



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 03:24 PM EDT

PDB ID : 3DIN / pdb_00003din
Title : Crystal structure of the protein-translocation complex formed by the SecY channel and the SecA ATPase
Authors : Zimmer, J.; Nam, Y.; Rapoport, T.A.
Deposited on : 2008-06-20
Resolution : 4.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

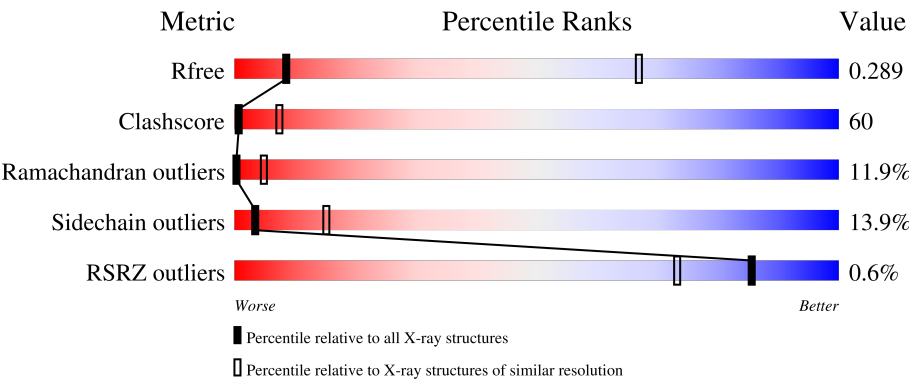
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1127 (5.10-3.90)
Clashscore	190562	1002 (5.06-3.94)
Ramachandran outliers	187476	1060 (5.10-3.90)
Sidechain outliers	187428	1043 (5.10-3.90)
RSRZ outliers	180081	1122 (5.10-3.90)

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	871	% 20%52%19%• 6%
1	B	871	% 20%52%19%• 6%
2	C	431	27%46%16%• 8%
2	F	431	27%46%16%• 8%
3	D	65	29%52%• • 14%

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Mol	Chain	Length	Quality of chain
3	G	65	
4	E	76	
4	H	76	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	ADP	A	873	-	-	X	-
6	ADP	B	873	-	-	X	-
7	BEF	A	874	-	-	X	-
7	BEF	B	874	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 21368 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 Protein translocase subunit secA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	816	Total	C	N	O	S	0	0	0
			6613	4215	1131	1239	28			
1	B	816	Total	C	N	O	S	0	0	0
			6613	4215	1131	1239	28			

- Molecule 2 is a protein called Preprotein translocase subunit SecY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	396	Total	C	N	O	S	0	0	0
			3124	2071	518	524	11			
2	F	396	Total	C	N	O	S	0	0	0
			3124	2071	518	524	11			

- Molecule 3 is a protein called Preprotein translocase subunit secE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	56	Total	C	N	O	0	0	0
			431	294	64	73			
3	G	56	Total	C	N	O	0	0	0
			431	294	64	73			

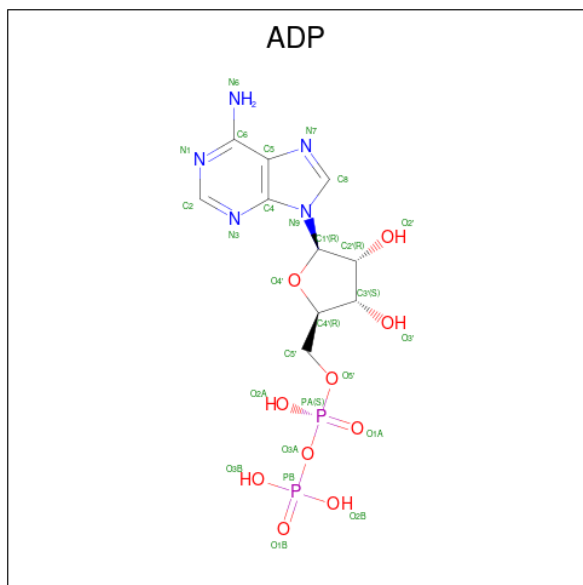
- Molecule 4 is a protein called Preprotein translocase subunit SecG.

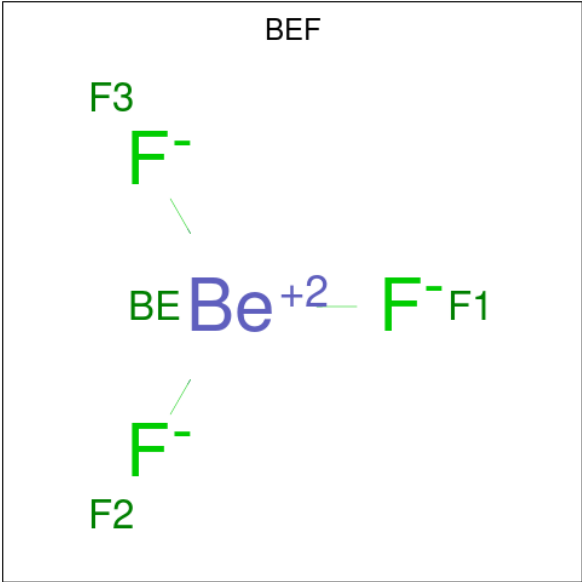
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	65	Total	C	N	O	S	0	0	0
			484	318	80	83	3			
4	H	65	Total	C	N	O	S	0	0	0
			484	318	80	83	3			

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0
5	B	1	Total Mg 1 1	0	0

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



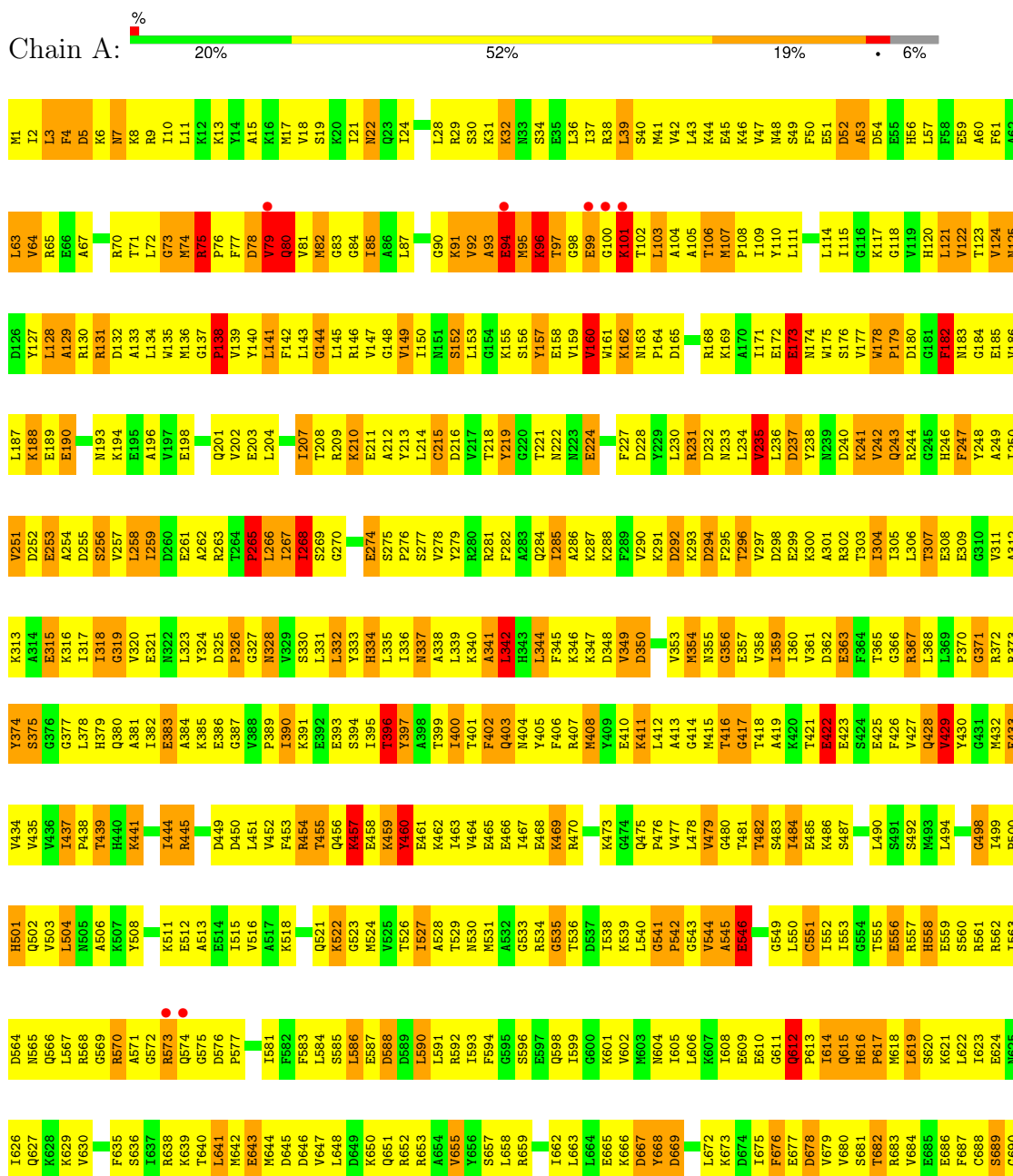


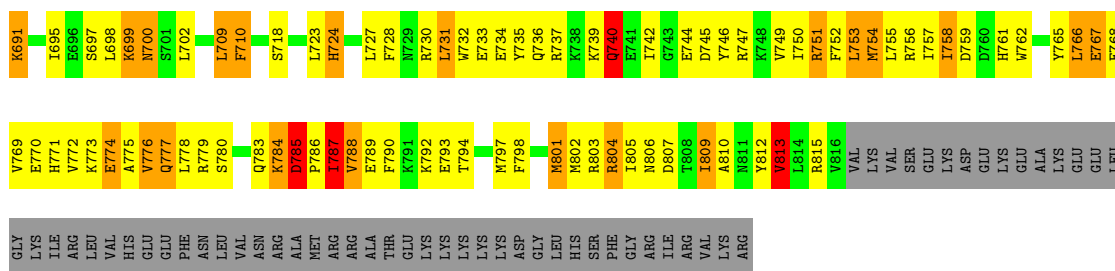
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	Be	F	0	0
			4	1	3		
7	B	1	Total	Be	F	0	0
			4	1	3		

3 Residue-property plots

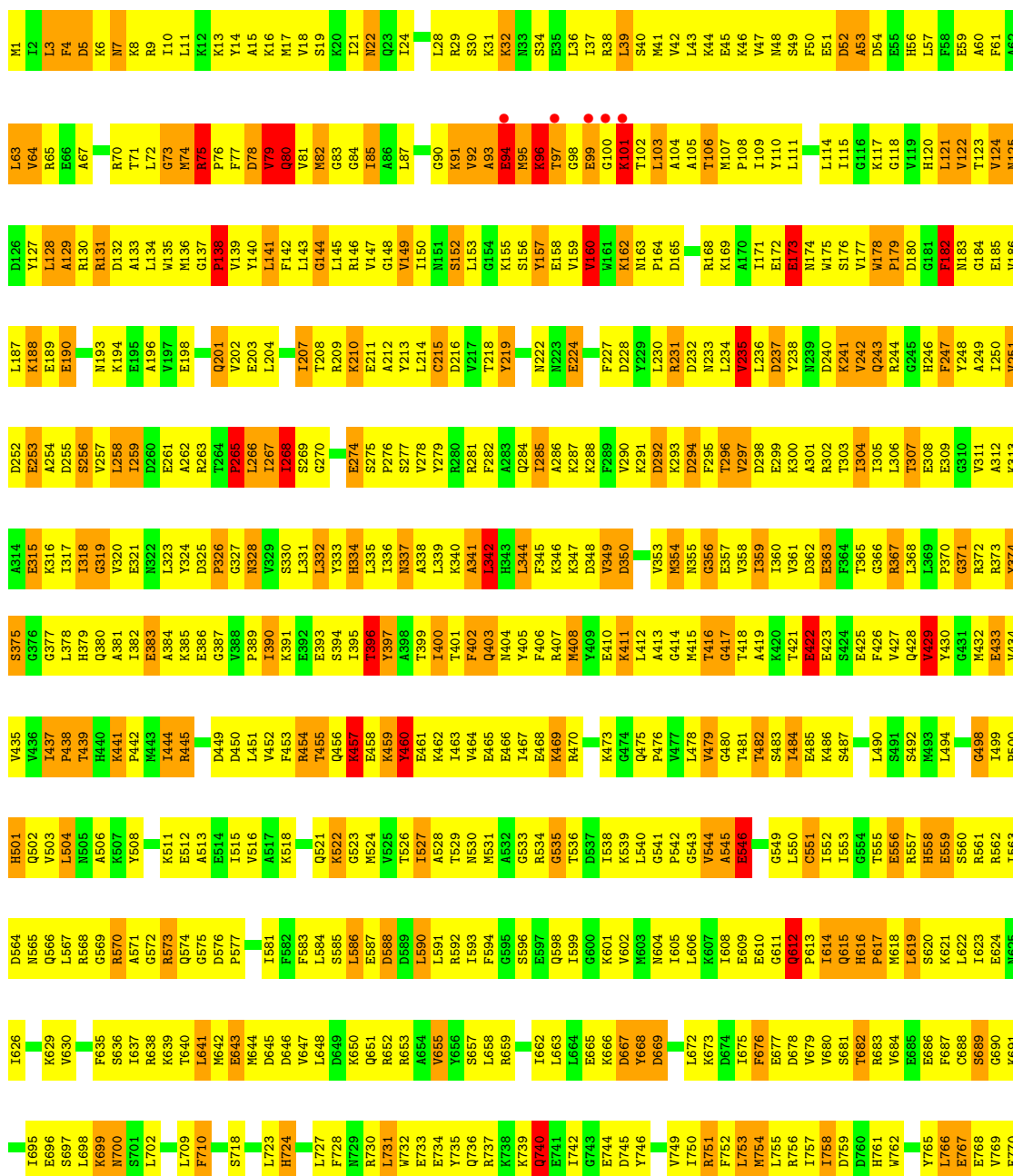
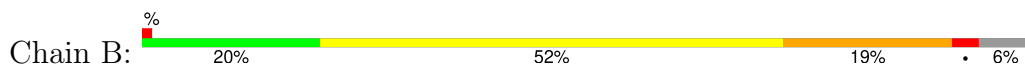
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

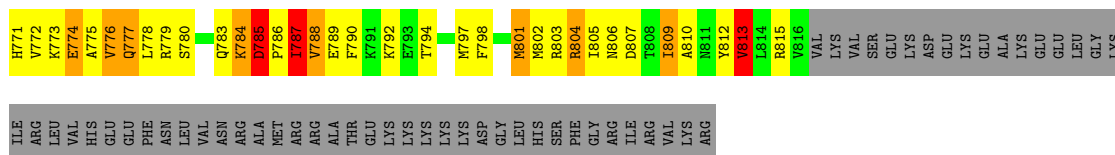
• Molecule 1: Protein translocase subunit secA



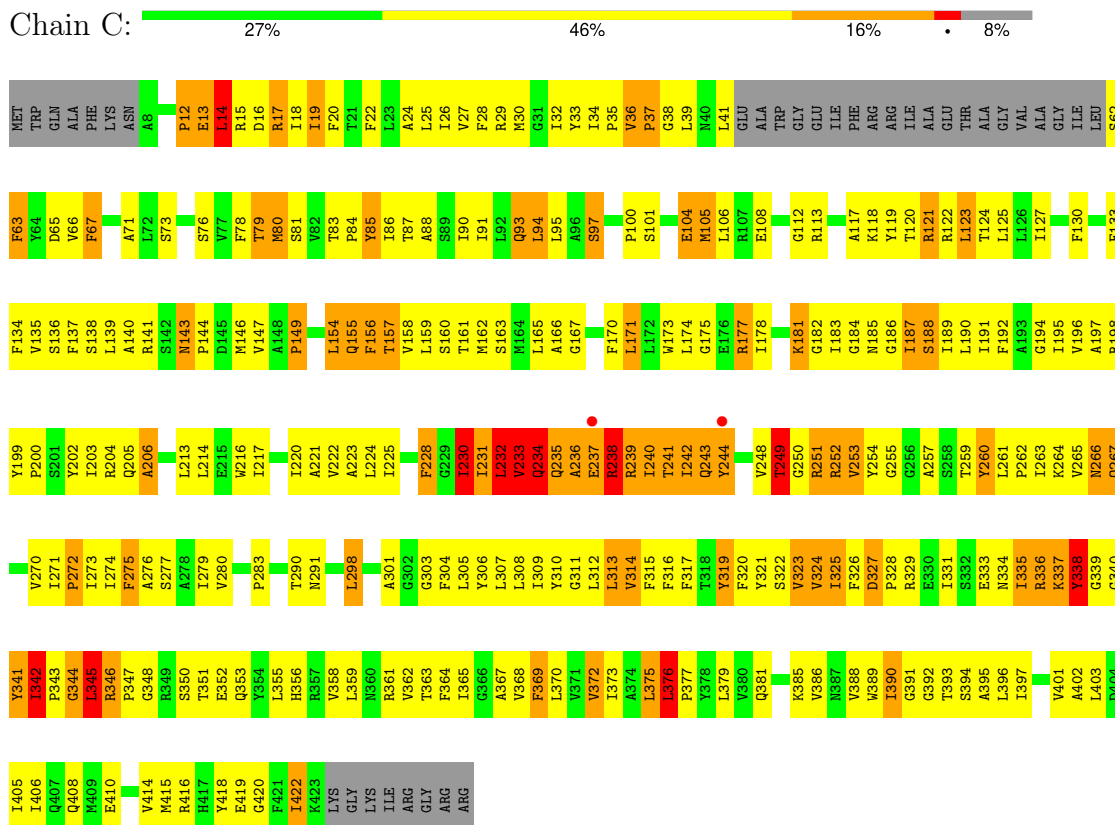


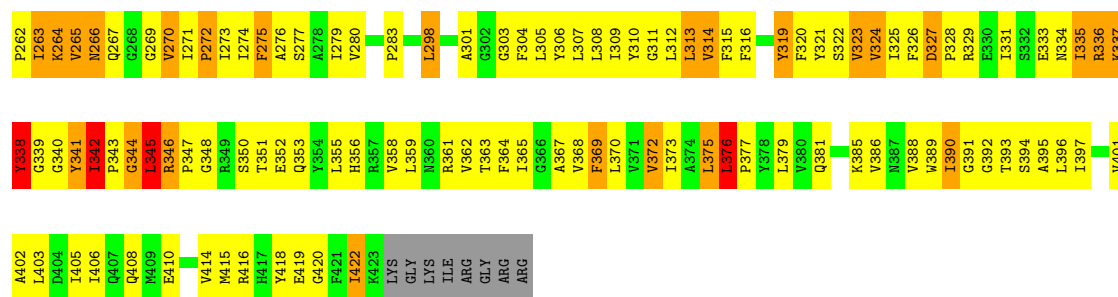
• Molecule 1: Protein translocase subunit secA



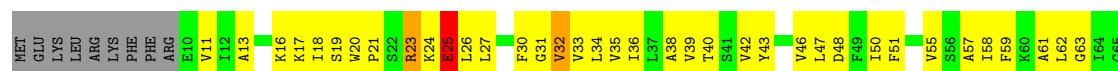


• Molecule 2: Preprotein translocase subunit SecY

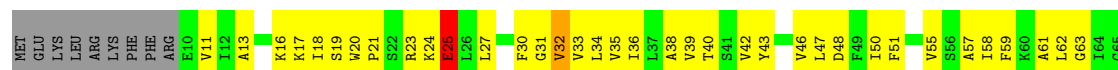




• Molecule 3: Preprotein translocase subunit secE



• Molecule 3: Preprotein translocase subunit secE

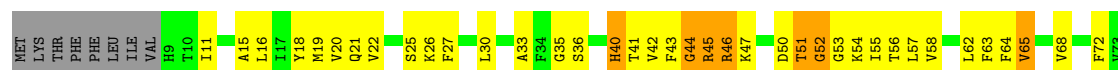
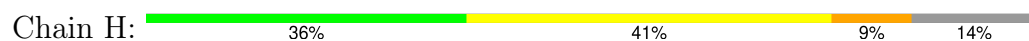


• Molecule 4: Preprotein translocase subunit SecG



LEU
THR
ARG

• Molecule 4: Preprotein translocase subunit SecG



LEU
THR
ARG

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.62Å 156.00Å 358.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 4.50 15.00 – 4.50	Depositor EDS
% Data completeness (in resolution range)	97.7 (15.00-4.50) 94.3 (15.00-4.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 4.54Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.279 , 0.303 0.286 , 0.289	Depositor DCC
R_{free} test set	1678 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	205.7	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 427.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	21368	wwPDB-VP
Average B, all atoms (Å ²)	356.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, BEF

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	0.37	1/6730 (0.0%)	0.98	46/9048 (0.5%)
1	B	0.37	1/6730 (0.0%)	0.98	44/9048 (0.5%)
2	C	0.65	7/3194 (0.2%)	1.11	25/4329 (0.6%)
2	F	0.60	6/3194 (0.2%)	1.10	25/4329 (0.6%)
3	D	0.31	0/440	0.92	3/596 (0.5%)
3	G	0.32	0/440	0.92	3/596 (0.5%)
4	E	0.29	0/492	0.97	5/662 (0.8%)
4	H	0.29	0/492	0.97	5/662 (0.8%)
All	All	0.46	15/21712 (0.1%)	1.02	156/29270 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	F	0	1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	235	GLN	C-N	11.04	1.43	1.33
2	C	235	GLN	N-CA	9.22	1.57	1.45
2	F	235	GLN	C-N	9.15	1.42	1.33
2	F	234	GLN	C-N	9.04	1.44	1.33
2	C	234	GLN	C-N	8.97	1.44	1.33
2	F	235	GLN	CA-C	7.93	1.62	1.52
2	C	235	GLN	CA-C	7.54	1.61	1.52
2	F	235	GLN	N-CA	7.31	1.55	1.45
1	A	79	VAL	C-O	6.54	1.31	1.24
1	B	79	VAL	C-O	6.51	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	237	GLU	N-CA	5.75	1.53	1.46
2	F	236	ALA	N-CA	5.59	1.54	1.46
2	C	236	ALA	CA-C	5.45	1.59	1.53
2	F	237	GLU	C-N	5.19	1.38	1.33
2	C	236	ALA	C-N	5.12	1.40	1.33

All (156) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	236	ALA	N-CA-C	13.42	125.50	108.19
2	F	236	ALA	N-CA-C	13.00	126.17	108.23
1	B	4	PHE	N-CA-C	-11.56	99.19	113.18
1	A	4	PHE	N-CA-C	-11.56	99.19	113.18
2	C	234	GLN	OE1-CD-NE2	-10.44	112.17	122.60
2	C	235	GLN	OE1-CD-NE2	-10.28	112.32	122.60
1	B	657	SER	N-CA-C	-9.97	99.67	112.23
1	A	657	SER	N-CA-C	-9.96	99.68	112.23
2	C	243	GLN	OE1-CD-NE2	-9.96	112.64	122.60
2	C	267	GLN	OE1-CD-NE2	-9.64	112.96	122.60
2	F	235	GLN	OE1-CD-NE2	-9.14	113.46	122.60
2	F	234	GLN	OE1-CD-NE2	-9.14	113.46	122.60
1	B	411	LYS	N-CA-C	8.75	122.29	109.69
1	A	411	LYS	N-CA-C	8.71	122.24	109.69
1	B	408	MET	N-CA-C	-8.70	101.70	111.71
1	A	408	MET	N-CA-C	-8.67	101.74	111.71
1	B	356	GLY	N-CA-C	-8.60	103.76	114.16
1	A	356	GLY	N-CA-C	-8.55	103.81	114.16
1	B	349	VAL	N-CA-C	-8.34	105.05	113.47
1	A	349	VAL	N-CA-C	-8.29	105.09	113.47
2	F	252	ARG	N-CA-C	8.15	121.28	109.14
2	C	252	ARG	N-CA-C	8.13	120.32	108.86
2	F	235	GLN	N-CA-C	7.80	120.93	109.07
3	G	57	ALA	N-CA-C	-7.72	102.94	111.36
3	D	57	ALA	N-CA-C	-7.67	103.00	111.36
1	B	777	GLN	N-CA-C	-7.54	104.08	113.28
1	A	777	GLN	N-CA-C	-7.54	104.08	113.28
1	B	124	VAL	N-CA-C	7.30	117.43	110.42
1	A	124	VAL	N-CA-C	7.22	117.36	110.42
1	A	350	ASP	N-CA-C	-7.19	99.69	109.54
1	B	350	ASP	N-CA-C	-7.17	99.72	109.54
2	C	238	ARG	N-CA-C	7.13	118.07	108.23
1	B	78	ASP	N-CA-C	7.09	122.61	113.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	ASP	N-CA-C	7.08	122.58	113.88
2	F	214	LEU	N-CA-C	-7.07	103.62	111.82
2	C	214	LEU	N-CA-C	-7.06	103.64	111.82
2	C	243	GLN	CG-CD-NE2	7.04	126.97	116.40
2	C	267	GLN	CG-CD-NE2	6.92	126.78	116.40
2	F	235	GLN	CG-CD-NE2	6.89	126.74	116.40
2	C	235	GLN	CG-CD-NE2	6.85	126.68	116.40
1	A	118	GLY	CA-C-N	-6.76	112.55	122.68
1	A	118	GLY	C-N-CA	-6.76	112.55	122.68
1	B	125	ASN	N-CA-C	6.71	119.37	109.24
1	A	125	ASN	N-CA-C	6.71	119.36	109.24
1	B	118	GLY	CA-C-N	-6.69	112.64	122.68
1	B	118	GLY	C-N-CA	-6.69	112.64	122.68
2	C	234	GLN	CG-CD-NE2	6.64	126.36	116.40
2	F	238	ARG	N-CA-C	6.64	117.39	108.23
2	F	105	MET	N-CA-C	6.52	120.09	109.59
2	C	105	MET	N-CA-C	6.52	120.08	109.59
2	F	266	ASN	N-CA-C	6.52	116.66	108.45
2	C	266	ASN	N-CA-C	6.50	116.64	108.45
3	G	31	GLY	N-CA-C	-6.49	104.74	113.24
3	D	31	GLY	N-CA-C	-6.46	104.78	113.24
1	A	740	GLN	N-CA-C	-6.33	105.42	113.01
1	B	173	GLU	N-CA-C	-6.32	103.69	111.40
1	A	173	GLU	N-CA-C	-6.30	103.72	111.40
1	B	740	GLN	N-CA-C	-6.29	105.46	113.01
1	A	96	LYS	N-CA-C	6.28	124.17	110.80
2	C	104	GLU	N-CA-C	6.28	124.17	110.80
1	B	96	LYS	N-CA-C	6.26	124.14	110.80
2	F	104	GLU	N-CA-C	6.24	124.08	110.80
1	B	82	MET	N-CA-C	-6.23	104.55	111.71
1	B	422	GLU	N-CA-C	6.23	120.95	113.23
1	A	82	MET	N-CA-C	-6.22	104.56	111.71
3	G	32	VAL	N-CA-C	-6.20	104.29	110.62
2	F	261	LEU	CA-C-N	6.19	127.58	119.84
2	F	261	LEU	C-N-CA	6.19	127.58	119.84
3	D	32	VAL	N-CA-C	-6.18	104.31	110.62
1	A	422	GLU	N-CA-C	6.18	120.89	113.23
2	F	376	LEU	CA-C-N	-6.16	112.50	119.28
2	F	376	LEU	C-N-CA	-6.16	112.50	119.28
2	C	376	LEU	CA-C-N	-6.16	112.51	119.28
2	C	376	LEU	C-N-CA	-6.16	112.51	119.28
2	F	234	GLN	CG-CD-NE2	6.14	125.60	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	541	GLY	CA-C-N	6.13	127.51	119.84
1	A	541	GLY	C-N-CA	6.13	127.51	119.84
1	B	541	GLY	CA-C-N	6.13	127.50	119.84
1	B	541	GLY	C-N-CA	6.13	127.50	119.84
1	A	304	ILE	N-CA-C	6.11	117.16	108.42
1	B	304	ILE	N-CA-C	6.06	117.09	108.42
1	B	80	GLN	N-CA-C	-6.06	104.62	112.68
2	C	235	GLN	N-CA-C	6.06	118.28	109.07
1	A	80	GLN	N-CA-C	-6.05	104.64	112.68
1	A	460	TYR	N-CA-C	-6.03	104.77	111.71
1	B	460	TYR	N-CA-C	-6.01	104.79	111.71
1	A	767	GLU	N-CA-C	-5.99	104.75	111.28
1	B	767	GLU	N-CA-C	-5.98	104.76	111.28
1	B	766	LEU	N-CA-C	-5.97	104.71	112.23
1	A	766	LEU	N-CA-C	-5.94	104.75	112.23
4	E	52	GLY	N-CA-C	-5.93	108.15	114.67
1	B	94	GLU	N-CA-C	5.92	123.41	110.80
4	E	56	THR	N-CA-C	-5.91	104.76	111.14
4	H	56	THR	N-CA-C	-5.90	104.77	111.14
1	A	94	GLU	N-CA-C	5.89	123.36	110.80
1	A	251	VAL	N-CA-C	5.87	116.56	107.99
1	B	251	VAL	N-CA-C	5.86	116.55	107.99
4	H	52	GLY	N-CA-C	-5.86	108.22	114.67
1	A	5	ASP	N-CA-C	-5.84	104.99	111.71
1	B	668	TYR	N-CA-C	-5.83	106.22	113.15
1	B	682	THR	N-CA-C	-5.82	105.02	111.71
1	A	668	TYR	N-CA-C	-5.81	106.24	113.15
1	B	5	ASP	N-CA-C	-5.80	105.04	111.71
1	A	682	THR	N-CA-C	-5.79	105.05	111.71
2	F	346	ARG	CA-C-N	5.76	127.03	119.84
2	F	346	ARG	C-N-CA	5.76	127.03	119.84
1	A	129	ALA	N-CA-C	-5.75	105.01	111.28
2	F	264	LYS	N-CA-C	5.71	122.96	110.80
2	F	249	THR	N-CA-C	5.67	115.72	108.24
2	F	251	ARG	N-CA-C	5.65	117.13	108.42
1	B	129	ALA	N-CA-C	-5.65	105.12	111.28
1	B	93	ALA	N-CA-C	-5.63	102.57	110.35
1	A	93	ALA	N-CA-C	-5.62	102.59	110.35
1	B	667	ASP	N-CA-C	5.56	118.20	108.52
1	A	667	ASP	N-CA-C	5.55	118.17	108.52
1	B	141	LEU	N-CA-C	-5.52	105.80	112.54
1	A	141	LEU	N-CA-C	-5.50	105.83	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	65	VAL	N-CA-C	-5.48	104.36	112.04
4	E	65	VAL	N-CA-C	-5.48	104.37	112.04
1	B	268	ILE	N-CA-C	5.47	120.72	109.34
1	A	268	ILE	N-CA-C	5.45	120.68	109.34
4	E	43	PHE	N-CA-C	-5.41	105.84	113.20
2	F	263	ILE	N-CA-C	5.41	115.91	108.12
2	C	346	ARG	CA-C-N	5.40	126.59	119.84
2	C	346	ARG	C-N-CA	5.40	126.59	119.84
1	B	731	LEU	N-CA-C	-5.38	105.53	111.71
4	H	43	PHE	N-CA-C	-5.36	105.91	113.20
1	A	731	LEU	N-CA-C	-5.30	105.50	111.28
2	F	237	GLU	N-CA-C	5.30	122.10	110.80
1	A	454	ARG	N-CA-C	5.27	118.02	109.86
1	B	454	ARG	N-CA-C	5.27	118.02	109.86
1	B	235	VAL	N-CA-C	5.26	111.84	106.21
1	A	94	GLU	CB-CA-C	-5.22	100.04	110.42
1	B	94	GLU	CB-CA-C	-5.21	100.05	110.42
1	A	235	VAL	N-CA-C	5.20	111.78	106.21
2	C	369	PHE	N-CA-C	5.20	117.94	111.24
2	F	369	PHE	N-CA-C	5.19	117.93	111.24
2	C	249	THR	N-CA-C	5.18	114.67	107.73
4	E	55	ILE	N-CA-C	-5.16	104.64	111.09
4	H	55	ILE	N-CA-C	-5.15	104.65	111.09
1	A	255	ASP	N-CA-C	-5.12	106.72	112.87
1	A	375	SER	N-CA-C	5.12	116.08	108.60
2	C	251	ARG	N-CA-C	5.12	116.31	108.42
1	B	255	ASP	N-CA-C	-5.12	106.73	112.87
2	F	336	ARG	N-CA-C	5.11	116.92	108.13
1	B	683	ARG	N-CA-C	-5.10	105.72	111.28
1	A	683	ARG	N-CA-C	-5.10	105.72	111.28
2	C	336	ARG	N-CA-C	5.09	116.89	108.13
1	B	375	SER	N-CA-C	5.09	116.03	108.60
2	C	237	GLU	N-CA-C	5.08	121.61	110.80
1	B	441	LYS	CA-C-N	5.04	125.82	120.13
1	B	441	LYS	C-N-CA	5.04	125.82	120.13
1	A	107	MET	CA-C-N	-5.02	113.87	119.19
1	A	107	MET	C-N-CA	-5.02	113.87	119.19
1	A	441	LYS	CA-C-N	5.00	125.78	120.13
1	A	441	LYS	C-N-CA	5.00	125.78	120.13

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	260	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6613	0	6689	952	2
1	B	6613	0	6689	926	2
2	C	3124	0	3275	363	0
2	F	3124	0	3275	349	0
3	D	431	0	460	31	0
3	G	431	0	460	34	0
4	E	484	0	508	34	0
4	H	484	0	508	30	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	27	0	12	41	0
6	B	27	0	12	39	0
7	A	4	0	0	4	0
7	B	4	0	0	5	0
All	All	21368	0	21888	2609	2

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 60.

All (2609) 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:A:76:PRO:HD2	6:A:873:ADP:N6	1.34	1.40
1:A:76:PRO:CD	6:A:873:ADP:HN62	1.40	1.34
1:B:76:PRO:HD2	6:B:873:ADP:N6	1.45	1.30
1:B:76:PRO:CD	6:B:873:ADP:HN62	1.50	1.25
1:B:101:LYS:HE2	7:B:874:BEF:F2	1.31	1.21
2:C:232:LEU:HB3	2:C:267:GLN:HB2	1.22	1.17
1:B:101:LYS:HD3	1:B:415:MET:CB	1.77	1.14
1:A:187:LEU:HD11	6:A:873:ADP:H2	1.09	1.13
1:B:101:LYS:HD3	1:B:415:MET:HB3	1.25	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:MET:HA	6:B:873:ADP:N1	1.64	1.11
1:A:74:MET:HA	6:A:873:ADP:N1	1.66	1.11
2:F:35:PRO:HG2	4:H:68:VAL:HA	1.31	1.10
1:A:187:LEU:HD11	6:A:873:ADP:C2	1.88	1.09
2:F:232:LEU:HB3	2:F:267:GLN:HB2	1.17	1.07
2:C:261:LEU:HB3	2:C:262:PRO:HD2	1.38	1.04
1:B:187:LEU:HD11	6:B:873:ADP:H2	1.19	1.04
1:A:74:MET:HE2	6:A:873:ADP:N3	1.72	1.03
2:F:232:LEU:HB3	2:F:267:GLN:CB	1.89	1.02
1:A:778:LEU:HD13	2:C:263:ILE:H	1.24	1.01
1:B:76:PRO:HD2	6:B:873:ADP:HN62	0.88	1.00
1:A:373:ARG:HE	1:A:374:TYR:H	1.03	0.99
2:F:261:LEU:HB3	2:F:262:PRO:HD2	1.42	0.99
1:A:93:ALA:O	1:A:94:GLU:HG2	1.60	0.99
1:A:251:VAL:HG11	1:A:257:VAL:HB	1.46	0.96
1:B:187:LEU:HD11	6:B:873:ADP:C2	2.01	0.95
1:B:251:VAL:HG11	1:B:257:VAL:HB	1.46	0.94
2:C:232:LEU:HB3	2:C:267:GLN:CB	1.96	0.94
2:C:377:PRO:HG3	2:C:389:TRP:HE1	1.32	0.94
1:B:74:MET:HE2	6:B:873:ADP:N3	1.83	0.94
1:A:160:VAL:HG11	1:A:169:LYS:HE2	1.51	0.93
1:B:778:LEU:HD13	2:F:263:ILE:H	1.33	0.93
2:C:14:LEU:HD22	2:C:17:ARG:HG3	1.50	0.93
1:A:75:ARG:HE	1:A:76:PRO:HD3	1.32	0.93
1:A:76:PRO:HD2	6:A:873:ADP:HN62	0.76	0.93
1:B:349:VAL:HG12	1:B:363:GLU:HG2	1.48	0.93
2:F:183:ILE:HG13	2:F:185:ASN:H	1.32	0.93
1:A:187:LEU:CD1	6:A:873:ADP:H2	1.82	0.93
2:C:309:ILE:HG22	2:C:313:LEU:CD1	1.99	0.93
1:B:75:ARG:HE	1:B:76:PRO:HD3	1.32	0.92
1:A:349:VAL:HG12	1:A:363:GLU:HG2	1.48	0.92
1:B:230:LEU:HD23	1:B:397:TYR:HB3	1.52	0.92
1:B:160:VAL:HG11	1:B:169:LYS:HE2	1.51	0.92
2:F:14:LEU:HD22	2:F:17:ARG:HG3	1.49	0.92
2:F:309:ILE:HG22	2:F:313:LEU:CD1	1.99	0.92
1:B:373:ARG:HE	1:B:374:TYR:H	1.03	0.92
1:A:230:LEU:HD23	1:A:397:TYR:HB3	1.51	0.92
2:F:233:VAL:HA	3:G:25:GLU:HG3	1.52	0.91
1:A:302:ARG:HB3	1:A:344:LEU:HD12	1.52	0.91
1:B:302:ARG:HB3	1:B:344:LEU:HD12	1.52	0.91
2:F:377:PRO:HG3	2:F:389:TRP:HE1	1.32	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:183:ILE:HG13	2:C:185:ASN:H	1.32	0.90
2:F:231:ILE:C	2:F:232:LEU:HD22	1.96	0.90
2:F:249:THR:HG22	2:F:250:GLY:H	1.36	0.89
2:C:239:ARG:HD3	2:C:251:ARG:HH12	1.37	0.88
1:B:101:LYS:CE	7:B:874:BEF:F2	2.12	0.88
1:A:340:LYS:HZ2	2:C:251:ARG:HE	1.17	0.88
1:B:57:LEU:HD23	1:B:111:LEU:HG	1.54	0.88
1:B:410:GLU:HG3	1:B:411:LYS:H	1.39	0.88
1:A:410:GLU:HG3	1:A:411:LYS:H	1.39	0.87
1:A:57:LEU:HD23	1:A:111:LEU:HG	1.54	0.87
2:C:230:ILE:O	2:C:232:LEU:HD13	1.75	0.86
2:C:35:PRO:HG2	4:E:68:VAL:HA	1.56	0.86
1:B:779:ARG:NH2	1:B:788:VAL:H	1.73	0.86
1:A:779:ARG:NH2	1:A:788:VAL:H	1.73	0.86
2:F:251:ARG:HH21	2:F:335:ILE:HD13	1.40	0.86
2:C:231:ILE:C	2:C:232:LEU:HD22	2.01	0.86
2:C:329:ARG:O	2:C:333:GLU:HB2	1.76	0.86
1:A:115:ILE:HG13	1:A:117:LYS:H	1.41	0.85
2:C:125:LEU:HD22	4:E:26:LYS:HE2	1.56	0.85
2:F:329:ARG:O	2:F:333:GLU:HB2	1.76	0.85
2:C:222:VAL:HG22	2:C:376:LEU:HD13	1.58	0.85
2:C:275:PHE:CD2	2:C:276:ALA:N	2.45	0.85
2:C:280:VAL:O	2:C:283:PRO:HD2	1.76	0.85
1:B:94:GLU:OE1	1:B:94:GLU:HA	1.74	0.84
1:A:612:GLN:H	1:A:613:PRO:HD2	1.42	0.84
2:F:222:VAL:HG22	2:F:376:LEU:HD13	1.58	0.84
2:C:261:LEU:HB3	2:C:262:PRO:CD	2.07	0.84
2:F:275:PHE:CD2	2:F:276:ALA:N	2.45	0.84
1:A:97:THR:H	1:A:573:ARG:HH12	1.25	0.84
1:B:115:ILE:HG13	1:B:117:LYS:H	1.41	0.84
2:F:25:LEU:HD21	3:G:47:LEU:HD22	1.59	0.84
1:B:101:LYS:HD3	1:B:415:MET:HB2	1.60	0.84
2:F:231:ILE:HD11	3:G:27:LEU:HD12	1.57	0.83
2:F:239:ARG:HD3	2:F:251:ARG:HH12	1.42	0.83
1:B:76:PRO:HD2	6:B:873:ADP:C6	2.13	0.83
1:A:460:TYR:O	1:A:463:ILE:HG22	1.79	0.83
2:F:275:PHE:CE2	2:F:314:VAL:HG22	2.14	0.83
1:A:306:LEU:HD21	1:A:309:GLU:HG3	1.59	0.82
1:A:502:GLN:HG2	1:A:526:THR:HG23	1.60	0.82
1:A:74:MET:HA	6:A:873:ADP:C6	2.13	0.82
1:B:292:ASP:HB2	1:B:313:LYS:HD3	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:275:PHE:CE2	2:C:314:VAL:HG22	2.14	0.82
1:A:101:LYS:HD3	1:A:415:MET:HB3	1.62	0.82
1:B:187:LEU:CD1	6:B:873:ADP:H2	1.92	0.82
1:A:159:VAL:HG12	1:A:160:VAL:H	1.45	0.82
1:A:786:PRO:HB3	4:E:41:THR:HB	1.62	0.82
1:A:76:PRO:HD2	6:A:873:ADP:C6	2.13	0.81
1:B:306:LEU:HD21	1:B:309:GLU:HG3	1.59	0.81
1:B:502:GLN:HG2	1:B:526:THR:HG23	1.60	0.81
1:B:460:TYR:O	1:B:463:ILE:HG22	1.79	0.81
1:B:75:ARG:H	1:B:76:PRO:CD	1.94	0.81
1:A:292:ASP:HB2	1:A:313:LYS:HD3	1.62	0.81
2:C:309:ILE:CG2	2:C:313:LEU:HD11	2.11	0.81
1:B:612:GLN:H	1:B:613:PRO:HD2	1.42	0.81
1:A:75:ARG:H	1:A:76:PRO:CD	1.94	0.81
1:B:97:THR:H	1:B:573:ARG:HH12	1.25	0.81
1:B:159:VAL:HG12	1:B:160:VAL:H	1.45	0.81
1:B:403:GLN:HG3	1:B:429:VAL:HG12	1.63	0.81
1:A:94:GLU:O	1:A:95:MET:HB2	1.80	0.81
1:B:94:GLU:O	1:B:95:MET:HB2	1.80	0.80
1:A:403:GLN:HG3	1:A:429:VAL:HG12	1.63	0.80
1:B:334:HIS:HA	1:B:337:ASN:HD22	1.47	0.80
1:A:635:PHE:HA	1:A:638:ARG:HE	1.46	0.80
2:C:315:PHE:HZ	2:C:370:LEU:HB2	1.46	0.80
2:F:173:TRP:HE1	4:H:57:LEU:HD12	1.44	0.80
1:B:635:PHE:HA	1:B:638:ARG:HE	1.46	0.80
2:F:309:ILE:CG2	2:F:313:LEU:HD11	2.11	0.80
1:A:75:ARG:H	1:A:76:PRO:HD3	1.46	0.79
1:B:74:MET:H	1:B:187:LEU:HD13	1.47	0.79
2:F:315:PHE:HZ	2:F:370:LEU:HB2	1.45	0.79
1:B:557:ARG:HG3	1:B:584:LEU:HD21	1.65	0.79
1:B:313:LYS:HA	1:B:316:LYS:HB2	1.64	0.79
2:F:232:LEU:CB	2:F:267:GLN:HB2	2.08	0.79
1:B:445:ARG:HH22	1:B:569:GLY:HA2	1.47	0.79
1:A:285:ILE:HG12	1:A:334:HIS:HD2	1.48	0.79
1:B:285:ILE:HG12	1:B:334:HIS:HD2	1.47	0.79
1:A:115:ILE:HD12	1:A:117:LYS:HE3	1.65	0.79
1:A:101:LYS:HE3	1:A:416:THR:OG1	1.83	0.78
1:B:134:LEU:HD21	1:B:204:LEU:HD11	1.64	0.78
1:A:101:LYS:CD	1:A:415:MET:HB3	2.13	0.78
2:C:231:ILE:O	2:C:232:LEU:O	2.00	0.78
2:C:249:THR:HG22	2:C:250:GLY:H	1.45	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:ILE:H	1:B:359:ILE:HD12	1.48	0.78
1:A:373:ARG:HE	1:A:374:TYR:N	1.81	0.78
1:B:775:ALA:HA	1:B:778:LEU:HD12	1.65	0.78
1:A:313:LYS:HA	1:A:316:LYS:HB2	1.64	0.78
1:B:635:PHE:O	1:B:638:ARG:HB3	1.83	0.78
1:A:785:ASP:H	1:A:786:PRO:HD3	1.49	0.78
1:B:75:ARG:H	1:B:76:PRO:HD3	1.46	0.78
1:A:635:PHE:O	1:A:638:ARG:HB3	1.83	0.78
1:A:210:LYS:HG3	1:A:211:GLU:H	1.48	0.78
1:B:403:GLN:HG2	1:B:407:ARG:HD3	1.66	0.78
1:A:134:LEU:HD21	1:A:204:LEU:HD11	1.65	0.78
1:A:403:GLN:HG2	1:A:407:ARG:HD3	1.66	0.78
1:B:778:LEU:HD23	2:F:264:LYS:HE3	1.63	0.78
1:B:784:LYS:HB3	1:B:786:PRO:CD	2.13	0.78
1:A:80:GLN:HG3	1:A:81:VAL:H	1.49	0.77
1:B:373:ARG:HG2	1:B:379:HIS:HB2	1.66	0.77
1:A:359:ILE:H	1:A:359:ILE:HD12	1.48	0.77
1:B:115:ILE:HD12	1:B:117:LYS:HE3	1.65	0.77
2:F:35:PRO:CG	4:H:68:VAL:HA	2.11	0.77
1:A:784:LYS:HB3	1:A:786:PRO:CD	2.13	0.77
1:B:177:VAL:HG11	1:B:193:ASN:HD22	1.49	0.77
1:A:74:MET:H	1:A:187:LEU:HD13	1.48	0.77
1:A:373:ARG:HG2	1:A:379:HIS:HB2	1.66	0.77
1:A:445:ARG:HH22	1:A:569:GLY:HA2	1.47	0.77
1:A:557:ARG:HG3	1:A:584:LEU:HD21	1.65	0.77
2:C:18:ILE:HD12	2:C:18:ILE:H	1.49	0.77
2:C:25:LEU:HD21	3:D:47:LEU:HD22	1.66	0.77
1:B:74:MET:HA	6:B:873:ADP:C2	2.19	0.77
1:A:779:ARG:HH21	1:A:786:PRO:N	1.83	0.77
1:B:779:ARG:HH21	1:B:786:PRO:N	1.83	0.77
1:A:177:VAL:HG11	1:A:193:ASN:HD22	1.49	0.77
1:A:775:ALA:HA	1:A:778:LEU:HD12	1.65	0.77
1:A:574:GLN:CG	6:A:873:ADP:H1'	2.14	0.77
3:G:13:ALA:HB1	3:G:17:LYS:HE3	1.67	0.77
1:A:325:ASP:HB3	2:C:345:LEU:HG	1.67	0.77
1:A:334:HIS:HA	1:A:337:ASN:HD22	1.47	0.77
1:A:779:ARG:HH22	1:A:788:VAL:H	1.33	0.77
2:F:275:PHE:CD2	2:F:314:VAL:HG22	2.20	0.76
2:C:236:ALA:HB3	2:C:262:PRO:C	2.09	0.76
1:B:718:SER:HB2	1:B:723:LEU:HD13	1.67	0.76
1:A:785:ASP:H	1:A:786:PRO:CD	1.99	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:VAL:HG21	1:B:251:VAL:HG22	1.68	0.76
1:B:210:LYS:HG3	1:B:211:GLU:H	1.48	0.76
1:B:785:ASP:H	1:B:786:PRO:HD3	1.49	0.76
1:A:718:SER:HB2	1:A:723:LEU:HD13	1.67	0.76
1:A:459:LYS:HG2	1:A:585:SER:HB2	1.68	0.76
1:A:574:GLN:HG3	6:A:873:ADP:H1'	1.66	0.76
1:B:340:LYS:HZ2	2:F:251:ARG:HE	1.34	0.76
2:F:18:ILE:H	2:F:18:ILE:HD12	1.49	0.76
2:F:356:HIS:HA	2:F:359:LEU:HD12	1.68	0.76
3:D:13:ALA:HB1	3:D:17:LYS:HE3	1.67	0.76
1:B:134:LEU:HD22	1:B:202:VAL:HG13	1.67	0.76
2:F:125:LEU:HD22	4:H:26:LYS:HE2	1.67	0.76
1:A:476:PRO:HG3	1:A:523:GLY:H	1.50	0.76
1:B:470:ARG:HH21	1:B:475:GLN:HE22	1.34	0.76
1:A:134:LEU:HD22	1:A:202:VAL:HG13	1.66	0.75
1:B:761:HIS:HB3	1:B:801:MET:HE2	1.68	0.75
2:C:356:HIS:HA	2:C:359:LEU:HD12	1.68	0.75
1:B:785:ASP:H	1:B:786:PRO:CD	1.99	0.75
1:A:93:ALA:O	1:A:94:GLU:CG	2.33	0.75
1:A:470:ARG:HH21	1:A:475:GLN:HE22	1.34	0.75
1:B:80:GLN:HG3	1:B:81:VAL:H	1.49	0.75
1:B:412:LEU:HB2	1:B:432:MET:HE3	1.69	0.75
1:A:93:ALA:C	1:A:94:GLU:HG2	2.11	0.75
1:B:476:PRO:HG3	1:B:523:GLY:H	1.50	0.75
1:A:122:VAL:HG23	1:A:251:VAL:HA	1.68	0.75
1:A:761:HIS:HB3	1:A:801:MET:HE2	1.67	0.75
2:C:84:PRO:HA	2:C:87:THR:HB	1.69	0.75
1:A:122:VAL:HG21	1:A:251:VAL:HG22	1.68	0.74
1:A:155:LYS:HD2	1:A:208:THR:C	2.12	0.74
1:B:79:VAL:HG23	1:B:94:GLU:OE1	1.86	0.74
1:A:412:LEU:HB2	1:A:432:MET:HE3	1.69	0.74
1:B:74:MET:HA	6:B:873:ADP:C6	2.21	0.74
1:B:97:THR:N	1:B:573:ARG:HH12	1.85	0.74
1:B:222:ASN:HD22	1:B:401:THR:HG21	1.51	0.74
1:B:463:ILE:HD11	1:B:553:ILE:HB	1.69	0.74
1:B:94:GLU:OE1	1:B:94:GLU:CA	2.36	0.74
1:B:573:ARG:HB3	6:B:873:ADP:H4'	1.69	0.74
2:F:362:VAL:HA	2:F:365:ILE:HD12	1.69	0.74
2:F:236:ALA:HB3	2:F:262:PRO:C	2.12	0.74
2:C:275:PHE:CD2	2:C:314:VAL:HG22	2.20	0.74
1:B:122:VAL:HG23	1:B:251:VAL:HA	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:THR:N	1:A:573:ARG:HH12	1.85	0.74
1:A:222:ASN:HD22	1:A:401:THR:HG21	1.51	0.74
1:B:779:ARG:HH22	1:B:788:VAL:H	1.33	0.74
1:B:147:VAL:HG13	1:B:157:TYR:HB2	1.69	0.74
1:A:644:MET:O	1:A:647:VAL:HG12	1.87	0.74
2:F:238:ARG:HG3	2:F:239:ARG:HG2	1.68	0.74
1:A:93:ALA:C	1:A:94:GLU:CG	2.60	0.74
1:B:644:MET:O	1:B:647:VAL:HG12	1.87	0.74
1:B:207:ILE:HG22	1:B:208:THR:H	1.53	0.74
1:B:459:LYS:HG2	1:B:585:SER:HB2	1.68	0.74
2:F:84:PRO:HA	2:F:87:THR:HB	1.69	0.74
1:A:662:ILE:HD12	1:A:754:MET:HB3	1.69	0.73
1:A:784:LYS:HB3	1:A:786:PRO:HD2	1.69	0.73
1:B:373:ARG:HE	1:B:374:TYR:N	1.81	0.73
1:A:451:LEU:HG	1:A:581:ILE:HD11	1.70	0.73
1:B:662:ILE:HD12	1:B:754:MET:HB3	1.69	0.73
2:F:230:ILE:O	2:F:232:LEU:HD13	1.88	0.73
1:A:207:ILE:HG22	1:A:208:THR:H	1.53	0.73
2:C:342:ILE:HG23	2:C:343:PRO:HD2	1.71	0.73
2:C:362:VAL:HA	2:C:365:ILE:HD12	1.69	0.73
1:B:187:LEU:HD23	1:B:187:LEU:H	1.53	0.73
2:C:238:ARG:HG3	2:C:239:ARG:HG2	1.70	0.73
1:B:155:LYS:HD2	1:B:208:THR:C	2.12	0.73
1:B:784:LYS:HB3	1:B:786:PRO:HD2	1.69	0.73
2:C:373:ILE:HG21	2:C:396:LEU:HD21	1.71	0.72
1:A:187:LEU:H	1:A:187:LEU:HD23	1.53	0.72
1:A:54:ASP:HA	1:A:57:LEU:HD12	1.71	0.72
1:A:147:VAL:HG13	1:A:157:TYR:HB2	1.69	0.72
2:F:309:ILE:HG22	2:F:313:LEU:HD12	1.72	0.72
1:A:75:ARG:N	6:A:873:ADP:N6	2.37	0.72
1:A:773:LYS:O	1:A:776:VAL:HG22	1.90	0.72
1:B:451:LEU:HG	1:B:581:ILE:HD11	1.70	0.72
1:B:618:MET:HA	1:B:621:LYS:HD2	1.71	0.72
1:A:96:LYS:HE3	1:A:569:GLY:HA3	1.70	0.72
1:B:325:ASP:HB3	2:F:345:LEU:HG	1.71	0.72
1:A:545:ALA:HA	1:A:549:GLY:HA2	1.71	0.72
2:C:306:TYR:HA	2:C:309:ILE:HD12	1.72	0.72
1:B:478:LEU:HD12	1:B:479:VAL:H	1.55	0.72
2:C:35:PRO:O	2:C:36:VAL:HB	1.90	0.72
1:B:96:LYS:HE3	1:B:569:GLY:HA3	1.70	0.72
2:F:355:LEU:O	2:F:359:LEU:HG	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:35:PRO:O	2:F:36:VAL:HB	1.90	0.72
1:A:463:ILE:HD11	1:A:553:ILE:HB	1.69	0.72
2:C:355:LEU:O	2:C:359:LEU:HG	1.89	0.72
2:F:373:ILE:HG21	2:F:396:LEU:HD21	1.71	0.72
2:C:309:ILE:HG22	2:C:313:LEU:HD11	1.71	0.71
1:B:54:ASP:HA	1:B:57:LEU:HD12	1.71	0.71
4:H:11:ILE:O	4:H:15:ALA:HB2	1.90	0.71
1:B:247:PHE:C	1:B:410:GLU:HB3	2.15	0.71
2:F:231:ILE:O	2:F:232:LEU:O	2.09	0.71
2:F:306:TYR:HA	2:F:309:ILE:HD12	1.72	0.71
4:E:11:ILE:O	4:E:15:ALA:HB2	1.90	0.71
1:A:247:PHE:C	1:A:410:GLU:HB3	2.15	0.71
1:A:550:LEU:HD23	1:A:551:CYS:N	2.06	0.71
1:A:574:GLN:CB	6:A:873:ADP:H1'	2.20	0.71
4:E:51:THR:HG22	4:E:53:GLY:H	1.55	0.71
2:F:341:TYR:O	2:F:342:ILE:HB	1.89	0.71
1:A:247:PHE:O	1:A:410:GLU:HB3	1.91	0.70
1:A:573:ARG:HB3	6:A:873:ADP:H4'	1.72	0.70
1:B:98:GLY:H	1:B:574:GLN:N	1.88	0.70
1:B:550:LEU:HD23	1:B:551:CYS:N	2.06	0.70
1:B:247:PHE:O	1:B:410:GLU:HB3	1.91	0.70
1:B:773:LYS:O	1:B:776:VAL:HG22	1.90	0.70
1:A:618:MET:HA	1:A:621:LYS:HD2	1.71	0.70
2:C:309:ILE:HG22	2:C:313:LEU:HD12	1.71	0.70
1:A:98:GLY:H	1:A:574:GLN:N	1.88	0.70
2:C:341:TYR:O	2:C:342:ILE:HB	1.90	0.70
4:H:51:THR:HG22	4:H:53:GLY:H	1.55	0.70
1:A:785:ASP:N	1:A:786:PRO:CD	2.54	0.70
2:F:183:ILE:HG23	2:F:186:GLY:N	2.07	0.70
1:B:100:GLY:C	6:B:873:ADP:O1A	2.34	0.70
1:B:416:THR:HG22	1:B:417:GLY:H	1.55	0.70
1:B:457:LYS:HG2	1:B:460:TYR:HB3	1.73	0.70
1:B:635:PHE:HA	1:B:638:ARG:NE	2.06	0.70
1:B:785:ASP:N	1:B:786:PRO:CD	2.54	0.70
2:F:224:LEU:HD11	3:G:34:LEU:HD11	1.71	0.70
2:C:183:ILE:HG23	2:C:186:GLY:N	2.07	0.70
1:A:453:PHE:HB2	1:A:459:LYS:HB3	1.73	0.70
1:B:453:PHE:HB2	1:B:459:LYS:HB3	1.73	0.70
1:B:545:ALA:HA	1:B:549:GLY:HA2	1.71	0.70
1:B:6:LYS:O	1:B:10:ILE:HG12	1.91	0.69
1:A:478:LEU:HD12	1:A:479:VAL:H	1.55	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:174:LEU:O	2:F:178:ILE:HG12	1.93	0.69
2:C:174:LEU:O	2:C:178:ILE:HG12	1.93	0.69
2:F:232:LEU:HD22	2:F:232:LEU:N	2.07	0.69
2:F:261:LEU:HB3	2:F:262:PRO:CD	2.18	0.69
1:A:74:MET:HA	6:A:873:ADP:C2	2.28	0.69
1:B:75:ARG:N	6:B:873:ADP:N6	2.40	0.69
1:B:96:LYS:HB2	1:B:573:ARG:HH22	1.57	0.69
1:A:187:LEU:CD1	6:A:873:ADP:C2	2.64	0.69
1:A:778:LEU:HD23	2:C:264:LYS:HE3	1.74	0.69
2:F:233:VAL:O	2:F:265:VAL:HB	1.92	0.69
1:B:473:LYS:HE2	1:B:473:LYS:HA	1.74	0.69
1:A:6:LYS:O	1:A:10:ILE:HG12	1.91	0.69
1:B:247:PHE:HB2	1:B:410:GLU:HB2	1.75	0.69
1:A:247:PHE:HB2	1:A:410:GLU:HB2	1.75	0.69
1:A:473:LYS:HE2	1:A:473:LYS:HA	1.75	0.69
1:B:454:ARG:HG2	1:B:586:LEU:HD13	1.75	0.69
2:C:309:ILE:CG2	2:C:313:LEU:CD1	2.69	0.69
1:B:93:ALA:O	1:B:94:GLU:HB2	1.93	0.69
2:F:80:MET:HG3	2:F:84:PRO:HD3	1.75	0.69
1:A:669:ASP:O	1:A:672:LEU:HG	1.94	0.69
2:C:87:THR:O	2:C:91:ILE:HG12	1.93	0.69
1:B:141:LEU:HB2	1:B:159:VAL:HG11	1.75	0.69
1:A:416:THR:HG22	1:A:417:GLY:H	1.55	0.68
1:A:457:LYS:HG2	1:A:460:TYR:HB3	1.73	0.68
1:A:573:ARG:HA	1:A:573:ARG:HH11	1.59	0.68
2:C:125:LEU:HD13	4:E:26:LYS:HD3	1.75	0.68
2:C:328:PRO:HG3	2:C:352:GLU:HB2	1.74	0.68
1:A:529:THR:HB	1:A:531:MET:HG2	1.76	0.68
1:A:573:ARG:CZ	6:A:873:ADP:O1B	2.41	0.68
1:B:557:ARG:HD2	1:B:584:LEU:HD11	1.75	0.68
1:A:234:LEU:HD21	1:B:745:ASP:OD2	1.94	0.68
1:A:635:PHE:HA	1:A:638:ARG:NE	2.06	0.68
1:A:96:LYS:HB2	1:A:573:ARG:HH22	1.57	0.68
1:B:397:TYR:HE2	1:B:652:ARG:HG3	1.58	0.68
1:B:574:GLN:HG3	6:B:873:ADP:H1'	1.75	0.68
2:F:35:PRO:HG2	4:H:68:VAL:CA	2.17	0.68
2:F:87:THR:O	2:F:91:ILE:HG12	1.93	0.68
1:B:529:THR:HB	1:B:531:MET:HG2	1.76	0.68
1:A:141:LEU:HB2	1:A:159:VAL:HG11	1.75	0.68
1:A:284:GLN:O	1:A:288:LYS:HG2	1.94	0.68
2:C:377:PRO:HG3	2:C:389:TRP:NE1	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:GLN:O	1:B:288:LYS:HG2	1.94	0.68
1:B:573:ARG:CZ	6:B:873:ADP:O1B	2.42	0.68
2:F:251:ARG:NH2	2:F:335:ILE:HD13	2.08	0.68
2:F:377:PRO:HG3	2:F:389:TRP:NE1	2.08	0.68
1:A:146:ARG:HG2	1:A:215:CYS:SG	2.34	0.68
1:A:281:ARG:NE	1:A:285:ILE:HD11	2.09	0.68
2:C:230:ILE:O	2:C:232:LEU:CD1	2.42	0.68
1:B:669:ASP:O	1:B:672:LEU:HG	1.93	0.68
1:A:397:TYR:HE2	1:A:652:ARG:HG3	1.58	0.68
1:B:146:ARG:HG2	1:B:215:CYS:SG	2.34	0.68
1:B:478:LEU:HD12	1:B:479:VAL:N	2.09	0.68
1:A:43:LEU:HA	1:A:46:LYS:HB2	1.76	0.67
1:A:504:LEU:HG	1:A:528:ALA:HB2	1.77	0.67
2:C:403:LEU:HA	2:C:406:ILE:HD12	1.75	0.67
1:B:373:ARG:HG3	1:B:375:SER:H	1.60	0.67
1:A:478:LEU:HD12	1:A:479:VAL:N	2.09	0.67
1:A:74:MET:SD	6:A:873:ADP:H2'	2.35	0.67
2:C:80:MET:HG3	2:C:84:PRO:HD3	1.75	0.67
1:A:454:ARG:HG2	1:A:586:LEU:HD13	1.75	0.67
1:A:557:ARG:HD2	1:A:584:LEU:HD11	1.75	0.67
1:A:585:SER:HB3	1:A:588:ASP:OD2	1.94	0.67
1:B:476:PRO:HG3	1:B:523:GLY:N	2.09	0.67
2:F:274:ILE:HG12	2:F:393:THR:HG23	1.76	0.67
1:B:504:LEU:HG	1:B:528:ALA:HB2	1.77	0.67
2:F:403:LEU:HA	2:F:406:ILE:HD12	1.76	0.67
1:A:478:LEU:HA	1:A:526:THR:O	1.95	0.67
1:A:783:GLN:HG2	1:A:784:LYS:H	1.59	0.67
2:C:188:SER:HA	2:C:191:ILE:HD12	1.76	0.67
1:A:373:ARG:HG3	1:A:375:SER:H	1.60	0.67
1:A:476:PRO:HG3	1:A:523:GLY:N	2.09	0.67
1:B:298:ASP:O	1:B:299:GLU:HG3	1.95	0.67
1:B:478:LEU:HA	1:B:526:THR:O	1.95	0.67
1:A:74:MET:HE2	6:A:873:ADP:C2	2.30	0.67
1:A:296:THR:HA	1:A:306:LEU:HB2	1.77	0.67
1:B:281:ARG:NE	1:B:285:ILE:HD11	2.09	0.67
1:A:298:ASP:O	1:A:299:GLU:HG3	1.95	0.67
1:A:673:LYS:HE3	1:A:733:GLU:HA	1.77	0.67
2:C:232:LEU:HD22	2:C:232:LEU:N	2.09	0.67
1:B:573:ARG:HH11	1:B:573:ARG:HA	1.58	0.67
2:F:178:ILE:HG13	2:F:187:ILE:HG23	1.77	0.67
2:F:188:SER:HA	2:F:191:ILE:HD12	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:VAL:HG21	1:B:257:VAL:HG21	1.77	0.66
2:F:237:GLU:HB3	2:F:338:TYR:HA	1.76	0.66
2:C:155:GLN:C	2:C:157:THR:H	2.03	0.66
2:C:233:VAL:HA	3:D:25:GLU:HG3	1.76	0.66
2:C:274:ILE:HG12	2:C:393:THR:HG23	1.76	0.66
1:B:585:SER:HB3	1:B:588:ASP:OD2	1.94	0.66
1:A:75:ARG:HH22	1:A:187:LEU:HB3	1.60	0.66
2:C:237:GLU:HB3	2:C:338:TYR:HA	1.78	0.66
1:B:75:ARG:HH22	1:B:187:LEU:HB3	1.60	0.66
1:B:778:LEU:HA	2:F:264:LYS:HE3	1.77	0.66
2:F:155:GLN:C	2:F:157:THR:H	2.03	0.66
1:B:574:GLN:CG	6:B:873:ADP:HI'	2.26	0.66
1:B:71:THR:HB	1:B:138:PRO:HB3	1.77	0.66
1:B:765:TYR:HD2	1:B:797:MET:HG3	1.60	0.66
1:A:404:ASN:O	1:A:408:MET:HB2	1.94	0.66
1:A:765:TYR:HD2	1:A:797:MET:HG3	1.61	0.66
1:B:783:GLN:HG2	1:B:784:LYS:H	1.59	0.66
2:F:342:ILE:HG23	2:F:343:PRO:HD2	1.77	0.66
2:C:178:ILE:HG13	2:C:187:ILE:HG23	1.77	0.66
1:B:43:LEU:HA	1:B:46:LYS:HB2	1.76	0.66
1:B:80:GLN:HG3	1:B:81:VAL:N	2.11	0.66
1:B:84:GLY:HA2	1:B:87:LEU:HD12	1.77	0.66
1:B:673:LYS:HE3	1:B:733:GLU:HA	1.77	0.66
1:A:254:ALA:O	1:A:257:VAL:HG12	1.95	0.66
1:B:254:ALA:O	1:B:257:VAL:HG12	1.95	0.66
1:B:267:ILE:HG22	1:B:395:ILE:HA	1.77	0.66
1:A:71:THR:HB	1:A:138:PRO:HB3	1.77	0.65
1:A:645:ASP:HA	1:A:648:LEU:HD12	1.78	0.65
1:B:416:THR:HG22	1:B:417:GLY:N	2.11	0.65
1:A:416:THR:HG22	1:A:417:GLY:N	2.11	0.65
1:A:778:LEU:HB3	2:C:263:ILE:O	1.95	0.65
2:C:119:TYR:O	2:C:123:LEU:HB2	1.96	0.65
1:B:404:ASN:O	1:B:408:MET:HB2	1.94	0.65
2:F:237:GLU:HG3	2:F:336:ARG:HB3	1.77	0.65
1:B:131:ARG:NH2	7:B:874:BEF:F3	2.20	0.65
1:B:64:VAL:HG11	1:B:107:MET:HA	1.77	0.65
1:B:120:HIS:HB2	1:B:249:ALA:HB2	1.78	0.65
1:B:296:THR:HA	1:B:306:LEU:HB2	1.77	0.65
1:A:120:HIS:HB2	1:A:249:ALA:HB2	1.78	0.65
1:A:134:LEU:HD13	1:A:202:VAL:HG13	1.79	0.65
1:B:258:LEU:HD11	1:B:638:ARG:NH1	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:LYS:HE3	1:B:335:LEU:HD11	1.77	0.65
1:A:258:LEU:HD11	1:A:638:ARG:NH1	2.11	0.65
1:A:267:ILE:HG22	1:A:395:ILE:HA	1.77	0.65
1:A:275:SER:HB3	1:A:391:LYS:HB2	1.79	0.65
1:B:767:GLU:HA	2:F:252:ARG:HH12	1.62	0.65
1:B:134:LEU:HD13	1:B:202:VAL:HG13	1.79	0.65
1:B:275:SER:HB3	1:B:391:LYS:HB2	1.79	0.65
2:C:189:ILE:HB	2:C:401:VAL:HG11	1.78	0.65
1:B:155:LYS:HZ3	1:B:209:ARG:HD2	1.62	0.65
1:B:651:GLN:O	1:B:655:VAL:HG23	1.96	0.65
1:A:84:GLY:HA2	1:A:87:LEU:HD12	1.77	0.65
1:A:313:LYS:HE3	1:A:335:LEU:HD11	1.77	0.65
1:A:64:VAL:HG11	1:A:107:MET:HA	1.77	0.65
1:B:626:ILE:O	1:B:629:LYS:HB3	1.97	0.64
2:C:173:TRP:HE1	4:E:57:LEU:HD12	1.62	0.64
1:A:651:GLN:O	1:A:655:VAL:HG23	1.96	0.64
1:B:281:ARG:HE	1:B:285:ILE:HD11	1.63	0.64
1:B:786:PRO:HB3	4:H:41:THR:HB	1.80	0.64
2:F:35:PRO:O	2:F:37:PRO:HD3	1.97	0.64
2:F:232:LEU:HG	2:F:266:ASN:HA	1.78	0.64
1:B:188:LYS:HD2	1:B:189:GLU:H	1.62	0.64
1:B:574:GLN:CB	6:B:873:ADP:HI'	2.27	0.64
1:A:80:GLN:HG3	1:A:81:VAL:N	2.11	0.64
1:A:251:VAL:HG21	1:A:257:VAL:HG21	1.77	0.64
1:A:263:ARG:HH11	1:A:641:LEU:HD11	1.62	0.64
2:C:331:ILE:HG23	2:C:336:ARG:HD3	1.80	0.64
1:B:178:TRP:CG	1:B:194:LYS:HZ3	2.16	0.64
2:C:237:GLU:HG3	2:C:336:ARG:HB3	1.78	0.64
1:A:75:ARG:HH21	1:A:187:LEU:HD22	1.63	0.64
1:A:508:TYR:HB3	1:A:511:LYS:HG3	1.80	0.64
1:B:645:ASP:HA	1:B:648:LEU:HD12	1.78	0.64
2:F:217:ILE:HA	2:F:220:ILE:HD12	1.79	0.64
1:A:188:LYS:HB3	1:A:190:GLU:OE1	1.98	0.64
1:A:284:GLN:HG2	1:A:288:LYS:HZ2	1.63	0.64
2:F:108:GLU:HB2	2:F:112:GLY:H	1.63	0.64
2:F:119:TYR:O	2:F:123:LEU:HB2	1.96	0.64
2:F:309:ILE:CG2	2:F:313:LEU:CD1	2.69	0.64
2:C:76:SER:HB3	2:C:78:PHE:O	1.99	0.63
1:B:779:ARG:HH22	1:B:788:VAL:HG23	1.63	0.63
2:F:190:LEU:HD21	3:G:51:PHE:HZ	1.63	0.63
2:C:80:MET:HE2	2:C:83:THR:HG21	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:LYS:HD2	1:A:189:GLU:H	1.62	0.63
1:A:779:ARG:HH22	1:A:788:VAL:HG23	1.63	0.63
1:B:144:GLY:O	1:B:145:LEU:HD23	1.98	0.63
1:B:156:SER:HA	1:B:207:ILE:HD12	1.81	0.63
1:B:484:ILE:HD13	1:B:485:GLU:H	1.63	0.63
2:F:189:ILE:HB	2:F:401:VAL:HG11	1.78	0.63
1:A:5:ASP:O	1:A:9:ARG:HB2	1.99	0.63
1:A:74:MET:O	1:A:103:LEU:HD13	1.99	0.63
1:A:144:GLY:O	1:A:145:LEU:HD23	1.98	0.63
1:A:281:ARG:HE	1:A:285:ILE:HD11	1.63	0.63
1:A:626:ILE:O	1:A:629:LYS:HB3	1.97	0.63
2:C:35:PRO:O	2:C:37:PRO:HD3	1.97	0.63
1:B:5:ASP:O	1:B:9:ARG:HB2	1.99	0.63
1:B:187:LEU:CD1	6:B:873:ADP:C2	2.77	0.63
1:A:156:SER:HA	1:A:207:ILE:HD12	1.81	0.63
1:A:590:LEU:HD23	1:A:590:LEU:H	1.64	0.63
1:B:188:LYS:HB3	1:B:190:GLU:OE1	1.98	0.63
2:F:76:SER:HB3	2:F:78:PHE:O	1.99	0.63
1:A:410:GLU:CG	1:A:411:LYS:H	2.08	0.63
1:A:480:GLY:HA3	1:A:567:LEU:HD11	1.80	0.63
2:C:334:ASN:C	2:C:335:ILE:HD12	2.22	0.63
1:B:618:MET:H	1:B:621:LYS:NZ	1.97	0.63
2:F:331:ILE:HG23	2:F:336:ARG:HD3	1.80	0.63
1:B:590:LEU:HD23	1:B:590:LEU:H	1.64	0.63
1:B:730:ARG:O	1:B:734:GLU:HB2	1.99	0.63
1:A:359:ILE:HD13	1:A:383:GLU:CD	2.24	0.63
1:A:730:ARG:O	1:A:734:GLU:HB2	1.99	0.63
2:C:368:VAL:O	2:C:372:VAL:HB	1.99	0.63
1:B:155:LYS:HE2	1:B:209:ARG:HA	1.80	0.63
1:A:187:LEU:HD21	6:A:873:ADP:C2	2.33	0.63
1:A:323:LEU:HD23	1:A:323:LEU:H	1.64	0.63
1:A:737:ARG:HA	1:A:740:GLN:HB2	1.81	0.63
1:B:263:ARG:HH11	1:B:641:LEU:HD11	1.62	0.63
1:B:680:VAL:O	1:B:684:VAL:HG23	1.99	0.63
1:B:749:VAL:O	1:B:753:LEU:HD23	1.98	0.63
2:F:368:VAL:O	2:F:372:VAL:HB	1.99	0.63
1:A:484:ILE:HD13	1:A:485:GLU:H	1.63	0.62
1:A:618:MET:H	1:A:621:LYS:NZ	1.97	0.62
1:B:98:GLY:H	1:B:574:GLN:H	1.47	0.62
1:B:359:ILE:HD13	1:B:383:GLU:CD	2.24	0.62
1:B:679:VAL:CG1	1:B:803:ARG:HE	2.12	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:765:TYR:O	1:B:769:VAL:HG23	1.99	0.62
1:A:98:GLY:H	1:A:574:GLN:H	1.48	0.62
1:A:131:ARG:NH2	7:A:874:BEF:F3	2.22	0.62
1:A:178:TRP:HB2	1:A:194:LYS:HD3	1.82	0.62
1:A:456:GLN:C	1:A:458:GLU:H	2.07	0.62
2:C:217:ILE:HA	2:C:220:ILE:HD12	1.79	0.62
2:C:224:LEU:HD11	3:D:34:LEU:HD11	1.81	0.62
2:C:251:ARG:HH21	2:C:335:ILE:HD13	1.64	0.62
1:B:480:GLY:HA3	1:B:567:LEU:HD11	1.80	0.62
1:B:776:VAL:O	1:B:779:ARG:HG2	2.00	0.62
1:A:690:GLY:HA2	1:A:695:ILE:HG21	1.81	0.62
1:B:456:GLN:C	1:B:458:GLU:H	2.08	0.62
1:B:659:ARG:HG2	1:B:755:LEU:HG	1.81	0.62
2:F:80:MET:HE2	2:F:83:THR:HG21	1.79	0.62
2:F:369:PHE:O	2:F:372:VAL:HG12	2.00	0.62
1:A:679:VAL:CG1	1:A:803:ARG:HE	2.13	0.62
1:A:749:VAL:O	1:A:753:LEU:HD23	1.98	0.62
1:B:585:SER:C	1:B:587:GLU:H	2.07	0.62
1:A:155:LYS:HE2	1:A:209:ARG:HA	1.80	0.62
1:B:323:LEU:H	1:B:323:LEU:HD23	1.64	0.62
1:B:643:GLU:O	1:B:646:ASP:HB2	1.99	0.62
1:A:28:LEU:HA	1:A:32:LYS:NZ	2.15	0.62
1:A:573:ARG:HA	1:A:573:ARG:NH1	2.15	0.62
1:A:585:SER:C	1:A:587:GLU:H	2.08	0.62
1:A:765:TYR:O	1:A:769:VAL:HG23	1.99	0.62
1:B:236:LEU:HD11	1:B:752:PHE:HA	1.82	0.62
3:G:24:LYS:C	3:G:25:GLU:HG2	2.24	0.62
1:B:75:ARG:HH21	1:B:187:LEU:HD22	1.63	0.62
1:A:697:SER:O	1:A:700:ASN:HB3	2.00	0.62
1:B:508:TYR:HB3	1:B:511:LYS:HG3	1.80	0.62
2:F:276:ALA:HA	2:F:279:ILE:HD12	1.81	0.62
1:A:75:ARG:NH2	1:A:187:LEU:HD22	2.15	0.61
1:A:659:ARG:HG2	1:A:755:LEU:HG	1.81	0.61
1:A:680:VAL:O	1:A:684:VAL:HG23	1.99	0.61
1:A:776:VAL:O	1:A:779:ARG:HG2	2.00	0.61
2:C:315:PHE:CZ	2:C:367:ALA:HA	2.35	0.61
2:F:249:THR:HG22	2:F:250:GLY:N	2.13	0.61
1:A:643:GLU:O	1:A:646:ASP:HB2	1.99	0.61
1:A:784:LYS:HB3	1:A:786:PRO:HD3	1.81	0.61
1:B:74:MET:O	1:B:103:LEU:HD13	1.99	0.61
2:F:27:VAL:HG21	2:F:174:LEU:HD13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:GLY:C	6:A:873:ADP:O1A	2.43	0.61
1:A:535:GLY:H	1:A:570:ARG:CZ	2.13	0.61
2:C:108:GLU:HB2	2:C:112:GLY:H	1.63	0.61
1:B:164:PRO:O	1:B:168:ARG:HG3	2.00	0.61
2:F:159:LEU:HA	2:F:162:MET:HE3	1.82	0.61
1:A:103:LEU:HD23	1:A:103:LEU:H	1.65	0.61
1:A:346:LYS:HB3	1:A:349:VAL:HG23	1.82	0.61
2:C:173:TRP:HZ3	4:E:25:SER:HA	1.64	0.61
1:B:410:GLU:CG	1:B:411:LYS:H	2.08	0.61
1:B:697:SER:O	1:B:700:ASN:HB3	2.00	0.61
1:B:737:ARG:HA	1:B:740:GLN:HB2	1.81	0.61
1:A:38:ARG:O	1:A:42:VAL:HG23	2.01	0.61
1:A:164:PRO:O	1:A:168:ARG:HG3	2.00	0.61
1:A:178:TRP:CG	1:A:194:LYS:HZ3	2.18	0.61
2:C:276:ALA:HA	2:C:279:ILE:HD12	1.81	0.61
1:B:778:LEU:HB3	2:F:263:ILE:O	2.00	0.61
2:C:222:VAL:HA	2:C:225:ILE:HD12	1.83	0.61
1:B:28:LEU:HA	1:B:32:LYS:NZ	2.15	0.61
1:A:536:THR:HB	1:A:538:ILE:HD11	1.82	0.61
2:C:275:PHE:CE2	2:C:314:VAL:CG2	2.84	0.61
1:B:346:LYS:HB3	1:B:349:VAL:HG23	1.81	0.61
2:F:315:PHE:CZ	2:F:367:ALA:HA	2.35	0.61
1:A:285:ILE:HG22	1:A:338:ALA:HB2	1.83	0.61
1:A:330:SER:O	1:A:333:TYR:HB3	2.01	0.61
1:B:75:ARG:NH2	1:B:187:LEU:HD22	2.15	0.61
1:B:178:TRP:HB2	1:B:194:LYS:HD3	1.82	0.61
1:B:535:GLY:H	1:B:570:ARG:CZ	2.14	0.61
2:F:222:VAL:HA	2:F:225:ILE:HD12	1.83	0.61
2:F:267:GLN:HA	2:F:319:TYR:HE1	1.65	0.61
1:A:141:LEU:HD22	1:A:159:VAL:HG11	1.83	0.61
1:A:251:VAL:HG11	1:A:257:VAL:CB	2.28	0.61
2:C:259:THR:HG22	2:C:260:TYR:H	1.64	0.61
2:C:369:PHE:O	2:C:372:VAL:HG12	2.00	0.61
1:B:295:PHE:C	1:B:296:THR:HG1	2.09	0.61
1:B:540:LEU:HB2	1:B:544:VAL:HG11	1.83	0.61
1:A:535:GLY:H	1:A:570:ARG:NE	1.98	0.61
1:B:330:SER:O	1:B:333:TYR:HB3	2.01	0.61
1:B:659:ARG:HH12	1:B:759:ASP:CG	2.09	0.61
1:B:690:GLY:HA2	1:B:695:ILE:HG21	1.81	0.61
2:F:350:SER:HA	2:F:353:GLN:NE2	2.16	0.61
1:A:97:THR:CA	1:A:573:ARG:HH12	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ARG:O	1:B:42:VAL:HG23	2.01	0.60
1:B:573:ARG:HA	1:B:573:ARG:NH1	2.15	0.60
2:F:275:PHE:CE2	2:F:314:VAL:CG2	2.84	0.60
1:A:1:MET:SD	4:E:52:GLY:HA3	2.40	0.60
1:A:102:THR:OG1	1:A:103:LEU:HD23	2.01	0.60
1:A:494:LEU:HD12	1:A:499:ILE:HG21	1.84	0.60
1:A:512:GLU:O	1:A:516:VAL:HG23	2.01	0.60
1:A:573:ARG:HD3	6:A:873:ADP:O1B	2.01	0.60
1:B:535:GLY:H	1:B:570:ARG:NE	1.98	0.60
1:B:659:ARG:HH22	1:B:759:ASP:CG	2.09	0.60
1:A:586:LEU:H	1:A:586:LEU:HD12	1.67	0.60
1:A:659:ARG:HH22	1:A:759:ASP:CG	2.09	0.60
1:B:103:LEU:HD23	1:B:103:LEU:H	1.65	0.60
2:C:159:LEU:HA	2:C:162:MET:HE3	1.82	0.60
1:B:102:THR:OG1	1:B:103:LEU:HD23	2.01	0.60
1:B:784:LYS:HB3	1:B:786:PRO:HD3	1.81	0.60
1:A:236:LEU:HD11	1:A:752:PHE:HA	1.82	0.60
1:A:536:THR:O	1:A:573:ARG:HD2	2.02	0.60
2:C:27:VAL:HG21	2:C:174:LEU:HD13	1.82	0.60
1:B:74:MET:SD	6:B:873:ADP:H2'	2.41	0.60
2:F:338:TYR:O	2:F:344:GLY:HA3	2.01	0.60
1:A:659:ARG:HH12	1:A:759:ASP:CG	2.09	0.60
3:D:24:LYS:C	3:D:25:GLU:HG2	2.24	0.60
1:B:98:GLY:HA2	1:B:574:GLN:HA	1.84	0.60
1:B:141:LEU:HD22	1:B:159:VAL:HG11	1.83	0.60
1:B:284:GLN:HG2	1:B:288:LYS:HZ2	1.67	0.60
2:C:280:VAL:C	2:C:283:PRO:HD2	2.25	0.60
1:B:74:MET:HE2	6:B:873:ADP:C2	2.36	0.60
1:B:311:VAL:HG12	1:B:315:GLU:OE2	2.02	0.60
1:B:400:ILE:HG22	1:B:404:ASN:H	1.67	0.60
1:A:97:THR:HA	1:A:573:ARG:HH12	1.67	0.60
1:A:155:LYS:HZ3	1:A:209:ARG:HD2	1.66	0.60
1:A:311:VAL:HG12	1:A:315:GLU:OE2	2.02	0.60
1:A:540:LEU:HB2	1:A:544:VAL:HG11	1.83	0.60
1:A:745:ASP:OD2	1:B:234:LEU:HD21	2.02	0.60
2:C:309:ILE:O	2:C:313:LEU:HG	2.02	0.60
2:C:319:TYR:HE2	2:C:359:LEU:HB3	1.66	0.60
1:B:775:ALA:O	1:B:778:LEU:HB2	2.02	0.60
1:A:682:THR:O	1:A:686:GLU:HB2	2.02	0.60
1:B:96:LYS:HZ3	1:B:573:ARG:NH2	2.00	0.60
1:B:536:THR:HB	1:B:538:ILE:HD11	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:682:THR:O	1:B:686:GLU:HB2	2.02	0.60
2:F:405:ILE:O	2:F:408:GLN:HB2	2.02	0.60
1:A:724:HIS:HA	1:A:727:LEU:HD12	1.84	0.59
1:B:285:ILE:HG22	1:B:338:ALA:HB2	1.83	0.59
1:B:512:GLU:O	1:B:516:VAL:HG23	2.01	0.59
2:F:319:TYR:HE2	2:F:359:LEU:HB3	1.66	0.59
1:A:556:GLU:HA	1:A:584:LEU:HD23	1.84	0.59
1:B:586:LEU:HD12	1:B:586:LEU:H	1.67	0.59
1:B:774:GLU:HB3	2:F:240:ILE:HG22	1.84	0.59
2:F:230:ILE:O	2:F:232:LEU:HD22	2.02	0.59
1:A:92:VAL:HG12	1:A:414:GLY:CA	2.32	0.59
2:C:236:ALA:HB3	2:C:263:ILE:N	2.17	0.59
1:B:97:THR:CA	1:B:573:ARG:HH12	2.14	0.59
1:B:536:THR:O	1:B:573:ARG:HD2	2.02	0.59
1:A:425:GLU:C	1:A:427:VAL:H	2.10	0.59
2:C:350:SER:HA	2:C:353:GLN:NE2	2.16	0.59
1:B:405:TYR:O	1:B:408:MET:HB3	2.03	0.59
1:A:150:ILE:HG13	1:A:155:LYS:HZ2	1.67	0.59
1:A:155:LYS:NZ	1:A:209:ARG:HD2	2.18	0.59
1:A:487:SER:O	1:A:490:LEU:HB3	2.03	0.59
2:C:35:PRO:C	2:C:37:PRO:HD3	2.28	0.59
2:C:338:TYR:HE2	2:C:345:LEU:H	1.50	0.59
1:B:479:VAL:HB	1:B:553:ILE:HG13	1.85	0.59
1:A:98:GLY:HA2	1:A:574:GLN:HA	1.83	0.59
1:A:306:LEU:HD21	1:A:309:GLU:CG	2.32	0.59
1:A:400:ILE:HG22	1:A:404:ASN:H	1.67	0.59
1:B:92:VAL:HG12	1:B:414:GLY:CA	2.32	0.59
1:A:165:ASP:O	1:A:168:ARG:HB2	2.03	0.59
1:A:458:GLU:O	1:A:461:GLU:HB3	2.02	0.59
1:A:768:GLU:O	1:A:772:VAL:HG23	2.03	0.59
2:C:405:ILE:O	2:C:408:GLN:HB2	2.01	0.59
1:B:774:GLU:CB	2:F:240:ILE:HG22	2.33	0.59
1:A:94:GLU:CA	1:A:94:GLU:OE1	2.50	0.59
1:B:97:THR:HA	1:B:573:ARG:HH12	1.67	0.59
1:B:155:LYS:NZ	1:B:209:ARG:HD2	2.18	0.59
1:B:487:SER:O	1:B:490:LEU:HB3	2.03	0.59
1:B:768:GLU:O	1:B:772:VAL:HG23	2.03	0.59
2:F:309:ILE:O	2:F:313:LEU:HG	2.02	0.59
1:A:18:VAL:HA	1:A:21:ILE:HG22	1.85	0.59
1:A:57:LEU:O	1:A:61:PHE:HB2	2.03	0.59
1:A:251:VAL:HB	1:A:254:ALA:HB2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:PHE:HA	1:A:406:PHE:CD1	2.38	0.59
1:A:775:ALA:O	1:A:778:LEU:HB2	2.02	0.59
1:B:458:GLU:O	1:B:461:GLU:HB3	2.02	0.59
2:F:338:TYR:HE2	2:F:345:LEU:H	1.49	0.59
1:A:479:VAL:HB	1:A:553:ILE:HG13	1.85	0.58
2:C:393:THR:O	2:C:397:ILE:HG13	2.03	0.58
1:B:57:LEU:O	1:B:61:PHE:HB2	2.03	0.58
1:B:263:ARG:O	1:B:265:PRO:HD3	2.03	0.58
1:B:724:HIS:HA	1:B:727:LEU:HD12	1.84	0.58
2:F:125:LEU:HD13	4:H:26:LYS:HD3	1.84	0.58
2:F:276:ALA:HB2	2:F:314:VAL:HG23	1.85	0.58
1:A:148:GLY:HA2	1:A:157:TYR:CG	2.39	0.58
1:A:263:ARG:O	1:A:265:PRO:HD3	2.03	0.58
1:B:425:GLU:C	1:B:427:VAL:H	2.10	0.58
1:A:73:GLY:HA2	1:A:75:ARG:NH1	2.19	0.58
1:A:97:THR:HA	1:A:573:ARG:NH1	2.19	0.58
1:A:452:VAL:HG21	1:A:619:LEU:HD12	1.84	0.58
1:A:454:ARG:NH1	1:A:608:ILE:HA	2.18	0.58
2:C:322:SER:C	2:C:324:VAL:H	2.11	0.58
1:B:494:LEU:HD12	1:B:499:ILE:HG21	1.84	0.58
2:F:328:PRO:HG3	2:F:352:GLU:HB2	1.85	0.58
1:A:592:ARG:HH21	1:A:593:ILE:HD11	1.67	0.58
1:B:344:LEU:HD23	1:B:345:PHE:N	2.19	0.58
2:F:35:PRO:C	2:F:37:PRO:HD3	2.28	0.58
1:B:97:THR:HA	1:B:573:ARG:NH1	2.19	0.58
1:B:454:ARG:NH1	1:B:608:ILE:HA	2.18	0.58
1:B:592:ARG:HH21	1:B:593:ILE:HD11	1.67	0.58
1:A:188:LYS:CD	1:A:189:GLU:H	2.17	0.58
1:B:251:VAL:HB	1:B:254:ALA:HB2	1.83	0.58
1:B:556:GLU:HA	1:B:584:LEU:HD23	1.84	0.58
1:A:405:TYR:O	1:A:408:MET:HB3	2.03	0.58
1:B:165:ASP:O	1:B:168:ARG:HB2	2.03	0.58
1:B:470:ARG:NH2	1:B:475:GLN:HE22	2.02	0.58
2:F:402:ALA:O	2:F:406:ILE:HG13	2.03	0.58
1:A:326:PRO:HD3	2:C:345:LEU:HD11	1.84	0.58
2:C:232:LEU:CB	2:C:267:GLN:HB2	2.14	0.58
1:B:73:GLY:HA2	1:B:75:ARG:NH1	2.19	0.58
1:B:482:THR:HG23	1:B:483:SER:H	1.68	0.58
1:A:285:ILE:HG12	1:A:334:HIS:CD2	2.35	0.58
2:C:402:ALA:O	2:C:406:ILE:HG13	2.04	0.58
1:B:134:LEU:HD13	1:B:202:VAL:CG1	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:LYS:HB3	1:B:385:LYS:HE3	1.86	0.58
1:B:402:PHE:HA	1:B:406:PHE:CD1	2.38	0.58
1:B:452:VAL:HG21	1:B:619:LEU:HD12	1.84	0.58
2:F:237:GLU:CB	2:F:338:TYR:HA	2.33	0.58
2:F:333:GLU:C	2:F:335:ILE:H	2.12	0.58
1:A:80:GLN:NE2	1:A:103:LEU:HD12	2.18	0.58
1:A:347:LYS:HB3	1:A:385:LYS:HE3	1.86	0.58
1:A:97:THR:HG23	1:A:572:GLY:C	2.29	0.57
1:B:80:GLN:NE2	1:B:103:LEU:HD12	2.18	0.57
1:B:148:GLY:HA2	1:B:157:TYR:CG	2.39	0.57
1:B:735:TYR:O	1:B:739:LYS:HB2	2.04	0.57
1:B:771:HIS:HA	2:F:240:ILE:HG21	1.86	0.57
2:F:393:THR:O	2:F:397:ILE:HG13	2.03	0.57
1:A:92:VAL:HG12	1:A:414:GLY:C	2.30	0.57
1:A:96:LYS:HZ3	1:A:573:ARG:NH2	2.01	0.57
1:A:128:LEU:O	1:A:131:ARG:HB3	2.04	0.57
1:B:710:PHE:CE2	1:B:731:LEU:HD11	2.39	0.57
1:A:96:LYS:NZ	1:A:570:ARG:NH2	2.53	0.57
1:A:97:THR:HG22	1:A:575:GLY:HA2	1.85	0.57
1:A:295:PHE:HB2	1:A:309:GLU:OE1	2.03	0.57
1:A:482:THR:HG23	1:A:483:SER:H	1.68	0.57
2:C:237:GLU:CB	2:C:338:TYR:HA	2.35	0.57
2:C:333:GLU:C	2:C:335:ILE:H	2.12	0.57
2:C:350:SER:O	2:C:353:GLN:HB2	2.04	0.57
1:B:18:VAL:HA	1:B:21:ILE:HG22	1.85	0.57
1:B:295:PHE:HB2	1:B:309:GLU:OE1	2.03	0.57
1:B:556:GLU:HB2	1:B:590:LEU:HD21	1.87	0.57
1:A:32:LYS:O	1:A:36:LEU:HB2	2.04	0.57
2:C:267:GLN:HA	2:C:319:TYR:HE1	1.68	0.57
1:B:150:ILE:HD11	1:B:209:ARG:NH2	2.19	0.57
1:B:188:LYS:CD	1:B:189:GLU:H	2.17	0.57
1:B:345:PHE:HZ	2:F:248:VAL:HA	1.69	0.57
2:F:331:ILE:O	2:F:336:ARG:HB2	2.04	0.57
2:F:350:SER:O	2:F:353:GLN:HB2	2.04	0.57
1:A:333:TYR:OH	2:C:253:VAL:HG22	2.05	0.57
1:B:32:LYS:O	1:B:36:LEU:HB2	2.04	0.57
1:B:97:THR:HG22	1:B:575:GLY:HA2	1.85	0.57
1:B:779:ARG:NH2	1:B:788:VAL:N	2.51	0.57
1:A:344:LEU:HD23	1:A:345:PHE:N	2.19	0.57
1:B:76:PRO:N	6:B:873:ADP:HN62	2.01	0.57
1:B:96:LYS:NZ	1:B:570:ARG:NH2	2.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:ALA:O	1:B:290:VAL:HG23	2.05	0.57
2:F:16:ASP:O	2:F:19:ILE:HB	2.04	0.57
2:F:197:ALA:C	2:F:200:PRO:HD2	2.29	0.57
1:A:41:MET:HA	1:A:44:LYS:NZ	2.20	0.57
2:C:16:ASP:O	2:C:19:ILE:HB	2.04	0.57
2:C:303:GLY:O	2:C:307:LEU:HG	2.05	0.57
1:B:779:ARG:HH21	1:B:785:ASP:C	2.13	0.57
2:F:259:THR:HG22	2:F:260:TYR:H	1.70	0.57
2:F:265:VAL:HG12	2:F:266:ASN:H	1.70	0.57
1:A:710:PHE:CE2	1:A:731:LEU:HD11	2.39	0.57
1:A:790:PHE:O	1:A:794:THR:HG23	2.05	0.57
1:B:285:ILE:HG12	1:B:334:HIS:CD2	2.34	0.57
1:B:672:LEU:HD12	1:B:732:TRP:HZ3	1.69	0.57
2:F:279:ILE:O	2:F:283:PRO:HD2	2.05	0.57
1:A:556:GLU:HB2	1:A:590:LEU:HD21	1.86	0.57
1:A:610:GLU:HG2	1:A:611:GLY:H	1.70	0.57
1:B:53:ALA:HB1	1:B:56:HIS:ND1	2.20	0.57
1:B:152:SER:C	1:B:153:LEU:HD12	2.30	0.57
1:B:268:ILE:HG23	1:B:269:SER:H	1.70	0.57
1:A:134:LEU:HD13	1:A:202:VAL:CG1	2.34	0.56
1:A:672:LEU:HD12	1:A:732:TRP:HZ3	1.69	0.56
2:C:197:ALA:C	2:C:200:PRO:HD2	2.29	0.56
1:A:134:LEU:HD11	1:A:204:LEU:HD11	1.87	0.56
1:A:268:ILE:HG23	1:A:269:SER:H	1.70	0.56
2:C:159:LEU:O	2:C:162:MET:HB2	2.05	0.56
1:A:13:LYS:O	1:A:17:MET:HG3	2.06	0.56
1:A:101:LYS:CD	1:A:415:MET:CB	2.84	0.56
1:A:102:THR:HB	1:A:135:TRP:CD1	2.41	0.56
1:A:150:ILE:HD11	1:A:209:ARG:NH2	2.19	0.56
1:A:286:ALA:O	1:A:290:VAL:HG23	2.05	0.56
1:A:301:ALA:HA	2:C:243:GLN:OE1	2.05	0.56
1:A:801:MET:O	1:A:804:ARG:HB2	2.05	0.56
2:C:237:GLU:O	2:C:262:PRO:HG3	2.05	0.56
1:B:92:VAL:HG12	1:B:414:GLY:C	2.30	0.56
1:B:128:LEU:O	1:B:131:ARG:HB3	2.04	0.56
1:B:134:LEU:HD11	1:B:204:LEU:HD11	1.87	0.56
1:B:251:VAL:HG11	1:B:257:VAL:CB	2.28	0.56
1:B:610:GLU:HG2	1:B:611:GLY:H	1.70	0.56
1:B:753:LEU:HD12	1:B:812:TYR:HB3	1.88	0.56
2:F:159:LEU:O	2:F:162:MET:HB2	2.05	0.56
2:F:322:SER:C	2:F:324:VAL:H	2.11	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:ASP:O	1:A:327:GLY:N	2.39	0.56
2:C:238:ARG:HD3	2:C:337:LYS:HZ3	1.70	0.56
4:E:65:VAL:O	4:E:68:VAL:HB	2.06	0.56
1:B:13:LYS:O	1:B:17:MET:HG3	2.06	0.56
1:B:97:THR:HG23	1:B:572:GLY:C	2.29	0.56
2:F:303:GLY:O	2:F:307:LEU:HG	2.06	0.56
1:A:104:ALA:O	1:A:108:PRO:HD2	2.05	0.56
1:B:407:ARG:HD2	1:B:429:VAL:O	2.06	0.56
1:B:702:LEU:HD11	1:B:803:ARG:HH22	1.70	0.56
1:B:790:PHE:O	1:B:794:THR:HG23	2.05	0.56
2:F:267:GLN:HA	2:F:319:TYR:CE1	2.41	0.56
3:G:46:VAL:O	3:G:50:ILE:HG13	2.06	0.56
1:A:129:ALA:O	1:A:133:ALA:HB2	2.05	0.56
1:A:355:ASN:O	1:A:357:GLU:HG3	2.05	0.56
1:A:702:LEU:HD11	1:A:803:ARG:HH22	1.70	0.56
1:A:774:GLU:CB	2:C:240:ILE:HG22	2.35	0.56
1:B:147:VAL:HG22	1:B:148:GLY:N	2.21	0.56
1:B:355:ASN:O	1:B:357:GLU:HG3	2.06	0.56
1:B:753:LEU:CD1	1:B:812:TYR:HB3	2.36	0.56
1:A:152:SER:C	1:A:153:LEU:HD12	2.30	0.56
1:A:407:ARG:HD2	1:A:429:VAL:O	2.06	0.56
2:C:237:GLU:CA	2:C:338:TYR:HA	2.36	0.56
2:C:275:PHE:HE2	2:C:314:VAL:CG2	2.19	0.56
2:C:341:TYR:O	2:C:342:ILE:CB	2.54	0.56
3:D:46:VAL:O	3:D:50:ILE:HG13	2.06	0.56
1:B:75:ARG:N	6:B:873:ADP:HN62	2.03	0.56
1:B:94:GLU:HB2	1:B:416:THR:H	1.70	0.56
1:B:102:THR:HB	1:B:135:TRP:CD1	2.41	0.56
1:B:104:ALA:O	1:B:108:PRO:HD2	2.05	0.56
1:B:801:MET:O	1:B:804:ARG:HB2	2.05	0.56
2:F:194:GLY:O	2:F:198:ARG:HG3	2.06	0.56
2:F:403:LEU:O	2:F:406:ILE:HB	2.06	0.56
1:A:21:ILE:HA	1:A:24:ILE:HD12	1.88	0.56
1:A:235:VAL:HG12	1:A:237:ASP:O	2.06	0.56
1:A:735:TYR:O	1:A:739:LYS:HB2	2.04	0.56
2:C:231:ILE:HD11	3:D:27:LEU:HD12	1.87	0.56
1:B:462:LYS:O	1:B:465:GLU:HG2	2.06	0.56
1:B:470:ARG:HE	1:B:475:GLN:NE2	2.04	0.56
1:A:110:TYR:CE1	1:A:143:LEU:HD23	2.41	0.56
1:A:157:TYR:CE2	1:A:207:ILE:HD13	2.41	0.56
1:A:470:ARG:HE	1:A:475:GLN:NE2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:276:ALA:HB2	2:C:314:VAL:HG23	1.87	0.56
1:B:41:MET:HA	1:B:44:LYS:NZ	2.20	0.56
1:B:129:ALA:O	1:B:133:ALA:HB2	2.05	0.56
2:F:394:SER:HA	2:F:397:ILE:HD12	1.88	0.56
1:A:295:PHE:HB2	1:A:309:GLU:CD	2.31	0.56
1:A:454:ARG:HH12	1:A:608:ILE:HA	1.71	0.56
1:A:753:LEU:CD1	1:A:812:TYR:HB3	2.36	0.56
1:A:779:ARG:HH21	1:A:785:ASP:C	2.13	0.56
2:C:155:GLN:C	2:C:157:THR:N	2.64	0.56
2:C:323:VAL:HG11	2:C:359:LEU:HD21	1.88	0.56
1:B:454:ARG:HH12	1:B:608:ILE:HA	1.71	0.56
2:F:341:TYR:O	2:F:342:ILE:CB	2.54	0.56
1:A:306:LEU:HD12	1:A:307:THR:H	1.71	0.55
1:A:373:ARG:HB2	1:A:379:HIS:ND1	2.21	0.55
1:A:566:GLN:O	1:A:570:ARG:HD2	2.06	0.55
1:A:802:MET:HB2	2:C:422:ILE:HD12	1.88	0.55
2:C:231:ILE:O	2:C:232:LEU:C	2.49	0.55
1:B:325:ASP:O	1:B:327:GLY:N	2.39	0.55
1:B:490:LEU:HD12	1:B:527:ILE:HG13	1.88	0.55
1:A:148:GLY:O	1:A:218:THR:HA	2.07	0.55
1:A:303:THR:CG2	2:C:241:THR:HG21	2.37	0.55
1:A:502:GLN:OE1	1:A:515:ILE:HG22	2.06	0.55
1:A:573:ARG:NE	6:A:873:ADP:O1B	2.39	0.55
1:B:268:ILE:HG23	1:B:269:SER:N	2.21	0.55
1:B:373:ARG:HB2	1:B:379:HIS:ND1	2.21	0.55
1:B:778:LEU:HD13	2:F:263:ILE:N	2.13	0.55
1:A:53:ALA:HB1	1:A:56:HIS:ND1	2.20	0.55
1:A:400:ILE:HB	1:A:404:ASN:OD1	2.07	0.55
1:A:462:LYS:O	1:A:465:GLU:HG2	2.06	0.55
1:A:490:LEU:HD12	1:A:527:ILE:HG13	1.88	0.55
2:C:253:VAL:HG12	2:C:254:TYR:CD2	2.40	0.55
1:B:157:TYR:CE2	1:B:207:ILE:HD13	2.41	0.55
1:B:306:LEU:HD12	1:B:307:THR:H	1.71	0.55
2:F:275:PHE:HE2	2:F:314:VAL:CG2	2.19	0.55
1:A:67:ALA:O	1:A:71:THR:HG23	2.07	0.55
1:A:753:LEU:HD12	1:A:812:TYR:HB3	1.88	0.55
1:A:755:LEU:H	1:A:755:LEU:HD12	1.70	0.55
1:B:97:THR:HA	1:B:573:ARG:HA	1.88	0.55
2:F:233:VAL:CG2	2:F:362:VAL:HG11	2.36	0.55
1:A:97:THR:HA	1:A:573:ARG:HA	1.88	0.55
1:B:21:ILE:HA	1:B:24:ILE:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:755:LEU:H	1:B:755:LEU:HD12	1.70	0.55
1:A:46:LYS:HB3	1:A:56:HIS:CD2	2.42	0.55
2:C:122:ARG:HA	2:C:125:LEU:HD12	1.89	0.55
1:B:46:LYS:HB3	1:B:56:HIS:CD2	2.41	0.55
1:B:93:ALA:O	1:B:94:GLU:CB	2.53	0.55
1:B:150:ILE:HG13	1:B:155:LYS:HZ2	1.70	0.55
1:B:596:SER:HA	1:B:599:ILE:HG22	1.89	0.55
4:H:65:VAL:O	4:H:68:VAL:HB	2.06	0.55
1:A:93:ALA:O	1:A:94:GLU:CB	2.53	0.55
1:A:127:TYR:HA	1:A:130:ARG:HD3	1.89	0.55
1:A:494:LEU:HB3	1:A:499:ILE:HB	1.89	0.55
1:B:235:VAL:HG12	1:B:237:ASP:O	2.06	0.55
1:B:502:GLN:OE1	1:B:515:ILE:HG22	2.06	0.55
2:F:28:PHE:HE1	2:F:187:ILE:HG22	1.71	0.55
2:F:173:TRP:HZ3	4:H:25:SER:HA	1.72	0.55
2:F:187:ILE:HD12	2:F:188:SER:N	2.22	0.55
2:F:237:GLU:CA	2:F:338:TYR:HA	2.37	0.55
1:A:268:ILE:HG23	1:A:269:SER:N	2.21	0.55
2:C:249:THR:HG22	2:C:250:GLY:N	2.20	0.55
1:B:67:ALA:O	1:B:71:THR:HG23	2.07	0.55
1:B:158:GLU:HG2	1:B:159:VAL:H	1.71	0.55
1:B:325:ASP:OD1	2:F:337:LYS:HG3	2.06	0.55
1:B:400:ILE:HB	1:B:404:ASN:OD1	2.07	0.55
1:B:421:THR:HG21	1:B:562:ARG:NH1	2.22	0.55
1:A:612:GLN:H	1:A:613:PRO:CD	2.18	0.55
1:B:110:TYR:CE1	1:B:143:LEU:HD23	2.41	0.55
1:B:295:PHE:HB2	1:B:309:GLU:CD	2.31	0.55
1:B:494:LEU:HB3	1:B:499:ILE:HB	1.89	0.55
1:B:566:GLN:O	1:B:570:ARG:HD2	2.06	0.55
1:B:770:GLU:CD	1:B:773:LYS:HD2	2.31	0.55
1:A:421:THR:HG21	1:A:562:ARG:NH1	2.21	0.55
1:A:504:LEU:HD13	1:A:515:ILE:HD13	1.89	0.55
1:A:767:GLU:HA	2:C:252:ARG:HH12	1.72	0.55
2:C:187:ILE:HD12	2:C:188:SER:N	2.22	0.55
1:B:8:LYS:O	1:B:11:LEU:HB3	2.07	0.55
1:B:240:ASP:C	1:B:242:VAL:H	2.15	0.55
1:B:347:LYS:HB3	1:B:385:LYS:CE	2.37	0.55
1:B:423:GLU:O	1:B:427:VAL:HG23	2.07	0.55
2:F:14:LEU:HD13	2:F:17:ARG:HB2	1.88	0.55
1:A:158:GLU:HG2	1:A:159:VAL:H	1.71	0.54
1:A:347:LYS:HB3	1:A:385:LYS:CE	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:35:PRO:O	2:C:36:VAL:CB	2.55	0.54
1:B:336:ILE:O	1:B:339:LEU:HB3	2.08	0.54
1:B:429:VAL:HG23	1:B:430:TYR:HD2	1.72	0.54
2:F:122:ARG:HA	2:F:125:LEU:HD12	1.89	0.54
1:A:76:PRO:CD	6:A:873:ADP:N6	2.20	0.54
1:A:99:GLU:H	1:A:439:THR:HG21	1.72	0.54
1:A:423:GLU:O	1:A:427:VAL:HG23	2.07	0.54
2:C:403:LEU:O	2:C:406:ILE:HB	2.06	0.54
1:B:306:LEU:HD21	1:B:309:GLU:CG	2.32	0.54
1:B:573:ARG:C	1:B:575:GLY:H	2.15	0.54
2:F:62:SER:O	2:F:66:VAL:HG23	2.08	0.54
2:F:280:VAL:HG21	2:F:306:TYR:HB3	1.89	0.54
2:F:351:THR:O	2:F:355:LEU:HG	2.08	0.54
1:A:147:VAL:HG22	1:A:148:GLY:N	2.21	0.54
1:A:770:GLU:CD	1:A:773:LYS:HD2	2.31	0.54
2:C:194:GLY:O	2:C:198:ARG:HG3	2.06	0.54
2:C:394:SER:HA	2:C:397:ILE:HD12	1.88	0.54
1:B:98:GLY:O	6:B:873:ADP:H8	1.91	0.54
1:B:99:GLU:H	1:B:439:THR:HG21	1.72	0.54
1:B:504:LEU:HD13	1:B:515:ILE:HD13	1.89	0.54
1:B:406:PHE:CG	1:B:412:LEU:HD11	2.43	0.54
1:A:178:TRP:H	1:A:179:PRO:HD2	1.73	0.54
1:A:240:ASP:C	1:A:242:VAL:H	2.15	0.54
1:A:475:GLN:HB3	1:A:551:CYS:SG	2.47	0.54
1:A:573:ARG:C	1:A:575:GLY:H	2.15	0.54
2:C:14:LEU:HD13	2:C:17:ARG:HB2	1.88	0.54
1:B:146:ARG:O	1:B:216:ASP:HB2	2.08	0.54
1:B:400:ILE:HD12	1:B:402:PHE:CE2	2.43	0.54
2:F:35:PRO:O	2:F:36:VAL:CB	2.55	0.54
2:F:375:LEU:HD22	2:F:379:LEU:HG	1.89	0.54
1:A:8:LYS:O	1:A:11:LEU:HB3	2.07	0.54
1:A:75:ARG:N	6:A:873:ADP:HN62	2.02	0.54
1:A:163:ASN:H	1:A:164:PRO:HD2	1.73	0.54
1:A:400:ILE:HD12	1:A:402:PHE:CE2	2.43	0.54
1:A:429:VAL:HG23	1:A:430:TYR:HD2	1.72	0.54
1:A:652:ARG:O	1:A:655:VAL:HB	2.08	0.54
1:B:421:THR:HG21	1:B:562:ARG:HH12	1.71	0.54
1:B:475:GLN:HB3	1:B:551:CYS:SG	2.47	0.54
1:B:770:GLU:HG3	2:F:240:ILE:HD13	1.88	0.54
1:A:421:THR:HG21	1:A:562:ARG:HH12	1.71	0.54
1:A:688:CYS:HB3	1:A:698:LEU:HD22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:28:PHE:HE1	2:C:187:ILE:HG22	1.71	0.54
1:B:75:ARG:N	1:B:76:PRO:CD	2.67	0.54
1:B:688:CYS:HB3	1:B:698:LEU:HD22	1.90	0.54
1:A:159:VAL:HG12	1:A:160:VAL:HG22	1.90	0.54
1:A:247:PHE:CG	1:A:248:TYR:N	2.76	0.54
1:A:778:LEU:HA	2:C:264:LYS:HE3	1.90	0.54
2:C:62:SER:O	2:C:66:VAL:HG23	2.07	0.54
2:C:233:VAL:O	2:C:265:VAL:HB	2.08	0.54
1:B:148:GLY:O	1:B:218:THR:HA	2.07	0.54
1:B:163:ASN:H	1:B:164:PRO:HD2	1.73	0.54
1:B:652:ARG:O	1:B:655:VAL:HB	2.08	0.54
2:F:183:ILE:HG13	2:F:185:ASN:N	2.14	0.54
1:A:103:LEU:O	1:A:106:THR:HG22	2.07	0.54
1:A:128:LEU:HG	1:A:131:ARG:HD3	1.89	0.54
1:A:259:ILE:HD11	1:A:562:ARG:HH21	1.72	0.54
1:A:596:SER:HA	1:A:599:ILE:HG22	1.89	0.54
1:B:101:LYS:CD	1:B:415:MET:HB2	2.33	0.54
1:B:103:LEU:O	1:B:106:THR:HG22	2.07	0.54
1:B:178:TRP:H	1:B:179:PRO:HD2	1.73	0.54
1:B:275:SER:N	1:B:276:PRO:HD2	2.23	0.54
1:B:460:TYR:O	1:B:464:VAL:HG23	2.08	0.54
1:A:275:SER:N	1:A:276:PRO:HD2	2.23	0.54
2:C:237:GLU:HA	2:C:338:TYR:HA	1.90	0.54
1:B:159:VAL:HG12	1:B:160:VAL:HG22	1.90	0.54
1:B:278:VAL:HG13	1:B:282:PHE:CD1	2.43	0.54
1:B:651:GLN:HA	1:B:798:PHE:CE2	2.43	0.54
1:B:775:ALA:HA	1:B:778:LEU:CD1	2.38	0.54
4:H:42:VAL:C	4:H:44:GLY:H	2.16	0.54
1:A:131:ARG:NH1	7:A:874:BEF:F3	2.31	0.53
1:A:146:ARG:O	1:A:216:ASP:HB2	2.08	0.53
1:A:171:ILE:HG13	1:A:172:GLU:N	2.23	0.53
1:A:303:THR:HA	1:A:340:LYS:HE2	1.90	0.53
2:C:63:PHE:O	2:C:67:PHE:HB2	2.08	0.53
2:C:351:THR:O	2:C:355:LEU:HG	2.08	0.53
2:C:375:LEU:HD22	2:C:379:LEU:HG	1.88	0.53
1:B:121:LEU:HD22	1:B:250:ILE:HB	1.90	0.53
1:B:128:LEU:HG	1:B:131:ARG:HD3	1.89	0.53
1:B:296:THR:HG23	1:B:306:LEU:HB2	1.90	0.53
1:B:415:MET:O	1:B:416:THR:CB	2.57	0.53
2:F:155:GLN:C	2:F:157:THR:N	2.64	0.53
2:C:225:ILE:HG23	2:C:369:PHE:HD2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:VAL:HG11	1:B:193:ASN:ND2	2.21	0.53
1:B:324:TYR:O	1:B:328:ASN:HB3	2.08	0.53
1:B:545:ALA:CA	1:B:549:GLY:HA2	2.37	0.53
1:A:336:ILE:O	1:A:339:LEU:HB3	2.07	0.53
2:C:135:VAL:HG12	2:C:139:LEU:HD22	1.90	0.53
2:C:275:PHE:CD2	2:C:275:PHE:C	2.86	0.53
3:D:35:VAL:O	3:D:39:VAL:HG23	2.08	0.53
2:F:237:GLU:O	2:F:262:PRO:HG3	2.09	0.53
3:G:35:VAL:O	3:G:39:VAL:HG23	2.08	0.53
1:A:278:VAL:HG13	1:A:282:PHE:CD1	2.43	0.53
1:A:406:PHE:CG	1:A:412:LEU:HD11	2.43	0.53
2:C:416:ARG:HD3	2:C:418:TYR:OH	2.09	0.53
1:B:127:TYR:HA	1:B:130:ARG:HD3	1.89	0.53
1:B:128:LEU:HD21	1:B:131:ARG:CZ	2.39	0.53
1:A:75:ARG:H	6:A:873:ADP:HN62	1.57	0.53
1:A:762:TRP:HA	1:A:801:MET:SD	2.49	0.53
2:C:331:ILE:O	2:C:336:ARG:HB2	2.09	0.53
1:B:303:THR:HA	1:B:340:LYS:HE2	1.89	0.53
1:B:557:ARG:HA	1:B:564:ASP:OD2	2.09	0.53
1:B:612:GLN:N	1:B:613:PRO:HD2	2.19	0.53
2:F:253:VAL:HG12	2:F:254:TYR:CD2	2.43	0.53
1:A:121:LEU:HD22	1:A:250:ILE:HB	1.90	0.53
1:A:163:ASN:N	1:A:164:PRO:HD2	2.24	0.53
1:A:460:TYR:O	1:A:464:VAL:HG23	2.08	0.53
1:A:689:SER:O	1:A:695:ILE:HG23	2.08	0.53
2:C:280:VAL:HG21	2:C:306:TYR:HB3	1.89	0.53
1:A:30:SER:HB2	1:A:32:LYS:HD2	1.91	0.53
1:A:177:VAL:HG11	1:A:193:ASN:ND2	2.21	0.53
2:C:304:PHE:HA	2:C:307:LEU:HD12	1.89	0.53
1:B:21:ILE:HA	1:B:24:ILE:CD1	2.39	0.53
1:B:259:ILE:HD11	1:B:562:ARG:HH21	1.73	0.53
1:B:689:SER:O	1:B:695:ILE:HG23	2.08	0.53
1:B:750:ILE:CD1	1:B:751:ARG:HH22	2.22	0.53
1:A:75:ARG:N	1:A:75:ARG:NE	2.57	0.53
1:A:128:LEU:HD21	1:A:131:ARG:CZ	2.39	0.53
1:A:139:VAL:HG23	1:A:140:TYR:HD2	1.73	0.53
1:A:573:ARG:CD	6:A:873:ADP:O1B	2.57	0.53
1:A:733:GLU:O	1:A:736:GLN:HB3	2.09	0.53
2:C:88:ALA:HA	2:C:124:THR:HB	1.89	0.53
2:C:335:ILE:O	2:C:336:ARG:HG3	2.09	0.53
1:B:43:LEU:HD12	1:B:110:TYR:OH	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:ILE:HG13	1:B:172:GLU:N	2.23	0.53
1:B:247:PHE:CG	1:B:248:TYR:N	2.76	0.53
1:B:618:MET:HA	1:B:621:LYS:CD	2.39	0.53
1:B:623:ILE:HG13	1:B:624:GLU:N	2.24	0.53
2:F:88:ALA:HA	2:F:124:THR:HB	1.89	0.53
2:F:416:ARG:HD3	2:F:418:TYR:OH	2.09	0.53
1:B:127:TYR:OH	1:B:516:VAL:HG22	2.09	0.53
1:B:590:LEU:O	1:B:594:PHE:HB2	2.09	0.53
2:F:71:ALA:HB1	2:F:138:SER:HB2	1.91	0.53
2:F:275:PHE:CD2	2:F:275:PHE:C	2.86	0.53
2:F:306:TYR:O	2:F:309:ILE:HB	2.09	0.53
4:H:64:PHE:O	4:H:68:VAL:HG23	2.09	0.53
1:A:569:GLY:C	1:A:571:ALA:H	2.16	0.53
1:A:574:GLN:N	6:A:873:ADP:O4'	2.42	0.53
1:A:770:GLU:O	1:A:773:LYS:HB2	2.09	0.53
2:C:85:TYR:CE2	2:C:171:LEU:HD12	2.44	0.53
1:B:569:GLY:C	1:B:571:ALA:H	2.16	0.53
2:F:63:PHE:O	2:F:67:PHE:HB2	2.08	0.53
2:F:192:PHE:O	2:F:196:VAL:HG23	2.09	0.53
1:A:470:ARG:NH2	1:A:475:GLN:HE22	2.02	0.52
1:A:750:ILE:CD1	1:A:751:ARG:HH22	2.22	0.52
1:B:110:TYR:CE1	1:B:114:LEU:HD21	2.44	0.52
1:B:139:VAL:HG23	1:B:140:TYR:HD2	1.73	0.52
1:B:165:ASP:O	1:B:169:LYS:HD2	2.09	0.52
1:B:397:TYR:CE2	1:B:652:ARG:HG3	2.43	0.52
2:F:85:TYR:CE2	2:F:171:LEU:HD12	2.44	0.52
2:F:335:ILE:O	2:F:336:ARG:HG3	2.09	0.52
1:A:324:TYR:O	1:A:328:ASN:HB3	2.08	0.52
1:A:400:ILE:CG2	1:A:404:ASN:H	2.22	0.52
1:A:651:GLN:HA	1:A:798:PHE:CE2	2.43	0.52
2:C:265:VAL:HG12	2:C:266:ASN:H	1.73	0.52
3:D:40:THR:O	3:D:43:TYR:HB2	2.10	0.52
4:E:42:VAL:C	4:E:44:GLY:H	2.16	0.52
1:B:30:SER:HB2	1:B:32:LYS:HD2	1.91	0.52
1:B:254:ALA:C	1:B:256:SER:N	2.65	0.52
1:B:762:TRP:HA	1:B:801:MET:SD	2.49	0.52
1:B:809:ILE:O	1:B:809:ILE:HD13	2.09	0.52
1:A:809:ILE:O	1:A:809:ILE:HD13	2.09	0.52
2:C:418:TYR:HD1	2:C:419:GLU:HG3	1.74	0.52
4:E:64:PHE:O	4:E:68:VAL:HG23	2.09	0.52
1:B:695:ILE:O	1:B:699:LYS:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:733:GLU:O	1:B:736:GLN:HB3	2.09	0.52
2:F:190:LEU:HD21	3:G:51:PHE:CZ	2.42	0.52
2:F:237:GLU:HA	2:F:338:TYR:HA	1.91	0.52
2:F:304:PHE:HA	2:F:307:LEU:HD12	1.89	0.52
2:F:323:VAL:HG11	2:F:359:LEU:HD21	1.92	0.52
1:A:101:LYS:CE	1:A:416:THR:OG1	2.55	0.52
1:A:110:TYR:CE1	1:A:114:LEU:HD21	2.44	0.52
1:A:127:TYR:OH	1:A:516:VAL:HG22	2.09	0.52
1:A:162:LYS:HB3	1:A:164:PRO:HD2	1.91	0.52
1:A:254:ALA:C	1:A:256:SER:N	2.65	0.52
1:A:387:GLY:O	1:A:389:PRO:HD3	2.09	0.52
1:A:415:MET:O	1:A:416:THR:CB	2.57	0.52
1:A:774:GLU:HB3	2:C:240:ILE:HG22	1.92	0.52
2:C:183:ILE:HG13	2:C:185:ASN:N	2.13	0.52
2:C:231:ILE:C	2:C:232:LEU:O	2.52	0.52
1:B:400:ILE:CG2	1:B:404:ASN:H	2.22	0.52
1:B:410:GLU:CG	1:B:411:LYS:N	2.73	0.52
2:F:235:GLN:C	2:F:264:LYS:H	2.18	0.52
2:F:418:TYR:HD1	2:F:419:GLU:HG3	1.75	0.52
1:A:43:LEU:HD12	1:A:110:TYR:OH	2.09	0.52
1:A:75:ARG:NE	1:A:76:PRO:HD3	2.15	0.52
1:A:105:ALA:O	1:A:109:ILE:HG13	2.10	0.52
1:A:165:ASP:O	1:A:169:LYS:HD2	2.09	0.52
1:A:623:ILE:HG13	1:A:624:GLU:N	2.24	0.52
2:C:162:MET:HG2	4:E:19:MET:HE3	1.92	0.52
1:B:75:ARG:N	1:B:75:ARG:NE	2.57	0.52
1:B:163:ASN:N	1:B:164:PRO:HD2	2.24	0.52
1:B:317:ILE:O	1:B:318:ILE:C	2.53	0.52
2:F:358:VAL:O	2:F:361:ARG:HG2	2.10	0.52
1:A:21:ILE:HA	1:A:24:ILE:CD1	2.39	0.52
1:A:482:THR:CG2	1:A:486:LYS:HD2	2.39	0.52
1:B:75:ARG:HE	1:B:75:ARG:H	1.58	0.52
1:B:778:LEU:HA	2:F:264:LYS:CE	2.38	0.52
1:A:74:MET:CE	6:A:873:ADP:N3	2.61	0.52
1:A:373:ARG:NH1	1:A:378:LEU:HD22	2.25	0.52
1:A:419:ALA:O	1:A:422:GLU:HG3	2.10	0.52
1:A:590:LEU:O	1:A:594:PHE:HB2	2.09	0.52
2:C:267:GLN:HA	2:C:319:TYR:CE1	2.45	0.52
1:B:187:LEU:HD21	6:B:873:ADP:C2	2.45	0.52
2:F:135:VAL:HG12	2:F:139:LEU:HD22	1.90	0.52
2:F:231:ILE:C	2:F:232:LEU:CD2	2.78	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:VAL:HG13	1:A:125:ASN:N	2.25	0.52
1:A:141:LEU:CB	1:A:159:VAL:HG11	2.40	0.52
1:A:157:TYR:CD2	1:A:207:ILE:HD13	2.45	0.52
1:A:304:ILE:HB	1:A:339:LEU:HD21	1.92	0.52
1:A:778:LEU:HD11	2:C:262:PRO:HA	1.92	0.52
1:B:75:ARG:NE	1:B:76:PRO:HD3	2.15	0.52
1:B:203:GLU:O	1:B:204:LEU:HG	2.10	0.52
2:F:186:GLY:O	2:F:189:ILE:HG22	2.10	0.52
1:A:101:LYS:HD2	1:A:415:MET:HB3	1.90	0.52
1:A:296:THR:HG23	1:A:306:LEU:HB2	1.91	0.52
1:A:406:PHE:CB	1:A:412:LEU:HD11	2.40	0.52
1:A:453:PHE:O	1:A:585:SER:HA	2.10	0.52
1:A:557:ARG:HA	1:A:564:ASP:OD2	2.09	0.52
2:C:205:GLN:OE1	2:C:388:VAL:HG11	2.10	0.52
2:C:232:LEU:HG	2:C:266:ASN:HA	1.91	0.52
1:B:72:LEU:HD12	1:B:138:PRO:HG2	1.92	0.52
1:B:286:ALA:HA	1:B:338:ALA:HB1	1.92	0.52
3:G:40:THR:O	3:G:43:TYR:HB2	2.10	0.52
1:A:74:MET:N	1:A:187:LEU:HD13	2.23	0.52
1:A:345:PHE:HZ	2:C:248:VAL:HA	1.75	0.52
1:A:383:GLU:HG2	1:A:390:ILE:H	1.75	0.52
1:A:463:ILE:O	1:A:466:GLU:HB3	2.10	0.52
1:A:545:ALA:CA	1:A:549:GLY:HA2	2.37	0.52
1:A:766:LEU:O	1:A:766:LEU:HD23	2.10	0.52
1:A:778:LEU:HD13	2:C:263:ILE:N	2.08	0.52
2:C:192:PHE:O	2:C:196:VAL:HG23	2.09	0.52
1:B:453:PHE:O	1:B:585:SER:HA	2.10	0.52
1:B:482:THR:CG2	1:B:486:LYS:HD2	2.39	0.52
2:F:225:ILE:HG23	2:F:369:PHE:HD2	1.74	0.52
2:F:238:ARG:HD2	2:F:337:LYS:HG2	1.91	0.52
1:A:100:GLY:O	1:A:102:THR:N	2.43	0.51
1:A:155:LYS:HD3	1:A:212:ALA:HB2	1.91	0.51
1:A:203:GLU:O	1:A:204:LEU:HG	2.10	0.51
1:A:278:VAL:O	1:A:282:PHE:HB2	2.10	0.51
1:A:410:GLU:CG	1:A:411:LYS:N	2.73	0.51
1:A:695:ILE:O	1:A:699:LYS:HB3	2.09	0.51
1:B:15:ALA:C	1:B:18:VAL:HG12	2.35	0.51
1:B:96:LYS:HZ1	1:B:570:ARG:CZ	2.23	0.51
1:B:383:GLU:HG2	1:B:390:ILE:H	1.75	0.51
1:B:770:GLU:O	1:B:773:LYS:HB2	2.09	0.51
1:A:96:LYS:HZ1	1:A:570:ARG:CZ	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:71:ALA:HB1	2:C:138:SER:HB2	1.91	0.51
2:C:101:SER:HB2	2:C:106:LEU:HD21	1.93	0.51
2:C:338:TYR:O	2:C:344:GLY:HA3	2.11	0.51
2:C:358:VAL:O	2:C:361:ARG:HG2	2.10	0.51
1:B:100:GLY:O	1:B:102:THR:N	2.43	0.51
1:B:110:TYR:O	1:B:114:LEU:HG	2.10	0.51
2:F:205:GLN:OE1	2:F:388:VAL:HG11	2.10	0.51
2:F:236:ALA:HB3	2:F:263:ILE:N	2.26	0.51
1:A:165:ASP:HA	1:A:168:ARG:HD2	1.92	0.51
1:A:230:LEU:C	1:A:232:ASP:N	2.66	0.51
1:A:779:ARG:HH22	1:A:788:VAL:N	2.06	0.51
2:C:186:GLY:O	2:C:189:ILE:HG22	2.10	0.51
1:B:105:ALA:O	1:B:109:ILE:HG13	2.10	0.51
1:B:162:LYS:HB3	1:B:164:PRO:HD2	1.91	0.51
1:B:178:TRP:N	1:B:179:PRO:HD2	2.26	0.51
1:B:304:ILE:HB	1:B:339:LEU:HD21	1.92	0.51
1:B:557:ARG:HG2	1:B:564:ASP:OD1	2.10	0.51
1:A:28:LEU:C	1:A:30:SER:H	2.19	0.51
1:A:317:ILE:O	1:A:318:ILE:C	2.53	0.51
2:C:306:TYR:O	2:C:309:ILE:HB	2.09	0.51
1:B:92:VAL:HG22	1:B:433:GLU:O	2.11	0.51
1:B:230:LEU:C	1:B:232:ASP:N	2.66	0.51
1:B:373:ARG:NH1	1:B:378:LEU:HD22	2.25	0.51
2:F:101:SER:HB2	2:F:106:LEU:HD21	1.93	0.51
2:F:312:LEU:O	2:F:316:PHE:HB2	2.10	0.51
2:F:373:ILE:O	2:F:377:PRO:HD2	2.10	0.51
1:A:7:ASN:O	1:A:10:ILE:HB	2.10	0.51
1:A:286:ALA:HA	1:A:338:ALA:HB1	1.92	0.51
1:A:324:TYR:C	1:A:326:PRO:HD2	2.36	0.51
1:A:557:ARG:HG2	1:A:564:ASP:OD1	2.10	0.51
2:C:274:ILE:HD13	2:C:397:ILE:HG12	1.92	0.51
2:C:373:ILE:O	2:C:377:PRO:HD2	2.10	0.51
1:B:79:VAL:CG2	1:B:94:GLU:OE1	2.57	0.51
1:B:160:VAL:HB	1:B:165:ASP:HB3	1.92	0.51
1:B:387:GLY:O	1:B:389:PRO:HD3	2.09	0.51
1:B:419:ALA:O	1:B:422:GLU:HG3	2.10	0.51
1:B:766:LEU:O	1:B:766:LEU:HD23	2.10	0.51
4:H:42:VAL:HG12	4:H:44:GLY:H	1.76	0.51
1:A:15:ALA:C	1:A:18:VAL:HG12	2.35	0.51
1:A:110:TYR:O	1:A:114:LEU:HG	2.10	0.51
1:A:178:TRP:N	1:A:179:PRO:HD2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:ASP:N	1:A:326:PRO:CD	2.74	0.51
1:B:165:ASP:HA	1:B:168:ARG:HD2	1.92	0.51
1:B:406:PHE:CB	1:B:412:LEU:HD11	2.40	0.51
1:B:573:ARG:NE	6:B:873:ADP:O1B	2.43	0.51
1:A:79:VAL:HB	1:A:437:ILE:HB	1.91	0.51
1:A:284:GLN:HG2	1:A:288:LYS:NZ	2.26	0.51
1:A:341:ALA:HB2	1:A:381:ALA:HB1	1.92	0.51
1:A:463:ILE:O	1:A:467:ILE:HG13	2.11	0.51
2:C:196:VAL:O	2:C:196:VAL:HG12	2.11	0.51
2:C:352:GLU:O	2:C:356:HIS:HB2	2.11	0.51
1:B:101:LYS:CD	1:B:415:MET:CB	2.70	0.51
1:B:131:ARG:NH1	7:B:874:BEF:F3	2.34	0.51
1:B:157:TYR:CD2	1:B:207:ILE:HD13	2.45	0.51
1:B:319:GLY:C	1:B:321:GLU:H	2.19	0.51
2:F:30:MET:O	2:F:34:ILE:HG13	2.11	0.51
2:F:232:LEU:HG	2:F:266:ASN:CA	2.40	0.51
1:A:298:ASP:CG	1:A:304:ILE:HG12	2.36	0.51
1:A:755:LEU:HD12	1:A:755:LEU:N	2.26	0.51
2:C:71:ALA:HB2	2:C:139:LEU:HD13	1.91	0.51
2:C:319:TYR:HA	2:C:322:SER:HB3	1.93	0.51
1:B:79:VAL:HB	1:B:437:ILE:HB	1.92	0.51
1:B:284:GLN:HG2	1:B:288:LYS:NZ	2.26	0.51
1:B:410:GLU:HG3	1:B:411:LYS:N	2.18	0.51
1:B:558:HIS:HD1	1:B:564:ASP:HA	1.75	0.51
1:B:676:PHE:O	1:B:680:VAL:HG23	2.10	0.51
2:F:71:ALA:HB2	2:F:139:LEU:HD13	1.92	0.51
2:F:274:ILE:HD13	2:F:397:ILE:HG12	1.93	0.51
1:A:107:MET:HB2	1:A:108:PRO:CD	2.41	0.51
1:A:337:ASN:O	1:A:338:ALA:C	2.54	0.51
1:A:373:ARG:CG	1:A:379:HIS:HB2	2.39	0.51
1:A:612:GLN:N	1:A:613:PRO:HD2	2.19	0.51
1:A:618:MET:H	1:A:621:LYS:HZ2	1.57	0.51
1:A:676:PHE:O	1:A:680:VAL:HG23	2.10	0.51
1:A:779:ARG:NH2	1:A:788:VAL:N	2.51	0.51
4:E:42:VAL:HG12	4:E:44:GLY:H	1.76	0.51
1:B:155:LYS:HD3	1:B:212:ALA:HB2	1.91	0.51
1:B:278:VAL:O	1:B:282:PHE:HB2	2.10	0.51
1:B:312:ALA:C	1:B:316:LYS:HD3	2.36	0.51
2:F:196:VAL:O	2:F:196:VAL:HG12	2.11	0.51
1:A:72:LEU:HD12	1:A:138:PRO:HG2	1.92	0.51
1:A:312:ALA:C	1:A:316:LYS:HD3	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:GLY:O	1:A:372:ARG:HB2	2.11	0.51
1:A:606:LEU:HD21	1:A:617:PRO:CG	2.41	0.51
2:C:238:ARG:HD2	2:C:337:LYS:HG2	1.93	0.51
1:B:7:ASN:O	1:B:10:ILE:HB	2.10	0.51
1:B:60:ALA:O	1:B:64:VAL:HG23	2.11	0.51
1:B:324:TYR:C	1:B:326:PRO:HD2	2.36	0.51
1:B:325:ASP:N	1:B:326:PRO:CD	2.74	0.51
1:B:366:GLY:O	1:B:531:MET:HB2	2.10	0.51
1:B:415:MET:O	1:B:416:THR:HB	2.11	0.51
2:F:234:GLN:HG3	2:F:234:GLN:O	2.11	0.51
1:A:397:TYR:CE2	1:A:652:ARG:HG3	2.43	0.50
2:C:123:LEU:O	2:C:127:ILE:HG12	2.11	0.50
2:C:233:VAL:CG2	2:C:362:VAL:HG11	2.41	0.50
1:B:124:VAL:HG13	1:B:125:ASN:N	2.25	0.50
1:B:529:THR:HG22	1:B:530:ASN:OD1	2.12	0.50
1:A:60:ALA:O	1:A:64:VAL:HG23	2.11	0.50
1:A:92:VAL:HG22	1:A:433:GLU:O	2.11	0.50
1:A:282:PHE:HA	1:A:285:ILE:CG1	2.41	0.50
1:B:104:ALA:O	1:B:105:ALA:C	2.54	0.50
1:B:303:THR:CG2	2:F:241:THR:HG21	2.41	0.50
1:B:373:ARG:CG	1:B:379:HIS:HB2	2.39	0.50
1:B:463:ILE:O	1:B:467:ILE:HG13	2.11	0.50
1:A:75:ARG:N	1:A:76:PRO:CD	2.67	0.50
1:A:96:LYS:NZ	1:A:573:ARG:NH2	2.58	0.50
1:A:160:VAL:HB	1:A:165:ASP:HB3	1.93	0.50
1:A:172:GLU:HA	1:A:175:TRP:HB3	1.94	0.50
1:A:362:ASP:CG	1:A:368:LEU:HA	2.36	0.50
1:A:529:THR:HG22	1:A:530:ASN:OD1	2.12	0.50
1:A:673:LYS:HZ1	1:A:736:GLN:HG3	1.77	0.50
1:A:779:ARG:HH22	1:A:788:VAL:CG2	2.24	0.50
2:C:30:MET:O	2:C:34:ILE:HG13	2.11	0.50
2:C:312:LEU:O	2:C:316:PHE:HB2	2.10	0.50
1:B:28:LEU:C	1:B:30:SER:H	2.19	0.50
1:B:67:ALA:HA	1:B:142:PHE:HE1	1.77	0.50
1:B:91:LYS:NZ	1:B:433:GLU:HB2	2.26	0.50
1:B:228:ASP:O	1:B:231:ARG:HB3	2.11	0.50
1:B:326:PRO:HD3	2:F:345:LEU:HD11	1.93	0.50
1:B:341:ALA:HB2	1:B:381:ALA:HB1	1.92	0.50
1:B:371:GLY:O	1:B:372:ARG:HB2	2.11	0.50
1:B:402:PHE:HA	1:B:406:PHE:HD1	1.76	0.50
1:B:450:ASP:HB3	1:B:584:LEU:HD12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:755:LEU:HD12	1:B:755:LEU:N	2.26	0.50
1:B:802:MET:HA	1:B:805:ILE:HD12	1.93	0.50
1:A:84:GLY:HA2	1:A:87:LEU:HB2	1.94	0.50
2:C:32:ILE:HG22	2:C:41:LEU:HD23	1.94	0.50
2:C:271:ILE:HG22	2:C:271:ILE:O	2.11	0.50
1:B:96:LYS:NZ	1:B:573:ARG:NH2	2.58	0.50
1:B:172:GLU:HA	1:B:175:TRP:HB3	1.94	0.50
1:B:282:PHE:HA	1:B:285:ILE:CG1	2.41	0.50
1:B:534:ARG:HA	1:B:570:ARG:HD3	1.93	0.50
1:A:75:ARG:HE	1:A:75:ARG:H	1.58	0.50
1:A:104:ALA:O	1:A:105:ALA:C	2.54	0.50
1:A:410:GLU:HG3	1:A:411:LYS:N	2.18	0.50
1:A:534:ARG:HA	1:A:570:ARG:HD3	1.93	0.50
1:A:802:MET:HA	1:A:805:ILE:HD12	1.93	0.50
1:B:298:ASP:CG	1:B:304:ILE:HG12	2.36	0.50
1:B:606:LEU:HD21	1:B:617:PRO:CG	2.41	0.50
1:A:402:PHE:HA	1:A:406:PHE:HD1	1.76	0.50
2:C:33:TYR:OH	3:D:55:VAL:HG11	2.11	0.50
1:B:96:LYS:HZ1	1:B:570:ARG:NH2	2.10	0.50
1:B:254:ALA:HA	1:B:257:VAL:HB	1.94	0.50
1:B:337:ASN:O	1:B:338:ALA:C	2.54	0.50
1:B:463:ILE:O	1:B:466:GLU:HB3	2.11	0.50
1:B:779:ARG:HH22	1:B:788:VAL:CG2	2.24	0.50
2:F:32:ILE:HG22	2:F:41:LEU:HD23	1.94	0.50
2:F:352:GLU:O	2:F:356:HIS:HB2	2.11	0.50
1:A:228:ASP:O	1:A:231:ARG:HB3	2.11	0.50
1:A:400:ILE:HB	1:A:404:ASN:CG	2.37	0.50
1:A:558:HIS:HD1	1:A:564:ASP:HA	1.75	0.50
1:B:3:LEU:HB2	1:B:5:ASP:HB2	1.94	0.50
1:B:254:ALA:C	1:B:256:SER:H	2.18	0.50
1:B:481:THR:HG22	1:B:555:THR:OG1	2.12	0.50
2:F:91:ILE:HD11	2:F:127:ILE:HG21	1.93	0.50
2:F:231:ILE:O	2:F:232:LEU:C	2.54	0.50
1:A:67:ALA:HA	1:A:142:PHE:HE1	1.77	0.50
1:A:230:LEU:HD11	1:A:399:THR:HG21	1.94	0.50
1:A:254:ALA:C	1:A:256:SER:H	2.18	0.50
1:A:366:GLY:O	1:A:531:MET:HB2	2.10	0.50
1:A:406:PHE:HB3	1:A:412:LEU:HD11	1.93	0.50
1:A:415:MET:O	1:A:416:THR:HB	2.11	0.50
1:A:450:ASP:HB3	1:A:584:LEU:HD12	1.92	0.50
2:C:182:GLY:HA2	2:C:408:GLN:OE1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:MET:HB2	1:B:108:PRO:CD	2.41	0.50
1:B:132:ASP:O	1:B:136:MET:HG2	2.12	0.50
1:B:160:VAL:HG13	1:B:201:GLN:HA	1.93	0.50
1:B:249:ALA:O	1:B:412:LEU:HA	2.11	0.50
1:B:303:THR:O	1:B:304:ILE:HG13	2.12	0.50
1:B:361:VAL:HG21	1:B:373:ARG:CZ	2.42	0.50
1:B:362:ASP:CG	1:B:368:LEU:HA	2.36	0.50
1:B:400:ILE:HB	1:B:404:ASN:CG	2.36	0.50
1:B:612:GLN:H	1:B:613:PRO:CD	2.18	0.50
2:F:113:ARG:HD3	4:H:40:HIS:NE2	2.26	0.50
2:F:334:ASN:C	2:F:335:ILE:HD12	2.37	0.50
1:A:84:GLY:O	1:A:87:LEU:HB2	2.12	0.50
1:A:91:LYS:NZ	1:A:433:GLU:HB2	2.26	0.50
1:A:94:GLU:HB3	1:A:99:GLU:OE2	2.12	0.50
1:A:101:LYS:NZ	7:A:874:BEF:F2	2.34	0.50
1:A:149:VAL:H	1:A:157:TYR:HB3	1.77	0.50
1:A:382:ILE:HG13	1:A:385:LYS:HE2	1.94	0.50
1:B:188:LYS:CE	1:B:189:GLU:H	2.24	0.50
1:B:230:LEU:CD2	1:B:397:TYR:HB3	2.35	0.50
1:B:331:LEU:O	1:B:334:HIS:ND1	2.42	0.50
2:F:123:LEU:O	2:F:127:ILE:HG12	2.11	0.50
2:F:182:GLY:HA2	2:F:408:GLN:OE1	2.12	0.50
1:A:160:VAL:HG13	1:A:201:GLN:HA	1.93	0.49
1:A:361:VAL:HG21	1:A:373:ARG:CZ	2.42	0.49
1:A:775:ALA:HA	1:A:778:LEU:CD1	2.38	0.49
2:C:202:TYR:CE1	2:C:206:ALA:HB2	2.46	0.49
1:B:98:GLY:O	1:B:100:GLY:N	2.45	0.49
1:B:282:PHE:HA	1:B:285:ILE:HD12	1.93	0.49
1:B:406:PHE:HB3	1:B:412:LEU:HD11	1.94	0.49
2:F:90:ILE:O	2:F:93:GLN:HB3	2.12	0.49
2:F:189:ILE:HA	2:F:192:PHE:CD1	2.47	0.49
1:A:80:GLN:HE22	1:A:103:LEU:HD12	1.77	0.49
1:B:84:GLY:HA2	1:B:87:LEU:HB2	1.94	0.49
1:B:230:LEU:HD11	1:B:399:THR:HG21	1.94	0.49
1:B:382:ILE:HG13	1:B:385:LYS:HE2	1.94	0.49
2:F:327:ASP:N	2:F:328:PRO:HD2	2.26	0.49
1:A:159:VAL:HG12	1:A:160:VAL:N	2.23	0.49
1:A:306:LEU:HD12	1:A:307:THR:N	2.28	0.49
1:A:333:TYR:CZ	2:C:253:VAL:HG13	2.46	0.49
1:A:620:SER:HA	1:A:623:ILE:HD11	1.94	0.49
1:A:778:LEU:CD1	2:C:262:PRO:HA	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:86:ILE:O	2:C:90:ILE:HD13	2.13	0.49
2:C:91:ILE:HD11	2:C:127:ILE:HG21	1.93	0.49
2:C:419:GLU:HA	2:C:422:ILE:HG13	1.95	0.49
2:F:202:TYR:CE1	2:F:206:ALA:HB2	2.46	0.49
1:A:303:THR:O	1:A:304:ILE:HG13	2.12	0.49
2:C:230:ILE:O	2:C:232:LEU:HD22	2.12	0.49
2:C:235:GLN:C	2:C:264:LYS:H	2.20	0.49
2:C:270:VAL:HG12	2:C:271:ILE:N	2.28	0.49
2:F:86:ILE:O	2:F:90:ILE:HD13	2.13	0.49
2:F:230:ILE:O	2:F:232:LEU:CD1	2.59	0.49
2:F:319:TYR:HA	2:F:322:SER:HB3	1.93	0.49
1:A:188:LYS:CE	1:A:189:GLU:H	2.25	0.49
1:A:249:ALA:O	1:A:412:LEU:HA	2.11	0.49
1:A:484:ILE:HD13	1:A:484:ILE:N	2.28	0.49
1:A:515:ILE:C	1:A:515:ILE:HD12	2.38	0.49
1:A:739:LYS:O	1:A:742:ILE:HD13	2.12	0.49
1:B:84:GLY:O	1:B:87:LEU:HB2	2.12	0.49
1:B:484:ILE:HD13	1:B:484:ILE:N	2.28	0.49
1:B:574:GLN:N	6:B:873:ADP:O4'	2.46	0.49
2:F:418:TYR:C	2:F:420:GLY:H	2.20	0.49
1:A:274:GLU:O	1:A:278:VAL:HG23	2.13	0.49
1:A:282:PHE:HA	1:A:285:ILE:HD12	1.93	0.49
1:A:330:SER:HB2	2:C:254:TYR:CZ	2.48	0.49
1:A:598:GLN:O	1:A:602:VAL:HG23	2.13	0.49
2:C:216:TRP:O	2:C:220:ILE:HG13	2.13	0.49
1:B:38:ARG:HA	1:B:41:MET:HE2	1.94	0.49
1:B:659:ARG:CG	1:B:755:LEU:HG	2.43	0.49
1:B:699:LYS:HB3	1:B:699:LYS:NZ	2.28	0.49
1:B:779:ARG:HH22	1:B:788:VAL:N	2.06	0.49
2:F:25:LEU:HB3	2:F:29:ARG:HH12	1.77	0.49
2:F:311:GLY:HA2	2:F:315:PHE:CD1	2.48	0.49
1:A:103:LEU:O	1:A:104:ALA:C	2.55	0.49
1:A:150:ILE:HD13	1:A:228:ASP:OD2	2.13	0.49
1:A:254:ALA:HA	1:A:257:VAL:HB	1.94	0.49
1:A:298:ASP:OD2	1:A:304:ILE:HG21	2.13	0.49
2:C:187:ILE:HD12	2:C:188:SER:H	1.78	0.49
1:B:150:ILE:HD13	1:B:228:ASP:OD2	2.13	0.49
1:B:185:GLU:CD	1:B:185:GLU:H	2.21	0.49
1:B:805:ILE:O	1:B:809:ILE:HG22	2.13	0.49
1:A:132:ASP:O	1:A:136:MET:HG2	2.12	0.49
1:A:319:GLY:C	1:A:321:GLU:H	2.19	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:ARG:HD3	1:A:378:LEU:HB3	1.95	0.49
3:D:18:ILE:C	3:D:21:PRO:HD2	2.38	0.49
1:B:94:GLU:HB3	1:B:95:MET:H	1.41	0.49
1:B:149:VAL:H	1:B:157:TYR:HB3	1.77	0.49
1:B:592:ARG:NH2	1:B:593:ILE:HD11	2.28	0.49
1:A:115:ILE:HD12	1:A:117:LYS:CE	2.41	0.49
1:A:149:VAL:HA	1:A:219:TYR:O	2.13	0.49
2:C:184:GLY:O	2:C:187:ILE:HD11	2.13	0.49
1:B:141:LEU:CB	1:B:159:VAL:HG11	2.40	0.49
1:B:298:ASP:OD2	1:B:304:ILE:HG21	2.13	0.49
2:F:231:ILE:C	2:F:232:LEU:O	2.55	0.49
1:A:38:ARG:HA	1:A:41:MET:HE2	1.94	0.49
1:A:659:ARG:CG	1:A:755:LEU:HG	2.42	0.49
2:C:189:ILE:HA	2:C:192:PHE:CD1	2.47	0.49
1:B:80:GLN:HE22	1:B:103:LEU:HD12	1.77	0.49
1:B:585:SER:H	1:B:588:ASP:CG	2.21	0.49
1:B:620:SER:HA	1:B:623:ILE:HD11	1.94	0.49
1:B:739:LYS:O	1:B:742:ILE:HD13	2.12	0.49
2:F:91:ILE:HG21	2:F:123:LEU:HG	1.95	0.49
3:G:18:ILE:C	3:G:21:PRO:HD2	2.38	0.49
1:A:333:TYR:CE1	2:C:253:VAL:HG13	2.48	0.48
1:A:490:LEU:C	1:A:490:LEU:HD13	2.38	0.48
1:A:535:GLY:HA2	1:A:570:ARG:NH2	2.28	0.48
1:A:618:MET:HA	1:A:621:LYS:CD	2.39	0.48
2:C:323:VAL:HG11	2:C:359:LEU:CD2	2.43	0.48
2:C:418:TYR:C	2:C:420:GLY:H	2.20	0.48
2:F:184:GLY:O	2:F:187:ILE:HD11	2.13	0.48
1:A:53:ALA:HB1	1:A:56:HIS:CE1	2.48	0.48
1:A:98:GLY:O	1:A:100:GLY:N	2.45	0.48
1:A:131:ARG:CZ	7:A:874:BEF:F3	2.51	0.48
1:A:666:LYS:NZ	1:A:666:LYS:HB3	2.28	0.48
2:C:90:ILE:O	2:C:93:GLN:HB3	2.12	0.48
2:C:199:TYR:N	2:C:200:PRO:HD2	2.28	0.48
1:B:97:THR:HG22	1:B:575:GLY:CA	2.43	0.48
1:B:103:LEU:O	1:B:104:ALA:C	2.55	0.48
1:B:535:GLY:HA2	1:B:570:ARG:NH2	2.28	0.48
2:F:154:LEU:O	2:F:158:VAL:HB	2.13	0.48
4:H:45:ARG:O	4:H:46:ARG:HG2	2.13	0.48
1:A:732:TRP:CZ2	1:A:810:ALA:HB1	2.48	0.48
1:A:805:ILE:O	1:A:809:ILE:HG22	2.13	0.48
2:C:25:LEU:HB3	2:C:29:ARG:HH12	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:VAL:HG12	1:B:437:ILE:CG2	2.43	0.48
1:B:270:GLY:CA	1:B:394:SER:HB3	2.43	0.48
1:B:296:THR:HA	1:B:306:LEU:HD13	1.95	0.48
1:B:306:LEU:HD12	1:B:307:THR:N	2.28	0.48
1:B:313:LYS:O	1:B:317:ILE:HG12	2.14	0.48
1:B:513:ALA:O	1:B:516:VAL:HB	2.14	0.48
2:F:25:LEU:HD22	3:G:51:PHE:CE1	2.48	0.48
3:G:30:PHE:HA	3:G:33:VAL:HG23	1.95	0.48
1:A:146:ARG:HG2	1:A:146:ARG:HH11	1.79	0.48
1:A:313:LYS:O	1:A:317:ILE:HG12	2.14	0.48
1:A:573:ARG:HB3	6:A:873:ADP:C4'	2.43	0.48
1:A:592:ARG:NH2	1:A:593:ILE:HD11	2.28	0.48
1:A:614:ILE:HG12	1:A:615:GLN:N	2.28	0.48
2:C:394:SER:HA	2:C:397:ILE:CD1	2.44	0.48
4:E:45:ARG:O	4:E:46:ARG:HG2	2.13	0.48
1:B:76:PRO:HB2	1:B:185:GLU:HG3	1.96	0.48
1:B:274:GLU:O	1:B:278:VAL:HG23	2.12	0.48
1:B:346:LYS:C	1:B:348:ASP:N	2.71	0.48
1:B:425:GLU:C	1:B:427:VAL:N	2.72	0.48
1:B:576:ASP:HB2	1:B:577:PRO:HD2	1.96	0.48
1:B:614:ILE:HG12	1:B:615:GLN:N	2.28	0.48
1:A:28:LEU:HA	1:A:32:LYS:HZ3	1.78	0.48
1:A:481:THR:HG22	1:A:555:THR:OG1	2.12	0.48
1:A:585:SER:C	1:A:587:GLU:N	2.71	0.48
1:B:96:LYS:H	1:B:99:GLU:CD	2.22	0.48
1:B:97:THR:HG22	1:B:575:GLY:N	2.29	0.48
1:B:786:PRO:C	1:B:787:ILE:HD12	2.39	0.48
2:F:356:HIS:O	2:F:359:LEU:HB2	2.14	0.48
1:A:94:GLU:HB2	1:A:416:THR:H	1.78	0.48
1:A:97:THR:HG22	1:A:575:GLY:CA	2.43	0.48
1:A:618:MET:N	1:A:621:LYS:HZ2	2.11	0.48
2:C:232:LEU:HB3	2:C:267:GLN:N	2.29	0.48
2:C:416:ARG:HB3	2:C:418:TYR:CE2	2.48	0.48
4:E:33:ALA:HA	4:E:36:SER:OG	2.14	0.48
1:B:53:ALA:HB1	1:B:56:HIS:CE1	2.48	0.48
1:B:213:TYR:CG	1:B:243:GLN:HA	2.49	0.48
2:F:199:TYR:N	2:F:200:PRO:HD2	2.29	0.48
2:F:216:TRP:O	2:F:220:ILE:HG13	2.13	0.48
1:A:145:LEU:HD22	1:A:216:ASP:OD2	2.14	0.48
1:A:149:VAL:HG13	1:A:156:SER:O	2.14	0.48
1:A:157:TYR:CZ	1:A:212:ALA:HA	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:SER:OG	1:A:331:LEU:HD12	2.13	0.48
1:A:585:SER:H	1:A:588:ASP:CG	2.21	0.48
1:A:659:ARG:HH12	1:A:759:ASP:CB	2.27	0.48
1:A:699:LYS:HB3	1:A:699:LYS:NZ	2.28	0.48
2:C:162:MET:SD	4:E:15:ALA:HB1	2.53	0.48
1:B:101:LYS:N	6:B:873:ADP:O1A	2.47	0.48
1:B:145:LEU:HD22	1:B:216:ASP:OD2	2.14	0.48
1:B:149:VAL:HG13	1:B:156:SER:O	2.14	0.48
1:B:490:LEU:HD13	1:B:490:LEU:C	2.38	0.48
1:B:732:TRP:CZ2	1:B:810:ALA:HB1	2.48	0.48
2:F:154:LEU:O	2:F:155:GLN:HB2	2.13	0.48
1:A:3:LEU:HB2	1:A:5:ASP:HB2	1.94	0.48
1:A:79:VAL:HG12	1:A:437:ILE:CG2	2.43	0.48
1:A:270:GLY:CA	1:A:394:SER:HB3	2.43	0.48
1:A:766:LEU:O	1:A:769:VAL:HB	2.13	0.48
1:B:515:ILE:C	1:B:515:ILE:HD12	2.38	0.48
1:B:766:LEU:O	1:B:769:VAL:HB	2.13	0.48
2:F:416:ARG:HB3	2:F:418:TYR:CE2	2.48	0.48
3:G:13:ALA:O	3:G:17:LYS:HG3	2.14	0.48
1:A:97:THR:HG22	1:A:575:GLY:N	2.29	0.48
1:A:134:LEU:HB3	1:A:202:VAL:HG22	1.96	0.48
1:A:422:GLU:HG3	1:A:422:GLU:H	1.33	0.48
1:A:450:ASP:HB3	1:A:584:LEU:CD1	2.44	0.48
2:C:339:GLY:HA2	2:C:344:GLY:H	1.79	0.48
1:B:515:ILE:O	1:B:516:VAL:C	2.56	0.48
1:B:598:GLN:O	1:B:602:VAL:HG23	2.13	0.48
1:B:636:SER:O	1:B:639:LYS:HB3	2.14	0.48
2:F:339:GLY:HA2	2:F:344:GLY:H	1.79	0.48
2:F:386:VAL:C	2:F:388:VAL:H	2.22	0.48
2:F:419:GLU:HA	2:F:422:ILE:HG13	1.95	0.48
1:A:75:ARG:HE	1:A:75:ARG:N	2.12	0.48
1:A:76:PRO:HB2	1:A:185:GLU:HG3	1.96	0.48
1:A:185:GLU:H	1:A:185:GLU:CD	2.21	0.48
1:A:230:LEU:CD2	1:A:397:TYR:HB3	2.35	0.48
1:A:334:HIS:ND1	1:A:335:LEU:N	2.62	0.48
1:A:515:ILE:O	1:A:516:VAL:C	2.55	0.48
1:A:536:THR:O	1:A:538:ILE:HD12	2.14	0.48
1:A:636:SER:O	1:A:639:LYS:HB3	2.14	0.48
2:C:154:LEU:O	2:C:158:VAL:HB	2.13	0.48
2:C:356:HIS:O	2:C:359:LEU:HB2	2.14	0.48
3:D:30:PHE:HA	3:D:33:VAL:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:SER:OG	1:B:331:LEU:HD12	2.13	0.48
1:B:659:ARG:HH12	1:B:759:ASP:CB	2.27	0.48
2:F:270:VAL:HG12	2:F:271:ILE:N	2.29	0.48
2:F:305:LEU:O	2:F:309:ILE:HG13	2.14	0.48
2:F:392:GLY:O	2:F:396:LEU:HG	2.14	0.48
1:A:3:LEU:C	1:A:5:ASP:N	2.71	0.47
1:A:757:ILE:HD11	1:A:812:TYR:CE1	2.49	0.47
1:A:786:PRO:C	1:A:787:ILE:HD12	2.39	0.47
2:C:91:ILE:HG21	2:C:123:LEU:HG	1.95	0.47
1:B:156:SER:HA	1:B:207:ILE:CD1	2.44	0.47
2:F:85:TYR:OH	2:F:175:GLY:HA3	2.14	0.47
2:F:323:VAL:O	2:F:324:VAL:C	2.57	0.47
2:F:394:SER:HA	2:F:397:ILE:CD1	2.44	0.47
1:A:576:ASP:HB2	1:A:577:PRO:HD2	1.96	0.47
2:C:13:GLU:C	2:C:13:GLU:CD	2.82	0.47
2:C:305:LEU:O	2:C:309:ILE:HG13	2.14	0.47
2:C:327:ASP:N	2:C:328:PRO:HD2	2.29	0.47
1:B:148:GLY:HA2	1:B:157:TYR:CB	2.44	0.47
1:B:149:VAL:HA	1:B:219:TYR:O	2.13	0.47
1:A:94:GLU:OE1	1:A:94:GLU:HA	2.13	0.47
1:A:121:LEU:CD2	1:A:250:ILE:HB	2.43	0.47
1:A:148:GLY:HA2	1:A:157:TYR:CB	2.44	0.47
1:A:184:GLY:C	1:A:186:VAL:H	2.22	0.47
1:A:346:LYS:C	1:A:348:ASP:N	2.71	0.47
1:A:425:GLU:C	1:A:427:VAL:N	2.72	0.47
1:A:513:ALA:O	1:A:516:VAL:HB	2.14	0.47
1:B:41:MET:HA	1:B:44:LYS:HZ1	1.80	0.47
1:B:121:LEU:CD2	1:B:250:ILE:HB	2.43	0.47
1:B:503:VAL:HG13	1:B:527:ILE:HG23	1.96	0.47
2:F:227:ILE:HG21	3:G:30:PHE:HD1	1.79	0.47
2:F:277:SER:HA	2:F:310:TYR:CZ	2.49	0.47
1:A:101:LYS:HD2	1:A:415:MET:CB	2.44	0.47
1:A:213:TYR:CG	1:A:243:GLN:HA	2.49	0.47
1:A:484:ILE:HD13	1:A:484:ILE:H	1.80	0.47
2:C:85:TYR:OH	2:C:175:GLY:HA3	2.14	0.47
2:C:161:THR:O	2:C:165:LEU:HD13	2.15	0.47
2:C:237:GLU:HB3	2:C:338:TYR:CA	2.44	0.47
2:C:358:VAL:HA	2:C:361:ARG:HG2	1.96	0.47
2:C:392:GLY:O	2:C:396:LEU:HG	2.14	0.47
1:B:339:LEU:HD23	1:B:340:LYS:N	2.30	0.47
1:B:806:ASN:HA	1:B:809:ILE:CG2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:161:THR:O	2:F:165:LEU:HD13	2.15	0.47
1:A:78:ASP:O	1:A:82:MET:N	2.46	0.47
1:A:339:LEU:HD23	1:A:340:LYS:N	2.30	0.47
1:A:452:VAL:HG12	1:A:453:PHE:N	2.30	0.47
3:D:47:LEU:HA	3:D:50:ILE:HD12	1.97	0.47
1:B:294:ASP:O	1:B:295:PHE:C	2.57	0.47
1:B:639:LYS:O	1:B:640:THR:C	2.57	0.47
1:B:666:LYS:NZ	1:B:666:LYS:HB3	2.28	0.47
1:B:757:ILE:HD11	1:B:812:TYR:CE1	2.49	0.47
3:G:21:PRO:O	3:G:24:LYS:HE3	2.15	0.47
1:A:78:ASP:C	1:A:80:GLN:H	2.23	0.47
1:A:81:VAL:O	1:A:85:ILE:HG12	2.15	0.47
1:A:96:LYS:H	1:A:99:GLU:CD	2.22	0.47
1:A:484:ILE:HG12	1:A:485:GLU:N	2.30	0.47
1:A:639:LYS:O	1:A:640:THR:C	2.57	0.47
2:C:154:LEU:O	2:C:155:GLN:HB2	2.13	0.47
1:B:429:VAL:HG23	1:B:430:TYR:H	1.79	0.47
1:B:450:ASP:HB3	1:B:584:LEU:CD1	2.44	0.47
1:B:574:GLN:CA	6:B:873:ADP:H1'	2.44	0.47
1:B:650:LYS:O	1:B:653:ARG:HB3	2.15	0.47
2:F:187:ILE:HD12	2:F:188:SER:H	1.77	0.47
1:A:233:ASN:C	1:A:235:VAL:H	2.23	0.47
1:A:294:ASP:O	1:A:295:PHE:C	2.57	0.47
1:A:368:LEU:HD23	1:A:368:LEU:O	2.15	0.47
2:C:91:ILE:HG22	2:C:95:LEU:HD12	1.97	0.47
2:C:187:ILE:H	2:C:187:ILE:HG13	1.46	0.47
2:C:238:ARG:HD3	2:C:337:LYS:NZ	2.29	0.47
3:D:13:ALA:O	3:D:17:LYS:HG3	2.14	0.47
1:B:28:LEU:HA	1:B:32:LYS:HZ2	1.80	0.47
1:B:78:ASP:O	1:B:82:MET:N	2.46	0.47
1:B:233:ASN:C	1:B:235:VAL:H	2.23	0.47
1:B:373:ARG:HD3	1:B:378:LEU:HB3	1.95	0.47
1:B:422:GLU:HG3	1:B:422:GLU:H	1.33	0.47
1:B:452:VAL:HG12	1:B:453:PHE:N	2.30	0.47
1:B:770:GLU:HG3	2:F:240:ILE:CD1	2.45	0.47
2:F:12:PRO:O	2:F:13:GLU:HB2	2.14	0.47
2:F:36:VAL:HG13	2:F:156:PHE:CE1	2.50	0.47
2:F:220:ILE:O	2:F:223:ALA:HB3	2.15	0.47
2:F:230:ILE:O	2:F:232:LEU:N	2.48	0.47
2:F:272:PRO:HG2	2:F:273:ILE:H	1.80	0.47
2:F:321:TYR:O	2:F:324:VAL:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:16:LYS:HA	3:G:19:SER:OG	2.14	0.47
1:A:96:LYS:HZ1	1:A:570:ARG:NH2	2.11	0.47
1:A:100:GLY:O	1:A:101:LYS:C	2.58	0.47
1:A:212:ALA:O	1:A:215:CYS:HB2	2.15	0.47
1:A:806:ASN:HA	1:A:809:ILE:CG2	2.45	0.47
2:C:232:LEU:HD23	2:C:234:GLN:HB3	1.97	0.47
1:B:75:ARG:HE	1:B:76:PRO:CD	2.15	0.47
1:B:96:LYS:HZ3	1:B:573:ARG:HH21	1.63	0.47
1:B:459:LYS:HZ2	1:B:584:LEU:C	2.23	0.47
1:B:573:ARG:HD3	6:B:873:ADP:O1B	2.15	0.47
1:B:614:ILE:HA	1:B:616:HIS:CE1	2.50	0.47
1:B:638:ARG:HG2	1:B:642:MET:HE2	1.97	0.47
2:F:33:TYR:OH	3:G:55:VAL:HG11	2.15	0.47
1:A:75:ARG:HA	1:A:103:LEU:HD13	1.96	0.47
1:A:331:LEU:O	1:A:334:HIS:ND1	2.42	0.47
1:A:484:ILE:H	1:A:484:ILE:CD1	2.28	0.47
2:C:277:SER:HA	2:C:310:TYR:CZ	2.49	0.47
3:D:16:LYS:HA	3:D:19:SER:OG	2.15	0.47
1:B:146:ARG:HG2	1:B:146:ARG:HH11	1.79	0.47
1:B:157:TYR:CZ	1:B:212:ALA:HA	2.49	0.47
1:B:214:LEU:H	1:B:214:LEU:HD12	1.80	0.47
1:B:368:LEU:O	1:B:368:LEU:HD23	2.15	0.47
1:B:626:ILE:O	1:B:630:VAL:HG23	2.15	0.47
3:G:47:LEU:HA	3:G:50:ILE:HD12	1.97	0.47
4:H:33:ALA:HA	4:H:36:SER:OG	2.14	0.47
1:A:296:THR:HA	1:A:306:LEU:HD13	1.96	0.47
1:B:81:VAL:O	1:B:85:ILE:HG12	2.15	0.47
1:B:334:HIS:ND1	1:B:335:LEU:N	2.62	0.47
1:B:484:ILE:CD1	1:B:484:ILE:H	2.28	0.47
2:F:358:VAL:HA	2:F:361:ARG:HG2	1.96	0.47
1:A:650:LYS:O	1:A:653:ARG:HB3	2.15	0.46
2:C:118:LYS:HA	2:C:121:ARG:HD3	1.96	0.46
1:B:326:PRO:C	1:B:328:ASN:N	2.72	0.46
1:B:402:PHE:O	1:B:406:PHE:N	2.48	0.46
1:B:574:GLN:HA	6:B:873:ADP:H1'	1.98	0.46
1:B:645:ASP:O	1:B:648:LEU:HB2	2.15	0.46
1:B:732:TRP:O	1:B:736:GLN:N	2.48	0.46
1:A:198:GLU:O	1:A:201:GLN:HB2	2.15	0.46
1:A:638:ARG:HG2	1:A:642:MET:HE2	1.97	0.46
1:A:699:LYS:HA	1:A:702:LEU:HB3	1.97	0.46
2:C:36:VAL:HG13	2:C:156:PHE:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:121:ARG:O	2:C:125:LEU:HG	2.16	0.46
2:C:323:VAL:O	2:C:324:VAL:C	2.57	0.46
1:B:75:ARG:HE	1:B:75:ARG:N	2.12	0.46
1:B:75:ARG:HA	1:B:103:LEU:HD13	1.96	0.46
1:B:78:ASP:C	1:B:80:GLN:H	2.23	0.46
1:B:101:LYS:NZ	1:B:416:THR:OG1	2.47	0.46
1:B:184:GLY:C	1:B:186:VAL:H	2.22	0.46
1:B:484:ILE:HG12	1:B:485:GLU:N	2.30	0.46
1:B:538:ILE:HG22	1:B:539:LYS:N	2.30	0.46
2:F:118:LYS:HA	2:F:121:ARG:HD3	1.96	0.46
2:F:163:SER:O	2:F:167:GLY:HA3	2.15	0.46
2:F:321:TYR:O	2:F:324:VAL:N	2.48	0.46
1:A:90:GLY:O	1:A:432:MET:HB3	2.16	0.46
1:A:238:TYR:C	1:A:240:ASP:N	2.72	0.46
1:A:367:ARG:NH2	1:A:506:ALA:H	2.14	0.46
1:A:521:GLN:H	1:A:524:MET:HB3	1.81	0.46
1:A:614:ILE:HA	1:A:616:HIS:CE1	2.50	0.46
1:A:732:TRP:O	1:A:736:GLN:N	2.48	0.46
2:C:12:PRO:O	2:C:13:GLU:HB2	2.14	0.46
2:C:275:PHE:CE2	2:C:276:ALA:HB2	2.51	0.46
2:C:275:PHE:O	2:C:279:ILE:HG13	2.16	0.46
2:C:311:GLY:HA2	2:C:315:PHE:CD1	2.51	0.46
1:B:100:GLY:O	1:B:101:LYS:C	2.58	0.46
1:B:198:GLU:O	1:B:201:GLN:HB2	2.15	0.46
1:B:212:ALA:O	1:B:215:CYS:HB2	2.15	0.46
2:F:270:VAL:HG12	2:F:271:ILE:H	1.79	0.46
1:A:75:ARG:HE	1:A:76:PRO:CD	2.15	0.46
1:A:134:LEU:CD2	1:A:202:VAL:HG13	2.43	0.46
1:A:527:ILE:C	1:A:527:ILE:HD13	2.40	0.46
1:A:645:ASP:O	1:A:648:LEU:HB2	2.15	0.46
2:C:279:ILE:O	2:C:283:PRO:HD3	2.15	0.46
2:C:315:PHE:CE2	2:C:370:LEU:HD12	2.50	0.46
3:D:21:PRO:O	3:D:24:LYS:HE3	2.15	0.46
1:B:134:LEU:CD2	1:B:202:VAL:HG13	2.43	0.46
1:B:504:LEU:HD13	1:B:515:ILE:CD1	2.46	0.46
1:B:749:VAL:HG12	1:B:753:LEU:HD23	1.97	0.46
2:F:13:GLU:CD	2:F:13:GLU:C	2.82	0.46
2:F:275:PHE:O	2:F:279:ILE:HG13	2.16	0.46
1:A:28:LEU:HA	1:A:32:LYS:HZ2	1.80	0.46
1:A:76:PRO:N	6:A:873:ADP:HN62	2.04	0.46
1:A:77:PHE:O	1:A:81:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:SER:HA	1:A:207:ILE:CD1	2.44	0.46
1:A:536:THR:HB	1:A:538:ILE:CD1	2.46	0.46
1:A:619:LEU:O	1:A:623:ILE:HG12	2.15	0.46
2:C:163:SER:O	2:C:167:GLY:HA3	2.15	0.46
2:C:236:ALA:HB2	2:C:264:LYS:HB2	1.96	0.46
2:C:270:VAL:HG12	2:C:271:ILE:H	1.80	0.46
1:B:28:LEU:HA	1:B:32:LYS:HZ3	1.79	0.46
1:B:306:LEU:CD2	1:B:309:GLU:HG3	2.39	0.46
1:B:367:ARG:NH2	1:B:506:ALA:H	2.14	0.46
1:B:500:PRO:O	1:B:501:HIS:HB3	2.16	0.46
2:F:91:ILE:HG22	2:F:95:LEU:HD12	1.97	0.46
2:F:315:PHE:CE2	2:F:370:LEU:HD12	2.50	0.46
3:G:59:PHE:O	3:G:63:GLY:HA3	2.15	0.46
1:A:115:ILE:CD1	1:A:117:LYS:HB2	2.46	0.46
1:A:503:VAL:HG13	1:A:527:ILE:HG23	1.97	0.46
1:A:655:VAL:HG11	1:A:762:TRP:CD1	2.50	0.46
1:A:802:MET:CB	2:C:422:ILE:HD12	2.45	0.46
2:C:35:PRO:CG	4:E:68:VAL:HA	2.39	0.46
2:C:189:ILE:HB	2:C:401:VAL:CG1	2.44	0.46
2:C:386:VAL:C	2:C:388:VAL:H	2.22	0.46
3:D:55:VAL:HA	3:D:58:ILE:HD12	1.98	0.46
1:B:287:LYS:O	1:B:290:VAL:HB	2.16	0.46
1:B:574:GLN:HA	6:B:873:ADP:C1'	2.46	0.46
1:B:753:LEU:O	1:B:754:MET:C	2.59	0.46
1:A:34:SER:HA	1:A:37:ILE:HD12	1.98	0.46
1:A:96:LYS:HZ3	1:A:573:ARG:HH21	1.63	0.46
1:A:626:ILE:O	1:A:630:VAL:HG23	2.15	0.46
1:A:749:VAL:HG12	1:A:753:LEU:HD23	1.97	0.46
2:C:14:LEU:HD13	2:C:17:ARG:CB	2.46	0.46
3:D:59:PHE:O	3:D:63:GLY:HA3	2.15	0.46
1:B:3:LEU:C	1:B:5:ASP:N	2.71	0.46
1:B:74:MET:N	1:B:187:LEU:HD13	2.23	0.46
1:B:281:ARG:O	1:B:285:ILE:HG13	2.16	0.46
1:B:295:PHE:O	1:B:306:LEU:HD22	2.16	0.46
1:B:400:ILE:HB	1:B:404:ASN:HB2	1.98	0.46
1:A:43:LEU:HD23	1:A:46:LYS:HD2	1.98	0.46
1:A:175:TRP:HE1	1:A:177:VAL:HB	1.81	0.46
1:A:214:LEU:HD12	1:A:214:LEU:H	1.80	0.46
1:A:281:ARG:O	1:A:285:ILE:HG13	2.16	0.46
1:A:402:PHE:O	1:A:406:PHE:N	2.48	0.46
1:A:500:PRO:O	1:A:501:HIS:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:GLU:O	1:A:681:SER:N	2.38	0.46
2:C:220:ILE:O	2:C:223:ALA:HB3	2.15	0.46
2:C:342:ILE:HG23	2:C:343:PRO:CD	2.43	0.46
2:C:364:PHE:O	2:C:368:VAL:HG23	2.16	0.46
1:B:115:ILE:CD1	1:B:117:LYS:HB2	2.46	0.46
1:B:175:TRP:HE1	1:B:177:VAL:HB	1.81	0.46
1:B:178:TRP:CD1	1:B:194:LYS:HZ3	2.34	0.46
1:B:400:ILE:HG23	1:B:402:PHE:CD2	2.50	0.46
1:B:536:THR:O	1:B:538:ILE:HD12	2.14	0.46
1:B:655:VAL:HG11	1:B:762:TRP:CD1	2.50	0.46
2:F:108:GLU:HB2	2:F:112:GLY:N	2.28	0.46
1:A:427:VAL:HG12	4:E:47:LYS:HD2	1.96	0.46
2:C:326:PHE:C	2:C:328:PRO:HD2	2.41	0.46
2:C:340:GLY:C	2:C:342:ILE:N	2.74	0.46
1:B:619:LEU:O	1:B:623:ILE:HG12	2.16	0.46
2:F:14:LEU:HD13	2:F:17:ARG:CB	2.46	0.46
2:F:121:ARG:O	2:F:125:LEU:HG	2.16	0.46
2:F:364:PHE:O	2:F:368:VAL:HG23	2.16	0.46
1:A:2:ILE:HD11	4:E:52:GLY:HA3	1.98	0.46
1:A:324:TYR:OH	2:C:337:LYS:HD2	2.16	0.46
1:A:400:ILE:HG23	1:A:402:PHE:CD2	2.50	0.46
1:A:479:VAL:HG13	1:A:527:ILE:HG12	1.98	0.46
1:B:332:LEU:O	1:B:336:ILE:HG13	2.16	0.46
1:B:521:GLN:H	1:B:524:MET:HB3	1.81	0.46
1:B:585:SER:C	1:B:587:GLU:N	2.71	0.46
1:B:699:LYS:HA	1:B:702:LEU:HB3	1.97	0.46
1:B:779:ARG:HH22	1:B:788:VAL:CB	2.29	0.46
2:F:14:LEU:HB2	2:F:17:ARG:HB2	1.97	0.46
2:F:156:PHE:CE1	2:F:159:LEU:HD23	2.51	0.46
2:F:326:PHE:HD2	2:F:329:ARG:HD2	1.81	0.46
1:A:29:ARG:C	1:A:31:LYS:H	2.24	0.45
1:A:288:LYS:O	1:A:291:LYS:HB3	2.16	0.45
1:A:295:PHE:O	1:A:306:LEU:HD22	2.16	0.45
1:A:745:ASP:OD2	1:B:756:ARG:NH1	2.49	0.45
2:C:326:PHE:HD2	2:C:329:ARG:HD2	1.81	0.45
1:B:74:MET:CA	6:B:873:ADP:C6	2.98	0.45
1:B:134:LEU:HB3	1:B:202:VAL:HG22	1.96	0.45
1:B:160:VAL:HA	1:B:203:GLU:OE1	2.16	0.45
1:B:527:ILE:HD13	1:B:527:ILE:C	2.41	0.45
2:F:217:ILE:O	2:F:220:ILE:HB	2.16	0.45
1:A:139:VAL:O	1:A:142:PHE:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:LEU:H	1:A:590:LEU:CD2	2.26	0.45
2:C:232:LEU:CB	2:C:266:ASN:C	2.89	0.45
3:D:20:TRP:HB3	3:D:21:PRO:HD3	1.98	0.45
1:B:43:LEU:HD23	1:B:46:LYS:HD2	1.98	0.45
1:B:102:THR:HG23	6:B:873:ADP:O2A	2.16	0.45
1:B:545:ALA:O	1:B:546:GLU:C	2.59	0.45
1:B:550:LEU:HD13	1:B:571:ALA:HA	1.97	0.45
1:B:669:ASP:HA	1:B:672:LEU:HD21	1.98	0.45
1:A:249:ALA:O	1:A:412:LEU:HD23	2.15	0.45
1:A:504:LEU:HD13	1:A:515:ILE:CD1	2.46	0.45
1:A:771:HIS:HA	2:C:240:ILE:HG21	1.99	0.45
2:C:242:ILE:O	2:C:249:THR:HG23	2.17	0.45
1:B:679:VAL:HG11	1:B:803:ARG:HG2	1.98	0.45
1:B:746:TYR:HA	1:B:749:VAL:HG23	1.98	0.45
1:A:133:ALA:HA	1:A:219:TYR:CD1	2.52	0.45
1:A:538:ILE:HG22	1:A:539:LYS:N	2.31	0.45
2:C:381:GLN:O	2:C:385:LYS:HE2	2.16	0.45
1:B:185:GLU:O	1:B:187:LEU:HD23	2.16	0.45
1:B:235:VAL:HG11	1:B:240:ASP:HB2	1.99	0.45
1:B:238:TYR:C	1:B:240:ASP:N	2.72	0.45
1:B:238:TYR:HB2	1:B:663:LEU:CD2	2.47	0.45
1:B:249:ALA:O	1:B:412:LEU:HD23	2.15	0.45
2:F:319:TYR:O	2:F:323:VAL:HG23	2.16	0.45
2:F:345:LEU:O	2:F:346:ARG:C	2.59	0.45
4:H:16:LEU:O	4:H:20:VAL:HG23	2.16	0.45
1:A:259:ILE:HA	1:A:261:GLU:OE1	2.17	0.45
1:A:306:LEU:CD2	1:A:309:GLU:HG3	2.39	0.45
1:A:550:LEU:HD13	1:A:571:ALA:HA	1.97	0.45
1:A:779:ARG:HH22	1:A:788:VAL:CB	2.29	0.45
1:B:77:PHE:O	1:B:81:VAL:HG23	2.16	0.45
2:F:81:SER:C	2:F:84:PRO:HD2	2.41	0.45
2:F:381:GLN:O	2:F:385:LYS:HE2	2.16	0.45
1:A:342:LEU:N	1:A:342:LEU:HD23	2.32	0.45
1:A:429:VAL:HG23	1:A:430:TYR:H	1.80	0.45
1:A:789:GLU:HA	1:A:792:LYS:HG2	1.99	0.45
2:C:81:SER:C	2:C:84:PRO:HD2	2.41	0.45
2:C:108:GLU:HB2	2:C:112:GLY:N	2.28	0.45
2:C:301:ALA:C	2:C:303:GLY:H	2.24	0.45
2:C:315:PHE:CZ	2:C:370:LEU:HB2	2.37	0.45
2:C:370:LEU:O	2:C:373:ILE:HB	2.17	0.45
4:E:27:PHE:HA	4:E:30:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ARG:HA	1:B:41:MET:CE	2.47	0.45
1:B:139:VAL:O	1:B:142:PHE:HB3	2.16	0.45
1:B:306:LEU:HD11	1:B:309:GLU:HG3	1.99	0.45
1:B:484:ILE:HD13	1:B:484:ILE:H	1.80	0.45
1:B:565:ASN:O	1:B:568:ARG:HB3	2.17	0.45
1:B:673:LYS:HZ1	1:B:736:GLN:HG3	1.82	0.45
1:B:771:HIS:O	1:B:774:GLU:HB3	2.17	0.45
3:G:55:VAL:HA	3:G:58:ILE:HD12	1.98	0.45
4:H:45:ARG:C	4:H:47:LYS:N	2.75	0.45
1:A:38:ARG:HA	1:A:41:MET:CE	2.47	0.45
1:A:74:MET:CA	6:A:873:ADP:C6	2.93	0.45
1:A:690:GLY:HA2	1:A:695:ILE:HD13	1.98	0.45
4:E:16:LEU:O	4:E:20:VAL:HG23	2.15	0.45
1:B:29:ARG:C	1:B:31:LYS:H	2.24	0.45
1:B:761:HIS:HB3	1:B:801:MET:CE	2.44	0.45
2:F:189:ILE:HB	2:F:401:VAL:CG1	2.44	0.45
3:G:20:TRP:HB3	3:G:21:PRO:HD3	1.98	0.45
1:A:160:VAL:HA	1:A:203:GLU:OE1	2.16	0.45
1:A:185:GLU:O	1:A:187:LEU:HD23	2.16	0.45
1:A:287:LYS:O	1:A:290:VAL:HB	2.16	0.45
1:A:332:LEU:O	1:A:336:ILE:HG13	2.16	0.45
1:A:403:GLN:HG3	1:A:429:VAL:CG1	2.40	0.45
1:A:536:THR:HG22	1:A:538:ILE:HG13	1.99	0.45
2:C:265:VAL:HG12	2:C:266:ASN:N	2.32	0.45
2:C:272:PRO:CB	2:C:314:VAL:HG11	2.46	0.45
4:E:58:VAL:O	4:E:62:LEU:HB2	2.17	0.45
1:B:61:PHE:O	1:B:64:VAL:HB	2.17	0.45
1:B:121:LEU:HG	1:B:219:TYR:CE2	2.52	0.45
1:B:296:THR:O	1:B:296:THR:HG22	2.17	0.45
1:B:359:ILE:HD13	1:B:383:GLU:OE1	2.17	0.45
1:B:360:ILE:HD12	1:B:368:LEU:HG	1.99	0.45
1:B:690:GLY:HA2	1:B:695:ILE:HD13	1.98	0.45
2:F:233:VAL:HG22	2:F:362:VAL:HG11	1.99	0.45
1:A:45:GLU:HA	1:A:48:ASN:OD1	2.17	0.45
1:A:80:GLN:HB2	1:A:104:ALA:HB2	1.99	0.45
1:A:771:HIS:O	1:A:774:GLU:HB3	2.17	0.45
2:C:14:LEU:HB2	2:C:17:ARG:HB2	1.97	0.45
2:C:319:TYR:O	2:C:323:VAL:HG23	2.16	0.45
2:C:327:ASP:N	2:C:328:PRO:CD	2.80	0.45
2:C:373:ILE:HG21	2:C:396:LEU:HD11	1.99	0.45
3:D:38:ALA:O	3:D:42:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:48:ASP:O	3:D:51:PHE:HB2	2.17	0.45
1:B:45:GLU:HA	1:B:48:ASN:OD1	2.17	0.45
1:B:75:ARG:HA	1:B:103:LEU:CD1	2.47	0.45
1:B:133:ALA:HA	1:B:219:TYR:CD1	2.52	0.45
1:B:259:ILE:HA	1:B:261:GLU:OE1	2.17	0.45
1:B:299:GLU:O	1:B:301:ALA:N	2.50	0.45
1:B:342:LEU:N	1:B:342:LEU:HD23	2.31	0.45
1:B:479:VAL:HG13	1:B:527:ILE:HG12	1.98	0.45
2:F:143:ASN:ND2	2:F:144:PRO:HD2	2.31	0.45
1:A:178:TRP:CD1	1:A:194:LYS:HZ3	2.34	0.45
1:A:340:LYS:NZ	2:C:251:ARG:HE	2.01	0.45
1:A:444:ILE:HD13	1:A:576:ASP:O	2.16	0.45
1:A:609:GLU:H	1:A:609:GLU:HG2	1.54	0.45
1:A:774:GLU:HB2	2:C:240:ILE:HG22	1.98	0.45
2:C:143:ASN:ND2	2:C:144:PRO:HD2	2.31	0.45
2:C:217:ILE:O	2:C:220:ILE:HB	2.16	0.45
2:C:321:TYR:O	2:C:324:VAL:N	2.50	0.45
1:B:444:ILE:HD13	1:B:576:ASP:O	2.16	0.45
1:B:573:ARG:HB3	6:B:873:ADP:C4'	2.44	0.45
2:F:265:VAL:HG12	2:F:266:ASN:N	2.31	0.45
3:G:38:ALA:O	3:G:42:VAL:HG23	2.17	0.45
1:A:21:ILE:HD11	1:A:61:PHE:HB3	1.99	0.44
1:A:238:TYR:HB2	1:A:663:LEU:CD2	2.46	0.44
1:A:753:LEU:O	1:A:754:MET:C	2.59	0.44
2:C:83:THR:N	2:C:84:PRO:HD2	2.32	0.44
2:C:156:PHE:CE1	2:C:159:LEU:HD23	2.51	0.44
2:C:321:TYR:O	2:C:324:VAL:HA	2.17	0.44
1:B:67:ALA:HA	1:B:142:PHE:CE1	2.52	0.44
1:B:75:ARG:H	6:B:873:ADP:HN62	1.64	0.44
1:B:288:LYS:O	1:B:291:LYS:HB3	2.16	0.44
1:B:304:ILE:HG22	1:B:305:ILE:N	2.32	0.44
1:B:416:THR:O	1:B:417:GLY:O	2.35	0.44
1:B:536:THR:HG22	1:B:538:ILE:HG13	1.99	0.44
1:B:677:GLU:O	1:B:681:SER:N	2.38	0.44
2:F:173:TRP:O	2:F:177:ARG:HD2	2.17	0.44
2:F:231:ILE:HD11	3:G:27:LEU:CD1	2.38	0.44
2:F:370:LEU:O	2:F:373:ILE:HB	2.17	0.44
1:A:155:LYS:HZ1	1:A:209:ARG:CZ	2.30	0.44
1:A:303:THR:C	1:A:304:ILE:HD12	2.42	0.44
1:A:566:GLN:O	1:A:567:LEU:C	2.61	0.44
2:C:15:ARG:O	2:C:15:ARG:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:VAL:HG13	1:B:19:SER:N	2.32	0.44
1:B:332:LEU:HD12	1:B:336:ILE:HD11	2.00	0.44
1:B:621:LYS:O	1:B:624:GLU:HB2	2.17	0.44
1:B:677:GLU:OE1	1:B:681:SER:HB3	2.17	0.44
1:B:750:ILE:O	1:B:754:MET:HG2	2.17	0.44
2:F:187:ILE:H	2:F:187:ILE:HG13	1.46	0.44
1:A:75:ARG:HA	1:A:103:LEU:CD1	2.47	0.44
1:A:81:VAL:C	1:A:83:GLY:N	2.75	0.44
1:A:543:GLY:O	1:A:545:ALA:N	2.50	0.44
1:A:565:ASN:O	1:A:568:ARG:HB3	2.17	0.44
1:A:621:LYS:O	1:A:624:GLU:HB2	2.17	0.44
1:A:807:ASP:O	1:A:810:ALA:HB3	2.17	0.44
2:C:158:VAL:O	2:C:162:MET:HG3	2.18	0.44
1:B:65:ARG:HG2	1:B:75:ARG:HB2	2.00	0.44
1:B:80:GLN:HB2	1:B:104:ALA:HB2	1.99	0.44
1:B:90:GLY:O	1:B:432:MET:HB3	2.16	0.44
1:B:131:ARG:CZ	7:B:874:BEF:F3	2.54	0.44
1:B:150:ILE:HG13	1:B:155:LYS:NZ	2.33	0.44
1:B:334:HIS:HA	1:B:337:ASN:ND2	2.24	0.44
1:B:456:GLN:C	1:B:458:GLU:N	2.75	0.44
2:F:117:ALA:O	2:F:120:THR:HB	2.18	0.44
2:F:323:VAL:HG11	2:F:359:LEU:CD2	2.47	0.44
2:F:381:GLN:O	2:F:385:LYS:HG2	2.17	0.44
3:G:48:ASP:O	3:G:51:PHE:HB2	2.17	0.44
1:A:235:VAL:HG11	1:A:240:ASP:HB2	1.98	0.44
1:A:299:GLU:O	1:A:301:ALA:N	2.50	0.44
1:A:306:LEU:HD11	1:A:309:GLU:HG3	1.99	0.44
1:A:360:ILE:HD12	1:A:368:LEU:HG	1.99	0.44
1:A:400:ILE:HB	1:A:404:ASN:HB2	1.98	0.44
1:A:508:TYR:O	1:A:511:LYS:HB2	2.17	0.44
1:A:545:ALA:O	1:A:546:GLU:C	2.59	0.44
1:A:658:LEU:O	1:A:662:ILE:HG23	2.18	0.44
1:A:750:ILE:O	1:A:754:MET:HG2	2.17	0.44
1:A:779:ARG:HH12	1:A:789:GLU:N	2.16	0.44
2:C:104:GLU:HB3	2:C:105:MET:HE2	2.00	0.44
2:C:173:TRP:O	2:C:177:ARG:HD2	2.17	0.44
2:C:327:ASP:OD2	2:C:328:PRO:HD3	2.17	0.44
1:B:75:ARG:NH2	1:B:187:LEU:HD13	2.32	0.44
1:B:101:LYS:HZ2	1:B:101:LYS:HG3	1.62	0.44
1:B:115:ILE:HD12	1:B:117:LYS:CE	2.41	0.44
1:B:338:ALA:O	1:B:342:LEU:HG	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:GLY:O	1:B:358:VAL:HG23	2.18	0.44
1:B:403:GLN:HG3	1:B:429:VAL:CG1	2.40	0.44
2:F:83:THR:N	2:F:84:PRO:HD2	2.32	0.44
2:F:117:ALA:O	2:F:121:ARG:HD2	2.18	0.44
2:F:272:PRO:CB	2:F:314:VAL:HG11	2.48	0.44
2:F:340:GLY:C	2:F:342:ILE:N	2.74	0.44
1:A:18:VAL:HG13	1:A:19:SER:N	2.32	0.44
1:A:97:THR:H	1:A:573:ARG:NH1	2.04	0.44
1:A:122:VAL:CG2	1:A:251:VAL:HG22	2.43	0.44
1:A:379:HIS:O	1:A:383:GLU:HB2	2.18	0.44
1:A:677:GLU:OE1	1:A:681:SER:HB3	2.17	0.44
1:A:679:VAL:HG11	1:A:803:ARG:HG2	1.98	0.44
1:A:806:ASN:HA	1:A:809:ILE:HG22	1.99	0.44
2:C:67:PHE:CE1	2:C:390:ILE:HD11	2.53	0.44
1:B:34:SER:HA	1:B:37:ILE:HD12	1.98	0.44
1:B:303:THR:C	1:B:304:ILE:HD12	2.43	0.44
1:B:465:GLU:HG3	1:B:466:GLU:N	2.33	0.44
1:B:508:TYR:O	1:B:511:LYS:HB2	2.17	0.44
1:B:522:LYS:C	1:B:524:MET:H	2.25	0.44
4:H:27:PHE:HA	4:H:30:LEU:HD12	1.99	0.44
1:A:22:ASN:HD22	1:A:22:ASN:HA	1.54	0.44
1:A:61:PHE:O	1:A:64:VAL:HB	2.17	0.44
1:A:150:ILE:HD11	1:A:209:ARG:CZ	2.48	0.44
1:A:321:GLU:OE2	1:A:324:TYR:HA	2.18	0.44
1:A:338:ALA:O	1:A:342:LEU:HG	2.17	0.44
1:A:338:ALA:O	1:A:339:LEU:C	2.60	0.44
1:A:416:THR:O	1:A:417:GLY:O	2.35	0.44
1:A:465:GLU:HG3	1:A:466:GLU:N	2.33	0.44
1:A:522:LYS:C	1:A:524:MET:H	2.25	0.44
1:A:574:GLN:CA	6:A:873:ADP:H1'	2.47	0.44
1:A:669:ASP:O	1:A:673:LYS:HG3	2.17	0.44
1:A:746:TYR:HA	1:A:749:VAL:HG23	1.98	0.44
2:C:25:LEU:HD11	3:D:47:LEU:HD22	1.99	0.44
2:C:319:TYR:OH	2:C:359:LEU:HA	2.18	0.44
1:B:172:GLU:O	1:B:176:SER:N	2.50	0.44
1:B:338:ALA:O	1:B:339:LEU:C	2.60	0.44
2:F:94:LEU:HA	2:F:97:SER:HB2	1.99	0.44
1:A:121:LEU:HG	1:A:219:TYR:CE2	2.52	0.44
1:A:459:LYS:HZ2	1:A:584:LEU:C	2.25	0.44
2:C:381:GLN:O	2:C:385:LYS:HG2	2.17	0.44
4:E:45:ARG:C	4:E:47:LYS:N	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:HIS:O	1:B:383:GLU:HB2	2.18	0.44
1:B:543:GLY:O	1:B:545:ALA:N	2.50	0.44
2:F:104:GLU:HB3	2:F:105:MET:HE2	1.99	0.44
2:F:237:GLU:HB3	2:F:338:TYR:CA	2.45	0.44
2:F:242:ILE:O	2:F:249:THR:HG23	2.18	0.44
1:A:3:LEU:HB3	1:A:4:PHE:H	1.63	0.44
1:A:172:GLU:O	1:A:176:SER:N	2.50	0.44
1:A:304:ILE:HG22	1:A:305:ILE:N	2.32	0.44
1:A:356:GLY:O	1:A:358:VAL:HG23	2.18	0.44
1:A:504:LEU:HG	1:A:528:ALA:CB	2.47	0.44
1:A:601:LYS:HB3	1:A:605:ILE:HD12	2.00	0.44
1:A:669:ASP:HA	1:A:672:LEU:HD21	1.98	0.44
1:A:723:LEU:O	1:A:727:LEU:HG	2.17	0.44
2:C:94:LEU:HA	2:C:97:SER:HB2	1.99	0.44
1:B:1:MET:SD	4:H:52:GLY:HA3	2.58	0.44
1:B:63:LEU:HD21	1:B:143:LEU:HD21	2.00	0.44
1:B:159:VAL:HG12	1:B:160:VAL:N	2.23	0.44
1:B:282:PHE:HB3	1:B:384:ALA:HB2	2.00	0.44
1:B:340:LYS:O	1:B:344:LEU:N	2.50	0.44
1:B:504:LEU:HG	1:B:528:ALA:CB	2.47	0.44
2:F:275:PHE:CE2	2:F:276:ALA:HB2	2.52	0.44
3:G:39:VAL:O	3:G:43:TYR:HD1	2.01	0.44
1:A:157:TYR:OH	1:A:207:ILE:HG21	2.18	0.44
1:A:261:GLU:O	1:A:262:ALA:C	2.60	0.44
1:A:336:ILE:HG13	1:A:336:ILE:H	1.65	0.44
1:A:574:GLN:HA	6:A:873:ADP:CI'	2.47	0.44
1:A:651:GLN:NE2	1:A:794:THR:HB	2.33	0.44
1:A:728:PHE:HA	1:A:731:LEU:HD12	2.00	0.44
2:C:127:ILE:HA	2:C:130:PHE:CD2	2.53	0.44
2:C:199:TYR:N	2:C:200:PRO:CD	2.81	0.44
1:B:21:ILE:HD11	1:B:61:PHE:HB3	1.99	0.44
1:B:334:HIS:O	1:B:337:ASN:HB2	2.18	0.44
2:F:71:ALA:HB3	2:F:135:VAL:HA	2.00	0.44
2:F:199:TYR:N	2:F:200:PRO:CD	2.81	0.44
2:F:222:VAL:HG11	2:F:373:ILE:HG23	2.00	0.44
2:F:358:VAL:HG13	2:F:361:ARG:HE	1.83	0.44
4:H:45:ARG:C	4:H:47:LYS:H	2.26	0.44
1:A:63:LEU:HD21	1:A:143:LEU:HD21	2.00	0.43
1:A:262:ALA:HB1	1:A:374:TYR:OH	2.18	0.43
1:A:334:HIS:O	1:A:337:ASN:HB2	2.18	0.43
1:A:340:LYS:O	1:A:344:LEU:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:761:HIS:HB3	1:A:801:MET:CE	2.44	0.43
2:C:71:ALA:HB3	2:C:135:VAL:HA	2.00	0.43
1:B:81:VAL:C	1:B:83:GLY:N	2.75	0.43
1:B:122:VAL:CG2	1:B:251:VAL:HG22	2.43	0.43
1:B:157:TYR:OH	1:B:207:ILE:HG21	2.18	0.43
1:B:262:ALA:HB1	1:B:374:TYR:OH	2.18	0.43
1:B:609:GLU:H	1:B:609:GLU:HG2	1.54	0.43
1:B:789:GLU:HA	1:B:792:LYS:HG2	1.99	0.43
2:F:104:GLU:C	2:F:105:MET:HE2	2.43	0.43
2:F:127:ILE:HA	2:F:130:PHE:CD2	2.53	0.43
4:H:58:VAL:O	4:H:62:LEU:HB2	2.17	0.43
1:A:313:LYS:CA	1:A:316:LYS:HB2	2.43	0.43
1:A:586:LEU:HA	1:A:591:LEU:HD11	2.00	0.43
2:C:290:THR:HG22	2:C:291:ASN:H	1.83	0.43
2:C:358:VAL:HG13	2:C:361:ARG:HE	1.83	0.43
1:B:292:ASP:CB	1:B:313:LYS:HD3	2.42	0.43
1:B:669:ASP:O	1:B:673:LYS:HG3	2.17	0.43
1:B:723:LEU:O	1:B:727:LEU:HG	2.17	0.43
2:F:232:LEU:N	2:F:232:LEU:CD2	2.80	0.43
1:A:18:VAL:O	1:A:22:ASN:HB2	2.18	0.43
1:A:152:SER:HA	1:A:224:GLU:OE2	2.19	0.43
1:A:456:GLN:C	1:A:458:GLU:N	2.75	0.43
2:C:117:ALA:O	2:C:121:ARG:HD2	2.18	0.43
2:C:197:ALA:HB2	3:D:48:ASP:OD2	2.18	0.43
2:C:358:VAL:HA	2:C:361:ARG:CD	2.48	0.43
1:B:150:ILE:HD11	1:B:209:ARG:CZ	2.48	0.43
1:B:288:LYS:HE2	1:B:318:ILE:HG12	2.00	0.43
1:B:346:LYS:C	1:B:348:ASP:H	2.27	0.43
1:B:425:GLU:OE1	1:B:425:GLU:HA	2.18	0.43
1:B:533:GLY:C	1:B:570:ARG:HG2	2.44	0.43
1:B:566:GLN:O	1:B:567:LEU:C	2.61	0.43
1:B:586:LEU:HA	1:B:591:LEU:HD11	2.00	0.43
1:B:673:LYS:HA	1:B:732:TRP:CZ3	2.53	0.43
1:B:798:PHE:O	1:B:802:MET:HG2	2.18	0.43
2:F:28:PHE:CD1	2:F:190:LEU:HD13	2.53	0.43
2:F:183:ILE:HG23	2:F:186:GLY:CA	2.49	0.43
2:F:373:ILE:HG21	2:F:396:LEU:HD11	1.99	0.43
1:A:75:ARG:NH2	1:A:187:LEU:HD13	2.32	0.43
1:A:296:THR:HG22	1:A:296:THR:O	2.17	0.43
1:A:786:PRO:HG2	1:A:788:VAL:HG23	2.01	0.43
2:C:166:ALA:HA	4:E:22:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:340:GLY:O	2:C:342:ILE:N	2.52	0.43
3:D:39:VAL:O	3:D:43:TYR:HD1	2.01	0.43
1:B:281:ARG:HH22	1:B:333:TYR:HE1	1.62	0.43
1:B:558:HIS:ND1	1:B:564:ASP:HA	2.33	0.43
1:B:612:GLN:N	1:B:613:PRO:CD	2.81	0.43
1:B:778:LEU:CD1	2:F:262:PRO:HA	2.48	0.43
1:B:786:PRO:HG2	1:B:788:VAL:HG23	2.01	0.43
1:B:806:ASN:HA	1:B:809:ILE:HG22	1.99	0.43
2:F:15:ARG:O	2:F:15:ARG:HG3	2.17	0.43
1:A:65:ARG:HG2	1:A:75:ARG:HB2	2.00	0.43
1:A:359:ILE:HD13	1:A:383:GLU:OE1	2.17	0.43
1:A:468:GLU:O	1:A:469:LYS:C	2.61	0.43
1:A:659:ARG:HA	1:A:662:ILE:CD1	2.48	0.43
2:C:228:PHE:CZ	3:D:26:LEU:HD22	2.53	0.43
1:B:182:PHE:HB2	1:B:183:ASN:H	1.56	0.43
1:B:651:GLN:NE2	1:B:794:THR:HB	2.33	0.43
1:B:659:ARG:HA	1:B:662:ILE:CD1	2.48	0.43
1:B:784:LYS:HB3	1:B:785:ASP:H	1.72	0.43
2:F:37:PRO:HG3	2:F:163:SER:OG	2.19	0.43
2:F:158:VAL:O	2:F:162:MET:HG3	2.18	0.43
1:A:67:ALA:HA	1:A:142:PHE:CE1	2.52	0.43
1:A:92:VAL:HA	1:A:414:GLY:O	2.18	0.43
1:A:561:ARG:HA	1:A:561:ARG:NE	2.34	0.43
1:A:690:GLY:HA2	1:A:695:ILE:CG2	2.49	0.43
1:A:798:PHE:O	1:A:802:MET:HG2	2.18	0.43
2:C:183:ILE:HG23	2:C:186:GLY:CA	2.49	0.43
2:C:191:ILE:O	2:C:195:ILE:HG13	2.18	0.43
1:B:178:TRP:O	1:B:180:ASP:N	2.52	0.43
1:B:333:TYR:OH	2:F:253:VAL:HG22	2.18	0.43
1:B:334:HIS:CG	1:B:335:LEU:N	2.85	0.43
1:B:755:LEU:H	1:B:755:LEU:CD1	2.31	0.43
1:B:779:ARG:HH12	1:B:789:GLU:N	2.16	0.43
1:B:807:ASP:O	1:B:810:ALA:HB3	2.17	0.43
2:F:162:MET:SD	4:H:15:ALA:HB1	2.59	0.43
2:F:304:PHE:O	2:F:308:LEU:HG	2.19	0.43
2:F:358:VAL:HA	2:F:361:ARG:CD	2.48	0.43
1:A:41:MET:O	1:A:44:LYS:HB3	2.19	0.43
1:A:187:LEU:CD2	6:A:873:ADP:C2	3.02	0.43
1:A:326:PRO:C	1:A:328:ASN:N	2.72	0.43
1:A:334:HIS:CG	1:A:335:LEU:N	2.85	0.43
1:A:425:GLU:HA	1:A:425:GLU:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:PRO:HB2	1:A:543:GLY:H	1.71	0.43
1:A:770:GLU:OE2	1:A:773:LYS:HD2	2.18	0.43
1:A:809:ILE:O	1:A:813:VAL:HG23	2.19	0.43
2:C:244:TYR:CD1	2:C:244:TYR:N	2.86	0.43
1:B:74:MET:H	1:B:75:ARG:NH2	2.17	0.43
1:B:298:ASP:OD2	1:B:304:ILE:HG12	2.19	0.43
1:B:645:ASP:HA	1:B:648:LEU:HB2	2.01	0.43
1:B:658:LEU:O	1:B:662:ILE:HG23	2.18	0.43
1:B:728:PHE:HA	1:B:731:LEU:HD12	2.00	0.43
1:B:809:ILE:O	1:B:813:VAL:HG23	2.19	0.43
2:F:191:ILE:O	2:F:195:ILE:HG13	2.18	0.43
1:A:178:TRP:O	1:A:180:ASP:N	2.52	0.43
1:A:319:GLY:C	1:A:321:GLU:N	2.77	0.43
1:A:502:GLN:CD	1:A:515:ILE:HG22	2.44	0.43
1:A:541:GLY:HA3	1:A:542:PRO:HD2	1.78	0.43
1:A:544:VAL:C	1:A:546:GLU:H	2.27	0.43
1:A:555:THR:O	1:A:556:GLU:HB3	2.19	0.43
1:A:684:VAL:HG12	1:A:684:VAL:O	2.18	0.43
2:C:117:ALA:O	2:C:120:THR:HB	2.18	0.43
1:B:100:GLY:O	1:B:103:LEU:HG	2.19	0.43
1:B:261:GLU:O	1:B:262:ALA:C	2.60	0.43
1:B:321:GLU:OE2	1:B:324:TYR:HA	2.18	0.43
1:B:637:ILE:HG21	2:F:244:TYR:HB3	2.01	0.43
1:B:672:LEU:O	1:B:676:PHE:HB3	2.18	0.43
1:B:750:ILE:O	1:B:754:MET:N	2.51	0.43
2:F:67:PHE:CE1	2:F:390:ILE:HD11	2.53	0.43
2:F:199:TYR:HA	2:F:203:ILE:HG22	2.01	0.43
2:F:419:GLU:CA	2:F:422:ILE:HG13	2.49	0.43
3:G:51:PHE:O	3:G:55:VAL:HG23	2.19	0.43
1:A:123:THR:HG22	1:A:252:ASP:HB3	2.00	0.43
1:A:210:LYS:HG3	1:A:211:GLU:N	2.27	0.43
1:A:332:LEU:HD12	1:A:336:ILE:HD11	2.00	0.43
1:A:770:GLU:HG3	2:C:240:ILE:HD13	2.00	0.43
2:C:28:PHE:CD1	2:C:190:LEU:HD13	2.54	0.43
2:C:37:PRO:HG3	2:C:163:SER:OG	2.19	0.43
2:C:104:GLU:C	2:C:105:MET:HE2	2.43	0.43
2:C:186:GLY:HA2	2:C:189:ILE:HG22	2.01	0.43
2:C:222:VAL:HG11	2:C:373:ILE:HG23	2.00	0.43
1:B:136:MET:O	1:B:139:VAL:HG22	2.19	0.43
1:B:155:LYS:HZ1	1:B:209:ARG:CZ	2.31	0.43
1:B:596:SER:HA	1:B:599:ILE:CG2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:618:MET:H	1:B:621:LYS:HZ3	1.67	0.43
2:F:143:ASN:HD22	2:F:143:ASN:HA	1.53	0.43
2:F:173:TRP:HE1	4:H:57:LEU:CD1	2.24	0.43
1:A:622:LEU:O	1:A:623:ILE:C	2.61	0.43
1:A:673:LYS:HA	1:A:732:TRP:CZ3	2.53	0.43
2:C:199:TYR:HA	2:C:203:ILE:HG22	2.01	0.43
3:D:51:PHE:O	3:D:55:VAL:HG23	2.19	0.43
4:E:45:ARG:O	4:E:47:LYS:N	2.52	0.43
4:E:45:ARG:C	4:E:47:LYS:H	2.26	0.43
1:B:83:GLY:O	1:B:87:LEU:HG	2.19	0.43
1:B:97:THR:H	1:B:573:ARG:NH1	2.05	0.43
1:B:171:ILE:C	1:B:173:GLU:H	2.26	0.43
1:B:400:ILE:HD12	1:B:402:PHE:HE2	1.82	0.43
1:B:601:LYS:HB3	1:B:605:ILE:HD12	2.00	0.43
1:B:622:LEU:O	1:B:623:ILE:C	2.61	0.43
1:B:770:GLU:OE2	1:B:773:LYS:HD2	2.18	0.43
1:A:31:LYS:HA	1:A:70:ARG:HH22	1.84	0.42
1:A:63:LEU:HD23	1:A:63:LEU:C	2.44	0.42
1:A:83:GLY:O	1:A:87:LEU:HG	2.19	0.42
1:A:282:PHE:HB3	1:A:384:ALA:HB2	2.00	0.42
1:A:302:ARG:HG2	2:C:249:THR:OG1	2.19	0.42
1:A:400:ILE:HD12	1:A:402:PHE:HE2	1.82	0.42
1:A:533:GLY:C	1:A:570:ARG:HG2	2.44	0.42
1:A:672:LEU:O	1:A:676:PHE:HB3	2.18	0.42
2:C:333:GLU:C	2:C:335:ILE:N	2.77	0.42
1:B:41:MET:O	1:B:44:LYS:HB3	2.19	0.42
1:B:92:VAL:HA	1:B:414:GLY:O	2.18	0.42
1:B:152:SER:HA	1:B:224:GLU:OE2	2.19	0.42
1:B:277:SER:O	1:B:278:VAL:C	2.63	0.42
1:B:536:THR:HB	1:B:538:ILE:CD1	2.46	0.42
1:B:551:CYS:O	1:B:552:ILE:HD13	2.19	0.42
1:B:559:GLU:HB3	2:F:246:ARG:HD2	2.00	0.42
1:B:561:ARG:NE	1:B:561:ARG:HA	2.34	0.42
1:B:592:ARG:HH21	1:B:593:ILE:CD1	2.31	0.42
1:B:774:GLU:HB2	2:F:240:ILE:HG22	2.02	0.42
2:F:319:TYR:OH	2:F:359:LEU:HA	2.18	0.42
2:F:340:GLY:O	2:F:342:ILE:N	2.52	0.42
1:A:82:MET:O	1:A:85:ILE:HB	2.19	0.42
1:A:91:LYS:O	1:A:92:VAL:HG13	2.19	0.42
1:A:298:ASP:OD2	1:A:304:ILE:HG12	2.19	0.42
1:A:315:GLU:HA	1:A:319:GLY:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:CYS:O	1:A:552:ILE:HD13	2.18	0.42
1:A:558:HIS:ND1	1:A:564:ASP:HA	2.34	0.42
1:A:560:SER:HB2	1:A:563:ILE:HD12	2.01	0.42
1:A:573:ARG:NH1	6:A:873:ADP:O1B	2.52	0.42
1:A:645:ASP:HA	1:A:648:LEU:HB2	2.01	0.42
1:A:750:ILE:HD11	1:A:751:ARG:HH22	1.83	0.42
2:C:104:GLU:O	2:C:105:MET:HE2	2.19	0.42
2:C:345:LEU:O	2:C:346:ARG:C	2.61	0.42
3:D:24:LYS:O	3:D:25:GLU:C	2.62	0.42
3:D:32:VAL:O	3:D:36:ILE:HG13	2.19	0.42
1:B:684:VAL:O	1:B:684:VAL:HG12	2.18	0.42
1:A:18:VAL:HA	1:A:21:ILE:CG2	2.48	0.42
1:A:74:MET:H	1:A:75:ARG:NH2	2.17	0.42
1:A:76:PRO:HB2	1:A:185:GLU:CG	2.50	0.42
1:A:91:LYS:O	1:A:413:ALA:HA	2.19	0.42
1:A:346:LYS:C	1:A:348:ASP:H	2.27	0.42
1:A:347:LYS:HD2	1:A:386:GLU:OE2	2.19	0.42
1:A:592:ARG:HH21	1:A:593:ILE:CD1	2.31	0.42
2:C:331:ILE:C	2:C:333:GLU:H	2.28	0.42
1:B:18:VAL:O	1:B:22:ASN:HB2	2.18	0.42
1:B:67:ALA:HB1	1:B:142:PHE:HD1	1.84	0.42
1:B:137:GLY:N	1:B:138:PRO:CD	2.82	0.42
1:B:359:ILE:HD12	1:B:359:ILE:N	2.26	0.42
1:B:465:GLU:O	1:B:468:GLU:HB3	2.20	0.42
1:B:802:MET:CB	2:F:422:ILE:HD12	2.49	0.42
3:G:32:VAL:O	3:G:36:ILE:HG13	2.18	0.42
4:H:45:ARG:O	4:H:47:LYS:N	2.52	0.42
1:A:94:GLU:HB2	1:A:416:THR:N	2.34	0.42
1:A:94:GLU:CD	1:A:94:GLU:N	2.78	0.42
1:A:465:GLU:O	1:A:468:GLU:HB3	2.20	0.42
1:A:484:ILE:CG1	1:A:485:GLU:N	2.82	0.42
2:C:20:PHE:HB3	2:C:181:LYS:HB2	2.02	0.42
2:C:232:LEU:HG	2:C:266:ASN:CA	2.50	0.42
2:C:238:ARG:CD	2:C:337:LYS:HG2	2.49	0.42
2:C:273:ILE:H	2:C:273:ILE:HG13	1.65	0.42
2:C:345:LEU:HB3	2:C:346:ARG:H	1.70	0.42
1:B:91:LYS:HB3	1:B:433:GLU:O	2.19	0.42
1:B:91:LYS:O	1:B:92:VAL:HG13	2.19	0.42
1:B:402:PHE:CG	1:B:403:GLN:N	2.86	0.42
1:B:555:THR:O	1:B:556:GLU:HB3	2.20	0.42
2:F:232:LEU:O	3:G:25:GLU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:301:ALA:C	2:F:303:GLY:H	2.27	0.42
1:A:28:LEU:HD12	1:A:32:LYS:CE	2.50	0.42
1:A:91:LYS:HB3	1:A:433:GLU:O	2.19	0.42
1:A:96:LYS:HZ3	1:A:570:ARG:NH2	2.18	0.42
1:A:171:ILE:C	1:A:173:GLU:H	2.27	0.42
1:A:209:ARG:NH2	1:A:228:ASP:OD1	2.53	0.42
1:A:281:ARG:HH21	1:A:334:HIS:CB	2.33	0.42
1:A:779:ARG:NH2	1:A:788:VAL:HG23	2.32	0.42
2:C:71:ALA:HB2	2:C:139:LEU:CD1	2.50	0.42
2:C:304:PHE:O	2:C:308:LEU:HG	2.20	0.42
1:B:39:LEU:O	1:B:43:LEU:HG	2.19	0.42
1:B:63:LEU:HD23	1:B:63:LEU:C	2.44	0.42
1:B:91:LYS:O	1:B:413:ALA:HA	2.19	0.42
1:B:502:GLN:CD	1:B:515:ILE:HG22	2.44	0.42
2:F:147:VAL:O	2:F:149:PRO:HD3	2.20	0.42
1:A:37:ILE:HD11	1:A:173:GLU:OE1	2.19	0.42
1:A:54:ASP:HA	1:A:57:LEU:CD1	2.47	0.42
1:A:67:ALA:HB1	1:A:142:PHE:HD1	1.84	0.42
1:A:100:GLY:O	1:A:103:LEU:HG	2.19	0.42
1:A:136:MET:O	1:A:139:VAL:HG22	2.19	0.42
1:A:137:GLY:N	1:A:138:PRO:CD	2.82	0.42
1:A:277:SER:O	1:A:278:VAL:C	2.63	0.42
1:A:755:LEU:H	1:A:755:LEU:CD1	2.31	0.42
2:C:315:PHE:HB3	2:C:363:THR:CG2	2.49	0.42
1:B:14:TYR:C	1:B:16:LYS:N	2.77	0.42
1:B:79:VAL:HG12	1:B:437:ILE:HG22	2.00	0.42
1:B:315:GLU:HA	1:B:319:GLY:O	2.19	0.42
1:B:345:PHE:HB3	1:B:350:ASP:OD2	2.20	0.42
2:F:37:PRO:O	2:F:38:GLY:C	2.62	0.42
1:A:246:HIS:NE2	1:A:408:MET:SD	2.93	0.42
1:A:784:LYS:HB3	1:A:785:ASP:H	1.72	0.42
2:C:22:PHE:O	2:C:26:ILE:HG13	2.19	0.42
2:C:34:ILE:HA	2:C:35:PRO:HD3	1.78	0.42
2:C:306:TYR:HA	2:C:309:ILE:CD1	2.47	0.42
2:C:365:ILE:H	2:C:365:ILE:HG13	1.67	0.42
1:B:82:MET:O	1:B:85:ILE:HB	2.19	0.42
1:B:302:ARG:HG2	2:F:249:THR:OG1	2.19	0.42
1:B:326:PRO:O	1:B:327:GLY:C	2.61	0.42
1:B:403:GLN:HA	1:B:407:ARG:HB2	2.02	0.42
1:B:435:VAL:O	1:B:437:ILE:HG13	2.20	0.42
1:B:690:GLY:HA2	1:B:695:ILE:CG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:22:PHE:O	2:F:26:ILE:HG13	2.19	0.42
2:F:88:ALA:HA	2:F:124:THR:CB	2.50	0.42
2:F:250:GLY:O	2:F:251:ARG:HG2	2.18	0.42
1:A:39:LEU:O	1:A:43:LEU:HG	2.19	0.42
1:A:79:VAL:HG12	1:A:437:ILE:HG22	2.00	0.42
1:A:288:LYS:HE2	1:A:318:ILE:HG12	2.00	0.42
1:A:334:HIS:HA	1:A:337:ASN:ND2	2.24	0.42
1:A:345:PHE:HB3	1:A:350:ASP:OD2	2.20	0.42
1:A:435:VAL:HG12	1:A:437:ILE:HD11	2.02	0.42
2:C:147:VAL:O	2:C:149:PRO:HD3	2.20	0.42
2:C:406:ILE:O	2:C:410:GLU:HG3	2.20	0.42
2:C:419:GLU:CA	2:C:422:ILE:HG13	2.49	0.42
1:B:18:VAL:HA	1:B:21:ILE:CG2	2.48	0.42
1:B:28:LEU:HD12	1:B:32:LYS:CE	2.50	0.42
1:B:92:VAL:CG2	1:B:434:VAL:HA	2.50	0.42
1:B:149:VAL:HG23	1:B:219:TYR:O	2.20	0.42
1:B:251:VAL:O	1:B:415:MET:HG3	2.20	0.42
1:B:502:GLN:CG	1:B:526:THR:HG23	2.40	0.42
1:B:544:VAL:C	1:B:546:GLU:H	2.27	0.42
1:B:612:GLN:HB2	1:B:613:PRO:HD3	2.01	0.42
1:B:659:ARG:O	1:B:662:ILE:HG12	2.20	0.42
1:B:750:ILE:HD11	1:B:751:ARG:HH22	1.83	0.42
2:F:186:GLY:HA2	2:F:189:ILE:HG22	2.01	0.42
1:A:367:ARG:HG3	1:A:531:MET:SD	2.60	0.42
1:A:403:GLN:O	1:A:407:ARG:HB2	2.20	0.42
1:A:435:VAL:O	1:A:437:ILE:HG13	2.20	0.42
1:A:518:LYS:HG2	1:A:518:LYS:O	2.19	0.42
1:A:659:ARG:O	1:A:662:ILE:HG12	2.20	0.42
1:A:667:ASP:C	1:A:669:ASP:H	2.27	0.42
1:A:758:ILE:HG22	1:A:759:ASP:N	2.34	0.42
2:C:325:ILE:H	2:C:325:ILE:HG13	1.70	0.42
1:B:123:THR:HG22	1:B:252:ASP:HB3	2.00	0.42
1:B:209:ARG:NH2	1:B:228:ASP:OD1	2.53	0.42
1:B:758:ILE:HG22	1:B:759:ASP:N	2.34	0.42
2:F:358:VAL:O	2:F:362:VAL:HG13	2.20	0.42
3:G:20:TRP:N	3:G:21:PRO:HD2	2.35	0.42
3:G:24:LYS:O	3:G:25:GLU:C	2.62	0.42
4:H:50:ASP:OD1	4:H:54:LYS:HD2	2.20	0.42
1:A:37:ILE:HD11	1:A:173:GLU:HG3	2.02	0.42
1:A:47:VAL:HG12	1:A:49:SER:O	2.20	0.42
1:A:64:VAL:O	1:A:67:ALA:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:LYS:O	1:A:414:GLY:N	2.53	0.42
1:A:98:GLY:O	6:A:873:ADP:H8	2.03	0.42
1:A:102:THR:HG23	6:A:873:ADP:O2A	2.20	0.42
1:A:187:LEU:HD21	6:A:873:ADP:H2	1.83	0.42
1:A:251:VAL:O	1:A:415:MET:HG3	2.20	0.42
1:A:326:PRO:O	1:A:327:GLY:C	2.61	0.42
1:A:430:TYR:HD2	1:A:430:TYR:H	1.68	0.42
1:A:456:GLN:O	1:A:458:GLU:N	2.52	0.42
1:A:543:GLY:HA3	1:A:546:GLU:OE2	2.20	0.42
2:C:156:PHE:O	2:C:160:SER:HB2	2.20	0.42
2:C:230:ILE:C	2:C:232:LEU:H	2.28	0.42
3:D:20:TRP:N	3:D:21:PRO:HD2	2.35	0.42
4:E:50:ASP:OD1	4:E:54:LYS:HD2	2.20	0.42
1:B:31:LYS:HA	1:B:70:ARG:HH22	1.84	0.42
1:B:347:LYS:HD2	1:B:386:GLU:OE2	2.19	0.42
1:B:403:GLN:HE21	1:B:403:GLN:HB3	1.66	0.42
1:B:468:GLU:O	1:B:469:LYS:C	2.61	0.42
1:B:581:ILE:HG23	1:B:583:PHE:HE1	1.85	0.42
1:B:604:ASN:HA	1:B:608:ILE:HG12	2.02	0.42
2:F:24:ALA:HB1	2:F:190:LEU:HD12	2.02	0.42
1:A:213:TYR:CE2	1:A:243:GLN:HG3	2.55	0.41
1:A:373:ARG:HH11	1:A:378:LEU:HD22	1.84	0.41
1:A:403:GLN:HA	1:A:407:ARG:HB2	2.02	0.41
1:A:503:VAL:HG13	1:A:527:ILE:HD12	2.02	0.41
1:A:569:GLY:C	1:A:571:ALA:N	2.78	0.41
1:A:596:SER:HA	1:A:599:ILE:CG2	2.49	0.41
1:A:612:GLN:N	1:A:613:PRO:CD	2.81	0.41
1:A:620:SER:HA	1:A:623:ILE:CD1	2.50	0.41
1:A:750:ILE:O	1:A:754:MET:N	2.51	0.41
2:C:240:ILE:C	2:C:240:ILE:HD12	2.44	0.41
1:B:22:ASN:HD22	1:B:22:ASN:HA	1.54	0.41
1:B:37:ILE:HD11	1:B:173:GLU:HG3	2.02	0.41
1:B:80:GLN:CB	1:B:104:ALA:HB2	2.50	0.41
1:B:241:LYS:O	1:B:243:GLN:N	2.54	0.41
1:B:287:LYS:HD3	1:B:287:LYS:HA	1.88	0.41
1:B:319:GLY:C	1:B:321:GLU:N	2.77	0.41
1:B:403:GLN:O	1:B:407:ARG:HB2	2.20	0.41
1:B:430:TYR:HD2	1:B:430:TYR:H	1.68	0.41
1:B:456:GLN:O	1:B:458:GLU:N	2.52	0.41
1:B:751:ARG:CZ	1:B:751:ARG:HA	2.50	0.41
2:F:21:THR:CG2	3:G:47:LEU:HD21	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:34:ILE:HA	2:F:35:PRO:HD3	1.78	0.41
2:F:71:ALA:HB2	2:F:139:LEU:CD1	2.50	0.41
2:F:101:SER:HB2	2:F:106:LEU:CD2	2.50	0.41
2:F:104:GLU:O	2:F:105:MET:HE2	2.19	0.41
1:A:92:VAL:CG2	1:A:434:VAL:HA	2.50	0.41
1:A:295:PHE:O	1:A:296:THR:OG1	2.38	0.41
1:A:395:ILE:HG22	1:A:396:THR:H	1.85	0.41
1:A:604:ASN:HA	1:A:608:ILE:HG12	2.02	0.41
1:A:709:LEU:HD12	1:A:709:LEU:O	2.20	0.41
2:C:251:ARG:NH2	2:C:335:ILE:HD13	2.34	0.41
1:B:76:PRO:HB2	1:B:185:GLU:CG	2.50	0.41
1:B:91:LYS:O	1:B:414:GLY:N	2.53	0.41
1:B:370:PRO:O	1:B:371:GLY:C	2.63	0.41
2:F:35:PRO:C	2:F:37:PRO:CD	2.93	0.41
2:F:156:PHE:O	2:F:160:SER:HB2	2.20	0.41
1:A:149:VAL:HG23	1:A:219:TYR:O	2.20	0.41
1:A:635:PHE:HA	1:A:638:ARG:CZ	2.50	0.41
2:C:88:ALA:HA	2:C:124:THR:CB	2.50	0.41
4:E:18:TYR:O	4:E:22:VAL:HG23	2.21	0.41
1:B:395:ILE:HG22	1:B:396:THR:H	1.85	0.41
1:B:484:ILE:CG1	1:B:485:GLU:N	2.82	0.41
1:B:696:GLU:HA	1:B:699:LYS:HZ3	1.84	0.41
2:F:20:PHE:HB3	2:F:181:LYS:HZ3	1.85	0.41
2:F:240:ILE:HD12	2:F:240:ILE:C	2.45	0.41
1:A:92:VAL:HG12	1:A:414:GLY:HA3	2.02	0.41
1:A:111:LEU:HA	1:A:114:LEU:HD12	2.02	0.41
1:A:120:HIS:O	1:A:249:ALA:HA	2.21	0.41
1:A:150:ILE:HG13	1:A:155:LYS:NZ	2.33	0.41
1:A:165:ASP:HA	1:A:168:ARG:CD	2.51	0.41
1:A:262:ALA:HB2	2:C:244:TYR:CE1	2.55	0.41
1:A:262:ALA:HA	2:C:244:TYR:CE2	2.55	0.41
1:A:281:ARG:HH22	1:A:333:TYR:HE1	1.62	0.41
1:A:295:PHE:C	1:A:306:LEU:HD13	2.45	0.41
1:A:428:GLN:O	4:E:46:ARG:HG3	2.20	0.41
2:C:27:VAL:CG1	2:C:174:LEU:HD22	2.50	0.41
1:B:40:SER:O	1:B:44:LYS:HB2	2.21	0.41
1:B:295:PHE:C	1:B:306:LEU:HD13	2.45	0.41
1:B:457:LYS:O	1:B:460:TYR:HB3	2.21	0.41
1:B:543:GLY:HA3	1:B:546:GLU:OE2	2.20	0.41
1:B:560:SER:HB2	1:B:563:ILE:HD12	2.01	0.41
1:B:675:ILE:H	1:B:675:ILE:HD12	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:802:MET:HB2	2:F:422:ILE:HD12	2.01	0.41
2:F:27:VAL:CG1	2:F:174:LEU:HD22	2.50	0.41
2:F:183:ILE:C	2:F:185:ASN:N	2.79	0.41
2:F:230:ILE:C	2:F:232:LEU:H	2.28	0.41
2:F:271:ILE:O	2:F:271:ILE:HG22	2.20	0.41
2:F:315:PHE:CZ	2:F:370:LEU:HB2	2.37	0.41
2:F:342:ILE:HG23	2:F:343:PRO:CD	2.46	0.41
1:A:136:MET:C	1:A:138:PRO:HD2	2.46	0.41
1:A:282:PHE:HA	1:A:285:ILE:CD1	2.51	0.41
1:A:348:ASP:O	1:A:484:ILE:HD11	2.20	0.41
1:A:370:PRO:O	1:A:371:GLY:C	2.63	0.41
1:A:405:TYR:O	1:A:408:MET:CB	2.68	0.41
1:A:457:LYS:O	1:A:460:TYR:HB3	2.21	0.41
1:A:515:ILE:HA	1:A:518:LYS:HB3	2.03	0.41
2:C:113:ARG:HD3	4:E:40:HIS:NE2	2.35	0.41
2:C:183:ILE:C	2:C:185:ASN:H	2.28	0.41
2:C:401:VAL:O	2:C:405:ILE:HG13	2.21	0.41
4:E:57:LEU:HD23	4:E:57:LEU:C	2.46	0.41
1:B:3:LEU:HB3	1:B:4:PHE:H	1.63	0.41
1:B:120:HIS:HB2	1:B:249:ALA:CB	2.50	0.41
1:B:136:MET:C	1:B:138:PRO:HD2	2.46	0.41
1:B:171:ILE:HA	1:B:174:ASN:OD1	2.20	0.41
1:B:213:TYR:CE2	1:B:243:GLN:HG3	2.55	0.41
1:B:246:HIS:NE2	1:B:408:MET:SD	2.93	0.41
1:B:455:THR:O	1:B:456:GLN:HB2	2.20	0.41
2:F:183:ILE:C	2:F:185:ASN:H	2.28	0.41
2:F:406:ILE:O	2:F:410:GLU:HG3	2.20	0.41
4:H:54:LYS:O	4:H:57:LEU:HB3	2.21	0.41
1:A:105:ALA:O	1:A:108:PRO:HD2	2.21	0.41
1:A:213:TYR:CD1	1:A:243:GLN:HA	2.56	0.41
1:A:227:PHE:CG	1:A:266:LEU:HD23	2.56	0.41
1:A:573:ARG:O	1:A:575:GLY:N	2.53	0.41
1:A:675:ILE:H	1:A:675:ILE:HD12	1.84	0.41
2:C:232:LEU:N	2:C:232:LEU:CD2	2.82	0.41
1:B:52:ASP:O	1:B:54:ASP:N	2.54	0.41
1:B:162:LYS:HB3	1:B:163:ASN:H	1.52	0.41
1:B:213:TYR:CD1	1:B:243:GLN:HA	2.56	0.41
1:B:367:ARG:HG3	1:B:531:MET:SD	2.60	0.41
1:B:403:GLN:CG	1:B:407:ARG:HD3	2.45	0.41
2:F:238:ARG:CD	2:F:337:LYS:HG2	2.51	0.41
2:F:326:PHE:O	2:F:329:ARG:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ASP:O	1:A:54:ASP:N	2.54	0.41
1:A:81:VAL:HA	1:A:107:MET:HE1	2.03	0.41
1:A:171:ILE:HA	1:A:174:ASN:OD1	2.20	0.41
1:A:230:LEU:O	1:A:231:ARG:C	2.64	0.41
1:A:251:VAL:HG11	1:A:254:ALA:HA	2.02	0.41
1:A:353:VAL:HG22	1:A:354:MET:N	2.36	0.41
1:A:677:GLU:O	1:A:678:ASP:C	2.62	0.41
1:A:789:GLU:O	1:A:793:GLU:HG2	2.21	0.41
2:C:32:ILE:C	2:C:34:ILE:H	2.29	0.41
2:C:183:ILE:HG23	2:C:186:GLY:H	1.84	0.41
1:B:164:PRO:HB2	1:B:168:ARG:NH2	2.36	0.41
1:B:227:PHE:CG	1:B:266:LEU:HD23	2.56	0.41
1:B:259:ILE:CD1	1:B:562:ARG:HH21	2.34	0.41
1:B:281:ARG:HH21	1:B:334:HIS:CB	2.33	0.41
1:B:313:LYS:N	1:B:316:LYS:HD3	2.35	0.41
1:B:405:TYR:O	1:B:408:MET:CB	2.68	0.41
2:F:20:PHE:HB3	2:F:181:LYS:HB2	2.02	0.41
2:F:212:ASN:C	2:F:214:LEU:H	2.29	0.41
2:F:221:ALA:O	2:F:225:ILE:HG13	2.21	0.41
2:F:311:GLY:O	2:F:315:PHE:HD1	2.04	0.41
1:A:162:LYS:HB3	1:A:163:ASN:H	1.52	0.41
1:A:182:PHE:HB2	1:A:183:ASN:H	1.56	0.41
1:A:241:LYS:O	1:A:243:GLN:N	2.54	0.41
1:A:282:PHE:HA	1:A:285:ILE:HG13	2.03	0.41
1:A:323:LEU:HB2	2:C:345:LEU:CD1	2.51	0.41
1:A:459:LYS:HZ2	1:A:585:SER:N	2.18	0.41
1:A:751:ARG:HA	1:A:751:ARG:CZ	2.51	0.41
2:C:20:PHE:HB3	2:C:181:LYS:HZ3	1.85	0.41
2:C:37:PRO:O	2:C:38:GLY:C	2.62	0.41
2:C:236:ALA:HB2	2:C:263:ILE:C	2.45	0.41
2:C:358:VAL:O	2:C:362:VAL:HG13	2.20	0.41
1:B:96:LYS:HA	6:B:873:ADP:O3B	2.21	0.41
1:B:251:VAL:HG11	1:B:254:ALA:HA	2.02	0.41
1:B:438:PRO:HB2	1:B:442:PRO:HB3	2.03	0.41
1:B:518:LYS:HG2	1:B:518:LYS:O	2.19	0.41
1:B:573:ARG:O	1:B:575:GLY:N	2.53	0.41
2:F:331:ILE:C	2:F:333:GLU:H	2.27	0.41
1:A:50:PHE:C	1:A:52:ASP:H	2.28	0.41
1:A:75:ARG:HH22	1:A:187:LEU:CB	2.32	0.41
1:A:161:TRP:O	1:A:165:ASP:HB2	2.21	0.41
1:A:261:GLU:OE1	1:A:638:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:ASN:C	1:A:357:GLU:N	2.77	0.41
1:A:402:PHE:CG	1:A:403:GLN:N	2.86	0.41
1:A:459:LYS:C	1:A:461:GLU:N	2.78	0.41
1:A:612:GLN:HB2	1:A:613:PRO:HD3	2.01	0.41
1:A:659:ARG:C	1:A:662:ILE:HG12	2.45	0.41
1:A:757:ILE:HD13	1:A:757:ILE:HA	1.94	0.41
2:C:35:PRO:C	2:C:37:PRO:CD	2.94	0.41
2:C:83:THR:HB	2:C:84:PRO:CD	2.51	0.41
2:C:101:SER:HB2	2:C:106:LEU:CD2	2.50	0.41
2:C:195:ILE:HA	2:C:198:ARG:HD2	2.03	0.41
2:C:221:ALA:O	2:C:225:ILE:HG13	2.21	0.41
2:C:311:GLY:O	2:C:315:PHE:HD1	2.04	0.41
2:C:326:PHE:O	2:C:329:ARG:HB2	2.21	0.41
1:B:37:ILE:HD11	1:B:173:GLU:OE1	2.19	0.41
1:B:47:VAL:HG12	1:B:49:SER:O	2.20	0.41
1:B:74:MET:CE	6:B:873:ADP:N3	2.70	0.41
1:B:84:GLY:HA3	1:B:108:PRO:HD3	2.03	0.41
1:B:177:VAL:O	1:B:177:VAL:HG13	2.20	0.41
1:B:320:VAL:HG12	1:B:320:VAL:O	2.21	0.41
1:B:348:ASP:O	1:B:484:ILE:HD11	2.20	0.41
1:B:451:LEU:HA	1:B:615:GLN:OE1	2.21	0.41
1:B:573:ARG:CD	6:B:873:ADP:O1B	2.68	0.41
1:B:667:ASP:C	1:B:669:ASP:H	2.27	0.41
2:F:27:VAL:HG11	2:F:174:LEU:HD22	2.02	0.41
2:F:33:TYR:CE2	3:G:59:PHE:HE2	2.39	0.41
2:F:195:ILE:HA	2:F:198:ARG:HD2	2.03	0.41
2:F:244:TYR:CD1	2:F:244:TYR:N	2.87	0.41
2:F:271:ILE:N	2:F:272:PRO:CD	2.84	0.41
2:F:315:PHE:HB3	2:F:363:THR:CG2	2.51	0.41
2:F:345:LEU:HB3	2:F:346:ARG:H	1.62	0.41
4:H:18:TYR:O	4:H:22:VAL:HG23	2.21	0.41
1:A:177:VAL:O	1:A:177:VAL:HG13	2.20	0.41
1:A:313:LYS:N	1:A:316:LYS:HD3	2.35	0.41
1:A:320:VAL:O	1:A:320:VAL:HG12	2.21	0.41
1:A:581:ILE:HG23	1:A:583:PHE:HE1	1.85	0.41
1:A:659:ARG:HH12	1:A:759:ASP:HB2	1.86	0.41
1:A:677:GLU:CD	1:A:681:SER:HB3	2.45	0.41
1:B:50:PHE:C	1:B:52:ASP:H	2.28	0.41
1:B:96:LYS:HZ3	1:B:570:ARG:NH2	2.19	0.41
1:B:96:LYS:NZ	1:B:569:GLY:O	2.54	0.41
1:B:404:ASN:HD22	1:B:404:ASN:HA	1.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:457:LYS:C	1:B:459:LYS:H	2.29	0.41
1:B:620:SER:HA	1:B:623:ILE:CD1	2.50	0.41
1:B:659:ARG:HH12	1:B:759:ASP:HB2	1.86	0.41
1:B:797:MET:O	1:B:797:MET:HG2	2.21	0.41
2:F:365:ILE:O	2:F:368:VAL:HB	2.21	0.41
1:A:259:ILE:CD1	1:A:562:ARG:HH21	2.33	0.40
1:A:331:LEU:HD12	1:A:331:LEU:N	2.36	0.40
1:A:340:LYS:HZ2	2:C:251:ARG:NE	1.99	0.40
1:A:503:VAL:HG22	1:A:527:ILE:CG2	2.51	0.40
1:A:794:THR:O	1:A:797:MET:HE2	2.22	0.40
2:C:13:GLU:O	2:C:15:ARG:N	2.55	0.40
2:C:24:ALA:HB1	2:C:190:LEU:HD12	2.02	0.40
2:C:391:GLY:O	2:C:395:ALA:HB2	2.21	0.40
4:E:54:LYS:O	4:E:57:LEU:HB3	2.21	0.40
1:B:214:LEU:CD1	1:B:244:ARG:HB2	2.51	0.40
1:B:297:VAL:HG23	1:B:297:VAL:O	2.21	0.40
1:B:659:ARG:C	1:B:662:ILE:HG12	2.46	0.40
1:B:737:ARG:HA	1:B:740:GLN:CB	2.50	0.40
2:F:235:GLN:CD	2:F:340:GLY:HA3	2.46	0.40
2:F:401:VAL:O	2:F:405:ILE:HG13	2.21	0.40
1:A:40:SER:O	1:A:44:LYS:HB2	2.20	0.40
1:A:123:THR:O	1:A:221:THR:HA	2.21	0.40
1:A:131:ARG:HH21	1:A:132:ASP:CG	2.29	0.40
1:A:305:ILE:HG13	1:A:306:LEU:N	2.36	0.40
1:A:345:PHE:O	1:A:346:LYS:C	2.64	0.40
1:A:457:LYS:C	1:A:459:LYS:N	2.78	0.40
1:A:477:VAL:HG12	1:A:551:CYS:HB2	2.03	0.40
6:A:873:ADP:O1B	6:A:873:ADP:C5'	2.70	0.40
2:C:324:VAL:O	2:C:326:PHE:N	2.55	0.40
3:D:42:VAL:O	3:D:46:VAL:HG23	2.22	0.40
1:B:81:VAL:HA	1:B:107:MET:HE1	2.03	0.40
1:B:124:VAL:HG13	1:B:125:ASN:OD1	2.21	0.40
1:B:331:LEU:HD12	1:B:331:LEU:N	2.36	0.40
1:B:373:ARG:HH11	1:B:378:LEU:HD22	1.84	0.40
1:B:503:VAL:HG13	1:B:527:ILE:HD12	2.02	0.40
1:B:503:VAL:HG22	1:B:527:ILE:CG2	2.51	0.40
1:B:677:GLU:CD	1:B:681:SER:HB3	2.45	0.40
1:A:24:ILE:HG21	1:A:59:GLU:HA	2.03	0.40
1:A:164:PRO:HB2	1:A:168:ARG:NH2	2.36	0.40
1:A:455:THR:O	1:A:456:GLN:HB2	2.20	0.40
2:C:27:VAL:HG11	2:C:174:LEU:HD22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:162:MET:CG	4:E:19:MET:HE3	2.51	0.40
2:C:233:VAL:HG22	2:C:362:VAL:HG11	2.03	0.40
1:B:24:ILE:HG21	1:B:59:GLU:HA	2.03	0.40
1:B:64:VAL:O	1:B:67:ALA:HB3	2.20	0.40
1:B:71:THR:O	1:B:72:LEU:HG	2.21	0.40
1:B:285:ILE:O	1:B:288:LYS:N	2.54	0.40
1:B:305:ILE:HG13	1:B:306:LEU:N	2.36	0.40
2:F:391:GLY:O	2:F:395:ALA:HB2	2.21	0.40
4:H:57:LEU:HD23	4:H:57:LEU:C	2.46	0.40
1:A:96:LYS:NZ	1:A:569:GLY:O	2.54	0.40
1:A:122:VAL:HG23	1:A:250:ILE:O	2.22	0.40
1:A:124:VAL:HG13	1:A:125:ASN:OD1	2.21	0.40
1:A:233:ASN:O	1:A:659:ARG:NE	2.54	0.40
1:A:292:ASP:HB2	1:A:313:LYS:CD	2.44	0.40
1:A:332:LEU:HD22	1:A:332:LEU:HA	1.95	0.40
1:A:451:LEU:HA	1:A:615:GLN:OE1	2.21	0.40
1:A:482:THR:HG23	1:A:483:SER:N	2.36	0.40
1:A:561:ARG:HA	1:A:627:GLN:OE1	2.21	0.40
1:A:635:PHE:HA	1:A:638:ARG:NH2	2.37	0.40
2:C:183:ILE:C	2:C:185:ASN:N	2.79	0.40
2:C:307:LEU:HD23	2:C:310:TYR:CE1	2.57	0.40
3:D:23:ARG:C	3:D:24:LYS:HG3	2.46	0.40
1:B:93:ALA:HA	1:B:435:VAL:O	2.21	0.40
1:B:122:VAL:HG23	1:B:250:ILE:O	2.22	0.40
1:B:141:LEU:HD13	1:B:159:VAL:HG11	2.04	0.40
1:B:230:LEU:O	1:B:231:ARG:C	2.64	0.40
1:B:233:ASN:O	1:B:659:ARG:NE	2.54	0.40
1:B:282:PHE:HA	1:B:285:ILE:CD1	2.50	0.40
1:B:299:GLU:C	1:B:301:ALA:H	2.30	0.40
1:B:353:VAL:HG22	1:B:354:MET:N	2.36	0.40
1:B:435:VAL:HG12	1:B:437:ILE:HD11	2.02	0.40
1:B:662:ILE:HD12	1:B:754:MET:CB	2.46	0.40
1:B:755:LEU:O	1:B:756:ARG:C	2.64	0.40
1:B:778:LEU:HD22	2:F:264:LYS:HG3	2.04	0.40
1:B:794:THR:O	1:B:797:MET:HE2	2.22	0.40
2:F:129:GLY:O	2:F:132:ALA:HB3	2.21	0.40
2:F:136:SER:HB2	2:F:157:THR:HG23	2.03	0.40
1:A:214:LEU:CD1	1:A:244:ARG:HB2	2.51	0.40
1:A:402:PHE:CD2	1:A:402:PHE:N	2.89	0.40
1:A:457:LYS:C	1:A:459:LYS:H	2.29	0.40
1:A:666:LYS:HE2	1:A:747:ARG:HD2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:689:SER:HB3	1:A:691:LYS:HG2	2.03	0.40
1:A:755:LEU:O	1:A:756:ARG:C	2.64	0.40
1:A:785:ASP:N	1:A:786:PRO:HD2	2.35	0.40
1:A:787:ILE:O	1:A:787:ILE:HG22	2.21	0.40
1:A:809:ILE:HD13	1:A:809:ILE:C	2.47	0.40
2:C:136:SER:HB2	2:C:157:THR:HG23	2.03	0.40
2:C:230:ILE:O	2:C:232:LEU:CD2	2.69	0.40
2:C:317:PHE:HD1	2:C:317:PHE:H	1.69	0.40
1:B:111:LEU:HA	1:B:114:LEU:HD12	2.02	0.40
1:B:120:HIS:O	1:B:249:ALA:HA	2.21	0.40
1:B:155:LYS:HD2	1:B:209:ARG:N	2.37	0.40
1:B:187:LEU:O	1:B:187:LEU:HG	2.22	0.40
1:B:515:ILE:HD12	1:B:516:VAL:N	2.36	0.40
1:B:591:LEU:HA	1:B:594:PHE:O	2.22	0.40
2:F:83:THR:HB	2:F:84:PRO:CD	2.51	0.40
2:F:232:LEU:HB2	2:F:233:VAL:H	1.74	0.40
2:F:266:ASN:OD1	2:F:323:VAL:HG22	2.21	0.40

All (2) 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:A:498:GLY:O	1:B:518:LYS:NZ[1_455]	2.07	0.13
1:A:518:LYS:NZ	1:B:498:GLY:O[1_455]	2.17	0.03

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	814/871 (94%)	510 (63%)	207 (25%)	97 (12%)	0	5
1	B	814/871 (94%)	511 (63%)	206 (25%)	97 (12%)	0	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	392/431 (91%)	260 (66%)	80 (20%)	52 (13%)	0	3
2	F	392/431 (91%)	262 (67%)	78 (20%)	52 (13%)	0	3
3	D	54/65 (83%)	41 (76%)	9 (17%)	4 (7%)	1	10
3	G	54/65 (83%)	41 (76%)	9 (17%)	4 (7%)	1	10
4	E	63/76 (83%)	46 (73%)	12 (19%)	5 (8%)	1	10
4	H	63/76 (83%)	46 (73%)	12 (19%)	5 (8%)	1	10
All	All	2646/2886 (92%)	1717 (65%)	613 (23%)	316 (12%)	0	5

All (316) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	ARG
1	A	95	MET
1	A	131	ARG
1	A	152	SER
1	A	178	TRP
1	A	242	VAL
1	A	297	VAL
1	A	300	LYS
1	A	307	THR
1	A	318	ILE
1	A	326	PRO
1	A	371	GLY
1	A	396	THR
1	A	416	THR
1	A	542	PRO
1	A	544	VAL
1	A	558	HIS
1	A	588	ASP
1	A	615	GLN
1	A	655	VAL
1	A	665	GLU
1	A	784	LYS
1	A	788	VAL
2	C	13	GLU
2	C	14	LEU
2	C	17	ARG
2	C	36	VAL
2	C	37	PRO
2	C	79	THR

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Mol	Chain	Res	Type
2	C	97	SER
2	C	100	PRO
2	C	232	LEU
2	C	260	TYR
2	C	272	PRO
2	C	298	LEU
2	C	314	VAL
2	C	324	VAL
2	C	342	ILE
2	C	415	MET
3	D	61	ALA
1	B	75	ARG
1	B	95	MET
1	B	131	ARG
1	B	152	SER
1	B	178	TRP
1	B	242	VAL
1	B	297	VAL
1	B	300	LYS
1	B	307	THR
1	B	318	ILE
1	B	326	PRO
1	B	371	GLY
1	B	396	THR
1	B	416	THR
1	B	542	PRO
1	B	544	VAL
1	B	558	HIS
1	B	588	ASP
1	B	615	GLN
1	B	655	VAL
1	B	665	GLU
1	B	784	LYS
1	B	788	VAL
2	F	13	GLU
2	F	14	LEU
2	F	17	ARG
2	F	36	VAL
2	F	37	PRO
2	F	79	THR
2	F	97	SER
2	F	100	PRO

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Mol	Chain	Res	Type
2	F	232	LEU
2	F	272	PRO
2	F	298	LEU
2	F	314	VAL
2	F	324	VAL
2	F	342	ILE
2	F	415	MET
3	G	61	ALA
1	A	32	LYS
1	A	53	ALA
1	A	73	GLY
1	A	85	ILE
1	A	94	GLU
1	A	101	LYS
1	A	160	VAL
1	A	179	PRO
1	A	182	PHE
1	A	210	LYS
1	A	215	CYS
1	A	268	ILE
1	A	296	THR
1	A	337	ASN
1	A	354	MET
1	A	365	THR
1	A	367	ARG
1	A	417	GLY
1	A	418	THR
1	A	455	THR
1	A	457	LYS
1	A	498	GLY
1	A	535	GLY
1	A	556	GLU
1	A	669	ASP
1	A	753	LEU
2	C	93	GLN
2	C	146	MET
2	C	149	PRO
2	C	204	ARG
2	C	234	GLN
2	C	239	ARG
2	C	313	LEU
2	C	338	TYR

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Mol	Chain	Res	Type
2	C	345	LEU
4	E	45	ARG
1	B	32	LYS
1	B	53	ALA
1	B	73	GLY
1	B	85	ILE
1	B	94	GLU
1	B	101	LYS
1	B	179	PRO
1	B	182	PHE
1	B	210	LYS
1	B	215	CYS
1	B	268	ILE
1	B	296	THR
1	B	337	ASN
1	B	354	MET
1	B	365	THR
1	B	367	ARG
1	B	417	GLY
1	B	418	THR
1	B	455	THR
1	B	457	LYS
1	B	498	GLY
1	B	535	GLY
1	B	556	GLU
1	B	669	ASP
1	B	753	LEU
2	F	93	GLN
2	F	146	MET
2	F	149	PRO
2	F	204	ARG
2	F	234	GLN
2	F	239	ARG
2	F	260	TYR
2	F	313	LEU
2	F	338	TYR
2	F	345	LEU
4	H	45	ARG
1	A	99	GLU
1	A	157	TYR
1	A	265	PRO
1	A	279	TYR

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Mol	Chain	Res	Type
1	A	285	ILE
1	A	319	GLY
1	A	341	ALA
1	A	363	GLU
1	A	377	GLY
1	A	428	GLN
1	A	439	THR
1	A	449	ASP
1	A	522	LYS
1	A	545	ALA
1	A	612	GLN
1	A	617	PRO
1	A	785	ASP
1	A	815	ARG
2	C	39	LEU
2	C	73	SER
2	C	123	LEU
2	C	137	PHE
2	C	155	GLN
2	C	213	LEU
2	C	347	PRO
3	D	23	ARG
4	E	35	GLY
4	E	46	ARG
1	B	99	GLU
1	B	157	TYR
1	B	160	VAL
1	B	265	PRO
1	B	279	TYR
1	B	285	ILE
1	B	319	GLY
1	B	341	ALA
1	B	363	GLU
1	B	377	GLY
1	B	428	GLN
1	B	439	THR
1	B	449	ASP
1	B	522	LYS
1	B	545	ALA
1	B	612	GLN
1	B	617	PRO
1	B	785	ASP

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Mol	Chain	Res	Type
1	B	815	ARG
2	F	39	LEU
2	F	73	SER
2	F	123	LEU
2	F	137	PHE
2	F	155	GLN
2	F	213	LEU
2	F	255	GLY
2	F	344	GLY
2	F	347	PRO
3	G	23	ARG
4	H	35	GLY
4	H	44	GLY
4	H	46	ARG
1	A	91	LYS
1	A	97	THR
1	A	162	LYS
1	A	196	ALA
1	A	247	PHE
1	A	253	GLU
1	A	308	GLU
1	A	342	LEU
1	A	780	SER
2	C	121	ARG
2	C	206	ALA
2	C	253	VAL
2	C	255	GLY
2	C	323	VAL
2	C	325	ILE
2	C	341	TYR
2	C	390	ILE
3	D	11	VAL
4	E	44	GLY
1	B	91	LYS
1	B	97	THR
1	B	162	LYS
1	B	196	ALA
1	B	247	PHE
1	B	253	GLU
1	B	308	GLU
1	B	342	LEU
1	B	780	SER

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Mol	Chain	Res	Type
2	F	121	ARG
2	F	206	ALA
2	F	253	VAL
2	F	341	TYR
2	F	390	ILE
3	G	11	VAL
1	A	3	LEU
1	A	241	LYS
1	A	243	GLN
1	A	293	LYS
1	A	691	LYS
1	A	754	MET
2	C	140	ALA
2	C	319	TYR
2	C	414	VAL
3	D	25	GLU
4	E	51	THR
1	B	3	LEU
1	B	241	LYS
1	B	243	GLN
1	B	293	LYS
1	B	691	LYS
1	B	754	MET
2	F	140	ALA
2	F	319	TYR
2	F	323	VAL
2	F	325	ILE
2	F	414	VAL
3	G	25	GLU
1	A	144	GLY
1	A	390	ILE
1	A	393	GLU
1	A	426	PHE
1	A	546	GLU
1	A	586	LEU
2	C	19	ILE
2	C	257	ALA
2	C	335	ILE
2	C	348	GLY
1	B	144	GLY
1	B	390	ILE
1	B	393	GLU

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Mol	Chain	Res	Type
1	B	426	PHE
1	B	546	GLU
1	B	586	LEU
2	F	19	ILE
2	F	257	ALA
2	F	335	ILE
2	F	348	GLY
4	H	51	THR
1	A	138	PRO
1	A	429	VAL
1	A	438	PRO
1	A	787	ILE
2	C	12	PRO
2	C	230	ILE
2	C	233	VAL
1	B	138	PRO
1	B	429	VAL
1	B	438	PRO
1	B	787	ILE
2	F	12	PRO
2	F	230	ILE
2	F	233	VAL
1	A	813	VAL
2	C	231	ILE
2	C	344	GLY
1	B	813	VAL
1	A	441	LYS
1	B	441	LYS
1	A	64	VAL
1	A	92	VAL
1	B	64	VAL
1	B	92	VAL
2	F	269	GLY
1	A	259	ILE
1	B	259	ILE

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	717/766 (94%)	610 (85%)	107 (15%)	3	14
1	B	717/766 (94%)	609 (85%)	108 (15%)	3	13
2	C	331/356 (93%)	287 (87%)	44 (13%)	4	16
2	F	331/356 (93%)	284 (86%)	47 (14%)	3	15
3	D	47/56 (84%)	45 (96%)	2 (4%)	26	48
3	G	47/56 (84%)	45 (96%)	2 (4%)	26	48
4	E	53/64 (83%)	48 (91%)	5 (9%)	8	26
4	H	53/64 (83%)	48 (91%)	5 (9%)	8	26
All	All	2296/2484 (92%)	1976 (86%)	320 (14%)	3	15

All (320) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	22	ASN
1	A	39	LEU
1	A	51	GLU
1	A	52	ASP
1	A	63	LEU
1	A	74	MET
1	A	75	ARG
1	A	79	VAL
1	A	80	GLN
1	A	94	GLU
1	A	96	LYS
1	A	101	LYS
1	A	103	LEU
1	A	106	THR
1	A	121	LEU
1	A	122	VAL
1	A	128	LEU
1	A	138	PRO
1	A	149	VAL
1	A	160	VAL
1	A	173	GLU
1	A	182	PHE
1	A	188	LYS
1	A	190	GLU

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Mol	Chain	Res	Type
1	A	207	ILE
1	A	219	TYR
1	A	224	GLU
1	A	231	ARG
1	A	235	VAL
1	A	237	ASP
1	A	253	GLU
1	A	256	SER
1	A	258	LEU
1	A	265	PRO
1	A	266	LEU
1	A	267	ILE
1	A	274	GLU
1	A	292	ASP
1	A	294	ASP
1	A	315	GLU
1	A	328	ASN
1	A	332	LEU
1	A	334	HIS
1	A	342	LEU
1	A	344	LEU
1	A	359	ILE
1	A	374	TYR
1	A	380	GLN
1	A	383	GLU
1	A	396	THR
1	A	397	TYR
1	A	400	ILE
1	A	402	PHE
1	A	403	GLN
1	A	422	GLU
1	A	429	VAL
1	A	433	GLU
1	A	437	ILE
1	A	444	ILE
1	A	445	ARG
1	A	457	LYS
1	A	459	LYS
1	A	460	TYR
1	A	469	LYS
1	A	479	VAL
1	A	482	THR

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Mol	Chain	Res	Type
1	A	484	ILE
1	A	492	SER
1	A	501	HIS
1	A	504	LEU
1	A	527	ILE
1	A	546	GLU
1	A	551	CYS
1	A	559	GLU
1	A	570	ARG
1	A	573	ARG
1	A	590	LEU
1	A	612	GLN
1	A	614	ILE
1	A	616	HIS
1	A	619	LEU
1	A	641	LEU
1	A	643	GLU
1	A	668	TYR
1	A	676	PHE
1	A	678	ASP
1	A	687	PHE
1	A	689	SER
1	A	699	LYS
1	A	700	ASN
1	A	709	LEU
1	A	710	PHE
1	A	724	HIS
1	A	740	GLN
1	A	744	GLU
1	A	751	ARG
1	A	758	ILE
1	A	774	GLU
1	A	776	VAL
1	A	777	GLN
1	A	785	ASP
1	A	787	ILE
1	A	801	MET
1	A	804	ARG
1	A	809	ILE
1	A	813	VAL
2	C	14	LEU
2	C	63	PHE

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Mol	Chain	Res	Type
2	C	65	ASP
2	C	67	PHE
2	C	79	THR
2	C	80	MET
2	C	85	TYR
2	C	94	LEU
2	C	133	PHE
2	C	134	PHE
2	C	141	ARG
2	C	143	ASN
2	C	154	LEU
2	C	156	PHE
2	C	157	THR
2	C	170	PHE
2	C	171	LEU
2	C	177	ARG
2	C	181	LYS
2	C	187	ILE
2	C	188	SER
2	C	228	PHE
2	C	230	ILE
2	C	232	LEU
2	C	233	VAL
2	C	234	GLN
2	C	238	ARG
2	C	240	ILE
2	C	241	THR
2	C	242	ILE
2	C	244	TYR
2	C	249	THR
2	C	275	PHE
2	C	298	LEU
2	C	320	PHE
2	C	327	ASP
2	C	337	LYS
2	C	338	TYR
2	C	342	ILE
2	C	345	LEU
2	C	372	VAL
2	C	375	LEU
2	C	376	LEU
2	C	422	ILE

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Mol	Chain	Res	Type
3	D	25	GLU
3	D	62	LEU
4	E	19	MET
4	E	21	GLN
4	E	40	HIS
4	E	63	PHE
4	E	72	PHE
1	B	7	ASN
1	B	22	ASN
1	B	39	LEU
1	B	51	GLU
1	B	52	ASP
1	B	63	LEU
1	B	74	MET
1	B	75	ARG
1	B	79	VAL
1	B	80	GLN
1	B	94	GLU
1	B	96	LYS
1	B	101	LYS
1	B	103	LEU
1	B	106	THR
1	B	121	LEU
1	B	122	VAL
1	B	128	LEU
1	B	138	PRO
1	B	149	VAL
1	B	160	VAL
1	B	173	GLU
1	B	182	PHE
1	B	188	LYS
1	B	190	GLU
1	B	201	GLN
1	B	207	ILE
1	B	219	TYR
1	B	224	GLU
1	B	231	ARG
1	B	235	VAL
1	B	237	ASP
1	B	253	GLU
1	B	256	SER
1	B	258	LEU

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Mol	Chain	Res	Type
1	B	265	PRO
1	B	266	LEU
1	B	267	ILE
1	B	274	GLU
1	B	292	ASP
1	B	294	ASP
1	B	315	GLU
1	B	328	ASN
1	B	332	LEU
1	B	334	HIS
1	B	342	LEU
1	B	344	LEU
1	B	359	ILE
1	B	374	TYR
1	B	380	GLN
1	B	383	GLU
1	B	396	THR
1	B	397	TYR
1	B	400	ILE
1	B	402	PHE
1	B	403	GLN
1	B	422	GLU
1	B	429	VAL
1	B	433	GLU
1	B	437	ILE
1	B	444	ILE
1	B	445	ARG
1	B	457	LYS
1	B	459	LYS
1	B	460	TYR
1	B	469	LYS
1	B	479	VAL
1	B	482	THR
1	B	484	ILE
1	B	492	SER
1	B	501	HIS
1	B	504	LEU
1	B	527	ILE
1	B	546	GLU
1	B	551	CYS
1	B	559	GLU
1	B	570	ARG

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Mol	Chain	Res	Type
1	B	573	ARG
1	B	590	LEU
1	B	612	GLN
1	B	614	ILE
1	B	616	HIS
1	B	619	LEU
1	B	641	LEU
1	B	643	GLU
1	B	668	TYR
1	B	676	PHE
1	B	678	ASP
1	B	687	PHE
1	B	689	SER
1	B	699	LYS
1	B	700	ASN
1	B	709	LEU
1	B	710	PHE
1	B	724	HIS
1	B	740	GLN
1	B	744	GLU
1	B	751	ARG
1	B	758	ILE
1	B	774	GLU
1	B	776	VAL
1	B	777	GLN
1	B	785	ASP
1	B	787	ILE
1	B	801	MET
1	B	804	ARG
1	B	809	ILE
1	B	813	VAL
2	F	14	LEU
2	F	63	PHE
2	F	65	ASP
2	F	67	PHE
2	F	79	THR
2	F	80	MET
2	F	85	TYR
2	F	94	LEU
2	F	133	PHE
2	F	134	PHE
2	F	141	ARG

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Mol	Chain	Res	Type
2	F	143	ASN
2	F	154	LEU
2	F	156	PHE
2	F	157	THR
2	F	170	PHE
2	F	171	LEU
2	F	177	ARG
2	F	181	LYS
2	F	187	ILE
2	F	188	SER
2	F	228	PHE
2	F	232	LEU
2	F	233	VAL
2	F	234	GLN
2	F	238	ARG
2	F	240	ILE
2	F	241	THR
2	F	242	ILE
2	F	244	TYR
2	F	248	VAL
2	F	249	THR
2	F	253	VAL
2	F	265	VAL
2	F	270	VAL
2	F	275	PHE
2	F	298	LEU
2	F	320	PHE
2	F	327	ASP
2	F	337	LYS
2	F	338	TYR
2	F	342	ILE
2	F	345	LEU
2	F	372	VAL
2	F	375	LEU
2	F	376	LEU
2	F	422	ILE
3	G	25	GLU
3	G	62	LEU
4	H	19	MET
4	H	21	GLN
4	H	40	HIS
4	H	63	PHE

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Mol	Chain	Res	Type
4	H	72	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	80	GLN
1	A	163	ASN
1	A	183	ASN
1	A	193	ASN
1	A	222	ASN
1	A	223	ASN
1	A	328	ASN
1	A	337	ASN
1	A	403	GLN
1	A	448	HIS
1	A	475	GLN
1	A	502	GLN
1	A	509	HIS
1	A	565	ASN
1	A	574	GLN
1	A	598	GLN
1	A	604	ASN
1	A	612	GLN
1	A	692	ASN
1	A	740	GLN
1	A	761	HIS
1	A	777	GLN
2	C	93	GLN
2	C	143	ASN
2	C	152	ASN
2	C	235	GLN
2	C	353	GLN
2	C	360	ASN
2	C	407	GLN
1	B	22	ASN
1	B	80	GLN
1	B	163	ASN
1	B	183	ASN
1	B	193	ASN
1	B	222	ASN
1	B	223	ASN

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Mol	Chain	Res	Type
1	B	328	ASN
1	B	337	ASN
1	B	403	GLN
1	B	448	HIS
1	B	475	GLN
1	B	502	GLN
1	B	509	HIS
1	B	565	ASN
1	B	574	GLN
1	B	598	GLN
1	B	604	ASN
1	B	612	GLN
1	B	692	ASN
1	B	736	GLN
1	B	740	GLN
1	B	761	HIS
1	B	777	GLN
2	F	93	GLN
2	F	143	ASN
2	F	152	ASN
2	F	353	GLN
2	F	360	ASN
2	F	407	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	ADP	B	873	7	28,29,29	2.22	5 (17%)	43,45,45	2.01	13 (30%)
7	BEF	A	874	6	0,3,3	-	-	-	-	-
6	ADP	A	873	7	28,29,29	2.22	5 (17%)	43,45,45	2.01	12 (27%)
7	BEF	B	874	6	0,3,3	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ADP	B	873	7	-	0/16/32/32	0/3/3/3
6	ADP	A	873	7	-	0/16/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	873	ADP	C8-N7	6.75	1.44	1.31
6	B	873	ADP	C8-N7	6.75	1.44	1.31
6	B	873	ADP	C8-N9	5.96	1.47	1.37
6	A	873	ADP	C8-N9	5.93	1.47	1.37
6	A	873	ADP	PA-O3A	5.47	1.65	1.59
6	B	873	ADP	PA-O3A	5.43	1.65	1.59
6	A	873	ADP	C6-N6	2.59	1.40	1.34
6	B	873	ADP	C6-N6	2.58	1.40	1.34
6	A	873	ADP	PB-O1B	2.37	1.57	1.50
6	B	873	ADP	PB-O1B	2.36	1.57	1.50

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	873	ADP	N9-C8-N7	-7.14	103.81	113.94
6	A	873	ADP	N9-C8-N7	-7.12	103.83	113.94
6	B	873	ADP	N3-C2-N1	-4.28	122.11	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	873	ADP	N3-C2-N1	-4.26	122.13	128.58
6	B	873	ADP	C5-C4-N3	-4.13	121.03	126.72
6	A	873	ADP	C5-C4-N3	-4.11	121.05	126.72
6	B	873	ADP	C6-C5-C4	3.03	121.31	117.18
6	A	873	ADP	C6-C5-C4	3.01	121.29	117.18
6	B	873	ADP	C5-N7-C8	2.95	108.08	103.45
6	A	873	ADP	C5-N7-C8	2.92	108.04	103.45
6	A	873	ADP	C2'-C1'-N9	-2.78	106.40	113.30
6	B	873	ADP	C2'-C1'-N9	-2.77	106.43	113.30
6	A	873	ADP	O3B-PB-O2B	2.50	117.19	107.80
6	B	873	ADP	O3B-PB-O2B	2.49	117.15	107.80
6	B	873	ADP	C2-N3-C4	2.32	117.51	111.83
6	A	873	ADP	C2-N3-C4	2.32	117.50	111.83
6	B	873	ADP	O3A-PB-O1B	-2.25	99.21	111.04
6	A	873	ADP	O3A-PB-O1B	-2.25	99.21	111.04
6	B	873	ADP	C4-N9-C8	2.21	108.06	105.74
6	A	873	ADP	C4-N9-C8	2.20	108.05	105.74
6	B	873	ADP	N3-C4-N9	2.19	130.89	127.17
6	A	873	ADP	N3-C4-N9	2.18	130.88	127.17
6	B	873	ADP	C5-C4-N9	2.06	108.05	105.81
6	A	873	ADP	C5-C4-N9	2.05	108.04	105.81
6	B	873	ADP	C4-N9-C1'	-2.01	121.94	126.63

There are no chirality outliers.

There are no torsion outliers.

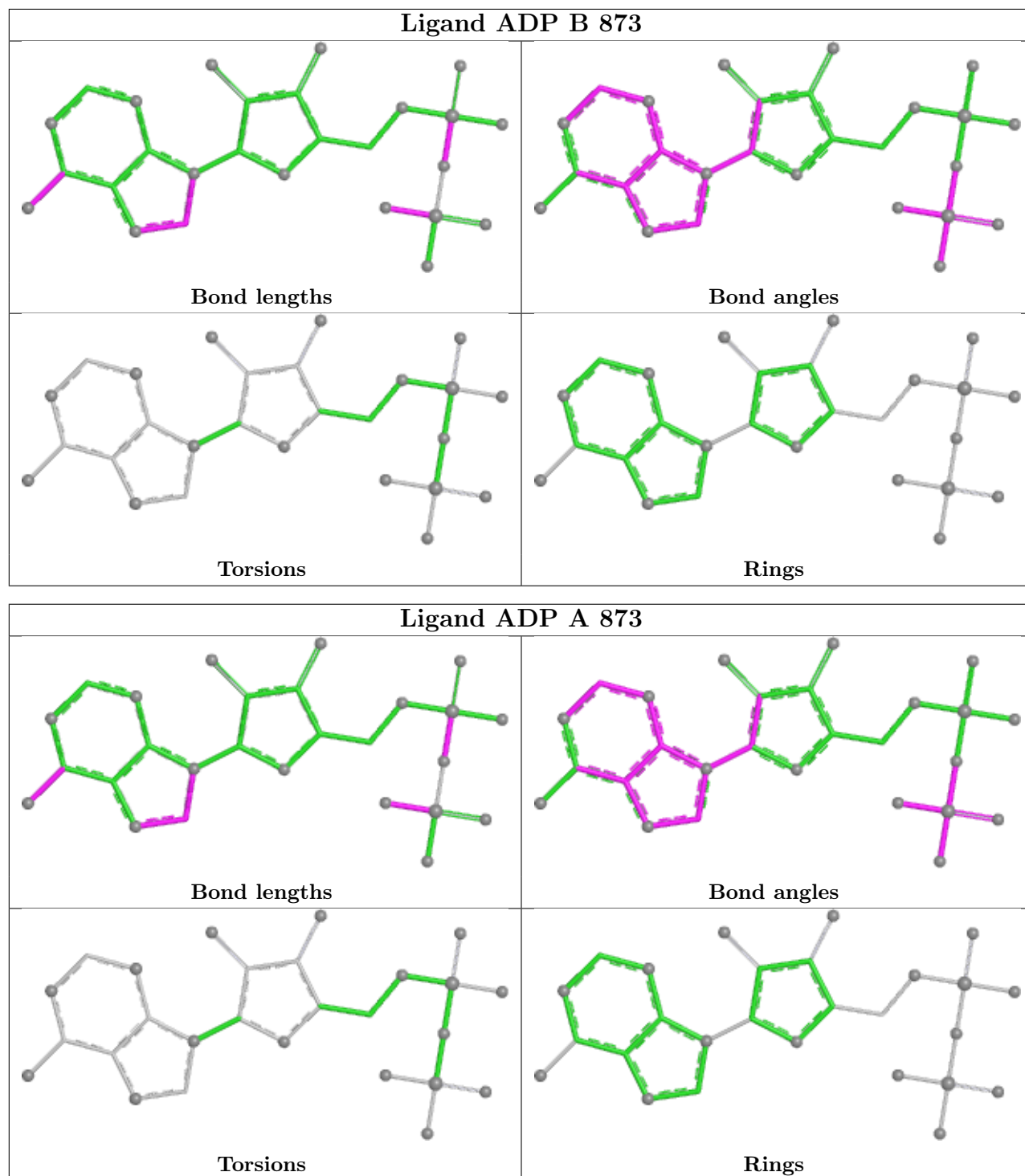
There are no ring outliers.

4 monomers are involved in 89 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	873	ADP	39	0
7	A	874	BEF	4	0
6	A	873	ADP	41	0
7	B	874	BEF	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	816/871 (93%)	-0.45	7 (0%) 81 67	108, 306, 457, 500	0
1	B	816/871 (93%)	-0.44	5 (0%) 85 73	108, 306, 457, 500	0
2	C	396/431 (91%)	-0.40	2 (0%) 87 75	223, 429, 500, 500	0
2	F	396/431 (91%)	-0.38	2 (0%) 87 75	223, 429, 500, 500	0
3	D	56/65 (86%)	-0.56	0 100 100	322, 414, 500, 500	0
3	G	56/65 (86%)	-0.48	0 100 100	322, 414, 500, 500	0
4	E	65/76 (85%)	-0.44	0 100 100	326, 444, 490, 500	0
4	H	65/76 (85%)	-0.46	0 100 100	326, 444, 490, 500	0
All	All	2666/2886 (92%)	-0.43	16 (0%) 85 73	108, 365, 489, 500	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	99	GLU	6.4
1	A	101	LYS	5.5
1	B	99	GLU	4.7
1	B	101	LYS	3.6
1	A	94	GLU	2.9
1	B	97	THR	2.8
1	A	573	ARG	2.7
1	B	100	GLY	2.6
1	A	100	GLY	2.5
1	A	574	GLN	2.5
1	A	79	VAL	2.5
2	C	244	TYR	2.3
2	C	237	GLU	2.2
2	F	140	ALA	2.2
1	B	94	GLU	2.2
2	F	228	PHE	2.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

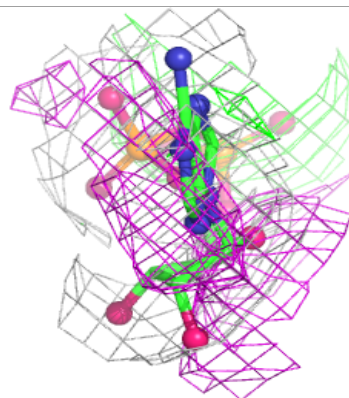
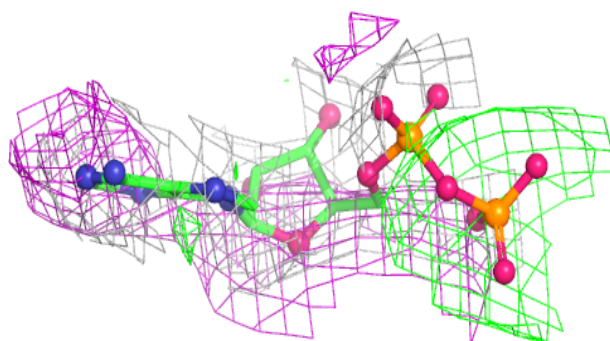
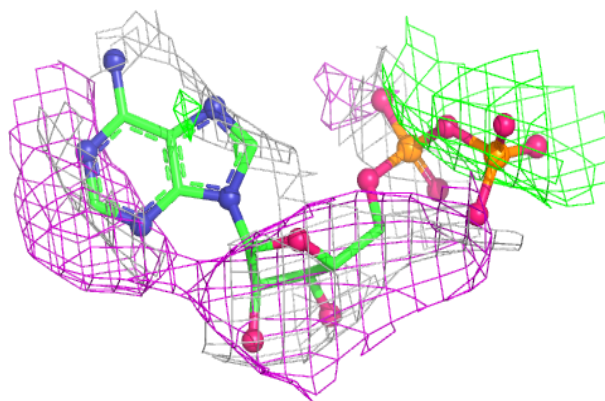
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	ADP	A	873	27/27	0.60	0.16	134,186,192,399	0
7	BEF	A	874	4/4	0.66	0.15	112,134,154,241	0
6	ADP	B	873	27/27	0.70	0.15	134,186,192,399	0
7	BEF	B	874	4/4	0.80	0.12	112,134,154,241	0
5	MG	A	872	1/1	0.82	0.18	130,130,130,130	0
5	MG	B	872	1/1	0.93	0.12	130,130,130,130	0

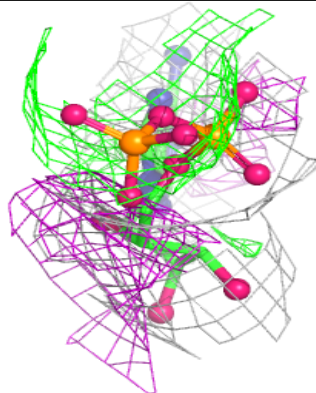
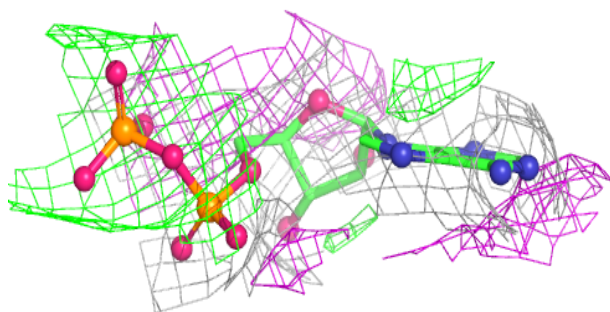
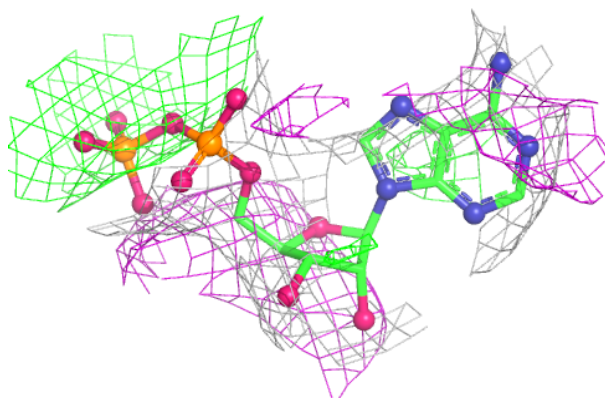
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ADP A 873:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ADP B 873:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.