



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 03:06 PM UTC

PDB ID : 3N6R / pdb_00003n6r
Title : CRYSTAL STRUCTURE OF the holoenzyme of PROPIONYL-COA CARBOXYLASE (PCC)
Authors : Huang, C.S.; Sadre-Bazzaz, K.; Tong, L.
Deposited on : 2010-05-26
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

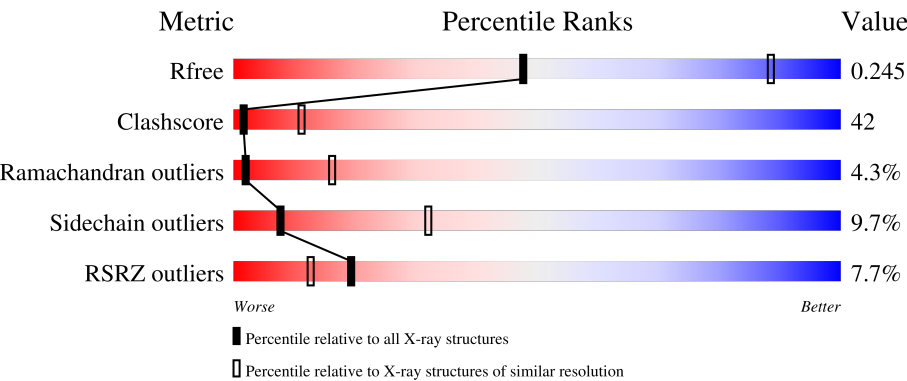
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	681	12% 29% 46% 11% • 13%
1	C	681	11% 28% 46% 12% • 13%
1	E	681	13% 30% 45% 12% • 13%
1	G	681	12% 31% 51% 12% • 5%
1	I	681	15% 30% 52% 12% • 5%

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Mol	Chain	Length	Quality of chain
1	K	681	12% 32% 51% 11% 5%
2	B	531	% 45% 43% 7% 5%
2	D	531	% 44% 45% 6% 5%
2	F	531	47% 40% 7% 5%
2	H	531	45% 43% 6% 5%
2	J	531	% 45% 43% 7% 5%
2	L	531	% 45% 44% 6% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 51921 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 Propionyl-CoA carboxylase, alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	591	Total	C	N	O	S	0	0	0
			4507	2828	794	857	28			
1	C	591	Total	C	N	O	S	0	0	0
			4507	2828	794	857	28			
1	E	591	Total	C	N	O	S	0	0	0
			4507	2828	794	857	28			
1	G	646	Total	C	N	O	S	0	0	0
			4950	3108	869	942	31			
1	I	646	Total	C	N	O	S	0	0	0
			4950	3108	869	942	31			
1	K	646	Total	C	N	O	S	0	0	0
			4950	3108	869	942	31			

- Molecule 2 is a protein called Propionyl-CoA carboxylase, beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	506	Total	C	N	O	S	0	0	0
			3910	2462	683	744	21			
2	D	506	Total	C	N	O	S	0	0	0
			3910	2462	683	744	21			
2	F	506	Total	C	N	O	S	0	0	0
			3910	2462	683	744	21			
2	H	506	Total	C	N	O	S	0	0	0
			3910	2462	683	744	21			
2	J	506	Total	C	N	O	S	0	0	0
			3910	2462	683	744	21			
2	L	506	Total	C	N	O	S	0	0	0
			3910	2462	683	744	21			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	11	MET	-	expression tag	UNP Q168G2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	12	GLY	-	expression tag	UNP Q168G2
B	13	SER	-	expression tag	UNP Q168G2
B	14	SER	-	expression tag	UNP Q168G2
B	15	HIS	-	expression tag	UNP Q168G2
B	16	HIS	-	expression tag	UNP Q168G2
B	17	HIS	-	expression tag	UNP Q168G2
B	18	HIS	-	expression tag	UNP Q168G2
B	19	HIS	-	expression tag	UNP Q168G2
B	20	HIS	-	expression tag	UNP Q168G2
B	21	SER	-	expression tag	UNP Q168G2
B	22	SER	-	expression tag	UNP Q168G2
B	23	GLY	-	expression tag	UNP Q168G2
B	24	LEU	-	expression tag	UNP Q168G2
B	25	VAL	-	expression tag	UNP Q168G2
B	26	PRO	-	expression tag	UNP Q168G2
B	27	ARG	-	expression tag	UNP Q168G2
B	28	GLY	-	expression tag	UNP Q168G2
B	29	SER	-	expression tag	UNP Q168G2
B	30	HIS	-	expression tag	UNP Q168G2
B	31	MET	-	expression tag	UNP Q168G2
D	11	MET	-	expression tag	UNP Q168G2
D	12	GLY	-	expression tag	UNP Q168G2
D	13	SER	-	expression tag	UNP Q168G2
D	14	SER	-	expression tag	UNP Q168G2
D	15	HIS	-	expression tag	UNP Q168G2
D	16	HIS	-	expression tag	UNP Q168G2
D	17	HIS	-	expression tag	UNP Q168G2
D	18	HIS	-	expression tag	UNP Q168G2
D	19	HIS	-	expression tag	UNP Q168G2
D	20	HIS	-	expression tag	UNP Q168G2
D	21	SER	-	expression tag	UNP Q168G2
D	22	SER	-	expression tag	UNP Q168G2
D	23	GLY	-	expression tag	UNP Q168G2
D	24	LEU	-	expression tag	UNP Q168G2
D	25	VAL	-	expression tag	UNP Q168G2
D	26	PRO	-	expression tag	UNP Q168G2
D	27	ARG	-	expression tag	UNP Q168G2
D	28	GLY	-	expression tag	UNP Q168G2
D	29	SER	-	expression tag	UNP Q168G2
D	30	HIS	-	expression tag	UNP Q168G2
D	31	MET	-	expression tag	UNP Q168G2
F	11	MET	-	expression tag	UNP Q168G2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	12	GLY	-	expression tag	UNP Q168G2
F	13	SER	-	expression tag	UNP Q168G2
F	14	SER	-	expression tag	UNP Q168G2
F	15	HIS	-	expression tag	UNP Q168G2
F	16	HIS	-	expression tag	UNP Q168G2
F	17	HIS	-	expression tag	UNP Q168G2
F	18	HIS	-	expression tag	UNP Q168G2
F	19	HIS	-	expression tag	UNP Q168G2
F	20	HIS	-	expression tag	UNP Q168G2
F	21	SER	-	expression tag	UNP Q168G2
F	22	SER	-	expression tag	UNP Q168G2
F	23	GLY	-	expression tag	UNP Q168G2
F	24	LEU	-	expression tag	UNP Q168G2
F	25	VAL	-	expression tag	UNP Q168G2
F	26	PRO	-	expression tag	UNP Q168G2
F	27	ARG	-	expression tag	UNP Q168G2
F	28	GLY	-	expression tag	UNP Q168G2
F	29	SER	-	expression tag	UNP Q168G2
F	30	HIS	-	expression tag	UNP Q168G2
F	31	MET	-	expression tag	UNP Q168G2
H	11	MET	-	expression tag	UNP Q168G2
H	12	GLY	-	expression tag	UNP Q168G2
H	13	SER	-	expression tag	UNP Q168G2
H	14	SER	-	expression tag	UNP Q168G2
H	15	HIS	-	expression tag	UNP Q168G2
H	16	HIS	-	expression tag	UNP Q168G2
H	17	HIS	-	expression tag	UNP Q168G2
H	18	HIS	-	expression tag	UNP Q168G2
H	19	HIS	-	expression tag	UNP Q168G2
H	20	HIS	-	expression tag	UNP Q168G2
H	21	SER	-	expression tag	UNP Q168G2
H	22	SER	-	expression tag	UNP Q168G2
H	23	GLY	-	expression tag	UNP Q168G2
H	24	LEU	-	expression tag	UNP Q168G2
H	25	VAL	-	expression tag	UNP Q168G2
H	26	PRO	-	expression tag	UNP Q168G2
H	27	ARG	-	expression tag	UNP Q168G2
H	28	GLY	-	expression tag	UNP Q168G2
H	29	SER	-	expression tag	UNP Q168G2
H	30	HIS	-	expression tag	UNP Q168G2
H	31	MET	-	expression tag	UNP Q168G2
J	11	MET	-	expression tag	UNP Q168G2

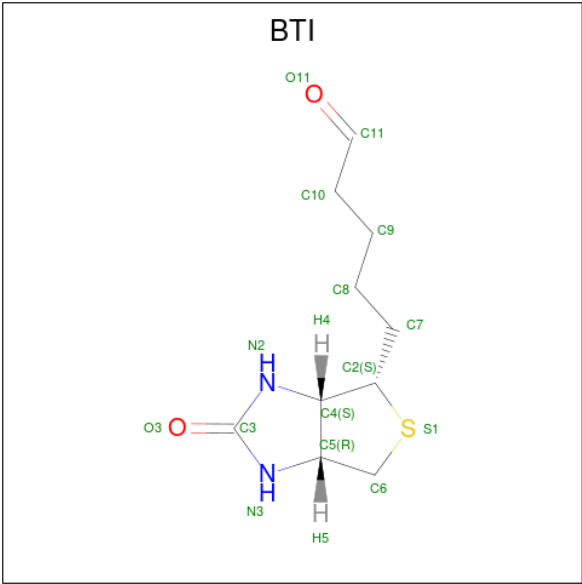
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Chain	Residue	Modelled	Actual	Comment	Reference
J	12	GLY	-	expression tag	UNP Q168G2
J	13	SER	-	expression tag	UNP Q168G2
J	14	SER	-	expression tag	UNP Q168G2
J	15	HIS	-	expression tag	UNP Q168G2
J	16	HIS	-	expression tag	UNP Q168G2
J	17	HIS	-	expression tag	UNP Q168G2
J	18	HIS	-	expression tag	UNP Q168G2
J	19	HIS	-	expression tag	UNP Q168G2
J	20	HIS	-	expression tag	UNP Q168G2
J	21	SER	-	expression tag	UNP Q168G2
J	22	SER	-	expression tag	UNP Q168G2
J	23	GLY	-	expression tag	UNP Q168G2
J	24	LEU	-	expression tag	UNP Q168G2
J	25	VAL	-	expression tag	UNP Q168G2
J	26	PRO	-	expression tag	UNP Q168G2
J	27	ARG	-	expression tag	UNP Q168G2
J	28	GLY	-	expression tag	UNP Q168G2
J	29	SER	-	expression tag	UNP Q168G2
J	30	HIS	-	expression tag	UNP Q168G2
J	31	MET	-	expression tag	UNP Q168G2
L	11	MET	-	expression tag	UNP Q168G2
L	12	GLY	-	expression tag	UNP Q168G2
L	13	SER	-	expression tag	UNP Q168G2
L	14	SER	-	expression tag	UNP Q168G2
L	15	HIS	-	expression tag	UNP Q168G2
L	16	HIS	-	expression tag	UNP Q168G2
L	17	HIS	-	expression tag	UNP Q168G2
L	18	HIS	-	expression tag	UNP Q168G2
L	19	HIS	-	expression tag	UNP Q168G2
L	20	HIS	-	expression tag	UNP Q168G2
L	21	SER	-	expression tag	UNP Q168G2
L	22	SER	-	expression tag	UNP Q168G2
L	23	GLY	-	expression tag	UNP Q168G2
L	24	LEU	-	expression tag	UNP Q168G2
L	25	VAL	-	expression tag	UNP Q168G2
L	26	PRO	-	expression tag	UNP Q168G2
L	27	ARG	-	expression tag	UNP Q168G2
L	28	GLY	-	expression tag	UNP Q168G2
L	29	SER	-	expression tag	UNP Q168G2
L	30	HIS	-	expression tag	UNP Q168G2
L	31	MET	-	expression tag	UNP Q168G2

- Molecule 3 is 5-(HEXAHYDRO-2-OXO-1H-THIENO[3,4-D]IMIDAZOL-6-YL)PENTANAL

(CCD ID: BTI) (formula: C₁₀H₁₆N₂O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
3	C	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
3	E	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
3	G	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
3	I	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
3	K	1	Total	C	N	O	S	0	0
			15	10	2	2	1		

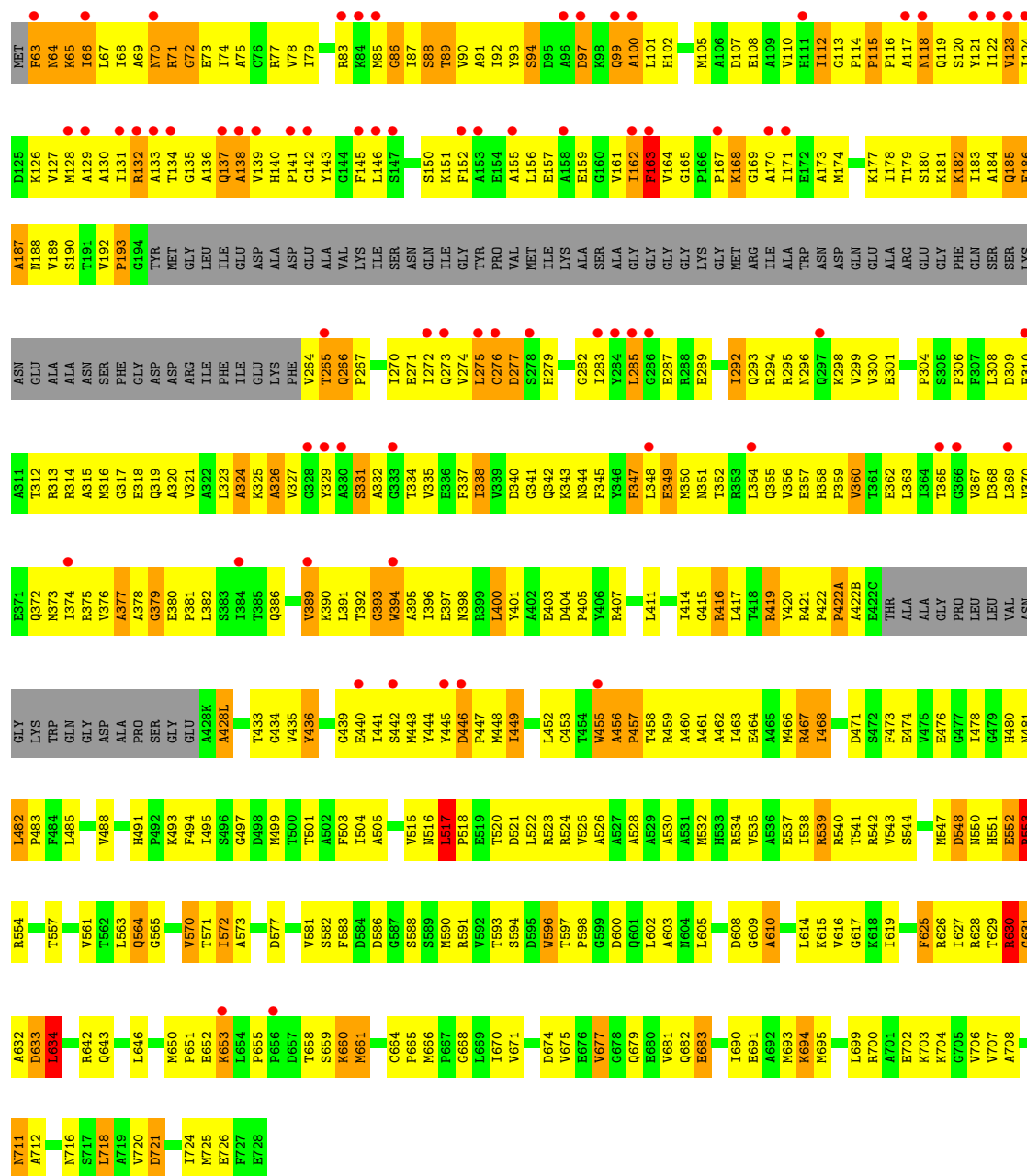
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- [illegible]

M725
E726
E727
E728

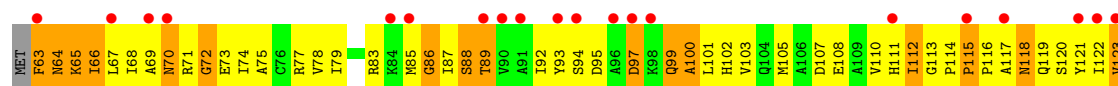
• Molecule 1: Propionyl-CoA carboxylase, alpha subunit

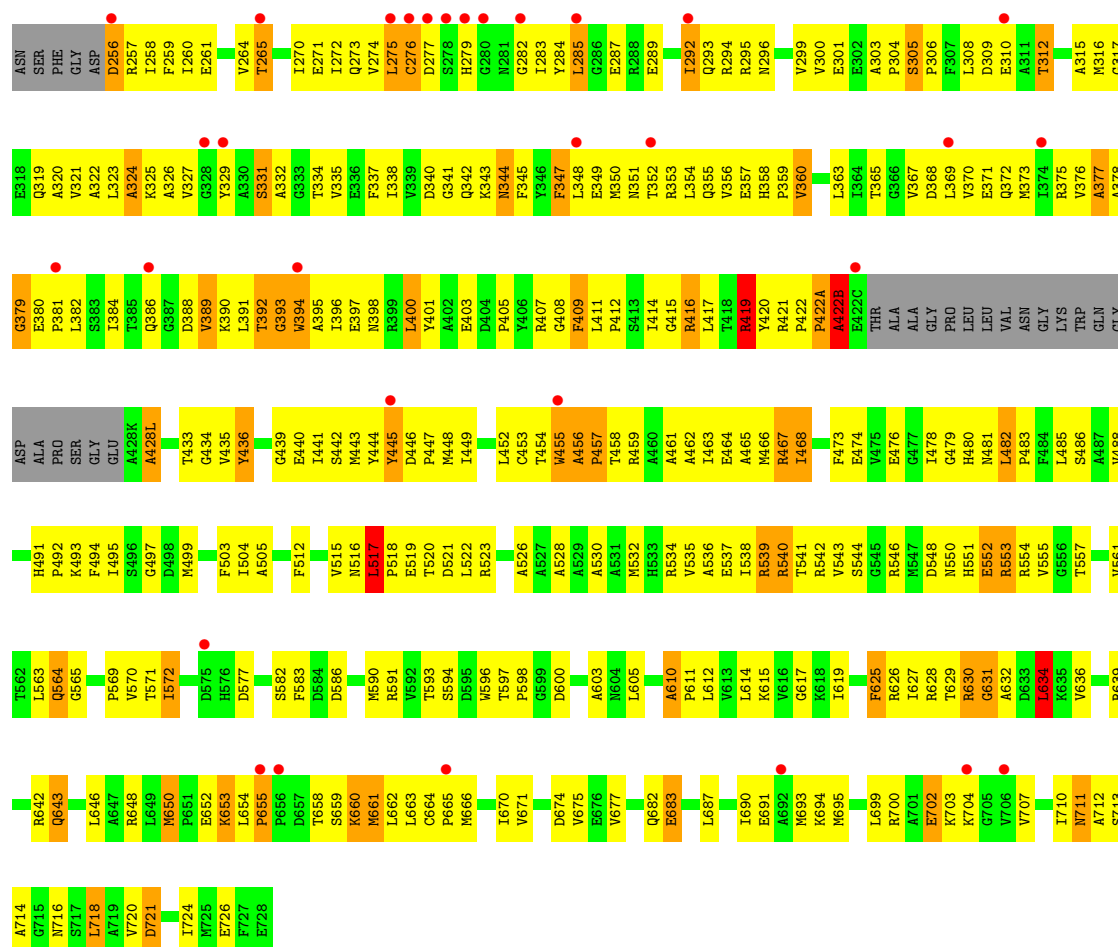
Chain C: 11% 28% 46% 12% 13%



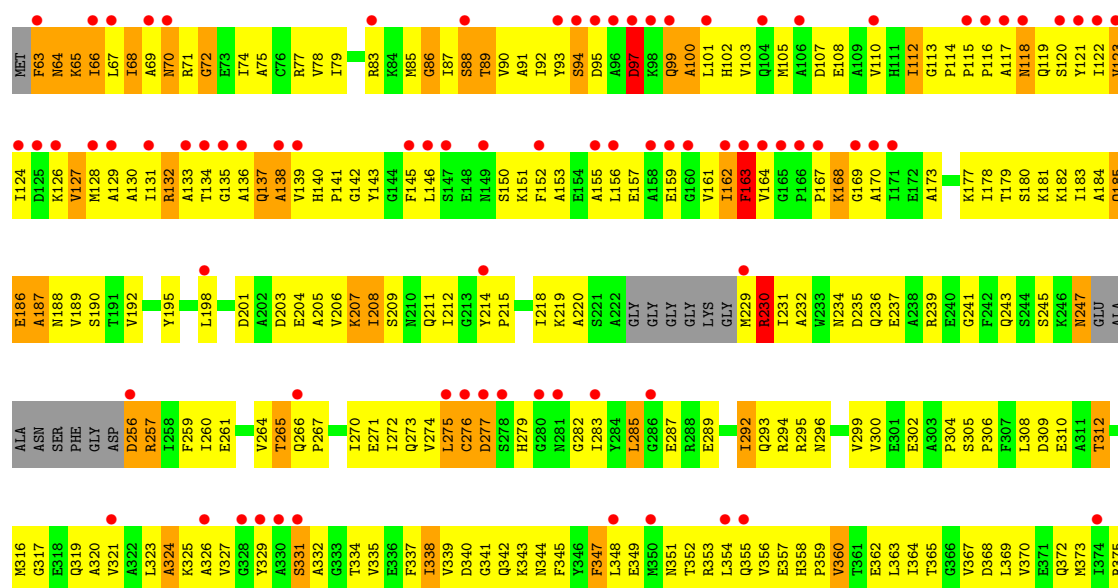
• Molecule 1: Propionyl-CoA carboxylase, alpha subunit

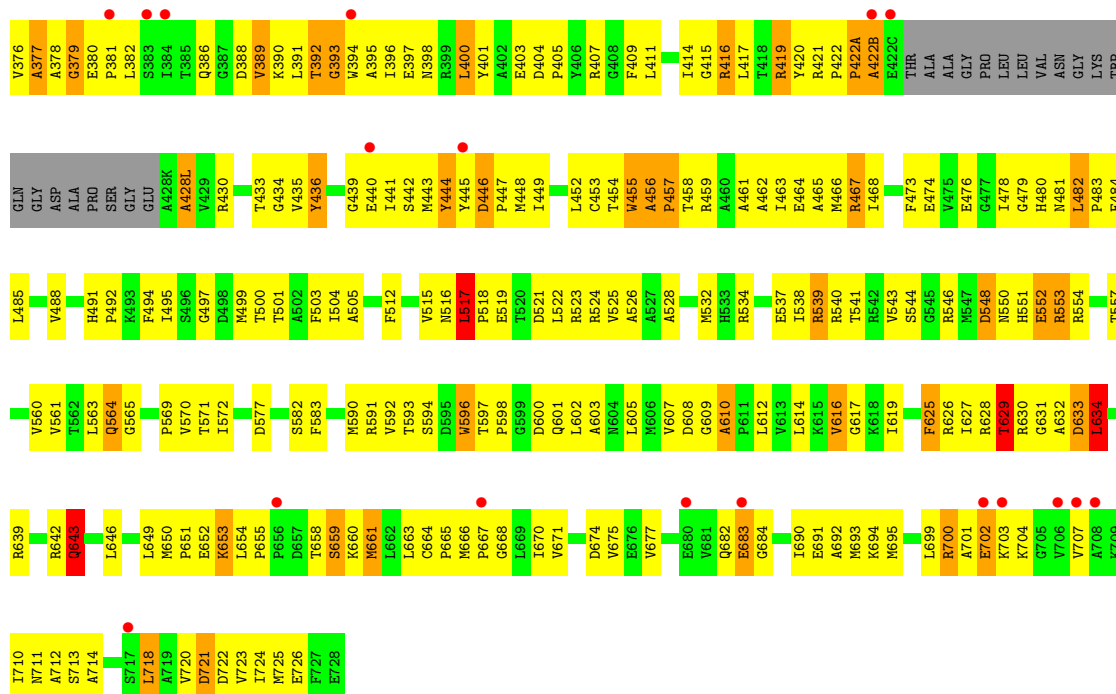
Chain E: 13% 30% 45% 12% 13%



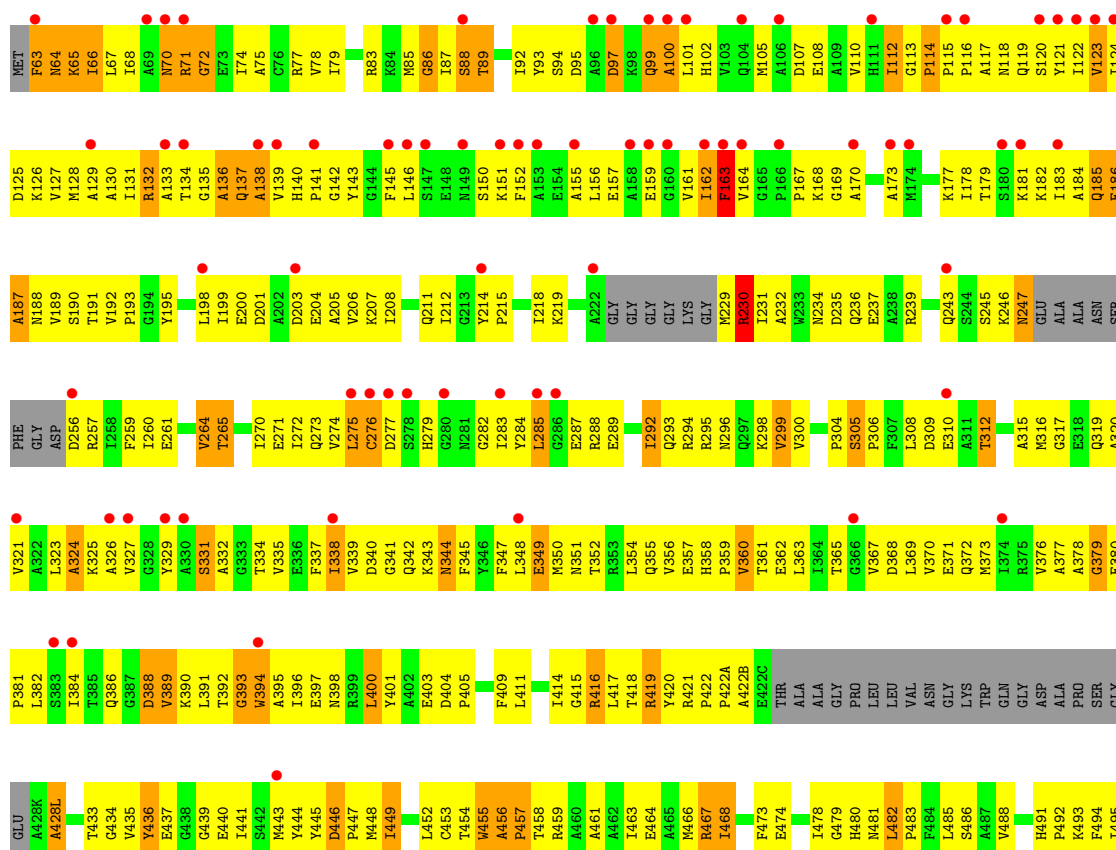


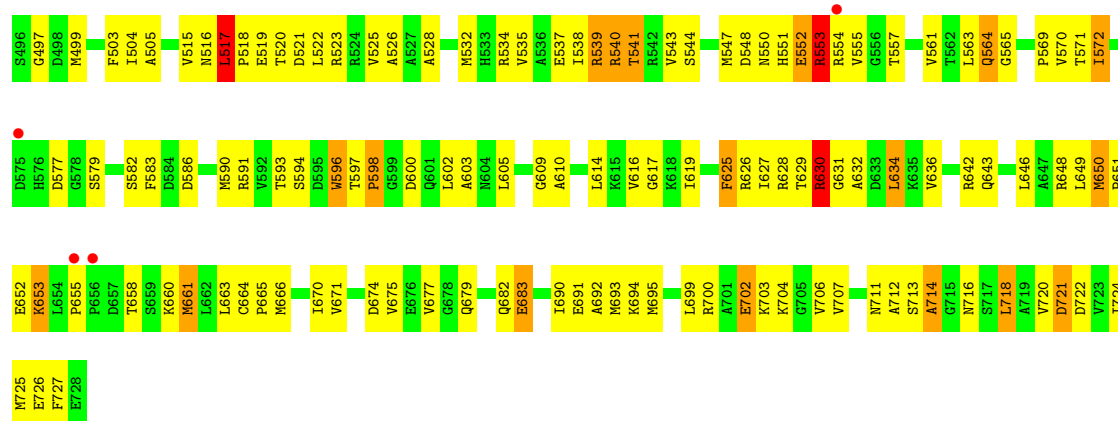
• Molecule 1: Propionyl-CoA carboxylase, alpha subunit



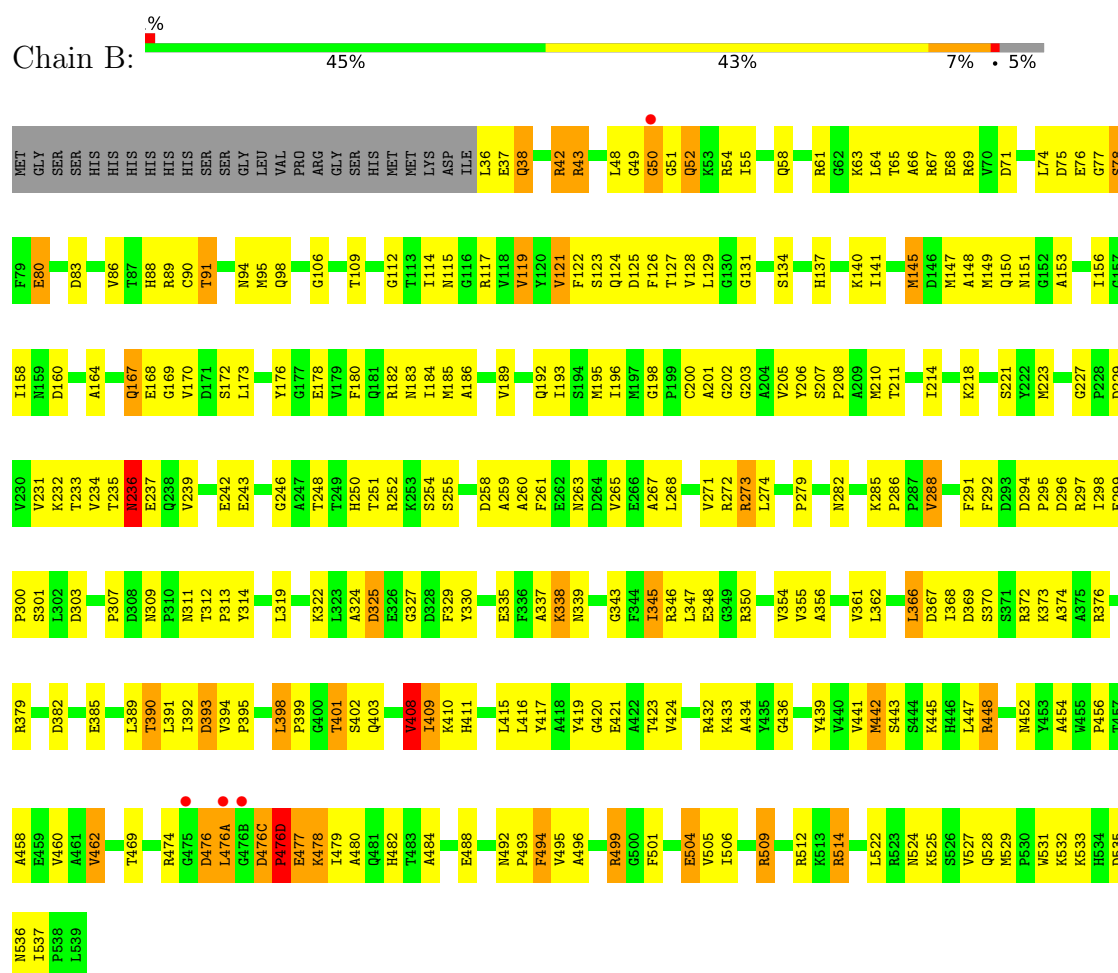


• Molecule 1: Propionyl-CoA carboxylase, alpha subunit

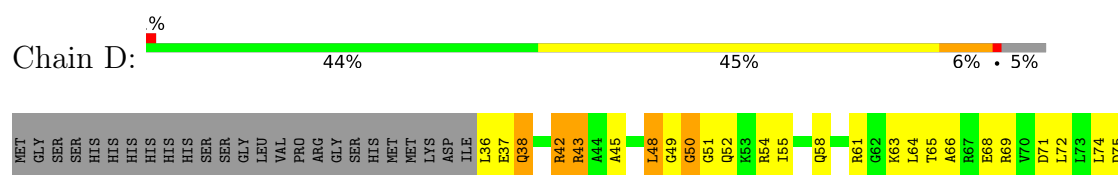


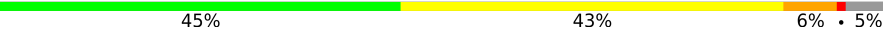


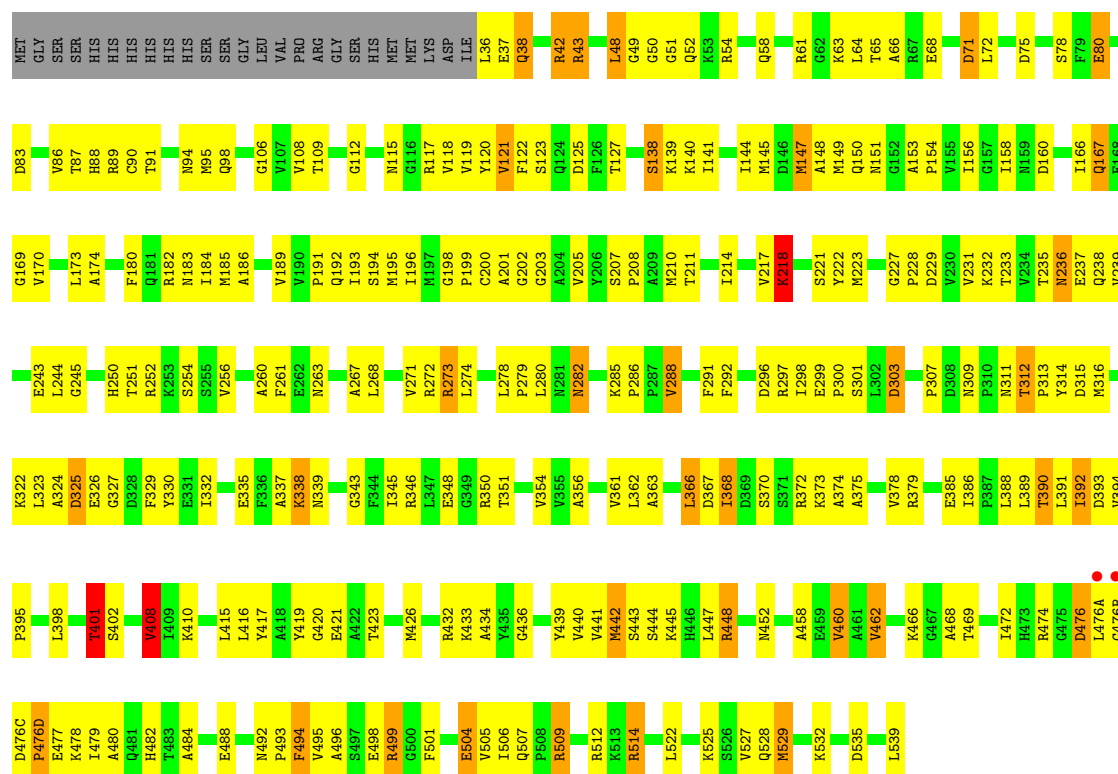
• Molecule 2: Propionyl-CoA carboxylase, beta subunit



• Molecule 2: Propionyl-CoA carboxylase, beta subunit

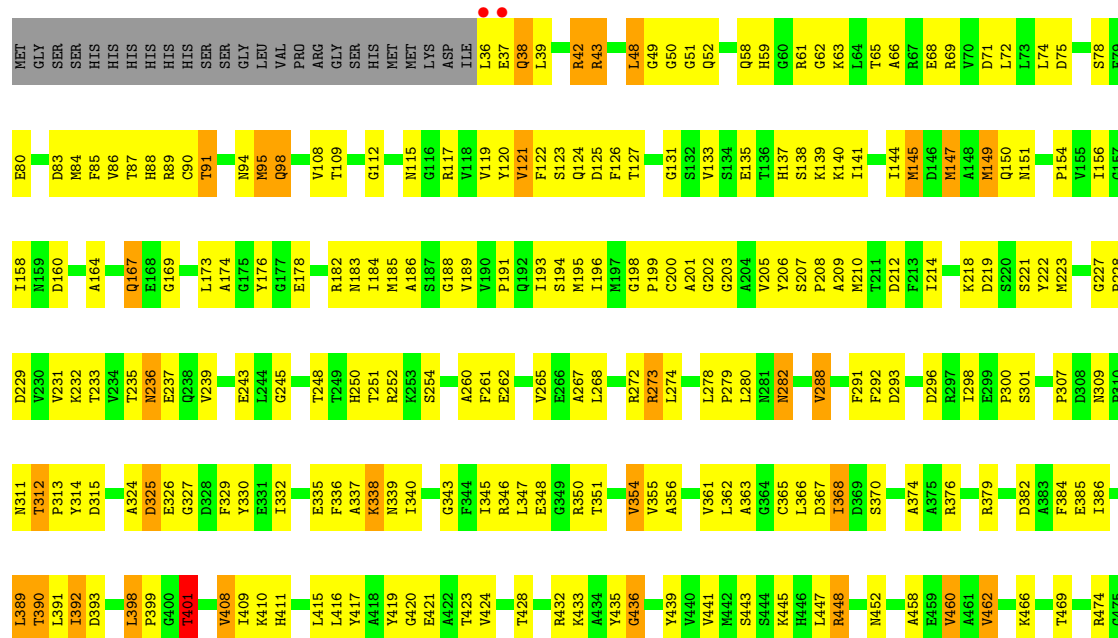


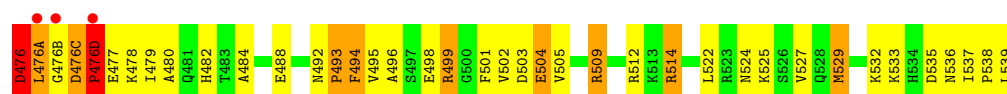
Chain H:  45% 43% 6% • 5%



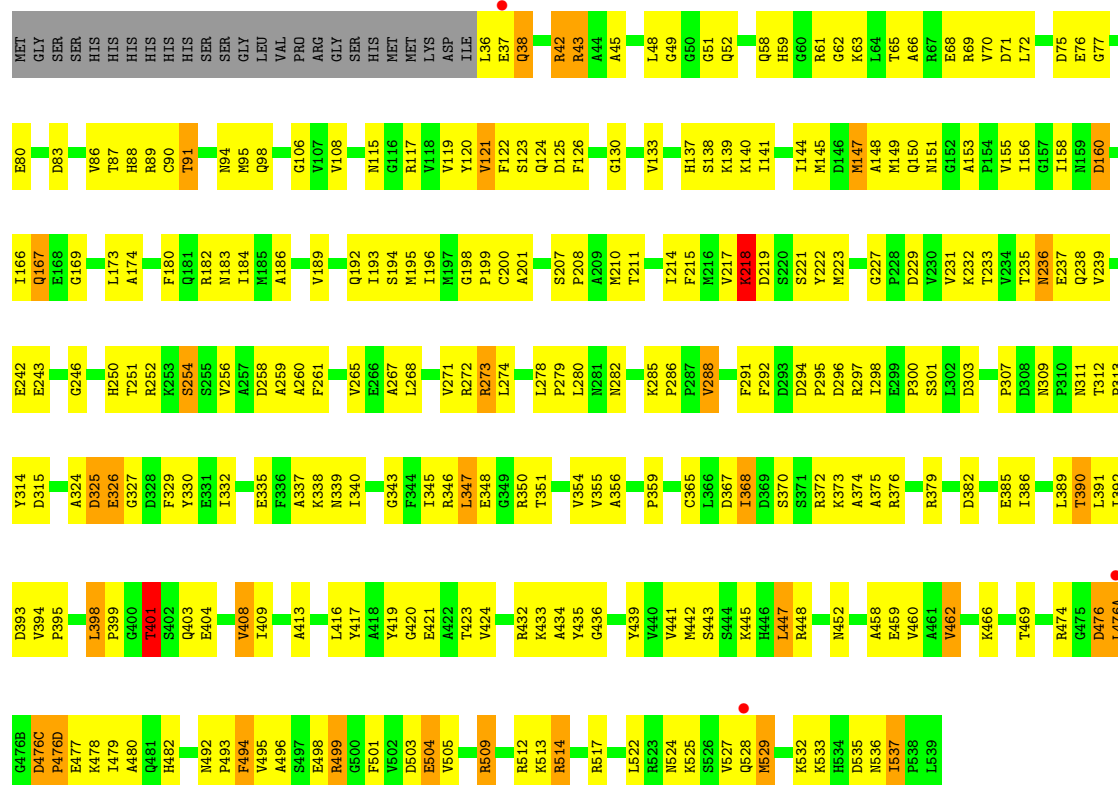
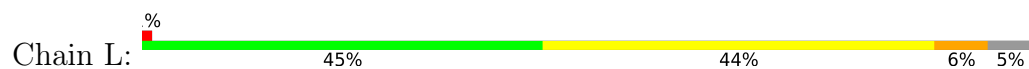
• Molecule 2: Propionyl-CoA carboxylase, beta subunit

Chain J:  45% 43% 7% • 5%





• Molecule 2: Propionyl-CoA carboxylase, beta subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	133.89Å 159.17Å 153.74Å 113.87° 101.03° 108.99°	Depositor
Resolution (Å)	29.36 – 3.20 29.36 – 3.20	Depositor EDS
% Data completeness (in resolution range)	92.4 (29.36-3.20) 92.3 (29.36-3.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 3.11Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.212 , 0.245 0.211 , 0.245	Depositor DCC
R_{free} test set	12641 reflections (7.45%)	wwPDB-VP
Wilson B-factor (Å ²)	44.8	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.017 for -h,h+k+l,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	51921	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

Bond lengths and bond angles in the following residue types are not validated in this section: BTI

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	0.65	0/4586	1.11	32/6209 (0.5%)
1	C	0.65	0/4586	1.12	35/6209 (0.6%)
1	E	0.66	1/4586 (0.0%)	1.10	26/6209 (0.4%)
1	G	0.68	1/5036 (0.0%)	1.13	39/6811 (0.6%)
1	I	0.68	0/5036	1.11	33/6811 (0.5%)
1	K	0.65	0/5036	1.12	37/6811 (0.5%)
2	B	0.77	0/3990	1.18	26/5399 (0.5%)
2	D	0.77	0/3990	1.20	32/5399 (0.6%)
2	F	0.77	0/3990	1.19	24/5399 (0.4%)
2	H	0.78	1/3990 (0.0%)	1.18	25/5399 (0.5%)
2	J	0.76	1/3990 (0.0%)	1.19	31/5399 (0.6%)
2	L	0.77	0/3990	1.19	33/5399 (0.6%)
All	All	0.71	4/52806 (0.0%)	1.15	373/71454 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	E	0	1
1	G	0	1
1	I	0	1
1	K	0	1
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	149	MET	SD-CE	-5.72	1.65	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	426	MET	SD-CE	5.34	1.92	1.79
1	E	629	THR	CA-C	-5.18	1.49	1.52
1	G	536	ALA	CA-CB	-5.15	1.45	1.53

All (373) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	517	LEU	CA-C-N	9.41	130.12	120.14
1	G	517	LEU	C-N-CA	9.41	130.12	120.14
1	I	517	LEU	CA-C-N	9.31	130.00	120.14
1	I	517	LEU	C-N-CA	9.31	130.00	120.14
2	L	392	ILE	N-CA-C	8.97	121.54	108.53
2	H	392	ILE	N-CA-C	8.96	122.06	108.71
1	K	113	GLY	CA-C-N	8.76	129.40	120.38
1	K	113	GLY	C-N-CA	8.76	129.40	120.38
2	B	392	ILE	N-CA-C	8.59	120.99	108.53
2	J	392	ILE	N-CA-C	8.55	121.45	108.71
2	L	494	PHE	N-CA-C	8.46	121.63	111.82
1	E	594	SER	N-CA-C	8.18	121.69	108.76
1	A	610	ALA	CA-C-N	8.04	128.51	119.83
1	A	610	ALA	C-N-CA	8.04	128.51	119.83
2	J	494	PHE	N-CA-C	8.00	121.10	111.82
2	D	494	PHE	N-CA-C	7.96	121.06	111.82
2	F	494	PHE	N-CA-C	7.96	121.05	111.82
1	G	192	VAL	CA-C-N	7.92	127.85	119.85
1	G	192	VAL	C-N-CA	7.92	127.85	119.85
1	I	192	VAL	CA-C-N	7.91	127.67	119.76
1	I	192	VAL	C-N-CA	7.91	127.67	119.76
2	F	392	ILE	N-CA-C	7.91	120.00	108.53
2	D	392	ILE	N-CA-C	7.85	120.40	108.71
2	J	398	LEU	CA-C-N	7.83	127.79	120.03
2	J	398	LEU	C-N-CA	7.83	127.79	120.03
1	I	428(L)	ALA	N-CA-C	7.78	119.98	110.41
1	C	118	ASN	N-CA-C	-7.73	104.32	113.21
1	E	517	LEU	CA-C-N	7.68	128.28	120.14
1	E	517	LEU	C-N-CA	7.68	128.28	120.14
1	I	113	GLY	CA-C-N	7.68	128.29	120.38
1	I	113	GLY	C-N-CA	7.68	128.29	120.38
1	A	422(B)	ALA	N-CA-C	7.64	127.07	110.80
1	C	113	GLY	CA-C-N	7.60	128.21	120.38
1	C	113	GLY	C-N-CA	7.60	128.21	120.38
1	C	428(L)	ALA	N-CA-C	7.50	120.43	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	594	SER	N-CA-C	7.42	120.47	108.76
2	H	401	THR	N-CA-C	-7.39	103.24	111.82
2	B	494	PHE	N-CA-C	7.37	120.37	111.82
1	K	310	GLU	N-CA-C	7.34	119.92	111.11
1	K	594	SER	N-CA-C	7.32	120.33	108.76
1	K	192	VAL	CA-C-N	7.27	127.19	119.85
1	K	192	VAL	C-N-CA	7.27	127.19	119.85
1	E	113	GLY	CA-C-N	7.27	127.86	120.38
1	E	113	GLY	C-N-CA	7.27	127.86	120.38
2	D	37	GLU	N-CA-C	-7.18	104.26	113.16
2	B	106	GLY	N-CA-C	7.14	124.20	114.92
1	A	113	GLY	CA-C-N	7.12	127.71	120.38
1	A	113	GLY	C-N-CA	7.12	127.71	120.38
1	E	118	ASN	N-CA-C	-7.09	105.06	113.21
1	C	187	ALA	N-CA-C	-7.02	104.83	113.19
1	A	594	SER	N-CA-C	7.02	119.85	108.76
1	K	422(B)	ALA	N-CA-C	7.02	125.75	110.80
1	G	422(B)	ALA	N-CA-C	6.99	125.69	110.80
2	L	278	LEU	N-CA-C	6.98	119.55	109.84
2	J	401	THR	N-CA-C	-6.94	103.15	111.69
1	I	422(B)	ALA	N-CA-C	6.89	125.48	110.80
1	C	517	LEU	CA-C-N	6.87	127.04	120.31
1	C	517	LEU	C-N-CA	6.87	127.04	120.31
2	L	398	LEU	CA-C-N	6.85	126.77	119.85
2	L	398	LEU	C-N-CA	6.85	126.77	119.85
2	F	256	VAL	N-CA-C	6.85	117.46	110.82
1	G	310	GLU	N-CA-C	6.82	119.29	111.11
2	B	201	ALA	N-CA-C	6.77	120.55	109.24
1	E	422(B)	ALA	N-CA-C	6.67	125.01	110.80
1	C	631	GLY	N-CA-C	-6.67	107.04	115.31
1	K	610	ALA	CA-C-N	6.61	126.97	119.83
1	K	610	ALA	C-N-CA	6.61	126.97	119.83
2	H	398	LEU	CA-C-N	6.60	126.99	119.92
2	H	398	LEU	C-N-CA	6.60	126.99	119.92
2	H	494	PHE	N-CA-C	6.60	120.55	112.23
1	C	422(B)	ALA	N-CA-C	6.59	124.83	110.80
1	K	616	VAL	N-CA-C	6.59	118.90	108.89
1	I	594	SER	N-CA-C	6.56	118.82	108.79
1	G	594	SER	N-CA-C	6.55	118.81	108.79
1	I	310	GLU	N-CA-C	6.54	118.96	111.11
2	F	201	ALA	N-CA-C	6.51	120.02	109.40
1	K	305	SER	CA-C-N	6.49	126.18	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	305	SER	C-N-CA	6.49	126.18	119.82
1	I	187	ALA	N-CA-C	-6.48	105.48	113.19
1	G	118	ASN	N-CA-C	-6.47	105.77	113.21
1	I	118	ASN	N-CA-C	-6.47	105.77	113.21
2	B	37	GLU	N-CA-C	-6.45	105.40	113.20
2	F	435	TYR	N-CA-C	6.45	119.45	109.07
2	B	131	GLY	N-CA-C	-6.45	104.37	114.10
2	L	37	GLU	N-CA-C	-6.44	105.39	113.18
2	B	366	LEU	N-CA-C	-6.43	99.21	109.76
2	F	385	GLU	N-CA-C	6.43	120.45	112.47
2	F	80	GLU	N-CA-C	-6.42	98.44	108.90
2	L	401	THR	N-CA-C	-6.42	104.37	111.36
2	F	366	LEU	N-CA-C	-6.41	99.25	109.76
2	H	37	GLU	N-CA-C	-6.38	105.48	113.20
2	F	416	LEU	N-CA-C	-6.37	104.27	111.14
1	A	616	VAL	N-CA-C	6.35	118.81	108.97
2	D	279	PRO	N-CA-C	-6.34	101.18	111.77
2	H	447	LEU	N-CA-C	-6.34	105.12	112.92
2	J	265	VAL	N-CA-C	6.32	116.47	110.53
2	B	121	VAL	N-CA-C	6.32	118.23	108.44
2	F	121	VAL	N-CA-C	6.31	118.22	108.44
1	G	428(L)	ALA	N-CA-C	6.31	118.86	110.53
1	E	700	ARG	N-CA-C	6.31	119.00	109.23
1	K	555	VAL	N-CA-C	6.30	117.18	109.30
2	D	435	TYR	N-CA-C	6.30	119.22	109.07
2	J	37	GLU	N-CA-C	-6.30	105.58	113.20
2	B	145	MET	N-CA-C	-6.28	103.97	111.69
2	D	385	GLU	N-CA-C	6.28	120.25	112.47
2	J	278	LEU	N-CA-C	6.27	118.73	110.08
2	J	219	ASP	N-CA-C	6.22	121.81	113.72
1	E	616	VAL	N-CA-C	6.21	117.53	108.53
2	J	38	GLN	N-CA-C	-6.20	104.60	111.36
2	J	201	ALA	N-CA-C	6.20	119.63	109.72
2	F	131	GLY	N-CA-C	-6.19	104.75	114.10
1	G	631	GLY	N-CA-C	-6.19	107.63	115.31
2	L	256	VAL	N-CA-C	6.19	116.82	110.82
1	A	428(L)	ALA	N-CA-C	6.19	118.70	110.53
2	J	279	PRO	N-CA-C	-6.18	101.35	111.68
1	K	553	ARG	N-CA-C	-6.18	101.33	110.48
1	G	419	ARG	N-CA-C	-6.18	99.62	109.76
1	A	631	GLY	N-CA-C	-6.17	107.66	115.31
1	G	113	GLY	CA-C-N	6.16	126.73	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	113	GLY	C-N-CA	6.16	126.73	120.38
2	D	201	ALA	N-CA-C	6.14	119.41	109.40
2	J	80	GLU	N-CA-C	-6.13	98.91	108.90
2	D	401	THR	N-CA-C	-6.12	104.69	111.36
1	A	517	LEU	CA-C-N	6.09	128.19	120.51
1	A	517	LEU	C-N-CA	6.09	128.19	120.51
1	G	479	GLY	N-CA-C	-6.09	101.64	112.54
2	H	121	VAL	N-CA-C	6.09	117.87	108.44
1	A	187	ALA	N-CA-C	-6.08	105.95	113.19
1	K	517	LEU	CA-C-N	6.07	128.44	120.25
1	K	517	LEU	C-N-CA	6.07	128.44	120.25
1	A	445	TYR	N-CA-C	6.07	116.25	108.24
1	K	446	ASP	CA-C-N	6.07	127.42	119.84
1	K	446	ASP	C-N-CA	6.07	127.42	119.84
1	K	428(L)	ALA	N-CA-C	6.05	118.52	110.53
2	D	80	GLU	N-CA-C	-6.05	99.03	108.90
1	A	555	VAL	N-CA-C	6.04	116.84	109.30
2	L	347	LEU	N-CA-C	-6.03	98.80	109.06
1	I	616	VAL	N-CA-C	6.01	118.02	108.89
1	C	299	VAL	CB-CA-C	-6.00	105.74	111.44
2	B	398	LEU	CA-C-N	6.00	126.33	119.92
2	B	398	LEU	C-N-CA	6.00	126.33	119.92
2	D	436	GLY	N-CA-C	5.99	121.90	111.78
1	C	700	ARG	N-CA-C	5.97	118.25	109.24
2	L	533	LYS	N-CA-C	-5.96	104.47	110.97
2	L	385	GLU	N-CA-C	5.95	119.76	111.90
2	B	265	VAL	N-CA-C	5.94	116.11	110.53
1	C	377	ALA	N-CA-C	-5.94	105.74	112.87
1	G	468	ILE	CB-CA-C	-5.92	104.26	112.02
2	L	219	ASP	N-CA-C	5.91	121.53	113.97
1	C	266	GLN	CA-C-N	-5.90	113.14	119.98
1	C	266	GLN	C-N-CA	-5.90	113.14	119.98
1	E	517	LEU	N-CA-C	5.90	118.04	109.84
1	E	187	ALA	N-CA-C	-5.89	105.24	113.37
1	G	394	TRP	N-CA-C	5.88	118.79	110.14
2	F	37	GLU	N-CA-C	-5.88	106.08	113.20
2	D	131	GLY	N-CA-C	-5.87	105.23	114.10
2	J	131	GLY	N-CA-C	-5.87	105.24	114.10
1	G	305	SER	CA-C-N	5.86	126.62	120.12
1	G	305	SER	C-N-CA	5.86	126.62	120.12
2	H	80	GLU	N-CA-C	-5.86	99.35	108.90
2	H	38	GLN	N-CA-C	-5.86	104.97	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	38	GLN	N-CA-C	-5.86	104.97	111.36
2	B	172	SER	N-CA-C	-5.85	104.49	111.69
2	D	38	GLN	N-CA-C	-5.84	105.00	111.36
1	C	446	ASP	CA-C-N	5.83	127.13	119.84
1	C	446	ASP	C-N-CA	5.83	127.13	119.84
2	J	133	VAL	N-CA-C	5.82	117.15	108.54
1	K	349	GLU	N-CA-C	5.82	117.09	107.73
2	B	389	LEU	N-CA-C	-5.81	98.94	108.41
1	A	299	VAL	CB-CA-C	-5.80	105.89	111.05
1	E	428(L)	ALA	N-CA-C	5.80	117.55	110.41
1	I	241	GLY	N-CA-C	-5.80	105.77	112.73
1	C	132	ARG	N-CA-C	-5.80	104.39	112.45
2	F	401	THR	N-CA-C	-5.79	105.05	111.36
2	H	366	LEU	N-CA-C	-5.79	100.26	109.76
2	F	345	ILE	N-CA-C	-5.78	101.48	108.53
2	D	106	GLY	N-CA-C	5.78	122.43	114.92
2	L	201	ALA	N-CA-C	5.78	118.89	109.24
2	D	121	VAL	N-CA-C	5.77	118.48	108.90
2	B	279	PRO	N-CA-C	-5.77	102.80	111.57
2	F	78	SER	N-CA-C	-5.77	105.62	114.16
2	B	385	GLU	N-CA-C	5.76	119.62	112.47
2	J	529	MET	N-CA-C	-5.76	102.64	110.36
2	H	385	GLU	N-CA-C	5.76	119.61	112.47
1	A	517	LEU	N-CA-C	5.74	117.82	109.84
2	H	256	VAL	N-CA-C	5.74	117.26	111.00
1	E	572	ILE	N-CA-C	5.74	116.86	108.53
2	D	265	VAL	N-CA-C	5.73	116.38	110.82
1	I	377	ALA	N-CA-C	-5.73	106.00	112.87
2	D	256	VAL	N-CA-C	5.72	116.77	111.45
1	A	310	GLU	N-CA-C	5.72	118.00	111.02
2	L	478	LYS	N-CA-C	-5.71	104.69	111.03
1	K	299	VAL	CB-CA-C	-5.70	106.02	111.44
1	E	377	ALA	N-CA-C	-5.70	106.03	112.87
1	G	555	VAL	N-CA-C	5.69	116.42	109.30
2	H	278	LEU	N-CA-C	5.69	117.94	110.08
1	I	132	ARG	N-CA-C	-5.68	104.55	112.45
1	A	377	ALA	N-CA-C	-5.68	106.05	112.87
2	D	366	LEU	N-CA-C	-5.67	100.47	109.76
2	L	70	VAL	N-CA-C	-5.67	104.98	110.42
2	L	279	PRO	N-CA-C	-5.66	102.97	111.57
2	F	227	GLY	CA-C-N	5.66	125.50	119.28
2	F	227	GLY	C-N-CA	5.66	125.50	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	299	VAL	CB-CA-C	-5.65	106.07	111.44
1	I	610	ALA	CA-C-N	5.65	125.58	119.76
1	I	610	ALA	C-N-CA	5.65	125.58	119.76
1	E	584	ASP	N-CA-C	5.64	118.16	111.33
2	F	172	SER	N-CA-C	-5.64	104.76	111.69
1	E	349	GLU	N-CA-C	5.63	116.79	107.73
2	B	478	LYS	N-CA-C	-5.63	104.79	111.03
2	J	262	GLU	N-CA-C	5.62	117.40	111.28
2	J	282	ASN	N-CA-C	5.61	119.86	113.19
1	K	572	ILE	N-CA-C	5.61	116.66	108.53
2	H	279	PRO	N-CA-C	-5.61	102.31	111.68
1	C	572	ILE	N-CA-C	5.59	116.63	108.53
1	K	187	ALA	N-CA-C	-5.59	106.54	113.19
2	B	80	GLU	N-CA-C	-5.59	99.18	108.34
1	C	349	GLU	N-CA-C	5.58	116.71	107.73
1	K	517	LEU	N-CA-C	5.57	117.77	110.08
1	G	236	GLN	N-CA-C	-5.57	106.44	113.18
2	D	528	GLN	N-CA-C	5.57	117.59	108.52
1	E	445	TYR	N-CA-C	5.57	115.59	108.24
2	J	366	LEU	N-CA-C	-5.56	100.64	109.76
1	I	548	ASP	N-CA-C	5.56	117.80	111.02
1	I	299	VAL	CB-CA-C	-5.55	106.17	111.44
2	H	106	GLY	N-CA-C	5.54	122.12	114.92
1	G	220	ALA	N-CA-C	-5.53	101.67	109.96
1	C	616	VAL	N-CA-C	5.53	117.29	108.89
2	J	121	VAL	N-CA-C	5.52	118.06	108.90
1	I	205	ALA	N-CA-C	-5.50	104.31	111.02
2	L	529	MET	N-CA-C	-5.50	102.98	110.36
1	K	125	ASP	N-CA-C	-5.50	104.93	111.03
2	D	118	VAL	N-CA-C	5.49	117.54	109.63
2	L	133	VAL	N-CA-C	5.48	116.07	108.84
1	A	305	SER	CA-C-N	5.47	126.67	119.84
1	A	305	SER	C-N-CA	5.47	126.67	119.84
1	C	394	TRP	N-CA-C	5.47	118.62	110.14
2	L	529	MET	CA-C-N	5.46	125.41	119.78
2	L	529	MET	C-N-CA	5.46	125.41	119.78
2	D	408	VAL	CB-CA-C	-5.46	103.69	112.16
2	D	455	TRP	N-CA-C	-5.46	103.05	110.36
1	K	540	ARG	N-CA-C	-5.46	105.33	111.28
2	L	435	TYR	N-CA-C	5.45	117.84	109.07
2	J	145	MET	N-CA-C	-5.44	105.26	111.14
2	L	218	LYS	CA-C-N	-5.43	113.21	122.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	218	LYS	C-N-CA	-5.43	113.21	122.11
2	H	389	LEU	N-CA-C	-5.43	99.56	108.41
1	A	660	LYS	N-CA-C	-5.42	106.51	113.02
2	F	106	GLY	N-CA-C	5.42	122.92	115.27
1	K	541	THR	N-CA-C	5.42	117.95	111.71
1	A	394	TRP	N-CA-C	5.42	118.54	110.14
1	E	362	GLU	N-CA-C	5.42	117.94	111.71
1	I	220	ALA	N-CA-C	-5.42	101.84	109.96
1	E	419	ARG	CB-CG-CD	5.41	123.75	111.30
1	G	187	ALA	N-CA-C	-5.41	105.90	113.37
1	A	132	ARG	N-CA-C	-5.41	104.93	112.45
2	D	172	SER	N-CA-C	-5.41	105.04	111.69
1	G	377	ALA	N-CA-C	-5.40	106.39	112.87
2	H	529	MET	N-CA-C	-5.40	103.12	110.36
1	K	700	ARG	N-CA-C	5.40	117.39	109.24
1	I	634	LEU	N-CA-C	5.39	117.59	109.23
1	K	569	PRO	N-CA-C	-5.39	102.04	110.50
2	L	106	GLY	N-CA-C	5.38	121.92	114.92
1	A	569	PRO	N-CA-C	-5.38	102.05	110.50
1	G	445	TYR	N-CA-C	5.38	115.34	108.24
1	E	451	LYS	N-CA-C	-5.38	99.64	108.41
1	C	660	LYS	N-CA-C	-5.37	106.92	112.93
2	H	201	ALA	N-CA-C	5.37	118.31	109.72
2	J	502	VAL	N-CA-C	-5.37	99.92	107.75
2	B	38	GLN	N-CA-C	-5.36	105.52	111.36
2	J	314	TYR	N-CA-C	-5.35	100.18	108.42
1	C	553	ARG	N-CA-C	-5.33	101.78	110.20
2	J	435	TYR	N-CA-C	5.33	118.16	109.59
2	D	529	MET	N-CA-C	-5.32	102.94	110.29
2	F	279	PRO	N-CA-C	-5.32	102.79	111.68
2	J	436	GLY	N-CA-C	5.32	120.93	111.73
1	E	660	LYS	N-CA-C	-5.31	106.98	112.93
1	A	573	ALA	N-CA-C	-5.30	98.93	108.48
1	G	517	LEU	N-CA-C	5.30	117.21	109.84
2	F	137	HIS	N-CA-C	-5.30	105.41	111.14
2	D	389	LEU	N-CA-C	-5.30	100.27	108.90
1	G	322	ALA	N-CA-C	-5.30	105.20	110.97
2	L	389	LEU	N-CA-C	-5.29	99.78	108.41
1	G	610	ALA	CA-C-N	5.29	125.30	119.90
1	G	610	ALA	C-N-CA	5.29	125.30	119.90
2	H	282	ASN	N-CA-C	5.29	119.61	113.20
2	J	478	LYS	N-CA-C	-5.29	105.42	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	468	ILE	N-CA-C	-5.28	105.56	110.53
1	C	517	LEU	N-CA-C	5.28	117.18	109.84
2	F	528	GLN	N-CA-C	5.27	117.56	109.07
1	K	479	GLY	N-CA-C	-5.27	102.29	111.62
1	G	650	MET	CA-C-N	5.27	125.21	119.78
1	G	650	MET	C-N-CA	5.27	125.21	119.78
1	I	479	GLY	N-CA-C	-5.27	102.30	111.62
1	K	468	ILE	CB-CA-C	-5.26	105.23	111.97
1	I	208	ILE	CB-CA-C	-5.26	105.13	112.02
1	E	643	GLN	N-CA-C	-5.26	105.44	111.07
2	H	506	ILE	N-CA-C	5.26	117.20	108.99
1	C	404	ASP	CA-C-N	5.25	125.31	119.32
1	C	404	ASP	C-N-CA	5.25	125.31	119.32
1	A	468	ILE	CB-CA-C	-5.25	105.14	112.02
1	K	132	ARG	N-CA-C	-5.25	105.15	112.45
1	I	659	SER	N-CA-C	-5.25	101.97	110.32
2	D	529	MET	CA-C-N	5.24	125.18	119.78
2	D	529	MET	C-N-CA	5.24	125.18	119.78
1	C	634	LEU	N-CA-C	5.24	117.22	108.99
1	I	446	ASP	CA-C-N	5.24	126.39	119.84
1	I	446	ASP	C-N-CA	5.24	126.39	119.84
1	A	479	GLY	N-CA-C	-5.24	102.35	111.62
2	H	528	GLN	N-CA-C	5.24	117.06	108.52
2	B	236	ASN	N-CA-C	-5.24	107.25	113.38
2	D	398	LEU	CA-C-N	5.23	125.52	119.92
2	D	398	LEU	C-N-CA	5.23	125.52	119.92
2	J	389	LEU	N-CA-C	-5.23	99.88	108.41
1	G	540	ARG	N-CA-C	-5.23	105.69	111.71
2	B	250	HIS	N-CA-C	5.23	118.82	112.23
1	G	132	ARG	N-CA-C	-5.22	105.19	112.45
2	J	529	MET	CA-C-N	5.21	125.15	119.78
2	J	529	MET	C-N-CA	5.21	125.15	119.78
1	G	241	GLY	N-CA-C	-5.21	106.45	112.50
2	B	408	VAL	CB-CA-C	-5.21	104.09	112.16
2	F	447	LEU	N-CA-C	-5.21	106.52	112.92
1	G	634	LEU	N-CA-C	5.21	117.30	109.23
1	K	264	VAL	N-CA-C	5.20	115.84	107.73
1	E	132	ARG	N-CA-C	-5.19	104.56	112.04
1	G	299	VAL	CB-CA-C	-5.19	106.51	111.44
1	K	114	PRO	N-CA-C	5.19	117.03	110.70
1	I	569	PRO	N-CA-C	-5.18	102.56	110.95
2	J	533	LYS	N-CA-C	-5.17	105.54	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	700	ARG	N-CA-C	5.16	117.23	109.23
1	I	643	GLN	N-CA-C	-5.16	105.30	111.03
1	I	629	THR	CB-CA-C	-5.15	105.20	114.52
2	L	254	SER	N-CA-C	5.15	118.83	112.54
1	C	681	VAL	N-CA-C	5.15	115.89	108.48
2	H	314	TYR	N-CA-C	-5.14	100.50	108.42
2	L	447	LEU	N-CA-C	-5.14	106.59	112.92
1	G	569	PRO	N-CA-C	-5.14	102.62	110.95
1	A	456	ALA	CA-C-N	-5.14	113.42	119.84
1	A	456	ALA	C-N-CA	-5.14	113.42	119.84
1	C	610	ALA	CA-C-N	5.13	125.04	119.76
1	C	610	ALA	C-N-CA	5.13	125.04	119.76
2	B	477	GLU	N-CA-C	-5.12	107.58	113.88
2	L	160	ASP	N-CA-C	-5.12	99.89	110.80
2	J	212	ASP	N-CA-C	5.10	118.76	112.54
2	L	528	GLN	N-CA-C	5.10	117.28	109.07
1	E	115	PRO	N-CA-C	5.09	116.92	110.70
2	F	529	MET	N-CA-C	-5.09	103.53	110.36
2	L	80	GLU	N-CA-C	-5.09	100.60	108.90
1	E	681	VAL	N-CA-C	5.09	115.81	108.48
1	C	310	GLU	N-CA-C	5.09	119.77	111.37
1	C	694	LYS	N-CA-C	-5.08	106.38	112.58
1	G	205	ALA	N-CA-C	-5.07	104.83	111.02
1	C	115	PRO	N-CA-C	5.07	116.89	110.70
2	H	408	VAL	CB-CA-C	-5.07	104.30	112.16
1	A	700	ARG	N-CA-C	5.07	117.08	109.23
2	B	345	ILE	N-CA-C	-5.06	100.99	108.23
2	D	478	LYS	N-CA-C	-5.06	105.41	111.03
2	D	278	LEU	N-CA-C	5.06	117.06	110.08
2	B	528	GLN	N-CA-C	5.05	117.21	109.07
1	K	394	TRP	N-CA-C	5.05	117.97	110.14
1	A	125	ASP	N-CA-C	-5.05	105.47	110.97
2	B	314	TYR	N-CA-C	-5.05	100.65	108.42
2	D	433	LYS	N-CA-C	5.05	117.78	109.76
1	K	650	MET	CA-C-N	5.04	125.32	119.92
1	K	650	MET	C-N-CA	5.04	125.32	119.92
2	D	416	LEU	N-CA-C	-5.04	105.67	111.07
1	C	468	ILE	CB-CA-C	-5.04	105.51	111.81
1	G	660	LYS	N-CA-C	-5.02	107.30	112.93
2	H	118	VAL	N-CA-C	5.02	116.86	109.63
1	G	572	ILE	N-CA-C	5.01	115.69	108.48
2	L	121	VAL	N-CA-C	5.00	116.20	108.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	517	LEU	N-CA-C	5.00	116.79	109.84
2	L	265	VAL	N-CA-C	5.00	115.15	110.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	420	TYR	Sidechain
1	E	420	TYR	Sidechain
1	G	420	TYR	Sidechain
1	I	420	TYR	Sidechain
1	K	420	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4507	0	4511	462	0
1	C	4507	0	4512	476	0
1	E	4507	0	4512	485	0
1	G	4950	0	4944	525	0
1	I	4950	0	4943	523	0
1	K	4950	0	4943	510	0
2	B	3910	0	3851	285	0
2	D	3910	0	3851	267	0
2	F	3910	0	3851	246	0
2	H	3910	0	3851	265	0
2	J	3910	0	3851	251	0
2	L	3910	0	3851	251	0
3	A	15	0	15	1	0
3	C	15	0	15	0	0
3	E	15	0	15	1	0
3	G	15	0	15	0	0
3	I	15	0	15	2	0
3	K	15	0	15	0	0
All	All	51921	0	51561	4296	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 42.

All (4296) 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:E:338:ILE:HD11	1:E:348:LEU:HB2	1.25	1.17
1:A:338:ILE:HD11	1:A:348:LEU:HB2	1.26	1.16
1:C:115:PRO:HG2	1:C:116:PRO:HD3	1.29	1.14
1:A:433:THR:HG22	1:A:435:VAL:H	1.06	1.11
1:G:400:LEU:HD13	1:G:449:ILE:HD11	1.33	1.11
1:K:338:ILE:HD11	1:K:348:LEU:HB2	1.22	1.10
1:I:400:LEU:HD13	1:I:449:ILE:HD11	1.32	1.10
1:A:665:PRO:HG2	1:A:666:MET:HE2	1.32	1.09
1:C:338:ILE:HD11	1:C:348:LEU:HB2	1.25	1.09
1:I:338:ILE:HD11	1:I:348:LEU:HB2	1.23	1.09
2:L:167:GLN:HE21	2:L:167:GLN:N	1.51	1.09
1:I:433:THR:HG22	1:I:435:VAL:H	1.10	1.09
1:E:400:LEU:HD13	1:E:449:ILE:HD11	1.35	1.08
2:L:167:GLN:H	2:L:167:GLN:NE2	1.51	1.08
1:A:79:ILE:HG23	1:A:89:THR:HG21	1.36	1.07
1:E:433:THR:HG22	1:E:435:VAL:H	1.12	1.07
2:H:167:GLN:HE21	2:H:167:GLN:N	1.53	1.06
1:A:400:LEU:HD13	1:A:449:ILE:HD11	1.34	1.06
1:G:338:ILE:HD11	1:G:348:LEU:HB2	1.35	1.06
1:C:400:LEU:HD13	1:C:449:ILE:HD11	1.34	1.06
1:E:115:PRO:HG2	1:E:116:PRO:HD3	1.34	1.04
1:I:665:PRO:HG2	1:I:666:MET:HE2	1.35	1.04
1:A:115:PRO:HG2	1:A:116:PRO:HD3	1.37	1.04
1:G:433:THR:HG22	1:G:435:VAL:H	1.23	1.04
1:K:433:THR:HG22	1:K:435:VAL:H	1.19	1.04
1:E:79:ILE:HG23	1:E:89:THR:HG21	1.38	1.03
1:C:433:THR:HG22	1:C:435:VAL:H	1.16	1.03
1:K:115:PRO:HG2	1:K:116:PRO:HD3	1.39	1.03
1:I:115:PRO:HG2	1:I:116:PRO:HD3	1.36	1.02
1:I:653:LYS:HD3	1:I:653:LYS:H	1.20	1.01
2:B:167:GLN:H	2:B:167:GLN:NE2	1.58	1.01
1:C:292:ILE:HD12	1:C:292:ILE:H	1.25	1.01
1:C:653:LYS:H	1:C:653:LYS:HD3	1.23	1.01
1:E:653:LYS:H	1:E:653:LYS:HD3	1.25	1.01
2:H:167:GLN:H	2:H:167:GLN:NE2	1.58	1.01
1:K:665:PRO:HG2	1:K:666:MET:HE2	1.42	0.99
2:B:167:GLN:N	2:B:167:GLN:HE21	1.60	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:167:GLN:HE21	2:J:167:GLN:N	1.60	0.99
1:E:162:ILE:HG21	1:E:377:ALA:O	1.62	0.99
1:G:292:ILE:H	1:G:292:ILE:HD12	1.27	0.99
1:G:653:LYS:HD3	1:G:653:LYS:H	1.26	0.99
1:G:309:ASP:OD1	1:G:312:THR:HG22	1.63	0.98
1:G:665:PRO:HG2	1:G:666:MET:HE2	1.43	0.98
1:E:308:LEU:HD22	1:E:316:MET:SD	2.03	0.98
1:I:309:ASP:OD1	1:I:312:THR:HG22	1.64	0.98
2:F:167:GLN:N	2:F:167:GLN:HE21	1.59	0.98
1:G:79:ILE:HG23	1:G:89:THR:HG21	1.44	0.98
1:A:653:LYS:HD3	1:A:653:LYS:H	1.23	0.98
1:C:79:ILE:HG23	1:C:89:THR:HG21	1.46	0.98
2:D:167:GLN:HE21	2:D:167:GLN:H	0.98	0.98
1:G:115:PRO:HG2	1:G:116:PRO:HD3	1.42	0.98
2:F:167:GLN:NE2	2:F:167:GLN:H	1.61	0.98
1:E:419:ARG:HD2	1:E:601:GLN:OE1	1.63	0.97
1:E:670:ILE:HG13	1:E:718:LEU:HD21	1.45	0.97
1:C:66:ILE:HD12	1:C:87:ILE:HG22	1.46	0.97
1:K:162:ILE:HG21	1:K:377:ALA:O	1.63	0.97
1:I:473:PHE:HB3	1:I:482:LEU:HD21	1.46	0.97
1:K:653:LYS:H	1:K:653:LYS:HD3	1.28	0.97
2:D:145:MET:HE1	2:D:183:ASN:ND2	1.78	0.97
1:C:178:ILE:H	1:C:178:ILE:HD12	1.30	0.96
1:G:178:ILE:H	1:G:178:ILE:HD12	1.30	0.96
1:K:540:ARG:O	1:K:543:VAL:HG23	1.65	0.96
2:J:167:GLN:H	2:J:167:GLN:NE2	1.62	0.96
1:I:670:ILE:HG13	1:I:718:LEU:HD21	1.48	0.95
1:G:162:ILE:HG21	1:G:377:ALA:O	1.67	0.95
1:K:292:ILE:HD12	1:K:292:ILE:H	1.30	0.95
1:K:400:LEU:HD13	1:K:449:ILE:HD11	1.45	0.95
1:I:528:ALA:O	1:I:532:MET:HG3	1.67	0.95
1:E:617:GLY:O	1:E:625:PHE:HB3	1.67	0.94
1:I:540:ARG:O	1:I:543:VAL:HG23	1.66	0.94
1:E:456:ALA:HB1	1:E:457:PRO:HD2	1.47	0.94
1:A:178:ILE:H	1:A:178:ILE:HD12	1.32	0.94
1:C:665:PRO:HG2	1:C:666:MET:HE2	1.47	0.94
1:K:456:ALA:HB1	1:K:457:PRO:HD2	1.48	0.94
1:C:456:ALA:HB1	1:C:457:PRO:HD2	1.50	0.94
1:I:162:ILE:HG21	1:I:377:ALA:O	1.66	0.94
1:E:665:PRO:HG2	1:E:666:MET:HE2	1.47	0.94
1:K:617:GLY:O	1:K:625:PHE:HB3	1.68	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:178:ILE:H	1:K:178:ILE:HD12	1.31	0.94
1:E:178:ILE:HD12	1:E:178:ILE:H	1.29	0.93
1:A:162:ILE:HG21	1:A:377:ALA:O	1.66	0.93
1:G:66:ILE:HD12	1:G:87:ILE:HG22	1.50	0.93
1:I:131:ILE:HG22	1:I:136:ALA:HB2	1.50	0.93
1:I:136:ALA:HB1	1:I:161:VAL:HG13	1.51	0.93
1:G:131:ILE:HG22	1:G:136:ALA:HB2	1.50	0.93
1:C:540:ARG:O	1:C:543:VAL:HG23	1.69	0.93
1:I:178:ILE:H	1:I:178:ILE:HD12	1.31	0.93
1:I:292:ILE:H	1:I:292:ILE:HD12	1.33	0.93
2:F:325:ASP:HA	2:F:512:ARG:HH12	1.32	0.93
1:A:670:ILE:HG13	1:A:718:LEU:HD21	1.51	0.93
1:K:309:ASP:OD1	1:K:312:THR:HG22	1.68	0.93
1:I:456:ALA:HB1	1:I:457:PRO:HD2	1.51	0.92
1:E:540:ARG:O	1:E:543:VAL:HG23	1.68	0.92
1:A:136:ALA:HB1	1:A:161:VAL:HG13	1.51	0.92
1:K:308:LEU:HD22	1:K:316:MET:SD	2.08	0.92
1:K:264:VAL:HG13	1:K:340:ASP:HB3	1.52	0.92
1:C:162:ILE:HG21	1:C:377:ALA:O	1.70	0.92
1:G:540:ARG:O	1:G:543:VAL:HG23	1.68	0.92
2:B:145:MET:HE1	2:B:183:ASN:ND2	1.85	0.92
1:K:131:ILE:HG22	1:K:136:ALA:HB2	1.52	0.92
1:K:528:ALA:O	1:K:532:MET:HG3	1.67	0.92
1:C:308:LEU:HD22	1:C:316:MET:SD	2.10	0.91
2:F:207:SER:HB3	2:F:208:PRO:HD3	1.50	0.91
1:K:136:ALA:HB1	1:K:161:VAL:HG13	1.51	0.91
2:L:479:ILE:HD12	2:L:480:ALA:N	1.84	0.91
1:I:79:ILE:HG23	1:I:89:THR:HG21	1.52	0.91
1:E:528:ALA:O	1:E:532:MET:HG3	1.71	0.91
1:K:66:ILE:HD12	1:K:87:ILE:HG22	1.53	0.91
2:F:499:ARG:HG2	2:F:499:ARG:HH11	1.34	0.91
1:E:66:ILE:HD12	1:E:87:ILE:HG22	1.53	0.91
1:E:136:ALA:HB1	1:E:161:VAL:HG13	1.51	0.91
2:F:420:GLY:HA3	2:H:184:ILE:HD12	1.53	0.90
2:B:36:LEU:HD22	2:B:38:GLN:HG3	1.53	0.90
2:D:167:GLN:HE21	2:D:167:GLN:N	1.69	0.90
1:A:66:ILE:HD12	1:A:87:ILE:HG22	1.54	0.90
2:J:479:ILE:HD12	2:J:480:ALA:N	1.85	0.90
1:A:265:THR:O	1:A:267:PRO:HD3	1.72	0.90
1:C:457:PRO:HG2	1:C:458:THR:H	1.37	0.90
2:J:145:MET:HE1	2:J:183:ASN:ND2	1.87	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:325:ASP:HA	2:D:512:ARG:HH12	1.37	0.90
1:G:456:ALA:HB1	1:G:457:PRO:HD2	1.51	0.90
1:A:617:GLY:O	1:A:625:PHE:HB3	1.72	0.89
2:B:88:HIS:HD2	2:B:90:CYS:H	1.17	0.89
2:F:83:ASP:HB2	2:F:140:LYS:HE3	1.52	0.89
2:B:325:ASP:HA	2:B:512:ARG:HH12	1.38	0.89
1:A:292:ILE:H	1:A:292:ILE:HD12	1.36	0.89
2:F:167:GLN:HE21	2:F:167:GLN:H	0.92	0.89
1:G:264:VAL:HG13	1:G:340:ASP:HB3	1.52	0.88
1:G:457:PRO:HG2	1:G:458:THR:H	1.38	0.88
1:G:390:LYS:HD3	1:G:391:LEU:N	1.87	0.88
1:G:136:ALA:HB1	1:G:161:VAL:HG13	1.55	0.88
2:L:207:SER:HB3	2:L:208:PRO:HD3	1.55	0.88
1:A:456:ALA:HB1	1:A:457:PRO:HD2	1.55	0.88
1:C:136:ALA:HB1	1:C:161:VAL:HG13	1.55	0.88
2:H:325:ASP:HA	2:H:512:ARG:HH12	1.36	0.88
2:H:499:ARG:HH21	2:J:89:ARG:HH11	1.21	0.88
1:G:528:ALA:O	1:G:532:MET:HG3	1.74	0.88
2:H:499:ARG:HH11	2:H:499:ARG:HG2	1.39	0.88
2:J:499:ARG:HG2	2:J:499:ARG:HH11	1.39	0.88
1:C:452:LEU:O	1:C:466:MET:HE1	1.72	0.88
2:D:167:GLN:H	2:D:167:GLN:NE2	1.70	0.88
2:B:207:SER:HB3	2:B:208:PRO:HD3	1.56	0.88
1:C:617:GLY:O	1:C:625:PHE:HB3	1.73	0.88
1:G:127:VAL:HG12	1:G:131:ILE:HD11	1.55	0.88
2:H:145:MET:HE1	2:H:183:ASN:ND2	1.90	0.87
1:E:457:PRO:HG2	1:E:458:THR:H	1.40	0.87
1:I:390:LYS:HD3	1:I:391:LEU:N	1.89	0.87
1:G:557:THR:HG23	1:G:572:ILE:O	1.74	0.87
1:A:127:VAL:HG12	1:A:131:ILE:HD11	1.56	0.87
2:B:189:VAL:HA	2:B:282:ASN:ND2	1.89	0.87
2:H:207:SER:HB3	2:H:208:PRO:HD3	1.55	0.86
1:I:66:ILE:HD12	1:I:87:ILE:HG22	1.55	0.86
2:B:151:ASN:HD21	2:D:522:LEU:HD23	1.37	0.86
2:F:184:ILE:HD12	2:H:420:GLY:HA3	1.57	0.86
1:C:390:LYS:HD3	1:C:391:LEU:N	1.90	0.86
2:H:479:ILE:HD12	2:H:480:ALA:N	1.90	0.86
1:I:127:VAL:HG12	1:I:131:ILE:HD11	1.58	0.86
1:K:390:LYS:HD3	1:K:391:LEU:N	1.90	0.86
1:A:665:PRO:HG2	1:A:666:MET:CE	2.06	0.86
2:B:479:ILE:HD12	2:B:480:ALA:N	1.90	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:499:ARG:HH21	2:F:89:ARG:HH11	1.23	0.86
1:A:433:THR:HG22	1:A:435:VAL:N	1.91	0.85
1:I:400:LEU:HB3	1:I:449:ILE:HG12	1.58	0.85
2:L:145:MET:HE1	2:L:183:ASN:ND2	1.89	0.85
1:A:517:LEU:HD22	1:A:517:LEU:H	1.38	0.85
2:J:499:ARG:HH21	2:L:89:ARG:HH11	1.23	0.85
1:A:131:ILE:HG22	1:A:136:ALA:HB2	1.58	0.85
1:A:308:LEU:HD22	1:A:316:MET:SD	2.16	0.85
1:C:517:LEU:HD22	1:C:517:LEU:H	1.40	0.85
1:E:665:PRO:HG2	1:E:666:MET:CE	2.06	0.85
2:L:504:GLU:HG3	2:L:505:VAL:N	1.89	0.85
1:E:131:ILE:HG22	1:E:136:ALA:HB2	1.56	0.85
1:E:156:LEU:HD12	1:E:163:PHE:HB2	1.59	0.85
1:G:396:ILE:HG12	1:G:463:ILE:HD13	1.58	0.84
1:E:557:THR:HG23	1:E:572:ILE:O	1.77	0.84
1:C:309:ASP:OD1	1:C:312:THR:HG22	1.76	0.84
2:B:499:ARG:HG2	2:B:499:ARG:HH11	1.41	0.84
2:H:417:TYR:OH	2:H:535:ASP:HB2	1.76	0.84
1:K:517:LEU:H	1:K:517:LEU:HD22	1.40	0.84
1:A:309:ASP:OD1	1:A:312:THR:HG22	1.78	0.84
1:E:421:ARG:HB3	1:E:474:GLU:HB2	1.59	0.84
1:C:131:ILE:HG22	1:C:136:ALA:HB2	1.56	0.84
1:K:112:ILE:HG13	1:K:120:SER:HB2	1.59	0.84
1:A:528:ALA:O	1:A:532:MET:HG3	1.78	0.84
2:D:420:GLY:HA3	2:L:184:ILE:HD12	1.59	0.84
2:J:207:SER:HB3	2:J:208:PRO:HD3	1.59	0.84
2:B:420:GLY:HA3	2:J:184:ILE:HD12	1.59	0.83
1:C:583:PHE:CZ	1:C:590:MET:HE3	2.13	0.83
2:J:417:TYR:OH	2:J:535:ASP:HB2	1.76	0.83
1:K:457:PRO:HG2	1:K:458:THR:H	1.43	0.83
1:A:583:PHE:CZ	1:A:590:MET:HE3	2.14	0.83
2:J:91:THR:HA	2:J:98:GLN:HG3	1.60	0.83
1:E:596:TRP:CZ3	1:E:600:ASP:O	2.32	0.83
1:G:665:PRO:HG2	1:G:666:MET:CE	2.09	0.83
1:G:400:LEU:HB3	1:G:449:ILE:HG12	1.59	0.83
2:J:36:LEU:HD22	2:J:38:GLN:HG3	1.60	0.83
2:J:42:ARG:HG2	2:J:42:ARG:HH11	1.42	0.83
1:K:665:PRO:HG2	1:K:666:MET:CE	2.07	0.83
2:B:167:GLN:H	2:B:167:GLN:HE21	0.85	0.83
1:C:357:GLU:O	1:C:360:VAL:HG23	1.78	0.83
1:E:292:ILE:H	1:E:292:ILE:HD12	1.44	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:499:ARG:HG2	2:L:499:ARG:HH11	1.42	0.83
1:K:79:ILE:HG23	1:K:89:THR:HG21	1.60	0.83
1:G:670:ILE:HG13	1:G:718:LEU:HD21	1.61	0.82
2:J:325:ASP:HA	2:J:512:ARG:HH12	1.44	0.82
1:K:321:VAL:O	1:K:324:ALA:HB3	1.79	0.82
2:F:479:ILE:HD12	2:F:480:ALA:N	1.94	0.82
1:G:473:PHE:HB3	1:G:482:LEU:HD21	1.61	0.82
1:A:419:ARG:HH11	1:A:421:ARG:HB2	1.45	0.82
1:I:112:ILE:HG13	1:I:120:SER:HB2	1.62	0.82
1:G:112:ILE:HG13	1:G:120:SER:HB2	1.62	0.82
2:B:416:LEU:HG	2:J:210:MET:HE1	1.61	0.82
1:C:127:VAL:HG12	1:C:131:ILE:HD11	1.61	0.82
1:C:528:ALA:O	1:C:532:MET:HG3	1.79	0.82
1:K:198:LEU:HD13	1:K:256:ASP:O	1.79	0.82
1:C:294:ARG:HB2	1:C:504:ILE:HG12	1.63	0.81
1:C:321:VAL:O	1:C:324:ALA:HB3	1.80	0.81
1:C:718:LEU:N	1:C:718:LEU:HD23	1.95	0.81
1:G:321:VAL:O	1:G:324:ALA:HB3	1.81	0.81
1:I:357:GLU:O	1:I:360:VAL:HG23	1.81	0.81
1:I:517:LEU:HD22	1:I:517:LEU:H	1.45	0.81
1:K:473:PHE:HB3	1:K:482:LEU:HD21	1.61	0.81
1:E:127:VAL:HG12	1:E:131:ILE:HD11	1.61	0.81
2:F:145:MET:HE1	2:F:183:ASN:ND2	1.96	0.81
1:C:156:LEU:HD12	1:C:163:PHE:HB2	1.62	0.81
1:A:338:ILE:CD1	1:A:348:LEU:HB2	2.09	0.81
2:F:184:ILE:HD13	2:H:417:TYR:HA	1.61	0.81
1:G:123:VAL:O	1:G:127:VAL:HG23	1.80	0.81
1:A:321:VAL:O	1:A:324:ALA:HB3	1.81	0.81
1:K:596:TRP:CZ3	1:K:600:ASP:O	2.34	0.81
1:K:497:GLY:HA2	1:K:499:MET:HE3	1.62	0.81
2:D:88:HIS:HD2	2:D:90:CYS:H	1.27	0.81
2:D:151:ASN:HD21	2:F:522:LEU:HD23	1.45	0.80
1:E:321:VAL:O	1:E:324:ALA:HB3	1.79	0.80
1:E:516:ASN:HB2	1:E:564:GLN:NE2	1.97	0.80
1:K:338:ILE:CD1	1:K:348:LEU:HB2	2.08	0.80
1:E:294:ARG:HB2	1:E:504:ILE:HG12	1.64	0.80
1:G:614:LEU:HD22	1:G:627:ILE:CG2	2.10	0.80
1:C:557:THR:HG23	1:C:572:ILE:O	1.80	0.80
1:E:718:LEU:HD23	1:E:718:LEU:N	1.97	0.80
1:I:293:GLN:O	1:I:504:ILE:HG21	1.80	0.80
1:C:665:PRO:HG2	1:C:666:MET:CE	2.10	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:LEU:CD1	1:C:163:PHE:HB2	2.12	0.80
1:C:661:MET:HE2	1:C:726:GLU:HA	1.63	0.80
1:I:156:LEU:HD12	1:I:163:PHE:HB2	1.62	0.80
1:E:517:LEU:H	1:E:517:LEU:HD22	1.47	0.80
1:I:321:VAL:O	1:I:324:ALA:HB3	1.81	0.80
1:E:156:LEU:CD1	1:E:163:PHE:HB2	2.12	0.80
1:E:596:TRP:HZ3	1:E:600:ASP:O	1.63	0.79
1:I:661:MET:HE2	1:I:726:GLU:HA	1.63	0.79
1:K:419:ARG:HH11	1:K:421:ARG:HB2	1.47	0.79
1:K:480:HIS:CD2	1:K:482:LEU:HB2	2.18	0.79
1:A:357:GLU:O	1:A:360:VAL:HG23	1.80	0.79
2:D:499:ARG:HG2	2:D:499:ARG:HH11	1.48	0.79
1:A:452:LEU:O	1:A:466:MET:HE1	1.82	0.79
1:I:308:LEU:HD22	1:I:316:MET:SD	2.22	0.79
1:E:130:ALA:HA	1:E:133:ALA:HB3	1.63	0.79
1:I:94:SER:HB2	1:I:114:PRO:O	1.82	0.79
1:A:540:ARG:O	1:A:543:VAL:HG23	1.82	0.79
1:K:294:ARG:HB2	1:K:504:ILE:HG12	1.65	0.79
2:D:207:SER:HB3	2:D:208:PRO:HD3	1.65	0.79
1:K:421:ARG:HB3	1:K:474:GLU:HB2	1.64	0.79
1:I:123:VAL:O	1:I:127:VAL:HG23	1.81	0.79
1:I:198:LEU:HD13	1:I:256:ASP:O	1.82	0.79
1:K:557:THR:HG23	1:K:572:ILE:O	1.83	0.79
1:A:497:GLY:HA2	1:A:499:MET:HE3	1.63	0.79
1:E:596:TRP:CZ3	1:E:600:ASP:HB2	2.17	0.79
1:I:419:ARG:HH11	1:I:421:ARG:HB2	1.47	0.78
1:I:421:ARG:HB3	1:I:474:GLU:HB2	1.63	0.78
1:K:614:LEU:HD22	1:K:627:ILE:CG2	2.13	0.78
1:C:115:PRO:CG	1:C:116:PRO:HD3	2.11	0.78
2:D:479:ILE:HD12	2:D:480:ALA:N	1.97	0.78
2:L:251:THR:HG21	2:L:260:ALA:HB2	1.64	0.78
1:A:396:ILE:HG12	1:A:463:ILE:HD13	1.66	0.78
2:B:409:ILE:HD13	2:J:205:VAL:HB	1.64	0.78
2:H:88:HIS:HD2	2:H:90:CYS:H	1.32	0.78
2:J:504:GLU:HG3	2:J:505:VAL:N	1.97	0.78
1:E:400:LEU:HB3	1:E:449:ILE:HG12	1.65	0.78
1:G:163:PHE:O	1:G:163:PHE:HD1	1.67	0.78
2:L:36:LEU:HD22	2:L:38:GLN:HG3	1.64	0.78
1:A:419:ARG:NH1	1:A:421:ARG:HB2	1.96	0.78
2:F:460:VAL:HG21	2:F:496:ALA:HB2	1.65	0.78
1:G:517:LEU:H	1:G:517:LEU:HD22	1.46	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:433:THR:HG22	1:I:435:VAL:N	1.95	0.78
2:F:337:ALA:HB3	2:F:373:LYS:HD2	1.65	0.78
1:K:123:VAL:O	1:K:127:VAL:HG23	1.84	0.78
1:A:433:THR:CG2	1:A:435:VAL:HG12	2.13	0.78
1:A:557:THR:HG23	1:A:572:ILE:O	1.82	0.78
1:A:614:LEU:HD22	1:A:627:ILE:CG2	2.13	0.78
1:C:400:LEU:HB3	1:C:449:ILE:HG12	1.66	0.78
1:E:433:THR:CG2	1:E:435:VAL:HG12	2.13	0.78
1:C:516:ASN:HB2	1:C:564:GLN:NE2	1.99	0.78
1:E:419:ARG:NH1	1:E:421:ARG:HB2	1.98	0.78
2:F:210:MET:HE2	2:H:417:TYR:HB2	1.63	0.78
2:B:88:HIS:CD2	2:B:90:CYS:H	2.00	0.78
1:E:653:LYS:HD3	1:E:653:LYS:N	1.98	0.78
1:G:419:ARG:HH11	1:G:421:ARG:HB2	1.48	0.78
1:K:357:GLU:O	1:K:360:VAL:HG23	1.84	0.78
1:K:433:THR:HG23	1:K:449:ILE:O	1.83	0.78
2:L:417:TYR:OH	2:L:535:ASP:HB2	1.83	0.78
2:D:89:ARG:HH11	2:F:499:ARG:HH21	1.31	0.77
1:I:457:PRO:HG2	1:I:458:THR:H	1.49	0.77
1:A:400:LEU:HB3	1:A:449:ILE:HG12	1.65	0.77
2:B:83:ASP:HB2	2:B:140:LYS:HE3	1.65	0.77
2:B:460:VAL:HG21	2:B:496:ALA:HB2	1.66	0.77
1:A:390:LYS:HD3	1:A:391:LEU:N	1.98	0.77
2:D:36:LEU:HD22	2:D:38:GLN:HG3	1.65	0.77
1:E:77:ARG:NH1	1:E:370:VAL:HG21	2.00	0.77
1:E:309:ASP:OD1	1:E:312:THR:HG22	1.83	0.77
1:I:557:THR:HG23	1:I:572:ILE:O	1.83	0.77
1:I:596:TRP:CZ3	1:I:600:ASP:O	2.37	0.77
2:D:145:MET:HE1	2:D:183:ASN:HD21	1.48	0.77
1:E:390:LYS:HD3	1:E:391:LEU:N	2.00	0.77
2:D:83:ASP:HB2	2:D:140:LYS:HE3	1.66	0.77
2:J:339:ASN:HD21	2:J:370:SER:HB3	1.49	0.77
1:C:130:ALA:HA	1:C:133:ALA:HB3	1.67	0.77
2:D:88:HIS:CD2	2:D:90:CYS:H	2.02	0.77
1:G:293:GLN:O	1:G:504:ILE:HG21	1.85	0.77
2:J:88:HIS:HD2	2:J:90:CYS:H	1.32	0.77
1:C:264:VAL:HG13	1:C:340:ASP:HB3	1.67	0.77
2:F:189:VAL:HG23	2:H:532:LYS:HE2	1.67	0.77
1:G:94:SER:HB2	1:G:114:PRO:O	1.85	0.77
1:I:653:LYS:HD3	1:I:653:LYS:N	2.00	0.77
1:E:115:PRO:CG	1:E:116:PRO:HD3	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:433:THR:CG2	1:C:435:VAL:HG12	2.15	0.76
2:D:184:ILE:HD13	2:L:417:TYR:HA	1.67	0.76
1:I:617:GLY:O	1:I:625:PHE:HB3	1.84	0.76
1:K:334:THR:HG21	1:K:355:GLN:NE2	2.01	0.76
1:A:163:PHE:HD1	1:A:163:PHE:O	1.67	0.76
1:G:583:PHE:CZ	1:G:590:MET:HE3	2.20	0.76
1:I:156:LEU:CD1	1:I:163:PHE:HB2	2.15	0.76
1:G:334:THR:HG21	1:G:355:GLN:NE2	1.99	0.76
1:G:433:THR:CG2	1:G:435:VAL:HG12	2.16	0.76
1:I:264:VAL:HG13	1:I:340:ASP:HB3	1.65	0.76
1:K:397:GLU:HG3	1:K:453:CYS:SG	2.25	0.76
1:E:163:PHE:O	1:E:163:PHE:HD1	1.69	0.76
1:G:308:LEU:HD22	1:G:316:MET:SD	2.25	0.76
1:I:665:PRO:HG2	1:I:666:MET:CE	2.12	0.76
2:D:492:ASN:HD22	2:D:494:PHE:H	1.34	0.76
1:K:419:ARG:NH1	1:K:421:ARG:HB2	2.01	0.76
1:K:433:THR:HG22	1:K:435:VAL:N	1.98	0.76
1:A:130:ALA:HA	1:A:133:ALA:HB3	1.68	0.76
1:A:467:ARG:HB3	1:A:467:ARG:HH11	1.51	0.76
1:I:130:ALA:HA	1:I:133:ALA:HB3	1.66	0.76
2:J:189:VAL:HA	2:J:282:ASN:ND2	2.00	0.76
1:E:94:SER:HB2	1:E:114:PRO:O	1.86	0.75
1:E:661:MET:HE2	1:E:726:GLU:HA	1.66	0.75
1:G:198:LEU:HD13	1:G:256:ASP:O	1.85	0.75
1:I:491:HIS:O	1:I:495:ILE:HG13	1.85	0.75
1:E:123:VAL:O	1:E:127:VAL:HG23	1.87	0.75
1:E:357:GLU:O	1:E:360:VAL:HG23	1.87	0.75
1:C:101:LEU:O	1:C:105:MET:HG3	1.87	0.75
1:G:130:ALA:HA	1:G:133:ALA:HB3	1.68	0.75
2:D:504:GLU:HG3	2:D:505:VAL:N	2.02	0.75
1:I:163:PHE:HD1	1:I:163:PHE:O	1.69	0.75
1:K:658:THR:HB	1:K:703:LYS:HD3	1.69	0.75
1:C:614:LEU:HD22	1:C:627:ILE:CG2	2.16	0.75
1:C:670:ILE:HG13	1:C:718:LEU:HD21	1.68	0.75
1:K:456:ALA:HB1	1:K:457:PRO:CD	2.16	0.75
1:A:294:ARG:HB2	1:A:504:ILE:HG12	1.69	0.75
1:C:596:TRP:CZ3	1:C:600:ASP:O	2.40	0.75
1:G:653:LYS:HD3	1:G:653:LYS:N	2.02	0.75
2:B:184:ILE:HD12	2:J:420:GLY:HA3	1.69	0.75
1:G:101:LEU:O	1:G:105:MET:HG3	1.87	0.75
1:G:398:ASN:HB3	1:G:485:LEU:HD13	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:614:LEU:HD22	1:G:627:ILE:HG23	1.67	0.75
2:H:288:VAL:HG13	2:H:350:ARG:HG3	1.67	0.75
2:J:492:ASN:HD22	2:J:494:PHE:H	1.33	0.75
1:A:128:MET:HA	1:A:131:ILE:HD12	1.69	0.74
2:B:522:LEU:HD23	2:F:151:ASN:HD21	1.52	0.74
1:I:66:ILE:HB	1:I:138:ALA:O	1.86	0.74
2:J:348:GLU:OE1	1:K:550:ASN:HB2	1.86	0.74
1:G:334:THR:HG21	1:G:355:GLN:HE21	1.49	0.74
1:A:115:PRO:CG	1:A:116:PRO:HD3	2.17	0.74
1:C:123:VAL:O	1:C:127:VAL:HG23	1.86	0.74
1:C:127:VAL:O	1:C:131:ILE:HG13	1.87	0.74
1:E:334:THR:HG21	1:E:355:GLN:NE2	2.02	0.74
1:I:596:TRP:HZ3	1:I:600:ASP:O	1.71	0.74
2:D:417:TYR:HA	2:L:184:ILE:HD13	1.70	0.74
2:H:251:THR:HG21	2:H:260:ALA:HB2	1.69	0.74
1:G:516:ASN:HB2	1:G:564:GLN:NE2	2.03	0.74
2:J:251:THR:HG21	2:J:260:ALA:HB2	1.70	0.74
1:K:234:ASN:ND2	1:K:236:GLN:HB2	2.03	0.74
1:K:401:TYR:HE2	1:K:448:MET:HB2	1.51	0.74
2:B:288:VAL:HG13	2:B:350:ARG:HG3	1.70	0.74
1:C:94:SER:HB2	1:C:114:PRO:O	1.88	0.74
2:D:173:LEU:HD21	2:L:436:GLY:HA2	1.68	0.74
1:I:528:ALA:HB1	1:I:605:LEU:HD22	1.69	0.74
1:A:661:MET:HE2	1:A:726:GLU:HA	1.68	0.74
1:C:66:ILE:HD12	1:C:87:ILE:CG2	2.18	0.74
1:E:583:PHE:CZ	1:E:590:MET:HE3	2.23	0.74
1:G:294:ARG:HB2	1:G:504:ILE:HG12	1.69	0.74
1:I:338:ILE:CD1	1:I:348:LEU:HB2	2.12	0.74
2:J:445:LYS:HE2	2:J:452:ASN:OD1	1.88	0.74
1:E:337:PHE:C	1:E:338:ILE:HD12	2.13	0.73
1:G:421:ARG:HB3	1:G:474:GLU:HB2	1.70	0.73
1:A:428(L):ALA:HB3	1:A:455:TRP:HD1	1.53	0.73
1:E:115:PRO:HB2	1:E:444:TYR:CD2	2.24	0.73
2:F:296:ASP:O	2:F:298:ILE:HD12	1.88	0.73
2:F:504:GLU:HG3	2:F:505:VAL:N	2.03	0.73
1:I:419:ARG:NH1	1:I:421:ARG:HB2	2.04	0.73
1:I:516:ASN:HB2	1:I:564:GLN:NE2	2.03	0.73
1:K:94:SER:HB2	1:K:114:PRO:O	1.87	0.73
1:K:334:THR:HG21	1:K:355:GLN:HE21	1.54	0.73
2:L:88:HIS:HD2	2:L:90:CYS:H	1.34	0.73
1:A:653:LYS:HD3	1:A:653:LYS:N	2.01	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:PRO:HB2	1:C:444:TYR:CD2	2.23	0.73
1:C:163:PHE:O	1:C:163:PHE:HD1	1.71	0.73
1:C:433:THR:HG22	1:C:435:VAL:N	1.99	0.73
1:C:658:THR:HB	1:C:703:LYS:HD3	1.71	0.73
2:F:83:ASP:HB3	2:F:86:VAL:CG2	2.18	0.73
1:A:115:PRO:HB2	1:A:444:TYR:CD2	2.23	0.73
1:A:264:VAL:HG13	1:A:340:ASP:HB3	1.71	0.73
2:D:75:ASP:OD1	2:D:272:ARG:NH2	2.20	0.73
1:E:189:VAL:HG21	1:E:323:LEU:HB2	1.69	0.73
1:E:433:THR:HG22	1:E:435:VAL:N	1.97	0.73
1:G:452:LEU:O	1:G:466:MET:HE1	1.88	0.73
1:A:473:PHE:HB3	1:A:482:LEU:HD21	1.68	0.73
1:I:614:LEU:HD22	1:I:627:ILE:HG23	1.70	0.73
1:C:419:ARG:HH11	1:C:421:ARG:HB2	1.54	0.73
2:F:65:THR:HG23	2:F:68:GLU:OE1	1.89	0.73
1:I:497:GLY:HA2	1:I:499:MET:HE3	1.69	0.73
2:L:58:GLN:OE1	2:L:63:LYS:HE3	1.89	0.73
2:L:460:VAL:HG21	2:L:496:ALA:HB2	1.71	0.73
1:A:614:LEU:HD22	1:A:627:ILE:HG23	1.71	0.73
1:C:159:GLU:HB2	1:C:161:VAL:HG23	1.71	0.73
1:C:110:VAL:HG21	1:C:130:ALA:HB1	1.71	0.72
1:E:419:ARG:HH11	1:E:421:ARG:HB2	1.52	0.72
2:F:36:LEU:HD22	2:F:38:GLN:HG3	1.71	0.72
2:F:379:ARG:NH2	2:H:535:ASP:OD2	2.22	0.72
1:G:74:ILE:HD13	1:G:143:TYR:CE2	2.23	0.72
1:I:159:GLU:HB2	1:I:161:VAL:HG23	1.71	0.72
2:H:36:LEU:HD22	2:H:38:GLN:HG3	1.70	0.72
1:K:122:ILE:HA	1:K:146:LEU:HD11	1.70	0.72
1:K:127:VAL:HG12	1:K:131:ILE:HD11	1.69	0.72
1:K:163:PHE:O	1:K:163:PHE:HD1	1.71	0.72
1:K:415:GLY:O	1:K:440:GLU:HG3	1.88	0.72
1:K:417:LEU:HD21	1:K:478:ILE:HD13	1.70	0.72
1:G:283:ILE:HD12	1:G:389:VAL:HG21	1.69	0.72
1:G:550:ASN:HB2	2:L:348:GLU:OE1	1.88	0.72
2:H:65:THR:HG23	2:H:68:GLU:OE1	1.89	0.72
2:H:504:GLU:HG3	2:H:505:VAL:N	2.03	0.72
1:I:276:CYS:HA	1:I:282:GLY:HA2	1.72	0.72
2:F:288:VAL:HG13	2:F:350:ARG:HG3	1.72	0.72
1:A:718:LEU:N	1:A:718:LEU:HD23	2.04	0.72
1:C:653:LYS:HD3	1:C:653:LYS:N	2.03	0.72
1:G:480:HIS:CD2	1:G:482:LEU:HB2	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:596:TRP:HZ3	1:K:600:ASP:O	1.71	0.72
1:E:473:PHE:HB3	1:E:482:LEU:HD21	1.70	0.72
1:G:456:ALA:HB1	1:G:457:PRO:CD	2.19	0.72
1:I:115:PRO:CG	1:I:116:PRO:HD3	2.16	0.72
1:K:66:ILE:H	1:K:66:ILE:HD13	1.52	0.72
1:E:419:ARG:CD	1:E:601:GLN:OE1	2.38	0.72
2:F:417:TYR:HA	2:H:184:ILE:HD13	1.70	0.72
2:J:83:ASP:HB2	2:J:140:LYS:HE3	1.70	0.72
1:A:596:TRP:CZ3	1:A:600:ASP:HB2	2.24	0.72
1:C:523:ARG:C	1:C:590:MET:HE1	2.15	0.72
2:D:417:TYR:OH	2:D:535:ASP:HB2	1.89	0.72
2:F:532:LYS:HE2	2:H:189:VAL:HG23	1.72	0.72
1:G:338:ILE:CD1	1:G:348:LEU:HB2	2.17	0.72
1:C:419:ARG:NH1	1:C:421:ARG:HB2	2.04	0.72
1:C:522:LEU:HD22	1:C:563:LEU:HD13	1.71	0.72
1:G:66:ILE:HD12	1:G:87:ILE:CG2	2.20	0.72
1:I:658:THR:HB	1:I:703:LYS:HD3	1.71	0.72
1:K:661:MET:HE2	1:K:726:GLU:HA	1.72	0.72
1:A:112:ILE:HG13	1:A:120:SER:HB2	1.72	0.71
1:A:457:PRO:HG2	1:A:458:THR:H	1.54	0.71
2:B:462:VAL:CG2	2:J:169:GLY:HA2	2.19	0.71
2:B:504:GLU:HG3	2:B:505:VAL:N	2.03	0.71
1:E:66:ILE:HD13	1:E:66:ILE:H	1.55	0.71
1:E:112:ILE:HG13	1:E:120:SER:HB2	1.71	0.71
1:G:419:ARG:NH1	1:G:421:ARG:HB2	2.05	0.71
1:I:101:LEU:O	1:I:105:MET:HG3	1.89	0.71
1:I:718:LEU:N	1:I:718:LEU:HD23	2.05	0.71
1:G:666:MET:HE3	1:G:690:ILE:HD12	1.71	0.71
1:K:452:LEU:O	1:K:466:MET:HE1	1.89	0.71
1:C:596:TRP:HZ3	1:C:600:ASP:O	1.73	0.71
1:G:156:LEU:CD1	1:G:163:PHE:HB2	2.20	0.71
1:G:156:LEU:HD12	1:G:163:PHE:HB2	1.72	0.71
1:K:400:LEU:HB3	1:K:449:ILE:HG12	1.71	0.71
2:F:492:ASN:HD22	2:F:494:PHE:H	1.36	0.71
1:E:338:ILE:CD1	1:E:348:LEU:HB2	2.15	0.71
1:I:452:LEU:O	1:I:466:MET:HE1	1.90	0.71
2:J:123:SER:HA	2:J:158:ILE:HB	1.73	0.71
1:A:117:ALA:C	1:A:119:GLN:H	1.96	0.71
1:I:219:LYS:HE2	1:I:229:MET:N	2.06	0.71
1:I:334:THR:HG21	1:I:355:GLN:NE2	2.05	0.71
1:K:293:GLN:O	1:K:504:ILE:HG21	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:550:ASN:HB2	2:F:348:GLU:OE1	1.90	0.71
1:K:115:PRO:HB2	1:K:444:TYR:CD2	2.25	0.71
1:A:179:THR:HG22	1:A:183:ILE:HD11	1.73	0.71
1:C:646:LEU:HD12	2:D:72:LEU:HD21	1.73	0.71
1:I:329:TYR:HE2	1:I:352:THR:HG22	1.56	0.71
1:K:66:ILE:HB	1:K:138:ALA:O	1.90	0.71
1:K:292:ILE:H	1:K:292:ILE:CD1	2.00	0.71
1:A:127:VAL:O	1:A:131:ILE:HG13	1.91	0.71
1:E:85:MET:O	1:E:87:ILE:HG13	1.91	0.71
1:E:456:ALA:HB1	1:E:457:PRO:CD	2.20	0.71
1:E:596:TRP:CE3	1:E:600:ASP:HB2	2.25	0.71
1:E:658:THR:HB	1:E:703:LYS:HD3	1.71	0.71
1:K:433:THR:CG2	1:K:435:VAL:HG12	2.20	0.71
1:C:112:ILE:HG13	1:C:120:SER:HB2	1.72	0.70
1:C:480:HIS:CD2	1:C:482:LEU:HB2	2.26	0.70
2:F:462:VAL:CG2	2:H:169:GLY:HA2	2.21	0.70
1:I:294:ARG:HB2	1:I:504:ILE:HG12	1.72	0.70
1:C:117:ALA:C	1:C:119:GLN:H	1.98	0.70
1:C:293:GLN:O	1:C:504:ILE:HG21	1.90	0.70
1:C:396:ILE:HG12	1:C:463:ILE:HD13	1.71	0.70
1:C:467:ARG:HH11	1:C:467:ARG:HB3	1.56	0.70
2:F:156:ILE:N	2:F:156:ILE:HD12	2.06	0.70
1:I:695:MET:SD	2:J:313:PRO:HG3	2.31	0.70
2:J:88:HIS:CD2	2:J:90:CYS:H	2.08	0.70
2:D:288:VAL:HG13	2:D:350:ARG:HG3	1.72	0.70
2:F:83:ASP:HB3	2:F:86:VAL:HG21	1.71	0.70
1:I:83:ARG:HG2	1:I:83:ARG:HH11	1.55	0.70
2:F:499:ARG:HG2	2:F:499:ARG:NH1	2.02	0.70
2:D:189:VAL:HG23	2:L:532:LYS:HE2	1.73	0.70
2:J:42:ARG:HG2	2:J:42:ARG:NH1	2.05	0.70
2:B:210:MET:HE2	2:J:417:TYR:HB2	1.71	0.70
1:C:337:PHE:C	1:C:338:ILE:HD12	2.16	0.70
1:G:329:TYR:HE2	1:G:352:THR:HG22	1.56	0.70
1:G:718:LEU:N	1:G:718:LEU:HD23	2.06	0.70
2:H:348:GLU:OE1	1:I:550:ASN:HB2	1.91	0.70
1:K:614:LEU:HD22	1:K:627:ILE:HG23	1.73	0.70
1:A:596:TRP:CZ3	1:A:600:ASP:O	2.45	0.70
1:C:456:ALA:HB1	1:C:457:PRO:CD	2.20	0.70
1:C:596:TRP:CZ3	1:C:600:ASP:HB2	2.27	0.70
2:D:460:VAL:HG21	2:D:496:ALA:HB2	1.72	0.70
1:K:130:ALA:HA	1:K:133:ALA:HB3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:219:LYS:HE2	1:K:229:MET:N	2.05	0.70
2:D:532:LYS:HE2	2:L:189:VAL:CG2	2.22	0.70
1:E:523:ARG:C	1:E:590:MET:HE1	2.17	0.70
2:F:417:TYR:OH	2:F:535:ASP:HB2	1.91	0.70
1:G:464:GLU:O	1:G:468:ILE:HG13	1.92	0.70
1:G:661:MET:HE2	1:G:726:GLU:HA	1.72	0.70
1:I:396:ILE:HG12	1:I:463:ILE:HD13	1.73	0.70
1:C:85:MET:O	1:C:87:ILE:HG13	1.92	0.70
1:K:543:VAL:HG11	2:L:117:ARG:HD2	1.74	0.70
1:E:110:VAL:HG21	1:E:130:ALA:HB1	1.72	0.70
1:G:234:ASN:ND2	1:G:236:GLN:HB2	2.07	0.70
1:I:329:TYR:CE2	1:I:352:THR:HG22	2.26	0.70
1:K:204:GLU:O	1:K:208:ILE:HG13	1.92	0.70
2:B:348:GLU:OE1	1:E:550:ASN:HB2	1.91	0.69
1:G:523:ARG:HB3	1:G:590:MET:HE1	1.72	0.69
1:K:670:ILE:HG13	1:K:718:LEU:HD21	1.73	0.69
1:A:123:VAL:O	1:A:127:VAL:HG23	1.92	0.69
1:K:218:ILE:HD12	1:K:260:ILE:HG12	1.73	0.69
2:D:379:ARG:NH2	2:L:535:ASP:OD2	2.25	0.69
1:E:639:ARG:HB3	1:E:643:GLN:HB3	1.74	0.69
1:G:617:GLY:O	1:G:625:PHE:HB3	1.93	0.69
1:I:583:PHE:CZ	1:I:590:MET:HE3	2.27	0.69
1:A:658:THR:HB	1:A:703:LYS:HD3	1.74	0.69
1:E:66:ILE:HB	1:E:138:ALA:O	1.92	0.69
1:E:117:ALA:C	1:E:119:GLN:H	2.00	0.69
1:G:66:ILE:HD13	1:G:66:ILE:H	1.58	0.69
1:A:630:ARG:C	1:A:632:ALA:H	2.01	0.69
2:D:210:MET:HE2	2:L:417:TYR:HB2	1.73	0.69
2:H:499:ARG:HG2	2:H:499:ARG:NH1	2.06	0.69
1:I:534:ARG:HG3	1:I:534:ARG:HH11	1.56	0.69
2:L:65:THR:HG23	2:L:68:GLU:OE1	1.91	0.69
2:B:89:ARG:HH11	2:D:499:ARG:HH21	1.40	0.69
1:E:396:ILE:HG22	1:E:466:MET:HE3	1.75	0.69
1:E:467:ARG:HB3	1:E:467:ARG:HH11	1.58	0.69
1:I:614:LEU:HD22	1:I:627:ILE:CG2	2.21	0.69
1:A:334:THR:HG21	1:A:355:GLN:NE2	2.08	0.69
1:A:550:ASN:HB2	2:D:348:GLU:OE1	1.93	0.69
2:D:49:GLY:C	2:D:51:GLY:H	2.00	0.69
1:E:159:GLU:HB2	1:E:161:VAL:HG23	1.73	0.69
1:E:614:LEU:HD22	1:E:627:ILE:CG2	2.21	0.69
1:G:159:GLU:HB2	1:G:161:VAL:HG23	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:219:LYS:HE2	1:G:229:MET:N	2.06	0.69
1:G:433:THR:HG22	1:G:435:VAL:N	2.03	0.69
1:K:695:MET:SD	2:L:313:PRO:HG3	2.33	0.69
1:A:66:ILE:HD13	1:A:66:ILE:H	1.57	0.69
1:A:516:ASN:HB2	1:A:564:GLN:NE2	2.07	0.69
2:B:417:TYR:OH	2:B:535:ASP:HB2	1.93	0.69
1:C:122:ILE:HA	1:C:146:LEU:HD11	1.74	0.69
1:E:128:MET:HA	1:E:131:ILE:HD12	1.74	0.69
2:F:445:LYS:HE2	2:F:452:ASN:OD1	1.92	0.69
1:G:74:ILE:HD13	1:G:143:TYR:HE2	1.57	0.69
1:G:596:TRP:CZ3	1:G:600:ASP:O	2.46	0.69
2:L:42:ARG:HG2	2:L:42:ARG:HH11	1.57	0.69
2:B:499:ARG:HH21	2:F:89:ARG:NH1	1.90	0.69
1:C:179:THR:HG22	1:C:183:ILE:HD11	1.73	0.69
1:E:117:ALA:HB1	1:E:121:TYR:HB2	1.75	0.69
1:G:658:THR:HB	1:G:703:LYS:HD3	1.75	0.69
1:A:74:ILE:HD13	1:A:143:TYR:CE2	2.27	0.69
2:B:184:ILE:HD13	2:J:417:TYR:HA	1.74	0.69
1:C:338:ILE:CD1	1:C:348:LEU:HB2	2.13	0.69
1:C:538:ILE:O	1:C:541:THR:HB	1.93	0.69
1:K:201:ASP:OD1	1:K:203:ASP:HB2	1.92	0.69
2:L:83:ASP:HB2	2:L:140:LYS:HE3	1.74	0.69
2:L:189:VAL:HA	2:L:282:ASN:ND2	2.08	0.69
2:L:445:LYS:HE2	2:L:452:ASN:OD1	1.93	0.69
1:A:334:THR:HG21	1:A:355:GLN:HE21	1.58	0.68
1:A:670:ILE:CG1	1:A:718:LEU:HD21	2.23	0.68
1:E:101:LEU:O	1:E:105:MET:HG3	1.93	0.68
1:I:337:PHE:C	1:I:338:ILE:HD12	2.19	0.68
2:L:149:MET:SD	2:L:186:ALA:HB2	2.32	0.68
1:A:110:VAL:HG21	1:A:130:ALA:HB1	1.73	0.68
1:A:156:LEU:CD1	1:A:163:PHE:HB2	2.22	0.68
2:B:50:GLY:O	2:B:54:ARG:HD2	1.94	0.68
1:I:74:ILE:O	1:I:77:ARG:HB3	1.93	0.68
1:K:115:PRO:CG	1:K:116:PRO:HD3	2.21	0.68
1:E:396:ILE:HG12	1:E:463:ILE:HD13	1.73	0.68
1:G:357:GLU:O	1:G:360:VAL:HG23	1.94	0.68
1:A:159:GLU:HB2	1:A:161:VAL:HG23	1.75	0.68
1:A:417:LEU:HD21	1:A:478:ILE:HD13	1.74	0.68
2:B:445:LYS:HE2	2:B:452:ASN:OD1	1.93	0.68
1:C:66:ILE:H	1:C:66:ILE:HD13	1.58	0.68
1:I:117:ALA:HB1	1:I:121:TYR:HB2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:235:ASP:O	1:K:239:ARG:HG2	1.93	0.68
2:H:329:PHE:CE1	2:H:343:GLY:HA3	2.28	0.68
1:I:129:ALA:O	1:I:133:ALA:HB2	1.93	0.68
1:I:456:ALA:HB1	1:I:457:PRO:CD	2.23	0.68
1:A:122:ILE:HA	1:A:146:LEU:HD11	1.74	0.68
1:A:140:HIS:CE1	1:A:142:GLY:H	2.12	0.68
2:B:65:THR:HG23	2:B:68:GLU:OE1	1.93	0.68
1:E:186:GLU:C	1:E:188:ASN:H	2.02	0.68
2:H:445:LYS:HE2	2:H:452:ASN:OD1	1.94	0.68
1:I:630:ARG:C	1:I:632:ALA:H	2.00	0.68
2:J:339:ASN:ND2	2:J:370:SER:HB3	2.08	0.68
1:K:159:GLU:HB2	1:K:161:VAL:HG23	1.76	0.68
2:D:65:THR:HG23	2:D:68:GLU:OE1	1.94	0.68
2:D:416:LEU:HG	2:L:210:MET:HE1	1.75	0.68
1:I:433:THR:CG2	1:I:435:VAL:HG12	2.24	0.68
1:I:538:ILE:O	1:I:541:THR:HB	1.93	0.68
1:K:179:THR:HG22	1:K:183:ILE:HD11	1.76	0.68
2:B:368:ILE:HG13	2:B:408:VAL:HG13	1.76	0.68
1:E:312:THR:O	1:E:316:MET:HG3	1.93	0.68
2:F:189:VAL:HA	2:F:282:ASN:ND2	2.08	0.68
1:I:596:TRP:CZ3	1:I:600:ASP:HB2	2.29	0.68
2:D:42:ARG:HG2	2:D:42:ARG:HH11	1.58	0.67
2:D:476(C):ASP:O	2:D:477:GLU:N	2.27	0.67
1:G:112:ILE:HD12	1:G:120:SER:O	1.93	0.67
1:I:464:GLU:O	1:I:468:ILE:HG13	1.95	0.67
1:A:77:ARG:NH1	1:A:370:VAL:HG21	2.09	0.67
1:E:397:GLU:HG3	1:E:453:CYS:SG	2.34	0.67
1:G:329:TYR:CE2	1:G:352:THR:HG22	2.30	0.67
2:J:499:ARG:HG2	2:J:499:ARG:NH1	2.06	0.67
1:K:140:HIS:CE1	1:K:142:GLY:H	2.12	0.67
1:K:276:CYS:HA	1:K:282:GLY:HA2	1.76	0.67
1:K:718:LEU:N	1:K:718:LEU:HD23	2.08	0.67
2:L:65:THR:OG1	2:L:68:GLU:HG3	1.93	0.67
1:A:480:HIS:CD2	1:A:482:LEU:HB2	2.30	0.67
2:B:83:ASP:HB3	2:B:86:VAL:CG2	2.24	0.67
1:C:186:GLU:C	1:C:188:ASN:H	2.02	0.67
2:F:532:LYS:HE2	2:H:189:VAL:CG2	2.25	0.67
1:G:115:PRO:CG	1:G:116:PRO:HD3	2.21	0.67
1:I:66:ILE:HD13	1:I:66:ILE:H	1.59	0.67
1:I:670:ILE:CG1	1:I:718:LEU:HD21	2.22	0.67
1:K:156:LEU:CD1	1:K:163:PHE:HB2	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:THR:HG21	2:L:91:THR:HG21	1.76	0.67
1:G:264:VAL:HG13	1:G:340:ASP:CB	2.23	0.67
1:G:528:ALA:HB1	1:G:605:LEU:HD22	1.75	0.67
2:J:167:GLN:HE21	2:J:167:GLN:H	0.79	0.67
1:A:642:ARG:HH11	2:B:71:ASP:HB3	1.60	0.67
2:F:58:GLN:CD	2:F:63:LYS:HE3	2.20	0.67
2:F:476(C):ASP:O	2:F:477:GLU:N	2.26	0.67
1:I:122:ILE:HA	1:I:146:LEU:HD11	1.76	0.67
2:J:58:GLN:OE1	2:J:63:LYS:HE3	1.94	0.67
1:A:66:ILE:HB	1:A:138:ALA:O	1.95	0.67
1:E:464:GLU:O	1:E:468:ILE:HG13	1.94	0.67
1:I:334:THR:HG21	1:I:355:GLN:HE21	1.57	0.67
1:K:117:ALA:C	1:K:119:GLN:H	1.99	0.67
2:B:83:ASP:HB3	2:B:86:VAL:HG21	1.76	0.67
1:E:630:ARG:C	1:E:632:ALA:H	2.00	0.67
1:I:204:GLU:O	1:I:208:ILE:HG13	1.95	0.67
1:A:329:TYR:HE2	1:A:352:THR:HG22	1.59	0.67
1:C:276:CYS:HA	1:C:282:GLY:HA2	1.75	0.67
2:D:169:GLY:HA2	2:L:462:VAL:CG2	2.24	0.67
2:D:329:PHE:CE1	2:D:343:GLY:HA3	2.30	0.67
2:F:210:MET:HE1	2:H:416:LEU:HG	1.76	0.67
1:G:117:ALA:HB1	1:G:121:TYR:HB2	1.76	0.67
2:L:423:THR:O	2:L:525:LYS:HE2	1.95	0.67
1:A:83:ARG:HG2	1:A:83:ARG:HH11	1.59	0.67
1:A:337:PHE:C	1:A:338:ILE:HD12	2.19	0.67
1:G:64:ASN:O	1:G:66:ILE:HG23	1.93	0.67
2:J:121:VAL:HG22	2:J:122:PHE:N	2.09	0.67
1:I:235:ASP:O	1:I:239:ARG:HG2	1.95	0.67
2:J:43:ARG:HH11	2:J:43:ARG:HG2	1.60	0.67
1:K:101:LEU:O	1:K:105:MET:HG3	1.95	0.67
1:K:396:ILE:HG12	1:K:463:ILE:HD13	1.76	0.67
1:K:401:TYR:CE2	1:K:448:MET:HB2	2.30	0.67
1:A:101:LEU:O	1:A:105:MET:HG3	1.94	0.66
2:H:492:ASN:HD22	2:H:494:PHE:H	1.41	0.66
1:I:92:ILE:HB	1:I:112:ILE:HG21	1.77	0.66
1:K:189:VAL:HG21	1:K:323:LEU:HB2	1.76	0.66
1:A:64:ASN:O	1:A:66:ILE:HG23	1.95	0.66
1:A:397:GLU:HG3	1:A:453:CYS:SG	2.35	0.66
1:C:443:MET:HG3	1:C:444:TYR:CD1	2.30	0.66
2:D:462:VAL:CG2	2:L:169:GLY:HA2	2.26	0.66
2:H:368:ILE:HG13	2:H:408:VAL:HG13	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:141:ILE:O	2:L:145:MET:HG3	1.96	0.66
1:C:329:TYR:HE2	1:C:352:THR:HG22	1.59	0.66
1:E:64:ASN:O	1:E:66:ILE:HG23	1.95	0.66
2:H:150:GLN:HG2	2:L:527:VAL:HG22	1.77	0.66
2:H:151:ASN:HD21	2:L:522:LEU:HD23	1.61	0.66
1:K:516:ASN:HB2	1:K:564:GLN:NE2	2.10	0.66
2:L:499:ARG:HG2	2:L:499:ARG:NH1	2.11	0.66
1:I:397:GLU:HG3	1:I:453:CYS:SG	2.35	0.66
1:C:358:HIS:ND1	1:C:359:PRO:HD3	2.11	0.66
2:D:291:PHE:CE1	2:D:348:GLU:HA	2.30	0.66
1:E:122:ILE:HA	1:E:146:LEU:HD11	1.78	0.66
1:G:110:VAL:HG21	1:G:130:ALA:HB1	1.77	0.66
2:J:368:ILE:HG13	2:J:408:VAL:HG13	1.77	0.66
1:A:156:LEU:HD12	1:A:163:PHE:HB2	1.76	0.66
1:G:232:ALA:HA	1:G:237:GLU:HG2	1.76	0.66
2:H:324:ALA:HA	2:H:345:ILE:HD12	1.78	0.66
1:C:140:HIS:CE1	1:C:142:GLY:H	2.13	0.66
1:C:614:LEU:HD22	1:C:627:ILE:HG23	1.77	0.66
2:D:339:ASN:HB3	2:D:361:VAL:HG12	1.77	0.66
1:G:129:ALA:O	1:G:133:ALA:HB2	1.95	0.66
1:G:276:CYS:HA	1:G:282:GLY:HA2	1.78	0.66
1:K:264:VAL:HG13	1:K:340:ASP:CB	2.23	0.66
1:A:456:ALA:HB1	1:A:457:PRO:CD	2.26	0.66
1:E:398:ASN:HB3	1:E:485:LEU:HD13	1.78	0.66
1:K:117:ALA:HB1	1:K:121:TYR:HB2	1.77	0.66
1:K:400:LEU:HD11	1:K:482:LEU:HD13	1.78	0.66
1:A:312:THR:O	1:A:316:MET:HG3	1.96	0.66
1:I:523:ARG:HB3	1:I:590:MET:HE1	1.77	0.66
1:K:265:THR:HB	1:K:341:GLY:H	1.61	0.66
2:H:231:VAL:O	2:H:235:THR:HB	1.96	0.66
2:B:231:VAL:O	2:B:235:THR:HB	1.96	0.65
1:E:270:ILE:HG12	1:E:289:GLU:HG3	1.76	0.65
1:E:276:CYS:HA	1:E:282:GLY:HA2	1.78	0.65
1:E:433:THR:HG21	1:E:435:VAL:HG12	1.77	0.65
1:G:235:ASP:O	1:G:239:ARG:HG2	1.96	0.65
1:I:117:ALA:C	1:I:119:GLN:H	2.03	0.65
2:L:339:ASN:HD21	2:L:370:SER:HB3	1.60	0.65
2:D:58:GLN:HE21	2:D:61:ARG:HH21	1.43	0.65
2:D:445:LYS:HE2	2:D:452:ASN:OD1	1.95	0.65
1:E:92:ILE:HB	1:E:112:ILE:HG21	1.79	0.65
1:I:115:PRO:HB2	1:I:444:TYR:CD2	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:480:HIS:CD2	1:I:482:LEU:HB2	2.31	0.65
1:K:376:VAL:C	1:K:378:ALA:H	2.04	0.65
1:K:596:TRP:CZ3	1:K:600:ASP:HB2	2.31	0.65
1:A:464:GLU:O	1:A:468:ILE:HG13	1.96	0.65
1:A:276:CYS:HA	1:A:282:GLY:HA2	1.77	0.65
1:C:117:ALA:HB1	1:C:121:TYR:HB2	1.76	0.65
2:D:123:SER:HA	2:D:158:ILE:HB	1.77	0.65
2:D:416:LEU:HB2	2:D:441:VAL:HG22	1.79	0.65
1:E:504:ILE:HG23	1:E:505:ALA:N	2.11	0.65
1:G:443:MET:HG3	1:G:444:TYR:CD1	2.32	0.65
1:K:232:ALA:HA	1:K:237:GLU:HG2	1.79	0.65
1:K:522:LEU:HD22	1:K:563:LEU:HD13	1.79	0.65
1:A:143:TYR:CZ	1:A:356:VAL:HG22	2.31	0.65
1:E:177:LYS:HB3	1:E:181:LYS:NZ	2.12	0.65
1:E:670:ILE:CG1	1:E:718:LEU:HD21	2.24	0.65
1:I:77:ARG:NH1	1:I:370:VAL:HG21	2.10	0.65
1:I:401:TYR:HE2	1:I:448:MET:HB2	1.61	0.65
1:I:411:LEU:HD22	1:I:682:GLN:HB2	1.78	0.65
1:I:634:LEU:HD23	1:I:634:LEU:N	2.11	0.65
1:K:110:VAL:HG21	1:K:130:ALA:HB1	1.77	0.65
1:K:619:ILE:HD12	1:K:625:PHE:C	2.21	0.65
2:F:189:VAL:CG2	2:H:532:LYS:HE2	2.26	0.65
2:F:199:PRO:HB3	2:F:222:TYR:CZ	2.31	0.65
1:C:428(L):ALA:HB3	1:C:455:TRP:HD1	1.61	0.65
1:E:107:ASP:O	1:E:108:GLU:HG3	1.97	0.65
1:G:265:THR:HB	1:G:341:GLY:H	1.61	0.65
2:B:156:ILE:HD12	2:B:156:ILE:N	2.12	0.65
2:D:532:LYS:HE2	2:L:189:VAL:HG23	1.78	0.65
2:F:123:SER:HA	2:F:158:ILE:HB	1.79	0.65
2:H:189:VAL:HA	2:H:282:ASN:ND2	2.12	0.65
1:K:312:THR:HG21	1:K:343:LYS:HD3	1.79	0.65
1:K:583:PHE:CZ	1:K:590:MET:HE3	2.31	0.65
1:C:66:ILE:HB	1:C:138:ALA:O	1.96	0.65
1:E:480:HIS:CD2	1:E:482:LEU:HB2	2.32	0.65
1:G:179:THR:HG22	1:G:183:ILE:HD11	1.78	0.65
2:H:65:THR:OG1	2:H:68:GLU:HG3	1.97	0.65
2:L:288:VAL:HG13	2:L:350:ARG:HG3	1.79	0.65
2:F:231:VAL:O	2:F:235:THR:HB	1.97	0.65
1:I:400:LEU:HD11	1:I:482:LEU:HD13	1.78	0.65
2:J:229:ASP:O	2:J:233:THR:HG23	1.97	0.65
1:A:94:SER:HB2	1:A:114:PRO:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:58:GLN:CD	2:D:63:LYS:HE3	2.22	0.64
2:F:325:ASP:HA	2:F:512:ARG:NH1	2.10	0.64
2:H:88:HIS:CD2	2:H:90:CYS:H	2.14	0.64
1:I:234:ASN:ND2	1:I:236:GLN:HB2	2.11	0.64
1:K:283:ILE:HD12	1:K:389:VAL:HG21	1.77	0.64
1:K:308:LEU:CD2	1:K:316:MET:SD	2.84	0.64
2:L:121:VAL:O	2:L:144:ILE:HD13	1.96	0.64
1:A:421:ARG:HB3	1:A:474:GLU:HB2	1.78	0.64
2:B:416:LEU:HB2	2:B:441:VAL:HG22	1.79	0.64
1:C:304:PRO:O	1:C:394:TRP:CH2	2.50	0.64
1:C:433:THR:HG23	1:C:449:ILE:O	1.97	0.64
1:C:630:ARG:C	1:C:632:ALA:H	2.02	0.64
2:D:296:ASP:O	2:D:298:ILE:HD12	1.97	0.64
2:D:401:THR:HB	2:L:237:GLU:OE1	1.98	0.64
1:E:293:GLN:O	1:E:504:ILE:HG21	1.96	0.64
1:E:634:LEU:N	1:E:634:LEU:HD23	2.12	0.64
2:H:83:ASP:HB2	2:H:140:LYS:HE3	1.78	0.64
1:I:308:LEU:HD12	1:I:308:LEU:O	1.97	0.64
2:L:325:ASP:HA	2:L:512:ARG:HH12	1.62	0.64
1:C:338:ILE:HD12	1:C:338:ILE:N	2.13	0.64
1:C:397:GLU:HG3	1:C:453:CYS:SG	2.37	0.64
1:E:83:ARG:HG2	1:E:83:ARG:HH11	1.61	0.64
1:E:127:VAL:O	1:E:131:ILE:HG13	1.97	0.64
2:F:291:PHE:CE1	2:F:348:GLU:HA	2.32	0.64
1:A:163:PHE:O	1:A:163:PHE:CD1	2.49	0.64
2:D:251:THR:HG21	2:D:260:ALA:HB2	1.79	0.64
2:F:227:GLY:O	2:F:231:VAL:HG23	1.98	0.64
2:H:460:VAL:HG21	2:H:496:ALA:HB2	1.78	0.64
1:I:186:GLU:C	1:I:188:ASN:H	2.04	0.64
1:K:443:MET:HG3	1:K:444:TYR:CD1	2.32	0.64
1:A:528:ALA:HB1	1:A:605:LEU:HD22	1.77	0.64
1:E:443:MET:HG3	1:E:444:TYR:CD1	2.32	0.64
1:E:619:ILE:HD12	1:E:625:PHE:C	2.23	0.64
2:F:88:HIS:CD2	2:F:90:CYS:H	2.15	0.64
2:F:169:GLY:HA2	2:H:462:VAL:CG2	2.27	0.64
1:G:66:ILE:HB	1:G:138:ALA:O	1.96	0.64
1:G:181:LYS:O	1:G:185:GLN:HG3	1.98	0.64
2:B:382:ASP:OD1	2:B:424:VAL:HG13	1.98	0.64
1:C:421:ARG:HB3	1:C:474:GLU:HB2	1.79	0.64
1:E:308:LEU:CD2	1:E:316:MET:SD	2.83	0.64
1:K:526:ALA:HA	1:K:561:VAL:HG11	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:358:HIS:ND1	1:E:359:PRO:HD3	2.12	0.64
1:E:666:MET:HE3	1:E:690:ILE:HD12	1.80	0.64
1:G:178:ILE:H	1:G:178:ILE:CD1	2.07	0.64
1:K:234:ASN:HD22	1:K:236:GLN:HB2	1.62	0.64
1:A:66:ILE:HD12	1:A:87:ILE:CG2	2.26	0.64
1:A:596:TRP:CE3	1:A:600:ASP:HB2	2.32	0.64
1:A:666:MET:HE3	1:A:690:ILE:HD12	1.80	0.64
2:F:346:ARG:HA	2:F:350:ARG:O	1.98	0.64
1:G:164:VAL:HG23	1:G:377:ALA:HB2	1.80	0.64
1:I:128:MET:HA	1:I:131:ILE:HD12	1.78	0.64
2:L:325:ASP:C	2:L:327:GLY:H	2.06	0.64
2:L:329:PHE:CE1	2:L:343:GLY:HA3	2.32	0.64
2:B:124:GLN:HE21	2:B:137:HIS:CE1	2.16	0.64
2:B:261:PHE:CD1	2:B:267:ALA:HA	2.33	0.64
1:C:83:ARG:HG2	1:C:83:ARG:HH11	1.63	0.64
1:E:338:ILE:HD12	1:E:338:ILE:N	2.13	0.64
2:F:346:ARG:HH11	2:F:346:ARG:HG3	1.61	0.64
2:F:419:TYR:CE1	2:F:443:SER:HB2	2.33	0.64
1:G:163:PHE:O	1:G:163:PHE:CD1	2.49	0.64
1:I:143:TYR:CZ	1:I:356:VAL:HG22	2.33	0.64
1:A:265:THR:O	1:A:267:PRO:CD	2.46	0.64
2:B:123:SER:HA	2:B:158:ILE:HB	1.78	0.64
1:C:189:VAL:HG21	1:C:323:LEU:HB2	1.79	0.64
2:F:339:ASN:HD21	2:F:370:SER:HB3	1.61	0.64
1:I:97:ASP:OD1	1:I:102:HIS:HE1	1.81	0.64
1:I:443:MET:HG3	1:I:444:TYR:CD1	2.33	0.64
1:K:275:LEU:HD23	1:K:331:SER:O	1.98	0.64
1:K:523:ARG:C	1:K:590:MET:HE1	2.23	0.64
2:B:476(C):ASP:O	2:B:477:GLU:N	2.31	0.63
1:C:329:TYR:CE2	1:C:352:THR:HG22	2.33	0.63
2:F:307:PRO:O	2:F:432:ARG:NH2	2.30	0.63
2:J:65:THR:HG23	2:J:68:GLU:OE1	1.98	0.63
1:K:329:TYR:HE2	1:K:352:THR:HG22	1.62	0.63
2:L:88:HIS:CD2	2:L:90:CYS:H	2.16	0.63
2:L:379:ARG:HD2	2:L:421:GLU:OE2	1.98	0.63
2:F:382:ASP:OD1	2:F:424:VAL:HG13	1.98	0.63
1:G:128:MET:HA	1:G:131:ILE:HD12	1.80	0.63
2:B:169:GLY:HA2	2:J:462:VAL:CG2	2.28	0.63
2:D:200:CYS:HB3	2:D:223:MET:HB3	1.79	0.63
2:H:273:ARG:HD2	2:H:330:TYR:HD1	1.64	0.63
1:I:316:MET:CE	1:I:337:PHE:HD1	2.11	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:110:VAL:HG21	1:I:130:ALA:HB1	1.81	0.63
1:A:85:MET:O	1:A:87:ILE:HG13	1.98	0.63
1:C:473:PHE:HB3	1:C:482:LEU:HD21	1.81	0.63
2:D:91:THR:HG21	2:H:91:THR:HG21	1.80	0.63
1:E:66:ILE:HD12	1:E:87:ILE:CG2	2.28	0.63
1:E:124:ILE:HG23	1:E:152:PHE:HD2	1.64	0.63
1:K:275:LEU:HG	1:K:332:ALA:HB2	1.81	0.63
1:K:329:TYR:CE2	1:K:352:THR:HG22	2.32	0.63
2:L:193:ILE:HD13	2:L:274:LEU:HD23	1.80	0.63
2:L:476(C):ASP:O	2:L:477:GLU:N	2.32	0.63
1:A:329:TYR:CE2	1:A:352:THR:HG22	2.33	0.63
2:B:532:LYS:HE2	2:J:189:VAL:CG2	2.28	0.63
1:C:64:ASN:O	1:C:66:ILE:HG23	1.98	0.63
1:C:143:TYR:CZ	1:C:356:VAL:HG22	2.33	0.63
1:E:163:PHE:O	1:E:163:PHE:CD1	2.49	0.63
1:E:411:LEU:HD22	1:E:682:GLN:HB2	1.81	0.63
1:G:177:LYS:HB3	1:G:181:LYS:NZ	2.14	0.63
1:G:414:ILE:HD11	1:G:443:MET:N	2.14	0.63
2:H:476(C):ASP:O	2:H:477:GLU:N	2.30	0.63
2:J:58:GLN:HE21	2:J:61:ARG:HH21	1.46	0.63
2:L:242:GLU:OE2	2:L:246:GLY:HA3	1.99	0.63
2:B:210:MET:HE1	2:J:416:LEU:HG	1.81	0.63
1:I:231:ILE:H	1:I:231:ILE:HD12	1.64	0.63
1:K:517:LEU:N	1:K:564:GLN:HE22	1.96	0.63
1:A:619:ILE:HD12	1:A:625:PHE:C	2.23	0.63
1:C:695:MET:SD	2:D:313:PRO:HG3	2.39	0.63
1:E:308:LEU:HD12	1:E:308:LEU:O	1.99	0.63
1:K:156:LEU:HD12	1:K:163:PHE:HB2	1.81	0.63
1:K:337:PHE:C	1:K:338:ILE:HD12	2.24	0.63
1:K:552:GLU:H	1:K:552:GLU:CD	2.07	0.63
2:B:65:THR:OG1	2:B:68:GLU:HG3	1.98	0.63
1:C:517:LEU:N	1:C:564:GLN:HE22	1.95	0.63
1:E:334:THR:HG21	1:E:355:GLN:HE21	1.63	0.63
1:E:526:ALA:HA	1:E:561:VAL:HG11	1.80	0.63
1:G:467:ARG:HB3	1:G:467:ARG:HH11	1.64	0.63
2:H:89:ARG:HH11	2:L:499:ARG:HH21	1.46	0.63
2:H:167:GLN:HE21	2:H:167:GLN:H	0.75	0.63
2:B:151:ASN:ND2	2:D:522:LEU:HD23	2.12	0.62
2:F:91:THR:HG21	2:J:91:THR:HG21	1.80	0.62
1:G:433:THR:HG23	1:G:449:ILE:O	1.98	0.62
1:G:522:LEU:HD22	1:G:563:LEU:HD13	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:64:ASN:O	1:I:66:ILE:HG23	1.99	0.62
1:I:398:ASN:HB3	1:I:485:LEU:HD13	1.81	0.62
1:I:494:PHE:HA	1:I:499:MET:HE2	1.81	0.62
2:J:419:TYR:CE1	2:J:443:SER:HB2	2.34	0.62
1:K:467:ARG:HB3	1:K:467:ARG:HH11	1.63	0.62
1:K:653:LYS:HD3	1:K:653:LYS:N	2.08	0.62
2:D:300:PRO:HA	2:D:509:ARG:NH1	2.14	0.62
2:H:527:VAL:HG22	2:J:150:GLN:HG2	1.81	0.62
1:I:66:ILE:HD12	1:I:87:ILE:CG2	2.28	0.62
1:I:157:GLU:C	1:I:159:GLU:H	2.06	0.62
1:I:259:PHE:CE2	1:I:261:GLU:HB2	2.34	0.62
1:E:304:PRO:HG2	1:E:394:TRP:CZ2	2.33	0.62
1:E:304:PRO:O	1:E:394:TRP:CH2	2.51	0.62
1:E:329:TYR:HE2	1:E:352:THR:HG22	1.65	0.62
1:I:177:LYS:HB3	1:I:181:LYS:NZ	2.14	0.62
2:J:43:ARG:HG2	2:J:43:ARG:NH1	2.13	0.62
1:A:157:GLU:C	1:A:159:GLU:H	2.05	0.62
1:A:433:THR:HG23	1:A:449:ILE:O	1.99	0.62
2:D:189:VAL:CG2	2:L:532:LYS:HE2	2.28	0.62
2:D:193:ILE:HD13	2:D:274:LEU:HD23	1.81	0.62
1:E:143:TYR:CZ	1:E:356:VAL:HG22	2.34	0.62
1:I:232:ALA:HA	1:I:237:GLU:HG2	1.80	0.62
2:B:499:ARG:HG2	2:B:499:ARG:NH1	2.07	0.62
1:E:179:THR:HG22	1:E:183:ILE:HD11	1.80	0.62
1:E:517:LEU:HD21	1:E:632:ALA:CB	2.30	0.62
1:G:292:ILE:HD13	1:G:300:VAL:O	1.99	0.62
1:I:146:LEU:HD23	1:I:152:PHE:CG	2.35	0.62
1:I:264:VAL:HG13	1:I:340:ASP:CB	2.29	0.62
1:K:181:LYS:O	1:K:185:GLN:HG3	2.00	0.62
1:K:415:GLY:C	1:K:440:GLU:HG3	2.24	0.62
1:K:517:LEU:HD21	1:K:632:ALA:CB	2.28	0.62
2:L:145:MET:HE1	2:L:183:ASN:HD21	1.62	0.62
1:G:117:ALA:C	1:G:119:GLN:H	2.06	0.62
1:G:259:PHE:CE2	1:G:261:GLU:HB2	2.35	0.62
1:G:400:LEU:HD11	1:G:482:LEU:HD13	1.82	0.62
1:G:596:TRP:CZ3	1:G:600:ASP:HB2	2.35	0.62
2:J:231:VAL:O	2:J:235:THR:HB	2.00	0.62
2:J:288:VAL:HG13	2:J:350:ARG:HG3	1.81	0.62
1:K:64:ASN:O	1:K:66:ILE:HG23	2.00	0.62
1:K:66:ILE:HD12	1:K:87:ILE:CG2	2.26	0.62
1:K:83:ARG:HG2	1:K:83:ARG:HH11	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:186:GLU:C	1:K:188:ASN:H	2.07	0.62
1:A:74:ILE:HD13	1:A:143:TYR:HE2	1.64	0.62
1:C:157:GLU:C	1:C:159:GLU:H	2.06	0.62
1:E:433:THR:HG23	1:E:449:ILE:O	2.00	0.62
1:G:170:ALA:O	1:G:173:ALA:HB3	1.99	0.62
2:B:529:MET:CE	2:J:185:MET:HE3	2.29	0.62
2:D:492:ASN:HB2	2:D:493:PRO:HD2	1.82	0.62
2:F:368:ILE:HG13	2:F:408:VAL:HG13	1.79	0.62
2:H:379:ARG:HD2	2:H:421:GLU:OE2	1.99	0.62
1:I:112:ILE:HD12	1:I:120:SER:O	2.00	0.62
1:I:275:LEU:HD23	1:I:276:CYS:N	2.14	0.62
1:K:164:VAL:HG22	1:K:373:MET:HE2	1.81	0.62
1:K:480:HIS:HD2	1:K:482:LEU:HB2	1.65	0.62
1:A:124:ILE:HG23	1:A:152:PHE:HD2	1.65	0.62
1:A:181:LYS:O	1:A:185:GLN:HG3	1.99	0.62
1:A:661:MET:HE2	1:A:726:GLU:CB	2.30	0.62
1:C:334:THR:HG21	1:C:355:GLN:NE2	2.14	0.62
2:D:499:ARG:HG2	2:D:499:ARG:NH1	2.12	0.62
1:G:397:GLU:HG3	1:G:453:CYS:SG	2.39	0.62
1:I:140:HIS:CE1	1:I:142:GLY:H	2.18	0.62
1:I:414:ILE:HD11	1:I:443:MET:N	2.14	0.62
1:C:128:MET:HA	1:C:131:ILE:HD12	1.82	0.62
1:C:401:TYR:HE2	1:C:448:MET:HB2	1.65	0.62
1:C:417:LEU:HD21	1:C:478:ILE:HD13	1.82	0.62
1:C:619:ILE:HD12	1:C:625:PHE:C	2.25	0.62
1:E:78:VAL:HG13	1:E:79:ILE:N	2.14	0.62
1:E:323:LEU:O	1:E:326:ALA:HB3	1.99	0.62
2:J:527:VAL:HG22	2:L:150:GLN:HG2	1.81	0.62
1:C:75:ALA:O	1:C:78:VAL:HG12	1.99	0.61
2:D:89:ARG:NH1	2:F:499:ARG:HH21	1.98	0.61
2:F:88:HIS:HD2	2:F:90:CYS:H	1.47	0.61
1:G:275:LEU:HG	1:G:332:ALA:HB2	1.80	0.61
1:G:403:GLU:O	1:G:405:PRO:HD3	1.99	0.61
2:H:325:ASP:HA	2:H:512:ARG:NH1	2.12	0.61
1:A:293:GLN:O	1:A:504:ILE:HG21	2.00	0.61
1:C:163:PHE:O	1:C:163:PHE:CD1	2.53	0.61
1:C:320:ALA:HB1	1:C:335:VAL:HG21	1.82	0.61
2:F:42:ARG:HG2	2:F:42:ARG:HH11	1.65	0.61
1:G:292:ILE:H	1:G:292:ILE:CD1	1.97	0.61
1:A:292:ILE:H	1:A:292:ILE:CD1	2.05	0.61
1:A:358:HIS:ND1	1:A:359:PRO:HD3	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:88:HIS:HD2	2:B:90:CYS:N	1.95	0.61
2:B:346:ARG:HA	2:B:350:ARG:O	2.00	0.61
2:B:532:LYS:HE2	2:J:189:VAL:HG23	1.82	0.61
1:G:74:ILE:O	1:G:77:ARG:HB3	1.99	0.61
1:G:395:ALA:C	1:G:396:ILE:HD12	2.25	0.61
1:G:642:ARG:HH11	2:H:71:ASP:HB3	1.66	0.61
2:H:229:ASP:O	2:H:233:THR:HG23	2.00	0.61
2:J:83:ASP:HB3	2:J:86:VAL:CG2	2.30	0.61
2:J:499:ARG:HH21	2:L:89:ARG:NH1	1.95	0.61
1:K:596:TRP:CE3	1:K:600:ASP:HB2	2.35	0.61
1:A:117:ALA:HB1	1:A:121:TYR:HB2	1.81	0.61
2:B:447:LEU:C	2:B:448:ARG:HG2	2.25	0.61
1:C:583:PHE:HZ	1:C:590:MET:HE3	1.64	0.61
2:D:58:GLN:OE1	2:D:63:LYS:HE3	2.00	0.61
1:C:275:LEU:HG	1:C:332:ALA:HB2	1.83	0.61
1:C:283:ILE:HD12	1:C:389:VAL:HG21	1.82	0.61
1:G:189:VAL:HA	1:G:319:GLN:OE1	2.01	0.61
2:J:83:ASP:HB3	2:J:86:VAL:HG21	1.81	0.61
1:A:596:TRP:HZ3	1:A:600:ASP:O	1.82	0.61
1:C:78:VAL:HG13	1:C:79:ILE:N	2.15	0.61
2:D:184:ILE:HD12	2:L:420:GLY:HA3	1.83	0.61
2:F:65:THR:OG1	2:F:68:GLU:HG3	2.00	0.61
2:H:95:MET:HE3	2:H:95:MET:HA	1.81	0.61
2:H:499:ARG:HH21	2:J:89:ARG:NH1	1.95	0.61
1:K:74:ILE:O	1:K:77:ARG:HB3	2.00	0.61
1:K:97:ASP:OD1	1:K:102:HIS:HE1	1.84	0.61
2:L:339:ASN:ND2	2:L:370:SER:HB3	2.15	0.61
1:A:275:LEU:HD11	1:A:372:GLN:HB2	1.82	0.61
1:C:661:MET:HE2	1:C:726:GLU:CA	2.30	0.61
2:F:184:ILE:CD1	2:H:417:TYR:HA	2.30	0.61
1:G:122:ILE:HA	1:G:146:LEU:HD11	1.81	0.61
2:H:156:ILE:HD12	2:H:156:ILE:N	2.14	0.61
1:K:494:PHE:HA	1:K:499:MET:HE2	1.82	0.61
1:K:538:ILE:O	1:K:541:THR:HB	2.00	0.61
1:I:163:PHE:O	1:I:163:PHE:CD1	2.52	0.61
1:I:400:LEU:HD23	1:I:481:ASN:OD1	2.00	0.61
2:L:346:ARG:HG3	2:L:346:ARG:HH11	1.64	0.61
1:A:184:ALA:HB1	1:A:189:VAL:HB	1.83	0.61
1:C:129:ALA:O	1:C:133:ALA:HB2	2.01	0.61
1:C:275:LEU:HD11	1:C:372:GLN:HB2	1.83	0.61
1:C:596:TRP:CE3	1:C:600:ASP:HB2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:164:VAL:HG23	1:E:377:ALA:HB2	1.82	0.61
2:F:535:ASP:OD2	2:H:379:ARG:NH2	2.33	0.61
1:G:77:ARG:NH1	1:G:370:VAL:HG21	2.16	0.61
1:C:433:THR:HG21	1:C:435:VAL:HG12	1.83	0.61
2:D:50:GLY:O	2:D:54:ARG:HD2	2.01	0.61
1:E:66:ILE:O	1:E:66:ILE:HG12	2.00	0.61
2:F:329:PHE:CE1	2:F:343:GLY:HA3	2.35	0.61
1:G:115:PRO:HB2	1:G:444:TYR:CD2	2.36	0.61
1:I:67:LEU:HG	1:I:68:ILE:H	1.64	0.61
2:L:123:SER:HA	2:L:158:ILE:HB	1.82	0.61
2:B:42:ARG:HG2	2:B:42:ARG:HH11	1.66	0.60
2:B:479:ILE:HD12	2:B:479:ILE:C	2.26	0.60
1:E:75:ALA:O	1:E:78:VAL:HG12	2.00	0.60
1:G:365:THR:HG22	1:G:391:LEU:CD2	2.31	0.60
1:G:376:VAL:C	1:G:378:ALA:H	2.09	0.60
1:I:201:ASP:OD1	1:I:203:ASP:HB2	2.01	0.60
2:J:460:VAL:HG21	2:J:496:ALA:HB2	1.82	0.60
2:L:324:ALA:HA	2:L:345:ILE:HD12	1.82	0.60
1:A:164:VAL:HG23	1:A:377:ALA:HB2	1.83	0.60
1:A:411:LEU:HD22	1:A:682:GLN:HB2	1.83	0.60
1:A:464:GLU:HA	1:A:464:GLU:OE2	2.01	0.60
1:E:157:GLU:C	1:E:159:GLU:H	2.08	0.60
2:F:409:ILE:HD13	2:H:205:VAL:HB	1.82	0.60
1:G:337:PHE:C	1:G:338:ILE:HD12	2.26	0.60
1:G:458:THR:O	1:G:461:ALA:HB3	2.02	0.60
2:H:95:MET:HE3	2:H:95:MET:CA	2.31	0.60
1:I:74:ILE:HD13	1:I:143:TYR:CE2	2.36	0.60
1:K:658:THR:OG1	1:K:702:GLU:HG2	2.00	0.60
1:C:494:PHE:HA	1:C:499:MET:HE2	1.82	0.60
2:D:307:PRO:O	2:D:432:ARG:NH2	2.34	0.60
2:D:436:GLY:HA2	2:L:173:LEU:HD21	1.82	0.60
2:D:535:ASP:OD2	2:L:379:ARG:NH2	2.34	0.60
1:E:74:ILE:O	1:E:77:ARG:HB3	2.01	0.60
1:E:552:GLU:CD	1:E:552:GLU:H	2.09	0.60
1:G:401:TYR:HE2	1:G:448:MET:HB2	1.66	0.60
2:H:337:ALA:HB1	2:H:370:SER:HA	1.83	0.60
2:H:423:THR:O	2:H:525:LYS:HE2	2.01	0.60
1:I:189:VAL:HG21	1:I:323:LEU:HB2	1.83	0.60
1:K:77:ARG:NH1	1:K:370:VAL:HG21	2.16	0.60
1:K:127:VAL:O	1:K:131:ILE:HG13	2.01	0.60
1:K:596:TRP:CG	1:K:597:THR:N	2.69	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:173:LEU:HD21	2:J:436:GLY:HA2	1.83	0.60
1:C:467:ARG:HE	1:C:630:ARG:HG3	1.66	0.60
2:D:417:TYR:HB2	2:L:210:MET:HE2	1.82	0.60
1:E:181:LYS:O	1:E:185:GLN:HG3	2.00	0.60
1:E:329:TYR:CE2	1:E:352:THR:HG22	2.37	0.60
1:I:215:PRO:HB2	1:I:231:ILE:CG2	2.32	0.60
1:I:492:PRO:HA	1:I:495:ILE:HD12	1.83	0.60
1:I:523:ARG:C	1:I:590:MET:HE1	2.26	0.60
1:I:526:ALA:HA	1:I:561:VAL:HG11	1.83	0.60
1:K:354:LEU:C	1:K:354:LEU:HD13	2.26	0.60
1:K:414:ILE:HD11	1:K:443:MET:N	2.15	0.60
1:K:517:LEU:H	1:K:564:GLN:HE22	1.46	0.60
2:L:231:VAL:O	2:L:235:THR:HB	2.01	0.60
1:C:504:ILE:HG23	1:C:505:ALA:N	2.15	0.60
1:C:653:LYS:H	1:C:653:LYS:CD	2.08	0.60
2:D:156:ILE:HD12	2:D:156:ILE:N	2.16	0.60
1:E:517:LEU:N	1:E:564:GLN:HE22	2.00	0.60
2:F:417:TYR:HB2	2:H:210:MET:HE2	1.82	0.60
1:G:157:GLU:C	1:G:159:GLU:H	2.09	0.60
1:I:316:MET:HE3	1:I:337:PHE:HD1	1.66	0.60
1:A:283:ILE:HD12	1:A:389:VAL:HG21	1.83	0.60
1:C:400:LEU:HD21	1:C:482:LEU:HD13	1.83	0.60
1:G:275:LEU:HD23	1:G:331:SER:O	2.01	0.60
1:G:417:LEU:HD21	1:G:478:ILE:HD13	1.83	0.60
1:G:538:ILE:O	1:G:541:THR:HB	2.02	0.60
1:G:670:ILE:CG1	1:G:718:LEU:HD21	2.29	0.60
1:I:543:VAL:HG12	1:I:544:SER:O	2.02	0.60
1:I:630:ARG:C	1:I:632:ALA:N	2.55	0.60
2:L:156:ILE:HD12	2:L:156:ILE:N	2.15	0.60
2:B:237:GLU:OE1	2:J:401:THR:HB	2.01	0.60
1:C:630:ARG:C	1:C:632:ALA:N	2.58	0.60
1:A:304:PRO:O	1:A:394:TRP:CH2	2.54	0.60
1:C:92:ILE:HB	1:C:112:ILE:HG21	1.83	0.60
1:E:97:ASP:OD1	1:E:102:HIS:HE1	1.85	0.60
1:E:265:THR:HG22	1:E:266:GLN:HG2	1.83	0.60
2:F:169:GLY:HA2	2:H:462:VAL:HG22	1.82	0.60
1:A:74:ILE:O	1:A:77:ARG:HB3	2.02	0.60
1:A:480:HIS:HD2	1:A:482:LEU:HB2	1.67	0.60
2:B:169:GLY:HA2	2:J:462:VAL:HG22	1.83	0.60
1:C:661:MET:HE2	1:C:726:GLU:CB	2.32	0.60
1:E:403:GLU:O	1:E:405:PRO:HD3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:339:ASN:ND2	2:F:370:SER:HB3	2.17	0.60
1:G:186:GLU:C	1:G:188:ASN:H	2.07	0.60
1:A:276:CYS:O	1:A:382:LEU:HD21	2.01	0.60
2:B:460:VAL:CG2	2:B:496:ALA:HB2	2.32	0.60
1:C:414:ILE:HD11	1:C:443:MET:N	2.16	0.60
1:C:464:GLU:O	1:C:468:ILE:HG13	2.02	0.60
2:D:337:ALA:HB3	2:D:373:LYS:HD2	1.84	0.60
1:G:97:ASP:OD1	1:G:102:HIS:HE1	1.85	0.60
1:K:128:MET:HA	1:K:131:ILE:HD12	1.83	0.60
1:K:163:PHE:O	1:K:163:PHE:CD1	2.54	0.60
1:C:276:CYS:O	1:C:382:LEU:HD21	2.01	0.59
1:C:392:THR:O	1:C:455:TRP:HZ3	1.84	0.59
1:E:118:ASN:HD21	1:E:119:GLN:HE21	1.50	0.59
2:L:42:ARG:HG2	2:L:42:ARG:NH1	2.17	0.59
2:L:124:GLN:HE21	2:L:137:HIS:CE1	2.19	0.59
2:L:337:ALA:HB3	2:L:373:LYS:HD2	1.84	0.59
1:A:186:GLU:C	1:A:188:ASN:H	2.09	0.59
1:A:267:PRO:O	1:A:501:THR:HG23	2.02	0.59
1:A:376:VAL:C	1:A:378:ALA:N	2.59	0.59
2:B:348:GLU:OE2	1:E:551:HIS:HE1	1.85	0.59
2:D:151:ASN:ND2	2:F:522:LEU:HD23	2.15	0.59
2:D:261:PHE:CD1	2:D:267:ALA:HA	2.37	0.59
1:E:129:ALA:O	1:E:133:ALA:HB2	2.01	0.59
2:F:50:GLY:O	2:F:54:ARG:HD2	2.01	0.59
2:H:83:ASP:HB3	2:H:86:VAL:CG2	2.32	0.59
2:H:273:ARG:HD2	2:H:330:TYR:CD1	2.37	0.59
2:J:476(C):ASP:O	2:J:477:GLU:N	2.35	0.59
2:L:193:ILE:CD1	2:L:274:LEU:HD23	2.33	0.59
1:E:414:ILE:HD11	1:E:443:MET:N	2.18	0.59
1:A:523:ARG:HB3	1:A:590:MET:HE1	1.84	0.59
1:A:695:MET:SD	2:B:313:PRO:HG3	2.43	0.59
2:B:121:VAL:HG22	2:B:122:PHE:N	2.17	0.59
2:B:417:TYR:HA	2:J:184:ILE:HD13	1.83	0.59
1:C:265:THR:HB	1:C:341:GLY:H	1.67	0.59
2:D:237:GLU:OE1	2:L:401:THR:HB	2.03	0.59
1:E:459:ARG:O	1:E:463:ILE:HG12	2.03	0.59
1:A:661:MET:HE2	1:A:726:GLU:CA	2.33	0.59
2:B:529:MET:HE2	2:J:185:MET:HE3	1.85	0.59
1:C:679:GLN:O	1:C:706:VAL:HG13	2.02	0.59
1:E:275:LEU:HG	1:E:332:ALA:HB2	1.84	0.59
2:F:239:VAL:HG22	2:F:243:GLU:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:42:ARG:HG2	2:H:42:ARG:HH11	1.67	0.59
2:H:149:MET:SD	2:H:186:ALA:HB2	2.43	0.59
1:I:164:VAL:HG23	1:I:377:ALA:HB2	1.84	0.59
2:J:160:ASP:OD1	2:J:198:GLY:HA3	2.03	0.59
1:K:178:ILE:H	1:K:178:ILE:CD1	2.07	0.59
1:K:577:ASP:HB2	1:K:591:ARG:NH2	2.16	0.59
2:D:160:ASP:OD1	2:D:198:GLY:HA3	2.02	0.59
1:E:179:THR:O	1:E:183:ILE:HG13	2.02	0.59
2:F:173:LEU:HD21	2:H:436:GLY:HA2	1.84	0.59
1:G:83:ARG:HG2	1:G:83:ARG:HH11	1.66	0.59
2:H:291:PHE:CE1	2:H:348:GLU:HA	2.36	0.59
2:J:65:THR:OG1	2:J:68:GLU:HG3	2.03	0.59
1:K:467:ARG:HE	1:K:630:ARG:HG3	1.67	0.59
1:K:528:ALA:HB1	1:K:605:LEU:HD22	1.84	0.59
1:A:630:ARG:C	1:A:632:ALA:N	2.58	0.59
2:B:54:ARG:HG2	2:B:54:ARG:HH11	1.67	0.59
2:B:462:VAL:HG22	2:J:169:GLY:HA2	1.85	0.59
2:B:527:VAL:HG22	2:F:150:GLN:HG2	1.84	0.59
2:D:83:ASP:HB3	2:D:86:VAL:CG2	2.32	0.59
1:G:167:PRO:O	1:G:169:GLY:N	2.36	0.59
1:G:189:VAL:HG21	1:G:323:LEU:HB2	1.83	0.59
1:G:275:LEU:HD23	1:G:276:CYS:N	2.18	0.59
2:J:492:ASN:HB2	2:J:493:PRO:HD2	1.83	0.59
1:K:598:PRO:HD2	2:L:292:PHE:CE1	2.38	0.59
2:B:61:ARG:HB2	2:B:63:LYS:HG3	1.85	0.59
1:E:334:THR:HG22	1:E:351:ASN:HB2	1.84	0.59
1:E:614:LEU:HD22	1:E:627:ILE:HG23	1.84	0.59
1:E:630:ARG:C	1:E:632:ALA:N	2.57	0.59
2:F:334:GLU:O	2:F:338:LYS:HD2	2.02	0.59
2:F:460:VAL:CG2	2:F:496:ALA:HB2	2.33	0.59
2:F:462:VAL:HG22	2:H:169:GLY:HA2	1.84	0.59
1:G:131:ILE:CG2	1:G:136:ALA:HB2	2.27	0.59
1:G:523:ARG:C	1:G:590:MET:HE1	2.27	0.59
1:G:634:LEU:N	1:G:634:LEU:HD23	2.17	0.59
2:H:346:ARG:HA	2:H:350:ARG:O	2.03	0.59
1:I:543:VAL:HG11	2:J:117:ARG:HD2	1.85	0.59
1:I:634:LEU:HD23	1:I:634:LEU:H	1.67	0.59
1:K:428(L):ALA:HB3	1:K:455:TRP:HD1	1.67	0.59
1:G:543:VAL:HG12	1:G:544:SER:O	2.03	0.59
1:K:358:HIS:ND1	1:K:359:PRO:HD3	2.18	0.59
1:K:378:ALA:O	1:K:379:GLY:C	2.46	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:THR:HG22	1:A:434:GLY:N	2.18	0.59
2:D:368:ILE:HG13	2:D:408:VAL:HG13	1.85	0.59
1:E:275:LEU:HD11	1:E:372:GLN:HB2	1.85	0.59
2:F:261:PHE:CD1	2:F:267:ALA:HA	2.38	0.59
1:G:229:MET:HG3	1:G:229:MET:O	2.01	0.59
1:G:234:ASN:HD22	1:G:236:GLN:HB2	1.66	0.59
1:K:400:LEU:HD23	1:K:481:ASN:OD1	2.02	0.59
1:C:181:LYS:O	1:C:185:GLN:HG3	2.03	0.58
2:F:436:GLY:HA2	2:H:173:LEU:HD21	1.85	0.58
1:G:132:ARG:HD3	1:G:159:GLU:OE1	2.03	0.58
1:G:378:ALA:O	1:G:379:GLY:C	2.46	0.58
1:G:392:THR:O	1:G:455:TRP:HZ3	1.86	0.58
2:J:145:MET:HE1	2:J:183:ASN:HD21	1.65	0.58
1:K:259:PHE:CE2	1:K:261:GLU:HB2	2.38	0.58
1:K:275:LEU:HD11	1:K:372:GLN:HB2	1.84	0.58
1:K:642:ARG:HH11	2:L:71:ASP:HB3	1.68	0.58
1:A:320:ALA:HB1	1:A:335:VAL:HG21	1.85	0.58
2:B:325:ASP:HA	2:B:512:ARG:NH1	2.15	0.58
1:C:178:ILE:H	1:C:178:ILE:CD1	2.08	0.58
2:D:436:GLY:O	2:D:439:TYR:HB3	2.03	0.58
1:E:492:PRO:HA	1:E:495:ILE:HD12	1.84	0.58
1:G:596:TRP:HZ3	1:G:600:ASP:O	1.86	0.58
1:I:78:VAL:HG23	1:I:370:VAL:CG1	2.33	0.58
1:I:338:ILE:HD12	1:I:338:ILE:N	2.19	0.58
1:I:653:LYS:H	1:I:653:LYS:CD	2.06	0.58
2:J:324:ALA:HA	2:J:345:ILE:HD12	1.85	0.58
1:K:157:GLU:C	1:K:159:GLU:H	2.07	0.58
1:K:365:THR:HG22	1:K:391:LEU:CD2	2.33	0.58
2:L:298:ILE:HG23	2:L:509:ARG:HB2	1.83	0.58
1:A:112:ILE:HD12	1:A:120:SER:O	2.03	0.58
1:A:189:VAL:HG21	1:A:323:LEU:HB2	1.85	0.58
1:A:433:THR:HG21	1:A:435:VAL:HG12	1.83	0.58
1:A:517:LEU:N	1:A:564:GLN:HE22	2.01	0.58
1:C:398:ASN:HB3	1:C:485:LEU:HD13	1.84	0.58
1:C:497:GLY:HA2	1:C:499:MET:HE3	1.83	0.58
2:F:58:GLN:OE1	2:F:63:LYS:HE3	2.03	0.58
1:G:124:ILE:HG23	1:G:152:PHE:HD2	1.68	0.58
2:H:43:ARG:HG2	2:H:43:ARG:HH11	1.69	0.58
1:I:170:ALA:O	1:I:173:ALA:HB3	2.03	0.58
1:I:181:LYS:O	1:I:185:GLN:HG3	2.02	0.58
1:K:245:SER:C	1:K:247:ASN:H	2.11	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:411:LEU:HD22	1:K:682:GLN:HB2	1.85	0.58
1:C:308:LEU:CD2	1:C:316:MET:SD	2.90	0.58
1:I:467:ARG:HE	1:I:630:ARG:HG3	1.68	0.58
2:J:199:PRO:HB3	2:J:222:TYR:CZ	2.38	0.58
1:K:128:MET:SD	1:K:131:ILE:HD12	2.44	0.58
1:A:376:VAL:C	1:A:378:ALA:H	2.10	0.58
1:A:724:ILE:HG22	1:A:725:MET:HG3	1.85	0.58
1:C:66:ILE:CD1	1:C:87:ILE:HG22	2.29	0.58
1:C:365:THR:HG22	1:C:391:LEU:HD22	1.85	0.58
1:E:400:LEU:HD21	1:E:482:LEU:HD13	1.84	0.58
2:H:348:GLU:OE2	1:I:551:HIS:HE1	1.86	0.58
1:I:467:ARG:HB3	1:I:467:ARG:HH11	1.68	0.58
1:I:553:ARG:NH1	2:J:115:ASN:OD1	2.37	0.58
1:A:78:VAL:HG13	1:A:79:ILE:N	2.18	0.58
1:C:264:VAL:CG1	1:C:340:ASP:HB3	2.34	0.58
1:C:526:ALA:HA	1:C:561:VAL:HG11	1.85	0.58
2:F:182:ARG:HH11	2:F:182:ARG:HG3	1.69	0.58
1:G:140:HIS:CE1	1:G:142:GLY:H	2.21	0.58
1:I:378:ALA:O	1:I:379:GLY:C	2.46	0.58
2:L:149:MET:CE	2:L:189:VAL:HG11	2.33	0.58
1:A:363:LEU:HD13	1:A:455:TRP:HB3	1.85	0.58
2:B:329:PHE:CE1	2:B:343:GLY:HA3	2.38	0.58
1:C:598:PRO:HD2	2:D:292:PHE:CE1	2.38	0.58
2:D:337:ALA:HB1	2:D:370:SER:HA	1.85	0.58
2:F:346:ARG:HG3	2:F:346:ARG:NH1	2.18	0.58
1:G:528:ALA:HB1	1:G:605:LEU:CD2	2.32	0.58
1:G:552:GLU:CD	1:G:552:GLU:H	2.12	0.58
1:I:179:THR:O	1:I:183:ILE:HG13	2.04	0.58
1:I:335:VAL:HG23	1:I:335:VAL:O	2.04	0.58
1:K:304:PRO:O	1:K:394:TRP:CH2	2.57	0.58
1:K:543:VAL:HG12	1:K:544:SER:O	2.04	0.58
1:A:128:MET:SD	1:A:131:ILE:HD12	2.44	0.58
1:C:312:THR:O	1:C:316:MET:HG3	2.03	0.58
1:C:577:ASP:HB2	1:C:591:ARG:NH2	2.19	0.58
1:C:634:LEU:N	1:C:634:LEU:HD23	2.18	0.58
2:D:95:MET:CA	2:D:95:MET:HE3	2.34	0.58
2:D:150:GLN:HG2	2:F:527:VAL:HG22	1.86	0.58
1:E:140:HIS:CE1	1:E:142:GLY:H	2.20	0.58
1:G:218:ILE:HD12	1:G:260:ILE:HG12	1.86	0.58
1:G:396:ILE:HG12	1:G:463:ILE:CD1	2.31	0.58
1:K:212:ILE:HD12	1:K:260:ILE:HG22	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:346:ARG:HG3	2:L:346:ARG:NH1	2.16	0.58
1:C:74:ILE:HD13	1:C:143:TYR:CE2	2.39	0.58
2:D:42:ARG:HG2	2:D:42:ARG:NH1	2.18	0.58
2:D:121:VAL:HG22	2:D:122:PHE:N	2.18	0.58
2:D:195:MET:SD	2:D:271:VAL:HG21	2.43	0.58
2:D:199:PRO:HB3	2:D:222:TYR:CZ	2.39	0.58
1:E:170:ALA:O	1:E:173:ALA:HB3	2.04	0.58
1:G:143:TYR:CZ	1:G:356:VAL:HG22	2.39	0.58
1:G:146:LEU:HD23	1:G:152:PHE:CG	2.38	0.58
1:G:619:ILE:HD12	1:G:625:PHE:C	2.29	0.58
2:H:43:ARG:HG2	2:H:43:ARG:NH1	2.18	0.58
1:I:128:MET:SD	1:I:131:ILE:HD12	2.44	0.58
1:K:78:VAL:HG23	1:K:370:VAL:CG1	2.33	0.58
1:A:380:GLU:CG	1:A:381:PRO:HD2	2.33	0.58
2:B:170:VAL:HG11	2:J:460:VAL:HG23	1.86	0.58
1:C:272:ILE:HB	1:C:335:VAL:HG23	1.85	0.58
1:C:365:THR:HG22	1:C:391:LEU:CD2	2.34	0.58
1:C:523:ARG:HB3	1:C:590:MET:HE1	1.85	0.58
1:G:204:GLU:O	1:G:208:ILE:HG13	2.04	0.58
1:G:630:ARG:C	1:G:632:ALA:H	2.11	0.58
2:H:87:THR:HG23	2:L:498:GLU:HG2	1.86	0.58
2:H:148:ALA:HB1	2:H:153:ALA:O	2.04	0.58
1:I:179:THR:HG22	1:I:183:ILE:HD11	1.85	0.58
1:I:275:LEU:HG	1:I:332:ALA:HB2	1.86	0.58
1:I:365:THR:HG22	1:I:391:LEU:CD2	2.34	0.58
1:A:504:ILE:HG23	1:A:505:ALA:N	2.19	0.57
1:E:543:VAL:HG12	1:E:544:SER:O	2.04	0.57
1:G:231:ILE:H	1:G:231:ILE:HD12	1.69	0.57
1:G:596:TRP:CE3	1:G:600:ASP:HB2	2.39	0.57
1:G:658:THR:OG1	1:G:702:GLU:HG2	2.04	0.57
1:I:376:VAL:C	1:I:378:ALA:H	2.12	0.57
1:K:67:LEU:HG	1:K:68:ILE:H	1.69	0.57
1:K:92:ILE:HB	1:K:112:ILE:HG21	1.86	0.57
1:K:184:ALA:HB1	1:K:189:VAL:HB	1.85	0.57
2:L:300:PRO:HA	2:L:509:ARG:NH1	2.18	0.57
1:C:304:PRO:HG2	1:C:394:TRP:CZ2	2.39	0.57
1:K:74:ILE:HD13	1:K:143:TYR:CE2	2.39	0.57
1:C:124:ILE:HG23	1:C:152:PHE:HD2	1.69	0.57
1:E:523:ARG:HB3	1:E:590:MET:HE1	1.85	0.57
2:F:178:GLU:O	2:F:182:ARG:HG3	2.04	0.57
1:G:128:MET:SD	1:G:131:ILE:HD12	2.44	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:358:HIS:HB2	1:G:369:LEU:HD12	1.85	0.57
2:L:58:GLN:HE21	2:L:61:ARG:HH21	1.52	0.57
1:A:551:HIS:HE1	2:D:348:GLU:OE2	1.86	0.57
2:B:401:THR:HB	2:J:237:GLU:OE1	2.04	0.57
1:C:74:ILE:O	1:C:77:ARG:HB3	2.03	0.57
1:G:275:LEU:HD11	1:G:372:GLN:HB2	1.85	0.57
1:I:596:TRP:CE3	1:I:600:ASP:HB2	2.39	0.57
1:A:275:LEU:HD23	1:A:331:SER:O	2.04	0.57
1:E:279:HIS:NE2	1:E:380:GLU:N	2.52	0.57
2:F:401:THR:HB	2:H:237:GLU:OE1	2.04	0.57
1:G:304:PRO:HG2	1:G:394:TRP:CZ2	2.40	0.57
2:H:325:ASP:C	2:H:327:GLY:H	2.12	0.57
1:I:137:GLN:O	1:I:138:ALA:HB2	2.03	0.57
1:I:670:ILE:HD11	1:I:718:LEU:HD11	1.85	0.57
2:J:307:PRO:O	2:J:432:ARG:NH2	2.37	0.57
1:K:230:ARG:HG2	1:K:230:ARG:HH11	1.69	0.57
1:K:398:ASN:HB3	1:K:485:LEU:HD13	1.86	0.57
1:K:464:GLU:O	1:K:468:ILE:HG13	2.05	0.57
1:K:504:ILE:HG23	1:K:505:ALA:N	2.19	0.57
1:A:400:LEU:HD21	1:A:482:LEU:HD13	1.85	0.57
1:A:491:HIS:O	1:A:495:ILE:HG13	2.04	0.57
1:A:517:LEU:HD22	1:A:517:LEU:N	2.15	0.57
1:A:526:ALA:HA	1:A:561:VAL:HG11	1.85	0.57
2:B:251:THR:HG21	2:B:260:ALA:HB2	1.86	0.57
2:B:501:PHE:CE1	2:J:174:ALA:HB2	2.40	0.57
1:C:279:HIS:NE2	1:C:380:GLU:N	2.53	0.57
2:D:193:ILE:CD1	2:D:274:LEU:HD23	2.35	0.57
1:E:131:ILE:CG2	1:E:136:ALA:HB2	2.32	0.57
2:F:210:MET:HE2	2:H:417:TYR:CB	2.34	0.57
2:L:419:TYR:CE1	2:L:443:SER:HB2	2.39	0.57
1:A:634:LEU:HD23	1:A:634:LEU:N	2.19	0.57
1:E:365:THR:HG22	1:E:391:LEU:HD22	1.86	0.57
1:E:494:PHE:HA	1:E:499:MET:HE2	1.87	0.57
1:G:400:LEU:HD21	1:G:482:LEU:HD13	1.85	0.57
2:H:75:ASP:OD1	2:H:272:ARG:NH2	2.38	0.57
1:I:78:VAL:HG13	1:I:79:ILE:N	2.19	0.57
1:I:121:TYR:HE2	1:I:445:TYR:HH	1.53	0.57
1:I:189:VAL:HA	1:I:319:GLN:OE1	2.04	0.57
1:K:137:GLN:O	1:K:138:ALA:HB2	2.04	0.57
1:K:177:LYS:O	1:K:181:LYS:HG2	2.04	0.57
1:K:661:MET:HE2	1:K:726:GLU:CB	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:VAL:HG23	1:C:377:ALA:HB2	1.86	0.57
2:F:207:SER:HB3	2:F:208:PRO:CD	2.26	0.57
1:G:85:MET:O	1:G:87:ILE:HG13	2.05	0.57
1:G:276:CYS:O	1:G:382:LEU:HD21	2.05	0.57
2:B:160:ASP:OD1	2:B:198:GLY:HA3	2.04	0.57
1:E:117:ALA:CB	1:E:121:TYR:HB2	2.35	0.57
1:E:264:VAL:CG1	1:E:340:ASP:HB3	2.35	0.57
1:E:417:LEU:HD21	1:E:478:ILE:HD13	1.87	0.57
1:G:400:LEU:HD23	1:G:481:ASN:OD1	2.05	0.57
1:G:683:GLU:HB2	1:G:704:LYS:HG3	1.86	0.57
1:I:283:ILE:HA	1:I:386:GLN:NE2	2.19	0.57
1:K:348:LEU:O	1:K:348:LEU:HD23	2.05	0.57
1:A:123:VAL:HG12	1:A:126:LYS:H	1.70	0.57
1:A:365:THR:HG22	1:A:391:LEU:CD2	2.35	0.57
2:F:200:CYS:HB3	2:F:223:MET:HB3	1.86	0.57
1:G:201:ASP:OD1	1:G:203:ASP:HB2	2.05	0.57
1:I:85:MET:O	1:I:87:ILE:HG13	2.05	0.57
1:K:112:ILE:HD12	1:K:120:SER:O	2.05	0.57
1:K:218:ILE:CD1	1:K:260:ILE:HG12	2.35	0.57
1:K:400:LEU:HD21	1:K:482:LEU:HD13	1.86	0.57
1:K:492:PRO:HA	1:K:495:ILE:HD12	1.85	0.57
1:C:270:ILE:HG12	1:C:289:GLU:HG3	1.87	0.56
1:C:376:VAL:C	1:C:378:ALA:H	2.13	0.56
1:E:190:SER:N	1:E:319:GLN:OE1	2.34	0.56
1:G:661:MET:HE2	1:G:726:GLU:CB	2.35	0.56
1:I:146:LEU:HD23	1:I:152:PHE:CD2	2.40	0.56
1:I:279:HIS:NE2	1:I:380:GLU:N	2.53	0.56
2:J:458:ALA:HB3	2:J:493:PRO:HB3	1.86	0.56
1:K:215:PRO:HB2	1:K:231:ILE:CG2	2.35	0.56
1:K:457:PRO:CG	1:K:458:THR:H	2.17	0.56
1:K:642:ARG:NH1	2:L:71:ASP:OD2	2.38	0.56
2:B:492:ASN:HB2	2:B:493:PRO:HD2	1.86	0.56
1:C:137:GLN:O	1:C:138:ALA:HB2	2.05	0.56
2:D:83:ASP:HB3	2:D:86:VAL:HG21	1.87	0.56
1:E:400:LEU:HD11	1:E:482:LEU:HD13	1.86	0.56
2:F:58:GLN:HE21	2:F:61:ARG:HH21	1.52	0.56
1:G:207:LYS:O	1:G:211:GLN:HB2	2.04	0.56
1:G:308:LEU:HD12	1:G:308:LEU:O	2.05	0.56
1:I:74:ILE:HD13	1:I:143:TYR:HE2	1.70	0.56
1:K:376:VAL:C	1:K:378:ALA:N	2.60	0.56
2:B:74:LEU:HD13	2:B:112:GLY:HA3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:MET:HE1	2:B:183:ASN:HD22	1.66	0.56
1:E:634:LEU:HD23	1:E:634:LEU:H	1.69	0.56
2:F:237:GLU:OE1	2:H:401:THR:HB	2.06	0.56
1:G:92:ILE:HB	1:G:112:ILE:HG21	1.88	0.56
1:G:712:ALA:HA	1:G:716:ASN:ND2	2.20	0.56
2:H:141:ILE:O	2:H:145:MET:HG3	2.06	0.56
2:H:337:ALA:HB3	2:H:373:LYS:HD2	1.86	0.56
1:I:66:ILE:HG12	1:I:66:ILE:O	2.05	0.56
1:I:395:ALA:C	1:I:396:ILE:HD12	2.30	0.56
1:I:401:TYR:CE2	1:I:448:MET:HB2	2.40	0.56
1:K:675:VAL:CG1	1:K:707:VAL:HG21	2.35	0.56
2:L:83:ASP:HB3	2:L:86:VAL:HG21	1.87	0.56
1:A:598:PRO:HD2	2:B:292:PHE:CE1	2.40	0.56
1:C:292:ILE:HD13	1:C:300:VAL:O	2.04	0.56
2:D:458:ALA:HB3	2:D:493:PRO:HB3	1.87	0.56
2:D:484:ALA:O	2:D:488:GLU:OE1	2.24	0.56
1:G:494:PHE:HA	1:G:499:MET:HE2	1.86	0.56
1:G:517:LEU:HB3	1:G:521:ASP:HB3	1.87	0.56
1:I:275:LEU:HD23	1:I:331:SER:O	2.05	0.56
1:K:167:PRO:O	1:K:169:GLY:N	2.38	0.56
1:A:275:LEU:HG	1:A:332:ALA:HB2	1.88	0.56
1:A:378:ALA:O	1:A:379:GLY:C	2.49	0.56
1:A:494:PHE:HA	1:A:499:MET:HE2	1.88	0.56
2:B:492:ASN:HD22	2:B:494:PHE:H	1.53	0.56
1:C:457:PRO:CG	1:C:458:THR:H	2.13	0.56
1:E:380:GLU:CG	1:E:381:PRO:HD2	2.36	0.56
1:E:497:GLY:HA2	1:E:499:MET:HE3	1.87	0.56
1:I:127:VAL:O	1:I:131:ILE:HG13	2.05	0.56
1:I:354:LEU:HD11	1:I:358:HIS:CE1	2.41	0.56
1:I:675:VAL:CG1	1:I:707:VAL:HG21	2.36	0.56
1:K:523:ARG:HB3	1:K:590:MET:HE1	1.86	0.56
1:K:553:ARG:NH1	2:L:115:ASN:OD1	2.39	0.56
2:L:291:PHE:CE1	2:L:348:GLU:HA	2.40	0.56
1:A:522:LEU:HD22	1:A:563:LEU:HD13	1.87	0.56
1:E:287:GLU:OE2	1:E:305:SER:N	2.38	0.56
1:E:358:HIS:HB2	1:E:369:LEU:HD12	1.87	0.56
1:G:441:ILE:HD12	1:G:478:ILE:HD13	1.88	0.56
1:I:415:GLY:C	1:I:440:GLU:HG3	2.30	0.56
1:I:666:MET:HE3	1:I:690:ILE:HD12	1.87	0.56
2:J:75:ASP:OD1	2:J:272:ARG:NH2	2.37	0.56
1:K:74:ILE:HD13	1:K:143:TYR:HE2	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:335:VAL:CG1	1:K:350:MET:HE3	2.35	0.56
2:L:367:ASP:O	2:L:368:ILE:C	2.49	0.56
2:B:501:PHE:N	2:B:501:PHE:CD2	2.69	0.56
1:C:186:GLU:C	1:C:188:ASN:N	2.63	0.56
1:C:272:ILE:HB	1:C:335:VAL:CG2	2.36	0.56
1:E:400:LEU:HD23	1:E:481:ASN:OD1	2.05	0.56
1:E:428(L):ALA:HB3	1:E:455:TRP:HD1	1.71	0.56
2:F:145:MET:HE1	2:F:183:ASN:HD21	1.69	0.56
1:I:92:ILE:HB	1:I:112:ILE:CG2	2.34	0.56
2:J:149:MET:SD	2:J:186:ALA:HB2	2.45	0.56
2:L:250:HIS:HA	2:L:254:SER:OG	2.06	0.56
1:A:67:LEU:HG	1:A:68:ILE:H	1.71	0.56
1:A:152:PHE:CE1	1:A:156:LEU:HD11	2.41	0.56
2:D:339:ASN:HD21	2:D:370:SER:HB3	1.71	0.56
1:G:163:PHE:CD1	1:G:163:PHE:C	2.84	0.56
2:H:154:PRO:HG3	2:H:191:PRO:HD2	1.88	0.56
2:H:296:ASP:O	2:H:298:ILE:HD12	2.06	0.56
2:L:120:TYR:HE2	2:L:147:MET:HE2	1.70	0.56
1:A:639:ARG:HB3	1:A:643:GLN:HB3	1.88	0.56
2:B:189:VAL:CG2	2:J:532:LYS:HE2	2.36	0.56
1:E:324:ALA:O	1:E:327:VAL:HG12	2.05	0.56
2:H:121:VAL:HG22	2:H:122:PHE:N	2.20	0.56
1:I:186:GLU:C	1:I:188:ASN:N	2.64	0.56
1:I:650:MET:HE2	1:I:650:MET:HA	1.88	0.56
1:K:517:LEU:HD21	1:K:632:ALA:HB1	1.87	0.56
2:L:460:VAL:CG2	2:L:496:ALA:HB2	2.36	0.56
1:A:92:ILE:HB	1:A:112:ILE:HG21	1.86	0.56
2:B:148:ALA:HB1	2:B:153:ALA:O	2.05	0.56
1:C:70:ASN:ND2	1:C:145:PHE:CD1	2.74	0.56
1:C:473:PHE:O	1:C:615:LYS:NZ	2.33	0.56
2:D:185:MET:HE3	2:L:529:MET:CE	2.36	0.56
1:E:363:LEU:HD13	1:E:455:TRP:HB3	1.88	0.56
2:F:436:GLY:O	2:F:439:TYR:HB3	2.05	0.56
1:G:683:GLU:H	1:G:704:LYS:HG2	1.71	0.56
2:H:492:ASN:ND2	2:H:494:PHE:H	2.03	0.56
1:I:117:ALA:CB	1:I:121:TYR:HB2	2.36	0.56
1:K:497:GLY:O	1:K:499:MET:HG2	2.05	0.56
1:K:537:GLU:HG3	1:K:553:ARG:NH2	2.21	0.56
1:A:523:ARG:C	1:A:590:MET:HE1	2.30	0.55
2:D:432:ARG:HG2	2:D:433:LYS:N	2.21	0.55
1:E:123:VAL:HG12	1:E:126:LYS:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:283:ILE:HG22	1:E:386:GLN:HG2	1.87	0.55
1:E:335:VAL:HG23	1:E:335:VAL:O	2.07	0.55
1:E:646:LEU:HD12	2:F:72:LEU:HD21	1.88	0.55
1:G:670:ILE:CD1	1:G:718:LEU:HD21	2.36	0.55
1:I:283:ILE:HD12	1:I:389:VAL:HG21	1.88	0.55
1:K:532:MET:HE1	1:K:603:ALA:CB	2.35	0.55
1:A:70:ASN:ND2	1:A:145:PHE:CD1	2.75	0.55
1:A:443:MET:HG3	1:A:444:TYR:CD1	2.41	0.55
2:B:189:VAL:HA	2:B:282:ASN:HD22	1.67	0.55
2:D:367:ASP:O	2:D:368:ILE:C	2.46	0.55
1:E:137:GLN:O	1:E:138:ALA:HB2	2.05	0.55
1:G:70:ASN:ND2	1:G:145:PHE:CD1	2.74	0.55
1:G:528:ALA:CB	1:G:605:LEU:HD22	2.36	0.55
1:I:376:VAL:C	1:I:378:ALA:N	2.64	0.55
1:K:177:LYS:HB3	1:K:181:LYS:NZ	2.21	0.55
2:L:307:PRO:HG3	2:L:312:THR:O	2.06	0.55
1:A:75:ALA:O	1:A:78:VAL:HG12	2.06	0.55
1:A:129:ALA:O	1:A:133:ALA:HB2	2.06	0.55
1:A:177:LYS:HB3	1:A:181:LYS:NZ	2.21	0.55
1:A:272:ILE:HB	1:A:335:VAL:CG2	2.35	0.55
1:A:538:ILE:O	1:A:541:THR:HB	2.06	0.55
1:E:378:ALA:O	1:E:379:GLY:C	2.50	0.55
1:E:421:ARG:HD2	1:E:474:GLU:HG3	1.87	0.55
1:E:484:PHE:O	1:E:487:ALA:HB3	2.06	0.55
2:H:78:SER:O	2:H:112:GLY:HA2	2.07	0.55
1:I:185:GLN:O	1:I:188:ASN:N	2.38	0.55
1:I:517:LEU:HD21	1:I:632:ALA:CB	2.36	0.55
1:K:75:ALA:O	1:K:78:VAL:HG12	2.06	0.55
1:K:394:TRP:CE3	1:K:459:ARG:HG3	2.41	0.55
1:A:338:ILE:HD12	1:A:338:ILE:N	2.21	0.55
1:A:683:GLU:H	1:A:704:LYS:HG2	1.70	0.55
2:F:492:ASN:HB2	2:F:493:PRO:HD2	1.88	0.55
1:G:283:ILE:HD12	1:G:389:VAL:CG2	2.37	0.55
1:G:376:VAL:C	1:G:378:ALA:N	2.62	0.55
1:G:380:GLU:CG	1:G:381:PRO:HD2	2.36	0.55
1:K:491:HIS:O	1:K:495:ILE:HG13	2.07	0.55
1:A:78:VAL:HA	1:A:370:VAL:HG11	1.88	0.55
1:A:517:LEU:HD21	1:A:632:ALA:CB	2.37	0.55
2:B:58:GLN:CD	2:B:63:LYS:HE3	2.31	0.55
2:B:419:TYR:CE1	2:B:443:SER:HB2	2.42	0.55
2:D:307:PRO:HG3	2:D:312:THR:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:346:ARG:HA	2:D:350:ARG:O	2.06	0.55
1:E:275:LEU:HD23	1:E:331:SER:O	2.06	0.55
1:G:92:ILE:HD12	1:G:112:ILE:HD13	1.87	0.55
1:G:443:MET:HG3	1:G:444:TYR:CE1	2.41	0.55
1:G:534:ARG:HH11	1:G:534:ARG:HG3	1.70	0.55
1:I:598:PRO:HD2	2:J:292:PHE:CE1	2.42	0.55
1:A:324:ALA:O	1:A:327:VAL:HG12	2.06	0.55
1:C:335:VAL:CG1	1:C:350:MET:HE3	2.37	0.55
2:D:65:THR:OG1	2:D:68:GLU:HG3	2.07	0.55
2:F:379:ARG:HD2	2:F:421:GLU:OE2	2.07	0.55
1:G:78:VAL:HG23	1:G:370:VAL:CG1	2.36	0.55
1:G:127:VAL:O	1:G:131:ILE:HG13	2.06	0.55
1:G:215:PRO:HB2	1:G:231:ILE:CG2	2.36	0.55
1:G:324:ALA:O	1:G:327:VAL:HG12	2.06	0.55
1:G:401:TYR:CD2	1:G:448:MET:HA	2.42	0.55
1:I:124:ILE:O	1:I:128:MET:HB2	2.05	0.55
1:I:661:MET:HE2	1:I:726:GLU:CA	2.35	0.55
1:K:229:MET:HG3	1:K:229:MET:O	2.06	0.55
1:C:123:VAL:HG12	1:C:126:LYS:H	1.70	0.55
2:D:154:PRO:HG3	2:D:191:PRO:HD2	1.89	0.55
2:F:160:ASP:OD1	2:F:198:GLY:HA3	2.06	0.55
2:F:196:ILE:HG22	2:F:221:SER:HB2	1.89	0.55
1:G:137:GLN:O	1:G:138:ALA:HB2	2.06	0.55
1:G:504:ILE:HG23	1:G:505:ALA:N	2.20	0.55
1:I:528:ALA:HB1	1:I:605:LEU:CD2	2.35	0.55
1:K:392:THR:O	1:K:455:TRP:HZ3	1.89	0.55
2:B:398:LEU:O	2:B:403:GLN:HG3	2.07	0.55
1:E:156:LEU:HD22	1:E:161:VAL:HB	1.89	0.55
1:G:517:LEU:HD21	1:G:632:ALA:CB	2.37	0.55
2:J:250:HIS:HA	2:J:254:SER:OG	2.07	0.55
1:A:358:HIS:HB2	1:A:369:LEU:HD12	1.88	0.55
1:C:163:PHE:CD1	1:C:163:PHE:C	2.85	0.55
1:C:334:THR:HG22	1:C:351:ASN:HB2	1.87	0.55
1:C:443:MET:HG3	1:C:444:TYR:CE1	2.42	0.55
1:E:275:LEU:HD23	1:E:276:CYS:N	2.21	0.55
1:E:401:TYR:HE2	1:E:448:MET:HB2	1.72	0.55
2:F:336:PHE:O	2:F:373:LYS:NZ	2.40	0.55
2:F:367:ASP:O	2:F:368:ILE:C	2.48	0.55
1:G:179:THR:O	1:G:183:ILE:HG13	2.07	0.55
1:G:401:TYR:HD2	1:G:448:MET:HA	1.71	0.55
1:G:464:GLU:HA	1:G:464:GLU:OE2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:517:LEU:HD22	1:K:517:LEU:N	2.17	0.55
1:A:117:ALA:C	1:A:119:GLN:N	2.65	0.55
2:B:235:THR:HG22	2:B:237:GLU:HB2	1.88	0.55
2:B:307:PRO:O	2:B:432:ARG:NH2	2.39	0.55
1:C:66:ILE:O	1:C:66:ILE:HG12	2.05	0.55
1:C:539:ARG:NH2	2:D:326:GLU:OE2	2.40	0.55
2:D:43:ARG:HG2	2:D:43:ARG:HH11	1.72	0.55
1:E:415:GLY:C	1:E:440:GLU:HG3	2.32	0.55
1:G:433:THR:HG22	1:G:434:GLY:N	2.21	0.55
2:H:498:GLU:HG2	2:J:87:THR:HG23	1.89	0.55
1:I:417:LEU:HD21	1:I:478:ILE:HD13	1.88	0.55
1:I:602:LEU:HD12	1:I:614:LEU:O	2.06	0.55
2:J:94:ASN:HA	2:J:98:GLN:OE1	2.06	0.55
1:K:433:THR:HG21	1:K:435:VAL:HG12	1.88	0.55
1:K:661:MET:HE2	1:K:726:GLU:CA	2.37	0.55
2:L:121:VAL:HG22	2:L:122:PHE:N	2.22	0.55
2:L:229:ASP:O	2:L:233:THR:HG23	2.06	0.55
2:L:382:ASP:OD1	2:L:424:VAL:HG13	2.06	0.55
2:B:324:ALA:HA	2:B:345:ILE:HD12	1.89	0.54
1:C:275:LEU:HD23	1:C:331:SER:O	2.06	0.54
1:C:316:MET:CE	1:C:337:PHE:HD1	2.19	0.54
1:C:598:PRO:HD2	2:D:292:PHE:CD1	2.42	0.54
2:D:309:ASN:HD21	2:D:311:ASN:HB2	1.72	0.54
1:E:405:PRO:HG2	1:E:481:ASN:HA	1.89	0.54
1:G:358:HIS:ND1	1:G:359:PRO:HD3	2.22	0.54
1:G:480:HIS:HD2	1:G:482:LEU:HB2	1.72	0.54
1:I:276:CYS:O	1:I:382:LEU:HD21	2.07	0.54
2:L:117:ARG:HH21	2:L:280:LEU:HG	1.72	0.54
1:A:97:ASP:OD1	1:A:102:HIS:HE1	1.90	0.54
1:A:264:VAL:HG13	1:A:340:ASP:CB	2.37	0.54
2:B:182:ARG:HG3	2:B:182:ARG:HH11	1.72	0.54
1:E:73:GLU:OE1	1:E:451:LYS:NZ	2.37	0.54
3:I:801:BTI:H63	2:J:399:PRO:HD3	1.89	0.54
2:J:522:LEU:HD23	2:L:151:ASN:HD21	1.71	0.54
1:K:563:LEU:O	1:K:565:GLY:N	2.40	0.54
1:A:543:VAL:HG12	1:A:544:SER:O	2.08	0.54
2:B:434:ALA:HB3	2:B:460:VAL:HG12	1.87	0.54
1:C:266:GLN:HG2	1:C:341:GLY:CA	2.38	0.54
2:D:43:ARG:HG2	2:D:43:ARG:NH1	2.22	0.54
1:E:283:ILE:HB	1:E:386:GLN:CD	2.32	0.54
1:E:365:THR:HG22	1:E:391:LEU:CD2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:335:VAL:CG1	1:G:350:MET:HE3	2.38	0.54
1:G:517:LEU:N	1:G:564:GLN:HE22	2.05	0.54
1:G:526:ALA:HA	1:G:561:VAL:HG11	1.90	0.54
1:G:646:LEU:HD12	2:H:72:LEU:HD11	1.89	0.54
1:I:458:THR:O	1:I:461:ALA:HB3	2.07	0.54
1:K:231:ILE:H	1:K:231:ILE:HD12	1.72	0.54
1:K:532:MET:O	1:K:535:VAL:HB	2.07	0.54
2:L:75:ASP:OD1	2:L:272:ARG:NH2	2.39	0.54
2:L:207:SER:HB3	2:L:208:PRO:CD	2.32	0.54
2:L:492:ASN:ND2	2:L:494:PHE:HB2	2.22	0.54
1:A:92:ILE:HD12	1:A:112:ILE:HD13	1.89	0.54
2:D:169:GLY:HA2	2:L:462:VAL:HG22	1.90	0.54
1:E:577:ASP:HB2	1:E:591:ARG:NH2	2.23	0.54
2:F:293:ASP:OD1	2:F:325:ASP:O	2.25	0.54
2:F:479:ILE:HD12	2:F:479:ILE:C	2.32	0.54
1:G:66:ILE:HD13	1:G:88:SER:O	2.06	0.54
1:G:78:VAL:HG13	1:G:79:ILE:N	2.21	0.54
1:G:415:GLY:C	1:G:440:GLU:HG3	2.32	0.54
1:G:491:HIS:O	1:G:495:ILE:HG13	2.06	0.54
2:J:156:ILE:HD12	2:J:156:ILE:N	2.21	0.54
1:K:304:PRO:HG2	1:K:394:TRP:CZ2	2.43	0.54
1:K:335:VAL:HG23	1:K:335:VAL:O	2.08	0.54
1:A:287:GLU:OE2	1:A:305:SER:N	2.36	0.54
1:C:411:LEU:HD22	1:C:682:GLN:HB2	1.90	0.54
2:D:492:ASN:ND2	2:D:494:PHE:H	2.01	0.54
2:F:83:ASP:HB3	2:F:86:VAL:HG23	1.90	0.54
1:G:75:ALA:O	1:G:78:VAL:HG12	2.07	0.54
2:J:49:GLY:C	2:J:51:GLY:H	2.16	0.54
2:B:141:ILE:O	2:B:145:MET:HG3	2.06	0.54
2:B:200:CYS:HB3	2:B:223:MET:HB3	1.88	0.54
2:B:291:PHE:CE1	2:B:348:GLU:HA	2.43	0.54
2:B:436:GLY:O	2:B:439:TYR:HB3	2.07	0.54
1:C:347:PHE:CD1	1:C:347:PHE:C	2.85	0.54
1:G:312:THR:O	1:G:316:MET:HG3	2.08	0.54
1:I:670:ILE:HD12	1:I:712:ALA:HB1	1.88	0.54
2:L:95:MET:O	2:L:95:MET:HE3	2.08	0.54
2:B:376:ARG:HH11	2:J:410:LYS:HZ2	1.55	0.54
1:C:380:GLU:CG	1:C:381:PRO:HD2	2.38	0.54
2:D:88:HIS:CD2	2:D:88:HIS:C	2.85	0.54
1:E:178:ILE:H	1:E:178:ILE:CD1	2.06	0.54
2:F:193:ILE:CD1	2:F:274:LEU:HD23	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:316:MET:CE	1:G:337:PHE:HD1	2.21	0.54
1:I:683:GLU:HB2	1:I:704:LYS:HG3	1.88	0.54
2:J:296:ASP:O	2:J:298:ILE:HD12	2.08	0.54
1:K:444:TYR:O	1:K:445:TYR:CG	2.61	0.54
2:L:95:MET:HE3	2:L:95:MET:CA	2.38	0.54
2:L:325:ASP:O	2:L:327:GLY:N	2.40	0.54
1:C:184:ALA:HB1	1:C:189:VAL:HB	1.90	0.54
1:C:401:TYR:CE2	1:C:448:MET:HB2	2.43	0.54
1:C:543:VAL:HG12	1:C:544:SER:O	2.08	0.54
2:D:49:GLY:O	2:D:51:GLY:N	2.41	0.54
1:E:74:ILE:HD13	1:E:143:TYR:CE2	2.42	0.54
2:F:374:ALA:HB3	2:F:415:LEU:HD13	1.90	0.54
1:G:347:PHE:O	1:G:347:PHE:CD1	2.61	0.54
2:H:307:PRO:O	2:H:432:ARG:NH2	2.41	0.54
1:I:518:PRO:HD2	1:I:521:ASP:HB2	1.89	0.54
2:J:447:LEU:C	2:J:448:ARG:HG2	2.32	0.54
1:K:123:VAL:HG12	1:K:126:LYS:H	1.73	0.54
2:L:239:VAL:HG22	2:L:243:GLU:HB2	1.89	0.54
1:A:392:THR:O	1:A:455:TRP:HZ3	1.90	0.54
1:A:534:ARG:HG3	1:A:534:ARG:HH11	1.72	0.54
1:C:444:TYR:CD1	1:C:444:TYR:N	2.76	0.54
2:D:298:ILE:HG23	2:D:509:ARG:HB2	1.90	0.54
1:E:189:VAL:CG2	1:E:323:LEU:HB2	2.36	0.54
1:E:354:LEU:C	1:E:354:LEU:HD13	2.33	0.54
1:E:491:HIS:CE1	1:E:493:LYS:HB2	2.43	0.54
2:F:476(C):ASP:C	2:F:477:GLU:H	2.15	0.54
1:G:695:MET:SD	2:H:313:PRO:HG3	2.48	0.54
1:I:324:ALA:O	1:I:327:VAL:HG12	2.08	0.54
1:I:358:HIS:ND1	1:I:359:PRO:HD3	2.21	0.54
2:J:149:MET:CE	2:J:189:VAL:HG11	2.38	0.54
1:K:190:SER:N	1:K:319:GLN:OE1	2.34	0.54
2:L:285:LYS:HB3	2:L:286:PRO:HD2	1.89	0.54
2:L:479:ILE:HD12	2:L:479:ILE:C	2.33	0.54
1:C:464:GLU:HA	1:C:464:GLU:OE2	2.08	0.54
2:D:95:MET:HE3	2:D:95:MET:HA	1.89	0.54
1:E:92:ILE:HB	1:E:112:ILE:CG2	2.37	0.54
1:E:283:ILE:CG2	1:E:386:GLN:HG2	2.38	0.54
2:F:337:ALA:HB1	2:F:370:SER:HA	1.90	0.54
1:G:66:ILE:O	1:G:66:ILE:HG12	2.06	0.54
1:G:316:MET:HE3	1:G:337:PHE:HD1	1.73	0.54
1:G:335:VAL:O	1:G:335:VAL:HG23	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:155:ALA:O	1:I:159:GLU:HG2	2.08	0.54
1:I:367:VAL:HG12	1:I:368:ASP:N	2.22	0.54
1:K:441:ILE:HD12	1:K:478:ILE:HD13	1.89	0.54
1:A:444:TYR:CD1	1:A:444:TYR:N	2.76	0.53
1:A:552:GLU:H	1:A:552:GLU:CD	2.16	0.53
2:B:298:ILE:N	2:B:298:ILE:HD12	2.23	0.53
1:C:267:PRO:O	1:C:501:THR:HG23	2.07	0.53
1:C:517:LEU:H	1:C:564:GLN:HE22	1.55	0.53
2:D:42:ARG:O	2:D:45:ALA:HB3	2.08	0.53
1:E:63:PHE:N	1:E:63:PHE:CD1	2.76	0.53
1:E:515:VAL:HB	1:E:631:GLY:C	2.33	0.53
1:E:517:LEU:HD21	1:E:632:ALA:HB1	1.90	0.53
1:G:304:PRO:O	1:G:394:TRP:CH2	2.61	0.53
2:H:83:ASP:HB3	2:H:86:VAL:HG21	1.88	0.53
1:I:354:LEU:HD11	1:I:358:HIS:ND1	2.23	0.53
1:I:670:ILE:CD1	1:I:718:LEU:HD21	2.38	0.53
2:J:200:CYS:HB3	2:J:223:MET:HB3	1.90	0.53
1:K:143:TYR:CZ	1:K:356:VAL:HG22	2.43	0.53
1:K:670:ILE:CD1	1:K:718:LEU:HD21	2.38	0.53
2:L:436:GLY:O	2:L:439:TYR:HB3	2.07	0.53
1:A:99:GLN:HB2	1:A:436:TYR:OH	2.08	0.53
2:B:109:THR:HG22	2:B:122:PHE:CB	2.38	0.53
1:C:358:HIS:HB2	1:C:369:LEU:HD12	1.90	0.53
1:C:376:VAL:C	1:C:378:ALA:N	2.63	0.53
1:C:400:LEU:HD11	1:C:482:LEU:HD13	1.90	0.53
1:E:283:ILE:HD12	1:E:389:VAL:HG21	1.89	0.53
1:E:457:PRO:CG	1:E:458:THR:H	2.14	0.53
1:E:534:ARG:HH11	1:E:534:ARG:HG3	1.73	0.53
1:G:218:ILE:CD1	1:G:260:ILE:HG12	2.38	0.53
1:G:518:PRO:O	1:G:521:ASP:N	2.36	0.53
2:H:193:ILE:CD1	2:H:274:LEU:HD23	2.38	0.53
1:K:129:ALA:O	1:K:133:ALA:HB2	2.07	0.53
1:K:537:GLU:HG3	1:K:553:ARG:HH21	1.72	0.53
1:K:666:MET:HE3	1:K:690:ILE:HD12	1.89	0.53
1:A:463:ILE:HD12	1:A:494:PHE:CE1	2.44	0.53
1:E:272:ILE:HB	1:E:335:VAL:CG2	2.38	0.53
1:E:276:CYS:O	1:E:382:LEU:HD21	2.08	0.53
2:F:49:GLY:C	2:F:51:GLY:H	2.15	0.53
1:G:312:THR:HG21	1:G:343:LYS:HD3	1.90	0.53
1:G:457:PRO:HG2	1:G:458:THR:N	2.17	0.53
2:H:346:ARG:HH11	2:H:346:ARG:HG3	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:66:ILE:O	1:K:66:ILE:HG12	2.08	0.53
1:K:670:ILE:HD12	1:K:712:ALA:HB1	1.90	0.53
2:L:43:ARG:HG2	2:L:43:ARG:HH11	1.74	0.53
2:B:94:ASN:HA	2:B:98:GLN:OE1	2.08	0.53
2:B:145:MET:HE1	2:B:183:ASN:HD21	1.68	0.53
2:B:299:GLU:HG3	2:B:322:LYS:HB3	1.89	0.53
1:C:283:ILE:HB	1:C:386:GLN:CD	2.33	0.53
2:D:339:ASN:ND2	2:D:370:SER:HB3	2.24	0.53
1:E:118:ASN:C	1:E:119:GLN:HG3	2.34	0.53
1:E:136:ALA:HB1	1:E:161:VAL:CG1	2.33	0.53
1:E:186:GLU:C	1:E:188:ASN:N	2.63	0.53
1:E:334:THR:CG2	1:E:351:ASN:HB2	2.39	0.53
1:E:543:VAL:HG11	2:F:117:ARG:HD2	1.89	0.53
1:E:625:PHE:N	1:E:625:PHE:CD1	2.76	0.53
1:G:177:LYS:O	1:G:181:LYS:HG2	2.08	0.53
2:H:149:MET:CE	2:H:189:VAL:HG11	2.39	0.53
1:I:285:LEU:HD12	1:I:285:LEU:N	2.23	0.53
1:I:304:PRO:O	1:I:394:TRP:CH2	2.61	0.53
1:I:304:PRO:HG2	1:I:394:TRP:CZ2	2.44	0.53
1:I:523:ARG:HB3	1:I:590:MET:CE	2.38	0.53
1:K:71:ARG:HG3	1:K:72:GLY:N	2.24	0.53
1:A:272:ILE:HB	1:A:335:VAL:HG23	1.90	0.53
1:A:295:ARG:O	1:A:296:ASN:HB2	2.09	0.53
1:A:626:ARG:C	1:A:627:ILE:HD12	2.33	0.53
1:A:683:GLU:HB2	1:A:704:LYS:HG3	1.90	0.53
2:B:460:VAL:HG21	2:B:496:ALA:CB	2.35	0.53
1:C:334:THR:HG21	1:C:355:GLN:HE21	1.72	0.53
2:D:337:ALA:HB3	2:D:373:LYS:CD	2.39	0.53
1:E:312:THR:O	1:E:315:ALA:HB3	2.09	0.53
1:I:78:VAL:HG23	1:I:370:VAL:HG11	1.90	0.53
1:I:184:ALA:HB1	1:I:189:VAL:HB	1.91	0.53
1:I:392:THR:O	1:I:455:TRP:HZ3	1.91	0.53
1:K:132:ARG:HD3	1:K:159:GLU:OE1	2.08	0.53
1:K:338:ILE:HD12	1:K:338:ILE:N	2.23	0.53
1:A:380:GLU:HG2	1:A:381:PRO:HD2	1.90	0.53
1:A:400:LEU:HD11	1:A:482:LEU:HD13	1.90	0.53
1:A:670:ILE:HD12	1:A:712:ALA:HB1	1.90	0.53
1:E:67:LEU:HG	1:E:68:ILE:H	1.72	0.53
1:E:283:ILE:HA	1:E:386:GLN:NE2	2.24	0.53
1:E:292:ILE:HG23	1:E:503:PHE:CD2	2.43	0.53
1:E:443:MET:HG3	1:E:444:TYR:CE1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:54:ARG:O	2:F:57:ALA:HB3	2.07	0.53
2:F:251:THR:HG21	2:F:260:ALA:HB2	1.90	0.53
1:G:598:PRO:HD2	2:H:292:PHE:CE1	2.44	0.53
1:G:642:ARG:NH1	2:H:71:ASP:OD2	2.41	0.53
1:I:283:ILE:HB	1:I:386:GLN:CD	2.33	0.53
1:K:292:ILE:HD13	1:K:300:VAL:O	2.09	0.53
1:A:66:ILE:HG12	1:A:66:ILE:O	2.08	0.53
2:B:149:MET:CE	2:B:189:VAL:HG11	2.39	0.53
2:B:346:ARG:HH11	2:B:346:ARG:HG3	1.74	0.53
1:C:444:TYR:O	1:C:445:TYR:CG	2.62	0.53
2:D:184:ILE:CD1	2:L:417:TYR:HA	2.39	0.53
1:E:150:SER:O	1:E:151:LYS:C	2.51	0.53
1:E:279:HIS:HD2	1:E:380:GLU:O	1.92	0.53
1:E:376:VAL:C	1:E:378:ALA:H	2.15	0.53
2:F:469:THR:HG23	2:F:482:HIS:HB3	1.91	0.53
2:F:484:ALA:O	2:F:488:GLU:OE1	2.27	0.53
1:I:163:PHE:CD1	1:I:163:PHE:C	2.86	0.53
2:J:346:ARG:HA	2:J:350:ARG:O	2.08	0.53
1:K:117:ALA:C	1:K:119:GLN:N	2.66	0.53
1:K:279:HIS:NE2	1:K:380:GLU:N	2.57	0.53
1:A:140:HIS:ND1	1:A:141:PRO:HD2	2.24	0.53
1:A:458:THR:O	1:A:461:ALA:HB3	2.09	0.53
1:C:128:MET:SD	1:C:131:ILE:HD12	2.48	0.53
1:E:155:ALA:O	1:E:159:GLU:HG2	2.09	0.53
2:H:346:ARG:HG3	2:H:346:ARG:NH1	2.23	0.53
1:I:131:ILE:CG2	1:I:136:ALA:HB2	2.29	0.53
2:J:325:ASP:C	2:J:327:GLY:H	2.17	0.53
2:J:379:ARG:HD2	2:J:421:GLU:OE2	2.09	0.53
2:L:58:GLN:CD	2:L:63:LYS:HE3	2.32	0.53
1:A:308:LEU:HD12	1:A:308:LEU:O	2.09	0.53
1:C:289:GLU:OE1	1:C:306:PRO:HD2	2.08	0.53
1:C:534:ARG:HH11	1:C:534:ARG:HG3	1.74	0.53
1:E:70:ASN:OD1	1:E:74:ILE:HG21	2.09	0.53
1:E:532:MET:HE1	1:E:603:ALA:CB	2.39	0.53
1:G:338:ILE:HD12	1:G:338:ILE:N	2.23	0.53
1:G:444:TYR:O	1:G:445:TYR:CG	2.62	0.53
1:G:675:VAL:CG1	1:G:707:VAL:HG21	2.38	0.53
1:I:411:LEU:HD22	1:I:682:GLN:CB	2.38	0.53
1:I:504:ILE:HG23	1:I:505:ALA:N	2.24	0.53
1:I:528:ALA:CB	1:I:605:LEU:HD22	2.36	0.53
2:J:109:THR:HG22	2:J:122:PHE:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:85:MET:O	1:K:87:ILE:HG13	2.09	0.53
2:L:83:ASP:HB3	2:L:86:VAL:CG2	2.38	0.53
2:L:424:VAL:O	2:L:525:LYS:NZ	2.38	0.53
2:L:501:PHE:N	2:L:501:PHE:CD2	2.75	0.53
1:C:114:PRO:HB2	1:C:115:PRO:HD2	1.91	0.53
1:C:156:LEU:HD22	1:C:161:VAL:HB	1.91	0.53
1:C:393:GLY:HA2	1:C:457:PRO:O	2.09	0.53
1:G:66:ILE:CD1	1:G:87:ILE:HG22	2.33	0.53
1:G:146:LEU:HD23	1:G:152:PHE:CD2	2.43	0.53
2:H:160:ASP:OD1	2:H:198:GLY:HA3	2.09	0.53
2:H:390:THR:HG23	2:H:419:TYR:OH	2.09	0.53
1:I:444:TYR:O	1:I:445:TYR:CG	2.62	0.53
1:K:78:VAL:HG13	1:K:79:ILE:N	2.24	0.53
1:K:124:ILE:O	1:K:128:MET:HB2	2.09	0.53
2:B:58:GLN:HE21	2:B:61:ARG:HH21	1.58	0.52
2:B:469:THR:HG23	2:B:482:HIS:HB3	1.91	0.52
1:C:335:VAL:HG23	1:C:335:VAL:O	2.09	0.52
2:D:95:MET:HE3	2:D:95:MET:O	2.09	0.52
2:D:114:ILE:O	2:D:115:ASN:HB2	2.08	0.52
1:E:78:VAL:CG1	1:E:79:ILE:N	2.72	0.52
1:E:272:ILE:HB	1:E:335:VAL:HG23	1.90	0.52
2:F:458:ALA:HB3	2:F:493:PRO:HB3	1.90	0.52
2:F:476(A):LEU:C	2:F:476(C):ASP:H	2.16	0.52
1:G:71:ARG:HG3	1:G:72:GLY:N	2.24	0.52
2:H:58:GLN:HE21	2:H:61:ARG:HH21	1.57	0.52
1:I:65:LYS:HE2	1:I:134:THR:O	2.10	0.52
1:I:66:ILE:HD13	1:I:88:SER:O	2.09	0.52
1:I:112:ILE:O	1:I:120:SER:HA	2.09	0.52
1:I:517:LEU:HD21	1:I:632:ALA:HB1	1.92	0.52
2:J:207:SER:HB3	2:J:208:PRO:CD	2.34	0.52
2:J:501:PHE:N	2:J:501:PHE:CD2	2.75	0.52
1:K:271:GLU:O	1:K:287:GLU:HB2	2.10	0.52
1:K:393:GLY:HA2	1:K:457:PRO:O	2.09	0.52
2:B:297:ARG:HG2	2:B:297:ARG:HH11	1.74	0.52
2:B:535:ASP:OD2	2:J:379:ARG:NH2	2.41	0.52
1:C:517:LEU:HD22	1:C:517:LEU:N	2.17	0.52
2:D:185:MET:HE3	2:L:529:MET:HE2	1.90	0.52
1:E:289:GLU:OE1	1:E:306:PRO:HD2	2.09	0.52
2:F:300:PRO:HA	2:F:509:ARG:NH1	2.24	0.52
2:F:394:VAL:HG23	2:F:395:PRO:HD2	1.92	0.52
2:F:416:LEU:HG	2:H:210:MET:HE1	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:484:ALA:O	2:H:488:GLU:OE1	2.28	0.52
1:I:132:ARG:HD3	1:I:159:GLU:OE1	2.09	0.52
1:I:275:LEU:HD11	1:I:372:GLN:HB2	1.90	0.52
1:I:390:LYS:HD3	1:I:391:LEU:H	1.71	0.52
2:J:178:GLU:HB3	2:J:182:ARG:NH1	2.24	0.52
1:K:122:ILE:HA	1:K:146:LEU:CD1	2.39	0.52
1:K:312:THR:O	1:K:316:MET:HG3	2.09	0.52
1:K:528:ALA:HB1	1:K:605:LEU:CD2	2.39	0.52
1:K:543:VAL:CG1	2:L:117:ARG:HD2	2.37	0.52
1:K:670:ILE:CG1	1:K:718:LEU:HD21	2.39	0.52
2:L:416:LEU:HB2	2:L:441:VAL:HG22	1.91	0.52
1:A:132:ARG:HD3	1:A:159:GLU:OE1	2.09	0.52
1:A:658:THR:OG1	1:A:702:GLU:HG2	2.10	0.52
1:C:189:VAL:HA	1:C:319:GLN:OE1	2.09	0.52
1:C:317:GLY:O	1:C:321:VAL:HG12	2.10	0.52
1:C:378:ALA:O	1:C:379:GLY:C	2.51	0.52
2:D:239:VAL:HG22	2:D:243:GLU:HB2	1.91	0.52
1:E:393:GLY:HA3	1:E:455:TRP:CZ3	2.45	0.52
1:G:283:ILE:HA	1:G:386:GLN:NE2	2.24	0.52
2:H:239:VAL:HG22	2:H:243:GLU:HB2	1.92	0.52
1:I:646:LEU:HD12	2:J:72:LEU:HD21	1.92	0.52
1:K:70:ASN:ND2	1:K:145:PHE:CD1	2.78	0.52
1:K:464:GLU:OE2	1:K:464:GLU:HA	2.10	0.52
2:L:149:MET:CE	2:L:189:VAL:CG1	2.87	0.52
1:A:78:VAL:HG23	1:A:370:VAL:CG1	2.40	0.52
2:D:476(C):ASP:C	2:D:477:GLU:H	2.17	0.52
1:E:107:ASP:C	1:E:108:GLU:HG3	2.34	0.52
1:E:444:TYR:CD1	1:E:444:TYR:N	2.78	0.52
2:F:141:ILE:O	2:F:145:MET:HG3	2.08	0.52
2:F:193:ILE:HD13	2:F:274:LEU:HD23	1.90	0.52
2:H:123:SER:HA	2:H:158:ILE:HB	1.91	0.52
1:I:358:HIS:N	1:I:359:PRO:CD	2.72	0.52
2:J:492:ASN:ND2	2:J:494:PHE:H	2.06	0.52
1:K:458:THR:O	1:K:461:ALA:HB3	2.09	0.52
1:A:163:PHE:CD1	1:A:163:PHE:C	2.87	0.52
1:A:401:TYR:HE2	1:A:448:MET:HB2	1.74	0.52
1:A:543:VAL:HG11	2:B:117:ARG:HD2	1.91	0.52
2:B:192:GLN:O	2:B:211:THR:HB	2.10	0.52
2:B:296:ASP:O	2:B:298:ILE:HD12	2.09	0.52
2:B:416:LEU:CG	2:J:210:MET:HE1	2.37	0.52
1:C:68:ILE:HG22	1:C:70:ASN:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:LYS:O	1:C:181:LYS:HG2	2.10	0.52
1:C:614:LEU:HD22	1:C:627:ILE:HG21	1.91	0.52
1:C:646:LEU:HD13	2:D:64:LEU:HD13	1.92	0.52
1:E:376:VAL:C	1:E:378:ALA:N	2.66	0.52
2:F:309:ASN:HD21	2:F:311:ASN:HB2	1.74	0.52
1:G:661:MET:HE2	1:G:726:GLU:CA	2.38	0.52
1:I:401:TYR:CD2	1:I:448:MET:HA	2.44	0.52
1:A:316:MET:CE	1:A:337:PHE:HD1	2.23	0.52
1:C:92:ILE:HB	1:C:112:ILE:CG2	2.38	0.52
1:C:292:ILE:H	1:C:292:ILE:CD1	1.96	0.52
1:E:70:ASN:ND2	1:E:145:PHE:CD1	2.77	0.52
1:E:78:VAL:HG23	1:E:370:VAL:CG1	2.39	0.52
1:E:163:PHE:CD1	1:E:163:PHE:C	2.87	0.52
1:E:628:ARG:HG3	1:E:633:ASP:HA	1.90	0.52
2:F:254:SER:OG	2:F:256:VAL:HG23	2.10	0.52
1:G:405:PRO:HG2	1:G:481:ASN:HA	1.90	0.52
1:I:140:HIS:ND1	1:I:141:PRO:HD2	2.25	0.52
1:I:295:ARG:O	1:I:296:ASN:HB2	2.10	0.52
1:I:428(L):ALA:HB3	1:I:455:TRP:HD1	1.75	0.52
1:I:480:HIS:HD2	1:I:482:LEU:HB2	1.73	0.52
1:A:283:ILE:HA	1:A:386:GLN:NE2	2.24	0.52
1:A:517:LEU:H	1:A:564:GLN:HE22	1.58	0.52
2:B:42:ARG:HG2	2:B:42:ARG:NH1	2.24	0.52
1:C:543:VAL:HG11	2:D:117:ARG:HD2	1.92	0.52
1:C:712:ALA:HA	1:C:716:ASN:ND2	2.25	0.52
1:E:189:VAL:HA	1:E:319:GLN:OE1	2.09	0.52
1:E:362:GLU:HG2	1:E:367:VAL:O	2.09	0.52
2:F:42:ARG:HG2	2:F:42:ARG:NH1	2.24	0.52
1:G:630:ARG:C	1:G:632:ALA:N	2.65	0.52
2:H:492:ASN:HB2	2:H:493:PRO:HD2	1.91	0.52
1:I:75:ALA:O	1:I:78:VAL:HG12	2.10	0.52
2:J:58:GLN:CD	2:J:63:LYS:HE3	2.34	0.52
1:K:99:GLN:HB2	1:K:436:TYR:OH	2.09	0.52
1:A:66:ILE:HD13	1:A:88:SER:O	2.09	0.52
1:C:117:ALA:CB	1:C:121:TYR:HB2	2.40	0.52
1:C:131:ILE:CG2	1:C:136:ALA:HB2	2.34	0.52
1:C:156:LEU:HD13	1:C:163:PHE:HB2	1.91	0.52
1:C:164:VAL:HG23	1:C:373:MET:O	2.09	0.52
2:D:51:GLY:O	2:D:55:ILE:HG13	2.10	0.52
2:D:109:THR:HG22	2:D:122:PHE:HB2	1.90	0.52
2:D:180:PHE:O	2:D:184:ILE:HG13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:189:VAL:HA	2:D:282:ASN:ND2	2.24	0.52
2:D:417:TYR:HA	2:L:184:ILE:CD1	2.39	0.52
1:E:504:ILE:CG2	1:E:505:ALA:N	2.73	0.52
1:G:283:ILE:HB	1:G:386:GLN:CD	2.35	0.52
1:G:444:TYR:CD1	1:G:444:TYR:N	2.77	0.52
2:H:200:CYS:HB3	2:H:223:MET:HB3	1.92	0.52
1:I:596:TRP:CG	1:I:597:THR:N	2.77	0.52
1:K:463:ILE:HD12	1:K:494:PHE:CE1	2.44	0.52
1:K:634:LEU:N	1:K:634:LEU:HD23	2.24	0.52
1:A:137:GLN:O	1:A:138:ALA:HB2	2.08	0.52
1:C:177:LYS:HB3	1:C:181:LYS:NZ	2.25	0.52
1:C:185:GLN:O	1:C:188:ASN:N	2.41	0.52
2:D:124:GLN:HE21	2:D:137:HIS:CE1	2.27	0.52
2:D:231:VAL:O	2:D:235:THR:HB	2.10	0.52
1:E:320:ALA:HB1	1:E:335:VAL:HG21	1.91	0.52
2:F:117:ARG:HH21	2:F:280:LEU:HG	1.74	0.52
2:H:261:PHE:CD1	2:H:267:ALA:HA	2.45	0.52
1:K:140:HIS:ND1	1:K:141:PRO:HD2	2.24	0.52
1:K:163:PHE:CD1	1:K:163:PHE:C	2.88	0.52
1:K:534:ARG:HH11	1:K:534:ARG:HG3	1.74	0.52
2:L:261:PHE:CD1	2:L:267:ALA:HA	2.44	0.52
1:A:83:ARG:CZ	1:A:83:ARG:HB3	2.40	0.52
1:A:693:MET:HE1	2:B:398:LEU:HD13	1.92	0.52
1:C:93:TYR:HA	1:C:121:TYR:OH	2.10	0.52
1:E:71:ARG:HG3	1:E:72:GLY:N	2.24	0.52
1:E:117:ALA:C	1:E:119:GLN:N	2.68	0.52
2:F:185:MET:HE3	2:H:529:MET:CE	2.40	0.52
2:F:501:PHE:CD2	2:F:501:PHE:N	2.74	0.52
1:G:457:PRO:CG	1:G:458:THR:H	2.14	0.52
1:G:494:PHE:HA	1:G:499:MET:CE	2.40	0.52
1:G:577:ASP:HB2	1:G:591:ARG:NH2	2.24	0.52
2:H:335:GLU:HA	2:H:338:LYS:HE2	1.91	0.52
2:J:95:MET:HA	2:J:95:MET:HE3	1.92	0.52
1:K:289:GLU:OE1	1:K:306:PRO:HD2	2.10	0.52
1:K:630:ARG:C	1:K:632:ALA:H	2.17	0.52
2:B:51:GLY:O	2:B:55:ILE:HG13	2.09	0.51
2:B:78:SER:O	2:B:112:GLY:HA2	2.10	0.51
2:D:182:ARG:HH11	2:D:182:ARG:HG3	1.73	0.51
1:E:354:LEU:HD11	1:E:358:HIS:ND1	2.25	0.51
1:I:316:MET:HB3	1:I:337:PHE:CE1	2.44	0.51
1:I:403:GLU:O	1:I:405:PRO:HD3	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:340:ILE:HD13	2:J:374:ALA:HB2	1.92	0.51
1:K:189:VAL:HA	1:K:319:GLN:OE1	2.09	0.51
2:L:368:ILE:HG13	2:L:408:VAL:HG13	1.92	0.51
1:A:164:VAL:HG22	1:A:373:MET:HE2	1.92	0.51
1:A:190:SER:N	1:A:319:GLN:OE1	2.33	0.51
1:A:393:GLY:HA3	1:A:455:TRP:CZ3	2.45	0.51
1:A:415:GLY:C	1:A:440:GLU:HG3	2.34	0.51
1:A:653:LYS:H	1:A:653:LYS:CD	2.09	0.51
2:B:95:MET:CA	2:B:95:MET:HE3	2.41	0.51
2:B:232:LYS:O	2:B:236:ASN:N	2.37	0.51
2:B:458:ALA:HB3	2:B:493:PRO:HB3	1.93	0.51
1:E:146:LEU:HD23	1:E:152:PHE:CD2	2.44	0.51
1:G:117:ALA:CB	1:G:121:TYR:HB2	2.39	0.51
1:G:363:LEU:HD13	1:G:455:TRP:HB3	1.92	0.51
1:I:177:LYS:O	1:I:181:LYS:HG2	2.09	0.51
2:J:222:TYR:HB2	2:J:245:GLY:O	2.10	0.51
1:A:275:LEU:HD23	1:A:276:CYS:N	2.25	0.51
1:A:497:GLY:O	1:A:499:MET:HG2	2.11	0.51
1:A:660:LYS:C	1:A:661:MET:HE3	2.36	0.51
2:B:300:PRO:HA	2:B:509:ARG:NH1	2.26	0.51
2:D:210:MET:HE1	2:L:416:LEU:HG	1.91	0.51
1:E:538:ILE:O	1:E:541:THR:HB	2.11	0.51
2:F:94:ASN:HA	2:F:98:GLN:OE1	2.11	0.51
2:H:42:ARG:HG2	2:H:42:ARG:NH1	2.24	0.51
1:I:71:ARG:HG3	1:I:72:GLY:N	2.25	0.51
1:I:524:ARG:N	1:I:590:MET:HE1	2.25	0.51
1:I:639:ARG:HB3	1:I:643:GLN:HB3	1.90	0.51
2:J:382:ASP:OD1	2:J:424:VAL:HG13	2.10	0.51
2:J:445:LYS:HE3	2:J:503:ASP:OD1	2.10	0.51
1:K:63:PHE:CD1	1:K:63:PHE:N	2.78	0.51
1:K:124:ILE:HG23	1:K:152:PHE:HD2	1.74	0.51
1:K:189:VAL:CG2	1:K:323:LEU:HB2	2.40	0.51
1:A:467:ARG:O	1:A:467:ARG:HD2	2.11	0.51
2:B:522:LEU:HD23	2:F:151:ASN:ND2	2.24	0.51
1:C:347:PHE:CD1	1:C:347:PHE:O	2.63	0.51
1:E:464:GLU:HA	1:E:464:GLU:OE2	2.10	0.51
1:E:517:LEU:H	1:E:564:GLN:HE22	1.58	0.51
1:E:517:LEU:HD22	1:E:517:LEU:N	2.22	0.51
1:I:400:LEU:HD21	1:I:482:LEU:HD13	1.92	0.51
2:J:273:ARG:HD2	2:J:330:TYR:HD1	1.75	0.51
1:K:380:GLU:CG	1:K:381:PRO:HD2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:563:LEU:HD23	1:K:636:VAL:HG22	1.92	0.51
2:B:89:ARG:NH1	2:D:499:ARG:HH21	2.08	0.51
2:B:207:SER:HB3	2:B:208:PRO:CD	2.35	0.51
1:C:528:ALA:HB1	1:C:605:LEU:HD22	1.92	0.51
2:D:416:LEU:CG	2:L:210:MET:HE1	2.41	0.51
1:E:401:TYR:CE2	1:E:448:MET:HB2	2.46	0.51
2:F:185:MET:HE3	2:H:529:MET:HE2	1.92	0.51
1:G:123:VAL:HG12	1:G:126:LYS:H	1.76	0.51
1:G:400:LEU:HD11	1:G:482:LEU:CD1	2.39	0.51
1:I:124:ILE:HG22	1:I:128:MET:HE2	1.93	0.51
1:I:164:VAL:HG22	1:I:373:MET:HE2	1.92	0.51
1:I:441:ILE:HD12	1:I:478:ILE:HD13	1.91	0.51
1:I:658:THR:OG1	1:I:702:GLU:HG2	2.11	0.51
1:K:319:GLN:NE2	1:K:345:PHE:CE1	2.78	0.51
1:K:358:HIS:N	1:K:359:PRO:CD	2.74	0.51
1:A:189:VAL:HA	1:A:319:GLN:OE1	2.10	0.51
2:B:150:GLN:HG2	2:D:527:VAL:HG22	1.93	0.51
2:B:178:GLU:HB3	2:B:182:ARG:NH1	2.25	0.51
1:C:275:LEU:HD23	1:C:276:CYS:N	2.26	0.51
1:C:316:MET:HE2	1:C:337:PHE:HD1	1.76	0.51
1:C:403:GLU:O	1:C:405:PRO:HD3	2.11	0.51
1:G:303:ALA:HB3	1:G:360:VAL:HG12	1.93	0.51
1:G:390:LYS:HD3	1:G:390:LYS:C	2.34	0.51
2:J:108:VAL:O	2:J:122:PHE:HA	2.09	0.51
1:K:207:LYS:HD2	1:K:207:LYS:O	2.11	0.51
1:K:679:GLN:O	1:K:706:VAL:HG13	2.11	0.51
2:L:43:ARG:HG2	2:L:43:ARG:NH1	2.25	0.51
2:B:95:MET:HE3	2:B:95:MET:HA	1.92	0.51
1:C:304:PRO:HD2	1:C:394:TRP:CE2	2.46	0.51
1:C:433:THR:HG22	1:C:434:GLY:N	2.24	0.51
1:C:547:MET:O	1:C:548:ASP:C	2.52	0.51
1:C:551:HIS:HE1	2:F:348:GLU:OE2	1.94	0.51
1:G:497:GLY:HA2	1:G:499:MET:HE3	1.92	0.51
2:H:196:ILE:HD13	2:H:214:ILE:HG23	1.93	0.51
1:K:418:THR:O	1:K:437:GLU:HG3	2.11	0.51
2:B:379:ARG:HD2	2:B:421:GLU:OE2	2.11	0.51
1:C:362:GLU:HG2	1:C:367:VAL:O	2.11	0.51
1:C:400:LEU:HD21	1:C:482:LEU:CD1	2.41	0.51
2:D:501:PHE:N	2:D:501:PHE:CD2	2.77	0.51
1:E:124:ILE:O	1:E:128:MET:HB2	2.11	0.51
1:E:140:HIS:ND1	1:E:141:PRO:HD2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:264:VAL:O	1:E:267:PRO:HD3	2.11	0.51
1:E:392:THR:O	1:E:455:TRP:HZ3	1.94	0.51
2:H:356:ALA:CB	2:H:391:LEU:HB2	2.41	0.51
1:I:415:GLY:O	1:I:440:GLU:HG3	2.10	0.51
1:I:444:TYR:CD1	1:I:444:TYR:N	2.78	0.51
1:K:206:VAL:HG13	1:K:235:ASP:HB3	1.93	0.51
1:K:363:LEU:HD13	1:K:455:TRP:HB3	1.93	0.51
1:A:517:LEU:H	1:A:517:LEU:CD2	2.15	0.51
1:A:614:LEU:HD22	1:A:627:ILE:HG21	1.92	0.51
2:B:75:ASP:OD1	2:B:272:ARG:NH2	2.43	0.51
1:C:279:HIS:HD2	1:C:380:GLU:O	1.93	0.51
1:C:324:ALA:O	1:C:327:VAL:HG12	2.11	0.51
1:C:415:GLY:C	1:C:440:GLU:HG3	2.36	0.51
1:E:458:THR:O	1:E:461:ALA:HB3	2.10	0.51
1:E:517:LEU:H	1:E:517:LEU:CD2	2.21	0.51
2:F:43:ARG:HG2	2:F:43:ARG:NH1	2.26	0.51
2:H:416:LEU:HB2	2:H:441:VAL:HG22	1.92	0.51
2:J:307:PRO:HG3	2:J:312:THR:O	2.10	0.51
1:K:179:THR:O	1:K:183:ILE:HG13	2.11	0.51
1:K:316:MET:O	1:K:320:ALA:HB2	2.11	0.51
1:K:365:THR:HG22	1:K:391:LEU:HD22	1.92	0.51
1:K:403:GLU:O	1:K:405:PRO:HD3	2.10	0.51
1:A:139:VAL:O	1:A:164:VAL:HG12	2.11	0.51
1:A:515:VAL:HG21	1:A:631:GLY:HA3	1.93	0.51
2:B:49:GLY:C	2:B:51:GLY:H	2.18	0.51
1:C:85:MET:O	1:C:86:GLY:C	2.53	0.51
1:C:97:ASP:OD1	1:C:102:HIS:HE1	1.94	0.51
1:E:164:VAL:HG23	1:E:373:MET:O	2.10	0.51
1:E:547:MET:O	1:E:548:ASP:C	2.52	0.51
2:F:539:LEU:OXT	2:H:372:ARG:NH2	2.44	0.51
1:G:186:GLU:C	1:G:188:ASN:N	2.68	0.51
1:G:320:ALA:HB1	1:G:335:VAL:HG21	1.94	0.51
2:H:50:GLY:O	2:H:54:ARG:HD2	2.11	0.51
1:I:283:ILE:HG22	1:I:386:GLN:HG2	1.93	0.51
1:I:362:GLU:HG2	1:I:367:VAL:O	2.11	0.51
1:K:283:ILE:HA	1:K:386:GLN:NE2	2.24	0.51
2:L:346:ARG:HA	2:L:350:ARG:O	2.10	0.51
1:A:393:GLY:HA2	1:A:457:PRO:O	2.11	0.50
1:A:537:GLU:HG3	1:A:553:ARG:NH2	2.26	0.50
2:D:178:GLU:O	2:D:182:ARG:HG3	2.10	0.50
2:D:462:VAL:HG22	2:L:169:GLY:HA2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:801:BTI:HD3	2:F:399:PRO:HD3	1.92	0.50
1:G:100:ALA:HB3	1:G:103:VAL:HG23	1.93	0.50
1:G:275:LEU:HD23	1:G:276:CYS:H	1.75	0.50
1:G:400:LEU:HD21	1:G:482:LEU:CD1	2.40	0.50
1:I:272:ILE:HB	1:I:335:VAL:CG2	2.41	0.50
1:I:405:PRO:HG2	1:I:481:ASN:HA	1.92	0.50
1:K:206:VAL:HG13	1:K:235:ASP:CB	2.41	0.50
1:K:400:LEU:HD11	1:K:482:LEU:CD1	2.41	0.50
1:A:186:GLU:C	1:A:188:ASN:N	2.69	0.50
1:C:295:ARG:O	1:C:296:ASN:HB2	2.11	0.50
1:C:334:THR:CG2	1:C:351:ASN:HB2	2.41	0.50
1:C:348:LEU:O	1:C:348:LEU:HD23	2.11	0.50
1:E:185:GLN:O	1:E:188:ASN:N	2.42	0.50
1:E:292:ILE:HD13	1:E:300:VAL:O	2.11	0.50
1:G:139:VAL:O	1:G:164:VAL:HG12	2.12	0.50
2:H:232:LYS:O	2:H:236:ASN:N	2.36	0.50
2:H:476(C):ASP:C	2:H:477:GLU:H	2.19	0.50
1:I:625:PHE:N	1:I:625:PHE:CD1	2.79	0.50
1:K:283:ILE:HB	1:K:386:GLN:CD	2.36	0.50
1:K:316:MET:CE	1:K:337:PHE:HD1	2.24	0.50
2:L:148:ALA:HB1	2:L:153:ALA:O	2.11	0.50
1:A:334:THR:HG22	1:A:351:ASN:HB2	1.93	0.50
1:A:634:LEU:HD23	1:A:634:LEU:H	1.76	0.50
1:C:74:ILE:HD13	1:C:143:TYR:HE2	1.77	0.50
1:C:363:LEU:HD13	1:C:455:TRP:HB3	1.93	0.50
2:D:273:ARG:HD2	2:D:330:TYR:CD1	2.47	0.50
1:E:177:LYS:HB3	1:E:181:LYS:HZ1	1.76	0.50
1:E:693:MET:O	1:E:694:LYS:HB2	2.11	0.50
1:G:92:ILE:CD1	1:G:112:ILE:HD13	2.42	0.50
1:G:380:GLU:HG2	1:G:381:PRO:HD2	1.93	0.50
1:I:577:ASP:HB2	1:I:591:ARG:NH2	2.26	0.50
1:I:671:VAL:CG2	1:I:691:GLU:HB2	2.41	0.50
1:K:276:CYS:O	1:K:382:LEU:HD21	2.10	0.50
1:K:405:PRO:HG2	1:K:481:ASN:HA	1.93	0.50
1:K:683:GLU:HB2	1:K:704:LYS:HG3	1.92	0.50
1:K:713:SER:O	1:K:714:ALA:C	2.55	0.50
2:L:66:ALA:HB2	2:L:125:ASP:HA	1.93	0.50
2:L:94:ASN:HA	2:L:98:GLN:OE1	2.11	0.50
2:L:325:ASP:C	2:L:327:GLY:N	2.70	0.50
1:A:150:SER:O	1:A:151:LYS:C	2.55	0.50
1:A:335:VAL:HG23	1:A:335:VAL:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:ARG:HG3	1:C:72:GLY:N	2.26	0.50
1:C:155:ALA:O	1:C:159:GLU:HG2	2.11	0.50
1:E:433:THR:HG22	1:E:434:GLY:N	2.23	0.50
1:E:515:VAL:CG2	1:E:631:GLY:HA3	2.41	0.50
1:E:675:VAL:CG1	1:E:707:VAL:HG21	2.41	0.50
2:F:88:HIS:CD2	2:F:88:HIS:C	2.89	0.50
2:F:156:ILE:N	2:F:156:ILE:CD1	2.73	0.50
1:G:74:ILE:HG23	1:G:75:ALA:N	2.27	0.50
1:G:112:ILE:O	1:G:120:SER:HA	2.12	0.50
1:G:287:GLU:HG3	1:G:308:LEU:HD21	1.93	0.50
1:I:348:LEU:O	1:I:348:LEU:HD23	2.11	0.50
1:K:78:VAL:HG23	1:K:370:VAL:HG11	1.93	0.50
1:K:283:ILE:HG22	1:K:386:GLN:HG2	1.93	0.50
1:K:317:GLY:O	1:K:321:VAL:HG12	2.11	0.50
1:K:400:LEU:HD13	1:K:449:ILE:CD1	2.32	0.50
1:K:664:CYS:SG	1:K:690:ILE:HD13	2.51	0.50
1:A:304:PRO:HG2	1:A:394:TRP:CZ2	2.46	0.50
2:D:469:THR:HG23	2:D:482:HIS:HB3	1.92	0.50
1:E:74:ILE:HD13	1:E:143:TYR:HE2	1.76	0.50
1:G:67:LEU:HG	1:G:68:ILE:H	1.77	0.50
1:G:99:GLN:HB2	1:G:436:TYR:OH	2.10	0.50
1:G:354:LEU:HD11	1:G:358:HIS:ND1	2.27	0.50
1:G:467:ARG:HE	1:G:630:ARG:HG3	1.76	0.50
1:I:167:PRO:O	1:I:169:GLY:N	2.45	0.50
2:J:121:VAL:O	2:J:144:ILE:HD13	2.11	0.50
2:J:196:ILE:HG22	2:J:221:SER:HB2	1.93	0.50
2:J:423:THR:O	2:J:525:LYS:HE2	2.11	0.50
1:K:92:ILE:HB	1:K:112:ILE:CG2	2.42	0.50
1:K:380:GLU:HG2	1:K:381:PRO:HD2	1.93	0.50
1:K:393:GLY:HA3	1:K:455:TRP:CZ3	2.47	0.50
1:A:71:ARG:HG3	1:A:72:GLY:N	2.25	0.50
1:A:83:ARG:HH11	1:A:83:ARG:CG	2.23	0.50
1:A:395:ALA:C	1:A:396:ILE:HD12	2.37	0.50
2:B:356:ALA:CB	2:B:391:LEU:HB2	2.42	0.50
2:B:476(C):ASP:C	2:B:477:GLU:H	2.19	0.50
1:C:515:VAL:HB	1:C:631:GLY:C	2.36	0.50
1:E:661:MET:HE2	1:E:726:GLU:CA	2.38	0.50
2:F:229:ASP:O	2:F:233:THR:HG23	2.12	0.50
1:I:292:ILE:HG23	1:I:503:PHE:CD2	2.46	0.50
1:I:380:GLU:CG	1:I:381:PRO:HD2	2.41	0.50
1:K:65:LYS:HE2	1:K:134:THR:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:312:THR:O	1:K:315:ALA:HB3	2.10	0.50
1:A:95:ASP:OD2	1:A:114:PRO:HA	2.12	0.50
1:A:365:THR:HG22	1:A:391:LEU:HD22	1.93	0.50
1:A:625:PHE:N	1:A:625:PHE:CD1	2.77	0.50
2:B:54:ARG:HG2	2:B:54:ARG:NH1	2.27	0.50
2:B:335:GLU:HA	2:B:338:LYS:HE2	1.94	0.50
2:B:346:ARG:HG3	2:B:346:ARG:NH1	2.27	0.50
1:C:312:THR:O	1:C:315:ALA:HB3	2.12	0.50
1:C:660:LYS:C	1:C:661:MET:HE3	2.37	0.50
1:C:671:VAL:CG2	1:C:691:GLU:HB2	2.42	0.50
2:D:379:ARG:HD2	2:D:421:GLU:OE2	2.12	0.50
1:E:414:ILE:HD12	1:E:441:ILE:O	2.12	0.50
1:G:306:PRO:HG3	1:G:394:TRP:CH2	2.46	0.50
1:G:334:THR:HG22	1:G:351:ASN:HB2	1.93	0.50
1:G:612:LEU:C	1:G:612:LEU:HD12	2.37	0.50
2:H:207:SER:HB3	2:H:208:PRO:CD	2.33	0.50
1:I:83:ARG:HH11	1:I:83:ARG:CG	2.22	0.50
2:J:91:THR:HA	2:J:98:GLN:CG	2.39	0.50
1:K:358:HIS:HB2	1:K:369:LEU:HD12	1.92	0.50
1:K:456:ALA:CB	1:K:457:PRO:CD	2.90	0.50
1:K:579:SER:O	1:K:591:ARG:HD2	2.12	0.50
2:L:335:GLU:HA	2:L:338:LYS:HE2	1.94	0.50
1:A:63:PHE:N	1:A:63:PHE:CD1	2.79	0.50
1:A:293:GLN:HB3	1:A:298:LYS:HA	1.94	0.50
1:C:124:ILE:O	1:C:128:MET:HB2	2.12	0.50
1:C:455:TRP:CD1	1:C:455:TRP:C	2.87	0.50
2:D:347:LEU:O	2:D:348:GLU:C	2.54	0.50
2:D:474:ARG:O	2:D:476:ASP:N	2.45	0.50
1:E:167:PRO:O	1:E:169:GLY:N	2.44	0.50
1:E:369:LEU:O	1:E:373:MET:HB2	2.12	0.50
1:G:517:LEU:H	1:G:517:LEU:CD2	2.22	0.50
1:G:523:ARG:HB3	1:G:590:MET:CE	2.39	0.50
1:I:265:THR:HB	1:I:341:GLY:H	1.76	0.50
1:A:92:ILE:HB	1:A:112:ILE:CG2	2.42	0.50
1:A:185:GLN:O	1:A:188:ASN:N	2.44	0.50
1:A:376:VAL:HG23	1:A:377:ALA:N	2.26	0.50
1:A:405:PRO:HG2	1:A:481:ASN:HA	1.94	0.50
1:A:646:LEU:HD13	2:B:64:LEU:HD13	1.94	0.50
2:B:69:ARG:HA	2:B:268:LEU:HD11	1.94	0.50
2:B:239:VAL:HG22	2:B:243:GLU:HB2	1.93	0.50
1:C:117:ALA:C	1:C:119:GLN:N	2.66	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:380:GLU:HG2	1:C:381:PRO:HD2	1.93	0.50
1:C:642:ARG:HH11	2:D:71:ASP:HB3	1.77	0.50
1:C:661:MET:HE2	1:C:726:GLU:HB3	1.93	0.50
2:D:49:GLY:C	2:D:51:GLY:N	2.65	0.50
1:E:184:ALA:HB1	1:E:189:VAL:HB	1.93	0.50
2:F:95:MET:CA	2:F:95:MET:HE3	2.42	0.50
2:H:58:GLN:CD	2:H:63:LYS:HE3	2.37	0.50
1:I:114:PRO:HB2	1:I:115:PRO:HD2	1.94	0.50
1:I:312:THR:O	1:I:316:MET:HG3	2.12	0.50
1:I:320:ALA:HB1	1:I:335:VAL:HG21	1.94	0.50
1:K:170:ALA:O	1:K:173:ALA:HB3	2.11	0.50
1:K:334:THR:HG22	1:K:351:ASN:HB2	1.94	0.50
1:K:348:LEU:O	1:K:349:GLU:HB3	2.12	0.50
2:B:178:GLU:O	2:B:182:ARG:HG3	2.12	0.49
1:C:658:THR:HG22	1:C:659:SER:O	2.12	0.49
1:E:380:GLU:HG2	1:E:381:PRO:HD2	1.94	0.49
2:F:43:ARG:HG2	2:F:43:ARG:HH11	1.76	0.49
1:G:162:ILE:O	1:G:164:VAL:N	2.45	0.49
1:G:190:SER:N	1:G:319:GLN:OE1	2.36	0.49
1:G:369:LEU:O	1:G:373:MET:HB2	2.12	0.49
1:G:537:GLU:HG3	1:G:553:ARG:HH21	1.77	0.49
2:H:250:HIS:HA	2:H:254:SER:OG	2.11	0.49
2:H:390:THR:CG2	2:H:419:TYR:OH	2.60	0.49
1:I:207:LYS:O	1:I:211:GLN:HB2	2.12	0.49
1:I:234:ASN:HD22	1:I:236:GLN:HB2	1.74	0.49
1:I:467:ARG:HE	1:I:630:ARG:CG	2.25	0.49
2:J:88:HIS:CD2	2:J:88:HIS:C	2.90	0.49
1:K:185:GLN:O	1:K:188:ASN:N	2.45	0.49
1:K:517:LEU:H	1:K:517:LEU:CD2	2.18	0.49
2:L:252:ARG:NH2	2:L:335:GLU:HG3	2.27	0.49
1:A:65:LYS:HE2	1:A:134:THR:O	2.12	0.49
1:A:396:ILE:HD13	1:A:462:ALA:CB	2.42	0.49
1:C:150:SER:O	1:C:151:LYS:C	2.55	0.49
2:D:109:THR:HG22	2:D:122:PHE:CB	2.42	0.49
1:E:118:ASN:O	1:E:119:GLN:HG3	2.11	0.49
1:E:177:LYS:O	1:E:181:LYS:HG2	2.12	0.49
1:E:288:ARG:HD3	1:E:361:THR:OG1	2.12	0.49
2:F:210:MET:HE1	2:H:416:LEU:CG	2.42	0.49
2:F:417:TYR:HA	2:H:184:ILE:CD1	2.40	0.49
1:G:342:GLN:O	1:G:343:LYS:HB2	2.11	0.49
1:G:454:THR:HG21	1:G:466:MET:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:596:TRP:CG	1:G:597:THR:N	2.80	0.49
2:H:189:VAL:HA	2:H:282:ASN:HD22	1.76	0.49
1:I:117:ALA:C	1:I:119:GLN:N	2.71	0.49
1:I:407:ARG:HG2	1:I:407:ARG:HH11	1.77	0.49
1:I:619:ILE:HD12	1:I:625:PHE:C	2.37	0.49
2:J:120:TYR:HE2	2:J:147:MET:HE2	1.77	0.49
2:J:232:LYS:O	2:J:236:ASN:N	2.36	0.49
2:J:367:ASP:O	2:J:368:ILE:C	2.55	0.49
1:K:146:LEU:HD23	1:K:152:PHE:CG	2.47	0.49
1:K:155:ALA:O	1:K:159:GLU:HG2	2.12	0.49
1:K:630:ARG:C	1:K:632:ALA:N	2.69	0.49
2:L:432:ARG:HG2	2:L:433:LYS:N	2.27	0.49
2:L:492:ASN:HD22	2:L:494:PHE:HB2	1.77	0.49
1:A:177:LYS:O	1:A:181:LYS:HG2	2.12	0.49
1:C:395:ALA:C	1:C:396:ILE:HD12	2.37	0.49
1:C:491:HIS:O	1:C:495:ILE:HG13	2.12	0.49
2:D:382:ASP:OD1	2:D:424:VAL:HG13	2.13	0.49
1:E:69:ALA:HB3	1:E:141:PRO:HA	1.94	0.49
1:G:78:VAL:HA	1:G:370:VAL:HG11	1.94	0.49
1:G:83:ARG:HB3	1:G:83:ARG:CZ	2.42	0.49
1:G:92:ILE:HB	1:G:112:ILE:CG2	2.42	0.49
1:G:279:HIS:NE2	1:G:380:GLU:N	2.60	0.49
1:G:358:HIS:N	1:G:359:PRO:CD	2.75	0.49
2:H:351:THR:HG22	2:H:386:ILE:HG23	1.94	0.49
1:I:634:LEU:N	1:I:634:LEU:CD2	2.75	0.49
1:K:71:ARG:O	1:K:75:ALA:CB	2.60	0.49
1:K:670:ILE:HD11	1:K:718:LEU:HD11	1.94	0.49
1:K:712:ALA:HA	1:K:716:ASN:ND2	2.28	0.49
1:A:179:THR:O	1:A:183:ILE:HG13	2.13	0.49
1:A:444:TYR:O	1:A:445:TYR:CG	2.66	0.49
2:B:337:ALA:HB1	2:B:370:SER:HA	1.92	0.49
2:B:337:ALA:HB3	2:B:373:LYS:HD2	1.94	0.49
1:C:414:ILE:HD11	1:C:442:SER:C	2.37	0.49
1:G:415:GLY:O	1:G:440:GLU:HG3	2.13	0.49
1:G:455:TRP:CG	1:G:456:ALA:N	2.79	0.49
1:I:283:ILE:CG2	1:I:386:GLN:HG2	2.42	0.49
1:I:463:ILE:HD12	1:I:494:PHE:CE1	2.47	0.49
1:I:534:ARG:HG3	1:I:534:ARG:NH1	2.25	0.49
1:I:664:CYS:HB2	1:I:724:ILE:HD11	1.93	0.49
2:J:66:ALA:HB2	2:J:125:ASP:HA	1.95	0.49
1:K:245:SER:C	1:K:247:ASN:N	2.70	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:PHE:CD1	1:A:347:PHE:C	2.90	0.49
2:B:417:TYR:HA	2:J:184:ILE:CD1	2.42	0.49
1:G:245:SER:C	1:G:247:ASN:H	2.20	0.49
1:G:347:PHE:CD1	1:G:347:PHE:C	2.90	0.49
1:G:537:GLU:HG3	1:G:553:ARG:NH2	2.28	0.49
2:J:356:ALA:HB2	2:J:391:LEU:HB2	1.94	0.49
1:K:117:ALA:CB	1:K:121:TYR:HB2	2.40	0.49
1:K:324:ALA:O	1:K:327:VAL:HG12	2.12	0.49
2:L:189:VAL:HA	2:L:282:ASN:HD22	1.77	0.49
2:L:476(A):LEU:C	2:L:476(C):ASP:H	2.20	0.49
1:A:71:ARG:O	1:A:75:ALA:CB	2.61	0.49
1:A:650:MET:SD	2:B:263:ASN:HB2	2.53	0.49
2:B:300:PRO:HB3	2:B:509:ARG:HH12	1.77	0.49
1:C:78:VAL:CG1	1:C:79:ILE:N	2.76	0.49
2:D:204:ALA:O	2:D:205:VAL:C	2.54	0.49
2:D:273:ARG:HD2	2:D:330:TYR:HD1	1.78	0.49
1:E:317:GLY:O	1:E:321:VAL:HG12	2.12	0.49
1:E:518:PRO:O	1:E:519:GLU:C	2.55	0.49
2:F:492:ASN:ND2	2:F:494:PHE:H	2.05	0.49
1:G:416:ARG:HG3	1:G:439:GLY:O	2.12	0.49
1:G:639:ARG:HB3	1:G:643:GLN:HB3	1.93	0.49
1:G:693:MET:O	1:G:694:LYS:HB2	2.13	0.49
2:H:507:GLN:OE1	2:J:39:LEU:HD23	2.13	0.49
1:I:515:VAL:CG2	1:I:631:GLY:HA3	2.42	0.49
2:J:329:PHE:CE1	2:J:343:GLY:HA3	2.47	0.49
2:L:227:GLY:O	2:L:231:VAL:HG23	2.13	0.49
2:L:403:GLN:O	2:L:408:VAL:HG22	2.12	0.49
2:B:307:PRO:HG3	2:B:312:THR:O	2.13	0.49
1:C:107:ASP:C	1:C:108:GLU:HG3	2.38	0.49
1:C:107:ASP:O	1:C:108:GLU:HG3	2.11	0.49
1:C:411:LEU:HB2	1:C:682:GLN:HG3	1.94	0.49
1:E:265:THR:HB	1:E:341:GLY:H	1.76	0.49
1:E:347:PHE:CD1	1:E:347:PHE:C	2.90	0.49
1:E:394:TRP:CE3	1:E:459:ARG:HG3	2.48	0.49
1:E:658:THR:OG1	1:E:702:GLU:HG2	2.13	0.49
2:F:338:LYS:HB3	2:F:361:VAL:HG21	1.93	0.49
1:G:150:SER:O	1:G:151:LYS:C	2.56	0.49
2:H:109:THR:HG22	2:H:122:PHE:HB2	1.93	0.49
2:H:361:VAL:C	2:H:363:ALA:N	2.71	0.49
1:I:358:HIS:HB2	1:I:369:LEU:HD12	1.94	0.49
1:I:411:LEU:HB2	1:I:682:GLN:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:693:MET:O	1:I:694:LYS:HB2	2.11	0.49
2:J:78:SER:O	2:J:112:GLY:HA2	2.12	0.49
2:L:273:ARG:HD2	2:L:330:TYR:HD1	1.77	0.49
2:L:307:PRO:O	2:L:432:ARG:NH2	2.45	0.49
1:C:179:THR:O	1:C:183:ILE:HG13	2.13	0.49
1:C:283:ILE:HA	1:C:386:GLN:NE2	2.28	0.49
1:C:720:VAL:HG22	1:C:721:ASP:H	1.78	0.49
2:D:108:VAL:O	2:D:122:PHE:HA	2.12	0.49
1:E:517:LEU:HD21	1:E:632:ALA:HB2	1.93	0.49
1:E:518:PRO:O	1:E:521:ASP:HB2	2.13	0.49
1:G:563:LEU:O	1:G:565:GLY:N	2.46	0.49
2:J:235:THR:HG22	2:J:237:GLU:HB2	1.93	0.49
2:J:273:ARG:HD2	2:J:330:TYR:CD1	2.46	0.49
1:K:207:LYS:O	1:K:211:GLN:HB2	2.12	0.49
1:K:275:LEU:HD23	1:K:276:CYS:N	2.28	0.49
1:K:658:THR:CB	1:K:703:LYS:HD3	2.42	0.49
1:A:312:THR:O	1:A:315:ALA:HB3	2.13	0.49
1:A:342:GLN:O	1:A:343:LYS:HB2	2.12	0.49
1:A:467:ARG:HH11	1:A:467:ARG:CB	2.22	0.49
2:B:180:PHE:O	2:B:184:ILE:HG13	2.13	0.49
2:B:193:ILE:HD13	2:B:274:LEU:HD23	1.94	0.49
2:B:376:ARG:NH1	2:J:410:LYS:HZ2	2.11	0.49
2:B:499:ARG:NH2	2:F:89:ARG:HH11	2.01	0.49
1:C:63:PHE:CD1	1:C:63:PHE:N	2.81	0.49
1:C:532:MET:HE1	1:C:603:ALA:CB	2.43	0.49
1:C:615:LYS:HB2	1:C:628:ARG:HB2	1.95	0.49
1:C:675:VAL:CG1	1:C:707:VAL:HG21	2.42	0.49
2:D:325:ASP:C	2:D:327:GLY:H	2.21	0.49
1:E:271:GLU:O	1:E:287:GLU:HB2	2.12	0.49
1:E:414:ILE:HD11	1:E:442:SER:C	2.37	0.49
1:E:421:ARG:O	1:E:421:ARG:CD	2.61	0.49
1:G:411:LEU:HD22	1:G:682:GLN:HB2	1.95	0.49
2:H:460:VAL:HG23	2:H:460:VAL:O	2.13	0.49
1:I:206:VAL:HG13	1:I:235:ASP:HB3	1.95	0.49
1:I:517:LEU:N	1:I:564:GLN:HE22	2.09	0.49
2:L:339:ASN:ND2	2:L:367:ASP:OD1	2.45	0.49
2:L:434:ALA:HB3	2:L:460:VAL:HG12	1.95	0.49
1:A:155:ALA:O	1:A:159:GLU:HG2	2.12	0.49
1:A:396:ILE:HD12	1:A:396:ILE:N	2.28	0.49
1:C:283:ILE:HG22	1:C:386:GLN:HG2	1.95	0.49
2:D:149:MET:CE	2:D:189:VAL:HG11	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:325:ASP:HA	2:D:512:ARG:NH1	2.17	0.49
2:D:347:LEU:HD12	2:D:352:VAL:HG21	1.95	0.49
1:E:467:ARG:HE	1:E:630:ARG:HG3	1.77	0.49
2:F:376:ARG:HH11	2:H:410:LYS:HZ2	1.61	0.49
1:G:428(L):ALA:HB3	1:G:455:TRP:HD1	1.77	0.49
1:G:482:LEU:N	1:G:483:PRO:HD2	2.27	0.49
1:G:543:VAL:HG11	2:H:117:ARG:HD2	1.94	0.49
1:G:626:ARG:C	1:G:627:ILE:HD12	2.38	0.49
2:H:195:MET:SD	2:H:271:VAL:HG21	2.52	0.49
2:H:227:GLY:O	2:H:231:VAL:HG23	2.13	0.49
2:H:235:THR:HG22	2:H:237:GLU:HB2	1.94	0.49
1:I:348:LEU:O	1:I:349:GLU:HB3	2.11	0.49
2:J:43:ARG:HH11	2:J:43:ARG:CG	2.26	0.49
2:J:499:ARG:NH1	2:J:499:ARG:CG	2.76	0.49
1:K:186:GLU:C	1:K:188:ASN:N	2.68	0.49
1:K:367:VAL:HG12	1:K:368:ASP:N	2.28	0.49
1:K:396:ILE:HG22	1:K:466:MET:HE3	1.95	0.49
1:K:626:ARG:NE	1:K:628:ARG:HD2	2.27	0.49
1:A:348:LEU:O	1:A:348:LEU:HD23	2.12	0.48
2:B:376:ARG:NH1	2:J:410:LYS:NZ	2.60	0.48
1:E:452:LEU:O	1:E:466:MET:HE1	2.13	0.48
2:F:122:PHE:CD1	2:F:141:ILE:HG23	2.48	0.48
1:G:309:ASP:OD1	1:G:312:THR:CG2	2.50	0.48
1:I:275:LEU:HD23	1:I:276:CYS:H	1.76	0.48
2:J:398:LEU:HD12	2:J:399:PRO:HD2	1.95	0.48
1:K:156:LEU:HD13	1:K:163:PHE:HB2	1.94	0.48
1:K:195:TYR:O	1:K:259:PHE:HA	2.12	0.48
1:C:83:ARG:HB3	1:C:83:ARG:CZ	2.43	0.48
1:C:517:LEU:H	1:C:517:LEU:CD2	2.17	0.48
2:D:476(A):LEU:C	2:D:476(C):ASP:H	2.20	0.48
1:E:156:LEU:HD13	1:E:163:PHE:HB2	1.94	0.48
1:E:400:LEU:HD21	1:E:482:LEU:CD1	2.42	0.48
1:E:435:VAL:HG22	1:E:436:TYR:H	1.77	0.48
1:E:583:PHE:HZ	1:E:590:MET:HE3	1.74	0.48
2:F:61:ARG:HB2	2:F:63:LYS:HG3	1.95	0.48
1:G:304:PRO:HD2	1:G:394:TRP:CE2	2.48	0.48
1:G:443:MET:SD	1:G:444:TYR:CE1	3.06	0.48
1:I:123:VAL:HG12	1:I:126:LYS:H	1.79	0.48
1:K:653:LYS:H	1:K:653:LYS:CD	2.12	0.48
1:A:334:THR:CG2	1:A:351:ASN:HB2	2.43	0.48
1:A:358:HIS:N	1:A:359:PRO:CD	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:VAL:CG2	1:A:631:GLY:HA3	2.44	0.48
2:B:227:GLY:O	2:B:231:VAL:HG23	2.14	0.48
1:C:99:GLN:HB2	1:C:436:TYR:OH	2.13	0.48
2:D:69:ARG:HA	2:D:268:LEU:HD11	1.94	0.48
2:D:317:LYS:HG3	2:D:341:ILE:HD13	1.95	0.48
2:D:492:ASN:HB2	2:D:493:PRO:CD	2.43	0.48
1:E:295:ARG:O	1:E:296:ASN:HB2	2.13	0.48
1:E:400:LEU:HD13	1:E:449:ILE:CD1	2.25	0.48
1:E:596:TRP:CG	1:E:597:THR:N	2.81	0.48
1:E:670:ILE:HD12	1:E:712:ALA:HB1	1.94	0.48
2:F:232:LYS:O	2:F:236:ASN:N	2.42	0.48
1:I:625:PHE:HB2	1:I:627:ILE:CD1	2.43	0.48
2:J:469:THR:HG23	2:J:482:HIS:HB3	1.95	0.48
1:K:112:ILE:O	1:K:120:SER:HA	2.12	0.48
1:K:467:ARG:HE	1:K:630:ARG:CG	2.26	0.48
1:A:69:ALA:HB3	1:A:141:PRO:HA	1.96	0.48
1:A:283:ILE:HD12	1:A:389:VAL:CG2	2.43	0.48
1:A:414:ILE:HD11	1:A:443:MET:N	2.28	0.48
1:A:660:LYS:O	1:A:661:MET:HE3	2.13	0.48
1:A:675:VAL:CG1	1:A:707:VAL:HG21	2.43	0.48
2:B:325:ASP:C	2:B:327:GLY:H	2.20	0.48
2:B:462:VAL:HG21	2:J:169:GLY:HA2	1.95	0.48
1:C:66:ILE:HG22	1:C:137:GLN:HG3	1.95	0.48
1:C:400:LEU:HD11	1:C:482:LEU:CD1	2.44	0.48
1:C:523:ARG:HB3	1:C:590:MET:CE	2.44	0.48
1:C:619:ILE:HD11	1:C:626:ARG:HB2	1.95	0.48
2:D:479:ILE:HD12	2:D:479:ILE:C	2.39	0.48
1:E:457:PRO:HG2	1:E:458:THR:N	2.20	0.48
1:G:150:SER:O	1:G:153:ALA:N	2.47	0.48
1:G:334:THR:CG2	1:G:351:ASN:HB2	2.44	0.48
1:G:480:HIS:HD2	1:G:482:LEU:H	1.62	0.48
1:I:292:ILE:HD13	1:I:300:VAL:O	2.13	0.48
1:I:316:MET:CE	1:I:337:PHE:CD1	2.95	0.48
1:K:518:PRO:O	1:K:521:ASP:HB2	2.12	0.48
1:K:563:LEU:CD2	1:K:636:VAL:HG22	2.43	0.48
1:K:646:LEU:HD12	2:L:72:LEU:HD21	1.94	0.48
1:A:131:ILE:CG2	1:A:136:ALA:HB2	2.38	0.48
1:A:273:GLN:O	1:A:285:LEU:HD12	2.14	0.48
1:A:467:ARG:HB3	1:A:467:ARG:NH1	2.24	0.48
1:A:528:ALA:HB1	1:A:605:LEU:CD2	2.43	0.48
2:B:88:HIS:CD2	2:B:88:HIS:C	2.91	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:ARG:NH1	1:C:370:VAL:HG21	2.28	0.48
1:C:504:ILE:CG2	1:C:505:ALA:N	2.77	0.48
2:D:207:SER:HB3	2:D:208:PRO:CD	2.41	0.48
1:E:146:LEU:HD23	1:E:152:PHE:CG	2.49	0.48
1:E:528:ALA:HB1	1:E:605:LEU:HD22	1.95	0.48
2:F:474:ARG:HD3	2:F:474:ARG:HA	1.63	0.48
1:G:167:PRO:C	1:G:169:GLY:H	2.21	0.48
2:H:499:ARG:NH1	2:H:499:ARG:CG	2.77	0.48
1:I:124:ILE:HG23	1:I:152:PHE:HD2	1.77	0.48
1:I:421:ARG:HD3	1:I:421:ARG:C	2.38	0.48
1:I:537:GLU:HG3	1:I:553:ARG:HH21	1.78	0.48
2:J:69:ARG:HA	2:J:268:LEU:HD11	1.95	0.48
1:K:405:PRO:CG	1:K:481:ASN:HA	2.44	0.48
2:L:337:ALA:HB1	2:L:370:SER:HA	1.96	0.48
1:A:167:PRO:O	1:A:169:GLY:N	2.47	0.48
2:B:43:ARG:NH1	2:B:43:ARG:HG2	2.28	0.48
1:C:157:GLU:C	1:C:159:GLU:N	2.72	0.48
1:C:168:LYS:HA	1:C:171:ILE:HD12	1.96	0.48
1:C:283:ILE:HD12	1:C:389:VAL:CG2	2.44	0.48
1:C:552:GLU:H	1:C:552:GLU:CD	2.20	0.48
1:E:617:GLY:O	1:E:625:PHE:CB	2.50	0.48
2:F:149:MET:CE	2:F:189:VAL:HG11	2.43	0.48
1:G:517:LEU:H	1:G:564:GLN:HE22	1.60	0.48
1:G:517:LEU:HD21	1:G:632:ALA:HB1	1.96	0.48
2:H:58:GLN:OE1	2:H:63:LYS:HE3	2.13	0.48
2:H:501:PHE:CD2	2:H:501:PHE:N	2.78	0.48
1:I:71:ARG:O	1:I:75:ALA:CB	2.62	0.48
1:I:308:LEU:HD12	1:I:308:LEU:C	2.38	0.48
1:I:393:GLY:HA3	1:I:455:TRP:CZ3	2.49	0.48
2:B:309:ASN:HD21	2:B:311:ASN:HB2	1.79	0.48
1:C:186:GLU:N	1:C:186:GLU:CD	2.72	0.48
1:C:308:LEU:O	1:C:308:LEU:HD12	2.13	0.48
1:E:93:TYR:HA	1:E:121:TYR:OH	2.14	0.48
2:H:432:ARG:HG2	2:H:433:LYS:N	2.28	0.48
2:H:432:ARG:O	2:H:458:ALA:HA	2.13	0.48
1:I:189:VAL:CG2	1:I:323:LEU:HB2	2.44	0.48
1:I:245:SER:C	1:I:247:ASN:H	2.20	0.48
1:I:400:LEU:HD13	1:I:449:ILE:CD1	2.24	0.48
2:J:188:GLY:HA2	2:J:384:PHE:CE2	2.49	0.48
2:J:346:ARG:HH11	2:J:346:ARG:HG3	1.78	0.48
2:J:436:GLY:O	2:J:439:TYR:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:270:ILE:HG12	1:K:289:GLU:HG3	1.95	0.48
1:K:411:LEU:HB2	1:K:682:GLN:HG3	1.95	0.48
1:K:417:LEU:HD21	1:K:478:ILE:CD1	2.39	0.48
1:A:78:VAL:CG1	1:A:79:ILE:N	2.77	0.48
1:C:419:ARG:HB2	1:C:476:GLU:HB2	1.95	0.48
1:C:524:ARG:N	1:C:590:MET:HE1	2.28	0.48
1:E:95:ASP:OD2	1:E:114:PRO:HA	2.14	0.48
1:E:132:ARG:HD3	1:E:159:GLU:OE1	2.14	0.48
2:F:42:ARG:O	2:F:45:ALA:HB3	2.13	0.48
2:F:109:THR:HG22	2:F:122:PHE:HB2	1.95	0.48
2:F:376:ARG:NH1	2:H:410:LYS:NZ	2.62	0.48
1:G:136:ALA:HB1	1:G:161:VAL:CG1	2.38	0.48
1:G:411:LEU:HG	1:G:412:PRO:O	2.13	0.48
1:G:518:PRO:O	1:G:521:ASP:HB2	2.14	0.48
1:I:347:PHE:CD1	1:I:347:PHE:C	2.91	0.48
1:I:517:LEU:HD22	1:I:517:LEU:N	2.22	0.48
1:I:552:GLU:CD	1:I:552:GLU:H	2.21	0.48
2:J:95:MET:HE3	2:J:95:MET:CA	2.43	0.48
1:K:400:LEU:HD21	1:K:482:LEU:CD1	2.44	0.48
1:K:671:VAL:CG2	1:K:691:GLU:HB2	2.44	0.48
2:L:160:ASP:OD1	2:L:198:GLY:HA3	2.14	0.48
2:L:296:ASP:O	2:L:298:ILE:HD12	2.14	0.48
1:A:403:GLU:O	1:A:405:PRO:HD3	2.14	0.48
1:A:515:VAL:HB	1:A:631:GLY:C	2.39	0.48
2:B:90:CYS:HB2	2:B:168:GLU:OE2	2.14	0.48
2:B:492:ASN:ND2	2:B:494:PHE:H	2.11	0.48
1:C:390:LYS:HD3	1:C:391:LEU:H	1.75	0.48
1:E:441:ILE:HD12	1:E:478:ILE:HD13	1.95	0.48
1:G:85:MET:O	1:G:86:GLY:C	2.57	0.48
1:G:155:ALA:O	1:G:159:GLU:HG2	2.14	0.48
1:G:292:ILE:HG23	1:G:503:PHE:CD2	2.48	0.48
1:G:553:ARG:NH1	2:H:115:ASN:OD1	2.47	0.48
2:H:193:ILE:HD13	2:H:274:LEU:HD23	1.95	0.48
2:H:367:ASP:O	2:H:368:ILE:C	2.57	0.48
1:I:64:ASN:H	1:I:137:GLN:HG2	1.79	0.48
1:I:164:VAL:HG23	1:I:373:MET:O	2.14	0.48
2:J:91:THR:HG22	2:J:98:GLN:HG2	1.96	0.48
2:J:351:THR:HG22	2:J:386:ILE:HG23	1.96	0.48
1:K:131:ILE:CG2	1:K:136:ALA:HB2	2.32	0.48
1:K:283:ILE:CG2	1:K:386:GLN:HG2	2.44	0.48
1:K:316:MET:HE3	1:K:337:PHE:HD1	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:LEU:HD13	1:A:163:PHE:HB2	1.95	0.48
1:A:518:PRO:O	1:A:521:ASP:HB2	2.13	0.48
1:C:596:TRP:CG	1:C:597:THR:N	2.82	0.48
2:D:178:GLU:HB3	2:D:182:ARG:NH1	2.29	0.48
2:D:348:GLU:O	2:D:350:ARG:HD2	2.14	0.48
2:D:476(C):ASP:HB3	2:D:478:LYS:HG3	1.96	0.48
1:E:339:VAL:HG22	1:E:345:PHE:HB3	1.95	0.48
1:E:421:ARG:C	1:E:421:ARG:HD3	2.39	0.48
1:E:683:GLU:HB2	1:E:704:LYS:HG3	1.94	0.48
1:G:627:ILE:HD12	1:G:627:ILE:N	2.29	0.48
2:H:235:THR:HG22	2:H:237:GLU:CB	2.44	0.48
2:H:312:THR:HG22	2:H:313:PRO:O	2.14	0.48
2:H:339:ASN:HD21	2:H:370:SER:HB3	1.79	0.48
1:I:267:PRO:O	1:I:501:THR:HG23	2.14	0.48
1:I:454:THR:HG21	1:I:466:MET:HA	1.95	0.48
1:I:515:VAL:HB	1:I:631:GLY:C	2.39	0.48
1:I:583:PHE:HZ	1:I:590:MET:HE3	1.74	0.48
2:J:117:ARG:HB3	2:J:280:LEU:HD21	1.94	0.48
1:K:74:ILE:HG23	1:K:75:ALA:N	2.29	0.48
1:K:358:HIS:CD2	1:K:362:GLU:OE1	2.67	0.48
1:K:422:PRO:HG3	1:K:473:PHE:CZ	2.49	0.48
1:K:481:ASN:O	1:K:482:LEU:C	2.56	0.48
1:A:124:ILE:O	1:A:128:MET:HB2	2.14	0.47
1:A:136:ALA:HB1	1:A:161:VAL:CG1	2.35	0.47
1:A:325:LYS:O	1:A:327:VAL:N	2.46	0.47
1:A:347:PHE:CD1	1:A:347:PHE:O	2.67	0.47
1:A:401:TYR:CD2	1:A:448:MET:HA	2.49	0.47
2:B:339:ASN:ND2	2:B:370:SER:HB3	2.29	0.47
1:C:78:VAL:HA	1:C:370:VAL:HG11	1.96	0.47
1:E:393:GLY:HA2	1:E:457:PRO:O	2.14	0.47
1:E:634:LEU:N	1:E:634:LEU:CD2	2.76	0.47
1:E:712:ALA:HA	1:E:716:ASN:ND2	2.28	0.47
1:G:446:ASP:OD1	1:G:447:PRO:HD2	2.14	0.47
1:G:670:ILE:HD12	1:G:712:ALA:HB1	1.95	0.47
2:H:300:PRO:HA	2:H:509:ARG:NH1	2.28	0.47
2:H:339:ASN:ND2	2:H:370:SER:HB3	2.29	0.47
2:H:339:ASN:HB3	2:H:361:VAL:HG12	1.96	0.47
1:I:433:THR:HG22	1:I:434:GLY:N	2.26	0.47
1:I:443:MET:HG3	1:I:444:TYR:CE1	2.49	0.47
1:I:457:PRO:CG	1:I:458:THR:H	2.24	0.47
2:J:492:ASN:HB2	2:J:493:PRO:CD	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:139:VAL:O	1:K:164:VAL:HG12	2.14	0.47
1:K:433:THR:HG22	1:K:434:GLY:N	2.29	0.47
2:L:155:VAL:C	2:L:156:ILE:HD12	2.39	0.47
2:L:492:ASN:HD22	2:L:494:PHE:H	1.61	0.47
2:B:128:VAL:O	2:B:129:LEU:C	2.55	0.47
1:C:162:ILE:O	1:C:164:VAL:N	2.47	0.47
2:D:394:VAL:HG23	2:D:395:PRO:HD2	1.97	0.47
2:D:419:TYR:CE1	2:D:443:SER:HB2	2.48	0.47
1:E:653:LYS:N	1:E:653:LYS:CD	2.75	0.47
1:G:289:GLU:OE1	1:G:305:SER:OG	2.31	0.47
1:G:626:ARG:NE	1:G:628:ARG:HD2	2.28	0.47
1:I:416:ARG:HG3	1:I:439:GLY:O	2.13	0.47
1:I:522:LEU:HD22	1:I:563:LEU:HD13	1.96	0.47
2:J:356:ALA:CB	2:J:391:LEU:HB2	2.44	0.47
1:K:162:ILE:HD13	1:K:377:ALA:O	2.14	0.47
1:K:292:ILE:HG23	1:K:503:PHE:CD2	2.49	0.47
1:K:293:GLN:HB3	1:K:298:LYS:HA	1.96	0.47
1:K:308:LEU:HA	1:K:343:LYS:HE3	1.95	0.47
1:A:367:VAL:HG12	1:A:368:ASP:N	2.29	0.47
1:A:401:TYR:CE2	1:A:448:MET:HB2	2.49	0.47
2:B:368:ILE:CG1	2:B:408:VAL:HG13	2.43	0.47
1:C:139:VAL:HG11	1:C:156:LEU:HD21	1.96	0.47
1:C:718:LEU:HD23	1:C:718:LEU:H	1.76	0.47
2:D:148:ALA:HB1	2:D:153:ALA:O	2.14	0.47
1:E:308:LEU:HD12	1:E:308:LEU:C	2.38	0.47
2:F:325:ASP:C	2:F:327:GLY:H	2.21	0.47
1:G:83:ARG:HH11	1:G:83:ARG:CG	2.27	0.47
1:G:492:PRO:HA	1:G:495:ILE:HD12	1.95	0.47
1:G:494:PHE:CD2	1:G:499:MET:HE1	2.48	0.47
2:H:522:LEU:HD23	2:J:151:ASN:HD21	1.79	0.47
1:I:206:VAL:HG13	1:I:235:ASP:CB	2.44	0.47
1:I:517:LEU:H	1:I:517:LEU:CD2	2.20	0.47
2:J:126:PHE:HB2	2:J:160:ASP:OD2	2.13	0.47
2:J:222:TYR:C	2:J:222:TYR:CD1	2.93	0.47
1:K:85:MET:O	1:K:86:GLY:C	2.58	0.47
1:A:187:ALA:O	1:A:188:ASN:CG	2.58	0.47
1:A:467:ARG:HE	1:A:630:ARG:HG3	1.79	0.47
1:A:661:MET:HE2	1:A:726:GLU:HB3	1.96	0.47
1:C:67:LEU:HG	1:C:68:ILE:H	1.79	0.47
2:D:138:SER:OG	2:D:139:LYS:N	2.47	0.47
1:E:65:LYS:HE2	1:E:134:THR:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:283:ILE:HG22	1:G:386:GLN:HG2	1.96	0.47
1:G:309:ASP:OD2	1:G:343:LYS:HE2	2.14	0.47
1:G:317:GLY:O	1:G:321:VAL:HG12	2.14	0.47
1:I:316:MET:HE2	1:I:337:PHE:CD1	2.49	0.47
1:I:400:LEU:HD11	1:I:482:LEU:CD1	2.43	0.47
1:I:433:THR:HG23	1:I:449:ILE:O	2.14	0.47
2:J:355:VAL:O	2:J:390:THR:HA	2.14	0.47
1:K:358:HIS:HD2	1:K:362:GLU:OE1	1.97	0.47
1:A:484:PHE:O	1:A:487:ALA:HB3	2.14	0.47
2:B:58:GLN:HA	2:B:61:ARG:HH21	1.80	0.47
2:B:420:GLY:HA3	2:J:184:ILE:CD1	2.37	0.47
1:C:309:ASP:OD2	1:C:343:LYS:HE2	2.15	0.47
1:C:401:TYR:CD2	1:C:448:MET:HA	2.50	0.47
1:C:518:PRO:HD2	1:C:521:ASP:OD1	2.15	0.47
2:D:298:ILE:HD12	2:D:298:ILE:N	2.29	0.47
1:E:319:GLN:NE2	1:E:345:PHE:CE1	2.83	0.47
1:G:78:VAL:CG1	1:G:79:ILE:N	2.78	0.47
1:I:178:ILE:H	1:I:178:ILE:CD1	2.08	0.47
2:J:141:ILE:O	2:J:145:MET:HG3	2.14	0.47
1:K:140:HIS:ND1	1:K:141:PRO:N	2.62	0.47
1:K:390:LYS:HD3	1:K:391:LEU:H	1.75	0.47
1:A:146:LEU:HD23	1:A:152:PHE:CD2	2.50	0.47
1:A:285:LEU:HD12	1:A:285:LEU:N	2.29	0.47
1:C:164:VAL:HG22	1:C:373:MET:HE2	1.96	0.47
1:C:316:MET:HE2	1:C:337:PHE:CD1	2.50	0.47
1:E:670:ILE:HD11	1:E:718:LEU:HD11	1.96	0.47
2:F:108:VAL:O	2:F:122:PHE:HA	2.14	0.47
2:F:138:SER:O	2:F:139:LYS:C	2.57	0.47
1:G:195:TYR:O	1:G:259:PHE:HA	2.15	0.47
1:G:515:VAL:CG2	1:G:631:GLY:HA3	2.45	0.47
1:G:614:LEU:HD22	1:G:627:ILE:HG21	1.95	0.47
2:H:309:ASN:HD21	2:H:311:ASN:HB2	1.80	0.47
1:I:231:ILE:HD12	1:I:231:ILE:N	2.27	0.47
2:J:298:ILE:HG23	2:J:509:ARG:HB2	1.96	0.47
2:J:479:ILE:HD12	2:J:479:ILE:C	2.37	0.47
1:A:283:ILE:HB	1:A:386:GLN:CD	2.40	0.47
1:A:289:GLU:OE1	1:A:306:PRO:HD2	2.15	0.47
1:A:400:LEU:HD11	1:A:482:LEU:CD1	2.45	0.47
1:A:617:GLY:O	1:A:625:PHE:CB	2.53	0.47
2:B:193:ILE:CD1	2:B:274:LEU:HD23	2.45	0.47
2:B:403:GLN:O	2:B:408:VAL:HG22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:484:ALA:O	2:B:488:GLU:OE1	2.33	0.47
2:B:522:LEU:HA	2:F:151:ASN:ND2	2.30	0.47
1:C:358:HIS:N	1:C:359:PRO:CD	2.77	0.47
1:C:400:LEU:HD23	1:C:481:ASN:OD1	2.15	0.47
1:C:658:THR:CB	1:C:703:LYS:HD3	2.40	0.47
1:E:358:HIS:CG	1:E:359:PRO:HD3	2.49	0.47
2:F:347:LEU:O	2:F:348:GLU:C	2.58	0.47
1:G:140:HIS:ND1	1:G:141:PRO:HD2	2.30	0.47
1:G:354:LEU:HD13	1:G:354:LEU:C	2.40	0.47
1:G:367:VAL:HG12	1:G:368:ASP:N	2.29	0.47
1:G:663:LEU:O	1:G:665:PRO:HD3	2.15	0.47
1:G:720:VAL:HG22	1:G:721:ASP:H	1.80	0.47
2:H:229:ASP:OD1	2:H:229:ASP:N	2.47	0.47
2:H:299:GLU:O	2:H:509:ARG:HA	2.15	0.47
1:I:63:PHE:N	1:I:63:PHE:CD1	2.82	0.47
1:I:115:PRO:HG2	1:I:444:TYR:CE2	2.50	0.47
1:I:515:VAL:HG21	1:I:631:GLY:HA3	1.97	0.47
1:I:517:LEU:HB3	1:I:521:ASP:HB3	1.96	0.47
2:J:121:VAL:CG2	2:J:122:PHE:N	2.76	0.47
2:J:261:PHE:CD1	2:J:267:ALA:HA	2.49	0.47
1:K:152:PHE:CE1	1:K:156:LEU:HD11	2.49	0.47
1:K:275:LEU:HD23	1:K:276:CYS:H	1.80	0.47
2:L:492:ASN:HB2	2:L:493:PRO:HD2	1.95	0.47
2:L:536:ASN:O	2:L:537:ILE:C	2.58	0.47
1:C:66:ILE:HD13	1:C:88:SER:O	2.14	0.47
1:G:184:ALA:HB1	1:G:189:VAL:HB	1.96	0.47
1:G:551:HIS:HE1	2:L:348:GLU:OE2	1.97	0.47
2:H:195:MET:HE1	2:H:268:LEU:HD23	1.97	0.47
2:H:307:PRO:HG3	2:H:312:THR:HG22	1.97	0.47
2:H:458:ALA:HB3	2:H:493:PRO:HB3	1.97	0.47
1:I:229:MET:O	1:I:229:MET:HG3	2.15	0.47
1:I:414:ILE:HD11	1:I:442:SER:C	2.40	0.47
1:K:157:GLU:C	1:K:159:GLU:N	2.72	0.47
1:K:515:VAL:HB	1:K:631:GLY:C	2.39	0.47
1:A:583:PHE:CE1	1:A:590:MET:HE3	2.49	0.47
2:B:379:ARG:NH2	2:J:535:ASP:OD2	2.47	0.47
1:C:78:VAL:HG23	1:C:370:VAL:CG1	2.45	0.47
1:C:517:LEU:HD21	1:C:632:ALA:CB	2.45	0.47
2:D:434:ALA:HB3	2:D:460:VAL:HG12	1.97	0.47
2:F:124:GLN:HE21	2:F:137:HIS:CE1	2.32	0.47
2:F:202:GLY:O	2:F:205:VAL:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:432:ARG:HG2	2:F:433:LYS:N	2.30	0.47
2:F:442:MET:O	2:F:443:SER:C	2.58	0.47
1:G:71:ARG:O	1:G:75:ALA:CB	2.63	0.47
1:G:107:ASP:O	1:G:108:GLU:HG3	2.15	0.47
1:G:235:ASP:OD1	1:G:235:ASP:N	2.46	0.47
1:I:187:ALA:O	1:I:188:ASN:CG	2.58	0.47
1:I:518:PRO:O	1:I:521:ASP:HB2	2.15	0.47
1:I:626:ARG:NE	1:I:628:ARG:HD2	2.30	0.47
2:J:476(D):PRO:HA	2:J:479:ILE:HD11	1.97	0.47
1:K:390:LYS:HD3	1:K:390:LYS:C	2.39	0.47
2:L:524:ASN:O	2:L:525:LYS:C	2.58	0.47
1:A:85:MET:O	1:A:86:GLY:C	2.58	0.47
1:A:436:TYR:HE1	1:A:439:GLY:CA	2.28	0.47
1:A:658:THR:HG22	1:A:659:SER:O	2.14	0.47
2:B:195:MET:SD	2:B:271:VAL:HG21	2.54	0.47
2:B:355:VAL:O	2:B:390:THR:HA	2.14	0.47
1:C:666:MET:HE3	1:C:690:ILE:HD12	1.97	0.47
2:D:501:PHE:CE1	2:L:174:ALA:HB2	2.49	0.47
1:E:683:GLU:H	1:E:704:LYS:HG2	1.78	0.47
2:F:170:VAL:HG11	2:H:460:VAL:HG23	1.96	0.47
2:F:390:THR:CG2	2:F:419:TYR:OH	2.63	0.47
1:G:63:PHE:N	1:G:63:PHE:CD1	2.83	0.47
1:G:371:GLU:O	1:G:372:GLN:C	2.58	0.47
1:G:436:TYR:HE1	1:G:439:GLY:CA	2.28	0.47
2:H:80:GLU:HB2	2:L:517:ARG:NH2	2.30	0.47
1:I:85:MET:O	1:I:86:GLY:C	2.57	0.47
1:I:136:ALA:HB1	1:I:161:VAL:CG1	2.34	0.47
1:I:394:TRP:CE3	1:I:459:ARG:HG3	2.50	0.47
1:I:396:ILE:HG22	1:I:466:MET:HE3	1.95	0.47
1:I:537:GLU:HG3	1:I:553:ARG:NH2	2.30	0.47
1:K:515:VAL:HG21	1:K:631:GLY:HA3	1.97	0.47
1:K:552:GLU:CD	1:K:552:GLU:N	2.73	0.47
1:K:625:PHE:CD1	1:K:627:ILE:HD11	2.49	0.47
2:L:48:LEU:HD23	2:L:48:LEU:HA	1.63	0.47
2:L:390:THR:CG2	2:L:419:TYR:OH	2.63	0.47
2:L:469:THR:HG23	2:L:482:HIS:HB3	1.96	0.47
1:A:117:ALA:CB	1:A:121:TYR:HB2	2.43	0.46
1:A:279:HIS:NE2	1:A:380:GLU:N	2.62	0.46
1:A:354:LEU:HD11	1:A:358:HIS:ND1	2.31	0.46
1:A:665:PRO:CG	1:A:666:MET:HE2	2.24	0.46
2:B:432:ARG:HG2	2:B:433:LYS:N	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:292:ILE:HG23	1:C:503:PHE:CD2	2.50	0.46
1:C:396:ILE:HG12	1:C:463:ILE:CD1	2.40	0.46
1:E:292:ILE:H	1:E:292:ILE:CD1	2.07	0.46
2:F:192:GLN:O	2:F:211:THR:HB	2.15	0.46
1:G:71:ARG:CA	1:G:75:ALA:HB2	2.45	0.46
1:G:245:SER:C	1:G:247:ASN:N	2.72	0.46
1:G:455:TRP:CD1	1:G:455:TRP:C	2.87	0.46
1:G:625:PHE:CD1	1:G:627:ILE:HD11	2.50	0.46
2:H:196:ILE:HG22	2:H:221:SER:HB2	1.97	0.46
1:I:245:SER:C	1:I:247:ASN:N	2.72	0.46
1:I:467:ARG:HH21	1:I:630:ARG:NE	2.14	0.46
2:J:291:PHE:CE1	2:J:348:GLU:HA	2.51	0.46
2:J:309:ASN:HD21	2:J:311:ASN:HB2	1.80	0.46
2:J:382:ASP:HA	2:J:424:VAL:CG1	2.45	0.46
2:J:432:ARG:HG2	2:J:433:LYS:N	2.31	0.46
1:K:444:TYR:CD1	1:K:444:TYR:N	2.83	0.46
1:K:515:VAL:CG2	1:K:631:GLY:HA3	2.45	0.46
1:A:164:VAL:HG23	1:A:373:MET:O	2.16	0.46
1:A:189:VAL:CG2	1:A:323:LEU:HB2	2.45	0.46
1:A:321:VAL:O	1:A:324:ALA:CB	2.60	0.46
1:A:335:VAL:CG1	1:A:350:MET:HE3	2.44	0.46
2:B:367:ASP:O	2:B:368:ILE:C	2.58	0.46
1:C:190:SER:N	1:C:319:GLN:OE1	2.36	0.46
1:C:515:VAL:CG2	1:C:631:GLY:HA3	2.44	0.46
1:C:627:ILE:HD12	1:C:627:ILE:N	2.30	0.46
2:D:229:ASP:O	2:D:233:THR:HG23	2.16	0.46
1:E:85:MET:O	1:E:86:GLY:C	2.58	0.46
1:E:660:LYS:C	1:E:661:MET:HE3	2.40	0.46
1:G:164:VAL:HG23	1:G:377:ALA:CB	2.44	0.46
1:G:167:PRO:C	1:G:169:GLY:N	2.73	0.46
1:G:186:GLU:CD	1:G:186:GLU:N	2.74	0.46
1:G:419:ARG:HB2	1:G:476:GLU:HB2	1.97	0.46
1:I:285:LEU:HB3	1:I:365:THR:HG21	1.97	0.46
1:I:543:VAL:HG12	1:I:544:SER:N	2.31	0.46
1:I:649:LEU:HD13	2:J:59:HIS:CD2	2.50	0.46
2:J:307:PRO:HG3	2:J:312:THR:HG22	1.95	0.46
1:K:287:GLU:OE2	1:K:305:SER:N	2.44	0.46
2:L:91:THR:O	2:L:98:GLN:NE2	2.45	0.46
2:L:458:ALA:HB3	2:L:493:PRO:HB3	1.97	0.46
1:A:327:VAL:O	1:A:327:VAL:HG22	2.15	0.46
1:A:411:LEU:HB2	1:A:682:GLN:HG3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:LEU:HD21	1:A:632:ALA:HB1	1.97	0.46
1:A:670:ILE:CD1	1:A:718:LEU:HD21	2.46	0.46
1:A:675:VAL:HG12	1:A:707:VAL:HG21	1.98	0.46
1:C:73:GLU:HG3	1:C:74:ILE:H	1.80	0.46
1:C:83:ARG:HH11	1:C:83:ARG:CG	2.26	0.46
1:C:146:LEU:HD23	1:C:152:PHE:CG	2.51	0.46
2:D:378:VAL:HG13	2:D:388:LEU:CD1	2.45	0.46
1:E:400:LEU:HD11	1:E:482:LEU:CD1	2.45	0.46
1:E:614:LEU:HD22	1:E:627:ILE:HG21	1.96	0.46
1:E:619:ILE:HD11	1:E:626:ARG:HB2	1.98	0.46
1:E:664:CYS:HB2	1:E:724:ILE:HD11	1.96	0.46
2:F:69:ARG:HA	2:F:268:LEU:HD11	1.97	0.46
1:G:319:GLN:NE2	1:G:345:PHE:CE1	2.83	0.46
1:G:543:VAL:HG12	1:G:544:SER:N	2.29	0.46
2:H:94:ASN:HA	2:H:98:GLN:OE1	2.16	0.46
2:H:235:THR:HG22	2:H:235:THR:O	2.15	0.46
1:I:78:VAL:CG1	1:I:79:ILE:N	2.77	0.46
1:I:532:MET:HE1	1:I:603:ALA:CB	2.46	0.46
1:I:675:VAL:HG12	1:I:707:VAL:HG21	1.96	0.46
2:J:239:VAL:HG22	2:J:243:GLU:HB2	1.97	0.46
2:J:346:ARG:HG3	2:J:346:ARG:NH1	2.30	0.46
1:K:541:THR:O	1:K:541:THR:HG22	2.14	0.46
2:L:200:CYS:HB3	2:L:223:MET:HB3	1.96	0.46
2:L:215:PHE:HD2	2:L:259:ALA:HB3	1.81	0.46
2:L:232:LYS:O	2:L:236:ASN:N	2.42	0.46
1:A:74:ILE:HG23	1:A:75:ALA:N	2.30	0.46
1:A:157:GLU:C	1:A:159:GLU:N	2.72	0.46
1:A:528:ALA:CB	1:A:605:LEU:HD22	2.43	0.46
2:B:149:MET:SD	2:B:186:ALA:HB2	2.56	0.46
2:B:469:THR:CG2	2:B:482:HIS:HB3	2.46	0.46
1:C:626:ARG:NE	1:C:628:ARG:HD2	2.30	0.46
2:D:119:VAL:HG13	2:D:156:ILE:HD13	1.96	0.46
2:D:135:GLU:OE1	2:H:89:ARG:NH2	2.48	0.46
2:D:410:LYS:HZ2	2:L:376:ARG:HH11	1.63	0.46
1:E:78:VAL:HA	1:E:370:VAL:HG11	1.98	0.46
1:E:83:ARG:HH11	1:E:83:ARG:CG	2.26	0.46
1:E:348:LEU:HD23	1:E:348:LEU:O	2.16	0.46
1:E:563:LEU:HB3	1:E:564:GLN:H	1.38	0.46
2:F:89:ARG:NH2	2:J:135:GLU:OE1	2.48	0.46
2:F:252:ARG:NH2	2:F:335:GLU:HG3	2.31	0.46
2:F:314:TYR:CE1	2:F:359:PRO:HG2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:339:ASN:HB3	2:F:361:VAL:HG12	1.96	0.46
2:F:382:ASP:HA	2:F:424:VAL:CG1	2.46	0.46
2:F:460:VAL:HG23	2:H:170:VAL:HG11	1.97	0.46
1:G:273:GLN:O	1:G:285:LEU:HD12	2.16	0.46
2:H:108:VAL:O	2:H:122:PHE:HA	2.14	0.46
2:H:458:ALA:O	2:H:493:PRO:HD3	2.15	0.46
1:I:195:TYR:CD2	1:I:208:ILE:HD13	2.51	0.46
1:I:401:TYR:HD2	1:I:448:MET:HA	1.80	0.46
1:I:539:ARG:NH2	2:J:326:GLU:OE2	2.49	0.46
1:I:563:LEU:O	1:I:565:GLY:N	2.48	0.46
1:K:334:THR:CG2	1:K:351:ASN:HB2	2.46	0.46
1:K:401:TYR:CD2	1:K:448:MET:HA	2.49	0.46
1:K:539:ARG:NH2	2:L:326:GLU:OE2	2.49	0.46
2:L:329:PHE:HE1	2:L:343:GLY:HA3	1.77	0.46
1:A:619:ILE:O	1:A:620:SER:C	2.59	0.46
1:C:457:PRO:HG2	1:C:458:THR:N	2.18	0.46
1:C:661:MET:CE	1:C:726:GLU:HB3	2.46	0.46
1:E:114:PRO:HB2	1:E:115:PRO:HD2	1.97	0.46
1:E:139:VAL:HG11	1:E:156:LEU:HD21	1.98	0.46
1:E:316:MET:O	1:E:320:ALA:HB2	2.15	0.46
1:E:515:VAL:HG21	1:E:631:GLY:HA3	1.97	0.46
1:G:517:LEU:HA	1:G:518:PRO:HD3	1.58	0.46
2:H:138:SER:OG	2:H:139:LYS:N	2.47	0.46
2:H:469:THR:HG23	2:H:482:HIS:HB3	1.96	0.46
1:I:93:TYR:HA	1:I:121:TYR:OH	2.15	0.46
1:I:419:ARG:HD2	1:I:601:GLN:OE1	2.15	0.46
1:I:690:ILE:CD1	1:I:699:LEU:HD11	2.46	0.46
1:K:164:VAL:HG23	1:K:373:MET:O	2.15	0.46
1:K:283:ILE:HD12	1:K:389:VAL:CG2	2.44	0.46
1:K:436:TYR:HE1	1:K:439:GLY:CA	2.28	0.46
2:L:52:GLN:OE1	2:L:52:GLN:O	2.34	0.46
2:L:88:HIS:CD2	2:L:88:HIS:C	2.94	0.46
2:L:315:ASP:C	2:L:315:ASP:OD1	2.58	0.46
1:A:93:TYR:HD1	1:A:94:SER:O	1.99	0.46
1:A:308:LEU:CD2	1:A:316:MET:SD	2.97	0.46
2:B:492:ASN:ND2	2:B:494:PHE:HB2	2.31	0.46
1:C:602:LEU:HD12	1:C:614:LEU:O	2.15	0.46
1:E:140:HIS:ND1	1:E:141:PRO:N	2.64	0.46
1:E:264:VAL:HG13	1:E:340:ASP:HB3	1.97	0.46
1:E:547:MET:HE3	1:E:551:HIS:HB2	1.98	0.46
1:E:596:TRP:CH2	1:E:600:ASP:O	2.67	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:299:GLU:HB2	2:F:302:LEU:CD1	2.45	0.46
2:F:299:GLU:O	2:F:509:ARG:HA	2.15	0.46
2:F:376:ARG:HH11	2:H:410:LYS:NZ	2.13	0.46
2:F:417:TYR:CB	2:H:210:MET:HE2	2.45	0.46
1:G:515:VAL:HG21	1:G:631:GLY:HA3	1.96	0.46
1:I:658:THR:HG22	1:I:659:SER:O	2.16	0.46
1:K:518:PRO:O	1:K:521:ASP:N	2.36	0.46
1:K:626:ARG:C	1:K:627:ILE:HD12	2.40	0.46
2:L:108:VAL:O	2:L:122:PHE:HA	2.15	0.46
2:L:340:ILE:HG23	2:L:373:LYS:HD3	1.97	0.46
1:A:140:HIS:ND1	1:A:141:PRO:N	2.63	0.46
1:A:268:ARG:NH2	1:A:497:GLY:O	2.43	0.46
1:A:414:ILE:HD12	1:A:441:ILE:O	2.15	0.46
1:A:541:THR:O	1:A:541:THR:HG22	2.15	0.46
1:A:596:TRP:CG	1:A:597:THR:N	2.83	0.46
1:A:640:THR:OG1	1:A:643:GLN:HB2	2.15	0.46
2:B:210:MET:HE2	2:J:417:TYR:CB	2.41	0.46
2:B:423:THR:O	2:B:525:LYS:HE2	2.16	0.46
1:C:68:ILE:CG2	1:C:70:ASN:H	2.29	0.46
1:C:93:TYR:HD1	1:C:94:SER:O	1.98	0.46
1:C:530:ALA:HB2	1:C:561:VAL:HG21	1.97	0.46
1:G:118:ASN:C	1:G:119:GLN:HG3	2.41	0.46
1:G:396:ILE:HG22	1:G:466:MET:HE3	1.97	0.46
1:G:539:ARG:NH2	2:H:326:GLU:OE2	2.48	0.46
2:H:474:ARG:HD3	2:H:474:ARG:HA	1.65	0.46
2:H:479:ILE:HD12	2:H:479:ILE:C	2.39	0.46
1:I:150:SER:O	1:I:151:LYS:C	2.58	0.46
1:I:157:GLU:C	1:I:159:GLU:N	2.73	0.46
1:I:363:LEU:HD13	1:I:455:TRP:HB3	1.96	0.46
2:J:50:GLY:HA3	2:J:127:THR:O	2.15	0.46
2:J:145:MET:HE1	2:J:183:ASN:HD22	1.76	0.46
1:K:528:ALA:CB	1:K:605:LEU:HD22	2.45	0.46
1:A:316:MET:HE2	1:A:337:PHE:CD1	2.51	0.46
1:A:517:LEU:HA	1:A:518:PRO:HD3	1.59	0.46
1:A:577:ASP:HB2	1:A:591:ARG:NH2	2.31	0.46
2:B:235:THR:HG22	2:B:235:THR:O	2.16	0.46
2:B:529:MET:HE1	2:J:185:MET:HE3	1.97	0.46
1:C:357:GLU:CD	1:C:357:GLU:H	2.23	0.46
1:C:491:HIS:CE1	1:C:493:LYS:HB2	2.51	0.46
1:E:150:SER:O	1:E:153:ALA:N	2.48	0.46
1:E:164:VAL:HG22	1:E:373:MET:HE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:455:TRP:CD1	1:E:455:TRP:C	2.91	0.46
1:E:724:ILE:HG22	1:E:725:MET:HG3	1.98	0.46
1:G:93:TYR:HA	1:G:121:TYR:OH	2.15	0.46
1:G:396:ILE:HD12	1:G:396:ILE:N	2.30	0.46
2:H:192:GLN:O	2:H:211:THR:HB	2.16	0.46
1:I:70:ASN:ND2	1:I:145:PHE:CD1	2.84	0.46
1:I:162:ILE:O	1:I:164:VAL:N	2.49	0.46
1:I:186:GLU:CD	1:I:186:GLU:N	2.73	0.46
1:I:661:MET:HG3	1:I:723:VAL:HG13	1.98	0.46
2:J:416:LEU:HB2	2:J:441:VAL:HG22	1.96	0.46
1:K:65:LYS:HA	1:K:88:SER:O	2.16	0.46
1:K:335:VAL:HG12	1:K:350:MET:HE3	1.98	0.46
1:C:132:ARG:HD3	1:C:159:GLU:OE1	2.15	0.46
1:C:167:PRO:O	1:C:169:GLY:N	2.49	0.46
1:C:414:ILE:HD12	1:C:441:ILE:O	2.16	0.46
1:E:444:TYR:O	1:E:445:TYR:CG	2.69	0.46
1:G:285:LEU:HD12	1:G:285:LEU:N	2.31	0.46
1:G:295:ARG:O	1:G:296:ASN:HB2	2.16	0.46
1:G:485:LEU:O	1:G:486:SER:C	2.57	0.46
1:I:334:THR:CG2	1:I:351:ASN:HB2	2.46	0.46
2:J:227:GLY:O	2:J:231:VAL:HG23	2.16	0.46
2:L:45:ALA:O	2:L:48:LEU:HB2	2.16	0.46
2:L:199:PRO:HB3	2:L:222:TYR:CZ	2.51	0.46
1:A:170:ALA:O	1:A:173:ALA:HB3	2.16	0.46
1:A:658:THR:CB	1:A:703:LYS:HD3	2.46	0.46
2:B:347:LEU:O	2:B:348:GLU:C	2.58	0.46
1:C:189:VAL:CG2	1:C:323:LEU:HB2	2.45	0.46
2:D:222:TYR:C	2:D:222:TYR:CD1	2.94	0.46
2:D:232:LYS:O	2:D:236:ASN:N	2.42	0.46
2:F:195:MET:SD	2:F:271:VAL:HG21	2.56	0.46
1:G:92:ILE:CG1	1:G:112:ILE:HD13	2.46	0.46
1:G:156:LEU:HD13	1:G:163:PHE:HB2	1.95	0.46
2:J:124:GLN:HE21	2:J:137:HIS:CE1	2.34	0.46
1:K:229:MET:O	1:K:230:ARG:HB2	2.13	0.46
1:K:661:MET:HE2	1:K:726:GLU:HB3	1.96	0.46
1:K:690:ILE:CD1	1:K:699:LEU:HD11	2.45	0.46
2:L:474:ARG:HD3	2:L:474:ARG:HA	1.60	0.46
2:B:43:ARG:HG2	2:B:43:ARG:HH11	1.80	0.45
1:C:112:ILE:O	1:C:120:SER:HA	2.16	0.45
1:C:293:GLN:HB3	1:C:298:LYS:HA	1.97	0.45
1:E:99:GLN:O	1:E:100:ALA:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:162:ILE:O	1:E:164:VAL:N	2.49	0.45
1:E:304:PRO:HD2	1:E:394:TRP:CE2	2.51	0.45
1:E:347:PHE:CD1	1:E:347:PHE:O	2.69	0.45
2:F:307:PRO:HG3	2:F:312:THR:O	2.16	0.45
1:G:396:ILE:CG1	1:G:463:ILE:HD13	2.38	0.45
1:G:713:SER:H	1:G:716:ASN:CG	2.24	0.45
2:H:66:ALA:HB2	2:H:125:ASP:HA	1.98	0.45
2:H:394:VAL:HG23	2:H:395:PRO:HD2	1.98	0.45
2:H:419:TYR:CE1	2:H:443:SER:HB2	2.51	0.45
2:H:476(A):LEU:C	2:H:476(C):ASP:H	2.22	0.45
1:I:334:THR:HG22	1:I:351:ASN:HB2	1.98	0.45
2:J:476(C):ASP:C	2:J:477:GLU:H	2.24	0.45
1:K:78:VAL:HA	1:K:370:VAL:HG11	1.97	0.45
1:K:265:THR:HG21	1:K:342:GLN:NE2	2.31	0.45
2:L:295:PRO:O	2:L:513:LYS:HA	2.16	0.45
1:C:390:LYS:HD3	1:C:390:LYS:C	2.40	0.45
2:D:207:SER:O	2:D:208:PRO:C	2.59	0.45
2:D:476(C):ASP:N	2:D:476(D):PRO:HD3	2.31	0.45
1:E:358:HIS:N	1:E:359:PRO:CD	2.79	0.45
1:E:690:ILE:CD1	1:E:699:LEU:HD11	2.46	0.45
1:E:718:LEU:HD23	1:E:718:LEU:H	1.80	0.45
1:G:365:THR:HG22	1:G:391:LEU:HD22	1.98	0.45
1:G:518:PRO:O	1:G:519:GLU:C	2.58	0.45
1:G:583:PHE:HZ	1:G:590:MET:HE3	1.79	0.45
1:G:646:LEU:HD13	2:H:64:LEU:HD13	1.97	0.45
1:I:68:ILE:HG12	1:I:78:VAL:HG11	1.97	0.45
1:I:124:ILE:HG22	1:I:128:MET:CE	2.46	0.45
1:I:190:SER:N	1:I:319:GLN:OE1	2.36	0.45
1:I:661:MET:HE2	1:I:726:GLU:CB	2.46	0.45
2:J:348:GLU:OE2	1:K:551:HIS:HE1	2.00	0.45
1:K:71:ARG:CA	1:K:75:ALA:HB2	2.46	0.45
1:K:436:TYR:HD1	1:K:436:TYR:C	2.24	0.45
1:K:517:LEU:HD21	1:K:632:ALA:HB2	1.97	0.45
1:K:660:LYS:O	1:K:661:MET:HE3	2.16	0.45
2:B:119:VAL:HG13	2:B:156:ILE:HD13	1.98	0.45
2:B:134:SER:H	2:B:137:HIS:HB3	1.81	0.45
2:B:298:ILE:HG23	2:B:509:ARG:HB2	1.98	0.45
1:C:112:ILE:HD12	1:C:120:SER:O	2.16	0.45
1:C:272:ILE:HG22	1:C:274:VAL:HG13	1.98	0.45
1:C:525:VAL:O	1:C:526:ALA:C	2.57	0.45
1:C:537:GLU:HG3	1:C:553:ARG:NH2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:693:MET:HE1	2:D:398:LEU:HD13	1.98	0.45
1:E:92:ILE:HG13	1:E:112:ILE:HD13	1.98	0.45
1:E:598:PRO:HD2	2:F:292:PHE:CE1	2.50	0.45
1:G:124:ILE:HG22	1:G:128:MET:CE	2.46	0.45
1:G:497:GLY:O	1:G:499:MET:HG2	2.16	0.45
1:G:713:SER:O	1:G:714:ALA:C	2.59	0.45
2:H:43:ARG:HH11	2:H:43:ARG:CG	2.30	0.45
2:H:337:ALA:HB3	2:H:373:LYS:CD	2.46	0.45
1:I:139:VAL:O	1:I:164:VAL:HG12	2.16	0.45
1:I:317:GLY:O	1:I:321:VAL:HG12	2.17	0.45
1:I:353:ARG:HH11	1:I:353:ARG:HG3	1.82	0.45
1:I:411:LEU:HD22	1:I:682:GLN:HG3	1.99	0.45
1:I:484:PHE:HZ	1:I:504:ILE:HD11	1.80	0.45
2:J:195:MET:HE1	2:J:268:LEU:HD23	1.98	0.45
2:J:522:LEU:HD23	2:L:151:ASN:ND2	2.30	0.45
1:K:136:ALA:HB1	1:K:161:VAL:CG1	2.36	0.45
1:K:265:THR:HB	1:K:341:GLY:N	2.30	0.45
1:K:436:TYR:C	1:K:436:TYR:CD1	2.93	0.45
1:A:396:ILE:HG22	1:A:466:MET:HE3	1.98	0.45
1:A:443:MET:HG3	1:A:444:TYR:CE1	2.52	0.45
2:B:208:PRO:O	2:B:214:ILE:HD11	2.16	0.45
2:B:242:GLU:OE2	2:B:246:GLY:HA3	2.17	0.45
1:C:118:ASN:C	1:C:119:GLN:HG3	2.41	0.45
1:C:146:LEU:HD23	1:C:152:PHE:CD2	2.51	0.45
1:C:287:GLU:OE1	1:C:313:ARG:CD	2.64	0.45
2:D:117:ARG:HH21	2:D:280:LEU:HG	1.81	0.45
2:D:336:PHE:O	2:D:337:ALA:C	2.58	0.45
2:D:390:THR:CG2	2:D:419:TYR:OH	2.65	0.45
1:E:316:MET:CE	1:E:337:PHE:HD1	2.29	0.45
1:E:367:VAL:HG12	1:E:368:ASP:N	2.31	0.45
1:G:189:VAL:CG2	1:G:323:LEU:HB2	2.47	0.45
2:H:149:MET:CE	2:H:186:ALA:HA	2.45	0.45
1:I:83:ARG:CG	1:I:83:ARG:NH1	2.79	0.45
1:I:396:ILE:HG12	1:I:463:ILE:CD1	2.44	0.45
1:I:517:LEU:H	1:I:564:GLN:HE22	1.65	0.45
1:I:683:GLU:H	1:I:704:LYS:HG2	1.82	0.45
2:J:337:ALA:HB1	2:J:370:SER:HA	1.99	0.45
2:J:536:ASN:O	2:J:537:ILE:C	2.58	0.45
1:K:279:HIS:HD2	1:K:380:GLU:O	1.99	0.45
1:K:320:ALA:HB1	1:K:335:VAL:HG21	1.98	0.45
1:K:650:MET:HA	1:K:651:PRO:HD3	1.86	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:273:ARG:HD2	2:L:330:TYR:CD1	2.52	0.45
2:L:460:VAL:O	2:L:460:VAL:HG23	2.16	0.45
1:A:285:LEU:HB3	1:A:365:THR:HG21	1.99	0.45
1:A:348:LEU:O	1:A:349:GLU:HB3	2.16	0.45
1:A:482:LEU:N	1:A:483:PRO:HD2	2.32	0.45
2:B:126:PHE:HB2	2:B:160:ASP:OD2	2.17	0.45
2:B:149:MET:CE	2:B:189:VAL:CG1	2.95	0.45
2:B:189:VAL:HG23	2:J:532:LYS:HE2	1.98	0.45
2:B:474:ARG:HD3	2:B:474:ARG:HA	1.66	0.45
1:C:170:ALA:O	1:C:173:ALA:HB3	2.17	0.45
1:C:675:VAL:HG12	1:C:707:VAL:HG21	1.98	0.45
2:D:291:PHE:CZ	2:D:348:GLU:HA	2.51	0.45
2:D:335:GLU:HA	2:D:338:LYS:HE2	1.98	0.45
1:E:128:MET:SD	1:E:131:ILE:HD12	2.56	0.45
1:E:157:GLU:C	1:E:159:GLU:N	2.74	0.45
1:E:186:GLU:CD	1:E:186:GLU:N	2.75	0.45
1:G:65:LYS:HE2	1:G:134:THR:O	2.16	0.45
1:G:73:GLU:HG3	1:G:74:ILE:H	1.82	0.45
1:G:512:PHE:CZ	1:G:515:VAL:HG23	2.51	0.45
1:G:532:MET:HE1	1:G:603:ALA:CB	2.46	0.45
2:H:228:PRO:HB3	2:H:239:VAL:O	2.17	0.45
2:H:299:GLU:HG3	2:H:322:LYS:HB3	1.98	0.45
2:J:228:PRO:HB3	2:J:239:VAL:O	2.17	0.45
2:J:398:LEU:HA	2:J:399:PRO:HD3	1.80	0.45
1:K:124:ILE:HG22	1:K:128:MET:HE2	1.97	0.45
1:K:308:LEU:O	1:K:308:LEU:HD12	2.16	0.45
2:L:180:PHE:O	2:L:184:ILE:HG13	2.17	0.45
1:A:178:ILE:H	1:A:178:ILE:CD1	2.10	0.45
2:B:69:ARG:HH12	2:B:160:ASP:CG	2.25	0.45
2:B:492:ASN:HB2	2:B:493:PRO:CD	2.46	0.45
1:C:192:VAL:O	1:C:193:PRO:C	2.59	0.45
1:C:646:LEU:HD12	2:D:72:LEU:HD11	1.98	0.45
2:D:61:ARG:HB2	2:D:63:LYS:HG3	1.98	0.45
2:D:126:PHE:O	2:D:130:GLY:HA2	2.16	0.45
2:D:410:LYS:NZ	2:L:376:ARG:NH1	2.63	0.45
1:E:516:ASN:CB	1:E:564:GLN:NE2	2.76	0.45
1:E:675:VAL:HG12	1:E:707:VAL:HG21	1.97	0.45
2:F:84:MET:O	2:F:84:MET:HG2	2.15	0.45
1:G:287:GLU:OE1	1:G:287:GLU:N	2.47	0.45
1:G:354:LEU:HD11	1:G:358:HIS:CE1	2.52	0.45
1:G:491:HIS:CE1	1:G:493:LYS:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:514:ARG:HA	2:H:514:ARG:HD2	1.68	0.45
1:I:369:LEU:O	1:I:373:MET:HB2	2.16	0.45
2:J:149:MET:CE	2:J:189:VAL:CG1	2.95	0.45
2:J:355:VAL:HB	2:J:390:THR:HG23	1.98	0.45
2:J:460:VAL:CG2	2:J:496:ALA:HB2	2.47	0.45
1:K:504:ILE:CG2	1:K:505:ALA:N	2.80	0.45
1:K:614:LEU:HD22	1:K:627:ILE:HG21	1.96	0.45
1:K:627:ILE:HD12	1:K:627:ILE:N	2.31	0.45
2:L:156:ILE:N	2:L:156:ILE:CD1	2.80	0.45
2:L:390:THR:HG23	2:L:419:TYR:OH	2.17	0.45
1:A:71:ARG:CA	1:A:75:ALA:HB2	2.47	0.45
1:A:517:LEU:HB3	1:A:521:ASP:HB3	1.98	0.45
1:C:625:PHE:N	1:C:625:PHE:CD1	2.85	0.45
2:D:410:LYS:HZ2	2:L:376:ARG:NH1	2.14	0.45
2:D:423:THR:O	2:D:525:LYS:HE2	2.17	0.45
1:E:83:ARG:HB3	1:E:83:ARG:CZ	2.47	0.45
1:E:165:GLY:HA2	1:E:331:SER:OG	2.16	0.45
1:E:267:PRO:O	1:E:501:THR:HG23	2.17	0.45
1:E:537:GLU:HG3	1:E:553:ARG:HH21	1.82	0.45
1:E:537:GLU:HG3	1:E:553:ARG:NH2	2.31	0.45
1:E:660:LYS:O	1:E:661:MET:HE3	2.16	0.45
2:F:337:ALA:HB3	2:F:373:LYS:CD	2.43	0.45
2:F:476(C):ASP:O	2:F:478:LYS:N	2.44	0.45
1:G:164:VAL:HG23	1:G:373:MET:O	2.17	0.45
1:G:407:ARG:HG2	1:G:407:ARG:HH11	1.81	0.45
1:G:433:THR:HG21	1:G:435:VAL:HG12	1.94	0.45
2:H:476(C):ASP:CG	2:H:478:LYS:HG2	2.42	0.45
1:I:272:ILE:HB	1:I:335:VAL:HG23	1.99	0.45
1:I:302:GLU:OE2	1:I:394:TRP:HZ3	2.00	0.45
1:I:339:VAL:HG22	1:I:345:PHE:HB3	1.99	0.45
1:I:342:GLN:O	1:I:343:LYS:HB2	2.17	0.45
1:I:455:TRP:CG	1:I:456:ALA:N	2.80	0.45
1:I:543:VAL:CG1	2:J:117:ARG:HD2	2.45	0.45
1:I:642:ARG:HH11	2:J:71:ASP:HB3	1.82	0.45
2:J:154:PRO:HG3	2:J:191:PRO:HD2	1.99	0.45
1:K:376:VAL:HG23	1:K:377:ALA:N	2.31	0.45
1:K:650:MET:HA	1:K:650:MET:HE2	1.99	0.45
2:L:235:THR:HG22	2:L:237:GLU:HB2	1.99	0.45
1:A:491:HIS:CE1	1:A:493:LYS:HB2	2.51	0.45
1:A:653:LYS:N	1:A:653:LYS:CD	2.75	0.45
2:B:66:ALA:HB2	2:B:125:ASP:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:ARG:NH1	2:B:67:ARG:HG2	2.31	0.45
2:B:195:MET:HE1	2:B:268:LEU:HD23	1.99	0.45
2:B:514:ARG:HA	2:B:514:ARG:HD2	1.72	0.45
1:C:436:TYR:HE1	1:C:439:GLY:CA	2.30	0.45
1:C:467:ARG:HH11	1:C:467:ARG:CB	2.28	0.45
1:C:670:ILE:CG1	1:C:718:LEU:HD21	2.42	0.45
2:D:340:ILE:HD13	2:D:374:ALA:HB2	1.99	0.45
1:E:436:TYR:HE1	1:E:439:GLY:CA	2.29	0.45
2:F:121:VAL:HG22	2:F:122:PHE:N	2.31	0.45
2:F:509:ARG:HB3	2:F:509:ARG:HH11	1.81	0.45
1:G:107:ASP:C	1:G:108:GLU:HG3	2.41	0.45
1:G:598:PRO:HD2	2:H:292:PHE:CD1	2.52	0.45
2:H:145:MET:HE1	2:H:183:ASN:HD21	1.73	0.45
2:H:356:ALA:HB2	2:H:391:LEU:HB2	1.97	0.45
1:I:494:PHE:CD2	1:I:499:MET:HE1	2.52	0.45
1:I:642:ARG:NH1	2:J:71:ASP:OD2	2.50	0.45
1:K:214:TYR:HB2	1:K:215:PRO:HA	1.99	0.45
1:A:369:LEU:O	1:A:373:MET:HB2	2.17	0.45
2:B:151:ASN:ND2	2:D:522:LEU:HA	2.32	0.45
1:C:342:GLN:O	1:C:343:LYS:HB2	2.15	0.45
1:C:468:ILE:O	1:C:471:ASP:HB2	2.17	0.45
1:E:272:ILE:HG22	1:E:274:VAL:HG13	1.99	0.45
1:E:485:LEU:O	1:E:486:SER:C	2.59	0.45
2:F:180:PHE:O	2:F:183:ASN:HB2	2.17	0.45
1:G:308:LEU:HD12	1:G:308:LEU:C	2.42	0.45
1:G:393:GLY:HA3	1:G:455:TRP:CZ3	2.52	0.45
2:H:495:VAL:HG13	2:H:496:ALA:N	2.32	0.45
1:I:414:ILE:HD12	1:I:441:ILE:O	2.17	0.45
1:I:666:MET:O	1:I:668:GLY:N	2.50	0.45
1:I:720:VAL:HG22	1:I:721:ASP:H	1.82	0.45
2:J:164:ALA:HB2	2:J:176:TYR:HE2	1.82	0.45
2:J:300:PRO:HA	2:J:509:ARG:NH1	2.31	0.45
2:J:484:ALA:O	2:J:488:GLU:OE1	2.35	0.45
1:K:83:ARG:HH11	1:K:83:ARG:CG	2.28	0.45
1:K:596:TRP:CH2	1:K:600:ASP:O	2.69	0.45
1:A:71:ARG:O	1:A:75:ALA:HB2	2.17	0.45
1:A:98:LYS:O	1:A:98:LYS:HG3	2.17	0.45
1:A:122:ILE:HA	1:A:146:LEU:CD1	2.45	0.45
1:A:270:ILE:HG12	1:A:289:GLU:HG3	1.98	0.45
1:A:435:VAL:HG22	1:A:436:TYR:H	1.80	0.45
1:A:537:GLU:HG3	1:A:553:ARG:HH21	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:650:MET:HE2	1:A:650:MET:HA	1.98	0.45
2:B:83:ASP:HB3	2:B:86:VAL:HG23	1.97	0.45
2:B:524:ASN:O	2:B:525:LYS:C	2.59	0.45
1:C:92:ILE:HD12	1:C:112:ILE:HD13	1.99	0.45
1:C:515:VAL:HG21	1:C:631:GLY:HA3	1.99	0.45
2:D:121:VAL:O	2:D:144:ILE:HD13	2.17	0.45
2:D:235:THR:HG22	2:D:237:GLU:HB2	1.99	0.45
1:E:165:GLY:CA	1:E:331:SER:OG	2.65	0.45
1:E:358:HIS:O	1:E:359:PRO:C	2.60	0.45
2:F:66:ALA:HB2	2:F:125:ASP:HA	1.98	0.45
1:G:376:VAL:HG23	1:G:377:ALA:N	2.31	0.45
1:G:396:ILE:HD13	1:G:462:ALA:CB	2.47	0.45
1:K:598:PRO:HD2	2:L:292:PHE:CD1	2.51	0.45
2:L:460:VAL:HG21	2:L:496:ALA:CB	2.44	0.45
1:A:517:LEU:HD21	1:A:632:ALA:HB2	1.98	0.44
2:B:460:VAL:O	2:B:460:VAL:HG23	2.18	0.44
1:C:537:GLU:HG3	1:C:553:ARG:HH21	1.82	0.44
2:D:50:GLY:HA3	2:D:127:THR:O	2.17	0.44
2:D:474:ARG:HD3	2:D:474:ARG:HA	1.63	0.44
2:D:509:ARG:HB3	2:D:509:ARG:HH11	1.82	0.44
1:E:99:GLN:HB2	1:E:436:TYR:OH	2.16	0.44
1:E:390:LYS:HD3	1:E:391:LEU:H	1.78	0.44
1:E:405:PRO:CG	1:E:481:ASN:HA	2.45	0.44
2:F:149:MET:SD	2:F:186:ALA:HB2	2.57	0.44
2:F:393:ASP:CG	2:F:432:ARG:HB3	2.41	0.44
1:G:124:ILE:HG22	1:G:128:MET:HE2	1.99	0.44
1:G:124:ILE:O	1:G:128:MET:HB2	2.17	0.44
1:G:283:ILE:CG2	1:G:386:GLN:HG2	2.47	0.44
2:H:89:ARG:NH1	2:L:499:ARG:HH21	2.13	0.44
2:H:109:THR:HG22	2:H:122:PHE:CB	2.47	0.44
1:I:517:LEU:HA	1:I:518:PRO:HD3	1.57	0.44
1:I:596:TRP:CH2	1:I:600:ASP:O	2.70	0.44
2:J:537:ILE:HG13	2:J:538:PRO:HD2	1.99	0.44
1:K:305:SER:HA	1:K:306:PRO:HD3	1.81	0.44
1:K:627:ILE:HD13	1:K:636:VAL:HB	1.98	0.44
2:L:504:GLU:HG3	2:L:505:VAL:H	1.77	0.44
1:A:288:ARG:HD3	1:A:361:THR:OG1	2.17	0.44
1:A:292:ILE:HG23	1:A:503:PHE:CD2	2.52	0.44
2:B:229:ASP:OD1	2:B:229:ASP:N	2.49	0.44
2:B:329:PHE:HD1	2:B:345:ILE:HG22	1.83	0.44
2:B:436:GLY:HA2	2:J:173:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:456:ALA:CB	1:C:457:PRO:CD	2.94	0.44
1:E:335:VAL:CG1	1:E:350:MET:HE3	2.47	0.44
1:E:494:PHE:CD2	1:E:499:MET:HE1	2.52	0.44
1:G:117:ALA:C	1:G:119:GLN:N	2.73	0.44
1:G:186:GLU:CD	1:G:186:GLU:H	2.26	0.44
1:I:69:ALA:HB3	1:I:141:PRO:HA	1.99	0.44
1:I:93:TYR:HD1	1:I:94:SER:O	2.00	0.44
1:I:229:MET:O	1:I:230:ARG:HB2	2.18	0.44
1:I:627:ILE:N	1:I:627:ILE:HD12	2.33	0.44
1:I:704:LYS:HG3	1:I:704:LYS:H	1.58	0.44
2:J:335:GLU:HA	2:J:338:LYS:HE2	1.99	0.44
1:K:118:ASN:HD21	1:K:119:GLN:HE21	1.65	0.44
1:K:167:PRO:C	1:K:169:GLY:H	2.25	0.44
1:K:271:GLU:C	1:K:272:ILE:HD12	2.42	0.44
1:K:443:MET:HG3	1:K:444:TYR:CE1	2.52	0.44
1:A:95:ASP:C	1:A:97:ASP:H	2.26	0.44
1:A:390:LYS:HD3	1:A:390:LYS:C	2.43	0.44
1:A:713:SER:O	1:A:714:ALA:C	2.59	0.44
2:B:67:ARG:HG2	2:B:67:ARG:HH11	1.82	0.44
1:C:683:GLU:H	1:C:704:LYS:HG2	1.82	0.44
2:D:139:LYS:HB3	2:D:139:LYS:HE2	1.74	0.44
2:D:196:ILE:HD13	2:D:214:ILE:HG23	1.99	0.44
1:E:74:ILE:HG23	1:E:75:ALA:N	2.32	0.44
1:G:650:MET:HE2	1:G:650:MET:HA	1.99	0.44
1:G:664:CYS:HB2	1:G:724:ILE:HD11	2.00	0.44
2:H:49:GLY:C	2:H:51:GLY:H	2.26	0.44
1:I:68:ILE:HG12	1:I:78:VAL:CG1	2.47	0.44
1:I:256:ASP:OD1	1:I:256:ASP:N	2.50	0.44
1:K:187:ALA:O	1:K:188:ASN:CG	2.61	0.44
1:K:491:HIS:CE1	1:K:493:LYS:HB2	2.52	0.44
1:K:653:LYS:N	1:K:653:LYS:CD	2.78	0.44
1:A:115:PRO:HG2	1:A:444:TYR:CE2	2.52	0.44
1:A:325:LYS:O	1:A:328:GLY:N	2.41	0.44
1:A:405:PRO:CG	1:A:481:ASN:HA	2.47	0.44
1:A:419:ARG:HD2	1:A:601:GLN:OE1	2.17	0.44
1:A:518:PRO:O	1:A:519:GLU:C	2.60	0.44
1:C:71:ARG:CA	1:C:75:ALA:HB2	2.48	0.44
1:C:271:GLU:O	1:C:287:GLU:HB2	2.18	0.44
1:C:400:LEU:HD13	1:C:449:ILE:CD1	2.25	0.44
1:C:563:LEU:HB3	1:C:564:GLN:H	1.33	0.44
2:D:447:LEU:O	2:D:448:ARG:HB2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:157:GLU:C	1:G:159:GLU:N	2.74	0.44
1:G:517:LEU:HD22	1:G:517:LEU:N	2.23	0.44
2:H:88:HIS:CD2	2:H:88:HIS:C	2.95	0.44
1:I:77:ARG:HE	1:I:430:ARG:HH22	1.66	0.44
1:I:83:ARG:CZ	1:I:83:ARG:HB3	2.47	0.44
1:I:177:LYS:HE3	1:I:181:LYS:HZ1	1.81	0.44
1:I:302:GLU:OE2	1:I:394:TRP:CZ3	2.70	0.44
1:K:518:PRO:O	1:K:519:GLU:C	2.60	0.44
2:L:69:ARG:HA	2:L:268:LEU:HD11	1.98	0.44
2:L:476(C):ASP:C	2:L:477:GLU:H	2.25	0.44
1:A:164:VAL:HG23	1:A:377:ALA:CB	2.48	0.44
1:A:308:LEU:HD12	1:A:308:LEU:C	2.43	0.44
2:B:156:ILE:N	2:B:156:ILE:CD1	2.81	0.44
2:B:258:ASP:O	2:B:259:ALA:HB2	2.18	0.44
2:B:297:ARG:HG2	2:B:297:ARG:NH1	2.32	0.44
2:B:368:ILE:HG23	2:B:411:HIS:CG	2.53	0.44
1:C:165:GLY:CA	1:C:331:SER:OG	2.66	0.44
1:C:401:TYR:HD2	1:C:448:MET:HA	1.83	0.44
2:D:425:PRO:HB3	2:D:522:LEU:HB3	2.00	0.44
1:E:93:TYR:HD1	1:E:94:SER:O	2.01	0.44
1:E:167:PRO:C	1:E:169:GLY:N	2.76	0.44
1:E:264:VAL:HG12	1:E:340:ASP:HB3	2.00	0.44
1:E:457:PRO:CG	1:E:458:THR:N	2.80	0.44
1:E:563:LEU:O	1:E:565:GLY:N	2.50	0.44
2:F:121:VAL:O	2:F:144:ILE:HD13	2.18	0.44
2:F:355:VAL:O	2:F:390:THR:HA	2.16	0.44
1:G:321:VAL:O	1:G:324:ALA:CB	2.60	0.44
1:G:515:VAL:HB	1:G:631:GLY:C	2.42	0.44
2:H:325:ASP:C	2:H:327:GLY:N	2.76	0.44
2:H:442:MET:O	2:H:443:SER:C	2.58	0.44
1:I:122:ILE:HA	1:I:146:LEU:CD1	2.46	0.44
1:I:388:ASP:O	1:I:390:LYS:N	2.51	0.44
1:I:713:SER:O	1:I:714:ALA:C	2.60	0.44
1:K:139:VAL:HG11	1:K:156:LEU:CD2	2.48	0.44
1:K:285:LEU:N	1:K:285:LEU:HD12	2.32	0.44
1:A:275:LEU:HD23	1:A:276:CYS:H	1.82	0.44
1:C:467:ARG:HE	1:C:630:ARG:CG	2.29	0.44
1:C:516:ASN:CB	1:C:564:GLN:NE2	2.76	0.44
2:D:75:ASP:CG	2:D:115:ASN:H	2.26	0.44
1:E:273:GLN:O	1:E:285:LEU:HD12	2.18	0.44
1:E:275:LEU:HD23	1:E:276:CYS:H	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:491:HIS:O	1:E:495:ILE:HG13	2.17	0.44
2:F:174:ALA:HB2	2:H:501:PHE:CE1	2.53	0.44
2:F:196:ILE:HD12	2:F:196:ILE:N	2.33	0.44
2:F:401:THR:CG2	2:F:402:SER:N	2.80	0.44
1:G:99:GLN:O	1:G:100:ALA:O	2.36	0.44
1:G:156:LEU:HD22	1:G:161:VAL:HB	1.99	0.44
1:G:534:ARG:HG3	1:G:534:ARG:NH1	2.33	0.44
1:G:662:LEU:HD22	1:G:687:LEU:HD12	2.00	0.44
1:G:704:LYS:HG3	1:G:704:LYS:H	1.63	0.44
1:I:92:ILE:HG13	1:I:112:ILE:HD13	1.98	0.44
1:I:92:ILE:CG1	1:I:112:ILE:HD13	2.48	0.44
1:I:354:LEU:HD13	1:I:355:GLN:O	2.17	0.44
2:J:474:ARG:O	2:J:476:ASP:N	2.47	0.44
1:K:71:ARG:O	1:K:75:ALA:HB2	2.17	0.44
1:K:115:PRO:HG2	1:K:444:TYR:CE2	2.52	0.44
2:L:149:MET:HE1	2:L:189:VAL:HG11	2.00	0.44
1:A:99:GLN:O	1:A:100:ALA:C	2.60	0.44
1:A:400:LEU:HD21	1:A:482:LEU:CD1	2.48	0.44
1:A:421:ARG:O	1:A:421:ARG:CD	2.66	0.44
2:B:58:GLN:NE2	2:B:63:LYS:HE3	2.32	0.44
2:B:229:ASP:O	2:B:233:THR:HG23	2.18	0.44
1:C:182:LYS:HA	1:C:185:GLN:HG3	2.00	0.44
1:C:347:PHE:O	1:C:347:PHE:HD1	2.00	0.44
1:C:629:THR:HB	1:C:630:ARG:H	1.71	0.44
2:D:303:ASP:OD1	2:D:508:PRO:HB2	2.18	0.44
1:E:168:LYS:O	1:E:172:GLU:OE1	2.36	0.44
1:E:523:ARG:HB3	1:E:590:MET:CE	2.48	0.44
1:E:615:LYS:HB2	1:E:628:ARG:HB2	2.00	0.44
2:F:447:LEU:O	2:F:448:ARG:HB2	2.17	0.44
2:F:501:PHE:CE1	2:H:174:ALA:HB2	2.53	0.44
1:G:414:ILE:HD11	1:G:442:SER:C	2.42	0.44
2:H:378:VAL:HG13	2:H:388:LEU:CD1	2.47	0.44
1:I:393:GLY:HA2	1:I:457:PRO:O	2.17	0.44
2:J:206:TYR:O	2:J:209:ALA:HB3	2.17	0.44
1:K:212:ILE:HD12	1:K:260:ILE:CG2	2.47	0.44
1:K:272:ILE:HG22	1:K:274:VAL:HG13	2.00	0.44
2:L:49:GLY:C	2:L:51:GLY:H	2.25	0.44
2:L:258:ASP:O	2:L:259:ALA:HB2	2.17	0.44
2:L:356:ALA:HB2	2:L:391:LEU:HB2	1.99	0.44
1:A:414:ILE:CD1	1:A:441:ILE:O	2.64	0.44
1:A:441:ILE:HD12	1:A:478:ILE:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:184:ILE:CD1	2:J:417:TYR:HA	2.44	0.44
1:C:186:GLU:OE2	1:C:187:ALA:N	2.51	0.44
2:D:94:ASN:HA	2:D:98:GLN:OE1	2.18	0.44
2:D:312:THR:HG22	2:D:313:PRO:O	2.17	0.44
2:D:417:TYR:CB	2:L:210:MET:HE2	2.48	0.44
1:E:539:ARG:NH2	2:F:326:GLU:OE2	2.51	0.44
1:E:640:THR:OG1	1:E:643:GLN:HB2	2.18	0.44
1:E:661:MET:HE2	1:E:726:GLU:CB	2.46	0.44
2:F:45:ALA:O	2:F:48:LEU:HB2	2.18	0.44
2:F:95:MET:HE3	2:F:95:MET:HA	2.00	0.44
2:F:529:MET:HE2	2:H:185:MET:HE3	2.00	0.44
1:G:653:LYS:N	1:G:653:LYS:CD	2.78	0.44
2:H:374:ALA:HB3	2:H:415:LEU:HD13	1.99	0.44
2:H:440:VAL:O	2:H:444:SER:HB3	2.18	0.44
1:I:156:LEU:HD13	1:I:163:PHE:HB2	1.96	0.44
1:I:209:SER:O	1:I:212:ILE:N	2.51	0.44
1:I:684:GLY:N	1:I:701:ALA:O	2.48	0.44
2:J:498:GLU:HG2	2:L:87:THR:HG23	2.00	0.44
1:K:199:ILE:HD13	1:K:205:ALA:HA	1.99	0.44
1:K:388:ASP:O	1:K:390:LYS:N	2.51	0.44
1:K:651:PRO:CG	2:L:62:GLY:HA3	2.48	0.44
2:L:514:ARG:HA	2:L:514:ARG:HD2	1.67	0.44
1:A:316:MET:HE2	1:A:337:PHE:HD1	1.83	0.44
2:B:356:ALA:HB2	2:B:391:LEU:HB2	1.99	0.44
1:C:67:LEU:C	1:C:68:ILE:HD12	2.43	0.44
1:C:376:VAL:HG23	1:C:377:ALA:N	2.33	0.44
1:C:455:TRP:CG	1:C:456:ALA:N	2.82	0.44
1:C:518:PRO:O	1:C:521:ASP:HB2	2.17	0.44
1:C:634:LEU:HD23	1:C:634:LEU:H	1.83	0.44
1:C:660:LYS:O	1:C:661:MET:HE3	2.17	0.44
1:E:112:ILE:O	1:E:120:SER:HA	2.18	0.44
1:E:411:LEU:HD22	1:E:682:GLN:CB	2.46	0.44
2:F:366:LEU:HD23	2:F:366:LEU:HA	1.81	0.44
1:G:70:ASN:OD1	1:G:74:ILE:HG21	2.17	0.44
1:G:177:LYS:HB3	1:G:181:LYS:HZ1	1.81	0.44
1:G:660:LYS:O	1:G:661:MET:HE3	2.18	0.44
1:I:71:ARG:NH1	1:I:445:TYR:CG	2.86	0.44
1:I:140:HIS:ND1	1:I:141:PRO:N	2.66	0.44
1:I:150:SER:O	1:I:153:ALA:N	2.51	0.44
1:I:271:GLU:O	1:I:287:GLU:HB2	2.18	0.44
1:I:276:CYS:HB2	1:I:277:ASP:H	1.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:109:THR:HG22	2:J:122:PHE:CB	2.47	0.44
2:J:374:ALA:HB3	2:J:415:LEU:HD13	1.99	0.44
1:K:93:TYR:HD1	1:K:94:SER:O	2.01	0.44
1:K:334:THR:HG21	1:K:355:GLN:CG	2.47	0.44
1:K:347:PHE:CD1	1:K:347:PHE:C	2.94	0.44
3:A:801:BTI:H63	2:B:399:PRO:HD3	2.00	0.43
2:B:205:VAL:HB	2:J:409:ILE:HG23	2.00	0.43
2:B:339:ASN:HB3	2:B:361:VAL:HG12	2.00	0.43
1:E:117:ALA:HA	1:E:121:TYR:H	1.82	0.43
1:E:139:VAL:O	1:E:164:VAL:HG12	2.18	0.43
1:E:411:LEU:HB2	1:E:682:GLN:HG3	1.99	0.43
2:F:492:ASN:HB2	2:F:493:PRO:CD	2.46	0.43
1:G:92:ILE:HG13	1:G:112:ILE:HD13	1.99	0.43
1:G:422:PRO:HA	1:G:422(A):PRO:HD3	1.82	0.43
1:G:615:LYS:HB2	1:G:628:ARG:HB2	2.00	0.43
1:I:71:ARG:O	1:I:75:ALA:HB2	2.18	0.43
1:I:272:ILE:HG22	1:I:274:VAL:HG13	2.00	0.43
1:I:279:HIS:HD2	1:I:380:GLU:O	2.00	0.43
1:I:390:LYS:HD3	1:I:390:LYS:C	2.42	0.43
1:I:446:ASP:OD1	1:I:447:PRO:HD2	2.17	0.43
1:I:598:PRO:HD2	2:J:292:PHE:CD1	2.53	0.43
1:K:107:ASP:O	1:K:108:GLU:HG3	2.19	0.43
1:K:455:TRP:CD1	1:K:455:TRP:C	2.93	0.43
1:A:150:SER:O	1:A:153:ALA:N	2.51	0.43
1:A:287:GLU:HG3	1:A:308:LEU:HD21	2.00	0.43
1:A:418:THR:O	1:A:437:GLU:HG3	2.18	0.43
1:A:492:PRO:HA	1:A:495:ILE:HD12	2.00	0.43
1:C:179:THR:HG22	1:C:183:ILE:CD1	2.46	0.43
1:C:279:HIS:CD2	1:C:380:GLU:O	2.71	0.43
1:C:283:ILE:CG2	1:C:386:GLN:HG2	2.48	0.43
1:C:482:LEU:N	1:C:483:PRO:HD2	2.32	0.43
1:C:583:PHE:N	1:C:583:PHE:CD1	2.86	0.43
1:E:285:LEU:HD12	1:E:285:LEU:N	2.33	0.43
1:E:467:ARG:HH11	1:E:467:ARG:CB	2.27	0.43
1:E:658:THR:CB	1:E:703:LYS:HD3	2.43	0.43
2:F:134:SER:H	2:F:137:HIS:HB3	1.82	0.43
2:F:372:ARG:NH2	2:H:539:LEU:OXT	2.50	0.43
1:G:99:GLN:O	1:G:100:ALA:C	2.61	0.43
1:G:258:ILE:HG22	1:G:259:PHE:N	2.33	0.43
1:G:272:ILE:HB	1:G:335:VAL:CG2	2.48	0.43
1:G:436:TYR:C	1:G:436:TYR:CD1	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:436:TYR:C	1:G:436:TYR:HD1	2.26	0.43
1:G:532:MET:O	1:G:535:VAL:HB	2.18	0.43
1:G:596:TRP:CH2	1:G:600:ASP:O	2.71	0.43
1:G:682:GLN:OE1	1:G:682:GLN:HA	2.19	0.43
2:H:120:TYR:HE2	2:H:147:MET:HE2	1.83	0.43
2:H:180:PHE:O	2:H:183:ASN:HB2	2.18	0.43
2:H:315:ASP:C	2:H:315:ASP:OD1	2.60	0.43
2:H:460:VAL:O	2:H:460:VAL:CG2	2.66	0.43
1:I:92:ILE:HD12	1:I:112:ILE:HD13	1.99	0.43
1:I:100:ALA:HB3	1:I:103:VAL:HG23	1.99	0.43
1:I:626:ARG:C	1:I:627:ILE:HD12	2.43	0.43
2:J:514:ARG:HA	2:J:514:ARG:HD2	1.74	0.43
1:K:164:VAL:HG23	1:K:377:ALA:HB2	1.99	0.43
1:K:619:ILE:HD11	1:K:626:ARG:HB2	2.00	0.43
2:L:196:ILE:HD12	2:L:196:ILE:N	2.33	0.43
2:L:298:ILE:HD12	2:L:298:ILE:N	2.33	0.43
1:A:93:TYR:HA	1:A:121:TYR:OH	2.17	0.43
1:A:162:ILE:O	1:A:164:VAL:N	2.51	0.43
2:B:164:ALA:HB2	2:B:176:TYR:HE2	1.83	0.43
2:B:394:VAL:HG23	2:B:395:PRO:HD2	2.00	0.43
1:C:285:LEU:N	1:C:285:LEU:HD12	2.33	0.43
2:D:460:VAL:CG2	2:D:496:ALA:HB2	2.43	0.43
1:E:414:ILE:CD1	1:E:441:ILE:O	2.66	0.43
2:F:423:THR:O	2:F:525:LYS:HE2	2.18	0.43
1:G:188:ASN:OD1	1:G:188:ASN:O	2.36	0.43
1:G:563:LEU:HD23	1:G:636:VAL:HG22	2.00	0.43
2:H:180:PHE:O	2:H:184:ILE:HG13	2.18	0.43
1:I:287:GLU:OE2	1:I:305:SER:N	2.45	0.43
1:I:289:GLU:OE1	1:I:306:PRO:HD2	2.18	0.43
1:K:124:ILE:HG22	1:K:128:MET:CE	2.48	0.43
1:K:660:LYS:C	1:K:661:MET:HE3	2.44	0.43
1:K:675:VAL:HG11	1:K:707:VAL:HG21	1.98	0.43
2:L:196:ILE:HD13	2:L:214:ILE:HG23	1.99	0.43
2:L:351:THR:HG22	2:L:386:ILE:HG23	2.00	0.43
1:A:70:ASN:ND2	1:A:145:PHE:CE1	2.87	0.43
2:B:80:GLU:HB2	2:D:517:ARG:NH2	2.33	0.43
1:C:273:GLN:HG2	1:C:369:LEU:HD11	2.00	0.43
1:C:327:VAL:HG22	1:C:327:VAL:O	2.18	0.43
1:C:480:HIS:HD2	1:C:482:LEU:H	1.66	0.43
2:D:476(D):PRO:HA	2:D:479:ILE:HD11	2.00	0.43
1:E:95:ASP:C	1:E:97:ASP:H	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:285:LEU:HB3	1:E:365:THR:HG21	2.00	0.43
1:E:467:ARG:HD2	1:E:467:ARG:O	2.19	0.43
2:F:258:ASP:O	2:F:259:ALA:HB2	2.17	0.43
1:G:70:ASN:ND2	1:G:145:PHE:CE1	2.86	0.43
1:G:206:VAL:HG13	1:G:235:ASP:CB	2.49	0.43
1:G:229:MET:O	1:G:230:ARG:HB2	2.17	0.43
1:G:256:ASP:N	1:G:256:ASP:OD1	2.52	0.43
1:G:417:LEU:HD21	1:G:478:ILE:CD1	2.46	0.43
2:H:208:PRO:C	2:H:214:ILE:HD11	2.44	0.43
1:I:118:ASN:C	1:I:119:GLN:HG3	2.43	0.43
1:I:376:VAL:HG23	1:I:377:ALA:N	2.33	0.43
1:K:325:LYS:O	1:K:327:VAL:N	2.52	0.43
1:K:369:LEU:O	1:K:373:MET:HB2	2.17	0.43
2:L:126:PHE:HB2	2:L:160:ASP:OD2	2.18	0.43
2:L:347:LEU:O	2:L:348:GLU:C	2.61	0.43
1:A:99:GLN:O	1:A:100:ALA:O	2.36	0.43
2:B:476(A):LEU:C	2:B:476(C):ASP:H	2.27	0.43
1:C:421:ARG:O	1:C:421:ARG:CD	2.67	0.43
1:C:650:MET:HA	1:C:651:PRO:HD3	1.87	0.43
2:D:149:MET:SD	2:D:186:ALA:HB2	2.59	0.43
2:D:202:GLY:HA2	2:D:225:VAL:O	2.18	0.43
2:D:208:PRO:C	2:D:214:ILE:HD11	2.43	0.43
2:D:458:ALA:O	2:D:492:ASN:HA	2.19	0.43
1:E:164:VAL:HG23	1:E:377:ALA:CB	2.47	0.43
1:E:327:VAL:O	1:E:327:VAL:HG22	2.19	0.43
1:E:401:TYR:CD2	1:E:448:MET:HA	2.53	0.43
1:E:421:ARG:O	1:E:421:ARG:HD3	2.19	0.43
1:E:518:PRO:HD2	1:E:521:ASP:OD1	2.18	0.43
1:E:532:MET:HE2	1:E:596:TRP:CG	2.53	0.43
2:F:117:ARG:NH2	2:F:280:LEU:HG	2.33	0.43
1:G:348:LEU:HD23	1:G:348:LEU:O	2.19	0.43
1:G:393:GLY:HA2	1:G:457:PRO:O	2.19	0.43
1:G:625:PHE:HB2	1:G:627:ILE:CD1	2.48	0.43
1:G:634:LEU:HD23	1:G:634:LEU:H	1.82	0.43
2:H:235:THR:C	2:H:237:GLU:N	2.74	0.43
2:H:323:LEU:O	2:H:324:ALA:C	2.60	0.43
1:I:396:ILE:HD13	1:I:462:ALA:CB	2.49	0.43
1:I:633:ASP:OD1	1:I:633:ASP:C	2.62	0.43
2:J:251:THR:HG21	2:J:260:ALA:CB	2.46	0.43
2:J:476(A):LEU:C	2:J:476(C):ASP:H	2.25	0.43
1:K:150:SER:O	1:K:151:LYS:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:167:PRO:C	1:K:169:GLY:N	2.74	0.43
1:K:354:LEU:HD13	1:K:355:GLN:O	2.17	0.43
1:K:401:TYR:HD2	1:K:448:MET:HA	1.84	0.43
2:L:126:PHE:O	2:L:130:GLY:HA2	2.19	0.43
2:L:200:CYS:O	2:L:223:MET:HA	2.18	0.43
1:A:283:ILE:HG22	1:A:386:GLN:HG2	2.01	0.43
2:B:202:GLY:O	2:B:203:GLY:C	2.61	0.43
1:C:287:GLU:OE1	1:C:313:ARG:HD2	2.19	0.43
1:C:517:LEU:HD21	1:C:632:ALA:HB1	2.00	0.43
1:C:617:GLY:O	1:C:625:PHE:CB	2.55	0.43
1:C:693:MET:O	1:C:694:LYS:HB2	2.18	0.43
2:D:74:LEU:HD13	2:D:112:GLY:HA3	2.00	0.43
1:E:93:TYR:O	1:E:112:ILE:HG12	2.19	0.43
1:E:324:ALA:O	1:E:325:LYS:C	2.61	0.43
1:E:521:ASP:O	1:E:522:LEU:C	2.62	0.43
1:E:552:GLU:CD	1:E:552:GLU:N	2.76	0.43
2:F:531:TRP:CG	2:F:532:LYS:N	2.86	0.43
1:G:287:GLU:OE2	1:G:305:SER:N	2.48	0.43
1:G:325:LYS:O	1:G:327:VAL:N	2.51	0.43
1:G:388:ASP:O	1:G:390:LYS:N	2.52	0.43
1:G:435:VAL:HG22	1:G:436:TYR:N	2.34	0.43
2:H:401:THR:CG2	2:H:402:SER:N	2.80	0.43
1:I:157:GLU:OE1	1:I:168:LYS:NZ	2.52	0.43
1:I:660:LYS:C	1:I:661:MET:HE3	2.44	0.43
1:K:118:ASN:C	1:K:119:GLN:HG3	2.44	0.43
1:K:675:VAL:HG12	1:K:707:VAL:HG21	1.99	0.43
2:L:235:THR:HG22	2:L:235:THR:O	2.18	0.43
1:A:401:TYR:HD2	1:A:448:MET:HA	1.84	0.43
1:A:704:LYS:HG3	1:A:704:LYS:H	1.64	0.43
2:B:121:VAL:CG2	2:B:122:PHE:N	2.81	0.43
2:B:339:ASN:HD21	2:B:370:SER:HB3	1.83	0.43
2:D:393:ASP:CG	2:D:432:ARG:HB3	2.43	0.43
2:D:460:VAL:O	2:D:460:VAL:HG23	2.19	0.43
2:D:492:ASN:ND2	2:D:494:PHE:HB2	2.33	0.43
1:E:162:ILE:HD13	1:E:377:ALA:O	2.19	0.43
1:E:524:ARG:N	1:E:590:MET:HE1	2.33	0.43
2:F:346:ARG:HH11	2:F:346:ARG:CG	2.28	0.43
1:G:68:ILE:CG1	1:G:78:VAL:HG11	2.49	0.43
1:G:271:GLU:O	1:G:287:GLU:HB2	2.18	0.43
1:G:464:GLU:O	1:G:465:ALA:C	2.62	0.43
1:G:546:ARG:H	1:G:546:ARG:HG2	1.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:563:LEU:HB3	1:G:564:GLN:H	1.30	0.43
1:I:70:ASN:ND2	1:I:145:PHE:CE1	2.87	0.43
1:I:71:ARG:CA	1:I:75:ALA:HB2	2.48	0.43
1:I:411:LEU:HD22	1:I:682:GLN:CG	2.49	0.43
2:J:392:ILE:HD12	2:J:428:THR:CG2	2.48	0.43
1:K:95:ASP:C	1:K:97:ASP:H	2.25	0.43
1:K:354:LEU:HD11	1:K:358:HIS:ND1	2.33	0.43
1:K:371:GLU:O	1:K:372:GLN:C	2.61	0.43
1:K:517:LEU:HA	1:K:518:PRO:HD3	1.62	0.43
1:K:563:LEU:HB3	1:K:564:GLN:H	1.37	0.43
1:A:164:VAL:HA	1:A:377:ALA:HB1	2.00	0.43
1:A:308:LEU:HD11	1:A:313:ARG:HD3	2.00	0.43
1:A:504:ILE:CG2	1:A:505:ALA:N	2.81	0.43
1:A:563:LEU:HB3	1:A:564:GLN:H	1.25	0.43
2:B:291:PHE:CZ	2:B:348:GLU:HA	2.54	0.43
1:C:110:VAL:HG21	1:C:130:ALA:CB	2.46	0.43
1:C:270:ILE:HG21	1:C:308:LEU:HD21	2.01	0.43
1:C:405:PRO:CG	1:C:481:ASN:HA	2.49	0.43
1:C:605:LEU:CD1	1:C:614:LEU:HD12	2.49	0.43
1:C:690:ILE:CD1	1:C:699:LEU:HD11	2.48	0.43
2:D:196:ILE:HG22	2:D:221:SER:HB2	2.01	0.43
1:E:167:PRO:C	1:E:169:GLY:H	2.26	0.43
1:E:679:GLN:O	1:E:706:VAL:HG13	2.19	0.43
1:G:292:ILE:HD12	1:G:292:ILE:N	2.11	0.43
1:G:675:VAL:HG11	1:G:707:VAL:HG21	2.00	0.43
2:H:297:ARG:HG2	2:H:297:ARG:HH11	1.83	0.43
1:I:724:ILE:C	1:I:725:MET:HG3	2.43	0.43
2:J:498:GLU:HA	2:L:86:VAL:HA	1.99	0.43
1:K:231:ILE:HD12	1:K:231:ILE:N	2.32	0.43
1:K:245:SER:O	1:K:247:ASN:N	2.52	0.43
2:L:356:ALA:CB	2:L:391:LEU:HB2	2.49	0.43
1:A:340:ASP:C	1:A:340:ASP:OD1	2.62	0.43
1:A:358:HIS:CG	1:A:359:PRO:HD3	2.54	0.43
2:B:137:HIS:C	2:B:137:HIS:CD2	2.97	0.43
2:B:531:TRP:CG	2:B:532:LYS:N	2.87	0.43
1:C:74:ILE:HG23	1:C:75:ALA:N	2.33	0.43
1:C:354:LEU:C	1:C:354:LEU:HD13	2.44	0.43
1:C:670:ILE:HD12	1:C:712:ALA:HB1	2.01	0.43
2:D:54:ARG:HG2	2:D:54:ARG:HH11	1.82	0.43
2:D:300:PRO:HB3	2:D:509:ARG:HH12	1.83	0.43
1:E:102:HIS:CG	1:E:103:VAL:N	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:661:MET:HG3	1:E:723:VAL:HG13	2.00	0.43
1:G:348:LEU:O	1:G:349:GLU:HB3	2.19	0.43
2:J:196:ILE:HD13	2:J:214:ILE:HG23	2.00	0.43
2:J:315:ASP:C	2:J:315:ASP:OD1	2.61	0.43
1:K:64:ASN:H	1:K:137:GLN:HG2	1.83	0.43
1:K:443:MET:SD	1:K:444:TYR:CE1	3.11	0.43
1:K:664:CYS:HB2	1:K:724:ILE:HD11	2.00	0.43
2:L:95:MET:HE3	2:L:95:MET:HA	1.99	0.43
2:L:297:ARG:HG2	2:L:297:ARG:HH11	1.84	0.43
1:A:128:MET:O	1:A:129:ALA:C	2.62	0.43
1:A:712:ALA:HA	1:A:716:ASN:ND2	2.34	0.43
2:B:109:THR:HG22	2:B:122:PHE:HB2	2.00	0.43
2:B:183:ASN:OD1	2:B:207:SER:OG	2.26	0.43
2:B:501:PHE:N	2:B:501:PHE:HD2	2.13	0.43
1:C:586:ASP:OD1	1:C:588:SER:OG	2.32	0.43
1:C:664:CYS:HB2	1:C:724:ILE:HD11	2.01	0.43
1:E:316:MET:HG2	1:E:345:PHE:CD2	2.54	0.43
2:F:75:ASP:OD1	2:F:272:ARG:NH2	2.48	0.43
2:F:235:THR:O	2:F:235:THR:HG22	2.18	0.43
2:H:117:ARG:HH21	2:H:280:LEU:HG	1.84	0.43
2:H:217:VAL:O	2:H:218:LYS:C	2.61	0.43
2:H:303:ASP:OD2	2:H:509:ARG:HD2	2.19	0.43
2:H:361:VAL:O	2:H:362:LEU:C	2.61	0.43
2:H:434:ALA:HB3	2:H:460:VAL:HG12	2.01	0.43
2:H:468:ALA:O	2:H:472:ILE:HG13	2.18	0.43
2:H:476(D):PRO:HA	2:H:479:ILE:HD11	2.00	0.43
1:I:456:ALA:CB	1:I:457:PRO:CD	2.95	0.43
1:K:693:MET:O	1:K:694:LYS:HB2	2.19	0.43
1:A:388:ASP:O	1:A:390:LYS:N	2.52	0.42
1:C:71:ARG:O	1:C:75:ALA:CB	2.67	0.42
2:D:460:VAL:HG21	2:D:496:ALA:CB	2.47	0.42
1:E:309:ASP:OD2	1:E:343:LYS:HE2	2.19	0.42
1:E:390:LYS:C	1:E:391:LEU:HD23	2.43	0.42
1:E:543:VAL:CG1	2:F:117:ARG:HD2	2.49	0.42
2:F:58:GLN:HA	2:F:61:ARG:HH21	1.84	0.42
2:F:206:TYR:O	2:F:209:ALA:HB3	2.18	0.42
2:F:293:ASP:OD2	2:F:294:ASP:N	2.52	0.42
2:F:403:GLN:O	2:F:408:VAL:HG22	2.19	0.42
1:G:212:ILE:HD12	1:G:260:ILE:HG22	2.01	0.42
1:G:231:ILE:HD12	1:G:231:ILE:N	2.31	0.42
1:G:661:MET:HE2	1:G:726:GLU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:95:MET:HE3	2:H:95:MET:O	2.19	0.42
2:H:392:ILE:HG12	2:H:442:MET:HB3	2.01	0.42
2:H:499:ARG:HD3	2:H:499:ARG:HA	1.88	0.42
1:I:266:GLN:HB3	1:I:500:THR:HG22	2.01	0.42
1:I:455:TRP:CD1	1:I:455:TRP:C	2.91	0.42
1:K:78:VAL:CG1	1:K:79:ILE:N	2.82	0.42
1:K:319:GLN:NE2	1:K:345:PHE:HE1	2.16	0.42
1:K:395:ALA:C	1:K:396:ILE:HD12	2.44	0.42
1:K:454:THR:HG21	1:K:466:MET:HA	2.00	0.42
1:K:459:ARG:O	1:K:463:ILE:HG12	2.19	0.42
2:L:251:THR:HG21	2:L:260:ALA:CB	2.43	0.42
2:L:340:ILE:CG2	2:L:373:LYS:HD3	2.49	0.42
1:A:317:GLY:O	1:A:321:VAL:HG12	2.19	0.42
1:C:130:ALA:HA	1:C:133:ALA:CB	2.45	0.42
1:C:319:GLN:NE2	1:C:345:PHE:CE1	2.87	0.42
1:E:68:ILE:HG12	1:E:78:VAL:HG11	2.01	0.42
1:E:176:ASP:OD1	1:E:178:ILE:HD13	2.19	0.42
1:E:553:ARG:NH1	2:F:115:ASN:OD1	2.52	0.42
2:F:355:VAL:HB	2:F:390:THR:HG23	2.01	0.42
2:F:424:VAL:O	2:F:525:LYS:NZ	2.47	0.42
1:G:75:ALA:O	1:G:79:ILE:HG13	2.18	0.42
1:G:411:LEU:HB2	1:G:682:GLN:HG3	2.00	0.42
2:H:50:GLY:HA3	2:H:127:THR:O	2.19	0.42
1:I:118:ASN:HD21	1:I:119:GLN:HE21	1.67	0.42
1:I:608:ASP:C	1:I:610:ALA:H	2.27	0.42
1:K:128:MET:O	1:K:129:ALA:C	2.61	0.42
1:K:191:THR:O	1:K:193:PRO:HD3	2.18	0.42
1:K:396:ILE:HG12	1:K:463:ILE:CD1	2.45	0.42
1:K:625:PHE:CD1	1:K:625:PHE:N	2.87	0.42
1:K:649:LEU:HD13	2:L:59:HIS:CD2	2.54	0.42
1:K:713:SER:H	1:K:716:ASN:CG	2.27	0.42
2:L:94:ASN:C	2:L:98:GLN:OE1	2.62	0.42
2:L:382:ASP:HA	2:L:424:VAL:CG1	2.50	0.42
1:A:353:ARG:HH11	1:A:353:ARG:HG3	1.83	0.42
2:B:52:GLN:OE1	2:B:52:GLN:O	2.37	0.42
2:B:303:ASP:OD2	2:B:509:ARG:HD2	2.19	0.42
2:B:533:LYS:HD2	2:J:385:GLU:OE2	2.18	0.42
1:C:118:ASN:O	1:C:119:GLN:HG3	2.19	0.42
1:C:186:GLU:CD	1:C:186:GLU:H	2.26	0.42
1:C:323:LEU:O	1:C:326:ALA:HB3	2.19	0.42
2:D:252:ARG:HE	2:D:252:ARG:HB2	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:66:ILE:HG22	1:E:137:GLN:HG3	2.01	0.42
2:F:281:ASN:OD1	2:F:281:ASN:C	2.63	0.42
1:G:68:ILE:HG12	1:G:78:VAL:CG1	2.50	0.42
1:G:191:THR:O	1:G:193:PRO:HD3	2.19	0.42
1:G:646:LEU:C	1:G:648:ARG:N	2.76	0.42
2:H:460:VAL:CG2	2:H:496:ALA:HB2	2.46	0.42
1:I:464:GLU:HA	1:I:464:GLU:OE2	2.19	0.42
1:I:628:ARG:HG3	1:I:633:ASP:HA	2.01	0.42
2:J:84:MET:SD	2:J:85:PHE:CE1	3.13	0.42
1:K:66:ILE:HD13	1:K:88:SER:O	2.19	0.42
1:K:272:ILE:HB	1:K:335:VAL:CG2	2.49	0.42
1:K:273:GLN:HG2	1:K:369:LEU:HD11	2.01	0.42
1:K:354:LEU:HD13	1:K:355:GLN:N	2.34	0.42
1:K:518:PRO:HD2	1:K:521:ASP:OD1	2.20	0.42
1:K:617:GLY:O	1:K:625:PHE:CB	2.52	0.42
2:L:416:LEU:HD13	2:L:441:VAL:HG22	2.01	0.42
1:A:107:ASP:O	1:A:108:GLU:HG3	2.19	0.42
1:A:156:LEU:HD22	1:A:161:VAL:HB	2.02	0.42
1:A:292:ILE:HD13	1:A:300:VAL:O	2.19	0.42
1:A:388:ASP:OD2	1:A:388:ASP:N	2.52	0.42
1:A:525:VAL:O	1:A:526:ALA:C	2.59	0.42
1:A:625:PHE:CD1	1:A:627:ILE:HD11	2.54	0.42
2:B:208:PRO:C	2:B:214:ILE:HD11	2.43	0.42
2:B:234:VAL:CG2	3:I:801:BTI:H83	2.50	0.42
2:B:410:LYS:NZ	2:J:376:ARG:HH11	2.17	0.42
2:B:417:TYR:HB2	2:J:210:MET:HE2	2.00	0.42
2:B:442:MET:O	2:B:443:SER:C	2.62	0.42
1:C:285:LEU:HB3	1:C:365:THR:HG21	2.02	0.42
1:C:690:ILE:HD12	1:C:699:LEU:HD11	2.01	0.42
2:D:66:ALA:HB2	2:D:125:ASP:HA	2.02	0.42
2:D:200:CYS:O	2:D:223:MET:HA	2.20	0.42
2:D:355:VAL:O	2:D:390:THR:HA	2.19	0.42
1:E:325:LYS:O	1:E:328:GLY:N	2.45	0.42
1:G:71:ARG:HA	1:G:75:ALA:HB2	2.01	0.42
1:G:467:ARG:HD2	1:G:467:ARG:O	2.19	0.42
1:I:130:ALA:HA	1:I:133:ALA:CB	2.43	0.42
1:I:419:ARG:HB2	1:I:476:GLU:HB2	2.00	0.42
1:I:629:THR:H	1:I:632:ALA:HB3	1.84	0.42
1:I:651:PRO:CG	2:J:62:GLY:HA3	2.50	0.42
2:J:447:LEU:HD23	2:J:447:LEU:HA	1.75	0.42
1:K:421:ARG:C	1:K:421:ARG:HD3	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:421:ARG:O	1:K:421:ARG:CD	2.67	0.42
2:L:398:LEU:HD12	2:L:399:PRO:HD2	2.00	0.42
1:A:186:GLU:OE2	1:A:187:ALA:N	2.52	0.42
1:A:358:HIS:O	1:A:359:PRO:C	2.62	0.42
1:A:411:LEU:HD22	1:A:682:GLN:CB	2.49	0.42
1:A:583:PHE:N	1:A:583:PHE:CD1	2.88	0.42
1:A:596:TRP:CH2	1:A:600:ASP:O	2.72	0.42
2:B:48:LEU:HA	2:B:48:LEU:HD23	1.61	0.42
2:B:185:MET:HE3	2:J:529:MET:CE	2.49	0.42
2:B:476(C):ASP:O	2:B:478:LYS:N	2.44	0.42
2:B:479:ILE:C	2:B:479:ILE:CD1	2.92	0.42
1:C:321:VAL:O	1:C:324:ALA:CB	2.61	0.42
1:C:421:ARG:C	1:C:421:ARG:HD3	2.44	0.42
1:C:532:MET:O	1:C:535:VAL:HB	2.20	0.42
1:C:563:LEU:O	1:C:565:GLY:N	2.52	0.42
1:C:642:ARG:NH1	2:D:71:ASP:OD2	2.53	0.42
2:D:81:GLU:OE1	2:D:84:MET:HE3	2.19	0.42
2:D:149:MET:CE	2:D:186:ALA:HA	2.50	0.42
2:D:408:VAL:O	2:D:409:ILE:C	2.58	0.42
2:D:471:ILE:HG21	2:L:166:ILE:HG13	2.02	0.42
1:E:65:LYS:HA	1:E:88:SER:O	2.19	0.42
1:E:347:PHE:CZ	1:E:349:GLU:HA	2.54	0.42
1:G:74:ILE:CD1	1:G:143:TYR:CE2	2.99	0.42
1:G:671:VAL:CG2	1:G:691:GLU:HB2	2.49	0.42
1:G:690:ILE:CD1	1:G:699:LEU:HD11	2.49	0.42
2:H:182:ARG:HH11	2:H:182:ARG:HG3	1.84	0.42
2:H:436:GLY:O	2:H:439:TYR:HB3	2.18	0.42
1:I:214:TYR:HB2	1:I:215:PRO:HA	2.00	0.42
1:I:218:ILE:CD1	1:I:260:ILE:HG12	2.49	0.42
1:I:654:LEU:HD23	1:I:654:LEU:HA	1.89	0.42
1:K:455:TRP:CG	1:K:456:ALA:N	2.85	0.42
1:A:140:HIS:ND1	1:A:141:PRO:CD	2.82	0.42
1:C:325:LYS:O	1:C:327:VAL:N	2.52	0.42
1:C:347:PHE:CZ	1:C:349:GLU:HA	2.55	0.42
2:D:351:THR:HG22	2:D:386:ILE:HG23	2.02	0.42
1:E:283:ILE:HD12	1:E:389:VAL:CG2	2.50	0.42
1:E:305:SER:C	1:E:307:PHE:H	2.28	0.42
1:E:627:ILE:HD12	1:E:627:ILE:N	2.34	0.42
1:E:695:MET:SD	2:F:313:PRO:HG3	2.59	0.42
1:G:530:ALA:HB2	1:G:561:VAL:HG21	2.01	0.42
2:H:48:LEU:HA	2:H:48:LEU:HD23	1.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:188:ASN:OD1	1:I:188:ASN:O	2.38	0.42
1:I:380:GLU:HG2	1:I:381:PRO:HD2	2.01	0.42
1:I:422:PRO:HA	1:I:422(A):PRO:HD3	1.85	0.42
2:J:202:GLY:O	2:J:203:GLY:C	2.62	0.42
1:K:195:TYR:CD2	1:K:208:ILE:HD13	2.54	0.42
2:L:499:ARG:NH1	2:L:499:ARG:CG	2.80	0.42
1:A:99:GLN:HG3	1:A:100:ALA:H	1.84	0.42
1:A:107:ASP:C	1:A:108:GLU:HG3	2.45	0.42
1:A:186:GLU:CD	1:A:186:GLU:N	2.78	0.42
1:A:274:VAL:HA	1:A:284:TYR:HA	2.02	0.42
1:A:455:TRP:CD1	1:A:455:TRP:C	2.93	0.42
2:B:69:ARG:HH12	2:B:160:ASP:CB	2.33	0.42
2:B:109:THR:HG22	2:B:122:PHE:HB3	2.01	0.42
2:B:180:PHE:O	2:B:183:ASN:HB2	2.19	0.42
1:C:99:GLN:O	1:C:100:ALA:C	2.62	0.42
1:C:463:ILE:HD12	1:C:494:PHE:CE1	2.54	0.42
2:D:301:SER:HB2	2:D:322:LYS:NZ	2.35	0.42
1:E:276:CYS:HB2	1:E:277:ASP:H	1.41	0.42
1:E:718:LEU:N	1:E:718:LEU:CD2	2.69	0.42
2:F:315:ASP:OD1	2:F:317:LYS:HB2	2.19	0.42
1:G:301:GLU:OE2	1:G:397:GLU:OE1	2.37	0.42
1:G:384:ILE:HB	1:G:388:ASP:HB2	2.01	0.42
1:G:583:PHE:CD1	1:G:583:PHE:N	2.87	0.42
2:H:235:THR:C	2:H:237:GLU:H	2.26	0.42
2:H:476(B):GLY:C	2:H:476(D):PRO:HD3	2.44	0.42
1:I:231:ILE:HG22	1:I:232:ALA:N	2.33	0.42
1:I:287:GLU:HG3	1:I:308:LEU:HD21	2.02	0.42
1:I:304:PRO:HD2	1:I:394:TRP:CE2	2.55	0.42
1:I:421:ARG:O	1:I:421:ARG:CD	2.68	0.42
1:I:650:MET:HA	1:I:651:PRO:HD3	1.90	0.42
2:J:193:ILE:CD1	2:J:274:LEU:HD23	2.50	0.42
1:K:146:LEU:HD23	1:K:152:PHE:CD2	2.54	0.42
2:L:196:ILE:HG22	2:L:221:SER:HB2	2.02	0.42
2:L:355:VAL:O	2:L:390:THR:HA	2.20	0.42
2:B:285:LYS:HB3	2:B:286:PRO:HD2	2.01	0.42
2:D:141:ILE:O	2:D:145:MET:HG3	2.19	0.42
2:D:299:GLU:HG3	2:D:322:LYS:HB3	2.02	0.42
2:D:539:LEU:OXT	2:L:372:ARG:NH2	2.52	0.42
1:E:85:MET:HB2	1:E:87:ILE:HD11	2.02	0.42
1:E:279:HIS:CD2	1:E:380:GLU:O	2.71	0.42
1:E:480:HIS:HD2	1:E:482:LEU:HB2	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:666:MET:HG2	1:E:666:MET:O	2.18	0.42
2:F:49:GLY:C	2:F:51:GLY:N	2.77	0.42
1:G:92:ILE:HD12	1:G:112:ILE:CD1	2.50	0.42
1:G:675:VAL:HG12	1:G:707:VAL:HG21	2.01	0.42
1:I:67:LEU:HG	1:I:68:ILE:N	2.32	0.42
1:I:421:ARG:C	1:I:421:ARG:CD	2.92	0.42
1:I:457:PRO:HG2	1:I:458:THR:N	2.27	0.42
1:I:504:ILE:CG2	1:I:505:ALA:N	2.82	0.42
1:I:518:PRO:O	1:I:519:GLU:C	2.61	0.42
1:I:541:THR:O	1:I:541:THR:HG22	2.20	0.42
1:I:625:PHE:HB2	1:I:627:ILE:HD12	2.02	0.42
1:K:93:TYR:HA	1:K:121:TYR:OH	2.19	0.42
1:K:292:ILE:HD12	1:K:292:ILE:N	2.14	0.42
1:K:358:HIS:O	1:K:359:PRO:C	2.63	0.42
1:K:446:ASP:HA	1:K:447:PRO:HD2	1.87	0.42
1:A:302:GLU:OE2	1:A:394:TRP:CZ3	2.73	0.42
1:A:371:GLU:O	1:A:374:ILE:HG12	2.20	0.42
1:A:661:MET:HG3	1:A:723:VAL:HG13	2.02	0.42
2:B:319:LEU:CD2	2:B:391:LEU:HD13	2.50	0.42
2:B:393:ASP:CG	2:B:432:ARG:HB3	2.44	0.42
1:C:140:HIS:ND1	1:C:141:PRO:HD2	2.35	0.42
1:C:266:GLN:HG2	1:C:341:GLY:HA2	2.02	0.42
1:C:354:LEU:HD11	1:C:358:HIS:ND1	2.35	0.42
1:C:367:VAL:HG12	1:C:368:ASP:N	2.34	0.42
2:D:120:TYR:HE2	2:D:147:MET:HE2	1.85	0.42
2:D:537:ILE:HA	2:D:538:PRO:HD3	1.91	0.42
1:E:71:ARG:O	1:E:75:ALA:CB	2.68	0.42
1:E:358:HIS:CE1	1:E:359:PRO:HD3	2.55	0.42
1:E:421:ARG:CD	1:E:421:ARG:C	2.93	0.42
1:E:515:VAL:HB	1:E:631:GLY:HA3	2.02	0.42
2:F:126:PHE:O	2:F:130:GLY:HA2	2.20	0.42
2:F:361:VAL:C	2:F:363:ALA:N	2.76	0.42
1:G:64:ASN:H	1:G:137:GLN:HG2	1.85	0.42
1:G:279:HIS:NE2	1:G:379:GLY:HA2	2.35	0.42
1:G:408:GLY:O	1:G:409:PHE:C	2.62	0.42
1:G:494:PHE:HD2	1:G:499:MET:HE1	1.84	0.42
1:G:670:ILE:HD11	1:G:718:LEU:HD11	2.02	0.42
2:H:325:ASP:O	2:H:327:GLY:N	2.53	0.42
2:H:476(C):ASP:N	2:H:476(D):PRO:HD3	2.35	0.42
1:I:78:VAL:HA	1:I:370:VAL:HG11	2.02	0.42
1:I:235:ASP:OD1	1:I:235:ASP:N	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:283:ILE:HD12	1:I:389:VAL:CG2	2.49	0.42
1:I:347:PHE:CD1	1:I:347:PHE:O	2.72	0.42
2:J:354:VAL:HA	2:J:389:LEU:O	2.20	0.42
1:K:140:HIS:ND1	1:K:141:PRO:CD	2.82	0.42
2:L:374:ALA:O	2:L:375:ALA:C	2.63	0.42
1:A:111:HIS:O	1:A:112:ILE:HG23	2.19	0.42
2:B:50:GLY:HA3	2:B:127:THR:O	2.19	0.42
1:C:69:ALA:HB3	1:C:141:PRO:HA	2.01	0.42
1:C:524:ARG:HA	1:C:590:MET:SD	2.60	0.42
2:D:138:SER:O	2:D:139:LYS:C	2.61	0.42
2:D:141:ILE:O	2:D:144:ILE:HG13	2.20	0.42
1:E:325:LYS:O	1:E:327:VAL:N	2.53	0.42
1:E:400:LEU:HD23	1:E:400:LEU:HA	1.74	0.42
2:F:222:TYR:CD1	2:F:222:TYR:C	2.97	0.42
1:G:304:PRO:HD2	1:G:394:TRP:CD2	2.55	0.42
1:G:422(A):PRO:O	1:G:422(B):ALA:HB2	2.19	0.42
1:G:504:ILE:CG2	1:G:505:ALA:N	2.82	0.42
2:H:222:TYR:HB2	2:H:245:GLY:O	2.20	0.42
2:H:315:ASP:O	2:H:316:MET:C	2.63	0.42
1:I:682:GLN:OE1	1:I:682:GLN:HA	2.20	0.42
2:J:42:ARG:HH11	2:J:42:ARG:CG	2.18	0.42
2:J:205:VAL:O	2:J:208:PRO:HD2	2.20	0.42
1:K:99:GLN:O	1:K:100:ALA:C	2.62	0.42
1:K:140:HIS:CE1	1:K:142:GLY:N	2.84	0.42
1:K:485:LEU:O	1:K:486:SER:C	2.61	0.42
1:K:583:PHE:N	1:K:583:PHE:CD1	2.88	0.42
1:K:724:ILE:HG22	1:K:725:MET:HG3	2.01	0.42
1:A:146:LEU:HD23	1:A:152:PHE:CG	2.55	0.41
1:A:165:GLY:CA	1:A:331:SER:OG	2.68	0.41
1:A:279:HIS:HD2	1:A:380:GLU:O	2.03	0.41
2:B:205:VAL:HG23	2:B:206:TYR:N	2.34	0.41
2:B:319:LEU:HD23	2:B:391:LEU:HD13	2.02	0.41
2:B:454:ALA:O	2:B:505:VAL:HA	2.20	0.41
1:C:177:LYS:HB3	1:C:181:LYS:HZ1	1.84	0.41
2:D:315:ASP:C	2:D:315:ASP:OD1	2.60	0.41
2:D:425:PRO:HB3	2:D:522:LEU:HD13	2.01	0.41
1:E:68:ILE:CG2	1:E:70:ASN:H	2.33	0.41
1:E:75:ALA:O	1:E:79:ILE:HG13	2.20	0.41
1:E:93:TYR:C	1:E:112:ILE:HG12	2.45	0.41
1:E:334:THR:HG21	1:E:355:GLN:CD	2.45	0.41
1:E:455:TRP:CG	1:E:456:ALA:N	2.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:482:LEU:N	1:E:483:PRO:HD2	2.35	0.41
1:E:515:VAL:HB	1:E:631:GLY:CA	2.50	0.41
1:G:78:VAL:HG23	1:G:370:VAL:HG11	2.01	0.41
1:G:335:VAL:HG12	1:G:350:MET:HE3	2.02	0.41
2:H:202:GLY:O	2:H:205:VAL:HG22	2.20	0.41
2:H:285:LYS:O	2:H:286:PRO:C	2.62	0.41
2:H:522:LEU:HA	2:J:151:ASN:ND2	2.34	0.41
1:I:68:ILE:CG1	1:I:78:VAL:HG11	2.50	0.41
1:I:77:ARG:NH1	1:I:370:VAL:CG2	2.80	0.41
1:I:140:HIS:CE1	1:I:142:GLY:N	2.88	0.41
1:I:358:HIS:CG	1:I:359:PRO:HD3	2.55	0.41
1:I:518:PRO:HD2	1:I:521:ASP:OD1	2.20	0.41
1:I:663:LEU:O	1:I:665:PRO:HD3	2.20	0.41
2:J:476(B):GLY:C	2:J:476(D):PRO:HD3	2.45	0.41
1:K:186:GLU:OE2	1:K:187:ALA:N	2.53	0.41
1:K:394:TRP:O	1:K:455:TRP:HA	2.20	0.41
1:K:456:ALA:CB	1:K:457:PRO:HD2	2.34	0.41
1:K:482:LEU:N	1:K:483:PRO:HD2	2.35	0.41
2:L:75:ASP:O	2:L:76:GLU:C	2.63	0.41
2:L:138:SER:OG	2:L:139:LYS:N	2.53	0.41
2:L:183:ASN:HD22	2:L:183:ASN:HA	1.67	0.41
2:L:217:VAL:O	2:L:218:LYS:C	2.63	0.41
2:L:239:VAL:CG2	2:L:243:GLU:HB2	2.50	0.41
1:A:136:ALA:O	1:A:137:GLN:CB	2.69	0.41
1:A:304:PRO:HD2	1:A:394:TRP:CE2	2.56	0.41
1:C:65:LYS:HE2	1:C:134:THR:O	2.19	0.41
1:C:570:VAL:HG22	1:C:581:VAL:HG12	2.02	0.41
1:C:711:ASN:O	1:C:712:ALA:HB2	2.20	0.41
1:E:186:GLU:CD	1:E:186:GLU:H	2.28	0.41
1:E:312:THR:HG21	1:E:343:LYS:HD3	2.01	0.41
1:E:710:ILE:HG22	1:E:711:ASN:N	2.35	0.41
2:F:180:PHE:O	2:F:184:ILE:HG13	2.19	0.41
2:F:181:GLN:CD	2:H:448:ARG:HD3	2.45	0.41
2:F:462:VAL:HG22	2:H:169:GLY:CA	2.50	0.41
1:G:128:MET:O	1:G:131:ILE:N	2.53	0.41
1:G:394:TRP:CE3	1:G:459:ARG:HG3	2.55	0.41
2:H:83:ASP:HB3	2:H:86:VAL:HG23	2.00	0.41
1:I:404:ASP:OD2	1:I:404:ASP:C	2.62	0.41
1:I:523:ARG:O	1:I:524:ARG:C	2.63	0.41
1:I:546:ARG:H	1:I:546:ARG:HG2	1.55	0.41
1:I:660:LYS:O	1:I:661:MET:HE3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:534:ARG:HG3	1:K:534:ARG:NH1	2.35	0.41
1:K:642:ARG:NH1	2:L:71:ASP:CG	2.78	0.41
2:L:222:TYR:CD1	2:L:222:TYR:C	2.97	0.41
1:A:271:GLU:O	1:A:287:GLU:HB2	2.21	0.41
1:C:140:HIS:ND1	1:C:141:PRO:N	2.68	0.41
1:C:314:ARG:O	1:C:318:GLU:HG3	2.19	0.41
1:C:368:ASP:C	1:C:368:ASP:OD2	2.63	0.41
1:C:407:ARG:HH11	1:C:407:ARG:HG2	1.85	0.41
1:C:428(L):ALA:HB3	1:C:455:TRP:CD1	2.49	0.41
1:C:446:ASP:OD1	1:C:447:PRO:HD2	2.19	0.41
1:C:724:ILE:HG22	1:C:725:MET:HG3	2.02	0.41
2:D:48:LEU:HD23	2:D:48:LEU:HA	1.63	0.41
2:D:138:SER:O	2:D:141:ILE:N	2.53	0.41
1:E:268:ARG:NH2	1:E:497:GLY:O	2.45	0.41
1:E:490:ASP:OD2	1:E:630:ARG:NH1	2.53	0.41
1:E:517:LEU:HA	1:E:518:PRO:HD3	1.62	0.41
1:G:195:TYR:CD2	1:G:208:ILE:HD13	2.56	0.41
1:G:234:ASN:O	1:G:237:GLU:HB3	2.19	0.41
1:G:293:GLN:O	1:G:504:ILE:CG2	2.64	0.41
1:G:334:THR:HG21	1:G:355:GLN:CG	2.50	0.41
1:G:695:MET:HG3	2:H:313:PRO:HG3	2.01	0.41
1:I:156:LEU:HD22	1:I:161:VAL:HB	2.02	0.41
1:I:195:TYR:O	1:I:259:PHE:HA	2.21	0.41
1:I:270:ILE:HG21	1:I:308:LEU:HD21	2.02	0.41
1:I:325:LYS:O	1:I:327:VAL:N	2.53	0.41
1:I:364:ILE:HG22	1:I:392:THR:O	2.20	0.41
1:I:368:ASP:C	1:I:368:ASP:OD2	2.63	0.41
2:J:248:THR:O	2:J:252:ARG:HG2	2.20	0.41
1:K:83:ARG:CZ	1:K:83:ARG:HB3	2.50	0.41
1:K:107:ASP:C	1:K:108:GLU:HG3	2.44	0.41
1:K:156:LEU:HD22	1:K:161:VAL:HB	2.03	0.41
2:L:309:ASN:HD21	2:L:311:ASN:HB2	1.86	0.41
2:L:432:ARG:O	2:L:459:GLU:N	2.54	0.41
2:L:447:LEU:HA	2:L:447:LEU:HD23	1.78	0.41
1:A:118:ASN:HD21	1:A:119:GLN:HE21	1.68	0.41
1:A:376:VAL:CG2	1:A:377:ALA:N	2.83	0.41
1:A:398:ASN:HB3	1:A:485:LEU:HD13	2.02	0.41
1:A:634:LEU:N	1:A:634:LEU:CD2	2.82	0.41
1:A:661:MET:CE	1:A:726:GLU:HB3	2.50	0.41
2:B:248:THR:O	2:B:252:ARG:HG2	2.20	0.41
2:B:369:ASP:O	2:B:370:SER:C	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:401:THR:CG2	2:B:402:SER:N	2.83	0.41
2:B:476(C):ASP:CG	2:B:478:LYS:HG2	2.45	0.41
1:C:174:MET:HA	1:C:180:SER:OG	2.20	0.41
1:C:275:LEU:HD23	1:C:276:CYS:H	1.85	0.41
1:C:338:ILE:CD1	1:C:338:ILE:N	2.82	0.41
1:C:358:HIS:CG	1:C:359:PRO:HD3	2.54	0.41
1:C:363:LEU:O	1:C:455:TRP:CE3	2.73	0.41
1:C:633:ASP:C	1:C:633:ASP:OD1	2.63	0.41
2:D:206:TYR:O	2:D:209:ALA:HB3	2.20	0.41
1:E:302:GLU:OE2	1:E:394:TRP:CZ3	2.73	0.41
1:E:456:ALA:CB	1:E:457:PRO:HD2	2.35	0.41
1:E:670:ILE:CD1	1:E:718:LEU:HD21	2.50	0.41
1:G:358:HIS:O	1:G:359:PRO:C	2.63	0.41
1:G:481:ASN:O	1:G:482:LEU:C	2.63	0.41
1:G:541:THR:O	1:G:541:THR:HG22	2.21	0.41
1:I:90:VAL:HG12	1:I:91:ALA:N	2.35	0.41
2:J:229:ASP:OD1	2:J:229:ASP:N	2.52	0.41
1:K:191:THR:O	1:K:193:PRO:CD	2.69	0.41
1:K:295:ARG:O	1:K:296:ASN:HB2	2.20	0.41
1:A:114:PRO:HB2	1:A:115:PRO:HD2	2.02	0.41
1:A:428(L):ALA:HB3	1:A:455:TRP:CD1	2.44	0.41
2:B:356:ALA:HA	2:B:391:LEU:O	2.19	0.41
2:B:476(C):ASP:N	2:B:476(D):PRO:HD3	2.35	0.41
2:B:509:ARG:HB3	2:B:509:ARG:HH11	1.86	0.41
1:C:396:ILE:HD12	1:C:396:ILE:N	2.36	0.41
2:D:134:SER:H	2:D:137:HIS:HB3	1.85	0.41
2:D:476(A):LEU:C	2:D:476(C):ASP:N	2.79	0.41
1:E:107:ASP:O	1:E:108:GLU:CG	2.68	0.41
1:E:563:LEU:CD2	1:E:636:VAL:HG22	2.51	0.41
2:F:67:ARG:HG2	2:F:67:ARG:HH11	1.84	0.41
2:F:417:TYR:N	2:H:210:MET:CE	2.83	0.41
1:G:563:LEU:CD2	1:G:636:VAL:HG22	2.50	0.41
2:H:375:ALA:HA	2:H:415:LEU:HD12	2.03	0.41
2:J:74:LEU:O	2:J:75:ASP:C	2.64	0.41
2:J:293:ASP:OD1	2:J:325:ASP:O	2.38	0.41
2:J:336:PHE:O	2:J:337:ALA:C	2.62	0.41
1:K:274:VAL:HA	1:K:284:TYR:HA	2.02	0.41
1:K:285:LEU:HB3	1:K:365:THR:HG21	2.02	0.41
1:K:358:HIS:O	1:K:361:THR:N	2.54	0.41
1:K:543:VAL:HG12	1:K:544:SER:N	2.35	0.41
2:L:117:ARG:NH2	2:L:280:LEU:HG	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:ASN:C	1:A:119:GLN:HG3	2.45	0.41
1:A:140:HIS:CE1	1:A:142:GLY:N	2.85	0.41
1:A:168:LYS:O	1:A:172:GLU:OE1	2.38	0.41
1:A:394:TRP:O	1:A:455:TRP:HA	2.21	0.41
1:A:404:ASP:OD2	1:A:404:ASP:C	2.63	0.41
2:B:75:ASP:O	2:B:76:GLU:C	2.62	0.41
1:C:114:PRO:CB	1:C:115:PRO:HD2	2.50	0.41
1:C:396:ILE:HD13	1:C:462:ALA:CB	2.51	0.41
2:D:90:CYS:HB2	2:D:168:GLU:OE2	2.21	0.41
2:D:182:ARG:HG3	2:D:182:ARG:NH1	2.35	0.41
2:D:244:LEU:HA	2:D:244:LEU:HD12	1.85	0.41
2:D:295:PRO:O	2:D:513:LYS:HA	2.20	0.41
2:D:347:LEU:HA	2:D:347:LEU:HD23	1.84	0.41
2:D:476(B):GLY:C	2:D:476(D):PRO:HD3	2.45	0.41
1:E:83:ARG:CG	1:E:83:ARG:NH1	2.83	0.41
2:F:182:ARG:HG3	2:F:182:ARG:NH1	2.36	0.41
2:F:347:LEU:HD23	2:F:347:LEU:HA	1.86	0.41
1:G:316:MET:HB3	1:G:337:PHE:CE1	2.55	0.41
2:H:199:PRO:HB3	2:H:222:TYR:CZ	2.56	0.41
1:I:116:PRO:HG3	1:I:444:TYR:CE2	2.55	0.41
1:I:347:PHE:CZ	1:I:349:GLU:HA	2.56	0.41
1:I:482:LEU:N	1:I:483:PRO:HD2	2.35	0.41
1:I:675:VAL:HG11	1:I:707:VAL:HG21	2.02	0.41
2:J:121:VAL:HG22	2:J:122:PHE:H	1.84	0.41
2:J:312:THR:HG22	2:J:313:PRO:O	2.21	0.41
2:J:361:VAL:C	2:J:363:ALA:N	2.78	0.41
1:K:114:PRO:HB2	1:K:115:PRO:HD2	2.03	0.41
1:K:164:VAL:HA	1:K:377:ALA:CB	2.51	0.41
1:K:342:GLN:O	1:K:343:LYS:HB2	2.21	0.41
1:K:720:VAL:HG22	1:K:721:ASP:H	1.85	0.41
2:L:192:GLN:O	2:L:211:THR:HB	2.20	0.41
2:L:285:LYS:O	2:L:286:PRO:C	2.61	0.41
1:A:111:HIS:O	1:A:112:ILE:CG2	2.69	0.41
1:A:112:ILE:O	1:A:120:SER:HA	2.19	0.41
1:A:422:PRO:HA	1:A:422(A):PRO:HD3	1.86	0.41
1:A:459:ARG:O	1:A:460:ALA:C	2.63	0.41
1:A:532:MET:HE1	1:A:603:ALA:CB	2.49	0.41
1:A:547:MET:O	1:A:548:ASP:C	2.63	0.41
1:A:553:ARG:NH1	2:B:115:ASN:OD1	2.53	0.41
1:A:610:ALA:HA	1:A:611:PRO:HD3	1.78	0.41
2:B:64:LEU:HD23	2:B:64:LEU:HA	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:ARG:HA	2:B:268:LEU:CD1	2.51	0.41
2:B:252:ARG:NH2	2:B:335:GLU:HG3	2.35	0.41
2:B:300:PRO:HB3	2:B:509:ARG:NH1	2.35	0.41
2:B:372:ARG:NH2	2:J:539:LEU:OXT	2.52	0.41
2:B:382:ASP:HA	2:B:424:VAL:CG1	2.51	0.41
2:B:495:VAL:HG13	2:B:496:ALA:N	2.36	0.41
1:C:139:VAL:O	1:C:164:VAL:HG12	2.20	0.41
1:C:165:GLY:HA2	1:C:331:SER:OG	2.21	0.41
1:C:348:LEU:O	1:C:349:GLU:HB3	2.21	0.41
1:C:421:ARG:O	1:C:421:ARG:HD3	2.21	0.41
1:C:446:ASP:HA	1:C:447:PRO:HD2	1.91	0.41
1:C:458:THR:O	1:C:461:ALA:HB3	2.20	0.41
1:C:537:GLU:HA	1:C:540:ARG:HG3	2.01	0.41
1:C:596:TRP:CH2	1:C:600:ASP:O	2.73	0.41
1:C:650:MET:HA	1:C:650:MET:HE2	2.01	0.41
2:D:300:PRO:O	2:D:303:ASP:HB2	2.20	0.41
1:E:71:ARG:NH1	1:E:445:TYR:CG	2.89	0.41
1:E:132:ARG:C	1:E:135:GLY:H	2.29	0.41
1:E:140:HIS:ND1	1:E:141:PRO:CD	2.84	0.41
1:E:273:GLN:HG2	1:E:369:LEU:HD11	2.03	0.41
1:E:658:THR:HG22	1:E:659:SER:O	2.20	0.41
2:F:476(A):LEU:C	2:F:476(C):ASP:N	2.76	0.41
1:I:74:ILE:HG23	1:I:75:ALA:N	2.35	0.41
1:I:140:HIS:ND1	1:I:141:PRO:CD	2.84	0.41
1:I:324:ALA:O	1:I:325:LYS:C	2.64	0.41
1:I:422:PRO:HG3	1:I:473:PHE:CZ	2.56	0.41
2:J:479:ILE:HD12	2:J:480:ALA:H	1.79	0.41
1:K:77:ARG:HH11	1:K:77:ARG:HG3	1.85	0.41
1:K:602:LEU:HD12	1:K:614:LEU:O	2.19	0.41
1:K:627:ILE:HD13	1:K:636:VAL:CG2	2.51	0.41
1:A:266:GLN:H	1:A:266:GLN:HG2	1.49	0.41
1:A:421:ARG:HD3	1:A:421:ARG:C	2.45	0.41
1:C:459:ARG:O	1:C:460:ALA:C	2.64	0.41
1:C:494:PHE:CD2	1:C:499:MET:HE1	2.56	0.41
1:C:517:LEU:HD11	1:C:632:ALA:HB2	2.02	0.41
1:E:64:ASN:H	1:E:137:GLN:HG2	1.85	0.41
1:E:316:MET:HB3	1:E:337:PHE:CE1	2.56	0.41
1:E:713:SER:O	1:E:714:ALA:C	2.64	0.41
2:F:135:GLU:OE1	2:J:89:ARG:NH2	2.54	0.41
2:F:149:MET:CE	2:F:189:VAL:CG1	2.99	0.41
1:G:95:ASP:C	1:G:97:ASP:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:118:ASN:HD21	1:G:119:GLN:HE21	1.69	0.41
1:G:207:LYS:O	1:G:207:LYS:HD3	2.20	0.41
1:G:390:LYS:HD3	1:G:391:LEU:H	1.77	0.41
1:G:421:ARG:CD	1:G:421:ARG:C	2.94	0.41
2:H:167:GLN:N	2:H:167:GLN:NE2	2.37	0.41
2:H:252:ARG:NH2	2:H:335:GLU:HG3	2.36	0.41
2:H:361:VAL:O	2:H:363:ALA:N	2.53	0.41
1:I:70:ASN:OD1	1:I:74:ILE:HG21	2.20	0.41
1:I:107:ASP:C	1:I:108:GLU:HG3	2.45	0.41
1:I:121:TYR:HE2	1:I:445:TYR:OH	2.04	0.41
1:I:124:ILE:CG2	1:I:128:MET:CE	2.99	0.41
1:I:325:LYS:H	1:I:325:LYS:HG3	1.74	0.41
1:I:455:TRP:CD2	1:I:456:ALA:N	2.89	0.41
1:I:612:LEU:C	1:I:612:LEU:HD12	2.45	0.41
1:K:339:VAL:HG22	1:K:345:PHE:HB3	2.02	0.41
1:K:416:ARG:HG3	1:K:439:GLY:O	2.21	0.41
1:K:467:ARG:HD2	1:K:467:ARG:O	2.21	0.41
1:K:663:LEU:O	1:K:665:PRO:HD3	2.21	0.41
2:L:303:ASP:OD2	2:L:509:ARG:HD2	2.20	0.41
1:A:83:ARG:CG	1:A:83:ARG:NH1	2.80	0.41
1:A:191:THR:O	1:A:193:PRO:HD3	2.21	0.41
1:A:384:ILE:HB	1:A:388:ASP:HB2	2.02	0.41
1:A:543:VAL:HG12	1:A:544:SER:N	2.36	0.41
1:A:721:ASP:O	1:A:722:ASP:C	2.64	0.41
2:B:205:VAL:HB	2:J:409:ILE:HD13	2.02	0.41
2:B:254:SER:O	2:B:255:SER:CB	2.68	0.41
2:B:366:LEU:HD23	2:B:366:LEU:HA	1.87	0.41
2:B:456:PRO:HD3	2:B:506:ILE:O	2.21	0.41
2:B:536:ASN:O	2:B:537:ILE:C	2.63	0.41
1:C:90:VAL:HG12	1:C:91:ALA:N	2.36	0.41
1:C:276:CYS:HB2	1:C:277:ASP:H	1.42	0.41
1:C:331:SER:HB3	1:C:332:ALA:H	1.61	0.41
1:C:461:ALA:O	1:C:464:GLU:HB3	2.21	0.41
1:C:608:ASP:C	1:C:610:ALA:H	2.29	0.41
1:C:626:ARG:C	1:C:627:ILE:HD12	2.46	0.41
2:D:156:ILE:N	2:D:156:ILE:CD1	2.82	0.41
2:D:205:VAL:HB	2:L:409:ILE:HD13	2.03	0.41
2:D:205:VAL:O	2:D:208:PRO:HD2	2.21	0.41
2:D:250:HIS:HA	2:D:254:SER:OG	2.20	0.41
1:E:68:ILE:CG1	1:E:78:VAL:HG11	2.50	0.41
1:E:270:ILE:HG21	1:E:308:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:396:ILE:CG1	1:E:463:ILE:HD13	2.46	0.41
1:E:504:ILE:CG2	1:E:505:ALA:H	2.32	0.41
1:E:717:SER:C	1:E:718:LEU:HD23	2.46	0.41
2:F:118:VAL:HG12	2:F:119:VAL:N	2.36	0.41
2:F:173:LEU:HD13	2:H:439:TYR:CD2	2.56	0.41
2:F:273:ARG:HD2	2:F:330:TYR:HD1	1.86	0.41
2:F:392:ILE:HG22	2:F:393:ASP:N	2.35	0.41
2:F:471:ILE:HG21	2:H:166:ILE:HG13	2.03	0.41
1:G:69:ALA:HB3	1:G:141:PRO:HA	2.02	0.41
1:G:99:GLN:HG3	1:G:100:ALA:H	1.86	0.41
1:G:191:THR:O	1:G:192:VAL:C	2.62	0.41
1:G:270:ILE:HG21	1:G:308:LEU:HD21	2.02	0.41
1:G:274:VAL:HA	1:G:284:TYR:HA	2.03	0.41
1:G:340:ASP:OD1	1:G:344:ASN:HB2	2.21	0.41
1:G:444:TYR:C	1:G:445:TYR:CG	2.98	0.41
1:G:658:THR:HG22	1:G:659:SER:O	2.20	0.41
1:G:660:LYS:C	1:G:661:MET:HE3	2.45	0.41
2:H:244:LEU:HD12	2:H:244:LEU:HA	1.83	0.41
2:H:366:LEU:HD23	2:H:366:LEU:HA	1.79	0.41
1:I:95:ASP:C	1:I:97:ASP:H	2.28	0.41
1:I:180:SER:O	1:I:181:LYS:C	2.64	0.41
1:I:283:ILE:HG22	1:I:386:GLN:CG	2.51	0.41
1:I:327:VAL:O	1:I:327:VAL:HG22	2.20	0.41
1:I:334:THR:HG21	1:I:355:GLN:CG	2.51	0.41
1:I:467:ARG:HH21	1:I:630:ARG:HE	1.68	0.41
1:I:532:MET:HE2	1:I:596:TRP:CG	2.56	0.41
1:I:690:ILE:HD12	1:I:699:LEU:HD11	2.02	0.41
1:I:718:LEU:HD23	1:I:718:LEU:H	1.79	0.41
2:J:48:LEU:HD23	2:J:48:LEU:HA	1.71	0.41
2:J:98:GLN:OE1	2:J:98:GLN:N	2.50	0.41
2:J:347:LEU:HD23	2:J:347:LEU:HA	1.87	0.41
1:K:162:ILE:O	1:K:164:VAL:N	2.54	0.41
1:K:293:GLN:HA	1:K:299:VAL:HG23	2.02	0.41
1:K:340:ASP:OD1	1:K:344:ASN:HB2	2.21	0.41
1:K:517:LEU:HB3	1:K:521:ASP:HB3	2.03	0.41
1:K:660:LYS:O	1:K:727:PHE:N	2.51	0.41
2:L:182:ARG:HG3	2:L:182:ARG:HH11	1.86	0.41
2:L:294:ASP:HA	2:L:295:PRO:HD2	1.94	0.41
2:L:314:TYR:CE1	2:L:359:PRO:HG2	2.56	0.41
1:A:598:PRO:HD2	2:B:292:PHE:CD1	2.55	0.41
1:A:626:ARG:NE	1:A:628:ARG:HD2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:122:PHE:CD1	2:B:141:ILE:HG23	2.56	0.41
2:B:476(D):PRO:O	2:B:480:ALA:HB2	2.20	0.41
1:C:457:PRO:CG	1:C:458:THR:N	2.79	0.41
1:C:517:LEU:HB3	1:C:521:ASP:HB3	2.02	0.41
1:C:634:LEU:N	1:C:634:LEU:CD2	2.82	0.41
2:D:120:TYR:CD1	2:D:148:ALA:HA	2.56	0.41
2:D:524:ASN:O	2:D:525:LYS:C	2.64	0.41
1:E:283:ILE:HG22	1:E:386:GLN:CG	2.49	0.41
1:G:272:ILE:HB	1:G:335:VAL:HG23	2.03	0.41
1:G:353:ARG:HH11	1:G:353:ARG:HG3	1.86	0.41
1:G:378:ALA:O	1:G:379:GLY:O	2.38	0.41
1:G:543:VAL:CG1	2:H:117:ARG:HD2	2.51	0.41
2:H:346:ARG:HH11	2:H:346:ARG:CG	2.32	0.41
1:I:77:ARG:NH1	1:I:77:ARG:O	2.50	0.41
1:I:99:GLN:HB2	1:I:436:TYR:OH	2.21	0.41
1:I:292:ILE:H	1:I:292:ILE:CD1	2.01	0.41
1:I:464:GLU:O	1:I:465:ALA:C	2.64	0.41
1:I:512:PHE:CZ	1:I:515:VAL:HG23	2.56	0.41
1:I:592:VAL:HG13	1:I:607:VAL:HG22	2.03	0.41
2:J:49:GLY:C	2:J:51:GLY:N	2.78	0.41
2:J:524:ASN:O	2:J:525:LYS:C	2.64	0.41
1:K:272:ILE:HB	1:K:335:VAL:HG23	2.03	0.41
1:K:288:ARG:HD3	1:K:361:THR:OG1	2.21	0.41
1:K:309:ASP:OD2	1:K:343:LYS:HE2	2.20	0.41
1:K:521:ASP:O	1:K:522:LEU:C	2.63	0.41
1:A:68:ILE:CG2	1:A:70:ASN:H	2.34	0.40
1:A:436:TYR:C	1:A:436:TYR:CD1	2.99	0.40
2:B:49:GLY:C	2:B:51:GLY:N	2.79	0.40
2:B:205:VAL:O	2:B:208:PRO:HD2	2.21	0.40
2:B:374:ALA:HB3	2:B:415:LEU:HD13	2.03	0.40
1:C:140:HIS:CE1	1:C:142:GLY:N	2.85	0.40
1:C:164:VAL:HG23	1:C:377:ALA:CB	2.51	0.40
1:C:187:ALA:O	1:C:188:ASN:CG	2.64	0.40
1:C:301:GLU:HG2	1:C:357:GLU:HB3	2.03	0.40
1:C:415:GLY:O	1:C:440:GLU:HG3	2.21	0.40
1:C:583:PHE:CE1	1:C:590:MET:HE3	2.54	0.40
2:D:366:LEU:HD23	2:D:366:LEU:HA	1.97	0.40
2:D:499:ARG:HD3	2:D:499:ARG:HA	1.92	0.40
1:E:78:VAL:HG23	1:E:370:VAL:HG11	2.02	0.40
1:E:187:ALA:O	1:E:188:ASN:CG	2.64	0.40
1:E:292:ILE:HD12	1:E:292:ILE:N	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:468:ILE:O	1:E:471:ASP:HB2	2.20	0.40
1:E:583:PHE:N	1:E:583:PHE:CD1	2.88	0.40
1:E:626:ARG:C	1:E:627:ILE:HD12	2.45	0.40
2:F:298:ILE:HG23	2:F:509:ARG:HB2	2.03	0.40
2:F:514:ARG:HA	2:F:514:ARG:HD2	1.73	0.40
1:G:71:ARG:O	1:G:75:ALA:HB2	2.21	0.40
1:G:74:ILE:CG2	1:G:75:ALA:N	2.84	0.40
1:G:597:THR:O	1:G:598:PRO:C	2.63	0.40
1:I:358:HIS:O	1:I:359:PRO:C	2.64	0.40
1:I:497:GLY:O	1:I:499:MET:HG2	2.21	0.40
1:I:517:LEU:HD21	1:I:632:ALA:HB2	2.02	0.40
1:I:630:ARG:O	1:I:632:ALA:N	2.54	0.40
2:J:368:ILE:HG23	2:J:411:HIS:CG	2.56	0.40
1:K:321:VAL:O	1:K:324:ALA:CB	2.61	0.40
1:A:67:LEU:HG	1:A:68:ILE:N	2.35	0.40
1:A:92:ILE:CD1	1:A:112:ILE:HD13	2.49	0.40
1:A:421:ARG:CD	1:A:421:ARG:C	2.94	0.40
1:A:433:THR:CG2	1:A:434:GLY:N	2.83	0.40
2:B:273:ARG:HD2	2:B:330:TYR:CD1	2.57	0.40
1:C:139:VAL:HG11	1:C:156:LEU:CD2	2.51	0.40
2:D:537:ILE:HG13	2:D:538:PRO:HD2	2.03	0.40
1:E:124:ILE:HG22	1:E:128:MET:CE	2.51	0.40
1:E:384:ILE:HB	1:E:388:ASP:HB2	2.04	0.40
2:F:390:THR:HG21	2:F:419:TYR:OH	2.21	0.40
1:G:68:ILE:HG12	1:G:78:VAL:HG11	2.03	0.40
1:G:114:PRO:HB2	1:G:115:PRO:HD2	2.03	0.40
1:G:405:PRO:CG	1:G:481:ASN:HA	2.51	0.40
1:G:455:TRP:CD2	1:G:456:ALA:N	2.89	0.40
1:G:597:THR:OG1	2:H:292:PHE:CG	2.74	0.40
2:H:120:TYR:CD1	2:H:148:ALA:HA	2.56	0.40
1:I:137:GLN:O	1:I:138:ALA:CB	2.69	0.40
1:I:273:GLN:HG2	1:I:369:LEU:HD11	2.04	0.40
1:I:710:ILE:HG12	1:I:725:MET:HG2	2.02	0.40
2:J:325:ASP:HA	2:J:512:ARG:NH1	2.25	0.40
1:K:139:VAL:HG11	1:K:156:LEU:HD21	2.02	0.40
1:K:404:ASP:OD2	1:K:404:ASP:C	2.63	0.40
2:L:195:MET:SD	2:L:271:VAL:HG21	2.61	0.40
1:A:444:TYR:HD1	1:A:444:TYR:H	1.69	0.40
1:A:491:HIS:HA	1:A:492:PRO:HD2	1.92	0.40
2:B:294:ASP:HA	2:B:295:PRO:HD2	1.92	0.40
1:C:124:ILE:HG22	1:C:128:MET:HE2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:369:LEU:O	1:C:373:MET:HB2	2.21	0.40
1:C:392:THR:O	1:C:455:TRP:CZ3	2.71	0.40
1:C:572:ILE:HG22	1:C:573:ALA:N	2.36	0.40
1:C:666:MET:O	1:C:668:GLY:N	2.54	0.40
2:D:121:VAL:CG2	2:D:122:PHE:N	2.83	0.40
2:D:225:VAL:N	2:L:404:GLU:OE2	2.52	0.40
1:E:78:VAL:CG1	1:E:79:ILE:H	2.33	0.40
1:E:92:ILE:CG1	1:E:112:ILE:HD13	2.50	0.40
1:E:329:TYR:HE2	1:E:352:THR:HA	1.86	0.40
1:G:152:PHE:CE1	1:G:156:LEU:HD11	2.56	0.40
1:G:168:LYS:O	1:G:172:GLU:OE1	2.39	0.40
1:G:319:GLN:NE2	1:G:345:PHE:CZ	2.89	0.40
1:G:461:ALA:O	1:G:464:GLU:HB3	2.22	0.40
1:G:610:ALA:HA	1:G:611:PRO:HD3	1.89	0.40
1:G:654:LEU:O	1:G:655:PRO:O	2.38	0.40
1:I:71:ARG:HD3	1:I:445:TYR:CD2	2.56	0.40
1:I:720:VAL:C	1:I:722:ASP:H	2.29	0.40
2:J:139:LYS:HE2	2:J:139:LYS:HB3	1.85	0.40
2:J:182:ARG:O	2:J:183:ASN:C	2.64	0.40
1:K:324:ALA:O	1:K:325:LYS:C	2.65	0.40
2:L:413:ALA:O	2:L:416:LEU:HB3	2.21	0.40
2:B:114:ILE:O	2:B:115:ASN:HB2	2.21	0.40
2:B:196:ILE:HG22	2:B:221:SER:HB2	2.02	0.40
1:C:374:ILE:O	1:C:375:ARG:C	2.64	0.40
1:C:416:ARG:HG3	1:C:439:GLY:O	2.21	0.40
1:C:422:PRO:HA	1:C:422(A):PRO:HD3	1.85	0.40
1:C:435:VAL:HG22	1:C:436:TYR:H	1.87	0.40
1:C:625:PHE:CD1	1:C:627:ILE:HD11	2.56	0.40
2:D:132:SER:HA	2:D:163:GLY:O	2.20	0.40
2:D:298:ILE:CG2	2:D:509:ARG:HB2	2.51	0.40
1:E:456:ALA:CB	1:E:457:PRO:CD	2.94	0.40
2:F:78:SER:O	2:F:112:GLY:HA2	2.20	0.40
2:F:476(C):ASP:N	2:F:476(D):PRO:HD3	2.35	0.40
1:G:400:LEU:HD23	1:G:400:LEU:HA	1.68	0.40
1:G:463:ILE:HD12	1:G:494:PHE:CE1	2.56	0.40
1:G:650:MET:SD	2:H:263:ASN:HB2	2.62	0.40
1:G:710:ILE:HG22	1:G:711:ASN:N	2.37	0.40
2:H:202:GLY:O	2:H:203:GLY:C	2.65	0.40
2:H:329:PHE:CZ	2:H:343:GLY:HA3	2.55	0.40
1:I:68:ILE:CG2	1:I:70:ASN:H	2.34	0.40
1:I:99:GLN:O	1:I:100:ALA:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:257:ARG:HE	1:I:257:ARG:HB2	1.58	0.40
2:J:499:ARG:NH2	2:L:89:ARG:HH11	2.04	0.40
1:K:308:LEU:HD12	1:K:308:LEU:C	2.47	0.40
1:K:319:GLN:NE2	1:K:345:PHE:CZ	2.89	0.40
1:K:384:ILE:HB	1:K:388:ASP:HB2	2.03	0.40
1:K:713:SER:O	1:K:714:ALA:O	2.38	0.40
1:K:720:VAL:O	1:K:722:ASP:N	2.54	0.40
2:L:442:MET:O	2:L:443:SER:C	2.64	0.40
2:L:445:LYS:HE3	2:L:503:ASP:OD1	2.22	0.40
1:A:167:PRO:C	1:A:169:GLY:N	2.80	0.40
1:A:319:GLN:NE2	1:A:345:PHE:CE1	2.89	0.40
1:A:334:THR:HG21	1:A:355:GLN:CG	2.51	0.40
1:A:374:ILE:O	1:A:375:ARG:C	2.64	0.40
1:A:396:ILE:HG12	1:A:463:ILE:CD1	2.45	0.40
1:A:414:ILE:HD11	1:A:442:SER:C	2.47	0.40
1:A:490:ASP:OD2	1:A:630:ARG:NH1	2.55	0.40
1:A:720:VAL:HG22	1:A:721:ASP:H	1.87	0.40
1:C:534:ARG:HG3	1:C:534:ARG:NH1	2.37	0.40
1:C:677:VAL:CG1	1:C:708:ALA:O	2.69	0.40
2:D:75:ASP:OD2	2:D:115:ASN:N	2.55	0.40
2:D:185:MET:HE3	2:L:529:MET:HE1	2.04	0.40
1:E:110:VAL:HG21	1:E:130:ALA:CB	2.46	0.40
1:E:111:HIS:C	1:E:112:ILE:HG23	2.46	0.40
1:E:525:VAL:O	1:E:526:ALA:C	2.64	0.40
2:F:462:VAL:HG22	2:H:169:GLY:C	2.46	0.40
1:G:185:GLN:O	1:G:188:ASN:N	2.49	0.40
1:G:186:GLU:OE2	1:G:187:ALA:N	2.54	0.40
1:G:312:THR:O	1:G:315:ALA:HB3	2.22	0.40
1:G:619:ILE:HD11	1:G:626:ARG:HB2	2.03	0.40
2:H:222:TYR:CD1	2:H:222:TYR:C	3.00	0.40
2:H:474:ARG:O	2:H:476:ASP:N	2.51	0.40
1:I:107:ASP:O	1:I:108:GLU:HG3	2.21	0.40
1:K:77:ARG:NH1	1:K:77:ARG:O	2.53	0.40
1:K:231:ILE:HG22	1:K:232:ALA:N	2.37	0.40
2:L:394:VAL:HG23	2:L:395:PRO:HD2	2.03	0.40
2:L:476(A):LEU:C	2:L:476(C):ASP:N	2.80	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	585/681 (86%)	451 (77%)	99 (17%)	35 (6%)	1	10
1	C	585/681 (86%)	456 (78%)	94 (16%)	35 (6%)	1	10
1	E	585/681 (86%)	449 (77%)	98 (17%)	38 (6%)	1	8
1	G	638/681 (94%)	502 (79%)	100 (16%)	36 (6%)	1	11
1	I	638/681 (94%)	504 (79%)	94 (15%)	40 (6%)	1	8
1	K	638/681 (94%)	505 (79%)	92 (14%)	41 (6%)	1	8
2	B	504/531 (95%)	444 (88%)	49 (10%)	11 (2%)	5	29
2	D	504/531 (95%)	445 (88%)	47 (9%)	12 (2%)	4	28
2	F	504/531 (95%)	451 (90%)	43 (8%)	10 (2%)	6	31
2	H	504/531 (95%)	451 (90%)	43 (8%)	10 (2%)	6	31
2	J	504/531 (95%)	452 (90%)	43 (8%)	9 (2%)	6	34
2	L	504/531 (95%)	455 (90%)	39 (8%)	10 (2%)	6	31
All	All	6693/7272 (92%)	5565 (83%)	841 (13%)	287 (4%)	2	16

All (287) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	ALA
1	A	137	GLN
1	A	138	ALA
1	A	277	ASP
1	A	331	SER
1	A	389	VAL
2	B	218	LYS
2	B	325	ASP
2	B	476(D)	PRO
1	C	64	ASN
1	C	100	ALA
1	C	137	GLN

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Mol	Chain	Res	Type
1	C	138	ALA
1	C	265	THR
1	C	331	SER
1	C	389	VAL
2	D	218	LYS
2	D	325	ASP
2	D	476(D)	PRO
1	E	64	ASN
1	E	100	ALA
1	E	137	GLN
1	E	138	ALA
1	E	193	PRO
1	E	265	THR
1	E	277	ASP
1	E	331	SER
1	E	389	VAL
1	E	564	GLN
2	F	218	LYS
2	F	325	ASP
2	F	476(D)	PRO
1	G	100	ALA
1	G	137	GLN
1	G	138	ALA
1	G	331	SER
1	G	389	VAL
1	G	409	PHE
1	G	456	ALA
2	H	218	LYS
2	H	325	ASP
2	H	476(D)	PRO
1	I	100	ALA
1	I	137	GLN
1	I	138	ALA
1	I	331	SER
1	I	389	VAL
2	J	218	LYS
2	J	325	ASP
2	J	476(D)	PRO
1	K	100	ALA
1	K	137	GLN
1	K	138	ALA
1	K	277	ASP

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Mol	Chain	Res	Type
1	K	331	SER
1	K	389	VAL
1	K	456	ALA
1	K	564	GLN
2	L	218	LYS
2	L	325	ASP
2	L	476(D)	PRO
1	A	64	ASN
1	A	65	LYS
1	A	72	GLY
1	A	163	PHE
1	A	168	LYS
1	A	265	THR
1	A	326	ALA
1	A	379	GLY
1	A	393	GLY
1	A	596	TRP
2	B	476	ASP
1	C	65	LYS
1	C	162	ILE
1	C	163	PHE
1	C	185	GLN
1	C	277	ASP
1	C	324	ALA
1	C	326	ALA
1	C	379	GLY
1	C	393	GLY
1	C	457	PRO
1	C	564	GLN
1	C	721	ASP
2	D	476	ASP
1	E	65	LYS
1	E	72	GLY
1	E	88	SER
1	E	163	PHE
1	E	168	LYS
1	E	324	ALA
1	E	326	ALA
1	E	379	GLY
1	E	393	GLY
1	E	457	PRO
2	F	476	ASP

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Mol	Chain	Res	Type
1	G	64	ASN
1	G	65	LYS
1	G	163	PHE
1	G	168	LYS
1	G	230	ARG
1	G	265	THR
1	G	277	ASP
1	G	324	ALA
1	G	326	ALA
1	G	379	GLY
1	G	393	GLY
1	G	457	PRO
1	G	564	GLN
1	G	655	PRO
1	G	721	ASP
2	H	476	ASP
1	I	64	ASN
1	I	65	LYS
1	I	162	ILE
1	I	163	PHE
1	I	168	LYS
1	I	185	GLN
1	I	230	ARG
1	I	277	ASP
1	I	324	ALA
1	I	326	ALA
1	I	379	GLY
1	I	393	GLY
1	I	409	PHE
1	I	456	ALA
1	I	457	PRO
1	I	564	GLN
1	I	721	ASP
2	J	476	ASP
1	K	64	ASN
1	K	65	LYS
1	K	163	PHE
1	K	168	LYS
1	K	185	GLN
1	K	230	ARG
1	K	324	ALA
1	K	326	ALA

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Mol	Chain	Res	Type
1	K	379	GLY
1	K	409	PHE
1	K	457	PRO
1	K	596	TRP
1	K	721	ASP
2	L	476	ASP
1	A	112	ILE
1	A	185	GLN
1	A	324	ALA
1	A	457	PRO
1	A	721	ASP
2	B	78	SER
2	B	362	LEU
2	B	393	ASP
2	B	442	MET
1	C	72	GLY
1	C	88	SER
1	C	168	LYS
1	C	630	ARG
1	C	655	PRO
1	E	112	ILE
1	E	162	ILE
1	E	185	GLN
1	E	422(A)	PRO
1	E	519	GLU
1	E	596	TRP
1	E	633	ASP
1	E	655	PRO
1	E	721	ASP
2	F	338	LYS
2	F	393	ASP
1	G	72	GLY
1	G	185	GLN
1	G	630	ARG
2	H	338	LYS
1	I	88	SER
1	I	265	THR
1	I	422(A)	PRO
1	I	655	PRO
2	J	338	LYS
2	J	362	LEU
2	J	393	ASP

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Mol	Chain	Res	Type
1	K	88	SER
1	K	136	ALA
1	K	393	GLY
1	K	422(A)	PRO
1	K	655	PRO
1	K	714	ALA
2	L	393	ASP
2	L	466	LYS
1	A	136	ALA
1	A	193	PRO
1	A	633	ASP
1	C	86	GLY
1	C	94	SER
1	C	112	ILE
1	C	135	GLY
1	C	422(A)	PRO
1	C	456	ALA
1	C	596	TRP
1	C	633	ASP
2	D	78	SER
2	D	393	ASP
1	E	456	ALA
2	F	76	GLU
1	G	112	ILE
1	G	135	GLY
1	G	422(A)	PRO
2	H	393	ASP
2	H	442	MET
2	H	466	LYS
1	I	72	GLY
1	I	97	ASP
1	I	112	ILE
1	I	596	TRP
1	I	609	GLY
1	K	112	ILE
1	K	162	ILE
1	K	200	GLU
1	K	246	LYS
1	K	265	THR
1	K	586	ASP
1	K	630	ARG
1	K	692	ALA

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Mol	Chain	Res	Type
2	L	326	GLU
2	L	368	ILE
1	A	135	GLY
1	A	162	ILE
1	A	266	GLN
1	A	422(A)	PRO
1	A	456	ALA
1	A	630	ARG
1	A	655	PRO
1	A	714	ALA
2	B	77	GLY
2	B	338	LYS
1	C	609	GLY
2	D	76	GLU
1	E	135	GLY
1	E	136	ALA
1	E	190	SER
1	G	88	SER
1	G	136	ALA
1	G	162	ILE
1	G	422(B)	ALA
1	G	586	ASP
2	H	303	ASP
1	I	86	GLY
1	I	633	ASP
1	I	692	ALA
2	J	466	LYS
1	K	71	ARG
1	K	72	GLY
1	K	135	GLY
1	A	123	VAL
1	C	71	ARG
2	F	368	ILE
1	G	94	SER
1	G	97	ASP
1	I	94	SER
1	I	135	GLY
1	I	422(B)	ALA
1	K	123	VAL
1	K	609	GLY
1	A	86	GLY
2	D	50	GLY

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Mol	Chain	Res	Type
2	D	368	ILE
1	E	86	GLY
1	E	123	VAL
1	G	86	GLY
2	D	77	GLY
1	E	447	PRO
2	J	368	ILE
1	K	86	GLY
1	E	609	GLY
2	H	368	ILE
1	I	123	VAL
1	I	127	VAL
1	I	667	PRO
1	A	609	GLY
1	C	123	VAL
2	D	395	PRO
2	D	475	GLY
2	F	154	PRO
2	F	395	PRO
2	L	77	GLY
2	L	537	ILE
2	B	50	GLY
1	E	280	GLY

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	474/540 (88%)	415 (88%)	59 (12%)	4	21
1	C	474/540 (88%)	422 (89%)	52 (11%)	6	26
1	E	474/540 (88%)	419 (88%)	55 (12%)	5	24
1	G	520/540 (96%)	462 (89%)	58 (11%)	6	25
1	I	520/540 (96%)	457 (88%)	63 (12%)	5	22
1	K	520/540 (96%)	460 (88%)	60 (12%)	5	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	415/437 (95%)	389 (94%)	26 (6%)	16	48
2	D	415/437 (95%)	386 (93%)	29 (7%)	14	45
2	F	415/437 (95%)	382 (92%)	33 (8%)	11	40
2	H	415/437 (95%)	385 (93%)	30 (7%)	13	44
2	J	415/437 (95%)	379 (91%)	36 (9%)	9	36
2	L	415/437 (95%)	385 (93%)	30 (7%)	13	44
All	All	5472/5862 (93%)	4941 (90%)	531 (10%)	8	32

All (531) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	PHE
1	A	66	ILE
1	A	70	ASN
1	A	89	THR
1	A	97	ASP
1	A	99	GLN
1	A	163	PHE
1	A	182	LYS
1	A	186	GLU
1	A	265	THR
1	A	266	GLN
1	A	275	LEU
1	A	276	CYS
1	A	285	LEU
1	A	292	ILE
1	A	338	ILE
1	A	344	ASN
1	A	347	PHE
1	A	360	VAL
1	A	375	ARG
1	A	388	ASP
1	A	400	LEU
1	A	416	ARG
1	A	419	ARG
1	A	436	TYR
1	A	443	MET
1	A	444	TYR
1	A	449	ILE
1	A	455	TRP

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Mol	Chain	Res	Type
1	A	467	ARG
1	A	482	LEU
1	A	488	VAL
1	A	517	LEU
1	A	520	THR
1	A	539	ARG
1	A	542	ARG
1	A	547	MET
1	A	548	ASP
1	A	552	GLU
1	A	553	ARG
1	A	554	ARG
1	A	570	VAL
1	A	571	THR
1	A	582	SER
1	A	593	THR
1	A	616	VAL
1	A	625	PHE
1	A	629	THR
1	A	634	LEU
1	A	643	GLN
1	A	652	GLU
1	A	653	LYS
1	A	661	MET
1	A	674	ASP
1	A	677	VAL
1	A	683	GLU
1	A	702	GLU
1	A	711	ASN
1	A	718	LEU
2	B	42	ARG
2	B	43	ARG
2	B	52	GLN
2	B	91	THR
2	B	119	VAL
2	B	147	MET
2	B	167	GLN
2	B	236	ASN
2	B	273	ARG
2	B	288	VAL
2	B	301	SER
2	B	354	VAL

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Mol	Chain	Res	Type
2	B	390	THR
2	B	401	THR
2	B	408	VAL
2	B	409	ILE
2	B	448	ARG
2	B	462	VAL
2	B	476	ASP
2	B	476(A)	LEU
2	B	476(C)	ASP
2	B	476(D)	PRO
2	B	499	ARG
2	B	504	GLU
2	B	509	ARG
2	B	514	ARG
1	C	63	PHE
1	C	66	ILE
1	C	70	ASN
1	C	89	THR
1	C	97	ASP
1	C	99	GLN
1	C	163	PHE
1	C	182	LYS
1	C	186	GLU
1	C	193	PRO
1	C	275	LEU
1	C	276	CYS
1	C	285	LEU
1	C	292	ILE
1	C	338	ILE
1	C	344	ASN
1	C	347	PHE
1	C	360	VAL
1	C	400	LEU
1	C	416	ARG
1	C	419	ARG
1	C	436	TYR
1	C	449	ILE
1	C	455	TRP
1	C	467	ARG
1	C	482	LEU
1	C	488	VAL
1	C	517	LEU

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Mol	Chain	Res	Type
1	C	520	THR
1	C	539	ARG
1	C	542	ARG
1	C	548	ASP
1	C	552	GLU
1	C	553	ARG
1	C	554	ARG
1	C	570	VAL
1	C	571	THR
1	C	582	SER
1	C	593	THR
1	C	625	PHE
1	C	630	ARG
1	C	634	LEU
1	C	643	GLN
1	C	652	GLU
1	C	653	LYS
1	C	661	MET
1	C	674	ASP
1	C	677	VAL
1	C	683	GLU
1	C	702	GLU
1	C	711	ASN
1	C	718	LEU
2	D	42	ARG
2	D	43	ARG
2	D	48	LEU
2	D	52	GLN
2	D	119	VAL
2	D	138	SER
2	D	139	LYS
2	D	147	MET
2	D	167	GLN
2	D	194	SER
2	D	218	LYS
2	D	273	ARG
2	D	288	VAL
2	D	301	SER
2	D	332	ILE
2	D	354	VAL
2	D	401	THR
2	D	408	VAL

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Mol	Chain	Res	Type
2	D	448	ARG
2	D	462	VAL
2	D	476	ASP
2	D	476(A)	LEU
2	D	476(C)	ASP
2	D	476(D)	PRO
2	D	493	PRO
2	D	495	VAL
2	D	504	GLU
2	D	509	ARG
2	D	514	ARG
1	E	63	PHE
1	E	66	ILE
1	E	70	ASN
1	E	89	THR
1	E	97	ASP
1	E	99	GLN
1	E	163	PHE
1	E	178	ILE
1	E	182	LYS
1	E	186	GLU
1	E	275	LEU
1	E	276	CYS
1	E	285	LEU
1	E	292	ILE
1	E	338	ILE
1	E	344	ASN
1	E	347	PHE
1	E	360	VAL
1	E	373	MET
1	E	400	LEU
1	E	416	ARG
1	E	419	ARG
1	E	435	VAL
1	E	436	TYR
1	E	449	ILE
1	E	455	TRP
1	E	467	ARG
1	E	482	LEU
1	E	488	VAL
1	E	517	LEU
1	E	520	THR

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Mol	Chain	Res	Type
1	E	539	ARG
1	E	548	ASP
1	E	552	GLU
1	E	553	ARG
1	E	554	ARG
1	E	570	VAL
1	E	571	THR
1	E	582	SER
1	E	593	THR
1	E	598	PRO
1	E	625	PHE
1	E	629	THR
1	E	630	ARG
1	E	634	LEU
1	E	643	GLN
1	E	652	GLU
1	E	653	LYS
1	E	661	MET
1	E	674	ASP
1	E	677	VAL
1	E	683	GLU
1	E	702	GLU
1	E	711	ASN
1	E	718	LEU
2	F	42	ARG
2	F	43	ARG
2	F	48	LEU
2	F	52	GLN
2	F	119	VAL
2	F	138	SER
2	F	147	MET
2	F	156	ILE
2	F	167	GLN
2	F	194	SER
2	F	236	ASN
2	F	238	GLN
2	F	273	ARG
2	F	288	VAL
2	F	301	SER
2	F	332	ILE
2	F	338	LYS
2	F	390	THR

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Mol	Chain	Res	Type
2	F	401	THR
2	F	408	VAL
2	F	409	ILE
2	F	448	ARG
2	F	460	VAL
2	F	462	VAL
2	F	476	ASP
2	F	476(A)	LEU
2	F	476(C)	ASP
2	F	476(D)	PRO
2	F	495	VAL
2	F	499	ARG
2	F	504	GLU
2	F	509	ARG
2	F	514	ARG
1	G	63	PHE
1	G	66	ILE
1	G	70	ASN
1	G	89	THR
1	G	97	ASP
1	G	99	GLN
1	G	163	PHE
1	G	182	LYS
1	G	186	GLU
1	G	207	LYS
1	G	243	GLN
1	G	247	ASN
1	G	256	ASP
1	G	257	ARG
1	G	275	LEU
1	G	276	CYS
1	G	285	LEU
1	G	292	ILE
1	G	312	THR
1	G	344	ASN
1	G	347	PHE
1	G	360	VAL
1	G	375	ARG
1	G	392	THR
1	G	400	LEU
1	G	416	ARG
1	G	419	ARG

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Mol	Chain	Res	Type
1	G	436	TYR
1	G	455	TRP
1	G	467	ARG
1	G	482	LEU
1	G	488	VAL
1	G	517	LEU
1	G	520	THR
1	G	539	ARG
1	G	542	ARG
1	G	548	ASP
1	G	552	GLU
1	G	553	ARG
1	G	554	ARG
1	G	570	VAL
1	G	571	THR
1	G	582	SER
1	G	593	THR
1	G	625	PHE
1	G	629	THR
1	G	634	LEU
1	G	643	GLN
1	G	652	GLU
1	G	653	LYS
1	G	661	MET
1	G	674	ASP
1	G	677	VAL
1	G	683	GLU
1	G	700	ARG
1	G	702	GLU
1	G	711	ASN
1	G	718	LEU
2	H	42	ARG
2	H	43	ARG
2	H	48	LEU
2	H	52	GLN
2	H	71	ASP
2	H	119	VAL
2	H	138	SER
2	H	144	ILE
2	H	147	MET
2	H	167	GLN
2	H	194	SER

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Mol	Chain	Res	Type
2	H	218	LYS
2	H	236	ASN
2	H	238	GLN
2	H	273	ARG
2	H	288	VAL
2	H	301	SER
2	H	312	THR
2	H	332	ILE
2	H	354	VAL
2	H	390	THR
2	H	401	THR
2	H	408	VAL
2	H	448	ARG
2	H	460	VAL
2	H	462	VAL
2	H	499	ARG
2	H	504	GLU
2	H	509	ARG
2	H	514	ARG
1	I	63	PHE
1	I	66	ILE
1	I	68	ILE
1	I	70	ASN
1	I	89	THR
1	I	97	ASP
1	I	99	GLN
1	I	163	PHE
1	I	182	LYS
1	I	186	GLU
1	I	207	LYS
1	I	230	ARG
1	I	243	GLN
1	I	247	ASN
1	I	256	ASP
1	I	257	ARG
1	I	275	LEU
1	I	276	CYS
1	I	285	LEU
1	I	292	ILE
1	I	312	THR
1	I	338	ILE
1	I	344	ASN

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Mol	Chain	Res	Type
1	I	347	PHE
1	I	360	VAL
1	I	375	ARG
1	I	392	THR
1	I	400	LEU
1	I	416	ARG
1	I	419	ARG
1	I	436	TYR
1	I	444	TYR
1	I	455	TRP
1	I	467	ARG
1	I	482	LEU
1	I	488	VAL
1	I	517	LEU
1	I	525	VAL
1	I	539	ARG
1	I	548	ASP
1	I	552	GLU
1	I	553	ARG
1	I	554	ARG
1	I	560	VAL
1	I	570	VAL
1	I	571	THR
1	I	582	SER
1	I	593	THR
1	I	616	VAL
1	I	625	PHE
1	I	629	THR
1	I	634	LEU
1	I	643	GLN
1	I	652	GLU
1	I	653	LYS
1	I	661	MET
1	I	674	ASP
1	I	677	VAL
1	I	683	GLU
1	I	700	ARG
1	I	702	GLU
1	I	711	ASN
1	I	718	LEU
2	J	42	ARG
2	J	43	ARG

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Mol	Chain	Res	Type
2	J	48	LEU
2	J	52	GLN
2	J	91	THR
2	J	95	MET
2	J	98	GLN
2	J	119	VAL
2	J	138	SER
2	J	147	MET
2	J	167	GLN
2	J	194	SER
2	J	236	ASN
2	J	273	ARG
2	J	288	VAL
2	J	301	SER
2	J	312	THR
2	J	332	ILE
2	J	354	VAL
2	J	365	CYS
2	J	390	THR
2	J	401	THR
2	J	408	VAL
2	J	448	ARG
2	J	460	VAL
2	J	462	VAL
2	J	476	ASP
2	J	476(A)	LEU
2	J	476(C)	ASP
2	J	476(D)	PRO
2	J	493	PRO
2	J	495	VAL
2	J	499	ARG
2	J	504	GLU
2	J	509	ARG
2	J	514	ARG
1	K	63	PHE
1	K	66	ILE
1	K	70	ASN
1	K	89	THR
1	K	97	ASP
1	K	99	GLN
1	K	163	PHE
1	K	182	LYS

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Mol	Chain	Res	Type
1	K	186	GLU
1	K	230	ARG
1	K	243	GLN
1	K	247	ASN
1	K	257	ARG
1	K	275	LEU
1	K	276	CYS
1	K	285	LEU
1	K	292	ILE
1	K	312	THR
1	K	338	ILE
1	K	344	ASN
1	K	360	VAL
1	K	388	ASP
1	K	400	LEU
1	K	416	ARG
1	K	419	ARG
1	K	436	TYR
1	K	449	ILE
1	K	455	TRP
1	K	467	ARG
1	K	482	LEU
1	K	488	VAL
1	K	517	LEU
1	K	520	THR
1	K	525	VAL
1	K	539	ARG
1	K	547	MET
1	K	548	ASP
1	K	552	GLU
1	K	553	ARG
1	K	554	ARG
1	K	570	VAL
1	K	571	THR
1	K	582	SER
1	K	593	THR
1	K	598	PRO
1	K	625	PHE
1	K	629	THR
1	K	630	ARG
1	K	634	LEU
1	K	643	GLN

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Mol	Chain	Res	Type
1	K	648	ARG
1	K	652	GLU
1	K	653	LYS
1	K	661	MET
1	K	674	ASP
1	K	677	VAL
1	K	683	GLU
1	K	702	GLU
1	K	711	ASN
1	K	718	LEU
2	L	42	ARG
2	L	43	ARG
2	L	91	THR
2	L	119	VAL
2	L	147	MET
2	L	167	GLN
2	L	194	SER
2	L	218	LYS
2	L	236	ASN
2	L	238	GLN
2	L	273	ARG
2	L	288	VAL
2	L	301	SER
2	L	332	ILE
2	L	354	VAL
2	L	365	CYS
2	L	390	THR
2	L	401	THR
2	L	408	VAL
2	L	448	ARG
2	L	462	VAL
2	L	476	ASP
2	L	476(A)	LEU
2	L	476(C)	ASP
2	L	476(D)	PRO
2	L	495	VAL
2	L	499	ARG
2	L	504	GLU
2	L	509	ARG
2	L	514	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (153) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	99	GLN
1	A	102	HIS
1	A	104	GLN
1	A	119	GLN
1	A	137	GLN
1	A	188	ASN
1	A	266	GLN
1	A	293	GLN
1	A	551	HIS
1	A	564	GLN
1	A	637	HIS
1	A	697	ASN
2	B	52	GLN
2	B	58	GLN
2	B	88	HIS
2	B	100	GLN
2	B	124	GLN
2	B	137	HIS
2	B	151	ASN
2	B	167	GLN
2	B	309	ASN
2	B	482	HIS
2	B	492	ASN
2	B	528	GLN
2	B	536	ASN
1	C	70	ASN
1	C	99	GLN
1	C	102	HIS
1	C	104	GLN
1	C	119	GLN
1	C	137	GLN
1	C	188	ASN
1	C	293	GLN
1	C	480	HIS
1	C	551	HIS
1	C	564	GLN
1	C	637	HIS
1	C	716	ASN
2	D	58	GLN
2	D	88	HIS
2	D	100	GLN
2	D	124	GLN

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Mol	Chain	Res	Type
2	D	151	ASN
2	D	167	GLN
2	D	309	ASN
2	D	473	HIS
2	D	482	HIS
2	D	492	ASN
2	D	536	ASN
1	E	70	ASN
1	E	99	GLN
1	E	102	HIS
1	E	119	GLN
1	E	137	GLN
1	E	188	ASN
1	E	551	HIS
1	E	564	GLN
1	E	637	HIS
1	E	643	GLN
1	E	716	ASN
2	F	58	GLN
2	F	88	HIS
2	F	100	GLN
2	F	151	ASN
2	F	167	GLN
2	F	183	ASN
2	F	238	GLN
2	F	309	ASN
2	F	482	HIS
2	F	492	ASN
2	F	536	ASN
1	G	70	ASN
1	G	99	GLN
1	G	102	HIS
1	G	104	GLN
1	G	119	GLN
1	G	137	GLN
1	G	188	ASN
1	G	342	GLN
1	G	480	HIS
1	G	516	ASN
1	G	551	HIS
1	G	564	GLN
1	G	637	HIS

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Mol	Chain	Res	Type
1	G	697	ASN
2	H	58	GLN
2	H	88	HIS
2	H	100	GLN
2	H	151	ASN
2	H	167	GLN
2	H	183	ASN
2	H	238	GLN
2	H	309	ASN
2	H	446	HIS
2	H	482	HIS
2	H	492	ASN
2	H	528	GLN
2	H	536	ASN
1	I	70	ASN
1	I	99	GLN
1	I	102	HIS
1	I	104	GLN
1	I	119	GLN
1	I	137	GLN
1	I	188	ASN
1	I	210	ASN
1	I	516	ASN
1	I	551	HIS
1	I	564	GLN
1	I	637	HIS
1	I	697	ASN
1	I	716	ASN
2	J	58	GLN
2	J	88	HIS
2	J	100	GLN
2	J	151	ASN
2	J	159	ASN
2	J	167	GLN
2	J	183	ASN
2	J	309	ASN
2	J	403	GLN
2	J	473	HIS
2	J	482	HIS
2	J	492	ASN
2	J	536	ASN
1	K	70	ASN

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Mol	Chain	Res	Type
1	K	99	GLN
1	K	102	HIS
1	K	104	GLN
1	K	119	GLN
1	K	137	GLN
1	K	188	ASN
1	K	210	ASN
1	K	236	GLN
1	K	293	GLN
1	K	342	GLN
1	K	480	HIS
1	K	516	ASN
1	K	551	HIS
1	K	564	GLN
2	L	58	GLN
2	L	88	HIS
2	L	100	GLN
2	L	151	ASN
2	L	167	GLN
2	L	238	GLN
2	L	309	ASN
2	L	333	GLN
2	L	473	HIS
2	L	482	HIS
2	L	492	ASN
2	L	536	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 oligosaccharides in this entry.

5.6 Ligand geometry

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BTI	G	801	1	15,16,16	1.86	1 (6%)	20,21,21	2.33	7 (35%)
3	BTI	K	801	1	15,16,16	1.76	1 (6%)	20,21,21	2.08	5 (25%)
3	BTI	C	801	1	15,16,16	1.72	1 (6%)	20,21,21	2.10	6 (30%)
3	BTI	I	801	1	15,16,16	1.77	1 (6%)	20,21,21	2.11	6 (30%)
3	BTI	A	801	1	15,16,16	1.72	1 (6%)	20,21,21	2.05	7 (35%)
3	BTI	E	801	1	15,16,16	1.76	1 (6%)	20,21,21	2.22	7 (35%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BTI	G	801	1	-	5/6/27/27	0/2/2/2
3	BTI	K	801	1	-	3/6/27/27	0/2/2/2
3	BTI	C	801	1	-	0/6/27/27	0/2/2/2
3	BTI	I	801	1	-	3/6/27/27	0/2/2/2
3	BTI	A	801	1	-	2/6/27/27	0/2/2/2
3	BTI	E	801	1	-	1/6/27/27	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	801	BTI	O3-C3	6.63	1.37	1.23
3	I	801	BTI	O3-C3	6.37	1.36	1.23
3	E	801	BTI	O3-C3	6.36	1.36	1.23
3	K	801	BTI	O3-C3	6.31	1.36	1.23
3	C	801	BTI	O3-C3	6.22	1.36	1.23
3	A	801	BTI	O3-C3	6.18	1.36	1.23

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	801	BTI	C6-C5-N3	-4.53	107.34	113.18
3	E	801	BTI	C6-C5-N3	-4.24	107.72	113.18
3	G	801	BTI	C4-N2-C3	-4.09	107.49	112.56
3	I	801	BTI	C6-S1-C2	4.03	98.37	89.98
3	E	801	BTI	C4-N2-C3	-3.98	107.62	112.56
3	C	801	BTI	C6-C5-N3	-3.98	108.06	113.18
3	K	801	BTI	C6-C5-N3	-3.96	108.08	113.18
3	C	801	BTI	C4-N2-C3	-3.95	107.66	112.56
3	I	801	BTI	C6-C5-N3	-3.93	108.11	113.18
3	G	801	BTI	C5-N3-C3	-3.90	106.64	112.38
3	G	801	BTI	C6-S1-C2	3.90	98.09	89.98
3	E	801	BTI	C4-C2-S1	-3.88	100.63	105.03
3	A	801	BTI	C6-S1-C2	3.81	97.91	89.98
3	A	801	BTI	C6-C5-N3	-3.79	108.29	113.18
3	I	801	BTI	C4-N2-C3	-3.73	107.93	112.56
3	K	801	BTI	C4-N2-C3	-3.72	107.94	112.56
3	C	801	BTI	N2-C3-N3	3.71	113.13	108.85
3	G	801	BTI	N2-C3-N3	3.67	113.08	108.85
3	K	801	BTI	C6-S1-C2	3.66	97.60	89.98
3	E	801	BTI	N2-C3-N3	3.57	112.98	108.85
3	K	801	BTI	N2-C3-N3	3.44	112.82	108.85
3	C	801	BTI	C6-S1-C2	3.38	97.02	89.98
3	I	801	BTI	N2-C3-N3	3.35	112.72	108.85
3	A	801	BTI	N2-C3-N3	3.25	112.60	108.85
3	I	801	BTI	C5-N3-C3	-3.22	107.64	112.38
3	A	801	BTI	C4-N2-C3	-3.09	108.72	112.56
3	E	801	BTI	C6-S1-C2	2.98	96.19	89.98
3	K	801	BTI	C5-N3-C3	-2.94	108.06	112.38
3	C	801	BTI	C5-N3-C3	-2.77	108.31	112.38
3	A	801	BTI	C5-N3-C3	-2.72	108.39	112.38
3	E	801	BTI	C5-N3-C3	-2.62	108.53	112.38
3	A	801	BTI	C6-C5-C4	2.39	112.84	109.06
3	A	801	BTI	C2-C4-C5	2.20	111.59	108.89
3	G	801	BTI	C4-C5-N3	-2.19	100.00	102.43
3	I	801	BTI	C4-C5-N3	-2.15	100.04	102.43
3	C	801	BTI	C4-C2-S1	-2.12	102.62	105.03
3	G	801	BTI	C4-C2-S1	-2.09	102.66	105.03
3	E	801	BTI	C2-C4-N2	-2.03	111.20	113.34

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	801	BTI	S1-C2-C7-C8
3	G	801	BTI	C4-C2-C7-C8
3	I	801	BTI	C9-C10-C11-O11
3	K	801	BTI	C2-C7-C8-C9
3	A	801	BTI	C2-C7-C8-C9
3	I	801	BTI	C2-C7-C8-C9
3	G	801	BTI	C7-C8-C9-C10
3	A	801	BTI	C11-C10-C9-C8
3	I	801	BTI	C11-C10-C9-C8
3	K	801	BTI	C11-C10-C9-C8
3	K	801	BTI	C7-C8-C9-C10
3	E	801	BTI	C7-C8-C9-C10
3	G	801	BTI	C11-C10-C9-C8
3	G	801	BTI	C2-C7-C8-C9

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	801	BTI	2	0
3	A	801	BTI	1	0
3	E	801	BTI	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	A	591/681 (86%)	0.79	83 (14%) 6 5	17, 65, 113, 128	0
1	C	591/681 (86%)	0.77	72 (12%) 8 6	17, 65, 113, 128	0
1	E	591/681 (86%)	0.82	86 (14%) 6 4	17, 66, 113, 128	0
1	G	646/681 (94%)	0.79	79 (12%) 8 6	15, 67, 112, 128	0
1	I	646/681 (94%)	0.85	99 (15%) 5 4	16, 67, 112, 127	0
1	K	646/681 (94%)	0.76	79 (12%) 8 6	16, 68, 112, 128	0
2	B	506/531 (95%)	-0.44	4 (0%) 82 67	10, 26, 57, 101	0
2	D	506/531 (95%)	-0.43	3 (0%) 85 73	11, 26, 58, 101	0
2	F	506/531 (95%)	-0.42	2 (0%) 88 79	12, 27, 58, 100	0
2	H	506/531 (95%)	-0.44	2 (0%) 88 79	10, 26, 58, 101	0
2	J	506/531 (95%)	-0.45	5 (0%) 79 63	11, 26, 58, 100	0
2	L	506/531 (95%)	-0.47	3 (0%) 85 73	11, 26, 57, 100	0
All	All	6747/7272 (92%)	0.24	517 (7%) 19 13	10, 43, 108, 128	0

All (517) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	162	ILE	6.9
1	E	162	ILE	6.1
1	C	162	ILE	6.0
1	C	286	GLY	6.0
1	I	70	ASN	5.2
1	E	138	ALA	5.1
1	A	138	ALA	5.0
1	C	138	ALA	4.9
1	I	122	ILE	4.7
1	E	152	PHE	4.7
1	G	214	TYR	4.7

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Mol	Chain	Res	Type	RSRZ
1	E	384	ILE	4.6
1	A	275	LEU	4.5
1	E	286	GLY	4.4
1	E	329	TYR	4.4
1	A	330	ALA	4.3
1	I	96	ALA	4.3
1	C	124	ILE	4.3
1	A	63	PHE	4.3
1	I	280	GLY	4.3
1	I	384	ILE	4.2
1	I	152	PHE	4.2
1	A	329	TYR	4.2
1	I	214	TYR	4.2
1	C	152	PHE	4.1
2	B	476(A)	LEU	4.0
1	G	63	PHE	4.0
1	C	134	THR	3.9
1	A	122	ILE	3.8
1	G	66	ILE	3.8
1	C	158	ALA	3.8
1	I	146	LEU	3.8
1	G	96	ALA	3.7
1	A	286	GLY	3.7
1	I	63	PHE	3.7
1	G	278	SER	3.7
1	I	162	ILE	3.7
1	E	283	ILE	3.7
1	K	122	ILE	3.7
1	I	121	TYR	3.7
1	E	122	ILE	3.7
1	C	63	PHE	3.7
1	I	129	ALA	3.6
1	I	331	SER	3.6
1	K	278	SER	3.6
1	A	366	GLY	3.6
1	E	276	CYS	3.6
1	K	162	ILE	3.6
1	E	278	SER	3.5
1	A	96	ALA	3.5
1	A	331	SER	3.5
1	C	139	VAL	3.5
1	G	256	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	G	94	SER	3.5
1	I	147	SER	3.5
1	I	171	ILE	3.5
1	K	384	ILE	3.5
1	A	147	SER	3.4
1	K	374	ILE	3.4
1	E	147	SER	3.4
1	K	63	PHE	3.4
1	K	123	VAL	3.4
2	D	476(A)	LEU	3.4
1	K	70	ASN	3.4
1	E	171	ILE	3.4
1	C	117	ALA	3.4
1	E	166	PRO	3.4
1	A	277	ASP	3.4
2	F	476(A)	LEU	3.4
1	G	147	SER	3.3
1	I	97	ASP	3.3
2	H	476(B)	GLY	3.3
1	I	166	PRO	3.3
1	E	374	ILE	3.3
1	I	329	TYR	3.3
1	A	166	PRO	3.3
1	C	122	ILE	3.3
1	G	374	ILE	3.3
1	E	310	GLU	3.2
1	G	329	TYR	3.2
1	C	278	SER	3.2
1	K	97	ASP	3.2
1	C	374	ILE	3.2
1	G	706	VAL	3.1
1	K	152	PHE	3.1
1	G	115	PRO	3.1
1	G	99	GLN	3.1
1	A	170	ALA	3.1
1	I	134	THR	3.1
1	K	170	ALA	3.1
1	G	146	LEU	3.1
1	I	139	VAL	3.1
1	C	132	ARG	3.1
1	C	656	PRO	3.1
1	K	214	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	K	348	LEU	3.1
1	C	163	PHE	3.1
1	I	708	ALA	3.1
1	I	135	GLY	3.1
1	G	97	ASP	3.1
1	G	276	CYS	3.1
1	K	158	ALA	3.0
1	G	265	THR	3.0
1	I	707	VAL	3.0
1	G	152	PHE	3.0
1	G	166	PRO	3.0
2	D	476(B)	GLY	3.0
1	G	98	LYS	3.0
1	A	150	SER	3.0
1	A	69	ALA	3.0
1	I	276	CYS	3.0
1	G	352	THR	3.0
1	K	174	MET	3.0
1	I	115	PRO	3.0
1	K	180	SER	3.0
1	C	133	ALA	3.0
1	I	123	VAL	3.0
1	K	163	PHE	3.0
1	A	448	MET	3.0
1	G	162	ILE	3.0
1	K	275	LEU	3.0
1	K	285	LEU	3.0
1	K	164	VAL	3.0
1	E	350	MET	3.0
1	C	96	ALA	2.9
1	I	120	SER	2.9
1	G	122	ILE	2.9
1	G	171	ILE	2.9
1	E	67	LEU	2.9
1	G	285	LEU	2.9
1	I	330	ALA	2.9
1	G	88	SER	2.9
1	G	121	TYR	2.9
1	I	94	SER	2.9
1	A	276	CYS	2.9
1	I	138	ALA	2.9
1	A	121	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	134	THR	2.9
1	K	134	THR	2.9
1	A	161	VAL	2.9
1	E	123	VAL	2.9
1	A	152	PHE	2.9
1	A	156	LEU	2.9
1	E	331	SER	2.9
1	A	134	THR	2.9
1	I	706	VAL	2.9
1	E	145	PHE	2.9
1	G	328	GLY	2.9
1	C	84	LYS	2.9
1	G	174	MET	2.9
1	A	97	ASP	2.8
1	C	100	ALA	2.8
1	K	115	PRO	2.8
1	G	704	LYS	2.8
1	K	146	LEU	2.8
1	G	134	THR	2.8
1	K	276	CYS	2.8
1	G	138	ALA	2.8
1	I	158	ALA	2.8
1	E	381	PRO	2.8
1	E	139	VAL	2.8
1	C	348	LEU	2.8
1	K	69	ALA	2.8
1	A	455	TRP	2.8
1	C	66	ILE	2.8
1	E	63	PHE	2.8
1	K	256	ASP	2.8
1	A	282	GLY	2.8
2	J	476(B)	GLY	2.8
1	K	329	TYR	2.8
1	K	138	ALA	2.8
1	I	98	LYS	2.8
1	I	67	LEU	2.8
1	G	163	PHE	2.7
1	I	374	ILE	2.8
1	C	366	GLY	2.7
1	I	69	ALA	2.7
1	A	273	GLN	2.7
1	C	455	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	277	ASP	2.7
1	E	121	TYR	2.7
1	G	70	ASN	2.7
1	E	328	GLY	2.7
1	G	245	SER	2.7
1	I	88	SER	2.7
1	I	256	ASP	2.7
1	A	111	HIS	2.7
1	A	158	ALA	2.7
1	A	163	PHE	2.7
1	E	131	ILE	2.7
1	I	163	PHE	2.7
1	E	93	TYR	2.7
1	C	70	ASN	2.7
1	G	275	LEU	2.7
1	K	149	ASN	2.7
1	E	124	ILE	2.7
1	G	167	PRO	2.7
1	G	169	GLY	2.7
1	I	136	ALA	2.7
1	K	100	ALA	2.7
1	A	164	VAL	2.7
1	E	354	LEU	2.7
1	E	163	PHE	2.6
1	E	455	TRP	2.6
1	I	101	LEU	2.6
1	I	445	TYR	2.6
1	A	171	ILE	2.6
1	E	85	MET	2.6
2	J	37	GLU	2.6
1	G	455	TRP	2.6
1	C	123	VAL	2.6
1	C	147	SER	2.6
1	E	150	SER	2.6
1	A	283	ILE	2.6
1	K	111	HIS	2.6
1	A	333	GLY	2.6
1	I	328	GLY	2.6
1	E	327	VAL	2.6
1	E	330	ALA	2.6
1	I	164	VAL	2.6
1	K	121	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	I	116	PRO	2.6
1	C	146	LEU	2.6
1	K	394	TRP	2.6
1	C	384	ILE	2.6
1	A	94	SER	2.6
1	C	442	SER	2.6
1	I	145	PHE	2.6
1	G	282	GLY	2.6
1	A	281	ASN	2.6
1	C	275	LEU	2.6
1	C	365	THR	2.6
1	G	92	ILE	2.5
1	A	99	GLN	2.5
1	C	97	ASP	2.5
1	I	149	ASN	2.5
1	A	440	GLU	2.5
1	E	337	PHE	2.5
1	G	111	HIS	2.5
1	C	142	GLY	2.5
1	I	160	GLY	2.5
1	G	83	ARG	2.5
1	A	153	ALA	2.5
1	I	124	ILE	2.5
1	I	283	ILE	2.5
1	A	394	TRP	2.5
1	A	279	HIS	2.5
1	C	276	CYS	2.5
1	K	286	GLY	2.5
1	K	383	SER	2.5
1	I	440	GLU	2.5
1	I	354	LEU	2.5
1	A	123	VAL	2.5
1	E	137	GLN	2.5
1	K	327	VAL	2.5
1	I	170	ALA	2.5
1	A	98	LYS	2.5
1	E	156	LEU	2.5
1	G	381	PRO	2.5
1	E	282	GLY	2.5
1	C	170	ALA	2.4
1	C	171	ILE	2.4
1	K	124	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	394	TRP	2.4
1	C	167	PRO	2.4
1	C	329	TYR	2.4
1	E	111	HIS	2.4
1	I	93	TYR	2.4
2	B	476(B)	GLY	2.4
1	A	100	ALA	2.4
1	K	96	ALA	2.4
1	I	278	SER	2.4
1	E	151	LYS	2.4
1	G	246	LYS	2.4
1	I	703	LYS	2.4
1	C	354	LEU	2.4
1	I	348	LEU	2.4
1	C	265	THR	2.4
1	C	394	TRP	2.4
1	I	118	ASN	2.4
1	I	281	ASN	2.4
1	I	667	PRO	2.4
1	E	165	GLY	2.4
1	E	333	GLY	2.4
2	B	50	GLY	2.4
1	G	117	ALA	2.4
1	K	106	ALA	2.4
1	C	137	GLN	2.4
1	E	372	GLN	2.4
1	I	717	SER	2.4
1	E	70	ASN	2.4
1	A	189	VAL	2.4
1	E	90	VAL	2.4
1	E	153	ALA	2.4
1	G	124	ILE	2.4
1	C	297	GLN	2.4
1	E	146	LEU	2.4
1	I	125	ASP	2.4
1	K	280	GLY	2.4
1	A	124	ILE	2.4
1	E	91	ALA	2.4
1	E	554	ARG	2.4
1	I	104	GLN	2.4
1	I	683	GLU	2.4
1	A	321	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	665	PRO	2.4
1	A	194	GLY	2.3
1	C	111	HIS	2.3
1	K	203	ASP	2.3
2	D	474	ARG	2.3
1	C	145	PHE	2.3
1	I	99	GLN	2.3
1	I	156	LEU	2.3
1	K	159	GLU	2.3
2	L	37	GLU	2.3
1	G	161	VAL	2.3
1	K	321	VAL	2.3
1	A	265	THR	2.3
1	C	333	GLY	2.3
1	E	366	GLY	2.3
1	I	326	ALA	2.3
1	I	277	ASP	2.3
1	G	145	PHE	2.3
1	I	198	LEU	2.3
1	K	145	PHE	2.3
1	K	198	LEU	2.3
1	G	386	GLN	2.3
1	G	123	VAL	2.3
1	I	83	ARG	2.3
1	K	71	ARG	2.3
1	A	86	GLY	2.3
1	E	394	TRP	2.3
1	A	191	THR	2.3
1	G	222	ALA	2.3
1	K	101	LEU	2.3
1	I	95	ASP	2.3
1	K	575	ASP	2.3
1	C	273	GLN	2.3
1	C	83	ARG	2.3
1	A	381	PRO	2.3
1	C	155	ALA	2.3
1	K	129	ALA	2.3
1	C	445	TYR	2.3
1	G	247	ASN	2.3
1	K	139	VAL	2.3
1	E	115	PRO	2.3
1	I	66	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	183	ILE	2.3
1	E	117	ALA	2.3
1	G	100	ALA	2.3
1	G	133	ALA	2.3
1	I	133	ALA	2.3
1	K	222	ALA	2.3
1	E	89	THR	2.3
2	H	476(A)	LEU	2.3
1	A	120	SER	2.3
1	G	71	ARG	2.3
1	G	575	ASP	2.3
1	A	112	ILE	2.2
1	I	381	PRO	2.2
1	I	656	PRO	2.2
1	A	350	MET	2.2
1	I	155	ALA	2.2
1	K	330	ALA	2.2
1	G	369	LEU	2.2
2	J	476(A)	LEU	2.2
1	A	143	TYR	2.2
1	G	180	SER	2.2
1	C	99	GLN	2.2
1	E	161	VAL	2.2
1	K	99	GLN	2.2
1	K	243	GLN	2.2
1	C	272	ILE	2.2
1	K	283	ILE	2.2
1	G	160	GLY	2.2
1	G	170	ALA	2.2
1	E	140	HIS	2.2
1	K	88	SER	2.2
1	E	149	ASN	2.2
1	A	108	GLU	2.2
1	G	183	ILE	2.2
1	A	67	LEU	2.2
1	A	280	GLY	2.2
1	A	328	GLY	2.2
1	C	129	ALA	2.2
1	C	153	ALA	2.2
1	C	285	LEU	2.2
1	K	141	PRO	2.2
2	J	36	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	65	LYS	2.2
1	E	98	LYS	2.2
1	C	121	TYR	2.2
1	G	131	ILE	2.2
1	A	149	ASN	2.2
1	C	369	LEU	2.2
1	E	323	LEU	2.2
1	I	275	LEU	2.2
1	I	422(C)	GLU	2.2
1	A	133	ALA	2.2
1	E	448	MET	2.2
1	C	141	PRO	2.2
1	G	153	ALA	2.2
1	G	280	GLY	2.2
1	K	326	ALA	2.2
1	A	168	LYS	2.2
1	I	394	TRP	2.2
1	A	274	VAL	2.2
1	A	92	ILE	2.2
1	A	137	GLN	2.2
1	A	278	SER	2.2
1	E	94	SER	2.2
1	I	266	GLN	2.2
1	I	383	SER	2.2
1	C	85	MET	2.2
1	A	70	ASN	2.2
1	E	155	ALA	2.2
1	K	155	ALA	2.2
1	G	655	PRO	2.2
1	I	167	PRO	2.2
1	K	655	PRO	2.2
1	K	277	ASP	2.2
1	G	292	ILE	2.1
2	L	528	GLN	2.1
1	E	84	LYS	2.1
1	K	443	MET	2.1
1	C	330	ALA	2.1
1	E	158	ALA	2.1
1	E	320	ALA	2.1
1	E	440	GLU	2.1
1	I	159	GLU	2.1
1	C	328	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	281	ASN	2.1
1	G	656	PRO	2.1
1	K	656	PRO	2.1
1	E	309	ASP	2.1
1	G	279	HIS	2.1
1	I	110	VAL	2.1
1	I	321	VAL	2.1
1	A	374	ILE	2.1
1	C	283	ILE	2.1
1	K	338	ILE	2.1
1	G	692	ALA	2.1
1	K	120	SER	2.1
1	K	160	GLY	2.1
2	B	475	GLY	2.1
2	J	476(D)	PRO	2.1
1	E	365	THR	2.1
1	I	131	ILE	2.1
1	A	91	ALA	2.1
1	E	69	ALA	2.1
1	E	386	GLN	2.1
1	K	173	ALA	2.1
1	E	186	GLU	2.1
1	A	88	SER	2.1
1	K	147	SER	2.1
1	C	118	ASN	2.1
1	C	446	ASP	2.1
2	F	36	LEU	2.1
2	L	476(A)	LEU	2.1
1	C	284	TYR	2.1
1	E	334	THR	2.1
1	E	346	TYR	2.1
1	G	445	TYR	2.1
1	K	133	ALA	2.1
1	K	104	GLN	2.1
1	A	317	GLY	2.1
1	I	169	GLY	2.1
1	G	422(C)	GLU	2.1
1	A	716	ASN	2.1
1	I	126	LYS	2.1
1	K	181	LYS	2.1
1	A	131	ILE	2.1
1	I	229	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	350	MET	2.1
1	A	284	TYR	2.1
1	A	117	ALA	2.1
1	E	96	ALA	2.1
1	I	106	ALA	2.1
1	C	440	GLU	2.1
1	I	680	GLU	2.1
1	K	116	PRO	2.1
1	E	274	VAL	2.0
1	A	64	ASN	2.0
1	A	382	LEU	2.0
1	A	554	ARG	2.0
1	C	131	ILE	2.0
1	K	554	ARG	2.0
1	C	128	MET	2.0
1	E	174	MET	2.0
1	A	692	ALA	2.0
1	E	133	ALA	2.0
1	E	385	THR	2.0
1	G	158	ALA	2.0
1	I	422(B)	ALA	2.0
1	K	153	ALA	2.0
1	I	286	GLY	2.0
1	K	366	GLY	2.0
1	K	166	PRO	2.0
1	C	653	LYS	2.0
1	K	151	LYS	2.0
1	E	275	LEU	2.0
1	E	596	TRP	2.0
1	G	140	HIS	2.0
1	I	128	MET	2.0
1	A	334	THR	2.0
1	I	117	ALA	2.0
1	E	97	ASP	2.0
1	E	575	ASP	2.0
1	I	165	GLY	2.0
1	E	667	PRO	2.0
1	I	355	GLN	2.0
1	C	310	GLU	2.0
1	C	389	VAL	2.0
1	G	310	GLU	2.0
1	I	702	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	K	310	GLU	2.0
1	G	348	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BTI	I	801	15/15	0.92	0.12	57,65,68,69	0
3	BTI	E	801	15/15	0.94	0.10	31,39,49,50	0
3	BTI	G	801	15/15	0.94	0.14	43,49,56,60	0
3	BTI	A	801	15/15	0.94	0.11	30,42,56,62	0
3	BTI	K	801	15/15	0.94	0.12	39,50,57,62	0
3	BTI	C	801	15/15	0.96	0.08	30,38,46,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.