



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:15 PM UTC

PDB ID : 3ZQJ / pdb_00003zqj
Title : Mycobacterium tuberculosis UvrA
Authors : Rossi, F.; Khanduja, J.S.; Bortoluzzi, A.; Houghton, J.; Sander, P.; Guthlein, C.; Davis, E.O.; Springer, B.; Bottger, E.C.; Relini, A.; Penco, A.; Muniyappa, K.; Rizzi, M.
Deposited on : 2011-06-09
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

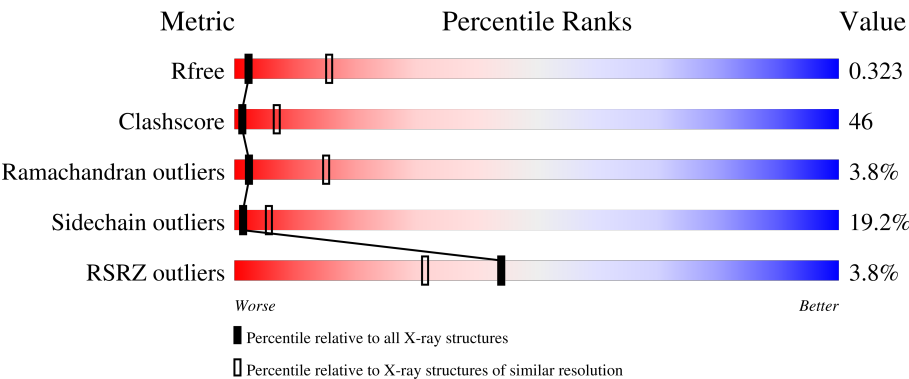
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	993	4% 40%40%13%• 5%
1	B	993	5% 39%41%12%• 8%
1	C	993	3% 37%39%12%• 10%
1	D	993	3% 37%43%12%• 7%
1	E	993	2% 37%40%13%• 7%

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Mol	Chain	Length	Quality of chain
1	F	993	3%16%30%14%.39%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 39998 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 UVRABC SYSTEM PROTEIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	944	Total	C	N	O	S	0	0	0
			7267	4550	1310	1385	22			
1	B	918	Total	C	N	O	S	0	0	0
			7067	4428	1272	1345	22			
1	C	890	Total	C	N	O	S	0	0	0
			6832	4277	1234	1299	22			
1	D	921	Total	C	N	O	S	0	0	0
			7095	4444	1276	1353	22			
1	E	919	Total	C	N	O	S	0	0	0
			7073	4434	1271	1347	21			
1	F	607	Total	C	N	O	S	0	0	0
			4650	2906	844	890	10			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP P63380
A	-19	GLY	-	expression tag	UNP P63380
A	-18	HIS	-	expression tag	UNP P63380
A	-17	HIS	-	expression tag	UNP P63380
A	-16	HIS	-	expression tag	UNP P63380
A	-15	HIS	-	expression tag	UNP P63380
A	-14	HIS	-	expression tag	UNP P63380
A	-13	HIS	-	expression tag	UNP P63380
A	-12	HIS	-	expression tag	UNP P63380
A	-11	HIS	-	expression tag	UNP P63380
A	-10	HIS	-	expression tag	UNP P63380
A	-9	HIS	-	expression tag	UNP P63380
A	-8	SER	-	expression tag	UNP P63380
A	-7	SER	-	expression tag	UNP P63380
A	-6	GLY	-	expression tag	UNP P63380
A	-5	HIS	-	expression tag	UNP P63380
A	-4	ILE	-	expression tag	UNP P63380

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLU	-	expression tag	UNP P63380
A	-2	GLY	-	expression tag	UNP P63380
A	-1	ARG	-	expression tag	UNP P63380
A	0	HIS	-	expression tag	UNP P63380
B	-20	MET	-	expression tag	UNP P63380
B	-19	GLY	-	expression tag	UNP P63380
B	-18	HIS	-	expression tag	UNP P63380
B	-17	HIS	-	expression tag	UNP P63380
B	-16	HIS	-	expression tag	UNP P63380
B	-15	HIS	-	expression tag	UNP P63380
B	-14	HIS	-	expression tag	UNP P63380
B	-13	HIS	-	expression tag	UNP P63380
B	-12	HIS	-	expression tag	UNP P63380
B	-11	HIS	-	expression tag	UNP P63380
B	-10	HIS	-	expression tag	UNP P63380
B	-9	HIS	-	expression tag	UNP P63380
B	-8	SER	-	expression tag	UNP P63380
B	-7	SER	-	expression tag	UNP P63380
B	-6	GLY	-	expression tag	UNP P63380
B	-5	HIS	-	expression tag	UNP P63380
B	-4	ILE	-	expression tag	UNP P63380
B	-3	GLU	-	expression tag	UNP P63380
B	-2	GLY	-	expression tag	UNP P63380
B	-1	ARG	-	expression tag	UNP P63380
B	0	HIS	-	expression tag	UNP P63380
C	-20	MET	-	expression tag	UNP P63380
C	-19	GLY	-	expression tag	UNP P63380
C	-18	HIS	-	expression tag	UNP P63380
C	-17	HIS	-	expression tag	UNP P63380
C	-16	HIS	-	expression tag	UNP P63380
C	-15	HIS	-	expression tag	UNP P63380
C	-14	HIS	-	expression tag	UNP P63380
C	-13	HIS	-	expression tag	UNP P63380
C	-12	HIS	-	expression tag	UNP P63380
C	-11	HIS	-	expression tag	UNP P63380
C	-10	HIS	-	expression tag	UNP P63380
C	-9	HIS	-	expression tag	UNP P63380
C	-8	SER	-	expression tag	UNP P63380
C	-7	SER	-	expression tag	UNP P63380
C	-6	GLY	-	expression tag	UNP P63380
C	-5	HIS	-	expression tag	UNP P63380
C	-4	ILE	-	expression tag	UNP P63380

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLU	-	expression tag	UNP P63380
C	-2	GLY	-	expression tag	UNP P63380
C	-1	ARG	-	expression tag	UNP P63380
C	0	HIS	-	expression tag	UNP P63380
D	-20	MET	-	expression tag	UNP P63380
D	-19	GLY	-	expression tag	UNP P63380
D	-18	HIS	-	expression tag	UNP P63380
D	-17	HIS	-	expression tag	UNP P63380
D	-16	HIS	-	expression tag	UNP P63380
D	-15	HIS	-	expression tag	UNP P63380
D	-14	HIS	-	expression tag	UNP P63380
D	-13	HIS	-	expression tag	UNP P63380
D	-12	HIS	-	expression tag	UNP P63380
D	-11	HIS	-	expression tag	UNP P63380
D	-10	HIS	-	expression tag	UNP P63380
D	-9	HIS	-	expression tag	UNP P63380
D	-8	SER	-	expression tag	UNP P63380
D	-7	SER	-	expression tag	UNP P63380
D	-6	GLY	-	expression tag	UNP P63380
D	-5	HIS	-	expression tag	UNP P63380
D	-4	ILE	-	expression tag	UNP P63380
D	-3	GLU	-	expression tag	UNP P63380
D	-2	GLY	-	expression tag	UNP P63380
D	-1	ARG	-	expression tag	UNP P63380
D	0	HIS	-	expression tag	UNP P63380
E	-20	MET	-	expression tag	UNP P63380
E	-19	GLY	-	expression tag	UNP P63380
E	-18	HIS	-	expression tag	UNP P63380
E	-17	HIS	-	expression tag	UNP P63380
E	-16	HIS	-	expression tag	UNP P63380
E	-15	HIS	-	expression tag	UNP P63380
E	-14	HIS	-	expression tag	UNP P63380
E	-13	HIS	-	expression tag	UNP P63380
E	-12	HIS	-	expression tag	UNP P63380
E	-11	HIS	-	expression tag	UNP P63380
E	-10	HIS	-	expression tag	UNP P63380
E	-9	HIS	-	expression tag	UNP P63380
E	-8	SER	-	expression tag	UNP P63380
E	-7	SER	-	expression tag	UNP P63380
E	-6	GLY	-	expression tag	UNP P63380
E	-5	HIS	-	expression tag	UNP P63380
E	-4	ILE	-	expression tag	UNP P63380

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	GLU	-	expression tag	UNP P63380
E	-2	GLY	-	expression tag	UNP P63380
E	-1	ARG	-	expression tag	UNP P63380
E	0	HIS	-	expression tag	UNP P63380
F	-20	MET	-	expression tag	UNP P63380
F	-19	GLY	-	expression tag	UNP P63380
F	-18	HIS	-	expression tag	UNP P63380
F	-17	HIS	-	expression tag	UNP P63380
F	-16	HIS	-	expression tag	UNP P63380
F	-15	HIS	-	expression tag	UNP P63380
F	-14	HIS	-	expression tag	UNP P63380
F	-13	HIS	-	expression tag	UNP P63380
F	-12	HIS	-	expression tag	UNP P63380
F	-11	HIS	-	expression tag	UNP P63380
F	-10	HIS	-	expression tag	UNP P63380
F	-9	HIS	-	expression tag	UNP P63380
F	-8	SER	-	expression tag	UNP P63380
F	-7	SER	-	expression tag	UNP P63380
F	-6	GLY	-	expression tag	UNP P63380
F	-5	HIS	-	expression tag	UNP P63380
F	-4	ILE	-	expression tag	UNP P63380
F	-3	GLU	-	expression tag	UNP P63380
F	-2	GLY	-	expression tag	UNP P63380
F	-1	ARG	-	expression tag	UNP P63380
F	0	HIS	-	expression tag	UNP P63380

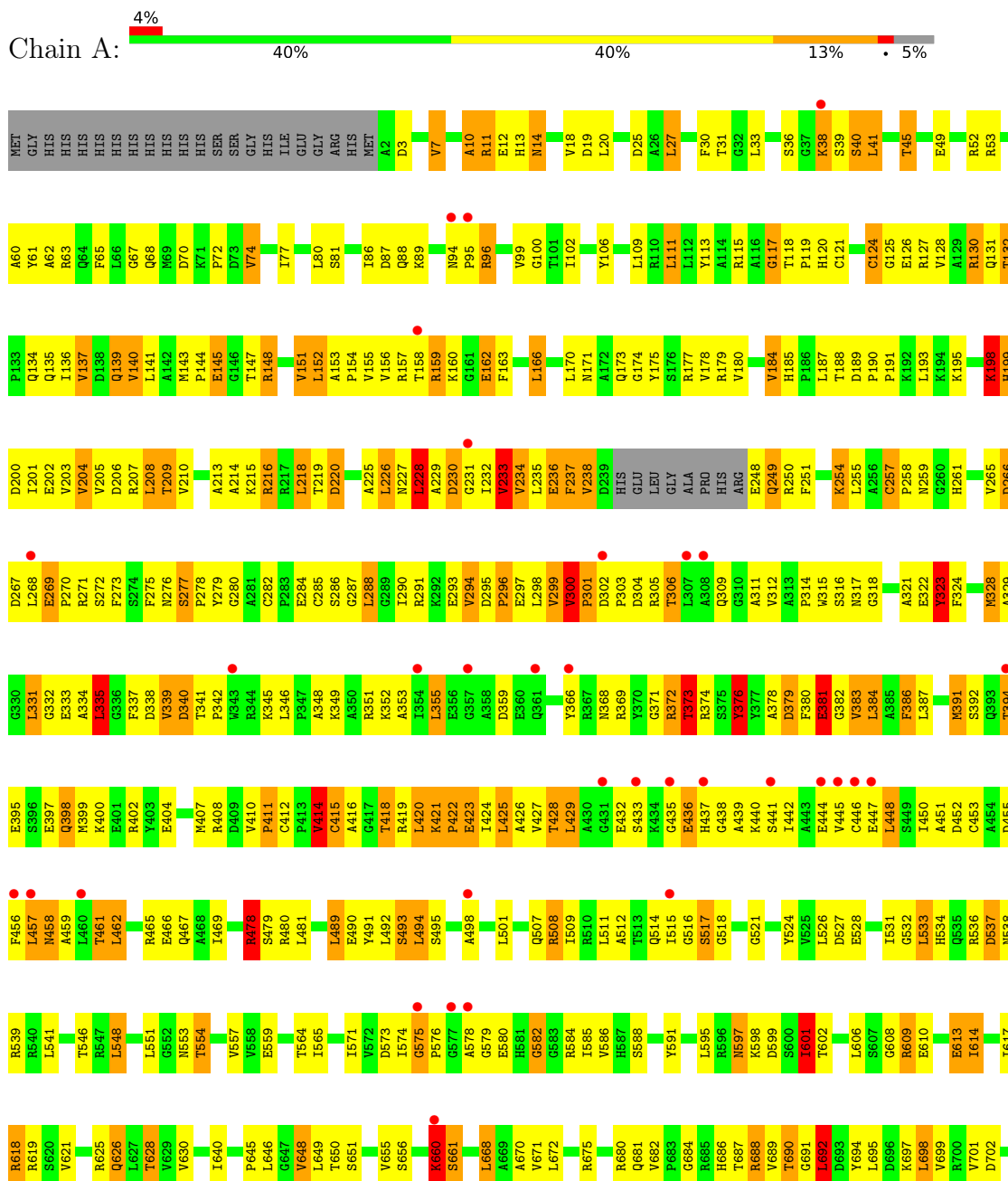
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

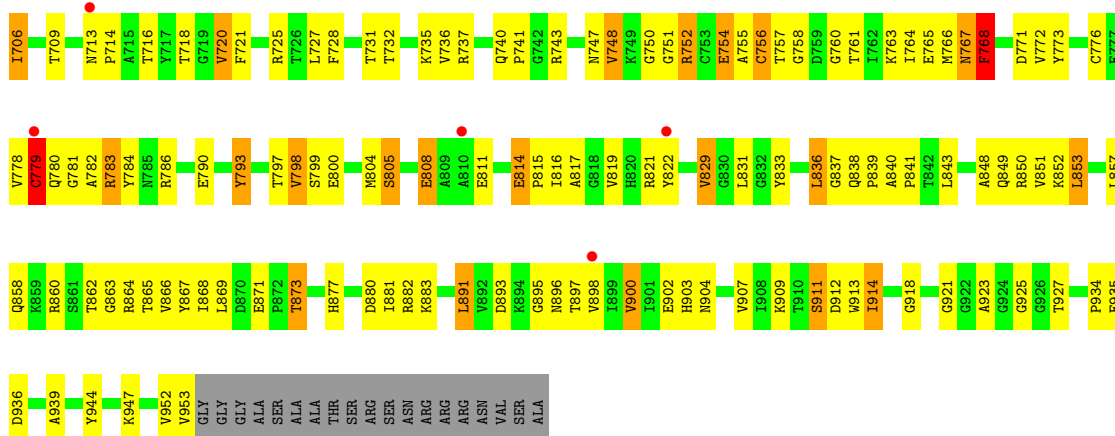
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total 3	Zn 3	0	0
2	B	3	Total 3	Zn 3	0	0
2	C	3	Total 3	Zn 3	0	0
2	D	3	Total 3	Zn 3	0	0
2	E	2	Total 2	Zn 2	0	0

3 Residue-property plots

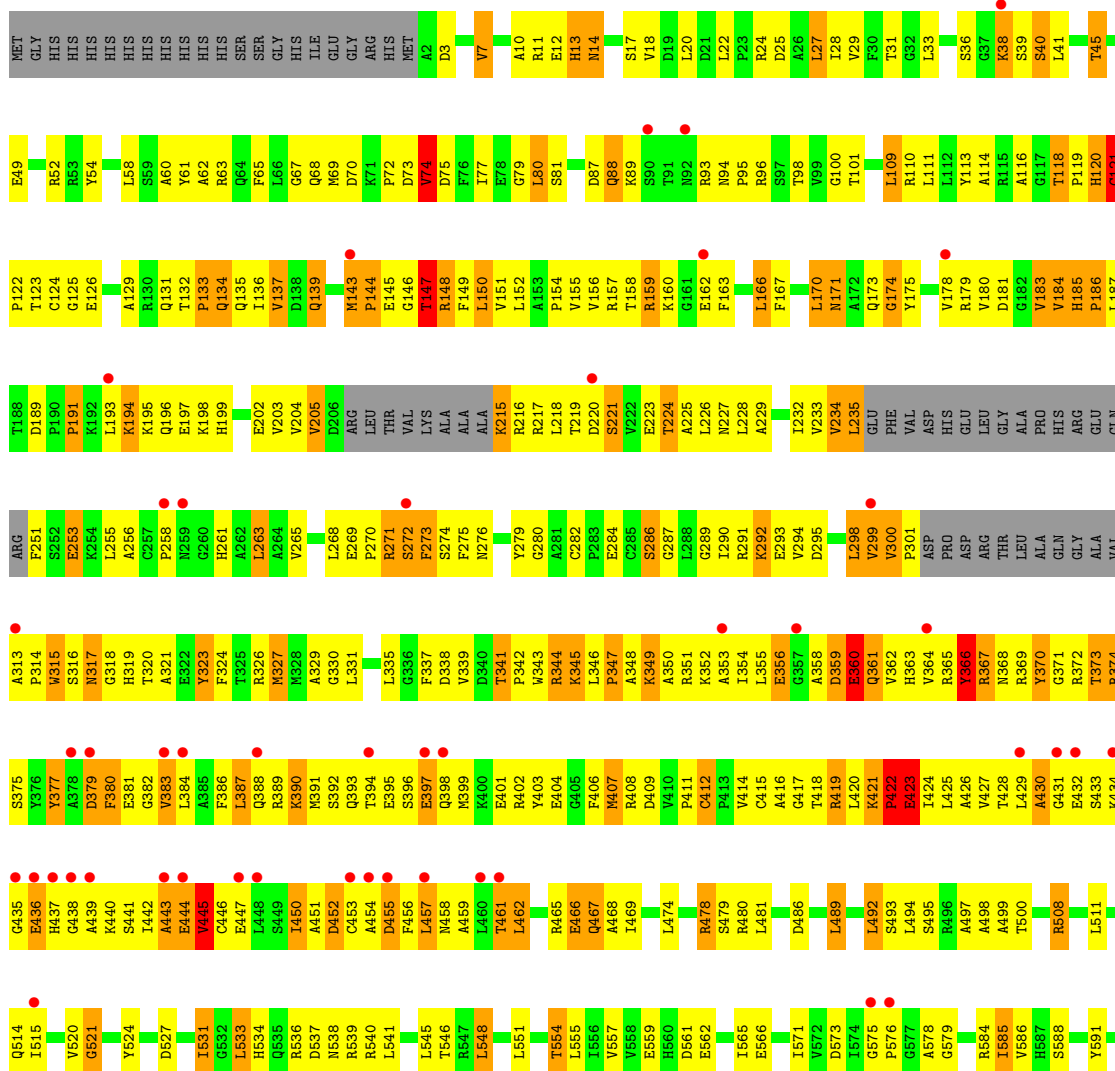
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

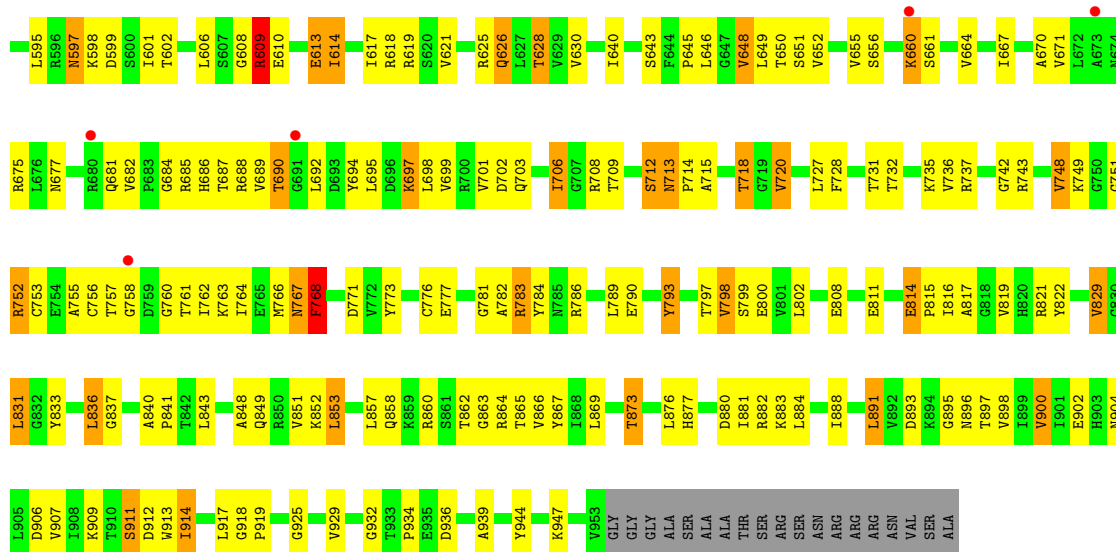
• Molecule 1: UVRABC SYSTEM PROTEIN A



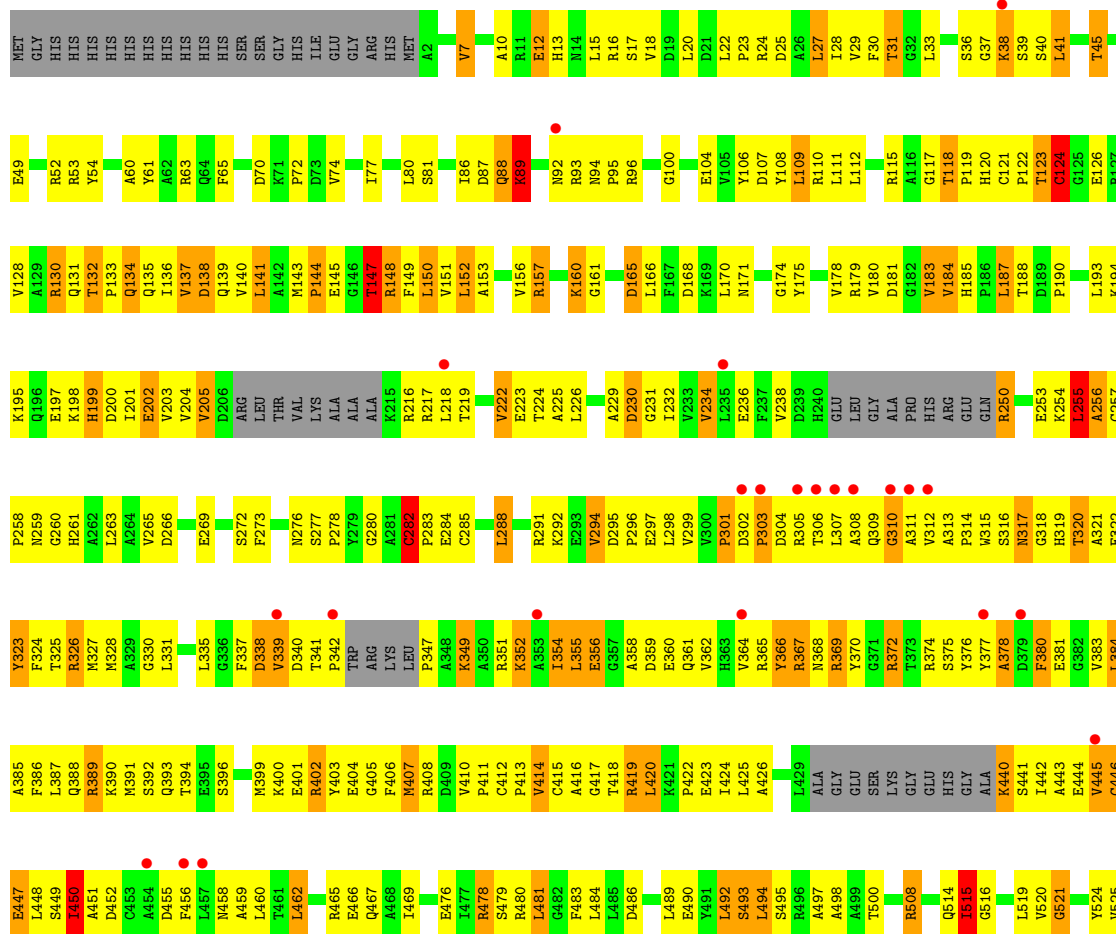


• Molecule 1: UVRABC SYSTEM PROTEIN A

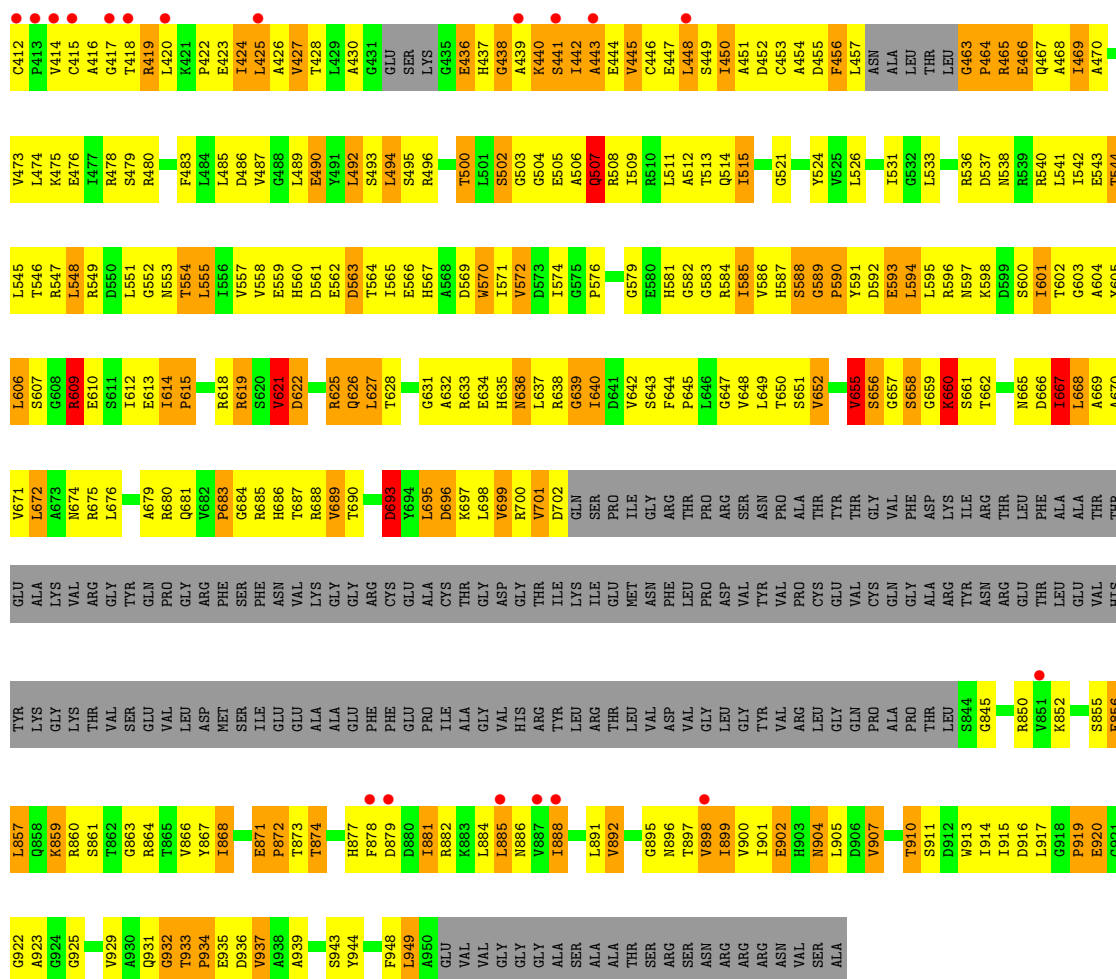




• Molecule 1: UVRABC SYSTEM PROTEIN A







4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	258.23Å 258.23Å 204.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.40 30.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-3.40) 98.3 (30.00-3.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 3.41Å)	Xtriage
Refinement program	REFMAC 5.5.0044	Depositor
R, R_{free}	0.273 , 0.324 0.268 , 0.323	Depositor DCC
R_{free} test set	1067 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å ²)	83.7	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 62.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.034 for -h,-k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	39998	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.18% 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: ZN

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	0.92	11/7394 (0.1%)	1.27	80/10021 (0.8%)
1	B	0.89	7/7190 (0.1%)	1.23	63/9741 (0.6%)
1	C	0.87	3/6945 (0.0%)	1.24	58/9406 (0.6%)
1	D	0.97	8/7217 (0.1%)	1.23	53/9779 (0.5%)
1	E	0.90	7/7196 (0.1%)	1.27	66/9753 (0.7%)
1	F	0.89	3/4721 (0.1%)	1.34	55/6385 (0.9%)
All	All	0.91	39/40663 (0.1%)	1.26	375/55085 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	1
1	C	0	6
1	D	0	4
1	E	0	4
1	F	0	6
All	All	0	27

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	126	GLU	C-N	-19.18	1.07	1.33
1	A	415	CYS	C-N	18.98	1.59	1.33
1	F	11	ARG	C-N	16.47	1.56	1.33
1	D	124	CYS	C-N	16.23	1.56	1.33
1	D	123	THR	C-N	15.40	1.53	1.33
1	B	261	HIS	C-N	14.87	1.53	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	11	ARG	C-N	-14.10	1.15	1.33
1	B	412	CYS	C-N	11.31	1.46	1.34
1	D	256	ALA	C-N	-9.87	1.02	1.33
1	D	260	GLY	C-N	-9.80	1.19	1.33
1	A	411	PRO	C-N	-9.46	1.11	1.33
1	B	273	PHE	C-N	8.76	1.45	1.33
1	C	285	CYS	C-N	-8.71	1.21	1.33
1	A	414	VAL	C-N	-8.39	1.21	1.33
1	B	120	HIS	C-N	-8.36	1.07	1.33
1	F	341	THR	CA-CB	8.35	1.66	1.53
1	A	778	VAL	C-N	-7.78	1.23	1.33
1	A	461	THR	CA-CB	7.50	1.64	1.53
1	B	461	THR	CA-CB	7.34	1.63	1.53
1	A	779	CYS	C-N	7.24	1.44	1.33
1	C	190	PRO	CA-C	6.89	1.58	1.52
1	C	233	VAL	CA-C	6.19	1.60	1.52
1	D	525	VAL	CA-CB	-6.03	1.46	1.53
1	B	445	VAL	CA-CB	5.82	1.62	1.54
1	D	205	VAL	CA-CB	5.67	1.61	1.54
1	E	130	ARG	N-CA	5.61	1.53	1.45
1	B	422	PRO	CA-C	5.57	1.60	1.52
1	F	36	SER	N-CA	5.56	1.53	1.46
1	E	233	VAL	CA-C	5.55	1.57	1.52
1	A	660	LYS	CE-NZ	-5.48	1.32	1.49
1	E	238	VAL	CA-CB	5.38	1.60	1.54
1	D	23	PRO	CA-C	-5.29	1.47	1.52
1	A	306	THR	CA-CB	5.24	1.61	1.53
1	E	261	HIS	CA-C	5.20	1.59	1.52
1	A	660	LYS	CG-CD	5.11	1.67	1.52
1	A	238	VAL	CA-C	5.09	1.57	1.52
1	E	150	LEU	CA-C	5.04	1.57	1.52
1	E	234	VAL	CA-C	5.03	1.59	1.52
1	E	397	GLU	CA-C	5.02	1.59	1.52

All (375) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	443	ALA	N-CA-C	19.10	132.23	111.03
1	F	622	ASP	N-CA-C	16.32	132.88	109.71
1	B	261	HIS	O-C-N	16.18	141.23	123.11
1	F	11	ARG	CA-C-N	14.47	149.19	121.54
1	F	11	ARG	C-N-CA	14.47	149.19	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	147	THR	N-CA-C	14.43	141.53	110.80
1	C	767	ASN	N-CA-C	14.35	126.64	111.14
1	E	767	ASN	N-CA-C	13.94	126.19	111.14
1	C	285	CYS	CA-C-N	-13.85	101.30	123.05
1	C	285	CYS	C-N-CA	-13.85	101.30	123.05
1	E	151	VAL	N-CA-C	13.68	137.79	109.34
1	D	124	CYS	N-CA-C	13.65	128.28	112.72
1	C	456	PHE	N-CA-C	13.60	125.82	111.14
1	F	443	ALA	N-CA-C	12.83	125.34	111.36
1	C	285	CYS	O-C-N	12.76	139.14	122.42
1	A	421	LYS	CA-C-N	12.43	135.38	119.84
1	A	421	LYS	C-N-CA	12.43	135.38	119.84
1	E	307	LEU	CB-CA-C	-12.40	86.66	110.35
1	A	374	ARG	N-CA-CB	12.24	125.46	110.53
1	F	58	LEU	N-CA-C	12.11	124.03	111.07
1	F	11	ARG	O-C-N	-11.83	109.02	123.33
1	A	14	ASN	N-CA-C	-11.76	97.13	112.41
1	B	261	HIS	CA-C-N	-11.58	104.43	120.87
1	B	261	HIS	C-N-CA	-11.58	104.43	120.87
1	E	282	CYS	O-C-N	11.46	130.78	121.38
1	C	130	ARG	N-CA-C	11.22	134.71	110.80
1	A	373	THR	N-CA-C	11.15	134.56	110.80
1	C	190	PRO	N-CA-C	11.13	124.28	110.70
1	A	415	CYS	O-C-N	11.03	136.13	122.34
1	B	361	GLN	N-CA-C	-10.94	92.78	109.41
1	D	380	PHE	N-CA-CB	-10.73	94.72	110.17
1	F	463	GLY	CA-C-N	10.70	133.22	119.84
1	F	463	GLY	C-N-CA	10.70	133.22	119.84
1	E	415	CYS	O-C-N	-10.61	111.06	122.09
1	E	348	ALA	N-CA-C	-10.60	99.87	113.12
1	C	190	PRO	CA-C-N	10.26	132.66	119.84
1	C	190	PRO	C-N-CA	10.26	132.66	119.84
1	F	696	ASP	N-CA-C	10.25	122.21	111.14
1	D	126	GLU	O-C-N	-10.15	111.31	123.19
1	C	421	LYS	CA-C-N	10.14	132.52	119.84
1	C	421	LYS	C-N-CA	10.14	132.52	119.84
1	E	317	ASN	N-CA-C	9.74	127.09	107.41
1	F	621	VAL	CB-CA-C	-9.67	95.43	111.29
1	A	89	LYS	N-CA-C	9.64	121.87	111.36
1	E	354	ILE	CB-CA-C	-9.62	95.51	111.29
1	C	395	GLU	N-CA-C	-9.62	100.11	112.23
1	D	393	GLN	N-CA-C	9.41	121.23	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	412	CYS	N-CA-C	-9.37	98.82	109.60
1	B	229	ALA	N-CA-C	-9.31	97.37	110.50
1	C	449	SER	N-CA-C	9.31	130.63	110.80
1	E	265	VAL	N-CA-C	9.28	121.48	108.12
1	B	444	GLU	N-CA-C	-9.23	101.92	113.55
1	E	234	VAL	N-CA-C	8.99	120.84	107.80
1	D	126	GLU	CA-C-N	8.96	134.00	120.82
1	D	126	GLU	C-N-CA	8.96	134.00	120.82
1	F	456	PHE	N-CA-C	-8.87	101.30	110.97
1	E	130	ARG	N-CA-C	8.82	121.26	110.41
1	E	355	LEU	N-CA-CB	8.66	122.71	110.67
1	D	132	THR	CA-C-N	8.66	128.24	119.24
1	D	132	THR	C-N-CA	8.66	128.24	119.24
1	B	374	ARG	CB-CA-C	8.51	127.35	110.42
1	A	11	ARG	O-C-N	-8.50	110.61	122.26
1	E	151	VAL	CB-CA-C	-8.46	97.42	111.29
1	B	366	TYR	N-CA-C	8.46	122.67	108.13
1	F	675	ARG	N-CA-C	8.38	120.20	111.14
1	A	767	ASN	N-CA-C	8.36	121.60	111.40
1	B	157	ARG	N-CA-C	8.33	122.54	112.38
1	D	13	HIS	N-CA-CB	8.27	124.47	110.49
1	A	411	PRO	O-C-N	-8.27	112.76	123.01
1	A	12	GLU	O-C-N	-8.26	113.37	122.12
1	B	360	GLU	CB-CA-C	8.26	126.86	110.42
1	E	118	THR	CA-C-N	8.07	128.02	120.03
1	E	118	THR	C-N-CA	8.07	128.02	120.03
1	E	13	HIS	N-CA-CB	8.04	124.08	110.49
1	E	459	ALA	N-CA-C	8.04	119.67	111.07
1	A	458	ASN	N-CA-C	8.02	127.88	110.80
1	F	589	GLY	CA-C-N	7.90	129.72	119.84
1	F	589	GLY	C-N-CA	7.90	129.72	119.84
1	E	233	VAL	N-CA-C	7.89	114.65	106.21
1	C	354	ILE	N-CA-C	-7.84	105.68	113.20
1	E	152	LEU	N-CA-C	7.82	120.42	110.33
1	A	754	GLU	N-CA-C	7.74	122.57	113.20
1	A	478	ARG	NE-CZ-NH2	-7.74	112.23	119.20
1	A	436	GLU	N-CA-CB	-7.74	98.66	110.04
1	B	317	ASN	N-CA-C	7.72	127.25	110.80
1	E	57	SER	N-CA-C	7.71	119.76	111.36
1	E	150	LEU	N-CA-C	-7.69	101.60	112.13
1	B	40	SER	N-CA-C	-7.62	102.97	111.28
1	C	232	ILE	N-CA-C	7.61	120.15	106.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	444	GLU	N-CA-C	7.52	122.91	113.43
1	A	381	GLU	N-CA-C	-7.52	98.33	109.15
1	E	341	THR	CA-C-N	7.43	127.48	119.90
1	E	341	THR	C-N-CA	7.43	127.48	119.90
1	A	296	PRO	N-CA-C	-7.43	104.25	114.80
1	E	309	GLN	N-CA-C	-7.42	102.48	113.61
1	A	478	ARG	NE-CZ-NH1	7.33	128.83	121.50
1	B	123	THR	N-CA-C	7.32	119.33	111.36
1	F	357	GLY	N-CA-C	-7.31	100.71	110.58
1	D	148	ARG	N-CA-C	7.26	121.77	112.34
1	A	779	CYS	O-C-N	-7.25	112.06	122.36
1	A	768	PHE	N-CA-C	-7.21	103.09	112.68
1	B	768	PHE	N-CA-C	-7.19	103.11	112.68
1	E	120	HIS	N-CA-C	-7.18	98.73	108.86
1	A	392	SER	N-CA-C	-7.17	103.40	111.07
1	C	752	ARG	CB-CG-CD	7.14	127.72	111.30
1	C	387	LEU	N-CA-C	-7.11	104.72	113.19
1	C	191	PRO	N-CA-C	7.02	126.92	112.47
1	C	89	LYS	N-CA-C	7.01	118.92	111.28
1	B	377	TYR	N-CA-C	7.01	121.09	108.69
1	B	341	THR	CA-C-N	7.00	128.59	119.84
1	B	341	THR	C-N-CA	7.00	128.59	119.84
1	D	12	GLU	N-CA-C	7.00	125.72	110.80
1	D	89	LYS	N-CA-C	6.98	125.67	110.80
1	E	256	ALA	N-CA-C	6.94	125.58	110.80
1	E	460	LEU	N-CA-C	-6.94	103.93	112.88
1	B	423	GLU	N-CA-C	-6.93	103.33	111.03
1	B	394	THR	N-CA-C	6.93	118.83	111.28
1	A	688	ARG	N-CA-C	6.93	117.01	107.73
1	E	688	ARG	N-CA-C	6.91	117.00	107.73
1	B	193	LEU	CB-CA-C	-6.88	95.74	109.35
1	E	423	GLU	N-CA-C	-6.87	103.48	110.97
1	A	162	GLU	CA-C-N	-6.87	112.93	123.17
1	A	162	GLU	C-N-CA	-6.87	112.93	123.17
1	C	768	PHE	N-CA-C	-6.86	104.91	113.55
1	B	443	ALA	CB-CA-C	-6.83	100.37	110.95
1	A	118	THR	CA-C-N	6.83	127.00	120.31
1	A	118	THR	C-N-CA	6.83	127.00	120.31
1	A	478	ARG	CD-NE-CZ	6.80	133.92	124.40
1	B	370	TYR	N-CA-C	-6.77	96.01	107.99
1	C	286	SER	N-CA-C	6.76	121.11	112.86
1	C	440	LYS	N-CA-C	6.73	118.70	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	159	ARG	N-CA-C	6.73	119.63	110.55
1	B	767	ASN	N-CA-C	6.72	119.92	111.24
1	F	3	ASP	N-CA-C	6.71	119.87	107.99
1	A	3	ASP	N-CA-C	-6.68	103.16	112.25
1	F	881	ILE	N-CA-C	6.67	118.22	110.62
1	A	10	ALA	N-CA-C	-6.65	98.41	109.46
1	A	752	ARG	NE-CZ-NH2	-6.65	113.21	119.20
1	E	354	ILE	N-CA-C	6.65	123.18	109.34
1	F	932	GLY	N-CA-C	6.64	119.59	110.56
1	B	688	ARG	N-CA-C	6.63	116.61	107.73
1	D	23	PRO	CB-CA-C	-6.62	106.31	111.87
1	A	228	LEU	N-CA-C	-6.61	105.35	113.41
1	A	779	CYS	CA-C-N	6.59	134.08	123.93
1	A	779	CYS	C-N-CA	6.59	134.08	123.93
1	A	143	MET	CA-C-N	6.58	128.06	119.84
1	A	143	MET	C-N-CA	6.58	128.06	119.84
1	D	688	ARG	N-CA-C	6.57	116.53	107.73
1	E	414	VAL	CA-C-N	6.56	129.40	120.54
1	E	414	VAL	C-N-CA	6.56	129.40	120.54
1	F	36	SER	N-CA-C	6.56	120.38	112.38
1	E	282	CYS	N-CA-C	-6.54	101.52	109.57
1	E	300	VAL	CB-CA-C	6.54	116.48	110.13
1	B	360	GLU	N-CA-C	-6.53	96.89	110.80
1	F	383	VAL	N-CA-C	6.53	122.92	109.34
1	C	40	SER	N-CA-C	-6.52	104.17	111.28
1	C	219	THR	N-CA-C	-6.52	105.48	113.50
1	A	754	GLU	CB-CA-C	-6.51	97.73	110.11
1	F	695	LEU	N-CA-C	6.49	119.88	110.28
1	B	421	LYS	CA-C-N	-6.43	111.80	119.84
1	B	421	LYS	C-N-CA	-6.43	111.80	119.84
1	D	414	VAL	N-CA-C	6.42	116.91	110.23
1	D	767	ASN	N-CA-C	6.41	120.97	111.04
1	C	423	GLU	N-CA-C	-6.41	104.38	111.36
1	A	414	VAL	CA-C-N	6.40	133.10	122.54
1	A	414	VAL	C-N-CA	6.40	133.10	122.54
1	E	454	ALA	N-CA-C	-6.40	105.51	113.38
1	B	194	LYS	N-CA-C	6.40	118.36	109.15
1	D	420	LEU	N-CA-C	6.39	119.94	109.72
1	D	126	GLU	N-CA-C	6.38	120.23	109.76
1	A	214	ALA	N-CA-C	-6.35	103.85	113.89
1	B	436	GLU	CB-CA-C	-6.35	98.80	110.62
1	F	102	ILE	CB-CA-C	-6.35	103.70	112.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	748	VAL	N-CA-C	6.33	116.98	108.11
1	A	228	LEU	CA-CB-CG	6.32	138.41	116.30
1	A	414	VAL	O-C-N	-6.32	115.33	121.90
1	E	440	LYS	N-CA-C	6.32	119.10	111.40
1	A	372	ARG	N-CA-C	6.29	118.94	111.33
1	B	319	HIS	CB-CA-C	-6.28	100.37	110.79
1	E	12	GLU	N-CA-C	6.25	124.11	110.80
1	E	447	GLU	N-CA-C	-6.24	104.17	110.97
1	A	316	SER	CB-CA-C	-6.23	101.17	111.51
1	C	448	LEU	N-CA-C	-6.21	97.57	110.80
1	E	188	THR	CB-CA-C	-6.21	98.07	110.42
1	F	440	LYS	N-CA-C	6.21	121.18	112.93
1	C	152	LEU	N-CA-C	6.20	119.57	109.59
1	F	35	GLY	CA-C-N	6.19	130.51	120.60
1	F	35	GLY	C-N-CA	6.19	130.51	120.60
1	C	437	HIS	CB-CA-C	-6.19	98.34	110.10
1	A	780	GLN	CA-C-N	-6.15	110.94	120.91
1	A	780	GLN	C-N-CA	-6.15	110.94	120.91
1	E	375	SER	N-CA-C	6.15	119.31	107.44
1	C	449	SER	N-CA-CB	-6.14	100.11	110.49
1	D	256	ALA	N-CA-C	6.13	116.53	107.88
1	E	355	LEU	N-CA-C	-6.13	106.12	113.97
1	B	436	GLU	N-CA-CB	-6.13	102.06	111.56
1	A	778	VAL	O-C-N	6.11	128.70	121.80
1	C	269	GLU	CA-C-N	6.09	127.46	119.84
1	C	269	GLU	C-N-CA	6.09	127.46	119.84
1	B	193	LEU	N-CA-C	6.06	119.36	109.24
1	C	682	VAL	CA-C-N	-6.05	113.74	119.85
1	C	682	VAL	C-N-CA	-6.05	113.74	119.85
1	A	323	TYR	N-CA-C	6.03	117.85	111.28
1	E	131	GLN	N-CA-C	6.03	116.20	108.24
1	B	748	VAL	N-CA-C	6.03	116.55	108.11
1	E	196	GLN	N-CA-C	6.03	117.54	110.97
1	C	351	ARG	N-CA-C	6.02	116.91	108.00
1	E	89	LYS	N-CA-C	6.01	117.83	111.28
1	A	316	SER	N-CA-C	6.00	120.45	107.49
1	A	376	TYR	N-CA-C	5.99	123.56	110.80
1	C	628	THR	N-CA-C	5.98	118.15	108.34
1	F	419	ARG	N-CA-C	5.97	123.52	110.80
1	A	257	CYS	N-CA-C	-5.96	102.25	109.83
1	F	660	LYS	N-CA-C	5.96	118.27	111.11
1	B	121	CYS	CB-CA-C	5.96	118.84	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	67	GLY	N-CA-C	-5.96	105.58	112.73
1	F	345	LYS	N-CA-C	-5.94	106.12	113.19
1	F	94	ASN	CA-C-N	5.94	125.64	119.64
1	F	94	ASN	C-N-CA	5.94	125.64	119.64
1	A	755	ALA	N-CA-C	-5.94	105.69	113.12
1	F	438	GLY	N-CA-C	-5.94	105.60	112.73
1	D	147	THR	CB-CA-C	-5.91	98.66	110.42
1	D	396	SER	N-CA-C	5.90	123.36	110.80
1	D	447	GLU	N-CA-C	-5.89	104.04	111.11
1	A	805	SER	N-CA-C	-5.88	102.21	110.50
1	E	453	CYS	CB-CA-C	5.87	120.21	110.81
1	B	455	ASP	N-CA-C	5.87	119.98	112.12
1	D	258	PRO	CA-C-N	-5.86	113.10	122.66
1	D	258	PRO	C-N-CA	-5.86	113.10	122.66
1	A	411	PRO	CA-C-N	5.84	132.04	120.94
1	A	411	PRO	C-N-CA	5.84	132.04	120.94
1	C	430	ALA	N-CA-C	5.84	118.28	108.23
1	E	682	VAL	CA-C-N	-5.84	113.95	120.14
1	E	682	VAL	C-N-CA	-5.84	113.95	120.14
1	B	218	LEU	N-CA-C	-5.84	105.99	113.23
1	A	767	ASN	CB-CA-C	-5.83	100.99	110.79
1	A	628	THR	N-CA-C	5.83	117.89	108.34
1	B	14	ASN	N-CA-C	5.82	117.63	111.28
1	B	173	GLN	N-CA-C	-5.82	104.35	113.02
1	C	392	SER	N-CA-C	-5.79	105.41	112.88
1	C	131	GLN	N-CA-C	5.79	117.73	108.41
1	B	234	VAL	N-CA-C	5.78	121.37	109.34
1	D	366	TYR	N-CA-C	5.78	118.47	109.52
1	F	317	ASN	N-CA-C	5.78	118.52	108.76
1	A	748	VAL	N-CA-CB	-5.76	103.11	111.52
1	D	748	VAL	N-CA-C	5.75	116.16	108.11
1	A	373	THR	CB-CA-C	-5.75	98.98	110.42
1	F	667	ILE	CB-CA-C	5.75	120.71	111.29
1	B	3	ASP	N-CA-C	-5.74	103.68	111.55
1	F	475	LYS	N-CA-C	-5.72	104.73	110.97
1	D	450	ILE	CB-CA-C	-5.72	104.42	112.14
1	C	318	GLY	N-CA-C	-5.72	105.93	112.79
1	D	805	SER	N-CA-C	-5.72	102.57	110.35
1	C	420	LEU	N-CA-C	5.71	118.54	109.81
1	D	282	CYS	CA-C-N	5.70	125.37	119.56
1	D	282	CYS	C-N-CA	5.70	125.37	119.56
1	D	89	LYS	CB-CA-C	-5.69	99.09	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	397	GLU	N-CA-C	5.69	116.59	108.74
1	A	661	SER	N-CA-C	5.69	117.56	111.36
1	E	427	VAL	N-CA-C	-5.68	99.94	108.12
1	D	682	VAL	CA-C-N	-5.68	114.12	120.14
1	D	682	VAL	C-N-CA	-5.68	114.12	120.14
1	B	89	LYS	N-CA-C	5.67	117.46	111.28
1	B	379	ASP	N-CA-C	5.67	118.64	109.40
1	F	622	ASP	N-CA-CB	-5.67	97.71	109.28
1	A	420	LEU	N-CA-C	5.66	118.70	109.24
1	C	321	ALA	N-CA-C	5.64	117.11	111.07
1	D	589	GLY	CA-C-N	5.64	125.96	119.92
1	D	589	GLY	C-N-CA	5.64	125.96	119.92
1	B	143	MET	C-N-CD	-5.64	101.89	125.00
1	A	601	ILE	N-CA-C	-5.63	105.03	110.72
1	B	121	CYS	N-CA-C	-5.63	102.81	110.36
1	D	521	GLY	N-CA-C	-5.63	107.42	115.64
1	D	393	GLN	CB-CA-C	-5.63	102.29	110.96
1	B	13	HIS	CB-CA-C	-5.62	110.11	116.63
1	C	748	VAL	N-CA-C	5.62	115.97	108.11
1	D	124	CYS	N-CA-CB	-5.61	102.34	110.70
1	F	406	PHE	N-CA-C	-5.61	106.48	113.55
1	C	229	ALA	N-CA-C	-5.61	106.44	113.28
1	A	384	LEU	N-CA-C	5.59	117.07	110.97
1	A	752	ARG	NE-CZ-NH1	5.59	127.09	121.50
1	B	272	SER	N-CA-C	-5.59	106.81	113.97
1	A	752	ARG	CD-NE-CZ	5.58	132.21	124.40
1	B	253	GLU	N-CA-C	5.58	117.36	111.28
1	F	884	LEU	N-CA-C	-5.57	105.78	113.18
1	B	682	VAL	CA-C-N	-5.53	114.28	120.14
1	B	682	VAL	C-N-CA	-5.53	114.28	120.14
1	F	94	ASN	N-CA-C	5.52	117.55	109.71
1	A	692	LEU	CA-CB-CG	5.51	135.60	116.30
1	F	859	LYS	N-CA-C	5.50	117.36	111.36
1	F	658	SER	N-CA-C	-5.50	106.77	112.93
1	E	333	GLU	N-CA-C	-5.49	104.22	111.96
1	C	559	GLU	N-CA-C	5.46	117.37	109.07
1	A	40	SER	N-CA-C	-5.46	105.33	111.28
1	A	394	THR	N-CA-C	5.45	117.22	111.28
1	C	574	ILE	CA-C-N	5.45	130.43	121.87
1	C	574	ILE	C-N-CA	5.45	130.43	121.87
1	A	13	HIS	CA-C-N	-5.44	113.95	122.49
1	A	13	HIS	C-N-CA	-5.44	113.95	122.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	423	GLU	N-CA-C	-5.44	105.43	111.36
1	C	123	THR	N-CA-C	5.44	117.01	111.14
1	E	74	VAL	CB-CA-C	-5.44	103.73	111.34
1	D	184	VAL	N-CA-C	5.43	115.72	108.11
1	E	628	THR	N-CA-C	5.43	117.25	108.34
1	F	97	SER	N-CA-C	5.43	117.81	109.07
1	A	300	VAL	N-CA-CB	5.43	118.81	111.21
1	D	446	CYS	CA-C-N	5.42	127.85	120.54
1	D	446	CYS	C-N-CA	5.42	127.85	120.54
1	C	13	HIS	CB-CA-C	-5.41	110.35	116.63
1	A	230	ASP	N-CA-C	5.39	118.88	111.54
1	B	273	PHE	N-CA-C	5.39	119.71	113.18
1	C	688	ARG	N-CA-C	5.39	114.95	107.73
1	D	118	THR	CA-C-N	5.39	126.86	120.23
1	D	118	THR	C-N-CA	5.39	126.86	120.23
1	E	275	PHE	N-CA-C	-5.38	106.68	113.20
1	E	398	GLN	N-CA-C	-5.38	106.21	112.89
1	B	319	HIS	N-CA-C	-5.38	105.42	111.28
1	D	258	PRO	N-CA-C	-5.36	106.08	113.53
1	F	311	ALA	N-CA-C	5.36	122.21	110.80
1	E	132	THR	CA-C-N	5.35	124.54	118.97
1	E	132	THR	C-N-CA	5.35	124.54	118.97
1	C	14	ASN	CA-C-N	5.35	131.76	121.54
1	C	14	ASN	C-N-CA	5.35	131.76	121.54
1	D	118	THR	N-CA-C	5.35	118.09	109.15
1	C	169	LYS	N-CA-C	-5.34	106.69	114.12
1	B	274	SER	N-CA-C	-5.34	103.34	110.55
1	E	589	GLY	CA-C-N	5.34	126.51	119.84
1	E	589	GLY	C-N-CA	5.34	126.51	119.84
1	C	445	VAL	N-CA-C	-5.32	98.28	109.34
1	A	233	VAL	CB-CA-C	-5.30	102.75	110.81
1	C	74	VAL	CB-CA-C	-5.30	103.92	111.19
1	F	71	LYS	N-CA-C	-5.30	104.04	110.13
1	E	359	ASP	N-CA-C	5.29	122.07	110.80
1	B	430	ALA	N-CA-C	5.27	117.00	108.41
1	F	14	ASN	N-CA-C	5.23	117.06	111.36
1	C	357	GLY	N-CA-C	5.21	118.78	112.48
1	A	199	HIS	N-CA-C	5.20	117.09	109.24
1	E	356	GLU	N-CA-C	5.19	118.53	110.17
1	B	450	ILE	N-CA-C	5.19	115.91	110.62
1	D	574	ILE	N-CA-C	5.18	116.04	108.53
1	E	364	VAL	N-CA-C	5.18	115.94	108.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	LYS	N-CA-C	-5.17	103.70	110.53
1	F	66	LEU	N-CA-C	5.17	121.89	114.39
1	E	13	HIS	N-CA-C	-5.17	99.79	110.80
1	F	367	ARG	N-CA-C	-5.15	103.73	110.53
1	F	507	GLN	N-CA-C	-5.15	105.74	112.23
1	D	559	GLU	N-CA-C	5.13	116.64	108.79
1	F	341	THR	CA-C-N	-5.13	113.43	119.84
1	F	341	THR	C-N-CA	-5.13	113.43	119.84
1	F	939	ALA	N-CA-C	-5.13	106.18	112.90
1	D	260	GLY	O-C-N	-5.12	116.04	122.70
1	E	313	ALA	CA-C-N	-5.11	113.45	119.84
1	E	313	ALA	C-N-CA	-5.11	113.45	119.84
1	B	74	VAL	CB-CA-C	-5.11	104.19	111.19
1	F	441	SER	N-CA-C	5.10	116.53	110.97
1	A	335	LEU	N-CA-C	-5.09	106.62	114.16
1	B	353	ALA	N-CA-C	-5.09	105.73	111.28
1	B	805	SER	N-CA-C	-5.09	103.43	110.35
1	B	444	GLU	N-CA-CB	5.09	117.78	110.40
1	C	3	ASP	N-CA-C	-5.09	104.58	111.55
1	A	682	VAL	CA-C-N	-5.08	114.76	120.14
1	A	682	VAL	C-N-CA	-5.08	114.76	120.14
1	A	582	GLY	N-CA-C	5.07	119.85	112.55
1	F	609	ARG	N-CA-C	-5.07	105.83	111.36
1	B	143	MET	CA-C-N	5.06	126.17	119.84
1	B	143	MET	C-N-CA	5.06	126.17	119.84
1	D	628	THR	N-CA-C	5.06	116.64	108.34
1	F	38	LYS	N-CA-C	5.05	117.44	111.33
1	D	190	PRO	CA-C-N	-5.04	115.16	120.66
1	D	190	PRO	C-N-CA	-5.04	115.16	120.66
1	E	355	LEU	CA-CB-CG	5.03	133.91	116.30
1	C	574	ILE	N-CA-C	5.03	115.82	108.53
1	D	926	GLY	N-CA-C	-5.02	107.34	115.08
1	B	521	GLY	N-CA-C	-5.01	108.37	115.43
1	A	151	VAL	CB-CA-C	5.00	119.50	111.29

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	ARG	Mainchain
1	A	148	ARG	Sidechain
1	A	213	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	A	373	THR	Peptide
1	A	411	PRO	Mainchain
1	A	779	CYS	Mainchain
1	B	366	TYR	Peptide
1	C	190	PRO	Peptide
1	C	232	ILE	Peptide
1	C	443	ALA	Peptide
1	C	448	LEU	Peptide
1	C	449	SER	Peptide
1	C	575	GLY	Peptide
1	D	124	CYS	Mainchain
1	D	256	ALA	Mainchain
1	D	338	ASP	Peptide
1	D	575	GLY	Peptide
1	E	347	PRO	Peptide
1	E	415	CYS	Mainchain
1	E	452	ASP	Peptide
1	E	575	GLY	Peptide
1	F	346	LEU	Peptide
1	F	35	GLY	Peptide
1	F	380	PHE	Peptide
1	F	382	GLY	Peptide
1	F	396	SER	Peptide
1	F	621	VAL	Peptide

5.2 Too-close contacts [i](#)

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	7267	0	7282	649	1
1	B	7067	0	7080	721	3
1	C	6832	0	6855	576	0
1	D	7095	0	7101	606	0
1	E	7073	0	7081	633	4
1	F	4650	0	4667	591	1
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3	0	0	0	0
2	E	2	0	0	0	0
All	All	39998	0	40066	3710	5

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 46.

All (3710) 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:442:ILE:HA	1:E:495:SER:CB	1.23	1.62
1:B:299:VAL:HG23	1:B:313:ALA:CB	1.23	1.58
1:D:305:ARG:HA	1:D:311:ALA:CB	1.28	1.57
1:B:299:VAL:CG2	1:B:313:ALA:HB2	1.29	1.56
1:F:412:CYS:SG	1:F:414:VAL:HG22	1.47	1.52
1:B:295:ASP:HB3	1:B:298:LEU:CD2	1.38	1.51
1:D:305:ARG:CD	1:D:311:ALA:HB1	1.06	1.50
1:E:88:GLN:HE22	1:E:531:ILE:CG2	1.22	1.50
1:D:305:ARG:HD2	1:D:311:ALA:CB	1.01	1.49
1:E:442:ILE:CA	1:E:495:SER:HB3	1.37	1.48
1:D:305:ARG:NH1	1:D:312:VAL:CG2	1.76	1.45
1:D:305:ARG:CA	1:D:311:ALA:HB2	1.47	1.41
1:B:576:PRO:HD3	1:B:586:VAL:CG2	1.51	1.39
1:B:515:ILE:CD1	1:B:548:LEU:HG	1.52	1.39
1:B:432:GLU:OE1	1:B:453:CYS:CB	1.69	1.37
1:E:352:LYS:HD2	1:E:356:GLU:CB	1.55	1.36
1:E:412:CYS:HB3	1:E:415:CYS:SG	1.66	1.35
1:F:882:ARG:NH1	1:F:886:ASN:HD21	0.89	1.34
1:B:428:THR:CG2	1:B:435:GLY:O	1.75	1.34
1:F:882:ARG:NH1	1:F:886:ASN:ND2	1.71	1.33
1:D:305:ARG:CA	1:D:311:ALA:CB	2.05	1.32
1:F:882:ARG:HH12	1:F:886:ASN:ND2	1.22	1.32
1:C:388:GLN:HA	1:C:391:MET:SD	1.67	1.32
1:F:695:LEU:CD2	1:F:864:ARG:O	1.78	1.31
1:B:451:ALA:O	1:B:455:ASP:HB2	1.27	1.31
1:C:151:VAL:O	1:C:204:VAL:HG12	1.15	1.30
1:D:305:ARG:NH1	1:D:312:VAL:HG23	0.99	1.29
1:C:441:SER:O	1:C:444:GLU:CG	1.83	1.27
1:D:305:ARG:CG	1:D:311:ALA:HB1	1.65	1.27
1:C:284:GLU:OE2	1:C:291:ARG:NH1	1.66	1.26
1:D:305:ARG:CD	1:D:311:ALA:CB	1.76	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:920:GLU:O	1:B:924:GLY:O	1.53	1.25
1:E:88:GLN:NE2	1:E:531:ILE:HG22	1.53	1.24
1:F:560:HIS:O	1:F:878:PHE:CZ	1.91	1.23
1:B:113:TYR:OH	1:B:436:GLU:O	1.54	1.22
1:A:282:CYS:SG	1:A:415:CYS:HB3	1.80	1.22
1:B:139:GLN:O	1:B:143:MET:HG3	1.38	1.22
1:E:65:PHE:HE2	1:E:767:ASN:ND2	1.38	1.21
1:D:305:ARG:HA	1:D:311:ALA:CA	1.71	1.21
1:B:139:GLN:HG2	1:B:143:MET:CE	1.69	1.21
1:D:301:PRO:C	1:D:303:PRO:HD3	1.63	1.21
1:F:440:LYS:O	1:F:445:VAL:HG23	1.35	1.21
1:D:284:GLU:HG3	1:D:414:VAL:HG21	1.23	1.19
1:E:440:LYS:HD2	1:E:454:ALA:CB	1.72	1.19
1:F:856:GLU:HG2	1:F:867:TYR:OH	1.43	1.19
1:F:412:CYS:SG	1:F:414:VAL:CG2	2.30	1.19
1:A:776:CYS:HB3	1:A:779:CYS:SG	1.83	1.19
1:B:428:THR:HB	1:B:435:GLY:C	1.68	1.19
1:E:440:LYS:O	1:E:444:GLU:HB2	1.04	1.19
1:E:121:CYS:SG	1:E:261:HIS:ND1	2.16	1.18
1:E:88:GLN:NE2	1:E:531:ILE:CG2	2.01	1.18
1:B:109:LEU:HD23	1:B:442:ILE:HD11	1.24	1.17
1:B:139:GLN:HG2	1:B:143:MET:HE3	1.25	1.16
1:A:576:PRO:HD3	1:A:586:VAL:CG2	1.74	1.15
1:E:451:ALA:HB1	1:E:456:PHE:CE1	1.81	1.15
1:B:451:ALA:C	1:B:455:ASP:HB2	1.70	1.14
1:B:109:LEU:CD2	1:B:442:ILE:HD11	1.76	1.14
1:D:183:VAL:CG1	1:D:184:VAL:H	1.54	1.14
1:F:340:ASP:O	1:F:342:PRO:HD3	1.44	1.14
1:C:437:HIS:CD2	1:C:440:LYS:NZ	2.15	1.14
1:E:444:GLU:OE2	1:E:450:ILE:CA	1.95	1.14
1:F:381:GLU:OE1	1:F:381:GLU:HA	1.48	1.14
1:A:508:ARG:HH11	1:A:508:ARG:HG3	1.08	1.13
1:C:356:GLU:HG2	1:C:381:GLU:CB	1.79	1.13
1:B:562:GLU:O	1:B:566:GLU:HG3	1.48	1.13
1:B:183:VAL:HG12	1:B:184:VAL:N	1.55	1.13
1:E:177:ARG:HD3	1:E:184:VAL:HG23	1.30	1.13
1:F:355:LEU:O	1:F:383:VAL:CG1	1.96	1.13
1:B:428:THR:CB	1:B:435:GLY:O	1.96	1.12
1:B:436:GLU:HG3	1:B:440:LYS:CG	1.79	1.12
1:C:11:ARG:NH1	1:C:17:SER:OG	1.80	1.12
1:D:305:ARG:HD3	1:D:311:ALA:HB1	1.26	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:317:ASN:HB3	1:C:321:ALA:CB	1.79	1.12
1:E:54:TYR:O	1:E:57:SER:OG	1.66	1.12
1:F:695:LEU:HD23	1:F:864:ARG:CB	1.80	1.12
1:D:809:ALA:O	1:D:813:PHE:HD1	1.32	1.12
1:F:695:LEU:HD22	1:F:864:ARG:C	1.74	1.12
1:D:508:ARG:HH11	1:D:508:ARG:HG3	1.15	1.12
1:E:442:ILE:O	1:E:495:SER:OG	1.65	1.12
1:E:444:GLU:OE2	1:E:450:ILE:HA	1.46	1.12
1:F:332:GLY:HA2	1:F:338:ASP:HB3	1.13	1.11
1:A:425:LEU:HA	1:A:437:HIS:CE1	1.83	1.11
1:A:315:TRP:HE1	1:A:387:LEU:HD22	1.13	1.11
1:B:273:PHE:HB3	1:B:437:HIS:NE2	1.65	1.11
1:C:441:SER:O	1:C:444:GLU:HG2	1.46	1.11
1:A:342:PRO:HD2	1:A:345:LYS:HD3	1.33	1.10
1:B:143:MET:HB3	1:B:144:PRO:CD	1.79	1.10
1:A:300:VAL:HG13	1:A:303:PRO:HD2	1.27	1.10
1:A:425:LEU:HA	1:A:437:HIS:ND1	1.67	1.10
1:B:183:VAL:CG1	1:B:184:VAL:H	1.56	1.10
1:C:425:LEU:CD2	1:C:439:ALA:HB2	1.82	1.10
1:C:430:ALA:CB	1:C:461:THR:HG21	1.82	1.10
1:E:65:PHE:CE2	1:E:767:ASN:ND2	2.19	1.10
1:E:440:LYS:O	1:E:444:GLU:CB	1.99	1.10
1:E:315:TRP:HE1	1:E:387:LEU:HD13	1.05	1.10
1:F:576:PRO:O	1:F:582:GLY:HA3	1.49	1.10
1:B:508:ARG:HH11	1:B:508:ARG:HG3	1.17	1.09
1:A:442:ILE:HG22	1:A:495:SER:CB	1.81	1.09
1:B:295:ASP:HB3	1:B:298:LEU:HD21	1.27	1.09
1:D:312:VAL:O	1:D:316:SER:OG	1.68	1.09
1:C:442:ILE:HG22	1:C:495:SER:HB3	1.32	1.09
1:A:317:ASN:H	1:A:321:ALA:HB2	1.06	1.09
1:B:428:THR:HB	1:B:435:GLY:O	1.53	1.09
1:C:284:GLU:CG	1:C:291:ARG:NH1	2.16	1.09
1:B:295:ASP:CB	1:B:298:LEU:CD2	2.29	1.08
1:F:345:LYS:HB2	1:F:347:PRO:HG3	1.32	1.08
1:B:576:PRO:HD3	1:B:586:VAL:HG23	1.34	1.08
1:D:448:LEU:HD11	1:D:490:GLU:HG2	1.25	1.08
1:B:215:LYS:HE2	1:B:215:LYS:HA	1.13	1.08
1:B:323:TYR:HE1	1:B:327:MET:HG3	1.15	1.08
1:A:335:LEU:HD21	1:A:352:LYS:HE3	1.12	1.08
1:C:356:GLU:HG2	1:C:381:GLU:HB3	1.08	1.08
1:E:352:LYS:HD2	1:E:356:GLU:HB2	1.16	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:368:ASN:HD21	1:E:372:ARG:HB3	0.94	1.07
1:F:381:GLU:HB3	1:F:383:VAL:HG23	1.29	1.07
1:A:20:LEU:HD21	1:A:585:ILE:HG12	1.23	1.07
1:C:441:SER:O	1:C:444:GLU:HG3	1.51	1.07
1:A:295:ASP:HB3	1:A:297:GLU:HG3	1.08	1.07
1:F:437:HIS:O	1:F:442:ILE:HG22	1.52	1.07
1:A:445:VAL:CG1	1:A:923:ALA:HB2	1.85	1.06
1:C:508:ARG:HG3	1:C:508:ARG:HH11	1.19	1.06
1:E:440:LYS:CE	1:E:454:ALA:HB3	1.84	1.06
1:B:432:GLU:CD	1:B:453:CYS:HB3	1.80	1.06
1:E:440:LYS:HE3	1:E:455:ASP:OD1	1.54	1.06
1:D:183:VAL:HG12	1:D:184:VAL:N	1.47	1.06
1:A:299:VAL:HG22	1:A:300:VAL:H	1.14	1.05
1:A:442:ILE:HG22	1:A:495:SER:HB3	1.09	1.05
1:C:317:ASN:HB3	1:C:321:ALA:HB1	1.31	1.05
1:E:368:ASN:HD21	1:E:372:ARG:CB	1.68	1.05
1:B:295:ASP:HB3	1:B:298:LEU:HD23	1.08	1.05
1:E:351:ARG:HH21	1:E:355:LEU:HD21	1.19	1.05
1:B:441:SER:HA	1:B:445:VAL:CG2	1.87	1.05
1:F:355:LEU:C	1:F:383:VAL:HG11	1.82	1.05
1:F:695:LEU:CD2	1:F:864:ARG:HB3	1.86	1.05
1:A:298:LEU:HD12	1:A:298:LEU:O	1.57	1.05
1:D:312:VAL:HG21	1:D:315:TRP:HE3	1.15	1.05
1:E:440:LYS:HD2	1:E:454:ALA:HB3	1.38	1.05
1:F:11:ARG:HG2	1:F:73:ASP:O	1.56	1.04
1:B:171:ASN:HA	1:B:187:LEU:HD21	1.33	1.04
1:B:383:VAL:HG23	1:B:387:LEU:N	1.70	1.04
1:F:652:VAL:HB	1:F:901:ILE:HG22	1.38	1.04
1:B:436:GLU:HG3	1:B:440:LYS:HG3	1.35	1.04
1:F:18:VAL:HG13	1:F:585:ILE:HD11	1.40	1.04
1:B:110:ARG:HA	1:B:437:HIS:HE1	1.17	1.03
1:F:695:LEU:HD23	1:F:864:ARG:HB3	1.06	1.03
1:A:353:ALA:O	1:A:384:LEU:HB3	1.58	1.03
1:C:136:ILE:HG23	1:C:139:GLN:NE2	1.72	1.03
1:F:380:PHE:HB2	1:F:382:GLY:H	1.16	1.03
1:A:335:LEU:CD2	1:A:352:LYS:HE3	1.88	1.03
1:D:152:LEU:O	1:D:234:VAL:HG12	1.59	1.03
1:E:440:LYS:CD	1:E:454:ALA:HB3	1.88	1.02
1:D:341:THR:HB	1:D:342:PRO:HD2	1.37	1.02
1:A:126:GLU:HB2	1:A:258:PRO:HG3	1.42	1.02
1:D:179:ARG:HG2	1:D:183:VAL:O	1.57	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:349:LYS:HA	1:D:352:LYS:HZ2	1.24	1.02
1:B:295:ASP:CB	1:B:298:LEU:HD23	1.90	1.02
1:B:428:THR:HG22	1:B:435:GLY:O	1.55	1.01
1:D:305:ARG:CZ	1:D:312:VAL:HG23	1.90	1.01
1:E:368:ASN:ND2	1:E:372:ARG:HB3	1.75	1.01
1:B:752:ARG:NH2	1:D:165:ASP:OD1	1.93	1.01
1:C:284:GLU:CD	1:C:291:ARG:NH1	2.18	1.01
1:D:305:ARG:CB	1:D:311:ALA:HB1	1.90	1.01
1:F:315:TRP:HE1	1:F:387:LEU:HD22	1.25	1.01
1:A:576:PRO:HD3	1:A:586:VAL:HG23	1.37	1.01
1:B:143:MET:HB3	1:B:144:PRO:HD2	1.36	1.01
1:D:312:VAL:HG12	1:D:315:TRP:H	1.22	1.01
1:B:323:TYR:HE1	1:B:327:MET:CG	1.74	1.01
1:B:515:ILE:HD11	1:B:548:LEU:HG	1.39	1.01
1:E:257:CYS:SG	1:E:261:HIS:ND1	2.34	1.01
1:B:145:GLU:HB2	1:B:148:ARG:CZ	1.90	1.00
1:B:382:GLY:O	1:B:383:VAL:HG13	1.61	1.00
1:E:281:ALA:HB1	1:E:287:GLY:HA3	1.43	1.00
1:F:368:ASN:HB3	1:F:372:ARG:O	1.60	1.00
1:B:438:GLY:HA2	1:B:442:ILE:HG12	1.41	1.00
1:C:388:GLN:HB2	1:C:389:ARG:NH1	1.74	1.00
1:D:349:LYS:HA	1:D:352:LYS:NZ	1.77	1.00
1:C:701:VAL:HG12	1:C:849:GLN:HG2	1.42	1.00
1:B:109:LEU:HD23	1:B:442:ILE:CD1	1.91	1.00
1:F:355:LEU:O	1:F:383:VAL:HG11	1.57	1.00
1:E:383:VAL:HB	1:E:386:PHE:HB2	1.41	1.00
1:C:383:VAL:HB	1:C:386:PHE:HB2	1.42	0.99
1:E:312:VAL:HG11	1:E:384:LEU:CD1	1.91	0.99
1:E:442:ILE:HA	1:E:495:SER:HB2	1.41	0.99
1:B:436:GLU:HG3	1:B:440:LYS:CD	1.91	0.99
1:C:136:ILE:HG23	1:C:139:GLN:HE21	1.22	0.99
1:C:445:VAL:HG12	1:C:448:LEU:H	1.26	0.99
1:F:695:LEU:HD22	1:F:864:ARG:O	0.82	0.99
1:F:75:ASP:O	1:F:76:PHE:O	1.78	0.99
1:B:451:ALA:O	1:B:455:ASP:CB	2.09	0.99
1:B:576:PRO:HD3	1:B:586:VAL:HG21	1.43	0.99
1:B:382:GLY:O	1:B:383:VAL:HG22	1.61	0.99
1:C:356:GLU:CG	1:C:381:GLU:HB3	1.92	0.99
1:E:226:LEU:HD13	1:E:231:GLY:HA2	1.44	0.99
1:A:323:TYR:C	1:A:323:TYR:HD1	1.71	0.98
1:D:349:LYS:H	1:D:349:LYS:HD3	1.26	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:281:ALA:HB1	1:E:287:GLY:CA	1.94	0.98
1:F:8:LYS:HD3	1:F:76:PHE:HD1	1.23	0.98
1:D:701:VAL:HG12	1:D:849:GLN:HG2	1.44	0.98
1:D:147:THR:O	1:D:147:THR:HG22	1.58	0.98
1:F:576:PRO:O	1:F:582:GLY:CA	2.11	0.98
1:B:299:VAL:CG2	1:B:313:ALA:CB	2.09	0.98
1:C:151:VAL:O	1:C:204:VAL:CG1	2.11	0.97
1:B:434:LYS:HD3	1:B:440:LYS:HD3	1.46	0.97
1:C:430:ALA:HB3	1:C:461:THR:HG21	1.00	0.97
1:B:299:VAL:HG23	1:B:313:ALA:CA	1.95	0.97
1:F:315:TRP:NE1	1:F:387:LEU:HD22	1.78	0.97
1:A:102:ILE:HD11	1:A:498:ALA:HB1	1.47	0.97
1:B:354:ILE:HG12	1:B:384:LEU:HD23	1.47	0.97
1:B:185:HIS:CE1	1:B:191:PRO:HB3	1.99	0.97
1:C:31:THR:HG23	1:C:573:ASP:OD1	1.65	0.97
1:E:451:ALA:CB	1:E:456:PHE:CE1	2.26	0.97
1:F:106:TYR:HD1	1:F:442:ILE:HG13	1.27	0.97
1:D:150:LEU:HD22	1:D:236:GLU:HB2	1.47	0.96
1:C:437:HIS:NE2	1:C:440:LYS:NZ	2.12	0.96
1:F:544:THR:HG23	1:F:547:ARG:NH1	1.79	0.96
1:C:222:VAL:O	1:C:226:LEU:HD23	1.66	0.96
1:E:412:CYS:CB	1:E:415:CYS:SG	2.53	0.96
1:D:305:ARG:C	1:D:311:ALA:HB2	1.89	0.96
1:D:326:ARG:HH11	1:D:326:ARG:HG2	1.28	0.96
1:B:131:GLN:NE2	1:B:256:ALA:HB2	1.80	0.96
1:B:139:GLN:O	1:B:143:MET:CG	2.14	0.95
1:E:88:GLN:NE2	1:E:531:ILE:HG21	1.80	0.95
1:B:436:GLU:CG	1:B:440:LYS:HD2	1.96	0.95
1:C:132:THR:HB	1:C:135:GLN:HB2	1.48	0.95
1:B:515:ILE:HD13	1:B:548:LEU:HG	1.48	0.95
1:A:318:GLY:O	1:A:322:GLU:HG3	1.67	0.95
1:E:441:SER:O	1:E:495:SER:N	1.99	0.95
1:D:312:VAL:HG21	1:D:315:TRP:CE3	2.00	0.95
1:E:65:PHE:CE2	1:E:767:ASN:CG	2.43	0.95
1:A:96:ARG:HH21	1:A:288:LEU:HD23	1.32	0.95
1:B:432:GLU:OE1	1:B:453:CYS:HB3	0.77	0.95
1:D:342:PRO:HB2	1:D:347:PRO:HG3	1.45	0.95
1:A:424:ILE:C	1:A:437:HIS:HE1	1.73	0.95
1:D:96:ARG:HH21	1:D:288:LEU:HD23	1.32	0.95
1:A:102:ILE:HD11	1:A:498:ALA:CB	1.97	0.94
1:D:31:THR:HG23	1:D:573:ASP:OD1	1.67	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:357:GLY:HA2	1:F:383:VAL:HB	1.49	0.94
1:B:712:SER:O	1:B:840:ALA:HB2	1.67	0.94
1:C:355:LEU:HA	1:C:383:VAL:HG12	1.49	0.94
1:A:442:ILE:CG2	1:A:495:SER:HB3	1.98	0.94
1:C:425:LEU:HD23	1:C:439:ALA:HB2	1.45	0.94
1:C:430:ALA:HB3	1:C:461:THR:CG2	1.94	0.94
1:A:323:TYR:C	1:A:323:TYR:CD1	2.43	0.94
1:A:295:ASP:CB	1:A:297:GLU:HG3	1.97	0.94
1:A:445:VAL:HG11	1:A:923:ALA:HB2	1.47	0.94
1:F:349:LYS:HD3	1:F:349:LYS:H	1.30	0.94
1:A:304:ASP:H	1:A:309:GLN:HG2	1.32	0.94
1:A:315:TRP:NE1	1:A:387:LEU:HD22	1.83	0.94
1:B:143:MET:CB	1:B:144:PRO:HD2	1.94	0.94
1:B:395:GLU:HG2	1:B:399:MET:SD	2.07	0.94
1:A:404:GLU:HA	1:A:407:MET:HE2	1.50	0.94
1:B:113:TYR:CZ	1:B:436:GLU:O	2.20	0.94
1:C:442:ILE:HG22	1:C:495:SER:CB	1.95	0.94
1:E:65:PHE:CZ	1:E:767:ASN:CG	2.46	0.93
1:E:305:ARG:HD3	1:E:305:ARG:H	1.30	0.93
1:A:106:TYR:CE1	1:A:442:ILE:HD11	2.03	0.93
1:A:445:VAL:HG11	1:A:923:ALA:CB	1.97	0.93
1:B:215:LYS:HE2	1:B:215:LYS:CA	1.97	0.93
1:D:305:ARG:HH12	1:D:312:VAL:CG2	1.61	0.93
1:B:515:ILE:CD1	1:B:548:LEU:CG	2.46	0.93
1:B:10:ALA:HB3	1:B:18:VAL:CG2	1.99	0.93
1:D:448:LEU:HD11	1:D:490:GLU:CG	1.97	0.93
1:B:292:LYS:HA	1:B:408:ARG:O	1.69	0.93
1:F:38:LYS:HD3	1:F:558:VAL:CG1	1.99	0.93
1:B:299:VAL:HG22	1:B:313:ALA:HB2	1.49	0.93
1:D:313:ALA:HB3	1:D:314:PRO:HD3	1.51	0.93
1:E:150:LEU:HB3	1:E:236:GLU:HB2	1.50	0.93
1:E:177:ARG:HD3	1:E:184:VAL:CG2	1.99	0.93
1:F:445:VAL:HG12	1:F:449:SER:CB	1.98	0.93
1:F:447:GLU:HB2	1:F:490:GLU:HA	1.51	0.93
1:E:352:LYS:HD2	1:E:356:GLU:HB3	1.48	0.92
1:F:483:PHE:O	1:F:487:VAL:HG23	1.69	0.92
1:C:437:HIS:CD2	1:C:440:LYS:HZ2	1.81	0.92
1:A:346:LEU:HB2	1:A:349:LYS:CG	2.00	0.92
1:E:445:VAL:HB	1:E:449:SER:HB2	1.49	0.92
1:E:446:CYS:SG	1:E:448:LEU:HB3	2.09	0.92
1:E:442:ILE:CA	1:E:495:SER:CB	2.12	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:437:HIS:CE1	1:C:440:LYS:HZ2	1.88	0.92
1:E:352:LYS:CD	1:E:356:GLU:HB2	1.99	0.92
1:E:508:ARG:HH11	1:E:508:ARG:HG3	1.33	0.92
1:A:96:ARG:HA	1:A:419:ARG:NH2	1.85	0.92
1:A:786:ARG:H	1:A:786:ARG:HD3	1.35	0.92
1:D:134:GLN:HE21	1:D:134:GLN:H	0.95	0.92
1:E:312:VAL:HG11	1:E:384:LEU:HD11	1.52	0.91
1:E:352:LYS:HA	1:E:356:GLU:HB3	1.51	0.91
1:F:18:VAL:CG1	1:F:585:ILE:HD11	2.00	0.91
1:B:755:ALA:HB2	1:B:778:VAL:HG21	1.50	0.91
1:A:422:PRO:HA	1:A:425:LEU:HD12	1.51	0.91
1:B:323:TYR:CE1	1:B:327:MET:HG3	2.06	0.91
1:E:216:ARG:HG2	1:E:216:ARG:O	1.69	0.91
1:B:185:HIS:ND1	1:B:191:PRO:HB3	1.85	0.91
1:E:88:GLN:HE22	1:E:531:ILE:HG22	0.75	0.91
1:A:106:TYR:HE1	1:A:442:ILE:CD1	1.82	0.91
1:B:183:VAL:HG12	1:B:184:VAL:H	0.74	0.91
1:B:777:GLU:OE2	1:D:160:LYS:NZ	2.04	0.91
1:A:20:LEU:HD21	1:A:585:ILE:CG1	2.01	0.91
1:D:305:ARG:HD2	1:D:311:ALA:HB3	0.91	0.91
1:A:425:LEU:CA	1:A:437:HIS:CE1	2.54	0.90
1:A:295:ASP:HB3	1:A:297:GLU:CG	2.00	0.90
1:A:701:VAL:HG12	1:A:849:GLN:HG2	1.52	0.90
1:E:440:LYS:HB3	1:E:440:LYS:HZ3	1.36	0.90
1:F:355:LEU:O	1:F:383:VAL:HG12	1.68	0.90
1:B:313:ALA:N	1:B:314:PRO:HD2	1.86	0.90
1:D:171:ASN:HD21	1:D:188:THR:HA	1.34	0.90
1:A:437:HIS:HD2	1:A:439:ALA:H	1.18	0.90
1:A:132:THR:H	1:A:135:GLN:HE21	1.19	0.90
1:E:315:TRP:NE1	1:E:387:LEU:HD13	1.85	0.90
1:F:52:ARG:HG2	1:F:66:LEU:HD22	1.53	0.90
1:F:660:LYS:HZ2	1:F:660:LYS:HB3	1.35	0.90
1:A:298:LEU:HD12	1:A:298:LEU:C	1.96	0.90
1:D:156:VAL:HG13	1:D:157:ARG:N	1.86	0.90
1:E:256:ALA:HA	1:E:263:LEU:HD11	1.53	0.90
1:F:412:CYS:O	1:F:415:CYS:SG	2.30	0.90
1:B:441:SER:HA	1:B:445:VAL:HG22	1.53	0.90
1:F:560:HIS:O	1:F:878:PHE:CE2	2.24	0.90
1:A:96:ARG:HA	1:A:419:ARG:HH21	1.35	0.90
1:A:346:LEU:HB2	1:A:349:LYS:CD	2.02	0.90
1:A:298:LEU:O	1:A:299:VAL:HG12	1.72	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:351:ARG:NH2	1:E:355:LEU:HD21	1.85	0.89
1:A:160:LYS:HB3	1:A:198:LYS:HA	1.53	0.89
1:C:918:GLY:O	1:C:925:GLY:HA2	1.72	0.89
1:B:110:ARG:HA	1:B:437:HIS:CE1	2.06	0.89
1:A:351:ARG:HE	1:A:355:LEU:CD1	1.86	0.89
1:B:346:LEU:HA	1:B:349:LYS:HZ1	1.34	0.89
1:F:24:ARG:HG3	1:F:24:ARG:HH11	1.38	0.89
1:F:410:VAL:HB	1:F:411:PRO:HD2	1.55	0.89
1:D:312:VAL:HB	1:D:315:TRP:HB2	1.55	0.89
1:F:8:LYS:HD3	1:F:76:PHE:CD1	2.08	0.89
1:E:312:VAL:CG1	1:E:384:LEU:HD11	2.03	0.89
1:C:437:HIS:CG	1:C:440:LYS:HZ2	1.91	0.88
1:C:444:GLU:OE1	1:C:444:GLU:HA	1.70	0.88
1:D:183:VAL:HG12	1:D:184:VAL:H	0.75	0.88
1:F:877:HIS:CD2	1:F:879:ASP:H	1.91	0.88
1:D:809:ALA:O	1:D:813:PHE:CD1	2.24	0.88
1:F:380:PHE:HB2	1:F:382:GLY:N	1.88	0.88
1:A:171:ASN:HD21	1:A:188:THR:HA	1.39	0.88
1:D:918:GLY:O	1:D:925:GLY:HA2	1.73	0.88
1:A:295:ASP:OD1	1:A:296:PRO:HD2	1.73	0.88
1:B:455:ASP:O	1:B:478:ARG:NH1	2.05	0.88
1:E:305:ARG:CZ	1:E:308:ALA:HB1	2.03	0.88
1:D:445:VAL:O	1:D:493:SER:HA	1.74	0.88
1:E:701:VAL:HG12	1:E:849:GLN:HG2	1.54	0.88
1:A:366:TYR:HE1	1:A:376:TYR:HB2	1.38	0.88
1:A:455:ASP:HA	1:A:478:ARG:HE	1.36	0.88
1:C:317:ASN:CB	1:C:321:ALA:HB2	2.03	0.88
1:B:273:PHE:CD1	1:B:437:HIS:CG	2.62	0.88
1:A:346:LEU:HB2	1:A:349:LYS:HD3	1.56	0.87
1:B:196:GLN:OE1	1:D:764:ILE:HD12	1.72	0.87
1:B:438:GLY:CA	1:B:442:ILE:HG12	2.04	0.87
1:C:445:VAL:HG11	1:C:448:LEU:HB2	1.53	0.87
1:B:397:GLU:HG2	1:B:398:GLN:H	1.39	0.87
1:E:442:ILE:C	1:E:495:SER:HG	1.82	0.87
1:B:215:LYS:HA	1:B:215:LYS:CE	2.02	0.87
1:E:727:LEU:HD22	1:E:793:TYR:HE2	1.39	0.87
1:A:20:LEU:HD11	1:A:41:LEU:HD11	1.56	0.87
1:A:424:ILE:O	1:A:437:HIS:CE1	2.28	0.87
1:B:701:VAL:HG12	1:B:849:GLN:HG2	1.55	0.87
1:C:448:LEU:O	1:C:449:SER:HB2	1.72	0.87
1:F:14:ASN:ND2	1:F:579:GLY:O	2.07	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:437:HIS:CD2	1:C:440:LYS:HZ3	1.87	0.87
1:E:444:GLU:CD	1:E:450:ILE:HG13	1.99	0.87
1:F:440:LYS:O	1:F:445:VAL:CG2	2.22	0.87
1:C:203:VAL:HG12	1:C:204:VAL:N	1.88	0.87
1:C:578:ALA:HB1	1:C:833:TYR:HB3	1.56	0.87
1:E:346:LEU:O	1:E:349:LYS:HE3	1.75	0.87
1:A:298:LEU:C	1:A:299:VAL:HG12	1.99	0.87
1:A:297:GLU:OE1	1:A:298:LEU:N	2.07	0.87
1:A:448:LEU:O	1:A:448:LEU:HD23	1.75	0.86
1:E:49:GLU:CD	1:E:52:ARG:HH12	1.84	0.86
1:A:424:ILE:C	1:A:437:HIS:CE1	2.53	0.86
1:D:446:CYS:HB2	1:D:448:LEU:HD12	1.57	0.86
1:E:462:LEU:HD22	1:E:466:GLU:HB2	1.57	0.86
1:A:18:VAL:HB	1:A:585:ILE:CD1	2.05	0.86
1:D:305:ARG:CB	1:D:311:ALA:CB	2.48	0.86
1:E:306:THR:O	1:E:307:LEU:HB3	1.72	0.86
1:A:106:TYR:HE1	1:A:442:ILE:HD11	1.36	0.86
1:C:425:LEU:HD23	1:C:439:ALA:CB	2.05	0.86
1:C:317:ASN:CB	1:C:321:ALA:CB	2.54	0.86
1:A:88:GLN:NE2	1:A:507:GLN:OE1	2.09	0.86
1:B:273:PHE:HB3	1:B:437:HIS:HE2	1.39	0.86
1:E:286:SER:HB2	1:E:288:LEU:CD2	2.04	0.86
1:C:351:ARG:CG	1:C:352:LYS:H	1.88	0.86
1:D:349:LYS:HD3	1:D:349:LYS:N	1.90	0.85
1:D:305:ARG:HA	1:D:311:ALA:HB2	0.87	0.85
1:B:323:TYR:HD1	1:B:323:TYR:C	1.84	0.85
1:E:307:LEU:O	1:E:307:LEU:HG	1.75	0.85
1:E:440:LYS:CE	1:E:455:ASP:OD1	2.24	0.85
1:F:11:ARG:HG3	1:F:73:ASP:HB3	1.59	0.85
1:A:144:PRO:HB2	1:A:147:THR:CG2	2.07	0.85
1:A:317:ASN:N	1:A:321:ALA:HB2	1.92	0.85
1:B:132:THR:O	1:B:135:GLN:HB2	1.75	0.85
1:B:284:GLU:HG2	1:B:412:CYS:SG	2.16	0.85
1:D:298:LEU:CD1	1:D:408:ARG:HH21	1.89	0.85
1:E:81:SER:HB3	1:E:521:GLY:O	1.77	0.85
1:F:868:ILE:HG13	1:F:899:ILE:HD13	1.58	0.85
1:B:428:THR:HB	1:B:435:GLY:CA	2.06	0.85
1:E:575:GLY:CA	1:E:584:ARG:O	2.24	0.85
1:F:415:CYS:SG	1:F:417:GLY:N	2.49	0.85
1:B:755:ALA:CB	1:B:778:VAL:HG21	2.06	0.85
1:D:304:ASP:CG	1:D:306:THR:HG23	2.01	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:ASP:HB2	1:A:303:PRO:HD3	1.58	0.84
1:C:431:GLY:HA2	1:C:457:LEU:HD12	1.59	0.84
1:A:175:TYR:HB2	1:A:187:LEU:HD13	1.59	0.84
1:B:363:HIS:HE1	1:B:365:ARG:HG3	1.41	0.84
1:D:134:GLN:H	1:D:134:GLN:NE2	1.75	0.84
1:A:323:TYR:CD1	1:A:323:TYR:O	2.31	0.84
1:D:305:ARG:HH11	1:D:312:VAL:HG23	1.07	0.84
1:E:88:GLN:CD	1:E:531:ILE:HG21	2.01	0.84
1:E:284:GLU:HG2	1:E:414:VAL:HG11	1.59	0.84
1:F:445:VAL:HG12	1:F:449:SER:HB2	1.57	0.84
1:A:299:VAL:HG22	1:A:300:VAL:N	1.88	0.84
1:B:272:SER:O	1:B:280:GLY:HA3	1.77	0.84
1:B:727:LEU:HD22	1:B:793:TYR:HE2	1.43	0.84
1:F:11:ARG:CG	1:F:73:ASP:O	2.25	0.84
1:B:273:PHE:CD1	1:B:437:HIS:CE1	2.65	0.84
1:F:10:ALA:HA	1:F:74:VAL:HG12	1.60	0.84
1:A:106:TYR:CE1	1:A:442:ILE:CD1	2.58	0.84
1:A:305:ARG:HB2	1:A:339:VAL:HG13	1.59	0.84
1:A:508:ARG:HG3	1:A:508:ARG:NH1	1.88	0.84
1:F:448:LEU:HD23	1:F:448:LEU:C	2.03	0.84
1:A:269:GLU:OE1	1:A:269:GLU:HA	1.77	0.84
1:A:346:LEU:HD13	1:A:349:LYS:HE2	1.58	0.84
1:B:143:MET:HB3	1:B:144:PRO:HD3	1.55	0.84
1:C:448:LEU:O	1:C:449:SER:CB	2.25	0.84
1:E:452:ASP:HA	1:E:456:PHE:HB2	1.60	0.84
1:A:668:LEU:HD13	1:A:668:LEU:C	2.01	0.84
1:C:356:GLU:OE2	1:C:360:GLU:HB2	1.77	0.84
1:D:123:THR:HG1	1:D:261:HIS:HD1	1.25	0.84
1:E:31:THR:HG23	1:E:573:ASP:OD1	1.78	0.84
1:E:440:LYS:HB3	1:E:440:LYS:NZ	1.93	0.84
1:B:436:GLU:HG2	1:B:440:LYS:HD2	1.59	0.84
1:D:442:ILE:HG22	1:D:495:SER:HB3	1.58	0.84
1:E:282:CYS:HB3	1:E:285:CYS:SG	2.18	0.84
1:A:346:LEU:O	1:A:349:LYS:HG2	1.78	0.84
1:A:441:SER:O	1:A:444:GLU:HG2	1.78	0.84
1:C:12:GLU:OE1	1:C:12:GLU:HA	1.78	0.84
1:F:649:LEU:HD23	1:F:911:SER:HA	1.60	0.84
1:B:397:GLU:HG2	1:B:398:GLN:N	1.93	0.83
1:B:660:LYS:HE2	1:B:661:SER:H	1.41	0.83
1:C:203:VAL:HG12	1:C:204:VAL:H	1.42	0.83
1:B:184:VAL:HG12	1:B:185:HIS:N	1.91	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:VAL:HA	1:B:313:ALA:CB	2.08	0.83
1:D:306:THR:C	1:D:307:LEU:CD1	2.51	0.83
1:A:304:ASP:HA	1:A:311:ALA:HB2	1.60	0.83
1:B:270:PRO:HD2	1:B:271:ARG:HG3	1.60	0.83
1:B:315:TRP:HE1	1:B:387:LEU:HD12	1.41	0.83
1:B:441:SER:HA	1:B:445:VAL:HG21	1.59	0.83
1:C:96:ARG:HB2	1:C:276:ASN:OD1	1.78	0.83
1:A:157:ARG:NH1	1:A:267:ASP:OD2	2.11	0.83
1:B:109:LEU:CD2	1:B:442:ILE:CD1	2.55	0.83
1:C:94:ASN:OD1	1:C:95:PRO:HD2	1.78	0.83
1:D:134:GLN:HE21	1:D:134:GLN:N	1.74	0.83
1:C:597:ASN:HD22	1:C:599:ASP:H	1.27	0.82
1:C:49:GLU:CD	1:C:52:ARG:HH12	1.86	0.82
1:A:351:ARG:CG	1:A:355:LEU:HD12	2.08	0.82
1:C:7:VAL:HG13	1:C:20:LEU:HB2	1.61	0.82
1:D:130:ARG:HA	1:D:254:LYS:HA	1.60	0.82
1:D:597:ASN:HD22	1:D:599:ASP:H	1.28	0.82
1:D:918:GLY:C	1:D:925:GLY:HA2	2.04	0.82
1:E:346:LEU:N	1:E:349:LYS:HZ2	1.77	0.82
1:A:342:PRO:CD	1:A:345:LYS:HD3	2.08	0.82
1:B:158:THR:HG21	1:B:271:ARG:HH12	1.43	0.82
1:B:576:PRO:CD	1:B:586:VAL:CG2	2.48	0.82
1:B:49:GLU:CD	1:B:52:ARG:HH12	1.86	0.82
1:D:940:VAL:HG13	1:F:638:ARG:HD3	1.62	0.82
1:E:286:SER:HB2	1:E:288:LEU:HD23	1.60	0.82
1:B:158:THR:HG21	1:B:271:ARG:NH1	1.95	0.82
1:B:428:THR:CB	1:B:435:GLY:C	2.46	0.82
1:E:312:VAL:CG1	1:E:384:LEU:CD1	2.57	0.82
1:E:312:VAL:HG12	1:E:314:PRO:HD2	1.60	0.82
1:B:7:VAL:HG13	1:B:20:LEU:HB2	1.61	0.82
1:D:7:VAL:HG13	1:D:20:LEU:HB2	1.59	0.82
1:B:786:ARG:HD3	1:B:786:ARG:H	1.43	0.82
1:C:284:GLU:CD	1:C:291:ARG:HH12	1.83	0.82
1:B:428:THR:HG21	1:B:435:GLY:O	1.80	0.81
1:D:132:THR:O	1:D:135:GLN:HB2	1.79	0.81
1:B:273:PHE:CG	1:B:437:HIS:CE1	2.68	0.81
1:C:284:GLU:CG	1:C:291:ARG:HH11	1.91	0.81
1:C:767:ASN:C	1:C:767:ASN:HD22	1.87	0.81
1:E:575:GLY:N	1:E:584:ARG:O	2.12	0.81
1:A:144:PRO:HB2	1:A:147:THR:HG21	1.61	0.81
1:A:158:THR:O	1:A:158:THR:HG22	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:PHE:CD1	1:B:437:HIS:ND1	2.48	0.81
1:C:361:GLN:HB3	1:C:378:ALA:C	2.05	0.81
1:D:367:ARG:HA	1:D:372:ARG:O	1.81	0.81
1:B:152:LEU:HB2	1:B:234:VAL:CG2	2.10	0.81
1:D:49:GLU:CD	1:D:52:ARG:HH12	1.88	0.81
1:F:337:PHE:CZ	1:F:347:PRO:HB3	2.15	0.81
1:A:31:THR:HG23	1:A:573:ASP:OD1	1.81	0.81
1:B:81:SER:HA	1:D:520:VAL:O	1.80	0.81
1:B:299:VAL:HA	1:B:313:ALA:HB3	1.63	0.81
1:B:382:GLY:C	1:B:383:VAL:HG13	2.05	0.81
1:C:193:LEU:HD22	1:C:199:HIS:CE1	2.16	0.81
1:C:442:ILE:HG22	1:C:495:SER:CA	2.10	0.81
1:D:150:LEU:CD2	1:D:236:GLU:HB2	2.09	0.81
1:F:10:ALA:HB3	1:F:18:VAL:HB	1.63	0.81
1:F:332:GLY:CA	1:F:338:ASP:HB3	2.06	0.81
1:B:713:ASN:ND2	1:B:837:GLY:HA2	1.95	0.81
1:A:346:LEU:HB2	1:A:349:LYS:HG2	1.62	0.81
1:B:166:LEU:O	1:B:170:LEU:HB2	1.79	0.81
1:F:397:GLU:HB3	1:F:400:LYS:H	1.45	0.81
1:D:282:CYS:SG	1:D:415:CYS:HB3	2.21	0.81
1:A:456:PHE:O	1:A:458:ASN:N	2.14	0.80
1:D:302:ASP:N	1:D:303:PRO:HD3	1.95	0.80
1:D:372:ARG:HD3	1:D:374:ARG:HB2	1.61	0.80
1:E:178:VAL:HG22	1:E:203:VAL:HG12	1.63	0.80
1:E:314:PRO:HG2	1:E:384:LEU:HD21	1.62	0.80
1:F:660:LYS:HB3	1:F:660:LYS:NZ	1.92	0.80
1:D:763:LYS:HB2	1:D:773:TYR:HE1	1.46	0.80
1:D:763:LYS:HD3	1:D:773:TYR:CE1	2.16	0.80
1:A:298:LEU:O	1:A:299:VAL:CG1	2.30	0.80
1:A:448:LEU:HD23	1:A:448:LEU:C	2.05	0.80
1:B:139:GLN:HG2	1:B:143:MET:HE2	1.60	0.80
1:E:444:GLU:OE2	1:E:450:ILE:N	2.15	0.80
1:F:445:VAL:HG12	1:F:449:SER:HB3	1.64	0.80
1:B:12:GLU:HG3	1:B:13:HIS:CD2	2.17	0.80
1:D:302:ASP:N	1:D:303:PRO:CD	2.44	0.80
1:D:305:ARG:HA	1:D:311:ALA:HA	1.63	0.80
1:E:412:CYS:SG	1:E:414:VAL:HG12	2.21	0.80
1:A:432:GLU:HG3	1:A:433:SER:H	1.47	0.80
1:B:143:MET:CB	1:B:144:PRO:CD	2.47	0.80
1:D:349:LYS:H	1:D:349:LYS:CD	1.86	0.80
1:F:885:LEU:O	1:F:885:LEU:HD13	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:GLU:CG	1:B:440:LYS:CD	2.57	0.80
1:B:447:GLU:HA	1:B:450:ILE:HG22	1.63	0.80
1:D:301:PRO:C	1:D:303:PRO:CD	2.53	0.80
1:F:695:LEU:HD11	1:F:897:THR:OG1	1.80	0.80
1:A:300:VAL:HG13	1:A:303:PRO:CD	2.12	0.80
1:A:618:ARG:NH2	1:A:909:LYS:O	2.15	0.80
1:C:388:GLN:CA	1:C:391:MET:SD	2.62	0.80
1:A:236:GLU:O	1:A:236:GLU:HG2	1.82	0.79
1:B:354:ILE:HG12	1:B:384:LEU:CD2	2.11	0.79
1:B:382:GLY:O	1:B:383:VAL:CG1	2.30	0.79
1:B:438:GLY:CA	1:B:442:ILE:CG1	2.60	0.79
1:B:578:ALA:HB1	1:B:833:TYR:HB3	1.62	0.79
1:E:65:PHE:HZ	1:E:767:ASN:OD1	1.65	0.79
1:A:432:GLU:HG3	1:A:433:SER:N	1.96	0.79
1:B:299:VAL:HG23	1:B:313:ALA:HB3	1.57	0.79
1:C:437:HIS:CD2	1:C:440:LYS:HD2	2.16	0.79
1:A:258:PRO:HG2	1:A:259:ASN:OD1	1.81	0.79
1:A:445:VAL:CG1	1:A:923:ALA:CB	2.59	0.79
1:C:388:GLN:HB2	1:C:389:ARG:HH12	1.47	0.79
1:A:425:LEU:CA	1:A:437:HIS:ND1	2.44	0.79
1:C:61:TYR:HE2	1:E:767:ASN:O	1.65	0.79
1:A:727:LEU:HD22	1:A:793:TYR:HE2	1.48	0.79
1:B:382:GLY:O	1:B:383:VAL:CG2	2.30	0.79
1:B:575:GLY:HA2	1:B:586:VAL:HG23	1.64	0.79
1:D:291:ARG:HD2	1:D:413:PRO:HD2	1.64	0.79
1:E:7:VAL:HG13	1:E:20:LEU:HB2	1.63	0.79
1:F:612:ILE:HD11	1:F:882:ARG:HG2	1.64	0.79
1:A:424:ILE:O	1:A:437:HIS:HE1	1.62	0.79
1:D:33:LEU:HD12	1:D:577:GLY:HA2	1.64	0.79
1:F:412:CYS:HB3	1:F:415:CYS:HB3	1.64	0.79
1:A:298:LEU:O	1:A:298:LEU:CD1	2.30	0.79
1:B:25:ASP:H	1:B:554:THR:HB	1.48	0.79
1:A:335:LEU:HD21	1:A:352:LYS:CE	2.05	0.79
1:B:96:ARG:NH2	1:B:286:SER:O	2.16	0.79
1:C:442:ILE:CG2	1:C:495:SER:HB3	2.13	0.79
1:D:337:PHE:HB3	1:D:349:LYS:HG3	1.63	0.79
1:E:578:ALA:HB1	1:E:833:TYR:HB3	1.65	0.79
1:A:119:PRO:HG3	1:A:268:LEU:CD1	2.11	0.78
1:A:436:GLU:HA	1:A:440:LYS:HD2	1.64	0.78
1:A:438:GLY:O	1:A:442:ILE:HG13	1.84	0.78
1:B:597:ASN:HD22	1:B:599:ASP:H	1.30	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:855:SER:O	1:F:859:LYS:HB3	1.83	0.78
1:C:444:GLU:HB3	1:C:450:ILE:HG22	1.63	0.78
1:F:672:LEU:HD23	1:F:676:LEU:HD12	1.66	0.78
1:B:441:SER:O	1:B:445:VAL:HG23	1.83	0.78
1:B:515:ILE:HD12	1:B:548:LEU:HG	1.63	0.78
1:C:425:LEU:HD21	1:C:439:ALA:HB2	1.65	0.78
1:C:446:CYS:HA	1:C:450:ILE:HG23	1.66	0.78
1:A:786:ARG:HD3	1:A:786:ARG:N	1.98	0.78
1:B:323:TYR:C	1:B:323:TYR:CD1	2.56	0.78
1:B:438:GLY:HA2	1:B:442:ILE:CG1	2.14	0.78
1:D:147:THR:O	1:D:147:THR:CG2	2.31	0.78
1:D:306:THR:O	1:D:307:LEU:HD13	1.84	0.78
1:A:299:VAL:HG22	1:A:301:PRO:HD3	1.65	0.78
1:D:578:ALA:HB1	1:D:833:TYR:HB3	1.64	0.78
1:E:88:GLN:OE1	1:E:531:ILE:HG21	1.84	0.78
1:F:448:LEU:HD23	1:F:448:LEU:O	1.82	0.78
1:B:156:VAL:O	1:B:156:VAL:HG12	1.82	0.78
1:E:177:ARG:CD	1:E:184:VAL:HG23	2.13	0.78
1:E:383:VAL:CB	1:E:386:PHE:HB2	2.13	0.78
1:A:342:PRO:O	1:A:345:LYS:HB2	1.84	0.78
1:C:437:HIS:HB2	1:C:440:LYS:HD2	1.65	0.78
1:C:575:GLY:HA2	1:C:586:VAL:HG23	1.66	0.78
1:D:301:PRO:O	1:D:303:PRO:HD3	1.84	0.78
1:F:106:TYR:CD1	1:F:442:ILE:HG13	2.17	0.78
1:F:313:ALA:O	1:F:316:SER:HB2	1.82	0.78
1:D:388:GLN:O	1:D:392:SER:HB2	1.83	0.78
1:D:727:LEU:HD22	1:D:793:TYR:HE2	1.49	0.78
1:B:215:LYS:O	1:B:217:ARG:N	2.14	0.78
1:B:354:ILE:CG1	1:B:384:LEU:HD23	2.14	0.78
1:C:437:HIS:CD2	1:C:440:LYS:CD	2.67	0.78
1:C:918:GLY:C	1:C:925:GLY:HA2	2.08	0.78
1:D:338:ASP:HB3	1:D:340:ASP:H	1.49	0.78
1:A:660:LYS:HE2	1:A:661:SER:H	1.49	0.77
1:B:397:GLU:CG	1:B:398:GLN:H	1.97	0.77
1:D:156:VAL:HG13	1:D:157:ARG:H	1.49	0.77
1:D:601:ILE:H	1:D:601:ILE:HD12	1.49	0.77
1:F:115:ARG:HD2	1:F:470:ALA:HB2	1.66	0.77
1:B:300:VAL:HG12	1:B:301:PRO:N	1.97	0.77
1:D:315:TRP:HE1	1:D:387:LEU:CD2	1.96	0.77
1:F:11:ARG:NH1	1:F:75:ASP:OD1	2.15	0.77
1:A:437:HIS:CD2	1:A:439:ALA:H	2.01	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:668:LEU:HD13	1:A:668:LEU:O	1.83	0.77
1:C:284:GLU:HG3	1:C:291:ARG:HH11	1.50	0.77
1:C:425:LEU:CD2	1:C:439:ALA:CB	2.61	0.77
1:D:284:GLU:HG3	1:D:414:VAL:CG2	2.11	0.77
1:A:381:GLU:O	1:A:381:GLU:HG3	1.83	0.77
1:A:786:ARG:H	1:A:786:ARG:CD	1.98	0.77
1:E:306:THR:O	1:E:339:VAL:HG13	1.84	0.77
1:B:377:TYR:HB2	1:B:379:ASP:OD1	1.85	0.77
1:C:359:ASP:O	1:C:360:GLU:HG2	1.84	0.77
1:E:446:CYS:HB2	1:E:490:GLU:O	1.84	0.77
1:A:226:LEU:HD22	1:A:231:GLY:O	1.85	0.77
1:C:81:SER:HB3	1:C:521:GLY:O	1.84	0.77
1:D:296:PRO:HA	1:D:299:VAL:HG22	1.67	0.77
1:B:383:VAL:CG2	1:B:387:LEU:N	2.47	0.77
1:B:447:GLU:HA	1:B:450:ILE:CG2	2.14	0.77
1:C:136:ILE:O	1:C:139:GLN:HG2	1.85	0.77
1:D:306:THR:C	1:D:307:LEU:HD12	2.11	0.77
1:A:442:ILE:HG22	1:A:495:SER:CA	2.15	0.76
1:B:920:GLU:C	1:B:924:GLY:O	2.28	0.76
1:C:220:ASP:C	1:C:222:VAL:H	1.93	0.76
1:D:341:THR:HB	1:D:342:PRO:CD	2.15	0.76
1:A:597:ASN:HD22	1:A:599:ASP:H	1.33	0.76
1:C:422:PRO:HB2	1:C:423:GLU:OE1	1.85	0.76
1:C:136:ILE:CG2	1:C:139:GLN:HE21	1.97	0.76
1:C:602:THR:HG22	1:C:606:LEU:HD12	1.66	0.76
1:F:52:ARG:CG	1:F:66:LEU:HD22	2.15	0.76
1:C:701:VAL:HG21	1:C:853:LEU:HD23	1.68	0.76
1:D:767:ASN:HB3	1:D:768:PHE:HD1	1.51	0.76
1:D:940:VAL:CG1	1:F:638:ARG:HD3	2.15	0.76
1:F:446:CYS:O	1:F:450:ILE:HG22	1.85	0.76
1:A:298:LEU:O	1:A:299:VAL:CB	2.30	0.76
1:D:865:THR:H	1:D:896:ASN:ND2	1.83	0.76
1:B:398:GLN:O	1:B:401:GLU:N	2.18	0.76
1:B:442:ILE:HD13	1:B:494:LEU:HD12	1.66	0.76
1:C:441:SER:C	1:C:444:GLU:HG2	2.11	0.76
1:C:628:THR:HB	1:C:690:THR:HB	1.68	0.76
1:F:440:LYS:N	1:F:440:LYS:HD2	2.00	0.76
1:F:440:LYS:C	1:F:445:VAL:HG23	2.10	0.76
1:A:412:CYS:SG	1:A:414:VAL:HG23	2.26	0.76
1:B:363:HIS:CE1	1:B:365:ARG:HG3	2.21	0.76
1:C:767:ASN:ND2	1:C:767:ASN:O	2.17	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:763:LYS:HD3	1:A:773:TYR:CE1	2.20	0.76
1:A:351:ARG:HG2	1:A:355:LEU:HD12	1.68	0.76
1:B:295:ASP:CB	1:B:298:LEU:HD21	2.10	0.76
1:B:786:ARG:HD3	1:B:786:ARG:N	2.00	0.76
1:C:312:VAL:HG23	1:C:315:TRP:HB2	1.68	0.76
1:D:763:LYS:HB2	1:D:773:TYR:CE1	2.19	0.76
1:E:444:GLU:HG2	1:E:450:ILE:HD12	1.68	0.76
1:A:126:GLU:CB	1:A:258:PRO:HG3	2.14	0.76
1:A:323:TYR:HD1	1:A:323:TYR:O	1.65	0.76
1:A:628:THR:HB	1:A:690:THR:HB	1.68	0.76
1:B:713:ASN:HD22	1:B:837:GLY:HA2	1.50	0.76
1:E:231:GLY:O	1:E:232:ILE:HG12	1.86	0.76
1:E:458:ASN:HA	1:E:461:THR:OG1	1.86	0.76
1:D:786:ARG:H	1:D:786:ARG:HD3	1.51	0.75
1:A:177:ARG:O	1:A:204:VAL:HG23	1.85	0.75
1:A:300:VAL:CG1	1:A:303:PRO:HD2	2.13	0.75
1:B:180:VAL:HG12	1:B:181:ASP:H	1.51	0.75
1:B:184:VAL:CG1	1:B:185:HIS:N	2.49	0.75
1:B:263:LEU:HD12	1:B:263:LEU:H	1.50	0.75
1:B:752:ARG:HH21	1:D:165:ASP:CG	1.94	0.75
1:D:597:ASN:ND2	1:D:599:ASP:H	1.83	0.75
1:F:66:LEU:HD23	1:F:69:MET:HB3	1.66	0.75
1:F:560:HIS:O	1:F:878:PHE:HZ	1.64	0.75
1:A:38:LYS:H	1:A:38:LYS:HD3	1.51	0.75
1:C:575:GLY:CA	1:C:584:ARG:O	2.35	0.75
1:D:338:ASP:C	1:D:339:VAL:HG12	2.11	0.75
1:B:94:ASN:OD1	1:B:95:PRO:HD2	1.86	0.75
1:B:354:ILE:HA	1:B:384:LEU:HB3	1.68	0.75
1:C:137:VAL:HG22	1:C:222:VAL:CG1	2.16	0.75
1:D:305:ARG:NH1	1:D:312:VAL:HG21	2.00	0.75
1:B:511:LEU:O	1:B:515:ILE:HG12	1.85	0.75
1:D:575:GLY:N	1:D:584:ARG:O	2.19	0.75
1:F:68:GLN:C	1:F:68:GLN:OE1	2.30	0.75
1:E:295:ASP:HB3	1:E:298:LEU:HG	1.67	0.75
1:B:10:ALA:HB3	1:B:18:VAL:HG23	1.68	0.75
1:B:185:HIS:CE1	1:B:191:PRO:CB	2.69	0.75
1:E:257:CYS:SG	1:E:261:HIS:CE1	2.80	0.75
1:E:401:GLU:HA	1:E:404:GLU:HB2	1.69	0.75
1:A:508:ARG:HH11	1:A:508:ARG:CG	1.94	0.75
1:A:767:ASN:HB3	1:A:768:PHE:HD1	1.50	0.75
1:C:25:ASP:H	1:C:554:THR:HB	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:CYS:O	1:C:125:GLY:HA2	1.86	0.75
1:C:428:THR:HG21	1:C:437:HIS:ND1	2.01	0.75
1:C:763:LYS:HD3	1:C:773:TYR:CE1	2.22	0.75
1:D:575:GLY:HA2	1:D:586:VAL:HG23	1.69	0.75
1:A:391:MET:HE3	1:A:394:THR:CG2	2.17	0.74
1:B:158:THR:HG23	1:B:159:ARG:NH1	2.02	0.74
1:B:767:ASN:HB3	1:B:768:PHE:HD1	1.50	0.74
1:C:119:PRO:HA	1:C:427:VAL:HG22	1.68	0.74
1:D:377:TYR:O	1:D:378:ALA:HB3	1.85	0.74
1:A:180:VAL:HG12	1:A:201:ILE:HG12	1.68	0.74
1:A:445:VAL:HG13	1:A:923:ALA:HB2	1.68	0.74
1:B:368:ASN:HD22	1:B:372:ARG:CB	2.00	0.74
1:F:885:LEU:HD13	1:F:885:LEU:C	2.11	0.74
1:A:226:LEU:HD22	1:A:231:GLY:C	2.12	0.74
1:D:446:CYS:SG	1:D:449:SER:OG	2.45	0.74
1:F:75:ASP:O	1:F:76:PHE:C	2.28	0.74
1:A:300:VAL:N	1:A:301:PRO:CD	2.48	0.74
1:B:300:VAL:HG13	1:B:301:PRO:HD2	1.68	0.74
1:B:459:ALA:HB2	1:B:478:ARG:NH1	2.01	0.74
1:C:445:VAL:CG1	1:C:448:LEU:H	2.00	0.74
1:D:96:ARG:HA	1:D:419:ARG:NH2	2.02	0.74
1:D:183:VAL:CG1	1:D:184:VAL:N	2.23	0.74
1:D:368:ASN:HB2	1:D:372:ARG:HG2	1.70	0.74
1:A:49:GLU:CD	1:A:52:ARG:HH12	1.95	0.74
1:A:297:GLU:OE1	1:A:297:GLU:C	2.30	0.74
1:A:584:ARG:HD3	1:D:584:ARG:HD3	1.69	0.74
1:B:159:ARG:HD2	1:D:777:GLU:HB2	1.69	0.74
1:C:190:PRO:HB2	1:C:191:PRO:HD2	1.70	0.74
1:D:867:TYR:HB2	1:D:898:VAL:HG22	1.70	0.74
1:E:323:TYR:HE1	1:E:327:MET:HG2	1.51	0.74
1:E:363:HIS:HD2	1:E:378:ALA:HA	1.52	0.74
1:F:672:LEU:CD2	1:F:676:LEU:HD12	2.18	0.74
1:B:294:VAL:HA	1:B:407:MET:HA	1.69	0.74
1:B:315:TRP:NE1	1:B:387:LEU:HD12	2.03	0.74
1:E:177:ARG:HA	1:E:185:HIS:O	1.87	0.74
1:A:157:ARG:NH2	1:A:266:ASP:HB2	2.02	0.74
1:C:575:GLY:N	1:C:584:ARG:O	2.20	0.74
1:E:602:THR:HG22	1:E:606:LEU:HD12	1.68	0.74
1:E:625:ARG:HE	1:E:694:TYR:HE2	1.36	0.74
1:F:38:LYS:HD3	1:F:558:VAL:HG13	1.69	0.74
1:F:89:LYS:HA	1:F:89:LYS:HE2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:695:LEU:CD2	1:F:864:ARG:CB	2.55	0.74
1:C:727:LEU:HD22	1:C:793:TYR:HE2	1.52	0.74
1:D:312:VAL:HG11	1:D:315:TRP:CG	2.22	0.74
1:C:33:LEU:HD12	1:C:577:GLY:HA2	1.70	0.74
1:C:38:LYS:H	1:C:38:LYS:HD3	1.53	0.74
1:C:442:ILE:HG22	1:C:495:SER:N	2.03	0.74
1:D:814:GLU:N	1:D:815:PRO:HD2	2.03	0.74
1:F:867:TYR:HB2	1:F:898:VAL:HG22	1.70	0.74
1:A:160:LYS:HB3	1:A:198:LYS:CA	2.18	0.74
1:A:298:LEU:O	1:A:299:VAL:HB	1.88	0.74
1:A:444:GLU:HB2	1:A:450:ILE:CG1	2.18	0.74
1:B:597:ASN:ND2	1:B:599:ASP:H	1.85	0.74
1:F:914:ILE:HD11	1:F:937:VAL:HG21	1.69	0.74
1:D:312:VAL:CB	1:D:315:TRP:HB2	2.17	0.73
1:D:575:GLY:CA	1:D:584:ARG:O	2.36	0.73
1:E:575:GLY:HA2	1:E:586:VAL:HG23	1.69	0.73
1:E:628:THR:HB	1:E:690:THR:HB	1.70	0.73
1:E:763:LYS:HD3	1:E:773:TYR:CE1	2.23	0.73
1:A:511:LEU:O	1:A:515:ILE:HG13	1.88	0.73
1:A:584:ARG:CD	1:D:584:ARG:HD3	2.18	0.73
1:C:11:ARG:HB2	1:C:11:ARG:CZ	2.18	0.73
1:C:284:GLU:HG3	1:C:291:ARG:NH1	2.03	0.73
1:C:442:ILE:HG23	1:C:494:LEU:HB3	1.68	0.73
1:D:120:HIS:O	1:D:426:ALA:HB1	1.87	0.73
1:D:866:VAL:HG23	1:D:897:THR:HB	1.71	0.73
1:E:442:ILE:C	1:E:495:SER:CB	2.61	0.73
1:E:442:ILE:C	1:E:495:SER:HB3	2.13	0.73
1:F:344:ARG:C	1:F:346:LEU:H	1.96	0.73
1:C:203:VAL:CG1	1:C:204:VAL:H	2.00	0.73
1:F:11:ARG:O	1:F:12:GLU:HG2	1.87	0.73
1:E:618:ARG:NH2	1:E:909:LYS:O	2.22	0.73
1:D:447:GLU:OE1	1:D:447:GLU:HA	1.87	0.73
1:C:767:ASN:C	1:C:767:ASN:ND2	2.44	0.73
1:A:337:PHE:CB	1:A:346:LEU:HD22	2.19	0.73
1:B:61:TYR:CE2	1:D:767:ASN:O	2.42	0.73
1:E:882:ARG:HH22	1:E:883:LYS:HE2	1.53	0.73
1:A:391:MET:HE3	1:A:394:THR:HG21	1.69	0.73
1:A:437:HIS:H	1:A:440:LYS:HD2	1.52	0.73
1:B:674:ASN:ND2	1:B:681:GLN:O	2.22	0.73
1:C:614:ILE:HD12	1:C:614:ILE:H	1.53	0.73
1:D:138:ASP:HA	1:D:141:LEU:HD22	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:786:ARG:HD3	1:E:786:ARG:H	1.53	0.73
1:B:273:PHE:HD1	1:B:437:HIS:CG	2.06	0.73
1:B:396:SER:O	1:B:397:GLU:HB3	1.89	0.73
1:D:25:ASP:H	1:D:554:THR:HB	1.54	0.73
1:E:307:LEU:O	1:E:307:LEU:CG	2.31	0.73
1:D:156:VAL:CG1	1:D:157:ARG:N	2.52	0.72
1:E:65:PHE:CZ	1:E:767:ASN:OD1	2.42	0.72
1:A:159:ARG:HH11	1:A:159:ARG:HG3	1.53	0.72
1:B:139:GLN:CG	1:B:143:MET:HE3	2.12	0.72
1:E:25:ASP:H	1:E:554:THR:HB	1.54	0.72
1:E:383:VAL:HB	1:E:386:PHE:CB	2.17	0.72
1:A:158:THR:HA	1:A:199:HIS:O	1.89	0.72
1:B:786:ARG:H	1:B:786:ARG:CD	2.02	0.72
1:C:660:LYS:HE2	1:C:661:SER:H	1.53	0.72
1:D:342:PRO:HB2	1:D:347:PRO:CG	2.19	0.72
1:E:150:LEU:CB	1:E:236:GLU:HB2	2.18	0.72
1:F:78:GLU:HG2	1:F:79:GLY:H	1.55	0.72
1:A:291:ARG:HB3	1:A:291:ARG:HH11	1.53	0.72
1:B:601:ILE:H	1:B:601:ILE:HD12	1.54	0.72
1:E:918:GLY:O	1:E:925:GLY:HA2	1.90	0.72
1:F:674:ASN:HA	1:F:679:ALA:O	1.90	0.72
1:A:232:ILE:HD12	1:A:266:ASP:HB3	1.70	0.72
1:C:282:CYS:SG	1:C:415:CYS:HB3	2.29	0.72
1:C:444:GLU:OE2	1:C:449:SER:OG	2.07	0.72
1:D:88:GLN:OE1	1:D:531:ILE:HG21	1.90	0.72
1:F:337:PHE:HZ	1:F:347:PRO:HA	1.54	0.72
1:C:867:TYR:HB2	1:C:898:VAL:HG22	1.72	0.72
1:A:25:ASP:H	1:A:554:THR:HB	1.55	0.72
1:A:155:VAL:HA	1:A:229:ALA:HA	1.72	0.72
1:A:425:LEU:N	1:A:437:HIS:CE1	2.58	0.72
1:B:431:GLY:CA	1:B:458:ASN:HB3	2.20	0.72
1:B:713:ASN:HD22	1:B:837:GLY:CA	2.02	0.72
1:E:177:ARG:CD	1:E:184:VAL:CG2	2.67	0.72
1:F:40:SER:HA	1:F:44:ASP:OD2	1.89	0.72
1:C:508:ARG:HH11	1:C:508:ARG:CG	2.02	0.71
1:D:295:ASP:HB3	1:D:298:LEU:HD13	1.72	0.71
1:D:305:ARG:CA	1:D:311:ALA:CA	2.59	0.71
1:E:151:VAL:O	1:E:151:VAL:HG12	1.90	0.71
1:E:281:ALA:HB1	1:E:287:GLY:HA2	1.72	0.71
1:A:124:CYS:HB3	1:A:261:HIS:CE1	2.25	0.71
1:A:453:CYS:HA	1:A:457:LEU:HB2	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:TYR:CE1	1:B:327:MET:CG	2.65	0.71
1:B:602:THR:HG22	1:B:606:LEU:HD12	1.70	0.71
1:C:597:ASN:ND2	1:C:599:ASP:H	1.86	0.71
1:A:208:LEU:HD13	1:A:218:LEU:HD12	1.70	0.71
1:B:373:THR:HG22	1:B:374:ARG:N	2.05	0.71
1:B:508:ARG:HH11	1:B:508:ARG:CG	1.99	0.71
1:D:156:VAL:CG1	1:D:157:ARG:H	2.03	0.71
1:B:219:THR:O	1:B:223:GLU:HG3	1.91	0.71
1:C:284:GLU:HG2	1:C:291:ARG:NH1	2.04	0.71
1:D:96:ARG:HB2	1:D:276:ASN:OD1	1.90	0.71
1:D:156:VAL:HB	1:D:201:ILE:H	1.55	0.71
1:F:439:ALA:C	1:F:440:LYS:HD2	2.15	0.71
1:A:398:GLN:HG2	1:A:399:MET:N	2.06	0.71
1:C:767:ASN:O	1:E:61:TYR:HE2	1.73	0.71
1:D:156:VAL:HG21	1:D:199:HIS:O	1.90	0.71
1:E:269:GLU:HB3	1:E:270:PRO:HD2	1.72	0.71
1:E:784:TYR:CE2	1:E:798:VAL:HB	2.25	0.71
1:F:543:GLU:HG3	1:F:547:ARG:NH2	2.06	0.71
1:A:447:GLU:HB2	1:A:490:GLU:HA	1.72	0.71
1:B:10:ALA:HB3	1:B:18:VAL:HG22	1.71	0.71
1:B:383:VAL:HG23	1:B:387:LEU:H	1.54	0.71
1:C:61:TYR:CE2	1:E:767:ASN:O	2.43	0.71
1:C:137:VAL:HG22	1:C:222:VAL:HG11	1.72	0.71
1:F:319:HIS:C	1:F:321:ALA:H	1.98	0.71
1:A:300:VAL:O	1:A:302:ASP:N	2.21	0.71
1:A:342:PRO:HD2	1:A:345:LYS:CD	2.17	0.71
1:A:763:LYS:HB2	1:A:773:TYR:HE1	1.56	0.71
1:C:777:GLU:OE2	1:E:160:LYS:HG2	1.88	0.71
1:D:306:THR:O	1:D:307:LEU:HB2	1.91	0.71
1:D:444:GLU:OE2	1:D:449:SER:HB3	1.90	0.71
1:D:508:ARG:HH11	1:D:508:ARG:CG	1.99	0.71
1:E:18:VAL:HB	1:E:585:ILE:CD1	2.20	0.71
1:E:129:ALA:O	1:E:255:LEU:O	2.08	0.71
1:D:410:VAL:HB	1:D:411:PRO:HD2	1.72	0.71
1:F:354:ILE:HG12	1:F:381:GLU:HG2	1.73	0.71
1:F:415:CYS:O	1:F:416:ALA:HB3	1.91	0.71
1:B:438:GLY:HA3	1:B:442:ILE:CG1	2.20	0.71
1:B:441:SER:O	1:B:445:VAL:CG2	2.38	0.71
1:E:352:LYS:CD	1:E:356:GLU:CB	2.52	0.71
1:F:443:ALA:HA	1:F:495:SER:OG	1.90	0.71
1:F:684:GLY:O	1:F:686:HIS:HD2	1.74	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:VAL:CG2	1:A:300:VAL:H	1.97	0.71
1:A:381:GLU:O	1:A:383:VAL:N	2.24	0.71
1:C:203:VAL:CG1	1:C:204:VAL:N	2.54	0.70
1:C:410:VAL:HB	1:C:411:PRO:CD	2.21	0.70
1:C:625:ARG:HE	1:C:694:TYR:HE2	1.39	0.70
1:C:767:ASN:O	1:E:61:TYR:CE2	2.44	0.70
1:D:156:VAL:HG11	1:D:200:ASP:HA	1.73	0.70
1:E:462:LEU:CD2	1:E:466:GLU:HB2	2.21	0.70
1:F:544:THR:HG23	1:F:547:ARG:HH12	1.56	0.70
1:A:216:ARG:HA	1:A:216:ARG:NE	2.06	0.70
1:C:290:ILE:HG12	1:C:409:ASP:HB3	1.73	0.70
1:C:763:LYS:HB2	1:C:773:TYR:HE1	1.55	0.70
1:F:651:SER:HA	1:F:900:VAL:O	1.91	0.70
1:A:578:ALA:HB1	1:A:833:TYR:HB3	1.72	0.70
1:C:275:PHE:CD1	1:C:419:ARG:HD3	2.26	0.70
1:D:602:THR:HG22	1:D:606:LEU:HD12	1.73	0.70
1:E:865:THR:H	1:E:896:ASN:ND2	1.88	0.70
1:C:139:GLN:O	1:C:143:MET:HG2	1.90	0.70
1:E:597:ASN:HD22	1:E:599:ASP:H	1.38	0.70
1:E:732:THR:HA	1:E:735:LYS:HE2	1.74	0.70
1:B:179:ARG:HD3	1:B:183:VAL:HG22	1.72	0.70
1:C:131:GLN:OE1	1:C:131:GLN:HA	1.91	0.70
1:C:453:CYS:C	1:C:455:ASP:H	1.98	0.70
1:A:576:PRO:HD3	1:A:586:VAL:HG21	1.73	0.70
1:B:777:GLU:CD	1:D:160:LYS:HZ2	1.97	0.70
1:D:298:LEU:HD12	1:D:408:ARG:HH21	1.55	0.70
1:E:760:GLY:O	1:E:781:GLY:HA2	1.92	0.70
1:B:129:ALA:O	1:B:255:LEU:HA	1.91	0.70
1:B:171:ASN:CA	1:B:187:LEU:HD21	2.16	0.70
1:B:628:THR:HB	1:B:690:THR:HB	1.73	0.70
1:C:359:ASP:O	1:C:360:GLU:CG	2.40	0.70
1:D:312:VAL:CG1	1:D:315:TRP:H	2.01	0.70
1:D:497:ALA:HB3	1:D:500:THR:HG23	1.73	0.70
1:F:439:ALA:O	1:F:444:GLU:HB2	1.92	0.70
1:F:11:ARG:NH2	1:F:75:ASP:OD1	2.24	0.70
1:F:315:TRP:HE3	1:F:328:MET:HE1	1.56	0.70
1:F:907:VAL:HA	1:F:910:THR:OG1	1.91	0.70
1:C:462:LEU:HD13	1:C:467:GLN:HA	1.73	0.70
1:E:614:ILE:H	1:E:614:ILE:HD12	1.57	0.70
1:F:418:THR:O	1:F:419:ARG:HB2	1.89	0.70
1:B:364:VAL:HG21	1:B:379:ASP:OD2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:GLY:O	1:B:442:ILE:HB	1.91	0.70
1:C:455:ASP:HA	1:C:478:ARG:HH11	1.56	0.70
1:C:618:ARG:NH2	1:C:909:LYS:O	2.25	0.69
1:D:767:ASN:HB3	1:D:768:PHE:CD1	2.26	0.69
1:D:811:GLU:HA	1:D:814:GLU:HG3	1.73	0.69
1:F:9:GLY:HA2	1:F:18:VAL:O	1.91	0.69
1:F:29:VAL:O	1:F:29:VAL:HG12	1.90	0.69
1:B:298:LEU:O	1:B:299:VAL:HB	1.92	0.69
1:C:445:VAL:CG1	1:C:448:LEU:HB2	2.22	0.69
1:C:865:THR:H	1:C:896:ASN:ND2	1.89	0.69
1:F:54:TYR:HB2	1:F:82:PRO:HB3	1.74	0.69
1:F:538:ASN:O	1:F:542:ILE:HG12	1.92	0.69
1:A:141:LEU:HD13	1:A:218:LEU:HD23	1.74	0.69
1:B:152:LEU:HD13	1:B:202:GLU:HG2	1.74	0.69
1:B:295:ASP:O	1:B:298:LEU:HD23	1.92	0.69
1:C:422:PRO:HB2	1:C:423:GLU:CD	2.18	0.69
1:D:315:TRP:HE1	1:D:387:LEU:HD23	1.56	0.69
1:E:575:GLY:O	1:E:582:GLY:HA2	1.92	0.69
1:B:273:PHE:HD1	1:B:437:HIS:CD2	2.11	0.69
1:B:299:VAL:CA	1:B:313:ALA:CB	2.71	0.69
1:F:436:GLU:HG2	1:F:438:GLY:H	1.56	0.69
1:A:299:VAL:HG22	1:A:301:PRO:CD	2.22	0.69
1:B:145:GLU:HB2	1:B:148:ARG:NE	2.07	0.69
1:B:352:LYS:HA	1:B:356:GLU:O	1.93	0.69
1:C:786:ARG:H	1:C:786:ARG:HD3	1.56	0.69
1:D:285:CYS:O	1:D:288:LEU:HB2	1.93	0.69
1:A:300:VAL:O	1:A:300:VAL:HG22	1.93	0.69
1:B:625:ARG:HE	1:B:694:TYR:HE2	1.40	0.69
1:D:305:ARG:CG	1:D:311:ALA:CB	2.46	0.69
1:D:312:VAL:HG11	1:D:315:TRP:CD2	2.26	0.69
1:A:179:ARG:HG3	1:A:184:VAL:HG13	1.75	0.69
1:A:584:ARG:HD3	1:D:584:ARG:CD	2.22	0.69
1:B:441:SER:CA	1:B:445:VAL:CG2	2.69	0.69
1:B:575:GLY:N	1:B:584:ARG:O	2.26	0.69
1:C:190:PRO:CB	1:C:191:PRO:CD	2.71	0.69
1:C:351:ARG:HG2	1:C:352:LYS:H	1.57	0.69
1:F:441:SER:O	1:F:450:ILE:HD12	1.92	0.69
1:F:864:ARG:HB2	1:F:864:ARG:NH1	2.08	0.69
1:A:728:PHE:O	1:A:731:THR:HG22	1.93	0.69
1:B:439:ALA:O	1:B:443:ALA:HB3	1.93	0.69
1:B:760:GLY:O	1:B:781:GLY:HA2	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:ASP:HB3	1:C:190:PRO:HD3	1.75	0.69
1:D:660:LYS:HE2	1:D:661:SER:H	1.57	0.69
1:F:332:GLY:HA2	1:F:338:ASP:CB	2.07	0.69
1:F:882:ARG:CZ	1:F:886:ASN:HD21	1.95	0.69
1:B:292:LYS:CA	1:B:408:ARG:O	2.41	0.69
1:B:767:ASN:HB3	1:B:768:PHE:CD1	2.28	0.69
1:C:285:CYS:O	1:C:288:LEU:HB2	1.92	0.69
1:D:305:ARG:NH1	1:D:312:VAL:CB	2.54	0.69
1:E:324:PHE:O	1:E:327:MET:HB2	1.92	0.69
1:E:651:SER:HB2	1:E:914:ILE:HG22	1.75	0.69
1:E:918:GLY:C	1:E:925:GLY:HA2	2.16	0.69
1:F:99:VAL:HA	1:F:102:ILE:HD12	1.74	0.69
1:F:399:MET:HA	1:F:402:ARG:HB3	1.74	0.69
1:F:695:LEU:HD11	1:F:897:THR:CB	2.22	0.69
1:A:126:GLU:HB2	1:A:258:PRO:CG	2.23	0.68
1:A:602:THR:HG22	1:A:606:LEU:HD12	1.73	0.68
1:B:313:ALA:N	1:B:314:PRO:CD	2.55	0.68
1:C:437:HIS:CE1	1:C:440:LYS:NZ	2.56	0.68
1:D:338:ASP:CB	1:D:340:ASP:H	2.06	0.68
1:D:383:VAL:HB	1:D:386:PHE:HB2	1.75	0.68
1:E:38:LYS:HD3	1:E:38:LYS:H	1.58	0.68
1:A:597:ASN:ND2	1:A:599:ASP:H	1.89	0.68
1:B:618:ARG:NH2	1:B:909:LYS:O	2.26	0.68
1:C:701:VAL:CG1	1:C:849:GLN:HG2	2.21	0.68
1:F:78:GLU:HG2	1:F:79:GLY:N	2.07	0.68
1:F:88:GLN:HB3	1:F:507:GLN:NE2	2.09	0.68
1:B:763:LYS:HB2	1:B:773:TYR:HE1	1.57	0.68
1:C:601:ILE:H	1:C:601:ILE:HD12	1.57	0.68
1:D:701:VAL:HB	1:D:869:LEU:HD23	1.76	0.68
1:F:487:VAL:HG21	1:F:512:ALA:HB2	1.76	0.68
1:A:300:VAL:HG11	1:A:303:PRO:HG2	1.75	0.68
1:A:346:LEU:H	1:A:349:LYS:HE3	1.58	0.68
1:C:394:THR:HG23	1:C:396:SER:HA	1.76	0.68
1:E:114:ALA:HB2	1:E:270:PRO:HA	1.75	0.68
1:A:300:VAL:H	1:A:301:PRO:CD	2.06	0.68
1:B:451:ALA:HA	1:B:455:ASP:OD2	1.92	0.68
1:B:865:THR:H	1:B:896:ASN:ND2	1.91	0.68
1:C:294:VAL:HA	1:C:407:MET:HA	1.76	0.68
1:C:866:VAL:HG23	1:C:897:THR:HB	1.74	0.68
1:D:234:VAL:HG23	1:D:250:ARG:HG2	1.75	0.68
1:D:304:ASP:O	1:D:305:ARG:HB3	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:LEU:HD21	1:A:179:ARG:HH12	1.59	0.68
1:A:158:THR:O	1:A:158:THR:CG2	2.41	0.68
1:C:575:GLY:O	1:C:582:GLY:HA2	1.94	0.68
1:D:296:PRO:HA	1:D:299:VAL:CG2	2.23	0.68
1:E:136:ILE:O	1:E:140:VAL:HG23	1.94	0.68
1:F:337:PHE:CE1	1:F:347:PRO:HB3	2.28	0.68
1:B:299:VAL:CB	1:B:313:ALA:CB	2.72	0.68
1:B:354:ILE:HA	1:B:384:LEU:HD23	1.74	0.68
1:C:763:LYS:HB2	1:C:773:TYR:CE1	2.29	0.68
1:D:445:VAL:O	1:D:493:SER:CA	2.40	0.68
1:E:728:PHE:O	1:E:731:THR:HG22	1.94	0.68
1:A:760:GLY:O	1:A:781:GLY:HA2	1.94	0.68
1:C:360:GLU:O	1:C:361:GLN:CD	2.37	0.68
1:D:308:ALA:O	1:D:309:GLN:HB2	1.92	0.68
1:D:347:PRO:N	1:D:349:LYS:HE2	2.09	0.68
1:D:621:VAL:HG13	1:D:645:PRO:HB3	1.76	0.68
1:F:98:THR:HG23	1:F:419:ARG:HH12	1.59	0.68
1:A:33:LEU:O	1:A:36:SER:HB2	1.93	0.68
1:A:575:GLY:N	1:A:584:ARG:O	2.27	0.68
1:B:158:THR:HG23	1:B:159:ARG:HH11	1.59	0.68
1:B:158:THR:HB	1:B:279:TYR:OH	1.93	0.68
1:C:784:TYR:CE2	1:C:798:VAL:HB	2.29	0.68
1:F:576:PRO:HG2	1:F:583:GLY:N	2.08	0.68
1:B:346:LEU:HA	1:B:349:LYS:NZ	2.08	0.67
1:D:575:GLY:O	1:D:582:GLY:HA2	1.93	0.67
1:E:442:ILE:N	1:E:495:SER:HB3	2.06	0.67
1:A:444:GLU:HB2	1:A:450:ILE:HG13	1.76	0.67
1:B:38:LYS:HD3	1:B:38:LYS:H	1.58	0.67
1:C:452:ASP:HA	1:C:456:PHE:CD1	2.29	0.67
1:E:597:ASN:ND2	1:E:599:ASP:H	1.92	0.67
1:F:442:ILE:O	1:F:494:LEU:HB2	1.94	0.67
1:F:668:LEU:O	1:F:672:LEU:HD12	1.94	0.67
1:D:351:ARG:HB2	1:D:352:LYS:HE3	1.75	0.67
1:E:388:GLN:O	1:E:392:SER:HB2	1.93	0.67
1:F:340:ASP:O	1:F:342:PRO:CD	2.33	0.67
1:F:349:LYS:HD3	1:F:349:LYS:N	2.04	0.67
1:B:299:VAL:HG23	1:B:313:ALA:HB2	0.71	0.67
1:B:784:TYR:CE2	1:B:798:VAL:HB	2.30	0.67
1:D:625:ARG:HG2	1:D:694:TYR:CE2	2.29	0.67
1:A:315:TRP:HE1	1:A:387:LEU:CD2	2.00	0.67
1:B:763:LYS:HD3	1:B:773:TYR:CE1	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:386:PHE:C	1:C:388:GLN:H	2.01	0.67
1:D:231:GLY:O	1:D:253:GLU:HB2	1.95	0.67
1:D:298:LEU:HD21	1:D:682:VAL:HG13	1.74	0.67
1:B:24:ARG:HG3	1:B:554:THR:HG21	1.76	0.67
1:B:706:ILE:HD11	1:B:851:VAL:HG11	1.77	0.67
1:D:18:VAL:HB	1:D:585:ILE:CD1	2.25	0.67
1:F:395:GLU:O	1:F:397:GLU:HB2	1.94	0.67
1:B:752:ARG:NE	1:D:165:ASP:OD2	2.23	0.67
1:B:442:ILE:CD1	1:B:494:LEU:HD12	2.24	0.67
1:C:33:LEU:O	1:C:36:SER:HB2	1.95	0.67
1:D:614:ILE:H	1:D:614:ILE:HD12	1.60	0.67
1:E:404:GLU:HG2	1:E:407:MET:HE2	1.75	0.67
1:B:389:ARG:O	1:B:393:GLN:HG2	1.95	0.67
1:F:380:PHE:HD2	1:F:382:GLY:HA2	1.60	0.67
1:A:297:GLU:CD	1:A:298:LEU:N	2.51	0.67
1:D:298:LEU:HD11	1:D:408:ARG:NH2	2.09	0.67
1:F:18:VAL:HG13	1:F:585:ILE:CD1	2.22	0.67
1:F:877:HIS:HD2	1:F:879:ASP:HB3	1.60	0.67
1:A:81:SER:HB3	1:A:521:GLY:O	1.95	0.66
1:A:155:VAL:HG23	1:A:156:VAL:HG23	1.76	0.66
1:A:455:ASP:HA	1:A:478:ARG:NE	2.10	0.66
1:A:763:LYS:HB2	1:A:773:TYR:CE1	2.29	0.66
1:B:114:ALA:HB2	1:B:270:PRO:HA	1.76	0.66
1:E:285:CYS:O	1:E:286:SER:HB2	1.95	0.66
1:E:452:ASP:HA	1:E:456:PHE:CB	2.25	0.66
1:F:11:ARG:HA	1:F:15:LEU:HD12	1.76	0.66
1:B:763:LYS:HB2	1:B:773:TYR:CE1	2.29	0.66
1:C:625:ARG:HG2	1:C:694:TYR:CE2	2.30	0.66
1:D:124:CYS:HB3	1:D:261:HIS:CE1	2.30	0.66
1:D:760:GLY:O	1:D:781:GLY:HA2	1.95	0.66
1:B:224:THR:HA	1:B:227:ASN:HB3	1.78	0.66
1:B:441:SER:CA	1:B:445:VAL:HG22	2.24	0.66
1:C:428:THR:CG2	1:C:437:HIS:ND1	2.57	0.66
1:C:437:HIS:CG	1:C:440:LYS:HD2	2.29	0.66
1:C:452:ASP:HA	1:C:456:PHE:HD1	1.60	0.66
1:E:352:LYS:CA	1:E:356:GLU:HB3	2.25	0.66
1:E:768:PHE:N	1:E:768:PHE:CD1	2.63	0.66
1:F:331:LEU:HG	1:F:335:LEU:HD12	1.76	0.66
1:F:660:LYS:NZ	1:F:660:LYS:CB	2.58	0.66
1:D:352:LYS:O	1:D:356:GLU:HA	1.95	0.66
1:B:269:GLU:HB3	1:B:270:PRO:CD	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:648:VAL:HG22	1:B:912:ASP:OD2	1.94	0.66
1:C:18:VAL:HB	1:C:585:ILE:CD1	2.26	0.66
1:C:760:GLY:O	1:C:781:GLY:HA2	1.96	0.66
1:A:867:TYR:HB2	1:A:898:VAL:HG22	1.78	0.66
1:B:649:LEU:HD23	1:B:911:SER:HA	1.76	0.66
1:D:81:SER:HB3	1:D:521:GLY:O	1.96	0.66
1:D:628:THR:HB	1:D:690:THR:HB	1.78	0.66
1:E:367:ARG:HA	1:E:373:THR:HA	1.78	0.66
1:E:445:VAL:HB	1:E:449:SER:CB	2.24	0.66
1:E:450:ILE:HG22	1:E:451:ALA:N	2.11	0.66
1:F:323:TYR:CD1	1:F:323:TYR:C	2.74	0.66
1:A:767:ASN:HB3	1:A:768:PHE:CD1	2.30	0.66
1:B:368:ASN:HD22	1:B:372:ARG:HB2	1.59	0.66
1:B:625:ARG:HG2	1:B:694:TYR:CE2	2.30	0.66
1:C:701:VAL:HB	1:C:869:LEU:HD23	1.78	0.66
1:A:145:GLU:CD	1:A:145:GLU:H	2.03	0.66
1:A:351:ARG:HE	1:A:355:LEU:HD12	1.60	0.66
1:B:614:ILE:H	1:B:614:ILE:HD12	1.61	0.66
1:D:38:LYS:H	1:D:38:LYS:HD3	1.61	0.66
1:D:342:PRO:CB	1:D:347:PRO:HG3	2.24	0.66
1:F:9:GLY:CA	1:F:18:VAL:O	2.44	0.66
1:F:24:ARG:HG3	1:F:24:ARG:NH1	2.10	0.66
1:B:81:SER:HB3	1:B:521:GLY:O	1.95	0.66
1:B:355:LEU:O	1:B:356:GLU:HB3	1.95	0.66
1:C:442:ILE:CG2	1:C:495:SER:CA	2.73	0.66
1:D:326:ARG:HG2	1:D:326:ARG:NH1	2.05	0.66
1:E:335:LEU:HD21	1:E:360:GLU:OE1	1.95	0.66
1:F:354:ILE:HA	1:F:383:VAL:HG21	1.76	0.66
1:B:31:THR:HG23	1:B:573:ASP:OD1	1.95	0.66
1:B:109:LEU:CG	1:B:442:ILE:HD11	2.26	0.66
1:B:273:PHE:CD1	1:B:437:HIS:CD2	2.84	0.66
1:B:447:GLU:CA	1:B:450:ILE:HG22	2.26	0.66
1:E:649:LEU:HD23	1:E:911:SER:HA	1.78	0.66
1:F:347:PRO:HB2	1:F:350:ALA:CB	2.26	0.66
1:F:381:GLU:OE1	1:F:381:GLU:CA	2.33	0.66
1:E:224:THR:HA	1:E:227:ASN:HB2	1.78	0.65
1:F:445:VAL:CG1	1:F:449:SER:HB3	2.24	0.65
1:F:856:GLU:HG3	1:F:860:ARG:HB2	1.77	0.65
1:B:273:PHE:CB	1:B:437:HIS:NE2	2.52	0.65
1:D:304:ASP:OD1	1:D:306:THR:HG23	1.96	0.65
1:D:349:LYS:O	1:D:352:LYS:HD2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:728:PHE:O	1:D:731:THR:HG22	1.95	0.65
1:E:440:LYS:HE2	1:E:454:ALA:HB3	1.76	0.65
1:F:380:PHE:CB	1:F:382:GLY:H	1.99	0.65
1:A:625:ARG:HG2	1:A:694:TYR:CE2	2.30	0.65
1:B:180:VAL:HG12	1:B:181:ASP:N	2.11	0.65
1:B:418:THR:C	1:B:419:ARG:HG3	2.20	0.65
1:C:452:ASP:CA	1:C:456:PHE:HD1	2.08	0.65
1:D:305:ARG:CA	1:D:311:ALA:HA	2.25	0.65
1:F:354:ILE:HA	1:F:383:VAL:CG2	2.25	0.65
1:A:113:TYR:CE1	1:A:429:LEU:HD22	2.32	0.65
1:E:444:GLU:OE2	1:E:450:ILE:CB	2.45	0.65
1:F:87:ASP:HB3	1:F:89:LYS:HE3	1.77	0.65
1:F:648:VAL:HA	1:F:892:VAL:HG13	1.78	0.65
1:F:699:VAL:O	1:F:867:TYR:HA	1.96	0.65
1:A:304:ASP:HB2	1:A:305:ARG:HD3	1.78	0.65
1:D:338:ASP:O	1:D:339:VAL:HG12	1.97	0.65
1:D:670:ALA:HA	1:D:681:GLN:HE21	1.61	0.65
1:E:763:LYS:HB2	1:E:773:TYR:HE1	1.61	0.65
1:A:294:VAL:HA	1:A:407:MET:HA	1.78	0.65
1:A:300:VAL:N	1:A:301:PRO:HD2	2.12	0.65
1:B:918:GLY:O	1:B:925:GLY:HA2	1.97	0.65
1:D:307:LEU:HD12	1:D:307:LEU:N	2.11	0.65
1:A:459:ALA:HB2	1:A:478:ARG:HH12	1.60	0.65
1:A:601:ILE:H	1:A:601:ILE:HD12	1.62	0.65
1:A:614:ILE:H	1:A:614:ILE:HD12	1.61	0.65
1:D:625:ARG:HE	1:D:694:TYR:HE2	1.43	0.65
1:E:356:GLU:HG2	1:E:358:ALA:H	1.61	0.65
1:A:345:LYS:C	1:A:346:LEU:HD12	2.22	0.65
1:A:444:GLU:O	1:A:493:SER:HB2	1.97	0.65
1:B:315:TRP:HE1	1:B:387:LEU:CD1	2.09	0.65
1:C:670:ALA:HA	1:C:681:GLN:NE2	2.12	0.65
1:E:100:GLY:HA2	1:E:494:LEU:HD22	1.79	0.65
1:E:442:ILE:O	1:E:495:SER:CB	2.45	0.65
1:E:866:VAL:HG23	1:E:897:THR:HB	1.78	0.65
1:F:326:ARG:O	1:F:329:ALA:HB3	1.97	0.65
1:C:12:GLU:OE1	1:C:12:GLU:CA	2.43	0.64
1:C:646:LEU:HD22	1:C:695:LEU:HD21	1.79	0.64
1:D:304:ASP:OD2	1:D:306:THR:CG2	2.45	0.64
1:F:12:GLU:OE2	1:F:73:ASP:N	2.30	0.64
1:A:96:ARG:NH2	1:A:288:LEU:HD23	2.09	0.64
1:A:339:VAL:O	1:A:339:VAL:CG1	2.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:784:TYR:CE2	1:A:798:VAL:HB	2.32	0.64
1:B:186:PRO:HD2	1:B:189:ASP:O	1.97	0.64
1:B:273:PHE:HB3	1:B:437:HIS:CE1	2.32	0.64
1:B:342:PRO:HG2	1:B:345:LYS:HE3	1.79	0.64
1:B:452:ASP:O	1:B:455:ASP:N	2.28	0.64
1:E:439:ALA:HA	1:E:443:ALA:HB3	1.78	0.64
1:F:448:LEU:C	1:F:448:LEU:CD2	2.70	0.64
1:B:451:ALA:O	1:B:456:PHE:HD1	1.81	0.64
1:B:701:VAL:HG21	1:B:853:LEU:HD23	1.80	0.64
1:B:918:GLY:C	1:B:925:GLY:HA2	2.22	0.64
1:C:508:ARG:HG3	1:C:508:ARG:NH1	2.00	0.64
1:D:323:TYR:C	1:D:323:TYR:HD1	2.05	0.64
1:D:445:VAL:HA	1:D:493:SER:HB2	1.79	0.64
1:D:446:CYS:HB2	1:D:448:LEU:CD1	2.27	0.64
1:E:281:ALA:CB	1:E:287:GLY:HA3	2.26	0.64
1:F:882:ARG:NH1	1:F:886:ASN:CG	2.52	0.64
1:B:298:LEU:O	1:B:299:VAL:CB	2.45	0.64
1:C:728:PHE:O	1:C:731:THR:HG22	1.97	0.64
1:E:363:HIS:HA	1:E:377:TYR:O	1.98	0.64
1:B:148:ARG:NH1	1:B:148:ARG:HB2	2.11	0.64
1:E:575:GLY:HA3	1:E:584:ARG:H	1.63	0.64
1:F:92:ASN:HD21	1:F:94:ASN:HB3	1.60	0.64
1:B:866:VAL:HG23	1:B:897:THR:HB	1.80	0.64
1:B:132:THR:O	1:B:135:GLN:CB	2.45	0.64
1:B:439:ALA:O	1:B:443:ALA:CB	2.46	0.64
1:D:646:LEU:HD22	1:D:695:LEU:HD21	1.79	0.64
1:E:732:THR:O	1:E:736:VAL:HG13	1.98	0.64
1:B:300:VAL:CG1	1:B:301:PRO:N	2.61	0.64
1:B:431:GLY:HA3	1:B:458:ASN:HB3	1.78	0.64
1:C:648:VAL:HG22	1:C:912:ASP:OD2	1.98	0.64
1:C:220:ASP:O	1:C:222:VAL:N	2.30	0.64
1:D:131:GLN:HE21	1:D:139:GLN:HE22	1.43	0.64
1:F:14:ASN:O	1:F:584:ARG:NH1	2.30	0.64
1:A:160:LYS:CB	1:A:198:LYS:HA	2.24	0.64
1:A:383:VAL:HG22	1:A:386:PHE:HB2	1.79	0.64
1:B:368:ASN:HB3	1:B:372:ARG:H	1.62	0.64
1:D:306:THR:C	1:D:307:LEU:HD13	2.22	0.64
1:E:284:GLU:CG	1:E:414:VAL:HG11	2.26	0.64
1:A:668:LEU:C	1:A:668:LEU:CD1	2.72	0.63
1:C:420:LEU:HD22	1:C:424:ILE:HG21	1.79	0.63
1:E:178:VAL:O	1:E:185:HIS:HB2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:698:LEU:HD12	1:F:866:VAL:HG13	1.80	0.63
1:F:914:ILE:CD1	1:F:937:VAL:HG21	2.27	0.63
1:A:757:THR:O	1:A:757:THR:HG22	1.98	0.63
1:C:317:ASN:CA	1:C:321:ALA:HB2	2.28	0.63
1:D:768:PHE:CD1	1:D:768:PHE:N	2.66	0.63
1:E:460:LEU:HD22	1:E:460:LEU:N	2.12	0.63
1:F:612:ILE:CD1	1:F:882:ARG:HG2	2.29	0.63
1:F:872:PRO:HG2	1:F:873:THR:H	1.63	0.63
1:B:728:PHE:O	1:B:731:THR:HG22	1.99	0.63
1:C:232:ILE:HD13	1:C:266:ASP:HB3	1.80	0.63
1:C:621:VAL:HG13	1:C:645:PRO:HB3	1.81	0.63
1:D:96:ARG:HA	1:D:419:ARG:HH22	1.63	0.63
1:A:119:PRO:HG3	1:A:268:LEU:HD13	1.80	0.63
1:A:269:GLU:OE1	1:A:269:GLU:CA	2.47	0.63
1:A:441:SER:C	1:A:444:GLU:HG2	2.22	0.63
1:B:576:PRO:CD	1:B:586:VAL:HG23	2.19	0.63
1:E:412:CYS:O	1:E:415:CYS:SG	2.56	0.63
1:F:450:ILE:O	1:F:450:ILE:HG12	1.97	0.63
1:F:657:GLY:H	1:F:660:LYS:CD	2.11	0.63
1:A:163:PHE:HB3	1:A:166:LEU:HB3	1.79	0.63
1:A:304:ASP:C	1:A:305:ARG:HG2	2.23	0.63
1:B:508:ARG:HG3	1:B:508:ARG:NH1	1.98	0.63
1:C:171:ASN:OD1	1:C:187:LEU:HB3	1.98	0.63
1:C:444:GLU:HB3	1:C:450:ILE:CG2	2.28	0.63
1:C:520:VAL:O	1:E:81:SER:HA	1.99	0.63
1:D:784:TYR:CE2	1:D:798:VAL:HB	2.34	0.63
1:E:706:ILE:HD11	1:E:851:VAL:HG11	1.80	0.63
1:E:763:LYS:HB2	1:E:773:TYR:CE1	2.34	0.63
1:A:159:ARG:HH11	1:A:159:ARG:CG	2.12	0.63
1:A:404:GLU:HA	1:A:407:MET:CE	2.27	0.63
1:A:441:SER:O	1:A:450:ILE:HG12	1.98	0.63
1:C:190:PRO:HB2	1:C:191:PRO:CD	2.28	0.63
1:C:429:LEU:HD13	1:C:458:ASN:HD21	1.63	0.63
1:D:178:VAL:CG2	1:D:187:LEU:HD13	2.29	0.63
1:E:305:ARG:O	1:E:308:ALA:CB	2.47	0.63
1:E:601:ILE:HD12	1:E:601:ILE:H	1.64	0.63
1:F:344:ARG:O	1:F:344:ARG:HG2	1.99	0.63
1:A:94:ASN:OD1	1:A:95:PRO:HD2	1.99	0.63
1:A:148:ARG:HB3	1:A:238:VAL:HG12	1.81	0.63
1:C:226:LEU:O	1:C:231:GLY:N	2.28	0.63
1:A:346:LEU:HD12	1:A:346:LEU:N	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:ILE:CG2	1:A:495:SER:CB	2.69	0.63
1:B:397:GLU:HG2	1:B:398:GLN:HG2	1.80	0.63
1:B:749:LYS:NZ	1:D:168:ASP:HB3	2.14	0.63
1:E:440:LYS:CD	1:E:454:ALA:CB	2.53	0.63
1:F:384:LEU:HA	1:F:387:LEU:HB3	1.81	0.63
1:B:533:LEU:CD2	1:B:537:ASP:HB2	2.29	0.63
1:D:178:VAL:HG21	1:D:187:LEU:HD13	1.81	0.63
1:D:882:ARG:HH22	1:D:883:LYS:HE2	1.64	0.63
1:A:625:ARG:HE	1:A:694:TYR:HE2	1.45	0.62
1:A:648:VAL:HG22	1:A:912:ASP:OD2	1.98	0.62
1:B:891:LEU:O	1:B:896:ASN:HB2	1.99	0.62
1:C:446:CYS:HA	1:C:450:ILE:CG2	2.29	0.62
1:E:150:LEU:HD22	1:E:236:GLU:O	1.99	0.62
1:F:453:CYS:HA	1:F:456:PHE:HD2	1.62	0.62
1:F:871:GLU:HA	1:F:902:GLU:OE2	1.99	0.62
1:A:346:LEU:CB	1:A:349:LYS:HD3	2.28	0.62
1:A:873:THR:HB	1:A:902:GLU:OE2	1.99	0.62
1:B:315:TRP:HZ2	1:B:383:VAL:O	1.81	0.62
1:B:375:SER:C	1:B:377:TYR:H	2.07	0.62
1:C:312:VAL:C	1:C:314:PRO:HD2	2.23	0.62
1:C:466:GLU:HA	1:C:469:ILE:HG22	1.80	0.62
1:E:286:SER:HB2	1:E:288:LEU:HD21	1.80	0.62
1:E:701:VAL:HG21	1:E:853:LEU:HD23	1.81	0.62
1:F:542:ILE:CD1	1:F:564:THR:HA	2.28	0.62
1:B:298:LEU:HD22	1:B:298:LEU:N	2.14	0.62
1:E:323:TYR:CD1	1:E:323:TYR:C	2.76	0.62
1:E:444:GLU:CD	1:E:450:ILE:CG1	2.72	0.62
1:A:456:PHE:C	1:A:458:ASN:N	2.58	0.62
1:B:428:THR:HB	1:B:435:GLY:HA3	1.81	0.62
1:B:578:ALA:HB1	1:B:833:TYR:CB	2.29	0.62
1:B:814:GLU:N	1:B:815:PRO:HD2	2.13	0.62
1:C:459:ALA:HB2	1:C:478:ARG:HH12	1.65	0.62
1:C:732:THR:O	1:C:736:VAL:HG13	1.99	0.62
1:D:585:ILE:O	1:D:585:ILE:HG22	1.98	0.62
1:E:358:ALA:O	1:E:360:GLU:N	2.22	0.62
1:F:347:PRO:HB2	1:F:350:ALA:HB2	1.80	0.62
1:F:354:ILE:HG22	1:F:354:ILE:O	1.99	0.62
1:B:18:VAL:HB	1:B:585:ILE:CD1	2.29	0.62
1:B:68:GLN:NE2	1:B:764:ILE:HD11	2.14	0.62
1:E:323:TYR:CE1	1:E:327:MET:HG2	2.33	0.62
1:E:534:HIS:HB2	1:E:655:VAL:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:625:ARG:HG2	1:E:694:TYR:CE2	2.35	0.62
1:A:210:VAL:O	1:A:210:VAL:HG12	1.99	0.62
1:B:382:GLY:O	1:B:383:VAL:CB	2.45	0.62
1:B:727:LEU:HD11	1:B:816:ILE:HG12	1.82	0.62
1:D:670:ALA:HA	1:D:681:GLN:NE2	2.14	0.62
1:D:701:VAL:HG12	1:D:849:GLN:CG	2.26	0.62
1:E:162:GLU:HB2	1:E:195:LYS:HG2	1.81	0.62
1:E:450:ILE:CG2	1:E:451:ALA:N	2.62	0.62
1:F:453:CYS:HA	1:F:456:PHE:CD2	2.34	0.62
1:A:858:GLN:HG3	1:A:858:GLN:O	2.00	0.62
1:D:706:ILE:HD11	1:D:851:VAL:HG11	1.81	0.62
1:D:801:VAL:CG2	1:D:813:PHE:HZ	2.12	0.62
1:E:429:LEU:H	1:E:435:GLY:HA3	1.64	0.62
1:F:118:THR:CB	1:F:119:PRO:HD2	2.29	0.62
1:F:328:MET:SD	1:F:354:ILE:HD13	2.39	0.62
1:F:857:LEU:C	1:F:857:LEU:HD13	2.24	0.62
1:A:515:ILE:HG12	1:A:548:LEU:HG	1.82	0.62
1:B:299:VAL:HG23	1:B:313:ALA:N	2.14	0.62
1:C:437:HIS:CB	1:C:440:LYS:HD2	2.29	0.62
1:E:352:LYS:HD2	1:E:356:GLU:CG	2.28	0.62
1:E:533:LEU:CD2	1:E:537:ASP:HB2	2.29	0.62
1:A:255:LEU:HD11	1:A:268:LEU:HD11	1.80	0.62
1:B:12:GLU:HG3	1:B:13:HIS:HD2	1.65	0.62
1:B:233:VAL:O	1:B:251:PHE:HB3	2.00	0.62
1:C:575:GLY:HA3	1:C:584:ARG:H	1.65	0.62
1:D:422:PRO:HA	1:D:425:LEU:HB2	1.81	0.62
1:F:872:PRO:HD2	1:F:902:GLU:OE2	1.99	0.62
1:F:916:ASP:OD2	1:F:943:SER:OG	2.09	0.62
1:A:424:ILE:HG22	1:A:437:HIS:CE1	2.34	0.62
1:A:451:ALA:O	1:A:455:ASP:HB3	2.00	0.62
1:B:767:ASN:O	1:D:61:TYR:CE2	2.53	0.62
1:C:275:PHE:CE1	1:C:419:ARG:HD3	2.35	0.62
1:C:449:SER:O	1:C:452:ASP:N	2.27	0.62
1:C:651:SER:HB2	1:C:914:ILE:HG22	1.80	0.62
1:D:194:LYS:HB3	1:D:197:GLU:OE1	1.99	0.62
1:D:451:ALA:O	1:D:455:ASP:N	2.20	0.62
1:E:305:ARG:NE	1:E:308:ALA:CB	2.63	0.62
1:C:701:VAL:HG12	1:C:849:GLN:CG	2.23	0.61
1:D:621:VAL:CG1	1:D:645:PRO:HB3	2.30	0.61
1:E:701:VAL:HB	1:E:869:LEU:HD23	1.82	0.61
1:F:118:THR:HA	1:F:427:VAL:HG22	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:695:LEU:HD23	1:F:864:ARG:CG	2.30	0.61
1:A:148:ARG:HH21	1:A:207:ARG:HD3	1.64	0.61
1:A:378:ALA:C	1:A:380:PHE:H	2.08	0.61
1:A:448:LEU:C	1:A:448:LEU:CD2	2.72	0.61
1:B:152:LEU:HD22	1:B:202:GLU:HB3	1.82	0.61
1:B:561:ASP:O	1:B:565:ILE:HG13	1.99	0.61
1:B:936:ASP:O	1:B:939:ALA:HB3	2.00	0.61
1:F:323:TYR:CE1	1:F:327:MET:HG2	2.35	0.61
1:A:216:ARG:HA	1:A:216:ARG:HE	1.62	0.61
1:A:346:LEU:H	1:A:349:LYS:CE	2.13	0.61
1:A:732:THR:O	1:A:736:VAL:HG13	2.00	0.61
1:B:184:VAL:CG1	1:B:185:HIS:H	2.11	0.61
1:B:706:ILE:HD11	1:B:851:VAL:CG1	2.30	0.61
1:D:377:TYR:O	1:D:378:ALA:CB	2.47	0.61
1:D:858:GLN:HG3	1:D:858:GLN:O	1.99	0.61
1:E:383:VAL:CG1	1:E:386:PHE:HB2	2.30	0.61
1:E:452:ASP:O	1:E:455:ASP:N	2.33	0.61
1:F:30:PHE:N	1:F:30:PHE:HD1	1.98	0.61
1:F:319:HIS:C	1:F:321:ALA:N	2.58	0.61
1:A:60:ALA:O	1:A:63:ARG:HB3	2.00	0.61
1:B:621:VAL:HG13	1:B:645:PRO:HB3	1.83	0.61
1:C:186:PRO:O	1:C:190:PRO:HD2	2.01	0.61
1:C:291:ARG:HG3	1:C:412:CYS:HB2	1.81	0.61
1:D:33:LEU:O	1:D:36:SER:HB2	2.01	0.61
1:E:444:GLU:HG2	1:E:450:ILE:HB	1.82	0.61
1:E:462:LEU:HB3	1:E:467:GLN:HG2	1.82	0.61
1:F:355:LEU:O	1:F:385:ALA:HB3	2.00	0.61
1:A:466:GLU:HA	1:A:469:ILE:HG22	1.83	0.61
1:A:585:ILE:O	1:A:585:ILE:HG22	1.99	0.61
1:D:120:HIS:O	1:D:426:ALA:CB	2.48	0.61
1:F:412:CYS:HB3	1:F:415:CYS:CB	2.30	0.61
1:F:602:THR:HG22	1:F:606:LEU:HD12	1.83	0.61
1:A:337:PHE:HB3	1:A:346:LEU:HD22	1.82	0.61
1:A:918:GLY:C	1:A:925:GLY:HA2	2.25	0.61
1:B:347:PRO:HD2	1:B:349:LYS:NZ	2.16	0.61
1:E:621:VAL:HG13	1:E:645:PRO:HB3	1.83	0.61
1:F:15:LEU:HD12	1:F:15:LEU:O	2.00	0.61
1:A:346:LEU:HD13	1:A:349:LYS:HD3	1.83	0.61
1:B:148:ARG:HB2	1:B:148:ARG:HH11	1.65	0.61
1:E:462:LEU:HD13	1:E:467:GLN:HA	1.81	0.61
1:A:533:LEU:CD2	1:A:537:ASP:HB2	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:816:ILE:H	1:A:816:ILE:HD12	1.66	0.61
1:C:670:ALA:HA	1:C:681:GLN:HE21	1.66	0.61
1:D:305:ARG:HH12	1:D:312:VAL:CB	2.11	0.61
1:D:446:CYS:SG	1:D:449:SER:CB	2.88	0.61
1:E:350:ALA:O	1:E:354:ILE:HG13	2.01	0.61
1:F:30:PHE:CE2	1:F:41:LEU:HG	2.36	0.61
1:B:858:GLN:HG3	1:B:858:GLN:O	2.00	0.61
1:B:873:THR:HB	1:B:902:GLU:OE2	2.01	0.61
1:D:303:PRO:HB2	1:D:310:GLY:O	2.00	0.61
1:A:672:LEU:HD23	1:A:692:LEU:HD22	1.83	0.61
1:C:359:ASP:O	1:C:360:GLU:CD	2.44	0.61
1:D:445:VAL:CA	1:D:493:SER:HB2	2.31	0.61
1:D:618:ARG:NH2	1:D:909:LYS:O	2.34	0.61
1:F:503:GLY:O	1:F:504:GLY:C	2.43	0.61
1:F:593:GLU:O	1:F:597:ASN:HB2	2.00	0.61
1:B:121:CYS:SG	1:B:124:CYS:N	2.65	0.60
1:B:289:GLY:O	1:B:412:CYS:N	2.26	0.60
1:B:351:ARG:HG3	1:B:355:LEU:HD12	1.83	0.60
1:C:768:PHE:N	1:C:768:PHE:CD1	2.69	0.60
1:D:442:ILE:HG22	1:D:495:SER:CB	2.31	0.60
1:F:330:GLY:HA3	1:F:362:VAL:CG1	2.31	0.60
1:F:877:HIS:O	1:F:881:ILE:HG12	2.02	0.60
1:B:88:GLN:HE22	1:B:531:ILE:HD13	1.66	0.60
1:B:171:ASN:ND2	1:B:187:LEU:HG	2.16	0.60
1:C:437:HIS:CD2	1:C:440:LYS:CE	2.84	0.60
1:C:447:GLU:OE1	1:C:447:GLU:HA	1.99	0.60
1:D:118:THR:O	1:D:120:HIS:CD2	2.53	0.60
1:E:466:GLU:HA	1:E:469:ILE:HG22	1.83	0.60
1:F:533:LEU:HG	1:F:537:ASP:HB2	1.83	0.60
1:F:571:ILE:HG21	1:F:594:LEU:CD2	2.31	0.60
1:A:291:ARG:HH11	1:A:291:ARG:CB	2.14	0.60
1:A:346:LEU:HD13	1:A:349:LYS:CE	2.28	0.60
1:B:300:VAL:CG1	1:B:301:PRO:HD2	2.31	0.60
1:C:452:ASP:O	1:C:456:PHE:HB2	2.01	0.60
1:D:20:LEU:HD21	1:D:585:ILE:HG12	1.82	0.60
1:D:508:ARG:HG3	1:D:508:ARG:NH1	1.95	0.60
1:F:118:THR:HB	1:F:119:PRO:HD2	1.83	0.60
1:F:447:GLU:HB2	1:F:490:GLU:CA	2.28	0.60
1:B:702:ASP:HB3	1:B:852:LYS:HZ2	1.66	0.60
1:C:281:ALA:HB1	1:C:287:GLY:CA	2.31	0.60
1:C:793:TYR:CD1	1:C:793:TYR:C	2.79	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:ARG:CD	1:D:413:PRO:HD2	2.30	0.60
1:D:323:TYR:C	1:D:323:TYR:CD1	2.77	0.60
1:D:712:SER:O	1:D:713:ASN:HB3	2.01	0.60
1:E:187:LEU:C	1:E:189:ASP:H	2.09	0.60
1:A:20:LEU:CD1	1:A:41:LEU:HD11	2.28	0.60
1:C:533:LEU:CD2	1:C:537:ASP:HB2	2.31	0.60
1:D:455:ASP:OD1	1:D:478:ARG:HD2	2.01	0.60
1:D:466:GLU:HA	1:D:469:ILE:HG22	1.84	0.60
1:D:727:LEU:HD11	1:D:816:ILE:HG12	1.83	0.60
1:E:305:ARG:NH2	1:E:308:ALA:HB1	2.16	0.60
1:A:732:THR:HA	1:A:735:LYS:HE2	1.84	0.60
1:B:578:ALA:CB	1:B:833:TYR:HB3	2.31	0.60
1:B:712:SER:O	1:B:840:ALA:CB	2.46	0.60
1:B:732:THR:O	1:B:736:VAL:HG13	2.01	0.60
1:D:578:ALA:HB1	1:D:833:TYR:CB	2.31	0.60
1:E:372:ARG:CG	1:E:374:ARG:HG3	2.31	0.60
1:E:439:ALA:O	1:E:443:ALA:C	2.45	0.60
1:E:440:LYS:NZ	1:E:440:LYS:CB	2.64	0.60
1:F:12:GLU:OE2	1:F:73:ASP:HB2	2.01	0.60
1:C:127:ARG:HB3	1:C:127:ARG:CZ	2.30	0.60
1:C:381:GLU:O	1:C:383:VAL:N	2.28	0.60
1:C:578:ALA:HB1	1:C:833:TYR:CB	2.29	0.60
1:D:96:ARG:HH21	1:D:288:LEU:CD2	2.12	0.60
1:D:298:LEU:HD22	1:D:406:PHE:O	2.01	0.60
1:E:597:ASN:HD22	1:E:597:ASN:C	2.10	0.60
1:A:216:ARG:O	1:A:220:ASP:HB2	2.01	0.60
1:B:701:VAL:HB	1:B:869:LEU:HD23	1.84	0.60
1:C:585:ILE:HG22	1:C:585:ILE:O	2.00	0.60
1:C:727:LEU:HD11	1:C:816:ILE:HG12	1.83	0.60
1:D:306:THR:O	1:D:307:LEU:CD1	2.47	0.60
1:E:119:PRO:C	1:E:120:HIS:CD2	2.80	0.60
1:E:412:CYS:SG	1:E:414:VAL:CG1	2.89	0.60
1:F:30:PHE:N	1:F:30:PHE:CD1	2.69	0.60
1:A:701:VAL:HB	1:A:869:LEU:HD23	1.84	0.60
1:B:562:GLU:O	1:B:566:GLU:CG	2.39	0.60
1:D:793:TYR:CD1	1:D:793:TYR:C	2.79	0.60
1:D:893:ASP:C	1:D:895:GLY:H	2.10	0.60
1:E:221:SER:O	1:E:224:THR:N	2.35	0.60
1:E:737:ARG:NH1	1:E:790:GLU:OE1	2.35	0.60
1:B:300:VAL:CG1	1:B:301:PRO:CD	2.79	0.59
1:B:422:PRO:HA	1:B:425:LEU:HG	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:675:ARG:CZ	1:C:692:LEU:HD22	2.31	0.59
1:E:171:ASN:HD21	1:E:188:THR:HG22	1.66	0.59
1:F:12:GLU:CD	1:F:73:ASP:HB2	2.27	0.59
1:A:225:ALA:HB3	1:A:233:VAL:HG12	1.84	0.59
1:A:391:MET:CE	1:A:394:THR:HB	2.31	0.59
1:B:755:ALA:CB	1:B:778:VAL:CG2	2.80	0.59
1:C:87:ASP:HA	1:C:527:ASP:HB3	1.84	0.59
1:C:356:GLU:CG	1:C:381:GLU:CB	2.67	0.59
1:C:356:GLU:H	1:C:383:VAL:CG1	2.16	0.59
1:C:359:ASP:C	1:C:360:GLU:HG2	2.27	0.59
1:D:575:GLY:HA3	1:D:584:ARG:H	1.66	0.59
1:F:99:VAL:HG21	1:F:492:LEU:HD12	1.84	0.59
1:B:354:ILE:CA	1:B:384:LEU:HD23	2.33	0.59
1:B:368:ASN:HD22	1:B:372:ARG:HB3	1.66	0.59
1:C:120:HIS:HB2	1:C:426:ALA:HB1	1.84	0.59
1:C:143:MET:O	1:C:144:PRO:C	2.44	0.59
1:C:219:THR:HG23	1:C:220:ASP:OD1	2.03	0.59
1:C:284:GLU:CD	1:C:291:ARG:HH11	2.00	0.59
1:C:706:ILE:HD11	1:C:851:VAL:HG11	1.84	0.59
1:E:33:LEU:HD12	1:E:577:GLY:HA2	1.82	0.59
1:E:422:PRO:HA	1:E:425:LEU:HG	1.84	0.59
1:A:424:ILE:O	1:A:427:VAL:HG23	2.01	0.59
1:A:621:VAL:HG13	1:A:645:PRO:HB3	1.84	0.59
1:B:49:GLU:HG2	1:B:72:PRO:HG2	1.83	0.59
1:B:452:ASP:OD1	1:B:452:ASP:N	2.33	0.59
1:C:814:GLU:N	1:C:815:PRO:HD2	2.18	0.59
1:E:402:ARG:NH2	1:E:680:ARG:HH21	2.01	0.59
1:E:440:LYS:HD2	1:E:454:ALA:HB1	1.81	0.59
1:E:452:ASP:OD1	1:E:452:ASP:N	2.26	0.59
1:B:25:ASP:N	1:B:554:THR:HB	2.17	0.59
1:B:515:ILE:HD13	1:B:548:LEU:CG	2.23	0.59
1:D:444:GLU:OE2	1:D:449:SER:CB	2.50	0.59
1:E:366:TYR:H	1:E:375:SER:CB	2.14	0.59
1:E:459:ALA:HA	1:E:478:ARG:HH22	1.67	0.59
1:E:648:VAL:HG22	1:E:912:ASP:OD2	2.03	0.59
1:F:355:LEU:CA	1:F:383:VAL:HG11	2.31	0.59
1:A:257:CYS:SG	1:A:258:PRO:HD2	2.42	0.59
1:C:100:GLY:HA2	1:C:494:LEU:HD22	1.84	0.59
1:C:379:ASP:O	1:C:380:PHE:C	2.45	0.59
1:C:437:HIS:CG	1:C:440:LYS:NZ	2.61	0.59
1:C:712:SER:O	1:C:713:ASN:HB3	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:GLN:HG2	1:D:135:GLN:N	2.17	0.59
1:E:68:GLN:HE21	1:E:764:ILE:HG12	1.68	0.59
1:E:307:LEU:H	1:E:310:GLY:HA2	1.68	0.59
1:E:440:LYS:C	1:E:444:GLU:HB2	2.12	0.59
1:F:330:GLY:HA3	1:F:362:VAL:CG2	2.32	0.59
1:F:422:PRO:O	1:F:425:LEU:N	2.36	0.59
1:F:447:GLU:CB	1:F:490:GLU:HA	2.30	0.59
1:F:658:SER:HB2	1:F:917:LEU:O	2.02	0.59
1:E:867:TYR:HB2	1:E:898:VAL:HG22	1.84	0.59
1:F:381:GLU:HB3	1:F:383:VAL:CG2	2.19	0.59
1:F:443:ALA:C	1:F:444:GLU:OE1	2.45	0.59
1:A:865:THR:H	1:A:896:ASN:ND2	1.99	0.59
1:B:88:GLN:OE1	1:B:531:ILE:HG21	2.02	0.59
1:B:98:THR:OG1	1:B:101:THR:HG23	2.03	0.59
1:B:576:PRO:CD	1:B:586:VAL:HG21	2.24	0.59
1:C:444:GLU:CD	1:C:449:SER:OG	2.46	0.59
1:E:404:GLU:HG2	1:E:407:MET:CE	2.32	0.59
1:E:585:ILE:O	1:E:585:ILE:HG22	2.01	0.59
1:F:935:GLU:OE1	1:F:935:GLU:N	2.30	0.59
1:A:136:ILE:O	1:A:140:VAL:HG12	2.03	0.59
1:A:402:ARG:HD3	1:A:680:ARG:HB2	1.85	0.59
1:B:466:GLU:HA	1:B:469:ILE:HG22	1.85	0.59
1:D:87:ASP:HA	1:D:527:ASP:HB3	1.85	0.59
1:D:578:ALA:CB	1:D:833:TYR:HB3	2.32	0.59
1:D:732:THR:O	1:D:736:VAL:HG13	2.03	0.59
1:D:786:ARG:H	1:D:786:ARG:CD	2.16	0.59
1:F:11:ARG:HH12	1:F:75:ASP:CG	2.08	0.59
1:F:28:ILE:N	1:F:28:ILE:HD12	2.18	0.59
1:A:237:PHE:HD1	1:A:237:PHE:H	1.49	0.59
1:A:595:LEU:HB3	1:B:468:ALA:HB2	1.85	0.59
1:B:273:PHE:CB	1:B:437:HIS:CE1	2.86	0.59
1:B:816:ILE:H	1:B:816:ILE:HD12	1.68	0.59
1:D:701:VAL:CG1	1:D:849:GLN:HG2	2.24	0.59
1:E:459:ALA:HA	1:E:478:ARG:HH12	1.68	0.59
1:F:557:VAL:CG1	1:F:559:GLU:HG2	2.32	0.59
1:F:684:GLY:O	1:F:686:HIS:N	2.29	0.59
1:A:297:GLU:O	1:A:299:VAL:HG12	2.03	0.58
1:A:442:ILE:CG2	1:A:495:SER:CA	2.80	0.58
1:A:649:LEU:HD23	1:A:911:SER:HA	1.85	0.58
1:A:675:ARG:NH2	1:A:692:LEU:HG	2.17	0.58
1:B:27:LEU:C	1:B:27:LEU:CD2	2.76	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:767:ASN:O	1:D:61:TYR:HE2	1.86	0.58
1:C:360:GLU:C	1:C:361:GLN:CD	2.71	0.58
1:D:12:GLU:HB2	1:D:15:LEU:HD12	1.85	0.58
1:D:156:VAL:CB	1:D:201:ILE:H	2.15	0.58
1:D:651:SER:HB2	1:D:914:ILE:HG22	1.83	0.58
1:E:168:ASP:OD1	1:E:168:ASP:N	2.36	0.58
1:F:622:ASP:HB3	1:F:625:ARG:O	2.03	0.58
1:A:102:ILE:HD11	1:A:498:ALA:HB2	1.81	0.58
1:B:215:LYS:CA	1:B:215:LYS:CE	2.69	0.58
1:E:12:GLU:HB2	1:E:15:LEU:HD12	1.85	0.58
1:E:323:TYR:CE1	1:E:327:MET:CG	2.87	0.58
1:F:885:LEU:O	1:F:888:ILE:HG22	2.02	0.58
1:A:866:VAL:HG23	1:A:897:THR:HB	1.86	0.58
1:B:68:GLN:HE21	1:B:764:ILE:CD1	2.17	0.58
1:B:275:PHE:HB2	1:B:287:GLY:HA2	1.83	0.58
1:C:442:ILE:CG2	1:C:495:SER:N	2.66	0.58
1:C:858:GLN:HG3	1:C:858:GLN:O	2.02	0.58
1:F:444:GLU:OE1	1:F:444:GLU:N	2.37	0.58
1:A:126:GLU:O	1:A:127:ARG:C	2.44	0.58
1:A:337:PHE:HB2	1:A:346:LEU:HD22	1.86	0.58
1:D:303:PRO:CB	1:D:310:GLY:O	2.51	0.58
1:E:352:LYS:C	1:E:354:ILE:H	2.11	0.58
1:E:399:MET:HE2	1:E:403:TYR:CZ	2.38	0.58
1:A:456:PHE:C	1:A:458:ASN:H	2.10	0.58
1:D:306:THR:O	1:D:307:LEU:CB	2.51	0.58
1:E:706:ILE:HD11	1:E:851:VAL:CG1	2.33	0.58
1:E:727:LEU:HD22	1:E:793:TYR:CE2	2.30	0.58
1:F:619:ARG:NH2	1:F:892:VAL:HG12	2.18	0.58
1:B:768:PHE:CD1	1:B:768:PHE:N	2.71	0.58
1:B:882:ARG:HH22	1:B:883:LYS:HE2	1.68	0.58
1:C:134:GLN:NE2	1:C:138:ASP:OD1	2.35	0.58
1:C:786:ARG:H	1:C:786:ARG:CD	2.16	0.58
1:C:816:ILE:HD12	1:C:816:ILE:H	1.67	0.58
1:E:305:ARG:O	1:E:308:ALA:HB2	2.02	0.58
1:F:337:PHE:CZ	1:F:347:PRO:CB	2.87	0.58
1:F:455:ASP:OD1	1:F:478:ARG:HG2	2.03	0.58
1:F:684:GLY:O	1:F:686:HIS:CD2	2.56	0.58
1:A:20:LEU:CD2	1:A:585:ILE:HG12	2.16	0.58
1:A:702:ASP:O	1:A:849:GLN:HG3	2.04	0.58
1:A:706:ILE:HD11	1:A:851:VAL:HG11	1.85	0.58
1:B:354:ILE:CB	1:B:384:LEU:HD23	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:793:TYR:C	1:B:793:TYR:CD1	2.82	0.58
1:D:254:LYS:O	1:D:255:LEU:HB2	2.02	0.58
1:E:786:ARG:H	1:E:786:ARG:CD	2.16	0.58
1:F:40:SER:O	1:F:44:ASP:HB2	2.02	0.58
1:A:814:GLU:N	1:A:815:PRO:HD2	2.19	0.58
1:A:936:ASP:O	1:A:939:ALA:HB3	2.02	0.58
1:B:163:PHE:CE1	1:D:755:ALA:HB2	2.38	0.58
1:E:712:SER:O	1:E:713:ASN:HB3	2.03	0.58
1:E:814:GLU:N	1:E:815:PRO:HD2	2.18	0.58
1:F:612:ILE:HG23	1:F:614:ILE:HG12	1.85	0.58
1:F:622:ASP:OD2	1:F:625:ARG:HB2	2.03	0.58
1:A:119:PRO:HG3	1:A:268:LEU:HD11	1.84	0.58
1:A:234:VAL:HB	1:A:250:ARG:HG2	1.84	0.58
1:A:266:ASP:OD1	1:A:266:ASP:N	2.31	0.58
1:C:119:PRO:HB2	1:C:128:VAL:HG22	1.85	0.58
1:C:578:ALA:CB	1:C:833:TYR:HB3	2.33	0.58
1:E:134:GLN:O	1:E:137:VAL:HB	2.04	0.58
1:E:442:ILE:HA	1:E:495:SER:HB3	0.59	0.58
1:E:508:ARG:HH11	1:E:508:ARG:CG	2.13	0.58
1:E:533:LEU:HD23	1:E:537:ASP:HB2	1.85	0.58
1:A:306:THR:N	1:A:309:GLN:O	2.37	0.58
1:D:153:ALA:HB1	1:D:229:ALA:HB2	1.85	0.58
1:D:296:PRO:C	1:D:299:VAL:HG22	2.29	0.58
1:D:706:ILE:HD11	1:D:851:VAL:CG1	2.34	0.58
1:E:136:ILE:HA	1:E:139:GLN:HB3	1.84	0.58
1:E:578:ALA:CB	1:E:833:TYR:HB3	2.33	0.58
1:E:902:GLU:HG3	1:E:907:VAL:HG11	1.86	0.58
1:B:584:ARG:HD2	1:C:584:ARG:HD3	1.85	0.57
1:D:171:ASN:ND2	1:D:188:THR:HA	2.12	0.57
1:F:69:MET:HG2	1:F:70:ASP:N	2.18	0.57
1:A:285:CYS:O	1:A:288:LEU:HB2	2.04	0.57
1:A:701:VAL:HG21	1:A:853:LEU:HD23	1.85	0.57
1:D:65:PHE:CZ	1:D:767:ASN:HB2	2.39	0.57
1:E:675:ARG:CZ	1:E:692:LEU:HD22	2.34	0.57
1:E:793:TYR:C	1:E:793:TYR:CD1	2.81	0.57
1:F:337:PHE:CZ	1:F:347:PRO:HA	2.38	0.57
1:B:437:HIS:CD2	1:B:437:HIS:O	2.57	0.57
1:A:305:ARG:HD2	1:A:305:ARG:N	2.19	0.57
1:A:646:LEU:HD22	1:A:695:LEU:HD21	1.85	0.57
1:E:447:GLU:O	1:E:448:LEU:C	2.47	0.57
1:E:578:ALA:HB1	1:E:833:TYR:CB	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:51:GLN:O	1:F:55:VAL:HG23	2.04	0.57
1:F:451:ALA:O	1:F:455:ASP:HB2	2.04	0.57
1:B:438:GLY:HA3	1:B:442:ILE:HG13	1.86	0.57
1:B:534:HIS:HB2	1:B:655:VAL:HA	1.84	0.57
1:F:30:PHE:HE2	1:F:41:LEU:HG	1.68	0.57
1:F:331:LEU:HA	1:F:334:ALA:HB3	1.85	0.57
1:C:524:TYR:HB2	1:C:555:LEU:HD22	1.85	0.57
1:D:936:ASP:O	1:D:939:ALA:HB3	2.05	0.57
1:E:306:THR:O	1:E:307:LEU:CB	2.48	0.57
1:E:486:ASP:O	1:E:540:ARG:NH2	2.37	0.57
1:D:533:LEU:CD2	1:D:537:ASP:HB2	2.35	0.57
1:D:675:ARG:CZ	1:D:692:LEU:HD22	2.35	0.57
1:E:347:PRO:HA	1:E:349:LYS:HG2	1.87	0.57
1:F:39:SER:O	1:F:43:PHE:HB2	2.05	0.57
1:B:420:LEU:HB2	1:B:425:LEU:HD21	1.87	0.57
1:C:171:ASN:HD21	1:C:188:THR:HA	1.70	0.57
1:C:862:THR:O	1:C:864:ARG:N	2.38	0.57
1:D:27:LEU:C	1:D:27:LEU:CD2	2.78	0.57
1:D:349:LYS:HA	1:D:352:LYS:HZ1	1.67	0.57
1:D:534:HIS:HB2	1:D:655:VAL:HA	1.86	0.57
1:E:305:ARG:CZ	1:E:308:ALA:CB	2.80	0.57
1:F:357:GLY:CA	1:F:383:VAL:HB	2.30	0.57
1:F:442:ILE:HG23	1:F:443:ALA:N	2.20	0.57
1:A:233:VAL:HG23	1:A:251:PHE:HB2	1.86	0.57
1:A:528:GLU:HG2	1:A:531:ILE:HG13	1.87	0.57
1:A:891:LEU:O	1:A:896:ASN:HB2	2.05	0.57
1:B:299:VAL:CB	1:B:313:ALA:HB3	2.35	0.57
1:B:442:ILE:CD1	1:B:494:LEU:CD1	2.83	0.57
1:C:384:LEU:O	1:C:388:GLN:NE2	2.37	0.57
1:C:459:ALA:HB2	1:C:478:ARG:NH1	2.20	0.57
1:C:732:THR:HA	1:C:735:LYS:HE2	1.87	0.57
1:C:893:ASP:C	1:C:895:GLY:H	2.12	0.57
1:D:160:LYS:HB3	1:D:198:LYS:HB3	1.85	0.57
1:D:330:GLY:HA3	1:D:362:VAL:HG11	1.86	0.57
1:D:331:LEU:HD21	1:D:335:LEU:HD13	1.86	0.57
1:F:440:LYS:N	1:F:440:LYS:CD	2.67	0.57
1:B:315:TRP:CD2	1:B:324:PHE:CD2	2.92	0.57
1:B:373:THR:CG2	1:B:374:ARG:N	2.68	0.57
1:C:442:ILE:CG2	1:C:495:SER:CB	2.76	0.57
1:C:865:THR:H	1:C:896:ASN:HD22	1.50	0.57
1:E:380:PHE:HD1	1:E:380:PHE:H	1.51	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:33:LEU:CD2	1:F:877:HIS:CD2	2.88	0.57
1:F:384:LEU:O	1:F:388:GLN:HG2	2.05	0.57
1:A:282:CYS:O	1:A:286:SER:N	2.37	0.56
1:B:299:VAL:CA	1:B:313:ALA:HB3	2.31	0.56
1:C:354:ILE:O	1:C:355:LEU:HB2	2.05	0.56
1:D:296:PRO:CA	1:D:299:VAL:HG22	2.34	0.56
1:D:298:LEU:CD1	1:D:408:ARG:NH2	2.61	0.56
1:E:65:PHE:HE1	1:E:766:MET:HA	1.70	0.56
1:B:670:ALA:HA	1:B:681:GLN:NE2	2.20	0.56
1:D:94:ASN:OD1	1:D:95:PRO:HD2	2.06	0.56
1:D:341:THR:O	1:D:342:PRO:C	2.48	0.56
1:D:891:LEU:O	1:D:896:ASN:HB2	2.05	0.56
1:A:425:LEU:HA	1:A:437:HIS:CG	2.40	0.56
1:A:429:LEU:O	1:A:435:GLY:HA2	2.05	0.56
1:A:441:SER:O	1:A:444:GLU:CG	2.51	0.56
1:A:534:HIS:HB2	1:A:655:VAL:HA	1.86	0.56
1:B:139:GLN:C	1:B:143:MET:CG	2.77	0.56
1:B:702:ASP:HB3	1:B:852:LYS:NZ	2.20	0.56
1:D:331:LEU:HD11	1:D:358:ALA:HB2	1.87	0.56
1:D:621:VAL:HG13	1:D:645:PRO:CB	2.35	0.56
1:E:441:SER:O	1:E:495:SER:HB3	2.04	0.56
1:F:427:VAL:O	1:F:436:GLU:CB	2.53	0.56
1:F:885:LEU:C	1:F:885:LEU:CD1	2.79	0.56
1:F:920:GLU:O	1:F:925:GLY:HA3	2.06	0.56
1:A:96:ARG:HH21	1:A:288:LEU:CD2	2.13	0.56
1:A:447:GLU:N	1:A:490:GLU:O	2.32	0.56
1:A:768:PHE:CD1	1:A:768:PHE:N	2.72	0.56
1:B:442:ILE:HD12	1:B:494:LEU:CD1	2.36	0.56
1:D:30:PHE:CE2	1:D:41:LEU:HD13	2.40	0.56
1:D:124:CYS:HB3	1:D:261:HIS:HE1	1.67	0.56
1:D:304:ASP:CG	1:D:306:THR:CG2	2.76	0.56
1:D:337:PHE:CB	1:D:349:LYS:HG3	2.34	0.56
1:E:858:GLN:O	1:E:858:GLN:HG3	2.06	0.56
1:F:412:CYS:HB3	1:F:415:CYS:SG	2.45	0.56
1:F:863:GLY:O	1:F:895:GLY:HA3	2.06	0.56
1:A:187:LEU:HD23	1:A:187:LEU:O	2.04	0.56
1:B:171:ASN:HA	1:B:187:LEU:CD2	2.21	0.56
1:B:446:CYS:O	1:B:450:ILE:HG22	2.06	0.56
1:B:575:GLY:CA	1:B:584:ARG:O	2.53	0.56
1:D:312:VAL:CG1	1:D:315:TRP:HB2	2.36	0.56
1:D:862:THR:O	1:D:864:ARG:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:865:THR:H	1:D:896:ASN:HD22	1.52	0.56
1:F:410:VAL:HB	1:F:411:PRO:CD	2.34	0.56
1:A:459:ALA:HB2	1:A:478:ARG:HH22	1.71	0.56
1:B:120:HIS:HD2	1:B:125:GLY:O	1.88	0.56
1:B:867:TYR:HB2	1:B:898:VAL:HG22	1.88	0.56
1:D:175:TYR:HE2	1:D:205:VAL:HG22	1.70	0.56
1:E:217:ARG:HB2	1:E:217:ARG:HH11	1.69	0.56
1:E:217:ARG:HB2	1:E:217:ARG:NH1	2.20	0.56
1:F:549:ARG:NH1	1:F:569:ASP:OD2	2.39	0.56
1:F:881:ILE:HG21	1:F:904:ASN:HD21	1.69	0.56
1:A:236:GLU:O	1:A:236:GLU:CG	2.53	0.56
1:A:391:MET:HA	1:A:394:THR:HB	1.87	0.56
1:A:862:THR:O	1:A:864:ARG:N	2.38	0.56
1:A:893:ASP:C	1:A:895:GLY:H	2.14	0.56
1:B:462:LEU:HB3	1:B:467:GLN:HG2	1.86	0.56
1:C:882:ARG:HH22	1:C:883:LYS:HE2	1.69	0.56
1:D:441:SER:O	1:D:450:ILE:HD11	2.06	0.56
1:E:277:SER:OG	1:E:278:PRO:HD2	2.06	0.56
1:F:619:ARG:HH22	1:F:892:VAL:CG1	2.18	0.56
1:B:343:TRP:CH2	1:B:350:ALA:HB1	2.40	0.56
1:B:755:ALA:HA	1:D:161:GLY:HA3	1.86	0.56
1:D:49:GLU:HG2	1:D:72:PRO:HG2	1.87	0.56
1:E:257:CYS:SG	1:E:261:HIS:CG	2.99	0.56
1:F:457:LEU:C	1:F:457:LEU:HD13	2.31	0.56
1:A:226:LEU:CD2	1:A:231:GLY:O	2.53	0.56
1:A:651:SER:HB2	1:A:914:ILE:HG22	1.87	0.56
1:A:882:ARG:HH22	1:A:883:LYS:HE2	1.70	0.56
1:B:185:HIS:CG	1:B:191:PRO:HB3	2.40	0.56
1:C:936:ASP:O	1:C:939:ALA:HB3	2.05	0.56
1:D:648:VAL:HG22	1:D:912:ASP:OD2	2.05	0.56
1:F:538:ASN:O	1:F:542:ILE:CG1	2.54	0.56
1:B:275:PHE:HB2	1:B:287:GLY:CA	2.35	0.56
1:B:354:ILE:HA	1:B:384:LEU:CB	2.34	0.56
1:C:361:GLN:CB	1:C:378:ALA:HB1	2.36	0.56
1:D:415:CYS:C	1:D:417:GLY:H	2.13	0.56
1:E:176:SER:O	1:E:187:LEU:N	2.37	0.56
1:E:295:ASP:HB3	1:E:298:LEU:CG	2.36	0.56
1:F:319:HIS:HA	1:F:322:GLU:HB3	1.87	0.56
1:A:87:ASP:HA	1:A:527:ASP:HB3	1.89	0.55
1:A:113:TYR:CZ	1:A:429:LEU:HD22	2.41	0.55
1:B:646:LEU:HD22	1:B:695:LEU:HD21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:902:GLU:HG3	1:B:907:VAL:HG11	1.87	0.55
1:E:16:ARG:HG3	1:E:584:ARG:HG3	1.87	0.55
1:E:384:LEU:O	1:E:388:GLN:HG2	2.06	0.55
1:E:459:ALA:CA	1:E:478:ARG:HH22	2.18	0.55
1:A:353:ALA:O	1:A:384:LEU:CB	2.44	0.55
1:A:444:GLU:HB2	1:A:450:ILE:HG12	1.88	0.55
1:B:116:ALA:O	1:B:429:LEU:HD13	2.05	0.55
1:B:315:TRP:CE2	1:B:324:PHE:CE2	2.94	0.55
1:D:149:PHE:HA	1:D:236:GLU:O	2.06	0.55
1:F:11:ARG:CZ	1:F:75:ASP:OD1	2.53	0.55
1:F:396:SER:HA	1:F:400:LYS:HD2	1.88	0.55
1:F:427:VAL:O	1:F:436:GLU:HB3	2.06	0.55
1:F:447:GLU:CG	1:F:489:LEU:O	2.54	0.55
1:F:536:ARG:NH1	1:F:944:TYR:CZ	2.74	0.55
1:F:852:LYS:O	1:F:855:SER:HB3	2.06	0.55
1:B:391:MET:HE1	1:B:395:GLU:HB2	1.89	0.55
1:B:442:ILE:HG23	1:B:494:LEU:HB3	1.88	0.55
1:C:453:CYS:C	1:C:455:ASP:N	2.61	0.55
1:C:649:LEU:HD23	1:C:911:SER:HA	1.87	0.55
1:E:305:ARG:HD3	1:E:305:ARG:N	2.11	0.55
1:F:502:SER:HB3	1:F:505:GLU:OE2	2.05	0.55
1:B:732:THR:HA	1:B:735:LYS:HE2	1.88	0.55
1:C:317:ASN:HA	1:C:321:ALA:CB	2.37	0.55
1:C:446:CYS:CA	1:C:450:ILE:HG23	2.36	0.55
1:E:18:VAL:HB	1:E:585:ILE:HD12	1.89	0.55
1:E:284:GLU:CB	1:E:414:VAL:HG11	2.36	0.55
1:E:727:LEU:HD11	1:E:816:ILE:HG12	1.88	0.55
1:F:453:CYS:O	1:F:454:ALA:C	2.48	0.55
1:F:627:LEU:HD12	1:F:628:THR:N	2.22	0.55
1:A:304:ASP:OD2	1:A:341:THR:O	2.24	0.55
1:B:62:ALA:HB1	1:B:768:PHE:CZ	2.42	0.55
1:B:359:ASP:O	1:B:360:GLU:HB2	2.07	0.55
1:C:391:MET:HB3	1:C:403:TYR:CD2	2.42	0.55
1:F:695:LEU:HA	1:F:864:ARG:HB3	1.88	0.55
1:B:163:PHE:HE1	1:D:755:ALA:HB2	1.70	0.55
1:C:410:VAL:HB	1:C:411:PRO:HD2	1.88	0.55
1:C:446:CYS:SG	1:C:447:GLU:N	2.78	0.55
1:D:118:THR:HG23	1:D:119:PRO:HD2	1.89	0.55
1:E:356:GLU:HG2	1:E:358:ALA:N	2.21	0.55
1:E:440:LYS:HE3	1:E:454:ALA:HB3	1.80	0.55
1:E:862:THR:O	1:E:864:ARG:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:865:THR:H	1:E:896:ASN:HD22	1.51	0.55
1:F:7:VAL:HA	1:F:77:ILE:HG22	1.89	0.55
1:F:315:TRP:CE3	1:F:328:MET:HE1	2.39	0.55
1:F:442:ILE:CG2	1:F:443:ALA:N	2.70	0.55
1:A:130:ARG:HB3	1:A:254:LYS:HA	1.87	0.55
1:A:754:GLU:H	1:A:754:GLU:CD	2.15	0.55
1:C:94:ASN:OD1	1:C:95:PRO:CD	2.53	0.55
1:C:136:ILE:O	1:C:139:GLN:CG	2.55	0.55
1:D:143:MET:SD	1:D:144:PRO:HD2	2.47	0.55
1:E:701:VAL:CG1	1:E:849:GLN:HG2	2.33	0.55
1:F:319:HIS:O	1:F:321:ALA:N	2.39	0.55
1:A:312:VAL:HG12	1:A:314:PRO:HD2	1.88	0.55
1:B:456:PHE:O	1:B:459:ALA:HB3	2.07	0.55
1:C:10:ALA:HB3	1:C:18:VAL:HG22	1.87	0.55
1:C:902:GLU:HG3	1:C:907:VAL:HG11	1.89	0.55
1:D:304:ASP:OD2	1:D:306:THR:HG21	2.06	0.55
1:D:356:GLU:HG2	1:D:358:ALA:HB3	1.88	0.55
1:E:797:THR:HG22	1:E:800:GLU:OE2	2.07	0.55
1:F:41:LEU:O	1:F:46:ILE:HG13	2.07	0.55
1:F:92:ASN:ND2	1:F:94:ASN:HB3	2.22	0.55
1:F:643:SER:O	1:F:645:PRO:HD3	2.07	0.55
1:A:714:PRO:HD2	1:A:836:LEU:O	2.06	0.55
1:B:323:TYR:CE1	1:B:327:MET:HG2	2.42	0.55
1:B:438:GLY:HA2	1:B:442:ILE:H	1.72	0.55
1:B:447:GLU:HG2	1:B:492:LEU:O	2.07	0.55
1:B:584:ARG:HD3	1:C:584:ARG:HD2	1.88	0.55
1:C:404:GLU:O	1:C:406:PHE:N	2.38	0.55
1:D:354:ILE:HA	1:D:384:LEU:HB3	1.89	0.55
1:E:399:MET:HG3	1:E:403:TYR:CE2	2.42	0.55
1:E:816:ILE:H	1:E:816:ILE:HD12	1.72	0.55
1:F:669:ALA:HB2	1:F:868:ILE:HD13	1.89	0.55
1:A:304:ASP:H	1:A:309:GLN:CG	2.14	0.55
1:B:364:VAL:CG2	1:B:379:ASP:HB2	2.36	0.55
1:B:862:THR:O	1:B:864:ARG:N	2.40	0.55
1:C:295:ASP:OD2	1:C:297:GLU:HB3	2.06	0.55
1:C:891:LEU:O	1:C:896:ASN:HB2	2.07	0.55
1:D:152:LEU:HD12	1:D:202:GLU:HB2	1.88	0.55
1:F:487:VAL:HG11	1:F:508:ARG:HB3	1.89	0.55
1:A:304:ASP:N	1:A:309:GLN:HG2	2.12	0.54
1:A:306:THR:HB	1:A:309:GLN:H	1.71	0.54
1:A:565:ILE:HG21	1:A:606:LEU:HD11	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:383:VAL:HG13	1:F:384:LEU:N	2.23	0.54
1:A:346:LEU:HD22	1:A:349:LYS:HD3	1.87	0.54
1:B:411:PRO:HB3	1:B:417:GLY:CA	2.38	0.54
1:B:865:THR:H	1:B:896:ASN:HD22	1.55	0.54
1:C:27:LEU:C	1:C:27:LEU:CD2	2.81	0.54
1:F:570:TRP:CZ3	1:F:588:SER:HB3	2.42	0.54
1:F:587:HIS:NE2	1:F:589:GLY:O	2.17	0.54
1:F:873:THR:O	1:F:874:THR:C	2.49	0.54
1:A:304:ASP:C	1:A:305:ARG:CG	2.79	0.54
1:B:40:SER:O	1:B:45:THR:OG1	2.25	0.54
1:B:152:LEU:HB2	1:B:234:VAL:HG23	1.89	0.54
1:B:152:LEU:HB2	1:B:234:VAL:HG21	1.86	0.54
1:B:354:ILE:HA	1:B:384:LEU:CD2	2.36	0.54
1:B:706:ILE:HD11	1:B:851:VAL:CB	2.37	0.54
1:B:877:HIS:O	1:B:880:ASP:HB2	2.08	0.54
1:C:203:VAL:O	1:C:204:VAL:HB	2.05	0.54
1:C:444:GLU:OE1	1:C:444:GLU:CA	2.47	0.54
1:C:514:GLN:O	1:C:515:ILE:C	2.50	0.54
1:D:401:GLU:HA	1:D:404:GLU:HB2	1.88	0.54
1:E:575:GLY:HA3	1:E:584:ARG:O	2.04	0.54
1:F:415:CYS:O	1:F:416:ALA:CB	2.55	0.54
1:F:576:PRO:O	1:F:582:GLY:HA2	2.03	0.54
1:A:727:LEU:HD11	1:A:816:ILE:HG12	1.90	0.54
1:B:196:GLN:OE1	1:D:764:ILE:CD1	2.50	0.54
1:C:222:VAL:O	1:C:226:LEU:CD2	2.49	0.54
1:E:406:PHE:HE2	1:E:680:ARG:HD2	1.71	0.54
1:F:349:LYS:N	1:F:349:LYS:CD	2.70	0.54
1:A:160:LYS:CA	1:A:198:LYS:HA	2.36	0.54
1:A:793:TYR:CD1	1:A:793:TYR:C	2.86	0.54
1:C:163:PHE:HB2	1:C:193:LEU:HD12	1.88	0.54
1:E:444:GLU:HG3	1:E:446:CYS:O	2.08	0.54
1:E:450:ILE:HG22	1:E:451:ALA:H	1.72	0.54
1:E:670:ALA:HA	1:E:681:GLN:HE21	1.71	0.54
1:F:44:ASP:O	1:F:48:ALA:CB	2.56	0.54
1:F:640:ILE:H	1:F:640:ILE:HD13	1.71	0.54
1:B:183:VAL:CG1	1:B:184:VAL:N	2.30	0.54
1:B:715:ALA:HB2	1:B:836:LEU:HD22	1.89	0.54
1:C:356:GLU:N	1:C:383:VAL:HG13	2.22	0.54
1:D:100:GLY:HA2	1:D:494:LEU:HD22	1.90	0.54
1:E:415:CYS:O	1:E:416:ALA:HB3	2.07	0.54
1:F:76:PHE:HE2	1:F:78:GLU:HB3	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:570:TRP:CH2	1:F:588:SER:HB3	2.42	0.54
1:F:697:LYS:O	1:F:866:VAL:HG12	2.07	0.54
1:B:675:ARG:CZ	1:B:692:LEU:HD22	2.37	0.54
1:C:294:VAL:HA	1:C:407:MET:CA	2.37	0.54
1:D:145:GLU:CD	1:D:148:ARG:HB2	2.32	0.54
1:D:446:CYS:SG	1:D:449:SER:HB2	2.48	0.54
1:D:706:ILE:HD11	1:D:851:VAL:CB	2.38	0.54
1:E:148:ARG:CB	1:E:148:ARG:HH11	2.21	0.54
1:E:786:ARG:HA	1:E:789:LEU:HD12	1.89	0.54
1:F:10:ALA:CA	1:F:74:VAL:HG12	2.35	0.54
1:A:96:ARG:HD3	1:A:276:ASN:ND2	2.22	0.54
1:A:111:LEU:HD23	1:A:115:ARG:NH1	2.23	0.54
1:A:121:CYS:O	1:A:125:GLY:HA2	2.07	0.54
1:B:14:ASN:ND2	1:B:579:GLY:O	2.41	0.54
1:B:343:TRP:O	1:B:346:LEU:HD12	2.07	0.54
1:C:630:VAL:O	1:C:687:THR:HB	2.07	0.54
1:D:752:ARG:HG3	1:D:752:ARG:O	2.08	0.54
1:A:152:LEU:HD21	1:A:179:ARG:NH1	2.21	0.54
1:A:170:LEU:HD22	1:A:203:VAL:HG11	1.89	0.54
1:B:79:GLY:HA2	1:D:520:VAL:HG21	1.90	0.54
1:B:576:PRO:CB	1:B:601:ILE:HD11	2.38	0.54
1:C:536:ARG:HD3	1:C:944:TYR:CE1	2.43	0.54
1:D:133:PRO:HB3	1:D:226:LEU:HD13	1.89	0.54
1:D:701:VAL:HG21	1:D:853:LEU:HD23	1.88	0.54
1:E:363:HIS:CD2	1:E:378:ALA:HA	2.39	0.54
1:F:919:PRO:HD2	1:F:925:GLY:HA2	1.89	0.54
1:A:764:ILE:HG23	1:A:764:ILE:O	2.06	0.54
1:B:561:ASP:OD1	1:B:562:GLU:N	2.41	0.54
1:C:151:VAL:O	1:C:204:VAL:C	2.50	0.54
1:C:613:GLU:OE1	1:C:613:GLU:HA	2.07	0.54
1:D:515:ILE:HG22	1:D:516:GLY:N	2.23	0.54
1:E:87:ASP:HA	1:E:527:ASP:HB3	1.89	0.54
1:E:441:SER:O	1:E:495:SER:CA	2.56	0.54
1:A:185:HIS:CE1	1:A:191:PRO:HG3	2.43	0.53
1:B:100:GLY:HA2	1:B:494:LEU:HD22	1.90	0.53
1:B:139:GLN:C	1:B:143:MET:HG2	2.33	0.53
1:B:459:ALA:HB2	1:B:478:ARG:HH12	1.71	0.53
1:B:533:LEU:HD21	1:B:537:ASP:HB2	1.90	0.53
1:C:444:GLU:CD	1:C:449:SER:HG	2.14	0.53
1:E:304:ASP:HB2	1:E:305:ARG:NH1	2.23	0.53
1:E:441:SER:C	1:E:495:SER:HB3	2.32	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:660:LYS:HE2	1:E:661:SER:H	1.71	0.53
1:F:485:LEU:HD23	1:F:490:GLU:HB2	1.89	0.53
1:B:175:TYR:N	1:B:187:LEU:HD23	2.24	0.53
1:C:326:ARG:HG2	1:C:364:VAL:HG11	1.89	0.53
1:D:20:LEU:HD13	1:D:22:LEU:HD11	1.90	0.53
1:E:121:CYS:SG	1:E:261:HIS:CG	2.98	0.53
1:F:29:VAL:O	1:F:29:VAL:CG1	2.56	0.53
1:F:312:VAL:CG1	1:F:314:PRO:HD2	2.38	0.53
1:F:607:SER:OG	1:F:609:ARG:HG3	2.08	0.53
1:A:33:LEU:HD23	1:A:877:HIS:CG	2.44	0.53
1:B:370:TYR:O	1:B:372:ARG:N	2.40	0.53
1:B:562:GLU:HG2	1:B:566:GLU:OE2	2.07	0.53
1:C:25:ASP:N	1:C:554:THR:HB	2.21	0.53
1:C:158:THR:HG22	1:C:198:LYS:HD2	1.90	0.53
1:C:351:ARG:CG	1:C:352:LYS:N	2.59	0.53
1:D:156:VAL:CG1	1:D:201:ILE:H	2.21	0.53
1:D:384:LEU:C	1:D:384:LEU:HD12	2.33	0.53
1:D:565:ILE:HG21	1:D:606:LEU:HD11	1.89	0.53
1:E:10:ALA:HB3	1:E:18:VAL:HG22	1.90	0.53
1:E:290:ILE:HA	1:E:411:PRO:HA	1.90	0.53
1:E:355:LEU:C	1:E:383:VAL:HG13	2.33	0.53
1:F:52:ARG:CZ	1:F:71:LYS:HD2	2.37	0.53
1:F:487:VAL:CG1	1:F:508:ARG:HB3	2.38	0.53
1:A:391:MET:HE3	1:A:394:THR:CB	2.38	0.53
1:A:576:PRO:CD	1:A:586:VAL:HG23	2.26	0.53
1:B:20:LEU:HD21	1:B:585:ILE:HG12	1.90	0.53
1:B:65:PHE:O	1:B:65:PHE:HD1	1.91	0.53
1:B:377:TYR:HD2	1:B:379:ASP:OD2	1.91	0.53
1:B:865:THR:HG22	1:B:896:ASN:ND2	2.23	0.53
1:D:10:ALA:HB3	1:D:18:VAL:HG22	1.91	0.53
1:D:305:ARG:CD	1:D:311:ALA:HB3	1.83	0.53
1:F:330:GLY:CA	1:F:362:VAL:HG13	2.38	0.53
1:F:548:LEU:O	1:F:551:LEU:HB3	2.09	0.53
1:A:284:GLU:HB2	1:A:414:VAL:HG21	1.91	0.53
1:B:524:TYR:HB2	1:B:555:LEU:HD22	1.89	0.53
1:D:445:VAL:HA	1:D:493:SER:CB	2.39	0.53
1:D:597:ASN:HD22	1:D:597:ASN:C	2.17	0.53
1:D:732:THR:HA	1:D:735:LYS:HE2	1.91	0.53
1:D:902:GLU:HG3	1:D:907:VAL:HG11	1.90	0.53
1:E:31:THR:O	1:E:573:ASP:HA	2.07	0.53
1:E:312:VAL:HG12	1:E:384:LEU:HD11	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:330:GLY:HA3	1:F:362:VAL:HG22	1.90	0.53
1:A:144:PRO:HB2	1:A:147:THR:HG23	1.87	0.53
1:D:150:LEU:HG	1:D:204:VAL:HG12	1.91	0.53
1:D:649:LEU:HD23	1:D:911:SER:HA	1.90	0.53
1:E:235:LEU:HD12	1:E:235:LEU:O	2.09	0.53
1:E:670:ALA:HA	1:E:681:GLN:NE2	2.23	0.53
1:F:28:ILE:H	1:F:28:ILE:CD1	2.22	0.53
1:F:695:LEU:CD2	1:F:864:ARG:CA	2.87	0.53
1:F:701:VAL:HG12	1:F:702:ASP:H	1.73	0.53
1:A:756:CYS:O	1:A:757:THR:HB	2.08	0.53
1:B:156:VAL:O	1:B:156:VAL:CG1	2.53	0.53
1:B:452:ASP:HA	1:B:456:PHE:H	1.72	0.53
1:F:76:PHE:CE2	1:F:78:GLU:HB3	2.44	0.53
1:F:508:ARG:NH1	1:F:531:ILE:O	2.42	0.53
1:F:619:ARG:HH22	1:F:892:VAL:HG12	1.74	0.53
1:A:302:ASP:CB	1:A:303:PRO:HD3	2.32	0.53
1:B:113:TYR:CZ	1:B:437:HIS:HA	2.44	0.53
1:B:158:THR:CG2	1:B:159:ARG:NH1	2.72	0.53
1:B:451:ALA:O	1:B:456:PHE:CD1	2.62	0.53
1:C:41:LEU:HD12	1:C:574:ILE:HD11	1.90	0.53
1:C:360:GLU:O	1:C:361:GLN:CG	2.57	0.53
1:E:284:GLU:HG2	1:E:414:VAL:CG1	2.34	0.53
1:F:604:ALA:HA	1:F:609:ARG:HD2	1.90	0.53
1:F:657:GLY:H	1:F:660:LYS:HD2	1.74	0.53
1:F:864:ARG:HB2	1:F:864:ARG:HH11	1.72	0.53
1:A:65:PHE:HE1	1:A:766:MET:HA	1.74	0.53
1:A:516:GLY:O	1:A:518:GLY:N	2.41	0.53
1:A:579:GLY:O	1:A:580:GLU:C	2.51	0.53
1:A:706:ILE:HD11	1:A:851:VAL:CG1	2.39	0.53
1:C:361:GLN:HB3	1:C:378:ALA:HB1	1.91	0.53
1:C:865:THR:HG22	1:C:896:ASN:ND2	2.24	0.53
1:D:630:VAL:O	1:D:687:THR:HB	2.08	0.53
1:E:320:THR:O	1:E:323:TYR:HB3	2.08	0.53
1:E:557:VAL:HG12	1:E:559:GLU:HG2	1.91	0.53
1:E:674:ASN:ND2	1:E:679:ALA:O	2.42	0.53
1:F:699:VAL:HB	1:F:867:TYR:CE1	2.43	0.53
1:A:425:LEU:C	1:A:437:HIS:HD1	2.17	0.53
1:B:451:ALA:CA	1:B:455:ASP:HB2	2.36	0.53
1:B:508:ARG:CG	1:B:508:ARG:NH1	2.66	0.53
1:C:389:ARG:O	1:C:393:GLN:HB3	2.09	0.53
1:D:304:ASP:O	1:D:305:ARG:CB	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:305:ARG:HD3	1:D:311:ALA:CB	1.99	0.53
1:D:368:ASN:C	1:D:370:TYR:N	2.63	0.53
1:D:404:GLU:O	1:D:406:PHE:N	2.42	0.53
1:D:914:ILE:HG13	1:D:937:VAL:HG21	1.90	0.53
1:E:352:LYS:CD	1:E:356:GLU:HB3	2.33	0.53
1:E:372:ARG:HG2	1:E:374:ARG:HG3	1.91	0.53
1:E:873:THR:HB	1:E:902:GLU:OE2	2.09	0.53
1:F:323:TYR:CD1	1:F:323:TYR:O	2.62	0.53
1:F:867:TYR:O	1:F:899:ILE:HD12	2.08	0.53
1:A:68:GLN:HE21	1:A:764:ILE:CG1	2.22	0.52
1:B:298:LEU:HB3	1:B:406:PHE:HD1	1.73	0.52
1:B:396:SER:O	1:B:397:GLU:CB	2.55	0.52
1:B:585:ILE:O	1:B:585:ILE:HG22	2.09	0.52
1:D:137:VAL:HG23	1:D:222:VAL:HG11	1.91	0.52
1:D:305:ARG:CZ	1:D:312:VAL:CG2	2.63	0.52
1:D:557:VAL:HG12	1:D:559:GLU:HG2	1.91	0.52
1:E:305:ARG:H	1:E:305:ARG:CD	2.10	0.52
1:E:412:CYS:C	1:E:415:CYS:SG	2.91	0.52
1:E:865:THR:HG22	1:E:896:ASN:ND2	2.24	0.52
1:F:330:GLY:HA3	1:F:362:VAL:HG13	1.89	0.52
1:F:561:ASP:OD2	1:F:564:THR:OG1	2.24	0.52
1:F:614:ILE:O	1:F:615:PRO:C	2.52	0.52
1:B:442:ILE:HD12	1:B:494:LEU:HD13	1.92	0.52
1:D:25:ASP:N	1:D:554:THR:HB	2.23	0.52
1:D:358:ALA:CB	1:D:381:GLU:HG2	2.39	0.52
1:D:368:ASN:HB2	1:D:372:ARG:CG	2.37	0.52
1:E:96:ARG:HB2	1:E:276:ASN:OD1	2.10	0.52
1:E:285:CYS:O	1:E:286:SER:CB	2.58	0.52
1:E:329:ALA:HB2	1:E:339:VAL:HG23	1.90	0.52
1:F:45:THR:HG22	1:F:46:ILE:N	2.24	0.52
1:F:605:TYR:CE2	1:F:879:ASP:HA	2.45	0.52
1:A:20:LEU:HD21	1:A:585:ILE:CD1	2.39	0.52
1:A:99:VAL:CG2	1:A:501:LEU:HD11	2.39	0.52
1:A:391:MET:HE2	1:A:394:THR:HB	1.92	0.52
1:A:557:VAL:HG12	1:A:559:GLU:HG2	1.92	0.52
1:A:865:THR:H	1:A:896:ASN:HD22	1.56	0.52
1:B:185:HIS:CG	1:B:191:PRO:HG3	2.43	0.52
1:C:323:TYR:CD1	1:C:323:TYR:C	2.87	0.52
1:C:356:GLU:H	1:C:383:VAL:HG13	1.72	0.52
1:C:400:LYS:HD3	1:C:400:LYS:C	2.34	0.52
1:C:460:LEU:O	1:C:461:THR:C	2.51	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:565:ILE:HG21	1:E:606:LEU:HD11	1.91	0.52
1:F:315:TRP:HE1	1:F:387:LEU:CD2	2.10	0.52
1:F:367:ARG:HH11	1:F:373:THR:HB	1.74	0.52
1:F:576:PRO:HG2	1:F:584:ARG:H	1.74	0.52
1:A:7:VAL:HG13	1:A:20:LEU:HB2	1.91	0.52
1:A:99:VAL:HG22	1:A:501:LEU:HD11	1.91	0.52
1:A:721:PHE:O	1:A:725:ARG:HG3	2.09	0.52
1:D:361:GLN:HG3	1:D:380:PHE:HA	1.90	0.52
1:E:508:ARG:HG3	1:E:508:ARG:NH1	2.12	0.52
1:A:175:TYR:HB2	1:A:187:LEU:CD1	2.37	0.52
1:A:456:PHE:O	1:A:457:LEU:C	2.53	0.52
1:A:829:VAL:HG11	1:A:850:ARG:O	2.10	0.52
1:D:459:ALA:HB2	1:D:478:ARG:HH22	1.75	0.52
1:D:737:ARG:NH1	1:D:790:GLU:OE1	2.42	0.52
1:A:106:TYR:CE1	1:A:442:ILE:HD13	2.43	0.52
1:B:533:LEU:HD23	1:B:537:ASP:HB2	1.91	0.52
1:B:706:ILE:HD11	1:B:851:VAL:HB	1.92	0.52
1:C:455:ASP:O	1:C:459:ALA:HB2	2.10	0.52
1:C:557:VAL:HG12	1:C:559:GLU:HG2	1.90	0.52
1:D:684:GLY:O	1:D:686:HIS:HD2	1.93	0.52
1:D:742:GLY:O	1:D:748:VAL:CG2	2.57	0.52
1:D:865:THR:HG22	1:D:896:ASN:ND2	2.24	0.52
1:E:169:LYS:NZ	1:E:228:LEU:HD21	2.24	0.52
1:F:486:ASP:HB3	1:F:544:THR:HG21	1.91	0.52
1:F:695:LEU:CD1	1:F:897:THR:HB	2.39	0.52
1:A:784:TYR:HE2	1:A:798:VAL:HB	1.74	0.52
1:B:727:LEU:HD22	1:B:793:TYR:CE2	2.34	0.52
1:D:399:MET:HE3	1:D:403:TYR:CE2	2.45	0.52
1:E:447:GLU:HB2	1:E:485:LEU:CD2	2.40	0.52
1:A:584:ARG:HD2	1:D:584:ARG:HD3	1.92	0.52
1:B:275:PHE:HD1	1:B:276:ASN:OD1	1.93	0.52
1:C:132:THR:HG22	1:C:134:GLN:H	1.75	0.52
1:C:755:ALA:HB2	1:E:163:PHE:CE1	2.45	0.52
1:D:250:ARG:NH2	1:D:266:ASP:OD2	2.42	0.52
1:D:305:ARG:HH12	1:D:312:VAL:HG21	1.61	0.52
1:D:706:ILE:HD11	1:D:851:VAL:HB	1.92	0.52
1:E:444:GLU:OE2	1:E:450:ILE:HG13	2.08	0.52
1:E:906:ASP:O	1:E:909:LYS:HG2	2.10	0.52
1:F:6:ILE:O	1:F:6:ILE:HG22	2.10	0.52
1:F:415:CYS:SG	1:F:417:GLY:CA	2.98	0.52
1:F:657:GLY:N	1:F:660:LYS:HD2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:LEU:O	1:A:175:TYR:HD1	1.92	0.52
1:B:125:GLY:O	1:B:126:GLU:C	2.53	0.52
1:B:160:LYS:HG2	1:B:198:LYS:HG2	1.92	0.52
1:C:49:GLU:HG2	1:C:72:PRO:HG2	1.92	0.52
1:C:391:MET:HA	1:C:394:THR:HB	1.91	0.52
1:C:575:GLY:HA3	1:C:584:ARG:O	2.10	0.52
1:E:402:ARG:HH21	1:E:680:ARG:HH21	1.57	0.52
1:E:701:VAL:HG12	1:E:849:GLN:CG	2.34	0.52
1:A:299:VAL:CG2	1:A:301:PRO:HD3	2.39	0.52
1:B:68:GLN:HE21	1:B:764:ILE:HG12	1.74	0.52
1:C:533:LEU:HD21	1:C:537:ASP:HB2	1.92	0.52
1:D:782:ALA:O	1:D:783:ARG:HB2	2.10	0.52
1:D:816:ILE:H	1:D:816:ILE:HD12	1.75	0.52
1:E:366:TYR:HE2	1:E:377:TYR:CD2	2.27	0.52
1:F:545:LEU:O	1:F:546:THR:C	2.53	0.52
1:A:378:ALA:O	1:A:380:PHE:N	2.41	0.51
1:B:282:CYS:O	1:B:286:SER:N	2.42	0.51
1:C:189:ASP:HB3	1:C:190:PRO:CD	2.40	0.51
1:D:119:PRO:HB2	1:D:128:VAL:HG22	1.92	0.51
1:D:312:VAL:HG12	1:D:315:TRP:N	2.07	0.51
1:E:148:ARG:NH1	1:E:148:ARG:HB3	2.24	0.51
1:E:150:LEU:HB3	1:E:236:GLU:CB	2.34	0.51
1:E:355:LEU:CA	1:E:383:VAL:HG13	2.40	0.51
1:E:592:ASP:HB3	1:F:468:ALA:CB	2.39	0.51
1:F:412:CYS:HG	1:F:414:VAL:CG2	2.18	0.51
1:F:502:SER:O	1:F:505:GLU:N	2.43	0.51
1:A:533:LEU:HD23	1:A:537:ASP:HB2	1.91	0.51
1:A:877:HIS:O	1:A:881:ILE:HG12	2.09	0.51
1:B:126:GLU:HG2	1:B:258:PRO:CG	2.40	0.51
1:C:317:ASN:HA	1:C:321:ALA:HB2	1.91	0.51
1:C:702:ASP:HB3	1:C:852:LYS:NZ	2.25	0.51
1:C:737:ARG:NH1	1:C:790:GLU:OE1	2.43	0.51
1:D:18:VAL:HB	1:D:585:ILE:HD12	1.92	0.51
1:D:112:LEU:HD21	1:D:458:ASN:HD21	1.74	0.51
1:E:65:PHE:HE2	1:E:767:ASN:HD21	1.44	0.51
1:E:329:ALA:HB2	1:E:339:VAL:CG2	2.40	0.51
1:F:118:THR:HB	1:F:119:PRO:CD	2.39	0.51
1:A:462:LEU:CD2	1:A:466:GLU:HB2	2.40	0.51
1:C:713:ASN:O	1:C:714:PRO:C	2.53	0.51
1:D:452:ASP:O	1:D:456:PHE:HB2	2.09	0.51
1:D:814:GLU:N	1:D:815:PRO:CD	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:746:PHE:HA	1:E:752:ARG:HB3	1.93	0.51
1:F:474:LEU:HD21	1:F:478:ARG:NH2	2.26	0.51
1:F:544:THR:HG23	1:F:547:ARG:HH11	1.72	0.51
1:A:62:ALA:HB1	1:A:768:PHE:CZ	2.46	0.51
1:A:297:GLU:O	1:A:298:LEU:C	2.50	0.51
1:A:701:VAL:CG1	1:A:849:GLN:HG2	2.32	0.51
1:B:346:LEU:HB3	1:B:349:LYS:HG3	1.92	0.51
1:C:445:VAL:HB	1:C:448:LEU:HB3	1.92	0.51
1:C:867:TYR:CE2	1:C:891:LEU:HD12	2.46	0.51
1:D:342:PRO:HB2	1:D:347:PRO:HB3	1.92	0.51
1:A:27:LEU:C	1:A:27:LEU:CD2	2.83	0.51
1:A:346:LEU:N	1:A:346:LEU:CD1	2.74	0.51
1:A:346:LEU:CG	1:A:349:LYS:HD3	2.41	0.51
1:A:918:GLY:O	1:A:927:THR:OG1	2.21	0.51
1:B:295:ASP:CA	1:B:298:LEU:HD23	2.39	0.51
1:C:388:GLN:HB2	1:C:389:ARG:HH11	1.68	0.51
1:D:817:ALA:O	1:D:821:ARG:HG2	2.10	0.51
1:E:338:ASP:CB	1:E:341:THR:OG1	2.59	0.51
1:E:404:GLU:HA	1:E:407:MET:HE2	1.92	0.51
1:E:893:ASP:C	1:E:895:GLY:H	2.18	0.51
1:A:265:VAL:HG22	1:A:421:LYS:CE	2.41	0.51
1:A:351:ARG:NE	1:A:355:LEU:HD12	2.26	0.51
1:A:421:LYS:O	1:A:424:ILE:HB	2.11	0.51
1:B:318:GLY:H	1:B:321:ALA:HB2	1.75	0.51
1:B:370:TYR:O	1:B:372:ARG:HB2	2.10	0.51
1:B:768:PHE:CE1	1:D:768:PHE:HB3	2.46	0.51
1:C:706:ILE:HD11	1:C:851:VAL:CG1	2.40	0.51
1:E:412:CYS:CA	1:E:415:CYS:SG	2.98	0.51
1:E:782:ALA:O	1:E:783:ARG:HB2	2.10	0.51
1:F:504:GLY:O	1:F:508:ARG:HG3	2.10	0.51
1:A:346:LEU:HD13	1:A:349:LYS:CD	2.40	0.51
1:A:737:ARG:NH1	1:A:790:GLU:OE1	2.43	0.51
1:B:88:GLN:HE22	1:B:531:ILE:CD1	2.23	0.51
1:C:38:LYS:HD3	1:C:38:LYS:N	2.25	0.51
1:C:360:GLU:C	1:C:361:GLN:OE1	2.53	0.51
1:C:384:LEU:C	1:C:386:PHE:H	2.18	0.51
1:C:462:LEU:CD2	1:C:466:GLU:HB2	2.40	0.51
1:D:356:GLU:OE2	1:D:358:ALA:O	2.28	0.51
1:D:455:ASP:HA	1:D:478:ARG:HH11	1.75	0.51
1:E:305:ARG:NE	1:E:308:ALA:HB2	2.25	0.51
1:E:440:LYS:HD2	1:E:454:ALA:HB2	1.82	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:784:TYR:HE2	1:E:798:VAL:HB	1.73	0.51
1:F:542:ILE:HD12	1:F:564:THR:HA	1.93	0.51
1:A:428:THR:HG23	1:A:435:GLY:HA3	1.92	0.51
1:B:298:LEU:C	1:B:299:VAL:HG12	2.36	0.51
1:C:319:HIS:H	1:C:319:HIS:CD2	2.29	0.51
1:C:448:LEU:O	1:C:449:SER:HB3	2.10	0.51
1:D:178:VAL:HG23	1:D:187:LEU:HB2	1.91	0.51
1:D:338:ASP:C	1:D:339:VAL:CG1	2.83	0.51
1:D:355:LEU:O	1:D:383:VAL:HG13	2.10	0.51
1:E:255:LEU:O	1:E:255:LEU:HD23	2.10	0.51
1:E:706:ILE:HD11	1:E:851:VAL:CB	2.41	0.51
1:F:98:THR:CG2	1:F:419:ARG:HH12	2.22	0.51
1:F:418:THR:O	1:F:419:ARG:CB	2.59	0.51
1:F:594:LEU:HA	1:F:597:ASN:HB3	1.93	0.51
1:A:65:PHE:O	1:A:65:PHE:HD1	1.93	0.51
1:A:782:ALA:O	1:A:783:ARG:HB2	2.11	0.51
1:B:412:CYS:O	1:B:416:ALA:N	2.44	0.51
1:C:220:ASP:C	1:C:222:VAL:N	2.61	0.51
1:C:368:ASN:O	1:C:370:TYR:N	2.43	0.51
1:C:394:THR:OG1	1:C:395:GLU:N	2.44	0.51
1:C:400:LYS:O	1:C:403:TYR:HB2	2.10	0.51
1:C:534:HIS:HB2	1:C:655:VAL:HA	1.92	0.51
1:C:873:THR:HG21	1:C:904:ASN:HB2	1.93	0.51
1:D:356:GLU:HB2	1:D:383:VAL:HA	1.92	0.51
1:D:918:GLY:O	1:D:927:THR:OG1	2.21	0.51
1:F:29:VAL:HG22	1:F:557:VAL:HB	1.93	0.51
1:F:447:GLU:HB2	1:F:490:GLU:O	2.11	0.51
1:F:872:PRO:HD2	1:F:902:GLU:HG2	1.92	0.51
1:A:119:PRO:C	1:A:120:HIS:CD2	2.89	0.51
1:A:416:ALA:HB3	1:A:418:THR:HG23	1.93	0.51
1:B:358:ALA:O	1:B:359:ASP:HB2	2.11	0.51
1:B:651:SER:HB2	1:B:914:ILE:HG22	1.92	0.51
1:C:13:HIS:CD2	1:C:40:SER:OG	2.64	0.51
1:C:396:SER:O	1:C:397:GLU:HB2	2.11	0.51
1:D:272:SER:O	1:D:280:GLY:HA3	2.11	0.51
1:E:335:LEU:HB2	1:E:337:PHE:HE2	1.76	0.51
1:E:406:PHE:CE2	1:E:680:ARG:HD2	2.45	0.51
1:F:40:SER:HA	1:F:44:ASP:HB2	1.92	0.51
1:F:408:ARG:NH1	1:F:683:PRO:O	2.44	0.51
1:F:933:THR:C	1:F:935:GLU:N	2.68	0.51
1:A:65:PHE:HD1	1:A:766:MET:HE3	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:GLU:CG	1:B:398:GLN:N	2.57	0.50
1:B:431:GLY:HA3	1:B:458:ASN:N	2.25	0.50
1:B:515:ILE:HD13	1:B:548:LEU:CD2	2.41	0.50
1:C:96:ARG:HH21	1:C:288:LEU:HD23	1.75	0.50
1:C:368:ASN:C	1:C:370:TYR:H	2.19	0.50
1:D:399:MET:O	1:D:402:ARG:N	2.37	0.50
1:F:423:GLU:O	1:F:426:ALA:HB3	2.11	0.50
1:F:633:ARG:HG2	1:F:633:ARG:HH11	1.76	0.50
1:A:68:GLN:HE21	1:A:764:ILE:HG12	1.77	0.50
1:A:255:LEU:HD11	1:A:268:LEU:CD1	2.42	0.50
1:A:269:GLU:HG3	1:A:270:PRO:HD2	1.92	0.50
1:A:391:MET:HE3	1:A:394:THR:HB	1.93	0.50
1:A:397:GLU:HG3	1:A:399:MET:H	1.76	0.50
1:A:508:ARG:NH1	1:A:508:ARG:CG	2.62	0.50
1:B:87:ASP:HA	1:B:527:ASP:HB3	1.94	0.50
1:B:120:HIS:CD2	1:B:125:GLY:O	2.65	0.50
1:C:784:TYR:HE2	1:C:798:VAL:HB	1.72	0.50
1:D:533:LEU:HD23	1:D:537:ASP:HB2	1.92	0.50
1:E:174:GLY:O	1:E:175:TYR:HB2	2.11	0.50
1:E:185:HIS:CD2	1:E:191:PRO:HD3	2.47	0.50
1:E:515:ILE:HG22	1:E:516:GLY:N	2.27	0.50
1:E:702:ASP:HB3	1:E:852:LYS:NZ	2.26	0.50
1:F:343:TRP:O	1:F:345:LYS:N	2.45	0.50
1:F:436:GLU:N	1:F:436:GLU:OE1	2.45	0.50
1:F:627:LEU:O	1:F:644:PHE:N	2.37	0.50
1:A:148:ARG:HH21	1:A:207:ARG:CD	2.23	0.50
1:A:275:PHE:HB3	1:A:420:LEU:CD2	2.41	0.50
1:B:14:ASN:OD1	1:B:14:ASN:O	2.29	0.50
1:B:323:TYR:HE1	1:B:327:MET:HG2	1.68	0.50
1:C:621:VAL:CG1	1:C:645:PRO:HB3	2.40	0.50
1:D:92:ASN:OD1	1:D:93:ARG:N	2.44	0.50
1:D:699:VAL:HB	1:D:867:TYR:CD1	2.46	0.50
1:E:402:ARG:HH21	1:E:680:ARG:NH2	2.09	0.50
1:E:625:ARG:NE	1:E:694:TYR:HE2	2.06	0.50
1:A:424:ILE:HG22	1:A:437:HIS:HE1	1.75	0.50
1:A:442:ILE:HG22	1:A:495:SER:N	2.26	0.50
1:B:113:TYR:CB	1:B:437:HIS:ND1	2.74	0.50
1:C:317:ASN:CA	1:C:321:ALA:CB	2.89	0.50
1:C:873:THR:HB	1:C:902:GLU:OE2	2.12	0.50
1:D:257:CYS:SG	1:D:259:ASN:N	2.83	0.50
1:E:27:LEU:CD2	1:E:27:LEU:C	2.84	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:148:ARG:HH11	1:E:148:ARG:HB2	1.77	0.50
1:E:446:CYS:SG	1:E:448:LEU:CB	2.91	0.50
1:E:592:ASP:OD1	1:F:465:ARG:HA	2.10	0.50
1:E:613:GLU:OE1	1:E:613:GLU:HA	2.10	0.50
1:F:412:CYS:N	1:F:415:CYS:SG	2.84	0.50
1:F:933:THR:O	1:F:936:ASP:N	2.42	0.50
1:A:670:ALA:HA	1:A:681:GLN:NE2	2.27	0.50
1:B:126:GLU:HG2	1:B:258:PRO:HG3	1.94	0.50
1:B:131:GLN:HE21	1:B:256:ALA:HB2	1.73	0.50
1:C:181:ASP:N	1:C:200:ASP:O	2.44	0.50
1:D:178:VAL:HG12	1:D:180:VAL:HG23	1.94	0.50
1:D:444:GLU:O	1:D:445:VAL:C	2.55	0.50
1:D:746:PHE:HA	1:D:752:ARG:HB3	1.94	0.50
1:E:25:ASP:N	1:E:554:THR:HB	2.23	0.50
1:E:106:TYR:OH	1:E:437:HIS:HE1	1.94	0.50
1:E:351:ARG:HE	1:E:355:LEU:HD11	1.76	0.50
1:E:444:GLU:CG	1:E:450:ILE:HD12	2.39	0.50
1:E:702:ASP:HB3	1:E:852:LYS:HZ3	1.77	0.50
1:F:54:TYR:CZ	1:F:58:LEU:HD21	2.46	0.50
1:A:437:HIS:H	1:A:440:LYS:CD	2.21	0.50
1:A:619:ARG:HB2	1:A:912:ASP:CG	2.37	0.50
1:B:122:PRO:HG3	1:B:423:GLU:HA	1.93	0.50
1:B:151:VAL:O	1:B:205:VAL:HG23	2.11	0.50
1:C:357:GLY:O	1:C:358:ALA:HB3	2.12	0.50
1:C:390:LYS:C	1:C:391:MET:CG	2.83	0.50
1:D:123:THR:HG1	1:D:261:HIS:CG	2.29	0.50
1:D:715:ALA:HB2	1:D:836:LEU:HD22	1.94	0.50
1:E:317:ASN:N	1:E:321:ALA:HB2	2.26	0.50
1:E:877:HIS:O	1:E:880:ASP:HB2	2.11	0.50
1:F:30:PHE:CE2	1:F:42:ALA:HB2	2.47	0.50
1:F:328:MET:SD	1:F:354:ILE:CD1	2.99	0.50
1:F:337:PHE:HD1	1:F:349:LYS:HZ3	1.59	0.50
1:F:398:GLN:HG3	1:F:399:MET:N	2.26	0.50
1:F:586:VAL:O	1:F:587:HIS:HB2	2.11	0.50
1:A:49:GLU:OE1	1:A:53:ARG:NE	2.44	0.50
1:B:68:GLN:HE21	1:B:764:ILE:HD11	1.77	0.50
1:B:146:GLY:O	1:B:148:ARG:HD3	2.12	0.50
1:B:721:PHE:O	1:B:725:ARG:HG3	2.11	0.50
1:D:913:TRP:CH2	1:D:932:GLY:HA2	2.47	0.50
1:E:706:ILE:HD11	1:E:851:VAL:HB	1.94	0.50
1:F:11:ARG:HA	1:F:15:LEU:CD1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:436:GLU:OE1	1:F:436:GLU:O	2.29	0.50
1:F:613:GLU:OE2	1:F:615:PRO:HD3	2.11	0.50
1:A:275:PHE:HB3	1:A:420:LEU:HD23	1.93	0.50
1:A:743:ARG:HG3	1:A:751:GLY:HA3	1.92	0.50
1:B:113:TYR:HB2	1:B:437:HIS:ND1	2.27	0.50
1:B:175:TYR:O	1:B:187:LEU:HD23	2.11	0.50
1:B:431:GLY:HA3	1:B:458:ASN:CB	2.42	0.50
1:B:597:ASN:HD22	1:B:597:ASN:C	2.20	0.50
1:C:20:LEU:HD21	1:C:585:ILE:HG12	1.93	0.50
1:C:65:PHE:HD1	1:C:65:PHE:O	1.95	0.50
1:C:295:ASP:C	1:C:297:GLU:H	2.20	0.50
1:C:386:PHE:C	1:C:388:GLN:N	2.68	0.50
1:C:425:LEU:HD21	1:C:439:ALA:CB	2.38	0.50
1:E:307:LEU:HD23	1:E:307:LEU:C	2.37	0.50
1:E:404:GLU:C	1:E:406:PHE:H	2.20	0.50
1:E:592:ASP:CB	1:F:468:ALA:CB	2.90	0.50
1:F:391:MET:HB3	1:F:403:TYR:CE2	2.47	0.50
1:A:230:ASP:O	1:A:230:ASP:CG	2.55	0.50
1:A:298:LEU:O	1:A:298:LEU:CG	2.60	0.50
1:A:359:ASP:OD1	1:A:359:ASP:O	2.30	0.50
1:B:352:LYS:CA	1:B:356:GLU:O	2.60	0.50
1:B:364:VAL:HG23	1:B:379:ASP:HB2	1.94	0.50
1:C:282:CYS:CB	1:C:415:CYS:HB3	2.42	0.50
1:C:363:HIS:HB3	1:C:377:TYR:C	2.37	0.50
1:D:459:ALA:HB2	1:D:478:ARG:HH12	1.77	0.50
1:D:508:ARG:CG	1:D:508:ARG:NH1	2.66	0.50
1:D:601:ILE:H	1:D:601:ILE:CD1	2.23	0.50
1:D:801:VAL:HG21	1:D:813:PHE:HZ	1.75	0.50
1:E:186:PRO:HG2	1:E:189:ASP:HB3	1.93	0.50
1:E:380:PHE:HD1	1:E:380:PHE:N	2.10	0.50
1:E:474:LEU:O	1:E:478:ARG:HG2	2.12	0.50
1:E:742:GLY:O	1:E:748:VAL:CG2	2.60	0.50
1:E:817:ALA:O	1:E:821:ARG:HG2	2.12	0.50
1:F:380:PHE:C	1:F:382:GLY:H	2.20	0.50
1:F:437:HIS:HB2	1:F:442:ILE:H	1.77	0.50
1:B:329:ALA:HB2	1:B:339:VAL:HG13	1.93	0.49
1:B:351:ARG:HD2	1:B:352:LYS:NZ	2.27	0.49
1:B:486:ASP:O	1:B:540:ARG:NH2	2.46	0.49
1:B:625:ARG:NE	1:B:694:TYR:HE2	2.08	0.49
1:B:893:ASP:C	1:B:895:GLY:H	2.20	0.49
1:C:625:ARG:NE	1:C:694:TYR:HE2	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:384:LEU:HD12	1:D:384:LEU:O	2.12	0.49
1:D:671:VAL:HG11	1:D:689:VAL:HG21	1.93	0.49
1:E:402:ARG:NH2	1:E:680:ARG:NH2	2.60	0.49
1:F:28:ILE:HD12	1:F:28:ILE:H	1.75	0.49
1:F:49:GLU:OE2	1:F:52:ARG:NH1	2.45	0.49
1:F:86:ILE:HB	1:F:526:LEU:HG	1.93	0.49
1:F:576:PRO:HG3	1:F:584:ARG:O	2.12	0.49
1:A:701:VAL:HG12	1:A:849:GLN:CG	2.34	0.49
1:A:918:GLY:O	1:A:925:GLY:HA2	2.12	0.49
1:B:330:GLY:HA3	1:B:362:VAL:HG13	1.93	0.49
1:C:153:ALA:HB2	1:C:225:ALA:HA	1.95	0.49
1:C:447:GLU:OE1	1:C:447:GLU:CA	2.59	0.49
1:E:397:GLU:HB3	1:E:399:MET:H	1.76	0.49
1:E:625:ARG:NE	1:E:694:TYR:CE2	2.80	0.49
1:A:193:LEU:HD22	1:A:199:HIS:CE1	2.48	0.49
1:A:533:LEU:HD21	1:A:537:ASP:HB2	1.93	0.49
1:A:574:ILE:O	1:A:575:GLY:C	2.56	0.49
1:B:298:LEU:O	1:B:299:VAL:HG12	2.13	0.49
1:B:497:ALA:HB3	1:B:500:THR:HG23	1.93	0.49
1:B:520:VAL:HG11	1:D:24:ARG:NH1	2.26	0.49
1:C:13:HIS:HD2	1:C:40:SER:HB3	1.77	0.49
1:C:30:PHE:CE2	1:C:41:LEU:HD13	2.47	0.49
1:E:380:PHE:N	1:E:380:PHE:CD1	2.79	0.49
1:E:646:LEU:HD22	1:E:695:LEU:HD21	1.94	0.49
1:A:178:VAL:HG12	1:A:185:HIS:O	2.11	0.49
1:A:448:LEU:HD21	1:A:452:ASP:OD2	2.12	0.49
1:A:462:LEU:HD22	1:A:466:GLU:HB2	1.93	0.49
1:B:11:ARG:HG2	1:B:17:SER:HA	1.94	0.49
1:B:171:ASN:CG	1:B:187:LEU:HG	2.37	0.49
1:C:368:ASN:C	1:C:370:TYR:N	2.70	0.49
1:D:446:CYS:HG	1:D:449:SER:HG	1.46	0.49
1:E:49:GLU:HG2	1:E:72:PRO:HG2	1.95	0.49
1:E:130:ARG:HG2	1:E:130:ARG:HH11	1.77	0.49
1:F:68:GLN:OE1	1:F:68:GLN:O	2.30	0.49
1:F:503:GLY:O	1:F:506:ALA:N	2.45	0.49
1:A:670:ALA:HA	1:A:681:GLN:HE21	1.77	0.49
1:A:698:LEU:HD22	1:A:699:VAL:N	2.28	0.49
1:B:147:THR:O	1:B:148:ARG:HB2	2.12	0.49
1:B:438:GLY:CA	1:B:442:ILE:HB	2.42	0.49
1:B:784:TYR:HE2	1:B:798:VAL:HB	1.75	0.49
1:C:318:GLY:C	1:C:320:THR:H	2.19	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:342:PRO:HB2	1:D:347:PRO:CB	2.42	0.49
1:D:385:ALA:HB1	1:D:389:ARG:HH22	1.77	0.49
1:D:638:ARG:HH12	1:F:929:VAL:HG13	1.77	0.49
1:E:86:ILE:HB	1:E:526:LEU:HG	1.95	0.49
1:E:326:ARG:HH12	1:E:364:VAL:HG22	1.77	0.49
1:E:352:LYS:C	1:E:354:ILE:N	2.69	0.49
1:F:324:PHE:O	1:F:328:MET:HG2	2.13	0.49
1:A:230:ASP:O	1:A:230:ASP:OD1	2.30	0.49
1:A:848:ALA:O	1:A:852:LYS:HG3	2.12	0.49
1:A:877:HIS:O	1:A:880:ASP:HB2	2.13	0.49
1:B:68:GLN:HE21	1:B:764:ILE:CG1	2.26	0.49
1:B:156:VAL:HG13	1:B:159:ARG:HB2	1.94	0.49
1:B:576:PRO:HB3	1:B:601:ILE:HD11	1.95	0.49
1:B:584:ARG:CD	1:C:584:ARG:HD3	2.43	0.49
1:C:154:PRO:HD2	1:C:229:ALA:CB	2.43	0.49
1:D:27:LEU:C	1:D:27:LEU:HD23	2.37	0.49
1:D:65:PHE:HD1	1:D:766:MET:HE3	1.77	0.49
1:D:784:TYR:HE2	1:D:798:VAL:HB	1.78	0.49
1:E:93:ARG:HA	1:E:499:ALA:HB2	1.94	0.49
1:E:162:GLU:O	1:E:162:GLU:HG3	2.11	0.49
1:A:684:GLY:O	1:A:686:HIS:HD2	1.96	0.49
1:A:816:ILE:HD12	1:A:816:ILE:N	2.28	0.49
1:B:282:CYS:SG	1:B:415:CYS:HB3	2.52	0.49
1:C:667:ILE:HG12	1:C:684:GLY:O	2.13	0.49
1:D:277:SER:HB2	1:D:278:PRO:HD2	1.93	0.49
1:E:180:VAL:HG21	1:E:191:PRO:HG3	1.95	0.49
1:F:54:TYR:CB	1:F:82:PRO:HB3	2.42	0.49
1:F:353:ALA:O	1:F:357:GLY:O	2.31	0.49
1:F:856:GLU:HG2	1:F:867:TYR:CZ	2.42	0.49
1:A:25:ASP:N	1:A:554:THR:HB	2.26	0.49
1:A:155:VAL:HG23	1:A:156:VAL:N	2.27	0.49
1:B:45:THR:HG22	1:B:74:VAL:HG13	1.94	0.49
1:B:436:GLU:CD	1:B:440:LYS:HE3	2.37	0.49
1:B:670:ALA:HA	1:B:681:GLN:HE21	1.77	0.49
1:C:327:MET:HE2	1:C:327:MET:N	2.28	0.49
1:C:452:ASP:O	1:C:456:PHE:HD1	1.95	0.49
1:D:445:VAL:O	1:D:492:LEU:O	2.30	0.49
1:F:447:GLU:HG2	1:F:489:LEU:O	2.13	0.49
1:F:881:ILE:CG2	1:F:904:ASN:HD21	2.24	0.49
1:A:287:GLY:HA2	1:A:419:ARG:HB3	1.93	0.49
1:A:706:ILE:HD11	1:A:851:VAL:CB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:HIS:CD2	1:C:40:SER:CB	2.96	0.49
1:C:36:SER:OG	1:C:574:ILE:HG22	2.13	0.49
1:C:143:MET:HB3	1:C:144:PRO:HD2	1.95	0.49
1:C:322:GLU:O	1:C:323:TYR:C	2.52	0.49
1:D:368:ASN:ND2	1:D:372:ARG:HE	2.11	0.49
1:D:805:SER:OG	1:D:808:GLU:HB2	2.12	0.49
1:E:170:LEU:O	1:E:175:TYR:CD2	2.66	0.49
1:E:215:LYS:C	1:E:217:ARG:H	2.20	0.49
1:F:563:ASP:O	1:F:567:HIS:HD2	1.94	0.49
1:F:602:THR:HG22	1:F:606:LEU:CD1	2.42	0.49
1:F:856:GLU:CG	1:F:867:TYR:OH	2.37	0.49
1:A:145:GLU:OE1	1:A:145:GLU:N	2.46	0.49
1:B:383:VAL:HG23	1:B:387:LEU:CA	2.41	0.49
1:B:441:SER:HB3	1:B:454:ALA:CB	2.42	0.49
1:E:269:GLU:O	1:E:270:PRO:C	2.56	0.49
1:E:362:VAL:O	1:E:362:VAL:HG12	2.11	0.49
1:E:440:LYS:HZ3	1:E:450:ILE:CG1	2.26	0.49
1:E:805:SER:OG	1:E:808:GLU:HB2	2.13	0.49
1:F:655:VAL:CG2	1:F:656:SER:N	2.76	0.49
1:A:279:TYR:O	1:A:421:LYS:HE2	2.13	0.48
1:A:597:ASN:HD22	1:A:597:ASN:C	2.21	0.48
1:B:65:PHE:CZ	1:B:767:ASN:HB2	2.47	0.48
1:B:421:LYS:O	1:B:423:GLU:N	2.46	0.48
1:B:848:ALA:O	1:B:852:LYS:HG3	2.12	0.48
1:C:131:GLN:OE1	1:C:131:GLN:CA	2.61	0.48
1:C:533:LEU:HD23	1:C:537:ASP:HB2	1.93	0.48
1:C:742:GLY:O	1:C:748:VAL:CG2	2.61	0.48
1:D:450:ILE:HD12	1:D:494:LEU:HG	1.93	0.48
1:E:151:VAL:O	1:E:205:VAL:HG23	2.13	0.48
1:E:206:ASP:OD1	1:E:221:SER:HB2	2.12	0.48
1:E:698:LEU:HD22	1:E:699:VAL:N	2.28	0.48
1:F:334:ALA:HB1	1:F:360:GLU:OE1	2.13	0.48
1:F:496:ARG:HH21	1:F:500:THR:HB	1.78	0.48
1:F:576:PRO:HG2	1:F:583:GLY:H	1.77	0.48
1:A:145:GLU:CD	1:A:145:GLU:N	2.71	0.48
1:A:423:GLU:O	1:A:426:ALA:HB3	2.12	0.48
1:B:68:GLN:NE2	1:B:764:ILE:CD1	2.76	0.48
1:B:520:VAL:O	1:D:81:SER:HA	2.13	0.48
1:B:701:VAL:CG1	1:B:849:GLN:HG2	2.35	0.48
1:C:159:ARG:HE	1:C:271:ARG:HH12	1.61	0.48
1:C:497:ALA:HB3	1:C:500:THR:HG23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:591:TYR:CE1	1:C:595:LEU:HD11	2.48	0.48
1:C:671:VAL:HG11	1:C:689:VAL:HG21	1.94	0.48
1:C:762:ILE:HD12	1:E:160:LYS:CE	2.43	0.48
1:D:121:CYS:SG	1:D:122:PRO:HD2	2.53	0.48
1:D:305:ARG:HG3	1:D:305:ARG:O	2.13	0.48
1:D:703:GLN:HG2	1:D:849:GLN:HB2	1.94	0.48
1:D:763:LYS:HD3	1:D:773:TYR:CZ	2.48	0.48
1:E:98:THR:OG1	1:E:101:THR:HG23	2.13	0.48
1:E:447:GLU:HB2	1:E:485:LEU:HD21	1.94	0.48
1:A:38:LYS:HD3	1:A:38:LYS:N	2.24	0.48
1:A:368:ASN:HB2	1:A:373:THR:H	1.78	0.48
1:A:804:MET:HE3	1:A:808:GLU:OE1	2.13	0.48
1:B:343:TRP:CZ2	1:B:350:ALA:HB1	2.49	0.48
1:C:331:LEU:O	1:C:335:LEU:N	2.44	0.48
1:D:16:ARG:O	1:D:17:SER:C	2.56	0.48
1:D:222:VAL:HG12	1:D:223:GLU:N	2.28	0.48
1:D:571:ILE:O	1:D:588:SER:HA	2.13	0.48
1:E:372:ARG:HG3	1:E:374:ARG:HG3	1.94	0.48
1:F:15:LEU:HD12	1:F:15:LEU:C	2.37	0.48
1:F:542:ILE:HA	1:F:545:LEU:HD12	1.94	0.48
1:F:695:LEU:HD22	1:F:864:ARG:CA	2.42	0.48
1:A:188:THR:O	1:A:190:PRO:HD3	2.13	0.48
1:A:295:ASP:OD2	1:A:408:ARG:NE	2.33	0.48
1:A:297:GLU:OE1	1:A:298:LEU:CA	2.61	0.48
1:A:306:THR:HB	1:A:309:GLN:HB3	1.95	0.48
1:A:437:HIS:N	1:A:440:LYS:HD2	2.23	0.48
1:A:609:ARG:HG2	1:A:609:ARG:HH11	1.77	0.48
1:B:11:ARG:NH2	1:B:73:ASP:OD1	2.46	0.48
1:C:442:ILE:HD13	1:C:494:LEU:HD12	1.95	0.48
1:C:453:CYS:O	1:C:455:ASP:N	2.47	0.48
1:D:702:ASP:HB3	1:D:852:LYS:NZ	2.28	0.48
1:E:231:GLY:O	1:E:232:ILE:CG1	2.59	0.48
1:E:338:ASP:HB3	1:E:341:THR:H	1.78	0.48
1:B:178:VAL:HG13	1:B:187:LEU:HB2	1.95	0.48
1:B:557:VAL:HG12	1:B:559:GLU:HG2	1.95	0.48
1:B:621:VAL:HG13	1:B:645:PRO:CB	2.43	0.48
1:C:356:GLU:N	1:C:383:VAL:CG1	2.77	0.48
1:C:385:ALA:C	1:C:388:GLN:HG2	2.38	0.48
1:C:452:ASP:CA	1:C:456:PHE:CD1	2.92	0.48
1:C:848:ALA:O	1:C:852:LYS:HG3	2.12	0.48
1:D:132:THR:CB	1:D:133:PRO:HD2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:786:ARG:HA	1:D:789:LEU:HD12	1.95	0.48
1:E:349:LYS:CG	1:E:350:ALA:N	2.76	0.48
1:F:9:GLY:N	1:F:18:VAL:O	2.46	0.48
1:F:448:LEU:CD2	1:F:452:ASP:OD2	2.61	0.48
1:F:602:THR:O	1:F:606:LEU:HD12	2.13	0.48
1:A:451:ALA:O	1:A:455:ASP:CB	2.61	0.48
1:B:536:ARG:HD3	1:B:944:TYR:CE1	2.49	0.48
1:B:873:THR:HB	1:B:902:GLU:CD	2.39	0.48
1:C:45:THR:HG22	1:C:74:VAL:HG13	1.96	0.48
1:C:390:LYS:C	1:C:391:MET:HG3	2.38	0.48
1:C:701:VAL:HB	1:C:869:LEU:CD2	2.44	0.48
1:C:797:THR:HG22	1:C:800:GLU:OE2	2.13	0.48
1:D:312:VAL:HG11	1:D:315:TRP:CB	2.43	0.48
1:D:913:TRP:CZ3	1:D:932:GLY:HA2	2.48	0.48
1:E:608:GLY:C	1:E:610:GLU:N	2.71	0.48
1:F:612:ILE:CD1	1:F:882:ARG:CG	2.92	0.48
1:F:877:HIS:HD2	1:F:879:ASP:CB	2.26	0.48
1:F:914:ILE:HD11	1:F:934:PRO:HA	1.94	0.48
1:A:137:VAL:HG21	1:A:219:THR:HG23	1.96	0.48
1:A:621:VAL:HG13	1:A:645:PRO:CB	2.44	0.48
1:B:150:LEU:HD23	1:B:151:VAL:H	1.78	0.48
1:B:348:ALA:O	1:B:351:ARG:HB3	2.14	0.48
1:B:621:VAL:CG1	1:B:645:PRO:HB3	2.42	0.48
1:B:625:ARG:NE	1:B:694:TYR:CE2	2.82	0.48
1:C:356:GLU:HG3	1:C:357:GLY:N	2.28	0.48
1:C:597:ASN:HD22	1:C:597:ASN:C	2.22	0.48
1:D:609:ARG:HG2	1:D:609:ARG:HH11	1.78	0.48
1:D:869:LEU:HB2	1:D:900:VAL:CG2	2.44	0.48
1:E:40:SER:O	1:E:45:THR:OG1	2.32	0.48
1:E:451:ALA:HB1	1:E:456:PHE:CZ	2.40	0.48
1:E:592:ASP:CB	1:F:468:ALA:HB2	2.44	0.48
1:E:597:ASN:HD22	1:E:598:LYS:N	2.12	0.48
1:E:607:SER:OG	1:E:609:ARG:NE	2.46	0.48
1:F:667:ILE:O	1:F:669:ALA:N	2.47	0.48
1:A:528:GLU:O	1:A:531:ILE:HG13	2.13	0.48
1:A:619:ARG:HD2	1:A:912:ASP:OD2	2.14	0.48
1:B:284:GLU:CG	1:B:412:CYS:SG	2.98	0.48
1:B:626:GLN:HE21	1:B:626:GLN:HB3	1.51	0.48
1:B:638:ARG:NH2	1:B:925:GLY:H	2.11	0.48
1:C:455:ASP:HA	1:C:478:ARG:HD3	1.95	0.48
1:C:565:ILE:HG21	1:C:606:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:68:GLN:NE2	1:E:764:ILE:HD11	2.29	0.48
1:E:323:TYR:HE1	1:E:327:MET:CG	2.18	0.48
1:E:802:LEU:HG	1:E:837:GLY:HA3	1.96	0.48
1:F:521:GLY:N	1:F:553:ASN:OD1	2.47	0.48
1:F:587:HIS:CD2	1:F:588:SER:N	2.82	0.48
1:F:638:ARG:O	1:F:639:GLY:C	2.56	0.48
1:A:399:MET:HA	1:A:402:ARG:HB3	1.96	0.48
1:B:313:ALA:O	1:B:316:SER:CB	2.62	0.48
1:B:441:SER:C	1:B:445:VAL:CG2	2.87	0.48
1:C:16:ARG:O	1:C:17:SER:C	2.57	0.48
1:D:222:VAL:O	1:D:225:ALA:N	2.47	0.48
1:D:613:GLU:OE1	1:D:613:GLU:HA	2.13	0.48
1:D:822:TYR:CD1	1:D:858:GLN:HG2	2.49	0.48
1:E:335:LEU:HB2	1:E:337:PHE:CE2	2.49	0.48
1:E:346:LEU:O	1:E:348:ALA:N	2.46	0.48
1:E:363:HIS:HB3	1:E:365:ARG:NH2	2.28	0.48
1:E:609:ARG:HH11	1:E:609:ARG:HG2	1.79	0.48
1:E:891:LEU:O	1:E:896:ASN:HB2	2.13	0.48
1:B:737:ARG:NH1	1:B:790:GLU:OE1	2.46	0.48
1:C:335:LEU:HD13	1:C:352:LYS:HE2	1.96	0.48
1:D:12:GLU:HG2	1:D:45:THR:HG23	1.95	0.48
1:E:30:PHE:CE2	1:E:41:LEU:HD13	2.49	0.48
1:E:94:ASN:OD1	1:E:95:PRO:HD2	2.14	0.48
1:E:148:ARG:CB	1:E:148:ARG:NH1	2.76	0.48
1:E:456:PHE:O	1:E:459:ALA:N	2.47	0.48
1:E:456:PHE:O	1:E:457:LEU:C	2.56	0.48
1:F:118:THR:CB	1:F:119:PRO:CD	2.91	0.48
1:F:422:PRO:O	1:F:425:LEU:CA	2.62	0.48
1:F:571:ILE:HG22	1:F:572:VAL:N	2.29	0.48
1:F:640:ILE:HD13	1:F:640:ILE:N	2.28	0.48
1:A:536:ARG:HD3	1:A:944:TYR:CE1	2.48	0.47
1:B:65:PHE:CE2	1:B:767:ASN:HB2	2.48	0.47
1:B:314:PRO:C	1:B:316:SER:H	2.21	0.47
1:B:441:SER:HB3	1:B:454:ALA:HB2	1.95	0.47
1:C:919:PRO:HA	1:C:929:VAL:HG21	1.96	0.47
1:D:873:THR:HG21	1:D:904:ASN:HB2	1.95	0.47
1:E:92:ASN:OD1	1:E:93:ARG:N	2.47	0.47
1:E:428:THR:HA	1:E:435:GLY:O	2.13	0.47
1:E:450:ILE:CG2	1:E:481:LEU:HG	2.44	0.47
1:F:399:MET:HA	1:F:402:ARG:CB	2.44	0.47
1:F:447:GLU:HA	1:F:447:GLU:OE1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:ARG:CB	1:A:291:ARG:NH1	2.77	0.47
1:A:345:LYS:HB3	1:A:349:LYS:HE2	1.95	0.47
1:A:346:LEU:CD1	1:A:349:LYS:HE2	2.38	0.47
1:B:299:VAL:O	1:B:300:VAL:O	2.32	0.47
1:C:313:ALA:N	1:C:314:PRO:HD2	2.27	0.47
1:C:445:VAL:C	1:C:447:GLU:N	2.71	0.47
1:D:873:THR:HB	1:D:902:GLU:OE2	2.14	0.47
1:E:120:HIS:HB2	1:E:426:ALA:HB1	1.96	0.47
1:E:411:PRO:O	1:E:412:CYS:C	2.53	0.47
1:E:441:SER:O	1:E:494:LEU:C	2.55	0.47
1:F:436:GLU:C	1:F:436:GLU:CD	2.81	0.47
1:F:905:LEU:HD21	1:F:948:PHE:O	2.14	0.47
1:A:18:VAL:CG1	1:A:585:ILE:HD12	2.44	0.47
1:A:425:LEU:C	1:A:437:HIS:ND1	2.72	0.47
1:A:706:ILE:HD11	1:A:851:VAL:HB	1.95	0.47
1:B:120:HIS:HB2	1:B:426:ALA:HB1	1.96	0.47
1:B:373:THR:HG22	1:B:374:ARG:HB2	1.95	0.47
1:B:619:ARG:HD2	1:B:912:ASP:OD2	2.14	0.47
1:C:544:THR:HG22	1:C:547:ARG:HH11	1.78	0.47
1:D:65:PHE:CD1	1:D:766:MET:HE3	2.49	0.47
1:D:591:TYR:CE1	1:D:595:LEU:HD11	2.50	0.47
1:D:625:ARG:NE	1:D:694:TYR:HE2	2.11	0.47
1:E:355:LEU:HA	1:E:383:VAL:HG13	1.95	0.47
1:F:86:ILE:HD11	1:F:514:GLN:HG3	1.96	0.47
1:F:445:VAL:CG1	1:F:449:SER:CB	2.82	0.47
1:A:271:ARG:C	1:A:273:PHE:H	2.22	0.47
1:B:149:PHE:C	1:B:149:PHE:CD1	2.92	0.47
1:B:275:PHE:O	1:B:287:GLY:HA3	2.14	0.47
1:B:327:MET:HA	1:B:362:VAL:HG11	1.95	0.47
1:B:423:GLU:O	1:B:426:ALA:HB3	2.15	0.47
1:B:576:PRO:HD3	1:B:586:VAL:HG22	1.74	0.47
1:C:128:VAL:HB	1:C:256:ALA:O	2.14	0.47
1:C:264:ALA:HB3	1:C:423:GLU:OE1	2.14	0.47
1:C:354:ILE:O	1:C:354:ILE:HG22	2.15	0.47
1:C:743:ARG:HD2	1:C:751:GLY:HA3	1.97	0.47
1:C:786:ARG:HA	1:C:789:LEU:HD12	1.96	0.47
1:D:418:THR:O	1:D:420:LEU:N	2.44	0.47
1:E:256:ALA:CA	1:E:263:LEU:HD11	2.37	0.47
1:E:936:ASP:O	1:E:939:ALA:HB3	2.14	0.47
1:F:312:VAL:HG13	1:F:314:PRO:HD2	1.96	0.47
1:F:505:GLU:O	1:F:509:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:524:TYR:CE2	1:F:548:LEU:HD21	2.49	0.47
1:A:88:GLN:HG2	1:A:507:GLN:HB2	1.97	0.47
1:A:180:VAL:HA	1:A:200:ASP:O	2.14	0.47
1:A:822:TYR:CD1	1:A:858:GLN:HG2	2.49	0.47
1:B:119:PRO:HB3	1:B:427:VAL:HG22	1.96	0.47
1:B:160:LYS:HD3	1:B:196:GLN:O	2.14	0.47
1:B:355:LEU:O	1:B:356:GLU:CB	2.60	0.47
1:B:699:VAL:HG21	1:B:867:TYR:CE1	2.50	0.47
1:C:853:LEU:O	1:C:857:LEU:HD23	2.15	0.47
1:D:134:GLN:O	1:D:137:VAL:HG12	2.13	0.47
1:D:151:VAL:O	1:D:151:VAL:HG13	2.14	0.47
1:D:608:GLY:C	1:D:610:GLU:N	2.72	0.47
1:E:406:PHE:CE2	1:E:680:ARG:CD	2.98	0.47
1:E:497:ALA:O	1:E:498:ALA:C	2.57	0.47
1:F:440:LYS:C	1:F:445:VAL:CG2	2.81	0.47
1:F:476:GLU:OE1	1:F:476:GLU:HA	2.14	0.47
1:A:402:ARG:HD2	1:A:680:ARG:CZ	2.44	0.47
1:A:584:ARG:HD3	1:D:584:ARG:HD2	1.95	0.47
1:A:618:ARG:NH2	1:A:934:PRO:HG2	2.29	0.47
1:A:869:LEU:HB2	1:A:900:VAL:HG22	1.96	0.47
1:B:337:PHE:HB3	1:B:349:LYS:HD2	1.97	0.47
1:C:131:GLN:HG3	1:C:136:ILE:HD11	1.97	0.47
1:D:89:LYS:O	1:D:89:LYS:HG3	2.14	0.47
1:D:349:LYS:N	1:D:349:LYS:CD	2.56	0.47
1:D:651:SER:HA	1:D:900:VAL:O	2.14	0.47
1:E:286:SER:CB	1:E:288:LEU:HD23	2.38	0.47
1:E:349:LYS:CG	1:E:350:ALA:H	2.28	0.47
1:E:514:GLN:O	1:E:515:ILE:C	2.58	0.47
1:F:661:SER:OG	1:F:665:ASN:HB2	2.15	0.47
1:F:857:LEU:C	1:F:857:LEU:CD1	2.88	0.47
1:A:7:VAL:O	1:A:19:ASP:HA	2.14	0.47
1:A:157:ARG:HH22	1:A:267:ASP:CG	2.23	0.47
1:A:226:LEU:O	1:A:231:GLY:N	2.47	0.47
1:A:391:MET:CE	1:A:394:THR:CG2	2.90	0.47
1:A:797:THR:HG22	1:A:800:GLU:OE2	2.15	0.47
1:A:805:SER:OG	1:A:808:GLU:HB2	2.14	0.47
1:A:873:THR:HG21	1:A:904:ASN:HB2	1.97	0.47
1:B:65:PHE:HE1	1:B:766:MET:HA	1.80	0.47
1:B:93:ARG:HA	1:B:499:ALA:HB2	1.96	0.47
1:B:180:VAL:CG1	1:B:181:ASP:H	2.22	0.47
1:B:185:HIS:CD2	1:B:191:PRO:HG3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:ALA:O	1:B:316:SER:HB3	2.15	0.47
1:B:538:ASN:OD1	1:B:561:ASP:OD2	2.31	0.47
1:B:776:CYS:SG	1:B:778:VAL:HB	2.53	0.47
1:B:817:ALA:O	1:B:821:ARG:HG2	2.14	0.47
1:C:152:LEU:HD22	1:C:179:ARG:HH21	1.78	0.47
1:C:508:ARG:CG	1:C:508:ARG:NH1	2.69	0.47
1:C:651:SER:HA	1:C:900:VAL:O	2.14	0.47
1:C:793:TYR:C	1:C:793:TYR:HD1	2.22	0.47
1:D:22:LEU:HB3	1:D:28:ILE:CD1	2.44	0.47
1:D:308:ALA:O	1:D:309:GLN:CB	2.62	0.47
1:D:497:ALA:O	1:D:498:ALA:C	2.58	0.47
1:E:323:TYR:C	1:E:323:TYR:HD1	2.22	0.47
1:E:422:PRO:HG3	1:E:425:LEU:HD12	1.95	0.47
1:E:453:CYS:O	1:E:457:LEU:HD23	2.14	0.47
1:E:509:ILE:O	1:E:512:ALA:N	2.48	0.47
1:F:557:VAL:HG12	1:F:559:GLU:HG2	1.95	0.47
1:F:695:LEU:CD1	1:F:897:THR:CB	2.92	0.47
1:F:907:VAL:O	1:F:907:VAL:HG13	2.15	0.47
1:A:49:GLU:HG2	1:A:72:PRO:HG2	1.96	0.47
1:A:131:GLN:HE22	1:A:139:GLN:HE22	1.63	0.47
1:A:348:ALA:O	1:A:352:LYS:HG2	2.15	0.47
1:A:441:SER:HA	1:A:444:GLU:HG2	1.96	0.47
1:A:574:ILE:O	1:A:575:GLY:O	2.33	0.47
1:A:575:GLY:CA	1:A:584:ARG:O	2.63	0.47
1:A:865:THR:HG22	1:A:896:ASN:ND2	2.29	0.47
1:B:145:GLU:HB2	1:B:148:ARG:NH2	2.29	0.47
1:B:343:TRP:C	1:B:343:TRP:CE3	2.93	0.47
1:B:797:THR:HG22	1:B:800:GLU:OE2	2.15	0.47
1:C:226:LEU:HD13	1:C:232:ILE:N	2.29	0.47
1:C:354:ILE:O	1:C:355:LEU:CB	2.61	0.47
1:C:387:LEU:HB3	1:C:388:GLN:NE2	2.30	0.47
1:D:298:LEU:HD23	1:D:406:PHE:HA	1.97	0.47
1:D:404:GLU:C	1:D:406:PHE:H	2.23	0.47
1:D:575:GLY:O	1:D:582:GLY:CA	2.60	0.47
1:D:727:LEU:HD22	1:D:793:TYR:CE2	2.40	0.47
1:E:68:GLN:HE21	1:E:764:ILE:CG1	2.28	0.47
1:E:460:LEU:N	1:E:460:LEU:CD2	2.76	0.47
1:E:793:TYR:C	1:E:793:TYR:HD1	2.23	0.47
1:F:363:HIS:CD2	1:F:377:TYR:HB3	2.50	0.47
1:F:440:LYS:HB3	1:F:445:VAL:HG22	1.97	0.47
1:F:533:LEU:HD22	1:F:541:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:545:LEU:O	1:F:548:LEU:N	2.48	0.47
1:F:922:GLY:O	1:F:925:GLY:O	2.33	0.47
1:B:391:MET:HE2	1:B:403:TYR:OH	2.14	0.47
1:B:584:ARG:HD3	1:C:584:ARG:CD	2.45	0.47
1:C:474:LEU:O	1:C:478:ARG:HG2	2.14	0.47
1:C:545:LEU:HD23	1:C:545:LEU:HA	1.77	0.47
1:C:703:GLN:HG2	1:C:849:GLN:HB2	1.97	0.47
1:D:152:LEU:HD13	1:D:179:ARG:HH21	1.78	0.47
1:E:24:ARG:HG3	1:E:554:THR:HG21	1.97	0.47
1:E:171:ASN:ND2	1:E:188:THR:HG22	2.30	0.47
1:E:804:MET:HE3	1:E:808:GLU:OE1	2.15	0.47
1:F:337:PHE:CZ	1:F:347:PRO:CA	2.97	0.47
1:F:440:LYS:HA	1:F:444:GLU:HB2	1.97	0.47
1:F:470:ALA:O	1:F:473:VAL:HB	2.15	0.47
1:A:284:GLU:CB	1:A:414:VAL:HG21	2.45	0.47
1:A:630:VAL:O	1:A:687:THR:HB	2.15	0.47
1:A:873:THR:HB	1:A:902:GLU:CD	2.40	0.47
1:B:576:PRO:HB3	1:B:601:ILE:CD1	2.45	0.47
1:C:10:ALA:HB3	1:C:18:VAL:CG2	2.44	0.47
1:C:31:THR:O	1:C:573:ASP:HA	2.15	0.47
1:D:88:GLN:OE1	1:D:531:ILE:CG2	2.62	0.47
1:D:388:GLN:O	1:D:392:SER:CB	2.61	0.47
1:D:514:GLN:O	1:D:515:ILE:C	2.57	0.47
1:D:758:GLY:O	1:D:783:ARG:HG2	2.15	0.47
1:E:338:ASP:HB3	1:E:341:THR:OG1	2.15	0.47
1:F:511:LEU:O	1:F:515:ILE:HG22	2.15	0.47
1:F:515:ILE:HB	1:F:548:LEU:HG	1.97	0.47
1:A:106:TYR:CD1	1:A:442:ILE:CD1	2.98	0.46
1:A:758:GLY:O	1:A:783:ARG:HG2	2.15	0.46
1:B:300:VAL:HG13	1:B:301:PRO:CD	2.38	0.46
1:B:474:LEU:O	1:B:478:ARG:HG2	2.16	0.46
1:D:10:ALA:HB3	1:D:18:VAL:CG2	2.45	0.46
1:E:22:LEU:HB3	1:E:28:ILE:HD13	1.95	0.46
1:E:873:THR:HG21	1:E:904:ASN:HB2	1.97	0.46
1:F:357:GLY:HA2	1:F:383:VAL:CB	2.33	0.46
1:F:448:LEU:HD21	1:F:452:ASP:OD2	2.15	0.46
1:F:634:GLU:HB2	1:F:684:GLY:HA3	1.97	0.46
1:F:674:ASN:OD1	1:F:679:ALA:O	2.33	0.46
1:A:36:SER:OG	1:A:574:ILE:O	2.32	0.46
1:A:432:GLU:CG	1:A:433:SER:N	2.66	0.46
1:A:591:TYR:CE2	1:A:595:LEU:HD11	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:621:VAL:HG13	1:C:645:PRO:CB	2.45	0.46
1:D:180:VAL:HG22	1:D:201:ILE:HG12	1.97	0.46
1:D:229:ALA:O	1:D:230:ASP:O	2.32	0.46
1:D:294:VAL:HA	1:D:407:MET:HA	1.97	0.46
1:D:701:VAL:HB	1:D:869:LEU:CD2	2.43	0.46
1:E:33:LEU:O	1:E:36:SER:HB2	2.15	0.46
1:E:315:TRP:HE1	1:E:387:LEU:CD1	1.98	0.46
1:F:113:TYR:C	1:F:115:ARG:H	2.23	0.46
1:F:915:ILE:HG22	1:F:917:LEU:CD1	2.46	0.46
1:A:10:ALA:HB3	1:A:18:VAL:CG2	2.46	0.46
1:A:96:ARG:HD3	1:A:276:ASN:HD21	1.79	0.46
1:A:331:LEU:HA	1:A:334:ALA:HB3	1.96	0.46
1:A:338:ASP:OD1	1:A:340:ASP:N	2.48	0.46
1:A:339:VAL:O	1:A:339:VAL:HG12	2.15	0.46
1:B:215:LYS:C	1:B:217:ARG:N	2.73	0.46
1:C:811:GLU:OE2	1:C:814:GLU:OE1	2.34	0.46
1:D:194:LYS:O	1:D:195:LYS:C	2.59	0.46
1:D:745:SER:HB3	1:D:748:VAL:HG22	1.97	0.46
1:E:257:CYS:O	1:E:260:GLY:N	2.48	0.46
1:F:14:ASN:O	1:F:14:ASN:OD1	2.33	0.46
1:F:345:LYS:CB	1:F:347:PRO:HG3	2.23	0.46
1:F:420:LEU:HD13	1:F:424:ILE:HG21	1.95	0.46
1:A:277:SER:OG	1:A:278:PRO:HD2	2.15	0.46
1:A:294:VAL:HB	1:A:407:MET:HG2	1.97	0.46
1:A:650:THR:HA	1:A:913:TRP:O	2.15	0.46
1:C:294:VAL:HA	1:C:407:MET:CB	2.46	0.46
1:C:368:ASN:OD1	1:C:369:ARG:N	2.49	0.46
1:C:489:LEU:HD12	1:C:489:LEU:HA	1.77	0.46
1:D:448:LEU:HD21	1:D:490:GLU:HG3	1.97	0.46
1:D:483:PHE:O	1:D:486:ASP:HB2	2.15	0.46
1:D:536:ARG:HD3	1:D:944:TYR:CE1	2.50	0.46
1:E:14:ASN:O	1:E:583:GLY:HA3	2.15	0.46
1:E:350:ALA:HA	1:E:353:ALA:HB3	1.95	0.46
1:F:28:ILE:N	1:F:28:ILE:CD1	2.78	0.46
1:C:295:ASP:H	1:C:407:MET:HA	1.80	0.46
1:C:397:GLU:C	1:C:399:MET:H	2.24	0.46
1:E:350:ALA:O	1:E:354:ILE:CG1	2.63	0.46
1:F:10:ALA:C	1:F:15:LEU:CD1	2.88	0.46
1:A:141:LEU:CD1	1:A:218:LEU:HD23	2.44	0.46
1:A:446:CYS:HB3	1:A:490:GLU:O	2.15	0.46
1:A:511:LEU:HG	1:A:515:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:GLY:HA3	1:A:584:ARG:H	1.80	0.46
1:A:621:VAL:CG1	1:A:645:PRO:HB3	2.45	0.46
1:B:184:VAL:HG12	1:B:185:HIS:CG	2.50	0.46
1:B:195:LYS:HB2	1:B:195:LYS:HE3	1.78	0.46
1:B:375:SER:CB	1:B:377:TYR:H	2.28	0.46
1:C:186:PRO:O	1:C:190:PRO:CD	2.63	0.46
1:C:718:THR:HG22	1:C:822:TYR:HD1	1.81	0.46
1:D:132:THR:HB	1:D:133:PRO:HD2	1.97	0.46
1:F:115:ARG:NH1	1:F:469:ILE:O	2.49	0.46
1:F:467:GLN:O	1:F:468:ALA:C	2.58	0.46
1:A:432:GLU:HB2	1:A:457:LEU:HG	1.97	0.46
1:A:626:GLN:HE21	1:A:626:GLN:HB3	1.56	0.46
1:A:747:ASN:C	1:A:752:ARG:HH11	2.24	0.46
1:B:94:ASN:OD1	1:B:95:PRO:CD	2.59	0.46
1:B:159:ARG:CD	1:D:777:GLU:OE1	2.64	0.46
1:B:268:LEU:HD23	1:B:268:LEU:HA	1.61	0.46
1:B:323:TYR:HD1	1:B:324:PHE:N	2.14	0.46
1:C:403:TYR:O	1:C:404:GLU:C	2.59	0.46
1:C:782:ALA:O	1:C:783:ARG:HB2	2.16	0.46
1:D:366:TYR:HD2	1:D:367:ARG:O	1.99	0.46
1:D:869:LEU:HB2	1:D:900:VAL:HG22	1.96	0.46
1:D:877:HIS:O	1:D:881:ILE:HG12	2.14	0.46
1:E:177:ARG:NE	1:E:184:VAL:CG2	2.79	0.46
1:E:323:TYR:CE1	1:E:327:MET:HG3	2.51	0.46
1:F:463:GLY:HA2	1:F:464:PRO:HD2	1.69	0.46
1:A:298:LEU:C	1:A:298:LEU:CD1	2.68	0.46
1:A:455:ASP:C	1:A:455:ASP:OD1	2.58	0.46
1:A:528:GLU:HB3	1:A:531:ILE:HD11	1.96	0.46
1:A:675:ARG:HB3	1:A:692:LEU:HD11	1.98	0.46
1:B:269:GLU:HB3	1:B:270:PRO:HD3	1.97	0.46
1:B:324:PHE:HA	1:B:327:MET:HB2	1.96	0.46
1:B:329:ALA:HB2	1:B:339:VAL:CG1	2.46	0.46
1:B:440:LYS:O	1:B:445:VAL:HG22	2.16	0.46
1:B:660:LYS:H	1:B:660:LYS:HG3	1.46	0.46
1:C:189:ASP:CB	1:C:190:PRO:HD3	2.44	0.46
1:C:421:LYS:HA	1:C:422:PRO:HD2	1.33	0.46
1:C:421:LYS:HB2	1:C:424:ILE:HD13	1.97	0.46
1:D:305:ARG:NH2	1:D:328:MET:SD	2.89	0.46
1:D:320:THR:O	1:D:322:GLU:N	2.49	0.46
1:D:524:TYR:HB2	1:D:555:LEU:HD22	1.97	0.46
1:D:674:ASN:ND2	1:D:679:ALA:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:187:LEU:C	1:E:189:ASP:N	2.74	0.46
1:E:307:LEU:O	1:E:307:LEU:CD2	2.64	0.46
1:E:621:VAL:HG13	1:E:645:PRO:CB	2.45	0.46
1:F:110:ARG:O	1:F:111:LEU:C	2.58	0.46
1:F:427:VAL:O	1:F:436:GLU:HB2	2.16	0.46
1:F:672:LEU:HB3	1:F:698:LEU:HD22	1.98	0.46
1:A:317:ASN:CG	1:A:318:GLY:H	2.24	0.46
1:A:743:ARG:HA	1:A:750:GLY:O	2.16	0.46
1:B:298:LEU:O	1:B:299:VAL:CG1	2.64	0.46
1:B:451:ALA:O	1:B:456:PHE:N	2.49	0.46
1:B:489:LEU:HD12	1:B:489:LEU:HA	1.62	0.46
1:C:360:GLU:O	1:C:361:GLN:HG3	2.16	0.46
1:C:625:ARG:NE	1:C:694:TYR:CE2	2.84	0.46
1:D:148:ARG:NH1	1:D:238:VAL:HG13	2.31	0.46
1:D:451:ALA:O	1:D:452:ASP:C	2.56	0.46
1:D:674:ASN:O	1:D:678:GLY:HA2	2.15	0.46
1:D:811:GLU:HA	1:D:814:GLU:CG	2.42	0.46
1:E:55:VAL:C	1:E:57:SER:N	2.73	0.46
1:E:175:TYR:HB3	1:E:187:LEU:HD12	1.96	0.46
1:E:497:ALA:HB3	1:E:500:THR:HG23	1.96	0.46
1:E:514:GLN:OE1	1:E:514:GLN:HA	2.15	0.46
1:F:12:GLU:O	1:F:15:LEU:HG	2.16	0.46
1:F:320:THR:O	1:F:324:PHE:HE2	1.98	0.46
1:F:414:VAL:HG23	1:F:415:CYS:N	2.31	0.46
1:F:585:ILE:H	1:F:585:ILE:HG12	1.59	0.46
1:A:134:GLN:O	1:A:137:VAL:HG12	2.16	0.46
1:A:608:GLY:C	1:A:610:GLU:N	2.72	0.46
1:A:675:ARG:CZ	1:A:692:LEU:HG	2.46	0.46
1:B:545:LEU:HD23	1:B:545:LEU:HA	1.75	0.46
1:C:81:SER:HA	1:E:520:VAL:O	2.17	0.46
1:C:356:GLU:OE2	1:C:360:GLU:CB	2.56	0.46
1:D:106:TYR:CD1	1:D:442:ILE:HG12	2.50	0.46
1:D:322:GLU:O	1:D:323:TYR:C	2.59	0.46
1:E:384:LEU:C	1:E:386:PHE:H	2.24	0.46
1:E:420:LEU:HB2	1:E:425:LEU:HD21	1.97	0.46
1:E:450:ILE:O	1:E:451:ALA:C	2.59	0.46
1:E:452:ASP:O	1:E:456:PHE:N	2.49	0.46
1:F:571:ILE:HG21	1:F:594:LEU:HD23	1.97	0.46
1:A:157:ARG:CZ	1:A:267:ASP:OD2	2.64	0.45
1:B:158:THR:O	1:B:198:LYS:HE2	2.15	0.45
1:B:235:LEU:HD21	1:B:251:PHE:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:706:ILE:CD1	1:B:851:VAL:HG11	2.43	0.45
1:D:295:ASP:O	1:D:299:VAL:HG13	2.16	0.45
1:D:317:ASN:O	1:D:319:HIS:N	2.49	0.45
1:D:909:LYS:HD2	1:D:952:VAL:HG11	1.97	0.45
1:E:22:LEU:HB3	1:E:28:ILE:CD1	2.45	0.45
1:E:260:GLY:O	1:E:261:HIS:C	2.59	0.45
1:E:346:LEU:N	1:E:349:LYS:NZ	2.58	0.45
1:E:414:VAL:HG13	1:E:415:CYS:N	2.32	0.45
1:F:11:ARG:CA	1:F:15:LEU:CD1	2.94	0.45
1:F:12:GLU:OE1	1:F:12:GLU:HA	2.16	0.45
1:F:384:LEU:O	1:F:385:ALA:C	2.59	0.45
1:F:667:ILE:C	1:F:669:ALA:H	2.24	0.45
1:A:160:LYS:HD3	1:A:198:LYS:HD2	1.98	0.45
1:A:691:GLY:O	1:A:692:LEU:HB3	2.15	0.45
1:B:163:PHE:HB3	1:B:166:LEU:HD12	1.98	0.45
1:B:372:ARG:HD2	1:B:372:ARG:C	2.41	0.45
1:B:383:VAL:CG2	1:B:386:PHE:C	2.89	0.45
1:B:438:GLY:CA	1:B:442:ILE:CB	2.94	0.45
1:C:272:SER:O	1:C:280:GLY:HA3	2.16	0.45
1:C:394:THR:HG23	1:C:396:SER:CA	2.46	0.45
1:C:715:ALA:HB2	1:C:836:LEU:HD22	1.98	0.45
1:D:575:GLY:HA3	1:D:584:ARG:O	2.15	0.45
1:D:618:ARG:NH2	1:D:934:PRO:HG2	2.30	0.45
1:E:434:LYS:HD3	1:E:434:LYS:HA	1.66	0.45
1:E:520:VAL:HA	1:E:553:ASN:OD1	2.15	0.45
1:F:44:ASP:O	1:F:48:ALA:HB3	2.15	0.45
1:F:339:VAL:HG23	1:F:345:LYS:NZ	2.31	0.45
1:F:355:LEU:HD12	1:F:385:ALA:HB2	1.97	0.45
1:F:524:TYR:CE2	1:F:548:LEU:CD2	2.99	0.45
1:F:589:GLY:O	1:F:590:PRO:O	2.34	0.45
1:F:621:VAL:HB	1:F:622:ASP:H	1.41	0.45
1:F:882:ARG:HH12	1:F:886:ASN:HD21	0.46	0.45
1:A:455:ASP:OD1	1:A:455:ASP:O	2.35	0.45
1:A:534:HIS:HA	1:A:903:HIS:ND1	2.31	0.45
1:B:33:LEU:O	1:B:36:SER:HB2	2.16	0.45
1:D:331:LEU:HD23	1:D:335:LEU:HB2	1.98	0.45
1:D:699:VAL:HG21	1:D:867:TYR:CE1	2.51	0.45
1:D:809:ALA:HB1	1:D:813:PHE:CE1	2.51	0.45
1:E:16:ARG:O	1:E:17:SER:C	2.59	0.45
1:E:106:TYR:CZ	1:E:437:HIS:HE1	2.34	0.45
1:E:215:LYS:HD3	1:E:217:ARG:HE	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:422:PRO:HA	1:F:425:LEU:HB2	1.98	0.45
1:F:546:THR:O	1:F:547:ARG:C	2.60	0.45
1:F:882:ARG:CZ	1:F:886:ASN:ND2	2.65	0.45
1:A:203:VAL:CG2	1:A:228:LEU:HD11	2.47	0.45
1:A:346:LEU:CD1	1:A:349:LYS:HD3	2.46	0.45
1:A:763:LYS:HD3	1:A:773:TYR:CZ	2.51	0.45
1:B:143:MET:CB	1:B:144:PRO:HD3	2.33	0.45
1:B:167:PHE:O	1:B:187:LEU:HD11	2.16	0.45
1:B:175:TYR:H	1:B:187:LEU:CD2	2.30	0.45
1:B:205:VAL:HG21	1:B:225:ALA:HB2	1.99	0.45
1:B:347:PRO:HD2	1:B:349:LYS:HZ1	1.80	0.45
1:B:364:VAL:HG21	1:B:379:ASP:CG	2.42	0.45
1:C:514:GLN:OE1	1:C:514:GLN:HA	2.16	0.45
1:D:597:ASN:HD22	1:D:599:ASP:N	2.06	0.45
1:D:853:LEU:O	1:D:857:LEU:HD23	2.16	0.45
1:F:368:ASN:CB	1:F:372:ARG:O	2.48	0.45
1:A:18:VAL:HB	1:A:585:ILE:HD13	1.92	0.45
1:A:100:GLY:HA2	1:A:494:LEU:HD22	1.97	0.45
1:A:447:GLU:OE1	1:A:447:GLU:HA	2.16	0.45
1:B:171:ASN:HD22	1:B:174:GLY:HA2	1.81	0.45
1:B:183:VAL:O	1:B:184:VAL:HB	2.16	0.45
1:B:292:LYS:HA	1:B:409:ASP:HA	1.98	0.45
1:B:351:ARG:HD2	1:B:352:LYS:HZ2	1.81	0.45
1:B:618:ARG:NH2	1:B:934:PRO:HG2	2.31	0.45
1:C:160:LYS:HZ2	1:E:777:GLU:HG3	1.82	0.45
1:C:768:PHE:HB3	1:E:768:PHE:CD1	2.51	0.45
1:C:816:ILE:HD12	1:C:816:ILE:N	2.31	0.45
1:C:822:TYR:CD1	1:C:858:GLN:HG2	2.51	0.45
1:D:756:CYS:O	1:D:757:THR:C	2.59	0.45
1:E:307:LEU:O	1:E:307:LEU:HD23	2.17	0.45
1:E:440:LYS:NZ	1:E:450:ILE:HG12	2.31	0.45
1:E:533:LEU:HD21	1:E:537:ASP:HB2	1.97	0.45
1:A:18:VAL:CB	1:A:585:ILE:CD1	2.89	0.45
1:A:300:VAL:CG1	1:A:303:PRO:HG2	2.45	0.45
1:A:351:ARG:CG	1:A:355:LEU:CD1	2.89	0.45
1:B:293:GLU:N	1:B:408:ARG:O	2.49	0.45
1:B:684:GLY:O	1:B:686:HIS:HD2	1.99	0.45
1:C:194:LYS:HG3	1:C:197:GLU:OE1	2.17	0.45
1:C:297:GLU:O	1:C:297:GLU:HG2	2.16	0.45
1:C:391:MET:HE3	1:C:391:MET:HB2	1.91	0.45
1:C:456:PHE:O	1:C:460:LEU:HD23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:536:ARG:C	1:C:538:ASN:H	2.24	0.45
1:D:60:ALA:O	1:D:63:ARG:HB3	2.17	0.45
1:D:338:ASP:OD2	1:D:341:THR:HG23	2.16	0.45
1:E:33:LEU:HD23	1:E:877:HIS:CG	2.51	0.45
1:E:352:LYS:CB	1:E:356:GLU:HB3	2.47	0.45
1:E:444:GLU:HG2	1:E:450:ILE:CB	2.47	0.45
1:E:459:ALA:C	1:E:460:LEU:HD22	2.41	0.45
1:F:54:TYR:CE2	1:F:58:LEU:HD21	2.52	0.45
1:F:361:GLN:HG2	1:F:379:ASP:HA	1.99	0.45
1:F:604:ALA:HA	1:F:609:ARG:CD	2.46	0.45
1:A:117:GLY:HA3	1:A:429:LEU:HD12	1.99	0.45
1:A:351:ARG:HE	1:A:355:LEU:HD11	1.79	0.45
1:A:400:LYS:O	1:A:404:GLU:HG3	2.16	0.45
1:C:18:VAL:HB	1:C:585:ILE:HD12	1.95	0.45
1:C:873:THR:HB	1:C:902:GLU:CD	2.42	0.45
1:E:397:GLU:OE1	1:E:397:GLU:HA	2.17	0.45
1:F:3:ASP:O	1:F:4:ARG:CG	2.64	0.45
1:F:16:ARG:O	1:F:17:SER:C	2.60	0.45
1:F:339:VAL:HG23	1:F:345:LYS:HZ3	1.81	0.45
1:F:355:LEU:N	1:F:383:VAL:HG11	2.32	0.45
1:F:410:VAL:CB	1:F:411:PRO:HD2	2.37	0.45
1:F:648:VAL:HA	1:F:892:VAL:CG1	2.45	0.45
1:F:856:GLU:CD	1:F:860:ARG:HD2	2.41	0.45
1:A:226:LEU:CD2	1:A:231:GLY:C	2.88	0.45
1:A:249:GLN:HG2	1:A:251:PHE:CE1	2.51	0.45
1:A:444:GLU:OE1	1:A:444:GLU:HA	2.16	0.45
1:A:613:GLU:OE1	1:A:613:GLU:HA	2.16	0.45
1:A:764:ILE:HG22	1:A:772:VAL:O	2.17	0.45
1:A:902:GLU:HG3	1:A:907:VAL:HG11	1.99	0.45
1:B:27:LEU:C	1:B:27:LEU:HD23	2.41	0.45
1:B:375:SER:C	1:B:377:TYR:N	2.70	0.45
1:B:584:ARG:CD	1:C:584:ARG:CD	2.95	0.45
1:C:13:HIS:CD2	1:C:40:SER:HB3	2.51	0.45
1:C:176:SER:HA	1:C:187:LEU:HB2	1.97	0.45
1:C:609:ARG:HG2	1:C:609:ARG:HH11	1.82	0.45
1:D:178:VAL:HG22	1:D:203:VAL:HG12	1.99	0.45
1:D:514:GLN:OE1	1:D:514:GLN:HA	2.12	0.45
1:E:699:VAL:HG21	1:E:867:TYR:CE1	2.52	0.45
1:E:905:LEU:O	1:E:906:ASP:C	2.60	0.45
1:F:88:GLN:HB3	1:F:507:GLN:HE21	1.79	0.45
1:A:137:VAL:CG2	1:A:219:THR:HA	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:GLN:O	1:B:137:VAL:HG23	2.17	0.45
1:B:270:PRO:C	1:B:272:SER:H	2.25	0.45
1:B:514:GLN:HB3	1:B:524:TYR:CE2	2.51	0.45
1:C:93:ARG:O	1:C:94:ASN:C	2.58	0.45
1:C:626:GLN:NE2	1:C:643:SER:HB3	2.32	0.45
1:C:877:HIS:O	1:C:880:ASP:HB2	2.16	0.45
1:D:86:ILE:HB	1:D:526:LEU:HG	1.98	0.45
1:D:305:ARG:HH11	1:D:312:VAL:N	2.14	0.45
1:D:706:ILE:CD1	1:D:851:VAL:HG11	2.45	0.45
1:E:621:VAL:CG1	1:E:645:PRO:HB3	2.46	0.45
1:F:681:GLN:O	1:F:683:PRO:HD3	2.17	0.45
1:A:351:ARG:HG3	1:A:355:LEU:HD12	1.93	0.45
1:A:368:ASN:CB	1:A:372:ARG:HB2	2.47	0.45
1:A:378:ALA:C	1:A:380:PHE:N	2.75	0.45
1:A:516:GLY:O	1:A:517:SER:C	2.59	0.45
1:B:432:GLU:HG2	1:B:433:SER:H	1.82	0.45
1:C:318:GLY:C	1:C:320:THR:N	2.74	0.45
1:D:597:ASN:HD22	1:D:598:LYS:N	2.14	0.45
1:E:62:ALA:HB1	1:E:768:PHE:CZ	2.51	0.45
1:E:162:GLU:CB	1:E:195:LYS:HG2	2.45	0.45
1:E:163:PHE:C	1:E:165:ASP:N	2.75	0.45
1:E:444:GLU:HG2	1:E:450:ILE:CD1	2.41	0.45
1:E:713:ASN:O	1:E:714:PRO:C	2.60	0.45
1:E:919:PRO:HA	1:E:929:VAL:HG21	1.99	0.45
1:F:632:ALA:O	1:F:639:GLY:N	2.50	0.45
1:F:855:SER:OG	1:F:859:LYS:HD3	2.17	0.45
1:A:366:TYR:CE1	1:A:376:TYR:HB2	2.31	0.44
1:A:514:GLN:HB3	1:A:524:TYR:CE2	2.52	0.44
1:B:11:ARG:HH12	1:B:75:ASP:CG	2.25	0.44
1:B:787:GLU:HA	1:B:787:GLU:OE1	2.17	0.44
1:C:650:THR:HA	1:C:913:TRP:O	2.17	0.44
1:D:7:VAL:CG1	1:D:20:LEU:HB2	2.40	0.44
1:D:148:ARG:HH11	1:D:238:VAL:HG13	1.82	0.44
1:D:650:THR:HA	1:D:913:TRP:O	2.17	0.44
1:E:131:GLN:CG	1:E:132:THR:N	2.80	0.44
1:E:338:ASP:HB2	1:E:341:THR:OG1	2.18	0.44
1:E:489:LEU:HD12	1:E:489:LEU:HA	1.62	0.44
1:E:531:ILE:HD11	1:E:874:THR:HG23	1.99	0.44
1:E:745:SER:HB3	1:E:748:VAL:HG22	1.99	0.44
1:F:44:ASP:O	1:F:48:ALA:HB2	2.17	0.44
1:F:55:VAL:O	1:F:58:LEU:HG	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:447:GLU:HG3	1:F:489:LEU:O	2.16	0.44
1:F:877:HIS:CD2	1:F:879:ASP:N	2.73	0.44
1:A:233:VAL:CG2	1:A:251:PHE:HB2	2.46	0.44
1:A:415:CYS:O	1:A:418:THR:HG23	2.17	0.44
1:A:516:GLY:C	1:A:518:GLY:N	2.74	0.44
1:B:147:THR:HG22	1:B:148:ARG:H	1.82	0.44
1:B:382:GLY:C	1:B:383:VAL:CG1	2.76	0.44
1:B:743:ARG:HD2	1:B:751:GLY:HA3	1.99	0.44
1:C:120:HIS:HA	1:C:126:GLU:O	2.17	0.44
1:C:201:ILE:C	1:C:202:GLU:HG3	2.41	0.44
1:C:275:PHE:HB3	1:C:420:LEU:HG	1.99	0.44
1:C:442:ILE:CG2	1:C:495:SER:HA	2.45	0.44
1:C:652:VAL:HG21	1:C:664:VAL:HG21	1.98	0.44
1:C:677:ASN:OD1	1:C:697:LYS:HB2	2.17	0.44
1:D:848:ALA:O	1:D:852:LYS:HG3	2.16	0.44
1:E:436:GLU:OE1	1:E:439:ALA:HB2	2.18	0.44
1:E:650:THR:HA	1:E:913:TRP:O	2.17	0.44
1:F:672:LEU:HD23	1:F:676:LEU:CD1	2.43	0.44
1:A:442:ILE:HG23	1:A:494:LEU:HB3	1.98	0.44
1:A:804:MET:CE	1:A:808:GLU:OE1	2.66	0.44
1:A:952:VAL:HG12	1:A:952:VAL:O	2.17	0.44
1:B:877:HIS:O	1:B:881:ILE:HG12	2.16	0.44
1:C:86:ILE:HB	1:C:526:LEU:HG	2.00	0.44
1:C:361:GLN:HB3	1:C:378:ALA:O	2.17	0.44
1:D:368:ASN:C	1:D:370:TYR:H	2.24	0.44
1:D:372:ARG:CZ	1:D:372:ARG:HB2	2.47	0.44
1:E:414:VAL:HG13	1:E:415:CYS:H	1.82	0.44
1:E:742:GLY:O	1:E:748:VAL:HG21	2.18	0.44
1:F:866:VAL:HG23	1:F:897:THR:HB	1.99	0.44
1:A:509:ILE:O	1:A:512:ALA:N	2.51	0.44
1:B:38:LYS:HD3	1:B:38:LYS:N	2.31	0.44
1:B:359:ASP:HA	1:B:380:PHE:HE1	1.82	0.44
1:B:816:ILE:HD12	1:B:816:ILE:N	2.31	0.44
1:D:877:HIS:O	1:D:880:ASP:HB2	2.17	0.44
1:E:10:ALA:HB3	1:E:18:VAL:CG2	2.47	0.44
1:E:159:ARG:O	1:E:199:HIS:N	2.50	0.44
1:E:732:THR:HA	1:E:735:LYS:CE	2.45	0.44
1:E:822:TYR:CD1	1:E:858:GLN:HG2	2.52	0.44
1:F:549:ARG:O	1:F:552:GLY:N	2.44	0.44
1:A:298:LEU:C	1:A:299:VAL:CG1	2.69	0.44
1:A:528:GLU:HB3	1:A:531:ILE:CD1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:LEU:HG	1:B:442:ILE:HD11	1.98	0.44
1:B:295:ASP:C	1:B:298:LEU:HD23	2.41	0.44
1:B:412:CYS:SG	1:B:414:VAL:HB	2.58	0.44
1:B:441:SER:CB	1:B:454:ALA:CB	2.95	0.44
1:B:698:LEU:HD22	1:B:699:VAL:N	2.33	0.44
1:B:866:VAL:O	1:B:866:VAL:HG13	2.16	0.44
1:C:108:TYR:CZ	1:C:476:GLU:HG2	2.53	0.44
1:C:190:PRO:CB	1:C:191:PRO:HD3	2.47	0.44
1:C:356:GLU:HG2	1:C:381:GLU:HB2	1.84	0.44
1:D:175:TYR:CE2	1:D:205:VAL:HG22	2.52	0.44
1:E:269:GLU:O	1:E:271:ARG:N	2.50	0.44
1:E:536:ARG:C	1:E:538:ASN:H	2.26	0.44
1:E:914:ILE:HG13	1:E:937:VAL:HG21	2.00	0.44
1:F:447:GLU:HB2	1:F:490:GLU:C	2.43	0.44
1:F:610:GLU:OE1	1:F:610:GLU:HA	2.18	0.44
1:F:670:ALA:O	1:F:674:ASN:ND2	2.50	0.44
1:F:695:LEU:CG	1:F:864:ARG:O	2.60	0.44
1:A:45:THR:HG22	1:A:74:VAL:HG13	2.00	0.44
1:A:152:LEU:CD2	1:A:179:ARG:HH12	2.27	0.44
1:A:180:VAL:HG23	1:A:180:VAL:O	2.18	0.44
1:B:295:ASP:CG	1:B:298:LEU:CD2	2.87	0.44
1:B:298:LEU:CD2	1:B:298:LEU:N	2.80	0.44
1:B:651:SER:HA	1:B:900:VAL:O	2.18	0.44
1:B:807:GLU:O	1:B:810:ALA:HB3	2.18	0.44
1:C:4:ARG:NE	1:C:21:ASP:OD1	2.41	0.44
1:C:460:LEU:O	1:C:462:LEU:N	2.50	0.44
1:C:497:ALA:O	1:C:498:ALA:C	2.60	0.44
1:C:706:ILE:HD11	1:C:851:VAL:CB	2.48	0.44
1:C:877:HIS:O	1:C:881:ILE:HG12	2.17	0.44
1:D:303:PRO:HB3	1:D:310:GLY:O	2.17	0.44
1:E:877:HIS:O	1:E:881:ILE:HG12	2.17	0.44
1:F:344:ARG:C	1:F:346:LEU:N	2.63	0.44
1:F:347:PRO:HB2	1:F:350:ALA:HB3	1.96	0.44
1:F:464:PRO:O	1:F:467:GLN:N	2.50	0.44
1:F:540:ARG:HE	1:F:540:ARG:HB3	1.38	0.44
1:F:650:THR:O	1:F:900:VAL:HG12	2.17	0.44
1:F:914:ILE:O	1:F:931:GLN:HA	2.18	0.44
1:A:18:VAL:HB	1:A:585:ILE:HD12	1.94	0.44
1:A:102:ILE:CD1	1:A:498:ALA:HB2	2.47	0.44
1:C:152:LEU:HD23	1:C:202:GLU:HB3	1.99	0.44
1:C:356:GLU:CG	1:C:357:GLY:N	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:876:LEU:HD22	1:C:880:ASP:HB3	1.98	0.44
1:D:713:ASN:HB2	1:D:714:PRO:HD2	2.00	0.44
1:E:441:SER:O	1:E:495:SER:CB	2.66	0.44
1:E:444:GLU:OE1	1:E:444:GLU:HA	2.18	0.44
1:F:436:GLU:OE1	1:F:436:GLU:CA	2.66	0.44
1:F:533:LEU:CG	1:F:537:ASP:HB2	2.48	0.44
1:A:324:PHE:O	1:A:328:MET:HG2	2.17	0.44
1:B:388:GLN:O	1:B:392:SER:HB2	2.17	0.44
1:B:432:GLU:HG2	1:B:433:SER:N	2.32	0.44
1:B:447:GLU:C	1:B:450:ILE:HG22	2.43	0.44
1:B:452:ASP:C	1:B:455:ASP:H	2.23	0.44
1:C:22:LEU:HB3	1:C:28:ILE:CD1	2.48	0.44
1:C:626:GLN:HE21	1:C:626:GLN:HB3	1.54	0.44
1:D:331:LEU:CD2	1:D:335:LEU:HD13	2.46	0.44
1:D:619:ARG:HB2	1:D:912:ASP:CG	2.43	0.44
1:E:440:LYS:HA	1:E:444:GLU:OE1	2.17	0.44
1:E:667:ILE:O	1:E:668:LEU:C	2.60	0.44
1:E:713:ASN:HB2	1:E:714:PRO:HD2	2.00	0.44
1:E:763:LYS:HD3	1:E:773:TYR:CZ	2.52	0.44
1:F:89:LYS:O	1:F:90:SER:HB2	2.16	0.44
1:F:107:ASP:N	1:F:107:ASP:OD1	2.50	0.44
1:F:402:ARG:HD3	1:F:680:ARG:NH1	2.32	0.44
1:F:476:GLU:O	1:F:480:ARG:HG2	2.18	0.44
1:F:656:SER:HA	1:F:660:LYS:HD2	1.99	0.44
1:F:866:VAL:HG22	1:F:899:ILE:HD11	2.00	0.44
1:A:148:ARG:HB3	1:A:238:VAL:CG1	2.47	0.44
1:A:255:LEU:CD1	1:A:268:LEU:HG	2.48	0.44
1:B:80:LEU:O	1:D:519:LEU:HA	2.18	0.44
1:B:366:TYR:CE1	1:B:374:ARG:O	2.70	0.44
1:B:718:THR:HG22	1:B:822:TYR:HD1	1.82	0.44
1:C:359:ASP:C	1:C:360:GLU:CG	2.89	0.44
1:C:699:VAL:HG21	1:C:867:TYR:CE1	2.53	0.44
1:C:756:CYS:HB3	1:C:776:CYS:HB2	2.00	0.44
1:D:297:GLU:OE1	1:D:297:GLU:HA	2.18	0.44
1:D:712:SER:O	1:D:713:ASN:CB	2.64	0.44
1:D:793:TYR:C	1:D:793:TYR:HD1	2.24	0.44
1:E:115:ARG:NH1	1:E:469:ILE:O	2.51	0.44
1:E:366:TYR:HE2	1:E:377:TYR:CE2	2.36	0.44
1:F:14:ASN:ND2	1:F:579:GLY:C	2.75	0.44
1:F:422:PRO:O	1:F:425:LEU:HB2	2.18	0.44
1:F:443:ALA:HA	1:F:495:SER:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:576:PRO:CG	1:F:584:ARG:H	2.30	0.44
1:F:618:ARG:HD2	1:F:933:THR:HG22	2.00	0.44
1:A:339:VAL:HG13	1:A:339:VAL:O	2.17	0.43
1:A:346:LEU:CB	1:A:349:LYS:HG2	2.41	0.43
1:A:351:ARG:NE	1:A:355:LEU:CD1	2.67	0.43
1:A:444:GLU:CG	1:A:450:ILE:HG12	2.48	0.43
1:A:893:ASP:C	1:A:895:GLY:N	2.76	0.43
1:B:520:VAL:HG11	1:D:24:ARG:CZ	2.48	0.43
1:B:840:ALA:N	1:B:841:PRO:CD	2.81	0.43
1:C:397:GLU:O	1:C:400:LYS:HG3	2.17	0.43
1:C:477:ILE:HG22	1:C:481:LEU:CD2	2.48	0.43
1:C:618:ARG:NH2	1:C:934:PRO:HG2	2.33	0.43
1:C:626:GLN:HE21	1:C:643:SER:HB3	1.83	0.43
1:C:802:LEU:HG	1:C:837:GLY:HA3	2.00	0.43
1:C:893:ASP:C	1:C:895:GLY:N	2.76	0.43
1:E:65:PHE:O	1:E:65:PHE:HD1	2.01	0.43
1:E:368:ASN:ND2	1:E:368:ASN:C	2.74	0.43
1:E:395:GLU:HG2	1:E:399:MET:HG2	2.00	0.43
1:E:873:THR:HB	1:E:902:GLU:CD	2.43	0.43
1:F:10:ALA:C	1:F:15:LEU:HD13	2.43	0.43
1:F:464:PRO:O	1:F:466:GLU:N	2.51	0.43
1:A:154:PRO:HD3	1:A:234:VAL:CG1	2.48	0.43
1:A:265:VAL:HG22	1:A:421:LYS:HE3	2.00	0.43
1:A:536:ARG:C	1:A:538:ASN:H	2.26	0.43
1:A:853:LEU:O	1:A:857:LEU:HD23	2.18	0.43
1:B:12:GLU:OE1	1:B:12:GLU:HA	2.18	0.43
1:B:58:LEU:HD23	1:B:58:LEU:HA	1.82	0.43
1:B:381:GLU:OE1	1:B:381:GLU:HA	2.17	0.43
1:B:891:LEU:HD13	1:B:891:LEU:HA	1.84	0.43
1:C:22:LEU:HB3	1:C:28:ILE:HD13	1.99	0.43
1:C:154:PRO:HD2	1:C:229:ALA:HB1	2.00	0.43
1:C:601:ILE:H	1:C:601:ILE:CD1	2.29	0.43
1:C:702:ASP:O	1:C:849:GLN:HG3	2.18	0.43
1:C:884:LEU:O	1:C:888:ILE:HG13	2.17	0.43
1:D:312:VAL:HG11	1:D:315:TRP:CE3	2.53	0.43
1:D:324:PHE:O	1:D:325:THR:C	2.62	0.43
1:D:756:CYS:O	1:D:758:GLY:N	2.51	0.43
1:E:305:ARG:HB2	1:E:339:VAL:O	2.18	0.43
1:E:363:HIS:HB3	1:E:365:ARG:CZ	2.48	0.43
1:E:526:LEU:N	1:E:526:LEU:HD12	2.33	0.43
1:E:715:ALA:HB2	1:E:836:LEU:HD22	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:TYR:CD1	1:A:442:ILE:HD11	2.51	0.43
1:A:671:VAL:HG11	1:A:689:VAL:HG21	2.00	0.43
1:B:411:PRO:HB3	1:B:417:GLY:HA2	2.00	0.43
1:B:758:GLY:O	1:B:783:ARG:HG2	2.18	0.43
1:B:869:LEU:HB2	1:B:900:VAL:HG22	1.99	0.43
1:C:165:ASP:CG	1:E:752:ARG:NH1	2.76	0.43
1:C:840:ALA:N	1:C:841:PRO:CD	2.80	0.43
1:D:29:VAL:HG22	1:D:557:VAL:HB	2.00	0.43
1:D:170:LEU:HB3	1:D:187:LEU:HD21	2.00	0.43
1:D:440:LYS:O	1:D:441:SER:C	2.61	0.43
1:E:307:LEU:C	1:E:307:LEU:CD2	2.89	0.43
1:E:444:GLU:OE2	1:E:450:ILE:CG1	2.67	0.43
1:E:459:ALA:CA	1:E:478:ARG:HH12	2.31	0.43
1:F:98:THR:O	1:F:99:VAL:C	2.62	0.43
1:F:603:GLY:O	1:F:607:SER:OG	2.36	0.43
1:F:907:VAL:HA	1:F:910:THR:HG1	1.79	0.43
1:F:949:LEU:HD13	1:F:949:LEU:HA	1.73	0.43
1:A:153:ALA:HB2	1:A:225:ALA:CB	2.49	0.43
1:A:287:GLY:C	1:A:419:ARG:HB3	2.44	0.43
1:A:351:ARG:HG3	1:A:355:LEU:CD1	2.48	0.43
1:A:432:GLU:OE1	1:A:432:GLU:HA	2.17	0.43
1:B:133:PRO:C	1:B:135:GLN:H	2.27	0.43
1:B:273:PHE:CD1	1:B:437:HIS:NE2	2.85	0.43
1:B:494:LEU:HD23	1:B:494:LEU:HA	1.87	0.43
1:B:597:ASN:HD22	1:B:599:ASP:N	2.07	0.43
1:C:380:PHE:O	1:C:381:GLU:C	2.61	0.43
1:C:391:MET:N	1:C:394:THR:H	2.15	0.43
1:C:763:LYS:HD3	1:C:773:TYR:CZ	2.52	0.43
1:D:110:ARG:HB3	1:D:273:PHE:HB2	2.00	0.43
1:D:130:ARG:H	1:D:130:ARG:NE	2.16	0.43
1:D:312:VAL:CG1	1:D:315:TRP:CB	2.96	0.43
1:D:366:TYR:H	1:D:375:SER:CB	2.32	0.43
1:D:399:MET:CE	1:D:403:TYR:CE2	3.01	0.43
1:D:576:PRO:O	1:D:581:HIS:O	2.35	0.43
1:D:720:VAL:HG12	1:D:819:VAL:HG13	2.00	0.43
1:E:177:ARG:HE	1:E:184:VAL:CG2	2.31	0.43
1:F:354:ILE:HG23	1:F:383:VAL:HG22	2.00	0.43
1:F:618:ARG:NH2	1:F:934:PRO:HG2	2.33	0.43
1:F:695:LEU:HD21	1:F:897:THR:OG1	2.18	0.43
1:A:102:ILE:CD1	1:A:498:ALA:CB	2.85	0.43
1:A:441:SER:CA	1:A:444:GLU:HG2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:GLU:O	1:D:754:GLU:O	2.36	0.43
1:B:344:ARG:HB2	1:B:345:LYS:HE2	1.99	0.43
1:B:373:THR:CG2	1:B:374:ARG:H	2.32	0.43
1:B:782:ALA:O	1:B:783:ARG:HB2	2.18	0.43
1:C:383:VAL:CB	1:C:386:PHE:HB2	2.31	0.43
1:C:900:VAL:O	1:C:900:VAL:HG12	2.17	0.43
1:D:533:LEU:HD21	1:D:537:ASP:HB2	2.00	0.43
1:D:625:ARG:NE	1:D:694:TYR:CE2	2.86	0.43
1:D:739:TYR:CE1	1:D:743:ARG:NE	2.86	0.43
1:D:858:GLN:O	1:D:858:GLN:CG	2.65	0.43
1:E:357:GLY:O	1:E:358:ALA:C	2.62	0.43
1:E:418:THR:C	1:E:419:ARG:HG3	2.44	0.43
1:F:562:GLU:O	1:F:563:ASP:C	2.61	0.43
1:A:418:THR:C	1:A:419:ARG:HG3	2.43	0.43
1:B:20:LEU:HD23	1:B:20:LEU:HA	1.88	0.43
1:C:290:ILE:O	1:C:291:ARG:HG2	2.19	0.43
1:C:384:LEU:C	1:C:384:LEU:HD12	2.44	0.43
1:C:544:THR:CG2	1:C:547:ARG:HH11	2.31	0.43
1:C:597:ASN:HD21	1:C:599:ASP:HB2	1.84	0.43
1:C:684:GLY:O	1:C:686:HIS:HD2	2.01	0.43
1:C:742:GLY:O	1:C:748:VAL:HG21	2.19	0.43
1:D:109:LEU:HD13	1:D:109:LEU:HA	1.78	0.43
1:E:20:LEU:HD21	1:E:585:ILE:HG12	2.00	0.43
1:E:356:GLU:HG2	1:E:357:GLY:N	2.34	0.43
1:E:368:ASN:N	1:E:368:ASN:HD22	2.17	0.43
1:E:395:GLU:OE1	1:E:395:GLU:HA	2.19	0.43
1:E:450:ILE:O	1:E:452:ASP:N	2.52	0.43
1:E:867:TYR:CE2	1:E:891:LEU:HD12	2.54	0.43
1:F:6:ILE:O	1:F:77:ILE:HB	2.19	0.43
1:F:14:ASN:HD21	1:F:582:GLY:C	2.27	0.43
1:A:65:PHE:CD1	1:A:766:MET:HE3	2.51	0.43
1:A:65:PHE:CE1	1:A:766:MET:HA	2.52	0.43
1:A:337:PHE:HB3	1:A:346:LEU:CD2	2.48	0.43
1:A:489:LEU:HD12	1:A:489:LEU:HA	1.75	0.43
1:B:571:ILE:O	1:B:588:SER:HA	2.18	0.43
1:C:185:HIS:HA	1:C:186:PRO:HD2	1.76	0.43
1:D:458:ASN:O	1:D:462:LEU:N	2.51	0.43
1:D:702:ASP:O	1:D:849:GLN:HG3	2.18	0.43
1:F:113:TYR:OH	1:F:436:GLU:HA	2.19	0.43
1:F:441:SER:O	1:F:450:ILE:CD1	2.63	0.43
1:A:14:ASN:C	1:A:14:ASN:OD1	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:ASP:OD2	1:A:341:THR:N	2.51	0.43
1:B:154:PRO:HA	1:B:202:GLU:HA	2.01	0.43
1:B:372:ARG:O	1:B:373:THR:CB	2.67	0.43
1:C:216:ARG:O	1:C:219:THR:HG22	2.18	0.43
1:D:559:GLU:HG3	1:D:564:THR:HG21	2.01	0.43
1:D:906:ASP:O	1:D:909:LYS:HG2	2.19	0.43
1:D:942:ALA:HB2	1:F:923:ALA:O	2.19	0.43
1:E:486:ASP:C	1:E:488:GLY:H	2.26	0.43
1:F:40:SER:O	1:F:45:THR:N	2.44	0.43
1:F:315:TRP:HE3	1:F:328:MET:CE	2.29	0.43
1:F:695:LEU:HD13	1:F:866:VAL:HB	2.01	0.43
1:A:153:ALA:HB2	1:A:225:ALA:HB1	2.00	0.43
1:A:579:GLY:O	1:A:582:GLY:N	2.44	0.43
1:A:869:LEU:HB2	1:A:900:VAL:CG2	2.49	0.43
1:B:920:GLU:HA	1:B:920:GLU:OE1	2.19	0.43
1:C:88:GLN:OE1	1:C:531:ILE:HG21	2.19	0.43
1:C:394:THR:CG2	1:C:396:SER:HA	2.45	0.43
1:C:565:ILE:O	1:C:566:GLU:C	2.60	0.43
1:D:65:PHE:HD1	1:D:65:PHE:O	2.01	0.43
1:D:65:PHE:CE2	1:D:767:ASN:HB2	2.53	0.43
1:D:153:ALA:HB2	1:D:225:ALA:HB1	2.01	0.43
1:D:224:THR:C	1:D:226:LEU:H	2.27	0.43
1:D:742:GLY:O	1:D:748:VAL:HG21	2.18	0.43
1:E:575:GLY:O	1:E:582:GLY:CA	2.65	0.43
1:E:684:GLY:O	1:E:686:HIS:HD2	2.02	0.43
1:E:701:VAL:HB	1:E:869:LEU:CD2	2.49	0.43
1:F:118:THR:OG1	1:F:119:PRO:HD2	2.19	0.43
1:F:618:ARG:CZ	1:F:934:PRO:HG2	2.49	0.43
1:A:126:GLU:OE1	1:A:126:GLU:HA	2.18	0.43
1:A:713:ASN:OD1	1:A:837:GLY:O	2.36	0.43
1:B:22:LEU:HB3	1:B:28:ILE:CD1	2.49	0.43
1:C:232:ILE:O	1:C:233:VAL:HG22	2.19	0.43
1:C:284:GLU:OE1	1:C:284:GLU:HA	2.19	0.43
1:C:361:GLN:HB2	1:C:378:ALA:HB1	2.01	0.43
1:C:608:GLY:C	1:C:610:GLU:N	2.76	0.43
1:C:702:ASP:HB3	1:C:852:LYS:HZ3	1.84	0.43
1:C:706:ILE:HD11	1:C:851:VAL:HB	2.01	0.43
1:D:366:TYR:CD1	1:D:375:SER:HB2	2.54	0.43
1:D:367:ARG:CD	1:D:367:ARG:H	2.32	0.43
1:D:443:ALA:HA	1:D:495:SER:OG	2.19	0.43
1:D:718:THR:HG22	1:D:822:TYR:HD1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:797:THR:HG22	1:D:800:GLU:OE2	2.19	0.43
1:E:268:LEU:HD23	1:E:268:LEU:HA	1.60	0.43
1:F:20:LEU:HD21	1:F:585:ILE:HD12	2.01	0.43
1:F:37:GLY:O	1:F:40:SER:HB2	2.18	0.43
1:F:503:GLY:HA2	1:F:506:ALA:HB3	2.00	0.43
1:F:570:TRP:CE2	1:F:589:GLY:HA2	2.54	0.43
1:F:636:ASN:OD1	1:F:659:GLY:HA2	2.19	0.43
1:F:877:HIS:CG	1:F:878:PHE:N	2.86	0.43
1:A:61:TYR:OH	1:A:65:PHE:HD2	2.01	0.42
1:A:548:LEU:HD22	1:A:553:ASN:HD22	1.84	0.42
1:A:754:GLU:CD	1:A:754:GLU:N	2.77	0.42
1:B:701:VAL:HB	1:B:869:LEU:CD2	2.48	0.42
1:B:829:VAL:O	1:B:829:VAL:CG1	2.67	0.42
1:C:229:ALA:O	1:C:230:ASP:HB3	2.19	0.42
1:C:269:GLU:O	1:C:271:ARG:N	2.52	0.42
1:C:407:MET:HE3	1:C:407:MET:H	1.83	0.42
1:D:31:THR:HG22	1:D:573:ASP:HA	1.99	0.42
1:D:40:SER:O	1:D:45:THR:OG1	2.36	0.42
1:D:132:THR:O	1:D:135:GLN:CB	2.58	0.42
1:D:364:VAL:HB	1:D:376:TYR:O	2.19	0.42
1:D:520:VAL:HA	1:D:553:ASN:OD1	2.19	0.42
1:D:756:CYS:HB3	1:D:776:CYS:HB2	2.01	0.42
1:E:743:ARG:HD2	1:E:751:GLY:CA	2.49	0.42
1:E:829:VAL:HG22	1:E:853:LEU:HD12	1.99	0.42
1:F:403:TYR:C	1:F:405:GLY:N	2.76	0.42
1:A:160:LYS:HB3	1:A:198:LYS:N	2.34	0.42
1:A:237:PHE:N	1:A:237:PHE:CD1	2.84	0.42
1:A:255:LEU:HD13	1:A:268:LEU:HG	2.01	0.42
1:B:630:VAL:O	1:B:687:THR:HB	2.19	0.42
1:B:777:GLU:CD	1:D:160:LYS:HE3	2.44	0.42
1:B:873:THR:HG21	1:B:904:ASN:HB2	2.01	0.42
1:C:462:LEU:HD23	1:C:462:LEU:HA	1.60	0.42
1:C:548:LEU:HD22	1:C:553:ASN:HD22	1.84	0.42
1:C:743:ARG:HD2	1:C:751:GLY:CA	2.49	0.42
1:C:891:LEU:HA	1:C:891:LEU:HD13	1.88	0.42
1:D:112:LEU:HD21	1:D:458:ASN:ND2	2.34	0.42
1:D:748:VAL:O	1:D:750:GLY:N	2.52	0.42
1:E:65:PHE:HD1	1:E:766:MET:HE3	1.83	0.42
1:E:108:TYR:CZ	1:E:476:GLU:HG2	2.55	0.42
1:E:412:CYS:C	1:E:415:CYS:HG	2.23	0.42
1:E:548:LEU:HD22	1:E:553:ASN:HD22	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:604:ALA:O	1:F:607:SER:OG	2.33	0.42
1:A:867:TYR:CE2	1:A:891:LEU:HD12	2.55	0.42
1:C:319:HIS:H	1:C:319:HIS:HD2	1.66	0.42
1:D:829:VAL:HG22	1:D:853:LEU:HD12	2.00	0.42
1:E:370:TYR:C	1:E:372:ARG:N	2.76	0.42
1:E:415:CYS:O	1:E:416:ALA:CB	2.67	0.42
1:A:65:PHE:O	1:A:65:PHE:CD1	2.73	0.42
1:A:597:ASN:HD22	1:A:598:LYS:N	2.17	0.42
1:B:372:ARG:HD2	1:B:372:ARG:O	2.19	0.42
1:B:430:ALA:HB1	1:B:432:GLU:O	2.19	0.42
1:B:793:TYR:C	1:B:793:TYR:HD1	2.24	0.42
1:C:285:CYS:SG	1:C:289:GLY:HA2	2.60	0.42
1:C:551:LEU:HD12	1:C:551:LEU:HA	1.84	0.42
1:C:575:GLY:O	1:C:582:GLY:CA	2.65	0.42
1:D:12:GLU:CG	1:D:45:THR:HG23	2.50	0.42
1:D:312:VAL:CG2	1:D:315:TRP:CE3	2.88	0.42
1:D:331:LEU:HD11	1:D:358:ALA:CB	2.48	0.42
1:D:494:LEU:HD23	1:D:494:LEU:HA	1.90	0.42
1:E:119:PRO:C	1:E:120:HIS:HD2	2.25	0.42
1:E:156:VAL:HG21	1:E:201:ILE:HD12	2.00	0.42
1:E:157:ARG:HH11	1:E:157:ARG:HG3	1.84	0.42
1:E:674:ASN:O	1:E:678:GLY:HA2	2.19	0.42
1:F:368:ASN:CG	1:F:369:ARG:N	2.77	0.42
1:F:402:ARG:HD3	1:F:680:ARG:HH11	1.85	0.42
1:F:667:ILE:HG22	1:F:668:LEU:N	2.33	0.42
1:A:86:ILE:HB	1:A:526:LEU:HG	2.01	0.42
1:A:384:LEU:HD12	1:A:384:LEU:O	2.20	0.42
1:A:442:ILE:CG2	1:A:495:SER:N	2.82	0.42
1:B:14:ASN:OD1	1:B:14:ASN:C	2.62	0.42
1:B:131:GLN:NE2	1:B:256:ALA:CB	2.66	0.42
1:C:381:GLU:C	1:C:383:VAL:H	2.21	0.42
1:C:486:ASP:O	1:C:540:ARG:NH2	2.52	0.42
1:E:131:GLN:HG3	1:E:132:THR:N	2.35	0.42
1:E:294:VAL:HA	1:E:407:MET:HA	2.01	0.42
1:E:420:LEU:O	1:E:422:PRO:HD3	2.19	0.42
1:E:739:TYR:CE1	1:E:743:ARG:NE	2.87	0.42
1:F:451:ALA:O	1:F:455:ASP:N	2.27	0.42
1:F:872:PRO:CG	1:F:873:THR:H	2.30	0.42
1:A:226:LEU:HD23	1:A:226:LEU:HA	1.82	0.42
1:A:811:GLU:OE1	1:A:811:GLU:HA	2.20	0.42
1:B:22:LEU:HB3	1:B:28:ILE:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:PHE:O	1:B:65:PHE:CD1	2.71	0.42
1:B:80:LEU:O	1:D:520:VAL:N	2.44	0.42
1:B:119:PRO:HA	1:B:427:VAL:HA	2.00	0.42
1:C:123:THR:OG1	1:C:261:HIS:CG	2.73	0.42
1:C:232:ILE:CD1	1:C:266:ASP:HB3	2.49	0.42
1:C:597:ASN:HD22	1:C:598:LYS:N	2.17	0.42
1:E:310:GLY:O	1:E:311:ALA:C	2.62	0.42
1:E:565:ILE:O	1:E:566:GLU:C	2.62	0.42
1:F:649:LEU:CD2	1:F:911:SER:HA	2.42	0.42
1:A:346:LEU:CD2	1:A:349:LYS:HD3	2.50	0.42
1:B:31:THR:HG23	1:B:573:ASP:HA	2.02	0.42
1:B:345:LYS:O	1:B:346:LEU:HG	2.20	0.42
1:B:404:GLU:C	1:B:406:PHE:H	2.27	0.42
1:C:762:ILE:HD12	1:E:160:LYS:HE3	2.01	0.42
1:C:829:VAL:O	1:C:829:VAL:CG1	2.68	0.42
1:D:865:THR:HG22	1:D:896:ASN:HD21	1.84	0.42
1:D:867:TYR:CE2	1:D:891:LEU:HD12	2.54	0.42
1:E:365:ARG:HA	1:E:375:SER:OG	2.19	0.42
1:E:405:GLY:HA3	1:E:680:ARG:O	2.20	0.42
1:E:743:ARG:HD2	1:E:751:GLY:HA3	2.02	0.42
1:F:388:GLN:O	1:F:392:SER:N	2.46	0.42
1:F:487:VAL:HG12	1:F:508:ARG:HD2	2.02	0.42
1:A:571:ILE:O	1:A:588:SER:HA	2.20	0.42
1:B:61:TYR:OH	1:B:65:PHE:HD2	2.03	0.42
1:B:180:VAL:CG1	1:B:181:ASP:N	2.79	0.42
1:B:234:VAL:HB	1:B:235:LEU:H	1.68	0.42
1:B:295:ASP:O	1:B:298:LEU:CD2	2.66	0.42
1:B:438:GLY:C	1:B:442:ILE:HB	2.45	0.42
1:B:441:SER:C	1:B:445:VAL:HG22	2.44	0.42
1:B:652:VAL:HG21	1:B:664:VAL:HG21	2.02	0.42
1:C:31:THR:O	1:C:574:ILE:N	2.48	0.42
1:D:305:ARG:HH12	1:D:312:VAL:HB	1.82	0.42
1:D:372:ARG:CD	1:D:374:ARG:HB2	2.41	0.42
1:D:873:THR:HB	1:D:902:GLU:CD	2.44	0.42
1:E:524:TYR:HB2	1:E:555:LEU:HD22	2.01	0.42
1:E:557:VAL:CG1	1:E:559:GLU:HG2	2.50	0.42
1:E:804:MET:CE	1:E:808:GLU:OE1	2.68	0.42
1:F:321:ALA:HA	1:F:324:PHE:HD2	1.85	0.42
1:F:598:LYS:HA	1:F:598:LYS:HD3	1.89	0.42
1:F:913:TRP:CH2	1:F:932:GLY:HA2	2.54	0.42
1:A:424:ILE:C	1:A:426:ALA:N	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:TYR:HB3	1:B:273:PHE:CZ	2.54	0.42
1:B:119:PRO:HA	1:B:427:VAL:HG22	2.01	0.42
1:B:184:VAL:HG12	1:B:185:HIS:H	1.74	0.42
1:B:377:TYR:CD2	1:B:379:ASP:OD2	2.73	0.42
1:B:608:GLY:C	1:B:610:GLU:N	2.76	0.42
1:C:80:LEU:O	1:E:519:LEU:HA	2.20	0.42
1:C:360:GLU:HA	1:C:360:GLU:OE1	2.20	0.42
1:C:415:CYS:O	1:C:416:ALA:C	2.60	0.42
1:C:447:GLU:O	1:C:449:SER:N	2.53	0.42
1:D:106:TYR:HD1	1:D:442:ILE:HG12	1.84	0.42
1:D:156:VAL:HB	1:D:201:ILE:N	2.31	0.42
1:D:420:LEU:HD22	1:D:424:ILE:HG21	2.02	0.42
1:D:481:LEU:O	1:D:484:LEU:HB2	2.19	0.42
1:E:41:LEU:HD12	1:E:574:ILE:HD11	2.00	0.42
1:E:201:ILE:C	1:E:202:GLU:HG2	2.43	0.42
1:E:703:GLN:HG2	1:E:849:GLN:HB2	2.01	0.42
1:E:848:ALA:O	1:E:852:LYS:HG3	2.20	0.42
1:A:436:GLU:CA	1:A:440:LYS:HD2	2.40	0.42
1:A:441:SER:HA	1:A:444:GLU:CG	2.50	0.42
1:A:668:LEU:HD12	1:A:868:ILE:HD11	2.02	0.42
1:A:713:ASN:H	1:A:716:THR:HB	1.84	0.42
1:A:720:VAL:HG12	1:A:819:VAL:HG13	2.02	0.42
1:A:838:GLN:HA	1:A:839:PRO:HD3	1.97	0.42
1:B:175:TYR:N	1:B:187:LEU:CD2	2.83	0.42
1:B:438:GLY:HA2	1:B:442:ILE:CB	2.50	0.42
1:B:920:GLU:O	1:B:925:GLY:HA3	2.20	0.42
1:C:483:PHE:O	1:C:486:ASP:HB2	2.20	0.42
1:D:41:LEU:HD12	1:D:574:ILE:HD11	2.01	0.42
1:D:415:CYS:C	1:D:417:GLY:N	2.78	0.42
1:D:532:GLY:HA2	1:D:871:GLU:OE2	2.20	0.42
1:D:667:ILE:HG22	1:D:668:LEU:N	2.35	0.42
1:E:38:LYS:HD3	1:E:38:LYS:N	2.31	0.42
1:E:49:GLU:OE1	1:E:53:ARG:NE	2.44	0.42
1:E:152:LEU:HB2	1:E:234:VAL:HG21	2.01	0.42
1:E:156:VAL:HG12	1:E:199:HIS:O	2.20	0.42
1:E:219:THR:HG22	1:E:223:GLU:OE2	2.19	0.42
1:F:565:ILE:O	1:F:566:GLU:C	2.63	0.42
1:F:570:TRP:NE1	1:F:589:GLY:HA2	2.35	0.42
1:F:598:LYS:HE2	1:F:609:ARG:NE	2.34	0.42
1:A:817:ALA:O	1:A:821:ARG:HG2	2.19	0.41
1:B:69:MET:HE3	1:B:69:MET:HB3	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:LEU:HD13	1:B:109:LEU:HA	1.82	0.41
1:B:591:TYR:CE2	1:B:595:LEU:HD11	2.55	0.41
1:B:777:GLU:OE1	1:D:160:LYS:HE3	2.20	0.41
1:C:54:TYR:CE2	1:E:54:TYR:CD2	3.08	0.41
1:C:165:ASP:OD2	1:E:752:ARG:HD2	2.20	0.41
1:C:447:GLU:OE1	1:C:452:ASP:OD1	2.37	0.41
1:C:578:ALA:O	1:C:579:GLY:C	2.64	0.41
1:D:132:THR:O	1:D:136:ILE:HG13	2.20	0.41
1:D:619:ARG:NH2	1:D:892:VAL:HB	2.35	0.41
1:E:60:ALA:O	1:E:63:ARG:HB3	2.20	0.41
1:E:171:ASN:C	1:E:173:GLN:H	2.27	0.41
1:E:298:LEU:HD12	1:E:406:PHE:C	2.45	0.41
1:E:626:GLN:HE21	1:E:643:SER:HB3	1.85	0.41
1:F:436:GLU:CD	1:F:439:ALA:H	2.27	0.41
1:F:511:LEU:O	1:F:514:GLN:HB2	2.20	0.41
1:F:698:LEU:CD1	1:F:866:VAL:HG13	2.48	0.41
1:A:151:VAL:HG12	1:A:205:VAL:HB	2.02	0.41
1:A:272:SER:O	1:A:424:ILE:HG13	2.21	0.41
1:A:299:VAL:CG2	1:A:300:VAL:N	2.60	0.41
1:A:858:GLN:O	1:A:858:GLN:CG	2.67	0.41
1:B:299:VAL:HG13	1:B:300:VAL:N	2.34	0.41
1:B:437:HIS:CG	1:B:437:HIS:O	2.72	0.41
1:B:443:ALA:HA	1:B:495:SER:HB3	2.01	0.41
1:B:497:ALA:O	1:B:498:ALA:C	2.61	0.41
1:B:763:LYS:HD3	1:B:773:TYR:CZ	2.55	0.41
1:C:65:PHE:HD1	1:C:766:MET:HE3	1.84	0.41
1:C:152:LEU:CD2	1:C:179:ARG:HH21	2.32	0.41
1:C:758:GLY:O	1:C:783:ARG:HG2	2.20	0.41
1:C:817:ALA:O	1:C:821:ARG:HG2	2.20	0.41
1:D:802:LEU:HG	1:D:837:GLY:HA3	2.02	0.41
1:E:626:GLN:HE21	1:E:626:GLN:HB3	1.55	0.41
1:E:671:VAL:HG11	1:E:689:VAL:HG21	2.02	0.41
1:F:543:GLU:HG3	1:F:547:ARG:HH21	1.81	0.41
1:F:684:GLY:C	1:F:686:HIS:H	2.23	0.41
1:A:699:VAL:HG21	1:A:867:TYR:CE1	2.56	0.41
1:A:713:ASN:HB3	1:A:837:GLY:HA2	2.02	0.41
1:B:145:GLU:HA	1:B:145:GLU:OE1	2.21	0.41
1:B:154:PRO:HB3	1:B:202:GLU:HG3	2.01	0.41
1:B:331:LEU:HD21	1:B:335:LEU:HD12	2.02	0.41
1:C:571:ILE:O	1:C:588:SER:HA	2.20	0.41
1:C:699:VAL:HB	1:C:867:TYR:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:713:ASN:HB2	1:C:714:PRO:HD2	2.01	0.41
1:D:143:MET:HE3	1:D:145:GLU:HB2	2.02	0.41
1:D:269:GLU:OE1	1:D:269:GLU:HA	2.19	0.41
1:D:423:GLU:OE1	1:D:423:GLU:N	2.51	0.41
1:E:284:GLU:OE1	1:E:284:GLU:HA	2.20	0.41
1:E:559:GLU:HG3	1:E:564:THR:HG21	2.03	0.41
1:E:877:HIS:HB3	1:E:880:ASP:OD2	2.20	0.41
1:F:323:TYR:O	1:F:326:ARG:HB3	2.19	0.41
1:F:436:GLU:OE2	1:F:439:ALA:N	2.54	0.41
1:A:157:ARG:HH22	1:A:267:ASP:H	1.68	0.41
1:A:225:ALA:C	1:A:227:ASN:H	2.28	0.41
1:A:282:CYS:CB	1:A:415:CYS:HB3	2.49	0.41
1:A:287:GLY:CA	1:A:419:ARG:HB3	2.50	0.41
1:B:162:GLU:H	1:B:195:LYS:HG3	1.86	0.41
1:B:447:GLU:HA	1:B:447:GLU:OE1	2.20	0.41
1:B:822:TYR:CD1	1:B:858:GLN:HG2	2.55	0.41
1:B:866:VAL:O	1:B:866:VAL:CG1	2.69	0.41
1:C:455:ASP:CA	1:C:478:ARG:HH11	2.30	0.41
1:C:619:ARG:CB	1:C:648:VAL:HG23	2.50	0.41
1:D:27:LEU:CD2	1:D:29:VAL:HG23	2.51	0.41
1:D:104:GLU:O	1:D:107:ASP:HB2	2.20	0.41
1:D:307:LEU:HD11	1:D:325:THR:HG21	2.02	0.41
1:D:720:VAL:CG1	1:D:819:VAL:HG13	2.50	0.41
1:F:388:GLN:O	1:F:389:ARG:C	2.62	0.41
1:A:160:LYS:HA	1:A:198:LYS:HA	2.02	0.41
1:A:625:ARG:NE	1:A:694:TYR:CE2	2.89	0.41
1:B:220:ASP:O	1:B:221:SER:C	2.62	0.41
1:B:375:SER:HB2	1:B:377:TYR:H	1.85	0.41
1:B:817:ALA:HA	1:B:820:HIS:HB3	2.02	0.41
1:B:865:THR:HG22	1:B:896:ASN:HD21	1.85	0.41
1:C:65:PHE:CZ	1:C:767:ASN:HB2	2.56	0.41
1:C:130:ARG:NH1	1:C:130:ARG:HB3	2.35	0.41
1:C:271:ARG:NH2	1:C:279:TYR:CZ	2.88	0.41
1:D:156:VAL:HG21	1:D:200:ASP:HA	2.01	0.41
1:D:918:GLY:HA3	1:D:919:PRO:HA	1.91	0.41
1:E:312:VAL:CG1	1:E:384:LEU:HD13	2.47	0.41
1:E:371:GLY:C	1:E:373:THR:H	2.27	0.41
1:E:509:ILE:O	1:E:510:ARG:C	2.62	0.41
1:F:422:PRO:O	1:F:425:LEU:CB	2.68	0.41
1:F:473:VAL:O	1:F:476:GLU:CB	2.68	0.41
1:F:586:VAL:O	1:F:586:VAL:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:SER:O	1:A:45:THR:OG1	2.38	0.41
1:A:559:GLU:HG3	1:A:564:THR:HG21	2.02	0.41
1:B:299:VAL:CG2	1:B:313:ALA:HB3	2.26	0.41
1:B:534:HIS:HA	1:B:903:HIS:ND1	2.36	0.41
1:C:159:ARG:HA	1:C:159:ARG:HD3	1.80	0.41
1:C:278:PRO:HG2	1:C:279:TYR:H	1.86	0.41
1:C:362:VAL:HG12	1:C:363:HIS:N	2.34	0.41
1:D:877:HIS:ND1	1:D:878:PHE:N	2.68	0.41
1:E:37:GLY:O	1:E:38:LYS:C	2.63	0.41
1:E:418:THR:O	1:E:419:ARG:CB	2.68	0.41
1:E:478:ARG:HG2	1:E:478:ARG:H	1.60	0.41
1:F:41:LEU:O	1:F:45:THR:HB	2.20	0.41
1:F:94:ASN:HA	1:F:95:PRO:HD3	1.92	0.41
1:F:442:ILE:CG2	1:F:443:ALA:H	2.33	0.41
1:F:695:LEU:CD2	1:F:864:ARG:C	2.59	0.41
1:F:696:ASP:O	1:F:697:LYS:HG3	2.21	0.41
1:A:30:PHE:CE2	1:A:41:LEU:HD13	2.55	0.41
1:A:300:VAL:CG1	1:A:303:PRO:CD	2.89	0.41
1:A:459:ALA:HA	1:A:462:LEU:HB2	2.02	0.41
1:B:447:GLU:HA	1:B:450:ILE:HG21	1.98	0.41
1:B:802:LEU:HD12	1:B:802:LEU:HA	1.91	0.41
1:B:802:LEU:HG	1:B:837:GLY:HA3	2.03	0.41
1:C:60:ALA:O	1:C:63:ARG:HB3	2.19	0.41
1:E:608:GLY:C	1:E:610:GLU:H	2.26	0.41
1:E:913:TRP:CH2	1:E:932:GLY:HA2	2.55	0.41
1:F:345:LYS:C	1:F:347:PRO:N	2.79	0.41
1:F:380:PHE:C	1:F:382:GLY:N	2.78	0.41
1:F:612:ILE:HD12	1:F:882:ARG:HG3	2.03	0.41
1:F:625:ARG:O	1:F:626:GLN:HG3	2.21	0.41
1:A:119:PRO:HA	1:A:427:VAL:HA	2.03	0.41
1:A:418:THR:OG1	1:A:425:LEU:HD21	2.20	0.41
1:A:491:TYR:HB2	1:A:921:GLY:O	2.21	0.41
1:A:597:ASN:HD22	1:A:599:ASP:N	2.11	0.41
1:B:158:THR:CG2	1:B:271:ARG:HH12	2.24	0.41
1:B:368:ASN:OD1	1:B:369:ARG:N	2.53	0.41
1:B:478:ARG:HG2	1:B:478:ARG:H	1.63	0.41
1:C:55:VAL:C	1:C:57:SER:N	2.78	0.41
1:D:702:ASP:HB3	1:D:852:LYS:HZ3	1.86	0.41
1:E:69:MET:HE3	1:E:69:MET:HB3	1.86	0.41
1:E:349:LYS:HE2	1:E:349:LYS:HB3	1.87	0.41
1:E:421:LYS:O	1:E:424:ILE:HB	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:816:ILE:HD12	1:E:816:ILE:N	2.34	0.41
1:F:339:VAL:O	1:F:340:ASP:O	2.39	0.41
1:F:367:ARG:NH1	1:F:373:THR:HB	2.36	0.41
1:F:635:HIS:C	1:F:637:LEU:H	2.28	0.41
1:A:159:ARG:CG	1:A:159:ARG:NH1	2.78	0.41
1:A:294:VAL:CA	1:A:407:MET:HG2	2.51	0.41
1:A:424:ILE:C	1:A:426:ALA:H	2.28	0.41
1:A:935:GLU:HG3	1:A:953:VAL:CG1	2.51	0.41
1:B:29:VAL:HG22	1:B:557:VAL:HB	2.03	0.41
1:B:60:ALA:O	1:B:63:ARG:HB3	2.20	0.41
1:B:118:THR:HA	1:B:119:PRO:HD3	1.72	0.41
1:B:390:LYS:O	1:B:393:GLN:HB2	2.21	0.41
1:B:811:GLU:OE2	1:B:814:GLU:OE1	2.38	0.41
1:B:858:GLN:O	1:B:858:GLN:CG	2.68	0.41
1:C:27:LEU:C	1:C:27:LEU:HD23	2.45	0.41
1:C:36:SER:OG	1:C:574:ILE:O	2.39	0.41
1:C:54:TYR:CD2	1:E:54:TYR:CE2	3.09	0.41
1:C:178:VAL:HG12	1:C:185:HIS:O	2.21	0.41
1:C:292:LYS:HB3	1:C:407:MET:HG3	2.03	0.41
1:C:396:SER:O	1:C:397:GLU:CB	2.68	0.41
1:C:452:ASP:O	1:C:456:PHE:CD1	2.73	0.41
1:C:519:LEU:HA	1:E:80:LEU:O	2.21	0.41
1:C:913:TRP:CH2	1:C:932:GLY:HA2	2.55	0.41
1:D:108:TYR:CZ	1:D:476:GLU:HG2	2.56	0.41
1:D:411:PRO:O	1:D:413:PRO:HD3	2.21	0.41
1:D:619:ARG:HB3	1:D:648:VAL:HG23	2.03	0.41
1:D:804:MET:HE1	1:D:812:PHE:CB	2.51	0.41
1:D:891:LEU:HD13	1:D:891:LEU:HA	1.88	0.41
1:E:43:PHE:CE2	1:E:527:ASP:HB2	2.55	0.41
1:E:269:GLU:HB3	1:E:270:PRO:CD	2.48	0.41
1:E:363:HIS:NE2	1:E:378:ALA:HB2	2.36	0.41
1:E:368:ASN:ND2	1:E:372:ARG:CB	2.54	0.41
1:E:532:GLY:HA2	1:E:871:GLU:OE2	2.21	0.41
1:E:914:ILE:HD11	1:E:937:VAL:HB	2.03	0.41
1:E:935:GLU:HG3	1:E:953:VAL:CG1	2.50	0.41
1:F:14:ASN:OD1	1:F:14:ASN:C	2.63	0.41
1:F:20:LEU:CD1	1:F:41:LEU:HD11	2.51	0.41
1:F:554:THR:C	1:F:555:LEU:HD23	2.46	0.41
1:F:871:GLU:HA	1:F:872:PRO:HD2	1.94	0.41
1:F:877:HIS:O	1:F:878:PHE:C	2.61	0.41
1:F:885:LEU:HD23	1:F:907:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:TYR:HE1	1:A:376:TYR:CB	2.21	0.41
1:A:514:GLN:O	1:A:517:SER:OG	2.31	0.41
1:A:714:PRO:HB2	1:A:836:LEU:O	2.21	0.41
1:A:840:ALA:N	1:A:841:PRO:CD	2.84	0.41
1:B:61:TYR:HE2	1:D:767:ASN:O	1.95	0.41
1:B:113:TYR:CG	1:B:437:HIS:ND1	2.89	0.41
1:B:131:GLN:HG3	1:B:253:GLU:HA	2.03	0.41
1:B:149:PHE:CD1	1:B:149:PHE:O	2.74	0.41
1:B:315:TRP:CE2	1:B:324:PHE:CD2	3.10	0.41
1:C:40:SER:HA	1:C:44:ASP:HB2	2.03	0.41
1:C:418:THR:HG21	1:C:425:LEU:HD21	2.02	0.41
1:C:509:ILE:O	1:C:512:ALA:N	2.54	0.41
1:C:514:GLN:HG3	1:C:524:TYR:HE2	1.86	0.41
1:C:913:TRP:CZ3	1:C:932:GLY:HA2	2.56	0.41
1:D:61:TYR:OH	1:D:65:PHE:HD2	2.04	0.41
1:D:305:ARG:O	1:D:311:ALA:HB2	2.15	0.41
1:D:339:VAL:O	1:D:339:VAL:HG22	2.20	0.41
1:E:706:ILE:CD1	1:E:851:VAL:HG11	2.48	0.41
1:E:945:THR:O	1:E:949:LEU:HB2	2.21	0.41
1:F:644:PHE:O	1:F:645:PRO:C	2.64	0.41
1:F:933:THR:HG22	1:F:935:GLU:OE1	2.21	0.41
1:A:740:GLN:HB3	1:A:741:PRO:HD2	2.03	0.40
1:B:452:ASP:HA	1:B:456:PHE:HB2	2.03	0.40
1:B:660:LYS:HE2	1:B:660:LYS:N	2.36	0.40
1:B:701:VAL:HG12	1:B:849:GLN:CG	2.38	0.40
1:B:752:ARG:O	1:B:752:ARG:HG3	2.20	0.40
1:C:536:ARG:C	1:C:538:ASN:N	2.79	0.40
1:C:906:ASP:O	1:C:909:LYS:HG2	2.21	0.40
1:D:387:LEU:HD12	1:D:391:MET:HB2	2.02	0.40
1:D:390:LYS:HG3	1:D:391:MET:N	2.36	0.40
1:D:829:VAL:HG11	1:D:850:ARG:O	2.20	0.40
1:E:96:ARG:HA	1:E:419:ARG:NH2	2.36	0.40
1:E:829:VAL:HG11	1:E:850:ARG:O	2.21	0.40
1:F:436:GLU:OE1	1:F:436:GLU:C	2.64	0.40
1:F:437:HIS:CB	1:F:441:SER:HB2	2.51	0.40
1:F:473:VAL:O	1:F:476:GLU:HB3	2.21	0.40
1:F:933:THR:O	1:F:935:GLU:N	2.54	0.40
1:A:124:CYS:SG	1:A:125:GLY:N	2.94	0.40
1:A:601:ILE:H	1:A:601:ILE:CD1	2.32	0.40
1:A:608:GLY:C	1:A:610:GLU:H	2.27	0.40
1:B:404:GLU:HA	1:B:407:MET:SD	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:444:GLU:N	1:B:444:GLU:OE1	2.54	0.40
1:B:613:GLU:OE1	1:B:613:GLU:HA	2.20	0.40
1:B:687:THR:HG22	1:B:688:ARG:HG3	2.03	0.40
1:C:12:GLU:O	1:C:15:LEU:HB2	2.21	0.40
1:C:190:PRO:HB3	1:C:191:PRO:HD3	2.03	0.40
1:C:509:ILE:O	1:C:510:ARG:C	2.63	0.40
1:D:22:LEU:HB3	1:D:28:ILE:HD13	2.02	0.40
1:D:37:GLY:O	1:D:38:LYS:C	2.64	0.40
1:D:49:GLU:OE1	1:D:53:ARG:NE	2.42	0.40
1:D:183:VAL:CG1	1:D:184:VAL:HG23	2.52	0.40
1:D:743:ARG:HG3	1:D:788:THR:HG23	2.03	0.40
1:E:442:ILE:C	1:E:495:SER:OG	2.43	0.40
1:F:412:CYS:CA	1:F:415:CYS:SG	3.10	0.40
1:F:443:ALA:CB	1:F:444:GLU:OE1	2.69	0.40
1:A:280:GLY:O	1:A:421:LYS:HB2	2.22	0.40
1:A:345:LYS:HB3	1:A:346:LEU:HD12	2.03	0.40
1:B:323:TYR:CD1	1:B:324:PHE:N	2.89	0.40
1:B:338:ASP:OD2	1:B:341:THR:HG23	2.21	0.40
1:B:431:GLY:O	1:B:457:LEU:HB3	2.20	0.40
1:B:597:ASN:HD22	1:B:598:LYS:N	2.20	0.40
1:C:269:GLU:C	1:C:271:ARG:H	2.29	0.40
1:D:178:VAL:HG22	1:D:203:VAL:CG1	2.51	0.40
1:D:282:CYS:HA	1:D:283:PRO:HD3	1.92	0.40
1:E:175:TYR:CB	1:E:187:LEU:HD12	2.51	0.40
1:E:758:GLY:O	1:E:783:ARG:HG2	2.21	0.40
1:E:797:THR:HG23	1:E:800:GLU:H	1.85	0.40
1:E:869:LEU:HB2	1:E:900:VAL:HG22	2.02	0.40
1:F:40:SER:HA	1:F:44:ASP:CG	2.46	0.40
1:F:466:GLU:H	1:F:466:GLU:HG3	1.75	0.40
1:F:628:THR:HA	1:F:642:VAL:O	2.21	0.40
1:A:131:GLN:NE2	1:A:139:GLN:HE22	2.20	0.40
1:A:329:ALA:C	1:A:332:GLY:H	2.29	0.40
1:A:345:LYS:HB3	1:A:346:LEU:CD1	2.52	0.40
1:A:532:GLY:HA2	1:A:871:GLU:OE2	2.21	0.40
1:A:714:PRO:CD	1:A:836:LEU:O	2.68	0.40
1:C:38:LYS:H	1:C:38:LYS:CD	2.29	0.40
1:C:104:GLU:O	1:C:107:ASP:HB2	2.21	0.40
1:C:177:ARG:HG3	1:C:184:VAL:HG13	2.02	0.40
1:C:329:ALA:O	1:C:333:GLU:HG3	2.21	0.40
1:C:619:ARG:HB3	1:C:648:VAL:HG23	2.03	0.40
1:C:720:VAL:HG12	1:C:819:VAL:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:LEU:HD22	1:D:236:GLU:CB	2.32	0.40
1:D:184:VAL:C	1:D:185:HIS:CD2	3.00	0.40
1:D:313:ALA:N	1:D:314:PRO:CD	2.83	0.40
1:D:441:SER:O	1:D:444:GLU:HB3	2.22	0.40
1:D:445:VAL:O	1:D:492:LEU:C	2.65	0.40
1:D:661:SER:O	1:D:662:THR:C	2.63	0.40
1:E:877:HIS:ND1	1:E:878:PHE:N	2.69	0.40
1:F:397:GLU:HG3	1:F:399:MET:H	1.87	0.40
1:F:437:HIS:ND1	1:F:438:GLY:N	2.69	0.40
1:F:676:LEU:HD11	1:F:693:ASP:HB3	2.04	0.40
1:A:31:THR:O	1:A:573:ASP:HA	2.22	0.40
1:A:170:LEU:HB3	1:A:187:LEU:HD11	2.02	0.40
1:A:198:LYS:H	1:A:198:LYS:HG2	1.67	0.40
1:A:300:VAL:CG1	1:A:303:PRO:CG	3.00	0.40
1:B:54:TYR:CE2	1:D:54:TYR:CD2	3.10	0.40
1:B:269:GLU:HB3	1:B:270:PRO:HD2	2.03	0.40
1:B:287:GLY:O	1:B:419:ARG:NE	2.52	0.40
1:C:69:MET:HE3	1:C:69:MET:HB3	1.90	0.40
1:C:223:GLU:O	1:C:227:ASN:CG	2.65	0.40
1:C:447:GLU:HB2	1:C:490:GLU:HB2	2.03	0.40
1:D:352:LYS:O	1:D:356:GLU:CA	2.66	0.40
1:D:545:LEU:HA	1:D:545:LEU:HD23	1.78	0.40
1:E:98:THR:O	1:E:99:VAL:C	2.64	0.40
1:E:178:VAL:HG22	1:E:203:VAL:CG1	2.44	0.40
1:E:372:ARG:O	1:E:373:THR:C	2.63	0.40
1:E:721:PHE:O	1:E:725:ARG:HG3	2.21	0.40
1:E:752:ARG:O	1:E:752:ARG:HG3	2.22	0.40
1:F:600:SER:O	1:F:601:ILE:C	2.63	0.40
1:F:698:LEU:CD2	1:F:700:ARG:HH11	2.35	0.40
1:F:935:GLU:N	1:F:935:GLU:CD	2.80	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:597:ASN:OD1	1:F:16:ARG:NH1[4_554]	2.07	0.13
1:B:398:GLN:OE1	1:E:366:TYR:CB[6_444]	2.09	0.11
1:B:398:GLN:OE1	1:E:366:TYR:CD2[6_444]	2.09	0.11
1:B:398:GLN:OE1	1:E:366:TYR:CG[6_444]	2.09	0.11
1:A:61:TYR:CE2	1:A:767:ASN:O[4_555]	2.10	0.10

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	940/993 (95%)	814 (87%)	105 (11%)	21 (2%)	5	24
1	B	910/993 (92%)	768 (84%)	112 (12%)	30 (3%)	3	17
1	C	876/993 (88%)	730 (83%)	109 (12%)	37 (4%)	2	14
1	D	911/993 (92%)	758 (83%)	123 (14%)	30 (3%)	3	17
1	E	907/993 (91%)	750 (83%)	128 (14%)	29 (3%)	3	17
1	F	595/993 (60%)	449 (76%)	98 (16%)	48 (8%)	1	4
All	All	5139/5958 (86%)	4269 (83%)	675 (13%)	195 (4%)	2	15

All (195) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	299	VAL
1	A	300	VAL
1	A	301	PRO
1	A	382	GLY
1	A	457	LEU
1	A	863	GLY
1	B	133	PRO
1	B	144	PRO
1	B	184	VAL
1	B	186	PRO
1	B	216	ARG
1	B	299	VAL
1	B	371	GLY
1	B	373	THR
1	B	383	VAL
1	B	863	GLY
1	C	129	ALA
1	C	184	VAL
1	C	189	ASP
1	C	191	PRO

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Mol	Chain	Res	Type
1	C	221	SER
1	C	383	VAL
1	C	391	MET
1	C	397	GLU
1	C	422	PRO
1	C	449	SER
1	C	462	LEU
1	C	863	GLY
1	D	147	THR
1	D	230	ASP
1	D	301	PRO
1	D	318	GLY
1	D	321	ALA
1	D	339	VAL
1	D	445	VAL
1	D	749	LYS
1	E	145	GLU
1	E	183	VAL
1	E	188	THR
1	E	256	ALA
1	E	359	ASP
1	E	451	ALA
1	E	863	GLY
1	F	12	GLU
1	F	76	PHE
1	F	320	THR
1	F	340	ASP
1	F	341	THR
1	F	342	PRO
1	F	344	ARG
1	F	346	LEU
1	F	380	PHE
1	F	430	ALA
1	F	464	PRO
1	F	590	PRO
1	F	655	VAL
1	F	683	PRO
1	F	919	PRO
1	A	174	GLY
1	A	209	THR
1	A	215	LYS
1	A	379	ASP

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Mol	Chain	Res	Type
1	A	517	SER
1	A	575	GLY
1	B	147	THR
1	B	183	VAL
1	B	315	TRP
1	B	347	PRO
1	B	356	GLU
1	B	359	ASP
1	B	367	ARG
1	B	397	GLU
1	C	350	ALA
1	C	355	LEU
1	C	369	ARG
1	C	373	THR
1	C	380	PHE
1	C	382	GLY
1	C	405	GLY
1	C	454	ALA
1	C	749	LYS
1	D	89	LYS
1	D	117	GLY
1	D	219	THR
1	D	255	LEU
1	D	310	GLY
1	D	369	ARG
1	D	405	GLY
1	D	863	GLY
1	E	142	ALA
1	E	347	PRO
1	E	405	GLY
1	F	9	GLY
1	F	90	SER
1	F	109	LEU
1	F	117	GLY
1	F	339	VAL
1	F	465	ARG
1	F	631	GLY
1	F	639	GLY
1	F	685	ARG
1	F	845	GLY
1	F	904	ASN
1	A	537	ASP

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Mol	Chain	Res	Type
1	B	174	GLY
1	B	300	VAL
1	B	344	ARG
1	B	422	PRO
1	B	749	LYS
1	C	158	THR
1	C	230	ASP
1	D	378	ALA
1	D	713	ASN
1	E	172	ALA
1	E	261	HIS
1	E	353	ALA
1	E	358	ALA
1	E	609	ARG
1	E	749	LYS
1	F	17	SER
1	F	668	LEU
1	A	425	LEU
1	C	270	PRO
1	C	279	TYR
1	C	317	ASN
1	C	378	ALA
1	C	713	ASN
1	D	183	VAL
1	D	303	PRO
1	D	419	ARG
1	D	757	THR
1	E	258	PRO
1	E	311	ALA
1	E	713	ASN
1	F	34	SER
1	F	37	GLY
1	F	59	SER
1	F	336	GLY
1	F	337	PHE
1	F	861	SER
1	F	874	THR
1	F	934	PRO
1	A	206	ASP
1	A	783	ARG
1	B	185	HIS
1	B	317	ASN

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Mol	Chain	Res	Type
1	B	360	GLU
1	B	831	LEU
1	C	396	SER
1	C	537	ASP
1	C	609	ARG
1	C	783	ARG
1	C	831	LEU
1	D	187	LEU
1	D	356	GLU
1	D	400	LYS
1	D	416	ALA
1	E	67	GLY
1	E	232	ILE
1	E	373	THR
1	E	416	ALA
1	E	783	ARG
1	E	831	LEU
1	F	615	PRO
1	F	693	ASP
1	A	67	GLY
1	A	355	LEU
1	A	371	GLY
1	B	67	GLY
1	C	67	GLY
1	C	294	VAL
1	C	385	ALA
1	C	445	VAL
1	D	144	PRO
1	D	783	ARG
1	E	537	ASP
1	F	334	ALA
1	F	595	LEU
1	F	872	PRO
1	F	118	THR
1	F	647	GLY
1	A	117	GLY
1	E	413	PRO
1	F	572	VAL
1	B	445	VAL
1	D	174	GLY
1	F	347	PRO
1	A	422	PRO

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Mol	Chain	Res	Type
1	B	191	PRO
1	E	137	VAL
1	E	336	GLY
1	F	405	GLY
1	F	689	VAL
1	F	871	GLU
1	D	515	ILE

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	778/815 (96%)	637 (82%)	141 (18%)	2	7
1	B	758/815 (93%)	632 (83%)	126 (17%)	2	10
1	C	732/815 (90%)	588 (80%)	144 (20%)	1	5
1	D	763/815 (94%)	623 (82%)	140 (18%)	2	7
1	E	758/815 (93%)	607 (80%)	151 (20%)	1	5
1	F	492/815 (60%)	371 (75%)	121 (25%)	1	2
All	All	4281/4890 (88%)	3458 (81%)	823 (19%)	1	6

All (823) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	27	LEU
1	A	38	LYS
1	A	39	SER
1	A	41	LEU
1	A	45	THR
1	A	70	ASP
1	A	74	VAL
1	A	77	ILE
1	A	80	LEU
1	A	96	ARG

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Mol	Chain	Res	Type
1	A	109	LEU
1	A	111	LEU
1	A	124	CYS
1	A	128	VAL
1	A	130	ARG
1	A	132	THR
1	A	137	VAL
1	A	139	GLN
1	A	140	VAL
1	A	145	GLU
1	A	152	LEU
1	A	159	ARG
1	A	162	GLU
1	A	166	LEU
1	A	173	GLN
1	A	184	VAL
1	A	189	ASP
1	A	195	LYS
1	A	198	LYS
1	A	202	GLU
1	A	204	VAL
1	A	208	LEU
1	A	209	THR
1	A	216	ARG
1	A	218	LEU
1	A	220	ASP
1	A	226	LEU
1	A	228	LEU
1	A	233	VAL
1	A	234	VAL
1	A	235	LEU
1	A	236	GLU
1	A	237	PHE
1	A	248	GLU
1	A	249	GLN
1	A	254	LYS
1	A	266	ASP
1	A	269	GLU
1	A	277	SER
1	A	288	LEU
1	A	290	ILE
1	A	293	GLU

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Mol	Chain	Res	Type
1	A	294	VAL
1	A	323	TYR
1	A	328	MET
1	A	331	LEU
1	A	333	GLU
1	A	335	LEU
1	A	339	VAL
1	A	340	ASP
1	A	369	ARG
1	A	376	TYR
1	A	379	ASP
1	A	381	GLU
1	A	383	VAL
1	A	386	PHE
1	A	391	MET
1	A	395	GLU
1	A	398	GLN
1	A	410	VAL
1	A	414	VAL
1	A	418	THR
1	A	428	THR
1	A	429	LEU
1	A	448	LEU
1	A	461	THR
1	A	462	LEU
1	A	465	ARG
1	A	467	GLN
1	A	478	ARG
1	A	479	SER
1	A	480	ARG
1	A	481	LEU
1	A	489	LEU
1	A	492	LEU
1	A	493	SER
1	A	494	LEU
1	A	508	ARG
1	A	533	LEU
1	A	539	ARG
1	A	541	LEU
1	A	546	THR
1	A	548	LEU
1	A	551	LEU

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Mol	Chain	Res	Type
1	A	554	THR
1	A	597	ASN
1	A	601	ILE
1	A	609	ARG
1	A	613	GLU
1	A	614	ILE
1	A	617	ILE
1	A	618	ARG
1	A	626	GLN
1	A	640	ILE
1	A	648	VAL
1	A	656	SER
1	A	660	LYS
1	A	668	LEU
1	A	688	ARG
1	A	690	THR
1	A	692	LEU
1	A	697	LYS
1	A	698	LEU
1	A	706	ILE
1	A	709	THR
1	A	718	THR
1	A	720	VAL
1	A	748	VAL
1	A	756	CYS
1	A	761	THR
1	A	765	GLU
1	A	768	PHE
1	A	771	ASP
1	A	793	TYR
1	A	798	VAL
1	A	799	SER
1	A	808	GLU
1	A	814	GLU
1	A	829	VAL
1	A	831	LEU
1	A	836	LEU
1	A	843	LEU
1	A	853	LEU
1	A	860	ARG
1	A	873	THR
1	A	891	LEU

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Mol	Chain	Res	Type
1	A	900	VAL
1	A	911	SER
1	A	914	ILE
1	A	947	LYS
1	B	7	VAL
1	B	27	LEU
1	B	38	LYS
1	B	39	SER
1	B	41	LEU
1	B	45	THR
1	B	70	ASP
1	B	74	VAL
1	B	77	ILE
1	B	80	LEU
1	B	88	GLN
1	B	109	LEU
1	B	111	LEU
1	B	118	THR
1	B	121	CYS
1	B	134	GLN
1	B	136	ILE
1	B	137	VAL
1	B	139	GLN
1	B	147	THR
1	B	148	ARG
1	B	150	LEU
1	B	155	VAL
1	B	166	LEU
1	B	170	LEU
1	B	171	ASN
1	B	194	LYS
1	B	197	GLU
1	B	199	HIS
1	B	203	VAL
1	B	204	VAL
1	B	205	VAL
1	B	215	LYS
1	B	221	SER
1	B	224	THR
1	B	226	LEU
1	B	228	LEU
1	B	232	ILE

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Mol	Chain	Res	Type
1	B	235	LEU
1	B	263	LEU
1	B	265	VAL
1	B	271	ARG
1	B	286	SER
1	B	290	ILE
1	B	291	ARG
1	B	292	LYS
1	B	298	LEU
1	B	320	THR
1	B	323	TYR
1	B	326	ARG
1	B	327	MET
1	B	345	LYS
1	B	349	LYS
1	B	361	GLN
1	B	367	ARG
1	B	380	PHE
1	B	387	LEU
1	B	390	LYS
1	B	402	ARG
1	B	407	MET
1	B	419	ARG
1	B	423	GLU
1	B	424	ILE
1	B	452	ASP
1	B	457	LEU
1	B	461	THR
1	B	462	LEU
1	B	465	ARG
1	B	466	GLU
1	B	467	GLN
1	B	478	ARG
1	B	479	SER
1	B	480	ARG
1	B	481	LEU
1	B	489	LEU
1	B	492	LEU
1	B	493	SER
1	B	508	ARG
1	B	531	ILE
1	B	533	LEU

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Mol	Chain	Res	Type
1	B	539	ARG
1	B	541	LEU
1	B	546	THR
1	B	548	LEU
1	B	551	LEU
1	B	554	THR
1	B	585	ILE
1	B	597	ASN
1	B	609	ARG
1	B	613	GLU
1	B	614	ILE
1	B	617	ILE
1	B	626	GLN
1	B	640	ILE
1	B	648	VAL
1	B	656	SER
1	B	660	LYS
1	B	690	THR
1	B	697	LYS
1	B	698	LEU
1	B	706	ILE
1	B	708	ARG
1	B	709	THR
1	B	718	THR
1	B	720	VAL
1	B	753	CYS
1	B	761	THR
1	B	764	ILE
1	B	768	PHE
1	B	771	ASP
1	B	793	TYR
1	B	798	VAL
1	B	799	SER
1	B	814	GLU
1	B	829	VAL
1	B	831	LEU
1	B	836	LEU
1	B	843	LEU
1	B	853	LEU
1	B	860	ARG
1	B	873	THR
1	B	891	LEU

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Mol	Chain	Res	Type
1	B	900	VAL
1	B	911	SER
1	B	914	ILE
1	B	947	LYS
1	C	7	VAL
1	C	12	GLU
1	C	27	LEU
1	C	31	THR
1	C	38	LYS
1	C	39	SER
1	C	41	LEU
1	C	45	THR
1	C	70	ASP
1	C	77	ILE
1	C	80	LEU
1	C	91	THR
1	C	93	ARG
1	C	109	LEU
1	C	127	ARG
1	C	128	VAL
1	C	130	ARG
1	C	131	GLN
1	C	135	GLN
1	C	151	VAL
1	C	152	LEU
1	C	158	THR
1	C	162	GLU
1	C	165	ASP
1	C	166	LEU
1	C	170	LEU
1	C	173	GLN
1	C	176	SER
1	C	180	VAL
1	C	183	VAL
1	C	187	LEU
1	C	196	GLN
1	C	198	LYS
1	C	200	ASP
1	C	202	GLU
1	C	215	LYS
1	C	216	ARG
1	C	217	ARG

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Mol	Chain	Res	Type
1	C	218	LEU
1	C	222	VAL
1	C	224	THR
1	C	232	ILE
1	C	233	VAL
1	C	282	CYS
1	C	288	LEU
1	C	290	ILE
1	C	293	GLU
1	C	294	VAL
1	C	297	GLU
1	C	300	VAL
1	C	317	ASN
1	C	319	HIS
1	C	325	THR
1	C	365	ARG
1	C	372	ARG
1	C	379	ASP
1	C	380	PHE
1	C	381	GLU
1	C	383	VAL
1	C	384	LEU
1	C	387	LEU
1	C	391	MET
1	C	393	GLN
1	C	394	THR
1	C	395	GLU
1	C	400	LYS
1	C	401	GLU
1	C	407	MET
1	C	408	ARG
1	C	420	LEU
1	C	425	LEU
1	C	444	GLU
1	C	447	GLU
1	C	450	ILE
1	C	457	LEU
1	C	462	LEU
1	C	465	ARG
1	C	466	GLU
1	C	467	GLN
1	C	478	ARG

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Mol	Chain	Res	Type
1	C	479	SER
1	C	480	ARG
1	C	481	LEU
1	C	489	LEU
1	C	490	GLU
1	C	492	LEU
1	C	493	SER
1	C	494	LEU
1	C	508	ARG
1	C	515	ILE
1	C	531	ILE
1	C	533	LEU
1	C	539	ARG
1	C	541	LEU
1	C	546	THR
1	C	548	LEU
1	C	551	LEU
1	C	554	THR
1	C	585	ILE
1	C	597	ASN
1	C	609	ARG
1	C	613	GLU
1	C	614	ILE
1	C	617	ILE
1	C	626	GLN
1	C	640	ILE
1	C	648	VAL
1	C	656	SER
1	C	660	LYS
1	C	685	ARG
1	C	690	THR
1	C	697	LYS
1	C	698	LEU
1	C	706	ILE
1	C	708	ARG
1	C	709	THR
1	C	712	SER
1	C	718	THR
1	C	720	VAL
1	C	752	ARG
1	C	753	CYS
1	C	757	THR

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Mol	Chain	Res	Type
1	C	761	THR
1	C	764	ILE
1	C	768	PHE
1	C	771	ASP
1	C	793	TYR
1	C	798	VAL
1	C	799	SER
1	C	808	GLU
1	C	814	GLU
1	C	829	VAL
1	C	831	LEU
1	C	836	LEU
1	C	843	LEU
1	C	853	LEU
1	C	860	ARG
1	C	873	THR
1	C	891	LEU
1	C	900	VAL
1	C	911	SER
1	C	914	ILE
1	C	917	LEU
1	C	947	LYS
1	D	7	VAL
1	D	27	LEU
1	D	31	THR
1	D	38	LYS
1	D	39	SER
1	D	41	LEU
1	D	45	THR
1	D	70	ASP
1	D	74	VAL
1	D	77	ILE
1	D	80	LEU
1	D	88	GLN
1	D	109	LEU
1	D	111	LEU
1	D	115	ARG
1	D	130	ARG
1	D	134	GLN
1	D	137	VAL
1	D	138	ASP
1	D	140	VAL

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Mol	Chain	Res	Type
1	D	141	LEU
1	D	147	THR
1	D	150	LEU
1	D	152	LEU
1	D	157	ARG
1	D	160	LYS
1	D	165	ASP
1	D	166	LEU
1	D	181	ASP
1	D	193	LEU
1	D	199	HIS
1	D	202	GLU
1	D	216	ARG
1	D	217	ARG
1	D	218	LEU
1	D	222	VAL
1	D	232	ILE
1	D	234	VAL
1	D	250	ARG
1	D	255	LEU
1	D	263	LEU
1	D	265	VAL
1	D	282	CYS
1	D	288	LEU
1	D	292	LYS
1	D	294	VAL
1	D	317	ASN
1	D	320	THR
1	D	323	TYR
1	D	326	ARG
1	D	327	MET
1	D	349	LYS
1	D	352	LYS
1	D	354	ILE
1	D	355	LEU
1	D	359	ASP
1	D	360	GLU
1	D	365	ARG
1	D	367	ARG
1	D	369	ARG
1	D	372	ARG
1	D	384	LEU

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Mol	Chain	Res	Type
1	D	389	ARG
1	D	394	THR
1	D	402	ARG
1	D	407	MET
1	D	412	CYS
1	D	440	LYS
1	D	450	ILE
1	D	460	LEU
1	D	462	LEU
1	D	465	ARG
1	D	467	GLN
1	D	478	ARG
1	D	479	SER
1	D	480	ARG
1	D	481	LEU
1	D	489	LEU
1	D	492	LEU
1	D	493	SER
1	D	494	LEU
1	D	508	ARG
1	D	515	ILE
1	D	531	ILE
1	D	533	LEU
1	D	539	ARG
1	D	541	LEU
1	D	546	THR
1	D	548	LEU
1	D	551	LEU
1	D	554	THR
1	D	555	LEU
1	D	585	ILE
1	D	597	ASN
1	D	609	ARG
1	D	613	GLU
1	D	614	ILE
1	D	617	ILE
1	D	626	GLN
1	D	640	ILE
1	D	648	VAL
1	D	656	SER
1	D	660	LYS
1	D	685	ARG

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Mol	Chain	Res	Type
1	D	690	THR
1	D	697	LYS
1	D	698	LEU
1	D	706	ILE
1	D	708	ARG
1	D	709	THR
1	D	712	SER
1	D	718	THR
1	D	720	VAL
1	D	752	ARG
1	D	757	THR
1	D	761	THR
1	D	764	ILE
1	D	767	ASN
1	D	768	PHE
1	D	771	ASP
1	D	793	TYR
1	D	798	VAL
1	D	799	SER
1	D	808	GLU
1	D	811	GLU
1	D	829	VAL
1	D	831	LEU
1	D	836	LEU
1	D	843	LEU
1	D	853	LEU
1	D	859	LYS
1	D	860	ARG
1	D	873	THR
1	D	874	THR
1	D	891	LEU
1	D	900	VAL
1	D	911	SER
1	D	914	ILE
1	D	917	LEU
1	D	947	LYS
1	E	7	VAL
1	E	27	LEU
1	E	38	LYS
1	E	39	SER
1	E	41	LEU
1	E	45	THR

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Mol	Chain	Res	Type
1	E	70	ASP
1	E	74	VAL
1	E	77	ILE
1	E	80	LEU
1	E	109	LEU
1	E	111	LEU
1	E	121	CYS
1	E	130	ARG
1	E	131	GLN
1	E	132	THR
1	E	141	LEU
1	E	147	THR
1	E	151	VAL
1	E	155	VAL
1	E	158	THR
1	E	166	LEU
1	E	168	ASP
1	E	169	LYS
1	E	185	HIS
1	E	193	LEU
1	E	202	GLU
1	E	217	ARG
1	E	226	LEU
1	E	239	ASP
1	E	255	LEU
1	E	258	PRO
1	E	259	ASN
1	E	263	LEU
1	E	265	VAL
1	E	266	ASP
1	E	268	LEU
1	E	288	LEU
1	E	292	LYS
1	E	294	VAL
1	E	300	VAL
1	E	303	PRO
1	E	305	ARG
1	E	306	THR
1	E	307	LEU
1	E	309	GLN
1	E	312	VAL
1	E	319	HIS

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Mol	Chain	Res	Type
1	E	320	THR
1	E	323	TYR
1	E	327	MET
1	E	333	GLU
1	E	338	ASP
1	E	339	VAL
1	E	346	LEU
1	E	351	ARG
1	E	354	ILE
1	E	355	LEU
1	E	364	VAL
1	E	368	ASN
1	E	369	ARG
1	E	372	ARG
1	E	374	ARG
1	E	380	PHE
1	E	381	GLU
1	E	384	LEU
1	E	386	PHE
1	E	390	LYS
1	E	392	SER
1	E	397	GLU
1	E	398	GLN
1	E	400	LYS
1	E	401	GLU
1	E	410	VAL
1	E	420	LEU
1	E	429	LEU
1	E	434	LYS
1	E	446	CYS
1	E	450	ILE
1	E	452	ASP
1	E	457	LEU
1	E	458	ASN
1	E	460	LEU
1	E	461	THR
1	E	462	LEU
1	E	465	ARG
1	E	466	GLU
1	E	467	GLN
1	E	478	ARG
1	E	479	SER

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Mol	Chain	Res	Type
1	E	480	ARG
1	E	481	LEU
1	E	489	LEU
1	E	490	GLU
1	E	493	SER
1	E	494	LEU
1	E	508	ARG
1	E	515	ILE
1	E	531	ILE
1	E	533	LEU
1	E	539	ARG
1	E	541	LEU
1	E	546	THR
1	E	548	LEU
1	E	551	LEU
1	E	554	THR
1	E	585	ILE
1	E	597	ASN
1	E	609	ARG
1	E	613	GLU
1	E	614	ILE
1	E	617	ILE
1	E	618	ARG
1	E	626	GLN
1	E	640	ILE
1	E	648	VAL
1	E	656	SER
1	E	660	LYS
1	E	668	LEU
1	E	690	THR
1	E	697	LYS
1	E	698	LEU
1	E	706	ILE
1	E	708	ARG
1	E	709	THR
1	E	712	SER
1	E	718	THR
1	E	720	VAL
1	E	752	ARG
1	E	757	THR
1	E	761	THR
1	E	764	ILE

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Mol	Chain	Res	Type
1	E	768	PHE
1	E	771	ASP
1	E	780	GLN
1	E	793	TYR
1	E	798	VAL
1	E	799	SER
1	E	808	GLU
1	E	814	GLU
1	E	829	VAL
1	E	831	LEU
1	E	843	LEU
1	E	853	LEU
1	E	860	ARG
1	E	873	THR
1	E	891	LEU
1	E	900	VAL
1	E	911	SER
1	E	914	ILE
1	E	947	LYS
1	F	5	LEU
1	F	6	ILE
1	F	22	LEU
1	F	24	ARG
1	F	25	ASP
1	F	27	LEU
1	F	28	ILE
1	F	29	VAL
1	F	30	PHE
1	F	33	LEU
1	F	34	SER
1	F	40	SER
1	F	53	ARG
1	F	61	TYR
1	F	71	LYS
1	F	73	ASP
1	F	76	PHE
1	F	77	ILE
1	F	78	GLU
1	F	84	VAL
1	F	89	LYS
1	F	99	VAL
1	F	316	SER

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Mol	Chain	Res	Type
1	F	320	THR
1	F	325	THR
1	F	328	MET
1	F	343	TRP
1	F	345	LYS
1	F	346	LEU
1	F	368	ASN
1	F	373	THR
1	F	375	SER
1	F	380	PHE
1	F	381	GLU
1	F	383	VAL
1	F	387	LEU
1	F	389	ARG
1	F	392	SER
1	F	397	GLU
1	F	407	MET
1	F	424	ILE
1	F	425	LEU
1	F	427	VAL
1	F	428	THR
1	F	436	GLU
1	F	442	ILE
1	F	445	VAL
1	F	448	LEU
1	F	450	ILE
1	F	466	GLU
1	F	469	ILE
1	F	479	SER
1	F	490	GLU
1	F	492	LEU
1	F	493	SER
1	F	494	LEU
1	F	500	THR
1	F	502	SER
1	F	507	GLN
1	F	513	THR
1	F	515	ILE
1	F	544	THR
1	F	548	LEU
1	F	554	THR
1	F	555	LEU

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Mol	Chain	Res	Type
1	F	563	ASP
1	F	570	TRP
1	F	574	ILE
1	F	581	HIS
1	F	585	ILE
1	F	588	SER
1	F	591	TYR
1	F	592	ASP
1	F	593	GLU
1	F	594	LEU
1	F	596	ARG
1	F	601	ILE
1	F	606	LEU
1	F	609	ARG
1	F	614	ILE
1	F	619	ARG
1	F	621	VAL
1	F	625	ARG
1	F	626	GLN
1	F	627	LEU
1	F	636	ASN
1	F	640	ILE
1	F	652	VAL
1	F	655	VAL
1	F	656	SER
1	F	660	LYS
1	F	662	THR
1	F	666	ASP
1	F	667	ILE
1	F	671	VAL
1	F	672	LEU
1	F	687	THR
1	F	688	ARG
1	F	689	VAL
1	F	690	THR
1	F	693	ASP
1	F	699	VAL
1	F	701	VAL
1	F	850	ARG
1	F	856	GLU
1	F	857	LEU
1	F	868	ILE

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Mol	Chain	Res	Type
1	F	885	LEU
1	F	888	ILE
1	F	891	LEU
1	F	892	VAL
1	F	896	ASN
1	F	898	VAL
1	F	899	ILE
1	F	902	GLU
1	F	907	VAL
1	F	910	THR
1	F	920	GLU
1	F	933	THR
1	F	937	VAL
1	F	949	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (104) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	HIS
1	A	68	GLN
1	A	120	HIS
1	A	131	GLN
1	A	135	GLN
1	A	171	ASN
1	A	173	GLN
1	A	249	GLN
1	A	276	ASN
1	A	368	ASN
1	A	437	HIS
1	A	597	ASN
1	A	626	GLN
1	A	681	GLN
1	A	686	HIS
1	A	747	ASN
1	A	889	ASN
1	A	896	ASN
1	A	931	GLN
1	B	13	HIS
1	B	51	GLN
1	B	68	GLN
1	B	88	GLN
1	B	131	GLN

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Mol	Chain	Res	Type
1	B	171	ASN
1	B	185	HIS
1	B	261	HIS
1	B	363	HIS
1	B	368	ASN
1	B	472	GLN
1	B	538	ASN
1	B	567	HIS
1	B	597	ASN
1	B	626	GLN
1	B	681	GLN
1	B	686	HIS
1	B	747	ASN
1	B	889	ASN
1	B	896	ASN
1	C	13	HIS
1	C	68	GLN
1	C	139	GLN
1	C	259	ASN
1	C	319	HIS
1	C	458	ASN
1	C	597	ASN
1	C	626	GLN
1	C	674	ASN
1	C	681	GLN
1	C	686	HIS
1	C	747	ASN
1	C	767	ASN
1	C	780	GLN
1	C	889	ASN
1	C	896	ASN
1	D	51	GLN
1	D	68	GLN
1	D	120	HIS
1	D	134	GLN
1	D	139	GLN
1	D	171	ASN
1	D	199	HIS
1	D	317	ASN
1	D	368	ASN
1	D	597	ASN
1	D	626	GLN

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Mol	Chain	Res	Type
1	D	674	ASN
1	D	681	GLN
1	D	686	HIS
1	D	747	ASN
1	D	767	ASN
1	D	838	GLN
1	D	889	ASN
1	D	896	ASN
1	E	13	HIS
1	E	51	GLN
1	E	68	GLN
1	E	88	GLN
1	E	120	HIS
1	E	185	HIS
1	E	309	GLN
1	E	363	HIS
1	E	368	ASN
1	E	437	HIS
1	E	597	ASN
1	E	626	GLN
1	E	674	ASN
1	E	681	GLN
1	E	686	HIS
1	E	747	ASN
1	E	767	ASN
1	E	780	GLN
1	E	889	ASN
1	E	896	ASN
1	F	14	ASN
1	F	92	ASN
1	F	319	HIS
1	F	363	HIS
1	F	560	HIS
1	F	567	HIS
1	F	626	GLN
1	F	686	HIS
1	F	877	HIS
1	F	886	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 14 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	3
1	A	2
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	260:GLY	C	261:HIS	N	1.19
1	A	11:ARG	C	12:GLU	N	1.15
1	A	411:PRO	C	412:CYS	N	1.11
1	B	120:HIS	C	121:CYS	N	1.08
1	D	126:GLU	C	127:ARG	N	1.07

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	256:ALA	C	257:CYS	N	1.02

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	944/993 (95%)	0.14	38 (4%)	42	30	16, 55, 94, 112	0
1	B	918/993 (92%)	0.15	49 (5%)	32	24	16, 57, 102, 111	0
1	C	890/993 (89%)	0.09	27 (3%)	52	39	16, 60, 108, 118	0
1	D	921/993 (92%)	0.09	30 (3%)	49	36	16, 60, 103, 114	0
1	E	919/993 (92%)	0.02	21 (2%)	61	46	16, 57, 102, 127	0
1	F	607/993 (61%)	0.34	34 (5%)	30	23	45, 79, 112, 117	0
All	All	5199/5958 (87%)	0.13	199 (3%)	44	31	16, 61, 104, 127	0

All (199) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	454	ALA	8.1
1	B	437	HIS	7.4
1	A	437	HIS	7.3
1	C	439	ALA	6.8
1	A	445	VAL	6.2
1	D	445	VAL	5.9
1	A	446	CYS	5.7
1	A	577	GLY	5.6
1	E	442	ILE	5.4
1	B	454	ALA	5.3
1	C	437	HIS	5.3
1	C	353	ALA	5.2
1	F	355	LEU	5.0
1	B	162	GLU	4.7
1	A	361	GLN	4.5
1	E	440	LYS	4.5
1	A	713	ASN	4.3
1	B	460	LEU	4.2
1	F	341	THR	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	311	ALA	4.2
1	A	308	ALA	4.1
1	A	357	GLY	4.1
1	F	413	PRO	4.1
1	A	575	GLY	4.0
1	B	575	GLY	4.0
1	F	415	CYS	4.0
1	B	431	GLY	3.9
1	E	129	ALA	3.8
1	B	398	GLN	3.8
1	B	429	LEU	3.8
1	E	233	VAL	3.7
1	A	268	LEU	3.7
1	F	441	SER	3.7
1	E	437	HIS	3.6
1	B	453	CYS	3.6
1	F	448	LEU	3.6
1	F	388	GLN	3.5
1	E	455	ASP	3.5
1	F	395	GLU	3.4
1	C	438	GLY	3.4
1	B	388	GLN	3.4
1	D	307	LEU	3.4
1	D	303	PRO	3.4
1	C	234	VAL	3.4
1	B	438	GLY	3.4
1	F	425	LEU	3.3
1	A	444	GLU	3.3
1	A	498	ALA	3.3
1	C	456	PHE	3.3
1	B	434	LYS	3.3
1	F	888	ILE	3.2
1	E	453	CYS	3.2
1	A	394	THR	3.2
1	F	443	ALA	3.2
1	C	459	ALA	3.2
1	A	431	GLY	3.1
1	A	460	LEU	3.1
1	D	305	ARG	3.1
1	C	354	ILE	3.1
1	D	673	ALA	3.1
1	F	420	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	436	GLU	3.1
1	D	740	GLN	3.1
1	F	310	GLY	3.1
1	A	578	ALA	3.0
1	F	885	LEU	3.0
1	A	435	GLY	3.0
1	A	447	GLU	3.0
1	B	383	VAL	3.0
1	F	878	PHE	3.0
1	A	95	PRO	3.0
1	F	68	GLN	3.0
1	A	343	TRP	3.0
1	B	443	ALA	3.0
1	D	457	LEU	2.9
1	B	444	GLU	2.9
1	F	417	GLY	2.9
1	A	158	THR	2.9
1	B	432	GLU	2.9
1	A	457	LEU	2.9
1	D	865	THR	2.9
1	E	444	GLU	2.9
1	B	313	ALA	2.8
1	A	456	PHE	2.8
1	D	379	ASP	2.8
1	B	435	GLY	2.8
1	C	673	ALA	2.8
1	B	455	ASP	2.8
1	A	38	LYS	2.8
1	B	258	PRO	2.8
1	B	364	VAL	2.8
1	D	577	GLY	2.7
1	B	38	LYS	2.7
1	F	439	ALA	2.7
1	F	898	VAL	2.7
1	B	92	ASN	2.7
1	B	457	LEU	2.7
1	F	879	ASP	2.6
1	C	32	GLY	2.6
1	D	310	GLY	2.6
1	B	220	ASP	2.6
1	B	353	ALA	2.6
1	A	354	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	691	GLY	2.6
1	C	457	LEU	2.6
1	D	306	THR	2.6
1	D	377	TYR	2.6
1	C	691	GLY	2.6
1	B	394	THR	2.6
1	A	822	TYR	2.5
1	A	660	LYS	2.5
1	F	339	VAL	2.5
1	C	460	LEU	2.5
1	B	728	PHE	2.5
1	A	366	TYR	2.5
1	B	515	ILE	2.5
1	C	13	HIS	2.5
1	A	231	GLY	2.5
1	A	441	SER	2.5
1	A	94	ASN	2.4
1	B	379	ASP	2.4
1	C	204	VAL	2.4
1	B	143	MET	2.4
1	A	433	SER	2.4
1	B	461	THR	2.4
1	C	461	THR	2.4
1	A	898	VAL	2.4
1	B	448	LEU	2.4
1	E	379	ASP	2.4
1	D	456	PHE	2.4
1	A	307	LEU	2.4
1	D	342	PRO	2.4
1	E	394	THR	2.3
1	E	443	ALA	2.3
1	A	302	ASP	2.3
1	E	235	LEU	2.3
1	C	222	VAL	2.3
1	D	339	VAL	2.3
1	B	90	SER	2.3
1	E	347	PRO	2.3
1	A	515	ILE	2.3
1	F	75	ASP	2.3
1	F	851	VAL	2.3
1	F	887	VAL	2.3
1	C	758	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	261	HIS	2.3
1	B	193	LEU	2.3
1	D	235	LEU	2.3
1	D	698	LEU	2.3
1	B	178	VAL	2.3
1	C	660	LYS	2.3
1	B	384	LEU	2.3
1	B	259	ASN	2.3
1	B	357	GLY	2.3
1	E	691	GLY	2.3
1	B	299	VAL	2.3
1	F	354	ILE	2.2
1	A	810	ALA	2.2
1	B	439	ALA	2.2
1	C	335	LEU	2.2
1	F	16	ARG	2.2
1	F	343	TRP	2.2
1	B	660	LYS	2.2
1	E	660	LYS	2.2
1	D	454	ALA	2.2
1	E	719	GLY	2.2
1	B	397	GLU	2.2
1	D	660	LYS	2.2
1	D	302	ASP	2.2
1	F	418	THR	2.1
1	C	255	LEU	2.1
1	B	272	SER	2.1
1	D	38	LYS	2.1
1	E	435	GLY	2.1
1	F	65	PHE	2.1
1	F	35	GLY	2.1
1	F	412	CYS	2.1
1	F	414	VAL	2.1
1	E	150	LEU	2.1
1	D	308	ALA	2.1
1	B	447	GLU	2.1
1	C	289	GLY	2.1
1	D	92	ASN	2.1
1	C	233	VAL	2.1
1	D	364	VAL	2.1
1	D	218	LEU	2.1
1	C	680	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	460	LEU	2.1
1	D	312	VAL	2.0
1	C	317	ASN	2.0
1	C	350	ALA	2.0
1	B	691	GLY	2.0
1	F	14	ASN	2.0
1	B	378	ALA	2.0
1	D	353	ALA	2.0
1	F	348	ALA	2.0
1	C	377	TYR	2.0
1	A	779	CYS	2.0
1	B	576	PRO	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(Å ²)	Q<0.9
2	ZN	B	1955	1/1	0.84	0.14	116,116,116,116	0
2	ZN	A	1954	1/1	0.87	0.10	65,65,65,65	0
2	ZN	E	1955	1/1	0.89	0.17	116,116,116,116	0
2	ZN	C	1955	1/1	0.96	0.11	116,116,116,116	0
2	ZN	A	1955	1/1	0.96	0.09	116,116,116,116	0
2	ZN	A	1956	1/1	0.97	0.08	48,48,48,48	0
2	ZN	B	1956	1/1	0.97	0.04	44,44,44,44	0
2	ZN	D	1955	1/1	0.98	0.09	116,116,116,116	0
2	ZN	D	1954	1/1	0.99	0.03	66,66,66,66	0
2	ZN	B	1954	1/1	0.99	0.06	65,65,65,65	0
2	ZN	E	1954	1/1	0.99	0.03	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	C	1956	1/1	0.99	0.03	76,76,76,76	0
2	ZN	C	1954	1/1	1.00	0.03	65,65,65,65	0
2	ZN	D	1956	1/1	1.00	0.01	59,59,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.