



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2023 – 02:37 PM EDT

PDB ID : 3DIN
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

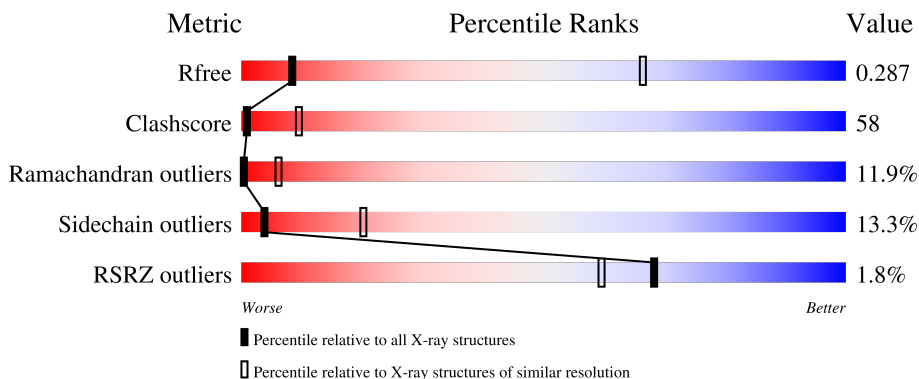
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	1055 (5.20-3.80)
Clashscore	141614	1123 (5.20-3.80)
Ramachandran outliers	138981	1069 (5.20-3.80)
Sidechain outliers	138945	1050 (5.20-3.80)
RSRZ outliers	127900	1101 (5.30-3.70)

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	 21% 55% 17% • 6%
1	B	871	 21% 54% 17% • 6%
2	C	431	 3% 27% 50% 13% • 8%
2	F	431	 3% 27% 51% 12% • 8%
3	D	65	 32% 51% • • 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 [i](#)

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
			Total	C	N	O	S			
1	A	816	Total 6613	C 4215	N 1131	O 1239	S 28	0	0	0
1	B	816	Total 6613	C 4215	N 1131	O 1239	S 28	0	0	0

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

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

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

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

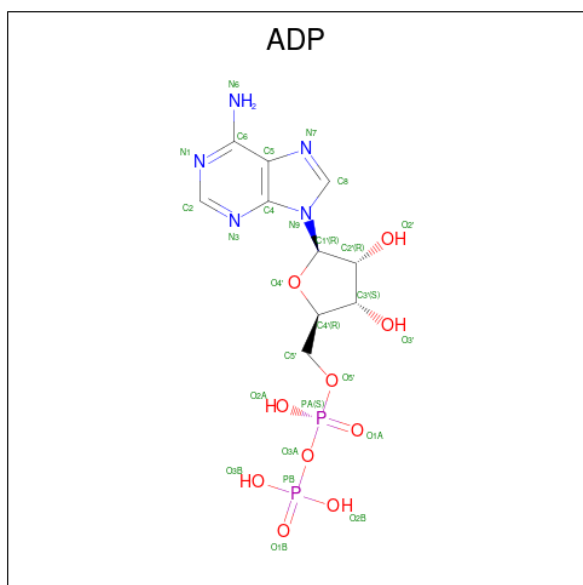
- Molecule 4 is a protein called Preprotein translocase subunit SecG.

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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

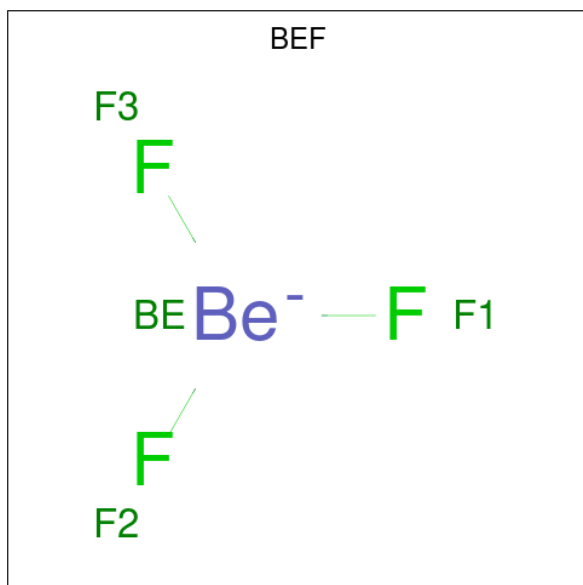
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0
5	B	1	Total Mg 1 1	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O P 27 10 5 10 2	0	0
6	B	1	Total C N O P 27 10 5 10 2	0	0

- Molecule 7 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3).

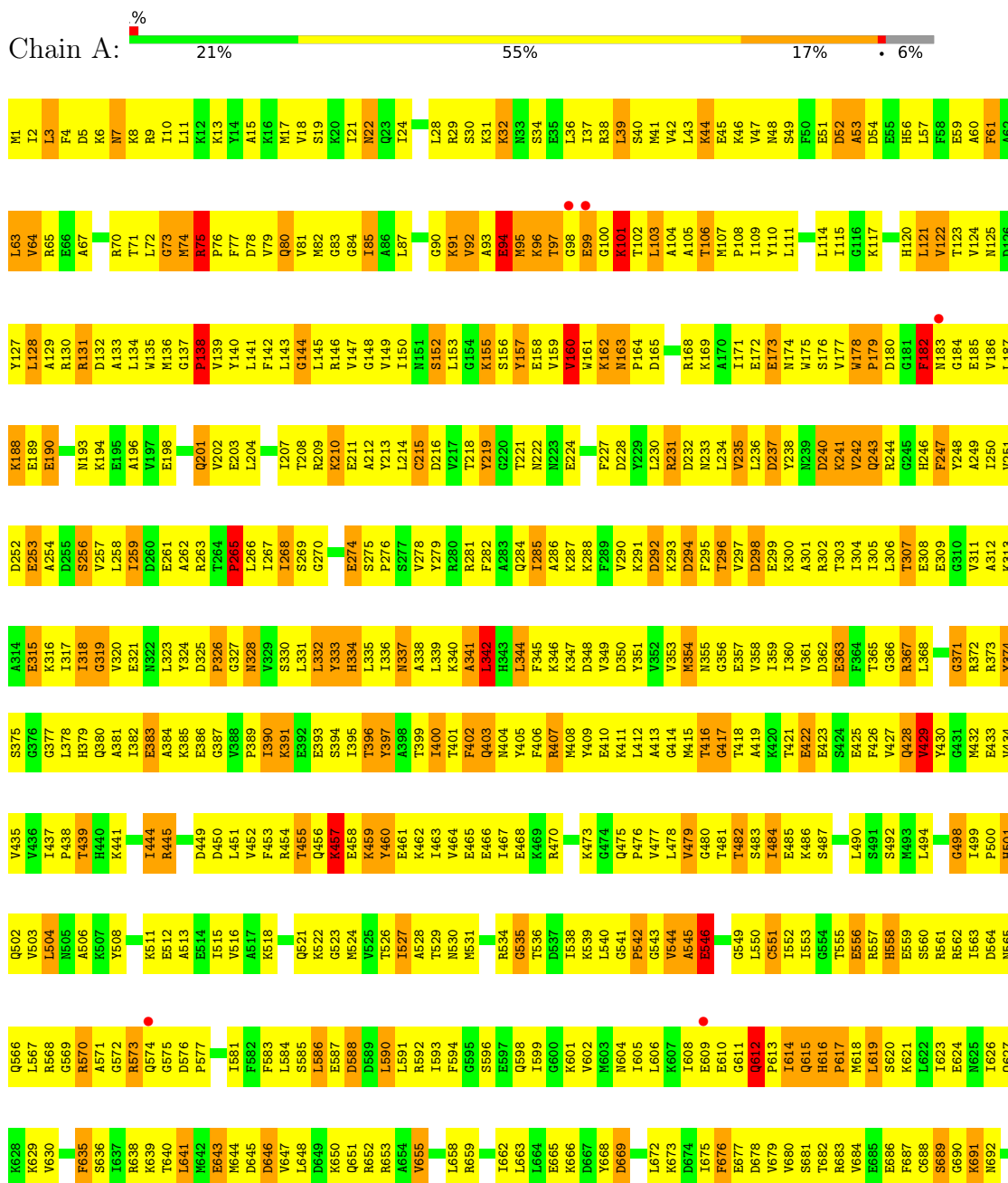


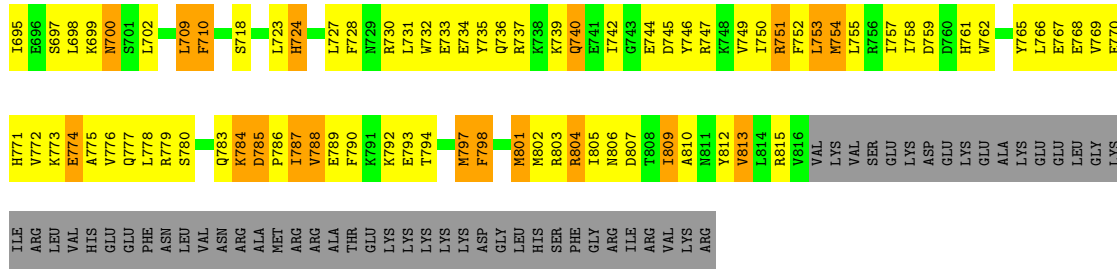
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Be	F		
7	A	1	4	1	3	0	0
7	B	1	4	1	3	0	0

3 Residue-property plots

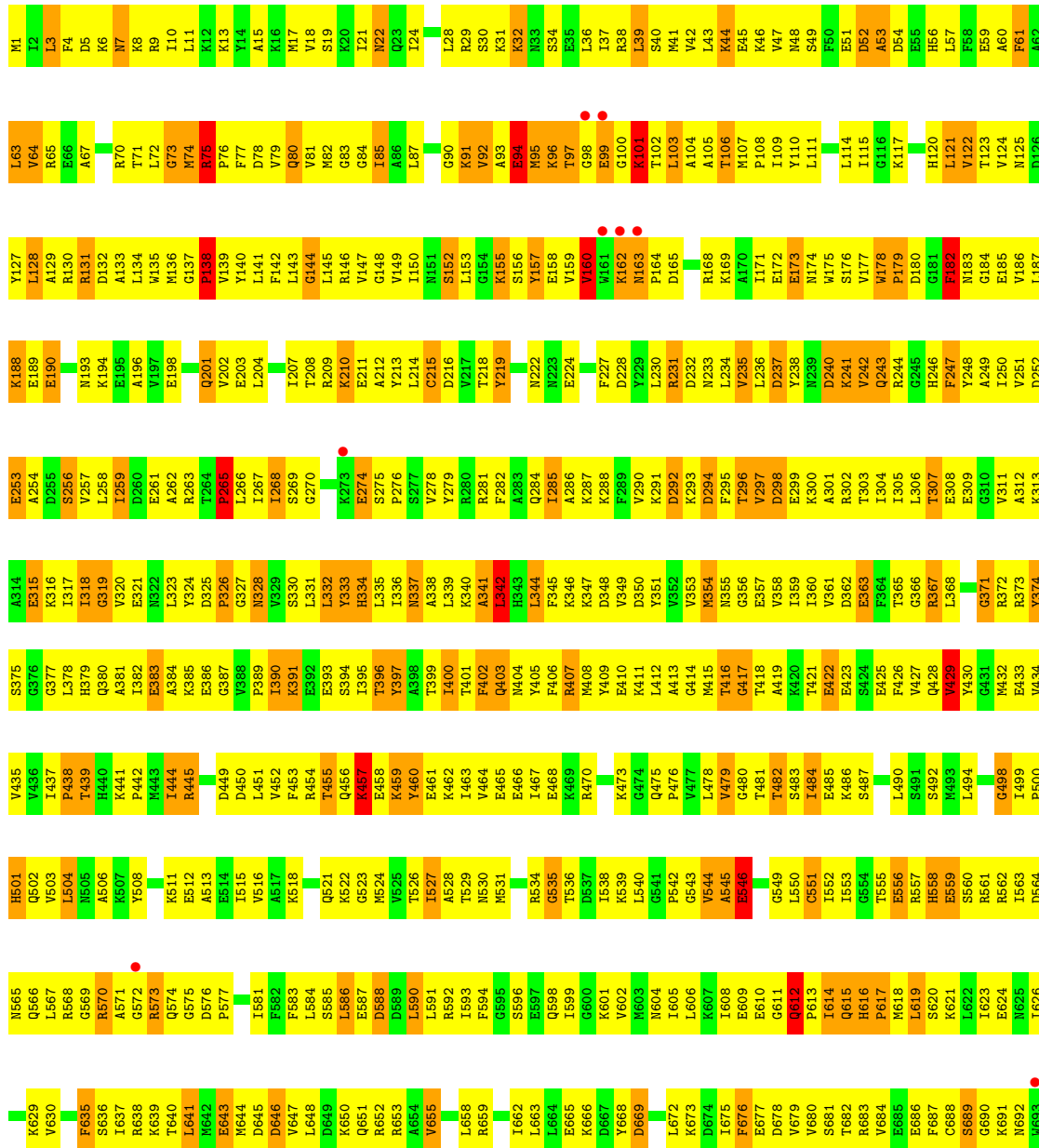
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

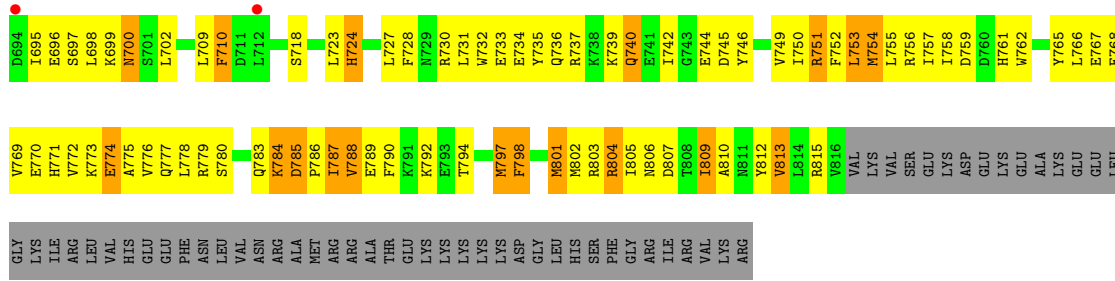
• Molecule 1: Protein translocase subunit secA



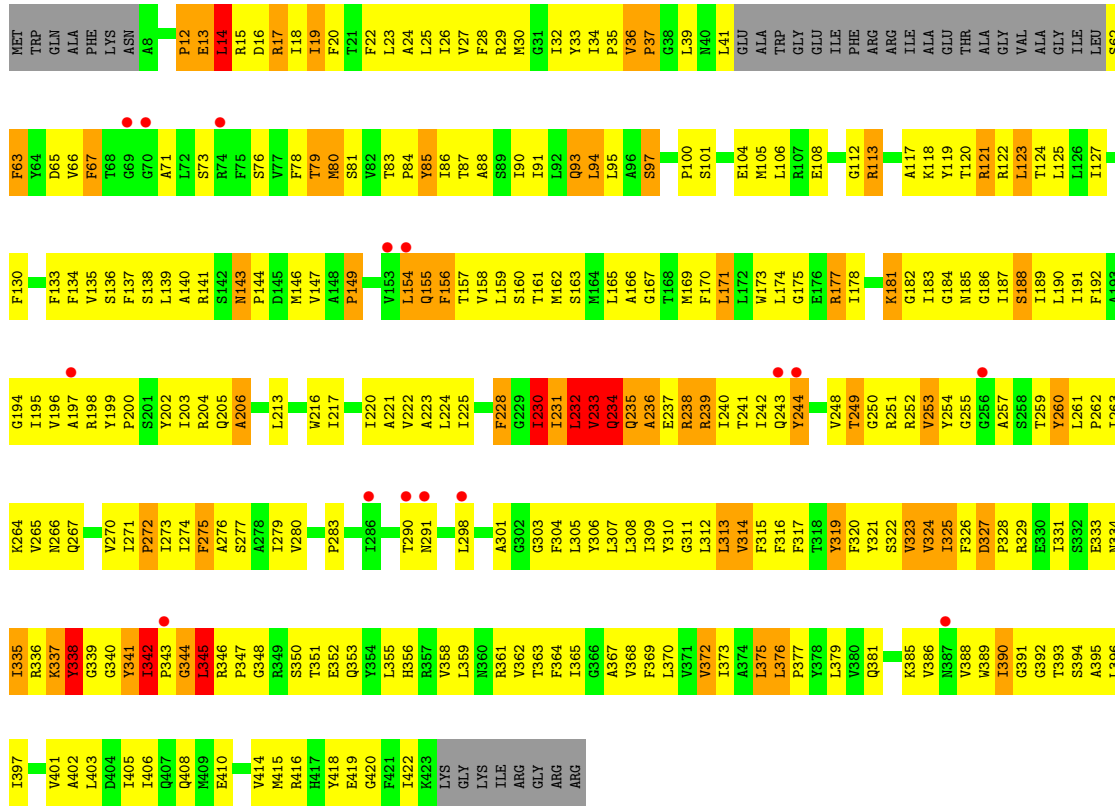


• Molecule 1: Protein translocase subunit secA

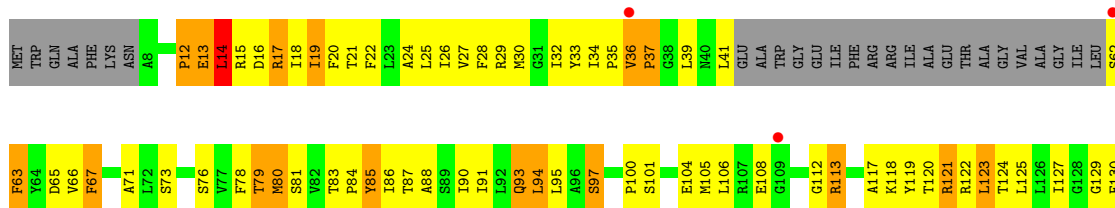


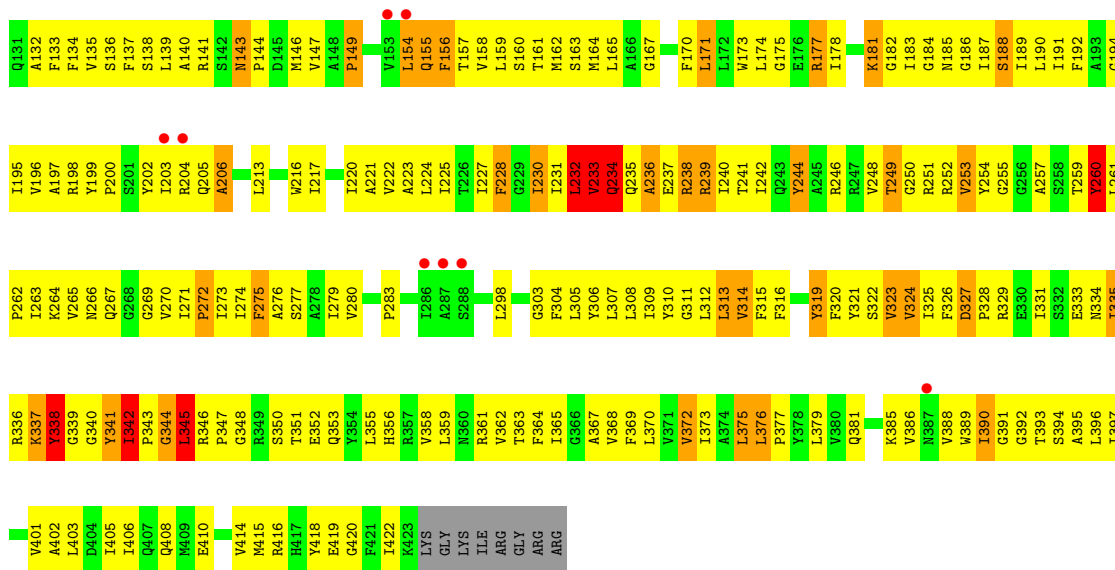


• Molecule 2: Preprotein translocase subunit SecY



• Molecule 2: Preprotein translocase subunit SecY

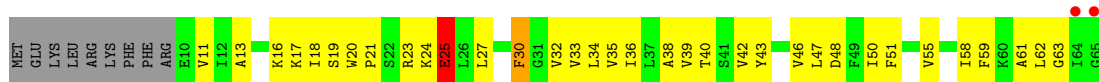
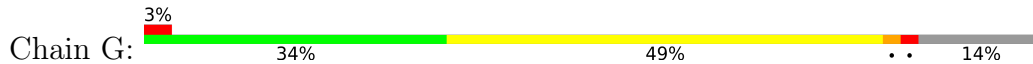




• Molecule 3: Preprotein translocase subunit secE



• Molecule 3: Preprotein translocase subunit secE



• Molecule 4: Preprotein translocase subunit SecG



• 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 19.97 – 4.50	Depositor EDS
% Data completeness (in resolution range)	97.7 (15.00-4.50) 97.2 (19.97-4.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 4.54Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.279 , 0.303 0.286 , 0.287	Depositor DCC
R_{free} test set	1678 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	205.7	Xtrriage
Anisotropy	0.402	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.17 , 253.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	21368	wwPDB-VP
Average B, all atoms (Å ²)	356.0	wwPDB-VP

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.31	0/6730	0.62	1/9048 (0.0%)
1	B	0.31	0/6730	0.62	1/9048 (0.0%)
2	C	0.44	1/3194 (0.0%)	0.68	1/4329 (0.0%)
2	F	0.42	0/3194	0.69	2/4329 (0.0%)
3	D	0.32	0/440	0.54	0/596
3	G	0.33	0/440	0.54	0/596
4	E	0.31	0/492	0.55	0/662
4	H	0.31	0/492	0.55	0/662
All	All	0.35	1/21712 (0.0%)	0.63	5/29270 (0.0%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	235	GLN	N-CA	5.64	1.57	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	236	ALA	N-CA-C	5.62	126.17	111.00
2	F	228	PHE	CB-CG-CD1	5.53	124.67	120.80
2	C	236	ALA	N-CA-C	5.37	125.50	111.00
1	A	94	GLU	CB-CA-C	-5.18	100.04	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	94	GLU	CB-CA-C	-5.18	100.05	110.40

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6613	0	6689	906	2
1	B	6613	0	6689	891	2
2	C	3124	0	3275	347	0
2	F	3124	0	3275	336	0
3	D	431	0	460	29	0
3	G	431	0	460	33	0
4	E	484	0	508	29	0
4	H	484	0	508	28	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	27	0	12	40	0
6	B	27	0	12	38	0
7	A	4	0	0	4	0
7	B	4	0	0	5	0
All	All	21368	0	21888	2490	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 58.

All (2490) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:340:LYS:HZ2	2:C:251:ARG:HE	1.18	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
2:C:183:ILE:HG13	2:C:185:ASN:H	1.32	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: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:B:94:GLU:OE1	1:B:94:GLU:HA	1.74	0.87
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: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
2:F:231:ILE:C	2:F:232:LEU:HD22	1.96	0.85
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:C:231:ILE:C	2:C:232:LEU:HD22	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
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: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
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:B:79:VAL:HG23	1:B:94:GLU:OE1	1.86	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:28:LEU:HA	1:B:32:LYS:HZ2	1.52	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
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:236:ALA:HB3	2:C:262:PRO:C	2.09	0.72
2:C:355:LEU:O	2:C:359:LEU:HG	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:A:93:ALA:C	1:A:94:GLU:HG2	2.11	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
1:A:74:MET:HE1	6:A:873:ADP:N3	2.07	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
2:F:236:ALA:HB3	2:F:262:PRO:C	2.12	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:155:LYS:HD2	1:A:208:THR:C	2.12	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:A:93:ALA:C	1:A:94:GLU:CG	2.60	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
2:C:232:LEU:HD22	2:C:232:LEU:N	2.09	0.68
1:B:155:LYS:HD2	1:B:208:THR:C	2.12	0.68
1:A:28:LEU:HA	1:A:32:LYS:HZ2	1.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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:247:PHE:C	1:B:410:GLU:HB3	2.15	0.66
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: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
1:A:247:PHE:C	1:A:410:GLU:HB3	2.15	0.66
1:B:574:GLN:CG	6:B:873:ADP:H1'	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:A:412:LEU:HB2	1:A:432:MET:HE3	1.77	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:100:GLY:C	6:B:873:ADP:O1A	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:313:LYS:HE3	1:B:335:LEU:HD11	1.77	0.65
1:A:155:LYS:HZ3	1:A:209:ARG:HD2	1.61	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: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
1:A:80:GLN:HG3	1:A:81:VAL:N	2.11	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:H1'	2.27	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:A:74:MET:CE	6:A:873:ADP:N3	2.61	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:B:155:LYS:HZ3	1:B:209:ARG:HD2	1.63	0.64
1:B:340:LYS:HZ2	2:F:251:ARG:HE	1.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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:679:VAL:CG1	1:B:803:ARG:HE	2.12	0.62
1:B:765:TYR:O	1:B:769:VAL:HG23	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:659:ARG:HG2	1:B:755:LEU:HG	1.81	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: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:573:ARG:HA	1:A:573:ARG:NH1	2.15	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
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:155:GLN:C	2:C:157:THR:H	2.03	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
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
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:74:MET:HE2	1:B:187:LEU:HD11	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:F:155:GLN:C	2:F:157:THR:H	2.03	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: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: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:28:LEU:HA	1:A:32:LYS:NZ	2.15	0.60
1:A:97:THR:CA	1:A:573:ARG:HH12	2.14	0.60
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:LEU:H	1:A:586:LEU:HD12	1.67	0.60
1:B:103:LEU:HD23	1:B:103:LEU:H	1.65	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: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: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: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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:284:GLN:HG2	1:B:288:LYS:HZ2	1.68	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
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:96:LYS:HZ3	1:A:573:ARG:NH2	2.00	0.58
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:ILE:HD13	1:A:383:GLU:CD	2.24	0.58
1:A:592:ARG:HH21	1:A:593:ILE:HD11	1.67	0.58
2:C:334:ASN:C	2:C:335:ILE:HD12	2.22	0.58
1:B:344:LEU:HD23	1:B:345:PHE:N	2.19	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:B:761:HIS:HB3	1:B:801:MET:HE2	1.84	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:359:ILE:HD13	1:B:383:GLU:CD	2.24	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
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
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
3:G:24:LYS:C	3:G:25:GLU:HG2	2.24	0.58
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:456:GLN:C	1:B:458:GLU:H	2.08	0.57
1:B:585:SER:C	1:B:587:GLU:H	2.07	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:585:SER:C	1:A:587:GLU:H	2.08	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:74:MET:HE2	1:A:187:LEU:HD11	1.86	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
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
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
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:100:GLY:C	6:A:873:ADP:O1A	2.43	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
3:D:24:LYS:C	3:D:25:GLU:HG2	2.24	0.57
1:B:53:ALA:HB1	1:B:56:HIS:ND1	2.20	0.57
1:B:268:ILE:HG23	1:B:269:SER:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:456:GLN:C	1:A:458:GLU:H	2.07	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: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
1:A:325:ASP:O	1:A:327:GLY:N	2.39	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
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:150:ILE:HG13	1:B:155:LYS:HZ2	1.69	0.56
1:B:407:ARG:HD2	1:B:429:VAL:O	2.06	0.56
1:B:412:LEU:HB2	1:B:432:MET:HE3	1.86	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:761:HIS:HB3	1:A:801:MET:HE2	1.86	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:407:ARG:HD2	1:A:429:VAL:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:454:ARG:HH12	1:A:608:ILE:HA	1.71	0.56
1:A:659:ARG:HH22	1:A:759:ASP:CG	2.09	0.56
1:A:753:LEU:CD1	1:A:812:TYR:HB3	2.36	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
1:B:659:ARG:HH22	1:B:759:ASP:CG	2.09	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:284:GLN:HG2	1:A:288:LYS:HZ2	1.72	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:659:ARG:HH12	1:A:759:ASP:CG	2.09	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
2:C:280:VAL:C	2:C:283:PRO:HD2	2.25	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
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
1:A:150:ILE:HG13	1:A:155:LYS:HZ2	1.71	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: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
1:A:425:GLU:C	1:A:427:VAL:H	2.10	0.55
2:C:249:THR:HG22	2:C:250:GLY:N	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:659:ARG:HH12	1:B:759:ASP:CG	2.09	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: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: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:74:MET:CE	6:B:873:ADP:N3	2.70	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
2:C:35:PRO:O	2:C:36:VAL:CB	2.55	0.54
2:C:35:PRO:C	2:C:37:PRO:HD3	2.28	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:TRP:H	1:A:179:PRO:HD2	1.73	0.54
1:A:475:GLN:HB3	1:A:551:CYS:SG	2.47	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:425:GLU:C	1:B:427:VAL:H	2.10	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
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
2:C:322:SER:C	2:C:324:VAL:H	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:F:35:PRO:C	2:F:37:PRO:HD3	2.28	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:C:225:ILE:HG23	2:C:369:PHE:HD2	1.74	0.53
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
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
2:F:333:GLU:C	2:F:335:ILE:H	2.12	0.53
1:A:121:LEU:HD22	1:A:250:ILE:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:97:THR:HG23	1:A:572:GLY:C	2.29	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:92:VAL:HG12	1:A:414:GLY:C	2.30	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
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:197:ALA:C	2:F:200:PRO:HD2	2.29	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:30:SER:HB2	1:B:32:LYS:HD2	1.91	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:96:LYS:HZ1	1:A:570:ARG:CZ	2.23	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
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: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
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
1:B:779:ARG:HH21	1:B:785:ASP:C	2.13	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:152:SER:C	1:A:153:LEU:HD12	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:333:GLU:C	2:C:335:ILE:H	2.12	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
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:152:SER:C	1:B:153:LEU:HD12	2.30	0.52
1:B:778:LEU:HA	2:F:264:LYS:CE	2.38	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
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:92:VAL:HG12	1:B:414:GLY:C	2.30	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
2:F:322:SER:C	2:F:324:VAL:H	2.11	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:340:LYS:HZ2	2:C:251:ARG:NE	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:197:ALA:C	2:C:200:PRO:HD2	2.29	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:96:LYS:HZ1	1:B:570:ARG:CZ	2.23	0.51
1:B:97:THR:HG23	1:B:572:GLY:C	2.29	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
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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:ALA:HA	1:A:338:ALA:HB1	1.92	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: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
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:295:PHE:HB2	1:A:309:GLU:CD	2.31	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
1:A:779:ARG:HH21	1:A:785:ASP:C	2.13	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
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: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:231:ILE:O	2:C:232:LEU:C	2.49	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:295:PHE:HB2	1:B:309:GLU:CD	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:MET:HB2	1:A:108:PRO:CD	2.41	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: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
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: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: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: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
2:F:155:GLN:C	2:F:157:THR:N	2.64	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:529:THR:HG22	1:A:530:ASN:OD1	2.12	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:606:LEU:HD21	1:B:617:PRO:CG	2.41	0.50
1:A:254:ALA:C	1:A:256:SER:N	2.65	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:463:ILE:O	1:B:466:GLU:HB3	2.11	0.50
1:B:770:GLU:CD	1:B:773:LYS:HD2	2.31	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: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:240:ASP:C	1:B:242:VAL:H	2.15	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:ASP:HB3	1:A:584:LEU:HD12	1.92	0.50
2:C:155:GLN:C	2:C:157:THR:N	2.64	0.50
2:C:182:GLY:HA2	2:C:408:GLN:OE1	2.12	0.50
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: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
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:240:ASP:C	1:A:242:VAL:H	2.15	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
1:B:573:ARG:C	1:B:575:GLY:H	2.15	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:770:GLU:CD	1:A:773:LYS:HD2	2.31	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:104:GLU:HB3	2:F:105:MET:HE2	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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
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:573:ARG:C	1:A:575:GLY:H	2.15	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: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: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: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:373:ARG:HD3	1:A:378:LEU:HB3	1.95	0.49
2:C:238:ARG:HD3	2:C:337:LYS:HZ3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
1:A:296:THR:HG1	1:A:306:LEU:HD22	1.78	0.48
1:A:333:TYR:CE1	2:C:253:VAL:HG13	2.48	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:275:PHE:CD2	2:C:275:PHE:C	2.86	0.48
2:C:323:VAL:HG11	2:C:359:LEU:CD2	2.43	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: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
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
1:B:569:GLY:C	1:B:571:ALA:H	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:481:THR:HG22	1:A:555:THR:OG1	2.12	0.48
1:B:97:THR:HG22	1:B:575:GLY:N	2.29	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:96:LYS:HZ1	1:A:570:ARG:NH2	2.10	0.48
1:A:97:THR:HG22	1:A:575:GLY:CA	2.43	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
1:A:330:SER:OG	1:A:331:LEU:HD12	2.13	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: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
2:F:275:PHE:CD2	2:F:275:PHE:C	2.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:GLY:CA	1:A:394:SER:HB3	2.43	0.48
1:A:569:GLY:C	1:A:571:ALA:H	2.16	0.48
1:A:766:LEU:O	1:A:769:VAL:HB	2.13	0.48
1:B:230:LEU:C	1:B:232:ASP:N	2.66	0.48
1:B:254:ALA:C	1:B:256:SER:N	2.65	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: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: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: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: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
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
4:H:42:VAL:C	4:H:44:GLY:H	2.16	0.48
1:A:757:ILE:HD11	1:A:812:TYR:CE1	2.49	0.47
2:C:91:ILE:HG21	2:C:123:LEU:HG	1.95	0.47
4:E:42:VAL:C	4:E:44:GLY:H	2.16	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:394:SER:HA	2:F:397:ILE:CD1	2.44	0.47
1:A:340:LYS:NZ	2:C:251:ARG:HE	2.01	0.47
1:A:576:ASP:HB2	1:A:577:PRO:HD2	1.96	0.47
1:A:761:HIS:HB3	1:A:801:MET:CE	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:513:ALA:O	1:A:516:VAL:HB	2.14	0.47
1:B:121:LEU:CD2	1:B:250:ILE:HB	2.43	0.47
1:B:317:ILE:O	1:B:318:ILE:C	2.53	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
2:F:158:VAL:O	2:F:162:MET:HE3	2.14	0.47
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: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
2:F:235:GLN:C	2:F:264:LYS:H	2.18	0.47
3:G:21:PRO:O	3:G:24:LYS:HE3	2.15	0.47
1:A:81:VAL:O	1:A:85:ILE:HG12	2.15	0.47
1:A:484:ILE:HG12	1:A:485:GLU:N	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:158:VAL:O	2:C:162:MET:HE3	2.14	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:78:ASP:O	1:B:82:MET:N	2.46	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:761:HIS:HB3	1:B:801:MET:CE	2.44	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
3:G:16:LYS:HA	3:G:19:SER:OG	2.14	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:15:ALA:C	1:B:18:VAL:HG12	2.35	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: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
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:230:LEU:C	1:A:232:ASP:N	2.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:THR:HA	1:A:306:LEU:HD13	1.96	0.47
1:B:74:MET:HE1	6:B:873:ADP:N3	2.29	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:317:ILE:O	1:A:318:ILE:C	2.53	0.46
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: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:324:TYR:C	1:A:326:PRO:HD2	2.36	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
2:C:121:ARG:O	2:C:125:LEU:HG	2.16	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:101:LYS:NZ	1:B:416:THR:OG1	2.47	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:15:ALA:C	1:A:18:VAL:HG12	2.35	0.46
1:A:90:GLY:O	1:A:432:MET:HB3	2.16	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:275:PHE:O	2:F:279:ILE:HG13	2.16	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
1:A:156:SER:HA	1:A:207:ILE:CD1	2.44	0.46
1:A:298:ASP:CG	1:A:304:ILE:HG12	2.36	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:306:LEU:CD2	1:B:309:GLU:HG3	2.39	0.46
1:B:324:TYR:C	1:B:326:PRO:HD2	2.36	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:96:LYS:HZ3	1:A:573:ARG:HH21	1.63	0.46
1:A:115:ILE:CD1	1:A:117:LYS:HB2	2.46	0.46
1:A:337:ASN:O	1:A:338:ALA:C	2.54	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
3:D:55:VAL:HA	3:D:58:ILE:HD12	1.98	0.46
1:B:254:ALA:C	1:B:256:SER:H	2.18	0.46
1:B:287:LYS:O	1:B:290:VAL:HB	2.16	0.46
1:B:312:ALA:C	1:B:316:LYS:HD3	2.36	0.46
1:B:574:GLN:HA	6:B:873:ADP:C1'	2.46	0.46
1:A:34:SER:HA	1:A:37:ILE:HD12	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:59:PHE:O	3:D:63:GLY:HA3	2.15	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:28:LEU:C	1:A:30:SER:H	2.19	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
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: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
1:A:618:MET:H	1:A:621:LYS:HZ3	1.62	0.46
1:B:104:ALA:O	1:B:105:ALA:C	2.54	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:362:ASP:CG	1:A:368:LEU:HA	2.36	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:28:LEU:C	1:B:30:SER:H	2.19	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
2:F:217:ILE:O	2:F:220:ILE:HB	2.16	0.45
1:A:104:ALA:O	1:A:105:ALA:C	2.54	0.45
1:A:139:VAL:O	1:A:142:PHE:HB3	2.16	0.45
1:A:312:ALA:C	1:A:316:LYS:HD3	2.36	0.45
1:A:590:LEU:H	1:A:590:LEU:CD2	2.26	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:298:ASP:CG	1:B:304:ILE:HG12	2.36	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:254:ALA:C	1:A:256:SER:H	2.18	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:104:GLU:HB3	2:C:105:MET:HE3	1.98	0.45
2:C:242:ILE:O	2:C:249:THR:HG23	2.17	0.45
1:B:337:ASN:O	1:B:338:ALA:C	2.54	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:400:ILE:HB	1:A:404:ASN:CG	2.37	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:HB2	1:B:663:LEU:CD2	2.47	0.45
1:B:249:ALA:O	1:B:412:LEU:HD23	2.15	0.45
1:B:362:ASP:CG	1:B:368:LEU:HA	2.36	0.45
2:F:231:ILE:O	2:F:232:LEU:C	2.54	0.45
2:F:319:TYR:O	2:F:323:VAL:HG23	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:400:ILE:HB	1:B:404:ASN:CG	2.36	0.45
2:F:231:ILE:C	2:F:232:LEU:CD2	2.78	0.45
2:F:334:ASN:C	2:F:335:ILE:HD12	2.37	0.45
2:F:381:GLN:O	2:F:385:LYS:HE2	2.16	0.45
2:F:418:TYR:C	2:F:420:GLY:H	2.20	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:108:GLU:HB2	2:C:112:GLY:N	2.28	0.45
2:C:231:ILE:C	2:C:232:LEU:O	2.52	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
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
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:319:GLY:C	1:A:321:GLU:H	2.19	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:235:GLN:C	2:C:264:LYS:H	2.20	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
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:41:MET:HA	1:B:44:LYS:HZ2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:319:GLY:C	1:B:321:GLU:H	2.19	0.44
1:B:416:THR:O	1:B:417:GLY:O	2.35	0.44
1:B:515:ILE:C	1:B:515:ILE:HD12	2.38	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:515:ILE:C	1:A:515:ILE:HD12	2.38	0.44
2:C:15:ARG:O	2:C:15:ARG:HG3	2.17	0.44
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:103:LEU:O	1:A:104:ALA:C	2.55	0.44
1:A:334:HIS:CG	1:A:335:LEU:N	2.85	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
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
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: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
2:F:231:ILE:C	2:F:232:LEU:O	2.55	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: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:574:GLN:CA	6:A:873:ADP:HI'	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:18:ILE:C	3:D:21:PRO:HD2	2.38	0.44
1:B:172:GLU:O	1:B:176:SER:N	2.50	0.44
2:F:94:LEU:HA	2:F:97:SER:HB2	1.99	0.44
3:G:18:ILE:C	3:G:21:PRO:HD2	2.38	0.44
1:A:121:LEU:HG	1:A:219:TYR:CE2	2.52	0.44
1:A:185:GLU:H	1:A:185:GLU:CD	2.21	0.44
1:A:490:LEU:C	1:A:490:LEU:HD13	2.38	0.44
2:C:381:GLN:O	2:C:385:LYS:HG2	2.17	0.44
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: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:103:LEU:O	1:B:104:ALA:C	2.55	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:412:LEU:H	1:B:432:MET:HE1	1.83	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:184:GLY:C	1:A:186:VAL:H	2.22	0.44
1:A:336:ILE:HG13	1:A:336:ILE:H	1.65	0.44
1:A:346:LYS:C	1:A:348:ASP:N	2.71	0.44
1:A:574:GLN:HA	6:A:873:ADP:C1'	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:HIS:O	1:B:337:ASN:HB2	2.18	0.44
1:B:794:THR:O	1:B:797:MET:HE2	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
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
1:A:794:THR:O	1:A:797:MET:HE2	2.18	0.43
2:C:71:ALA:HB3	2:C:135:VAL:HA	2.00	0.43
2:C:418:TYR:C	2:C:420:GLY:H	2.20	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:346:LYS:C	1:B:348:ASP:N	2.71	0.43
1:B:490:LEU:HD13	1:B:490:LEU:C	2.38	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: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:96:LYS:H	1:B:99:GLU:CD	2.22	0.43
1:B:292:ASP:CB	1:B:313:LYS:HD3	2.42	0.43
1:B:425:GLU:C	1:B:427:VAL:N	2.72	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
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:334:HIS:CG	1:B:335:LEU:N	2.85	0.43
1:B:425:GLU:OE1	1:B:425:GLU:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:155:LYS:HZ1	1:A:209:ARG:CZ	2.31	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
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:185:GLU:H	1:B:185:GLU:CD	2.21	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: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:617:PRO:HB2	1:B:618:MET:HE2	2.01	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:155:LYS:HZ1	1:B:209:ARG:CZ	2.31	0.43
1:B:178:TRP:O	1:B:180:ASP:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:TYR:OH	2:F:253:VAL:HG22	2.18	0.43
1:B:515:ILE:O	1:B:516:VAL:C	2.56	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
2:F:386:VAL:C	2:F:388:VAL:H	2.22	0.43
1:A:3:LEU:C	1:A:5:ASP:N	2.71	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:425:GLU:HA	1:A:425:GLU:OE1	2.18	0.43
1:A:515:ILE:O	1:A:516:VAL:C	2.55	0.43
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:786:PRO:C	1:A:787:ILE:HD12	2.39	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:425:GLU:C	1:A:427:VAL:N	2.72	0.43
1:A:541:GLY:HA3	1:A:542:PRO:HD2	1.78	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: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:323:VAL:O	2:F:324:VAL:C	2.57	0.43
2:F:419:GLU:CA	2:F:422:ILE:HG13	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:585:SER:C	1:A:587:GLU:N	2.71	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: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:596:SER:HA	1:B:599:ILE:CG2	2.49	0.43
1:B:618:MET:H	1:B:621:LYS:HZ3	1.67	0.43
1:B:786:PRO:C	1:B:787:ILE:HD12	2.39	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:639:LYS:O	1:A:640:THR:C	2.57	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
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: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: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:41:MET:HA	1:A:44:LYS:HZ2	1.82	0.42
1:A:78:ASP:C	1:A:80:GLN:H	2.23	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:326:PRO:C	1:A:328:ASN:N	2.72	0.42
1:A:400:ILE:HD12	1:A:402:PHE:HE2	1.82	0.42
1:A:672:LEU:O	1:A:676:PHE:HB3	2.18	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:D:32:VAL:O	3:D:36:ILE:HG13	2.19	0.42
1:B:294:ASP:O	1:B:295:PHE:C	2.57	0.42
1:B:639:LYS:O	1:B:640:THR:C	2.57	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:96:LYS:H	1:A:99:GLU:CD	2.22	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
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:150:ILE:HG13	1:A:155:LYS:NZ	2.33	0.42
1:A:233:ASN:C	1:A:235:VAL:H	2.23	0.42
1:A:294:ASP:O	1:A:295:PHE:C	2.57	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
1:A:585:SER:H	1:A:588:ASP:CG	2.21	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:91:LYS:O	1:B:413:ALA:HA	2.19	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:100:GLY:O	1:A:101:LYS:C	2.58	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: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: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
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:403:GLN:HA	1:B:407:ARG:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:184:GLY:C	1:B:186:VAL:H	2.22	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: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:132:ALA:HA	2:F:164:MET:HE1	2.01	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: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
2:C:386:VAL:C	2:C:388:VAL:H	2.22	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:233:ASN:C	1:B:235:VAL:H	2.23	0.42
1:B:326:PRO:C	1:B:328:ASN:N	2.72	0.42
1:B:585:SER:H	1:B:588:ASP:CG	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:20:TRP:N	3:G:21:PRO:HD2	2.35	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
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: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
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:581:ILE:HG23	1:B:583:PHE:HE1	1.85	0.42
1:B:585:SER:C	1:B:587:GLU:N	2.71	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:527:ILE:C	1:A:527:ILE:HD13	2.40	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:323:VAL:O	2:C:324:VAL:C	2.57	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:100:GLY:O	1:B:101:LYS:C	2.58	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:92:VAL:CG2	1:A:434:VAL:HA	2.50	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
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
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: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: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:457:LYS:O	1:B:460:TYR:HB3	2.21	0.41
1:B:459:LYS:HZ2	1:B:585:SER:N	2.18	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:401:VAL:O	2:C:405:ILE:HG13	2.21	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: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
1:B:753:LEU:O	1:B:754:MET:C	2.59	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:459:LYS:HZ2	1:A:585:SER:N	2.17	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
1:A:52:ASP:O	1:A:54:ASP:N	2.54	0.41
1:A:96:LYS:HZ3	1:A:570:ARG:NH2	2.19	0.41
1:A:171:ILE:HA	1:A:174:ASN:OD1	2.20	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:789:GLU:O	1:A:793:GLU:HG2	2.21	0.41
2:C:125:LEU:CD2	2:C:169:MET:HE1	2.51	0.41
2:C:183:ILE:HG23	2:C:186:GLY:H	1.84	0.41
2:C:326:PHE:C	2:C:328:PRO:HD2	2.41	0.41
2:C:340:GLY:C	2:C:342:ILE:N	2.74	0.41
1:B:78:ASP:C	1:B:80:GLN:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:751:ARG:HA	1:A:751:ARG:CZ	2.51	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
1:A:29:ARG:C	1:A:31:LYS:H	2.24	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
1:A:402:PHE:CG	1:A:403:GLN:N	2.86	0.41
1:A:612:GLN:HB2	1:A:613:PRO:HD3	2.01	0.41
1:A:757:ILE:HD13	1:A:757:ILE:HA	1.94	0.41
2:C:23:LEU:HD12	2:C:181:LYS:HZ1	1.86	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:232:LEU:CB	2:C:266:ASN:C	2.89	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: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:238:TYR:C	1:B:240:ASP:N	2.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:527:ILE:HD13	1:B:527:ILE:C	2.41	0.41
1:B:545:ALA:O	1:B:546:GLU:C	2.59	0.41
1:B:573:ARG:CD	6:B:873:ADP:O1B	2.68	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: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:296:THR:HG1	1:B:306:LEU:HD22	1.85	0.41
1:B:404:ASN:HD22	1:B:404:ASN:HA	1.71	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:305:ILE:HG13	1:A:306:LEU:N	2.36	0.40
1:A:331:LEU:HD12	1:A:331:LEU:N	2.36	0.40
1:A:455:THR:O	1:A:456:GLN:HB2	2.20	0.40
1:A:503:VAL:HG22	1:A:527:ILE:CG2	2.51	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:737:ARG:HA	1:B:740:GLN:CB	2.50	0.40
2:F:81:SER:C	2:F:84:PRO:HD2	2.41	0.40
2:F:345:LEU:O	2:F:346:ARG:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:24:ILE:HG21	1:A:59:GLU:HA	2.03	0.40
1:A:38:ARG:HA	1:A:41:MET:HE3	2.02	0.40
1:A:164:PRO:HB2	1:A:168:ARG:NH2	2.36	0.40
2:C:27:VAL:HG11	2:C:174:LEU:HD22	2.02	0.40
2:C:81:SER:C	2:C:84:PRO:HD2	2.41	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:20:PHE:HB3	2:F:181:LYS:HZ3	1.86	0.40
2:F:391:GLY:O	2:F:395:ALA:HB2	2.21	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
1:A:673:LYS:HZ1	1:A:736:GLN:HG3	1.87	0.40
2:C:307:LEU:HD23	2:C:310:TYR:CE1	2.57	0.40
1:B:29:ARG:C	1:B:31:LYS:H	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:340:LYS:NZ	2:F:251:ARG:HE	2.18	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:778:LEU:HD22	2:F:264:LYS:HG3	2.04	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
4:H:45:ARG:C	4:H:47:LYS:N	2.75	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:666:LYS:HE2	1:A:747:ARG:HD2	2.04	0.40
1:A:689:SER:HB3	1:A:691:LYS:HG2	2.03	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
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:301:ALA:C	2:C:303:GLY:H	2.24	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	6
1	B	814/871 (94%)	511 (63%)	206 (25%)	97 (12%)	0	6
2	C	392/431 (91%)	260 (66%)	80 (20%)	52 (13%)	0	5
2	F	392/431 (91%)	262 (67%)	78 (20%)	52 (13%)	0	5
3	D	54/65 (83%)	41 (76%)	9 (17%)	4 (7%)	1	16
3	G	54/65 (83%)	41 (76%)	9 (17%)	4 (7%)	1	16
4	E	63/76 (83%)	46 (73%)	12 (19%)	5 (8%)	1	14
4	H	63/76 (83%)	46 (73%)	12 (19%)	5 (8%)	1	14
All	All	2646/2886 (92%)	1717 (65%)	613 (23%)	316 (12%)	0	6

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	717/766 (94%)	610 (85%)	107 (15%)	3	17
1	B	717/766 (94%)	610 (85%)	107 (15%)	3	17
2	C	331/356 (93%)	293 (88%)	38 (12%)	5	23
2	F	331/356 (93%)	294 (89%)	37 (11%)	6	24
3	D	47/56 (84%)	44 (94%)	3 (6%)	17	44
3	G	47/56 (84%)	44 (94%)	3 (6%)	17	44
4	E	53/64 (83%)	48 (91%)	5 (9%)	8	30
4	H	53/64 (83%)	48 (91%)	5 (9%)	8	30
All	All	2296/2484 (92%)	1991 (87%)	305 (13%)	4	20

All (305) 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	44	LYS
1	A	51	GLU
1	A	52	ASP
1	A	61	PHE
1	A	63	LEU
1	A	74	MET
1	A	75	ARG

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Mol	Chain	Res	Type
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	155	LYS
1	A	160	VAL
1	A	163	ASN
1	A	173	GLU
1	A	182	PHE
1	A	188	LYS
1	A	190	GLU
1	A	201	GLN
1	A	219	TYR
1	A	231	ARG
1	A	235	VAL
1	A	237	ASP
1	A	240	ASP
1	A	253	GLU
1	A	256	SER
1	A	265	PRO
1	A	274	GLU
1	A	292	ASP
1	A	294	ASP
1	A	298	ASP
1	A	315	GLU
1	A	328	ASN
1	A	332	LEU
1	A	333	TYR
1	A	334	HIS
1	A	342	LEU
1	A	344	LEU
1	A	351	TYR
1	A	374	TYR
1	A	380	GLN
1	A	383	GLU
1	A	391	LYS

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Mol	Chain	Res	Type
1	A	397	TYR
1	A	400	ILE
1	A	402	PHE
1	A	403	GLN
1	A	407	ARG
1	A	409	TYR
1	A	422	GLU
1	A	429	VAL
1	A	444	ILE
1	A	445	ARG
1	A	457	LYS
1	A	459	LYS
1	A	460	TYR
1	A	479	VAL
1	A	482	THR
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	635	PHE
1	A	641	LEU
1	A	643	GLU
1	A	646	ASP
1	A	668	TYR
1	A	676	PHE
1	A	678	ASP
1	A	683	ARG
1	A	687	PHE
1	A	689	SER
1	A	692	ASN
1	A	700	ASN

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Mol	Chain	Res	Type
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	774	GLU
1	A	777	GLN
1	A	797	MET
1	A	798	PHE
1	A	801	MET
1	A	804	ARG
1	A	809	ILE
2	C	14	LEU
2	C	63	PHE
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	113	ARG
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	170	PHE
2	C	171	LEU
2	C	177	ARG
2	C	181	LYS
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	244	TYR
2	C	249	THR
2	C	275	PHE

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Mol	Chain	Res	Type
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
3	D	25	GLU
3	D	30	PHE
3	D	62	LEU
4	E	21	GLN
4	E	40	HIS
4	E	46	ARG
4	E	63	PHE
4	E	72	PHE
1	B	7	ASN
1	B	22	ASN
1	B	39	LEU
1	B	44	LYS
1	B	51	GLU
1	B	52	ASP
1	B	61	PHE
1	B	63	LEU
1	B	74	MET
1	B	75	ARG
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	155	LYS
1	B	160	VAL
1	B	163	ASN
1	B	173	GLU
1	B	182	PHE

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Mol	Chain	Res	Type
1	B	188	LYS
1	B	190	GLU
1	B	201	GLN
1	B	219	TYR
1	B	231	ARG
1	B	235	VAL
1	B	237	ASP
1	B	240	ASP
1	B	253	GLU
1	B	256	SER
1	B	265	PRO
1	B	274	GLU
1	B	292	ASP
1	B	294	ASP
1	B	298	ASP
1	B	315	GLU
1	B	328	ASN
1	B	332	LEU
1	B	333	TYR
1	B	334	HIS
1	B	342	LEU
1	B	344	LEU
1	B	351	TYR
1	B	374	TYR
1	B	380	GLN
1	B	383	GLU
1	B	391	LYS
1	B	397	TYR
1	B	400	ILE
1	B	402	PHE
1	B	403	GLN
1	B	407	ARG
1	B	409	TYR
1	B	422	GLU
1	B	429	VAL
1	B	444	ILE
1	B	445	ARG
1	B	457	LYS
1	B	459	LYS
1	B	460	TYR
1	B	479	VAL
1	B	482	THR

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Mol	Chain	Res	Type
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
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	635	PHE
1	B	641	LEU
1	B	643	GLU
1	B	646	ASP
1	B	668	TYR
1	B	676	PHE
1	B	678	ASP
1	B	683	ARG
1	B	687	PHE
1	B	689	SER
1	B	692	ASN
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	774	GLU
1	B	777	GLN
1	B	797	MET
1	B	798	PHE
1	B	801	MET
1	B	804	ARG
1	B	809	ILE
2	F	14	LEU
2	F	63	PHE

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Mol	Chain	Res	Type
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	113	ARG
2	F	133	PHE
2	F	134	PHE
2	F	141	ARG
2	F	143	ASN
2	F	154	LEU
2	F	156	PHE
2	F	170	PHE
2	F	171	LEU
2	F	177	ARG
2	F	181	LYS
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	244	TYR
2	F	249	THR
2	F	275	PHE
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
3	G	25	GLU
3	G	30	PHE
3	G	62	LEU
4	H	21	GLN
4	H	40	HIS
4	H	46	ARG
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 (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	80	GLN
1	A	112	ASN
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	475	GLN
1	A	509	HIS
1	A	565	ASN
1	A	598	GLN
1	A	612	GLN
1	A	692	ASN
1	A	729	ASN
1	A	740	GLN
1	A	777	GLN
2	C	93	GLN
2	C	143	ASN
2	C	353	GLN
2	C	360	ASN
2	C	407	GLN
1	B	22	ASN
1	B	80	GLN
1	B	112	ASN
1	B	163	ASN
1	B	183	ASN
1	B	193	ASN
1	B	222	ASN
1	B	223	ASN
1	B	328	ASN
1	B	337	ASN
1	B	403	GLN
1	B	475	GLN

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Mol	Chain	Res	Type
1	B	509	HIS
1	B	565	ASN
1	B	598	GLN
1	B	612	GLN
1	B	692	ASN
1	B	729	ASN
1	B	740	GLN
1	B	777	GLN
2	F	93	GLN
2	F	143	ASN
2	F	353	GLN
2	F	360	ASN
2	F	407	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	$\# Z > 2$
7	BEF	B	874	6	0,3,3	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	BEF	A	874	6	0,3,3	-	-	-		
6	ADP	B	873	7	24,29,29	1.59	3 (12%)	29,45,45	1.47	4 (13%)
6	ADP	A	873	7	24,29,29	1.59	3 (12%)	29,45,45	1.46	4 (13%)

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	-	0/12/32/32	0/3/3/3
6	ADP	A	873	7	-	0/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	873	ADP	C8-N7	5.58	1.44	1.34
6	B	873	ADP	C8-N7	5.58	1.44	1.34
6	A	873	ADP	PB-O1B	2.27	1.57	1.50
6	B	873	ADP	PB-O1B	2.26	1.57	1.50
6	B	873	ADP	C2-N3	2.20	1.35	1.32
6	A	873	ADP	C2-N3	2.19	1.35	1.32

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	873	ADP	N3-C2-N1	-4.21	122.11	128.68
6	A	873	ADP	N3-C2-N1	-4.19	122.13	128.68
6	B	873	ADP	C1'-N9-C4	-2.68	121.94	126.64
6	A	873	ADP	C1'-N9-C4	-2.67	121.96	126.64
6	A	873	ADP	O3B-PB-O2B	2.50	117.19	107.64
6	B	873	ADP	O3B-PB-O2B	2.49	117.15	107.64
6	B	873	ADP	O3A-PB-O1B	-2.16	99.21	111.19
6	A	873	ADP	O3A-PB-O1B	-2.16	99.21	111.19

There are no chirality outliers.

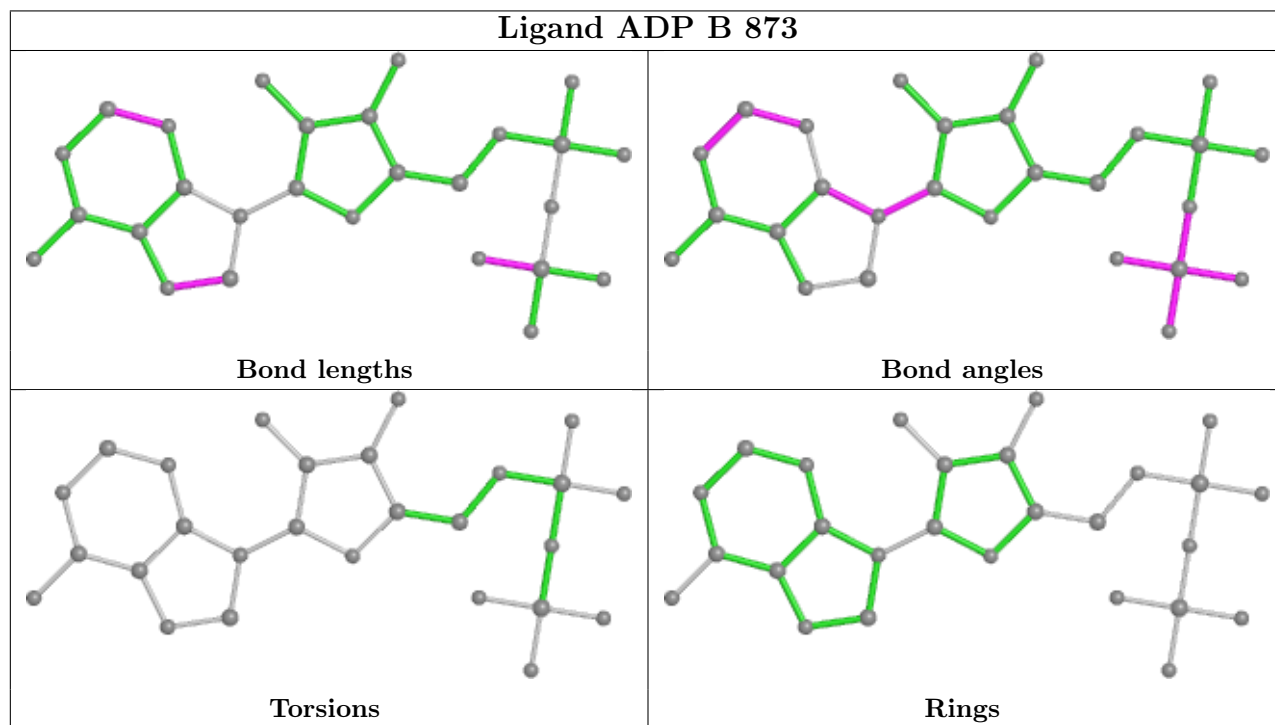
There are no torsion outliers.

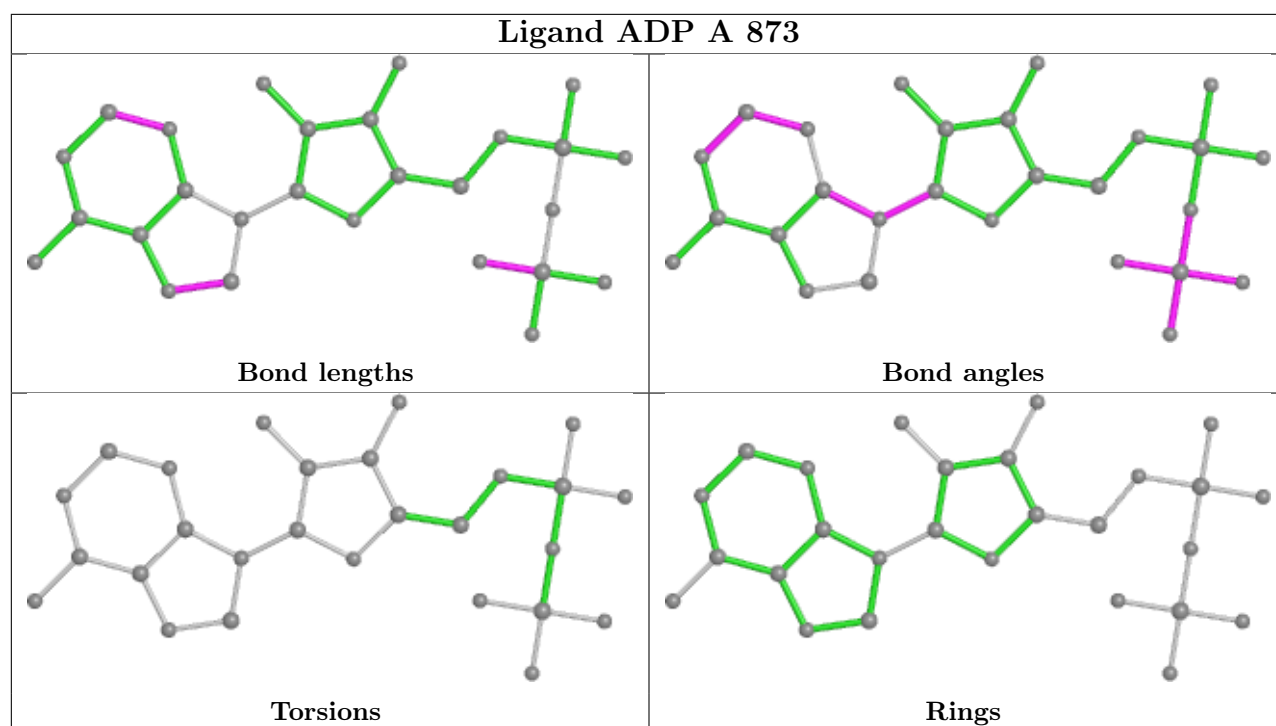
There are no ring outliers.

4 monomers are involved in 87 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	874	BEF	5	0
7	A	874	BEF	4	0
6	B	873	ADP	38	0
6	A	873	ADP	40	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	816/871 (93%)	-0.49	5 (0%) 89 84	108, 306, 457, 500	0
1	B	816/871 (93%)	-0.45	10 (1%) 79 70	108, 306, 457, 500	0
2	C	396/431 (91%)	-0.13	15 (3%) 40 32	223, 429, 500, 500	0
2	F	396/431 (91%)	-0.18	11 (2%) 53 43	223, 429, 500, 500	0
3	D	56/65 (86%)	-0.43	0 100 100	322, 414, 500, 500	0
3	G	56/65 (86%)	-0.43	2 (3%) 42 35	322, 414, 500, 500	0
4	E	65/76 (85%)	-0.05	2 (3%) 49 39	326, 444, 490, 500	0
4	H	65/76 (85%)	-0.09	2 (3%) 49 39	326, 444, 490, 500	0
All	All	2666/2886 (92%)	-0.36	47 (1%) 68 59	108, 365, 489, 500	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	162	LYS	5.7
2	C	69	GLY	5.4
1	A	98	GLY	5.2
1	B	572	GLY	5.0
2	C	197	ALA	4.6
3	G	65	GLY	4.5
2	C	387	ASN	4.4
2	C	70	GLY	4.3
1	B	693	TRP	3.9
4	E	73	VAL	3.9
2	C	290	THR	3.5
1	B	99	GLU	3.5
1	B	98	GLY	3.5
2	F	287	ALA	3.5
2	C	343	PRO	3.3
2	F	154	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
4	E	72	PHE	3.0
1	B	163	ASN	3.0
1	B	273	LYS	3.0
2	C	244	TYR	2.9
1	A	183	ASN	2.9
1	A	99	GLU	2.9
1	A	609	GLU	2.8
2	F	387	ASN	2.8
1	B	694	ASP	2.8
2	C	74	ARG	2.6
2	C	153	VAL	2.6
2	C	291	ASN	2.6
1	B	712	LEU	2.6
2	C	298	LEU	2.5
3	G	64	ILE	2.5
2	C	286	ILE	2.4
4	H	69	VAL	2.4
2	F	109	GLY	2.4
2	F	286	ILE	2.4
2	C	243	GLN	2.4
2	F	203	ILE	2.4
4	H	73	VAL	2.3
2	F	153	VAL	2.3
1	B	161	TRP	2.3
2	C	256	GLY	2.2
2	F	288	SER	2.2
2	F	36	VAL	2.1
2	C	154	LEU	2.1
1	A	574	GLN	2.1
2	F	62	SER	2.1
2	F	204	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

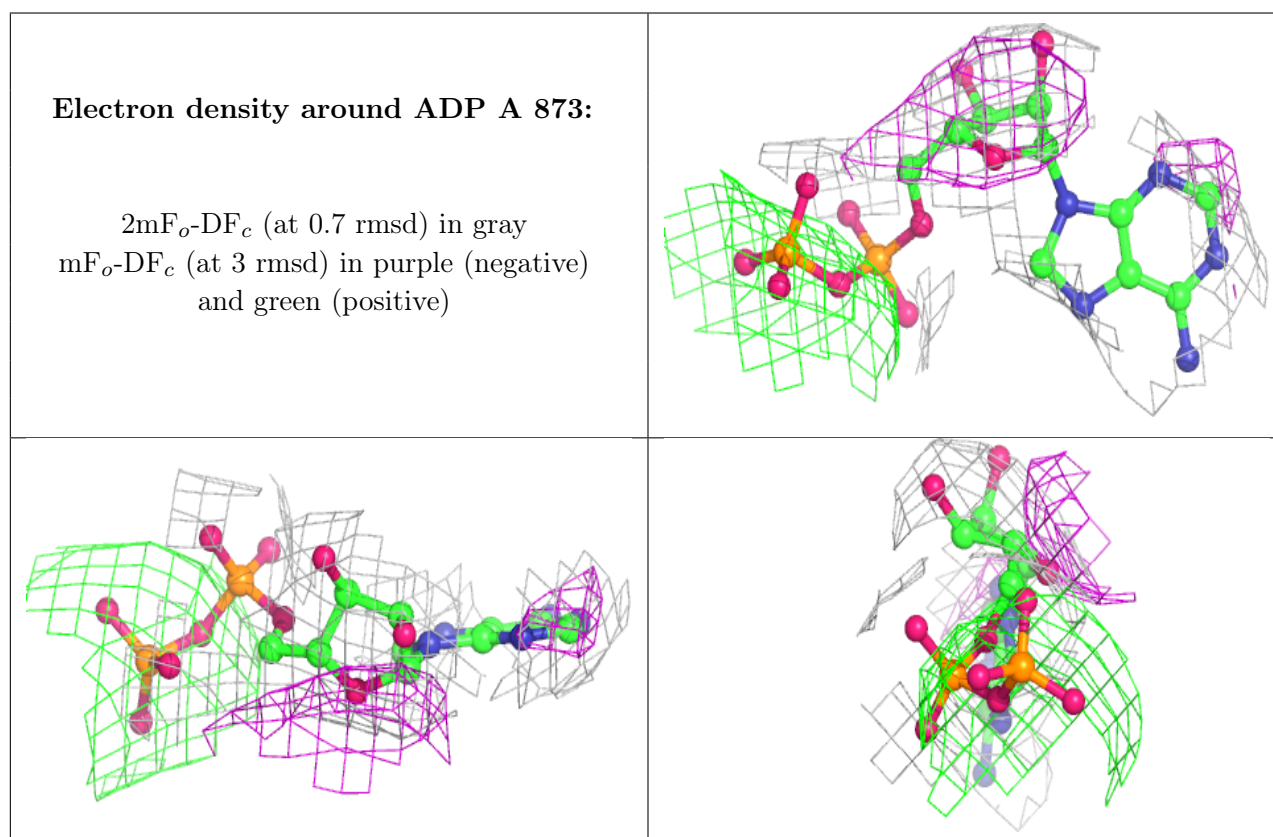
There are no monosaccharides in this entry.

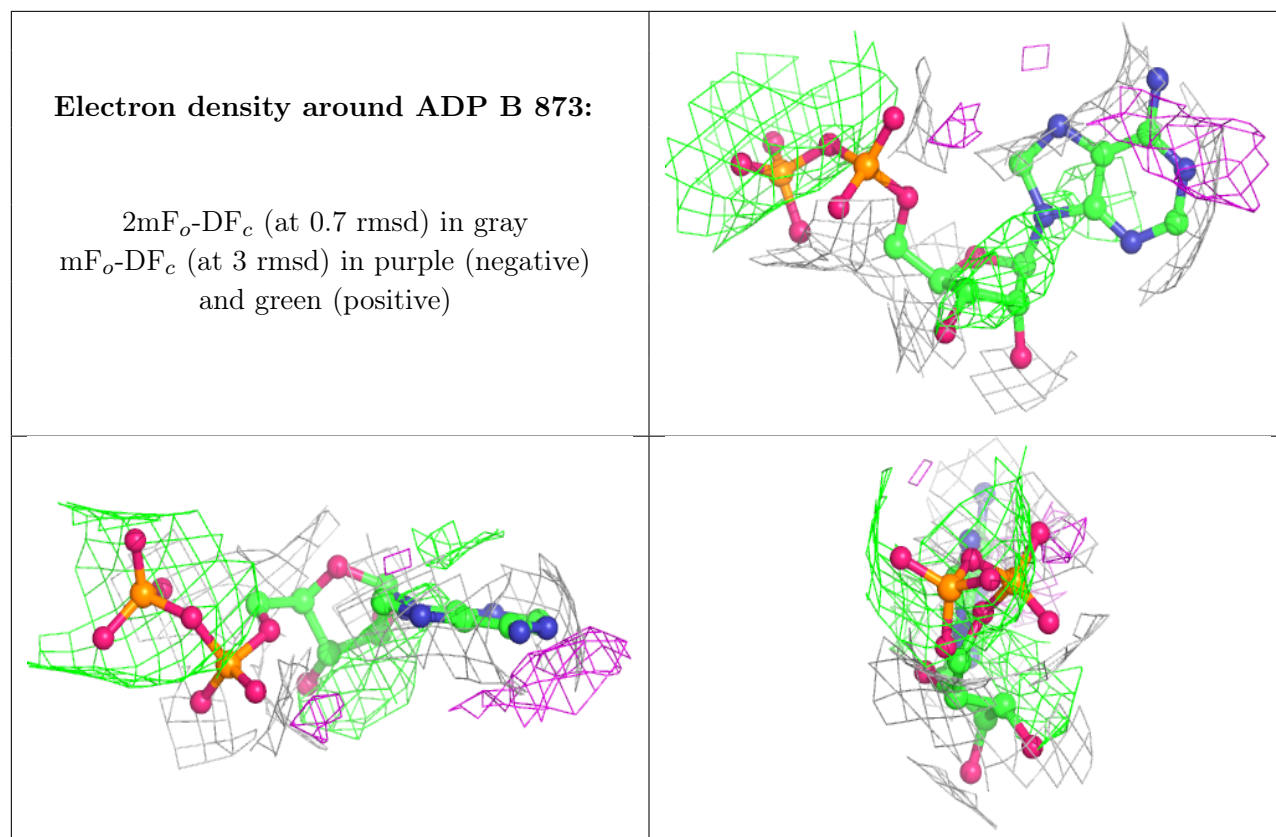
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	BEF	A	874	4/4	0.64	0.30	112,134,154,241	0
6	ADP	A	873	27/27	0.69	0.34	134,186,192,399	0
6	ADP	B	873	27/27	0.79	0.27	134,186,192,399	0
7	BEF	B	874	4/4	0.84	0.22	112,134,154,241	0
5	MG	A	872	1/1	0.90	0.29	130,130,130,130	0
5	MG	B	872	1/1	0.90	0.18	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.