



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 08:26 pm GMT

PDB ID : 3ZQJ
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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

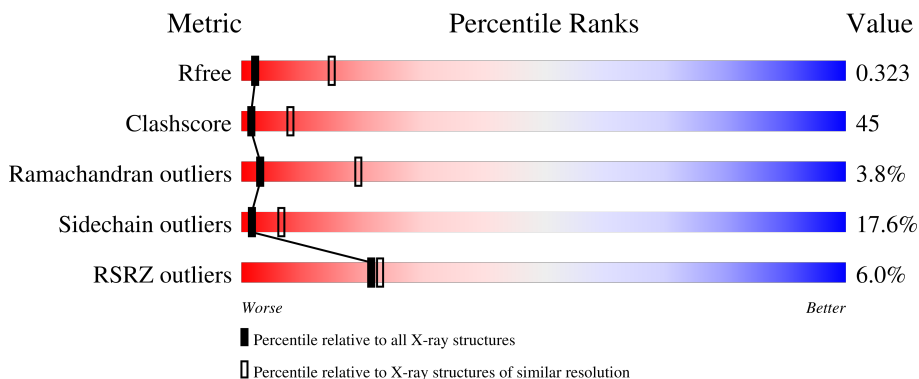
1 Overall quality at a glance

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}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	 5% 42% 42% 10% • 5%
1	B	993	 5% 41% 41% 10% • 8%
1	C	993	 4% 39% 39% 10% • 10%
1	D	993	 7% 39% 43% 10% • 7%
1	E	993	 7% 40% 41% 11% • 7%

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Mol	Chain	Length	Quality of chain
1	F	993	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into five segments: a red segment (5%), a green segment (18%), a yellow segment (32%), an orange segment (10%), and a grey segment (39%).</p>

2 Entry composition [i](#)

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

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

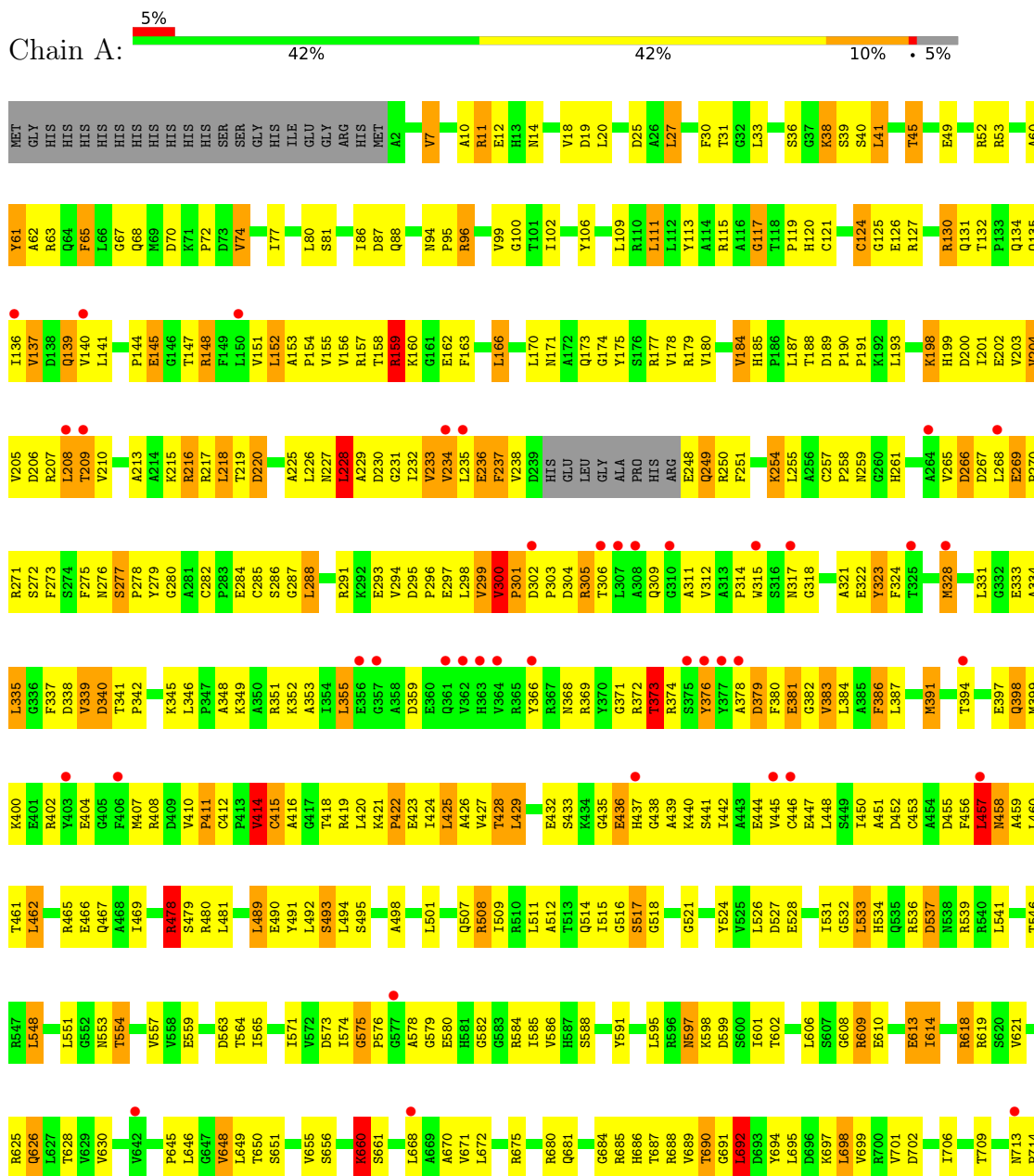
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

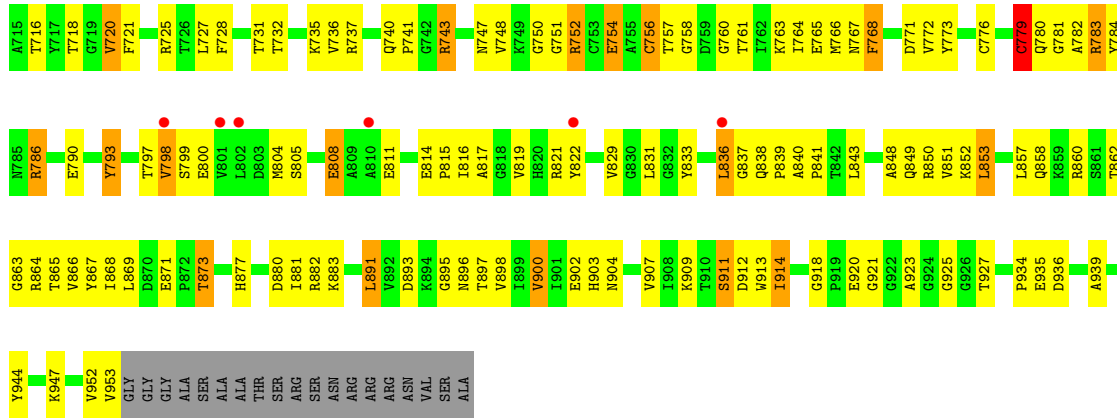
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Zn	0	0
			3	3		
2	B	3	Total	Zn	0	0
			3	3		
2	C	3	Total	Zn	0	0
			3	3		
2	D	3	Total	Zn	0	0
			3	3		
2	E	2	Total	Zn	0	0
			2	2		

3 Residue-property plots

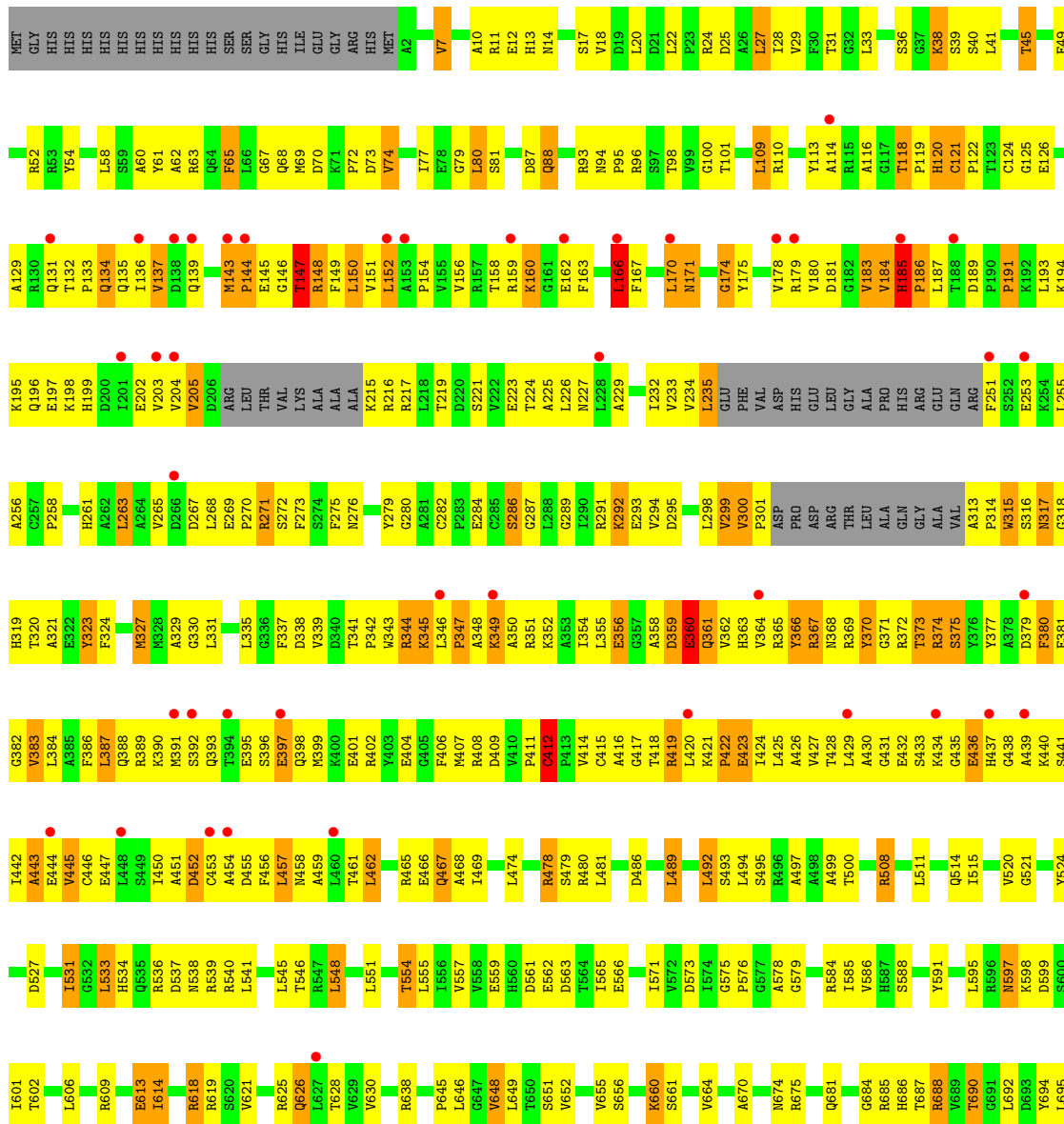
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

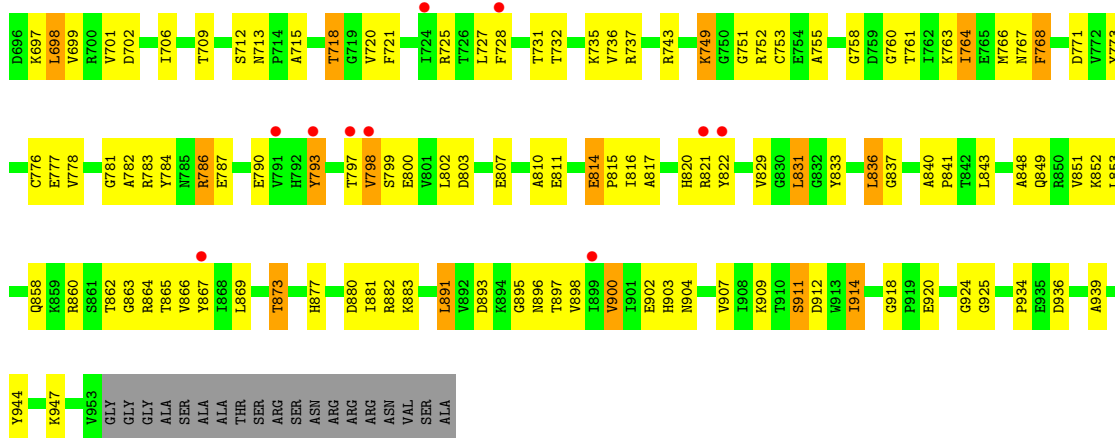
• Molecule 1: UVRABC SYSTEM PROTEIN A



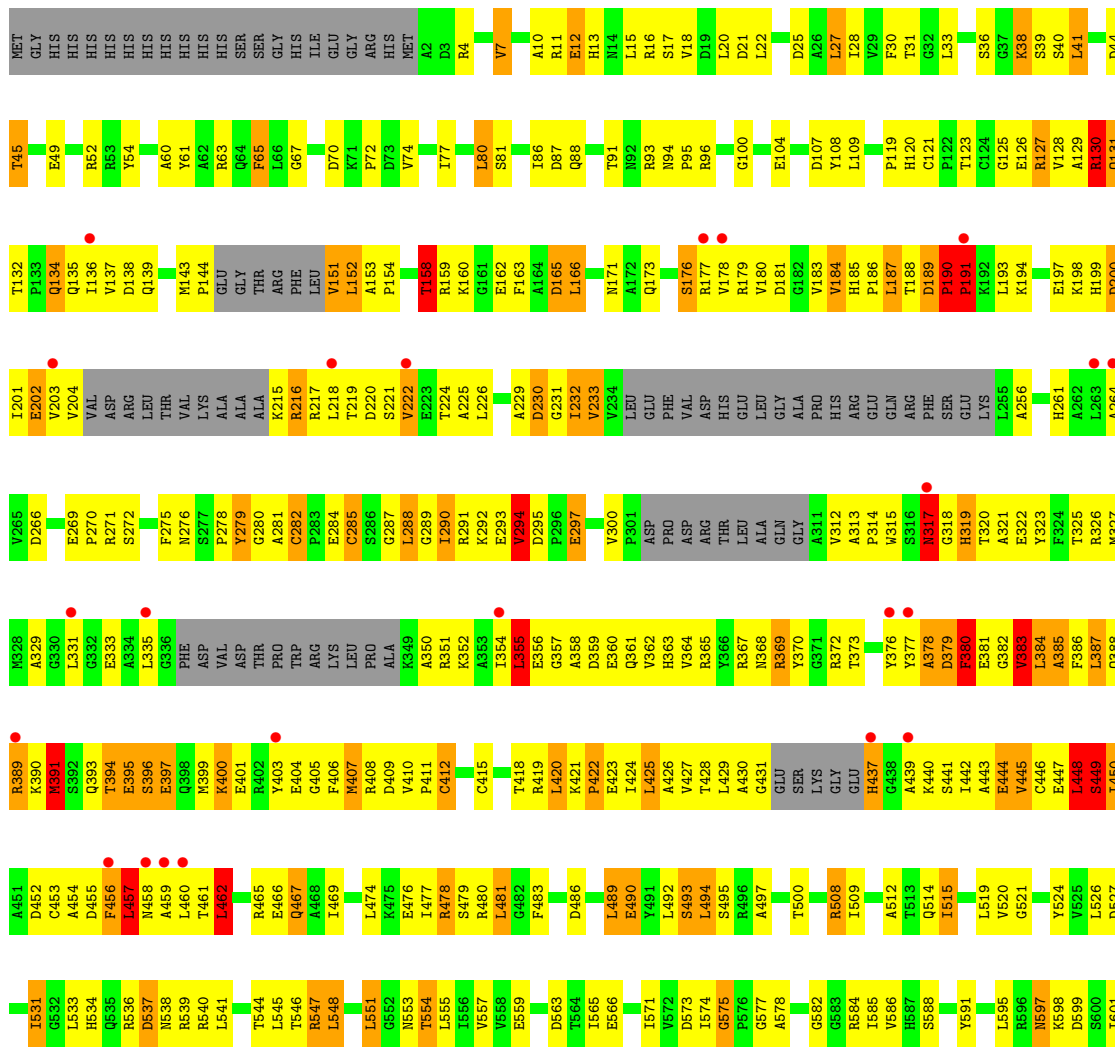


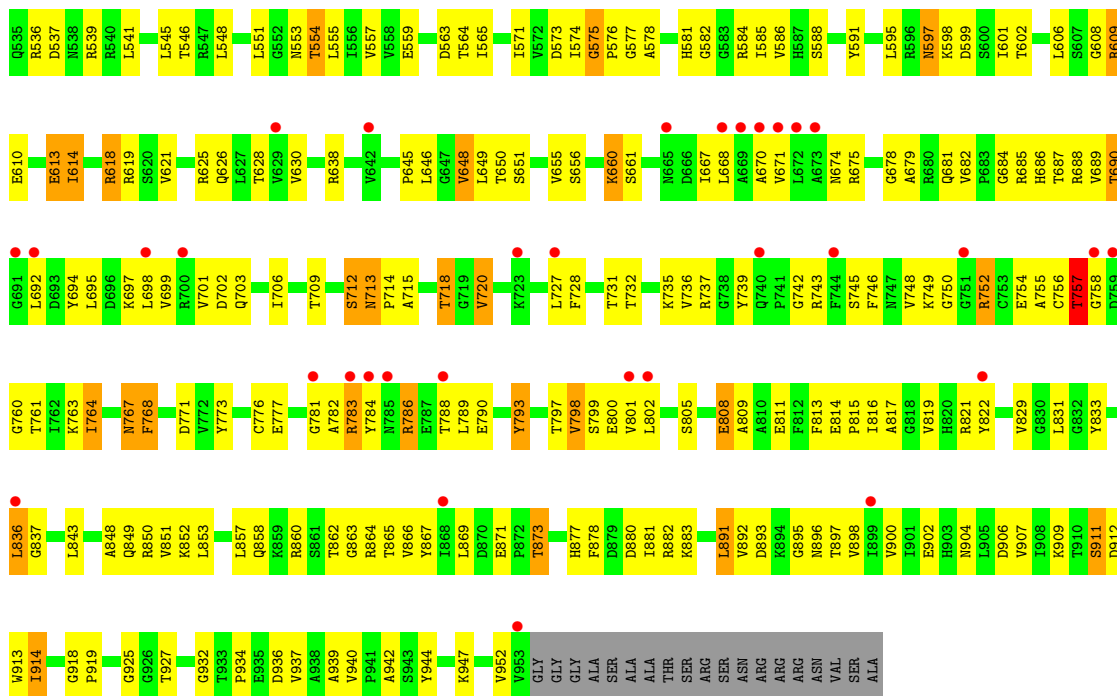
● Molecule 1: UVRABC SYSTEM PROTEIN A



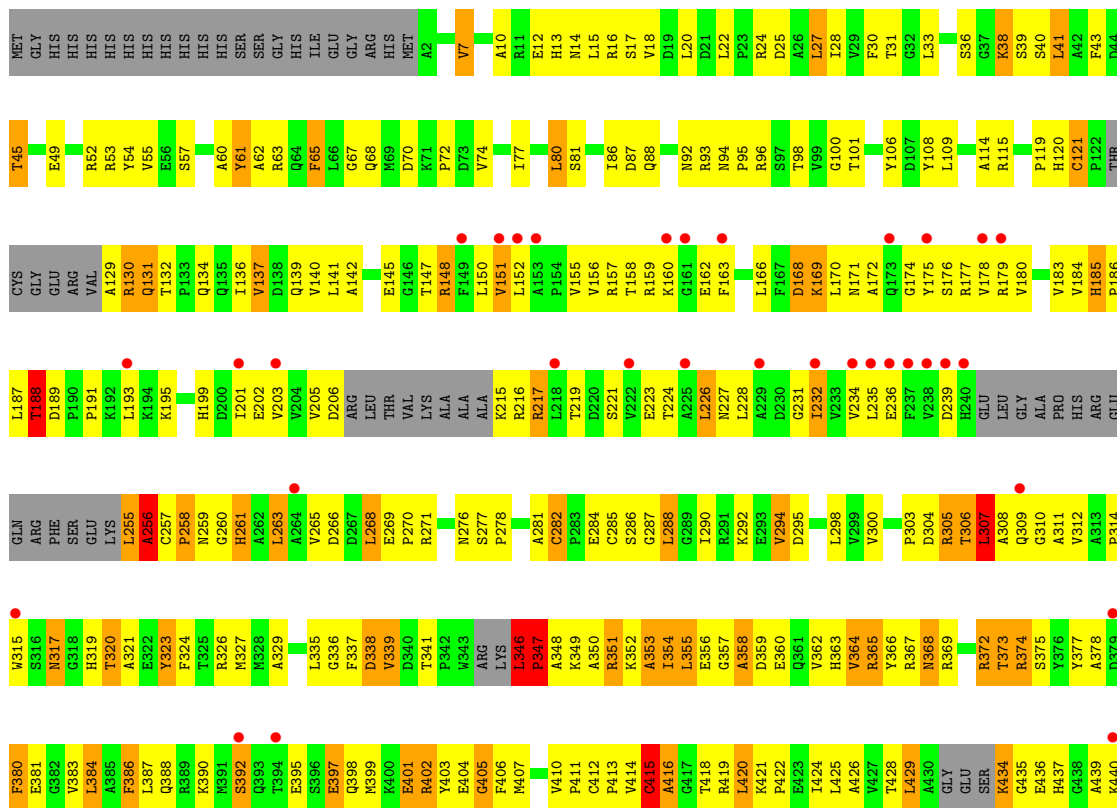


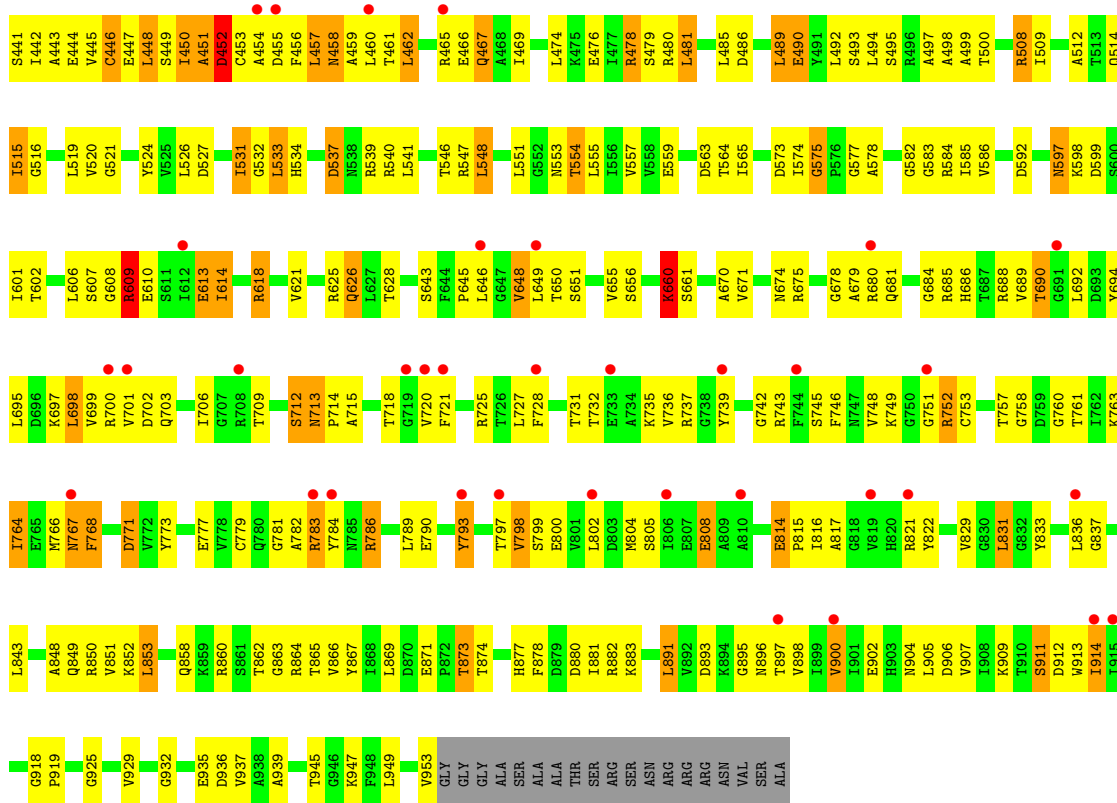
• Molecule 1: UVRABC SYSTEM PROTEIN A



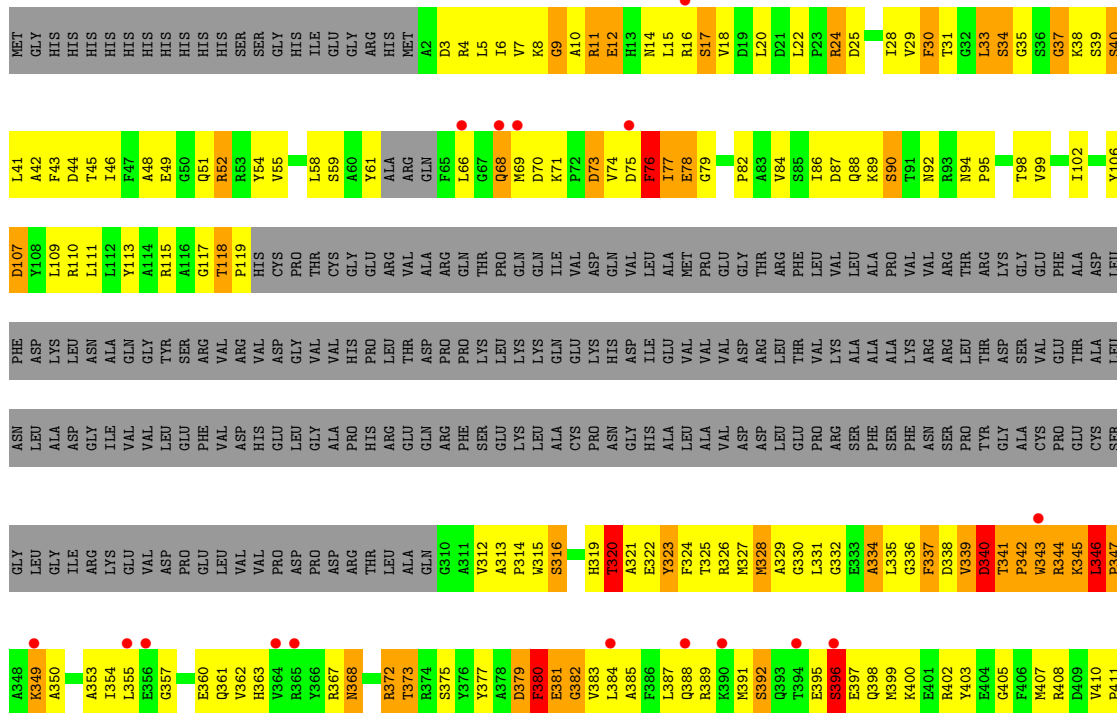


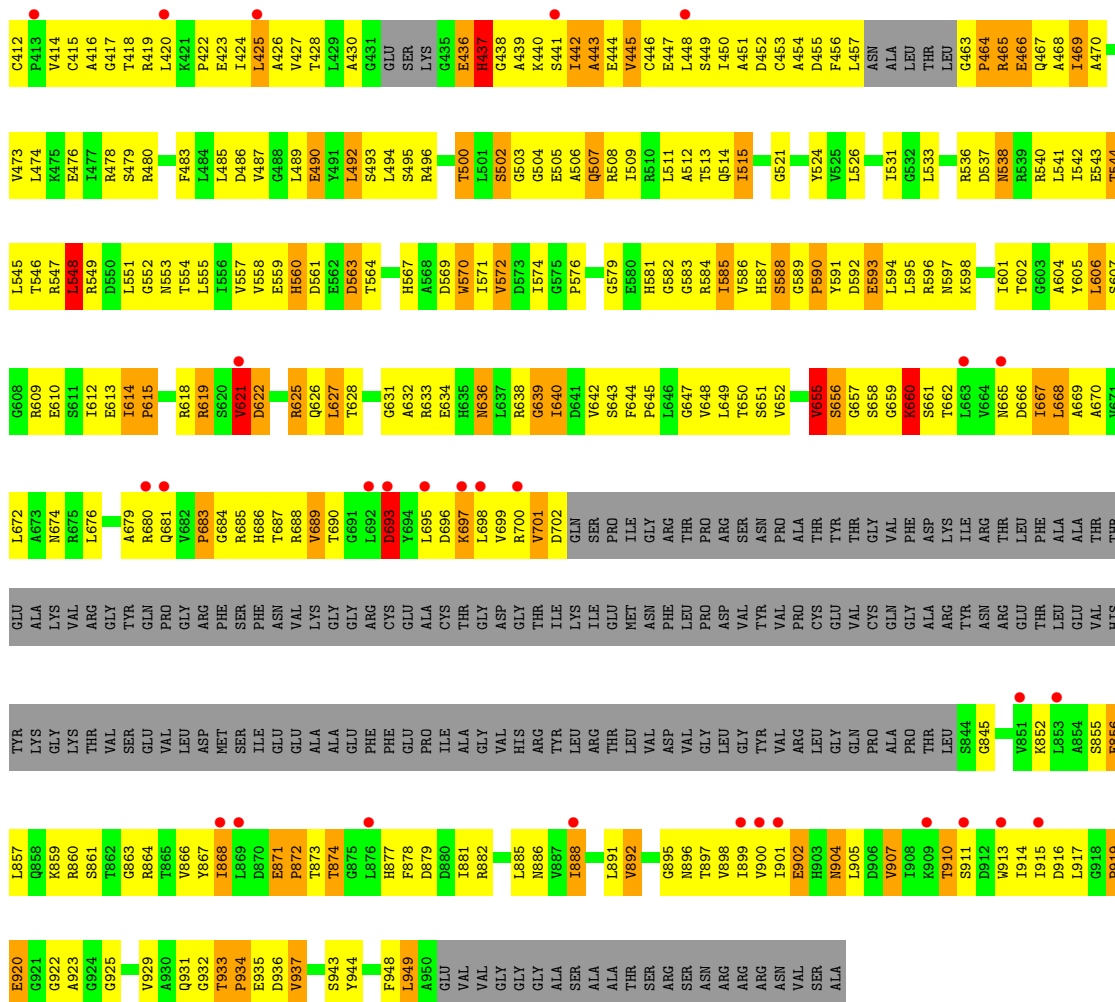
● Molecule 1: UVRABC SYSTEM PROTEIN A





● Molecule 1: UVRABC SYSTEM PROTEIN A





4 Data and refinement statistics i

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 84.52 – 3.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-3.40) 98.5 (84.52-3.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 3.41Å)	Xtrriage
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	Xtrriage
Anisotropy	0.229	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 69.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.034 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	39998	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

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	0.72	5/7394 (0.1%)	0.95	28/10021 (0.3%)
1	B	0.71	3/7190 (0.0%)	0.87	20/9741 (0.2%)
1	C	0.70	2/6945 (0.0%)	0.87	17/9406 (0.2%)
1	D	0.77	6/7217 (0.1%)	0.87	12/9779 (0.1%)
1	E	0.73	2/7196 (0.0%)	0.91	19/9753 (0.2%)
1	F	0.68	2/4721 (0.0%)	0.92	11/6385 (0.2%)
All	All	0.72	20/40663 (0.0%)	0.90	107/55085 (0.2%)

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 (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	256	ALA	C-N	-13.62	1.02	1.34
1	D	124	CYS	C-N	12.92	1.56	1.33
1	D	126	GLU	C-N	-11.61	1.07	1.34
1	B	120	HIS	C-N	-11.33	1.07	1.34
1	A	415	CYS	C-N	11.23	1.59	1.34
1	A	411	PRO	C-N	-9.89	1.11	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	11	ARG	C-N	9.87	1.56	1.34
1	D	123	THR	C-N	8.38	1.53	1.34
1	B	261	HIS	C-N	8.28	1.53	1.34
1	A	11	ARG	C-N	-8.08	1.15	1.34
1	B	412	CYS	C-N	6.53	1.46	1.34
1	A	660	LYS	CE-NZ	-6.46	1.32	1.49
1	D	260	GLY	C-N	-6.44	1.19	1.34
1	D	215	LYS	CE-NZ	5.63	1.63	1.49
1	C	285	CYS	C-N	-5.47	1.21	1.34
1	A	414	VAL	C-N	-5.42	1.21	1.34
1	C	566	GLU	CG-CD	5.38	1.60	1.51
1	E	660	LYS	CE-NZ	-5.38	1.35	1.49
1	F	341	THR	CA-CB	5.10	1.66	1.53
1	E	779	CYS	CB-SG	-5.03	1.73	1.81

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	478	ARG	NE-CZ-NH1	17.05	128.83	120.30
1	A	478	ARG	NE-CZ-NH2	-16.13	112.23	120.30
1	A	752	ARG	NE-CZ-NH2	-14.18	113.21	120.30
1	A	752	ARG	NE-CZ-NH1	13.59	127.09	120.30
1	E	307	LEU	CB-CA-C	-12.39	86.66	110.20
1	B	261	HIS	O-C-N	11.58	141.23	122.70
1	D	147	THR	N-CA-C	11.31	141.53	111.00
1	F	11	ARG	C-N-CA	10.99	149.19	121.70
1	C	285	CYS	O-C-N	10.28	139.14	122.70
1	A	228	LEU	CA-CB-CG	10.05	138.41	115.30
1	E	151	VAL	N-CA-C	9.92	137.79	111.00
1	C	285	CYS	CA-C-N	-9.37	96.58	117.20
1	B	261	HIS	CA-C-N	-9.33	96.68	117.20
1	A	692	LEU	CA-CB-CG	8.82	135.60	115.30
1	D	380	PHE	N-CA-CB	-8.82	94.72	110.60
1	C	130	ARG	N-CA-C	8.78	134.71	111.00
1	A	373	THR	N-CA-C	8.72	134.56	111.00
1	F	11	ARG	O-C-N	-8.55	109.02	122.70
1	B	143	MET	C-N-CD	-8.51	101.89	120.60
1	B	374	ARG	CB-CA-C	8.48	127.35	110.40
1	F	621	VAL	CB-CA-C	-8.41	95.43	111.40
1	A	415	CYS	O-C-N	8.39	136.13	122.70
1	A	374	ARG	N-CA-CB	8.26	125.46	110.60
1	B	360	GLU	CB-CA-C	8.23	126.86	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	285	CYS	C-N-CA	-8.16	101.30	121.70
1	F	622	ASP	N-CA-C	8.10	132.88	111.00
1	E	355	LEU	CA-CB-CG	8.09	133.91	115.30
1	E	354	ILE	CB-CA-C	-8.04	95.51	111.60
1	B	443	ALA	N-CA-C	7.86	132.23	111.00
1	D	13	HIS	N-CA-CB	7.70	124.47	110.60
1	B	193	LEU	CB-CA-C	-7.61	95.74	110.20
1	A	11	ARG	O-C-N	-7.55	110.61	122.70
1	E	13	HIS	N-CA-CB	7.49	124.08	110.60
1	A	478	ARG	CD-NE-CZ	7.37	133.92	123.60
1	E	151	VAL	CB-CA-C	-7.36	97.42	111.40
1	D	300	VAL	C-N-CD	-7.30	104.55	120.60
1	E	415	CYS	O-C-N	-7.28	111.06	122.70
1	C	449	SER	N-CA-C	7.27	130.63	111.00
1	F	622	ASP	N-CA-CB	-7.16	97.71	110.60
1	D	126	GLU	O-C-N	-7.12	111.31	122.70
1	D	166	LEU	CA-CB-CG	6.97	131.34	115.30
1	C	449	SER	N-CA-CB	-6.93	100.11	110.50
1	B	261	HIS	C-N-CA	-6.91	104.43	121.70
1	F	548	LEU	CA-CB-CG	6.75	130.84	115.30
1	B	361	GLN	N-CA-C	-6.75	92.78	111.00
1	A	457	LEU	CA-CB-CG	6.69	130.68	115.30
1	C	457	LEU	CA-CB-CG	6.68	130.68	115.30
1	A	779	CYS	O-C-N	-6.65	112.06	122.70
1	A	436	GLU	N-CA-CB	-6.63	98.66	110.60
1	A	159	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	B	443	ALA	CB-CA-C	-6.49	100.37	110.10
1	A	920	GLU	CB-CA-C	6.42	123.25	110.40
1	D	124	CYS	N-CA-C	6.40	128.28	111.00
1	A	415	CYS	CA-C-N	-6.36	103.22	117.20
1	A	754	GLU	CB-CA-C	-6.33	97.73	110.40
1	C	166	LEU	CA-CB-CG	6.32	129.84	115.30
1	E	255	LEU	CA-CB-CG	6.26	129.69	115.30
1	A	458	ASN	N-CA-C	6.25	127.88	111.00
1	C	190	PRO	C-N-CD	-6.23	106.89	120.60
1	A	411	PRO	O-C-N	-6.21	112.76	122.70
1	C	752	ARG	CB-CG-CD	6.20	127.72	111.60
1	B	166	LEU	CA-CB-CG	6.18	129.51	115.30
1	E	355	LEU	N-CA-CB	6.16	122.71	110.40
1	A	752	ARG	CD-NE-CZ	6.15	132.21	123.60
1	C	437	HIS	CB-CA-C	-6.03	98.34	110.40
1	B	317	ASN	N-CA-C	6.02	127.25	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	317	ASN	N-CA-C	5.96	127.09	111.00
1	C	448	LEU	CA-CB-CG	5.96	129.00	115.30
1	E	307	LEU	CA-CB-CG	5.89	128.86	115.30
1	A	692	LEU	CB-CG-CD1	5.84	120.93	111.00
1	A	12	GLU	O-C-N	-5.83	113.37	122.70
1	D	124	CYS	CA-C-N	-5.83	104.54	116.20
1	B	436	GLU	CB-CA-C	-5.80	98.80	110.40
1	C	767	ASN	N-CA-C	5.79	126.64	111.00
1	A	748	VAL	CG1-CB-CG2	5.77	120.14	110.90
1	C	191	PRO	N-CA-C	5.70	126.92	112.10
1	D	89	LYS	CB-CA-C	-5.66	99.09	110.40
1	E	767	ASN	N-CA-C	5.63	126.19	111.00
1	D	460	LEU	CA-CB-CG	5.62	128.23	115.30
1	F	660	LYS	CD-CE-NZ	5.58	124.53	111.70
1	B	370	TYR	N-CA-C	-5.55	96.01	111.00
1	A	460	LEU	CA-CB-CG	5.53	128.03	115.30
1	A	300	VAL	C-N-CD	-5.52	108.45	120.60
1	B	375	SER	N-CA-CB	5.49	118.74	110.50
1	C	456	PHE	N-CA-C	5.49	125.82	111.00
1	F	11	ARG	CA-C-N	5.46	129.22	117.20
1	D	12	GLU	N-CA-C	5.45	125.72	111.00
1	D	89	LYS	N-CA-C	5.43	125.67	111.00
1	A	780	GLN	C-N-CA	-5.41	110.94	122.30
1	E	256	ALA	N-CA-C	5.40	125.58	111.00
1	E	771	ASP	CB-CG-OD1	5.36	123.12	118.30
1	F	443	ALA	N-CA-C	5.31	125.34	111.00
1	F	346	LEU	CA-CB-CG	5.28	127.43	115.30
1	E	448	LEU	CA-CB-CG	5.23	127.33	115.30
1	B	360	GLU	N-CA-C	-5.23	96.89	111.00
1	C	355	LEU	CA-CB-CG	5.15	127.14	115.30
1	A	14	ASN	N-CA-C	-5.14	97.13	111.00
1	F	437	HIS	CB-CA-C	-5.13	100.14	110.40
1	E	282	CYS	O-C-N	5.09	130.78	121.10
1	C	771	ASP	CB-CG-OD1	5.07	122.86	118.30
1	B	229	ALA	N-CA-C	-5.05	97.37	111.00
1	E	346	LEU	CA-CB-CG	5.04	126.88	115.30
1	B	185	HIS	C-N-CD	-5.03	109.53	120.60
1	E	402	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	B	152	LEU	CA-CB-CG	5.02	126.84	115.30
1	B	319	HIS	CB-CA-C	-5.01	100.37	110.40
1	E	188	THR	CB-CA-C	-5.01	98.07	111.60

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
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	7280	633	1
1	B	7067	0	7080	707	3
1	C	6832	0	6855	556	0
1	D	7095	0	7100	590	0
1	E	7073	0	7081	602	4

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	4650	0	4667	567	1
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
2	E	2	0	0	0	0
All	All	39998	0	40063	3590	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 45.

All (3590) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:183:VAL:HG12	1:D:184:VAL:N	1.47	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: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: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:D:301:PRO:C	1:D:303:PRO:HD3	1.63	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: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:B:428:THR:HB	1:B:435:GLY:C	1.68	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:B:451:ALA:C	1:B:455:ASP:HB2	1.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:LEU:HD21	1:A:352:LYS:HE3	1.12	1.08
1:B:139:GLN:HG2	1:B:143:MET:HE3	1.10	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
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:F:695:LEU:HD22	1:F:864:ARG:C	1.74	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:E:440:LYS:HE3	1:E:455:ASP:OD1	1.54	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:349:LYS:HA	1:D:352:LYS:HZ2	1.24	1.02
1:F:355:LEU:O	1:F:383:VAL:HG11	1.57	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:B:432:GLU:CD	1:B:453:CYS:HB3	1.80	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: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:F:355:LEU:C	1:F:383:VAL:HG11	1.82	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:226:LEU:HD13	1:E:231:GLY:HA2	1.44	0.99
1:D:349:LYS:H	1:D:349:LYS:HD3	1.26	0.98
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:284:GLU:CD	1:C:291:ARG:NH1	2.18	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: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: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: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:295:ASP:CB	1:A:297:GLU:HG3	1.97	0.94
1:A:323:TYR:C	1:A:323:TYR:HD1	1.71	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:305:ARG:C	1:D:311:ALA:HB2	1.89	0.91
1:E:216:ARG:HG2	1:E:216:ARG:O	1.69	0.91
1:B:139:GLN:CG	1:B:143:MET:HE3	2.00	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:A:424:ILE:C	1:A:437:HIS:HE1	1.73	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:HB3	1:F:660:LYS:HZ3	1.35	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:E:65:PHE:CE2	1:E:767:ASN:CG	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:LEU:O	1:A:299:VAL:HG12	1.72	0.90
1:E:351:ARG:NH2	1:E:355:LEU:HD21	1.85	0.89
1:A:323:TYR:C	1:A:323:TYR:CD1	2.43	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:C:203:VAL:HG12	1:C:204:VAL:N	1.88	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:E:65:PHE:CZ	1:E:767:ASN:CG	2.46	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:437:HIS:CD2	1:C:440:LYS:HZ3	1.87	0.87
1:F:440:LYS:O	1:F:445:VAL:CG2	2.22	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: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: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:A:298:LEU:HD12	1:A:298:LEU:C	1.96	0.85
1:E:307:LEU:O	1:E:307:LEU:HG	1.75	0.85
1:E:346:LEU:N	1:E:349:LYS:HZ2	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:184:VAL:HG12	1:B:185:HIS:N	1.91	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:299:VAL:HA	1:B:313:ALA:CB	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:E:444:GLU:CD	1:E:450:ILE:HG13	1.99	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: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:A:298:LEU:C	1:A:299:VAL:HG12	1.99	0.82
1:B:158:THR:HG21	1:B:271:ARG:NH1	1.95	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:A:424:ILE:C	1:A:437:HIS:CE1	2.53	0.81
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:E:49:GLU:CD	1:E:52:ARG:HH12	1.84	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: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
1:B:273:PHE:CD1	1:B:437:HIS:ND1	2.48	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:323:TYR:HD1	1:B:323:TYR:C	1.84	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:B:346:LEU:HA	1:B:349:LYS:HZ1	1.43	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: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:304:ASP:CG	1:D:306:THR:HG23	2.01	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
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:E:88:GLN:CD	1:E:531:ILE:HG21	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:448:LEU:HD23	1:F:448:LEU:C	2.03	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:668:LEU:HD13	1:A:668:LEU:C	2.01	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:D:306:THR:C	1:D:307:LEU:CD1	2.51	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
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:D:918:GLY:C	1:D:925:GLY:HA2	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:404:GLU:HG2	1:E:407:MET:HE1	1.65	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:B:428:THR:CB	1:B:435:GLY:C	2.46	0.78
1:C:49:GLU:CD	1:C:52:ARG:HH12	1.86	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: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:49:GLU:CD	1:B:52:ARG:HH12	1.86	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:D:49:GLU:CD	1:D:52:ARG:HH12	1.88	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:284:GLU:CD	1:C:291:ARG:HH12	1.83	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:C:767:ASN:C	1:C:767:ASN:HD22	1.87	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:C:361:GLN:HB3	1:C:378:ALA:C	2.05	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:A:442:ILE:HG22	1:A:495:SER:CA	2.15	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:B:382:GLY:C	1:B:383:VAL:HG13	2.05	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:448:LEU:HD23	1:A:448:LEU:C	2.05	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: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: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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:391:MET:HE3	1:A:394:THR:CG2	2.17	0.74
1:D:446:CYS:SG	1:D:449:SER:OG	2.45	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: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
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:B:323:TYR:C	1:B:323:TYR:CD1	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:C:918:GLY:C	1:C:925:GLY:HA2	2.08	0.73
1:E:882:ARG:HH22	1:E:883:LYS:HE2	1.53	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
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:A:391:MET:HE3	1:A:394:THR:HG21	1.69	0.72
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: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:F:856:GLU:HG2	1:F:867:TYR:HH	1.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:220:ASP:C	1:C:222:VAL:H	1.93	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:D:306:THR:C	1:D:307:LEU:HD12	2.11	0.72
1:F:337:PHE:HZ	1:F:347:PRO:HA	1.54	0.72
1:B:920:GLU:C	1:B:924:GLY:O	2.28	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:E:442:ILE:C	1:E:495:SER:HG	1.89	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
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:C:441:SER:C	1:C:444:GLU:HG2	2.11	0.71
1:D:96:ARG:HB2	1:D:276:ASN:OD1	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:VAL:HB	1:D:201:ILE:H	1.55	0.71
1:F:440:LYS:C	1:F:445:VAL:HG23	2.10	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: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
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:B:752:ARG:HH21	1:D:165:ASP:CG	1.94	0.71
1:D:338:ASP:C	1:D:339:VAL:HG12	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:68:GLN:C	1:F:68:GLN:OE1	2.30	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:A:576:PRO:HD3	1:A:586:VAL:HG21	1.73	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:418:THR:O	1:F:419:ARG:HB2	1.89	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:885:LEU:HD13	1:F:885:LEU:C	2.11	0.70
1:B:364:VAL:HG21	1:B:379:ASP:OD2	1.91	0.70
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:A:226:LEU:HD22	1:A:231:GLY:C	2.12	0.69
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:F:75:ASP:O	1:F:76:PHE:C	2.28	0.69
1:A:297:GLU:OE1	1:A:297:GLU:C	2.30	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:E:442:ILE:C	1:E:495:SER:CB	2.61	0.69
1:E:442:ILE:C	1:E:495:SER:HB3	2.13	0.69
1:F:344:ARG:C	1:F:346:LEU:H	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:767:ASN:C	1:C:767:ASN:ND2	2.44	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:A:49:GLU:CD	1:A:52:ARG:HH12	1.95	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
1:D:308:ALA:O	1:D:309:GLN:HB2	1.92	0.68
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:E:285:CYS:O	1:E:286:SER:HB2	1.95	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:301:PRO:C	1:D:303:PRO:CD	2.53	0.67
1:D:614:ILE:H	1:D:614:ILE:HD12	1.60	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: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:439:ALA:C	1:F:440:LYS:HD2	2.15	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: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:319:HIS:C	1:F:321:ALA:H	1.98	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:777:GLU:CD	1:D:160:LYS:HZ2	1.97	0.65
1:C:453:CYS:C	1:C:455:ASP:H	1.98	0.65
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:307:LEU:HD12	1:D:307:LEU:N	2.11	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: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:C:422:PRO:HB2	1:C:423:GLU:CD	2.18	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:404:GLU:HA	1:A:407:MET:CE	2.27	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:439:ALA:HA	1:E:443:ALA:HB3	1.78	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:C:508:ARG:HG3	1:C:508:ARG:NH1	2.00	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: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:E:918:GLY:C	1:E:925:GLY:HA2	2.16	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:E:284:GLU:CG	1:E:414:VAL:HG11	2.26	0.64
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:360:GLU:O	1:C:361:GLN:CD	2.37	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:N	1:A:346:LEU:HD12	2.12	0.63
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:C:386:PHE:C	1:C:388:GLN:H	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:306:THR:O	1:D:307:LEU:CD1	2.47	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:GLU:CD	1:A:298:LEU:N	2.51	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:61:TYR:HH	1:A:65:PHE:HD2	1.48	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:A:145:GLU:CD	1:A:145:GLU:H	2.03	0.61
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:323:TYR:CD1	1:F:323:TYR:C	2.74	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: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
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:B:391:MET:HE1	1:B:395:GLU:HB2	1.82	0.61
1:B:418:THR:C	1:B:419:ARG:HG3	2.20	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:281:ALA:HB1	1:C:287:GLY:CA	2.31	0.60
1:D:291:ARG:CD	1:D:413:PRO:HD2	2.30	0.60
1:D:712:SER:O	1:D:713:ASN:HB3	2.01	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:C:858:GLN:HG3	1:C:858:GLN:O	2.02	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: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:A:345:LYS:C	1:A:346:LEU:HD12	2.22	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
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:882:ARG:NH1	1:F:886:ASN:CG	2.52	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:B:918:GLY:C	1:B:925:GLY:HA2	2.22	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: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:219:THR:HG23	1:C:220:ASP:OD1	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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: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: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:448:LEU:C	1:F:448:LEU:CD2	2.70	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:668:LEU:C	1:A:668:LEU:CD1	2.72	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:767:ASN:O	1:D:61:TYR:HE2	1.86	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:323:TYR:C	1:D:323:TYR:HD1	2.05	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:A:441:SER:C	1:A:444:GLU:HG2	2.22	0.58
1:B:61:TYR:HH	1:B:65:PHE:HD2	1.51	0.58
1:B:215:LYS:CA	1:B:215:LYS:CE	2.69	0.58
1:D:306:THR:C	1:D:307:LEU:HD13	2.22	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:304:ASP:C	1:A:305:ARG:HG2	2.23	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:B:347:PRO:HD2	1:B:349:LYS:HZ1	1.68	0.58
1:C:442:ILE:CG2	1:C:495:SER:N	2.66	0.58
1:F:444:GLU:OE1	1:F:444:GLU:N	2.37	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: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:712:SER:O	1:E:713:ASN:HB3	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:375:SER:C	1:B:377:TYR:H	2.07	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:A:448:LEU:C	1:A:448:LEU:CD2	2.72	0.58
1:C:119:PRO:HB2	1:C:128:VAL:HG22	1.85	0.58
1:C:312:VAL:C	1:C:314:PRO:HD2	2.23	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: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:323:TYR:CD1	1:E:323:TYR:C	2.76	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:A:456:PHE:C	1:A:458:ASN:N	2.58	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:319:HIS:C	1:F:321:ALA:N	2.58	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: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:578:ALA:HB1	1:E:833:TYR:CB	2.33	0.57
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:F:857:LEU:C	1:F:857:LEU:HD13	2.24	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:E:444:GLU:CD	1:E:450:ILE:CG1	2.72	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:A:918:GLY:C	1:A:925:GLY:HA2	2.25	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: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:378:ALA:C	1:A:380:PHE:H	2.08	0.57
1:A:528:GLU:HG2	1:A:531:ILE:HG13	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:203:VAL:O	1:C:204:VAL:HB	2.05	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:323:TYR:C	1:D:323:TYR:CD1	2.77	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
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: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:503:GLY:O	1:F:504:GLY:C	2.43	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:C:359:ASP:O	1:C:360:GLU:CD	2.44	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:187:LEU:C	1:E:189:ASP:H	2.09	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: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
1:B:902:GLU:HG3	1:B:907:VAL:HG11	1.87	0.55
1:C:284:GLU:CD	1:C:291:ARG:HH11	2.00	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:442:ILE:HG23	1:B:494:LEU:HB3	1.88	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:E:597:ASN:HD22	1:E:597:ASN:C	2.10	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:439:ALA:O	1:E:443:ALA:C	2.45	0.55
1:E:727:LEU:HD11	1:E:816:ILE:HG12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:119:PRO:C	1:E:120:HIS:CD2	2.80	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:D:793:TYR:CD1	1:D:793:TYR:C	2.79	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
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:12:GLU:CD	1:F:73:ASP:HB2	2.27	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: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:A:404:GLU:HA	1:A:407:MET:HE3	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:359:ASP:C	1:C:360:GLU:HG2	2.27	0.55
1:C:793:TYR:CD1	1:C:793:TYR:C	2.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:143:MET:O	1:C:144:PRO:C	2.44	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:D:893:ASP:C	1:D:895:GLY:H	2.10	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
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:379:ASP:O	1:C:380:PHE:C	2.45	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:A:391:MET:HE3	1:A:394:THR:CB	2.37	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:444:GLU:OE1	1:C:444:GLU:CA	2.47	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:443:ALA:C	1:F:444:GLU:OE1	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:VAL:O	1:C:226:LEU:CD2	2.49	0.54
1:C:444:GLU:CD	1:C:449:SER:OG	2.46	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: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:11:ARG:HH12	1:F:75:ASP:CG	2.08	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:220:ASP:C	1:C:222:VAL:N	2.61	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
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:27:LEU:C	1:B:27:LEU:CD2	2.76	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: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:A:764:ILE:HG23	1:A:764:ILE:O	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:352:LYS:C	1:E:354:ILE:H	2.11	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:126:GLU:O	1:A:127:ARG:C	2.44	0.54
1:A:456:PHE:C	1:A:458:ASN:H	2.10	0.54
1:B:561:ASP:OD1	1:B:562:GLU:N	2.41	0.54
1:B:793:TYR:C	1:B:793:TYR:CD1	2.82	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: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:E:304:ASP:HB2	1:E:305:ARG:NH1	2.23	0.53
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: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: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:576:PRO:CD	1:A:586:VAL:HG23	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:453:CYS:C	1:C:455:ASP:N	2.61	0.53
1:D:445:VAL:HA	1:D:493:SER:CB	2.39	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
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:296:PRO:C	1:D:299:VAL:HG22	2.29	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:E:793:TYR:C	1:E:793:TYR:CD1	2.81	0.53
1:F:604:ALA:HA	1:F:609:ARG:HD2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
1:D:305:ARG:HD3	1:D:311:ALA:CB	1.99	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:447:GLU:O	1:E:448:LEU:C	2.47	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:356:GLU:H	1:C:383:VAL:HG13	1.72	0.52
1:C:893:ASP:C	1:C:895:GLY:H	2.12	0.52
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:27:LEU:C	1:D:27:LEU:CD2	2.78	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:341:THR:O	1:D:342:PRO:C	2.48	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
1:A:170:LEU:O	1:A:175:TYR:HD1	1.92	0.52
1:A:391:MET:HE3	1:A:394:THR:HB	1.91	0.52
1:A:893:ASP:C	1:A:895:GLY:H	2.14	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:B:139:GLN:C	1:B:143:MET:CG	2.77	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:885:LEU:C	1:F:885:LEU:CD1	2.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:782:ALA:O	1:E:783:ARG:HB2	2.10	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:D:304:ASP:CG	1:D:306:THR:CG2	2.76	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
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: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:F:344:ARG:C	1:F:346:LEU:N	2.63	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:415:CYS:C	1:D:417:GLY:H	2.13	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:F:457:LEU:C	1:F:457:LEU:HD13	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:391:MET:HE2	1:A:394:THR:HB	1.93	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: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
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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:453:CYS:O	1:F:454:ALA:C	2.48	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: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:A:304:ASP:C	1:A:305:ARG:CG	2.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:754:GLU:H	1:A:754:GLU:CD	2.15	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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:407:MET:HE3	1:C:407:MET:H	1.76	0.50
1:C:425:LEU:HD21	1:C:439:ALA:CB	2.38	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: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:A:404:GLU:HA	1:A:407:MET:HE2	1.91	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: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:437:HIS:HB2	1:F:442:ILE:H	1.77	0.50
1:F:873:THR:O	1:F:874:THR:C	2.49	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:C:27:LEU:C	1:C:27:LEU:CD2	2.81	0.49
1:C:514:GLN:O	1:C:515:ILE:C	2.50	0.49
1:C:625:ARG:NE	1:C:694:TYR:HE2	2.10	0.49
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:793:TYR:CD1	1:A:793:TYR:C	2.86	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:C:360:GLU:C	1:C:361:GLN:CD	2.71	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:D:145:GLU:CD	1:D:148:ARG:HB2	2.32	0.49
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:151:VAL:O	1:C:204:VAL:C	2.50	0.49
1:C:154:PRO:HD2	1:C:229:ALA:CB	2.43	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:D:307:LEU:CD1	1:D:307:LEU:N	2.76	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:670:ALA:HA	1:B:681:GLN:HE21	1.77	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:441:SER:C	1:E:495:SER:HB3	2.32	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: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: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:444:GLU:CD	1:C:449:SER:HG	2.14	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: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:139:GLN:C	1:B:143:MET:HG2	2.33	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:355:LEU:C	1:E:383:VAL:HG13	2.33	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: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: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:D:597:ASN:HD22	1:D:597:ASN:C	2.17	0.48
1:E:372:ARG:HG3	1:E:374:ARG:HG3	1.94	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:B:702:ASP:HB3	1:B:852:LYS:HZ3	1.78	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:514:GLN:OE1	1:D:514:GLN:HA	2.12	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: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
1:D:368:ASN:C	1:D:370:TYR:N	2.63	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:THR:HG22	1:C:74:VAL:HG13	1.96	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:384:LEU:HD12	1:D:384:LEU:C	2.33	0.48
1:D:913:TRP:CZ3	1:D:932:GLY:HA2	2.48	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:579:GLY:O	1:A:580:GLU:C	2.51	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: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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:614:ILE:O	1:F:615:PRO:C	2.52	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:412:CYS:C	1:E:415:CYS:SG	2.91	0.48
1:E:456:PHE:O	1:E:459:ALA:N	2.47	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:139:GLN:HG2	1:B:143:MET:HE2	1.81	0.47
1:B:441:SER:HB3	1:B:454:ALA:HB2	1.95	0.47
1:C:323:TYR:CD1	1:C:323:TYR:C	2.87	0.47
1:C:400:LYS:HD3	1:C:400:LYS:C	2.34	0.47
1:C:460:LEU:O	1:C:461:THR:C	2.51	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
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: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:F:905:LEU:HD21	1:F:948:PHE:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:VAL:CG1	1:A:585:ILE:HD12	2.44	0.47
1:A:456:PHE:O	1:A:457:LEU:C	2.53	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: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: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:360:GLU:C	1:C:361:GLN:OE1	2.53	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
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:E:406:PHE:CE2	1:E:680:ARG:CD	2.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:661:SER:OG	1:F:665:ASN:HB2	2.15	0.47
1:A:7:VAL:O	1:A:19:ASP:HA	2.14	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:125:GLY:O	1:B:126:GLU:C	2.53	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
1:F:545:LEU:O	1:F:546:THR:C	2.53	0.47
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:584:ARG:HD3	1:C:584:ARG:CD	2.45	0.47
1:C:390:LYS:C	1:C:391:MET:CG	2.83	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: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: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:C:713:ASN:O	1:C:714:PRO:C	2.53	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:515:ILE:HB	1:F:548:LEU:HG	1.97	0.47
1:F:604:ALA:O	1:F:607:SER:OG	2.33	0.47
1:A:106:TYR:CD1	1:A:442:ILE:CD1	2.98	0.46
1:A:297:GLU:O	1:A:298:LEU:C	2.50	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:C:322:GLU:O	1:C:323:TYR:C	2.52	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:27:LEU:C	1:A:27:LEU:CD2	2.83	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
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:305:ARG:O	1:D:311:ALA:HB2	2.15	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: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:C:811:GLU:OE2	1:C:814:GLU:OE1	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:384:LEU:C	1:C:386:PHE:H	2.18	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:B:298:LEU:C	1:B:299:VAL:HG12	2.36	0.46
1:C:295:ASP:H	1:C:407:MET:HA	1.80	0.46
1:E:350:ALA:O	1:E:354:ILE:CG1	2.63	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
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:E:893:ASP:C	1:E:895:GLY:H	2.18	0.46
1:F:115:ARG:NH1	1:F:469:ILE:O	2.49	0.46
1:F:414:VAL:HG23	1:F:415:CYS:N	2.31	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:933:THR:C	1:F:935:GLU:N	2.68	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:368:ASN:C	1:C:370:TYR:H	2.19	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
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: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: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:160:LYS:HZ2	1:E:777:GLU:HG3	1.81	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: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: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:585:ILE:H	1:F:585:ILE:HG12	1.59	0.46
1:A:119:PRO:C	1:A:120:HIS:CD2	2.89	0.46
1:A:134:GLN:O	1:A:137:VAL:HG12	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:27:LEU:CD2	1:E:27:LEU:C	2.84	0.46
1:E:420:LEU:HB2	1:E:425:LEU:HD21	1.97	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
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: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:315:TRP:HE3	1:F:328:MET:CE	2.29	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: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:444:GLU:O	1:D:445:VAL:C	2.55	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:352:LYS:C	1:E:354:ILE:N	2.69	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:O	1:A:455:ASP:OD1	2.35	0.45
1:A:534:HIS:HA	1:A:903:HIS:ND1	2.31	0.45
1:A:619:ARG:HB2	1:A:912:ASP:CG	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:LEU:O	1:B:36:SER:HB2	2.16	0.45
1:C:386:PHE:C	1:C:388:GLN:N	2.68	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: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
1:F:422:PRO:HA	1:F:425:LEU:HB2	1.98	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:C:514:GLN:HA	1:C:514:GLN:OE1	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:E:307:LEU:HD23	1:E:307:LEU:C	2.37	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:597:ASN:HD22	1:B:597:ASN:C	2.20	0.45
1:B:618:ARG:NH2	1:B:934:PRO:HG2	2.31	0.45
1:B:893:ASP:C	1:B:895:GLY:H	2.20	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:E:307:LEU:O	1:E:307:LEU:HD23	2.17	0.45
1:E:404:GLU:C	1:E:406:PHE:H	2.20	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:F:380:PHE:C	1:F:382:GLY:H	2.20	0.45
1:A:18:VAL:CB	1:A:585:ILE:CD1	2.89	0.45
1:A:230:ASP:O	1:A:230:ASP:CG	2.55	0.45
1:A:300:VAL:CG1	1:A:303:PRO:HG2	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:295:ASP:C	1:C:297:GLU:H	2.20	0.45
1:C:297:GLU:HG2	1:C:297:GLU:O	2.16	0.45
1:C:363:HIS:HB3	1:C:377:TYR:C	2.37	0.45
1:C:456:PHE:O	1:C:460:LEU:HD23	2.16	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: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: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: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: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: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:E:699:VAL:HG21	1:E:867:TYR:CE1	2.52	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
1:A:574:ILE:O	1:A:575:GLY:C	2.56	0.45
1:A:804:MET:HE3	1:A:808:GLU:OE1	2.17	0.45
1:B:134:GLN:O	1:B:137:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:GLU:CD	1:B:440:LYS:HE3	2.37	0.45
1:B:514:GLN:HB3	1:B:524:TYR:CE2	2.51	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:B:432:GLU:HG2	1:B:433:SER:H	1.82	0.45
1:C:368:ASN:C	1:C:370:TYR:N	2.70	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:444:GLU:HG2	1:E:450:ILE:CD1	2.41	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: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
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:B:147:THR:HG22	1:B:148:ARG:H	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:275:PHE:HB3	1:C:420:LEU:HG	1.99	0.44
1:C:356:GLU:CG	1:C:357:GLY:N	2.81	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:27:LEU:C	1:D:27:LEU:HD23	2.37	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: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:C:318:GLY:C	1:C:320:THR:H	2.19	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:528:GLU:HB3	1:A:531:ILE:CD1	2.48	0.44
1:B:109:LEU:HG	1:B:442:ILE:HD11	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:215:LYS:C	1:E:217:ARG:H	2.20	0.44
1:E:269:GLU:O	1:E:271:ARG:N	2.50	0.44
1:E:914:ILE:HG13	1:E:937:VAL:HG21	2.00	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:A:298:LEU:C	1:A:298:LEU:CD1	2.68	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: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:269:GLU:O	1:E:270:PRO:C	2.56	0.44
1:E:877:HIS:O	1:E:881:ILE:HG12	2.17	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:A:597:ASN:HD22	1:A:597:ASN:C	2.21	0.44
1:C:152:LEU:HD23	1:C:202:GLU:HB3	1.99	0.44
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:145:GLU:CD	1:A:145:GLU:N	2.71	0.44
1:A:324:PHE:O	1:A:328:MET:HG2	2.17	0.44
1:B:171:ASN:CG	1:B:187:LEU:HG	2.37	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:C:22:LEU:HB3	1:C:28:ILE:CD1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:TYR:HE1	1:C:327:MET:HE1	1.83	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:E:440:LYS:HA	1:E:444:GLU:OE1	2.17	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:314:PRO:C	1:B:316:SER:H	2.21	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: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: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:E:608:GLY:C	1:E:610:GLU:N	2.71	0.44
1:F:15:LEU:HD12	1:F:15:LEU:C	2.37	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
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: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:385:ALA:C	1:C:388:GLN:HG2	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:702:ASP:HB3	1:C:852:LYS:HZ3	1.83	0.43
1:C:802:LEU:HG	1:C:837:GLY:HA3	2.00	0.43
1:D:16:ARG:O	1:D:17:SER:C	2.56	0.43
1:E:65:PHE:O	1:E:65:PHE:HD1	2.01	0.43
1:E:395:GLU:HG2	1:E:399:MET:HG2	2.00	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: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: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
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:B:873:THR:HB	1:B:902:GLU:CD	2.39	0.43
1:C:390:LYS:C	1:C:391:MET:HG3	2.38	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: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:315:TRP:HE3	1:F:328:MET:HE1	1.83	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:351:ARG:HG3	1:A:355:LEU:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:GLU:OE1	1:A:432:GLU:HA	2.17	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:391:MET:N	1:C:394:THR:H	2.15	0.43
1:C:597:ASN:HD22	1:C:597:ASN:C	2.22	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
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:F:638:ARG:O	1:F:639:GLY:C	2.56	0.43
1:B:20:LEU:HD23	1:B:20:LEU:HA	1.88	0.43
1:B:441:SER:C	1:B:445:VAL:CG2	2.87	0.43
1:C:16:ARG:O	1:C:17:SER:C	2.57	0.43
1:C:290:ILE:O	1:C:291:ARG:HG2	2.19	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:C:793:TYR:C	1:C:793:TYR:HD1	2.22	0.43
1:D:109:LEU:HD13	1:D:109:LEU:HA	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:749:LYS:HZ2	1:D:168:ASP:HB3	1.82	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:E:456:PHE:O	1:E:457:LEU:C	2.56	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: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:B:375:SER:C	1:B:377:TYR:N	2.70	0.43
1:C:216:ARG:O	1:C:219:THR:HG22	2.18	0.43
1:C:445:VAL:C	1:C:447:GLU:N	2.71	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:F:40:SER:O	1:F:45:THR:N	2.44	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:D:65:PHE:O	1:D:65:PHE:HD1	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:742:GLY:O	1:D:748:VAL:HG21	2.18	0.43
1:E:411:PRO:O	1:E:412:CYS:C	2.53	0.43
1:E:575:GLY:O	1:E:582:GLY:CA	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:E:441:SER:O	1:E:494:LEU:C	2.55	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:113:TYR:C	1:F:115:ARG:H	2.23	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:857:LEU:C	1:F:857:LEU:CD1	2.88	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:608:GLY:C	1:A:610:GLU:N	2.72	0.42
1:B:149:PHE:C	1:B:149:PHE:CD1	2.92	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:793:TYR:C	1:E:793:TYR:HD1	2.23	0.42
1:E:829:VAL:HG22	1:E:853:LEU:HD12	1.99	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:A:271:ARG:C	1:A:273:PHE:H	2.22	0.42
1:B:630:VAL:O	1:B:687:THR:HB	2.19	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:108:TYR:CZ	1:E:476:GLU:HG2	2.55	0.42
1:E:497:ALA:O	1:E:498:ALA:C	2.57	0.42
1:E:548:LEU:HD22	1:E:553:ASN:HD22	1.83	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:415:CYS:O	1:E:416:ALA:CB	2.67	0.42
1:E:514:GLN:O	1:E:515:ILE:C	2.58	0.42
1:F:31:THR:HA	1:F:38:LYS:HZ3	1.83	0.42
1:A:65:PHE:O	1:A:65:PHE:CD1	2.73	0.42
1:A:157:ARG:HH22	1:A:267:ASP:CG	2.23	0.42
1:A:597:ASN:HD22	1:A:598:LYS:N	2.17	0.42
1:B:372:ARG:O	1:B:372:ARG:HD2	2.19	0.42
1:B:430:ALA:HB1	1:B:432:GLU:O	2.19	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:D:608:GLY:C	1:D:610:GLU:N	2.72	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:131:GLN:NE2	1:B:256:ALA:CB	2.66	0.42
1:C:486:ASP:O	1:C:540:ARG:NH2	2.52	0.42
1:D:497:ALA:O	1:D:498:ALA:C	2.58	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:65:PHE:O	1:A:766:MET:HE1	2.20	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
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:362:VAL:HG12	1:C:363:HIS:N	2.34	0.42
1:C:597:ASN:HD22	1:C:598:LYS:N	2.17	0.42
1:D:404:GLU:C	1:D:406:PHE:H	2.23	0.42
1:F:339:VAL:HG23	1:F:345:LYS:HZ3	1.84	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:343:TRP:C	1:B:343:TRP:CE3	2.93	0.42
1:B:345:LYS:O	1:B:346:LEU:HG	2.20	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:A:873:THR:HB	1:A:902:GLU:CD	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:514:GLN:O	1:D:515:ILE:C	2.57	0.42
1:E:323:TYR:C	1:E:323:TYR:HD1	2.22	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:425:LEU:C	1:A:437:HIS:ND1	2.72	0.42
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:702:ASP:HB3	1:D:852:LYS:HZ3	1.85	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: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:61:TYR:OH	1:B:65:PHE:HD2	2.03	0.41
1:B:109:LEU:HD13	1:B:109:LEU:HA	1.82	0.41
1:B:215:LYS:C	1:B:217:ARG:N	2.73	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:D:132:THR:O	1:D:136:ILE:HG13	2.20	0.41
1:D:194:LYS:O	1:D:195:LYS:C	2.59	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:626:GLN:HE21	1:E:643:SER:HB3	1.85	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:763:LYS:HD3	1:B:773:TYR:CZ	2.55	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:10:ALA:C	1:F:15:LEU:CD1	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:543:GLU:HG3	1:F:547:ARG:HH21	1.81	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:397:GLU:C	1:C:399:MET:H	2.24	0.41
1:C:493:SER:HG	1:C:495:SER:H	1.68	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
1:C:713:ASN:HB2	1:C:714:PRO:HD2	2.01	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: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:467:GLN:O	1:F:468:ALA:C	2.58	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:A:747:ASN:C	1:A:752:ARG:HH11	2.24	0.41
1:B:351:ARG:HD2	1:B:352:LYS:HZ2	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:271:ARG:NH2	1:C:279:TYR:CZ	2.88	0.41
1:C:403:TYR:O	1:C:404:GLU:C	2.59	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:187:LEU:C	1:E:189:ASP:N	2.74	0.41
1:E:312:VAL:CG1	1:E:384:LEU:HD13	2.47	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
1:A:40:SER:O	1:A:45:THR:OG1	2.38	0.41
1:A:455:ASP:OD1	1:A:455:ASP:C	2.58	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:372:ARG:HD2	1:B:372:ARG:C	2.41	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:D:877:HIS:ND1	1:D:878:PHE:N	2.68	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:110:ARG:O	1:F:111:LEU:C	2.58	0.41
1:F:442:ILE:CG2	1:F:443:ALA:H	2.33	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:317:ASN:CG	1:A:318:GLY:H	2.24	0.41
1:A:459:ALA:HA	1:A:462:LEU:HB2	2.02	0.41
1:B:382:GLY:C	1:B:383:VAL:CG1	2.76	0.41
1:B:447:GLU:HA	1:B:450:ILE:HG21	1.98	0.41
1:B:793:TYR:C	1:B:793:TYR:HD1	2.24	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:55:VAL:C	1:E:57:SER:N	2.73	0.41
1:E:913:TRP:CH2	1:E:932:GLY:HA2	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:322:GLU:O	1:D:323:TYR:C	2.59	0.41
1:D:451:ALA:O	1:D:452:ASP:C	2.56	0.41
1:E:349:LYS:HE2	1:E:349:LYS:HB3	1.87	0.41
1:E:384:LEU:C	1:E:386:PHE:H	2.24	0.41
1:E:421:LYS:O	1:E:424:ILE:HB	2.21	0.41
1:E:450:ILE:O	1:E:451:ALA:C	2.59	0.41
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: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:935:GLU:HG3	1:A:953:VAL:CG1	2.51	0.41
1:B:27:LEU:C	1:B:27:LEU:HD23	2.41	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:383:VAL:CG2	1:B:386:PHE:C	2.89	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: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:418:THR:O	1:D:418:THR:OG1	2.38	0.41
1:D:619:ARG:HB3	1:D:648:VAL:HG23	2.03	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:260:GLY:O	1:E:261:HIS:C	2.59	0.41
1:E:269:GLU:HB3	1:E:270:PRO:CD	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:20:LEU:CD1	1:F:41:LEU:HD11	2.51	0.41
1:F:384:LEU:O	1:F:385:ALA:C	2.59	0.41
1:F:667:ILE:C	1:F:669:ALA:H	2.24	0.41
1:F:871:GLU:HA	1:F:872:PRO:HD2	1.94	0.41
1:F:885:LEU:HD23	1:F:907:VAL:HG22	2.02	0.41
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:339:VAL:O	1:D:339:VAL:HG22	2.20	0.41
1:E:16:ARG:O	1:E:17:SER:C	2.59	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:546:THR:O	1:F:547:ARG:C	2.60	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:364:VAL:HG21	1:B:379:ASP:CG	2.42	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:201:ILE:C	1:C:202:GLU:HG3	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:404:GLU:HA	1:B:407:MET:SD	2.60	0.40
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:318:GLY:C	1:C:320:THR:N	2.74	0.40
1:D:22:LEU:HB3	1:D:28:ILE:HD13	2.02	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:D:756:CYS:O	1:D:757:THR:C	2.59	0.40
1:F:342:PRO:HG2	1:F:345:LYS:HZ3	1.86	0.40
1:F:412:CYS:CA	1:F:415:CYS:SG	3.10	0.40
1:F:440:LYS:C	1:F:445:VAL:CG2	2.81	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:B:920:GLU:OE2	1:B:944:TYR:OH	2.23	0.40
1:C:536:ARG:C	1:C:538:ASN:H	2.24	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:459:ALA:C	1:E:460:LEU:HD22	2.41	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:GLN:NE2	1:A:139:GLN:HE22	2.20	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
1:C:873:THR:HB	1:C:902:GLU:CD	2.42	0.40
1:D:150:LEU:HD22	1:D:236:GLU:CB	2.32	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:E:877:HIS:ND1	1:E:878:PHE:N	2.69	0.40
1:F:16:ARG:O	1:F:17:SER:C	2.60	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:F:856:GLU:CD	1:F:860:ARG:HD2	2.41	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: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:119:PRO:O	1:E:120:HIS:CD2	2.75	0.40
1:E:178:VAL:HG22	1:E:203:VAL:CG1	2.44	0.40
1:E:713:ASN:O	1:E:714:PRO:C	2.60	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:E:905:LEU:O	1:E:906:ASP:C	2.60	0.40
1:F:698:LEU:CD2	1:F:700:ARG:HH11	2.35	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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	940/993 (95%)	814 (87%)	105 (11%)	21 (2%)	6	29
1	B	910/993 (92%)	768 (84%)	112 (12%)	30 (3%)	4	22
1	C	876/993 (88%)	730 (83%)	109 (12%)	37 (4%)	3	18
1	D	911/993 (92%)	758 (83%)	123 (14%)	30 (3%)	4	22
1	E	907/993 (91%)	750 (83%)	128 (14%)	29 (3%)	4	22
1	F	595/993 (60%)	449 (76%)	98 (16%)	48 (8%)	1	5
All	All	5139/5958 (86%)	4269 (83%)	675 (13%)	195 (4%)	3	19

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 [i](#)

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%)	648 (83%)	130 (17%)	2 8
1	B	758/815 (93%)	640 (84%)	118 (16%)	2 11
1	C	732/815 (90%)	594 (81%)	138 (19%)	1 4
1	D	763/815 (94%)	642 (84%)	121 (16%)	2 10
1	E	758/815 (93%)	616 (81%)	142 (19%)	1 5
1	F	492/815 (60%)	386 (78%)	106 (22%)	1 3
All	All	4281/4890 (88%)	3526 (82%)	755 (18%)	2 6

All (755) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	27	LEU

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Mol	Chain	Res	Type
1	A	38	LYS
1	A	39	SER
1	A	41	LEU
1	A	45	THR
1	A	61	TYR
1	A	65	PHE
1	A	70	ASP
1	A	74	VAL
1	A	77	ILE
1	A	80	LEU
1	A	96	ARG
1	A	109	LEU
1	A	111	LEU
1	A	124	CYS
1	A	130	ARG
1	A	137	VAL
1	A	139	GLN
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	198	LYS
1	A	202	GLU
1	A	204	VAL
1	A	208	LEU
1	A	209	THR
1	A	216	ARG
1	A	217	ARG
1	A	218	LEU
1	A	220	ASP
1	A	227	ASN
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

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Mol	Chain	Res	Type
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	293	GLU
1	A	305	ARG
1	A	323	TYR
1	A	328	MET
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	398	GLN
1	A	410	VAL
1	A	414	VAL
1	A	428	THR
1	A	429	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	508	ARG
1	A	533	LEU
1	A	539	ARG
1	A	541	LEU
1	A	546	THR

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Mol	Chain	Res	Type
1	A	548	LEU
1	A	551	LEU
1	A	554	THR
1	A	563	ASP
1	A	597	ASN
1	A	609	ARG
1	A	613	GLU
1	A	614	ILE
1	A	618	ARG
1	A	626	GLN
1	A	648	VAL
1	A	656	SER
1	A	660	LYS
1	A	685	ARG
1	A	688	ARG
1	A	690	THR
1	A	692	LEU
1	A	697	LYS
1	A	698	LEU
1	A	709	THR
1	A	718	THR
1	A	720	VAL
1	A	743	ARG
1	A	756	CYS
1	A	761	THR
1	A	765	GLU
1	A	768	PHE
1	A	771	ASP
1	A	786	ARG
1	A	793	TYR
1	A	798	VAL
1	A	799	SER
1	A	808	GLU
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
1	A	900	VAL
1	A	911	SER

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Mol	Chain	Res	Type
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	65	PHE
1	B	69	MET
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	118	THR
1	B	121	CYS
1	B	134	GLN
1	B	136	ILE
1	B	137	VAL
1	B	147	THR
1	B	148	ARG
1	B	150	LEU
1	B	160	LYS
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	221	SER
1	B	226	LEU
1	B	232	ILE
1	B	235	LEU
1	B	263	LEU
1	B	265	VAL
1	B	267	ASP
1	B	271	ARG

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Mol	Chain	Res	Type
1	B	286	SER
1	B	291	ARG
1	B	292	LYS
1	B	320	THR
1	B	323	TYR
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	402	ARG
1	B	412	CYS
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	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
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	563	ASP
1	B	597	ASN
1	B	609	ARG

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Mol	Chain	Res	Type
1	B	613	GLU
1	B	614	ILE
1	B	618	ARG
1	B	626	GLN
1	B	648	VAL
1	B	656	SER
1	B	660	LYS
1	B	685	ARG
1	B	688	ARG
1	B	690	THR
1	B	697	LYS
1	B	698	LEU
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	786	ARG
1	B	793	TYR
1	B	798	VAL
1	B	799	SER
1	B	803	ASP
1	B	814	GLU
1	B	831	LEU
1	B	836	LEU
1	B	843	LEU
1	B	860	ARG
1	B	873	THR
1	B	891	LEU
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	38	LYS
1	C	39	SER
1	C	41	LEU

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Mol	Chain	Res	Type
1	C	45	THR
1	C	65	PHE
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	130	ARG
1	C	131	GLN
1	C	134	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	173	GLN
1	C	176	SER
1	C	180	VAL
1	C	183	VAL
1	C	187	LEU
1	C	200	ASP
1	C	202	GLU
1	C	215	LYS
1	C	216	ARG
1	C	217	ARG
1	C	218	LEU
1	C	222	VAL
1	C	224	THR
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

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Mol	Chain	Res	Type
1	C	365	ARG
1	C	367	ARG
1	C	372	ARG
1	C	376	TYR
1	C	379	ASP
1	C	380	PHE
1	C	383	VAL
1	C	384	LEU
1	C	387	LEU
1	C	389	ARG
1	C	391	MET
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	412	CYS
1	C	420	LEU
1	C	425	LEU
1	C	444	GLU
1	C	450	ILE
1	C	457	LEU
1	C	462	LEU
1	C	465	ARG
1	C	467	GLN
1	C	478	ARG
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	539	ARG
1	C	541	LEU
1	C	546	THR
1	C	547	ARG

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Mol	Chain	Res	Type
1	C	548	LEU
1	C	551	LEU
1	C	554	THR
1	C	563	ASP
1	C	597	ASN
1	C	609	ARG
1	C	613	GLU
1	C	614	ILE
1	C	618	ARG
1	C	626	GLN
1	C	648	VAL
1	C	656	SER
1	C	660	LYS
1	C	685	ARG
1	C	688	ARG
1	C	690	THR
1	C	697	LYS
1	C	698	LEU
1	C	700	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
1	C	761	THR
1	C	764	ILE
1	C	767	ASN
1	C	768	PHE
1	C	771	ASP
1	C	786	ARG
1	C	793	TYR
1	C	798	VAL
1	C	799	SER
1	C	808	GLU
1	C	814	GLU
1	C	831	LEU
1	C	836	LEU
1	C	843	LEU
1	C	857	LEU
1	C	860	ARG

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Mol	Chain	Res	Type
1	C	873	THR
1	C	891	LEU
1	C	900	VAL
1	C	911	SER
1	C	914	ILE
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	65	PHE
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	115	ARG
1	D	130	ARG
1	D	134	GLN
1	D	137	VAL
1	D	138	ASP
1	D	140	VAL
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	181	ASP
1	D	193	LEU
1	D	199	HIS
1	D	202	GLU
1	D	216	ARG
1	D	222	VAL
1	D	232	ILE
1	D	234	VAL
1	D	250	ARG

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Mol	Chain	Res	Type
1	D	263	LEU
1	D	282	CYS
1	D	288	LEU
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	355	LEU
1	D	359	ASP
1	D	365	ARG
1	D	367	ARG
1	D	369	ARG
1	D	372	ARG
1	D	384	LEU
1	D	386	PHE
1	D	389	ARG
1	D	392	SER
1	D	394	THR
1	D	402	ARG
1	D	412	CYS
1	D	420	LEU
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	508	ARG
1	D	515	ILE
1	D	531	ILE
1	D	539	ARG
1	D	541	LEU
1	D	546	THR

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Mol	Chain	Res	Type
1	D	548	LEU
1	D	551	LEU
1	D	554	THR
1	D	563	ASP
1	D	597	ASN
1	D	609	ARG
1	D	613	GLU
1	D	614	ILE
1	D	618	ARG
1	D	626	GLN
1	D	648	VAL
1	D	656	SER
1	D	660	LYS
1	D	685	ARG
1	D	688	ARG
1	D	690	THR
1	D	697	LYS
1	D	698	LEU
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	786	ARG
1	D	793	TYR
1	D	798	VAL
1	D	799	SER
1	D	808	GLU
1	D	831	LEU
1	D	836	LEU
1	D	843	LEU
1	D	860	ARG
1	D	873	THR
1	D	891	LEU
1	D	911	SER
1	D	914	ILE

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Mol	Chain	Res	Type
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
1	E	61	TYR
1	E	65	PHE
1	E	70	ASP
1	E	74	VAL
1	E	77	ILE
1	E	80	LEU
1	E	109	LEU
1	E	121	CYS
1	E	130	ARG
1	E	131	GLN
1	E	141	LEU
1	E	147	THR
1	E	148	ARG
1	E	155	VAL
1	E	158	THR
1	E	166	LEU
1	E	168	ASP
1	E	169	LYS
1	E	179	ARG
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	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

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Mol	Chain	Res	Type
1	E	303	PRO
1	E	305	ARG
1	E	306	THR
1	E	307	LEU
1	E	309	GLN
1	E	319	HIS
1	E	320	THR
1	E	323	TYR
1	E	338	ASP
1	E	339	VAL
1	E	346	LEU
1	E	351	ARG
1	E	364	VAL
1	E	365	ARG
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	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	462	LEU
1	E	465	ARG
1	E	467	GLN
1	E	478	ARG
1	E	479	SER
1	E	480	ARG

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Mol	Chain	Res	Type
1	E	481	LEU
1	E	489	LEU
1	E	490	GLU
1	E	492	LEU
1	E	493	SER
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	547	ARG
1	E	548	LEU
1	E	551	LEU
1	E	554	THR
1	E	563	ASP
1	E	597	ASN
1	E	609	ARG
1	E	613	GLU
1	E	614	ILE
1	E	618	ARG
1	E	626	GLN
1	E	648	VAL
1	E	656	SER
1	E	660	LYS
1	E	685	ARG
1	E	688	ARG
1	E	690	THR
1	E	697	LYS
1	E	698	LEU
1	E	700	ARG
1	E	709	THR
1	E	712	SER
1	E	718	THR
1	E	720	VAL
1	E	752	ARG
1	E	753	CYS
1	E	757	THR
1	E	761	THR
1	E	764	ILE
1	E	768	PHE

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Mol	Chain	Res	Type
1	E	771	ASP
1	E	786	ARG
1	E	793	TYR
1	E	798	VAL
1	E	799	SER
1	E	808	GLU
1	E	814	GLU
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	22	LEU
1	F	24	ARG
1	F	25	ASP
1	F	30	PHE
1	F	33	LEU
1	F	34	SER
1	F	40	SER
1	F	52	ARG
1	F	61	TYR
1	F	68	GLN
1	F	73	ASP
1	F	76	PHE
1	F	77	ILE
1	F	78	GLU
1	F	84	VAL
1	F	107	ASP
1	F	316	SER
1	F	320	THR
1	F	323	TYR
1	F	325	THR
1	F	328	MET
1	F	340	ASP
1	F	343	TRP
1	F	345	LYS

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Mol	Chain	Res	Type
1	F	346	LEU
1	F	349	LYS
1	F	368	ASN
1	F	372	ARG
1	F	373	THR
1	F	375	SER
1	F	379	ASP
1	F	380	PHE
1	F	381	GLU
1	F	389	ARG
1	F	392	SER
1	F	396	SER
1	F	407	MET
1	F	425	LEU
1	F	428	THR
1	F	436	GLU
1	F	437	HIS
1	F	442	ILE
1	F	445	VAL
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	500	THR
1	F	502	SER
1	F	507	GLN
1	F	513	THR
1	F	515	ILE
1	F	538	ASN
1	F	544	THR
1	F	548	LEU
1	F	554	THR
1	F	555	LEU
1	F	560	HIS
1	F	563	ASP
1	F	570	TRP
1	F	574	ILE
1	F	581	HIS
1	F	585	ILE
1	F	588	SER

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Mol	Chain	Res	Type
1	F	591	TYR
1	F	592	ASP
1	F	593	GLU
1	F	596	ARG
1	F	601	ILE
1	F	606	LEU
1	F	614	ILE
1	F	619	ARG
1	F	621	VAL
1	F	625	ARG
1	F	627	LEU
1	F	636	ASN
1	F	640	ILE
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	687	THR
1	F	688	ARG
1	F	689	VAL
1	F	690	THR
1	F	693	ASP
1	F	697	LYS
1	F	701	VAL
1	F	856	GLU
1	F	868	ILE
1	F	888	ILE
1	F	891	LEU
1	F	892	VAL
1	F	896	ASN
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 (94) 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	398	GLN
1	A	437	HIS
1	A	597	ASN
1	A	626	GLN
1	A	681	GLN
1	A	686	HIS
1	A	889	ASN
1	A	896	ASN
1	B	13	HIS
1	B	68	GLN
1	B	88	GLN
1	B	131	GLN
1	B	134	GLN
1	B	171	ASN
1	B	185	HIS
1	B	227	ASN
1	B	261	HIS
1	B	363	HIS
1	B	368	ASN
1	B	538	ASN
1	B	597	ASN
1	B	626	GLN
1	B	681	GLN
1	B	686	HIS
1	B	886	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	437	HIS

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Mol	Chain	Res	Type
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	889	ASN
1	C	896	ASN
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	538	ASN
1	D	597	ASN
1	D	626	GLN
1	D	674	ASN
1	D	681	GLN
1	D	686	HIS
1	D	767	ASN
1	D	886	ASN
1	D	889	ASN
1	D	896	ASN
1	E	13	HIS
1	E	68	GLN
1	E	88	GLN
1	E	120	HIS
1	E	363	HIS
1	E	368	ASN
1	E	398	GLN
1	E	437	HIS
1	E	538	ASN
1	E	597	ASN
1	E	626	GLN
1	E	674	ASN
1	E	681	GLN
1	E	686	HIS
1	E	889	ASN
1	E	896	ASN

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Mol	Chain	Res	Type
1	F	14	ASN
1	F	92	ASN
1	F	363	HIS
1	F	560	HIS
1	F	567	HIS
1	F	686	HIS
1	F	849	GLN
1	F	877	HIS
1	F	886	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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

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
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%)	0.47	46 (4%) 29 29	16, 55, 94, 112	0
1	B	918/993 (92%)	0.44	53 (5%) 23 24	16, 57, 102, 111	0
1	C	890/993 (89%)	0.37	35 (3%) 39 38	16, 60, 108, 118	0
1	D	921/993 (92%)	0.43	65 (7%) 16 18	16, 60, 103, 114	0
1	E	919/993 (92%)	0.46	68 (7%) 14 16	16, 57, 102, 127	0
1	F	607/993 (61%)	0.53	45 (7%) 14 16	45, 79, 112, 117	0
All	All	5199/5958 (87%)	0.44	312 (6%) 21 23	16, 61, 104, 127	0

All (312) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	357	GLY	7.0
1	E	239	ASP	6.8
1	D	235	LEU	6.7
1	A	308	ALA	6.5
1	A	307	LEU	6.1
1	D	303	PRO	6.0
1	B	437	HIS	5.7
1	F	355	LEU	5.4
1	A	361	GLN	5.4
1	E	238	VAL	5.3
1	E	240	HIS	5.0
1	A	394	THR	5.0
1	D	310	GLY	4.9
1	D	307	LEU	4.8
1	D	306	THR	4.8
1	E	454	ALA	4.8
1	A	306	THR	4.8
1	E	178	VAL	4.7
1	B	162	GLU	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	728	PHE	4.6
1	C	377	TYR	4.6
1	D	740	GLN	4.6
1	A	325	THR	4.6
1	F	388	GLN	4.5
1	D	309	GLN	4.4
1	D	377	TYR	4.4
1	C	439	ALA	4.4
1	A	445	VAL	4.3
1	D	305	ARG	4.3
1	E	203	VAL	4.3
1	B	178	VAL	4.2
1	B	188	THR	4.2
1	F	851	VAL	4.2
1	F	899	ILE	4.2
1	D	379	ASP	4.1
1	D	953	VAL	4.0
1	C	758	GLY	4.0
1	B	454	ALA	4.0
1	D	784	TYR	4.0
1	D	311	ALA	4.0
1	C	178	VAL	3.9
1	E	235	LEU	3.9
1	D	234	VAL	3.8
1	F	868	ILE	3.8
1	C	459	ALA	3.8
1	D	700	ARG	3.8
1	D	308	ALA	3.8
1	C	746	PHE	3.8
1	D	751	GLY	3.8
1	D	788	THR	3.8
1	D	237	PHE	3.7
1	A	364	VAL	3.7
1	F	869	LEU	3.7
1	E	149	PHE	3.7
1	D	758	GLY	3.7
1	A	377	TYR	3.6
1	A	446	CYS	3.6
1	A	235	LEU	3.6
1	F	349	LYS	3.6
1	F	693	ASP	3.6
1	A	136	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	F	698	LEU	3.6
1	B	143	MET	3.6
1	F	911	SER	3.5
1	F	66	LEU	3.5
1	A	437	HIS	3.5
1	F	343	TRP	3.5
1	F	413	PRO	3.5
1	B	203	VAL	3.5
1	E	153	ALA	3.5
1	C	317	ASN	3.4
1	F	448	LEU	3.4
1	C	177	ARG	3.4
1	C	791	VAL	3.3
1	B	460	LEU	3.3
1	D	868	ILE	3.3
1	D	445	VAL	3.3
1	D	324	PHE	3.2
1	A	801	VAL	3.2
1	D	673	ALA	3.2
1	C	136	ILE	3.2
1	F	915	ILE	3.2
1	D	692	LEU	3.2
1	E	218	LEU	3.2
1	B	228	LEU	3.2
1	B	166	LEU	3.2
1	E	160	LYS	3.2
1	F	420	LEU	3.1
1	E	379	ASP	3.1
1	B	251	PHE	3.1
1	E	720	VAL	3.1
1	D	670	ALA	3.1
1	D	152	LEU	3.1
1	E	646	LEU	3.1
1	A	378	ALA	3.1
1	E	751	GLY	3.1
1	C	222	VAL	3.0
1	D	403	TYR	3.0
1	D	178	VAL	3.0
1	E	733	GLU	3.0
1	A	668	LEU	3.0
1	F	700	ARG	3.0
1	C	757	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	151	VAL	3.0
1	E	175	TYR	3.0
1	D	698	LEU	3.0
1	C	458	ASN	2.9
1	E	161	GLY	2.9
1	A	302	ASP	2.9
1	C	354	ILE	2.9
1	D	388	GLN	2.9
1	E	163	PHE	2.9
1	C	460	LEU	2.9
1	D	783	ARG	2.9
1	C	263	LEU	2.9
1	E	234	VAL	2.8
1	E	455	ASP	2.8
1	D	629	VAL	2.8
1	D	668	LEU	2.8
1	A	822	TYR	2.8
1	B	797	THR	2.8
1	E	897	THR	2.8
1	C	191	PRO	2.8
1	F	68	GLN	2.8
1	B	379	ASP	2.8
1	B	179	ARG	2.8
1	F	665	ASN	2.8
1	E	392	SER	2.8
1	E	237	PHE	2.8
1	D	759	ASP	2.8
1	B	138	ASP	2.7
1	D	836	LEU	2.7
1	A	802	LEU	2.7
1	B	391	MET	2.7
1	C	331	LEU	2.7
1	B	204	VAL	2.7
1	D	669	ALA	2.7
1	B	185	HIS	2.7
1	F	384	LEU	2.7
1	D	801	VAL	2.7
1	F	663	LEU	2.7
1	B	152	LEU	2.7
1	D	149	PHE	2.7
1	A	315	TRP	2.7
1	B	201	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	394	THR	2.6
1	E	819	VAL	2.6
1	E	784	TYR	2.6
1	C	335	LEU	2.6
1	A	376	TYR	2.6
1	B	364	VAL	2.6
1	B	793	TYR	2.6
1	E	728	PHE	2.6
1	D	363	HIS	2.6
1	E	222	VAL	2.6
1	D	218	LEU	2.6
1	F	900	VAL	2.6
1	C	728	PHE	2.6
1	F	69	MET	2.6
1	C	784	TYR	2.6
1	A	317	ASN	2.6
1	C	437	HIS	2.6
1	E	179	ARG	2.5
1	C	692	LEU	2.5
1	D	672	LEU	2.5
1	F	396	SER	2.5
1	C	456	PHE	2.5
1	E	701	VAL	2.5
1	F	876	LEU	2.5
1	E	836	LEU	2.5
1	A	406	PHE	2.5
1	F	441	SER	2.5
1	A	328	MET	2.5
1	F	888	ILE	2.5
1	A	375	SER	2.5
1	A	836	LEU	2.5
1	C	899	ILE	2.5
1	A	642	VAL	2.5
1	C	673	ALA	2.5
1	D	744	PHE	2.5
1	A	362	VAL	2.5
1	C	264	ALA	2.5
1	C	403	TYR	2.5
1	E	739	TYR	2.5
1	E	465	ARG	2.4
1	D	671	VAL	2.4
1	F	680	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	665	ASN	2.4
1	B	453	CYS	2.4
1	B	724	ILE	2.4
1	E	691	GLY	2.4
1	F	16	ARG	2.4
1	F	425	LEU	2.4
1	E	394	THR	2.4
1	E	201	ILE	2.4
1	D	691	GLY	2.4
1	D	642	VAL	2.4
1	E	229	ALA	2.4
1	F	692	LEU	2.4
1	F	901	ILE	2.4
1	E	193	LEU	2.4
1	A	150	LEU	2.4
1	B	448	LEU	2.4
1	E	232	ILE	2.3
1	D	325	THR	2.3
1	D	391	MET	2.3
1	E	810	ALA	2.3
1	A	140	VAL	2.3
1	F	364	VAL	2.3
1	E	309	GLN	2.3
1	A	366	TYR	2.3
1	A	208	LEU	2.3
1	D	822	TYR	2.3
1	E	460	LEU	2.3
1	B	434	LYS	2.3
1	A	713	ASN	2.3
1	B	439	ALA	2.3
1	D	298	LEU	2.3
1	B	867	TYR	2.3
1	C	203	VAL	2.3
1	D	252	SER	2.3
1	E	708	ARG	2.3
1	C	376	TYR	2.3
1	A	798	VAL	2.3
1	D	184	VAL	2.3
1	A	310	GLY	2.3
1	A	577	GLY	2.3
1	E	719	GLY	2.3
1	E	802	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	810	ALA	2.3
1	A	356	GLU	2.3
1	B	153	ALA	2.3
1	D	458	ASN	2.3
1	C	218	LEU	2.3
1	B	791	VAL	2.3
1	D	376	TYR	2.2
1	E	793	TYR	2.2
1	A	363	HIS	2.2
1	D	802	LEU	2.2
1	B	139	GLN	2.2
1	B	392	SER	2.2
1	C	389	ARG	2.2
1	F	390	LYS	2.2
1	B	627	LEU	2.2
1	F	697	LYS	2.2
1	E	649	LEU	2.2
1	B	821	ARG	2.2
1	E	236	GLU	2.2
1	F	75	ASP	2.2
1	F	909	LYS	2.2
1	B	131	GLN	2.2
1	B	346	LEU	2.2
1	F	681	GLN	2.2
1	E	680	ARG	2.2
1	F	356	GLU	2.2
1	D	151	VAL	2.2
1	E	806	ILE	2.2
1	B	144	PRO	2.2
1	E	721	PHE	2.1
1	B	136	ILE	2.1
1	B	253	GLU	2.1
1	E	914	ILE	2.1
1	E	915	ILE	2.1
1	D	723	LYS	2.1
1	F	365	ARG	2.1
1	E	700	ARG	2.1
1	E	783	ARG	2.1
1	D	781	GLY	2.1
1	C	744	PHE	2.1
1	C	668	LEU	2.1
1	F	695	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	375	SER	2.1
1	E	821	ARG	2.1
1	E	612	ILE	2.1
1	B	114	ALA	2.1
1	B	266	ASP	2.1
1	E	440	LYS	2.1
1	B	798	VAL	2.1
1	B	420	LEU	2.1
1	E	173	GLN	2.1
1	E	264	ALA	2.1
1	E	900	VAL	2.1
1	A	403	TYR	2.1
1	E	152	LEU	2.1
1	E	315	TRP	2.1
1	E	767	ASN	2.1
1	A	268	LEU	2.1
1	B	170	LEU	2.1
1	B	429	LEU	2.1
1	A	264	ALA	2.0
1	B	822	TYR	2.0
1	A	457	LEU	2.0
1	D	899	ILE	2.0
1	F	913	TRP	2.0
1	E	225	ALA	2.0
1	F	621	VAL	2.0
1	B	159	ARG	2.0
1	D	203	VAL	2.0
1	D	727	LEU	2.0
1	E	744	PHE	2.0
1	B	397	GLU	2.0
1	B	444	GLU	2.0
1	A	234	VAL	2.0
1	B	349	LYS	2.0
1	B	899	ILE	2.0
1	D	313	ALA	2.0
1	F	853	LEU	2.0
1	C	822	TYR	2.0
1	A	209	THR	2.0
1	B	394	THR	2.0
1	D	785	ASN	2.0
1	E	797	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
2	ZN	A	1954	1/1	0.75	0.20	65,65,65,65	0
2	ZN	B	1955	1/1	0.80	0.26	116,116,116,116	0
2	ZN	A	1955	1/1	0.83	0.21	116,116,116,116	0
2	ZN	E	1955	1/1	0.85	0.24	116,116,116,116	0
2	ZN	D	1955	1/1	0.89	0.23	116,116,116,116	0
2	ZN	C	1955	1/1	0.93	0.23	116,116,116,116	0
2	ZN	A	1956	1/1	0.94	0.21	48,48,48,48	0
2	ZN	B	1956	1/1	0.95	0.19	44,44,44,44	0
2	ZN	B	1954	1/1	0.95	0.21	65,65,65,65	0
2	ZN	D	1954	1/1	0.96	0.13	66,66,66,66	0
2	ZN	E	1954	1/1	0.98	0.17	66,66,66,66	0
2	ZN	D	1956	1/1	0.99	0.16	59,59,59,59	0
2	ZN	C	1954	1/1	0.99	0.17	65,65,65,65	0
2	ZN	C	1956	1/1	0.99	0.18	76,76,76,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.