



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 11:19 pm BST

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 X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

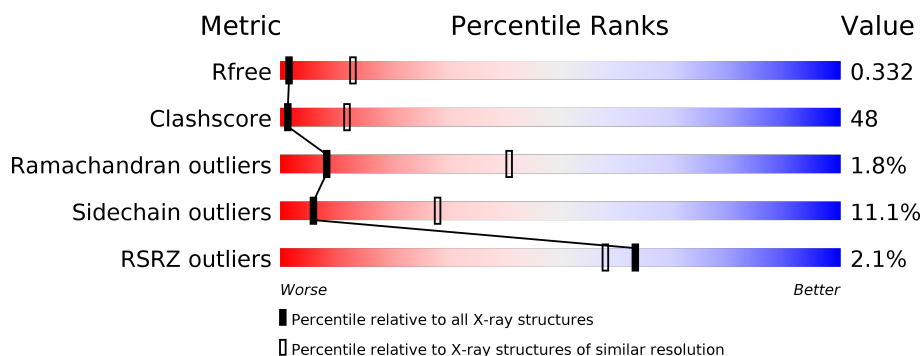
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	385	<div> <div>36%</div> <div>45%</div> <div>10%</div> <div>9%</div> </div>
1	B	385	<div>2%</div> <div>34%</div> <div>46%</div> <div>9%</div> <div>12%</div>
1	C	385	<div>2%</div> <div>33%</div> <div>51%</div> <div>6%</div> <div>9%</div>
1	D	385	<div>%</div> <div>30%</div> <div>49%</div> <div>8%</div> <div>13%</div>
1	E	385	<div>3%</div> <div>32%</div> <div>50%</div> <div>6%</div> <div>12%</div>
1	F	385	<div>3%</div> <div>36%</div> <div>46%</div> <div>6%</div> <div>12%</div>

2 Entry composition

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

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 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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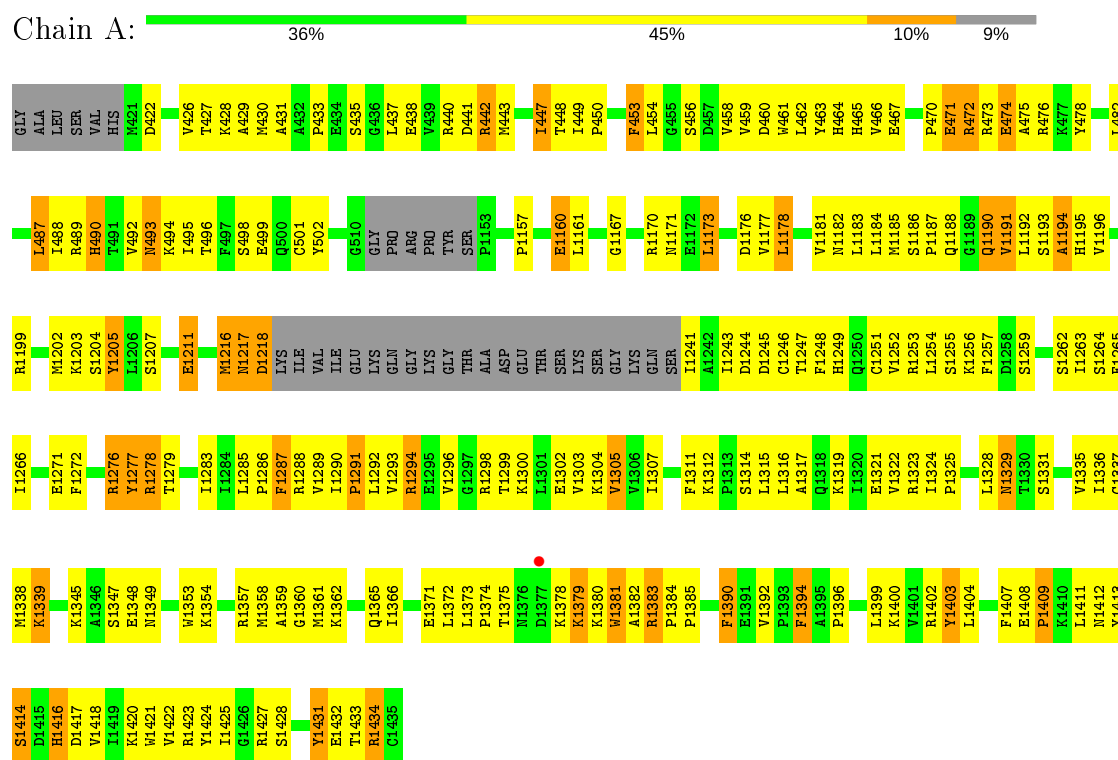
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Chain	Residue	Modelled	Actual	Comment	Reference
F	1162	GLU	-	LINKER	UNP P84092
F	1163	PHE	-	LINKER	UNP P84092
F	1164	GLY	-	LINKER	UNP P84092
F	1165	GLY	-	LINKER	UNP P84092
F	1166	SER	-	LINKER	UNP P84092
F	1167	GLY	-	LINKER	UNP P84092
F	1168	GLY	-	LINKER	UNP P84092
F	1169	SER	-	LINKER	UNP P84092

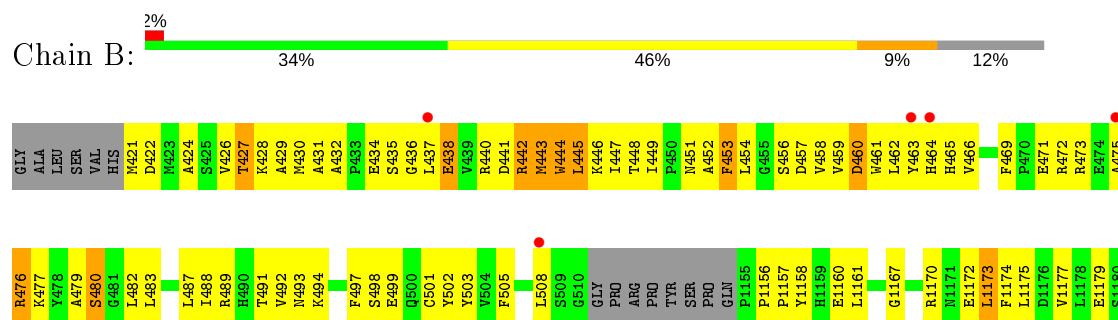
3 Residue-property plots

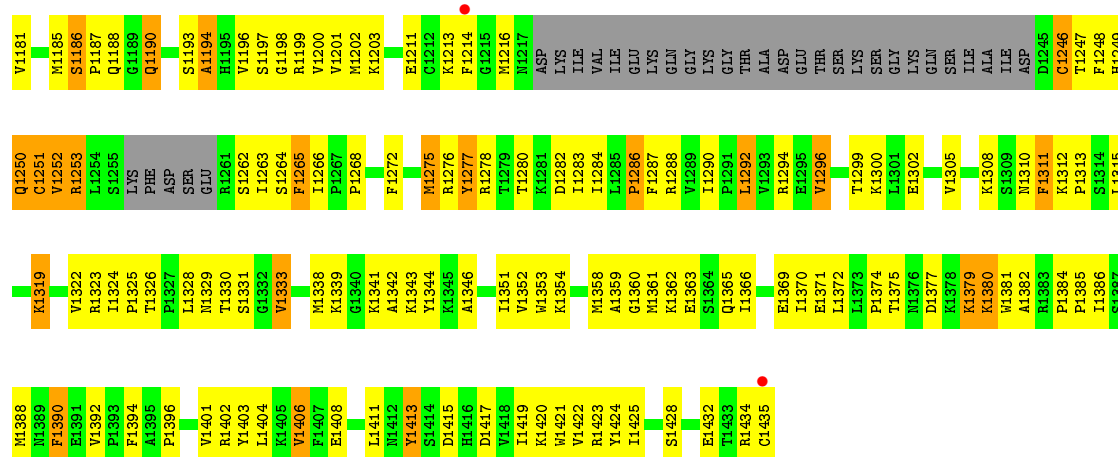
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

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

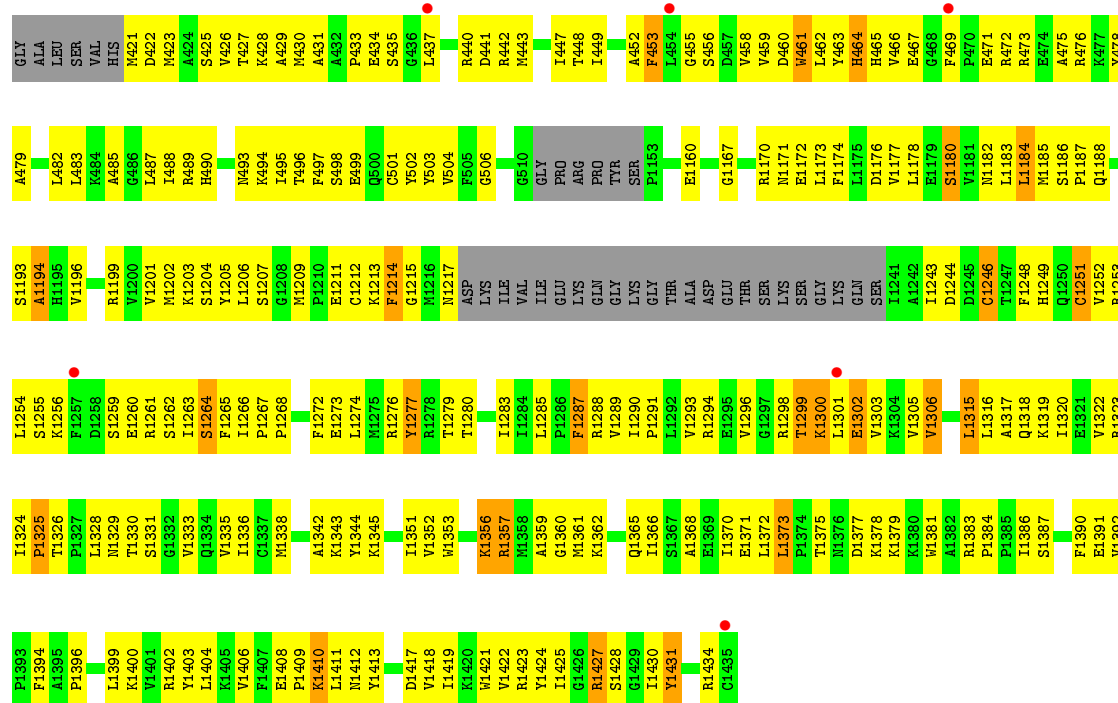


- Molecule 1: Chimeric complex between protein Dishevelled2 homolog dvl-2 and clathrin adaptor AP-2 complex subunit mu

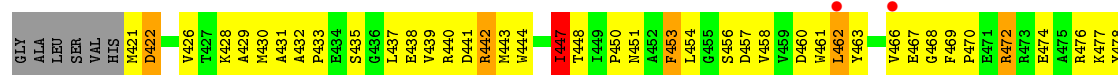


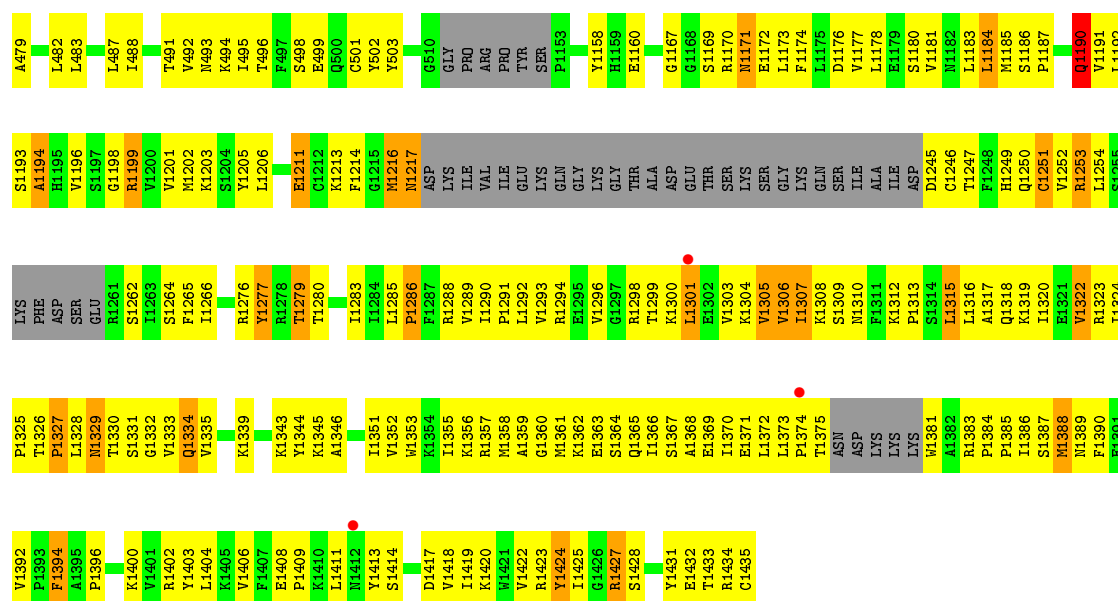


- Molecule 1: Chimeric complex between protein Dishevelled2 homolog dvl-2 and clathrin adaptor AP-2 complex subunit mu

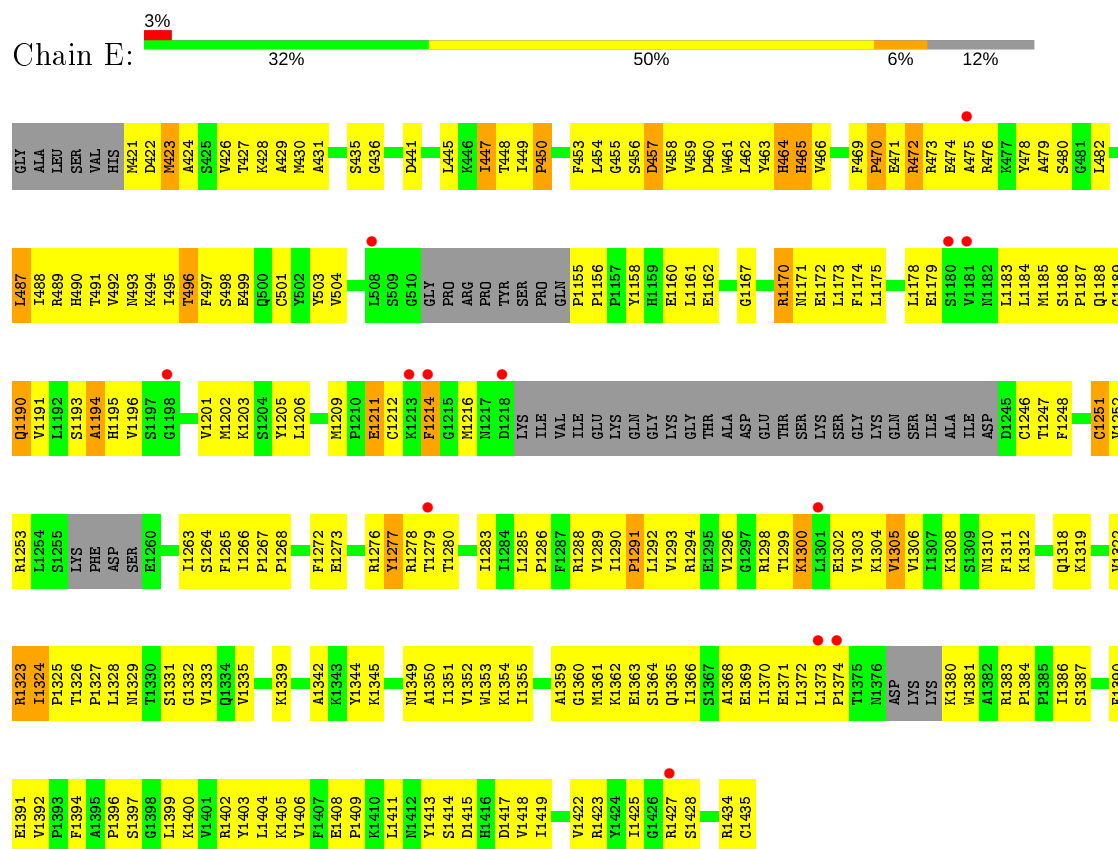


- Molecule 1: Chimeric complex between protein Dishevelled2 homolog dvl-2 and clathrin adaptor AP-2 complex subunit mu





- 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



L1399	K1400	V1401	R1402	Y1403	L1404	K1405	V1406	F1407	E1408	P1409	K1410	L1411	M1412	Y1413	S1414	D1415	H1416	D1417	V1418	I1419	K1420	W1421	V1422	R1423	Y1424	I1425	G1426	R1427	S1428	E1432	T1433	R1434	C1435																											
L1327	L1328	M1329	T1330	S1331	G1332	V1333	Q1334	I1336	C1337	M1338	K1339	A1342	K1345	I1351	V1352	K1353	K1354	R1357	M1358	A1359	G1360	M1361	K1362	E1363	S1364	Q1365	I1366	I1370	E1371	L1372	L1373	P1374	T1375	K1379	K1380	W1381	A1382	R1383	P1384	P1385	I1386	S1387	M1388	M1389	F1390	E1391	V1392	P1393	F1394	P1396										
ASP	SER	GLU	R1261	I1263	I1263	S1264	F1266	I1266	P1267	P1268	F1272	E1273	L1274	M1275	R1276	Y1277	R1278	T1279	I1283	I1284	L1285	P1286	F1287	R1288	V1289	P1291	L1292	V1293	R1294	E1295	V1296	G1297	R1298	T1299	K1300	L1301	E1302	L1303	I1307	N1310	F1311	K1312	L1316	A1317	Q1318	K1319	I1320	E1321	V1322	R1323	I1324	P1325	T1326							
G1189	Q1190	V1191	L1192	S1193	A1194	H1195	V1196	R1199	L1206	E1211	G1212	K1213	F1214	Y502	G1215	M1216	N1217	D1218	LYS	ILE	VAL	ILE	GLU	LYS	GLN	PRO	GLY	TYR	LYS	SER	PRO	GLN	P1155	P1156	P1157	Y1158	H1159	E1160	G1167	L1170	R1171	E1172	L1173	F1174	L1175	ASP	D1245	G1246	T1247	F1248	H1249	Q1250	V1181	M1182	L1183	L1184	M1185	S1186	P1187	Q1188
GLY	ALA	LEU	SER	SER	VAL	HIS	M421	D422	M423	A424	S425	T426	V427	K428	A429	M430	A431	A432	R433	E434	S435	G436	L437	E438	V439	R440	D441	R442	M443	I447	T448	I449	P450	N451	A452	F453	L454	G455	S456	D457	V458	V459	D460	W461	L462	Y463	H464	H465	V466	F469	P470	E471	A475	Y478	L482					

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 , 0.332	Depositor DCC
R_{free} test set	2576 reflections (5.01%)	wwPDB-VP
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 , 69.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	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.

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

5 Model quality

5.1 Standard geometry

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 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 48.

All (1588) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A: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:C:1406:VAL:HG11	1:C:1418:VAL:HG21	1.41	1.00
1:F:1323:ARG:HH12	1:F:1352:VAL:HG22	1.26	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:1183:LEU:HD21	1:D:1285:LEU:HD23	1.44	0.98
1:D:1324:ILE:HD12	1:D:1386:ILE:HG12	1.43	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:B:476:ARG:HB3	1:B:476:ARG:HH21	1.29	0.95
1:E:462:LEU:O	1:E:466:VAL:HB	1.65	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:464:HIS:ND1	1:B:465:HIS:NE2	2.14	0.93
1:F:1183:LEU:HD12	1:F:1184:LEU:H	1.28	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:D:1356:LYS:HD3	1:D:1357:ARG:HH12	1.34	0.90
1:F:1390:PHE:CE1	1:F:1428:SER:HB3	2.07	0.90
1:C:1174:PHE:HD2	1:C:1203:LYS:HD2	1.34	0.90
1:F:1408:GLU:HG2	1:F:1411:LEU:HB2	1.54	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:B:1305:VAL:HG21	1:B:1324:ILE:HD11	1.57	0.87
1:E:1327:PRO:HA	1:E:1381:TRP:CE2	2.10	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	Interatomic distance (Å)	Clash overlap (Å)
1:A:1378:LYS:HE3	1:A:1381:TRP:CZ2	2.11	0.86
1:E:1186:SER:HA	1:E:1434:ARG:HD2	1.57	0.86
1:E:462:LEU:HD22	1:E:475:ALA:O	1.74	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:B:1323:ARG:HB2	1:B:1323:ARG:NH1	1.93	0.83
1:D:1301:LEU:HB3	1:D:1370:ILE:HG13	1.60	0.83
1:A:1390:PHE:CE1	1:A:1428:SER:HB3	2.12	0.83
1:C:440:ARG:HG2	1:C:442:ARG:NH1	1.92	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:B:1294:ARG:HH12	1:B:1302:GLU:HG3	1.45	0.82
1:F:422:ASP:O	1:F:426:VAL:HG23	1.79	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: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:F:1408:GLU:CG	1:F:1411:LEU:HB2	2.09	0.82
1:B:442:ARG:NH2	1:B:453:PHE:HA	1.95	0.81
1:B:464:HIS:HD1	1:B:465:HIS:CD2	1.97	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:C:1249:HIS:CE1	1:C:1268:PRO:HG2	2.15	0.81
1:F:1329:ASN:ND2	1:F:1372:LEU:HB3	1.96	0.81
1:A:1173:LEU:HD12	1:A:1173:LEU:O	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:PHE:HZ	1:B:488:ILE:HD12	1.45	0.81
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:A:1305:VAL:HG12	1:A:1366:ILE:HG22	1.62	0.80
1:C:422:ASP:O	1:C:426:VAL:HG23	1.80	0.80
1:D:1408:GLU:HG2	1:D:1411:LEU:HB2	1.64	0.80
1:E:1203:LYS:HB3	1:E:1205:TYR:HE1	1.46	0.80
1:E:1339:LYS:NZ	1:E:1364:SER:HA	1.96	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:1339:LYS:NZ	1:A:1339:LYS:HB3	1.97	0.79
1:A:1345:LYS:HA	1:A:1345:LYS:HE2	1.64	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:1337:CYS:HB3	1:A:1366:ILE:HG13	1.64	0.78
1:A:430:MET:HE2	1:A:437:LEU:HD22	1.65	0.78
1:F:1177:VAL:HB	1:F:1424:TYR:HD1	1.47	0.78
1:B:473:ARG:O	1:B:477:LYS:HG3	1.84	0.78
1:C:1178:LEU:HD12	1:C:1178:LEU:N	1.99	0.78
1:E:1331:SER:HB3	1:E:1373:LEU:HG	1.64	0.78
1:F:1213:LYS:CE	1:F:1262:SER:OG	2.31	0.78
1:B:430:MET:CE	1:B:437:LEU:HD22	2.14	0.78
1:D:1301:LEU:HB2	1:D:1372:LEU:HD11	1.64	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:B:1214:PHE:HE1	1:B:1401:VAL:HG13	1.50	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:F:1324:ILE:HD12	1:F:1386:ILE:CG2	2.14	0.77
1:B:463:TYR:HB2	1:B:475:ALA:HB2	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:1318:GLN:HE21	1:C:1357:ARG:HH11	1.30	0.76
1:D:1434:ARG:HH11	1:D:1434:ARG:HG3	1.49	0.76
1:D:1301:LEU:CB	1:D:1370:ILE:HG13	2.15	0.76
1:A:422:ASP:O	1:A:426:VAL:HG23	1.86	0.76
1:D:1187:PRO:HD3	1:D:1434:ARG:HB2	1.67	0.76
1:E:1172:GLU:HB3	1:E:1419:ILE:HB	1.68	0.76
1:E:1318:GLN:HE21	1:E:1319:LYS:HE3	1.51	0.76
1:F:1422:VAL:HG12	1:F:1423:ARG:N	2.01	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:D:1408:GLU:OE2	1:D:1409:PRO:HD2	1.87	0.75
1:E:1325:PRO:HG3	1:E:1384:PRO:O	1.86	0.75
1:C:1217:ASN:HD21	1:C:1400:LYS:HB2	1.49	0.75
1:D:1289:VAL:HB	1:D:1433:THR:HG21	1.68	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:B:1425:ILE:O	1:B:1425:ILE:HG22	1.86	0.74
1:B:457:ASP:HA	1:B:460:ASP:OD2	1.87	0.74
1:E:1394:PHE:O	1:E:1396:PRO:HD3	1.86	0.74
1:F:1319:LYS:HE3	1:F:1391:GLU:OE1	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:C:1333:VAL:HG22	1:C:1370:ILE:HG12	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:433:PRO:HD3	1:D:1254:LEU:O	1.87	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
1:B:459:VAL:HA	1:B:462:LEU:HD12	1.70	0.74
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:F:1213:LYS:HE3	1:F:1262:SER:OG	1.87	0.74
1:B:1173:LEU:HD11	1:B:1420:LYS:HG2	1.68	0.73
1:B:1419:ILE:HD12	1:B:1419:ILE:N	2.03	0.73
1:D:1356:LYS:HB3	1:D:1357:ARG:NH1	2.03	0.73
1:B:1308:LYS:HG2	1:B:1363:GLU:HG2	1.70	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: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:A:490:HIS:CE1	1:A:494:LYS:HE2	2.23	0.73
1:B:1333:VAL:HG11	1:B:1344:TYR:CG	2.23	0.73
1:C:1318:GLN:HG2	1:C:1357:ARG:HB2	1.70	0.73
1:F:1217:ASN:HD21	1:F:1400:LYS:H	1.34	0.73
1:B:1160:GLU:HB3	1:B:1167:GLY:HA3	1.69	0.73
1:B:442:ARG:HG2	1:B:502:TYR:CZ	2.24	0.73
1:E:1173:LEU:HD12	1:E:1173:LEU:C	2.09	0.73
1:F:1402:ARG:HG3	1:F:1402:ARG:HH11	1.52	0.73
1:B:1408:GLU:CB	1:B:1413:TYR:CE2	2.72	0.72
1:D:1322:VAL:HG23	1:D:1353:TRP:HB3	1.71	0.72
1:F:1284:ILE:HG12	1:F:1396:PRO:O	1.88	0.72
1:A:1160:GLU:HB3	1:A:1167:GLY:HA3	1.71	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:1312:LYS:HB2	1:A:1315:LEU:HD12	1.71	0.72
1:B:440:ARG:HG2	1:B:441:ASP:H	1.54	0.72
1:A:1408:GLU:HG2	1:A:1411:LEU:HB2	1.71	0.72
1:A:1241:ILE:HD11	1:A:1399:LEU:HA	1.72	0.72
1:D:1318:GLN:HG2	1:D:1357:ARG:HB3	1.70	0.72
1:C:1409:PRO:HG2	1:C:1410:LYS:HD2	1.71	0.72
1:A:1422:VAL:HG23	1:E:1161:LEU:HB2	1.72	0.72
1:B:1425:ILE:HD11	1:F:1156:PRO:CG	2.20	0.72
1:F:1329:ASN:HD21	1:F:1372:LEU:HB3	1.55	0.72
1:A:1434:ARG:CG	1:A:1434:ARG:HH11	2.03	0.71
1:D:1320:ILE:CG2	1:D:1388:MET:HE1	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:422:ASP:OD2	1:E:424:ALA:HB3	1.90	0.71
1:F:1217:ASN:ND2	1:F:1400:LYS:H	1.89	0.71
1:C:1214:PHE:C	1:C:1214:PHE:HD2	1.94	0.71
1:C:440:ARG:H	1:C:442:ARG:NH1	1.87	0.71
1:C:462:LEU:HD11	1:C:479:ALA:HB2	1.73	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:HG22	1:F:1425:ILE:O	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:1301:LEU:HB3	1:D:1370:ILE:CD1	2.22	0.70
1:D:1187:PRO:HD3	1:D:1434:ARG:CB	2.21	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:D:1298:ARG:HH22	1:D:1372:LEU:HD22	1.56	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:C:1214:PHE:CD2	1:C:1214:PHE:C	2.65	0.69
1:F:1187:PRO:CD	1:F:1434:ARG:HB2	2.21	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: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:F:1324:ILE:HD12	1:F:1386:ILE:HG21	1.73	0.69
1:A:476:ARG:HG2	1:A:476:ARG:NH2	2.08	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:C:1357:ARG:HB3	1:C:1357:ARG:NH1	2.08	0.69
1:D:1333:VAL:CG2	1:D:1370:ILE:HG22	2.22	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:1214:PHE:HD1	1:F:1215:GLY:N	1.90	0.69
1:F:1211:GLU:HA	1:F:1266:ILE:HD13	1.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1211:GLU:HA	1:B:1266:ILE:HD13	1.74	0.69
1:C:498:SER:HB3	1:C:501:CYS:SG	2.33	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:D:1394:PHE:O	1:D:1396:PRO:HD3	1.91	0.69
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:1304:LYS:HD2	1:A:1365:GLN:NE2	2.08	0.68
1:B:1253:ARG:O	1:B:1263:ILE:HD11	1.93	0.68
1:D:1329:ASN:ND2	1:D:1372:LEU:HD23	2.07	0.68
1:A:1380:LYS:HB3	1:D:477:LYS:HE3	1.75	0.68
1:F:1196:VAL:HG23	1:F:1283:ILE:HD13	1.75	0.68
1:C:490:HIS:NE2	1:C:494:LYS:HB3	2.08	0.68
1:D:1217:ASN:HD21	1:D:1400:LYS:H	1.41	0.68
1:D:1285:LEU:N	1:D:1285:LEU:HD12	2.08	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: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: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:E:447:ILE:HG22	1:E:448:THR:H	1.59	0.68
1:B:1425:ILE:HD11	1:F:1156:PRO:HG2	1.76	0.68
1:B:1268:PRO:HD2	1:B:1272:PHE:CE2	2.29	0.68
1:C:1408:GLU:HG2	1:C:1411:LEU:HB2	1.75	0.68
1:A:487:LEU:HD23	1:A:487:LEU:N	2.08	0.68
1:B:1294:ARG:HH12	1:B:1302:GLU:CG	2.07	0.68
1:C:1180:SER:HB2	1:C:1427:ARG:NH1	2.08	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: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:B:424:ALA:O	1:B:428:LYS:HG3	1.93	0.67
1:C:471:GLU:HG2	1:C:473:ARG:NH2	2.09	0.67
1:C:1174:PHE:CE1	1:C:1421:TRP:CD1	2.80	0.67
1:C:463:TYR:CZ	1:C:464:HIS:ND1	2.63	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:1331:SER:HB2	1:F:1373:LEU:HD22	1.75	0.67
1:F:1345:LYS:CE	1:F:1352:VAL:HG21	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:454:LEU:HB3	1:E:457:ASP:OD2	1.95	0.66
1:A:492:VAL:HG13	1:C:1338:MET:HG2	1.76	0.66
1:B:464:HIS:CE1	1:B:465:HIS:NE2	2.62	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:A:1204:SER:C	1:A:1205:TYR:HD2	1.98	0.66
1:E:1335:VAL:HG12	1:E:1368:ALA:HB2	1.77	0.66
1:F:1187:PRO:HD3	1:F:1434:ARG:CB	2.25	0.66
1:A:1336:ILE:N	1:A:1336:ILE:HD12	2.10	0.66
1:D:1183:LEU:HD12	1:D:1193:SER:O	1.95	0.66
1:D:1246:CYS:HB2	1:D:1276:ARG:O	1.96	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:B:1408:GLU:CB	1:B:1413:TYR:HE2	2.09	0.66
1:C:469:PHE:HZ	1:C:478:TYR:CD2	2.12	0.66
1:C:483:LEU:HD22	1:C:488:ILE:HB	1.76	0.66
1:D:1434:ARG:NH1	1:D:1434:ARG:HG3	2.11	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:F:1311:PHE:CE1	1:F:1360:GLY:HA2	2.31	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:C:447:ILE:CG2	1:C:448:THR:N	2.59	0.66
1:D:1305:VAL:HG23	1:D:1366:ILE:HG23	1.76	0.66
1:D:1298:ARG:HH22	1:D:1372:LEU:CB	2.09	0.65
1:D:441:ASP:OD1	1:D:450:PRO:HA	1.96	0.65
1:E:1183:LEU:HD11	1:E:1191:VAL:HG13	1.78	0.65
1:A:1290:ILE:N	1:A:1290:ILE:HD12	2.11	0.65
1:A:453:PHE:CD2	1:A:453:PHE:N	2.64	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:454:LEU:HG	1:B:456:SER:H	1.61	0.65
1:D:1170:ARG:HH11	1:D:1172:GLU:CD	2.00	0.65
1:F:1294:ARG:HB3	1:F:1294:ARG:HH11	1.60	0.65
1:F:448:THR:O	1:F:448:THR:HG22	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:D:1250:GLN:HG3	1:D:1251:CYS:N	2.12	0.65
1:B:1170:ARG:HA	1:F:1421:TRP:CZ3	2.31	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:A:447:ILE:HG22	1:A:448:THR:H	1.61	0.65
1:C:1331:SER:HB3	1:C:1373:LEU:CD2	2.27	0.65
1:C:455:GLY:O	1:C:458:VAL:HG12	1.97	0.65
1:E:1342:ALA:HB2	1:E:1353:TRP:CD1	2.32	0.65
1:F:1384:PRO:O	1:F:1435:CYS:SG	2.54	0.65
1:B:442:ARG:HH21	1:B:453:PHE:HA	1.62	0.65
1:C:1177:VAL:C	1:C:1178:LEU:HD12	2.16	0.65
1:C:1326:THR:HG22	1:C:1370:ILE:HD11	1.79	0.65
1:C:1306:VAL:HG23	1:C:1365:GLN:HB2	1.79	0.65
1:D:1357:ARG:HH11	1:D:1357:ARG:HG2	1.61	0.65
1:D:462:LEU:HD23	1:D:466:VAL:HG21	1.77	0.65
1:E:466:VAL:CG1	1:E:469:PHE:HE2	2.10	0.65
1:F:1217:ASN:ND2	1:F:1400:LYS:HB2	2.12	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:D:491:THR:HG22	1:D:492:VAL:HG13	1.78	0.65
1:F:1312:LYS:HB2	1:F:1312:LYS:NZ	2.11	0.65
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:458:VAL:O	1:F:462:LEU:HB2	1.97	0.64
1:B:1338:MET:HE2	1:E:491:THR:HB	1.80	0.64
1:D:1319:LYS:O	1:D:1390:PHE:HA	1.98	0.64
1:E:441:ASP:OD1	1:E:450:PRO:HA	1.97	0.64
1:F:1293:VAL:CG2	1:F:1383:ARG:NH1	2.60	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:C:467:GLU:OE2	1:C:467:GLU:HA	1.96	0.64
1:D:1326:THR:HB	1:D:1327:PRO:HD2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:464:HIS:HB3	1:E:465:HIS:CD2	2.32	0.64
1:A:487:LEU:O	1:A:488:ILE:HD13	1.96	0.64
1:D:1323:ARG:O	1:D:1386:ILE:HG23	1.98	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:B:1325:PRO:HG3	1:B:1384:PRO:O	1.97	0.64
1:E:1435:CYS:O	1:E:1435:CYS:SG	2.56	0.64
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:1327:PRO:HG3	1:E:1381:TRP:CE3	2.33	0.64
1:E:1359:ALA:HB3	1:E:1362:LYS:HD2	1.80	0.64
1:C:1331:SER:HB3	1:C:1373:LEU:CG	2.28	0.64
1:D:1356:LYS:HB3	1:D:1357:ARG:HH11	1.62	0.64
1:D:1172:GLU:HB3	1:D:1419:ILE:HB	1.81	0.64
1:E:1183:LEU:HD12	1:E:1193:SER:O	1.98	0.64
1:D:1359:ALA:HB3	1:D:1362:LYS:HE2	1.79	0.63
1:E:1171:ASN:O	1:E:1418:VAL:HG13	1.98	0.63
1:A:1422:VAL:HG12	1:A:1423:ARG:H	1.63	0.63
1:B:1315:LEU:N	1:B:1315:LEU:HD12	2.13	0.63
1:C:1202:MET:HE1	1:C:1272:PHE:HZ	1.63	0.63
1:B:1311:PHE:CE1	1:B:1360:GLY:HA2	2.33	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:A:1187:PRO:HD3	1:A:1434:ARG:HB3	1.80	0.63
1:E:462:LEU:HD22	1:E:475:ALA:C	2.18	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: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:434:GLU:HA	1:B:434:GLU:OE1	1.99	0.63
1:D:453:PHE:CD2	1:D:453:PHE:N	2.67	0.63
1:F:1327:PRO:HG3	1:F:1381:TRP:CE3	2.33	0.63
1:F:1298:ARG:NH2	1:F:1379:LYS:HD2	2.13	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:C:1305:VAL:HG21	1:C:1324:ILE:HD13	1.81	0.63
1:F:1183:LEU:HD22	1:F:1285:LEU:HD22	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:B:483:LEU:HD13	1:B:503:TYR:CE1	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1184:LEU:HB3	1:D:1193:SER:HB3	1.79	0.62
1:D:476:ARG:HH11	1:D:499:GLU:HB2	1.64	0.62
1:E:1327:PRO:HA	1:E:1381:TRP:NE1	2.14	0.62
1:A:1171:ASN:HD21	1:A:1207:SER:H	1.46	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: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
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: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:E:1381:TRP:CZ3	1:E:1383:ARG:HG2	2.34	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: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:F:1184:LEU:HB3	1:F:1193:SER:HB3	1.80	0.62
1:B:449:ILE:HG22	1:B:452:ALA:HB2	1.81	0.62
1:B:476:ARG:HB3	1:B:476:ARG:NH2	2.09	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:A:1187:PRO:HD3	1:A:1434:ARG:CB	2.30	0.62
1:E:472:ARG:O	1:E:472:ARG:HD3	2.00	0.62
1:B:1319:LYS:O	1:B:1390:PHE:HA	2.00	0.62
1:F:1192:LEU:HD11	1:F:1434:ARG:NE	2.15	0.62
1:A:1170:ARG:NH1	1:A:1205:TYR:CD1	2.60	0.61
1:A:1276:ARG:HB2	1:A:1276:ARG:CZ	2.30	0.61
1:A:1427:ARG:HH11	1:A:1427:ARG:HG2	1.64	0.61
1:F:1325:PRO:HG3	1:F:1384:PRO:O	2.00	0.61
1:F:1422:VAL:HG12	1:F:1423:ARG:H	1.63	0.61
1:A:1422:VAL:HG12	1:A:1423:ARG:N	2.15	0.61
1:B:1408:GLU:HB3	1:B:1413:TYR:CE2	2.35	0.61
1:E:1196:VAL:HG23	1:E:1283:ILE:HD13	1.82	0.61
1:E:1298:ARG:HH21	1:E:1298:ARG:HG2	1.64	0.61
1:F:1158:TYR:HB2	1:F:1170:ARG:HD2	1.82	0.61
1:A:1170:ARG:HH12	1:A:1205:TYR:HD1	1.40	0.61
1:A:462:LEU:HD11	1:A:478:TYR:CD2	2.28	0.61
1:A:428:LYS:O	1:A:431:ALA:HB3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:480:SER:OG	1:B:497:PHE:HB3	2.00	0.61
1:A:1188:GLN:NE2	1:D:422:ASP:OD1	2.33	0.61
1:E:1184:LEU:HB2	1:E:1193:SER:HB3	1.83	0.61
1:C:1356:LYS:H	1:C:1356:LYS:HD2	1.64	0.61
1:F:491:THR:HG22	1:F:492:VAL:CG1	2.30	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
1:A:1255:SER:CB	1:A:1263:ILE:HA	2.30	0.60
1:C:1276:ARG:HG3	1:C:1276:ARG:HH11	1.66	0.60
1:C:1329:ASN:ND2	1:C:1372:LEU:HB3	2.16	0.60
1:A:462:LEU:HD23	1:A:475:ALA:CB	2.31	0.60
1:C:1214:PHE:HD2	1:C:1215:GLY:N	1.99	0.60
1:D:1183:LEU:HD11	1:D:1191:VAL:CG1	2.31	0.60
1:F:428:LYS:O	1:F:431:ALA:HB3	2.01	0.60
1:B:447:ILE:HG22	1:B:448:THR:N	2.16	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: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:A:1204:SER:C	1:A:1205:TYR:CD2	2.75	0.60
1:C:1214:PHE:CD2	1:C:1215:GLY:N	2.70	0.60
1:D:1186:SER:HA	1:D:1434:ARG:HB2	1.83	0.60
1:F:1333:VAL:HG13	1:F:1370:ILE:HG12	1.83	0.60
1:D:1424:TYR:N	1:D:1424:TYR:CD2	2.68	0.60
1:E:423:MET:HA	1:E:478:TYR:OH	2.01	0.60
1:A:442:ARG:NH1	1:A:442:ARG:HG3	2.03	0.60
1:B:483:LEU:HD13	1:B:503:TYR:HE1	1.65	0.60
1:C:1316:LEU:HD13	1:C:1357:ARG:HD2	1.84	0.60
1:E:465:HIS:N	1:E:465:HIS:CD2	2.68	0.60
1:F:1402:ARG:HG3	1:F:1402:ARG:NH1	2.17	0.60
1:D:1425:ILE:HG22	1:D:1425:ILE:O	2.00	0.60
1:A:442:ARG:CG	1:A:442:ARG:NH1	2.41	0.60
1:B:1253:ARG:NH2	1:B:1253:ARG:HG3	2.06	0.60
1:B:447:ILE:HG22	1:B:448:THR:H	1.67	0.60
1:F:1298:ARG:O	1:F:1372:LEU:HD12	2.01	0.60
1:A:467:GLU:HA	1:A:467:GLU:OE2	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1356:LYS:CD	1:D:1357:ARG:HH12	2.12	0.59
1:D:1359:ALA:HB3	1:D:1362:LYS:CE	2.31	0.59
1:E:470:PRO:HG2	1:E:471:GLU:H	1.67	0.59
1:B:1198:GLY:O	1:B:1276:ARG:HD3	2.02	0.59
1:F:1298:ARG:NH1	1:F:1375:THR:OG1	2.35	0.59
1:A:1276:ARG:HG3	1:A:1276:ARG:HH11	1.68	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: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
1:F:440:ARG:NH2	1:F:440:ARG:HB3	2.17	0.59
1:A:1408:GLU:CG	1:A:1411:LEU:HB2	2.33	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: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:F:1390:PHE:CZ	1:F:1428:SER:HB3	2.38	0.59
1:A:1243:ILE:HD12	1:A:1277:TYR:HD1	1.67	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:1183:LEU:HG	1:A:1184:LEU:N	2.17	0.59
1:A:1211:GLU:OE2	1:A:1253:ARG:NH2	2.36	0.59
1:C:1319:LYS:O	1:C:1390:PHE:HA	2.03	0.59
1:E:1279:THR:HG22	1:E:1280:THR:N	2.18	0.59
1:F:1324:ILE:HD12	1:F:1386:ILE:HG23	1.84	0.59
1:B:1305:VAL:HG21	1:B:1324:ILE:CD1	2.30	0.58
1:D:1185:MET:HB3	1:D:1433:THR:HG22	1.85	0.58
1:D:428:LYS:O	1:D:431:ALA:HB3	2.02	0.58
1:E:1186:SER:HA	1:E:1434:ARG:CD	2.30	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:B:1187:PRO:HB2	1:B:1188:GLN:HE21	1.68	0.58
1:C:1178:LEU:CD1	1:C:1178:LEU:N	2.66	0.58
1:C:497:PHE:O	1:C:497:PHE:CD1	2.55	0.58
1:B:453:PHE:CD2	1:B:453:PHE:N	2.71	0.58
1:B:462:LEU:HD11	1:B:479:ALA:HB2	1.85	0.58
1:C:489:ARG:HH21	1:C:1410:LYS:CE	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1298:ARG:NH2	1:D:1372:LEU:HD22	2.19	0.58
1:E:1423:ARG:CD	1:E:1425:ILE:HD11	2.33	0.58
1:E:1423:ARG:NE	1:E:1425:ILE:HD11	2.18	0.58
1:A:1298:ARG:HD3	1:A:1298:ARG:O	2.04	0.58
1:B:430:MET:HE2	1:B:437:LEU:HB2	1.85	0.58
1:D:1292:LEU:HD12	1:D:1304:LYS:CE	2.34	0.58
1:E:1279:THR:HG22	1:E:1280:THR:H	1.67	0.58
1:A:1241:ILE:CD1	1:A:1399:LEU:HA	2.33	0.58
1:B:1408:GLU:HB2	1:B:1413:TYR:CE2	2.38	0.58
1:E:1188:GLN:HB2	1:E:1190:GLN:HE21	1.67	0.58
1:A:1287:PHE:N	1:A:1287:PHE:HD1	2.02	0.58
1:A:1408:GLU:OE2	1:A:1409:PRO:HD2	2.04	0.58
1:C:1404:LEU:HD23	1:C:1404:LEU:C	2.24	0.58
1:D:1422:VAL:HG12	1:D:1423:ARG:H	1.66	0.58
1:A:1361:MET:O	1:A:1362:LYS:HG3	2.03	0.58
1:F:1394:PHE:CD1	1:F:1394:PHE:C	2.77	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: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: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:B:1246:CYS:SG	1:B:1276:ARG:O	2.62	0.57
1:C:1187:PRO:HD3	1:C:1434:ARG:HB2	1.86	0.57
1:C:483:LEU:HG	1:C:497:PHE:HD2	1.68	0.57
1:C:453:PHE:CE1	1:C:503:TYR:HB2	2.40	0.57
1:D:1335:VAL:HG12	1:D:1368:ALA:HB2	1.86	0.57
1:E:428:LYS:O	1:E:431:ALA:HB3	2.04	0.57
1:E:458:VAL:O	1:E:462:LEU:CB	2.47	0.57
1:A:449:ILE:HD12	1:A:1407:PHE:CZ	2.40	0.57
1:F:1181:VAL:HG11	1:F:1396:PRO:HB3	1.86	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:E:1381:TRP:CE3	1:E:1383:ARG:HG2	2.39	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:A:1287:PHE:CD1	1:A:1287:PHE:N	2.73	0.57
1:C:1202:MET:HE1	1:C:1272:PHE:CZ	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1276:ARG:HG2	1:C:1277:TYR:N	2.20	0.57
1:E:470:PRO:HG2	1:E:474:GLU:HG3	1.85	0.57
1:B:1173:LEU:HD12	1:B:1173:LEU:O	2.04	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:A:459:VAL:O	1:A:463:TYR:HD2	1.87	0.57
1:B:1408:GLU:HB3	1:B:1413:TYR:CD2	2.39	0.57
1:B:488:ILE:HG22	1:B:503:TYR:HD1	1.70	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:E:1328:LEU:HA	1:E:1349:ASN:HD21	1.69	0.56
1:E:489:ARG:NH2	1:E:1409:PRO:HG3	2.20	0.56
1:F:1381:TRP:CZ3	1:F:1383:ARG:HG2	2.40	0.56
1:B:1187:PRO:HD3	1:B:1434:ARG:HB2	1.85	0.56
1:D:1290:ILE:HG22	1:D:1290:ILE:O	2.05	0.56
1:E:471:GLU:OE2	1:E:473:ARG:HB2	2.04	0.56
1:F:1250:GLN:HG3	1:F:1251:CYS:N	2.20	0.56
1:B:1329:ASN:OD1	1:B:1372:LEU:HD22	2.05	0.56
1:B:463:TYR:HD1	1:B:469:PHE:CB	2.18	0.56
1:C:1381:TRP:CH2	1:C:1383:ARG:HG2	2.40	0.56
1:D:1277:TYR:N	1:D:1277:TYR:CD2	2.71	0.56
1:D:1298:ARG:NH2	1:D:1372:LEU:CB	2.68	0.56
1:D:1331:SER:OG	1:D:1371:GLU:HB3	2.04	0.56
1:D:440:ARG:HG2	1:D:442:ARG:NH2	2.21	0.56
1:F:1319:LYS:O	1:F:1390:PHE:HA	2.05	0.56
1:F:1324:ILE:CD1	1:F:1386:ILE:HG21	2.34	0.56
1:A:1392:VAL:HB	1:A:1394:PHE:HE2	1.66	0.56
1:E:495:ILE:HG23	1:E:496:THR:N	2.21	0.56
1:B:1202:MET:SD	1:B:1272:PHE:CZ	2.98	0.56
1:B:471:GLU:HG3	1:B:472:ARG: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:1156:PRO:HG2	1:F:1425:ILE:HD11	1.88	0.56
1:B:1326:THR:HG21	1:B:1344:TYR:CE1	2.40	0.56
1:A:462:LEU:CD1	1:A:478:TYR:HD2	2.16	0.56
1:C:422:ASP:OD1	1:C:425:SER:HB2	2.06	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:A:1331:SER:HB3	1:A:1373:LEU:HG	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1317:ALA:HB2	1:C:1392:VAL:HG12	1.87	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:1425:ILE:O	1:C:1425:ILE:HG23	2.06	0.56
1:E:462:LEU:CD2	1:E:475:ALA:CA	2.84	0.56
1:F:425:SER:HA	1:F:428:LYS:HD3	1.88	0.56
1:A:495:ILE:HG23	1:A:496:THR:N	2.20	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:C:1325:PRO:HG3	1:C:1384:PRO:O	2.06	0.56
1:C:426:VAL:HG21	1:C:478:TYR:OH	2.06	0.56
1:D:1343:LYS:HE3	1:D:1345:LYS:HZ3	1.71	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:C:1277:TYR:CD2	1:C:1277:TYR:N	2.74	0.55
1:A:1322:VAL:HB	1:A:1353:TRP:HB3	1.88	0.55
1:B:1333:VAL:HG21	1:B:1351:ILE:HD11	1.87	0.55
1:D:460:ASP:O	1:D:463:TYR:N	2.34	0.55
1:E:1175:LEU:HD11	1:E:1404:LEU:HD22	1.88	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:A:472:ARG:O	1:A:472:ARG:HD3	2.06	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: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: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:E:1296:VAL:HB	1:E:1300:LYS:HB3	1.88	0.55
1:E:1324:ILE:HD12	1:E:1386:ILE:CG2	2.36	0.55
1:F:478:TYR:CE1	1:F:482:LEU:HD21	2.41	0.55
1:B:438:GLU:HG3	1:B:438:GLU:O	2.05	0.55
1:C:1422:VAL:CG1	1:C:1423:ARG:N	2.70	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:A:1413:TYR:HB2	1:A:1417:ASP:HB2	1.88	0.55
1:C:1253:ARG:HH12	1:C:1266:ILE:CD1	2.11	0.55
1:C:447:ILE:CG2	1:C:448:THR:H	2.19	0.55
1:D:1211:GLU:OE1	1:D:1266:ILE:HD11	2.06	0.55
1:F:1183:LEU:CD1	1:F:1191:VAL:HG13	2.36	0.55
1:F:440:ARG:HG2	1:F:441:ASP:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:443:MET:HG3	1:F:447:ILE:O	2.07	0.55
1:B:1413:TYR:HB2	1:B:1417:ASP:HB2	1.87	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:E:1305:VAL:HG23	1:E:1366:ILE:CG2	2.36	0.55
1:E:421:MET:HG3	1:E:422:ASP:H	1.71	0.55
1:A:1182:ASN:ND2	1:A:1195:HIS:CE1	2.67	0.55
1:C:1294:ARG:O	1:C:1301:LEU:HD12	2.06	0.55
1:C:476:ARG:NH1	1:C:499:GLU:HG3	2.22	0.55
1:D:439:VAL:HG22	1:D:453:PHE:CD2	2.42	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:A:471:GLU:H	1:A:474:GLU:HG3	1.72	0.55
1:B:1294:ARG:NH1	1:B:1294:ARG:HB3	2.22	0.55
1:D:1356:LYS:HD3	1:D:1357:ARG:NH1	2.13	0.55
1:E:430:MET:HE1	1:E:458:VAL:HG23	1.88	0.55
1:F:454:LEU:HD23	1:F:456:SER:OG	2.07	0.55
1:C:1288:ARG:HH11	1:C:1290:ILE:HD11	1.72	0.54
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: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:D:1286:PRO:HG2	1:D:1390:PHE:CE1	2.42	0.54
1:F:1381:TRP:CE3	1:F:1383:ARG:HG2	2.42	0.54
1:D:1357:ARG:NH1	1:D:1357:ARG:HG2	2.22	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:HG23	1.88	0.54
1:D:495:ILE:HG13	1:D:496:THR:H	1.73	0.54
1:F:426:VAL:O	1:F:429:ALA:HB3	2.08	0.54
1:A:442:ARG:NH1	1:A:442:ARG:HG2	2.21	0.54
1:B:1290:ILE:O	1:B:1290:ILE:HG22	2.07	0.54
1:B:1408:GLU:CG	1:B:1411:LEU:HB2	2.36	0.54
1:B:1419:ILE:CD1	1:B:1419:ILE:N	2.70	0.54
1:C:440:ARG:N	1:C:442:ARG:NH1	2.55	0.54
1:F:1263:ILE:N	1:F:1263:ILE:CD1	2.71	0.54
1:A:1323:ARG:HG3	1:A:1323:ARG:HH11	1.73	0.54
1:F:1181:VAL:CG1	1:F:1396:PRO:CB	2.85	0.54
1:F:1324:ILE:O	1:F:1324:ILE:HG22	2.07	0.54
1:C:1273:GLU:OE2	1:C:1276:ARG:NH2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1264:SER:O	1:D:1265:PHE:HB3	2.08	0.54
1:E:1286:PRO:O	1:E:1310:ASN:HB3	2.07	0.54
1:E:1323:ARG:HH12	1:E:1352:VAL:HG13	1.73	0.54
1:B:463:TYR:HD1	1:B:469:PHE:HB2	1.71	0.54
1:E:479:ALA:HB3	1:E:497:PHE:HE2	1.72	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:F:1185:MET:HE2	1:F:1186:SER:O	2.08	0.54
1:F:463:TYR:HB2	1:F:475:ALA:HB2	1.90	0.54
1:A:1184:LEU:CB	1:A:1193:SER:OG	2.56	0.54
1:A:1359:ALA:HB3	1:A:1362:LYS:HD3	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:E:490:HIS:CD2	1:E:494:LYS:HB3	2.43	0.54
1:B:451:ASN:HD21	1:B:1213:LYS:HG3	1.73	0.54
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:1434:ARG:HG3	1:B:1434:ARG:HH11	1.73	0.53
1:C:453:PHE:HE1	1:C:503:TYR:HB2	1.72	0.53
1:D:1317:ALA:HB2	1:D:1392:VAL:HG12	1.90	0.53
1:F:1312:LYS:HB2	1:F:1312:LYS:HZ2	1.73	0.53
1:F:1408:GLU:OE2	1:F:1410:LYS:HB2	2.08	0.53
1:D:432:ALA:HB3	1:D:435:SER:OG	2.09	0.53
1:D:479:ALA:HA	1:D:482:LEU:HD12	1.90	0.53
1:E:1359:ALA:HB3	1:E:1362:LYS:CE	2.38	0.53
1:E:426:VAL:O	1:E:429:ALA:HB3	2.07	0.53
1:A:1244:ASP:HB2	1:A:1278:ARG:O	2.09	0.53
1:C:1323:ARG:HB3	1:C:1387:SER:OG	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:A:1253:ARG:HB2	1:A:1264:SER:OG	2.08	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:E:1293:VAL:HG21	1:E:1383:ARG:HH11	1.73	0.53
1:B:1277:TYR:N	1:B:1277:TYR:CD2	2.77	0.53
1:B:1341:LYS:NZ	1:B:1343:LYS:HE3	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1345:LYS:NZ	1:E:1354:LYS:NZ	2.56	0.53
1:E:1399:LEU:HD23	1:E:1400:LYS:N	2.23	0.53
1:F:1277:TYR:CD2	1:F:1277:TYR:N	2.76	0.53
1:A:1375:THR:CG2	1:A:1378:LYS:HD3	2.38	0.53
1:C:1183:LEU:HD22	1:C:1285:LEU:HD22	1.91	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: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:F:1188:GLN:NE2	1:F:1190:GLN:HG2	2.24	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:B:1202:MET:SD	1:B:1272:PHE:HZ	2.31	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:E:504:VAL:HB	1:E:1211:GLU:OE1	2.09	0.53
1:A:1241:ILE:O	1:A:1241:ILE:HG22	2.08	0.53
1:C:1276:ARG:HB2	1:C:1276:ARG:CZ	2.38	0.53
1:C:1288:ARG:NH1	1:C:1290:ILE:CD1	2.71	0.53
1:E:466:VAL:HG11	1:E:469:PHE:HE2	1.74	0.53
1:F:1217:ASN:HD22	1:F:1400:LYS:HB2	1.74	0.53
1:A:1403:TYR:CD1	1:A:1403:TYR:C	2.82	0.52
1:D:1196:VAL:HG23	1:D:1279:THR:HG22	1.90	0.52
1:D:1424:TYR:HD2	1:D:1424:TYR:N	2.05	0.52
1:D:422:ASP:O	1:D:426:VAL:HG23	2.09	0.52
1:E:491:THR:HG22	1:E:492:VAL:CG1	2.39	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:A:1434:ARG:CG	1:A:1434:ARG:NH1	2.65	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:F:1298:ARG:HH21	1:F:1298:ARG:HG3	1.74	0.52
1:F:1394:PHE:HD1	1:F:1394:PHE:C	2.11	0.52
1:A:1317:ALA:HB2	1:A:1392:VAL:HG12	1.92	0.52
1:C:1174:PHE:HD1	1:C:1421:TRP:HB2	1.73	0.52
1:E:462:LEU:HD13	1:E:479:ALA:HB2	1.91	0.52
1:B:1342:ALA:HB2	1:B:1353:TRP:CD1	2.44	0.52
1:F:1177:VAL:HB	1:F:1424:TYR:CD1	2.35	0.52
1:D:1183:LEU:HD11	1:D:1191:VAL:HG13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1301:LEU:O	1:D:1370:ILE:HG12	2.09	0.52
1:E:1203:LYS:HB3	1:E:1205:TYR:CE1	2.37	0.52
1:E:1329:ASN:OD1	1:E:1372:LEU:HD22	2.10	0.52
1:F:1323:ARG:NH1	1:F:1352:VAL:HG22	2.09	0.52
1:B:1300:LYS:NZ	1:B:1302:GLU:OE1	2.38	0.52
1:B:1322:VAL:HB	1:B:1353:TRP:HB3	1.91	0.52
1:B:426:VAL:O	1:B:429:ALA:HB3	2.09	0.52
1:C:487:LEU:HD12	1:C:487:LEU:H	1.73	0.52
1:D:1173:LEU:HD12	1:D:1173:LEU:C	2.29	0.52
1:D:1206:LEU:HD22	1:D:1406:VAL:HG11	1.90	0.52
1:A:1329:ASN:ND2	1:A:1372:LEU:HD13	2.25	0.52
1:A:487:LEU:H	1:A:487:LEU:HD23	1.74	0.52
1:B:1252:VAL:HG22	1:B:1263:ILE:CG1	2.40	0.52
1:C:1211:GLU:HG3	1:C:1253:ARG:HH11	1.73	0.52
1:E:1324:ILE:CG2	1:E:1324:ILE:O	2.57	0.52
1:F:460:ASP:C	1:F:464:HIS:HD2	2.14	0.52
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: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
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:D:430:MET:HE3	1:D:458:VAL:HG13	1.92	0.51
1:A:1423:ARG:HB2	1:E:1158:TYR:CD1	2.44	0.51
1:A:1247:THR:C	1:A:1248:PHE:CD1	2.84	0.51
1:A:430:MET:O	1:A:435:SER:OG	2.28	0.51
1:A:449:ILE:HD12	1:A:1407:PHE:CE1	2.45	0.51
1:B:1422:VAL:HG22	1:B:1423:ARG:H	1.75	0.51
1:D:1181:VAL:CG1	1:D:1396:PRO:HB3	2.41	0.51
1:E:430:MET:CE	1:E:458:VAL:HG23	2.39	0.51
1:F:1293:VAL:HG23	1:F:1383:ARG:HH12	1.74	0.51
1:B:1170:ARG:HA	1:F:1421:TRP:CH2	2.46	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:C:449:ILE:HG22	1:C:452:ALA:HB2	1.92	0.51
1:D:1392:VAL:HB	1:D:1394:PHE:HE2	1.76	0.51
1:F:1331:SER:HB2	1:F:1373:LEU:CD2	2.40	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:A:1253:ARG:CD	1:A:1264:SER:OG	2.49	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:427:THR:CG2	1:C:482:LEU:HD22	2.41	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:A:1296:VAL:O	1:A:1300:LYS:HB2	2.11	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:D:1289:VAL:HG22	1:D:1307:ILE:CG2	2.40	0.51
1:D:426:VAL:O	1:D:429:ALA:HB3	2.11	0.51
1:D:439:VAL:HG12	1:D:439:VAL:O	2.10	0.51
1:E:1268:PRO:HD2	1:E:1272:PHE:CE1	2.45	0.51
1:F:1296:VAL:HB	1:F:1300:LYS:HB2	1.93	0.51
1:A:1185:MET:CE	1:A:1288:ARG:HD2	2.41	0.51
1:A:454:LEU:HG	1:A:456:SER:H	1.76	0.51
1:D:1178:LEU:HD23	1:D:1425:ILE:HB	1.93	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:F:1422:VAL:CG1	1:F:1423:ARG:H	2.24	0.51
1:A:1319:LYS:O	1:A:1390:PHE:HA	2.11	0.51
1:D:1285:LEU:CD1	1:D:1285:LEU:N	2.73	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:F:462:LEU:HD12	1:F:475:ALA:O	2.11	0.51
1:D:1413:TYR:HB2	1:D:1417:ASP:HB2	1.91	0.51
1:A:426:VAL:O	1:A:429:ALA:HB3	2.11	0.50
1:C:1359:ALA:HB3	1:C:1362:LYS:HE2	1.92	0.50
1:C:495:ILE:HG23	1:C:496:THR:HG23	1.94	0.50
1:D:1320:ILE:HG23	1:D:1388:MET:CE	2.39	0.50
1:D:1324:ILE:CG2	1:D:1324:ILE:O	2.58	0.50
1:E:1179:GLU:OE2	1:E:1397:SER:OG	2.24	0.50
1:E:1300:LYS:HE2	1:E:1369:GLU:OE2	2.11	0.50
1:B:1359:ALA:HB3	1:B:1362:LYS:HD2	1.92	0.50
1:E:487:LEU:HD23	1:E:487:LEU:H	1.75	0.50
1:F:1329:ASN:OD1	1:F:1372:LEU:HD22	2.12	0.50
1:C:1174:PHE:CD1	1:C:1421:TRP:HB2	2.47	0.50
1:C:1375:THR:HG22	1:C:1378:LYS:H	1.75	0.50
1:C:460:ASP:HA	1:C:463:TYR:HE1	1.75	0.50
1:D:430:MET:HE2	1:D:437:LEU:HD22	1.93	0.50
1:A:1338:MET:HE2	1:F:492:VAL:HG13	1.92	0.50
1:C:1315:LEU:HD23	1:C:1315:LEU:N	2.26	0.50
1:C:443:MET:HG3	1:C:447:ILE:O	2.11	0.50
1:E:1170:ARG:NH2	1:E:1205:TYR:CD2	2.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1370:ILE:N	1:E:1370:ILE:HD12	2.25	0.50
1:E:1178:LEU:HB3	1:E:1427:ARG:HH12	1.76	0.50
1:F:440:ARG:O	1:F:442:ARG:HD3	2.11	0.50
1:A:1184:LEU:HB2	1:A:1193:SER:OG	2.12	0.50
1:A:1183:LEU:HB3	1:A:1431:TYR:CE1	2.47	0.50
1:D:1216:MET:HA	1:D:1402:ARG:HG3	1.92	0.50
1:E:1305:VAL:HG11	1:E:1324:ILE:HD11	1.94	0.50
1:E:479:ALA:HB3	1:E:497:PHE:CE2	2.47	0.50
1:F:1214:PHE:HD1	1:F:1214:PHE:C	2.15	0.50
1:F:1284:ILE:HG13	1:F:1396:PRO:HA	1.94	0.50
1:A:1202:MET:O	1:A:1271:GLU:HA	2.11	0.50
1:B:1249:HIS:CD2	1:B:1272:PHE:HB2	2.47	0.50
1:D:1296:VAL:HB	1:D:1300:LYS:HB2	1.94	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:F:441:ASP:OD1	1:F:450:PRO:HA	2.11	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
1:A:1298:ARG:HH21	1:A:1374:PRO:HA	1.77	0.50
1:B:1322:VAL:HG22	1:B:1388:MET:CE	2.42	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:E:1195:HIS:CE1	1:E:1278:ARG:HH12	2.29	0.50
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: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:C:463:TYR:CG	1:C:464:HIS:N	2.80	0.50
1:E:1299:THR:HG22	1:E:1300:LYS:HD2	1.93	0.50
1:E:1392:VAL:HB	1:E:1394:PHE:CE2	2.47	0.50
1:E:1419:ILE:N	1:E:1419:ILE:HD12	2.26	0.50
1:A:463:TYR:HB3	1:A:475:ALA:HB2	1.94	0.50
1:C:495:ILE:HG23	1:C:496:THR:N	2.27	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: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:A:1293:VAL:HG12	1:A:1303:VAL:HG13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1392:VAL:HB	1:A:1394:PHE:CD2	2.47	0.49
1:D:1185:MET:HG3	1:D:1191:VAL:HG22	1.94	0.49
1:D:1324:ILE:CD1	1:D:1386:ILE:HG12	2.30	0.49
1:E:1306:VAL:HG22	1:E:1365:GLN:HB2	1.93	0.49
1:B:1284:ILE:O	1:B:1286:PRO:HD3	2.12	0.49
1:C:489:ARG:HD2	1:C:1410:LYS:HE2	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:A:1328:LEU:HD13	1:A:1381:TRP:CZ3	2.48	0.49
1:A:1345:LYS:HA	1:A:1345:LYS:CE	2.37	0.49
1:A:472:ARG:NH2	1:A:472:ARG:CG	2.76	0.49
1:B:1415:ASP:OD2	1:B:1420:LYS:NZ	2.43	0.49
1:C:1264:SER:O	1:C:1265:PHE:HB3	2.12	0.49
1:C:458:VAL:CG1	1:C:459:VAL:N	2.76	0.49
1:D:1249:HIS:O	1:D:1252:VAL:HG23	2.11	0.49
1:D:494:LYS:HE2	1:D:498:SER:OG	2.13	0.49
1:B:1413:TYR:HA	1:B:1417:ASP:OD2	2.12	0.49
1:B:1421:TRP:CH2	1:F:1170:ARG:HA	2.48	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:E:1183:LEU:HD11	1:E:1191:VAL:CG1	2.42	0.49
1:B:1158:TYR:HD1	1:F:1421:TRP:HB3	1.78	0.49
1:A:1329:ASN:OD1	1:A:1378:LYS:HD2	2.13	0.49
1:F:1214:PHE:CD1	1:F:1214:PHE:C	2.85	0.49
1:F:1293:VAL:HG23	1:F:1383:ARG:NH1	2.27	0.49
1:F:439:VAL:HG13	1:F:453:PHE:HD2	1.77	0.49
1:B:1394:PHE:O	1:B:1396:PRO:HD3	2.13	0.49
1:B:458:VAL:O	1:B:462:LEU:CG	2.60	0.49
1:F:1323:ARG:HH11	1:F:1323:ARG:HG3	1.76	0.49
1:F:440:ARG:HG2	1:F:441:ASP:H	1.77	0.49
1:B:1375:THR:HG23	1:B:1375:THR:O	2.12	0.49
1:D:1250:GLN:HG3	1:D:1251:CYS:H	1.76	0.49
1:D:1181:VAL:HG11	1:D:1396:PRO:HB3	1.95	0.49
1:A:1182:ASN:HB2	1:A:1195:HIS:CE1	2.46	0.49
1:A:1286:PRO:C	1:A:1287:PHE:HD1	2.16	0.49
1:B:1272:PHE:CD1	1:B:1272:PHE:C	2.85	0.49
1:B:1422:VAL:HG22	1:B:1423:ARG:N	2.28	0.49
1:C:1174:PHE:CE1	1:C:1421:TRP:HD1	2.27	0.49
1:C:430:MET:HB3	1:C:437:LEU:CD2	2.43	0.49
1:E:459:VAL:HG11	1:E:472:ARG:HE	1.78	0.49
1:A:1328:LEU:HD13	1:A:1381:TRP:HZ3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1277:TYR:HD2	1:B:1277:TYR:N	2.11	0.48
1:B:1421:TRP:CZ3	1:F:1170:ARG:CB	2.96	0.48
1:B:483:LEU:HD12	1:B:488:ILE:O	2.13	0.48
1:C:472:ARG:CG	1:C:472:ARG:NH2	2.74	0.48
1:E:1173:LEU:HD12	1:E:1173:LEU:O	2.12	0.48
1:E:1298:ARG:HH21	1:E:1298:ARG:CG	2.26	0.48
1:E:1390:PHE:CE1	1:E:1428:SER:HB3	2.48	0.48
1:E:1413:TYR:HB2	1:E:1417:ASP:HB2	1.95	0.48
1:E:490:HIS:NE2	1:E:494:LYS:HB3	2.28	0.48
1:F:1277:TYR:CE1	1:F:1399:LEU:HD12	2.48	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: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:F:1289:VAL:O	1:F:1291:PRO:HD3	2.12	0.48
1:A:433:PRO:HG3	1:A:1256:LYS:HB2	1.94	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:1205:TYR:N	1:A:1205:TYR:HD2	2.11	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:B:1382:ALA:O	1:B:1384:PRO:HD3	2.13	0.48
1:B:440:ARG:HB3	1:B:442:ARG:NH1	2.29	0.48
1:C:1276:ARG:HH11	1:C:1276:ARG:CG	2.26	0.48
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: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:D:479:ALA:HA	1:D:482:LEU:CD1	2.43	0.48
1:F:1287:PHE:HD1	1:F:1388:MET:SD	2.36	0.48
1:A:1173:LEU:HD22	1:A:1404:LEU:CD2	2.44	0.48
1:B:494:LYS:NZ	1:B:498:SER:HB2	2.29	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:A:447:ILE:CG2	1:A:448:THR:N	2.77	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:CD1	1:E:1173:LEU:C	2.82	0.48
1:F:423:MET:HA	1:F:478:TYR:OH	2.14	0.48
1:C:1343:LYS:HG2	1:C:1344:TYR:N	2.28	0.48
1:C:460:ASP:HA	1:C:463:TYR:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1277:TYR:CD2	1:E:1277:TYR:N	2.82	0.48
1:A:1247:THR:O	1:A:1248:PHE:CD1	2.67	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: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:F:478:TYR:CZ	1:F:482:LEU:HD21	2.49	0.48
1:B:1185:MET:SD	1:B:1288:ARG:HD2	2.54	0.48
1:C:1329:ASN:HD21	1:C:1372:LEU:HB3	1.78	0.48
1:D:467:GLU:HG2	1:D:468:GLY:N	2.29	0.48
1:E:1345:LYS:NZ	1:E:1354:LYS:HZ1	2.12	0.48
1:F:424:ALA:O	1:F:428:LYS:HG3	2.14	0.48
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: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:B:1296:VAL:O	1:B:1300:LYS:HB2	2.14	0.47
1:E:1253:ARG:HG3	1:E:1253:ARG:NH2	2.30	0.47
1:E:1300:LYS:HG3	1:E:1369:GLU:OE2	2.14	0.47
1:A:1184:LEU:HA	1:A:1432:GLU:O	2.14	0.47
1:A:1277:TYR:N	1:A:1277:TYR:CD2	2.82	0.47
1:A:1421:TRP:CZ3	1:E:1170:ARG:HB2	2.50	0.47
1:B:1326:THR:HG21	1:B:1344:TYR:HE1	1.79	0.47
1:E:1293:VAL:CG2	1:E:1383:ARG:NH1	2.77	0.47
1:E:1299:THR:O	1:E:1371:GLU:HA	2.14	0.47
1:E:422:ASP:O	1:E:426:VAL:CG2	2.60	0.47
1:A:1193:SER:O	1:A:1194:ALA:HB2	2.14	0.47
1:A:1298:ARG:NH2	1:A:1375:THR:H	2.12	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:B:1158:TYR:CE2	1:F:1423:ARG:CZ	2.98	0.47
1:B:1305:VAL:CG2	1:B:1324:ILE:HD11	2.37	0.47
1:F:1177:VAL:HG21	1:F:1424:TYR:CE1	2.49	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: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:E:1413:TYR:HA	1:E:1417:ASP:OD2	2.14	0.47
1:F:1296:VAL:O	1:F:1300:LYS:HB2	2.15	0.47
1:F:430:MET:HE2	1:F:437:LEU:HD22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1218:ASP:HA	1:A:1241:ILE:HB	1.97	0.47
1:A:489:ARG:HH12	1:A:1211:GLU:HB2	1.80	0.47
1:B:463:TYR:CD1	1:B:469:PHE:HB2	2.49	0.47
1:C:1287:PHE:N	1:C:1287:PHE:HD1	2.13	0.47
1:C:463:TYR:OH	1:C:464:HIS:CE1	2.67	0.47
1:D:1181:VAL:CG1	1:D:1396:PRO:CB	2.93	0.47
1:D:456:SER:HA	1:D:499:GLU:CG	2.45	0.47
1:E:466:VAL:CG1	1:E:469:PHE:CE2	2.95	0.47
1:F:1182:ASN:HB2	1:F:1195:HIS:CE1	2.50	0.47
1:F:1250:GLN:CG	1:F:1251:CYS:N	2.77	0.47
1:A:1264:SER:O	1:A:1265:PHE:HB3	2.15	0.47
1:A:482:LEU:HD23	1:A:482:LEU:N	2.28	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:D:1353:TRP:CZ3	1:D:1366:ILE:HB	2.50	0.47
1:D:441:ASP:OD2	1:D:1213:LYS:NZ	2.39	0.47
1:E:1178:LEU:HB3	1:E:1427:ARG:NH1	2.29	0.47
1:E:1214:PHE:C	1:E:1214:PHE:HD2	2.18	0.47
1:F:460:ASP:O	1:F:464:HIS:CD2	2.66	0.47
1:A:1277:TYR:N	1:A:1277:TYR:HD2	2.12	0.47
1:A:1298:ARG:O	1:A:1372:LEU:HB2	2.15	0.47
1:A:1421:TRP:CH2	1:E:1170:ARG:HA	2.49	0.47
1:A:476:ARG:CG	1:A:476:ARG:HH21	2.24	0.47
1:B:1299:THR:O	1:B:1371:GLU:HA	2.14	0.47
1:C:1290:ILE:HD12	1:C:1290:ILE:N	2.30	0.47
1:C:1298:ARG:O	1:C:1372:LEU:HD12	2.15	0.47
1:D:1181:VAL:HG12	1:D:1196:VAL:HG12	1.95	0.47
1:D:1413:TYR:HA	1:D:1417:ASP:OD2	2.13	0.47
1:F:1425:ILE:CG2	1:F:1425:ILE:O	2.61	0.47
1:B:1408:GLU:O	1:B:1411:LEU:O	2.33	0.47
1:C:1402:ARG:O	1:C:1403:TYR:HB3	2.15	0.47
1:C:1427:ARG:CG	1:C:1428:SER:N	2.77	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:F:1264:SER:O	1:F:1265:PHE:HB3	2.14	0.47
1:F:453:PHE:HZ	1:F:488:ILE:HD12	1.80	0.47
1:C:1408:GLU:HG2	1:C:1411:LEU:CB	2.44	0.47
1:C:489:ARG:NH2	1:C:1410:LYS:HE3	2.29	0.47
1:D:1187:PRO:CD	1:D:1434:ARG:HB2	2.41	0.47
1:E:1305:VAL:HG21	1:E:1324:ILE:CD1	2.41	0.47
1:F:1277:TYR:HD2	1:F:1277:TYR:N	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:443:MET:HG3	1:A:447:ILE:O	2.15	0.47
1:B:428:LYS:HE2	1:B:508:LEU:O	2.15	0.47
1:C:1330:THR:HG21	1:C:1344:TYR:OH	2.15	0.47
1:C:497:PHE:O	1:C:497:PHE:HD1	1.98	0.47
1:E:426:VAL:HG21	1:E:478:TYR:OH	2.15	0.47
1:F:1276:ARG:HG2	1:F:1277:TYR:N	2.30	0.47
1:F:461:TRP:O	1:F:461:TRP:CE3	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:1199:ARG:N	1:B:1277:TYR:HE2	2.13	0.46
1:B:454:LEU:O	1:B:458:VAL:HG23	2.14	0.46
1:B:427:THR:HG21	1:B:487:LEU:HB3	1.97	0.46
1:C:1290:ILE:O	1:C:1290:ILE:HG22	2.14	0.46
1:D:1389:ASN:HA	1:D:1428:SER:OG	2.15	0.46
1:E:1201:VAL:HG12	1:E:1202:MET:N	2.30	0.46
1:E:1322:VAL:HB	1:E:1353:TRP:HB3	1.95	0.46
1:B:1193:SER:O	1:B:1194:ALA:HB2	2.16	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: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: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:A:1276:ARG:HH11	1:A:1276:ARG:CG	2.27	0.46
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:1263:ILE:HD11	1:C:1274:LEU:HD21	1.96	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:E:1355:ILE:HG22	1:E:1355:ILE:O	2.15	0.46
1:F:440:ARG:CB	1:F:440:ARG:NH2	2.78	0.46
1:A:1379:LYS:HD2	1:A:1379:LYS:N	2.19	0.46
1:A:1383:ARG:H	1:A:1383:ARG:NH1	2.14	0.46
1:A:460:ASP:HA	1:A:463:TYR:HE2	1.77	0.46
1:B:1366:ILE:HG23	1:B:1366:ILE:O	2.15	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:A:1339:LYS:HB3	1:A:1339:LYS:HZ3	1.78	0.46
1:A:461:TRP:CD1	1:A:465:HIS:CD2	3.04	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1173:LEU:O	1:F:1173:LEU:HD12	2.15	0.46
1:F:1247:THR:O	1:F:1248:PHE:CD2	2.69	0.46
1:F:1323:ARG:HH12	1:F:1352:VAL:CG2	2.11	0.46
1:F:1361:MET:CE	1:F:1361:MET:HA	2.44	0.46
1:F:1323:ARG:O	1:F:1386:ILE:HG23	2.15	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:A:1321:GLU:OE1	1:A:1354:LYS:HE3	2.16	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:HG3	1:B:1434:ARG:NH1	2.28	0.46
1:B:473:ARG:CG	1:B:473:ARG:HH21	2.28	0.46
1:C:1252:VAL:HA	1:C:1265:PHE:HB3	1.97	0.46
1:A:492:VAL:CG2	1:C:1338:MET:HB3	2.45	0.46
1:D:1304:LYS:HG3	1:D:1367:SER:OG	2.14	0.46
1:A:1185:MET:HE1	1:A:1288:ARG:HD2	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:B:1172:GLU:HB3	1:B:1419:ILE:HB	1.97	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:1402:ARG:O	1:A:1403:TYR:HB3	2.16	0.46
1:C:1217:ASN:HD21	1:C:1400:LYS:CB	2.23	0.46
1:C:1294:ARG:NH2	1:C:1302:GLU:OE2	2.48	0.46
1:C:433:PRO:CG	1:C:1256:LYS:HE2	2.46	0.46
1:D:1300:LYS:HD3	1:D:1300:LYS:HA	1.72	0.46
1:E:480:SER:HB2	1:E:497:PHE:HD2	1.81	0.46
1:F:447:ILE:HG22	1:F:448:THR:H	1.81	0.46
1:A:1316:LEU:CD2	1:A:1359:ALA:HA	2.45	0.46
1:C:1276:ARG:CG	1:C:1277:TYR:N	2.79	0.46
1:D:1199:ARG:N	1:D:1277:TYR:HE2	2.14	0.46
1:D:1315:LEU:HD23	1:D:1315:LEU:N	2.31	0.46
1:D:1390:PHE:CE2	1:D:1428:SER:HB3	2.51	0.46
1:D:1402:ARG:O	1:D:1403:TYR:HB3	2.16	0.46
1:D:1408:GLU:CG	1:D:1411:LEU:HB2	2.38	0.46
1:E:1246:CYS:HB2	1:E:1276:ARG:O	2.16	0.46
1:F:1410:LYS:HD3	1:F:1410:LYS:HA	1.71	0.46
1:A:1252:VAL:HG12	1:A:1253:ARG:O	2.16	0.46
1:A:447:ILE:CG2	1:A:448:THR:H	2.26	0.46
1:B:1371:GLU:O	1:B:1372:LEU:HD23	2.16	0.46
1:C:1390:PHE:HD1	1:C:1391:GLU:N	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:462:LEU:HD22	1:E:475:ALA:CB	2.45	0.46
1:E:449:ILE:HD13	1:E:491:THR:CG2	2.46	0.46
1:F:1188:GLN:HE21	1:F:1190:GLN:HG2	1.79	0.46
1:F:1328:LEU:HD23	1:F:1328:LEU:N	2.31	0.46
1:A:498:SER:OG	1:A:499:GLU:N	2.48	0.45
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:C:1287:PHE:CE2	1:C:1320:ILE:HD13	2.51	0.45
1:C:461:TRP:CD1	1:C:465:HIS:HD2	2.34	0.45
1:D:1202:MET:CE	1:D:1404:LEU:HD21	2.46	0.45
1:E:1335:VAL:HG11	1:E:1351:ILE:HG21	1.98	0.45
1:A:1316:LEU:HD22	1:A:1359:ALA:HA	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:E:1280:THR:HA	1:E:1283:ILE:HD11	1.98	0.45
1:E:1335:VAL:HG12	1:E:1368:ALA:CB	2.46	0.45
1:F:1298:ARG:O	1:F:1372:LEU:HB2	2.16	0.45
1:B:1186:SER:HB3	1:B:1190:GLN:HB2	1.99	0.45
1:C:1298:ARG:O	1:C:1372:LEU:HB2	2.16	0.45
1:C:490:HIS:CE1	1:C:494:LYS:HB3	2.51	0.45
1:D:1288:ARG:NH1	1:D:1310:ASN:OD1	2.48	0.45
1:D:437:LEU:HD12	1:D:438:GLU:N	2.31	0.45
1:F:1335:VAL:HG12	1:F:1351:ILE:HD13	1.97	0.45
1:B:1344:TYR:CD2	1:B:1344:TYR:O	2.69	0.45
1:B:1331:SER:OG	1:B:1371:GLU:HB3	2.16	0.45
1:C:1289:VAL:O	1:C:1291:PRO:HD3	2.17	0.45
1:C:469:PHE:CE1	1:C:475:ALA:HA	2.51	0.45
1:D:1198:GLY:C	1:D:1277:TYR:CE2	2.90	0.45
1:D:430:MET:CE	1:D:458:VAL:HG13	2.46	0.45
1:E:1359:ALA:HB3	1:E:1362:LYS:NZ	2.32	0.45
1:F:1299:THR:O	1:F:1371:GLU:HA	2.17	0.45
1:F:456:SER:HA	1:F:499:GLU:HG2	1.99	0.45
1:C:1182:ASN:OD1	1:C:1430:ILE:N	2.49	0.45
1:D:1286:PRO:HG2	1:D:1390:PHE:HE1	1.82	0.45
1:D:442:ARG:HD3	1:D:502:TYR:CE1	2.51	0.45
1:D:482:LEU:HD23	1:D:487:LEU:HD12	1.97	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1365:GLN:HG2	1:B:1366:ILE:N	2.31	0.45
1:B:1187:PRO:HD3	1:B:1434:ARG:CB	2.46	0.45
1:E:1247:THR:C	1:E:1248:PHE:CD1	2.90	0.45
1:F:1181:VAL:CG1	1:F:1396:PRO:HB3	2.46	0.45
1:A:1203:LYS:HB3	1:A:1205:TYR:HE2	1.82	0.45
1:A:1266:ILE:O	1:A:1266:ILE:HG22	2.16	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:B:442:ARG:NH2	1:B:452:ALA:O	2.49	0.45
1:D:1381:TRP:CG	1:D:1381:TRP:O	2.70	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:1179:GLU:OE2	1:B:1277:TYR:OH	2.26	0.45
1:C:1267:PRO:HA	1:C:1268:PRO:HD3	1.90	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:1324:ILE:O	1:F:1324:ILE:CG2	2.63	0.45
1:F:1316:LEU:CD2	1:F:1357:ARG:HD2	2.47	0.45
1:F:1298:ARG:HH12	1:F:1375:THR:H	1.64	0.45
1:A:1311:PHE:CE1	1:A:1360:GLY:HA2	2.51	0.45
1:B:1402:ARG:O	1:B:1403:TYR:HB3	2.17	0.45
1:D:1335:VAL:HG12	1:D:1368:ALA:CB	2.47	0.45
1:F:1434:ARG:NH1	1:F:1434:ARG:HG2	2.32	0.45
1:A:1249:HIS:CD2	1:A:1272:PHE:HD2	2.35	0.44
1:A:1375:THR:HG22	1:A:1378:LYS:HD3	1.99	0.44
1:A:1422:VAL:O	1:E:1158:TYR:HD1	2.01	0.44
1:B:1352:VAL:HG11	1:B:1354:LYS:HE3	1.99	0.44
1:C:1187:PRO:HD3	1:C:1434:ARG:CB	2.46	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
1:F:1172:GLU:HB2	1:F:1419:ILE:O	2.17	0.44
1:A:1171:ASN:ND2	1:A:1207:SER:H	2.14	0.44
1:A:1307:ILE:CD1	1:A:1358:MET:HE1	2.47	0.44
1:A:1413:TYR:HA	1:A:1417:ASP:OD2	2.18	0.44
1:B:1390:PHE:CD1	1:B:1390:PHE:C	2.91	0.44
1:A:494:LYS:NZ	1:C:1338:MET:O	2.39	0.44
1:E:1267:PRO:HA	1:E:1268:PRO:HD3	1.89	0.44
1:E:1327:PRO:HG3	1:E:1381:TRP:CD2	2.51	0.44
1:F:461:TRP:CE3	1:F:461:TRP:C	2.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1174:PHE:HB2	1:B:1203:LYS:HB2	1.99	0.44
1:B:463:TYR:CE1	1:B:469:PHE:O	2.61	0.44
1:C:458:VAL:HG13	1:C:459:VAL:N	2.32	0.44
1:D:1299:THR:O	1:D:1371:GLU:HA	2.18	0.44
1:E:1161:LEU:HD12	1:E:1162:GLU:N	2.32	0.44
1:E:1286:PRO:HG2	1:E:1390:PHE:CZ	2.52	0.44
1:F:1206:LEU:HD22	1:F:1406:VAL:HG11	1.99	0.44
1:F:442:ARG:HB3	1:F:502:TYR:CE2	2.52	0.44
1:C:1280:THR:HA	1:C:1283:ILE:HD11	1.99	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:D:1298:ARG:HE	1:D:1375:THR:H	1.64	0.44
1:F:463:TYR:HB2	1:F:475:ALA:CB	2.48	0.44
1:B:1330:THR:HG23	1:B:1370:ILE:CG2	2.48	0.44
1:B:1390:PHE:CZ	1:B:1428:SER:HB3	2.52	0.44
1:C:1185:MET:HE1	1:C:1289:VAL:O	2.18	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:E:476:ARG:HG2	1:E:476:ARG:NH2	2.32	0.44
1:A:1173:LEU:CD2	1:A:1404:LEU:HD23	2.47	0.44
1:A:1183:LEU:HB3	1:A:1431:TYR:HD1	1.82	0.44
1:A:1186:SER:OG	1:A:1190:GLN:HB2	2.17	0.44
1:A:1328:LEU:HD22	1:A:1381:TRP:CZ3	2.53	0.44
1:B:453:PHE:HZ	1:B:488:ILE:CD1	2.24	0.44
1:C:1193:SER:O	1:C:1194:ALA:HB2	2.18	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:A:1245:ASP:O	1:A:1246:CYS:HB3	2.18	0.44
1:A:430:MET:HB3	1:A:437:LEU:HD23	1.98	0.44
1:B:1315:LEU:N	1:B:1315:LEU:CD1	2.80	0.44
1:B:502:TYR:C	1:B:503:TYR:HD2	2.21	0.44
1:D:1170:ARG:NH1	1:D:1172:GLU:CG	2.80	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: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:1288:ARG:NH1	1:A:1290:ILE:HG13	2.32	0.44
1:A:1380:LYS:O	1:A:1381:TRP:HB3	2.18	0.44
1:A:495:ILE:CG2	1:A:496:THR:N	2.81	0.44
1:B:1425:ILE:HD11	1:F:1156:PRO:HG3	1.95	0.44
1:C:1260:GLU:O	1:C:1261:ARG:CB	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1170:ARG:NH1	1:D:1172:GLU:OE2	2.50	0.44
1:D:1184:LEU:HD23	1:D:1184:LEU:O	2.18	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:D:1326:THR:CG2	1:D:1344:TYR:CE1	2.99	0.44
1:E:1298:ARG:CZ	1:E:1298:ARG:HB3	2.47	0.44
1:E:1326:THR:HG23	1:E:1350:ALA:HA	1.99	0.44
1:F:1415:ASP:CG	1:F:1420:LYS:HZ1	2.20	0.44
1:A:433:PRO:HD3	1:A:1254:LEU:O	2.18	0.43
1:B:1360:GLY:O	1:B:1361:MET:C	2.56	0.43
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:1392:VAL:O	1:B:1392:VAL:HG23	2.17	0.43
1:C:1249:HIS:O	1:C:1252:VAL:HG23	2.17	0.43
1:C:469:PHE:HZ	1:C:478:TYR:HD2	1.61	0.43
1:D:1170:ARG:NH1	1:D:1172:GLU:CD	2.69	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:E:495:ILE:HG23	1:E:496:THR:HG22	1.99	0.43
1:F:1408:GLU:HG3	1:F:1411:LEU:N	2.33	0.43
1:A:1256:LYS:HE2	1:A:1259:SER:HB2	1.99	0.43
1:A:1338:MET:HE1	1:F:491:THR:HB	2.00	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:C:1206:LEU:HD13	1:C:1406:VAL:CG2	2.48	0.43
1:E:1178:LEU:C	1:E:1427:ARG:HH12	2.21	0.43
1:A:1336:ILE:CD1	1:A:1336:ILE:N	2.80	0.43
1:B:1252:VAL:HA	1:B:1265:PHE:HB3	2.01	0.43
1:C:1254:LEU:HD23	1:C:1254:LEU:N	2.33	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: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
1:F:1408:GLU:CD	1:F:1409:PRO:HD2	2.38	0.43
1:B:1173:LEU:HD11	1:B:1420:LYS:CG	2.43	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:E:1290:ILE:CD1	1:E:1308:LYS:HE3	2.48	0.43
1:F:1284:ILE:CD1	1:F:1396:PRO:HA	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1311:PHE:O	1:A:1312:LYS:C	2.57	0.43
1:C:449:ILE:CG2	1:C:452:ALA:HB2	2.49	0.43
1:E:1193:SER:O	1:E:1194:ALA:HB2	2.18	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:F:1360:GLY:O	1:F:1361:MET:C	2.57	0.43
1:A:1190:GLN:OE1	1:A:1190:GLN:HA	2.18	0.43
1:A:449:ILE:CD1	1:A:1407:PHE:CE1	3.01	0.43
1:B:1200:VAL:HB	1:B:1275:MET:HG3	2.01	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:1255:SER:HB2	1:A:1263:ILE:HG22	2.01	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:D:1298:ARG:O	1:D:1372:LEU:HB2	2.18	0.43
1:E:427:THR:HG21	1:E:487:LEU:CB	2.49	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:A:1360:GLY:O	1:A:1361:MET:C	2.56	0.43
1:B:1333:VAL:CG1	1:B:1344:TYR:CD2	3.02	0.43
1:B:488:ILE:HD13	1:B:505:PHE:HA	2.01	0.43
1:C:1277:TYR:CE1	1:C:1399:LEU:HD12	2.54	0.43
1:C:1408:GLU:HG2	1:C:1411:LEU:HD12	2.01	0.43
1:C:1378:LYS:HG2	1:C:1379:LYS:N	2.32	0.42
1:C:430:MET:HB3	1:C:437:LEU:HD22	2.01	0.42
1:D:1184:LEU:CD2	1:D:1192:LEU:HB2	2.49	0.42
1:E:1360:GLY:O	1:E:1361:MET:C	2.57	0.42
1:F:1390:PHE:CD1	1:F:1390:PHE:C	2.92	0.42
1:F:1173:LEU:HD11	1:F:1420:LYS:HG2	2.00	0.42
1:C:1202:MET:CE	1:C:1204:SER:HB2	2.49	0.42
1:C:1277:TYR:HE1	1:C:1399:LEU:HD12	1.84	0.42
1:D:1360:GLY:O	1:D:1361:MET:C	2.58	0.42
1:D:1306:VAL:HG23	1:D:1365:GLN:HB2	2.01	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:E:449:ILE:HG22	1:E:450:PRO:HD2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:ILE:HG23	1:A:1414:SER:HB3	2.01	0.42
1:B:1156:PRO:HA	1:B:1157:PRO:HD3	1.77	0.42
1:C:1196:VAL:HG23	1:C:1283:ILE:HD13	2.01	0.42
1:C:1360:GLY:O	1:C:1361:MET:C	2.58	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:E:427:THR:HG21	1:E:487:LEU:HB3	2.01	0.42
1:A:1345:LYS:CB	1:A:1348:GLU:OE2	2.68	0.42
1:A:1171:ASN:O	1:A:1418:VAL:HG13	2.20	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:F:1159:HIS:ND1	1:F:1167:GLY:O	2.52	0.42
1:F:1249:HIS:CE1	1:F:1250:GLN:HG2	2.54	0.42
1:A:1338:MET:CE	1:F:491:THR:HB	2.49	0.42
1:B:1177:VAL:CG2	1:B:1424:TYR:HD1	2.32	0.42
1:B:440:ARG:CG	1:B:441:ASP:N	2.83	0.42
1:B:443:MET:HE3	1:B:446:LYS:O	2.18	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:1211:GLU:HA	1:D:1266:ILE:HD13	2.01	0.42
1:D:1298:ARG:NH1	1:D:1375:THR:HG23	2.35	0.42
1:D:1422:VAL:CG1	1:D:1423:ARG:N	2.80	0.42
1:E:1251:CYS:SG	1:E:1268:PRO:HD3	2.60	0.42
1:E:1252:VAL:HA	1:E:1265:PHE:HB3	2.01	0.42
1:E:1273:GLU:OE2	1:E:1276:ARG:NH2	2.52	0.42
1:E:497:PHE:CD1	1:E:497:PHE:C	2.93	0.42
1:F:463:TYR:HD1	1:F:469:PHE:HB3	1.85	0.42
1:C:1335:VAL:HG11	1:C:1351:ILE:HG21	2.01	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:F:463:TYR:HE1	1:F:469:PHE:O	2.02	0.42
1:A:1245:ASP:O	1:A:1246:CYS:CB	2.66	0.42
1:A:1255:SER:HB3	1:A:1263:ILE:HA	2.02	0.42
1:B:1312:LYS:HA	1:B:1313:PRO:HD3	1.93	0.42
1:C:490:HIS:HA	1:C:503:TYR:HD1	1.84	0.42
1:D:1192:LEU:CD1	1:D:1434:ARG:HH12	2.33	0.42
1:D:1327:PRO:HA	1:D:1381:TRP:CE2	2.54	0.42
1:E:1304:LYS:HE2	1:E:1304:LYS:HB3	1.90	0.42
1:F:1179:GLU:OE1	1:F:1196:VAL:HG11	2.20	0.42
1:F:441:ASP:C	1:F:442:ARG:HD3	2.39	0.42
1:A:1290:ILE:CD1	1:A:1290:ILE:N	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1263:ILE:HA	1:B:1263:ILE:HD12	1.88	0.42
1:C:1188:GLN:N	1:C:1188:GLN:CD	2.73	0.42
1:D:1174:PHE:HB2	1:D:1203:LYS:HB2	2.02	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:A:462:LEU:O	1:A:466:VAL:CG2	2.68	0.42
1:A:473:ARG:HH21	1:A:473:ARG:HG2	1.85	0.42
1:B:1211:GLU:HA	1:B:1266:ILE:CD1	2.44	0.42
1:B:1276:ARG:CG	1:B:1277:TYR:N	2.76	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:F:462:LEU:HD23	1:F:462:LEU:HA	1.77	0.42
1:B:463:TYR:HD1	1:B:469:PHE:HB3	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:F:1184:LEU:HA	1:F:1432:GLU:O	2.20	0.42
1:A:1382:ALA:HB1	1:A:1383:ARG:HH22	1.85	0.41
1:B:471:GLU:HG3	1:B:473:ARG:H	1.85	0.41
1:C:1246:CYS:SG	1:C:1248:PHE:CZ	3.13	0.41
1:D:1184:LEU:HD13	1:D:1193:SER:HB2	2.02	0.41
1:D:1324:ILE:HA	1:D:1325:PRO:HD2	1.96	0.41
1:D:1334:GLN:HG3	1:D:1369:GLU:HB3	2.02	0.41
1:E:1276:ARG:CG	1:E:1277:TYR:N	2.83	0.41
1:E:1345:LYS:HD2	1:E:1352:VAL:HG21	2.02	0.41
1:F:435:SER:HG	1:F:461:TRP:HE1	1.67	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:C:1399:LEU:C	1:C:1399:LEU:CD2	2.88	0.41
1:D:443:MET:HE2	1:D:448:THR:HG23	2.02	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:E:1361:MET:O	1:E:1362:LYS:HG3	2.20	0.41
1:F:1392:VAL:HG21	1:F:1394:PHE:CE1	2.55	0.41
1:F:498:SER:O	1:F:503:TYR:OH	2.31	0.41
1:A:459:VAL:O	1:A:462:LEU:HB3	2.19	0.41
1:B:444:TRP:C	1:B:445:LEU:HG	2.40	0.41
1:C:1293:VAL:HG21	1:C:1383:ARG:NH1	2.34	0.41
1:C:1406:VAL:O	1:C:1406:VAL:CG1	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1187:PRO:HD3	1:D:1434:ARG:HB3	2.01	0.41
1:D:1312:LYS:HA	1:D:1313:PRO:HD3	1.88	0.41
1:E:1298:ARG:NE	1:E:1374:PRO:HA	2.35	0.41
1:F:1342:ALA:HB2	1:F:1353:TRP:CD1	2.56	0.41
1:F:440:ARG:CZ	1:F:440:ARG:HB3	2.50	0.41
1:A:1183:LEU:HD13	1:A:1285:LEU:CD2	2.50	0.41
1:B:1287:PHE:HE2	1:B:1358:MET:SD	2.43	0.41
1:E:1298:ARG:NH2	1:E:1298:ARG:CG	2.83	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:E:497:PHE:HD1	1:E:503:TYR:OH	2.03	0.41
1:F:1188:GLN:HB2	1:F:1190:GLN:HE21	1.86	0.41
1:F:1247:THR:CG2	1:F:1276:ARG:HD2	2.49	0.41
1:F:1298:ARG:O	1:F:1372:LEU:CD1	2.69	0.41
1:A:1323:ARG:HG3	1:A:1323:ARG:NH1	2.36	0.41
1:B:1179:GLU:HB3	1:B:1196:VAL:CG1	2.50	0.41
1:C:497:PHE:CD1	1:C:497:PHE:C	2.94	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:D:1214:PHE:O	1:D:1262:SER:HA	2.20	0.41
1:E:456:SER:HA	1:E:499:GLU:HG2	2.02	0.41
1:E:461:TRP:CE3	1:E:461:TRP:O	2.73	0.41
1:F:1323:ARG:HB2	1:F:1323:ARG:CZ	2.50	0.41
1:A:1292:LEU:HD12	1:A:1292:LEU:HA	1.66	0.41
1:B:1174:PHE:CD2	1:B:1421:TRP:HB2	2.55	0.41
1:B:1425:ILE:CD1	1:F:1156:PRO:HG3	2.50	0.41
1:B:447:ILE:CG2	1:B:448:THR:H	2.33	0.41
1:C:447:ILE:HG23	1:C:448:THR:H	1.84	0.41
1:F:1178:LEU:HD12	1:F:1199:ARG:NH1	2.36	0.41
1:F:1311:PHE:CE1	1:F:1360:GLY:CA	3.03	0.41
1:F:1339:LYS:HD3	1:F:1364:SER:OG	2.21	0.41
1:F:1213:LYS:HE2	1:F:1403:TYR:OH	2.21	0.41
1:A:1171:ASN:ND2	1:A:1413:TYR:CZ	2.89	0.41
1:A:1390:PHE:CD1	1:A:1428:SER:HB3	2.53	0.41
1:B:447:ILE:CG2	1:B:448:THR:N	2.83	0.41
1:C:460:ASP:O	1:C:463:TYR:CD1	2.73	0.41
1:D:488:ILE:HA	1:D:488:ILE:HD13	1.74	0.41
1:E:1289:VAL:O	1:E:1291:PRO:HD3	2.21	0.41
1:E:1402:ARG:NH2	1:E:1402:ARG:HG2	2.36	0.41
1:E:1402:ARG:HH21	1:E:1402:ARG:HG2	1.85	0.41
1:E:492:VAL:O	1:E:492:VAL:CG2	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1175:LEU:HD23	1:F:1175:LEU:HA	1.90	0.41
1:F:1312:LYS:NZ	1:F:1312:LYS:CB	2.83	0.41
1:A:1183:LEU:HD13	1:A:1285:LEU:HD21	2.03	0.41
1:B:1294:ARG:NH1	1:B:1302:GLU:CG	2.80	0.41
1:B:431:ALA:O	1:B:432:ALA:C	2.59	0.41
1:B:482:LEU:N	1:B:482:LEU:HD23	2.36	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:C:1381:TRP:CZ2	1:C:1383:ARG:HG2	2.55	0.41
1:D:1216:MET:C	1:D:1402:ARG:HG3	2.41	0.41
1:E:1174:PHE:HB2	1:E:1203:LYS:HB2	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:F:447:ILE:H	1:F:447:ILE:HG13	1.57	0.41
1:A:1305:VAL:HG12	1:A:1366:ILE:CG2	2.42	0.41
1:A:1416:HIS:N	1:A:1416:HIS:ND1	2.58	0.41
1:B:1250:GLN:OE1	1:B:1251:CYS:N	2.54	0.41
1:B:1353:TRP:CH2	1:B:1366:ILE:HB	2.56	0.41
1:B:1380:LYS:H	1:B:1380:LYS:HG2	1.62	0.41
1:B:1404:LEU:O	1:B:1420:LYS:NZ	2.50	0.41
1:C:434:GLU:HA	1:C:434:GLU:OE1	2.21	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:F:433:PRO:HD3	1:F:1254:LEU:O	2.20	0.41
1:F:458:VAL:O	1:F:462:LEU:CB	2.66	0.41
1:F:427:THR:HG21	1:F:487:LEU:HB3	2.03	0.41
1:B:1339:LYS:NZ	1:B:1363:GLU:O	2.54	0.41
1:C:1199:ARG:HG3	1:C:1273:GLU:HG3	2.03	0.41
1:C:490:HIS:NE2	1:C:494:LYS:HD3	2.36	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: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:A:1187:PRO:HD3	1:A:1434:ARG:HB2	2.00	0.41
1:A:1298:ARG:HG2	1:A:1298:ARG:HH21	1.85	0.41
1:A:1384:PRO:HA	1:A:1385:PRO:HD3	1.99	0.41
1:B:1292:LEU:C	1:B:1292:LEU:HD12	2.41	0.41
1:B:1322:VAL:HG22	1:B:1388:MET:HE2	2.02	0.41
1:B:1179:GLU:HB2	1:B:1396:PRO:HD2	2.02	0.41
1:C:1213:LYS:HE2	1:C:1262:SER:OG	2.21	0.41
1:D:1245:ASP:O	1:D:1246:CYS:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1296:VAL:O	1:E:1300:LYS:HB2	2.21	0.41
1:F:1311:PHE:O	1:F:1312:LYS:C	2.60	0.41
1:F:1414:SER:O	1:F:1415:ASP:C	2.59	0.41
1:A:1216:MET:HB3	1:A:1216:MET:HE2	1.80	0.40
1:B:1322:VAL:HG22	1:B:1388:MET:HE3	2.03	0.40
1:C:1202:MET:CE	1:C:1272:PHE:CZ	3.04	0.40
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:F:427:THR:OG1	1:F:487:LEU:HD13	2.21	0.40
1:B:1324:ILE:HG12	1:B:1386:ILE:HD13	2.03	0.40
1:B:436:GLY:HA3	1:B:465:HIS:HE1	1.85	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: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: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:C:1390:PHE:CD1	1:C:1391:GLU:N	2.89	0.40
1:D:1301:LEU:HB2	1:D:1370:ILE:HG13	2.00	0.40
1:F:1195:HIS:CD2	1:F:1278:ARG:NH2	2.90	0.40
1:F:442:ARG:N	1:F:442:ARG:HD3	2.37	0.40
1:F:478:TYR:O	1:F:482:LEU:HG	2.21	0.40
1:A:1378:LYS:HE3	1:A:1381:TRP:CE2	2.53	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:B:422:ASP:OD2	1:B:424:ALA:HB3	2.21	0.40
1:B:459:VAL:HG21	1:B:499:GLU:OE1	2.22	0.40
1:B:488:ILE:HA	1:B:488:ILE:HD13	1.84	0.40
1:D:1290:ILE:CB	1:D:1306:VAL:HG12	2.38	0.40
1:D:1324:ILE:HG22	1:D:1351:ILE:CB	2.48	0.40
1:E:1155:PRO:HA	1:E:1156:PRO:HD2	1.85	0.40
1:F:1192:LEU:CD1	1:F:1434:ARG:NE	2.81	0.40
1:F:1195:HIS:CD2	1:F:1278:ARG:HH21	2.39	0.40
1:A:1183:LEU:HD21	1:A:1185:MET:HB2	2.02	0.40
1:A:1325:PRO:HG3	1:A:1384:PRO:O	2.22	0.40
1:B:1177:VAL:HG21	1:B:1424:TYR:CD1	2.56	0.40
1:B:473:ARG:HB2	1:B:473:ARG:NH2	2.36	0.40
1:C:1317:ALA:CB	1:C:1392:VAL:HG12	2.51	0.40
1:D:1344:TYR:CE2	1:D:1346:ALA:HB2	2.56	0.40
1:E:1248:PHE:HE2	1:E:1263:ILE:HG21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:490:HIS:HA	1:E:503:TYR:CD1	2.57	0.40
1:F:1294:ARG:CZ	1:F:1302:GLU:CG	2.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	345/385 (90%)	294 (85%)	44 (13%)	7 (2%)	7	39
1	B	331/385 (86%)	284 (86%)	40 (12%)	7 (2%)	7	38
1	C	344/385 (89%)	288 (84%)	52 (15%)	4 (1%)	13	50
1	D	326/385 (85%)	279 (86%)	41 (13%)	6 (2%)	8	41
1	E	328/385 (85%)	282 (86%)	39 (12%)	7 (2%)	7	38
1	F	332/385 (86%)	289 (87%)	38 (11%)	5 (2%)	10	45
All	All	2006/2310 (87%)	1716 (86%)	254 (13%)	36 (2%)	8	41

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
1	A	493	ASN
1	A	1190	GLN

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Mol	Chain	Res	Type
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%)	3	17
1	B	298/337 (88%)	260 (87%)	38 (13%)	4	22
1	C	307/337 (91%)	275 (90%)	32 (10%)	7	31
1	D	295/337 (88%)	258 (88%)	37 (12%)	4	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	297/337 (88%)	276 (93%)	21 (7%)	14	46
1	F	299/337 (89%)	272 (91%)	27 (9%)	9	37
All	All	1804/2022 (89%)	1603 (89%)	201 (11%)	6	28

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 molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	351/385 (91%)	0.18	1 (0%) 94 91	91, 112, 131, 141	0
1	B	339/385 (88%)	0.20	7 (2%) 63 58	103, 117, 134, 145	0
1	C	350/385 (90%)	0.25	6 (1%) 70 64	99, 119, 132, 147	0
1	D	336/385 (87%)	0.20	5 (1%) 73 68	97, 117, 129, 136	0
1	E	338/385 (87%)	0.37	13 (3%) 40 36	98, 118, 132, 141	0
1	F	340/385 (88%)	0.32	12 (3%) 44 39	100, 120, 133, 140	0
All	All	2054/2310 (88%)	0.25	44 (2%) 63 58	91, 117, 132, 147	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1181	VAL	3.7
1	F	1296	VAL	3.5
1	F	487	LEU	3.4
1	C	1435	CYS	3.3
1	B	463	TYR	3.3
1	B	1435	CYS	3.2
1	E	1373	LEU	3.2
1	E	1180	SER	3.1
1	B	475	ALA	3.1
1	B	464	HIS	2.7
1	F	1435	CYS	2.7
1	E	508	LEU	2.7
1	D	1301	LEU	2.7
1	E	1301	LEU	2.6
1	C	1257	PHE	2.6
1	E	1427	ARG	2.6
1	B	508	LEU	2.5
1	D	1374	PRO	2.5
1	F	1370	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	1214	PHE	2.5
1	E	1213	LYS	2.5
1	D	466	VAL	2.4
1	E	1374	PRO	2.4
1	C	437	LEU	2.4
1	C	454	LEU	2.4
1	D	462	LEU	2.3
1	E	1279	THR	2.3
1	B	1214	PHE	2.3
1	F	1379	LYS	2.3
1	E	475	ALA	2.3
1	F	506	GLY	2.3
1	A	1377	ASP	2.2
1	F	1295	GLU	2.2
1	F	1177	VAL	2.2
1	F	1289	VAL	2.2
1	C	469	PHE	2.2
1	E	1198	GLY	2.1
1	F	1274	LEU	2.1
1	E	1218	ASP	2.0
1	C	1301	LEU	2.0
1	F	1302	GLU	2.0
1	F	1342	ALA	2.0
1	B	437	LEU	2.0
1	D	1412	ASN	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 [i](#)

There are no such residues in this entry.