:J:448:GLU:HG2	1.80	0.63
1:K:166:MET:CE	1:K:171:LYS:HA	2.27	0.63
1:M:183:LEU:HD13	1:M:184:GLN:N	2.13	0.63
1:C:176:THR:HG21	1:C:333:ILE:HD13	1.80	0.63
1:E:511:ALA:O	1:E:515:ILE:HG13	1.99	0.63
1:I:420:ILE:HG13	1:I:448:GLU:HG2	1.79	0.63
1:J:213:VAL:HG12	1:J:214:GLU:N	2.13	0.63
1:N:174:VAL:HG23	1:N:376:VAL:HA	1.79	0.63
1:N:247:LEU:HB3	1:N:273:VAL:HG12	1.80	0.63
1:C:482:THR:O	1:C:484:GLU:HG3	1.99	0.63
1:D:449:ALA:HB3	1:D:450:PRO:HD3	1.81	0.63
1:K:213:VAL:HG12	1:K:214:GLU:N	2.13	0.63
1:L:8:PHE:CE1	1:M:26:ALA:HA	2.31	0.63
1:M:496:PRO:O	1:M:499:VAL:HG13	1.99	0.63
1:N:199:TYR:HA	1:N:276:VAL:HG12	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:ALA:O	1:A:515:ILE:HG13	1.98	0.63
1:C:455:VAL:HG13	1:C:460:GLU:CB	2.29	0.63
1:A:297:GLY:O	1:A:318:GLY:HA2	1.99	0.63
1:F:230:ILE:HG22	1:F:257:GLU:OE1	1.99	0.63
1:D:228:SER:O	1:D:257:GLU:HB3	1.98	0.63
1:E:202:PRO:HB3	1:E:205:ILE:HD11	1.80	0.63
1:E:230:ILE:HG22	1:E:257:GLU:OE1	1.99	0.63
1:K:28:LYS:O	1:K:30:THR:N	2.32	0.63
1:K:420:ILE:HG13	1:K:448:GLU:HG2	1.81	0.63
1:B:7:LYS:HG3	1:B:66:PHE:CZ	2.34	0.62
1:E:517:THR:CG2	1:F:39:VAL:HG23	2.27	0.62
1:I:183:LEU:HD13	1:I:184:GLN:N	2.14	0.62
1:J:247:LEU:HB3	1:J:273:VAL:HG12	1.81	0.62
1:N:326:ASN:OD1	1:N:329:THR:HB	1.99	0.62
1:F:449:ALA:HB3	1:F:450:PRO:HD3	1.81	0.62
1:L:493:ILE:O	1:L:493:ILE:HG22	1.97	0.62
1:M:391:GLU:O	1:M:394:ALA:HB3	2.00	0.62
1:C:214:GLU:O	1:C:215:LEU:HD23	1.99	0.62
1:D:295:LEU:HA	1:D:342:ILE:HD11	1.81	0.62
1:D:326:ASN:HD22	1:D:329:THR:CB	1.97	0.62
1:F:228:SER:O	1:F:257:GLU:HB3	1.99	0.62
1:I:213:VAL:HG12	1:I:214:GLU:N	2.13	0.62
1:M:247:LEU:HB3	1:M:273:VAL:HG12	1.81	0.62
1:B:131:LEU:CD1	1:B:422:VAL:HG21	2.29	0.62
1:C:131:LEU:CD1	1:C:422:VAL:HG21	2.29	0.62
1:C:202:PRO:HB3	1:C:205:ILE:HD11	1.81	0.62
1:A:82:ASN:HB2	1:A:89:THR:OG1	1.99	0.62
1:C:69:MET:SD	1:D:41:ASP:HB2	2.40	0.62
1:C:222:LEU:HD23	1:C:250:ILE:HB	1.81	0.62
1:D:383:ALA:HB3	1:D:389:MET:HB2	1.80	0.62
1:H:247:LEU:HB3	1:H:273:VAL:HG12	1.82	0.62
1:H:493:ILE:HG22	1:H:493:ILE:O	1.99	0.62
1:D:214:GLU:O	1:D:215:LEU:HD23	2.00	0.62
1:D:230:ILE:HG22	1:D:257:GLU:OE1	1.99	0.62
1:H:183:LEU:O	1:H:184:GLN:HB2	1.99	0.62
1:J:17:LEU:HA	1:J:20:VAL:HG12	1.81	0.62
1:A:176:THR:HG21	1:A:333:ILE:HD13	1.82	0.62
1:C:455:VAL:HG11	1:C:462:PRO:HA	1.81	0.62
1:D:222:LEU:HD23	1:D:250:ILE:HB	1.80	0.62
1:G:90:THR:O	1:G:94:VAL:HG13	2.00	0.62
1:K:76:GLU:O	1:K:79:SER:HB3	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:349:ILE:O	1:K:353:ILE:HG13	2.00	0.62
1:N:213:VAL:HG12	1:N:214:GLU:N	2.15	0.62
1:D:482:THR:O	1:D:484:GLU:HG3	1.98	0.62
1:J:37:ASN:ND2	1:J:51:LYS:HG3	2.14	0.62
1:J:219:PHE:O	1:J:247:LEU:HD12	2.00	0.62
1:F:519:CYS:HB3	1:G:38:VAL:HG13	1.81	0.62
1:G:222:LEU:HD23	1:G:250:ILE:HB	1.82	0.62
1:G:321:LYS:O	1:G:322:ARG:HB2	1.99	0.62
1:H:76:GLU:O	1:H:79:SER:HB3	2.00	0.62
1:I:6:VAL:HG22	1:I:521:VAL:HG22	1.81	0.62
1:K:173:GLY:O	1:K:404:ARG:NH2	2.33	0.62
1:N:219:PHE:O	1:N:247:LEU:HD12	1.99	0.62
1:A:131:LEU:CD1	1:A:422:VAL:HG21	2.30	0.61
1:L:519:CYS:CB	1:M:38:VAL:HG13	2.29	0.61
1:M:321:LYS:O	1:M:322:ARG:HB2	2.00	0.61
1:E:449:ALA:HB3	1:E:450:PRO:HD3	1.81	0.61
1:F:383:ALA:HB3	1:F:389:MET:HB2	1.82	0.61
1:G:202:PRO:HB3	1:G:205:ILE:HD11	1.81	0.61
1:K:6:VAL:HG22	1:K:521:VAL:HG22	1.81	0.61
1:B:321:LYS:O	1:B:322:ARG:HB2	2.00	0.61
1:E:245:LYS:NZ	1:E:319:GLN:HE22	1.98	0.61
1:C:519:CYS:HB3	1:D:38:VAL:HG13	1.82	0.61
1:D:176:THR:HG21	1:D:333:ILE:HD13	1.82	0.61
1:C:383:ALA:HB3	1:C:389:MET:HB2	1.82	0.61
1:D:213:VAL:HG12	1:D:214:GLU:N	2.16	0.61
1:D:519:CYS:HB3	1:E:38:VAL:HG13	1.83	0.61
1:F:429:LEU:HD12	1:F:430:ARG:H	1.65	0.61
1:H:166:MET:CE	1:H:171:LYS:HA	2.31	0.61
1:M:493:ILE:HG22	1:M:493:ILE:O	2.01	0.61
1:I:183:LEU:O	1:I:184:GLN:HB2	2.00	0.61
1:L:173:GLY:O	1:L:404:ARG:NH2	2.34	0.61
1:L:174:VAL:HG21	1:L:376:VAL:HG22	1.82	0.61
1:C:228:SER:O	1:C:257:GLU:HB3	2.00	0.61
1:F:321:LYS:O	1:F:322:ARG:HB2	2.00	0.61
1:H:37:ASN:ND2	1:H:51:LYS:HG3	2.16	0.61
1:K:17:LEU:HA	1:K:20:VAL:HG12	1.81	0.61
1:N:37:ASN:ND2	1:N:51:LYS:HG3	2.16	0.61
1:A:383:ALA:HB3	1:A:389:MET:HB2	1.82	0.61
1:L:166:MET:CE	1:L:171:LYS:HA	2.30	0.61
1:C:213:VAL:HG12	1:C:214:GLU:N	2.16	0.61
1:D:8:PHE:HE1	1:E:26:ALA:HA	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:LYS:HD2	1:D:458:CYS:SG	2.40	0.61
1:F:202:PRO:HB3	1:F:205:ILE:HD11	1.82	0.61
1:H:213:VAL:HG12	1:H:214:GLU:N	2.16	0.61
1:J:183:LEU:O	1:J:184:GLN:HB2	2.00	0.61
1:A:254:VAL:HG12	1:A:259:LEU:HB2	1.82	0.61
1:G:383:ALA:HB3	1:G:389:MET:HB2	1.83	0.61
1:H:499:VAL:HG22	1:H:500:THR:N	2.16	0.61
1:M:174:VAL:HG21	1:M:376:VAL:HG22	1.83	0.61
1:B:449:ALA:HB3	1:B:450:PRO:HD3	1.82	0.60
1:G:449:ALA:HB3	1:G:450:PRO:HD3	1.82	0.60
1:H:219:PHE:O	1:H:247:LEU:HD12	2.00	0.60
1:I:16:MET:SD	1:I:73:MET:HE1	2.41	0.60
1:L:183:LEU:HD13	1:L:184:GLN:N	2.16	0.60
1:J:82:ASN:HB2	1:J:89:THR:OG1	2.01	0.60
1:L:82:ASN:HB2	1:L:89:THR:OG1	2.00	0.60
1:K:37:ASN:ND2	1:K:51:LYS:HG3	2.16	0.60
1:M:249:ILE:HB	1:M:275:ALA:CB	2.32	0.60
1:N:82:ASN:HB2	1:N:89:THR:OG1	2.01	0.60
1:H:279:PRO:O	1:H:285:ARG:HG3	2.01	0.60
1:I:166:MET:CE	1:I:171:LYS:HA	2.30	0.60
1:K:326:ASN:OD1	1:K:329:THR:HB	2.01	0.60
1:L:219:PHE:O	1:L:247:LEU:HD12	2.01	0.60
1:M:20:VAL:HG23	1:M:74:VAL:HG11	1.83	0.60
1:E:7:LYS:HG3	1:E:66:PHE:CZ	2.36	0.60
1:F:176:THR:HG21	1:F:333:ILE:HD13	1.83	0.60
1:I:200:LEU:CD1	1:I:254:VAL:HB	2.32	0.60
1:K:455:VAL:HG13	1:K:460:GLU:HB3	1.83	0.60
1:L:213:VAL:HG12	1:L:214:GLU:N	2.16	0.60
1:L:247:LEU:HB3	1:L:273:VAL:HG12	1.81	0.60
1:C:295:LEU:HA	1:C:342:ILE:HD11	1.84	0.60
1:G:213:VAL:HG12	1:G:214:GLU:N	2.16	0.60
1:I:174:VAL:HG21	1:I:376:VAL:HG22	1.84	0.60
1:K:213:VAL:HG12	1:K:214:GLU:H	1.65	0.60
1:L:166:MET:HE1	1:L:171:LYS:HA	1.82	0.60
1:N:166:MET:CE	1:N:171:LYS:HA	2.31	0.60
1:B:32:GLY:HA3	1:B:454:ILE:HG23	1.84	0.60
1:E:176:THR:HG21	1:E:333:ILE:HD13	1.82	0.60
1:E:254:VAL:HG12	1:E:259:LEU:HB2	1.83	0.60
1:F:214:GLU:O	1:F:215:LEU:HD23	2.01	0.60
1:H:236:VAL:O	1:H:236:VAL:HG12	2.01	0.60
1:L:37:ASN:ND2	1:L:51:LYS:HG3	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:LEU:HD23	1:B:250:ILE:HB	1.84	0.60
1:C:144:ILE:HD13	1:C:166:MET:SD	2.42	0.60
1:C:254:VAL:HG12	1:C:259:LEU:HB2	1.83	0.60
1:E:295:LEU:HA	1:E:342:ILE:HD11	1.83	0.60
1:F:131:LEU:CD1	1:F:422:VAL:HG21	2.31	0.60
1:H:34:LYS:HG3	1:H:458:CYS:HA	1.84	0.60
1:H:82:ASN:HB2	1:H:89:THR:OG1	2.02	0.60
1:J:349:ILE:O	1:J:353:ILE:HG13	2.02	0.60
1:K:247:LEU:HB3	1:K:273:VAL:HG12	1.82	0.60
1:E:222:LEU:HD23	1:E:250:ILE:HB	1.83	0.60
1:F:254:VAL:HG12	1:F:259:LEU:HB2	1.84	0.60
1:G:82:ASN:HB2	1:G:89:THR:OG1	2.01	0.60
1:J:173:GLY:O	1:J:404:ARG:NH2	2.34	0.60
1:K:183:LEU:O	1:K:184:GLN:HB2	2.01	0.60
1:L:114:MET:HG3	1:M:34:LYS:HD2	1.82	0.60
1:M:114:MET:HG3	1:N:34:LYS:HB3	1.83	0.60
1:A:7:LYS:HG3	1:A:66:PHE:CZ	2.36	0.59
1:B:254:VAL:HG12	1:B:259:LEU:HB2	1.83	0.59
1:I:82:ASN:HB2	1:I:89:THR:OG1	2.02	0.59
1:M:74:VAL:HA	1:M:510:VAL:HG21	1.84	0.59
1:A:31:LEU:O	1:A:457:ASN:ND2	2.31	0.59
1:B:144:ILE:HD13	1:B:166:MET:SD	2.42	0.59
1:D:69:MET:SD	1:E:41:ASP:HB2	2.42	0.59
1:D:321:LYS:O	1:D:322:ARG:HB2	2.01	0.59
1:J:249:ILE:HB	1:J:275:ALA:CB	2.32	0.59
1:K:16:MET:SD	1:K:514:MET:HE2	2.41	0.59
1:A:23:LEU:HD23	1:A:74:VAL:HG22	1.83	0.59
1:A:295:LEU:HA	1:A:342:ILE:HD11	1.83	0.59
1:E:455:VAL:HG13	1:E:460:GLU:CB	2.31	0.59
1:I:174:VAL:HG23	1:I:376:VAL:HA	1.83	0.59
1:I:249:ILE:HB	1:I:275:ALA:CB	2.31	0.59
1:K:202:PRO:O	1:K:203:TYR:HB2	2.02	0.59
1:L:183:LEU:O	1:L:184:GLN:HB2	2.03	0.59
1:A:30:THR:O	1:A:35:GLY:HA3	2.02	0.59
1:A:230:ILE:HG22	1:A:257:GLU:OE1	2.02	0.59
1:D:131:LEU:CD1	1:D:422:VAL:HG21	2.32	0.59
1:D:455:VAL:HG13	1:D:460:GLU:CB	2.30	0.59
1:F:223:ALA:O	1:F:251:ALA:HA	2.02	0.59
1:N:183:LEU:O	1:N:184:GLN:HB2	2.01	0.59
1:N:499:VAL:HG22	1:N:500:THR:N	2.17	0.59
1:D:511:ALA:O	1:D:515:ILE:HG13	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:23:LEU:HD23	1:E:74:VAL:CG2	2.32	0.59
1:J:213:VAL:HG12	1:J:214:GLU:H	1.67	0.59
1:J:279:PRO:O	1:J:285:ARG:HG3	2.02	0.59
1:L:37:ASN:HD21	1:L:51:LYS:NZ	2.00	0.59
1:M:16:MET:SD	1:M:514:MET:HE2	2.43	0.59
1:M:197:ARG:HG3	1:M:277:LYS:O	2.03	0.59
1:I:32:GLY:HA3	1:I:454:ILE:HG23	1.84	0.59
1:N:77:VAL:CG2	1:N:78:ALA:N	2.65	0.59
1:D:82:ASN:HB2	1:D:89:THR:OG1	2.02	0.59
1:E:321:LYS:O	1:E:322:ARG:HB2	2.03	0.59
1:C:223:ALA:O	1:C:251:ALA:HA	2.03	0.59
1:D:223:ALA:O	1:D:251:ALA:HA	2.03	0.59
1:F:23:LEU:HD23	1:F:74:VAL:CG2	2.33	0.59
1:J:444:LEU:HA	1:J:447:MET:HE3	1.85	0.59
1:J:493:ILE:HG22	1:J:493:ILE:O	2.03	0.59
1:L:326:ASN:OD1	1:L:329:THR:HB	2.03	0.59
1:M:279:PRO:O	1:M:285:ARG:HG3	2.03	0.59
1:C:213:VAL:HG12	1:C:214:GLU:H	1.68	0.59
1:D:245:LYS:NZ	1:D:319:GLN:HE22	2.01	0.59
1:E:32:GLY:O	1:E:35:GLY:N	2.36	0.59
1:H:3:ALA:HA	1:I:61:GLU:O	2.03	0.59
1:K:417:VAL:O	1:K:420:ILE:HG22	2.03	0.59
1:L:213:VAL:HG12	1:L:214:GLU:H	1.68	0.59
1:L:247:LEU:HD12	1:L:248:LEU:H	1.68	0.59
1:N:249:ILE:HB	1:N:275:ALA:CB	2.33	0.59
1:A:202:PRO:HB3	1:A:205:ILE:HD11	1.85	0.59
1:B:455:VAL:HG11	1:B:462:PRO:HA	1.85	0.59
1:D:7:LYS:HG3	1:D:66:PHE:CZ	2.38	0.59
1:E:213:VAL:HG12	1:E:214:GLU:N	2.18	0.59
1:F:482:THR:O	1:F:484:GLU:HG3	2.03	0.59
1:I:247:LEU:HB3	1:I:273:VAL:HG12	1.84	0.59
1:I:349:ILE:O	1:I:353:ILE:HG13	2.01	0.59
1:J:169:VAL:CG2	1:J:377:ALA:HB2	2.29	0.59
1:K:69:MET:CE	1:L:39:VAL:HG12	2.32	0.59
1:M:349:ILE:O	1:M:353:ILE:HG13	2.03	0.59
1:A:440:ILE:HG22	1:A:441:LYS:N	2.17	0.58
1:D:257:GLU:HB2	1:E:269:GLY:HA3	1.85	0.58
1:G:297:GLY:O	1:G:318:GLY:HA2	2.02	0.58
1:H:349:ILE:O	1:H:353:ILE:HG13	2.02	0.58
1:K:82:ASN:HB2	1:K:89:THR:OG1	2.03	0.58
1:N:279:PRO:O	1:N:285:ARG:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:VAL:HG12	1:A:214:GLU:N	2.17	0.58
1:B:237:LEU:HD23	1:B:237:LEU:O	2.03	0.58
1:C:237:LEU:O	1:C:237:LEU:HD23	2.02	0.58
1:M:82:ASN:HB2	1:M:89:THR:OG1	2.03	0.58
1:B:213:VAL:HG12	1:B:214:GLU:N	2.18	0.58
1:B:228:SER:O	1:B:257:GLU:HB3	2.02	0.58
1:I:202:PRO:O	1:I:203:TYR:HB2	2.04	0.58
1:L:236:VAL:O	1:L:236:VAL:HG12	2.02	0.58
1:L:279:PRO:O	1:L:285:ARG:HG3	2.03	0.58
1:N:247:LEU:HB3	1:N:273:VAL:CG1	2.33	0.58
1:A:213:VAL:HG12	1:A:214:GLU:H	1.68	0.58
1:A:326:ASN:HD22	1:A:329:THR:CB	1.97	0.58
1:G:344:GLY:O	1:G:347:ALA:HB3	2.03	0.58
1:I:326:ASN:OD1	1:I:329:THR:HB	2.04	0.58
1:J:236:VAL:O	1:J:236:VAL:HG12	2.03	0.58
1:K:236:VAL:O	1:K:236:VAL:HG12	2.04	0.58
1:K:247:LEU:HB3	1:K:273:VAL:CG1	2.33	0.58
1:M:213:VAL:HG12	1:M:214:GLU:N	2.18	0.58
1:M:236:VAL:O	1:M:236:VAL:HG12	2.03	0.58
1:M:252:GLU:O	1:M:253:ASP:HB2	2.03	0.58
1:A:23:LEU:HD23	1:A:74:VAL:CG2	2.33	0.58
1:F:222:LEU:HD23	1:F:250:ILE:HB	1.86	0.58
1:J:252:GLU:O	1:J:253:ASP:HB2	2.03	0.58
1:M:31:LEU:HB2	1:M:90:THR:HG21	1.86	0.58
1:M:202:PRO:O	1:M:203:TYR:HB2	2.02	0.58
1:H:202:PRO:O	1:H:203:TYR:HB2	2.03	0.58
1:G:176:THR:HG21	1:G:333:ILE:HD13	1.84	0.58
1:G:228:SER:OG	1:G:255:GLU:HB2	2.03	0.58
1:I:391:GLU:O	1:I:394:ALA:HB3	2.03	0.58
1:I:451:LEU:C	1:I:451:LEU:HD23	2.24	0.58
1:J:202:PRO:O	1:J:203:TYR:HB2	2.04	0.58
1:K:174:VAL:HG21	1:K:376:VAL:HG22	1.83	0.58
1:K:249:ILE:HB	1:K:275:ALA:CB	2.33	0.58
1:L:391:GLU:O	1:L:394:ALA:HB3	2.03	0.58
1:M:451:LEU:HD23	1:M:451:LEU:C	2.23	0.58
1:B:23:LEU:HD23	1:B:74:VAL:CG2	2.33	0.58
1:G:30:THR:HB	1:G:51:LYS:O	2.03	0.58
1:H:326:ASN:OD1	1:H:329:THR:HB	2.03	0.58
1:M:455:VAL:HG13	1:M:460:GLU:HB3	1.84	0.58
1:N:202:PRO:O	1:N:204:PHE:N	2.34	0.58
1:D:213:VAL:HG12	1:D:214:GLU:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:279:PRO:O	1:I:285:ARG:HG3	2.03	0.58
1:I:319:GLN:O	1:I:336:VAL:HG23	2.04	0.58
1:J:166:MET:CE	1:J:171:LYS:HA	2.33	0.58
1:K:319:GLN:O	1:K:336:VAL:HG23	2.03	0.58
1:B:36:ARG:HH11	1:B:36:ARG:HG3	1.69	0.58
1:C:36:ARG:HG3	1:C:36:ARG:HH11	1.69	0.58
1:G:223:ALA:O	1:G:251:ALA:HA	2.02	0.58
1:M:247:LEU:HB3	1:M:273:VAL:CG1	2.34	0.58
1:E:90:THR:O	1:E:94:VAL:HG13	2.04	0.57
1:F:144:ILE:HD13	1:F:166:MET:SD	2.44	0.57
1:G:31:LEU:HD23	1:G:453:GLN:HG2	1.86	0.57
1:I:455:VAL:HG13	1:I:460:GLU:HB3	1.86	0.57
1:J:247:LEU:HB3	1:J:273:VAL:CG1	2.34	0.57
1:L:249:ILE:HB	1:L:275:ALA:CB	2.33	0.57
1:N:174:VAL:HG21	1:N:376:VAL:HG22	1.86	0.57
1:E:8:PHE:CZ	1:F:26:ALA:HB2	2.39	0.57
1:F:455:VAL:HG13	1:F:460:GLU:CB	2.34	0.57
1:H:213:VAL:HG12	1:H:214:GLU:H	1.69	0.57
1:I:37:ASN:ND2	1:I:51:LYS:HG3	2.19	0.57
1:L:77:VAL:CG2	1:L:78:ALA:N	2.67	0.57
1:L:252:GLU:O	1:L:253:ASP:HB2	2.04	0.57
1:M:202:PRO:O	1:M:204:PHE:N	2.34	0.57
1:N:460:GLU:O	1:N:462:PRO:HD3	2.03	0.57
1:B:6:VAL:HG22	1:B:521:VAL:HG22	1.86	0.57
1:F:429:LEU:HD12	1:F:430:ARG:N	2.19	0.57
1:H:200:LEU:CD1	1:H:254:VAL:HB	2.34	0.57
1:I:77:VAL:CG2	1:I:78:ALA:N	2.67	0.57
1:J:499:VAL:HG22	1:J:500:THR:N	2.19	0.57
1:M:76:GLU:O	1:M:79:SER:HB3	2.03	0.57
1:N:139:SER:HB3	1:N:171:LYS:NZ	2.20	0.57
1:B:208:PRO:HG2	1:B:209:GLU:OE1	2.04	0.57
1:B:223:ALA:O	1:B:251:ALA:HA	2.04	0.57
1:D:297:GLY:O	1:D:318:GLY:HA2	2.05	0.57
1:F:440:ILE:HG22	1:F:441:LYS:N	2.18	0.57
1:I:252:GLU:O	1:I:253:ASP:HB2	2.04	0.57
1:F:511:ALA:O	1:F:515:ILE:HG13	2.04	0.57
1:H:63:GLU:HA	1:N:3:ALA:HB2	1.85	0.57
1:H:417:VAL:O	1:H:420:ILE:HG22	2.04	0.57
1:K:391:GLU:O	1:K:394:ALA:HB3	2.04	0.57
1:N:213:VAL:HG12	1:N:214:GLU:H	1.69	0.57
1:N:236:VAL:HG12	1:N:236:VAL:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:278:ALA:HB3	1:N:285:ARG:HD3	1.85	0.57
1:A:223:ALA:O	1:A:251:ALA:HA	2.04	0.57
1:F:245:LYS:NZ	1:F:319:GLN:HE22	2.03	0.57
1:J:76:GLU:O	1:J:79:SER:HB3	2.03	0.57
1:L:305:ILE:O	1:L:305:ILE:HG22	2.05	0.57
1:M:77:VAL:HG23	1:M:78:ALA:N	2.18	0.57
1:E:223:ALA:O	1:E:251:ALA:HA	2.04	0.57
1:H:221:LEU:HB3	1:H:249:ILE:HD13	1.87	0.57
1:I:305:ILE:O	1:I:305:ILE:HG22	2.04	0.57
1:J:77:VAL:CG2	1:J:78:ALA:N	2.67	0.57
1:L:76:GLU:O	1:L:79:SER:HB3	2.04	0.57
1:M:77:VAL:CG2	1:M:78:ALA:N	2.67	0.57
1:N:247:LEU:HD12	1:N:248:LEU:H	1.69	0.57
1:G:295:LEU:HA	1:G:342:ILE:HD11	1.86	0.57
1:H:203:TYR:HB3	1:H:267:MET:HE1	1.86	0.57
1:K:77:VAL:CG2	1:K:78:ALA:N	2.66	0.57
1:K:499:VAL:HG22	1:K:500:THR:N	2.20	0.57
1:M:223:ALA:O	1:M:251:ALA:HA	2.04	0.57
1:N:252:GLU:O	1:N:253:ASP:HB2	2.05	0.57
1:E:201:SER:O	1:E:202:PRO:O	2.23	0.57
1:H:249:ILE:HB	1:H:275:ALA:CB	2.34	0.57
1:K:155:ASP:OD1	1:K:157:THR:HB	2.05	0.57
1:N:259:LEU:O	1:N:263:VAL:HG23	2.05	0.57
1:B:90:THR:O	1:B:94:VAL:HG13	2.05	0.57
1:C:208:PRO:HG2	1:C:209:GLU:OE1	2.05	0.57
1:C:259:LEU:O	1:C:263:VAL:HG23	2.04	0.57
1:C:297:GLY:O	1:C:318:GLY:HA2	2.05	0.57
1:G:237:LEU:HD23	1:G:237:LEU:O	2.05	0.57
1:I:219:PHE:O	1:I:247:LEU:HD12	2.05	0.57
1:N:76:GLU:O	1:N:79:SER:HB3	2.05	0.57
1:C:511:ALA:O	1:C:515:ILE:HG13	2.05	0.56
1:D:90:THR:O	1:D:94:VAL:HG13	2.05	0.56
1:E:519:CYS:O	1:F:39:VAL:N	2.38	0.56
1:J:155:ASP:OD1	1:J:157:THR:HB	2.05	0.56
1:J:197:ARG:HG3	1:J:277:LYS:O	2.05	0.56
1:E:297:GLY:O	1:E:318:GLY:HA2	2.04	0.56
1:F:237:LEU:O	1:F:237:LEU:HD23	2.05	0.56
1:G:23:LEU:HD23	1:G:74:VAL:CG2	2.34	0.56
1:H:28:LYS:O	1:H:31:LEU:HB2	2.05	0.56
1:H:37:ASN:HD21	1:H:51:LYS:NZ	2.03	0.56
1:L:247:LEU:HB3	1:L:273:VAL:CG1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:349:ILE:O	1:L:353:ILE:HG13	2.05	0.56
1:M:499:VAL:HG22	1:M:500:THR:N	2.19	0.56
1:A:237:LEU:O	1:A:237:LEU:HD23	2.04	0.56
1:A:245:LYS:NZ	1:A:319:GLN:HE22	2.04	0.56
1:C:228:SER:OG	1:C:255:GLU:HB2	2.05	0.56
1:E:237:LEU:HD23	1:E:237:LEU:O	2.06	0.56
1:G:455:VAL:HG11	1:G:462:PRO:HA	1.87	0.56
1:H:77:VAL:CG2	1:H:78:ALA:N	2.69	0.56
1:H:391:GLU:O	1:H:394:ALA:HB3	2.05	0.56
1:I:213:VAL:HG12	1:I:214:GLU:H	1.67	0.56
1:I:236:VAL:O	1:I:236:VAL:HG12	2.05	0.56
1:M:183:LEU:O	1:M:184:GLN:HB2	2.05	0.56
1:M:305:ILE:O	1:M:305:ILE:HG22	2.05	0.56
1:N:155:ASP:OD1	1:N:157:THR:HB	2.05	0.56
1:N:391:GLU:O	1:N:394:ALA:HB3	2.04	0.56
1:B:214:GLU:O	1:B:215:LEU:HD23	2.05	0.56
1:D:201:SER:O	1:D:202:PRO:O	2.23	0.56
1:H:139:SER:HB3	1:H:171:LYS:NZ	2.20	0.56
1:L:455:VAL:HG13	1:L:460:GLU:HB3	1.87	0.56
1:E:23:LEU:HD23	1:E:74:VAL:HG22	1.86	0.56
1:J:200:LEU:CD1	1:J:254:VAL:HB	2.35	0.56
1:K:200:LEU:CD1	1:K:254:VAL:HB	2.35	0.56
1:M:203:TYR:HB3	1:M:267:MET:HE1	1.88	0.56
1:M:417:VAL:O	1:M:420:ILE:HG22	2.05	0.56
1:N:223:ALA:O	1:N:251:ALA:HA	2.04	0.56
1:A:90:THR:O	1:A:94:VAL:HG13	2.06	0.56
1:B:23:LEU:HD23	1:B:74:VAL:HG22	1.88	0.56
1:D:237:LEU:O	1:D:237:LEU:HD23	2.05	0.56
1:H:142:LYS:O	1:H:142:LYS:HD3	2.05	0.56
1:K:223:ALA:O	1:K:251:ALA:HA	2.06	0.56
1:L:202:PRO:O	1:L:203:TYR:HB2	2.04	0.56
1:L:460:GLU:O	1:L:462:PRO:HD3	2.05	0.56
1:M:20:VAL:CG2	1:M:74:VAL:HG11	2.34	0.56
1:N:455:VAL:HG13	1:N:460:GLU:HB3	1.87	0.56
1:H:278:ALA:HB3	1:H:285:ARG:HD3	1.86	0.56
1:L:69:MET:CE	1:M:39:VAL:HG12	2.35	0.56
1:N:77:VAL:HG23	1:N:78:ALA:N	2.19	0.56
1:N:349:ILE:O	1:N:353:ILE:HG13	2.05	0.56
1:C:23:LEU:HD23	1:C:74:VAL:CG2	2.35	0.56
1:I:169:VAL:CG2	1:I:377:ALA:HB2	2.34	0.56
1:J:391:GLU:O	1:J:394:ALA:HB3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:77:VAL:HG23	1:K:78:ALA:N	2.19	0.56
1:L:25:ASP:HA	1:L:28:LYS:HE2	1.87	0.56
1:L:319:GLN:O	1:L:336:VAL:HG23	2.05	0.56
1:N:496:PRO:O	1:N:499:VAL:HG13	2.06	0.56
1:A:131:LEU:HD13	1:A:422:VAL:HG21	1.88	0.56
1:C:131:LEU:HD13	1:C:422:VAL:HG21	1.87	0.56
1:D:218:PRO:HB3	1:D:246:PRO:HG2	1.88	0.56
1:D:429:LEU:HD12	1:D:430:ARG:N	2.21	0.56
1:E:213:VAL:HG12	1:E:214:GLU:H	1.71	0.56
1:F:23:LEU:HD23	1:F:74:VAL:HG22	1.87	0.56
1:H:202:PRO:O	1:H:204:PHE:N	2.36	0.56
1:H:247:LEU:HB3	1:H:273:VAL:CG1	2.35	0.56
1:H:451:LEU:HD23	1:H:451:LEU:C	2.26	0.56
1:I:242:LYS:O	1:I:243:ALA:HB3	2.06	0.56
1:J:32:GLY:HA3	1:J:454:ILE:HG23	1.86	0.56
1:J:305:ILE:O	1:J:305:ILE:HG22	2.06	0.56
1:L:413:ALA:HB2	1:L:475:ASN:HD22	1.71	0.56
1:M:219:PHE:O	1:M:247:LEU:HD12	2.05	0.56
1:B:174:VAL:HB	1:B:376:VAL:HG13	1.87	0.56
1:D:429:LEU:HD12	1:D:430:ARG:H	1.70	0.56
1:G:131:LEU:CD1	1:G:422:VAL:HG21	2.36	0.56
1:G:245:LYS:NZ	1:G:319:GLN:HE22	2.03	0.56
1:K:142:LYS:O	1:K:142:LYS:HD3	2.06	0.56
1:K:493:ILE:O	1:K:493:ILE:HG22	2.06	0.56
1:M:139:SER:HB3	1:M:171:LYS:NZ	2.21	0.56
1:C:440:ILE:HG22	1:C:441:LYS:N	2.20	0.55
1:E:429:LEU:HD12	1:E:430:ARG:H	1.72	0.55
1:H:223:ALA:O	1:H:251:ALA:HA	2.05	0.55
1:J:77:VAL:HG23	1:J:78:ALA:N	2.20	0.55
1:L:176:THR:HG21	1:L:333:ILE:HD13	1.87	0.55
1:N:305:ILE:HG22	1:N:305:ILE:O	2.06	0.55
1:B:69:MET:SD	1:C:41:ASP:HB2	2.46	0.55
1:E:389:MET:SD	1:E:389:MET:C	2.84	0.55
1:G:23:LEU:HD23	1:G:74:VAL:HG22	1.88	0.55
1:G:259:LEU:O	1:G:263:VAL:HG23	2.05	0.55
1:I:203:TYR:HB3	1:I:267:MET:HE1	1.88	0.55
1:K:139:SER:HB3	1:K:171:LYS:NZ	2.21	0.55
1:K:209:GLU:OE1	1:K:209:GLU:N	2.39	0.55
1:L:417:VAL:O	1:L:420:ILE:HG22	2.06	0.55
1:N:321:LYS:O	1:N:322:ARG:HB2	2.06	0.55
1:F:213:VAL:HG12	1:F:214:GLU:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:208:PRO:HG2	1:G:209:GLU:OE1	2.06	0.55
1:I:223:ALA:O	1:I:251:ALA:HA	2.07	0.55
1:K:197:ARG:HG3	1:K:277:LYS:O	2.06	0.55
1:K:305:ILE:HG22	1:K:305:ILE:O	2.06	0.55
1:L:517:THR:HG21	1:M:39:VAL:HG23	1.88	0.55
1:A:268:ARG:O	1:A:270:ILE:N	2.40	0.55
1:E:520:MET:HG2	1:F:39:VAL:HB	1.89	0.55
1:F:242:LYS:O	1:F:243:ALA:HB3	2.06	0.55
1:J:77:VAL:HG21	1:J:510:VAL:CG1	2.37	0.55
1:L:74:VAL:HA	1:L:510:VAL:HG21	1.88	0.55
1:L:77:VAL:HG21	1:L:510:VAL:CG1	2.36	0.55
1:M:37:ASN:ND2	1:M:51:LYS:HG3	2.21	0.55
1:N:169:VAL:CG2	1:N:377:ALA:HB2	2.31	0.55
1:G:201:SER:O	1:G:202:PRO:O	2.24	0.55
1:I:278:ALA:HB3	1:I:285:ARG:HD3	1.88	0.55
1:J:139:SER:HB3	1:J:171:LYS:NZ	2.22	0.55
1:J:247:LEU:HD12	1:J:248:LEU:H	1.71	0.55
1:K:25:ASP:HA	1:K:28:LYS:HE2	1.88	0.55
1:L:517:THR:CG2	1:M:39:VAL:HG23	2.36	0.55
1:N:202:PRO:O	1:N:203:TYR:HB2	2.06	0.55
1:B:297:GLY:O	1:B:318:GLY:HA2	2.07	0.55
1:C:201:SER:O	1:C:202:PRO:O	2.24	0.55
1:C:245:LYS:NZ	1:C:319:GLN:HE22	2.05	0.55
1:D:202:PRO:O	1:D:203:TYR:HB2	2.06	0.55
1:E:34:LYS:HB2	1:E:458:CYS:SG	2.47	0.55
1:I:139:SER:HB3	1:I:171:LYS:NZ	2.21	0.55
1:I:173:GLY:O	1:I:404:ARG:NH2	2.39	0.55
1:K:259:LEU:O	1:K:263:VAL:HG23	2.06	0.55
1:L:242:LYS:O	1:L:243:ALA:HB3	2.06	0.55
1:N:20:VAL:CG2	1:N:74:VAL:HG11	2.36	0.55
1:A:236:VAL:O	1:A:236:VAL:HG12	2.07	0.55
1:D:16:MET:HB3	1:D:514:MET:HE1	1.87	0.55
1:D:228:SER:OG	1:D:255:GLU:HB2	2.07	0.55
1:M:200:LEU:CD1	1:M:254:VAL:HB	2.36	0.55
1:E:131:LEU:CD1	1:E:422:VAL:HG21	2.37	0.55
1:H:197:ARG:HG3	1:H:277:LYS:O	2.07	0.55
1:I:77:VAL:HG23	1:I:78:ALA:N	2.20	0.55
1:I:247:LEU:HB3	1:I:273:VAL:CG1	2.37	0.55
1:I:247:LEU:HD12	1:I:248:LEU:H	1.71	0.55
1:J:176:THR:HG21	1:J:333:ILE:HD13	1.88	0.55
1:F:381:VAL:HG21	1:F:393:LYS:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:213:VAL:HG12	1:G:214:GLU:H	1.71	0.55
1:H:63:GLU:HB2	1:N:3:ALA:HB1	1.88	0.55
1:I:197:ARG:HG3	1:I:277:LYS:O	2.06	0.55
1:L:139:SER:HB3	1:L:171:LYS:NZ	2.21	0.55
1:I:493:ILE:O	1:I:493:ILE:HG22	2.07	0.55
1:K:27:VAL:O	1:K:30:THR:CG2	2.52	0.55
1:K:279:PRO:O	1:K:285:ARG:HG3	2.06	0.55
1:K:518:GLU:HG2	1:L:36:ARG:HG3	1.89	0.55
1:M:166:MET:HE1	1:M:171:LYS:HA	1.88	0.55
1:M:209:GLU:N	1:M:209:GLU:OE1	2.40	0.55
1:A:455:VAL:HG11	1:A:462:PRO:HA	1.88	0.54
1:B:213:VAL:HG12	1:B:214:GLU:H	1.71	0.54
1:E:311:LYS:HB3	1:I:311:LYS:CD	2.35	0.54
1:H:305:ILE:HG22	1:H:305:ILE:O	2.06	0.54
1:L:155:ASP:OD1	1:L:157:THR:HB	2.06	0.54
1:M:413:ALA:HB2	1:M:475:ASN:HD22	1.72	0.54
1:N:20:VAL:HG23	1:N:74:VAL:HG11	1.90	0.54
1:C:7:LYS:HG3	1:C:66:PHE:CZ	2.42	0.54
1:C:23:LEU:HD23	1:C:74:VAL:HG22	1.88	0.54
1:D:268:ARG:O	1:D:270:ILE:N	2.40	0.54
1:H:176:THR:HG21	1:H:333:ILE:HD13	1.89	0.54
1:N:215:LEU:HB2	1:N:323:VAL:HG22	1.89	0.54
1:A:228:SER:OG	1:A:255:GLU:HB2	2.07	0.54
1:C:349:ILE:O	1:C:353:ILE:HG13	2.06	0.54
1:D:174:VAL:HB	1:D:376:VAL:HG13	1.89	0.54
1:F:344:GLY:O	1:F:347:ALA:HB3	2.08	0.54
1:H:77:VAL:HG21	1:H:510:VAL:CG1	2.37	0.54
1:H:242:LYS:O	1:H:243:ALA:HB3	2.07	0.54
1:J:344:GLY:O	1:J:347:ALA:HB3	2.07	0.54
1:L:451:LEU:C	1:L:451:LEU:HD23	2.27	0.54
1:F:106:ALA:O	1:F:109:ALA:HB3	2.06	0.54
1:F:174:VAL:HB	1:F:376:VAL:HG13	1.88	0.54
1:F:259:LEU:O	1:F:263:VAL:HG23	2.07	0.54
1:H:74:VAL:HA	1:H:510:VAL:HG21	1.90	0.54
1:H:77:VAL:HG23	1:H:78:ALA:N	2.23	0.54
1:H:166:MET:HE2	1:H:171:LYS:HA	1.89	0.54
1:I:247:LEU:H	1:I:273:VAL:HG12	1.73	0.54
1:K:252:GLU:O	1:K:253:ASP:HB2	2.07	0.54
1:L:77:VAL:HG23	1:L:78:ALA:N	2.21	0.54
1:M:242:LYS:O	1:M:243:ALA:HB3	2.06	0.54
1:A:201:SER:O	1:A:202:PRO:O	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:511:ALA:O	1:G:515:ILE:HG13	2.07	0.54
1:H:252:GLU:O	1:H:253:ASP:HB2	2.08	0.54
1:H:444:LEU:HA	1:H:447:MET:HE3	1.90	0.54
1:H:479:ASN:ND2	1:H:482:THR:HG23	2.21	0.54
1:J:259:LEU:O	1:J:263:VAL:HG23	2.07	0.54
1:M:319:GLN:O	1:M:336:VAL:HG23	2.07	0.54
1:G:199:TYR:HA	1:G:276:VAL:HG12	1.89	0.54
1:G:311:LYS:HB3	1:N:311:LYS:HG2	1.90	0.54
1:N:25:ASP:HA	1:N:28:LYS:HE2	1.90	0.54
1:E:23:LEU:CD2	1:E:75:LYS:HG3	2.38	0.54
1:E:420:ILE:HG13	1:E:448:GLU:HG2	1.89	0.54
1:H:155:ASP:OD1	1:H:157:THR:HB	2.08	0.54
1:I:176:THR:HG21	1:I:333:ILE:HD13	1.89	0.54
1:J:393:LYS:O	1:J:397:GLU:HB2	2.07	0.54
1:N:200:LEU:CD1	1:N:254:VAL:HB	2.38	0.54
1:B:429:LEU:HD12	1:B:430:ARG:N	2.22	0.54
1:C:245:LYS:HZ2	1:C:319:GLN:HE22	1.55	0.54
1:D:236:VAL:O	1:D:236:VAL:HG12	2.07	0.54
1:F:208:PRO:HG2	1:F:209:GLU:OE1	2.08	0.54
1:H:455:VAL:HG13	1:H:460:GLU:HB3	1.89	0.54
1:J:417:VAL:O	1:J:420:ILE:HG22	2.08	0.54
1:M:213:VAL:HG12	1:M:214:GLU:H	1.73	0.54
1:B:131:LEU:HD13	1:B:422:VAL:HG21	1.90	0.54
1:B:440:ILE:HG22	1:B:441:LYS:N	2.22	0.54
1:C:174:VAL:HB	1:C:376:VAL:HG13	1.89	0.54
1:H:23:LEU:HD23	1:H:74:VAL:HG22	1.89	0.54
1:I:74:VAL:HA	1:I:510:VAL:HG21	1.89	0.54
1:I:259:LEU:O	1:I:263:VAL:HG23	2.07	0.54
1:J:221:LEU:HB3	1:J:249:ILE:HD13	1.90	0.54
1:J:278:ALA:HB3	1:J:285:ARG:HD3	1.90	0.54
1:J:319:GLN:O	1:J:336:VAL:HG23	2.08	0.54
1:L:202:PRO:O	1:L:204:PHE:N	2.35	0.54
1:L:209:GLU:OE1	1:L:209:GLU:N	2.41	0.54
1:B:245:LYS:NZ	1:B:319:GLN:HE22	2.05	0.54
1:B:248:LEU:HD12	1:B:274:ALA:O	2.08	0.54
1:B:429:LEU:HD12	1:B:430:ARG:H	1.72	0.54
1:D:259:LEU:O	1:D:263:VAL:HG23	2.08	0.54
1:E:344:GLY:O	1:E:347:ALA:HB3	2.08	0.54
1:F:25:ASP:O	1:F:29:VAL:HG13	2.08	0.54
1:G:155:ASP:OD1	1:G:157:THR:HB	2.08	0.54
1:G:429:LEU:HD12	1:G:430:ARG:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:209:GLU:OE1	1:H:209:GLU:N	2.41	0.54
1:H:269:GLY:HA3	1:N:257:GLU:CG	2.36	0.54
1:I:28:LYS:C	1:I:30:THR:H	2.12	0.54
1:J:8:PHE:HE1	1:K:26:ALA:HA	1.73	0.54
1:L:223:ALA:O	1:L:251:ALA:HA	2.07	0.54
1:A:199:TYR:HA	1:A:276:VAL:HG12	1.91	0.53
1:A:420:ILE:HG13	1:A:448:GLU:HG2	1.91	0.53
1:A:429:LEU:HD12	1:A:430:ARG:H	1.73	0.53
1:A:429:LEU:HD12	1:A:430:ARG:N	2.23	0.53
1:B:295:LEU:HA	1:B:342:ILE:HD11	1.90	0.53
1:F:268:ARG:O	1:F:270:ILE:N	2.40	0.53
1:G:77:VAL:HG23	1:G:78:ALA:N	2.23	0.53
1:H:34:LYS:HB3	1:N:114:MET:HG3	1.90	0.53
1:J:32:GLY:O	1:J:34:LYS:N	2.41	0.53
1:M:221:LEU:HB3	1:M:249:ILE:HD13	1.89	0.53
1:N:493:ILE:O	1:N:493:ILE:HG22	2.07	0.53
1:B:349:ILE:O	1:B:353:ILE:HG13	2.07	0.53
1:D:23:LEU:HD23	1:D:74:VAL:HG22	1.90	0.53
1:I:221:LEU:HB3	1:I:249:ILE:HD13	1.89	0.53
1:J:74:VAL:HA	1:J:510:VAL:HG21	1.91	0.53
1:J:234:LEU:N	1:J:235:PRO:HD2	2.23	0.53
1:J:242:LYS:O	1:J:243:ALA:HB3	2.08	0.53
1:J:247:LEU:H	1:J:273:VAL:HG12	1.73	0.53
1:K:221:LEU:HB3	1:K:249:ILE:HD13	1.90	0.53
1:B:242:LYS:C	1:B:244:GLY:H	2.12	0.53
1:C:6:VAL:HG22	1:C:521:VAL:HG22	1.91	0.53
1:C:268:ARG:O	1:C:270:ILE:N	2.40	0.53
1:D:440:ILE:HG22	1:D:441:LYS:N	2.23	0.53
1:H:234:LEU:N	1:H:235:PRO:HD2	2.23	0.53
1:K:18:ARG:HH11	1:K:18:ARG:CG	2.20	0.53
1:K:278:ALA:HB3	1:K:285:ARG:HD3	1.90	0.53
1:L:69:MET:CE	1:M:41:ASP:HB2	2.39	0.53
1:L:203:TYR:HB3	1:L:267:MET:HE1	1.90	0.53
1:A:77:VAL:HG23	1:A:78:ALA:N	2.22	0.53
1:A:174:VAL:HB	1:A:376:VAL:HG13	1.90	0.53
1:A:259:LEU:O	1:A:263:VAL:HG23	2.09	0.53
1:E:429:LEU:HD12	1:E:430:ARG:N	2.23	0.53
1:F:228:SER:OG	1:F:255:GLU:HB2	2.08	0.53
1:H:259:LEU:O	1:H:263:VAL:HG23	2.08	0.53
1:I:321:LYS:O	1:I:322:ARG:HB2	2.08	0.53
1:K:166:MET:HE2	1:K:171:LYS:HA	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:413:ALA:HB2	1:K:475:ASN:HD22	1.74	0.53
1:M:259:LEU:O	1:M:263:VAL:HG23	2.08	0.53
1:A:77:VAL:CG2	1:A:78:ALA:N	2.70	0.53
1:E:199:TYR:HA	1:E:276:VAL:HG12	1.91	0.53
1:K:485:TYR:HD1	1:K:485:TYR:H	1.55	0.53
1:B:122:LYS:HE2	1:B:429:LEU:HD11	1.91	0.53
1:B:202:PRO:O	1:B:204:PHE:N	2.41	0.53
1:D:496:PRO:HB2	1:D:499:VAL:HG13	1.91	0.53
1:E:32:GLY:O	1:E:34:LYS:N	2.42	0.53
1:G:77:VAL:CG2	1:G:78:ALA:N	2.72	0.53
1:I:7:LYS:HG3	1:I:66:PHE:CZ	2.44	0.53
1:J:25:ASP:HA	1:J:28:LYS:HE2	1.90	0.53
1:J:223:ALA:O	1:J:251:ALA:HA	2.08	0.53
1:K:247:LEU:HD12	1:K:248:LEU:H	1.73	0.53
1:M:247:LEU:HD12	1:M:248:LEU:H	1.72	0.53
1:D:199:TYR:HA	1:D:276:VAL:HG12	1.90	0.53
1:E:77:VAL:O	1:E:80:LYS:N	2.42	0.53
1:F:33:PRO:C	1:F:35:GLY:H	2.11	0.53
1:F:201:SER:O	1:F:202:PRO:O	2.26	0.53
1:G:429:LEU:HD12	1:G:430:ARG:H	1.73	0.53
1:H:25:ASP:HA	1:H:28:LYS:HE2	1.91	0.53
1:I:142:LYS:O	1:I:142:LYS:HD3	2.08	0.53
1:C:90:THR:O	1:C:94:VAL:HG13	2.09	0.53
1:C:242:LYS:C	1:C:244:GLY:H	2.12	0.53
1:E:122:LYS:HE2	1:E:429:LEU:HD11	1.91	0.53
1:E:236:VAL:O	1:E:236:VAL:HG12	2.09	0.53
1:E:517:THR:HG21	1:F:39:VAL:CG2	2.37	0.53
1:F:17:LEU:HA	1:F:20:VAL:HG12	1.91	0.53
1:K:169:VAL:CG2	1:K:377:ALA:HB2	2.31	0.53
1:K:234:LEU:N	1:K:235:PRO:HD2	2.24	0.53
1:K:247:LEU:H	1:K:273:VAL:HG12	1.74	0.53
1:M:247:LEU:H	1:M:273:VAL:HG12	1.74	0.53
1:N:209:GLU:OE1	1:N:209:GLU:N	2.42	0.53
1:B:199:TYR:HA	1:B:276:VAL:HG12	1.89	0.53
1:D:450:PRO:O	1:D:454:ILE:HG13	2.09	0.53
1:E:218:PRO:HB3	1:E:246:PRO:HG2	1.91	0.53
1:E:259:LEU:O	1:E:263:VAL:HG23	2.09	0.53
1:E:496:PRO:HB2	1:E:499:VAL:HG13	1.91	0.53
1:F:17:LEU:HA	1:F:20:VAL:CG1	2.39	0.53
1:G:31:LEU:HD23	1:G:453:GLN:CG	2.39	0.53
1:I:155:ASP:OD1	1:I:157:THR:HB	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:77:VAL:HG11	1:J:510:VAL:HB	1.91	0.53
1:J:209:GLU:N	1:J:209:GLU:OE1	2.41	0.53
1:J:455:VAL:HG13	1:J:460:GLU:HB3	1.90	0.53
1:J:460:GLU:O	1:J:462:PRO:HD3	2.09	0.53
1:K:73:MET:SD	1:L:49:ILE:HD11	2.49	0.53
1:K:451:LEU:HD23	1:K:451:LEU:C	2.28	0.53
1:L:485:TYR:H	1:L:485:TYR:HD1	1.57	0.53
1:N:197:ARG:HG3	1:N:277:LYS:O	2.08	0.53
1:B:118:ARG:HH22	1:C:34:LYS:HE2	1.73	0.53
1:D:122:LYS:HE2	1:D:429:LEU:HD11	1.89	0.53
1:E:440:ILE:HG22	1:E:441:LYS:N	2.23	0.53
1:I:118:ARG:NH2	1:J:34:LYS:HE3	2.23	0.53
1:L:247:LEU:H	1:L:273:VAL:HG12	1.74	0.53
1:A:242:LYS:O	1:A:243:ALA:HB3	2.09	0.52
1:G:7:LYS:HG3	1:G:66:PHE:CZ	2.44	0.52
1:G:440:ILE:HG22	1:G:441:LYS:N	2.24	0.52
1:I:20:VAL:CG2	1:I:74:VAL:HG11	2.39	0.52
1:L:28:LYS:C	1:L:30:THR:H	2.11	0.52
1:M:169:VAL:CG2	1:M:377:ALA:HB2	2.35	0.52
1:N:444:LEU:HA	1:N:447:MET:HE3	1.91	0.52
1:B:268:ARG:O	1:B:270:ILE:N	2.42	0.52
1:D:344:GLY:O	1:D:347:ALA:HB3	2.10	0.52
1:E:6:VAL:HG22	1:E:521:VAL:HG22	1.91	0.52
1:E:242:LYS:O	1:E:243:ALA:HB3	2.09	0.52
1:F:33:PRO:O	1:F:35:GLY:N	2.39	0.52
1:F:77:VAL:O	1:F:80:LYS:N	2.42	0.52
1:F:134:LEU:O	1:F:134:LEU:HD23	2.09	0.52
1:F:420:ILE:HG13	1:F:448:GLU:HG2	1.92	0.52
1:G:349:ILE:O	1:G:353:ILE:HG13	2.10	0.52
1:H:321:LYS:O	1:H:322:ARG:HB2	2.08	0.52
1:I:20:VAL:HG23	1:I:74:VAL:HG11	1.91	0.52
1:I:86:GLY:O	1:I:87:ASP:HB2	2.10	0.52
1:J:485:TYR:HD1	1:J:485:TYR:H	1.57	0.52
1:B:389:MET:SD	1:B:389:MET:C	2.88	0.52
1:F:479:ASN:OD1	1:F:481:ALA:HB3	2.09	0.52
1:I:166:MET:HE2	1:I:171:LYS:HA	1.90	0.52
1:J:166:MET:HE1	1:J:171:LYS:HA	1.90	0.52
1:L:200:LEU:CD1	1:L:254:VAL:HB	2.40	0.52
1:L:450:PRO:O	1:L:454:ILE:HG13	2.10	0.52
1:A:144:ILE:HD13	1:A:166:MET:SD	2.50	0.52
1:B:247:LEU:HB3	1:B:273:VAL:CG1	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:199:TYR:HA	1:F:276:VAL:HG12	1.91	0.52
1:G:174:VAL:HB	1:G:376:VAL:HG13	1.91	0.52
1:H:20:VAL:CG2	1:H:74:VAL:HG11	2.40	0.52
1:K:242:LYS:O	1:K:243:ALA:HB3	2.09	0.52
1:E:268:ARG:O	1:E:270:ILE:N	2.43	0.52
1:H:20:VAL:HG23	1:H:74:VAL:HG11	1.90	0.52
1:K:36:ARG:O	1:K:51:LYS:HG2	2.10	0.52
1:K:519:CYS:O	1:L:38:VAL:HA	2.10	0.52
1:L:221:LEU:HB3	1:L:249:ILE:HD13	1.92	0.52
1:N:247:LEU:H	1:N:273:VAL:HG12	1.75	0.52
1:B:202:PRO:O	1:B:203:TYR:HB2	2.10	0.52
1:B:344:GLY:O	1:B:347:ALA:HB3	2.09	0.52
1:E:25:ASP:HA	1:E:28:LYS:HE2	1.90	0.52
1:F:140:ASP:C	1:F:142:LYS:H	2.13	0.52
1:G:381:VAL:HG21	1:G:393:LYS:HA	1.92	0.52
1:H:499:VAL:CG2	1:H:500:THR:N	2.72	0.52
1:I:77:VAL:HG21	1:I:510:VAL:CG1	2.40	0.52
1:K:134:LEU:HD11	1:K:421:ARG:HG2	1.91	0.52
1:K:444:LEU:HA	1:K:447:MET:HE3	1.92	0.52
1:L:234:LEU:N	1:L:235:PRO:HD2	2.24	0.52
1:A:389:MET:SD	1:A:389:MET:C	2.87	0.52
1:B:77:VAL:CG2	1:B:78:ALA:N	2.73	0.52
1:B:259:LEU:O	1:B:263:VAL:HG23	2.10	0.52
1:C:429:LEU:HD12	1:C:430:ARG:H	1.74	0.52
1:D:242:LYS:O	1:D:243:ALA:HB3	2.10	0.52
1:D:389:MET:SD	1:D:389:MET:C	2.88	0.52
1:F:131:LEU:HD13	1:F:422:VAL:HG21	1.92	0.52
1:I:37:ASN:HD21	1:I:51:LYS:NZ	2.08	0.52
1:I:138:CYS:O	1:I:138:CYS:SG	2.68	0.52
1:I:234:LEU:N	1:I:235:PRO:HD2	2.25	0.52
1:J:451:LEU:HD23	1:J:451:LEU:C	2.29	0.52
1:M:393:LYS:O	1:M:397:GLU:HB2	2.08	0.52
1:M:460:GLU:O	1:M:462:PRO:HD3	2.09	0.52
1:N:77:VAL:HG21	1:N:510:VAL:CG1	2.40	0.52
1:A:349:ILE:O	1:A:353:ILE:HG13	2.10	0.52
1:B:131:LEU:HD12	1:B:422:VAL:HG21	1.91	0.52
1:D:144:ILE:HD13	1:D:166:MET:SD	2.50	0.52
1:E:228:SER:OG	1:E:255:GLU:HB2	2.10	0.52
1:H:319:GLN:O	1:H:336:VAL:HG23	2.10	0.52
1:M:160:LYS:O	1:M:164:GLU:HG3	2.10	0.52
1:M:485:TYR:HD1	1:M:485:TYR:H	1.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:247:LEU:HB3	1:D:273:VAL:CG1	2.39	0.52
1:F:202:PRO:O	1:F:204:PHE:N	2.38	0.52
1:G:242:LYS:O	1:G:243:ALA:HB3	2.09	0.52
1:G:245:LYS:HZ2	1:G:319:GLN:HE22	1.58	0.52
1:G:268:ARG:O	1:G:270:ILE:N	2.42	0.52
1:H:63:GLU:HA	1:N:3:ALA:CB	2.40	0.52
1:I:209:GLU:OE1	1:I:209:GLU:N	2.43	0.52
1:J:86:GLY:O	1:J:87:ASP:HB2	2.10	0.52
1:M:23:LEU:HD23	1:M:74:VAL:HG22	1.91	0.52
1:M:37:ASN:HD21	1:M:51:LYS:NZ	2.08	0.52
1:M:234:LEU:N	1:M:235:PRO:HD2	2.24	0.52
1:N:499:VAL:CG2	1:N:500:THR:N	2.73	0.52
1:A:208:PRO:HG2	1:A:209:GLU:OE1	2.09	0.52
1:D:33:PRO:O	1:D:35:GLY:N	2.38	0.52
1:D:77:VAL:O	1:D:80:LYS:N	2.43	0.52
1:E:174:VAL:HB	1:E:376:VAL:HG13	1.92	0.52
1:F:247:LEU:HB3	1:F:273:VAL:CG1	2.40	0.52
1:F:295:LEU:HA	1:F:342:ILE:HD11	1.92	0.52
1:F:389:MET:C	1:F:389:MET:SD	2.88	0.52
1:H:215:LEU:HB2	1:H:323:VAL:HG22	1.91	0.52
1:J:202:PRO:O	1:J:204:PHE:N	2.38	0.52
1:B:201:SER:O	1:B:202:PRO:O	2.28	0.51
1:B:218:PRO:HB3	1:B:246:PRO:HG2	1.93	0.51
1:D:17:LEU:HA	1:D:20:VAL:HG12	1.92	0.51
1:D:349:ILE:O	1:D:353:ILE:HG13	2.09	0.51
1:E:391:GLU:O	1:E:394:ALA:HB3	2.10	0.51
1:K:8:PHE:CE1	1:L:26:ALA:HA	2.43	0.51
1:K:160:LYS:O	1:K:164:GLU:HG3	2.10	0.51
1:A:412:VAL:HG13	1:A:497:THR:OG1	2.10	0.51
1:C:199:TYR:HA	1:C:276:VAL:HG12	1.91	0.51
1:D:8:PHE:CE1	1:E:26:ALA:HA	2.43	0.51
1:D:13:ARG:HD2	1:D:104:LEU:HD22	1.93	0.51
1:E:221:LEU:HD23	1:E:249:ILE:HG23	1.93	0.51
1:I:202:PRO:O	1:I:204:PHE:N	2.38	0.51
1:J:203:TYR:HB3	1:J:267:MET:HE1	1.93	0.51
1:K:215:LEU:HB2	1:K:323:VAL:HG22	1.92	0.51
1:B:242:LYS:O	1:B:243:ALA:HB3	2.10	0.51
1:E:247:LEU:HB3	1:E:273:VAL:CG1	2.41	0.51
1:H:61:GLU:O	1:N:3:ALA:HA	2.09	0.51
1:K:74:VAL:HA	1:K:510:VAL:HG21	1.93	0.51
1:L:444:LEU:HA	1:L:447:MET:HE3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:86:GLY:O	1:M:87:ASP:HB2	2.10	0.51
1:M:155:ASP:OD1	1:M:157:THR:HB	2.11	0.51
1:A:344:GLY:O	1:A:347:ALA:HB3	2.10	0.51
1:D:221:LEU:HB3	1:D:249:ILE:HD13	1.93	0.51
1:F:6:VAL:HG22	1:F:521:VAL:HG22	1.91	0.51
1:H:247:LEU:HD12	1:H:248:LEU:H	1.75	0.51
1:H:247:LEU:H	1:H:273:VAL:HG12	1.76	0.51
1:L:259:LEU:O	1:L:263:VAL:HG23	2.10	0.51
1:N:142:LYS:O	1:N:142:LYS:HD3	2.10	0.51
1:N:176:THR:HG21	1:N:333:ILE:HD13	1.93	0.51
1:N:234:LEU:N	1:N:235:PRO:HD2	2.24	0.51
1:A:313:THR:HG23	1:M:311:LYS:NZ	2.25	0.51
1:B:77:VAL:HG23	1:B:78:ALA:N	2.25	0.51
1:C:236:VAL:HG12	1:C:236:VAL:O	2.10	0.51
1:E:69:MET:CE	1:F:41:ASP:HB2	2.39	0.51
1:G:236:VAL:O	1:G:236:VAL:HG12	2.11	0.51
1:K:37:ASN:HD21	1:K:51:LYS:NZ	2.09	0.51
1:N:242:LYS:O	1:N:243:ALA:HB3	2.11	0.51
1:N:417:VAL:O	1:N:420:ILE:HG22	2.11	0.51
1:C:344:GLY:O	1:C:347:ALA:HB3	2.10	0.51
1:C:429:LEU:HD12	1:C:430:ARG:N	2.25	0.51
1:D:23:LEU:HD23	1:D:74:VAL:CG2	2.40	0.51
1:E:77:VAL:CG2	1:E:78:ALA:N	2.74	0.51
1:F:213:VAL:HG12	1:F:214:GLU:H	1.74	0.51
1:H:169:VAL:CG2	1:H:377:ALA:HB2	2.34	0.51
1:H:404:ARG:HG2	1:H:404:ARG:NH1	2.26	0.51
1:I:25:ASP:HA	1:I:28:LYS:HE2	1.92	0.51
1:K:20:VAL:HG23	1:K:74:VAL:HG11	1.93	0.51
1:L:321:LYS:O	1:L:322:ARG:HB2	2.10	0.51
1:N:413:ALA:HB2	1:N:475:ASN:HD22	1.76	0.51
1:H:207:LYS:O	1:H:209:GLU:N	2.44	0.51
1:H:460:GLU:O	1:H:462:PRO:HD3	2.11	0.51
1:J:28:LYS:C	1:J:30:THR:H	2.13	0.51
1:L:23:LEU:HD23	1:L:74:VAL:HG22	1.92	0.51
1:D:155:ASP:OD1	1:D:157:THR:HB	2.10	0.51
1:D:338:GLU:C	1:D:340:ALA:H	2.14	0.51
1:E:37:ASN:HD21	1:E:51:LYS:HE3	1.76	0.51
1:G:412:VAL:HG13	1:G:497:THR:OG1	2.10	0.51
1:I:499:VAL:HG22	1:I:500:THR:N	2.26	0.51
1:J:455:VAL:HG11	1:J:462:PRO:HA	1.91	0.51
1:K:166:MET:HE1	1:K:171:LYS:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:278:ALA:HB3	1:M:285:ARG:HD3	1.92	0.51
1:A:479:ASN:OD1	1:A:481:ALA:HB3	2.11	0.51
1:E:16:MET:HB3	1:E:514:MET:HE3	1.93	0.51
1:H:413:ALA:HB2	1:H:475:ASN:HD22	1.76	0.51
1:I:16:MET:HB3	1:I:514:MET:HE1	1.93	0.51
1:L:278:ALA:HB3	1:L:285:ARG:HD3	1.91	0.51
1:C:183:LEU:HD22	1:C:184:GLN:N	2.25	0.51
1:F:218:PRO:HB3	1:F:246:PRO:HG2	1.93	0.51
1:K:20:VAL:CG2	1:K:74:VAL:HG11	2.41	0.51
1:K:77:VAL:HG21	1:K:510:VAL:CG1	2.39	0.51
1:K:321:LYS:O	1:K:322:ARG:HB2	2.09	0.51
1:L:36:ARG:O	1:L:51:LYS:HG2	2.11	0.51
1:L:207:LYS:O	1:L:209:GLU:N	2.44	0.51
1:N:393:LYS:O	1:N:397:GLU:HB2	2.11	0.51
1:B:245:LYS:HZ2	1:B:319:GLN:HE22	1.58	0.50
1:E:479:ASN:OD1	1:E:481:ALA:HB3	2.10	0.50
1:F:77:VAL:CG2	1:F:78:ALA:N	2.74	0.50
1:D:519:CYS:O	1:E:38:VAL:HA	2.11	0.50
1:E:77:VAL:HG23	1:E:78:ALA:N	2.25	0.50
1:E:208:PRO:HG2	1:E:209:GLU:OE1	2.10	0.50
1:F:242:LYS:C	1:F:244:GLY:H	2.14	0.50
1:G:389:MET:SD	1:G:389:MET:C	2.90	0.50
1:N:36:ARG:O	1:N:51:LYS:HG2	2.12	0.50
1:A:16:MET:HB3	1:A:514:MET:HE3	1.93	0.50
1:D:131:LEU:HD12	1:D:422:VAL:HG21	1.93	0.50
1:D:219:PHE:O	1:D:247:LEU:HD12	2.11	0.50
1:E:202:PRO:O	1:E:203:TYR:HB2	2.11	0.50
1:I:134:LEU:HD11	1:I:421:ARG:HG2	1.93	0.50
1:I:233:MET:O	1:I:237:LEU:HB2	2.11	0.50
1:L:499:VAL:HG22	1:L:500:THR:N	2.25	0.50
1:A:17:LEU:HA	1:A:20:VAL:HG12	1.93	0.50
1:A:183:LEU:HD22	1:A:184:GLN:N	2.26	0.50
1:B:69:MET:CE	1:C:41:ASP:HB2	2.42	0.50
1:E:349:ILE:O	1:E:353:ILE:HG13	2.11	0.50
1:H:160:LYS:O	1:H:164:GLU:HG3	2.12	0.50
1:I:230:ILE:HD12	1:I:261:THR:CG2	2.38	0.50
1:J:321:LYS:O	1:J:322:ARG:HB2	2.12	0.50
1:J:413:ALA:HB2	1:J:475:ASN:HD22	1.76	0.50
1:L:344:GLY:O	1:L:347:ALA:HB3	2.11	0.50
1:B:108:ALA:C	1:B:110:GLY:H	2.15	0.50
1:D:208:PRO:HG2	1:D:209:GLU:OE1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:221:LEU:HB3	1:F:249:ILE:HD13	1.94	0.50
1:J:404:ARG:HG2	1:J:404:ARG:NH1	2.25	0.50
1:K:23:LEU:HD23	1:K:74:VAL:HG22	1.93	0.50
1:M:238:GLU:C	1:M:240:VAL:H	2.14	0.50
1:M:344:GLY:O	1:M:347:ALA:HB3	2.12	0.50
1:N:24:ALA:HA	1:N:27:VAL:HG12	1.94	0.50
1:A:17:LEU:HA	1:A:20:VAL:CG1	2.42	0.50
1:A:202:PRO:O	1:A:203:TYR:HB2	2.12	0.50
1:D:131:LEU:HD13	1:D:422:VAL:HG21	1.93	0.50
1:I:413:ALA:HB2	1:I:475:ASN:HD22	1.76	0.50
1:J:142:LYS:O	1:J:142:LYS:HD3	2.11	0.50
1:K:118:ARG:NH2	1:L:34:LYS:HE2	2.25	0.50
1:K:220:ILE:HG23	1:K:248:LEU:HD23	1.93	0.50
1:M:7:LYS:HG3	1:M:66:PHE:CZ	2.46	0.50
1:M:138:CYS:O	1:M:138:CYS:SG	2.69	0.50
1:N:134:LEU:HD11	1:N:421:ARG:HG2	1.92	0.50
1:N:166:MET:HE2	1:N:171:LYS:HA	1.94	0.50
1:D:420:ILE:HG13	1:D:448:GLU:HG2	1.93	0.50
1:B:412:VAL:HG13	1:B:497:THR:OG1	2.12	0.50
1:C:77:VAL:CG2	1:C:78:ALA:N	2.74	0.50
1:C:180:GLY:HA3	1:C:381:VAL:O	2.11	0.50
1:F:13:ARG:HD2	1:F:104:LEU:HD22	1.94	0.50
1:F:30:THR:O	1:F:31:LEU:C	2.50	0.50
1:F:77:VAL:HG23	1:F:78:ALA:N	2.26	0.50
1:F:349:ILE:O	1:F:353:ILE:HG13	2.11	0.50
1:I:238:GLU:C	1:I:240:VAL:H	2.15	0.50
1:J:238:GLU:C	1:J:240:VAL:H	2.15	0.50
1:A:369:VAL:HG23	1:A:370:ALA:N	2.27	0.50
1:D:517:THR:HG21	1:E:39:VAL:HG23	1.93	0.50
1:E:202:PRO:O	1:E:204:PHE:N	2.41	0.50
1:E:242:LYS:C	1:E:244:GLY:H	2.14	0.50
1:E:338:GLU:C	1:E:340:ALA:H	2.15	0.50
1:G:522:THR:OG1	1:G:523:ASP:N	2.45	0.50
1:J:198:GLY:HA3	1:J:327:LYS:O	2.12	0.50
1:M:142:LYS:O	1:M:142:LYS:HD3	2.11	0.50
1:M:335:GLY:C	1:M:337:GLY:H	2.14	0.50
1:N:201:SER:O	1:N:202:PRO:O	2.28	0.50
1:A:265:ASN:HD22	1:A:265:ASN:N	2.10	0.49
1:C:77:VAL:HG23	1:C:78:ALA:N	2.26	0.49
1:C:338:GLU:C	1:C:340:ALA:H	2.13	0.49
1:C:389:MET:C	1:C:389:MET:SD	2.91	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:391:GLU:O	1:D:394:ALA:HB3	2.11	0.49
1:G:369:VAL:HG23	1:G:370:ALA:N	2.27	0.49
1:H:34:LYS:HG2	1:H:458:CYS:SG	2.52	0.49
1:H:198:GLY:HA3	1:H:327:LYS:O	2.12	0.49
1:L:238:GLU:C	1:L:240:VAL:H	2.15	0.49
1:M:198:GLY:HA3	1:M:327:LYS:O	2.11	0.49
1:C:412:VAL:HG13	1:C:497:THR:OG1	2.12	0.49
1:D:17:LEU:HA	1:D:20:VAL:CG1	2.42	0.49
1:G:6:VAL:HG22	1:G:521:VAL:HG22	1.94	0.49
1:G:77:VAL:O	1:G:80:LYS:N	2.45	0.49
1:J:28:LYS:C	1:J:30:THR:N	2.63	0.49
1:K:176:THR:HG21	1:K:333:ILE:HD13	1.93	0.49
1:K:224:ASP:O	1:K:225:LYS:HB3	2.12	0.49
1:L:16:MET:SD	1:L:514:MET:HE2	2.52	0.49
1:N:166:MET:HE1	1:N:171:LYS:HA	1.94	0.49
1:B:36:ARG:HG3	1:B:36:ARG:NH1	2.27	0.49
1:B:221:LEU:HD23	1:B:249:ILE:HG23	1.94	0.49
1:B:228:SER:OG	1:B:255:GLU:HB2	2.12	0.49
1:C:131:LEU:HD12	1:C:422:VAL:HG21	1.94	0.49
1:F:236:VAL:HG12	1:F:236:VAL:O	2.13	0.49
1:G:221:LEU:HB3	1:G:249:ILE:HD13	1.95	0.49
1:G:242:LYS:C	1:G:244:GLY:H	2.14	0.49
1:I:166:MET:HE1	1:I:171:LYS:HA	1.94	0.49
1:J:215:LEU:HB2	1:J:323:VAL:HG22	1.93	0.49
1:M:18:ARG:HH11	1:M:18:ARG:CG	2.25	0.49
1:N:465:VAL:O	1:N:469:VAL:HG23	2.13	0.49
1:A:134:LEU:HD23	1:A:134:LEU:O	2.13	0.49
1:A:180:GLY:HA3	1:A:381:VAL:O	2.13	0.49
1:B:180:GLY:HA3	1:B:381:VAL:O	2.12	0.49
1:B:420:ILE:HG13	1:B:448:GLU:HG2	1.94	0.49
1:D:217:SER:N	1:D:218:PRO:CD	2.75	0.49
1:F:338:GLU:C	1:F:340:ALA:H	2.15	0.49
1:H:86:GLY:O	1:H:87:ASP:HB2	2.13	0.49
1:I:207:LYS:O	1:I:209:GLU:N	2.46	0.49
1:J:16:MET:HB3	1:J:514:MET:HE1	1.94	0.49
1:L:86:GLY:O	1:L:87:ASP:HB2	2.12	0.49
1:L:197:ARG:HG3	1:L:277:LYS:O	2.13	0.49
1:N:203:TYR:CD1	1:N:267:MET:HE3	2.47	0.49
1:A:217:SER:N	1:A:218:PRO:CD	2.76	0.49
1:B:265:ASN:HD22	1:B:265:ASN:N	2.11	0.49
1:C:247:LEU:HB3	1:C:273:VAL:CG1	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:ALA:C	1:D:110:GLY:H	2.15	0.49
1:D:240:VAL:HG11	1:D:247:LEU:HB2	1.95	0.49
1:E:144:ILE:HD13	1:E:166:MET:SD	2.52	0.49
1:G:33:PRO:HD2	1:G:454:ILE:HG23	1.94	0.49
1:G:202:PRO:O	1:G:203:TYR:HB2	2.11	0.49
1:G:218:PRO:HB3	1:G:246:PRO:HG2	1.93	0.49
1:H:129:GLU:C	1:H:131:LEU:H	2.15	0.49
1:I:460:GLU:O	1:I:462:PRO:HD3	2.12	0.49
1:M:215:LEU:HB2	1:M:323:VAL:HG22	1.94	0.49
1:N:86:GLY:O	1:N:87:ASP:HB2	2.12	0.49
1:N:319:GLN:O	1:N:336:VAL:HG23	2.12	0.49
1:B:338:GLU:C	1:B:340:ALA:H	2.16	0.49
1:C:25:ASP:HA	1:C:28:LYS:HE2	1.94	0.49
1:F:183:LEU:HD22	1:F:184:GLN:N	2.25	0.49
1:J:37:ASN:HD21	1:J:51:LYS:NZ	2.11	0.49
1:K:77:VAL:HG11	1:K:510:VAL:HB	1.93	0.49
1:K:202:PRO:O	1:K:204:PHE:N	2.39	0.49
1:L:169:VAL:CG2	1:L:377:ALA:HB2	2.33	0.49
1:M:176:THR:HG21	1:M:333:ILE:HD13	1.94	0.49
1:N:233:MET:O	1:N:237:LEU:HB2	2.13	0.49
1:C:122:LYS:HE2	1:C:429:LEU:HD11	1.94	0.49
1:C:369:VAL:HG23	1:C:370:ALA:N	2.28	0.49
1:E:245:LYS:HZ2	1:E:319:GLN:HE22	1.58	0.49
1:F:245:LYS:HZ2	1:F:319:GLN:HE22	1.59	0.49
1:G:202:PRO:O	1:G:204:PHE:N	2.40	0.49
1:L:129:GLU:C	1:L:131:LEU:H	2.15	0.49
1:N:74:VAL:HA	1:N:510:VAL:HG21	1.95	0.49
1:C:250:ILE:HG22	1:C:289:LEU:HD21	1.95	0.49
1:J:201:SER:O	1:J:202:PRO:O	2.30	0.49
1:L:393:LYS:O	1:L:397:GLU:HB2	2.13	0.49
1:M:77:VAL:HG21	1:M:510:VAL:CG1	2.42	0.49
1:N:207:LYS:O	1:N:209:GLU:N	2.46	0.49
1:A:325:ILE:N	1:A:325:ILE:HD12	2.27	0.49
1:B:451:LEU:O	1:B:451:LEU:HD23	2.13	0.49
1:C:77:VAL:O	1:C:80:LYS:N	2.46	0.49
1:D:369:VAL:HG23	1:D:370:ALA:N	2.28	0.49
1:G:391:GLU:O	1:G:394:ALA:HB3	2.12	0.49
1:H:241:ALA:CB	1:N:231:ARG:NH1	2.75	0.49
1:J:224:ASP:O	1:J:225:LYS:HB3	2.13	0.49
1:K:203:TYR:HB3	1:K:267:MET:HE1	1.93	0.49
1:K:207:LYS:O	1:K:209:GLU:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:344:GLY:O	1:K:347:ALA:HB3	2.13	0.49
1:L:24:ALA:HA	1:L:27:VAL:HG12	1.94	0.49
1:L:335:GLY:C	1:L:337:GLY:H	2.16	0.49
1:M:224:ASP:O	1:M:225:LYS:HB3	2.12	0.49
1:N:37:ASN:HD21	1:N:51:LYS:HZ3	1.61	0.49
1:N:238:GLU:C	1:N:240:VAL:H	2.14	0.49
1:N:451:LEU:HD23	1:N:451:LEU:C	2.33	0.49
1:A:271:VAL:HG12	1:A:273:VAL:HG13	1.95	0.49
1:C:202:PRO:O	1:C:204:PHE:N	2.43	0.49
1:D:494:LEU:C	1:D:494:LEU:HD12	2.32	0.49
1:E:25:ASP:O	1:E:29:VAL:HG22	2.12	0.49
1:E:501:ARG:O	1:E:505:GLN:HG3	2.12	0.49
1:F:127:ALA:HB1	1:F:422:VAL:HG11	1.95	0.49
1:F:217:SER:N	1:F:218:PRO:CD	2.76	0.49
1:G:122:LYS:HE2	1:G:429:LEU:HD11	1.95	0.49
1:J:224:ASP:HB3	1:J:302:SER:HB3	1.95	0.49
1:K:201:SER:O	1:K:202:PRO:O	2.31	0.49
1:K:460:GLU:O	1:K:462:PRO:HD3	2.12	0.49
1:L:404:ARG:HG2	1:L:404:ARG:NH1	2.24	0.49
1:N:221:LEU:HB3	1:N:249:ILE:HD13	1.93	0.49
1:N:335:GLY:C	1:N:337:GLY:H	2.16	0.49
1:A:338:GLU:C	1:A:340:ALA:H	2.15	0.48
1:B:134:LEU:HD23	1:B:134:LEU:O	2.12	0.48
1:C:8:PHE:HE1	1:D:26:ALA:HA	1.78	0.48
1:C:202:PRO:O	1:C:203:TYR:HB2	2.13	0.48
1:D:77:VAL:HG23	1:D:78:ALA:N	2.28	0.48
1:I:77:VAL:HG11	1:I:510:VAL:HB	1.95	0.48
1:N:160:LYS:O	1:N:164:GLU:HG3	2.13	0.48
1:A:106:ALA:O	1:A:109:ALA:HB3	2.13	0.48
1:A:131:LEU:HD12	1:A:422:VAL:HG21	1.94	0.48
1:A:242:LYS:C	1:A:244:GLY:H	2.15	0.48
1:B:319:GLN:O	1:B:336:VAL:HG23	2.13	0.48
1:C:242:LYS:O	1:C:243:ALA:HB3	2.13	0.48
1:E:31:LEU:HA	1:E:31:LEU:HD12	1.60	0.48
1:G:106:ALA:O	1:G:109:ALA:HB3	2.13	0.48
1:G:247:LEU:HB3	1:G:273:VAL:CG1	2.42	0.48
1:K:8:PHE:HZ	1:L:26:ALA:HB2	1.78	0.48
1:K:393:LYS:O	1:K:397:GLU:HB2	2.12	0.48
1:L:20:VAL:HG23	1:L:74:VAL:HG11	1.94	0.48
1:M:166:MET:HE2	1:M:171:LYS:HA	1.94	0.48
1:F:114:MET:HG3	1:G:34:LYS:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:202:PRO:O	1:F:203:TYR:HB2	2.13	0.48
1:G:338:GLU:C	1:G:340:ALA:H	2.17	0.48
1:H:393:LYS:O	1:H:397:GLU:HB2	2.12	0.48
1:I:200:LEU:HD13	1:I:254:VAL:HB	1.95	0.48
1:L:20:VAL:CG2	1:L:74:VAL:HG11	2.42	0.48
1:L:160:LYS:O	1:L:164:GLU:HG3	2.12	0.48
1:L:224:ASP:O	1:L:225:LYS:HB3	2.12	0.48
1:A:155:ASP:OD1	1:A:157:THR:HB	2.13	0.48
1:B:513:LEU:HD13	1:C:49:ILE:HD12	1.96	0.48
1:E:111:MET:SD	1:E:438:VAL:HG21	2.53	0.48
1:F:131:LEU:HD12	1:F:422:VAL:HG21	1.94	0.48
1:F:197:ARG:HE	1:F:279:PRO:HA	1.78	0.48
1:H:162:ILE:O	1:H:165:ALA:HB3	2.13	0.48
1:H:344:GLY:O	1:H:347:ALA:HB3	2.13	0.48
1:N:203:TYR:HB3	1:N:267:MET:HE1	1.93	0.48
1:B:496:PRO:HB2	1:B:499:VAL:HG13	1.95	0.48
1:D:77:VAL:CG2	1:D:78:ALA:N	2.76	0.48
1:D:369:VAL:O	1:D:373:ALA:N	2.46	0.48
1:G:219:PHE:O	1:G:247:LEU:HD12	2.13	0.48
1:H:134:LEU:HD11	1:H:421:ARG:HG2	1.96	0.48
1:J:7:LYS:HG3	1:J:66:PHE:CZ	2.49	0.48
1:N:200:LEU:HG	1:N:275:ALA:O	2.13	0.48
1:B:325:ILE:HD12	1:B:325:ILE:N	2.29	0.48
1:E:326:ASN:HD22	1:E:329:THR:CB	2.01	0.48
1:J:160:LYS:O	1:J:164:GLU:HG3	2.13	0.48
1:L:127:ALA:O	1:L:131:LEU:HB2	2.13	0.48
1:L:455:VAL:HG11	1:L:462:PRO:HA	1.95	0.48
1:M:162:ILE:O	1:M:165:ALA:HB3	2.13	0.48
1:M:499:VAL:CG2	1:M:500:THR:N	2.76	0.48
1:B:25:ASP:HA	1:B:28:LYS:HE2	1.95	0.48
1:C:155:ASP:OD1	1:C:157:THR:HB	2.14	0.48
1:D:33:PRO:C	1:D:35:GLY:H	2.17	0.48
1:D:242:LYS:C	1:D:244:GLY:H	2.17	0.48
1:E:153:ASN:O	1:E:154:SER:HB2	2.14	0.48
1:H:230:ILE:HD12	1:H:261:THR:CG2	2.38	0.48
1:I:248:LEU:CD1	1:I:325:ILE:HD11	2.44	0.48
1:J:111:MET:SD	1:J:438:VAL:HG21	2.54	0.48
1:N:37:ASN:HD21	1:N:51:LYS:HZ2	1.62	0.48
1:N:200:LEU:HG	1:N:276:VAL:HA	1.95	0.48
1:C:36:ARG:HG3	1:C:36:ARG:NH1	2.27	0.48
1:D:250:ILE:HG22	1:D:289:LEU:HD21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:319:GLN:O	1:D:336:VAL:HG23	2.13	0.48
1:E:450:PRO:O	1:E:454:ILE:HG13	2.14	0.48
1:G:265:ASN:N	1:G:265:ASN:HD22	2.11	0.48
1:H:18:ARG:HH11	1:H:18:ARG:CG	2.24	0.48
1:H:335:GLY:C	1:H:337:GLY:H	2.16	0.48
1:I:215:LEU:HB2	1:I:323:VAL:HG22	1.96	0.48
1:I:404:ARG:HG2	1:I:404:ARG:NH1	2.21	0.48
1:I:444:LEU:HA	1:I:447:MET:HE3	1.95	0.48
1:J:254:VAL:O	1:J:259:LEU:HD22	2.13	0.48
1:J:499:VAL:CG2	1:J:500:THR:N	2.77	0.48
1:K:24:ALA:HA	1:K:27:VAL:HG12	1.95	0.48
1:L:134:LEU:HD11	1:L:421:ARG:HG2	1.96	0.48
1:M:444:LEU:HA	1:M:447:MET:HE3	1.95	0.48
1:B:155:ASP:OD1	1:B:157:THR:HB	2.14	0.48
1:C:218:PRO:HB3	1:C:246:PRO:HG2	1.96	0.48
1:D:265:ASN:HD22	1:D:265:ASN:N	2.10	0.48
1:D:381:VAL:HG21	1:D:393:LYS:HA	1.95	0.48
1:E:520:MET:HA	1:F:39:VAL:O	2.14	0.48
1:F:311:LYS:O	1:H:311:LYS:HE2	2.14	0.48
1:G:25:ASP:HA	1:G:28:LYS:HE2	1.96	0.48
1:H:77:VAL:HG11	1:H:510:VAL:HB	1.96	0.48
1:H:238:GLU:C	1:H:240:VAL:H	2.16	0.48
1:K:69:MET:HE1	1:L:39:VAL:HG12	1.96	0.48
1:L:7:LYS:HG3	1:L:66:PHE:CZ	2.49	0.48
1:L:77:VAL:HG11	1:L:510:VAL:HB	1.95	0.48
1:L:418:ALA:O	1:L:422:VAL:HG22	2.14	0.48
1:M:25:ASP:HA	1:M:28:LYS:HE2	1.95	0.48
1:A:140:ASP:C	1:A:142:LYS:H	2.17	0.48
1:A:247:LEU:HB3	1:A:273:VAL:CG1	2.43	0.48
1:C:420:ILE:HG13	1:C:448:GLU:HG2	1.96	0.48
1:D:325:ILE:N	1:D:325:ILE:HD12	2.29	0.48
1:E:17:LEU:HA	1:E:20:VAL:CG1	2.44	0.48
1:I:252:GLU:O	1:I:277:LYS:HG3	2.14	0.48
1:A:36:ARG:HH11	1:A:36:ARG:HG3	1.79	0.47
1:C:391:GLU:O	1:C:394:ALA:HB3	2.14	0.47
1:F:311:LYS:HD3	1:H:311:LYS:HG2	1.96	0.47
1:G:131:LEU:HD13	1:G:422:VAL:HG21	1.95	0.47
1:J:23:LEU:HD23	1:J:74:VAL:HG22	1.95	0.47
1:K:86:GLY:O	1:K:87:ASP:HB2	2.13	0.47
1:L:118:ARG:NH2	1:M:34:LYS:HE3	2.29	0.47
1:M:22:VAL:HG11	1:M:62:LEU:CD2	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:194:GLN:O	1:M:194:GLN:HG2	2.14	0.47
1:B:236:VAL:O	1:B:236:VAL:HG12	2.14	0.47
1:C:221:LEU:HD23	1:C:249:ILE:HG23	1.95	0.47
1:G:17:LEU:HA	1:G:20:VAL:HG12	1.96	0.47
1:J:203:TYR:CD1	1:J:267:MET:HE3	2.50	0.47
1:K:30:THR:CG2	1:K:31:LEU:N	2.77	0.47
1:K:230:ILE:HD12	1:K:261:THR:CG2	2.38	0.47
1:L:70:GLY:HA2	1:L:73:MET:HE3	1.95	0.47
1:N:404:ARG:HG2	1:N:404:ARG:NH1	2.27	0.47
1:N:485:TYR:HD1	1:N:485:TYR:H	1.62	0.47
1:A:25:ASP:HA	1:A:28:LYS:HE2	1.96	0.47
1:B:494:LEU:C	1:B:494:LEU:HD12	2.35	0.47
1:C:17:LEU:HA	1:C:20:VAL:HG12	1.96	0.47
1:D:106:ALA:O	1:D:109:ALA:HB3	2.14	0.47
1:F:31:LEU:HD22	1:F:90:THR:CG2	2.44	0.47
1:F:485:TYR:N	1:F:485:TYR:CD1	2.82	0.47
1:G:134:LEU:HD23	1:G:134:LEU:O	2.13	0.47
1:G:153:ASN:O	1:G:154:SER:HB2	2.14	0.47
1:H:37:ASN:HD21	1:H:51:LYS:HZ3	1.61	0.47
1:H:180:GLY:HA3	1:H:381:VAL:O	2.14	0.47
1:J:207:LYS:O	1:J:209:GLU:N	2.47	0.47
1:K:404:ARG:HG2	1:K:404:ARG:NH1	2.25	0.47
1:L:18:ARG:HH11	1:L:18:ARG:CG	2.27	0.47
1:M:404:ARG:HG2	1:M:404:ARG:NH1	2.27	0.47
1:A:3:ALA:HA	1:B:61:GLU:O	2.14	0.47
1:C:226:LYS:HD3	1:C:255:GLU:OE2	2.15	0.47
1:D:271:VAL:HG12	1:D:273:VAL:HG13	1.97	0.47
1:F:226:LYS:HD3	1:F:255:GLU:OE2	2.15	0.47
1:G:17:LEU:HA	1:G:20:VAL:CG1	2.45	0.47
1:I:118:ARG:HH22	1:J:34:LYS:HE3	1.79	0.47
1:I:160:LYS:O	1:I:164:GLU:HG3	2.13	0.47
1:I:224:ASP:HB3	1:I:302:SER:HB3	1.96	0.47
1:I:451:LEU:HD23	1:I:451:LEU:O	2.14	0.47
1:K:129:GLU:C	1:K:131:LEU:H	2.16	0.47
1:K:201:SER:C	1:K:202:PRO:O	2.53	0.47
1:K:499:VAL:CG2	1:K:500:THR:N	2.77	0.47
1:L:103:GLY:O	1:L:107:VAL:HG23	2.14	0.47
1:A:233:MET:HB3	1:A:237:LEU:HD12	1.96	0.47
1:B:17:LEU:HA	1:B:20:VAL:CG1	2.45	0.47
1:B:23:LEU:CD2	1:B:75:LYS:HG3	2.45	0.47
1:C:265:ASN:HD22	1:C:265:ASN:N	2.11	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:494:LEU:C	1:C:494:LEU:HD12	2.35	0.47
1:F:369:VAL:HG23	1:F:370:ALA:N	2.29	0.47
1:I:23:LEU:HD23	1:I:74:VAL:HG22	1.96	0.47
1:K:103:GLY:O	1:K:107:VAL:HG23	2.14	0.47
1:K:335:GLY:C	1:K:337:GLY:H	2.16	0.47
1:L:128:VAL:O	1:L:132:LYS:HG3	2.14	0.47
1:L:142:LYS:O	1:L:142:LYS:HD3	2.14	0.47
1:M:139:SER:HB3	1:M:171:LYS:HZ3	1.79	0.47
1:A:221:LEU:HB3	1:A:249:ILE:HD13	1.96	0.47
1:B:127:ALA:HB1	1:B:422:VAL:HG11	1.96	0.47
1:B:198:GLY:O	1:B:276:VAL:HG12	2.15	0.47
1:E:180:GLY:HA3	1:E:381:VAL:O	2.14	0.47
1:E:485:TYR:N	1:E:485:TYR:CD1	2.82	0.47
1:F:250:ILE:HG22	1:F:289:LEU:HD21	1.97	0.47
1:G:226:LYS:HD3	1:G:255:GLU:OE2	2.14	0.47
1:G:240:VAL:HG11	1:G:247:LEU:HB2	1.96	0.47
1:H:451:LEU:HD23	1:H:451:LEU:O	2.14	0.47
1:L:162:ILE:O	1:L:165:ALA:HB3	2.15	0.47
1:L:201:SER:O	1:L:202:PRO:O	2.32	0.47
1:M:70:GLY:HA2	1:M:73:MET:HE3	1.95	0.47
1:N:224:ASP:HB3	1:N:302:SER:HB3	1.95	0.47
1:A:199:TYR:CE2	1:A:327:LYS:HA	2.49	0.47
1:D:140:ASP:C	1:D:142:LYS:H	2.18	0.47
1:E:17:LEU:HA	1:E:20:VAL:HG12	1.97	0.47
1:E:140:ASP:C	1:E:142:LYS:H	2.18	0.47
1:F:122:LYS:HE2	1:F:429:LEU:HD11	1.95	0.47
1:G:180:GLY:HA3	1:G:381:VAL:O	2.15	0.47
1:H:485:TYR:HD1	1:H:485:TYR:H	1.61	0.47
1:J:278:ALA:HB1	1:J:279:PRO:HD2	1.97	0.47
1:L:22:VAL:HG11	1:L:62:LEU:CD2	2.44	0.47
1:L:198:GLY:HA3	1:L:327:LYS:O	2.15	0.47
1:N:23:LEU:HD23	1:N:74:VAL:HG22	1.96	0.47
1:N:214:GLU:C	1:N:215:LEU:HD23	2.35	0.47
1:A:23:LEU:CD2	1:A:75:LYS:HG3	2.45	0.47
1:H:252:GLU:O	1:H:277:LYS:HG3	2.13	0.47
1:L:114:MET:HB3	1:M:34:LYS:HE2	1.97	0.47
1:L:180:GLY:HA3	1:L:381:VAL:O	2.15	0.47
1:M:34:LYS:HB2	1:M:458:CYS:SG	2.55	0.47
1:A:221:LEU:HD23	1:A:249:ILE:HG23	1.96	0.47
1:A:391:GLU:O	1:A:394:ALA:HB3	2.15	0.47
1:B:381:VAL:HG21	1:B:393:LYS:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:LEU:CD2	1:C:75:LYS:HG3	2.45	0.47
1:C:134:LEU:O	1:C:134:LEU:HD23	2.15	0.47
1:F:233:MET:HB3	1:F:237:LEU:HD12	1.97	0.47
1:G:233:MET:HB3	1:G:237:LEU:HD12	1.96	0.47
1:G:271:VAL:HG12	1:G:273:VAL:HG13	1.96	0.47
1:H:248:LEU:CD1	1:H:325:ILE:HD11	2.45	0.47
1:I:129:GLU:C	1:I:131:LEU:H	2.19	0.47
1:K:7:LYS:HG3	1:K:66:PHE:CZ	2.50	0.47
1:K:138:CYS:O	1:K:138:CYS:SG	2.73	0.47
1:K:139:SER:HB3	1:K:171:LYS:HZ1	1.79	0.47
1:K:140:ASP:C	1:K:142:LYS:H	2.18	0.47
1:K:291:ASP:OD2	1:K:368:ARG:HD2	2.15	0.47
1:M:201:SER:O	1:M:202:PRO:O	2.33	0.47
1:M:233:MET:O	1:M:237:LEU:HB2	2.15	0.47
1:N:349:ILE:HG21	1:N:369:VAL:HG13	1.97	0.47
1:A:451:LEU:O	1:A:451:LEU:HD23	2.15	0.47
1:C:197:ARG:HE	1:C:279:PRO:HA	1.80	0.47
1:C:271:VAL:HG12	1:C:273:VAL:HG13	1.96	0.47
1:C:479:ASN:OD1	1:C:481:ALA:HB3	2.15	0.47
1:D:16:MET:HB3	1:D:514:MET:CE	2.45	0.47
1:F:23:LEU:CD2	1:F:75:LYS:HG3	2.45	0.47
1:G:296:THR:O	1:G:297:GLY:O	2.33	0.47
1:H:233:MET:O	1:H:237:LEU:HB2	2.15	0.47
1:J:200:LEU:HD13	1:J:254:VAL:HB	1.96	0.47
1:K:22:VAL:HG11	1:K:62:LEU:CD2	2.45	0.47
1:K:200:LEU:HG	1:K:275:ALA:O	2.15	0.47
1:K:200:LEU:HD13	1:K:254:VAL:HB	1.96	0.47
1:K:238:GLU:C	1:K:240:VAL:H	2.18	0.47
1:M:451:LEU:HD23	1:M:451:LEU:O	2.15	0.47
1:N:201:SER:C	1:N:202:PRO:O	2.54	0.47
1:N:344:GLY:O	1:N:347:ALA:HB3	2.15	0.47
1:C:13:ARG:HD2	1:C:104:LEU:HD22	1.97	0.46
1:C:140:ASP:C	1:C:142:LYS:H	2.18	0.46
1:C:249:ILE:HB	1:C:275:ALA:CB	2.45	0.46
1:G:217:SER:N	1:G:218:PRO:CD	2.79	0.46
1:G:420:ILE:HG13	1:G:448:GLU:HG2	1.97	0.46
1:H:127:ALA:O	1:H:131:LEU:HB2	2.15	0.46
1:H:198:GLY:CA	1:H:328:ASP:HA	2.45	0.46
1:I:201:SER:O	1:I:202:PRO:O	2.33	0.46
1:L:349:ILE:HG21	1:L:369:VAL:HG13	1.97	0.46
1:M:31:LEU:HD12	1:M:90:THR:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:MET:CE	1:A:292:ILE:HG12	2.45	0.46
1:A:249:ILE:HB	1:A:275:ALA:CB	2.45	0.46
1:B:217:SER:N	1:B:218:PRO:CD	2.77	0.46
1:B:233:MET:HB3	1:B:237:LEU:HD12	1.97	0.46
1:B:369:VAL:HG23	1:B:370:ALA:N	2.30	0.46
1:D:34:LYS:HD2	1:D:458:CYS:HB3	1.94	0.46
1:E:131:LEU:HD12	1:E:422:VAL:HG21	1.96	0.46
1:E:369:VAL:HG23	1:E:370:ALA:N	2.30	0.46
1:M:103:GLY:O	1:M:107:VAL:HG23	2.15	0.46
1:A:108:ALA:C	1:A:110:GLY:H	2.18	0.46
1:C:233:MET:HB3	1:C:237:LEU:HD12	1.96	0.46
1:C:248:LEU:HD12	1:C:274:ALA:O	2.15	0.46
1:E:193:MET:HG2	1:E:194:GLN:N	2.30	0.46
1:E:265:ASN:HD22	1:E:265:ASN:N	2.11	0.46
1:E:487:ASN:O	1:E:491:MET:HG3	2.15	0.46
1:G:479:ASN:OD1	1:G:481:ALA:HB3	2.15	0.46
1:H:166:MET:HE1	1:H:171:LYS:HA	1.96	0.46
1:J:233:MET:O	1:J:237:LEU:HB2	2.15	0.46
1:K:349:ILE:HG21	1:K:369:VAL:HG13	1.98	0.46
1:K:520:MET:HG2	1:L:39:VAL:HB	1.97	0.46
1:L:73:MET:SD	1:M:49:ILE:HD11	2.56	0.46
1:L:139:SER:HB3	1:L:171:LYS:HZ1	1.80	0.46
1:N:77:VAL:HG11	1:N:510:VAL:HB	1.98	0.46
1:A:224:ASP:O	1:A:225:LYS:HB3	2.16	0.46
1:B:140:ASP:C	1:B:142:LYS:H	2.19	0.46
1:B:166:MET:CE	1:B:171:LYS:HA	2.45	0.46
1:F:140:ASP:O	1:F:142:LYS:N	2.48	0.46
1:F:209:GLU:OE1	1:F:209:GLU:N	2.48	0.46
1:F:391:GLU:O	1:F:394:ALA:HB3	2.16	0.46
1:G:465:VAL:O	1:G:469:VAL:HG23	2.15	0.46
1:H:70:GLY:HA2	1:H:73:MET:HE3	1.96	0.46
1:I:198:GLY:HA3	1:I:327:LYS:O	2.16	0.46
1:A:250:ILE:HG22	1:A:289:LEU:HD21	1.98	0.46
1:B:153:ASN:O	1:B:154:SER:HB2	2.15	0.46
1:B:391:GLU:O	1:B:394:ALA:HB3	2.16	0.46
1:E:250:ILE:HG22	1:E:289:LEU:HD21	1.97	0.46
1:G:140:ASP:C	1:G:142:LYS:H	2.16	0.46
1:G:201:SER:O	1:G:204:PHE:HD2	1.98	0.46
1:H:258:ALA:O	1:H:262:LEU:HG	2.16	0.46
1:I:393:LYS:O	1:I:397:GLU:HB2	2.14	0.46
1:I:417:VAL:O	1:I:420:ILE:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:17:LEU:HA	1:L:20:VAL:CG1	2.43	0.46
1:L:140:ASP:C	1:L:142:LYS:H	2.19	0.46
1:L:501:ARG:HG2	1:L:501:ARG:HH11	1.80	0.46
1:M:455:VAL:HG11	1:M:462:PRO:HA	1.98	0.46
1:M:479:ASN:ND2	1:M:482:THR:HG23	2.31	0.46
1:E:193:MET:CE	1:E:292:ILE:HG12	2.46	0.46
1:E:217:SER:N	1:E:218:PRO:CD	2.78	0.46
1:E:319:GLN:O	1:E:336:VAL:HG23	2.16	0.46
1:F:311:LYS:HD3	1:H:311:LYS:CB	2.46	0.46
1:H:224:ASP:HB3	1:H:302:SER:HB3	1.97	0.46
1:J:129:GLU:C	1:J:131:LEU:H	2.19	0.46
1:J:321:LYS:O	1:J:321:LYS:HG2	2.16	0.46
1:L:17:LEU:O	1:L:20:VAL:HG12	2.16	0.46
1:L:252:GLU:O	1:L:277:LYS:HG3	2.15	0.46
1:L:521:VAL:O	1:M:41:ASP:N	2.46	0.46
1:M:69:MET:HE2	1:N:39:VAL:CG1	2.45	0.46
1:B:250:ILE:HG22	1:B:289:LEU:HD21	1.97	0.46
1:C:369:VAL:O	1:C:373:ALA:N	2.49	0.46
1:D:127:ALA:O	1:D:131:LEU:HB2	2.16	0.46
1:H:278:ALA:HB1	1:H:279:PRO:HD2	1.98	0.46
1:K:265:ASN:HD22	1:K:265:ASN:N	2.14	0.46
1:K:336:VAL:HG12	1:K:336:VAL:O	2.16	0.46
1:L:265:ASN:HD22	1:L:265:ASN:N	2.14	0.46
1:N:198:GLY:HA3	1:N:327:LYS:O	2.16	0.46
1:A:197:ARG:HG3	1:A:277:LYS:O	2.16	0.46
1:B:166:MET:HE1	1:B:171:LYS:HA	1.98	0.46
1:B:385:THR:OG1	1:B:388:GLU:HG3	2.16	0.46
1:D:180:GLY:HA3	1:D:381:VAL:O	2.16	0.46
1:E:155:ASP:OD1	1:E:157:THR:HB	2.15	0.46
1:F:34:LYS:HG2	1:F:458:CYS:SG	2.56	0.46
1:G:248:LEU:HD12	1:G:274:ALA:O	2.15	0.46
1:H:200:LEU:HD13	1:H:254:VAL:HB	1.98	0.46
1:H:224:ASP:O	1:H:225:LYS:HB3	2.15	0.46
1:J:37:ASN:HD22	1:J:51:LYS:HG3	1.80	0.46
1:A:209:GLU:OE1	1:A:209:GLU:N	2.49	0.46
1:D:233:MET:HB3	1:D:237:LEU:HD12	1.97	0.46
1:D:485:TYR:N	1:D:485:TYR:CD1	2.83	0.46
1:E:485:TYR:HD1	1:E:485:TYR:H	1.64	0.46
1:F:108:ALA:C	1:F:110:GLY:H	2.20	0.46
1:I:28:LYS:C	1:I:30:THR:N	2.70	0.46
1:I:344:GLY:O	1:I:347:ALA:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:494:LEU:HD12	1:K:494:LEU:N	2.25	0.46
1:M:200:LEU:HG	1:M:276:VAL:HA	1.96	0.46
1:N:198:GLY:CA	1:N:328:ASP:HA	2.46	0.46
1:N:418:ALA:O	1:N:422:VAL:HG22	2.15	0.46
1:A:218:PRO:HB3	1:A:246:PRO:HG2	1.98	0.46
1:D:6:VAL:HG22	1:D:521:VAL:HG22	1.97	0.46
1:D:134:LEU:HD23	1:D:134:LEU:O	2.16	0.46
1:H:336:VAL:O	1:H:336:VAL:HG12	2.16	0.46
1:I:335:GLY:C	1:I:337:GLY:H	2.19	0.46
1:I:479:ASN:ND2	1:I:482:THR:HG23	2.31	0.46
1:L:201:SER:C	1:L:202:PRO:O	2.54	0.46
1:L:220:ILE:HG23	1:L:248:LEU:HD23	1.98	0.46
1:M:278:ALA:HB1	1:M:279:PRO:HD2	1.97	0.46
1:N:9:GLY:O	1:N:12:ALA:N	2.49	0.46
1:C:217:SER:N	1:C:218:PRO:CD	2.79	0.45
1:D:224:ASP:O	1:D:225:LYS:HB3	2.16	0.45
1:E:271:VAL:HG12	1:E:273:VAL:HG13	1.98	0.45
1:H:16:MET:SD	1:H:514:MET:CE	3.04	0.45
1:I:278:ALA:HB1	1:I:279:PRO:HD2	1.98	0.45
1:J:243:ALA:O	1:J:245:LYS:N	2.49	0.45
1:K:233:MET:O	1:K:237:LEU:HB2	2.17	0.45
1:K:252:GLU:O	1:K:277:LYS:HG3	2.17	0.45
1:K:455:VAL:HG13	1:K:460:GLU:CB	2.47	0.45
1:L:37:ASN:HD21	1:L:51:LYS:HZ2	1.63	0.45
1:N:126:ALA:O	1:N:129:GLU:N	2.49	0.45
1:N:138:CYS:O	1:N:138:CYS:SG	2.73	0.45
1:C:16:MET:HB3	1:C:514:MET:CE	2.46	0.45
1:C:17:LEU:HA	1:C:20:VAL:CG1	2.46	0.45
1:C:296:THR:O	1:C:297:GLY:O	2.34	0.45
1:C:501:ARG:O	1:C:505:GLN:HG3	2.16	0.45
1:D:201:SER:C	1:D:202:PRO:O	2.55	0.45
1:G:197:ARG:HE	1:G:279:PRO:HA	1.80	0.45
1:H:138:CYS:O	1:H:138:CYS:SG	2.74	0.45
1:J:430:ARG:HG2	1:J:430:ARG:HH11	1.81	0.45
1:M:180:GLY:HA3	1:M:381:VAL:O	2.15	0.45
1:M:200:LEU:HD13	1:M:254:VAL:HB	1.98	0.45
1:M:224:ASP:HB3	1:M:302:SER:HB3	1.98	0.45
1:A:77:VAL:O	1:A:80:LYS:N	2.48	0.45
1:C:82:ASN:HB2	1:C:89:THR:HG1	1.81	0.45
1:E:233:MET:HB3	1:E:237:LEU:HD12	1.97	0.45
1:E:248:LEU:HD12	1:E:274:ALA:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:296:THR:O	1:E:297:GLY:O	2.34	0.45
1:F:28:LYS:C	1:F:30:THR:H	2.18	0.45
1:F:140:ASP:C	1:F:142:LYS:N	2.69	0.45
1:G:249:ILE:HB	1:G:275:ALA:CB	2.46	0.45
1:K:127:ALA:O	1:K:131:LEU:HB2	2.15	0.45
1:M:265:ASN:HD22	1:M:265:ASN:N	2.13	0.45
1:N:7:LYS:HG3	1:N:66:PHE:CZ	2.50	0.45
1:A:16:MET:HB3	1:A:514:MET:CE	2.46	0.45
1:B:249:ILE:HB	1:B:275:ALA:CB	2.46	0.45
1:C:209:GLU:OE1	1:C:209:GLU:N	2.49	0.45
1:D:25:ASP:HA	1:D:28:LYS:HE2	1.98	0.45
1:D:36:ARG:HH11	1:D:36:ARG:HG3	1.81	0.45
1:E:13:ARG:HD3	1:E:104:LEU:HD22	1.98	0.45
1:E:493:ILE:HG22	1:E:493:ILE:O	2.16	0.45
1:F:249:ILE:HB	1:F:275:ALA:CB	2.47	0.45
1:G:131:LEU:HD12	1:G:422:VAL:HG21	1.98	0.45
1:J:248:LEU:CD1	1:J:325:ILE:HD11	2.47	0.45
1:J:291:ASP:OD2	1:J:368:ARG:HD2	2.16	0.45
1:J:335:GLY:C	1:J:337:GLY:H	2.18	0.45
1:L:200:LEU:HG	1:L:276:VAL:HA	1.98	0.45
1:N:64:ASP:OD1	1:N:66:PHE:HB2	2.16	0.45
1:N:220:ILE:HG23	1:N:248:LEU:HD23	1.97	0.45
1:B:519:CYS:HB3	1:C:38:VAL:HG13	1.98	0.45
1:E:16:MET:HB3	1:E:514:MET:CE	2.46	0.45
1:F:265:ASN:HD22	1:F:265:ASN:N	2.13	0.45
1:G:494:LEU:C	1:G:494:LEU:HD12	2.37	0.45
1:J:134:LEU:HD11	1:J:421:ARG:HG2	1.97	0.45
1:K:198:GLY:HA3	1:K:327:LYS:O	2.15	0.45
1:L:278:ALA:HB1	1:L:279:PRO:HD2	1.98	0.45
1:L:494:LEU:HD12	1:L:494:LEU:N	2.24	0.45
1:M:207:LYS:O	1:M:209:GLU:N	2.49	0.45
1:M:291:ASP:OD2	1:M:368:ARG:HD2	2.17	0.45
1:N:129:GLU:C	1:N:131:LEU:H	2.19	0.45
1:B:296:THR:O	1:B:297:GLY:O	2.33	0.45
1:B:451:LEU:HD23	1:B:451:LEU:C	2.37	0.45
1:C:221:LEU:HB3	1:C:249:ILE:HD13	1.97	0.45
1:D:52:ASP:OD1	1:D:54:VAL:HG23	2.17	0.45
1:G:183:LEU:HD22	1:G:184:GLN:N	2.26	0.45
1:J:127:ALA:O	1:J:131:LEU:HB2	2.17	0.45
1:J:235:PRO:HG3	1:J:310:GLU:CG	2.46	0.45
1:L:124:VAL:O	1:L:125:THR:C	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:18:ARG:HH11	1:N:18:ARG:CG	2.29	0.45
1:N:140:ASP:C	1:N:142:LYS:H	2.20	0.45
1:A:485:TYR:N	1:A:485:TYR:CD1	2.85	0.45
1:B:207:LYS:O	1:B:209:GLU:N	2.50	0.45
1:C:417:VAL:O	1:C:420:ILE:HG22	2.16	0.45
1:D:16:MET:SD	1:D:73:MET:CE	3.05	0.45
1:D:202:PRO:O	1:D:204:PHE:N	2.46	0.45
1:D:413:ALA:CB	1:D:417:VAL:CG2	2.94	0.45
1:E:23:LEU:HD22	1:E:75:LYS:HG3	1.97	0.45
1:E:412:VAL:HG13	1:E:497:THR:OG1	2.17	0.45
1:E:465:VAL:O	1:E:469:VAL:HG23	2.17	0.45
1:G:171:LYS:HB3	1:G:407:VAL:HG11	1.97	0.45
1:G:199:TYR:CE2	1:G:327:LYS:HA	2.52	0.45
1:J:200:LEU:HG	1:J:276:VAL:HA	1.98	0.45
1:M:482:THR:O	1:M:483:GLU:HB2	2.17	0.45
1:A:207:LYS:O	1:A:209:GLU:N	2.50	0.45
1:A:245:LYS:HZ2	1:A:319:GLN:HE22	1.63	0.45
1:A:381:VAL:HG21	1:A:393:LYS:HA	1.99	0.45
1:D:183:LEU:HD22	1:D:184:GLN:N	2.29	0.45
1:D:197:ARG:HE	1:D:279:PRO:HA	1.81	0.45
1:E:134:LEU:O	1:E:134:LEU:HD23	2.17	0.45
1:E:224:ASP:O	1:E:225:LYS:HB3	2.17	0.45
1:E:248:LEU:HA	1:E:274:ALA:O	2.17	0.45
1:F:193:MET:HG2	1:F:194:GLN:N	2.31	0.45
1:G:356:ALA:C	1:G:358:SER:H	2.21	0.45
1:G:505:GLN:HE21	1:G:505:GLN:HB3	1.58	0.45
1:H:455:VAL:HG13	1:H:460:GLU:CB	2.47	0.45
1:I:248:LEU:HD11	1:I:325:ILE:HD11	1.99	0.45
1:J:252:GLU:O	1:J:277:LYS:HG3	2.17	0.45
1:M:30:THR:OG1	1:M:31:LEU:N	2.50	0.45
1:M:128:VAL:O	1:M:132:LYS:HG3	2.16	0.45
1:M:198:GLY:CA	1:M:328:ASP:HA	2.47	0.45
1:M:258:ALA:O	1:M:262:LEU:HG	2.17	0.45
1:N:265:ASN:HD22	1:N:265:ASN:N	2.13	0.45
1:A:219:PHE:O	1:A:247:LEU:HD12	2.16	0.45
1:B:123:ALA:HB2	1:B:440:ILE:HG13	1.98	0.45
1:B:221:LEU:HB3	1:B:249:ILE:HD13	1.99	0.45
1:C:112:ASN:OD1	1:C:114:MET:N	2.50	0.45
1:C:237:LEU:HD23	1:C:237:LEU:C	2.37	0.45
1:D:183:LEU:O	1:D:184:GLN:CB	2.65	0.45
1:D:209:GLU:OE1	1:D:209:GLU:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:479:ASN:OD1	1:D:481:ALA:HB3	2.17	0.45
1:E:183:LEU:HD22	1:E:184:GLN:N	2.27	0.45
1:E:221:LEU:HB3	1:E:249:ILE:HD13	1.99	0.45
1:F:221:LEU:HD23	1:F:249:ILE:HG23	1.99	0.45
1:G:197:ARG:HG3	1:G:277:LYS:O	2.17	0.45
1:H:254:VAL:O	1:H:259:LEU:HD22	2.17	0.45
1:I:224:ASP:O	1:I:225:LYS:HB3	2.16	0.45
1:I:482:THR:O	1:I:483:GLU:HB2	2.17	0.45
1:J:128:VAL:O	1:J:132:LYS:HG3	2.16	0.45
1:J:198:GLY:CA	1:J:328:ASP:HA	2.46	0.45
1:J:220:ILE:HG23	1:J:248:LEU:HD23	1.99	0.45
1:J:479:ASN:ND2	1:J:482:THR:HG23	2.32	0.45
1:K:70:GLY:HA2	1:K:73:MET:HE3	1.99	0.45
1:L:200:LEU:HG	1:L:275:ALA:O	2.15	0.45
1:N:162:ILE:O	1:N:165:ALA:HB3	2.17	0.45
1:N:200:LEU:HD13	1:N:254:VAL:HB	1.98	0.45
1:A:6:VAL:HG22	1:A:521:VAL:HG22	1.99	0.45
1:B:305:ILE:O	1:B:305:ILE:HG22	2.17	0.45
1:C:201:SER:O	1:C:204:PHE:HD2	2.00	0.45
1:D:249:ILE:HB	1:D:275:ALA:CB	2.47	0.45
1:F:485:TYR:HD1	1:F:485:TYR:H	1.64	0.45
1:G:183:LEU:O	1:G:184:GLN:CB	2.64	0.45
1:G:501:ARG:O	1:G:505:GLN:HG3	2.17	0.45
1:H:265:ASN:HD22	1:H:265:ASN:N	2.14	0.45
1:H:349:ILE:HG21	1:H:369:VAL:HG13	1.98	0.45
1:I:321:LYS:O	1:I:321:LYS:HG2	2.17	0.45
1:I:349:ILE:HG21	1:I:369:VAL:HG13	1.97	0.45
1:K:518:GLU:CG	1:L:36:ARG:HG3	2.47	0.45
1:L:200:LEU:HD13	1:L:254:VAL:HB	1.99	0.45
1:L:215:LEU:HB2	1:L:323:VAL:HG22	1.98	0.45
1:L:224:ASP:HB3	1:L:302:SER:HB3	1.98	0.45
1:B:17:LEU:HA	1:B:20:VAL:HG12	1.98	0.44
1:C:108:ALA:C	1:C:110:GLY:H	2.20	0.44
1:C:381:VAL:HG21	1:C:393:LYS:HA	1.99	0.44
1:E:13:ARG:CD	1:E:104:LEU:HD22	2.47	0.44
1:E:28:LYS:C	1:E:30:THR:H	2.20	0.44
1:E:108:ALA:C	1:E:110:GLY:H	2.20	0.44
1:E:356:ALA:C	1:E:358:SER:H	2.20	0.44
1:F:77:VAL:O	1:F:80:LYS:HB2	2.17	0.44
1:H:9:GLY:O	1:H:12:ALA:N	2.50	0.44
1:I:17:LEU:HA	1:I:20:VAL:CG1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:417:VAL:HG21	1:K:488:MET:HG3	1.99	0.44
1:C:219:PHE:O	1:C:247:LEU:HD12	2.16	0.44
1:D:295:LEU:HA	1:D:342:ILE:CD1	2.47	0.44
1:F:487:ASN:O	1:F:491:MET:HG3	2.18	0.44
1:H:9:GLY:O	1:H:10:ASN:C	2.55	0.44
1:L:230:ILE:HD12	1:L:261:THR:CG2	2.41	0.44
1:L:291:ASP:OD2	1:L:368:ARG:HD2	2.17	0.44
1:M:220:ILE:HG23	1:M:248:LEU:HD23	1.98	0.44
1:A:122:LYS:HE2	1:A:429:LEU:HD11	1.98	0.44
1:A:153:ASN:O	1:A:154:SER:HB2	2.16	0.44
1:A:496:PRO:HB2	1:A:499:VAL:HG13	1.98	0.44
1:C:52:ASP:OD1	1:C:54:VAL:HG23	2.17	0.44
1:C:240:VAL:HG11	1:C:247:LEU:HB2	2.00	0.44
1:D:111:MET:SD	1:D:438:VAL:HG21	2.58	0.44
1:D:245:LYS:HZ2	1:D:319:GLN:HE22	1.66	0.44
1:E:219:PHE:O	1:E:247:LEU:HD12	2.17	0.44
1:F:451:LEU:O	1:F:451:LEU:HD23	2.17	0.44
1:G:77:VAL:O	1:G:80:LYS:HB2	2.17	0.44
1:H:494:LEU:HD12	1:H:494:LEU:N	2.20	0.44
1:K:200:LEU:HG	1:K:276:VAL:HA	1.99	0.44
1:L:64:ASP:OD1	1:L:66:PHE:HB2	2.17	0.44
1:A:36:ARG:O	1:A:51:LYS:HG2	2.17	0.44
1:A:296:THR:O	1:A:297:GLY:O	2.35	0.44
1:B:171:LYS:HB3	1:B:407:VAL:HG11	1.98	0.44
1:B:226:LYS:HD3	1:B:255:GLU:OE2	2.17	0.44
1:C:356:ALA:C	1:C:358:SER:H	2.21	0.44
1:D:16:MET:SD	1:D:73:MET:HE1	2.58	0.44
1:D:485:TYR:H	1:D:485:TYR:HD1	1.65	0.44
1:E:365:LEU:C	1:E:367:GLU:H	2.20	0.44
1:E:381:VAL:HG21	1:E:393:LYS:HA	1.99	0.44
1:F:201:SER:O	1:F:204:PHE:HD2	2.00	0.44
1:G:23:LEU:CD2	1:G:75:LYS:HG3	2.47	0.44
1:G:209:GLU:OE1	1:G:209:GLU:N	2.50	0.44
1:G:221:LEU:HD23	1:G:249:ILE:HG23	1.98	0.44
1:J:183:LEU:CD1	1:J:184:GLN:HG3	2.47	0.44
1:K:224:ASP:HB3	1:K:302:SER:HB3	1.98	0.44
1:L:479:ASN:CG	1:L:493:ILE:HD11	2.37	0.44
1:M:127:ALA:O	1:M:131:LEU:HB2	2.18	0.44
1:A:31:LEU:HD22	1:A:31:LEU:HA	1.61	0.44
1:A:201:SER:O	1:A:204:PHE:HD2	2.01	0.44
1:B:219:PHE:O	1:B:247:LEU:HD12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:GLU:C	1:C:340:ALA:N	2.70	0.44
1:D:417:VAL:O	1:D:420:ILE:HG22	2.17	0.44
1:E:112:ASN:OD1	1:E:114:MET:N	2.50	0.44
1:E:209:GLU:OE1	1:E:209:GLU:N	2.50	0.44
1:F:29:VAL:O	1:F:29:VAL:HG23	2.18	0.44
1:F:36:ARG:HG3	1:F:36:ARG:HH11	1.82	0.44
1:I:198:GLY:CA	1:I:328:ASP:HA	2.47	0.44
1:J:265:ASN:HD22	1:J:265:ASN:N	2.15	0.44
1:J:496:PRO:HB2	1:J:499:VAL:CG1	2.48	0.44
1:L:207:LYS:C	1:L:209:GLU:H	2.21	0.44
1:N:17:LEU:HA	1:N:20:VAL:CG1	2.46	0.44
1:N:74:VAL:O	1:N:74:VAL:HG23	2.17	0.44
1:A:28:LYS:C	1:A:30:THR:H	2.20	0.44
1:B:183:LEU:HD22	1:B:184:GLN:N	2.29	0.44
1:B:183:LEU:O	1:B:184:GLN:CB	2.66	0.44
1:B:193:MET:HG2	1:B:194:GLN:N	2.32	0.44
1:B:209:GLU:OE1	1:B:209:GLU:N	2.50	0.44
1:C:193:MET:HG2	1:C:194:GLN:N	2.33	0.44
1:C:207:LYS:O	1:C:209:GLU:N	2.51	0.44
1:D:42:LYS:O	1:D:43:SER:C	2.56	0.44
1:E:311:LYS:HG2	1:I:311:LYS:HG2	1.98	0.44
1:F:77:VAL:HG21	1:F:510:VAL:CG1	2.48	0.44
1:H:201:SER:O	1:H:202:PRO:O	2.36	0.44
1:I:162:ILE:O	1:I:165:ALA:HB3	2.17	0.44
1:J:201:SER:C	1:J:202:PRO:O	2.53	0.44
1:K:16:MET:SD	1:K:514:MET:CE	3.05	0.44
1:K:69:MET:HE1	1:L:39:VAL:CG1	2.47	0.44
1:L:198:GLY:CA	1:L:328:ASP:HA	2.48	0.44
1:L:521:VAL:N	1:M:39:VAL:O	2.45	0.44
1:M:77:VAL:C	1:M:79:SER:N	2.71	0.44
1:B:197:ARG:HE	1:B:279:PRO:HA	1.83	0.44
1:B:237:LEU:HD23	1:B:237:LEU:C	2.38	0.44
1:D:207:LYS:O	1:D:209:GLU:N	2.50	0.44
1:D:413:ALA:HB1	1:D:417:VAL:CG2	2.47	0.44
1:E:123:ALA:HB2	1:E:440:ILE:HG13	2.00	0.44
1:E:494:LEU:HD12	1:E:494:LEU:C	2.37	0.44
1:G:119:GLY:O	1:G:440:ILE:HD12	2.17	0.44
1:G:224:ASP:O	1:G:225:LYS:HB3	2.18	0.44
1:H:63:GLU:CA	1:N:3:ALA:HB1	2.47	0.44
1:H:201:SER:C	1:H:202:PRO:O	2.56	0.44
1:I:243:ALA:O	1:I:245:LYS:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:485:TYR:H	1:I:485:TYR:HD1	1.66	0.44
1:K:77:VAL:O	1:K:79:SER:N	2.51	0.44
1:L:111:MET:SD	1:L:438:VAL:HG21	2.58	0.44
1:M:201:SER:C	1:M:202:PRO:O	2.56	0.44
1:N:479:ASN:ND2	1:N:482:THR:HG23	2.31	0.44
1:A:221:LEU:HA	1:A:317:LEU:HD11	1.99	0.44
1:E:106:ALA:O	1:E:109:ALA:HB3	2.18	0.44
1:E:127:ALA:O	1:E:131:LEU:HB2	2.18	0.44
1:E:131:LEU:HD13	1:E:422:VAL:HG21	2.00	0.44
1:E:240:VAL:HG11	1:E:247:LEU:HB2	2.00	0.44
1:F:311:LYS:HD3	1:H:311:LYS:CA	2.44	0.44
1:G:417:VAL:O	1:G:420:ILE:HG22	2.18	0.44
1:G:496:PRO:HB2	1:G:499:VAL:HG13	1.98	0.44
1:H:220:ILE:HG23	1:H:248:LEU:HD23	1.99	0.44
1:I:140:ASP:C	1:I:142:LYS:H	2.21	0.44
1:J:17:LEU:O	1:J:20:VAL:HG12	2.18	0.44
1:J:336:VAL:O	1:J:336:VAL:HG12	2.18	0.44
1:K:77:VAL:C	1:K:79:SER:N	2.70	0.44
1:L:233:MET:O	1:L:237:LEU:HB2	2.17	0.44
1:A:319:GLN:O	1:A:336:VAL:HG23	2.17	0.44
1:B:201:SER:O	1:B:204:PHE:HD2	2.01	0.44
1:B:479:ASN:OD1	1:B:481:ALA:HB3	2.17	0.44
1:C:77:VAL:HG21	1:C:510:VAL:CG1	2.48	0.44
1:C:183:LEU:O	1:C:184:GLN:CB	2.66	0.44
1:D:27:VAL:O	1:D:30:THR:OG1	2.34	0.44
1:E:201:SER:C	1:E:202:PRO:O	2.56	0.44
1:E:237:LEU:HD23	1:E:237:LEU:C	2.39	0.44
1:F:450:PRO:O	1:F:454:ILE:HG13	2.18	0.44
1:G:325:ILE:N	1:G:325:ILE:HD12	2.33	0.44
1:H:22:VAL:HG11	1:H:62:LEU:CD2	2.46	0.44
1:H:111:MET:SD	1:H:438:VAL:HG21	2.58	0.44
1:H:441:LYS:O	1:H:445:ARG:HB2	2.18	0.44
1:H:524:LEU:HD12	1:H:524:LEU:HA	1.87	0.44
1:I:136:VAL:O	1:I:136:VAL:HG12	2.18	0.44
1:I:220:ILE:HG23	1:I:248:LEU:HD23	1.99	0.44
1:K:183:LEU:CD1	1:K:184:GLN:HG3	2.47	0.44
1:K:496:PRO:HB2	1:K:499:VAL:CG1	2.48	0.44
1:M:24:ALA:HA	1:M:27:VAL:HG12	1.99	0.44
1:M:243:ALA:O	1:M:245:LYS:N	2.51	0.44
1:N:243:ALA:O	1:N:245:LYS:N	2.50	0.44
1:C:485:TYR:N	1:C:485:TYR:CD1	2.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:73:MET:SD	1:E:49:ILE:HD11	2.58	0.43
1:D:77:VAL:HG21	1:D:510:VAL:CG1	2.48	0.43
1:D:338:GLU:C	1:D:340:ALA:N	2.71	0.43
1:E:201:SER:O	1:E:204:PHE:HD2	2.00	0.43
1:E:505:GLN:HE21	1:E:505:GLN:HB3	1.63	0.43
1:F:180:GLY:HA3	1:F:381:VAL:O	2.17	0.43
1:F:237:LEU:HD23	1:F:237:LEU:C	2.39	0.43
1:H:17:LEU:HA	1:H:20:VAL:CG1	2.47	0.43
1:J:214:GLU:C	1:J:215:LEU:HD23	2.39	0.43
1:J:485:TYR:CD1	1:J:485:TYR:N	2.86	0.43
1:K:198:GLY:CA	1:K:328:ASP:HA	2.48	0.43
1:L:10:ASN:HA	1:L:13:ARG:NH1	2.33	0.43
1:M:77:VAL:HG11	1:M:510:VAL:HB	2.00	0.43
1:M:418:ALA:O	1:M:422:VAL:HG22	2.18	0.43
1:M:450:PRO:O	1:M:454:ILE:HG13	2.18	0.43
1:N:224:ASP:O	1:N:225:LYS:HB3	2.17	0.43
1:A:32:GLY:O	1:A:34:LYS:N	2.51	0.43
1:A:112:ASN:OD1	1:A:114:MET:N	2.51	0.43
1:A:197:ARG:HE	1:A:279:PRO:HA	1.83	0.43
1:A:201:SER:C	1:A:202:PRO:O	2.57	0.43
1:B:224:ASP:O	1:B:225:LYS:HB3	2.18	0.43
1:B:248:LEU:HA	1:B:274:ALA:O	2.19	0.43
1:B:271:VAL:HG12	1:B:273:VAL:HG13	2.00	0.43
1:C:31:LEU:HD12	1:C:31:LEU:HA	1.79	0.43
1:C:197:ARG:HG3	1:C:277:LYS:O	2.18	0.43
1:D:221:LEU:HD23	1:D:249:ILE:HG23	2.00	0.43
1:F:248:LEU:HA	1:F:274:ALA:O	2.18	0.43
1:F:271:VAL:HG12	1:F:273:VAL:HG13	1.98	0.43
1:G:369:VAL:O	1:G:373:ALA:N	2.51	0.43
1:I:90:THR:O	1:I:94:VAL:HG12	2.18	0.43
1:K:321:LYS:O	1:K:321:LYS:HG2	2.19	0.43
1:L:243:ALA:O	1:L:245:LYS:N	2.50	0.43
1:L:248:LEU:CD1	1:L:325:ILE:HD11	2.47	0.43
1:L:482:THR:O	1:L:483:GLU:HB2	2.18	0.43
1:M:134:LEU:HD11	1:M:421:ARG:HG2	2.00	0.43
1:N:180:GLY:HA3	1:N:381:VAL:O	2.18	0.43
1:A:37:ASN:HD21	1:A:51:LYS:HE3	1.83	0.43
1:A:385:THR:OG1	1:A:388:GLU:HG3	2.18	0.43
1:B:106:ALA:O	1:B:109:ALA:HB3	2.17	0.43
1:B:112:ASN:OD1	1:B:114:MET:N	2.51	0.43
1:D:23:LEU:CD2	1:D:75:LYS:HG3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:SER:O	1:D:204:PHE:HD2	1.99	0.43
1:E:325:ILE:HD12	1:E:325:ILE:N	2.34	0.43
1:G:102:GLU:O	1:G:105:LYS:HB3	2.18	0.43
1:H:139:SER:HB3	1:H:171:LYS:HZ1	1.82	0.43
1:I:139:SER:HB3	1:I:171:LYS:HZ3	1.83	0.43
1:I:265:ASN:N	1:I:265:ASN:HD22	2.15	0.43
1:I:455:VAL:HG13	1:I:460:GLU:CB	2.48	0.43
1:L:336:VAL:O	1:L:336:VAL:HG12	2.18	0.43
1:M:77:VAL:O	1:M:79:SER:N	2.50	0.43
1:M:455:VAL:HG13	1:M:460:GLU:CB	2.47	0.43
1:A:123:ALA:HB2	1:A:440:ILE:HG13	2.00	0.43
1:B:493:ILE:HG22	1:B:493:ILE:O	2.18	0.43
1:D:501:ARG:O	1:D:505:GLN:HG3	2.19	0.43
1:E:207:LYS:O	1:E:209:GLU:N	2.52	0.43
1:E:338:GLU:C	1:E:340:ALA:N	2.72	0.43
1:F:23:LEU:HD22	1:F:75:LYS:HG3	1.99	0.43
1:F:325:ILE:N	1:F:325:ILE:HD12	2.34	0.43
1:H:183:LEU:CD1	1:H:184:GLN:HG3	2.49	0.43
1:H:450:PRO:O	1:H:454:ILE:HG13	2.18	0.43
1:J:140:ASP:C	1:J:142:LYS:H	2.21	0.43
1:M:501:ARG:HG2	1:M:501:ARG:HH11	1.83	0.43
1:A:183:LEU:O	1:A:184:GLN:CB	2.66	0.43
1:A:248:LEU:HD12	1:A:274:ALA:O	2.18	0.43
1:D:296:THR:O	1:D:297:GLY:O	2.36	0.43
1:E:521:VAL:HB	1:F:40:LEU:HD23	2.00	0.43
1:F:27:VAL:HG22	1:F:90:THR:HG23	2.01	0.43
1:H:140:ASP:C	1:H:142:LYS:H	2.21	0.43
1:I:479:ASN:CG	1:I:493:ILE:HD11	2.38	0.43
1:I:494:LEU:HD12	1:I:494:LEU:N	2.22	0.43
1:J:24:ALA:HA	1:J:27:VAL:HG12	2.00	0.43
1:J:77:VAL:O	1:J:79:SER:N	2.51	0.43
1:L:23:LEU:HD23	1:L:74:VAL:CG2	2.49	0.43
1:M:8:PHE:HE1	1:N:26:ALA:HA	1.82	0.43
1:M:124:VAL:O	1:M:125:THR:C	2.56	0.43
1:M:214:GLU:C	1:M:215:LEU:HD23	2.38	0.43
1:N:199:TYR:CZ	1:N:327:LYS:HA	2.54	0.43
1:A:102:GLU:O	1:A:105:LYS:HB3	2.18	0.43
1:A:417:VAL:O	1:A:420:ILE:HG22	2.19	0.43
1:D:32:GLY:HA3	1:D:33:PRO:HD2	1.81	0.43
1:D:127:ALA:HB1	1:D:422:VAL:HG11	2.00	0.43
1:E:166:MET:CE	1:E:171:LYS:HA	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:258:ALA:O	1:J:262:LEU:HG	2.18	0.43
1:K:126:ALA:O	1:K:129:GLU:N	2.52	0.43
1:K:248:LEU:CD1	1:K:325:ILE:HD11	2.48	0.43
1:L:31:LEU:HD13	1:L:31:LEU:HA	1.75	0.43
1:M:129:GLU:C	1:M:131:LEU:H	2.21	0.43
1:N:16:MET:HB3	1:N:514:MET:HE1	2.01	0.43
1:A:77:VAL:HG21	1:A:510:VAL:CG1	2.48	0.43
1:A:230:ILE:HD12	1:A:261:THR:CG2	2.48	0.43
1:E:197:ARG:HE	1:E:279:PRO:HA	1.83	0.43
1:E:451:LEU:HD23	1:E:451:LEU:O	2.18	0.43
1:F:477:GLY:HA3	1:F:488:MET:CG	2.49	0.43
1:G:311:LYS:HZ1	1:N:313:THR:HG23	1.75	0.43
1:I:36:ARG:O	1:I:51:LYS:HG2	2.19	0.43
1:I:235:PRO:HG3	1:I:310:GLU:CG	2.46	0.43
1:I:393:LYS:O	1:I:393:LYS:HG2	2.18	0.43
1:J:69:MET:CE	1:K:39:VAL:HG12	2.48	0.43
1:J:166:MET:HE2	1:J:171:LYS:HA	2.01	0.43
1:K:243:ALA:O	1:K:245:LYS:N	2.51	0.43
1:L:254:VAL:O	1:L:259:LEU:HD22	2.19	0.43
1:M:69:MET:CE	1:N:39:VAL:HG12	2.49	0.43
1:M:204:PHE:CE1	1:M:274:ALA:HA	2.53	0.43
1:N:207:LYS:C	1:N:209:GLU:H	2.22	0.43
1:A:166:MET:CE	1:A:171:LYS:HA	2.49	0.43
1:A:455:VAL:CG1	1:A:460:GLU:HB2	2.37	0.43
1:B:465:VAL:O	1:B:469:VAL:HG23	2.18	0.43
1:B:485:TYR:N	1:B:485:TYR:CD1	2.87	0.43
1:C:112:ASN:HA	1:C:113:PRO:HD3	1.79	0.43
1:C:119:GLY:O	1:C:440:ILE:HD12	2.19	0.43
1:C:249:ILE:HB	1:C:275:ALA:HB2	2.00	0.43
1:D:37:ASN:HD21	1:D:51:LYS:HE3	1.83	0.43
1:D:77:VAL:HG11	1:D:510:VAL:HB	2.01	0.43
1:D:230:ILE:HD12	1:D:261:THR:CG2	2.47	0.43
1:D:353:ILE:HG23	1:D:362:ARG:HG3	2.01	0.43
1:E:69:MET:SD	1:E:520:MET:HE2	2.59	0.43
1:E:77:VAL:O	1:E:80:LYS:HB2	2.19	0.43
1:E:521:VAL:O	1:F:41:ASP:N	2.46	0.43
1:F:240:VAL:HG11	1:F:247:LEU:HB2	2.01	0.43
1:G:123:ALA:HB2	1:G:440:ILE:HG13	1.99	0.43
1:G:140:ASP:C	1:G:142:LYS:N	2.72	0.43
1:G:237:LEU:HD23	1:G:237:LEU:C	2.39	0.43
1:H:36:ARG:O	1:H:51:LYS:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:214:GLU:C	1:H:215:LEU:HD23	2.38	0.43
1:I:126:ALA:O	1:I:127:ALA:C	2.57	0.43
1:K:455:VAL:HG11	1:K:462:PRO:HA	2.00	0.43
1:L:145:ALA:O	1:L:159:GLY:HA3	2.19	0.43
1:M:9:GLY:O	1:M:10:ASN:C	2.57	0.43
1:M:200:LEU:HG	1:M:275:ALA:O	2.19	0.43
1:A:194:GLN:HB2	1:A:331:THR:HB	2.00	0.43
1:A:501:ARG:O	1:A:505:GLN:HG3	2.18	0.43
1:B:16:MET:O	1:B:20:VAL:HG12	2.19	0.43
1:D:171:LYS:HB3	1:D:407:VAL:HG11	2.01	0.43
1:D:477:GLY:HA3	1:D:488:MET:CG	2.49	0.43
1:E:197:ARG:HG3	1:E:277:LYS:O	2.19	0.43
1:E:249:ILE:HB	1:E:275:ALA:CB	2.49	0.43
1:E:522:THR:OG1	1:E:523:ASP:N	2.52	0.43
1:F:112:ASN:OD1	1:F:114:MET:N	2.52	0.43
1:F:412:VAL:HG13	1:F:497:THR:OG1	2.19	0.43
1:I:258:ALA:O	1:I:262:LEU:HG	2.18	0.43
1:J:20:VAL:HG23	1:J:74:VAL:HG11	2.01	0.43
1:J:77:VAL:C	1:J:79:SER:N	2.72	0.43
1:K:449:ALA:HB3	1:K:450:PRO:CD	2.41	0.43
1:K:518:GLU:HB2	1:L:36:ARG:HB2	2.01	0.43
1:L:247:LEU:HD12	1:L:248:LEU:N	2.32	0.43
1:M:18:ARG:CG	1:M:18:ARG:NH1	2.82	0.43
1:M:140:ASP:C	1:M:142:LYS:H	2.21	0.43
1:N:127:ALA:O	1:N:131:LEU:HB2	2.19	0.43
1:B:42:LYS:O	1:B:43:SER:C	2.57	0.43
1:B:365:LEU:C	1:B:367:GLU:H	2.21	0.43
1:C:106:ALA:O	1:C:109:ALA:HB3	2.18	0.43
1:C:496:PRO:HB2	1:C:499:VAL:HG13	2.00	0.43
1:D:36:ARG:O	1:D:51:LYS:HG2	2.19	0.43
1:E:221:LEU:HB3	1:E:249:ILE:HA	2.01	0.43
1:F:193:MET:CE	1:F:292:ILE:HG12	2.49	0.43
1:H:9:GLY:O	1:H:11:ASP:N	2.51	0.43
1:I:180:GLY:HA3	1:I:381:VAL:O	2.18	0.43
1:J:349:ILE:HG21	1:J:369:VAL:HG13	2.01	0.43
1:K:126:ALA:O	1:K:127:ALA:C	2.56	0.43
1:N:336:VAL:HG12	1:N:336:VAL:O	2.18	0.43
1:A:269:GLY:O	1:G:229:ASN:OD1	2.37	0.42
1:C:224:ASP:O	1:C:225:LYS:HB3	2.19	0.42
1:C:305:ILE:HG22	1:C:305:ILE:O	2.19	0.42
1:D:112:ASN:OD1	1:D:114:MET:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:ALA:HB2	1:D:440:ILE:HG13	2.00	0.42
1:D:305:ILE:O	1:D:305:ILE:HG22	2.19	0.42
1:J:22:VAL:HG11	1:J:62:LEU:CD2	2.48	0.42
1:K:479:ASN:CG	1:K:493:ILE:HD11	2.39	0.42
1:L:9:GLY:O	1:L:12:ALA:N	2.51	0.42
1:L:258:ALA:O	1:L:262:LEU:HG	2.19	0.42
1:M:136:VAL:O	1:M:136:VAL:HG12	2.18	0.42
1:M:145:ALA:O	1:M:159:GLY:HA3	2.19	0.42
1:M:494:LEU:HD12	1:M:494:LEU:N	2.20	0.42
1:N:230:ILE:HD12	1:N:261:THR:CG2	2.40	0.42
1:N:252:GLU:O	1:N:277:LYS:HG3	2.19	0.42
1:A:493:ILE:O	1:A:493:ILE:HG22	2.18	0.42
1:B:16:MET:HB3	1:B:514:MET:HE1	2.00	0.42
1:B:77:VAL:HG11	1:B:510:VAL:HB	2.01	0.42
1:B:77:VAL:HG21	1:B:510:VAL:CG1	2.49	0.42
1:B:505:GLN:HE21	1:B:505:GLN:HB3	1.65	0.42
1:H:124:VAL:O	1:H:125:THR:C	2.57	0.42
1:I:77:VAL:C	1:I:79:SER:N	2.72	0.42
1:J:204:PHE:CD1	1:J:274:ALA:HA	2.54	0.42
1:J:230:ILE:HD12	1:J:261:THR:CG2	2.43	0.42
1:K:278:ALA:HB1	1:K:279:PRO:HD2	2.00	0.42
1:K:485:TYR:CD1	1:K:485:TYR:N	2.86	0.42
1:L:77:VAL:C	1:L:79:SER:N	2.71	0.42
1:M:65:LYS:HB3	1:M:65:LYS:NZ	2.34	0.42
1:N:258:ALA:O	1:N:262:LEU:HG	2.17	0.42
1:N:450:PRO:O	1:N:454:ILE:HG13	2.19	0.42
1:N:455:VAL:HG11	1:N:462:PRO:HA	2.00	0.42
1:A:36:ARG:HG3	1:A:36:ARG:NH1	2.34	0.42
1:A:499:VAL:CG2	1:A:500:THR:N	2.82	0.42
1:B:194:GLN:HB2	1:B:331:THR:HB	2.01	0.42
1:B:353:ILE:HG23	1:B:362:ARG:HG3	2.01	0.42
1:C:221:LEU:HB3	1:C:249:ILE:HA	2.01	0.42
1:C:365:LEU:C	1:C:367:GLU:H	2.23	0.42
1:D:31:LEU:HD13	1:D:31:LEU:HA	1.83	0.42
1:D:356:ALA:C	1:D:358:SER:H	2.23	0.42
1:E:32:GLY:HA3	1:E:454:ILE:HG23	2.00	0.42
1:F:219:PHE:O	1:F:247:LEU:HD12	2.18	0.42
1:F:296:THR:O	1:F:297:GLY:O	2.37	0.42
1:F:356:ALA:C	1:F:358:SER:H	2.23	0.42
1:G:37:ASN:HD21	1:G:51:LYS:HE3	1.84	0.42
1:H:77:VAL:C	1:H:79:SER:N	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:176:THR:HG21	1:H:333:ILE:CD1	2.49	0.42
1:H:207:LYS:C	1:H:209:GLU:H	2.22	0.42
1:H:221:LEU:HD23	1:H:249:ILE:CD1	2.43	0.42
1:H:366:GLN:O	1:H:369:VAL:HG22	2.20	0.42
1:I:111:MET:SD	1:I:438:VAL:HG21	2.59	0.42
1:J:20:VAL:CG2	1:J:74:VAL:HG11	2.49	0.42
1:K:254:VAL:O	1:K:259:LEU:HD22	2.20	0.42
1:L:235:PRO:HG3	1:L:310:GLU:CG	2.45	0.42
1:M:321:LYS:O	1:M:321:LYS:HG2	2.19	0.42
1:N:77:VAL:C	1:N:79:SER:N	2.73	0.42
1:N:112:ASN:HA	1:N:113:PRO:HD3	1.89	0.42
1:N:278:ALA:HB1	1:N:279:PRO:HD2	2.01	0.42
1:A:127:ALA:HB1	1:A:422:VAL:HG11	2.01	0.42
1:A:202:PRO:O	1:A:204:PHE:N	2.44	0.42
1:A:237:LEU:HD23	1:A:237:LEU:C	2.40	0.42
1:A:305:ILE:O	1:A:305:ILE:HG22	2.19	0.42
1:B:240:VAL:HG11	1:B:247:LEU:HB2	2.01	0.42
1:B:249:ILE:HB	1:B:275:ALA:HB2	2.02	0.42
1:B:356:ALA:C	1:B:358:SER:H	2.22	0.42
1:C:77:VAL:HG11	1:C:510:VAL:HB	2.01	0.42
1:D:34:LYS:HD2	1:D:458:CYS:CA	2.50	0.42
1:D:166:MET:CE	1:D:171:LYS:HA	2.49	0.42
1:F:228:SER:HA	1:F:255:GLU:O	2.19	0.42
1:G:193:MET:HG2	1:G:194:GLN:N	2.34	0.42
1:I:496:PRO:HB2	1:I:499:VAL:CG1	2.49	0.42
1:J:9:GLY:O	1:J:12:ALA:N	2.52	0.42
1:K:28:LYS:O	1:K:29:VAL:C	2.55	0.42
1:L:112:ASN:HA	1:L:113:PRO:HD3	1.88	0.42
1:M:204:PHE:CD1	1:M:274:ALA:HA	2.54	0.42
1:M:248:LEU:CD1	1:M:325:ILE:HD11	2.49	0.42
1:N:479:ASN:CG	1:N:493:ILE:HD11	2.40	0.42
1:A:42:LYS:O	1:A:43:SER:C	2.58	0.42
1:C:193:MET:CE	1:C:292:ILE:HG12	2.49	0.42
1:C:319:GLN:O	1:C:336:VAL:HG23	2.19	0.42
1:D:226:LYS:HD3	1:D:255:GLU:OE2	2.19	0.42
1:G:42:LYS:O	1:G:43:SER:C	2.58	0.42
1:G:105:LYS:HE3	1:G:105:LYS:HB2	1.90	0.42
1:G:166:MET:CE	1:G:171:LYS:HA	2.49	0.42
1:H:200:LEU:HG	1:H:276:VAL:HA	2.00	0.42
1:I:200:LEU:HG	1:I:276:VAL:HA	2.01	0.42
1:K:207:LYS:C	1:K:209:GLU:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:176:THR:HG21	1:L:333:ILE:CD1	2.49	0.42
1:L:204:PHE:CD1	1:L:274:ALA:HA	2.55	0.42
1:L:496:PRO:HB2	1:L:499:VAL:CG1	2.49	0.42
1:L:499:VAL:CG2	1:L:500:THR:N	2.82	0.42
1:M:64:ASP:OD1	1:M:66:PHE:HB2	2.18	0.42
1:M:69:MET:HE2	1:N:39:VAL:HG12	2.00	0.42
1:N:321:LYS:O	1:N:321:LYS:HG2	2.19	0.42
1:A:77:VAL:HG11	1:A:510:VAL:HB	2.01	0.42
1:A:119:GLY:O	1:A:440:ILE:HD12	2.19	0.42
1:A:171:LYS:HB3	1:A:407:VAL:HG11	2.02	0.42
1:A:450:PRO:O	1:A:454:ILE:HG13	2.19	0.42
1:B:221:LEU:HB3	1:B:249:ILE:HA	2.02	0.42
1:D:221:LEU:HA	1:D:317:LEU:HD11	2.02	0.42
1:D:308:GLU:C	1:D:310:GLU:H	2.23	0.42
1:D:493:ILE:O	1:D:493:ILE:HG22	2.19	0.42
1:E:230:ILE:HD12	1:E:261:THR:CG2	2.49	0.42
1:F:42:LYS:O	1:F:43:SER:C	2.58	0.42
1:F:505:GLN:HE21	1:F:505:GLN:HB3	1.57	0.42
1:I:24:ALA:HA	1:I:27:VAL:HG12	2.01	0.42
1:J:199:TYR:CZ	1:J:327:LYS:HA	2.54	0.42
1:J:482:THR:O	1:J:483:GLU:HB2	2.19	0.42
1:K:162:ILE:O	1:K:165:ALA:HB3	2.19	0.42
1:M:16:MET:SD	1:M:514:MET:CE	3.07	0.42
1:M:17:LEU:HA	1:M:20:VAL:CG1	2.47	0.42
1:N:37:ASN:HD22	1:N:51:LYS:HG3	1.82	0.42
1:N:248:LEU:CD1	1:N:325:ILE:HD11	2.48	0.42
1:A:226:LYS:HD3	1:A:255:GLU:OE2	2.19	0.42
1:A:338:GLU:C	1:A:340:ALA:N	2.73	0.42
1:A:477:GLY:HA3	1:A:488:MET:CG	2.50	0.42
1:B:339:GLU:H	1:B:339:GLU:HG2	1.56	0.42
1:B:369:VAL:O	1:B:373:ALA:N	2.51	0.42
1:B:501:ARG:O	1:B:505:GLN:HG3	2.18	0.42
1:C:140:ASP:C	1:C:142:LYS:N	2.73	0.42
1:C:199:TYR:CE2	1:C:327:LYS:HA	2.55	0.42
1:E:140:ASP:C	1:E:142:LYS:N	2.73	0.42
1:E:477:GLY:HA3	1:E:488:MET:CG	2.49	0.42
1:F:33:PRO:C	1:F:35:GLY:N	2.72	0.42
1:F:207:LYS:O	1:F:209:GLU:N	2.52	0.42
1:F:353:ILE:HG23	1:F:362:ARG:HG3	2.02	0.42
1:G:193:MET:CE	1:G:292:ILE:HG12	2.49	0.42
1:G:485:TYR:CD1	1:G:485:TYR:N	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:18:ARG:CG	1:H:18:ARG:NH1	2.83	0.42
1:H:243:ALA:O	1:H:245:LYS:N	2.52	0.42
1:I:37:ASN:HD21	1:I:51:LYS:HZ3	1.67	0.42
1:I:103:GLY:O	1:I:107:VAL:HG23	2.19	0.42
1:I:201:SER:C	1:I:202:PRO:O	2.55	0.42
1:I:213:VAL:CG1	1:I:214:GLU:H	2.33	0.42
1:J:77:VAL:HG21	1:J:510:VAL:HB	2.02	0.42
1:L:441:LYS:O	1:L:445:ARG:HB2	2.20	0.42
1:N:70:GLY:HA2	1:N:73:MET:HE3	2.01	0.42
1:N:482:THR:O	1:N:483:GLU:HB2	2.19	0.42
1:A:112:ASN:HA	1:A:113:PRO:HD3	1.80	0.42
1:D:34:LYS:HB2	1:D:458:CYS:SG	2.60	0.42
1:E:77:VAL:HG21	1:E:510:VAL:CG1	2.49	0.42
1:E:171:LYS:HB3	1:E:407:VAL:HG11	2.01	0.42
1:E:289:LEU:HD23	1:E:289:LEU:HA	1.93	0.42
1:F:127:ALA:O	1:F:131:LEU:HB2	2.19	0.42
1:H:199:TYR:CZ	1:H:327:LYS:HA	2.55	0.42
1:H:291:ASP:OD2	1:H:368:ARG:HD2	2.19	0.42
1:K:235:PRO:HG3	1:K:310:GLU:CG	2.46	0.42
1:L:419:LEU:O	1:L:422:VAL:HG23	2.18	0.42
1:L:451:LEU:HD23	1:L:451:LEU:O	2.19	0.42
1:M:254:VAL:O	1:M:259:LEU:HD22	2.20	0.42
1:N:111:MET:SD	1:N:438:VAL:HG21	2.60	0.42
1:N:194:GLN:O	1:N:194:GLN:HG2	2.20	0.42
1:A:485:TYR:HD1	1:A:485:TYR:H	1.67	0.42
1:B:338:GLU:C	1:B:340:ALA:N	2.73	0.42
1:C:16:MET:HB3	1:C:514:MET:HE1	2.01	0.42
1:C:270:ILE:O	1:C:271:VAL:HB	2.19	0.42
1:D:193:MET:CE	1:D:292:ILE:HG12	2.49	0.42
1:D:522:THR:OG1	1:D:523:ASP:N	2.52	0.42
1:F:279:PRO:O	1:F:285:ARG:HG3	2.19	0.42
1:F:338:GLU:C	1:F:340:ALA:N	2.72	0.42
1:G:365:LEU:C	1:G:367:GLU:H	2.23	0.42
1:H:24:ALA:HA	1:H:27:VAL:HG12	2.00	0.42
1:H:393:LYS:O	1:H:393:LYS:HG2	2.19	0.42
1:I:145:ALA:O	1:I:159:GLY:HA3	2.19	0.42
1:K:17:LEU:O	1:K:20:VAL:HG12	2.19	0.42
1:K:77:VAL:O	1:K:80:LYS:N	2.52	0.42
1:K:204:PHE:CD1	1:K:274:ALA:HA	2.55	0.42
1:L:288:MET:HG2	1:L:368:ARG:HD3	2.02	0.42
1:M:17:LEU:O	1:M:20:VAL:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:126:ALA:O	1:M:129:GLU:N	2.51	0.42
1:M:169:VAL:CG1	1:M:173:GLY:HA3	2.48	0.42
1:N:17:LEU:CA	1:N:20:VAL:HG12	2.50	0.42
1:N:136:VAL:O	1:N:136:VAL:HG12	2.20	0.42
1:N:201:SER:O	1:N:204:PHE:HD2	2.03	0.42
1:N:235:PRO:HG3	1:N:310:GLU:CG	2.45	0.42
1:A:68:ASN:O	1:A:69:MET:C	2.57	0.42
1:A:221:LEU:HA	1:A:317:LEU:CD1	2.50	0.42
1:A:240:VAL:HG11	1:A:247:LEU:HB2	2.01	0.42
1:C:450:PRO:O	1:C:454:ILE:HG13	2.19	0.42
1:D:140:ASP:C	1:D:142:LYS:N	2.73	0.42
1:D:197:ARG:HG3	1:D:277:LYS:O	2.20	0.42
1:D:245:LYS:HZ3	1:D:319:GLN:HE22	1.67	0.42
1:D:365:LEU:C	1:D:367:GLU:H	2.23	0.42
1:D:385:THR:OG1	1:D:388:GLU:HG3	2.19	0.42
1:E:102:GLU:O	1:E:105:LYS:HB3	2.20	0.42
1:E:226:LYS:HD3	1:E:255:GLU:OE2	2.19	0.42
1:F:86:GLY:O	1:F:87:ASP:HB2	2.20	0.42
1:F:197:ARG:HG3	1:F:277:LYS:O	2.20	0.42
1:F:230:ILE:HD12	1:F:261:THR:CG2	2.47	0.42
1:F:319:GLN:O	1:F:336:VAL:HG23	2.20	0.42
1:J:213:VAL:CG1	1:J:214:GLU:N	2.81	0.42
1:J:221:LEU:HD23	1:J:249:ILE:CD1	2.45	0.42
1:K:199:TYR:CZ	1:K:327:LYS:HA	2.54	0.42
1:L:129:GLU:C	1:L:131:LEU:N	2.73	0.42
1:M:336:VAL:O	1:M:336:VAL:HG12	2.19	0.42
1:A:140:ASP:C	1:A:142:LYS:N	2.73	0.41
1:B:108:ALA:C	1:B:110:GLY:N	2.74	0.41
1:B:199:TYR:CE2	1:B:327:LYS:HA	2.55	0.41
1:B:221:LEU:HA	1:B:317:LEU:HD11	2.02	0.41
1:C:465:VAL:O	1:C:469:VAL:HG23	2.21	0.41
1:D:153:ASN:O	1:D:154:SER:HB2	2.18	0.41
1:F:205:ILE:H	1:F:205:ILE:HG13	1.53	0.41
1:F:369:VAL:O	1:F:373:ALA:N	2.53	0.41
1:F:385:THR:OG1	1:F:388:GLU:HG3	2.20	0.41
1:H:64:ASP:OD1	1:H:66:PHE:HB2	2.20	0.41
1:H:441:LYS:HA	1:H:441:LYS:HD3	1.91	0.41
1:H:479:ASN:CG	1:H:493:ILE:HD11	2.40	0.41
1:I:127:ALA:O	1:I:131:LEU:HB2	2.20	0.41
1:I:404:ARG:NH1	1:I:404:ARG:CG	2.81	0.41
1:J:194:GLN:O	1:J:194:GLN:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:219:PHE:HB3	1:K:317:LEU:CD2	2.50	0.41
1:K:478:TYR:CE2	1:K:480:ALA:HA	2.55	0.41
1:K:524:LEU:HD12	1:K:524:LEU:HA	1.91	0.41
1:A:230:ILE:CD1	1:A:261:THR:HG21	2.49	0.41
1:A:240:VAL:O	1:A:240:VAL:HG12	2.19	0.41
1:A:248:LEU:HA	1:A:274:ALA:O	2.19	0.41
1:C:111:MET:SD	1:C:438:VAL:HG21	2.61	0.41
1:C:228:SER:HA	1:C:255:GLU:O	2.20	0.41
1:E:214:GLU:C	1:E:215:LEU:HD23	2.40	0.41
1:G:207:LYS:O	1:G:209:GLU:N	2.53	0.41
1:G:213:VAL:CG1	1:G:214:GLU:N	2.83	0.41
1:G:250:ILE:HG22	1:G:289:LEU:HD21	2.02	0.41
1:G:319:GLN:O	1:G:336:VAL:HG23	2.19	0.41
1:H:37:ASN:HD22	1:H:51:LYS:HG3	1.84	0.41
1:H:143:ALA:C	1:H:145:ALA:N	2.73	0.41
1:I:213:VAL:CG1	1:I:214:GLU:N	2.80	0.41
1:I:291:ASP:OD2	1:I:368:ARG:HD2	2.20	0.41
1:J:162:ILE:O	1:J:165:ALA:HB3	2.19	0.41
1:M:392:LYS:C	1:M:394:ALA:N	2.73	0.41
1:N:254:VAL:O	1:N:259:LEU:HD22	2.20	0.41
1:A:111:MET:SD	1:A:438:VAL:HG21	2.60	0.41
1:A:249:ILE:HB	1:A:275:ALA:HB2	2.02	0.41
1:B:201:SER:C	1:B:202:PRO:O	2.59	0.41
1:C:201:SER:C	1:C:202:PRO:O	2.56	0.41
1:D:36:ARG:HG3	1:D:36:ARG:NH1	2.35	0.41
1:I:42:LYS:HB3	1:I:42:LYS:HE2	1.86	0.41
1:J:450:PRO:O	1:J:454:ILE:HG13	2.20	0.41
1:K:413:ALA:HB1	1:K:417:VAL:CG2	2.50	0.41
1:K:468:THR:HG21	1:K:485:TYR:CE2	2.56	0.41
1:L:37:ASN:HD22	1:L:51:LYS:HG3	1.86	0.41
1:L:479:ASN:ND2	1:L:482:THR:HG23	2.35	0.41
1:N:22:VAL:HG11	1:N:62:LEU:CD2	2.46	0.41
1:N:77:VAL:O	1:N:79:SER:N	2.54	0.41
1:N:139:SER:HB3	1:N:171:LYS:HZ1	1.83	0.41
1:N:204:PHE:CD1	1:N:274:ALA:HA	2.54	0.41
1:B:16:MET:HB3	1:B:514:MET:CE	2.51	0.41
1:C:248:LEU:HA	1:C:274:ALA:O	2.20	0.41
1:D:494:LEU:HD12	1:D:494:LEU:O	2.20	0.41
1:E:117:LYS:O	1:E:120:ILE:N	2.53	0.41
1:E:199:TYR:HB3	1:E:325:ILE:HG21	2.02	0.41
1:E:305:ILE:HG22	1:E:305:ILE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:16:MET:SD	1:F:73:MET:CE	3.08	0.41
1:F:111:MET:SD	1:F:438:VAL:HG21	2.60	0.41
1:F:199:TYR:HB3	1:F:325:ILE:HG21	2.01	0.41
1:F:496:PRO:HB2	1:F:499:VAL:HG13	2.02	0.41
1:G:112:ASN:OD1	1:G:114:MET:N	2.53	0.41
1:G:214:GLU:C	1:G:215:LEU:HD23	2.40	0.41
1:H:136:VAL:O	1:H:136:VAL:HG12	2.19	0.41
1:I:254:VAL:O	1:I:259:LEU:HD22	2.20	0.41
1:J:69:MET:HE2	1:K:39:VAL:CG1	2.51	0.41
1:L:37:ASN:HD21	1:L:51:LYS:HZ3	1.68	0.41
1:L:204:PHE:CE1	1:L:274:ALA:HA	2.56	0.41
1:L:214:GLU:C	1:L:215:LEU:HD23	2.40	0.41
1:M:183:LEU:CD1	1:M:184:GLN:HG3	2.50	0.41
1:N:216:GLU:O	1:N:217:SER:C	2.58	0.41
1:N:430:ARG:HG2	1:N:430:ARG:HH11	1.85	0.41
1:N:449:ALA:HB3	1:N:450:PRO:CD	2.43	0.41
1:A:198:GLY:O	1:A:276:VAL:HG12	2.21	0.41
1:A:311:LYS:HB3	1:M:311:LYS:HB3	2.02	0.41
1:D:194:GLN:HB2	1:D:331:THR:HB	2.01	0.41
1:D:198:GLY:O	1:D:276:VAL:HG12	2.20	0.41
1:H:77:VAL:HG21	1:H:510:VAL:HB	2.03	0.41
1:H:129:GLU:C	1:H:131:LEU:N	2.73	0.41
1:H:194:GLN:O	1:H:194:GLN:HG2	2.19	0.41
1:H:288:MET:HG2	1:H:368:ARG:HD3	2.02	0.41
1:H:321:LYS:O	1:H:321:LYS:HG2	2.21	0.41
1:J:139:SER:HB3	1:J:171:LYS:HZ3	1.84	0.41
1:K:450:PRO:O	1:K:454:ILE:HG13	2.21	0.41
1:M:252:GLU:O	1:M:277:LYS:HG3	2.20	0.41
1:N:213:VAL:CG1	1:N:214:GLU:N	2.83	0.41
1:N:440:ILE:HG22	1:N:441:LYS:N	2.35	0.41
1:A:295:LEU:HD13	1:A:295:LEU:C	2.40	0.41
1:A:339:GLU:H	1:A:339:GLU:HG2	1.56	0.41
1:A:353:ILE:HD13	1:A:366:GLN:HG2	2.01	0.41
1:B:321:LYS:O	1:B:321:LYS:HG2	2.20	0.41
1:C:485:TYR:H	1:C:485:TYR:HD1	1.69	0.41
1:F:501:ARG:O	1:F:505:GLN:HG3	2.20	0.41
1:G:201:SER:C	1:G:202:PRO:O	2.58	0.41
1:K:18:ARG:HG2	1:K:18:ARG:NH1	2.29	0.41
1:L:77:VAL:O	1:L:79:SER:N	2.53	0.41
1:M:207:LYS:C	1:M:209:GLU:H	2.24	0.41
1:M:221:LEU:HD23	1:M:249:ILE:CD1	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:9:GLY:O	1:N:10:ASN:C	2.59	0.41
1:N:103:GLY:O	1:N:107:VAL:HG23	2.20	0.41
1:C:176:THR:HG21	1:C:333:ILE:CD1	2.48	0.41
1:C:310:GLU:C	1:C:312:ALA:H	2.24	0.41
1:D:108:ALA:C	1:D:110:GLY:N	2.73	0.41
1:D:451:LEU:O	1:D:451:LEU:HD23	2.21	0.41
1:E:37:ASN:ND2	1:E:51:LYS:HE3	2.35	0.41
1:F:155:ASP:OD1	1:F:157:THR:HB	2.21	0.41
1:F:224:ASP:O	1:F:225:LYS:HB3	2.21	0.41
1:G:127:ALA:HB1	1:G:422:VAL:HG11	2.03	0.41
1:G:140:ASP:O	1:G:142:LYS:N	2.54	0.41
1:I:207:LYS:C	1:I:209:GLU:H	2.23	0.41
1:I:524:LEU:HD12	1:I:524:LEU:HA	1.87	0.41
1:J:180:GLY:HA3	1:J:381:VAL:O	2.20	0.41
1:L:17:LEU:CA	1:L:20:VAL:HG12	2.45	0.41
1:L:213:VAL:CG1	1:L:214:GLU:N	2.84	0.41
1:L:393:LYS:O	1:L:393:LYS:HG2	2.20	0.41
1:M:440:ILE:HG22	1:M:441:LYS:N	2.36	0.41
1:N:455:VAL:HG13	1:N:460:GLU:CB	2.50	0.41
1:A:356:ALA:C	1:A:358:SER:H	2.23	0.41
1:B:176:THR:HG21	1:B:333:ILE:CD1	2.49	0.41
1:E:245:LYS:NZ	1:E:319:GLN:NE2	2.68	0.41
1:F:31:LEU:HD22	1:F:90:THR:HG22	2.03	0.41
1:F:216:GLU:C	1:F:218:PRO:HD3	2.41	0.41
1:G:36:ARG:HH11	1:G:36:ARG:HG3	1.84	0.41
1:G:86:GLY:O	1:G:87:ASP:HB2	2.21	0.41
1:G:493:ILE:O	1:G:493:ILE:HG22	2.21	0.41
1:I:214:GLU:C	1:I:215:LEU:HD23	2.41	0.41
1:J:18:ARG:HH11	1:J:18:ARG:CG	2.28	0.41
1:J:90:THR:O	1:J:94:VAL:HG12	2.21	0.41
1:J:288:MET:HG2	1:J:368:ARG:HD3	2.02	0.41
1:K:18:ARG:CG	1:K:18:ARG:NH1	2.79	0.41
1:K:224:ASP:O	1:K:225:LYS:CB	2.69	0.41
1:L:28:LYS:O	1:L:30:THR:N	2.54	0.41
1:A:114:MET:HG3	1:B:34:LYS:HB3	2.02	0.41
1:A:162:ILE:O	1:A:165:ALA:HB3	2.21	0.41
1:A:193:MET:HG2	1:A:194:GLN:N	2.36	0.41
1:A:369:VAL:O	1:A:373:ALA:N	2.49	0.41
1:B:77:VAL:O	1:B:80:LYS:N	2.52	0.41
1:B:140:ASP:C	1:B:142:LYS:N	2.74	0.41
1:C:30:THR:HB	1:C:51:LYS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:VAL:O	1:C:240:VAL:HG12	2.21	0.41
1:C:269:GLY:O	1:C:271:VAL:N	2.54	0.41
1:C:295:LEU:HA	1:C:342:ILE:CD1	2.50	0.41
1:C:494:LEU:HD12	1:C:494:LEU:O	2.21	0.41
1:D:105:LYS:HE3	1:D:105:LYS:HB2	1.92	0.41
1:D:237:LEU:HD23	1:D:237:LEU:C	2.40	0.41
1:E:205:ILE:H	1:E:205:ILE:HG13	1.53	0.41
1:F:25:ASP:HA	1:F:28:LYS:HE2	2.02	0.41
1:F:222:LEU:HD12	1:F:293:ALA:HB2	2.03	0.41
1:F:270:ILE:O	1:F:271:VAL:HB	2.21	0.41
1:F:289:LEU:HD23	1:F:289:LEU:HA	1.93	0.41
1:F:305:ILE:O	1:F:305:ILE:HG22	2.21	0.41
1:G:36:ARG:HG3	1:G:36:ARG:NH1	2.36	0.41
1:G:69:MET:SD	1:G:520:MET:HE2	2.60	0.41
1:G:221:LEU:HA	1:G:317:LEU:HD11	2.03	0.41
1:G:249:ILE:HB	1:G:275:ALA:HB2	2.02	0.41
1:G:308:GLU:C	1:G:310:GLU:H	2.24	0.41
1:G:326:ASN:HD22	1:G:329:THR:CB	1.97	0.41
1:G:338:GLU:C	1:G:340:ALA:N	2.74	0.41
1:G:353:ILE:HD13	1:G:366:GLN:HG2	2.03	0.41
1:H:204:PHE:CD1	1:H:274:ALA:HA	2.56	0.41
1:H:482:THR:O	1:H:483:GLU:HB2	2.21	0.41
1:I:18:ARG:HH11	1:I:18:ARG:CG	2.29	0.41
1:I:74:VAL:O	1:I:74:VAL:HG23	2.20	0.41
1:I:247:LEU:HD12	1:I:248:LEU:N	2.36	0.41
1:I:430:ARG:HH11	1:I:430:ARG:HG2	1.86	0.41
1:I:499:VAL:CG2	1:I:500:THR:N	2.82	0.41
1:J:247:LEU:HD12	1:J:248:LEU:N	2.35	0.41
1:K:129:GLU:C	1:K:131:LEU:N	2.74	0.41
1:K:207:LYS:C	1:K:209:GLU:N	2.75	0.41
1:K:247:LEU:HD12	1:K:248:LEU:N	2.36	0.41
1:K:257:GLU:CG	1:L:269:GLY:HA3	2.51	0.41
1:K:435:ASP:O	1:K:438:VAL:N	2.54	0.41
1:L:28:LYS:C	1:L:30:THR:N	2.74	0.41
1:L:194:GLN:O	1:L:194:GLN:HG2	2.21	0.41
1:L:224:ASP:O	1:L:225:LYS:CB	2.68	0.41
1:L:487:ASN:N	1:L:491:MET:HE2	2.36	0.41
1:M:441:LYS:O	1:M:445:ARG:HB2	2.21	0.41
1:C:194:GLN:HB2	1:C:331:THR:HB	2.02	0.41
1:D:34:LYS:HD2	1:D:458:CYS:HA	2.03	0.41
1:D:119:GLY:O	1:D:440:ILE:HD12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:108:ALA:C	1:G:110:GLY:H	2.23	0.41
1:H:392:LYS:C	1:H:394:ALA:N	2.74	0.41
1:I:108:ALA:C	1:I:110:GLY:H	2.25	0.41
1:I:194:GLN:O	1:I:194:GLN:HG2	2.21	0.41
1:I:225:LYS:HE2	1:I:226:LYS:O	2.20	0.41
1:J:28:LYS:O	1:J:30:THR:N	2.55	0.41
1:J:201:SER:O	1:J:204:PHE:HD2	2.04	0.41
1:J:204:PHE:CE1	1:J:274:ALA:HA	2.55	0.41
1:L:321:LYS:O	1:L:321:LYS:HG2	2.21	0.41
1:M:247:LEU:HD12	1:M:248:LEU:N	2.36	0.41
1:M:288:MET:HG2	1:M:368:ARG:HD3	2.03	0.41
1:M:349:ILE:HG21	1:M:369:VAL:HG13	2.03	0.41
1:M:520:MET:HG2	1:N:39:VAL:HB	2.02	0.41
1:N:104:LEU:HD23	1:N:104:LEU:HA	1.89	0.41
1:N:207:LYS:C	1:N:209:GLU:N	2.74	0.41
1:B:36:ARG:N	1:B:36:ARG:HD3	2.36	0.40
1:C:153:ASN:O	1:C:154:SER:HB2	2.21	0.40
1:C:325:ILE:HD12	1:C:325:ILE:N	2.35	0.40
1:C:517:THR:HG21	1:D:39:VAL:HG23	2.03	0.40
1:D:193:MET:HG2	1:D:194:GLN:N	2.36	0.40
1:D:245:LYS:HZ3	1:D:319:GLN:NE2	2.19	0.40
1:E:34:LYS:HA	1:E:34:LYS:HD3	1.86	0.40
1:E:194:GLN:HB2	1:E:331:THR:HB	2.03	0.40
1:F:102:GLU:O	1:F:105:LYS:HB3	2.22	0.40
1:F:308:GLU:C	1:F:310:GLU:H	2.25	0.40
1:G:68:ASN:O	1:G:69:MET:C	2.58	0.40
1:G:310:GLU:C	1:G:312:ALA:H	2.25	0.40
1:G:451:LEU:HD23	1:G:451:LEU:O	2.21	0.40
1:H:200:LEU:HG	1:H:275:ALA:O	2.22	0.40
1:I:77:VAL:HG21	1:I:510:VAL:HB	2.03	0.40
1:I:216:GLU:O	1:I:217:SER:C	2.60	0.40
1:J:225:LYS:HE2	1:J:226:LYS:O	2.22	0.40
1:K:65:LYS:NZ	1:K:65:LYS:HB3	2.36	0.40
1:K:339:GLU:H	1:K:339:GLU:HG2	1.68	0.40
1:K:413:ALA:CB	1:K:417:VAL:CG2	2.98	0.40
1:L:138:CYS:O	1:L:138:CYS:SG	2.78	0.40
1:L:207:LYS:C	1:L:209:GLU:N	2.73	0.40
1:M:37:ASN:HD21	1:M:51:LYS:HZ3	1.67	0.40
1:M:430:ARG:HG2	1:M:430:ARG:HH11	1.86	0.40
1:N:247:LEU:HD12	1:N:248:LEU:N	2.33	0.40
1:A:13:ARG:HD3	1:A:104:LEU:HD22	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:GLU:C	1:A:310:GLU:H	2.24	0.40
1:B:36:ARG:O	1:B:51:LYS:HG2	2.21	0.40
1:B:230:ILE:HD12	1:B:261:THR:CG2	2.49	0.40
1:C:127:ALA:O	1:C:131:LEU:HB2	2.21	0.40
1:C:199:TYR:HB3	1:C:325:ILE:HG21	2.04	0.40
1:C:230:ILE:HD12	1:C:261:THR:CG2	2.49	0.40
1:D:166:MET:HE1	1:D:171:LYS:HA	2.03	0.40
1:D:199:TYR:HB3	1:D:325:ILE:HG21	2.02	0.40
1:D:207:LYS:C	1:D:209:GLU:H	2.24	0.40
1:E:513:LEU:HD13	1:F:49:ILE:HD12	2.03	0.40
1:F:248:LEU:HD12	1:F:274:ALA:O	2.21	0.40
1:F:413:ALA:O	1:F:418:ALA:HB2	2.20	0.40
1:G:228:SER:HA	1:G:255:GLU:O	2.21	0.40
1:H:436:GLN:O	1:H:440:ILE:CD1	2.69	0.40
1:J:207:LYS:C	1:J:209:GLU:H	2.24	0.40
1:K:128:VAL:O	1:K:132:LYS:HG3	2.21	0.40
1:K:258:ALA:O	1:K:262:LEU:HG	2.20	0.40
1:K:479:ASN:ND2	1:K:482:THR:HG23	2.36	0.40
1:M:524:LEU:HD12	1:M:524:LEU:HA	1.89	0.40
1:N:17:LEU:O	1:N:20:VAL:HG12	2.21	0.40
1:N:128:VAL:O	1:N:132:LYS:HG3	2.21	0.40
1:A:140:ASP:O	1:A:142:LYS:N	2.55	0.40
1:A:353:ILE:HG23	1:A:362:ARG:HG3	2.04	0.40
1:B:494:LEU:HD12	1:B:494:LEU:O	2.21	0.40
1:D:350:ARG:HA	1:D:353:ILE:HD12	2.03	0.40
1:D:477:GLY:HA3	1:D:488:MET:HG2	2.04	0.40
1:E:308:GLU:C	1:E:310:GLU:H	2.24	0.40
1:F:295:LEU:HD13	1:F:295:LEU:C	2.41	0.40
1:G:230:ILE:CD1	1:G:261:THR:HG21	2.50	0.40
1:I:219:PHE:HB3	1:I:317:LEU:CD2	2.51	0.40
1:J:103:GLY:O	1:J:107:VAL:HG23	2.21	0.40
1:J:112:ASN:HA	1:J:113:PRO:HD3	1.89	0.40
1:K:418:ALA:O	1:K:422:VAL:HG22	2.21	0.40
1:L:30:THR:HG22	1:L:36:ARG:O	2.21	0.40
1:L:231:ARG:HH11	1:M:241:ALA:C	2.24	0.40
1:L:485:TYR:CD1	1:L:485:TYR:N	2.86	0.40
1:A:207:LYS:C	1:A:209:GLU:H	2.25	0.40
1:A:303:GLU:O	1:A:305:ILE:N	2.54	0.40
1:B:28:LYS:C	1:B:30:THR:H	2.23	0.40
1:B:236:VAL:HG22	1:B:312:ALA:O	2.21	0.40
1:C:321:LYS:O	1:C:321:LYS:HG2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:249:ILE:HB	1:F:275:ALA:HB2	2.04	0.40
1:F:353:ILE:HD13	1:F:366:GLN:HG2	2.02	0.40
1:G:248:LEU:HA	1:G:274:ALA:O	2.21	0.40
1:G:448:GLU:HB3	1:G:452:ARG:HD2	2.03	0.40
1:H:145:ALA:O	1:H:159:GLY:HA3	2.22	0.40
1:H:157:THR:O	1:H:161:LEU:HB2	2.22	0.40
1:H:449:ALA:HB3	1:H:450:PRO:CD	2.45	0.40
1:I:216:GLU:C	1:I:218:PRO:HD3	2.42	0.40
1:I:219:PHE:HB3	1:I:317:LEU:HD21	2.04	0.40
1:J:70:GLY:O	1:J:74:VAL:HG13	2.22	0.40
1:J:444:LEU:HD23	1:J:447:MET:CE	2.52	0.40
1:K:64:ASP:OD1	1:K:66:PHE:HB2	2.22	0.40
1:K:262:LEU:C	1:K:264:VAL:N	2.75	0.40
1:M:366:GLN:O	1:M:369:VAL:HG22	2.22	0.40
1:N:113:PRO:O	1:N:115:ASP:N	2.55	0.40
1:N:441:LYS:O	1:N:445:ARG:HB2	2.21	0.40
1:A:214:GLU:C	1:A:215:LEU:HD23	2.41	0.40
1:B:290:GLN:O	1:B:291:ASP:C	2.60	0.40
1:C:36:ARG:N	1:C:36:ARG:HD3	2.37	0.40
1:C:140:ASP:O	1:C:142:LYS:N	2.54	0.40
1:D:412:VAL:HG13	1:D:497:THR:OG1	2.20	0.40
1:E:221:LEU:HA	1:E:317:LEU:HD11	2.03	0.40
1:F:36:ARG:HG3	1:F:36:ARG:NH1	2.37	0.40
1:F:52:ASP:OD1	1:F:54:VAL:HG23	2.22	0.40
1:F:201:SER:C	1:F:202:PRO:O	2.60	0.40
1:F:221:LEU:HB3	1:F:249:ILE:HA	2.04	0.40
1:F:240:VAL:O	1:F:240:VAL:HG12	2.21	0.40
1:F:413:ALA:CB	1:F:417:VAL:CG2	3.00	0.40
1:F:482:THR:C	1:F:483:GLU:OE1	2.59	0.40
1:G:234:LEU:N	1:G:235:PRO:HD2	2.37	0.40
1:G:270:ILE:O	1:G:271:VAL:HB	2.21	0.40
1:G:413:ALA:CB	1:G:417:VAL:CG2	3.00	0.40
1:H:23:LEU:HD23	1:H:74:VAL:CG2	2.52	0.40
1:H:128:VAL:O	1:H:132:LYS:HG3	2.22	0.40
1:I:28:LYS:O	1:I:30:THR:N	2.54	0.40
1:I:207:LYS:C	1:I:209:GLU:N	2.75	0.40
1:J:198:GLY:HA3	1:J:328:ASP:HA	2.04	0.40
1:K:169:VAL:CG1	1:K:173:GLY:HA3	2.47	0.40
1:M:235:PRO:HG3	1:M:310:GLU:CG	2.47	0.40
1:N:20:VAL:HG22	1:N:20:VAL:O	2.22	0.40
1:N:169:VAL:CG1	1:N:173:GLY:HA3	2.48	0.40



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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:484:GLU:OE1	1:M:484:GLU:OE1[8_556]	2.13	0.07

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	522/548 (95%)	449 (86%)	54 (10%)	19 (4%)	3	20
1	B	522/548 (95%)	450 (86%)	51 (10%)	21 (4%)	3	18
1	C	522/548 (95%)	455 (87%)	49 (9%)	18 (3%)	3	22
1	D	522/548 (95%)	448 (86%)	54 (10%)	20 (4%)	3	19
1	E	522/548 (95%)	453 (87%)	50 (10%)	19 (4%)	3	20
1	F	522/548 (95%)	449 (86%)	52 (10%)	21 (4%)	3	18
1	G	522/548 (95%)	450 (86%)	56 (11%)	16 (3%)	4	23
1	H	522/548 (95%)	434 (83%)	69 (13%)	19 (4%)	3	20
1	I	522/548 (95%)	438 (84%)	67 (13%)	17 (3%)	4	22
1	J	522/548 (95%)	441 (84%)	58 (11%)	23 (4%)	2	16
1	K	522/548 (95%)	441 (84%)	60 (12%)	21 (4%)	3	18
1	L	522/548 (95%)	434 (83%)	63 (12%)	25 (5%)	2	14
1	M	522/548 (95%)	438 (84%)	62 (12%)	22 (4%)	3	17
1	N	522/548 (95%)	440 (84%)	61 (12%)	21 (4%)	3	18
All	All	7308/7672 (95%)	6220 (85%)	806 (11%)	282 (4%)	3	18

All (282) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	PRO

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Mol	Chain	Res	Type
1	A	43	SER
1	A	152	ALA
1	B	32	GLY
1	B	33	PRO
1	B	43	SER
1	B	152	ALA
1	C	43	SER
1	C	152	ALA
1	D	33	PRO
1	D	34	LYS
1	D	43	SER
1	D	152	ALA
1	E	33	PRO
1	E	43	SER
1	E	152	ALA
1	F	32	GLY
1	F	33	PRO
1	F	43	SER
1	G	43	SER
1	G	152	ALA
1	H	33	PRO
1	H	43	SER
1	H	244	GLY
1	H	256	GLY
1	H	313	THR
1	I	43	SER
1	I	244	GLY
1	I	256	GLY
1	I	313	THR
1	J	33	PRO
1	J	43	SER
1	J	244	GLY
1	J	256	GLY
1	J	313	THR
1	K	43	SER
1	K	244	GLY
1	K	256	GLY
1	K	313	THR
1	L	31	LEU
1	L	33	PRO
1	L	43	SER
1	L	244	GLY

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Mol	Chain	Res	Type
1	L	256	GLY
1	L	313	THR
1	M	43	SER
1	M	244	GLY
1	M	256	GLY
1	M	313	THR
1	N	43	SER
1	N	244	GLY
1	N	256	GLY
1	N	313	THR
1	A	202	PRO
1	A	269	GLY
1	A	297	GLY
1	B	202	PRO
1	B	269	GLY
1	B	297	GLY
1	C	202	PRO
1	C	269	GLY
1	C	297	GLY
1	D	202	PRO
1	D	269	GLY
1	D	297	GLY
1	E	202	PRO
1	E	269	GLY
1	E	297	GLY
1	F	152	ALA
1	F	202	PRO
1	F	269	GLY
1	F	297	GLY
1	F	304	GLU
1	G	202	PRO
1	G	269	GLY
1	G	297	GLY
1	H	9	GLY
1	H	10	ASN
1	H	32	GLY
1	H	297	GLY
1	I	257	GLU
1	I	297	GLY
1	J	9	GLY
1	J	32	GLY
1	J	141	SER

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Mol	Chain	Res	Type
1	J	257	GLU
1	J	297	GLY
1	K	141	SER
1	K	297	GLY
1	L	141	SER
1	L	257	GLU
1	L	297	GLY
1	M	35	GLY
1	M	297	GLY
1	N	114	MET
1	N	141	SER
1	N	202	PRO
1	N	257	GLU
1	N	297	GLY
1	A	271	VAL
1	A	304	GLU
1	B	271	VAL
1	B	304	GLU
1	C	253	ASP
1	C	271	VAL
1	C	304	GLU
1	D	271	VAL
1	D	304	GLU
1	D	483	GLU
1	E	271	VAL
1	E	304	GLU
1	F	141	SER
1	F	253	ASP
1	F	271	VAL
1	G	271	VAL
1	G	304	GLU
1	H	141	SER
1	H	202	PRO
1	H	225	LYS
1	H	257	GLU
1	H	334	ASP
1	I	141	SER
1	I	202	PRO
1	I	225	LYS
1	I	334	ASP
1	J	10	ASN
1	J	202	PRO

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Mol	Chain	Res	Type
1	J	225	LYS
1	K	202	PRO
1	K	225	LYS
1	K	257	GLU
1	K	334	ASP
1	L	9	GLY
1	L	32	GLY
1	L	114	MET
1	L	202	PRO
1	L	225	LYS
1	M	9	GLY
1	M	141	SER
1	M	202	PRO
1	M	225	LYS
1	M	257	GLU
1	N	9	GLY
1	N	10	ASN
1	N	225	LYS
1	A	141	SER
1	A	225	LYS
1	A	483	GLU
1	B	34	LYS
1	B	253	ASP
1	B	483	GLU
1	C	141	SER
1	C	322	ARG
1	C	483	GLU
1	D	141	SER
1	D	225	LYS
1	D	253	ASP
1	E	225	LYS
1	E	253	ASP
1	E	483	GLU
1	F	34	LYS
1	G	141	SER
1	G	253	ASP
1	I	9	GLY
1	J	171	LYS
1	J	334	ASP
1	K	9	GLY
1	K	10	ASN
1	L	10	ASN

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Mol	Chain	Res	Type
1	L	304	GLU
1	L	334	ASP
1	M	10	ASN
1	M	114	MET
1	M	304	GLU
1	M	334	ASP
1	N	334	ASP
1	A	253	ASP
1	A	313	THR
1	A	322	ARG
1	B	141	SER
1	B	225	LYS
1	B	313	THR
1	B	322	ARG
1	C	225	LYS
1	C	313	THR
1	C	334	ASP
1	D	322	ARG
1	D	334	ASP
1	E	141	SER
1	E	313	THR
1	E	322	ARG
1	E	334	ASP
1	E	357	THR
1	F	31	LEU
1	F	225	LYS
1	F	313	THR
1	F	322	ARG
1	G	225	LYS
1	G	256	GLY
1	G	313	THR
1	G	322	ARG
1	G	483	GLU
1	H	184	GLN
1	H	208	PRO
1	H	271	VAL
1	I	10	ASN
1	I	208	PRO
1	I	271	VAL
1	J	61	GLU
1	J	271	VAL
1	J	304	GLU

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Mol	Chain	Res	Type
1	K	61	GLU
1	K	184	GLN
1	K	271	VAL
1	K	304	GLU
1	L	208	PRO
1	L	271	VAL
1	M	61	GLU
1	M	271	VAL
1	N	23	LEU
1	N	34	LYS
1	N	208	PRO
1	N	271	VAL
1	N	304	GLU
1	A	201	SER
1	A	334	ASP
1	A	357	THR
1	B	201	SER
1	B	334	ASP
1	B	357	THR
1	C	201	SER
1	D	208	PRO
1	D	256	GLY
1	D	313	THR
1	D	357	THR
1	F	201	SER
1	F	256	GLY
1	F	334	ASP
1	G	201	SER
1	H	137	PRO
1	I	184	GLN
1	J	184	GLN
1	J	208	PRO
1	K	114	MET
1	K	208	PRO
1	L	47	PRO
1	L	184	GLN
1	M	137	PRO
1	M	184	GLN
1	M	208	PRO
1	N	113	PRO
1	N	184	GLN
1	A	208	PRO

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Mol	Chain	Res	Type
1	A	256	GLY
1	C	256	GLY
1	D	201	SER
1	E	208	PRO
1	E	256	GLY
1	F	29	VAL
1	H	113	PRO
1	I	137	PRO
1	L	113	PRO
1	L	137	PRO
1	N	137	PRO
1	B	208	PRO
1	B	256	GLY
1	C	208	PRO
1	E	201	SER
1	F	208	PRO
1	G	208	PRO
1	J	137	PRO
1	L	29	VAL
1	M	113	PRO
1	K	29	VAL
1	K	113	PRO
1	M	47	PRO
1	C	270	ILE
1	J	47	PRO
1	L	35	GLY
1	I	113	PRO
1	J	113	PRO
1	K	47	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	404/415 (97%)	381 (94%)	23 (6%)	20	51
1	B	404/415 (97%)	383 (95%)	21 (5%)	23	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	404/415 (97%)	383 (95%)	21 (5%)	23	54
1	D	404/415 (97%)	383 (95%)	21 (5%)	23	54
1	E	404/415 (97%)	383 (95%)	21 (5%)	23	54
1	F	404/415 (97%)	381 (94%)	23 (6%)	20	51
1	G	404/415 (97%)	384 (95%)	20 (5%)	24	55
1	H	404/415 (97%)	388 (96%)	16 (4%)	31	61
1	I	404/415 (97%)	391 (97%)	13 (3%)	39	67
1	J	404/415 (97%)	391 (97%)	13 (3%)	39	67
1	K	404/415 (97%)	389 (96%)	15 (4%)	34	63
1	L	404/415 (97%)	389 (96%)	15 (4%)	34	63
1	M	404/415 (97%)	391 (97%)	13 (3%)	39	67
1	N	404/415 (97%)	391 (97%)	13 (3%)	39	67
All	All	5656/5810 (97%)	5408 (96%)	248 (4%)	28	59

All (248) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	31	LEU
1	A	33	PRO
1	A	44	PHE
1	A	54	VAL
1	A	65	LYS
1	A	74	VAL
1	A	94	VAL
1	A	125	THR
1	A	161	LEU
1	A	174	VAL
1	A	183	LEU
1	A	209	GLU
1	A	310	GLU
1	A	328	ASP
1	A	331	THR
1	A	339	GLU
1	A	404	ARG
1	A	411	VAL
1	A	461	LYS
1	A	463	SER

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Mol	Chain	Res	Type
1	A	499	VAL
1	A	505	GLN
1	B	18	ARG
1	B	33	PRO
1	B	44	PHE
1	B	54	VAL
1	B	65	LYS
1	B	74	VAL
1	B	94	VAL
1	B	125	THR
1	B	161	LEU
1	B	174	VAL
1	B	183	LEU
1	B	209	GLU
1	B	310	GLU
1	B	328	ASP
1	B	331	THR
1	B	339	GLU
1	B	404	ARG
1	B	411	VAL
1	B	463	SER
1	B	499	VAL
1	B	505	GLN
1	C	18	ARG
1	C	31	LEU
1	C	44	PHE
1	C	54	VAL
1	C	65	LYS
1	C	74	VAL
1	C	94	VAL
1	C	125	THR
1	C	161	LEU
1	C	174	VAL
1	C	183	LEU
1	C	209	GLU
1	C	310	GLU
1	C	328	ASP
1	C	331	THR
1	C	339	GLU
1	C	404	ARG
1	C	411	VAL
1	C	463	SER

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Mol	Chain	Res	Type
1	C	499	VAL
1	C	505	GLN
1	D	18	ARG
1	D	31	LEU
1	D	44	PHE
1	D	54	VAL
1	D	65	LYS
1	D	74	VAL
1	D	94	VAL
1	D	125	THR
1	D	161	LEU
1	D	174	VAL
1	D	183	LEU
1	D	209	GLU
1	D	310	GLU
1	D	328	ASP
1	D	331	THR
1	D	339	GLU
1	D	404	ARG
1	D	411	VAL
1	D	463	SER
1	D	499	VAL
1	D	505	GLN
1	E	18	ARG
1	E	29	VAL
1	E	44	PHE
1	E	54	VAL
1	E	65	LYS
1	E	74	VAL
1	E	94	VAL
1	E	125	THR
1	E	161	LEU
1	E	174	VAL
1	E	183	LEU
1	E	209	GLU
1	E	310	GLU
1	E	328	ASP
1	E	331	THR
1	E	339	GLU
1	E	404	ARG
1	E	411	VAL
1	E	463	SER

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Mol	Chain	Res	Type
1	E	499	VAL
1	E	505	GLN
1	F	18	ARG
1	F	31	LEU
1	F	33	PRO
1	F	44	PHE
1	F	54	VAL
1	F	65	LYS
1	F	74	VAL
1	F	94	VAL
1	F	125	THR
1	F	161	LEU
1	F	174	VAL
1	F	183	LEU
1	F	209	GLU
1	F	310	GLU
1	F	328	ASP
1	F	331	THR
1	F	339	GLU
1	F	404	ARG
1	F	411	VAL
1	F	461	LYS
1	F	463	SER
1	F	499	VAL
1	F	505	GLN
1	G	18	ARG
1	G	44	PHE
1	G	54	VAL
1	G	65	LYS
1	G	74	VAL
1	G	94	VAL
1	G	125	THR
1	G	161	LEU
1	G	174	VAL
1	G	183	LEU
1	G	209	GLU
1	G	310	GLU
1	G	328	ASP
1	G	331	THR
1	G	339	GLU
1	G	404	ARG
1	G	411	VAL

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Mol	Chain	Res	Type
1	G	463	SER
1	G	499	VAL
1	G	505	GLN
1	H	31	LEU
1	H	33	PRO
1	H	44	PHE
1	H	65	LYS
1	H	74	VAL
1	H	134	LEU
1	H	174	VAL
1	H	310	GLU
1	H	328	ASP
1	H	331	THR
1	H	398	ASP
1	H	407	VAL
1	H	461	LYS
1	H	490	ASP
1	H	494	LEU
1	H	505	GLN
1	I	44	PHE
1	I	65	LYS
1	I	174	VAL
1	I	310	GLU
1	I	328	ASP
1	I	331	THR
1	I	398	ASP
1	I	407	VAL
1	I	411	VAL
1	I	461	LYS
1	I	490	ASP
1	I	494	LEU
1	I	505	GLN
1	J	44	PHE
1	J	65	LYS
1	J	174	VAL
1	J	231	ARG
1	J	310	GLU
1	J	328	ASP
1	J	331	THR
1	J	398	ASP
1	J	407	VAL
1	J	461	LYS

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Mol	Chain	Res	Type
1	J	490	ASP
1	J	494	LEU
1	J	505	GLN
1	K	31	LEU
1	K	44	PHE
1	K	65	LYS
1	K	134	LEU
1	K	174	VAL
1	K	310	GLU
1	K	328	ASP
1	K	331	THR
1	K	398	ASP
1	K	407	VAL
1	K	411	VAL
1	K	461	LYS
1	K	490	ASP
1	K	494	LEU
1	K	505	GLN
1	L	31	LEU
1	L	44	PHE
1	L	65	LYS
1	L	74	VAL
1	L	161	LEU
1	L	174	VAL
1	L	310	GLU
1	L	328	ASP
1	L	331	THR
1	L	398	ASP
1	L	407	VAL
1	L	461	LYS
1	L	490	ASP
1	L	494	LEU
1	L	505	GLN
1	M	34	LYS
1	M	44	PHE
1	M	65	LYS
1	M	174	VAL
1	M	310	GLU
1	M	328	ASP
1	M	331	THR
1	M	398	ASP
1	M	407	VAL

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Mol	Chain	Res	Type
1	M	461	LYS
1	M	490	ASP
1	M	494	LEU
1	M	505	GLN
1	N	44	PHE
1	N	65	LYS
1	N	134	LEU
1	N	174	VAL
1	N	310	GLU
1	N	328	ASP
1	N	331	THR
1	N	398	ASP
1	N	407	VAL
1	N	461	LYS
1	N	490	ASP
1	N	494	LEU
1	N	505	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	265	ASN
1	A	319	GLN
1	A	326	ASN
1	A	351	GLN
1	A	467	ASN
1	A	475	ASN
1	B	37	ASN
1	B	72	GLN
1	B	265	ASN
1	B	319	GLN
1	B	326	ASN
1	B	351	GLN
1	B	467	ASN
1	B	475	ASN
1	C	37	ASN
1	C	72	GLN
1	C	265	ASN
1	C	319	GLN
1	C	326	ASN
1	C	351	GLN

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Mol	Chain	Res	Type
1	C	467	ASN
1	C	475	ASN
1	D	37	ASN
1	D	72	GLN
1	D	265	ASN
1	D	319	GLN
1	D	326	ASN
1	D	351	GLN
1	D	467	ASN
1	D	475	ASN
1	E	72	GLN
1	E	265	ASN
1	E	319	GLN
1	E	326	ASN
1	E	351	GLN
1	E	467	ASN
1	E	475	ASN
1	F	72	GLN
1	F	265	ASN
1	F	319	GLN
1	F	326	ASN
1	F	351	GLN
1	F	467	ASN
1	F	475	ASN
1	F	505	GLN
1	G	37	ASN
1	G	229	ASN
1	G	265	ASN
1	G	319	GLN
1	G	326	ASN
1	G	351	GLN
1	G	467	ASN
1	G	475	ASN
1	G	505	GLN
1	H	37	ASN
1	H	265	ASN
1	H	319	GLN
1	H	467	ASN
1	H	475	ASN
1	I	37	ASN
1	I	265	ASN
1	I	319	GLN

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Mol	Chain	Res	Type
1	I	467	ASN
1	I	475	ASN
1	J	37	ASN
1	J	265	ASN
1	J	319	GLN
1	J	467	ASN
1	J	475	ASN
1	K	37	ASN
1	K	72	GLN
1	K	265	ASN
1	K	319	GLN
1	K	467	ASN
1	K	475	ASN
1	L	37	ASN
1	L	265	ASN
1	L	319	GLN
1	L	467	ASN
1	L	475	ASN
1	M	37	ASN
1	M	72	GLN
1	M	265	ASN
1	M	319	GLN
1	M	467	ASN
1	M	475	ASN
1	N	37	ASN
1	N	265	ASN
1	N	319	GLN
1	N	467	ASN
1	N	475	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	524/548 (95%)	0.01	11 (2%) 63 62	5, 52, 107, 117	0
1	B	524/548 (95%)	0.04	5 (0%) 82 82	3, 50, 106, 118	0
1	C	524/548 (95%)	-0.05	3 (0%) 89 90	3, 52, 106, 118	0
1	D	524/548 (95%)	0.11	16 (3%) 49 48	6, 52, 107, 118	0
1	E	524/548 (95%)	0.02	7 (1%) 77 77	8, 53, 107, 117	0
1	F	524/548 (95%)	-0.01	7 (1%) 77 77	7, 52, 107, 118	0
1	G	524/548 (95%)	-0.00	8 (1%) 73 72	6, 53, 107, 118	0
1	H	524/548 (95%)	0.17	21 (4%) 38 36	4, 56, 114, 120	0
1	I	524/548 (95%)	0.05	5 (0%) 82 82	8, 55, 113, 120	0
1	J	524/548 (95%)	-0.02	9 (1%) 70 68	4, 56, 113, 120	0
1	K	524/548 (95%)	-0.03	4 (0%) 86 86	9, 56, 112, 120	0
1	L	524/548 (95%)	-0.01	6 (1%) 80 81	10, 56, 112, 120	0
1	M	524/548 (95%)	0.03	7 (1%) 77 77	10, 56, 113, 120	0
1	N	524/548 (95%)	0.04	7 (1%) 77 77	9, 56, 113, 120	0
All	All	7336/7672 (95%)	0.02	116 (1%) 72 70	3, 54, 110, 120	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	357	THR	4.7
1	A	361	ASP	4.4
1	A	238	GLU	4.3
1	I	268	ARG	4.1
1	J	203	TYR	3.7
1	N	234	LEU	3.7
1	D	156	GLU	3.6
1	M	357	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	H	349	ILE	3.4
1	D	372	LEU	3.4
1	M	155	ASP	3.4
1	H	283	ASP	3.3
1	H	361	ASP	3.2
1	H	292	ILE	3.2
1	J	349	ILE	3.2
1	N	236	VAL	3.2
1	J	359	ASP	3.1
1	G	357	THR	3.1
1	A	355	GLU	3.1
1	M	525	PRO	3.0
1	A	357	THR	3.0
1	F	357	THR	3.0
1	D	267	MET	2.9
1	L	2	ALA	2.9
1	D	366	GLN	2.8
1	F	283	ASP	2.8
1	H	234	LEU	2.8
1	E	479	ASN	2.8
1	B	361	ASP	2.8
1	I	245	LYS	2.7
1	G	351	GLN	2.7
1	A	203	TYR	2.7
1	D	355	GLU	2.7
1	J	268	ARG	2.7
1	H	345	ARG	2.7
1	I	339	GLU	2.7
1	M	351	GLN	2.7
1	H	230	ILE	2.7
1	G	524	LEU	2.6
1	H	356	ALA	2.6
1	H	191	GLU	2.6
1	D	342	ILE	2.6
1	K	262	LEU	2.6
1	A	351	GLN	2.6
1	B	203	TYR	2.6
1	F	363	GLU	2.6
1	N	343	GLN	2.6
1	G	366	GLN	2.5
1	N	235	PRO	2.5
1	G	354	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	355	GLU	2.5
1	C	268	ARG	2.5
1	D	233	MET	2.5
1	J	361	ASP	2.4
1	M	311	LYS	2.4
1	N	233	MET	2.4
1	M	41	ASP	2.4
1	B	311	LYS	2.4
1	H	351	GLN	2.4
1	C	354	GLU	2.4
1	B	236	VAL	2.4
1	E	144	ILE	2.4
1	C	211	GLY	2.4
1	A	267	MET	2.3
1	E	154	SER	2.3
1	I	2	ALA	2.3
1	A	233	MET	2.3
1	D	312	ALA	2.3
1	F	361	ASP	2.3
1	H	332	ILE	2.3
1	J	357	THR	2.3
1	H	193	MET	2.3
1	H	2	ALA	2.3
1	H	299	THR	2.3
1	J	355	GLU	2.3
1	J	484	GLU	2.2
1	A	354	GLU	2.2
1	A	356	ALA	2.2
1	I	224	ASP	2.2
1	G	368	ARG	2.2
1	N	351	GLN	2.2
1	D	237	LEU	2.2
1	D	359	ASP	2.2
1	G	247	LEU	2.2
1	L	156	GLU	2.2
1	L	361	ASP	2.2
1	E	477	GLY	2.2
1	H	348	GLN	2.1
1	K	348	GLN	2.1
1	E	296	THR	2.1
1	H	357	THR	2.1
1	L	311	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	342	ILE	2.1
1	F	153	ASN	2.1
1	N	156	GLU	2.1
1	E	381	VAL	2.1
1	J	365	LEU	2.1
1	D	361	ASP	2.1
1	M	366	GLN	2.1
1	F	155	ASP	2.1
1	K	138	CYS	2.1
1	H	347	ALA	2.1
1	K	361	ASP	2.1
1	D	266	THR	2.0
1	A	365	LEU	2.0
1	F	284	ARG	2.0
1	D	319	GLN	2.0
1	G	352	GLN	2.0
1	H	360	TYR	2.0
1	L	381	VAL	2.0
1	D	349	ILE	2.0
1	H	192	GLY	2.0
1	D	313	THR	2.0
1	B	2	ALA	2.0
1	E	227	ILE	2.0
1	H	222	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.