



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:25 PM GMT

PDB ID : 3ML6
Title : a complex between Dishevelled2 and clathrin adaptor AP-2
Authors : Yu, A.; Xing, Y.; Harrison, S.C.; Kirchhausen, T.L.
Deposited on : 2010-04-16
Resolution : 3.50 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

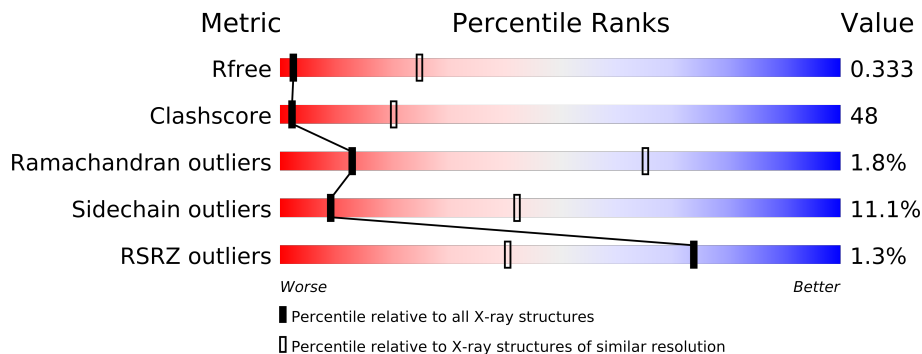
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.50 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}	66092	1243 (3.70-3.30)
Clashscore	79885	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)
RSRZ outliers	66119	1243 (3.70-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	385	
1	B	385	
1	C	385	
1	D	385	
1	E	385	
1	F	385	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 16319 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Chimeric complex between protein Dishevelled2 homolog dvl-2 and clathrin adaptor AP-2 complex subunit mu.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	351	Total	C	N	O	S	0	0	0
			2787	1790	480	498	19			
1	B	339	Total	C	N	O	S	0	0	0
			2695	1732	466	478	19			
1	C	350	Total	C	N	O	S	0	0	0
			2780	1785	479	497	19			
1	D	336	Total	C	N	O	S	0	0	0
			2668	1716	460	473	19			
1	E	338	Total	C	N	O	S	0	0	0
			2686	1725	463	479	19			
1	F	340	Total	C	N	O	S	0	0	0
			2703	1736	467	481	19			

There are 150 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	415	GLY	-	EXPRESSION TAG	UNP Q60838
A	416	ALA	-	EXPRESSION TAG	UNP Q60838
A	1147	GLY	-	LINKER	UNP P84092
A	1148	PRO	-	LINKER	UNP P84092
A	1149	ARG	-	LINKER	UNP P84092
A	1150	PRO	-	LINKER	UNP P84092
A	1151	TYR	-	LINKER	UNP P84092
A	1152	SER	-	LINKER	UNP P84092
A	1153	PRO	-	LINKER	UNP P84092
A	1154	GLN	-	LINKER	UNP P84092
A	1155	PRO	-	LINKER	UNP P84092
A	1156	PRO	-	LINKER	UNP P84092
A	1157	PRO	-	LINKER	UNP P84092
A	1158	TYR	-	LINKER	UNP P84092
A	1159	HIS	-	LINKER	UNP P84092
A	1160	GLU	-	LINKER	UNP P84092

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1161	LEU	-	LINKER	UNP P84092
A	1162	GLU	-	LINKER	UNP P84092
A	1163	PHE	-	LINKER	UNP P84092
A	1164	GLY	-	LINKER	UNP P84092
A	1165	GLY	-	LINKER	UNP P84092
A	1166	SER	-	LINKER	UNP P84092
A	1167	GLY	-	LINKER	UNP P84092
A	1168	GLY	-	LINKER	UNP P84092
A	1169	SER	-	LINKER	UNP P84092
B	415	GLY	-	EXPRESSION TAG	UNP Q60838
B	416	ALA	-	EXPRESSION TAG	UNP Q60838
B	1147	GLY	-	LINKER	UNP P84092
B	1148	PRO	-	LINKER	UNP P84092
B	1149	ARG	-	LINKER	UNP P84092
B	1150	PRO	-	LINKER	UNP P84092
B	1151	TYR	-	LINKER	UNP P84092
B	1152	SER	-	LINKER	UNP P84092
B	1153	PRO	-	LINKER	UNP P84092
B	1154	GLN	-	LINKER	UNP P84092
B	1155	PRO	-	LINKER	UNP P84092
B	1156	PRO	-	LINKER	UNP P84092
B	1157	PRO	-	LINKER	UNP P84092
B	1158	TYR	-	LINKER	UNP P84092
B	1159	HIS	-	LINKER	UNP P84092
B	1160	GLU	-	LINKER	UNP P84092
B	1161	LEU	-	LINKER	UNP P84092
B	1162	GLU	-	LINKER	UNP P84092
B	1163	PHE	-	LINKER	UNP P84092
B	1164	GLY	-	LINKER	UNP P84092
B	1165	GLY	-	LINKER	UNP P84092
B	1166	SER	-	LINKER	UNP P84092
B	1167	GLY	-	LINKER	UNP P84092
B	1168	GLY	-	LINKER	UNP P84092
B	1169	SER	-	LINKER	UNP P84092
C	415	GLY	-	EXPRESSION TAG	UNP Q60838
C	416	ALA	-	EXPRESSION TAG	UNP Q60838
C	1147	GLY	-	LINKER	UNP P84092
C	1148	PRO	-	LINKER	UNP P84092
C	1149	ARG	-	LINKER	UNP P84092
C	1150	PRO	-	LINKER	UNP P84092
C	1151	TYR	-	LINKER	UNP P84092
C	1152	SER	-	LINKER	UNP P84092

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1153	PRO	-	LINKER	UNP P84092
C	1154	GLN	-	LINKER	UNP P84092
C	1155	PRO	-	LINKER	UNP P84092
C	1156	PRO	-	LINKER	UNP P84092
C	1157	PRO	-	LINKER	UNP P84092
C	1158	TYR	-	LINKER	UNP P84092
C	1159	HIS	-	LINKER	UNP P84092
C	1160	GLU	-	LINKER	UNP P84092
C	1161	LEU	-	LINKER	UNP P84092
C	1162	GLU	-	LINKER	UNP P84092
C	1163	PHE	-	LINKER	UNP P84092
C	1164	GLY	-	LINKER	UNP P84092
C	1165	GLY	-	LINKER	UNP P84092
C	1166	SER	-	LINKER	UNP P84092
C	1167	GLY	-	LINKER	UNP P84092
C	1168	GLY	-	LINKER	UNP P84092
C	1169	SER	-	LINKER	UNP P84092
D	415	GLY	-	EXPRESSION TAG	UNP Q60838
D	416	ALA	-	EXPRESSION TAG	UNP Q60838
D	1147	GLY	-	LINKER	UNP P84092
D	1148	PRO	-	LINKER	UNP P84092
D	1149	ARG	-	LINKER	UNP P84092
D	1150	PRO	-	LINKER	UNP P84092
D	1151	TYR	-	LINKER	UNP P84092
D	1152	SER	-	LINKER	UNP P84092
D	1153	PRO	-	LINKER	UNP P84092
D	1154	GLN	-	LINKER	UNP P84092
D	1155	PRO	-	LINKER	UNP P84092
D	1156	PRO	-	LINKER	UNP P84092
D	1157	PRO	-	LINKER	UNP P84092
D	1158	TYR	-	LINKER	UNP P84092
D	1159	HIS	-	LINKER	UNP P84092
D	1160	GLU	-	LINKER	UNP P84092
D	1161	LEU	-	LINKER	UNP P84092
D	1162	GLU	-	LINKER	UNP P84092
D	1163	PHE	-	LINKER	UNP P84092
D	1164	GLY	-	LINKER	UNP P84092
D	1165	GLY	-	LINKER	UNP P84092
D	1166	SER	-	LINKER	UNP P84092
D	1167	GLY	-	LINKER	UNP P84092
D	1168	GLY	-	LINKER	UNP P84092
D	1169	SER	-	LINKER	UNP P84092

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Chain	Residue	Modelled	Actual	Comment	Reference
E	415	GLY	-	EXPRESSION TAG	UNP Q60838
E	416	ALA	-	EXPRESSION TAG	UNP Q60838
E	1147	GLY	-	LINKER	UNP P84092
E	1148	PRO	-	LINKER	UNP P84092
E	1149	ARG	-	LINKER	UNP P84092
E	1150	PRO	-	LINKER	UNP P84092
E	1151	TYR	-	LINKER	UNP P84092
E	1152	SER	-	LINKER	UNP P84092
E	1153	PRO	-	LINKER	UNP P84092
E	1154	GLN	-	LINKER	UNP P84092
E	1155	PRO	-	LINKER	UNP P84092
E	1156	PRO	-	LINKER	UNP P84092
E	1157	PRO	-	LINKER	UNP P84092
E	1158	TYR	-	LINKER	UNP P84092
E	1159	HIS	-	LINKER	UNP P84092
E	1160	GLU	-	LINKER	UNP P84092
E	1161	LEU	-	LINKER	UNP P84092
E	1162	GLU	-	LINKER	UNP P84092
E	1163	PHE	-	LINKER	UNP P84092
E	1164	GLY	-	LINKER	UNP P84092
E	1165	GLY	-	LINKER	UNP P84092
E	1166	SER	-	LINKER	UNP P84092
E	1167	GLY	-	LINKER	UNP P84092
E	1168	GLY	-	LINKER	UNP P84092
E	1169	SER	-	LINKER	UNP P84092
F	415	GLY	-	EXPRESSION TAG	UNP Q60838
F	416	ALA	-	EXPRESSION TAG	UNP Q60838
F	1147	GLY	-	LINKER	UNP P84092
F	1148	PRO	-	LINKER	UNP P84092
F	1149	ARG	-	LINKER	UNP P84092
F	1150	PRO	-	LINKER	UNP P84092
F	1151	TYR	-	LINKER	UNP P84092
F	1152	SER	-	LINKER	UNP P84092
F	1153	PRO	-	LINKER	UNP P84092
F	1154	GLN	-	LINKER	UNP P84092
F	1155	PRO	-	LINKER	UNP P84092
F	1156	PRO	-	LINKER	UNP P84092
F	1157	PRO	-	LINKER	UNP P84092
F	1158	TYR	-	LINKER	UNP P84092
F	1159	HIS	-	LINKER	UNP P84092
F	1160	GLU	-	LINKER	UNP P84092
F	1161	LEU	-	LINKER	UNP P84092

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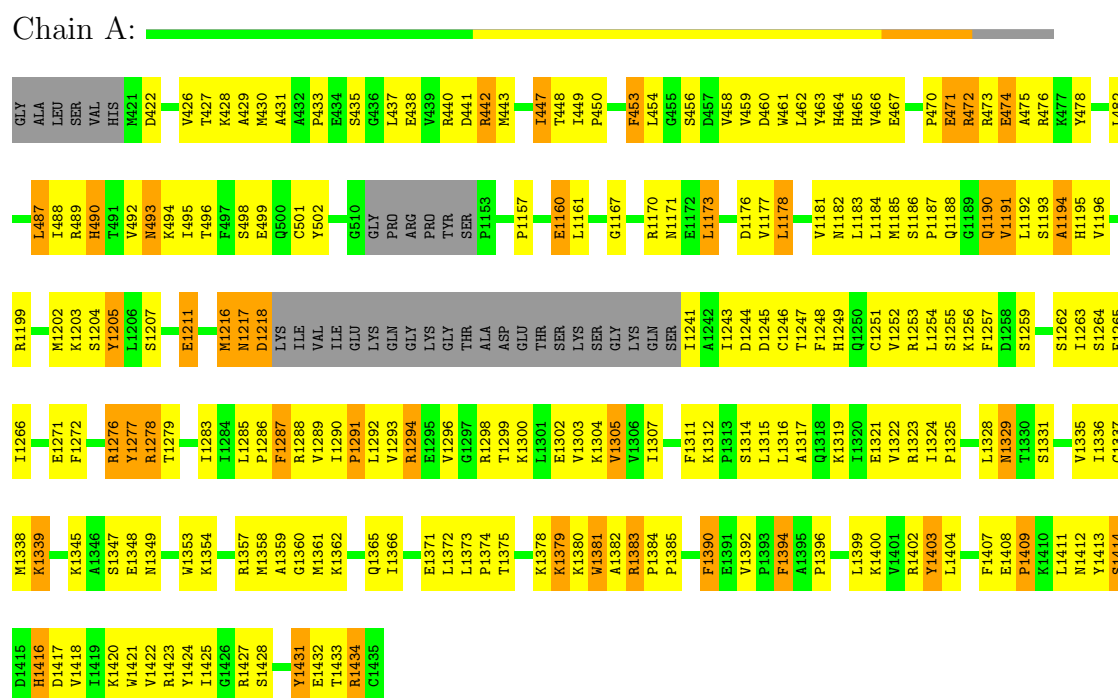
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Chain	Residue	Modelled	Actual	Comment	Reference
F	1162	GLU	-	LINKER	UNP P84092
F	1163	PHE	-	LINKER	UNP P84092
F	1164	GLY	-	LINKER	UNP P84092
F	1165	GLY	-	LINKER	UNP P84092
F	1166	SER	-	LINKER	UNP P84092
F	1167	GLY	-	LINKER	UNP P84092
F	1168	GLY	-	LINKER	UNP P84092
F	1169	SER	-	LINKER	UNP P84092

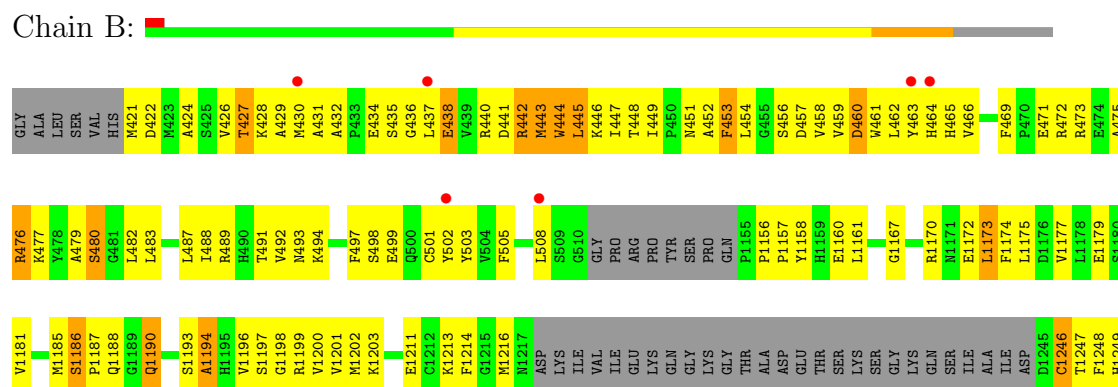
3 Residue-property plots

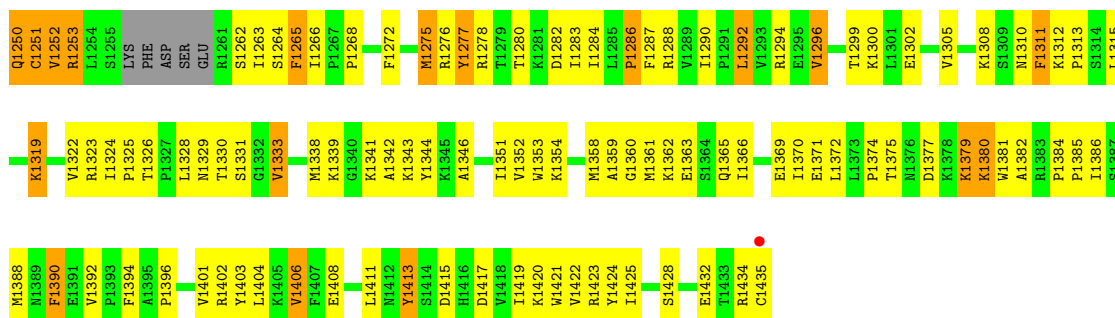
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Chimeric complex between protein Dishevelled2 homolog dvl-2 and clathrin adaptor AP-2 complex subunit mu



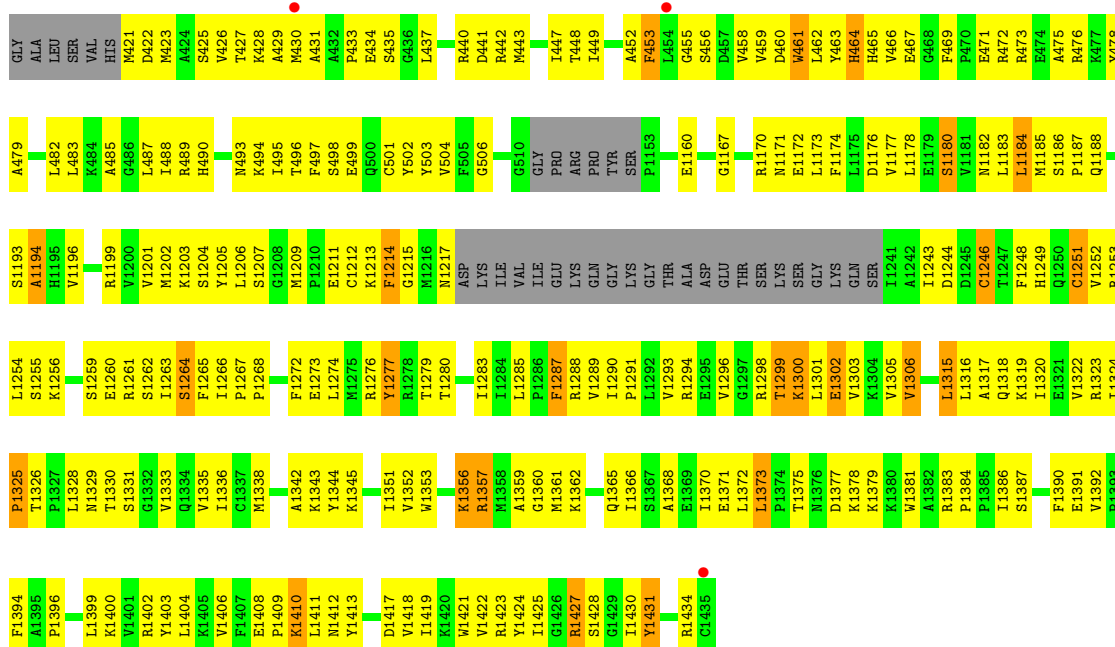
- Molecule 1: Chimeric complex between protein Dishevelled2 homolog dvl-2 and clathrin adaptor AP-2 complex subunit mu





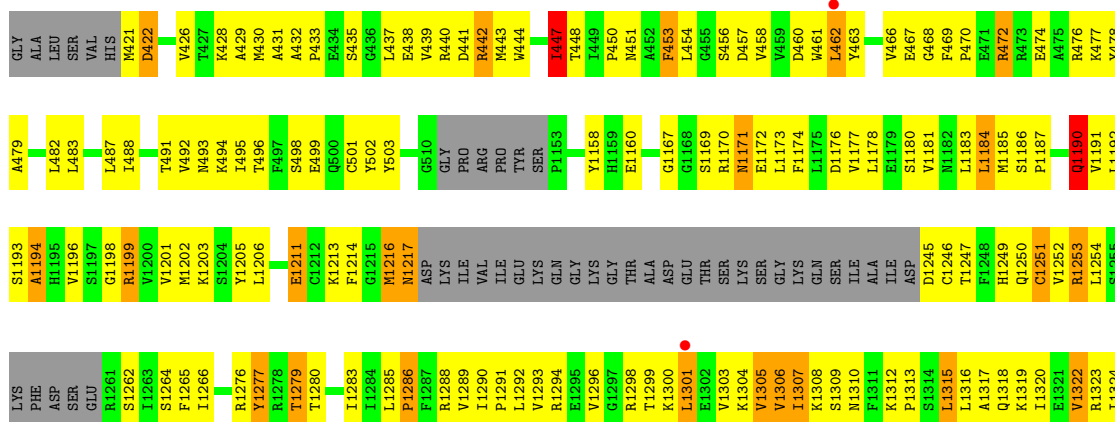
• Molecule 1: Chimeric complex between protein Dishevelled2 homolog dvl-2 and clathrin adaptor AP-2 complex subunit mu

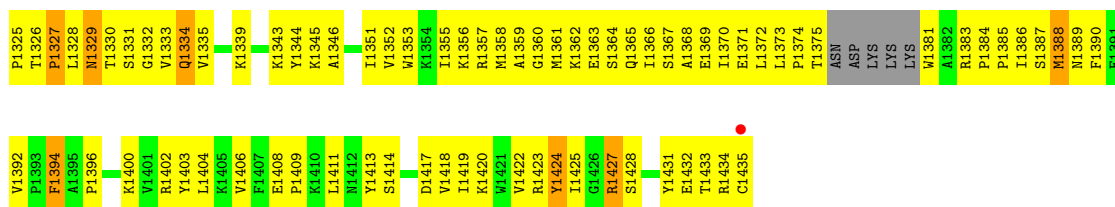
Chain C:



• Molecule 1: Chimeric complex between protein Dishevelled2 homolog dvl-2 and clathrin adaptor AP-2 complex subunit mu

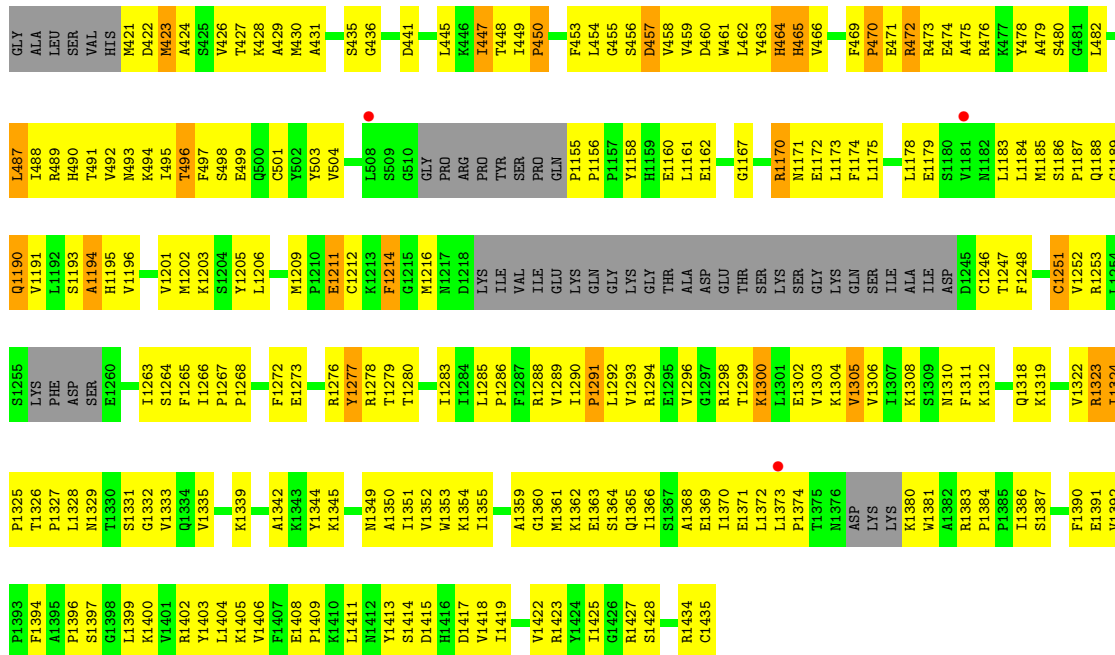
Chain D:





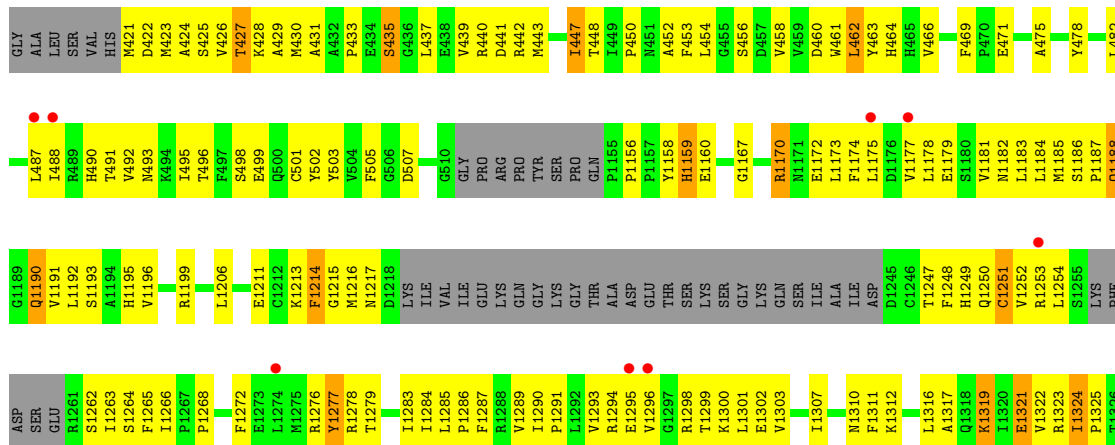
• Molecule 1: Chimeric complex between protein Dishevelled2 homolog dvl-2 and clathrin adaptor AP-2 complex subunit mu

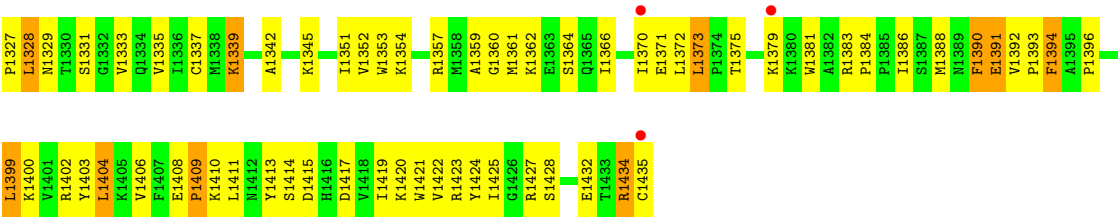
Chain E:



• Molecule 1: Chimeric complex between protein Dishevelled2 homolog dvl-2 and clathrin adaptor AP-2 complex subunit mu

Chain F:





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	292.37Å 98.14Å 171.32Å 90.00° 121.97° 90.00°	Depositor
Resolution (Å)	49.07 – 3.50 49.07 – 3.50	Depositor EDS
% Data completeness (in resolution range)	98.3 (49.07-3.50) 98.1 (49.07-3.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 3.48Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.308 , 0.335 0.308 , 0.333	Depositor DCC
R_{free} test set	2576 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	107.5	Xtriage
Anisotropy	0.646	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 66.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 51407 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	16319	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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	0.53	0/2851	0.67	0/3845
1	B	0.50	0/2756	0.66	0/3714
1	C	0.50	0/2844	0.69	2/3835 (0.1%)
1	D	0.53	1/2729 (0.0%)	0.69	2/3680 (0.1%)
1	E	0.52	0/2746	0.68	1/3701 (0.0%)
1	F	0.50	0/2764	0.67	1/3725 (0.0%)
All	All	0.51	1/16690 (0.0%)	0.68	6/22500 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	421	MET	CG-SD	5.74	1.96	1.81

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1184	LEU	CA-CB-CG	8.40	134.62	115.30
1	C	1373	LEU	CA-CB-CG	-6.66	99.99	115.30
1	F	1373	LEU	CA-CB-CG	5.83	128.72	115.30
1	C	461	TRP	O-C-N	-5.75	113.50	122.70
1	E	1170	ARG	CA-C-O	-5.20	109.17	120.10
1	D	421	MET	CB-CG-SD	5.05	127.55	112.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2787	0	2835	277	0
1	B	2695	0	2751	260	0
1	C	2780	0	2826	279	0
1	D	2668	0	2716	272	0
1	E	2686	0	2730	264	0
1	F	2703	0	2755	278	0
All	All	16319	0	16613	1588	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 48.

All (1588) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1244:ASP:OD1	1:A:1279:THR:HA	1.24	1.37
1:C:462:LEU:O	1:C:466:VAL:HB	1.22	1.28
1:C:458:VAL:O	1:C:462:LEU:HG	1.28	1.24
1:C:462:LEU:O	1:C:466:VAL:CB	1.94	1.15
1:A:462:LEU:O	1:A:466:VAL:HB	1.43	1.14
1:C:1256:LYS:HG3	1:C:1259:SER:HB2	1.17	1.10
1:D:1293:VAL:HG22	1:D:1303:VAL:HG22	1.25	1.10
1:A:1217:ASN:HD21	1:A:1400:LYS:HB2	1.04	1.10
1:A:1294:ARG:HB3	1:A:1294:ARG:HH11	1.15	1.05
1:A:442:ARG:CG	1:A:442:ARG:HH11	1.70	1.04
1:C:1183:LEU:HD12	1:C:1184:LEU:H	1.22	1.04
1:F:462:LEU:O	1:F:466:VAL:HB	1.56	1.03
1:C:459:VAL:HA	1:C:462:LEU:HD12	1.41	1.03
1:A:1196:VAL:HG23	1:A:1283:ILE:HD13	1.36	1.01
1:F:1323:ARG:HH12	1:F:1352:VAL:HG22	1.26	1.00
1:C:1406:VAL:HG11	1:C:1418:VAL:HG21	1.41	1.00
1:C:1253:ARG:HH12	1:C:1266:ILE:HD11	1.27	1.00
1:A:1328:LEU:HB2	1:A:1381:TRP:HH2	1.21	1.00
1:C:1244:ASP:OD2	1:C:1280:THR:HG23	1.62	0.99
1:A:442:ARG:HG3	1:A:442:ARG:HH11	1.23	0.99
1:A:1253:ARG:HD2	1:A:1264:SER:OG	1.63	0.99
1:D:1324:ILE:HD12	1:D:1386:ILE:HG12	1.43	0.98
1:D:1183:LEU:HD21	1:D:1285:LEU:HD23	1.44	0.98
1:A:1184:LEU:HD22	1:A:1192:LEU:HD12	1.47	0.96
1:C:440:ARG:HG2	1:C:442:ARG:HH11	1.32	0.95
1:E:1293:VAL:HG12	1:E:1303:VAL:HG13	1.48	0.95
1:E:462:LEU:O	1:E:466:VAL:HB	1.65	0.95

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:476:ARG:HB3	1:B:476:ARG:HH21	1.29	0.95
1:A:1182:ASN:HD22	1:A:1195:HIS:CE1	1.85	0.94
1:D:1196:VAL:CG2	1:D:1279:THR:HG22	1.97	0.94
1:C:1243:ILE:HA	1:C:1279:THR:HG22	1.47	0.94
1:F:1183:LEU:HD12	1:F:1184:LEU:H	1.28	0.93
1:B:464:HIS:ND1	1:B:465:HIS:NE2	2.14	0.93
1:A:1183:LEU:HD11	1:A:1191:VAL:HG22	1.50	0.93
1:E:1187:PRO:HD3	1:E:1434:ARG:HD3	1.50	0.93
1:B:491:THR:HG22	1:B:492:VAL:HG13	1.49	0.93
1:D:1333:VAL:HG22	1:D:1370:ILE:HG22	1.50	0.93
1:B:464:HIS:ND1	1:B:465:HIS:CD2	2.37	0.92
1:D:1217:ASN:HD21	1:D:1400:LYS:N	1.68	0.92
1:A:1244:ASP:OD1	1:A:1279:THR:CA	2.16	0.91
1:C:1256:LYS:CG	1:C:1259:SER:HB2	2.00	0.91
1:C:458:VAL:O	1:C:462:LEU:CG	2.19	0.91
1:A:1294:ARG:HB3	1:A:1294:ARG:NH1	1.85	0.91
1:E:1298:ARG:NH1	1:E:1374:PRO:HG3	1.87	0.90
1:D:1253:ARG:HB2	1:D:1253:ARG:HH21	1.36	0.90
1:B:1253:ARG:HG3	1:B:1253:ARG:HH21	1.36	0.90
1:F:1390:PHE:CE1	1:F:1428:SER:HB3	2.07	0.90
1:D:1356:LYS:HD3	1:D:1357:ARG:HH12	1.34	0.90
1:F:1408:GLU:HG2	1:F:1411:LEU:HB2	1.54	0.90
1:C:1174:PHE:HD2	1:C:1203:LYS:HD2	1.34	0.90
1:D:1325:PRO:HG3	1:D:1384:PRO:O	1.70	0.90
1:D:1180:SER:HB2	1:D:1427:ARG:HE	1.36	0.90
1:C:1246:CYS:HB2	1:C:1276:ARG:O	1.73	0.89
1:D:1290:ILE:HB	1:D:1306:VAL:HG12	1.55	0.89
1:F:1187:PRO:HD3	1:F:1434:ARG:HB2	1.53	0.89
1:E:1339:LYS:HZ1	1:E:1364:SER:HA	1.35	0.89
1:A:462:LEU:HD11	1:A:478:TYR:HD2	1.39	0.88
1:E:458:VAL:O	1:E:462:LEU:HB2	1.72	0.88
1:A:1289:VAL:HB	1:A:1433:THR:HG21	1.55	0.88
1:B:1312:LYS:HB2	1:B:1315:LEU:HD13	1.55	0.88
1:F:1294:ARG:NH2	1:F:1302:GLU:HG3	1.87	0.88
1:A:441:ASP:OD1	1:A:450:PRO:HA	1.73	0.88
1:E:1408:GLU:HG2	1:E:1411:LEU:HB2	1.56	0.87
1:A:1217:ASN:ND2	1:A:1400:LYS:HB2	1.90	0.87
1:C:479:ALA:HA	1:C:482:LEU:HD12	1.55	0.87
1:E:1327:PRO:HA	1:E:1381:TRP:CE2	2.10	0.87
1:B:1305:VAL:HG21	1:B:1324:ILE:HD11	1.57	0.87
1:B:462:LEU:O	1:B:466:VAL:HB	1.75	0.86
1:B:1161:LEU:HB2	1:F:1422:VAL:HG23	1.56	0.86

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1378:LYS:HE3	1:A:1381:TRP:CZ2	2.11	0.86
1:E:462:LEU:HD22	1:E:475:ALA:O	1.74	0.86
1:E:1186:SER:HA	1:E:1434:ARG:HD2	1.57	0.86
1:F:1217:ASN:HD21	1:F:1400:LYS:N	1.73	0.86
1:A:1294:ARG:HH11	1:A:1294:ARG:CB	1.89	0.85
1:B:476:ARG:HD2	1:B:499:GLU:OE2	1.76	0.85
1:A:472:ARG:HG3	1:A:472:ARG:HH21	1.41	0.85
1:A:1379:LYS:HD2	1:A:1379:LYS:H	1.40	0.85
1:B:1390:PHE:CE1	1:B:1428:SER:HB3	2.12	0.84
1:C:1256:LYS:HG3	1:C:1259:SER:CB	2.04	0.84
1:C:472:ARG:HG2	1:C:472:ARG:HH21	1.42	0.84
1:F:498:SER:HB2	1:F:501:CYS:SG	2.17	0.84
1:C:1256:LYS:HB2	1:C:1260:GLU:HG3	1.58	0.84
1:A:430:MET:CE	1:A:437:LEU:HD22	2.08	0.84
1:C:1174:PHE:HE1	1:C:1421:TRP:CD1	1.94	0.84
1:C:1399:LEU:HD23	1:C:1400:LYS:N	1.92	0.84
1:E:498:SER:HB2	1:E:501:CYS:SG	2.17	0.84
1:A:1294:ARG:HH12	1:A:1302:GLU:HG3	1.41	0.84
1:A:1422:VAL:HG21	1:E:1161:LEU:HD13	1.60	0.83
1:D:1301:LEU:HB3	1:D:1370:ILE:HG13	1.60	0.83
1:B:1323:ARG:HB2	1:B:1323:ARG:NH1	1.93	0.83
1:C:440:ARG:HG2	1:C:442:ARG:NH1	1.92	0.83
1:A:1390:PHE:CE1	1:A:1428:SER:HB3	2.12	0.83
1:A:1378:LYS:HE3	1:A:1381:TRP:HZ2	1.40	0.83
1:E:463:TYR:HB2	1:E:475:ALA:CB	2.09	0.83
1:A:460:ASP:HA	1:A:463:TYR:CE2	2.14	0.83
1:F:422:ASP:O	1:F:426:VAL:HG23	1.79	0.82
1:B:1294:ARG:HH12	1:B:1302:GLU:HG3	1.45	0.82
1:D:1171:ASN:O	1:D:1418:VAL:HG13	1.80	0.82
1:C:1171:ASN:O	1:C:1418:VAL:HG13	1.80	0.82
1:C:1318:GLN:HE21	1:C:1357:ARG:NH1	1.78	0.82
1:F:1408:GLU:CG	1:F:1411:LEU:HB2	2.09	0.82
1:C:1217:ASN:ND2	1:C:1400:LYS:HB2	1.95	0.82
1:E:1160:GLU:HB3	1:E:1167:GLY:HA3	1.61	0.82
1:B:464:HIS:HD1	1:B:465:HIS:CD2	1.97	0.81
1:B:442:ARG:NH2	1:B:453:PHE:HA	1.95	0.81
1:A:1161:LEU:HB2	1:E:1422:VAL:HG23	1.63	0.81
1:B:1408:GLU:HG2	1:B:1411:LEU:HB2	1.63	0.81
1:F:1329:ASN:ND2	1:F:1372:LEU:HB3	1.96	0.81
1:C:1249:HIS:CE1	1:C:1268:PRO:HG2	2.15	0.81
1:B:453:PHE:HZ	1:B:488:ILE:HD12	1.45	0.81
1:A:1173:LEU:HD12	1:A:1173:LEU:O	1.81	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:1183:LEU:HD22	1:E:1285:LEU:HD22	1.62	0.80
1:C:1293:VAL:HG12	1:C:1303:VAL:HG13	1.64	0.80
1:A:462:LEU:O	1:A:466:VAL:CB	2.28	0.80
1:B:1161:LEU:HD13	1:F:1422:VAL:HG21	1.63	0.80
1:B:422:ASP:O	1:B:426:VAL:HG23	1.81	0.80
1:D:458:VAL:O	1:D:462:LEU:HB2	1.79	0.80
1:C:1249:HIS:HE1	1:C:1268:PRO:HG2	1.45	0.80
1:F:1357:ARG:HG2	1:F:1357:ARG:HH11	1.46	0.80
1:C:422:ASP:O	1:C:426:VAL:HG23	1.80	0.80
1:E:1339:LYS:NZ	1:E:1364:SER:HA	1.96	0.80
1:E:1203:LYS:HB3	1:E:1205:TYR:HE1	1.46	0.80
1:D:1408:GLU:HG2	1:D:1411:LEU:HB2	1.64	0.80
1:A:1305:VAL:HG12	1:A:1366:ILE:HG22	1.62	0.80
1:C:462:LEU:O	1:C:466:VAL:CG2	2.29	0.80
1:C:1183:LEU:HD12	1:C:1184:LEU:N	1.95	0.79
1:D:1183:LEU:CD2	1:D:1285:LEU:HD23	2.13	0.79
1:D:1339:LYS:HD2	1:D:1364:SER:OG	1.81	0.79
1:A:1345:LYS:HA	1:A:1345:LYS:HE2	1.64	0.79
1:A:1339:LYS:NZ	1:A:1339:LYS:HB3	1.97	0.79
1:F:1160:GLU:HB3	1:F:1167:GLY:HA3	1.64	0.79
1:E:463:TYR:HB2	1:E:475:ALA:HB2	1.65	0.79
1:C:1160:GLU:HB3	1:C:1167:GLY:HA3	1.64	0.79
1:A:430:MET:HE2	1:A:437:LEU:HD22	1.65	0.78
1:A:1337:CYS:HB3	1:A:1366:ILE:HG13	1.64	0.78
1:F:1177:VAL:HB	1:F:1424:TYR:HD1	1.47	0.78
1:C:1178:LEU:HD12	1:C:1178:LEU:N	1.99	0.78
1:F:1213:LYS:CE	1:F:1262:SER:OG	2.31	0.78
1:B:473:ARG:O	1:B:477:LYS:HG3	1.84	0.78
1:E:1331:SER:HB3	1:E:1373:LEU:HG	1.64	0.78
1:D:1301:LEU:HB2	1:D:1372:LEU:HD11	1.64	0.78
1:B:430:MET:CE	1:B:437:LEU:HD22	2.14	0.78
1:A:442:ARG:HD2	1:A:502:TYR:CZ	2.19	0.78
1:B:1276:ARG:HG3	1:B:1277:TYR:N	1.98	0.78
1:E:1323:ARG:HB3	1:E:1387:SER:OG	1.83	0.78
1:D:1217:ASN:ND2	1:D:1400:LYS:HB2	1.99	0.77
1:F:1324:ILE:HD12	1:F:1386:ILE:CG2	2.14	0.77
1:B:462:LEU:HD13	1:B:475:ALA:O	1.85	0.77
1:C:1324:ILE:HG23	1:C:1386:ILE:HD11	1.64	0.77
1:B:1214:PHE:HE1	1:B:1401:VAL:HG13	1.50	0.77
1:B:463:TYR:HB2	1:B:475:ALA:HB2	1.65	0.77
1:D:1253:ARG:HB2	1:D:1253:ARG:NH2	1.98	0.77
1:A:1394:PHE:O	1:A:1396:PRO:HD3	1.85	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1434:ARG:HG2	1:A:1434:ARG:HH11	1.49	0.77
1:B:1323:ARG:HH11	1:B:1323:ARG:HB2	1.49	0.77
1:D:1298:ARG:HH22	1:D:1372:LEU:CD2	1.97	0.76
1:D:1312:LYS:HE3	1:D:1315:LEU:HD11	1.67	0.76
1:C:1176:ASP:HB3	1:C:1178:LEU:HD11	1.67	0.76
1:C:1290:ILE:HB	1:C:1306:VAL:HG12	1.67	0.76
1:A:1328:LEU:HB2	1:A:1381:TRP:CH2	2.14	0.76
1:D:1253:ARG:CB	1:D:1253:ARG:HH21	1.99	0.76
1:A:438:GLU:OE2	1:A:440:ARG:NH2	2.18	0.76
1:D:1434:ARG:HH11	1:D:1434:ARG:HG3	1.49	0.76
1:C:1318:GLN:HE21	1:C:1357:ARG:HH11	1.30	0.76
1:D:1301:LEU:CB	1:D:1370:ILE:HG13	2.15	0.76
1:D:1187:PRO:HD3	1:D:1434:ARG:HB2	1.67	0.76
1:F:1422:VAL:HG12	1:F:1423:ARG:N	2.01	0.76
1:A:422:ASP:O	1:A:426:VAL:HG23	1.86	0.76
1:E:1318:GLN:HE21	1:E:1319:LYS:HE3	1.51	0.76
1:E:1172:GLU:HB3	1:E:1419:ILE:HB	1.68	0.76
1:D:1301:LEU:HB3	1:D:1370:ILE:CG1	2.15	0.76
1:B:1344:TYR:CE2	1:B:1346:ALA:HB2	2.20	0.75
1:E:1325:PRO:HG3	1:E:1384:PRO:O	1.86	0.75
1:D:1408:GLU:OE2	1:D:1409:PRO:HD2	1.87	0.75
1:D:1289:VAL:HB	1:D:1433:THR:HG21	1.68	0.75
1:C:1217:ASN:HD21	1:C:1400:LYS:HB2	1.49	0.75
1:E:464:HIS:HB3	1:E:465:HIS:HD2	1.50	0.75
1:F:491:THR:HG22	1:F:492:VAL:HG13	1.68	0.75
1:F:1186:SER:HA	1:F:1434:ARG:HG3	1.67	0.75
1:C:1331:SER:HB3	1:C:1373:LEU:HD21	1.68	0.75
1:D:1330:THR:HG21	1:D:1344:TYR:OH	1.87	0.75
1:C:1296:VAL:HB	1:C:1300:LYS:HB3	1.67	0.74
1:A:1392:VAL:HB	1:A:1394:PHE:CE2	2.23	0.74
1:E:422:ASP:O	1:E:426:VAL:HG23	1.87	0.74
1:F:1319:LYS:HE3	1:F:1391:GLU:OE1	1.87	0.74
1:B:1425:ILE:O	1:B:1425:ILE:HG22	1.86	0.74
1:E:1394:PHE:O	1:E:1396:PRO:HD3	1.86	0.74
1:B:457:ASP:HA	1:B:460:ASP:OD2	1.87	0.74
1:B:463:TYR:HE1	1:B:469:PHE:O	1.70	0.74
1:C:1183:LEU:HD23	1:C:1431:TYR:CE1	2.22	0.74
1:D:1160:GLU:HB3	1:D:1167:GLY:HA3	1.70	0.74
1:D:433:PRO:HD3	1:D:1254:LEU:O	1.87	0.74
1:C:1333:VAL:HG22	1:C:1370:ILE:HG12	1.68	0.74
1:C:1357:ARG:HB3	1:C:1357:ARG:HH11	1.51	0.74
1:E:1422:VAL:HG12	1:E:1423:ARG:N	2.01	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:459:VAL:HG21	1:C:499:GLU:OE1	1.88	0.74
1:E:1383:ARG:HD2	1:E:1435:CYS:SG	2.28	0.74
1:B:459:VAL:HA	1:B:462:LEU:HD12	1.70	0.74
1:F:1213:LYS:HE3	1:F:1262:SER:OG	1.87	0.74
1:D:1356:LYS:HB3	1:D:1357:ARG:NH1	2.03	0.73
1:B:1419:ILE:HD12	1:B:1419:ILE:N	2.03	0.73
1:B:1173:LEU:HD11	1:B:1420:LYS:HG2	1.68	0.73
1:C:1422:VAL:HG12	1:C:1423:ARG:N	2.03	0.73
1:D:440:ARG:HG2	1:D:442:ARG:NH1	2.03	0.73
1:B:1308:LYS:HG2	1:B:1363:GLU:HG2	1.70	0.73
1:F:1188:GLN:NE2	1:F:1188:GLN:H	1.85	0.73
1:F:1192:LEU:HD11	1:F:1434:ARG:HE	1.51	0.73
1:E:455:GLY:O	1:E:458:VAL:HG12	1.89	0.73
1:C:1318:GLN:HG2	1:C:1357:ARG:HB2	1.70	0.73
1:B:1333:VAL:HG11	1:B:1344:TYR:CG	2.23	0.73
1:A:490:HIS:CE1	1:A:494:LYS:HE2	2.23	0.73
1:F:1217:ASN:HD21	1:F:1400:LYS:H	1.34	0.73
1:B:442:ARG:HG2	1:B:502:TYR:CZ	2.24	0.73
1:F:1402:ARG:HG3	1:F:1402:ARG:HH11	1.52	0.73
1:B:1160:GLU:HB3	1:B:1167:GLY:HA3	1.69	0.73
1:E:1173:LEU:HD12	1:E:1173:LEU:C	2.09	0.73
1:D:1322:VAL:HG23	1:D:1353:TRP:HB3	1.71	0.72
1:B:1408:GLU:CB	1:B:1413:TYR:CE2	2.72	0.72
1:F:1284:ILE:HG12	1:F:1396:PRO:O	1.88	0.72
1:A:1278:ARG:HH11	1:A:1278:ARG:HG3	1.53	0.72
1:B:1302:GLU:OE2	1:B:1369:GLU:HG2	1.89	0.72
1:A:1160:GLU:HB3	1:A:1167:GLY:HA3	1.71	0.72
1:B:440:ARG:HG2	1:B:441:ASP:H	1.54	0.72
1:A:1312:LYS:HB2	1:A:1315:LEU:HD12	1.71	0.72
1:A:1408:GLU:HG2	1:A:1411:LEU:HB2	1.71	0.72
1:D:1318:GLN:HG2	1:D:1357:ARG:HB3	1.70	0.72
1:A:1241:ILE:HD11	1:A:1399:LEU:HA	1.72	0.72
1:A:1422:VAL:HG23	1:E:1161:LEU:HB2	1.72	0.72
1:C:1409:PRO:HG2	1:C:1410:LYS:HD2	1.71	0.72
1:F:1329:ASN:HD21	1:F:1372:LEU:HB3	1.55	0.72
1:B:1425:ILE:HD11	1:F:1156:PRO:CG	2.20	0.72
1:F:1217:ASN:ND2	1:F:1400:LYS:H	1.89	0.71
1:A:1434:ARG:CG	1:A:1434:ARG:HH11	2.03	0.71
1:E:422:ASP:OD2	1:E:424:ALA:HB3	1.90	0.71
1:D:1320:ILE:CG2	1:D:1388:MET:HE1	2.20	0.71
1:C:1214:PHE:C	1:C:1214:PHE:HD2	1.94	0.71
1:C:462:LEU:HD11	1:C:479:ALA:HB2	1.73	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:440:ARG:H	1:C:442:ARG:NH1	1.87	0.71
1:D:1217:ASN:ND2	1:D:1400:LYS:N	2.38	0.71
1:E:470:PRO:CG	1:E:474:GLU:HG3	2.20	0.71
1:F:1425:ILE:O	1:F:1425:ILE:HG22	1.89	0.71
1:D:1158:TYR:HB2	1:D:1170:ARG:HD2	1.71	0.71
1:D:1324:ILE:HG22	1:D:1351:ILE:HB	1.73	0.70
1:D:444:TRP:O	1:D:447:ILE:HG13	1.90	0.70
1:E:462:LEU:HD22	1:E:475:ALA:CA	2.21	0.70
1:E:1305:VAL:HG21	1:E:1324:ILE:HD13	1.73	0.70
1:D:1187:PRO:HD3	1:D:1434:ARG:CB	2.21	0.70
1:D:1301:LEU:HB3	1:D:1370:ILE:CD1	2.22	0.70
1:D:1298:ARG:HH22	1:D:1372:LEU:HD22	1.56	0.70
1:A:1335:VAL:C	1:A:1336:ILE:HD12	2.12	0.70
1:D:1308:LYS:HE2	1:D:1363:GLU:OE2	1.91	0.70
1:C:1211:GLU:HG3	1:C:1253:ARG:NH1	2.07	0.70
1:D:1217:ASN:ND2	1:D:1400:LYS:H	1.90	0.70
1:F:1293:VAL:HG12	1:F:1303:VAL:HG22	1.73	0.70
1:B:430:MET:HE1	1:B:437:LEU:HD22	1.74	0.69
1:F:1187:PRO:CD	1:F:1434:ARG:HB2	2.21	0.69
1:C:1214:PHE:CD2	1:C:1214:PHE:C	2.65	0.69
1:E:1294:ARG:NH2	1:E:1302:GLU:HG3	2.07	0.69
1:A:1294:ARG:HH12	1:A:1302:GLU:CG	2.05	0.69
1:F:1324:ILE:HD12	1:F:1386:ILE:HG21	1.73	0.69
1:D:1305:VAL:HG23	1:D:1366:ILE:CG2	2.22	0.69
1:E:1298:ARG:HD2	1:E:1374:PRO:HA	1.74	0.69
1:F:1263:ILE:N	1:F:1263:ILE:HD12	2.07	0.69
1:D:440:ARG:HG2	1:D:442:ARG:CZ	2.22	0.69
1:E:1305:VAL:HG23	1:E:1366:ILE:HG23	1.73	0.69
1:A:476:ARG:HG2	1:A:476:ARG:NH2	2.08	0.69
1:D:1333:VAL:CG2	1:D:1370:ILE:HG22	2.22	0.69
1:C:1357:ARG:HB3	1:C:1357:ARG:NH1	2.08	0.69
1:E:1187:PRO:HD3	1:E:1434:ARG:CD	2.20	0.69
1:F:1375:THR:OG1	1:F:1379:LYS:HD3	1.92	0.69
1:F:1211:GLU:HA	1:F:1266:ILE:HD13	1.74	0.69
1:F:1214:PHE:HD1	1:F:1215:GLY:N	1.90	0.69
1:E:487:LEU:N	1:E:487:LEU:HD23	2.06	0.69
1:A:1278:ARG:NH1	1:A:1278:ARG:HG3	2.07	0.69
1:A:1161:LEU:HD13	1:E:1422:VAL:HG21	1.75	0.69
1:F:1213:LYS:HE2	1:F:1262:SER:OG	1.93	0.69
1:C:498:SER:HB3	1:C:501:CYS:SG	2.33	0.69
1:B:1211:GLU:HA	1:B:1266:ILE:HD13	1.74	0.69
1:D:1394:PHE:O	1:D:1396:PRO:HD3	1.91	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1158:TYR:CE1	1:F:1174:PHE:HD2	2.11	0.69
1:F:1178:LEU:HD22	1:F:1427:ARG:NH1	2.08	0.69
1:A:1380:LYS:HB3	1:D:477:LYS:HE3	1.75	0.68
1:D:1329:ASN:ND2	1:D:1372:LEU:HD23	2.07	0.68
1:B:1253:ARG:O	1:B:1263:ILE:HD11	1.93	0.68
1:F:1196:VAL:HG23	1:F:1283:ILE:HD13	1.75	0.68
1:A:1304:LYS:HD2	1:A:1365:GLN:NE2	2.08	0.68
1:D:1285:LEU:N	1:D:1285:LEU:HD12	2.08	0.68
1:D:1217:ASN:HD21	1:D:1400:LYS:H	1.41	0.68
1:E:1339:LYS:NZ	1:E:1363:GLU:O	2.27	0.68
1:F:1357:ARG:HG2	1:F:1357:ARG:NH1	2.07	0.68
1:C:490:HIS:NE2	1:C:494:LYS:HB3	2.08	0.68
1:C:1406:VAL:HG11	1:C:1418:VAL:CG2	2.22	0.68
1:F:1217:ASN:ND2	1:F:1400:LYS:N	2.42	0.68
1:A:1339:LYS:HZ2	1:A:1339:LYS:HB3	1.59	0.68
1:A:476:ARG:HG2	1:A:476:ARG:HH21	1.57	0.68
1:B:1425:ILE:HD11	1:F:1156:PRO:HG2	1.76	0.68
1:E:447:ILE:HG22	1:E:448:THR:H	1.59	0.68
1:C:1408:GLU:HG2	1:C:1411:LEU:HB2	1.75	0.68
1:B:1268:PRO:HD2	1:B:1272:PHE:CE2	2.29	0.68
1:B:1294:ARG:HH12	1:B:1302:GLU:CG	2.07	0.68
1:D:442:ARG:HD3	1:D:502:TYR:CZ	2.29	0.68
1:F:1359:ALA:HB3	1:F:1362:LYS:HD2	1.74	0.68
1:C:1180:SER:HB2	1:C:1427:ARG:NH1	2.08	0.68
1:A:487:LEU:HD23	1:A:487:LEU:N	2.08	0.68
1:A:1184:LEU:CD2	1:A:1192:LEU:HD12	2.21	0.67
1:C:1170:ARG:HH22	1:C:1205:TYR:HD2	1.42	0.67
1:C:471:GLU:HG2	1:C:473:ARG:NH2	2.09	0.67
1:B:424:ALA:O	1:B:428:LYS:HG3	1.93	0.67
1:C:463:TYR:CZ	1:C:464:HIS:ND1	2.63	0.67
1:C:1174:PHE:CE1	1:C:1421:TRP:CD1	2.80	0.67
1:D:1280:THR:HA	1:D:1283:ILE:HD11	1.74	0.67
1:C:1293:VAL:CG1	1:C:1303:VAL:HG13	2.23	0.67
1:B:1406:VAL:HG23	1:B:1415:ASP:OD1	1.94	0.67
1:F:1345:LYS:CE	1:F:1352:VAL:HG21	2.24	0.67
1:F:1331:SER:HB2	1:F:1373:LEU:HD22	1.75	0.67
1:A:447:ILE:HG22	1:A:448:THR:N	2.09	0.67
1:E:1211:GLU:HA	1:E:1266:ILE:HD13	1.75	0.67
1:E:1293:VAL:CG1	1:E:1303:VAL:HG13	2.23	0.67
1:D:1301:LEU:HD12	1:D:1372:LEU:HD21	1.75	0.67
1:F:1289:VAL:HG22	1:F:1307:ILE:HG22	1.76	0.67
1:A:492:VAL:HG21	1:C:1338:MET:HB3	1.76	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:454:LEU:HB3	1:E:457:ASP:OD2	1.95	0.66
1:B:464:HIS:CE1	1:B:465:HIS:NE2	2.62	0.66
1:A:492:VAL:HG13	1:C:1338:MET:HG2	1.76	0.66
1:C:447:ILE:HG22	1:C:448:THR:N	2.10	0.66
1:D:1323:ARG:HB2	1:D:1387:SER:OG	1.95	0.66
1:E:1323:ARG:HB2	1:E:1323:ARG:HH11	1.58	0.66
1:B:462:LEU:CD1	1:B:479:ALA:HB2	2.25	0.66
1:D:1326:THR:HG21	1:D:1344:TYR:CE1	2.31	0.66
1:F:1187:PRO:HD3	1:F:1434:ARG:CB	2.25	0.66
1:E:1335:VAL:HG12	1:E:1368:ALA:HB2	1.77	0.66
1:A:1204:SER:C	1:A:1205:TYR:HD2	1.98	0.66
1:D:1183:LEU:HD12	1:D:1193:SER:O	1.95	0.66
1:D:1196:VAL:HG21	1:D:1279:THR:HG22	1.75	0.66
1:D:1298:ARG:HH22	1:D:1372:LEU:HB3	1.60	0.66
1:E:1408:GLU:CG	1:E:1411:LEU:HB2	2.26	0.66
1:A:1336:ILE:N	1:A:1336:ILE:HD12	2.10	0.66
1:D:1246:CYS:HB2	1:D:1276:ARG:O	1.96	0.66
1:C:469:PHE:HZ	1:C:478:TYR:CD2	2.12	0.66
1:D:1434:ARG:NH1	1:D:1434:ARG:HG3	2.11	0.66
1:B:1408:GLU:CB	1:B:1413:TYR:HE2	2.09	0.66
1:C:483:LEU:HD22	1:C:488:ILE:HB	1.76	0.66
1:F:1311:PHE:CE1	1:F:1360:GLY:HA2	2.31	0.66
1:C:1378:LYS:HG2	1:C:1379:LYS:H	1.60	0.66
1:D:1331:SER:HB3	1:D:1373:LEU:HG	1.77	0.66
1:D:1345:LYS:HD2	1:D:1352:VAL:HG21	1.77	0.66
1:D:1386:ILE:HG13	1:D:1435:CYS:SG	2.36	0.66
1:D:478:TYR:O	1:D:482:LEU:HD12	1.95	0.66
1:F:1293:VAL:HG21	1:F:1383:ARG:NH1	2.10	0.66
1:D:1305:VAL:HG23	1:D:1366:ILE:HG23	1.76	0.66
1:C:447:ILE:CG2	1:C:448:THR:N	2.59	0.66
1:D:1298:ARG:HH22	1:D:1372:LEU:CB	2.09	0.65
1:E:1183:LEU:HD11	1:E:1191:VAL:HG13	1.78	0.65
1:D:441:ASP:OD1	1:D:450:PRO:HA	1.96	0.65
1:A:1290:ILE:N	1:A:1290:ILE:HD12	2.11	0.65
1:B:454:LEU:HG	1:B:456:SER:H	1.61	0.65
1:A:453:PHE:CD2	1:A:453:PHE:N	2.64	0.65
1:F:1294:ARG:HH11	1:F:1294:ARG:HB3	1.60	0.65
1:D:1170:ARG:HH11	1:D:1172:GLU:CD	2.00	0.65
1:F:448:THR:HG22	1:F:448:THR:O	1.97	0.65
1:E:1324:ILE:HD12	1:E:1386:ILE:HG21	1.77	0.65
1:F:430:MET:CE	1:F:437:LEU:HD22	2.26	0.65
1:B:1170:ARG:HA	1:F:1421:TRP:CZ3	2.31	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:1250:GLN:HG3	1:D:1251:CYS:N	2.12	0.65
1:C:471:GLU:HG3	1:C:472:ARG:N	2.11	0.65
1:D:443:MET:HG3	1:D:447:ILE:O	1.97	0.65
1:B:1338:MET:HB3	1:E:492:VAL:HG21	1.79	0.65
1:B:458:VAL:O	1:B:462:LEU:HG	1.96	0.65
1:D:1320:ILE:HG23	1:D:1388:MET:HE1	1.79	0.65
1:C:455:GLY:O	1:C:458:VAL:HG12	1.97	0.65
1:C:1331:SER:HB3	1:C:1373:LEU:CD2	2.27	0.65
1:A:447:ILE:HG22	1:A:448:THR:H	1.61	0.65
1:F:1384:PRO:O	1:F:1435:CYS:SG	2.54	0.65
1:E:1342:ALA:HB2	1:E:1353:TRP:CD1	2.32	0.65
1:E:466:VAL:CG1	1:E:469:PHE:HE2	2.10	0.65
1:D:1357:ARG:HH11	1:D:1357:ARG:HG2	1.61	0.65
1:F:1217:ASN:ND2	1:F:1400:LYS:HB2	2.12	0.65
1:B:442:ARG:HH21	1:B:453:PHE:HA	1.62	0.65
1:D:462:LEU:HD23	1:D:466:VAL:HG21	1.77	0.65
1:C:1177:VAL:C	1:C:1178:LEU:HD12	2.16	0.65
1:C:1306:VAL:HG23	1:C:1365:GLN:HB2	1.79	0.65
1:C:1326:THR:HG22	1:C:1370:ILE:HD11	1.79	0.65
1:A:472:ARG:HG3	1:A:472:ARG:NH2	2.11	0.65
1:D:440:ARG:O	1:D:442:ARG:NH1	2.30	0.65
1:F:1312:LYS:HB2	1:F:1312:LYS:NZ	2.11	0.65
1:D:491:THR:HG22	1:D:492:VAL:HG13	1.78	0.65
1:F:458:VAL:O	1:F:462:LEU:HB2	1.97	0.64
1:D:1422:VAL:HG12	1:D:1423:ARG:N	2.11	0.64
1:F:1295:GLU:OE2	1:F:1301:LEU:HD13	1.98	0.64
1:F:1293:VAL:CG2	1:F:1383:ARG:NH1	2.60	0.64
1:B:1338:MET:HE2	1:E:491:THR:HB	1.80	0.64
1:E:441:ASP:OD1	1:E:450:PRO:HA	1.97	0.64
1:D:1319:LYS:O	1:D:1390:PHE:HA	1.98	0.64
1:C:462:LEU:CD1	1:C:479:ALA:HB2	2.27	0.64
1:C:1174:PHE:CD2	1:C:1203:LYS:HD2	2.26	0.64
1:E:464:HIS:HB3	1:E:465:HIS:CD2	2.32	0.64
1:D:1326:THR:HB	1:D:1327:PRO:HD2	1.79	0.64
1:C:467:GLU:OE2	1:C:467:GLU:HA	1.96	0.64
1:D:1323:ARG:O	1:D:1386:ILE:HG23	1.98	0.64
1:A:487:LEU:O	1:A:488:ILE:HD13	1.96	0.64
1:F:1186:SER:HA	1:F:1434:ARG:CG	2.28	0.64
1:A:1183:LEU:HB3	1:A:1431:TYR:CD1	2.33	0.64
1:E:1435:CYS:O	1:E:1435:CYS:SG	2.56	0.64
1:B:1325:PRO:HG3	1:B:1384:PRO:O	1.97	0.64
1:E:1327:PRO:HG3	1:E:1381:TRP:CE3	2.33	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1170:ARG:NH1	1:B:1172:GLU:OE1	2.31	0.64
1:B:428:LYS:O	1:B:431:ALA:HB3	1.97	0.64
1:E:1359:ALA:HB3	1:E:1362:LYS:HD2	1.80	0.64
1:D:1356:LYS:HB3	1:D:1357:ARG:HH11	1.62	0.64
1:E:1183:LEU:HD12	1:E:1193:SER:O	1.98	0.64
1:C:1331:SER:HB3	1:C:1373:LEU:CG	2.28	0.64
1:D:1172:GLU:HB3	1:D:1419:ILE:HB	1.81	0.64
1:E:1171:ASN:O	1:E:1418:VAL:HG13	1.98	0.63
1:D:1359:ALA:HB3	1:D:1362:LYS:HE2	1.79	0.63
1:B:1315:LEU:N	1:B:1315:LEU:HD12	2.13	0.63
1:A:1422:VAL:HG12	1:A:1423:ARG:H	1.63	0.63
1:C:1202:MET:HE1	1:C:1272:PHE:HZ	1.63	0.63
1:C:463:TYR:CE2	1:C:464:HIS:ND1	2.62	0.63
1:E:1332:GLY:HA3	1:E:1371:GLU:OE1	1.98	0.63
1:B:1311:PHE:CE1	1:B:1360:GLY:HA2	2.33	0.63
1:E:462:LEU:HD22	1:E:475:ALA:C	2.18	0.63
1:A:1187:PRO:HD3	1:A:1434:ARG:HB3	1.80	0.63
1:F:1345:LYS:HE3	1:F:1352:VAL:HG21	1.80	0.63
1:F:1192:LEU:CD1	1:F:1434:ARG:HE	2.11	0.63
1:B:453:PHE:CZ	1:B:488:ILE:HD12	2.30	0.63
1:D:483:LEU:HD12	1:D:483:LEU:O	1.98	0.63
1:E:1185:MET:SD	1:E:1189:GLY:HA2	2.39	0.63
1:F:1298:ARG:NH2	1:F:1379:LYS:HD2	2.13	0.63
1:F:1327:PRO:HG3	1:F:1381:TRP:CE3	2.33	0.63
1:D:453:PHE:CD2	1:D:453:PHE:N	2.67	0.63
1:B:434:GLU:HA	1:B:434:GLU:OE1	1.99	0.63
1:F:460:ASP:O	1:F:464:HIS:HD2	1.81	0.63
1:B:462:LEU:O	1:B:466:VAL:CB	2.46	0.63
1:F:1183:LEU:HD22	1:F:1285:LEU:HD22	1.81	0.63
1:C:1305:VAL:HG21	1:C:1324:ILE:HD13	1.81	0.63
1:F:1186:SER:OG	1:F:1188:GLN:NE2	2.31	0.62
1:F:1294:ARG:HB3	1:F:1294:ARG:NH1	2.13	0.62
1:D:1184:LEU:HB3	1:D:1193:SER:HB3	1.79	0.62
1:E:1327:PRO:HA	1:E:1381:TRP:NE1	2.14	0.62
1:B:483:LEU:HD13	1:B:503:TYR:CE1	2.35	0.62
1:D:476:ARG:HH11	1:D:499:GLU:HB2	1.64	0.62
1:A:459:VAL:O	1:A:463:TYR:CD2	2.51	0.62
1:B:1312:LYS:HB2	1:B:1315:LEU:CD1	2.27	0.62
1:D:495:ILE:HG13	1:D:496:THR:N	2.14	0.62
1:A:1171:ASN:HD21	1:A:1207:SER:H	1.46	0.62
1:C:471:GLU:HG3	1:C:472:ARG:H	1.64	0.62
1:E:462:LEU:CD2	1:E:475:ALA:HA	2.30	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:442:ARG:HG2	1:A:442:ARG:HH11	1.62	0.62
1:D:1301:LEU:HB3	1:D:1370:ILE:HD11	1.81	0.62
1:F:1294:ARG:CZ	1:F:1302:GLU:HG3	2.29	0.62
1:E:1381:TRP:CZ3	1:E:1383:ARG:HG2	2.34	0.62
1:D:1392:VAL:HB	1:D:1394:PHE:CE2	2.34	0.62
1:E:1291:PRO:O	1:E:1292:LEU:HD12	1.99	0.62
1:F:1184:LEU:HB3	1:F:1193:SER:HB3	1.80	0.62
1:D:1298:ARG:NH2	1:D:1372:LEU:HB3	2.15	0.62
1:E:1319:LYS:O	1:E:1390:PHE:HA	2.00	0.62
1:C:1172:GLU:HB3	1:C:1419:ILE:HB	1.81	0.62
1:C:461:TRP:CD1	1:C:465:HIS:CD2	2.88	0.62
1:B:476:ARG:HB3	1:B:476:ARG:NH2	2.09	0.62
1:B:449:ILE:HG22	1:B:452:ALA:HB2	1.81	0.62
1:D:1203:LYS:HB3	1:D:1205:TYR:HE2	1.65	0.62
1:A:1329:ASN:ND2	1:A:1372:LEU:HD22	2.15	0.62
1:E:472:ARG:O	1:E:472:ARG:HD3	2.00	0.62
1:A:1187:PRO:HD3	1:A:1434:ARG:CB	2.30	0.62
1:F:1192:LEU:HD11	1:F:1434:ARG:NE	2.15	0.62
1:B:1319:LYS:O	1:B:1390:PHE:HA	2.00	0.62
1:F:1422:VAL:HG12	1:F:1423:ARG:H	1.63	0.61
1:A:1170:ARG:NH1	1:A:1205:TYR:CD1	2.60	0.61
1:F:1325:PRO:HG3	1:F:1384:PRO:O	2.00	0.61
1:A:1427:ARG:HH11	1:A:1427:ARG:HG2	1.64	0.61
1:A:1276:ARG:CZ	1:A:1276:ARG:HB2	2.30	0.61
1:A:1422:VAL:HG12	1:A:1423:ARG:N	2.15	0.61
1:E:1298:ARG:HH21	1:E:1298:ARG:HG2	1.64	0.61
1:B:1408:GLU:HB3	1:B:1413:TYR:CE2	2.35	0.61
1:F:1158:TYR:HB2	1:F:1170:ARG:HD2	1.82	0.61
1:E:1196:VAL:HG23	1:E:1283:ILE:HD13	1.82	0.61
1:A:462:LEU:HD11	1:A:478:TYR:CD2	2.28	0.61
1:A:1170:ARG:HH12	1:A:1205:TYR:HD1	1.40	0.61
1:E:1184:LEU:HB2	1:E:1193:SER:HB3	1.83	0.61
1:A:428:LYS:O	1:A:431:ALA:HB3	2.00	0.61
1:A:1188:GLN:NE2	1:D:422:ASP:OD1	2.33	0.61
1:B:480:SER:OG	1:B:497:PHE:HB3	2.00	0.61
1:F:491:THR:HG22	1:F:492:VAL:CG1	2.30	0.61
1:C:1356:LYS:HD2	1:C:1356:LYS:H	1.64	0.61
1:E:1325:PRO:O	1:E:1381:TRP:HH2	1.83	0.61
1:D:1315:LEU:C	1:D:1316:LEU:HD23	2.20	0.61
1:E:1318:GLN:NE2	1:E:1319:LYS:HE3	2.16	0.61
1:A:1305:VAL:HG11	1:A:1324:ILE:HD11	1.82	0.61
1:D:1176:ASP:CG	1:D:1423:ARG:HH21	2.05	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:1276:ARG:HH11	1:C:1276:ARG:HG3	1.66	0.60
1:C:1329:ASN:ND2	1:C:1372:LEU:HB3	2.16	0.60
1:A:1255:SER:CB	1:A:1263:ILE:HA	2.30	0.60
1:A:462:LEU:HD23	1:A:475:ALA:CB	2.31	0.60
1:D:1183:LEU:HD11	1:D:1191:VAL:CG1	2.31	0.60
1:C:1214:PHE:HD2	1:C:1215:GLY:N	1.99	0.60
1:F:428:LYS:O	1:F:431:ALA:HB3	2.01	0.60
1:C:427:THR:HG21	1:C:487:LEU:HB3	1.83	0.60
1:D:1184:LEU:HA	1:D:1432:GLU:O	2.02	0.60
1:B:447:ILE:HG22	1:B:448:THR:N	2.16	0.60
1:A:1328:LEU:HD12	1:A:1349:ASN:ND2	2.15	0.60
1:D:1277:TYR:N	1:D:1277:TYR:HD2	2.00	0.60
1:D:1186:SER:HA	1:D:1434:ARG:HB2	1.83	0.60
1:C:1214:PHE:CD2	1:C:1215:GLY:N	2.70	0.60
1:A:1204:SER:C	1:A:1205:TYR:CD2	2.75	0.60
1:F:1333:VAL:HG13	1:F:1370:ILE:HG12	1.83	0.60
1:E:423:MET:HA	1:E:478:TYR:OH	2.01	0.60
1:D:1424:TYR:N	1:D:1424:TYR:CD2	2.68	0.60
1:A:442:ARG:NH1	1:A:442:ARG:HG3	2.03	0.60
1:C:1316:LEU:HD13	1:C:1357:ARG:HD2	1.84	0.60
1:B:483:LEU:HD13	1:B:503:TYR:HE1	1.65	0.60
1:F:1402:ARG:HG3	1:F:1402:ARG:NH1	2.17	0.60
1:E:465:HIS:N	1:E:465:HIS:CD2	2.68	0.60
1:D:1425:ILE:O	1:D:1425:ILE:HG22	2.00	0.60
1:A:442:ARG:NH1	1:A:442:ARG:CG	2.41	0.60
1:B:1253:ARG:NH2	1:B:1253:ARG:HG3	2.06	0.60
1:F:1298:ARG:O	1:F:1372:LEU:HD12	2.01	0.60
1:B:447:ILE:HG22	1:B:448:THR:H	1.67	0.60
1:E:470:PRO:HG2	1:E:471:GLU:H	1.67	0.59
1:D:1356:LYS:CD	1:D:1357:ARG:HH12	2.12	0.59
1:C:1331:SER:CB	1:C:1373:LEU:HD21	2.32	0.59
1:C:1422:VAL:HG12	1:C:1423:ARG:H	1.66	0.59
1:D:1359:ALA:HB3	1:D:1362:LYS:CE	2.31	0.59
1:A:467:GLU:HA	1:A:467:GLU:OE2	2.02	0.59
1:F:1298:ARG:NH1	1:F:1375:THR:OG1	2.35	0.59
1:B:1198:GLY:O	1:B:1276:ARG:HD3	2.02	0.59
1:A:492:VAL:CG1	1:C:1338:MET:HG2	2.33	0.59
1:D:1158:TYR:HB2	1:D:1170:ARG:CD	2.32	0.59
1:A:1276:ARG:HG3	1:A:1276:ARG:HH11	1.68	0.59
1:D:498:SER:HB2	1:D:501:CYS:SG	2.41	0.59
1:A:462:LEU:HD23	1:A:475:ALA:HB1	1.83	0.59
1:B:442:ARG:HG2	1:B:502:TYR:CE2	2.38	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:440:ARG:NH2	1:F:440:ARG:HB3	2.17	0.59
1:B:440:ARG:HG2	1:B:441:ASP:N	2.17	0.59
1:E:1422:VAL:HG12	1:E:1423:ARG:H	1.68	0.59
1:A:1408:GLU:CG	1:A:1411:LEU:HB2	2.33	0.59
1:F:1390:PHE:CZ	1:F:1428:SER:HB3	2.38	0.59
1:A:1176:ASP:HB3	1:A:1178:LEU:HD21	1.85	0.59
1:A:1425:ILE:HG22	1:A:1425:ILE:O	2.03	0.59
1:F:1290:ILE:HD12	1:F:1290:ILE:N	2.18	0.59
1:A:430:MET:HE1	1:A:437:LEU:HD22	1.84	0.59
1:F:1394:PHE:O	1:F:1396:PRO:HD3	2.02	0.59
1:A:1243:ILE:HD12	1:A:1277:TYR:HD1	1.67	0.59
1:F:1324:ILE:HD12	1:F:1386:ILE:HG23	1.84	0.59
1:A:1211:GLU:OE2	1:A:1253:ARG:NH2	2.36	0.59
1:A:1183:LEU:HG	1:A:1184:LEU:N	2.17	0.59
1:E:1279:THR:HG22	1:E:1280:THR:N	2.18	0.59
1:C:1319:LYS:O	1:C:1390:PHE:HA	2.03	0.59
1:D:1185:MET:HB3	1:D:1433:THR:HG22	1.85	0.58
1:E:1186:SER:HA	1:E:1434:ARG:CD	2.30	0.58
1:B:1305:VAL:HG21	1:B:1324:ILE:CD1	2.30	0.58
1:D:428:LYS:O	1:D:431:ALA:HB3	2.02	0.58
1:C:1187:PRO:HB2	1:C:1188:GLN:NE2	2.19	0.58
1:C:1394:PHE:O	1:C:1396:PRO:HD3	2.03	0.58
1:C:1178:LEU:CD1	1:C:1178:LEU:N	2.66	0.58
1:C:497:PHE:CD1	1:C:497:PHE:O	2.55	0.58
1:B:1187:PRO:HB2	1:B:1188:GLN:HE21	1.68	0.58
1:B:462:LEU:HD11	1:B:479:ALA:HB2	1.85	0.58
1:B:453:PHE:CD2	1:B:453:PHE:N	2.71	0.58
1:C:489:ARG:HH21	1:C:1410:LYS:CE	2.16	0.58
1:D:1298:ARG:NH2	1:D:1372:LEU:HD22	2.19	0.58
1:E:1423:ARG:NE	1:E:1425:ILE:HD11	2.18	0.58
1:E:1423:ARG:CD	1:E:1425:ILE:HD11	2.33	0.58
1:A:1173:LEU:HD22	1:A:1404:LEU:HD23	1.85	0.58
1:B:1280:THR:HA	1:B:1283:ILE:HD11	1.84	0.58
1:A:1298:ARG:HD3	1:A:1298:ARG:O	2.04	0.58
1:D:1292:LEU:HD12	1:D:1304:LYS:CE	2.34	0.58
1:B:430:MET:HE2	1:B:437:LEU:HB2	1.85	0.58
1:E:1279:THR:HG22	1:E:1280:THR:H	1.67	0.58
1:B:1408:GLU:HB2	1:B:1413:TYR:CE2	2.38	0.58
1:A:1241:ILE:CD1	1:A:1399:LEU:HA	2.33	0.58
1:E:1188:GLN:HB2	1:E:1190:GLN:HE21	1.67	0.58
1:A:1408:GLU:OE2	1:A:1409:PRO:HD2	2.04	0.58
1:D:1422:VAL:HG12	1:D:1423:ARG:H	1.66	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1287:PHE:N	1:A:1287:PHE:HD1	2.02	0.58
1:C:1404:LEU:HD23	1:C:1404:LEU:C	2.24	0.58
1:F:1394:PHE:CD1	1:F:1394:PHE:C	2.77	0.58
1:A:1361:MET:O	1:A:1362:LYS:HG3	2.03	0.58
1:B:463:TYR:HB2	1:B:475:ALA:CB	2.33	0.58
1:D:472:ARG:HH21	1:D:472:ARG:HG3	1.69	0.58
1:E:462:LEU:CD2	1:E:475:ALA:O	2.50	0.57
1:F:1185:MET:O	1:F:1434:ARG:HG3	2.04	0.57
1:D:430:MET:CE	1:D:437:LEU:HD22	2.34	0.57
1:D:451:ASN:ND2	1:D:1264:SER:HB3	2.19	0.57
1:E:458:VAL:O	1:E:462:LEU:CB	2.47	0.57
1:B:1246:CYS:SG	1:B:1276:ARG:O	2.62	0.57
1:C:453:PHE:CE1	1:C:503:TYR:HB2	2.40	0.57
1:C:483:LEU:HG	1:C:497:PHE:HD2	1.68	0.57
1:C:1187:PRO:HD3	1:C:1434:ARG:HB2	1.86	0.57
1:E:428:LYS:O	1:E:431:ALA:HB3	2.04	0.57
1:D:1335:VAL:HG12	1:D:1368:ALA:HB2	1.86	0.57
1:F:1181:VAL:HG11	1:F:1396:PRO:HB3	1.86	0.57
1:A:449:ILE:HD12	1:A:1407:PHE:CZ	2.40	0.57
1:E:1381:TRP:CE3	1:E:1383:ARG:HG2	2.39	0.57
1:B:449:ILE:CG2	1:B:452:ALA:HB2	2.35	0.57
1:C:428:LYS:O	1:C:431:ALA:HB3	2.04	0.57
1:B:1252:VAL:HG22	1:B:1263:ILE:HG13	1.85	0.57
1:D:1304:LYS:HG3	1:D:1365:GLN:HE21	1.68	0.57
1:B:1338:MET:CE	1:E:491:THR:HB	2.34	0.57
1:E:491:THR:HG22	1:E:492:VAL:HG13	1.87	0.57
1:A:1183:LEU:HD11	1:A:1191:VAL:CG2	2.29	0.57
1:E:470:PRO:HG2	1:E:474:GLU:HG3	1.85	0.57
1:C:1276:ARG:HG2	1:C:1277:TYR:N	2.20	0.57
1:C:1202:MET:HE1	1:C:1272:PHE:CZ	2.40	0.57
1:A:1287:PHE:CD1	1:A:1287:PHE:N	2.73	0.57
1:D:1324:ILE:HD12	1:D:1386:ILE:CG1	2.28	0.57
1:F:1183:LEU:HD12	1:F:1184:LEU:N	2.08	0.57
1:B:1173:LEU:HD12	1:B:1173:LEU:O	2.04	0.57
1:A:459:VAL:O	1:A:463:TYR:HD2	1.87	0.57
1:B:488:ILE:HG22	1:B:503:TYR:HD1	1.70	0.57
1:B:1408:GLU:HB3	1:B:1413:TYR:CD2	2.39	0.57
1:C:1329:ASN:OD1	1:C:1372:LEU:HD22	2.05	0.57
1:C:1253:ARG:NH1	1:C:1266:ILE:HD11	2.10	0.56
1:F:1381:TRP:CZ3	1:F:1383:ARG:HG2	2.40	0.56
1:E:489:ARG:NH2	1:E:1409:PRO:HG3	2.20	0.56
1:E:1328:LEU:HA	1:E:1349:ASN:HD21	1.69	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:471:GLU:OE2	1:E:473:ARG:HB2	2.04	0.56
1:D:1290:ILE:HG22	1:D:1290:ILE:O	2.05	0.56
1:B:1187:PRO:HD3	1:B:1434:ARG:HB2	1.85	0.56
1:F:1250:GLN:HG3	1:F:1251:CYS:N	2.20	0.56
1:F:1324:ILE:CD1	1:F:1386:ILE:HG21	2.34	0.56
1:B:463:TYR:HD1	1:B:469:PHE:CB	2.18	0.56
1:D:1298:ARG:NH2	1:D:1372:LEU:CB	2.68	0.56
1:F:1319:LYS:O	1:F:1390:PHE:HA	2.05	0.56
1:C:1381:TRP:CH2	1:C:1383:ARG:HG2	2.40	0.56
1:A:1392:VAL:HB	1:A:1394:PHE:HE2	1.66	0.56
1:D:440:ARG:HG2	1:D:442:ARG:NH2	2.21	0.56
1:D:1331:SER:OG	1:D:1371:GLU:HB3	2.04	0.56
1:D:1277:TYR:N	1:D:1277:TYR:CD2	2.71	0.56
1:B:1329:ASN:OD1	1:B:1372:LEU:HD22	2.05	0.56
1:E:495:ILE:HG23	1:E:496:THR:N	2.21	0.56
1:C:462:LEU:HD13	1:C:475:ALA:O	2.05	0.56
1:D:1324:ILE:HG23	1:D:1324:ILE:O	2.04	0.56
1:D:1217:ASN:HD22	1:D:1400:LYS:HB2	1.69	0.56
1:E:1422:VAL:CG1	1:E:1423:ARG:N	2.68	0.56
1:B:471:GLU:HG3	1:B:472:ARG:N	2.21	0.56
1:B:1202:MET:SD	1:B:1272:PHE:CZ	2.98	0.56
1:B:1326:THR:HG21	1:B:1344:TYR:CE1	2.40	0.56
1:B:1156:PRO:HG2	1:F:1425:ILE:HD11	1.88	0.56
1:C:422:ASP:OD1	1:C:425:SER:HB2	2.06	0.56
1:A:462:LEU:CD1	1:A:478:TYR:HD2	2.16	0.56
1:B:498:SER:HB3	1:B:501:CYS:SG	2.45	0.56
1:A:1211:GLU:OE2	1:A:1253:ARG:CZ	2.53	0.56
1:D:1171:ASN:O	1:D:1418:VAL:CG1	2.53	0.56
1:B:1338:MET:HB3	1:E:492:VAL:CG2	2.36	0.56
1:C:1317:ALA:HB2	1:C:1392:VAL:HG12	1.87	0.56
1:A:1331:SER:HB3	1:A:1373:LEU:HG	1.88	0.56
1:E:462:LEU:CD2	1:E:475:ALA:CA	2.84	0.56
1:C:1425:ILE:O	1:C:1425:ILE:HG23	2.06	0.56
1:F:425:SER:HA	1:F:428:LYS:HD3	1.88	0.56
1:C:426:VAL:HG21	1:C:478:TYR:OH	2.06	0.56
1:C:1277:TYR:N	1:C:1277:TYR:HD2	2.03	0.56
1:C:1288:ARG:NH1	1:C:1290:ILE:HD11	2.21	0.56
1:E:436:GLY:HA3	1:E:465:HIS:HE1	1.71	0.56
1:F:1317:ALA:HB2	1:F:1392:VAL:HG12	1.88	0.56
1:D:1343:LYS:HE3	1:D:1345:LYS:HZ3	1.71	0.56
1:A:495:ILE:HG23	1:A:496:THR:N	2.20	0.56
1:C:1325:PRO:HG3	1:C:1384:PRO:O	2.06	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:1277:TYR:CD2	1:C:1277:TYR:N	2.74	0.55
1:B:1333:VAL:HG21	1:B:1351:ILE:HD11	1.87	0.55
1:F:1268:PRO:HD2	1:F:1272:PHE:CE1	2.41	0.55
1:F:1415:ASP:OD2	1:F:1420:LYS:NZ	2.36	0.55
1:E:1175:LEU:HD11	1:E:1404:LEU:HD22	1.88	0.55
1:D:460:ASP:O	1:D:463:TYR:N	2.34	0.55
1:A:1322:VAL:HB	1:A:1353:TRP:HB3	1.88	0.55
1:C:1212:CYS:SG	1:C:1406:VAL:HG23	2.46	0.55
1:E:453:PHE:CE1	1:E:503:TYR:HB2	2.42	0.55
1:A:472:ARG:HD3	1:A:472:ARG:O	2.06	0.55
1:B:1333:VAL:HG11	1:B:1344:TYR:CD2	2.42	0.55
1:C:1299:THR:HB	1:C:1371:GLU:OE2	2.06	0.55
1:E:1324:ILE:HD12	1:E:1386:ILE:CG2	2.36	0.55
1:E:1296:VAL:HB	1:E:1300:LYS:HB3	1.88	0.55
1:C:1413:TYR:HB2	1:C:1417:ASP:HB2	1.88	0.55
1:E:1206:LEU:HD23	1:E:1406:VAL:HG11	1.87	0.55
1:F:478:TYR:CE1	1:F:482:LEU:HD21	2.41	0.55
1:F:1183:LEU:CD1	1:F:1184:LEU:H	2.11	0.55
1:F:1422:VAL:CG1	1:F:1423:ARG:N	2.68	0.55
1:C:1422:VAL:CG1	1:C:1423:ARG:N	2.70	0.55
1:B:438:GLU:HG3	1:B:438:GLU:O	2.05	0.55
1:C:1253:ARG:HH12	1:C:1266:ILE:CD1	2.11	0.55
1:F:1183:LEU:CD1	1:F:1191:VAL:HG13	2.36	0.55
1:C:447:ILE:CG2	1:C:448:THR:H	2.19	0.55
1:F:443:MET:HG3	1:F:447:ILE:O	2.07	0.55
1:A:1413:TYR:HB2	1:A:1417:ASP:HB2	1.88	0.55
1:F:440:ARG:HG2	1:F:441:ASP:N	2.21	0.55
1:D:1211:GLU:OE1	1:D:1266:ILE:HD11	2.06	0.55
1:C:472:ARG:HG2	1:C:472:ARG:NH2	2.16	0.55
1:D:1298:ARG:HH12	1:D:1329:ASN:ND2	2.03	0.55
1:B:1413:TYR:HB2	1:B:1417:ASP:HB2	1.87	0.55
1:E:421:MET:HG3	1:E:422:ASP:H	1.71	0.55
1:E:1305:VAL:HG23	1:E:1366:ILE:CG2	2.36	0.55
1:C:476:ARG:NH1	1:C:499:GLU:HG3	2.22	0.55
1:A:1182:ASN:ND2	1:A:1195:HIS:CE1	2.67	0.55
1:D:439:VAL:HG22	1:D:453:PHE:CD2	2.42	0.55
1:C:1294:ARG:O	1:C:1301:LEU:HD12	2.06	0.55
1:E:1214:PHE:CD2	1:E:1214:PHE:C	2.80	0.55
1:B:501:CYS:SG	1:B:503:TYR:HE2	2.29	0.55
1:E:1323:ARG:HH11	1:E:1323:ARG:CB	2.20	0.55
1:E:430:MET:HE1	1:E:458:VAL:HG23	1.88	0.55
1:D:1356:LYS:HD3	1:D:1357:ARG:NH1	2.13	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1294:ARG:NH1	1:B:1294:ARG:HB3	2.22	0.55
1:A:471:GLU:H	1:A:474:GLU:HG3	1.72	0.55
1:F:454:LEU:HD23	1:F:456:SER:OG	2.07	0.55
1:D:1291:PRO:HA	1:D:1305:VAL:HG12	1.89	0.54
1:F:1252:VAL:HG13	1:F:1263:ILE:CG2	2.37	0.54
1:C:1288:ARG:HH11	1:C:1290:ILE:HD11	1.72	0.54
1:F:1284:ILE:CG1	1:F:1396:PRO:HA	2.36	0.54
1:C:433:PRO:HG2	1:C:1256:LYS:HE2	1.89	0.54
1:D:1322:VAL:CG2	1:D:1353:TRP:HB3	2.36	0.54
1:F:1381:TRP:CE3	1:F:1383:ARG:HG2	2.42	0.54
1:D:1286:PRO:HG2	1:D:1390:PHE:CE1	2.42	0.54
1:D:1357:ARG:NH1	1:D:1357:ARG:HG2	2.22	0.54
1:F:426:VAL:O	1:F:429:ALA:HB3	2.08	0.54
1:D:430:MET:HB3	1:D:437:LEU:HD23	1.89	0.54
1:D:495:ILE:HG13	1:D:496:THR:H	1.73	0.54
1:D:495:ILE:HG13	1:D:496:THR:HG23	1.88	0.54
1:A:442:ARG:NH1	1:A:442:ARG:HG2	2.21	0.54
1:C:440:ARG:N	1:C:442:ARG:NH1	2.55	0.54
1:B:1419:ILE:CD1	1:B:1419:ILE:N	2.70	0.54
1:B:1408:GLU:CG	1:B:1411:LEU:HB2	2.36	0.54
1:F:1263:ILE:N	1:F:1263:ILE:CD1	2.71	0.54
1:B:1290:ILE:O	1:B:1290:ILE:HG22	2.07	0.54
1:F:1324:ILE:O	1:F:1324:ILE:HG22	2.07	0.54
1:F:1181:VAL:CG1	1:F:1396:PRO:CB	2.85	0.54
1:A:1323:ARG:HG3	1:A:1323:ARG:HH11	1.73	0.54
1:C:1273:GLU:OE2	1:C:1276:ARG:NH2	2.41	0.54
1:E:1323:ARG:HH12	1:E:1352:VAL:HG13	1.73	0.54
1:E:1286:PRO:O	1:E:1310:ASN:HB3	2.07	0.54
1:D:1264:SER:O	1:D:1265:PHE:HB3	2.08	0.54
1:E:479:ALA:HB3	1:E:497:PHE:HE2	1.72	0.54
1:B:463:TYR:HD1	1:B:469:PHE:HB2	1.71	0.54
1:F:463:TYR:HB2	1:F:475:ALA:HB2	1.90	0.54
1:F:1185:MET:HE2	1:F:1186:SER:O	2.08	0.54
1:B:488:ILE:CG2	1:B:503:TYR:HD1	2.19	0.54
1:C:1288:ARG:HH11	1:C:1290:ILE:CD1	2.20	0.54
1:E:447:ILE:HG22	1:E:448:THR:N	2.21	0.54
1:E:449:ILE:HD13	1:E:491:THR:HG21	1.90	0.54
1:A:458:VAL:O	1:A:462:LEU:HB2	2.07	0.54
1:D:1183:LEU:HB2	1:D:1431:TYR:CE2	2.43	0.54
1:A:1184:LEU:CB	1:A:1193:SER:OG	2.56	0.54
1:E:490:HIS:CD2	1:E:494:LYS:HB3	2.43	0.54
1:A:1359:ALA:HB3	1:A:1362:LYS:HD3	1.90	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:489:ARG:HH21	1:C:1410:LYS:HE3	1.73	0.54
1:F:1286:PRO:O	1:F:1310:ASN:HB3	2.07	0.54
1:F:1322:VAL:HB	1:F:1353:TRP:HB3	1.90	0.54
1:B:451:ASN:HD21	1:B:1213:LYS:HG3	1.73	0.54
1:D:1317:ALA:HB2	1:D:1392:VAL:HG12	1.90	0.53
1:F:1408:GLU:OE2	1:F:1410:LYS:HB2	2.08	0.53
1:C:453:PHE:HE1	1:C:503:TYR:HB2	1.72	0.53
1:F:1312:LYS:HB2	1:F:1312:LYS:HZ2	1.73	0.53
1:B:1434:ARG:HH11	1:B:1434:ARG:HG3	1.73	0.53
1:D:479:ALA:HA	1:D:482:LEU:HD12	1.90	0.53
1:E:426:VAL:O	1:E:429:ALA:HB3	2.07	0.53
1:E:1359:ALA:HB3	1:E:1362:LYS:CE	2.38	0.53
1:D:432:ALA:HB3	1:D:435:SER:OG	2.09	0.53
1:A:1244:ASP:HB2	1:A:1278:ARG:O	2.09	0.53
1:C:427:THR:OG1	1:C:487:LEU:HD23	2.08	0.53
1:F:1408:GLU:HG3	1:F:1411:LEU:HB2	1.89	0.53
1:C:1323:ARG:HB3	1:C:1387:SER:OG	2.09	0.53
1:A:1253:ARG:HB2	1:A:1264:SER:OG	2.08	0.53
1:E:1293:VAL:HG21	1:E:1383:ARG:HH11	1.73	0.53
1:B:1294:ARG:HB3	1:B:1294:ARG:HH11	1.73	0.53
1:C:490:HIS:CD2	1:C:494:LYS:HB3	2.42	0.53
1:B:1277:TYR:N	1:B:1277:TYR:CD2	2.77	0.53
1:E:1345:LYS:NZ	1:E:1354:LYS:NZ	2.56	0.53
1:B:1384:PRO:O	1:B:1435:CYS:SG	2.66	0.53
1:D:1309:SER:OG	1:D:1358:MET:SD	2.67	0.53
1:E:1399:LEU:HD23	1:E:1400:LYS:N	2.23	0.53
1:B:1341:LYS:NZ	1:B:1343:LYS:HE3	2.24	0.53
1:F:1277:TYR:CD2	1:F:1277:TYR:N	2.76	0.53
1:C:1183:LEU:HD22	1:C:1285:LEU:HD22	1.91	0.53
1:A:1375:THR:CG2	1:A:1378:LYS:HD3	2.38	0.53
1:C:1399:LEU:C	1:C:1399:LEU:HD23	2.29	0.53
1:E:1206:LEU:CD2	1:E:1406:VAL:HG11	2.38	0.53
1:F:1188:GLN:NE2	1:F:1190:GLN:HG2	2.24	0.53
1:C:1318:GLN:NE2	1:C:1357:ARG:NH1	2.51	0.53
1:E:1333:VAL:HG22	1:E:1370:ILE:HG13	1.91	0.53
1:D:1324:ILE:CG2	1:D:1351:ILE:HB	2.36	0.53
1:E:1298:ARG:CD	1:E:1374:PRO:HA	2.39	0.53
1:F:1402:ARG:O	1:F:1403:TYR:HB3	2.09	0.53
1:C:462:LEU:O	1:C:466:VAL:HG23	2.09	0.53
1:D:1289:VAL:O	1:D:1291:PRO:HD3	2.08	0.53
1:D:1292:LEU:HD12	1:D:1304:LYS:HE2	1.91	0.53
1:B:1202:MET:SD	1:B:1272:PHE:HZ	2.31	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:504:VAL:HB	1:E:1211:GLU:OE1	2.09	0.53
1:E:466:VAL:HG11	1:E:469:PHE:HE2	1.74	0.53
1:C:1276:ARG:CZ	1:C:1276:ARG:HB2	2.38	0.53
1:F:1217:ASN:HD22	1:F:1400:LYS:HB2	1.74	0.53
1:C:1288:ARG:NH1	1:C:1290:ILE:CD1	2.71	0.53
1:A:1241:ILE:O	1:A:1241:ILE:HG22	2.08	0.53
1:D:1196:VAL:HG23	1:D:1279:THR:HG22	1.90	0.52
1:E:491:THR:HG22	1:E:492:VAL:CG1	2.39	0.52
1:D:422:ASP:O	1:D:426:VAL:HG23	2.09	0.52
1:D:1424:TYR:N	1:D:1424:TYR:HD2	2.05	0.52
1:A:1403:TYR:CD1	1:A:1403:TYR:C	2.82	0.52
1:C:426:VAL:O	1:C:429:ALA:HB3	2.09	0.52
1:E:1319:LYS:HD2	1:E:1391:GLU:OE2	2.09	0.52
1:F:1298:ARG:HH21	1:F:1298:ARG:HG3	1.74	0.52
1:A:1434:ARG:CG	1:A:1434:ARG:NH1	2.65	0.52
1:F:1394:PHE:HD1	1:F:1394:PHE:C	2.11	0.52
1:B:489:ARG:NH1	1:B:1211:GLU:HB2	2.25	0.52
1:C:1345:LYS:HD2	1:C:1352:VAL:HG21	1.91	0.52
1:E:462:LEU:HD13	1:E:479:ALA:HB2	1.91	0.52
1:C:1174:PHE:HD1	1:C:1421:TRP:HB2	1.73	0.52
1:A:1317:ALA:HB2	1:A:1392:VAL:HG12	1.92	0.52
1:F:1177:VAL:HB	1:F:1424:TYR:CD1	2.35	0.52
1:B:1342:ALA:HB2	1:B:1353:TRP:CD1	2.44	0.52
1:F:1323:ARG:NH1	1:F:1352:VAL:HG22	2.09	0.52
1:D:1183:LEU:HD11	1:D:1191:VAL:HG13	1.92	0.52
1:D:1301:LEU:O	1:D:1370:ILE:HG12	2.09	0.52
1:E:1329:ASN:OD1	1:E:1372:LEU:HD22	2.10	0.52
1:E:1203:LYS:HB3	1:E:1205:TYR:CE1	2.37	0.52
1:C:487:LEU:HD12	1:C:487:LEU:H	1.73	0.52
1:B:1300:LYS:NZ	1:B:1302:GLU:OE1	2.38	0.52
1:D:1206:LEU:HD22	1:D:1406:VAL:HG11	1.90	0.52
1:B:426:VAL:O	1:B:429:ALA:HB3	2.09	0.52
1:B:1322:VAL:HB	1:B:1353:TRP:HB3	1.91	0.52
1:D:1173:LEU:HD12	1:D:1173:LEU:C	2.29	0.52
1:C:1211:GLU:HG3	1:C:1253:ARG:HH11	1.73	0.52
1:A:1329:ASN:ND2	1:A:1372:LEU:HD13	2.25	0.52
1:B:1252:VAL:HG22	1:B:1263:ILE:CG1	2.40	0.52
1:E:1324:ILE:CG2	1:E:1324:ILE:O	2.57	0.52
1:A:487:LEU:H	1:A:487:LEU:HD23	1.74	0.52
1:F:460:ASP:C	1:F:464:HIS:HD2	2.14	0.52
1:E:458:VAL:CG1	1:E:459:VAL:N	2.73	0.52
1:F:1294:ARG:HH11	1:F:1294:ARG:CB	2.22	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:1201:VAL:HG12	1:C:1202:MET:N	2.23	0.52
1:E:1264:SER:O	1:E:1265:PHE:HB3	2.10	0.52
1:A:1423:ARG:HB2	1:E:1158:TYR:CD1	2.44	0.51
1:D:430:MET:HE3	1:D:458:VAL:HG13	1.92	0.51
1:A:1399:LEU:C	1:A:1399:LEU:HD23	2.30	0.51
1:C:1322:VAL:HB	1:C:1353:TRP:HB3	1.91	0.51
1:E:430:MET:CE	1:E:458:VAL:HG23	2.39	0.51
1:D:1181:VAL:CG1	1:D:1396:PRO:HB3	2.41	0.51
1:B:1170:ARG:HA	1:F:1421:TRP:CH2	2.46	0.51
1:A:430:MET:O	1:A:435:SER:OG	2.28	0.51
1:F:1293:VAL:HG23	1:F:1383:ARG:HH12	1.74	0.51
1:A:449:ILE:HD12	1:A:1407:PHE:CE1	2.45	0.51
1:A:1247:THR:C	1:A:1248:PHE:CD1	2.84	0.51
1:B:1422:VAL:HG22	1:B:1423:ARG:H	1.75	0.51
1:D:1392:VAL:HB	1:D:1394:PHE:HE2	1.76	0.51
1:B:473:ARG:HG3	1:B:473:ARG:HH21	1.75	0.51
1:C:1299:THR:O	1:C:1371:GLU:HA	2.11	0.51
1:F:1331:SER:HB2	1:F:1373:LEU:CD2	2.40	0.51
1:C:449:ILE:HG22	1:C:452:ALA:HB2	1.92	0.51
1:D:1183:LEU:HD11	1:D:1191:VAL:HG11	1.93	0.51
1:F:1158:TYR:O	1:F:1159:HIS:CD2	2.64	0.51
1:F:1335:VAL:CG1	1:F:1351:ILE:HD13	2.41	0.51
1:C:427:THR:CG2	1:C:482:LEU:HD22	2.41	0.51
1:A:1253:ARG:CD	1:A:1264:SER:OG	2.49	0.51
1:D:1183:LEU:HD21	1:D:1285:LEU:CD2	2.29	0.51
1:E:497:PHE:HD1	1:E:503:TYR:HH	1.57	0.51
1:C:1331:SER:HB3	1:C:1373:LEU:HG	1.92	0.51
1:F:1214:PHE:CD1	1:F:1215:GLY:N	2.74	0.51
1:A:1296:VAL:O	1:A:1300:LYS:HB2	2.11	0.51
1:D:1289:VAL:HG22	1:D:1307:ILE:CG2	2.40	0.51
1:D:439:VAL:HG12	1:D:439:VAL:O	2.10	0.51
1:D:426:VAL:O	1:D:429:ALA:HB3	2.11	0.51
1:F:1296:VAL:HB	1:F:1300:LYS:HB2	1.93	0.51
1:E:1268:PRO:HD2	1:E:1272:PHE:CE1	2.45	0.51
1:A:1185:MET:CE	1:A:1288:ARG:HD2	2.41	0.51
1:F:1422:VAL:CG1	1:F:1423:ARG:H	2.24	0.51
1:F:1298:ARG:NH1	1:F:1375:THR:HG23	2.26	0.51
1:F:1284:ILE:HD11	1:F:1396:PRO:HA	1.93	0.51
1:D:1178:LEU:HD23	1:D:1425:ILE:HB	1.93	0.51
1:A:454:LEU:HG	1:A:456:SER:H	1.76	0.51
1:F:462:LEU:HD12	1:F:475:ALA:O	2.11	0.51
1:D:1285:LEU:CD1	1:D:1285:LEU:N	2.73	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1319:LYS:O	1:A:1390:PHE:HA	2.11	0.51
1:D:454:LEU:HB3	1:D:457:ASP:OD2	2.11	0.51
1:E:1253:ARG:HG3	1:E:1253:ARG:HH21	1.76	0.51
1:D:1413:TYR:HB2	1:D:1417:ASP:HB2	1.91	0.51
1:D:1324:ILE:CG2	1:D:1324:ILE:O	2.58	0.50
1:A:426:VAL:O	1:A:429:ALA:HB3	2.11	0.50
1:D:1320:ILE:HG23	1:D:1388:MET:CE	2.39	0.50
1:E:1300:LYS:HE2	1:E:1369:GLU:OE2	2.11	0.50
1:E:1179:GLU:OE2	1:E:1397:SER:OG	2.24	0.50
1:C:495:ILE:HG23	1:C:496:THR:HG23	1.94	0.50
1:C:1359:ALA:HB3	1:C:1362:LYS:HE2	1.92	0.50
1:F:1329:ASN:OD1	1:F:1372:LEU:HD22	2.12	0.50
1:E:487:LEU:H	1:E:487:LEU:HD23	1.75	0.50
1:B:1359:ALA:HB3	1:B:1362:LYS:HD2	1.92	0.50
1:C:460:ASP:HA	1:C:463:TYR:HE1	1.75	0.50
1:C:1174:PHE:CD1	1:C:1421:TRP:HB2	2.47	0.50
1:D:430:MET:HE2	1:D:437:LEU:HD22	1.93	0.50
1:C:1375:THR:HG22	1:C:1378:LYS:H	1.75	0.50
1:E:1170:ARG:NH2	1:E:1205:TYR:CD2	2.79	0.50
1:A:1338:MET:HE2	1:F:492:VAL:HG13	1.92	0.50
1:C:443:MET:HG3	1:C:447:ILE:O	2.11	0.50
1:F:440:ARG:O	1:F:442:ARG:HD3	2.11	0.50
1:E:1370:ILE:N	1:E:1370:ILE:HD12	2.25	0.50
1:C:1315:LEU:N	1:C:1315:LEU:HD23	2.26	0.50
1:E:1178:LEU:HB3	1:E:1427:ARG:HH12	1.76	0.50
1:A:1183:LEU:HB3	1:A:1431:TYR:CE1	2.47	0.50
1:A:1184:LEU:HB2	1:A:1193:SER:OG	2.12	0.50
1:E:479:ALA:HB3	1:E:497:PHE:CE2	2.47	0.50
1:F:1284:ILE:HG13	1:F:1396:PRO:HA	1.94	0.50
1:E:1305:VAL:HG11	1:E:1324:ILE:HD11	1.94	0.50
1:F:1214:PHE:C	1:F:1214:PHE:HD1	2.15	0.50
1:D:1216:MET:HA	1:D:1402:ARG:HG3	1.92	0.50
1:E:1327:PRO:HA	1:E:1381:TRP:CZ2	2.47	0.50
1:E:1186:SER:CA	1:E:1434:ARG:HD2	2.37	0.50
1:F:1177:VAL:HG21	1:F:1424:TYR:HE1	1.77	0.50
1:B:1249:HIS:CD2	1:B:1272:PHE:HB2	2.47	0.50
1:F:441:ASP:OD1	1:F:450:PRO:HA	2.11	0.50
1:D:1296:VAL:HB	1:D:1300:LYS:HB2	1.94	0.50
1:A:1202:MET:O	1:A:1271:GLU:HA	2.11	0.50
1:A:1298:ARG:HH21	1:A:1374:PRO:HA	1.77	0.50
1:A:1161:LEU:HB2	1:E:1422:VAL:CG2	2.38	0.50
1:A:1173:LEU:C	1:A:1173:LEU:HD12	2.30	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:1262:SER:C	1:F:1263:ILE:HD12	2.32	0.50
1:F:430:MET:HE1	1:F:437:LEU:HD22	1.94	0.50
1:B:1322:VAL:HG22	1:B:1388:MET:CE	2.42	0.50
1:E:1195:HIS:CE1	1:E:1278:ARG:HH12	2.29	0.50
1:C:1287:PHE:N	1:C:1287:PHE:CD1	2.80	0.50
1:C:1335:VAL:HG12	1:C:1368:ALA:HB2	1.93	0.50
1:C:463:TYR:CG	1:C:464:HIS:N	2.80	0.50
1:B:1323:ARG:HH11	1:B:1323:ARG:CB	2.22	0.50
1:C:1288:ARG:HG2	1:C:1288:ARG:HH11	1.76	0.50
1:E:1419:ILE:HD12	1:E:1419:ILE:N	2.26	0.50
1:E:1392:VAL:HB	1:E:1394:PHE:CE2	2.47	0.50
1:E:1299:THR:HG22	1:E:1300:LYS:HD2	1.93	0.50
1:A:463:TYR:HB3	1:A:475:ALA:HB2	1.94	0.50
1:E:458:VAL:HG13	1:E:459:VAL:N	2.27	0.50
1:E:462:LEU:HD22	1:E:475:ALA:HB1	1.92	0.50
1:F:1183:LEU:HD22	1:F:1285:LEU:CD2	2.42	0.50
1:C:495:ILE:HG23	1:C:496:THR:N	2.27	0.50
1:F:1413:TYR:HB2	1:F:1417:ASP:HB2	1.94	0.49
1:A:1205:TYR:CD2	1:A:1205:TYR:N	2.79	0.49
1:C:1419:ILE:HD12	1:C:1419:ILE:N	2.26	0.49
1:D:1324:ILE:CD1	1:D:1386:ILE:HG12	2.30	0.49
1:D:1185:MET:HG3	1:D:1191:VAL:HG22	1.94	0.49
1:A:1392:VAL:HB	1:A:1394:PHE:CD2	2.47	0.49
1:A:1293:VAL:HG12	1:A:1303:VAL:HG13	1.94	0.49
1:E:1306:VAL:HG22	1:E:1365:GLN:HB2	1.93	0.49
1:D:1294:ARG:O	1:D:1301:LEU:HD23	2.12	0.49
1:D:440:ARG:HG2	1:D:442:ARG:HH12	1.76	0.49
1:C:489:ARG:HD2	1:C:1410:LYS:HE2	1.93	0.49
1:B:1284:ILE:O	1:B:1286:PRO:HD3	2.12	0.49
1:C:458:VAL:CG1	1:C:459:VAL:N	2.76	0.49
1:A:1328:LEU:HD13	1:A:1381:TRP:CZ3	2.48	0.49
1:A:472:ARG:CG	1:A:472:ARG:NH2	2.76	0.49
1:C:1264:SER:O	1:C:1265:PHE:HB3	2.12	0.49
1:A:1345:LYS:HA	1:A:1345:LYS:CE	2.37	0.49
1:B:1415:ASP:OD2	1:B:1420:LYS:NZ	2.43	0.49
1:D:494:LYS:HE2	1:D:498:SER:OG	2.13	0.49
1:D:1249:HIS:O	1:D:1252:VAL:HG23	2.11	0.49
1:C:427:THR:HG23	1:C:482:LEU:HD22	1.94	0.49
1:D:1180:SER:CB	1:D:1427:ARG:HE	2.16	0.49
1:B:1158:TYR:HD1	1:F:1421:TRP:HB3	1.78	0.49
1:B:1413:TYR:HA	1:B:1417:ASP:OD2	2.12	0.49
1:E:1183:LEU:HD11	1:E:1191:VAL:CG1	2.42	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1421:TRP:CH2	1:F:1170:ARG:HA	2.48	0.49
1:A:1329:ASN:OD1	1:A:1378:LYS:HD2	2.13	0.49
1:F:1293:VAL:HG23	1:F:1383:ARG:NH1	2.27	0.49
1:F:1214:PHE:CD1	1:F:1214:PHE:C	2.85	0.49
1:F:439:VAL:HG13	1:F:453:PHE:HD2	1.77	0.49
1:F:1323:ARG:HH11	1:F:1323:ARG:HG3	1.76	0.49
1:B:458:VAL:O	1:B:462:LEU:CG	2.60	0.49
1:B:1394:PHE:O	1:B:1396:PRO:HD3	2.13	0.49
1:F:440:ARG:HG2	1:F:441:ASP:H	1.77	0.49
1:D:1181:VAL:HG11	1:D:1396:PRO:HB3	1.95	0.49
1:D:1250:GLN:HG3	1:D:1251:CYS:H	1.76	0.49
1:B:1375:THR:HG23	1:B:1375:THR:O	2.12	0.49
1:E:459:VAL:HG11	1:E:472:ARG:HE	1.78	0.49
1:A:1182:ASN:HB2	1:A:1195:HIS:CE1	2.46	0.49
1:C:1174:PHE:CE1	1:C:1421:TRP:HD1	2.27	0.49
1:B:1272:PHE:CD1	1:B:1272:PHE:C	2.85	0.49
1:A:1286:PRO:C	1:A:1287:PHE:HD1	2.16	0.49
1:B:1422:VAL:HG22	1:B:1423:ARG:N	2.28	0.49
1:C:430:MET:HB3	1:C:437:LEU:CD2	2.43	0.49
1:C:472:ARG:CG	1:C:472:ARG:NH2	2.74	0.48
1:A:1328:LEU:HD13	1:A:1381:TRP:HZ3	1.78	0.48
1:E:490:HIS:NE2	1:E:494:LYS:HB3	2.28	0.48
1:E:1298:ARG:HH21	1:E:1298:ARG:CG	2.26	0.48
1:B:483:LEU:HD12	1:B:488:ILE:O	2.13	0.48
1:B:1421:TRP:CZ3	1:F:1170:ARG:CB	2.96	0.48
1:B:1277:TYR:HD2	1:B:1277:TYR:N	2.11	0.48
1:E:1390:PHE:CE1	1:E:1428:SER:HB3	2.48	0.48
1:E:1173:LEU:HD12	1:E:1173:LEU:O	2.12	0.48
1:F:1277:TYR:CE1	1:F:1399:LEU:HD12	2.48	0.48
1:E:1413:TYR:HB2	1:E:1417:ASP:HB2	1.95	0.48
1:C:1244:ASP:OD2	1:C:1280:THR:CG2	2.48	0.48
1:C:440:ARG:HG2	1:C:442:ARG:HD2	1.95	0.48
1:F:1289:VAL:O	1:F:1291:PRO:HD3	2.12	0.48
1:D:1343:LYS:HE3	1:D:1345:LYS:NZ	2.27	0.48
1:E:1359:ALA:HB3	1:E:1362:LYS:CD	2.43	0.48
1:C:1251:CYS:SG	1:C:1268:PRO:HD3	2.54	0.48
1:E:457:ASP:HA	1:E:460:ASP:OD2	2.14	0.48
1:A:433:PRO:HG3	1:A:1256:LYS:HB2	1.94	0.48
1:B:1252:VAL:CG1	1:B:1252:VAL:O	2.62	0.48
1:B:1264:SER:O	1:B:1265:PHE:HB3	2.14	0.48
1:C:1276:ARG:HH11	1:C:1276:ARG:CG	2.26	0.48
1:B:440:ARG:HB3	1:B:442:ARG:NH1	2.29	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:1381:TRP:CZ3	1:C:1383:ARG:HG2	2.49	0.48
1:C:1422:VAL:CG1	1:C:1423:ARG:H	2.26	0.48
1:A:1205:TYR:HD2	1:A:1205:TYR:N	2.11	0.48
1:B:1382:ALA:O	1:B:1384:PRO:HD3	2.13	0.48
1:D:479:ALA:HA	1:D:482:LEU:CD1	2.43	0.48
1:A:1408:GLU:CD	1:A:1409:PRO:HD2	2.34	0.48
1:D:447:ILE:HG22	1:D:1414:SER:OG	2.14	0.48
1:F:1287:PHE:HD1	1:F:1388:MET:SD	2.36	0.48
1:B:494:LYS:NZ	1:B:498:SER:HB2	2.29	0.48
1:A:1173:LEU:HD22	1:A:1404:LEU:CD2	2.44	0.48
1:C:1178:LEU:HG	1:C:1425:ILE:CG2	2.44	0.48
1:E:1326:THR:HG21	1:E:1344:TYR:CE1	2.49	0.48
1:C:434:GLU:OE2	1:C:1256:LYS:NZ	2.38	0.48
1:D:1217:ASN:ND2	1:D:1400:LYS:CB	2.76	0.48
1:E:1173:LEU:C	1:E:1173:LEU:CD1	2.82	0.48
1:A:447:ILE:CG2	1:A:448:THR:N	2.77	0.48
1:F:423:MET:HA	1:F:478:TYR:OH	2.14	0.48
1:C:460:ASP:HA	1:C:463:TYR:CE1	2.48	0.48
1:C:1343:LYS:HG2	1:C:1344:TYR:N	2.28	0.48
1:E:1277:TYR:CD2	1:E:1277:TYR:N	2.82	0.48
1:C:1183:LEU:CD1	1:C:1184:LEU:N	2.72	0.48
1:A:1422:VAL:CG2	1:E:1161:LEU:HB2	2.42	0.48
1:E:1423:ARG:HD2	1:E:1425:ILE:HD11	1.94	0.48
1:A:1291:PRO:HA	1:A:1305:VAL:HG23	1.96	0.48
1:B:1249:HIS:ND1	1:B:1250:GLN:HG3	2.29	0.48
1:F:478:TYR:CZ	1:F:482:LEU:HD21	2.49	0.48
1:A:1247:THR:O	1:A:1248:PHE:CD1	2.67	0.48
1:E:1345:LYS:NZ	1:E:1354:LYS:HZ1	2.12	0.48
1:C:1329:ASN:HD21	1:C:1372:LEU:HB3	1.78	0.48
1:F:424:ALA:O	1:F:428:LYS:HG3	2.14	0.48
1:B:1185:MET:SD	1:B:1288:ARG:HD2	2.54	0.48
1:D:467:GLU:HG2	1:D:468:GLY:N	2.29	0.48
1:C:1211:GLU:CG	1:C:1253:ARG:HH11	2.27	0.47
1:E:1422:VAL:CG1	1:E:1423:ARG:H	2.26	0.47
1:A:1304:LYS:HD2	1:A:1365:GLN:HE22	1.79	0.47
1:A:1177:VAL:HB	1:A:1424:TYR:HD1	1.79	0.47
1:B:1296:VAL:O	1:B:1300:LYS:HB2	2.14	0.47
1:E:1300:LYS:HG3	1:E:1369:GLU:OE2	2.14	0.47
1:E:1253:ARG:HG3	1:E:1253:ARG:NH2	2.30	0.47
1:A:1184:LEU:HA	1:A:1432:GLU:O	2.14	0.47
1:E:1293:VAL:CG2	1:E:1383:ARG:NH1	2.77	0.47
1:A:1421:TRP:CZ3	1:E:1170:ARG:HB2	2.50	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1326:THR:HG21	1:B:1344:TYR:HE1	1.79	0.47
1:E:422:ASP:O	1:E:426:VAL:CG2	2.60	0.47
1:E:1299:THR:O	1:E:1371:GLU:HA	2.14	0.47
1:A:1277:TYR:N	1:A:1277:TYR:CD2	2.82	0.47
1:A:1298:ARG:NH2	1:A:1375:THR:H	2.12	0.47
1:A:1193:SER:O	1:A:1194:ALA:HB2	2.14	0.47
1:B:1305:VAL:CG2	1:B:1324:ILE:HD11	2.37	0.47
1:B:1158:TYR:CE2	1:F:1423:ARG:CZ	2.98	0.47
1:F:1177:VAL:HG21	1:F:1424:TYR:CE1	2.49	0.47
1:A:1299:THR:O	1:A:1371:GLU:HA	2.13	0.47
1:A:498:SER:HB3	1:A:501:CYS:SG	2.54	0.47
1:A:1289:VAL:HG22	1:A:1307:ILE:HG22	1.96	0.47
1:B:1198:GLY:C	1:B:1277:TYR:CE2	2.87	0.47
1:F:430:MET:HE2	1:F:437:LEU:HD22	1.95	0.47
1:F:1296:VAL:O	1:F:1300:LYS:HB2	2.15	0.47
1:E:1413:TYR:HA	1:E:1417:ASP:OD2	2.14	0.47
1:B:1377:ASP:OD2	1:B:1379:LYS:HE3	2.13	0.47
1:D:461:TRP:CE3	1:D:461:TRP:O	2.67	0.47
1:C:463:TYR:OH	1:C:464:HIS:CE1	2.67	0.47
1:A:489:ARG:HH12	1:A:1211:GLU:HB2	1.80	0.47
1:E:466:VAL:CG1	1:E:469:PHE:CE2	2.95	0.47
1:B:463:TYR:CD1	1:B:469:PHE:HB2	2.49	0.47
1:D:1181:VAL:CG1	1:D:1396:PRO:CB	2.93	0.47
1:A:1218:ASP:HA	1:A:1241:ILE:HB	1.97	0.47
1:D:456:SER:HA	1:D:499:GLU:CG	2.45	0.47
1:F:1250:GLN:CG	1:F:1251:CYS:N	2.77	0.47
1:C:1287:PHE:N	1:C:1287:PHE:HD1	2.13	0.47
1:F:1182:ASN:HB2	1:F:1195:HIS:CE1	2.50	0.47
1:A:1298:ARG:O	1:A:1372:LEU:HB2	2.15	0.47
1:A:1264:SER:O	1:A:1265:PHE:HB3	2.15	0.47
1:D:1353:TRP:CZ3	1:D:1366:ILE:HB	2.50	0.47
1:D:1181:VAL:HG12	1:D:1196:VAL:HG12	1.95	0.47
1:A:1421:TRP:CH2	1:E:1170:ARG:HA	2.49	0.47
1:C:1290:ILE:HD12	1:C:1290:ILE:N	2.30	0.47
1:C:1326:THR:HG22	1:C:1370:ILE:CD1	2.44	0.47
1:D:1320:ILE:CG2	1:D:1388:MET:CE	2.91	0.47
1:F:1425:ILE:O	1:F:1425:ILE:CG2	2.61	0.47
1:A:476:ARG:CG	1:A:476:ARG:HH21	2.24	0.47
1:D:441:ASP:OD2	1:D:1213:LYS:NZ	2.39	0.47
1:F:460:ASP:O	1:F:464:HIS:CD2	2.66	0.47
1:C:1298:ARG:O	1:C:1372:LEU:HD12	2.15	0.47
1:A:1277:TYR:N	1:A:1277:TYR:HD2	2.12	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1299:THR:O	1:B:1371:GLU:HA	2.14	0.47
1:E:1214:PHE:C	1:E:1214:PHE:HD2	2.18	0.47
1:D:1413:TYR:HA	1:D:1417:ASP:OD2	2.13	0.47
1:E:1178:LEU:HB3	1:E:1427:ARG:NH1	2.29	0.47
1:A:482:LEU:HD23	1:A:482:LEU:N	2.28	0.47
1:D:1329:ASN:HD22	1:D:1372:LEU:HD23	1.77	0.47
1:F:1185:MET:HE1	1:F:1289:VAL:O	2.14	0.47
1:B:1408:GLU:O	1:B:1411:LEU:O	2.33	0.47
1:C:1427:ARG:CG	1:C:1428:SER:N	2.77	0.47
1:F:453:PHE:HZ	1:F:488:ILE:HD12	1.80	0.47
1:F:1264:SER:O	1:F:1265:PHE:HB3	2.14	0.47
1:C:1402:ARG:O	1:C:1403:TYR:HB3	2.15	0.47
1:D:1187:PRO:CD	1:D:1434:ARG:HB2	2.41	0.47
1:C:489:ARG:NH2	1:C:1410:LYS:HE3	2.29	0.47
1:E:1305:VAL:HG21	1:E:1324:ILE:CD1	2.41	0.47
1:C:1408:GLU:HG2	1:C:1411:LEU:CB	2.44	0.47
1:F:1277:TYR:HD2	1:F:1277:TYR:N	2.12	0.47
1:F:495:ILE:HG13	1:F:496:THR:H	1.78	0.47
1:A:1181:VAL:HG23	1:A:1196:VAL:HG22	1.96	0.47
1:B:428:LYS:HE2	1:B:508:LEU:O	2.15	0.47
1:E:426:VAL:HG21	1:E:478:TYR:OH	2.15	0.47
1:A:443:MET:HG3	1:A:447:ILE:O	2.15	0.47
1:C:497:PHE:HD1	1:C:497:PHE:O	1.98	0.47
1:F:1276:ARG:HG2	1:F:1277:TYR:N	2.30	0.47
1:C:1330:THR:HG21	1:C:1344:TYR:OH	2.15	0.47
1:F:461:TRP:CE3	1:F:461:TRP:O	2.67	0.47
1:F:505:PHE:HB2	1:F:1253:ARG:NH2	2.30	0.47
1:A:442:ARG:HD2	1:A:502:TYR:OH	2.15	0.46
1:B:454:LEU:O	1:B:458:VAL:HG23	2.14	0.46
1:B:1199:ARG:N	1:B:1277:TYR:HE2	2.13	0.46
1:C:1290:ILE:O	1:C:1290:ILE:HG22	2.14	0.46
1:E:1322:VAL:HB	1:E:1353:TRP:HB3	1.95	0.46
1:D:1389:ASN:HA	1:D:1428:SER:OG	2.15	0.46
1:B:427:THR:HG21	1:B:487:LEU:HB3	1.97	0.46
1:E:1201:VAL:HG12	1:E:1202:MET:N	2.30	0.46
1:B:440:ARG:HD2	1:B:441:ASP:O	2.14	0.46
1:B:501:CYS:SG	1:B:503:TYR:CE2	3.06	0.46
1:B:1251:CYS:SG	1:B:1268:PRO:HD3	2.55	0.46
1:B:1325:PRO:O	1:B:1381:TRP:HH2	1.98	0.46
1:D:1296:VAL:O	1:D:1300:LYS:HB2	2.15	0.46
1:F:495:ILE:HG13	1:F:496:THR:N	2.31	0.46
1:B:1193:SER:O	1:B:1194:ALA:HB2	2.16	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:437:LEU:N	1:A:461:TRP:CD1	2.83	0.46
1:C:1265:PHE:HE1	1:C:1267:PRO:HB3	1.81	0.46
1:C:1365:GLN:HG2	1:C:1366:ILE:N	2.31	0.46
1:D:1381:TRP:CD2	1:D:1381:TRP:O	2.68	0.46
1:A:1276:ARG:HH11	1:A:1276:ARG:CG	2.27	0.46
1:F:440:ARG:CB	1:F:440:ARG:NH2	2.78	0.46
1:C:1263:ILE:HD11	1:C:1274:LEU:HD21	1.96	0.46
1:E:1355:ILE:HG22	1:E:1355:ILE:O	2.15	0.46
1:A:460:ASP:HA	1:A:463:TYR:HE2	1.77	0.46
1:A:1379:LYS:HD2	1:A:1379:LYS:N	2.19	0.46
1:B:473:ARG:CZ	1:B:473:ARG:HB2	2.45	0.46
1:D:1316:LEU:N	1:D:1316:LEU:HD23	2.30	0.46
1:B:1366:ILE:HG23	1:B:1366:ILE:O	2.15	0.46
1:A:1383:ARG:H	1:A:1383:ARG:NH1	2.14	0.46
1:F:1323:ARG:HH12	1:F:1352:VAL:CG2	2.11	0.46
1:F:1323:ARG:O	1:F:1386:ILE:HG23	2.15	0.46
1:A:461:TRP:CD1	1:A:465:HIS:CD2	3.04	0.46
1:A:1339:LYS:HB3	1:A:1339:LYS:HZ3	1.78	0.46
1:F:1361:MET:CE	1:F:1361:MET:HA	2.44	0.46
1:F:1173:LEU:HD12	1:F:1173:LEU:O	2.15	0.46
1:F:1247:THR:O	1:F:1248:PHE:CD2	2.69	0.46
1:F:1413:TYR:HA	1:F:1417:ASP:OD2	2.16	0.46
1:A:489:ARG:NH1	1:A:1211:GLU:HB2	2.30	0.46
1:D:1304:LYS:HG3	1:D:1367:SER:OG	2.14	0.46
1:C:1252:VAL:HA	1:C:1265:PHE:HB3	1.97	0.46
1:B:473:ARG:CG	1:B:473:ARG:HH21	2.28	0.46
1:A:492:VAL:CG2	1:C:1338:MET:HB3	2.45	0.46
1:B:1201:VAL:HG12	1:B:1202:MET:N	2.29	0.46
1:B:1268:PRO:HD2	1:B:1272:PHE:CD2	2.50	0.46
1:B:1434:ARG:NH1	1:B:1434:ARG:HG3	2.28	0.46
1:A:1321:GLU:OE1	1:A:1354:LYS:HE3	2.16	0.46
1:C:1211:GLU:CG	1:C:1253:ARG:NH1	2.78	0.46
1:D:1324:ILE:HG21	1:D:1351:ILE:HD12	1.96	0.46
1:A:1185:MET:HE1	1:A:1288:ARG:HD2	1.97	0.46
1:B:1172:GLU:HB3	1:B:1419:ILE:HB	1.97	0.46
1:A:1186:SER:HA	1:A:1434:ARG:HB2	1.98	0.46
1:B:1286:PRO:O	1:B:1310:ASN:HB3	2.16	0.46
1:C:433:PRO:CG	1:C:1256:LYS:HE2	2.46	0.46
1:E:480:SER:HB2	1:E:497:PHE:HD2	1.81	0.46
1:C:1217:ASN:HD21	1:C:1400:LYS:CB	2.23	0.46
1:F:447:ILE:HG22	1:F:448:THR:H	1.81	0.46
1:C:1294:ARG:NH2	1:C:1302:GLU:OE2	2.48	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1402:ARG:O	1:A:1403:TYR:HB3	2.16	0.46
1:D:1300:LYS:HD3	1:D:1300:LYS:HA	1.72	0.46
1:F:1410:LYS:HD3	1:F:1410:LYS:HA	1.71	0.46
1:C:1276:ARG:CG	1:C:1277:TYR:N	2.79	0.46
1:D:1408:GLU:CG	1:D:1411:LEU:HB2	2.38	0.46
1:D:1315:LEU:HD23	1:D:1315:LEU:N	2.31	0.46
1:A:1316:LEU:CD2	1:A:1359:ALA:HA	2.45	0.46
1:D:1390:PHE:CE2	1:D:1428:SER:HB3	2.51	0.46
1:D:1199:ARG:N	1:D:1277:TYR:HE2	2.14	0.46
1:D:1402:ARG:O	1:D:1403:TYR:HB3	2.16	0.46
1:E:1246:CYS:HB2	1:E:1276:ARG:O	2.16	0.46
1:A:1252:VAL:HG12	1:A:1253:ARG:O	2.16	0.46
1:E:462:LEU:HD22	1:E:475:ALA:CB	2.45	0.46
1:F:1188:GLN:HE21	1:F:1190:GLN:HG2	1.79	0.46
1:A:447:ILE:CG2	1:A:448:THR:H	2.26	0.46
1:E:449:ILE:HD13	1:E:491:THR:CG2	2.46	0.46
1:C:1390:PHE:HD1	1:C:1391:GLU:N	2.14	0.46
1:B:1371:GLU:O	1:B:1372:LEU:HD23	2.16	0.46
1:F:1328:LEU:HD23	1:F:1328:LEU:N	2.31	0.46
1:B:1394:PHE:C	1:B:1394:PHE:CD1	2.90	0.45
1:B:1425:ILE:O	1:B:1425:ILE:CG2	2.57	0.45
1:E:1335:VAL:HG11	1:E:1351:ILE:HG21	1.98	0.45
1:C:461:TRP:CD1	1:C:465:HIS:HD2	2.34	0.45
1:C:1287:PHE:CE2	1:C:1320:ILE:HD13	2.51	0.45
1:A:498:SER:OG	1:A:499:GLU:N	2.48	0.45
1:D:1202:MET:CE	1:D:1404:LEU:HD21	2.46	0.45
1:F:1298:ARG:O	1:F:1372:LEU:HB2	2.16	0.45
1:A:1316:LEU:HD22	1:A:1359:ALA:HA	1.98	0.45
1:E:1335:VAL:HG12	1:E:1368:ALA:CB	2.46	0.45
1:E:1280:THR:HA	1:E:1283:ILE:HD11	1.98	0.45
1:C:1173:LEU:HD11	1:C:1404:LEU:HD13	1.97	0.45
1:C:1342:ALA:HB2	1:C:1353:TRP:CD1	2.52	0.45
1:D:437:LEU:HD12	1:D:438:GLU:N	2.31	0.45
1:C:490:HIS:CE1	1:C:494:LYS:HB3	2.51	0.45
1:C:1298:ARG:O	1:C:1372:LEU:HB2	2.16	0.45
1:F:1335:VAL:HG12	1:F:1351:ILE:HD13	1.97	0.45
1:B:1186:SER:HB3	1:B:1190:GLN:HB2	1.99	0.45
1:D:1288:ARG:NH1	1:D:1310:ASN:OD1	2.48	0.45
1:C:469:PHE:CE1	1:C:475:ALA:HA	2.51	0.45
1:D:430:MET:CE	1:D:458:VAL:HG13	2.46	0.45
1:B:1344:TYR:CD2	1:B:1344:TYR:O	2.69	0.45
1:E:1359:ALA:HB3	1:E:1362:LYS:NZ	2.32	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:1198:GLY:C	1:D:1277:TYR:CE2	2.90	0.45
1:B:1331:SER:OG	1:B:1371:GLU:HB3	2.16	0.45
1:F:456:SER:HA	1:F:499:GLU:HG2	1.99	0.45
1:F:1299:THR:O	1:F:1371:GLU:HA	2.17	0.45
1:C:1289:VAL:O	1:C:1291:PRO:HD3	2.17	0.45
1:D:482:LEU:HD23	1:D:487:LEU:HD12	1.97	0.45
1:D:442:ARG:HD3	1:D:502:TYR:CE1	2.51	0.45
1:D:1286:PRO:HG2	1:D:1390:PHE:HE1	1.82	0.45
1:C:1182:ASN:OD1	1:C:1430:ILE:N	2.49	0.45
1:C:506:GLY:O	1:C:1253:ARG:NH2	2.49	0.45
1:D:1290:ILE:HB	1:D:1306:VAL:CG1	2.36	0.45
1:D:456:SER:OG	1:D:457:ASP:N	2.50	0.45
1:B:1290:ILE:N	1:B:1290:ILE:HD12	2.31	0.45
1:B:1330:THR:HG23	1:B:1370:ILE:HG23	1.97	0.45
1:A:1183:LEU:HG	1:A:1184:LEU:H	1.81	0.45
1:A:1288:ARG:HH12	1:A:1290:ILE:HG13	1.80	0.45
1:F:1181:VAL:CG1	1:F:1396:PRO:HB3	2.46	0.45
1:B:1187:PRO:HD3	1:B:1434:ARG:CB	2.46	0.45
1:B:1365:GLN:HG2	1:B:1366:ILE:N	2.31	0.45
1:E:1247:THR:C	1:E:1248:PHE:CD1	2.90	0.45
1:E:471:GLU:HG2	1:E:472:ARG:N	2.32	0.45
1:E:497:PHE:CE1	1:E:498:SER:O	2.70	0.45
1:B:442:ARG:NH2	1:B:452:ALA:O	2.49	0.45
1:A:1345:LYS:HB3	1:A:1348:GLU:OE2	2.17	0.45
1:B:1275:MET:HE3	1:B:1276:ARG:O	2.16	0.45
1:D:1381:TRP:CG	1:D:1381:TRP:O	2.70	0.45
1:A:1203:LYS:HB3	1:A:1205:TYR:HE2	1.82	0.45
1:A:1266:ILE:HG22	1:A:1266:ILE:O	2.16	0.45
1:F:1324:ILE:O	1:F:1324:ILE:CG2	2.63	0.45
1:F:1298:ARG:HH12	1:F:1375:THR:H	1.64	0.45
1:C:1267:PRO:HA	1:C:1268:PRO:HD3	1.90	0.45
1:F:1316:LEU:CD2	1:F:1357:ARG:HD2	2.47	0.45
1:B:1179:GLU:OE2	1:B:1277:TYR:OH	2.26	0.45
1:E:1195:HIS:CE1	1:E:1278:ARG:NH1	2.85	0.45
1:F:1321:GLU:OE1	1:F:1354:LYS:HG2	2.17	0.45
1:F:1434:ARG:NH1	1:F:1434:ARG:HG2	2.32	0.45
1:A:1311:PHE:CE1	1:A:1360:GLY:HA2	2.51	0.45
1:D:1335:VAL:HG12	1:D:1368:ALA:CB	2.47	0.45
1:B:1402:ARG:O	1:B:1403:TYR:HB3	2.17	0.45
1:A:1375:THR:HG22	1:A:1378:LYS:HD3	1.99	0.44
1:D:1192:LEU:CD1	1:D:1434:ARG:HH22	2.31	0.44
1:E:453:PHE:HZ	1:E:488:ILE:HD12	1.82	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1422:VAL:O	1:E:1158:TYR:HD1	2.01	0.44
1:C:1187:PRO:HD3	1:C:1434:ARG:CB	2.46	0.44
1:A:1249:HIS:CD2	1:A:1272:PHE:HD2	2.35	0.44
1:B:1352:VAL:HG11	1:B:1354:LYS:HE3	1.99	0.44
1:F:1172:GLU:HB2	1:F:1419:ILE:O	2.17	0.44
1:E:1327:PRO:HG3	1:E:1381:TRP:CD2	2.51	0.44
1:A:1307:ILE:CD1	1:A:1358:MET:HE1	2.47	0.44
1:B:1390:PHE:C	1:B:1390:PHE:CD1	2.91	0.44
1:A:494:LYS:NZ	1:C:1338:MET:O	2.39	0.44
1:A:1171:ASN:ND2	1:A:1207:SER:H	2.14	0.44
1:A:1413:TYR:HA	1:A:1417:ASP:OD2	2.18	0.44
1:E:1267:PRO:HA	1:E:1268:PRO:HD3	1.89	0.44
1:F:461:TRP:C	1:F:461:TRP:CE3	2.91	0.44
1:C:458:VAL:HG13	1:C:459:VAL:N	2.32	0.44
1:B:463:TYR:CE1	1:B:469:PHE:O	2.61	0.44
1:E:1161:LEU:HD12	1:E:1162:GLU:N	2.32	0.44
1:B:1174:PHE:HB2	1:B:1203:LYS:HB2	1.99	0.44
1:E:1286:PRO:HG2	1:E:1390:PHE:CZ	2.52	0.44
1:D:1299:THR:O	1:D:1371:GLU:HA	2.18	0.44
1:F:442:ARG:HB3	1:F:502:TYR:CE2	2.52	0.44
1:F:1206:LEU:HD22	1:F:1406:VAL:HG11	1.99	0.44
1:F:463:TYR:HB2	1:F:475:ALA:CB	2.48	0.44
1:C:1280:THR:HA	1:C:1283:ILE:HD11	1.99	0.44
1:D:1298:ARG:HE	1:D:1375:THR:H	1.64	0.44
1:C:1287:PHE:CZ	1:C:1320:ILE:HD13	2.52	0.44
1:C:423:MET:CE	1:C:485:ALA:HB2	2.48	0.44
1:B:1390:PHE:CZ	1:B:1428:SER:HB3	2.52	0.44
1:D:469:PHE:HZ	1:D:478:TYR:CG	2.36	0.44
1:E:1324:ILE:HG22	1:E:1351:ILE:HB	1.99	0.44
1:C:1185:MET:HE1	1:C:1289:VAL:O	2.18	0.44
1:B:1330:THR:HG23	1:B:1370:ILE:CG2	2.48	0.44
1:E:476:ARG:HG2	1:E:476:ARG:NH2	2.32	0.44
1:C:1193:SER:O	1:C:1194:ALA:HB2	2.18	0.44
1:A:1328:LEU:HD22	1:A:1381:TRP:CZ3	2.53	0.44
1:A:1183:LEU:HB3	1:A:1431:TYR:HD1	1.82	0.44
1:B:453:PHE:HZ	1:B:488:ILE:CD1	2.24	0.44
1:A:1173:LEU:CD2	1:A:1404:LEU:HD23	2.47	0.44
1:A:1186:SER:OG	1:A:1190:GLN:HB2	2.17	0.44
1:D:1201:VAL:HG12	1:D:1202:MET:N	2.31	0.44
1:E:1402:ARG:O	1:E:1403:TYR:HB3	2.17	0.44
1:B:1315:LEU:N	1:B:1315:LEU:CD1	2.80	0.44
1:A:430:MET:HB3	1:A:437:LEU:HD23	1.98	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:502:TYR:C	1:B:503:TYR:HD2	2.21	0.44
1:E:1170:ARG:NH2	1:E:1205:TYR:HD2	2.16	0.44
1:E:461:TRP:C	1:E:461:TRP:CE3	2.91	0.44
1:D:1170:ARG:NH1	1:D:1172:GLU:CG	2.80	0.44
1:F:1293:VAL:HG21	1:F:1383:ARG:HH11	1.81	0.44
1:F:442:ARG:CB	1:F:502:TYR:CE2	3.01	0.44
1:A:1245:ASP:O	1:A:1246:CYS:HB3	2.18	0.44
1:C:1260:GLU:O	1:C:1261:ARG:CB	2.66	0.44
1:A:1380:LYS:O	1:A:1381:TRP:HB3	2.18	0.44
1:D:1184:LEU:HD23	1:D:1184:LEU:O	2.18	0.44
1:A:1288:ARG:NH1	1:A:1290:ILE:HG13	2.32	0.44
1:B:1425:ILE:HD11	1:F:1156:PRO:HG3	1.95	0.44
1:D:1170:ARG:NH1	1:D:1172:GLU:OE2	2.50	0.44
1:A:495:ILE:CG2	1:A:496:THR:N	2.81	0.44
1:F:1276:ARG:CG	1:F:1277:TYR:N	2.81	0.44
1:F:1366:ILE:O	1:F:1366:ILE:HG23	2.18	0.44
1:E:1298:ARG:CZ	1:E:1298:ARG:HB3	2.47	0.44
1:D:1326:THR:CG2	1:D:1344:TYR:CE1	2.99	0.44
1:F:1415:ASP:CG	1:F:1420:LYS:HZ1	2.20	0.44
1:E:1326:THR:HG23	1:E:1350:ALA:HA	1.99	0.44
1:C:1183:LEU:HD22	1:C:1285:LEU:CD2	2.47	0.43
1:E:471:GLU:HG2	1:E:472:ARG:H	1.83	0.43
1:B:1360:GLY:O	1:B:1361:MET:C	2.56	0.43
1:A:433:PRO:HD3	1:A:1254:LEU:O	2.18	0.43
1:C:469:PHE:HZ	1:C:478:TYR:HD2	1.61	0.43
1:D:1289:VAL:HG22	1:D:1307:ILE:HG23	2.00	0.43
1:E:1293:VAL:HG21	1:E:1383:ARG:NH1	2.33	0.43
1:E:1298:ARG:O	1:E:1372:LEU:HB2	2.18	0.43
1:F:1408:GLU:HG3	1:F:1411:LEU:N	2.33	0.43
1:C:1249:HIS:O	1:C:1252:VAL:HG23	2.17	0.43
1:D:1170:ARG:NH1	1:D:1172:GLU:CD	2.69	0.43
1:E:495:ILE:HG23	1:E:496:THR:HG22	1.99	0.43
1:B:1392:VAL:O	1:B:1392:VAL:HG23	2.17	0.43
1:C:1206:LEU:HD13	1:C:1406:VAL:CG2	2.48	0.43
1:A:1328:LEU:CD1	1:A:1349:ASN:ND2	2.81	0.43
1:B:1248:PHE:HB3	1:B:1252:VAL:HG11	1.99	0.43
1:B:437:LEU:N	1:B:461:TRP:CD1	2.87	0.43
1:A:1338:MET:HE1	1:F:491:THR:HB	2.00	0.43
1:E:1178:LEU:C	1:E:1427:ARG:HH12	2.21	0.43
1:A:1256:LYS:HE2	1:A:1259:SER:HB2	1.99	0.43
1:C:442:ARG:HG2	1:C:502:TYR:CE1	2.53	0.43
1:E:459:VAL:CG1	1:E:472:ARG:HE	2.32	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1252:VAL:HA	1:B:1265:PHE:HB3	2.01	0.43
1:F:1408:GLU:CD	1:F:1409:PRO:HD2	2.38	0.43
1:C:1331:SER:OG	1:C:1371:GLU:HB3	2.18	0.43
1:C:1333:VAL:CG2	1:C:1370:ILE:HG12	2.45	0.43
1:A:1336:ILE:N	1:A:1336:ILE:CD1	2.80	0.43
1:C:1254:LEU:HD23	1:C:1254:LEU:N	2.33	0.43
1:D:1186:SER:OG	1:D:1190:GLN:HB3	2.18	0.43
1:D:1301:LEU:O	1:D:1370:ILE:CG1	2.67	0.43
1:B:1173:LEU:HD11	1:B:1420:LYS:CG	2.43	0.43
1:F:1284:ILE:CD1	1:F:1396:PRO:HA	2.49	0.43
1:E:1290:ILE:CD1	1:E:1308:LYS:HE3	2.48	0.43
1:F:1404:LEU:C	1:F:1404:LEU:CD2	2.86	0.43
1:C:459:VAL:O	1:C:463:TYR:HD1	2.01	0.43
1:D:1192:LEU:HD11	1:D:1434:ARG:HH12	1.82	0.43
1:D:462:LEU:HA	1:D:462:LEU:HD23	1.83	0.43
1:D:470:PRO:CG	1:D:474:GLU:HG3	2.48	0.43
1:F:1183:LEU:HD12	1:F:1193:SER:O	2.19	0.43
1:F:1298:ARG:HH12	1:F:1375:THR:CB	2.32	0.43
1:E:1193:SER:O	1:E:1194:ALA:HB2	2.18	0.43
1:A:1311:PHE:O	1:A:1312:LYS:C	2.57	0.43
1:F:1360:GLY:O	1:F:1361:MET:C	2.57	0.43
1:C:449:ILE:CG2	1:C:452:ALA:HB2	2.49	0.43
1:B:1200:VAL:HB	1:B:1275:MET:HG3	2.01	0.43
1:A:1190:GLN:OE1	1:A:1190:GLN:HA	2.18	0.43
1:D:1332:GLY:O	1:D:1371:GLU:HB2	2.19	0.43
1:F:440:ARG:CB	1:F:440:ARG:HH21	2.31	0.43
1:A:449:ILE:CD1	1:A:1407:PHE:CE1	3.01	0.43
1:D:1298:ARG:O	1:D:1372:LEU:HB2	2.18	0.43
1:A:1422:VAL:CG2	1:E:1161:LEU:HD22	2.48	0.43
1:B:440:ARG:HB3	1:B:442:ARG:HH11	1.84	0.43
1:E:427:THR:HG21	1:E:487:LEU:CB	2.49	0.43
1:A:1255:SER:HB2	1:A:1263:ILE:HG22	2.01	0.43
1:F:456:SER:HA	1:F:499:GLU:CG	2.48	0.43
1:F:495:ILE:HG13	1:F:496:THR:HG23	2.00	0.43
1:C:1277:TYR:CE1	1:C:1399:LEU:HD12	2.54	0.43
1:B:488:ILE:HD13	1:B:505:PHE:HA	2.01	0.43
1:B:1333:VAL:CG1	1:B:1344:TYR:CD2	3.02	0.43
1:A:1360:GLY:O	1:A:1361:MET:C	2.56	0.43
1:C:1408:GLU:HG2	1:C:1411:LEU:HD12	2.01	0.43
1:D:1184:LEU:CD2	1:D:1192:LEU:HB2	2.49	0.42
1:F:1390:PHE:CD1	1:F:1390:PHE:C	2.92	0.42
1:C:1378:LYS:HG2	1:C:1379:LYS:N	2.32	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:1360:GLY:O	1:E:1361:MET:C	2.57	0.42
1:F:1173:LEU:HD11	1:F:1420:LYS:HG2	2.00	0.42
1:C:430:MET:HB3	1:C:437:LEU:HD22	2.01	0.42
1:C:1277:TYR:HE1	1:C:1399:LEU:HD12	1.84	0.42
1:D:1306:VAL:HG23	1:D:1365:GLN:HB2	2.01	0.42
1:E:449:ILE:HG22	1:E:450:PRO:HD2	2.00	0.42
1:C:1202:MET:CE	1:C:1204:SER:HB2	2.49	0.42
1:D:483:LEU:HD22	1:D:503:TYR:CE1	2.54	0.42
1:E:1212:CYS:SG	1:E:1267:PRO:HD3	2.59	0.42
1:D:1360:GLY:O	1:D:1361:MET:C	2.58	0.42
1:C:1196:VAL:HG23	1:C:1283:ILE:HD13	2.01	0.42
1:D:1298:ARG:HE	1:D:1375:THR:N	2.17	0.42
1:D:1408:GLU:HG3	1:D:1411:LEU:H	1.85	0.42
1:B:1156:PRO:HA	1:B:1157:PRO:HD3	1.77	0.42
1:E:427:THR:HG21	1:E:487:LEU:HB3	2.01	0.42
1:A:447:ILE:HG23	1:A:1414:SER:HB3	2.01	0.42
1:C:1360:GLY:O	1:C:1361:MET:C	2.58	0.42
1:B:1296:VAL:HB	1:B:1300:LYS:HB2	2.01	0.42
1:D:478:TYR:CD2	1:D:482:LEU:HD11	2.55	0.42
1:A:1345:LYS:CB	1:A:1348:GLU:OE2	2.68	0.42
1:F:1159:HIS:ND1	1:F:1167:GLY:O	2.52	0.42
1:A:1338:MET:CE	1:F:491:THR:HB	2.49	0.42
1:A:1171:ASN:O	1:A:1418:VAL:HG13	2.20	0.42
1:F:1249:HIS:CE1	1:F:1250:GLN:HG2	2.54	0.42
1:F:463:TYR:HD1	1:F:469:PHE:HB3	1.85	0.42
1:E:497:PHE:CD1	1:E:497:PHE:C	2.93	0.42
1:D:1298:ARG:NH1	1:D:1375:THR:HG23	2.35	0.42
1:B:440:ARG:CG	1:B:441:ASP:N	2.83	0.42
1:C:1177:VAL:HB	1:C:1424:TYR:HD1	1.84	0.42
1:C:1324:ILE:HA	1:C:1386:ILE:HG12	2.00	0.42
1:D:1422:VAL:CG1	1:D:1423:ARG:N	2.80	0.42
1:D:1211:GLU:HA	1:D:1266:ILE:HD13	2.01	0.42
1:E:1252:VAL:HA	1:E:1265:PHE:HB3	2.01	0.42
1:E:1251:CYS:SG	1:E:1268:PRO:HD3	2.60	0.42
1:E:1273:GLU:OE2	1:E:1276:ARG:NH2	2.52	0.42
1:B:1177:VAL:CG2	1:B:1424:TYR:HD1	2.32	0.42
1:B:443:MET:HE3	1:B:446:LYS:O	2.18	0.42
1:F:463:TYR:HE1	1:F:469:PHE:O	2.02	0.42
1:D:1171:ASN:OD1	1:D:1206:LEU:HA	2.20	0.42
1:E:450:PRO:O	1:E:450:PRO:HG2	2.19	0.42
1:C:1335:VAL:HG11	1:C:1351:ILE:HG21	2.01	0.42
1:D:1192:LEU:CD1	1:D:1434:ARG:HH12	2.33	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1312:LYS:HA	1:B:1313:PRO:HD3	1.93	0.42
1:D:1327:PRO:HA	1:D:1381:TRP:CE2	2.54	0.42
1:F:1179:GLU:OE1	1:F:1196:VAL:HG11	2.20	0.42
1:C:490:HIS:HA	1:C:503:TYR:HD1	1.84	0.42
1:A:1255:SER:HB3	1:A:1263:ILE:HA	2.02	0.42
1:F:441:ASP:C	1:F:442:ARG:HD3	2.39	0.42
1:A:1245:ASP:O	1:A:1246:CYS:CB	2.66	0.42
1:E:1304:LYS:HE2	1:E:1304:LYS:HB3	1.90	0.42
1:A:1290:ILE:CD1	1:A:1290:ILE:N	2.78	0.42
1:B:1263:ILE:HA	1:B:1263:ILE:HD12	1.88	0.42
1:D:462:LEU:CD1	1:D:478:TYR:HD2	2.33	0.42
1:F:1402:ARG:CG	1:F:1402:ARG:NH1	2.81	0.42
1:D:1174:PHE:HB2	1:D:1203:LYS:HB2	2.02	0.42
1:C:1188:GLN:CD	1:C:1188:GLN:N	2.73	0.42
1:A:462:LEU:O	1:A:466:VAL:CG2	2.68	0.42
1:F:462:LEU:HA	1:F:462:LEU:HD23	1.77	0.42
1:B:1276:ARG:CG	1:B:1277:TYR:N	2.76	0.42
1:B:1211:GLU:HA	1:B:1266:ILE:CD1	2.44	0.42
1:C:1201:VAL:CG1	1:C:1202:MET:N	2.82	0.42
1:C:1403:TYR:CD1	1:C:1403:TYR:C	2.93	0.42
1:C:423:MET:HE1	1:C:485:ALA:HB2	2.01	0.42
1:F:1404:LEU:C	1:F:1404:LEU:HD23	2.40	0.42
1:A:473:ARG:HH21	1:A:473:ARG:HG2	1.85	0.42
1:C:459:VAL:HG11	1:C:472:ARG:NH2	2.34	0.42
1:C:463:TYR:HB3	1:C:475:ALA:HB2	2.01	0.42
1:B:463:TYR:HD1	1:B:469:PHE:HB3	1.85	0.42
1:F:1184:LEU:HA	1:F:1432:GLU:O	2.20	0.42
1:D:1324:ILE:HA	1:D:1325:PRO:HD2	1.96	0.41
1:D:1184:LEU:HD13	1:D:1193:SER:HB2	2.02	0.41
1:C:1246:CYS:SG	1:C:1248:PHE:CZ	3.13	0.41
1:B:471:GLU:HG3	1:B:473:ARG:H	1.85	0.41
1:E:1345:LYS:HD2	1:E:1352:VAL:HG21	2.02	0.41
1:E:1276:ARG:CG	1:E:1277:TYR:N	2.83	0.41
1:F:435:SER:HG	1:F:461:TRP:HE1	1.67	0.41
1:A:1382:ALA:HB1	1:A:1383:ARG:HH22	1.85	0.41
1:D:1334:GLN:HG3	1:D:1369:GLU:HB3	2.02	0.41
1:C:1399:LEU:C	1:C:1399:LEU:CD2	2.88	0.41
1:F:498:SER:O	1:F:503:TYR:OH	2.31	0.41
1:A:437:LEU:HD12	1:A:438:GLU:N	2.35	0.41
1:B:1174:PHE:O	1:B:1175:LEU:HD23	2.20	0.41
1:B:1181:VAL:HG22	1:B:1396:PRO:CB	2.50	0.41
1:F:1392:VAL:HG21	1:F:1394:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:443:MET:HE2	1:D:448:THR:HG23	2.02	0.41
1:E:1361:MET:O	1:E:1362:LYS:HG3	2.20	0.41
1:E:1216:MET:HE1	1:E:1399:LEU:HD11	2.02	0.41
1:E:1311:PHE:O	1:E:1312:LYS:C	2.57	0.41
1:A:459:VAL:O	1:A:462:LEU:HB3	2.19	0.41
1:C:1406:VAL:O	1:C:1406:VAL:CG1	2.67	0.41
1:D:1187:PRO:HD3	1:D:1434:ARG:HB3	2.01	0.41
1:E:1298:ARG:NE	1:E:1374:PRO:HA	2.35	0.41
1:C:1293:VAL:HG21	1:C:1383:ARG:NH1	2.34	0.41
1:D:1312:LYS:HA	1:D:1313:PRO:HD3	1.88	0.41
1:F:440:ARG:CZ	1:F:440:ARG:HB3	2.50	0.41
1:F:1342:ALA:HB2	1:F:1353:TRP:CD1	2.56	0.41
1:B:444:TRP:C	1:B:445:LEU:HG	2.40	0.41
1:A:1183:LEU:HD13	1:A:1285:LEU:CD2	2.50	0.41
1:E:497:PHE:HD1	1:E:503:TYR:OH	2.03	0.41
1:E:1298:ARG:NH2	1:E:1298:ARG:CG	2.83	0.41
1:F:1188:GLN:HB2	1:F:1190:GLN:HE21	1.86	0.41
1:F:1298:ARG:O	1:F:1372:LEU:CD1	2.69	0.41
1:E:482:LEU:CD2	1:E:487:LEU:HD12	2.50	0.41
1:E:489:ARG:NH2	1:E:1409:PRO:CG	2.84	0.41
1:F:1247:THR:CG2	1:F:1276:ARG:HD2	2.49	0.41
1:B:1287:PHE:HE2	1:B:1358:MET:SD	2.43	0.41
1:F:1323:ARG:HB2	1:F:1323:ARG:CZ	2.50	0.41
1:D:1193:SER:O	1:D:1194:ALA:HB2	2.21	0.41
1:D:1181:VAL:HG12	1:D:1196:VAL:CG1	2.50	0.41
1:B:1179:GLU:HB3	1:B:1196:VAL:CG1	2.50	0.41
1:E:461:TRP:CE3	1:E:461:TRP:O	2.73	0.41
1:C:497:PHE:CD1	1:C:497:PHE:C	2.94	0.41
1:A:1323:ARG:HG3	1:A:1323:ARG:NH1	2.36	0.41
1:E:456:SER:HA	1:E:499:GLU:HG2	2.02	0.41
1:D:1214:PHE:O	1:D:1262:SER:HA	2.20	0.41
1:B:1174:PHE:CD2	1:B:1421:TRP:HB2	2.55	0.41
1:F:1213:LYS:HE2	1:F:1403:TYR:OH	2.21	0.41
1:B:1425:ILE:CD1	1:F:1156:PRO:HG3	2.50	0.41
1:F:1178:LEU:HD12	1:F:1199:ARG:NH1	2.36	0.41
1:C:447:ILE:HG23	1:C:448:THR:H	1.84	0.41
1:F:1311:PHE:CE1	1:F:1360:GLY:CA	3.03	0.41
1:B:447:ILE:CG2	1:B:448:THR:H	2.33	0.41
1:F:1339:LYS:HD3	1:F:1364:SER:OG	2.21	0.41
1:A:1292:LEU:HD12	1:A:1292:LEU:HA	1.66	0.41
1:C:460:ASP:O	1:C:463:TYR:CD1	2.73	0.41
1:A:1390:PHE:CD1	1:A:1428:SER:HB3	2.53	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:1312:LYS:NZ	1:F:1312:LYS:CB	2.83	0.41
1:E:492:VAL:O	1:E:492:VAL:CG2	2.69	0.41
1:A:1171:ASN:ND2	1:A:1413:TYR:CZ	2.89	0.41
1:E:1289:VAL:O	1:E:1291:PRO:HD3	2.21	0.41
1:B:447:ILE:CG2	1:B:448:THR:N	2.83	0.41
1:E:1402:ARG:HH21	1:E:1402:ARG:HG2	1.85	0.41
1:E:1402:ARG:NH2	1:E:1402:ARG:HG2	2.36	0.41
1:F:1175:LEU:HD23	1:F:1175:LEU:HA	1.90	0.41
1:D:488:ILE:HD13	1:D:488:ILE:HA	1.74	0.41
1:C:1184:LEU:CB	1:C:1193:SER:HB2	2.50	0.41
1:C:1206:LEU:HD13	1:C:1406:VAL:HG21	2.03	0.41
1:A:1183:LEU:HD13	1:A:1285:LEU:HD21	2.03	0.41
1:E:1298:ARG:O	1:E:1372:LEU:HD12	2.21	0.41
1:F:1186:SER:HB3	1:F:1192:LEU:HD21	2.02	0.41
1:B:1294:ARG:NH1	1:B:1302:GLU:CG	2.80	0.41
1:C:1381:TRP:CZ2	1:C:1383:ARG:HG2	2.55	0.41
1:B:431:ALA:O	1:B:432:ALA:C	2.59	0.41
1:E:1174:PHE:HB2	1:E:1203:LYS:HB2	2.03	0.41
1:F:447:ILE:H	1:F:447:ILE:HG13	1.57	0.41
1:D:1216:MET:C	1:D:1402:ARG:HG3	2.41	0.41
1:B:482:LEU:N	1:B:482:LEU:HD23	2.36	0.41
1:C:434:GLU:HA	1:C:434:GLU:OE1	2.21	0.41
1:F:458:VAL:O	1:F:462:LEU:CB	2.66	0.41
1:D:1366:ILE:O	1:D:1366:ILE:HG23	2.21	0.41
1:E:462:LEU:CD2	1:E:475:ALA:HB1	2.51	0.41
1:C:1199:ARG:HG3	1:C:1273:GLU:HG3	2.03	0.41
1:A:1305:VAL:HG12	1:A:1366:ILE:CG2	2.42	0.41
1:B:1404:LEU:O	1:B:1420:LYS:NZ	2.50	0.41
1:B:1339:LYS:NZ	1:B:1363:GLU:O	2.54	0.41
1:C:490:HIS:NE2	1:C:494:LYS:HD3	2.36	0.41
1:B:1250:GLN:OE1	1:B:1251:CYS:N	2.54	0.41
1:F:442:ARG:N	1:F:442:ARG:CD	2.83	0.41
1:F:442:ARG:HG2	1:F:452:ALA:HB3	2.03	0.41
1:B:1353:TRP:CH2	1:B:1366:ILE:HB	2.56	0.41
1:D:461:TRP:CE3	1:D:461:TRP:C	2.95	0.41
1:E:1403:TYR:CE1	1:E:1405:LYS:HE3	2.55	0.41
1:F:427:THR:HG21	1:F:487:LEU:HB3	2.03	0.41
1:A:1416:HIS:N	1:A:1416:HIS:ND1	2.58	0.41
1:B:1380:LYS:H	1:B:1380:LYS:HG2	1.62	0.41
1:F:433:PRO:HD3	1:F:1254:LEU:O	2.20	0.41
1:A:1298:ARG:HG2	1:A:1298:ARG:HH21	1.85	0.41
1:B:1179:GLU:HB2	1:B:1396:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1187:PRO:HD3	1:A:1434:ARG:HB2	2.00	0.41
1:D:1245:ASP:O	1:D:1246:CYS:HB3	2.21	0.41
1:F:1311:PHE:O	1:F:1312:LYS:C	2.60	0.41
1:E:1296:VAL:O	1:E:1300:LYS:HB2	2.21	0.41
1:F:1414:SER:O	1:F:1415:ASP:C	2.59	0.41
1:B:1322:VAL:HG22	1:B:1388:MET:HE2	2.02	0.41
1:C:1213:LYS:HE2	1:C:1262:SER:OG	2.21	0.41
1:B:1292:LEU:C	1:B:1292:LEU:HD12	2.41	0.41
1:A:1384:PRO:HA	1:A:1385:PRO:HD3	1.99	0.41
1:E:430:MET:H	1:E:430:MET:HG3	1.70	0.40
1:E:461:TRP:CD1	1:E:465:HIS:CE1	3.09	0.40
1:C:1202:MET:CE	1:C:1272:PHE:CZ	3.04	0.40
1:B:1322:VAL:HG22	1:B:1388:MET:HE3	2.03	0.40
1:F:427:THR:OG1	1:F:487:LEU:HD13	2.21	0.40
1:A:1216:MET:HB3	1:A:1216:MET:HE2	1.80	0.40
1:B:436:GLY:HA3	1:B:465:HIS:HE1	1.85	0.40
1:B:1324:ILE:HG12	1:B:1386:ILE:HD13	2.03	0.40
1:F:1174:PHE:N	1:F:1174:PHE:CD1	2.89	0.40
1:B:1170:ARG:CA	1:F:1421:TRP:CZ3	3.02	0.40
1:B:1158:TYR:CE2	1:F:1423:ARG:NH2	2.90	0.40
1:C:1177:VAL:HG21	1:C:1424:TYR:CE1	2.56	0.40
1:E:1179:GLU:HB3	1:E:1196:VAL:CG1	2.51	0.40
1:D:1301:LEU:HB2	1:D:1370:ILE:HG13	2.00	0.40
1:A:1173:LEU:HD11	1:A:1420:LYS:HB3	2.03	0.40
1:B:1363:GLU:OE1	1:E:445:LEU:HD13	2.21	0.40
1:F:442:ARG:N	1:F:442:ARG:HD3	2.37	0.40
1:C:1390:PHE:CD1	1:C:1391:GLU:N	2.89	0.40
1:F:478:TYR:O	1:F:482:LEU:HG	2.21	0.40
1:F:1195:HIS:CD2	1:F:1278:ARG:NH2	2.90	0.40
1:A:1378:LYS:HE3	1:A:1381:TRP:CE2	2.53	0.40
1:D:1324:ILE:HG22	1:D:1351:ILE:CB	2.48	0.40
1:B:459:VAL:HG21	1:B:499:GLU:OE1	2.22	0.40
1:D:1290:ILE:CB	1:D:1306:VAL:HG12	2.38	0.40
1:F:1192:LEU:CD1	1:F:1434:ARG:NE	2.81	0.40
1:B:488:ILE:HA	1:B:488:ILE:HD13	1.84	0.40
1:B:422:ASP:OD2	1:B:424:ALA:HB3	2.21	0.40
1:B:1344:TYR:HE2	1:B:1346:ALA:HB2	1.81	0.40
1:B:1384:PRO:HA	1:B:1385:PRO:HD3	1.98	0.40
1:F:1195:HIS:CD2	1:F:1278:ARG:HH21	2.39	0.40
1:E:1155:PRO:HA	1:E:1156:PRO:HD2	1.85	0.40
1:A:1183:LEU:HD21	1:A:1185:MET:HB2	2.02	0.40
1:E:490:HIS:HA	1:E:503:TYR:CD1	2.57	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:1294:ARG:CZ	1:F:1302:GLU:CG	2.99	0.40
1:B:473:ARG:NH2	1:B:473:ARG:HB2	2.36	0.40
1:D:1344:TYR:CE2	1:D:1346:ALA:HB2	2.56	0.40
1:C:1317:ALA:CB	1:C:1392:VAL:HG12	2.51	0.40
1:E:1248:PHE:HE2	1:E:1263:ILE:HG21	1.86	0.40
1:B:1177:VAL:HG21	1:B:1424:TYR:CD1	2.56	0.40
1:A:1325:PRO:HG3	1:A:1384:PRO:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	345/385 (90%)	294 (85%)	44 (13%)	7 (2%)	11	63
1	B	331/385 (86%)	284 (86%)	40 (12%)	7 (2%)	11	62
1	C	344/385 (89%)	288 (84%)	52 (15%)	4 (1%)	19	75
1	D	326/385 (85%)	279 (86%)	41 (13%)	6 (2%)	13	65
1	E	328/385 (85%)	282 (86%)	39 (12%)	7 (2%)	11	62
1	F	332/385 (86%)	289 (87%)	38 (11%)	5 (2%)	15	69
All	All	2006/2310 (87%)	1716 (86%)	254 (13%)	36 (2%)	13	65

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1251	CYS
1	B	493	ASN
1	B	1379	LYS
1	C	493	ASN
1	E	493	ASN
1	E	1251	CYS
1	F	493	ASN
1	F	1190	GLN

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Mol	Chain	Res	Type
1	A	493	ASN
1	A	1190	GLN
1	A	1251	CYS
1	B	1194	ALA
1	B	1251	CYS
1	B	1262	SER
1	C	435	SER
1	C	1194	ALA
1	D	493	ASN
1	D	1190	GLN
1	D	1194	ALA
1	D	1251	CYS
1	E	435	SER
1	E	1190	GLN
1	F	435	SER
1	A	1194	ALA
1	B	435	SER
1	B	1190	GLN
1	E	1194	ALA
1	F	1251	CYS
1	D	1286	PRO
1	A	1409	PRO
1	D	447	ILE
1	E	447	ILE
1	F	1409	PRO
1	A	447	ILE
1	A	470	PRO
1	E	470	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	308/337 (91%)	262 (85%)	46 (15%)	4	26
1	B	298/337 (88%)	260 (87%)	38 (13%)	6	33
1	C	307/337 (91%)	275 (90%)	32 (10%)	10	47
1	D	295/337 (88%)	258 (88%)	37 (12%)	7	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	297/337 (88%)	276 (93%)	21 (7%)	21	67
1	F	299/337 (89%)	272 (91%)	27 (9%)	14	55
All	All	1804/2022 (89%)	1603 (89%)	201 (11%)	9	42

All (201) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	427	THR
1	A	442	ARG
1	A	453	PHE
1	A	464	HIS
1	A	471	GLU
1	A	472	ARG
1	A	474	GLU
1	A	487	LEU
1	A	490	HIS
1	A	493	ASN
1	A	1157	PRO
1	A	1160	GLU
1	A	1173	LEU
1	A	1178	LEU
1	A	1191	VAL
1	A	1199	ARG
1	A	1205	TYR
1	A	1211	GLU
1	A	1216	MET
1	A	1217	ASN
1	A	1218	ASP
1	A	1257	PHE
1	A	1262	SER
1	A	1276	ARG
1	A	1277	TYR
1	A	1278	ARG
1	A	1287	PHE
1	A	1291	PRO
1	A	1294	ARG
1	A	1305	VAL
1	A	1314	SER
1	A	1329	ASN
1	A	1339	LYS
1	A	1347	SER

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Mol	Chain	Res	Type
1	A	1357	ARG
1	A	1379	LYS
1	A	1381	TRP
1	A	1383	ARG
1	A	1390	PHE
1	A	1394	PHE
1	A	1403	TYR
1	A	1412	ASN
1	A	1414	SER
1	A	1416	HIS
1	A	1431	TYR
1	A	1434	ARG
1	B	421	MET
1	B	427	THR
1	B	438	GLU
1	B	442	ARG
1	B	443	MET
1	B	444	TRP
1	B	445	LEU
1	B	453	PHE
1	B	460	ASP
1	B	476	ARG
1	B	480	SER
1	B	1173	LEU
1	B	1186	SER
1	B	1197	SER
1	B	1216	MET
1	B	1246	CYS
1	B	1247	THR
1	B	1250	GLN
1	B	1252	VAL
1	B	1253	ARG
1	B	1265	PHE
1	B	1275	MET
1	B	1277	TYR
1	B	1278	ARG
1	B	1282	ASP
1	B	1286	PRO
1	B	1292	LEU
1	B	1296	VAL
1	B	1311	PHE
1	B	1319	LYS

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Mol	Chain	Res	Type
1	B	1328	LEU
1	B	1333	VAL
1	B	1374	PRO
1	B	1380	LYS
1	B	1390	PHE
1	B	1406	VAL
1	B	1413	TYR
1	B	1432	GLU
1	C	421	MET
1	C	441	ASP
1	C	453	PHE
1	C	456	SER
1	C	464	HIS
1	C	504	VAL
1	C	1180	SER
1	C	1184	LEU
1	C	1186	SER
1	C	1207	SER
1	C	1209	MET
1	C	1214	PHE
1	C	1246	CYS
1	C	1255	SER
1	C	1264	SER
1	C	1277	TYR
1	C	1287	PHE
1	C	1299	THR
1	C	1300	LYS
1	C	1302	GLU
1	C	1306	VAL
1	C	1315	LEU
1	C	1325	PRO
1	C	1328	LEU
1	C	1336	ILE
1	C	1356	LYS
1	C	1357	ARG
1	C	1377	ASP
1	C	1410	LYS
1	C	1412	ASN
1	C	1427	ARG
1	C	1431	TYR
1	D	422	ASP
1	D	442	ARG

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Mol	Chain	Res	Type
1	D	447	ILE
1	D	453	PHE
1	D	462	LEU
1	D	472	ARG
1	D	1169	SER
1	D	1171	ASN
1	D	1177	VAL
1	D	1190	GLN
1	D	1199	ARG
1	D	1211	GLU
1	D	1216	MET
1	D	1217	ASN
1	D	1247	THR
1	D	1253	ARG
1	D	1277	TYR
1	D	1279	THR
1	D	1301	LEU
1	D	1305	VAL
1	D	1306	VAL
1	D	1307	ILE
1	D	1315	LEU
1	D	1322	VAL
1	D	1327	PRO
1	D	1328	LEU
1	D	1329	ASN
1	D	1334	GLN
1	D	1355	ILE
1	D	1374	PRO
1	D	1383	ARG
1	D	1385	PRO
1	D	1388	MET
1	D	1394	PHE
1	D	1420	LYS
1	D	1424	TYR
1	D	1427	ARG
1	E	423	MET
1	E	450	PRO
1	E	457	ASP
1	E	464	HIS
1	E	465	HIS
1	E	472	ARG
1	E	487	LEU

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Mol	Chain	Res	Type
1	E	496	THR
1	E	1209	MET
1	E	1211	GLU
1	E	1214	PHE
1	E	1277	TYR
1	E	1288	ARG
1	E	1291	PRO
1	E	1300	LYS
1	E	1305	VAL
1	E	1323	ARG
1	E	1324	ILE
1	E	1380	LYS
1	E	1414	SER
1	E	1415	ASP
1	F	421	MET
1	F	427	THR
1	F	447	ILE
1	F	462	LEU
1	F	471	GLU
1	F	490	HIS
1	F	507	ASP
1	F	1159	HIS
1	F	1170	ARG
1	F	1188	GLN
1	F	1214	PHE
1	F	1216	MET
1	F	1277	TYR
1	F	1279	THR
1	F	1319	LYS
1	F	1321	GLU
1	F	1324	ILE
1	F	1328	LEU
1	F	1337	CYS
1	F	1339	LYS
1	F	1390	PHE
1	F	1391	GLU
1	F	1393	PRO
1	F	1394	PHE
1	F	1399	LEU
1	F	1404	LEU
1	F	1434	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	465	HIS
1	A	490	HIS
1	A	500	GLN
1	A	1159	HIS
1	A	1171	ASN
1	A	1182	ASN
1	A	1195	HIS
1	A	1250	GLN
1	A	1349	ASN
1	A	1365	GLN
1	B	451	ASN
1	B	1188	GLN
1	C	451	ASN
1	C	465	HIS
1	C	1190	GLN
1	C	1217	ASN
1	C	1318	GLN
1	D	451	ASN
1	D	465	HIS
1	D	1217	ASN
1	D	1318	GLN
1	D	1329	ASN
1	D	1365	GLN
1	E	465	HIS
1	E	500	GLN
1	E	1190	GLN
1	E	1195	HIS
1	E	1318	GLN
1	F	464	HIS
1	F	1159	HIS
1	F	1188	GLN
1	F	1190	GLN
1	F	1195	HIS
1	F	1217	ASN
1	F	1250	GLN
1	F	1318	GLN
1	F	1412	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	351/385 (91%)	0.32	0	100	100	91, 112, 131, 141	0
1	B	339/385 (88%)	0.36	7 (2%)	60	29	103, 117, 134, 145	0
1	C	350/385 (90%)	0.35	3 (0%)	81	51	99, 119, 132, 147	0
1	D	336/385 (87%)	0.32	3 (0%)	81	51	97, 117, 129, 136	0
1	E	338/385 (87%)	0.40	3 (0%)	81	51	98, 118, 132, 141	0
1	F	340/385 (88%)	0.42	11 (3%)	45	21	100, 120, 133, 140	0
All	All	2054/2310 (88%)	0.36	27 (1%)	74	40	91, 117, 132, 147	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1435	CYS	3.6
1	B	1435	CYS	3.1
1	F	487	LEU	3.0
1	F	1435	CYS	3.0
1	B	430	MET	2.8
1	B	463	TYR	2.7
1	F	1295	GLU	2.7
1	B	508	LEU	2.7
1	F	1296	VAL	2.6
1	C	454	LEU	2.6
1	E	508	LEU	2.5
1	D	1301	LEU	2.4
1	B	464	HIS	2.3
1	B	437	LEU	2.2
1	E	1373	LEU	2.2
1	F	488	ILE	2.2
1	F	1175	LEU	2.2
1	D	1435	CYS	2.1
1	F	1253	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	1274	LEU	2.1
1	F	1370	ILE	2.1
1	E	1181	VAL	2.1
1	F	1177	VAL	2.1
1	B	502	TYR	2.0
1	F	1379	LYS	2.0
1	C	430	MET	2.0
1	D	462	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.