



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 07:15 AM GMT

PDB ID : 2B39
Title : Structure of mammalian C3 with an intact thioester at 3Å resolution
Authors : Fredslund, F.; Jenner, L.; Husted, L.B.; Nyborg, J.; Andersen, G.R.; Sottrup-Jensen, L.
Deposited on : 2005-09-20
Resolution : 3.00 Å(reported)

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

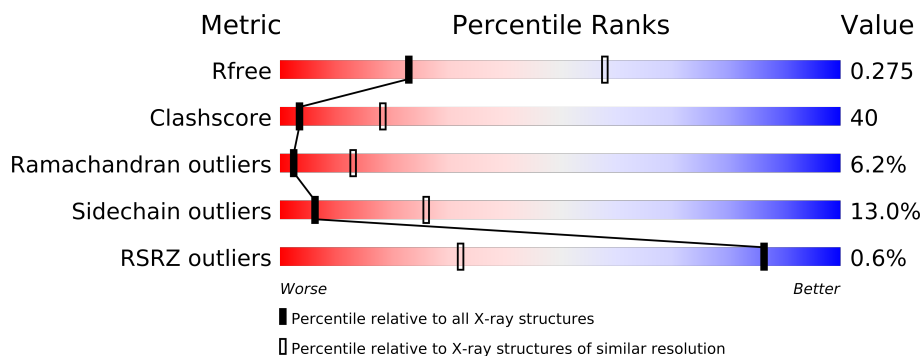
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	1661	
1	B	1661	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25624 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a protein called C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1610	Total	C	N	O	S	0	0	0
			12773	8093	2187	2439	54			
1	B	1610	Total	C	N	O	S	0	0	0
			12773	8093	2187	2439	54			

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

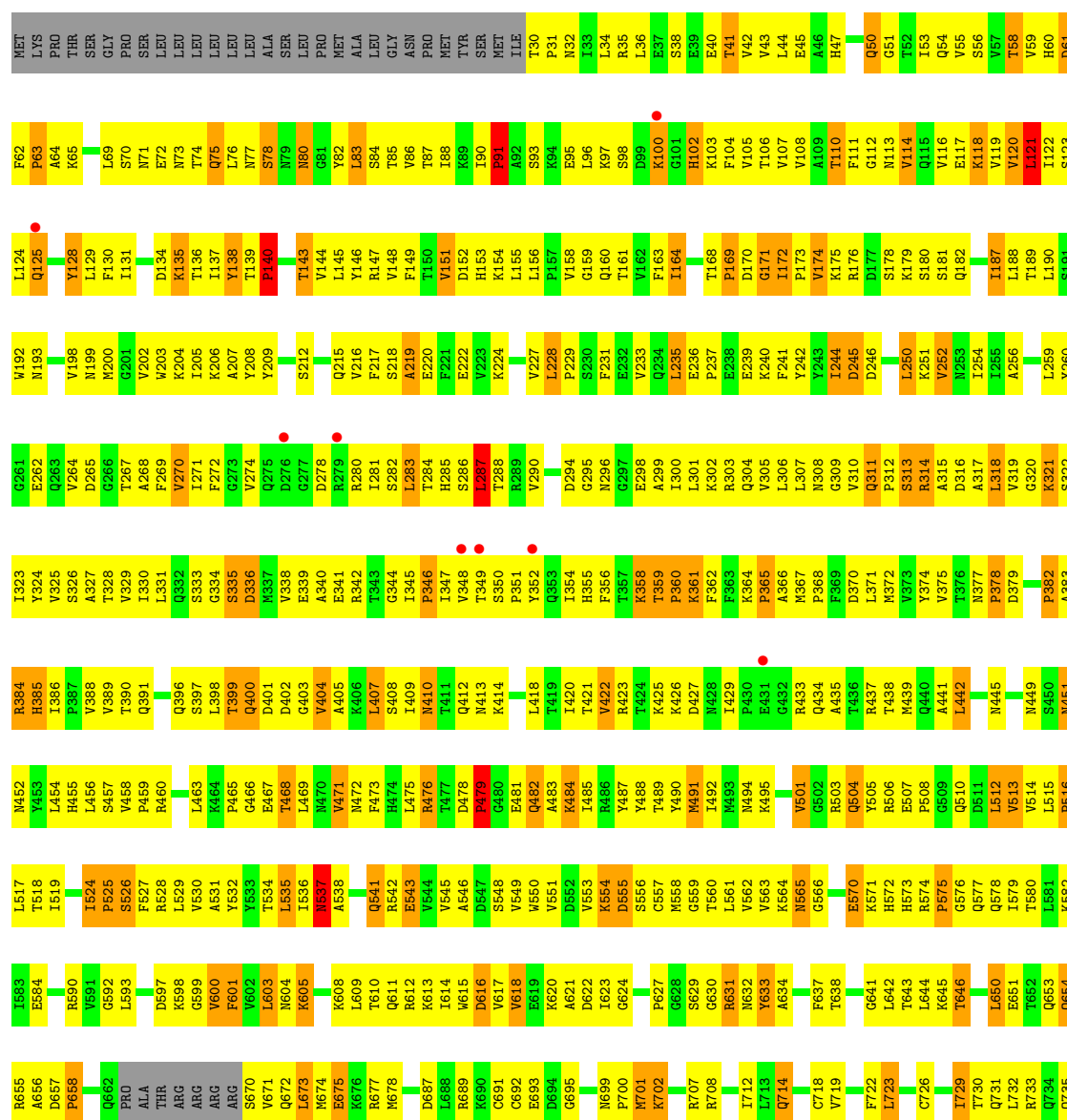
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	3	Total	C	N	O	0	0
			39	22	2	15		
2	B	3	Total	C	N	O	0	0
			39	22	2	15		

3 Residue-property plots

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

• Molecule 1: C3

Chain A: 



L1318	E1137	K1035	V931	E864	I798	P661	K598	R528	P459	Q396	G334	A268	T188
R1319	K1138	E1039	P932	L865	I799	Q652	G599	L529	R460	S397	S335	F269	L190
E1322	D1139	K1040	E933	L866	W801	PRD	V600	A531	E461	L399	S336	F270	S191
T1323	S1141	R1041	T940	Y867	E902	THR	L603	Y532	E462	T339	E462	I271	W192
R1328	L1142	Q1042	T945	A870	I903	ARG	N604	Y533	K463	Q400	K337	G272	L197
K1332	L1147	E1043	L946	F871	L804	ARG	K605	T534	P465	D401	A340	G273	L198
Q1338	A1153	S1044	R958	C872	A805	ARG	K606	L535	P466	Q403	E341	Q275	V198
G1339	E1046	L1045	T876	T876	V806	ARG	N607	L536	G466	Y404	R342	D276	M200
T1340	L1048	L1047	A877	A877	L808	ARG	K608	L537	T468	G277	G344	G277	W203
L1341	C1157	R1049	K878	K878	S807	GLU	L609	A538	L469	K406	G344	R279	K204
Q1358	Q1160	L1056	V961	K879	LEU	ALA	T610	K539	N470	L407	I345	R280	I205
R1359	V1161	A1057	P962	K880	ALA	ARG	Q611	G540	P346	S408	I347	E281	Y208
F1344	F1162	F1058	P971	H881	SER	ARG	R612	Q541	N471	I409	I347	I281	S282
T1345	S1163	R1059	D972	A881	ASP	ARG	K613	R542	M472	N410	V348	S282	L283
V1346	L1164	Q1060	E976	T886	LEU	LEU	W615	V545	L475	L475	T349	S282	Y208
Y1347	K1061	K1061	T977	T887	D750	ASP	W617	V549	R476	N413	K350	T284	P213
H1348	S1167	A1064	Q982	P888	D751	LEU	D616	S548	T477	K414	P351	H285	Q214
A1349	T1168	A1064	P985	S891	D752	ARG	W619	V549	R478	R415	P352	S286	Q215
K1350	R1183	P1073	P986	T892	E821	ARG	E619	W550	P479	D416	Q353	L287	V216
L1351	R1184	A1086	Q988	V895	E822	ARG	E620	V551	G480	I420	I354	R289	F217
C1357	R1188	L1077	Q988	T896	E823	ARG	E621	V552	Q482	T421	F356	S218	A219
K1358	R1189	L1078	Q989	T897	E824	ARG	E622	V553	Q483	V422	T357	V290	
K1359	R1190	T1078	T990	P896	E825	ARG	E623	V554	K484	R423	K358	D284	K224
Q1362	A1191	V1081	E991	V898	E826	ARG	E624	C557	I485	T424	T359	G295	E225
R1363	L1193	A1082	E992	V900	E827	ARG	E625	R558	Y487	K426	P361	G296	E226
L1366	A1194	A1086	E993	P901	E828	ARG	E626	R559	Y488	D427	F362	T288	L228
I1367	L1201	L1091	E994	P901	E829	ARG	E627	T560	Y489	Q434	F363	A299	P229
R1367	L1202	L1092	E995	P901	E830	ARG	E628	T561	Y490	I429	K364	I300	
P1368	G1203	A1093	E996	P901	E831	ARG	E629	T562	M491	P430	P365	L301	Q234
A1369	G1204	L1094	E997	P901	E832	ARG	E630	T563	I492	E431	P368	R303	L235
P1370	D1204	I1094	E998	P901	E833	ARG	E631	T564	M493	Q432	E236	Q304	E237
E1371	R1205	D1095	E999	P901	E834	ARG	E632	T565	L498	Q433	V305	V305	E238
T1372	L1206	D1098	E1003	P901	E835	ARG	E633	T566	L499	T436	E239	L306	E239
K1375	L1207	D1098	E1004	P901	E836	ARG	E634	T567	K500	R437	K372	L307	Y240
P1376	L1208	D1098	E1005	P901	E837	ARG	E635	T568	R503	T438	V373	N308	F241
Q1377	L1209	D1098	E1006	P901	E838	ARG	E636	T569	Q504	Y374	V375	Q310	Y242
S1382	L1210	D1098	E1007	P901	E839	ARG	E637	T570	Y505	M439	T376	Q311	I244
M1383	L1211	D1098	E1008	P901	E840	ARG	E638	T571	R506	Q440	A441	D245	D245
L1385	L1212	D1098	E1009	P901	E841	ARG	E639	T572	E507	Q442	P378	P312	
L1386	L1213	D1098	E1010	P901	E842	ARG	E640	T573	E508	L442	D378	D316	F247
L1387	L1214	D1098	E1011	P901	E843	ARG	E641	T574	E509	P508	G380	A317	D248
L1388	L1215	D1098	E1012	P901	E844	ARG	E642	T575	Q509	Q509	S381	L318	G249
L1389	L1216	D1098	E1013	P901	E845	ARG	E643	T576	Q510	T444	P382	V319	L250
L1390	L1217	D1098	E1014	P901	E846	ARG	E644	T577	V514	Q447	A383	G320	K251
L1391	L1218	D1098	E1015	P901	E847	ARG	E645	T578	L581	G448	R384	K321	
L1392	L1219	D1098	E1016	P901	E848	ARG	E646	T579	L582	N449	R385	S322	A256
L1393	L1220	D1098	E1017	P901	E849	ARG	E647	T580	L583	S450	I386	I323	R257
L1394	L1221	D1098	E1018	P901	E850	ARG	E648	T581	L584	I519	P387	Y324	F258
L1395	L1222	D1098	E1019	P901	E851	ARG	E649	T582	L585	T520	N451	V325	L259
L1396	L1223	D1098	E1020	P901	E852	ARG	E650	T583	L586	S521	R389	S326	Y260
L1397	L1224	D1098	E1021	P901	E853	ARG	E651	T584	L587	I524	V390	A327	
L1398	L1225	D1098	E1022	P901	E854	ARG	E652	T585	L588	I525	Q391	T328	Q263
L1399	L1226	D1098	E1023	P901	E855	ARG	E653	T586	L589	P525	N394	V329	V264
L1400	L1227	D1098	E1024	P901	E856	ARG	E654	T587	L590	S526	V395	I330	D265
L1401	L1228	D1098	E1025	P901	E857	ARG	E655	T588	L591	F527	V395	L331	
L1402	L1229	D1098	E1026	P901	E858	ARG	E656	T589	L592				
L1403	L1230	D1098	E1027	P901	E859	ARG	E657	T590	L593				
L1404	L1231	D1098	E1028	P901	E860	ARG	E658	T591	L594				
L1405	L1232	D1098	E1029	P901	E861	ARG	E659	T592	L595				
L1406	L1233	D1098	E1030	P901	E862	ARG	E660	T593	L596				
L1407	L1234	D1098	E1031	P901	E863	ARG	E661	T594	L597				
L1408	L1235	D1098	E1032	P901	E864	ARG	E662	T595	L598				
L1409	L1236	D1098	E1033	P901	E865	ARG	E663	T596	L599				
L1410	L1237	D1098	E1034	P901	E866	ARG	E664	T597	L600				



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	254.25Å 246.86Å 113.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.00 37.85 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.00) 97.2 (37.85-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.278 , 0.286 0.267 , 0.275	Depositor DCC
R_{free} test set	1392 reflections (1.01%)	DCC
Wilson B-factor (Å ²)	69.3	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 46.0	EDS
Estimated twinning fraction	0.008 for k,h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	2 of 138964 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	25624	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG

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	0.58	1/13020 (0.0%)	0.82	15/17632 (0.1%)
1	B	0.57	0/13020	0.81	11/17632 (0.1%)
All	All	0.57	1/26040 (0.0%)	0.82	26/35264 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
2	A	1	0
2	B	1	0
All	All	2	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	102	HIS	CB-CG	6.64	1.61	1.50

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	121	LEU	CA-CB-CG	-9.75	92.87	115.30
1	A	91	PRO	N-CA-C	7.91	132.66	112.10
1	B	1362	LEU	CA-CB-CG	6.57	130.40	115.30
1	A	1362	LEU	CA-CB-CG	6.54	130.34	115.30
1	A	1130	GLY	N-CA-C	-6.49	96.87	113.10
1	B	228	LEU	CA-CB-CG	6.41	130.03	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	SER	N-CA-C	6.32	128.07	111.00
1	B	1502	LYS	N-CA-C	-6.08	94.59	111.00
1	B	815	CYS	CA-CB-SG	-6.02	103.16	114.00
1	B	82	TYR	CB-CG-CD1	5.92	124.55	121.00
1	A	524	ILE	C-N-CD	5.86	140.70	128.40
1	B	77	ASN	C-N-CA	5.84	136.29	121.70
1	A	780	ALA	N-CA-C	5.74	126.50	111.00
1	A	121	LEU	CA-CB-CG	-5.62	102.38	115.30
1	A	171	GLY	N-CA-C	-5.54	99.24	113.10
1	A	1436	ASP	CB-CG-OD1	5.52	123.27	118.30
1	B	185	PHE	N-CA-C	5.50	125.84	111.00
1	B	558	MET	N-CA-C	5.50	125.84	111.00
1	A	123	SER	N-CA-C	-5.34	96.59	111.00
1	A	860	LYS	N-CA-C	-5.31	96.66	111.00
1	B	80	ASN	CB-CA-C	-5.28	99.84	110.40
1	B	127	GLY	N-CA-C	5.25	126.22	113.10
1	A	940	THR	N-CA-C	-5.21	96.92	111.00
1	A	287	LEU	CA-CB-CG	5.17	127.18	115.30
1	A	525	PRO	N-CA-C	-5.11	98.81	112.10
1	A	245	ASP	N-CA-C	5.06	124.67	111.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	2001	NAG	C1
2	B	2001	NAG	C1

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	138	TYR	Sidechain
1	B	820	TYR	Sidechain

5.2 Close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	12773	0	12782	1027	0
1	B	12773	0	12782	1002	0
2	A	39	0	34	3	0
2	B	39	0	34	3	0
All	All	25624	0	25632	2029	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 40.

All (2029) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:117:GLU:O	1:B:118:LYS:HG2	1.47	1.14
1:B:369:PHE:HB3	1:B:409:ILE:HD12	1.32	1.10
1:A:44:LEU:HD13	1:A:55:VAL:HG11	1.34	1.09
1:B:244:ILE:HD11	1:B:319:VAL:CG2	1.84	1.08
1:B:116:VAL:HG13	1:B:645:LYS:HG2	1.28	1.06
1:A:1575:GLN:HB3	1:A:1578:GLN:NE2	1.70	1.05
1:B:116:VAL:CG1	1:B:645:LYS:HG2	1.87	1.04
1:A:55:VAL:HG13	1:A:111:PHE:HB3	1.39	1.04
1:A:651:GLU:HB3	1:A:653:GLN:HE22	1.18	1.04
1:B:558:MET:HB2	1:B:812:LYS:HE2	1.38	1.03
1:B:118:LYS:HD3	1:B:645:LYS:HE2	1.40	1.03
1:B:227:VAL:HG12	1:B:229:PRO:HD3	1.39	1.03
1:A:281:ILE:HD13	1:A:310:VAL:HG22	1.41	1.02
1:A:244:ILE:HD11	1:A:319:VAL:HG22	1.39	1.02
1:A:61:ASP:HB2	1:A:63:PRO:HD2	1.40	1.02
1:A:55:VAL:HG23	1:A:75:GLN:HA	1.39	1.02
1:A:256:ALA:O	1:A:264:VAL:HB	1.61	1.01
1:B:503:ARG:HE	1:B:503:ARG:H	1.05	1.00
1:B:1493:PRO:HB2	1:B:1497:ASP:OD2	1.61	0.99
1:A:359:THR:HG22	1:A:360:PRO:HD2	1.44	0.98
1:A:800:THR:HG23	1:A:823:THR:HG22	1.45	0.97
1:B:244:ILE:HD11	1:B:319:VAL:HG22	1.44	0.96
1:B:272:PHE:HD1	1:B:325:VAL:HG21	1.30	0.96
1:A:272:PHE:HD1	1:A:325:VAL:HG21	1.29	0.94
1:B:442:LEU:HD13	1:B:631:ARG:HH21	1.32	0.94
1:A:700:PRO:HB2	1:A:701:MET:HE3	1.49	0.94
1:B:243:TYR:CZ	1:B:245:ASP:HB2	2.03	0.94
1:A:574:ARG:NH1	1:A:920:ILE:HB	1.82	0.94
1:B:808:LEU:HB2	1:B:814:ILE:HG12	1.47	0.93
1:B:276:ASP:HB2	1:B:279:ARG:HB2	1.51	0.93
1:B:396:GLN:HE21	1:B:407:LEU:HA	1.30	0.93
1:A:1492:HIS:ND1	1:A:1493:PRO:HD2	1.84	0.93

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:904:ILE:HG22	1:A:905:GLY:H	1.31	0.92
1:B:1415:GLU:HA	1:B:1415:GLU:OE1	1.66	0.92
1:A:524:ILE:HG23	1:A:525:PRO:HD3	1.51	0.92
1:B:382:PRO:HB3	1:B:403:GLY:HA3	1.52	0.91
1:A:339:GLU:HG3	1:A:759:ILE:HG23	1.52	0.91
1:B:371:LEU:HD23	1:B:371:LEU:H	1.34	0.91
1:A:118:LYS:NZ	1:A:645:LYS:HD2	1.85	0.90
1:B:1547:LEU:HD22	1:B:1596:GLU:HA	1.53	0.90
1:B:234:GLN:HE22	1:B:257:ARG:NH2	1.67	0.90
1:B:398:LEU:HD11	1:B:403:GLY:O	1.72	0.90
1:A:83:LEU:HD12	1:A:83:LEU:C	1.91	0.90
1:B:1415:GLU:OE1	1:B:1418:LYS:HE2	1.72	0.89
1:A:118:LYS:HZ3	1:A:645:LYS:HD2	1.34	0.89
1:B:1311:LEU:HD12	1:B:1313:GLU:HB3	1.53	0.89
1:B:852:ASN:HD22	1:B:859:LEU:HD23	1.34	0.89
1:B:66:LYS:NZ	1:B:94:LYS:HG2	1.88	0.89
1:A:1147:LEU:HD23	1:A:1194:ALA:HB1	1.55	0.88
1:A:1435:ARG:O	1:A:1436:ASP:OD1	1.91	0.88
1:A:476:ARG:HB3	1:A:476:ARG:HH11	1.36	0.88
1:B:117:GLU:O	1:B:118:LYS:CG	2.21	0.88
1:A:72:GLU:HG2	1:A:86:VAL:HG13	1.56	0.88
1:A:1289:LYS:HD3	1:A:1289:LYS:H	1.36	0.88
1:A:458:VAL:HG13	1:A:469:LEU:HD11	1.56	0.87
1:B:421:THR:HG22	1:B:438:THR:HB	1.53	0.87
1:B:1563:ILE:HD12	1:B:1563:ILE:H	1.40	0.87
1:B:700:PRO:HB2	1:B:701:MET:HE2	1.56	0.87
1:A:290:VAL:HG11	1:A:298:GLU:H	1.39	0.86
1:B:530:VAL:HG21	1:B:642:LEU:HD11	1.56	0.86
1:B:110:THR:HB	1:B:115:GLN:HB3	1.58	0.86
1:B:161:THR:HG22	1:B:180:SER:HB2	1.59	0.85
1:B:60:HIS:HB3	1:B:65:LYS:HB3	1.59	0.85
1:B:129:LEU:HB2	1:B:217:PHE:CD2	2.12	0.85
1:B:573:HIS:ND1	1:B:579:ILE:HD11	1.90	0.85
1:B:1573:GLU:HG2	1:B:1580:ARG:HH21	1.42	0.85
1:B:977:THR:HG23	1:B:1323:THR:HG23	1.58	0.84
1:A:43:VAL:HA	1:A:85:THR:HG22	1.59	0.84
1:B:611:GLN:NE2	1:B:815:CYS:HA	1.91	0.84
1:A:1494:ASP:OD2	1:B:1203:GLY:HA2	1.77	0.84
1:A:812:LYS:O	1:A:812:LYS:HD3	1.77	0.84
1:B:272:PHE:HD1	1:B:325:VAL:CG2	1.90	0.84
1:A:700:PRO:HB2	1:A:701:MET:CE	2.07	0.84
1:B:633:TYR:O	1:B:637:PHE:HD2	1.60	0.84

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:407:LEU:HD23	1:A:408:SER:H	1.42	0.83
1:A:1217:ASN:HD21	1:A:1218:ARG:HD3	1.43	0.83
1:B:398:LEU:HD12	1:B:405:ALA:H	1.44	0.83
1:B:846:ILE:HD12	1:B:899:ILE:HD12	1.58	0.83
1:A:368:PRO:HA	1:A:410:ASN:HA	1.60	0.83
1:A:228:LEU:HG	1:A:228:LEU:O	1.77	0.83
1:B:458:VAL:HG13	1:B:469:LEU:HD11	1.61	0.82
1:B:442:LEU:HD13	1:B:631:ARG:NH2	1.92	0.82
1:A:271:ILE:HG12	1:A:287:LEU:HB3	1.61	0.82
1:B:992:ASP:HB2	1:B:998:ARG:HB3	1.59	0.82
1:B:271:ILE:HG12	1:B:287:LEU:HB3	1.62	0.82
1:A:260:TYR:HB3	1:A:853:TYR:CE1	2.14	0.82
1:A:808:LEU:HD23	1:A:808:LEU:O	1.80	0.82
1:A:242:TYR:CD1	1:A:250:LEU:HD11	2.14	0.81
1:B:398:LEU:HA	1:B:405:ALA:HB2	1.59	0.81
1:A:558:MET:C	1:A:812:LYS:HZ2	1.83	0.81
1:B:374:TYR:HE2	1:B:376:THR:HG23	1.44	0.81
1:B:1217:ASN:ND2	1:B:1218:ARG:HD3	1.96	0.81
1:B:105:VAL:HB	1:B:122:ILE:HD11	1.60	0.81
1:A:1579:GLU:O	1:A:1580:ARG:HG2	1.81	0.81
1:A:1566:ILE:HG13	1:A:1576:VAL:HG22	1.62	0.81
1:A:36:LEU:HD12	1:A:124:LEU:HB3	1.61	0.81
1:A:532:TYR:HB3	1:A:546:ALA:HB2	1.61	0.80
1:B:384:ARG:HA	1:B:400:GLN:HB2	1.64	0.80
1:A:809:SER:OG	1:A:812:LYS:HB3	1.80	0.80
1:A:1573:GLU:CD	1:A:1580:ARG:HE	1.83	0.80
1:A:859:LEU:H	1:A:859:LEU:HD22	1.45	0.80
1:A:846:ILE:HD12	1:A:899:ILE:HD12	1.63	0.80
1:A:83:LEU:O	1:A:83:LEU:HG	1.81	0.80
1:B:1112:LYS:HB3	1:B:1113:PRO:HD2	1.64	0.80
1:B:398:LEU:HD12	1:B:405:ALA:N	1.97	0.80
1:A:272:PHE:HA	1:A:325:VAL:HG22	1.63	0.80
1:A:904:ILE:HG22	1:A:905:GLY:N	1.97	0.80
1:B:1571:SER:O	1:B:1572:ASP:HB2	1.82	0.79
1:A:314:ARG:HA	1:A:314:ARG:HE	1.47	0.79
1:A:314:ARG:O	1:A:318:LEU:HB2	1.82	0.79
1:A:1605:VAL:HG12	1:A:1607:SER:H	1.46	0.79
1:A:346:PRO:HB2	1:A:348:VAL:HG23	1.65	0.79
1:A:846:ILE:CD1	1:A:899:ILE:HD12	2.12	0.79
1:B:593:LEU:HD11	1:B:774:ILE:HD11	1.62	0.79
1:B:888:PRO:HB2	1:B:891:SER:HB2	1.63	0.79
1:A:281:ILE:CD1	1:A:310:VAL:HG22	2.13	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:610:THR:HG22	1:A:613:LYS:HD2	1.65	0.79
1:A:32:ASN:HB2	1:A:641:GLY:HA2	1.64	0.79
1:A:829:PHE:HD2	1:A:853:TYR:HE2	1.29	0.78
1:A:375:VAL:HG11	1:A:386:ILE:HD12	1.62	0.78
1:B:359:THR:HG22	1:B:360:PRO:HD2	1.63	0.78
1:B:389:VAL:HG13	1:B:394:ASN:O	1.82	0.78
1:B:530:VAL:HG13	1:B:548:SER:HB3	1.63	0.78
1:B:369:PHE:HB3	1:B:409:ILE:CD1	2.11	0.78
1:B:396:GLN:HG2	1:B:407:LEU:HG	1.65	0.78
1:A:260:TYR:HB3	1:A:853:TYR:HE1	1.48	0.78
1:B:714:GLN:HE21	1:B:1424:VAL:HG13	1.49	0.78
1:B:44:LEU:HD11	1:B:86:VAL:HG23	1.64	0.78
1:B:234:GLN:HE22	1:B:257:ARG:HH22	1.32	0.78
1:B:1217:ASN:HD21	1:B:1218:ARG:HD3	1.48	0.78
1:B:995:ASP:HB3	1:B:998:ARG:HB2	1.67	0.77
1:A:605:LYS:HB3	1:A:608:LYS:HE2	1.66	0.77
1:B:503:ARG:H	1:B:503:ARG:NE	1.83	0.77
1:A:611:GLN:HG2	1:A:816:VAL:HB	1.67	0.77
1:A:106:THR:HG22	1:A:119:VAL:HG22	1.66	0.77
1:A:271:ILE:HG23	1:A:287:LEU:HD22	1.65	0.77
1:B:270:VAL:HG13	1:B:327:ALA:HB2	1.66	0.77
1:B:208:TYR:HD2	1:B:213:PRO:HA	1.50	0.77
1:B:373:VAL:HG11	1:B:388:VAL:HG11	1.66	0.77
1:B:272:PHE:CE2	1:B:301:LEU:HB2	2.20	0.77
1:A:458:VAL:HG13	1:A:459:PRO:HD2	1.65	0.77
1:B:1498:GLY:O	1:B:1501:SER:HB3	1.84	0.77
1:B:852:ASN:HD22	1:B:859:LEU:CD2	1.97	0.76
1:B:62:PHE:HA	1:B:106:THR:HG23	1.67	0.76
1:B:1285:VAL:N	1:B:1286:PRO:HD3	2.00	0.76
1:A:1204:ASP:HB2	1:A:1205:ARG:HH21	1.49	0.76
1:B:243:TYR:OH	1:B:245:ASP:HB2	1.86	0.76
1:B:700:PRO:HB2	1:B:701:MET:CE	2.14	0.76
1:A:274:VAL:HG23	1:A:283:LEU:HD11	1.68	0.76
1:B:701:MET:O	1:B:702:LYS:HB2	1.86	0.76
1:A:245:ASP:OD1	1:A:246:ASP:N	2.17	0.76
1:B:336:ASP:CG	1:B:1377:GLN:HE22	1.89	0.76
1:A:1237:LEU:HD21	1:A:1277:ALA:HA	1.68	0.76
1:A:852:ASN:HB2	1:A:859:LEU:HD23	1.67	0.75
1:B:1610:TRP:HB3	1:B:1617:SER:HB2	1.68	0.75
1:B:537:ASN:ND2	1:B:538:ALA:H	1.84	0.75
1:A:651:GLU:HB3	1:A:653:GLN:NE2	2.00	0.75
1:B:301:LEU:HD13	1:B:301:LEU:O	1.86	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:382:PRO:HB3	1:A:403:GLY:HA3	1.67	0.75
1:B:344:GLY:O	1:B:346:PRO:HD3	1.86	0.75
1:B:977:THR:HB	1:B:1345:THR:HB	1.68	0.75
1:A:507:GLU:HB3	1:A:510:GLN:NE2	2.02	0.75
1:A:1630:PRO:HD3	1:A:1643:GLN:HE21	1.52	0.75
1:B:46:ALA:HB2	1:B:76:LEU:HD13	1.67	0.75
1:B:256:ALA:O	1:B:264:VAL:HB	1.86	0.75
1:B:208:TYR:CD2	1:B:213:PRO:HA	2.21	0.74
1:A:359:THR:HG23	1:A:371:LEU:HA	1.69	0.74
1:B:323:ILE:CG1	1:B:347:ILE:HD11	2.17	0.74
1:B:871:PHE:HB3	1:B:901:PRO:HA	1.67	0.74
1:A:691:CYS:HA	1:A:1424:VAL:HG21	1.69	0.74
1:B:611:GLN:HE21	1:B:815:CYS:HA	1.50	0.74
1:A:149:PHE:CZ	1:A:806:VAL:HG11	2.23	0.74
1:A:1492:HIS:ND1	1:A:1493:PRO:CD	2.51	0.74
1:B:1630:PRO:HD3	1:B:1643:GLN:HE21	1.51	0.74
1:B:611:GLN:HE21	1:B:816:VAL:H	1.34	0.74
1:A:1217:ASN:ND2	1:A:1218:ARG:HD3	2.02	0.74
1:A:827:ASP:HB2	1:A:854:ARG:HH21	1.53	0.74
1:B:503:ARG:HE	1:B:503:ARG:N	1.83	0.73
1:A:272:PHE:HD1	1:A:325:VAL:CG2	2.01	0.73
1:A:364:LYS:O	1:A:367:MET:HB2	1.88	0.73
1:B:931:VAL:HG11	1:B:1438:ASN:HB3	1.68	0.73
1:A:1636:GLN:HA	1:A:1641:GLN:HE22	1.54	0.73
1:A:598:LYS:HB2	1:A:800:THR:O	1.89	0.73
1:A:1036:PHE:HB3	1:A:1040:LYS:HG3	1.69	0.72
1:A:131:ILE:HG12	1:A:148:VAL:HG22	1.71	0.72
1:B:915:VAL:HB	1:B:920:ILE:HB	1.71	0.72
1:B:895:VAL:HG23	1:B:895:VAL:O	1.88	0.72
1:A:871:PHE:HB3	1:A:901:PRO:HA	1.70	0.72
1:B:1255:LEU:HD22	1:B:1274:VAL:HG23	1.71	0.72
1:B:1368:PRO:HA	1:B:1383:MET:HG2	1.71	0.72
1:B:319:VAL:HG13	1:B:347:ILE:O	1.89	0.72
1:B:251:LYS:HG2	1:B:300:ILE:HG12	1.71	0.72
1:A:614:ILE:O	1:A:617:VAL:HB	1.89	0.72
1:A:442:LEU:HD22	1:A:631:ARG:HH22	1.54	0.72
1:A:323:ILE:HD11	1:A:347:ILE:HD11	1.70	0.72
1:B:492:ILE:HG22	1:B:499:LEU:HB3	1.70	0.72
1:B:1147:LEU:HD23	1:B:1194:ALA:HB1	1.70	0.72
1:A:830:ILE:HD11	1:A:911:VAL:HG12	1.72	0.72
1:A:1003:ILE:HG12	1:A:1268:THR:HG22	1.70	0.72
1:A:314:ARG:HE	1:A:314:ARG:CA	2.03	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:359:THR:CG2	1:B:360:PRO:HD2	2.20	0.72
1:A:1575:GLN:HB3	1:A:1578:GLN:CD	2.10	0.72
1:B:330:ILE:HG22	1:B:337:MET:HB3	1.70	0.72
1:A:910:GLU:HG3	1:A:925:LYS:HB3	1.70	0.71
1:B:391:GLN:HA	1:B:423:ARG:HH22	1.55	0.71
1:A:876:THR:HB	1:A:879:LYS:HG3	1.71	0.71
1:A:377:ASN:HD21	1:A:383:ALA:HA	1.54	0.71
1:B:904:ILE:HG22	1:B:905:GLY:N	2.03	0.71
1:A:850:LEU:HD12	1:A:885:ILE:HD11	1.73	0.71
1:A:80:ASN:ND2	1:A:83:LEU:H	1.88	0.71
1:A:359:THR:CG2	1:A:360:PRO:HD2	2.20	0.71
1:A:118:LYS:HA	1:A:118:LYS:HE3	1.73	0.71
1:A:274:VAL:O	1:A:281:ILE:HG22	1.91	0.71
1:A:610:THR:CG2	1:A:613:LYS:HG3	2.19	0.71
1:B:228:LEU:O	1:B:228:LEU:HD23	1.89	0.71
1:B:1566:ILE:CD1	1:B:1576:VAL:HG22	2.21	0.71
1:B:611:GLN:HG2	1:B:816:VAL:HB	1.72	0.71
1:A:848:ALA:HB3	1:A:895:VAL:CG2	2.21	0.71
1:A:359:THR:HG22	1:A:360:PRO:CD	2.21	0.71
1:A:580:THR:HB	1:A:791:ASN:ND2	2.05	0.70
1:A:284:THR:HG22	1:A:678:MET:HE2	1.73	0.70
1:A:134:ASP:HB2	1:A:145:LEU:HB2	1.72	0.70
1:B:227:VAL:CG1	1:B:229:PRO:HD3	2.20	0.70
1:A:270:VAL:HG21	1:A:299:ALA:HB2	1.73	0.70
1:A:605:LYS:HE2	1:A:605:LYS:H	1.55	0.70
1:B:1401:ILE:HD12	1:B:1480:TYR:HD1	1.57	0.70
1:A:1156:ILE:HD12	1:A:1156:ILE:H	1.56	0.70
1:A:564:LYS:HG2	1:A:565:ASN:N	2.06	0.70
1:A:339:GLU:HB2	1:A:759:ILE:HD12	1.73	0.70
1:B:806:VAL:HG22	1:B:816:VAL:HA	1.72	0.70
1:A:1354:LYS:HA	1:A:1489:ARG:NH2	2.07	0.70
1:A:835:PRO:HG3	1:A:844:VAL:HG11	1.73	0.70
1:B:62:PHE:CD2	1:B:63:PRO:HD3	2.27	0.70
1:A:386:ILE:H	1:A:398:LEU:HB3	1.55	0.70
1:A:377:ASN:HB3	1:A:378:PRO:HD2	1.73	0.70
1:B:1545:THR:HG22	1:B:1563:ILE:HG23	1.74	0.70
1:A:532:TYR:CB	1:A:546:ALA:HB2	2.21	0.70
1:A:1610:TRP:HB3	1:A:1617:SER:HB2	1.74	0.70
1:A:1061:LYS:HD2	1:A:1061:LYS:H	1.56	0.70
1:A:537:ASN:ND2	1:A:538:ALA:H	1.90	0.70
1:B:528:ARG:NH2	1:B:623:ILE:HD11	2.06	0.70
1:A:610:THR:HG22	1:A:613:LYS:CD	2.22	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:418:LEU:HB3	1:A:441:ALA:HB3	1.74	0.70
1:B:1287:ASP:HA	1:B:1290:GLU:OE1	1.91	0.70
1:B:1605:VAL:HG12	1:B:1606:SER:H	1.56	0.70
1:B:407:LEU:HD23	1:B:408:SER:H	1.56	0.69
1:B:134:ASP:HB2	1:B:145:LEU:HB2	1.74	0.69
1:A:491:MET:HG3	1:A:501:VAL:HG12	1.73	0.69
1:B:986:VAL:O	1:B:990:THR:HG23	1.92	0.69
1:B:892:SER:O	1:B:893:VAL:HG23	1.91	0.69
1:B:852:ASN:ND2	1:B:859:LEU:HD23	2.07	0.69
1:B:520:THR:HG22	1:B:521:SER:H	1.57	0.69
1:A:573:HIS:CD2	1:A:579:ILE:HD11	2.28	0.69
1:B:1566:ILE:HD12	1:B:1576:VAL:HG22	1.74	0.69
1:B:504:GLN:HG3	1:B:515:LEU:HB2	1.75	0.69
1:B:118:LYS:CD	1:B:645:LYS:HE2	2.22	0.69
1:A:673:LEU:HD12	1:A:674:MET:H	1.56	0.69
1:A:611:GLN:HE21	1:A:815:CYS:HA	1.58	0.69
1:A:852:ASN:ND2	1:A:859:LEU:CD2	2.56	0.69
1:B:691:CYS:HA	1:B:1424:VAL:HG21	1.74	0.69
1:B:358:LYS:HD2	1:B:550:TRP:CZ3	2.28	0.69
1:A:152:ASP:HB3	1:A:158:VAL:HG21	1.74	0.69
1:A:593:LEU:HD12	1:A:772:THR:HG23	1.73	0.69
1:B:616:ASP:O	1:B:620:LYS:HB2	1.93	0.69
1:A:155:LEU:O	1:A:813:GLY:HA2	1.93	0.69
1:B:524:ILE:HG22	1:B:525:PRO:HD3	1.74	0.69
1:B:63:PRO:HG2	1:B:64:ALA:H	1.57	0.69
1:A:600:VAL:HG22	1:A:765:PHE:CG	2.28	0.69
1:A:616:ASP:O	1:A:620:LYS:HB2	1.93	0.68
1:B:1156:ILE:HD12	1:B:1156:ILE:H	1.58	0.68
1:B:429:ILE:HG22	1:B:430:PRO:HD2	1.73	0.68
1:A:250:LEU:N	1:A:250:LEU:HD12	2.07	0.68
1:B:1498:GLY:O	1:B:1501:SER:CB	2.41	0.68
1:A:83:LEU:CG	1:A:83:LEU:O	2.41	0.68
1:A:904:ILE:CG2	1:A:905:GLY:H	2.05	0.68
1:A:1435:ARG:C	1:A:1436:ASP:OD1	2.32	0.68
1:A:859:LEU:HD22	1:A:859:LEU:N	2.08	0.68
1:B:1613:LYS:HE2	1:B:1614:PRO:HD3	1.74	0.68
1:B:561:LEU:HD13	1:B:807:SER:HB3	1.76	0.68
1:B:128:TYR:HE2	1:B:617:VAL:HG12	1.58	0.68
1:B:753:ILE:C	1:B:754:ILE:HD12	2.14	0.68
1:A:1470:ILE:HG21	1:A:1499:MET:HG2	1.76	0.68
1:B:1585:HIS:HB3	1:B:1587:LYS:HG2	1.76	0.68
1:B:499:LEU:HG	1:B:500:LYS:HG2	1.75	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:940:THR:HB	1:B:1344:VAL:HG22	1.75	0.68
1:A:846:ILE:HD13	1:A:846:ILE:H	1.59	0.68
1:A:336:ASP:CG	1:A:1377:GLN:HE22	1.96	0.68
1:B:996:GLY:HA2	1:B:1047:LEU:HD11	1.75	0.68
1:B:244:ILE:HD11	1:B:319:VAL:HG21	1.73	0.68
1:A:423:ARG:HD2	1:A:425:LYS:HZ1	1.59	0.68
1:A:750:ASP:HB2	1:A:752:ASP:OD1	1.93	0.67
1:A:794:LEU:HD21	1:A:824:VAL:CG2	2.24	0.67
1:A:794:LEU:HG	1:A:795:LYS:H	1.59	0.67
1:A:524:ILE:O	1:A:553:VAL:HG23	1.94	0.67
1:B:241:PHE:HD2	1:B:378:PRO:HG3	1.59	0.67
1:B:62:PHE:CB	1:B:104:PHE:HB2	2.25	0.67
1:B:605:LYS:O	1:B:608:LYS:HG2	1.93	0.67
1:B:1223:ASN:O	1:B:1224:GLN:HG2	1.94	0.67
1:B:237:PRO:HG2	1:B:239:GLU:O	1.93	0.67
1:A:307:LEU:C	1:A:308:ASN:HD22	1.98	0.67
1:B:781:ASP:C	1:B:783:ASN:H	1.96	0.67
1:A:601:PHE:HD2	1:A:802:GLU:HG3	1.58	0.67
1:A:524:ILE:HG23	1:A:525:PRO:CD	2.24	0.67
1:B:1577:LYS:HE2	1:B:1577:LYS:HA	1.77	0.67
1:A:854:ARG:CD	1:A:857:GLU:HB2	2.25	0.67
1:A:876:THR:HG22	1:A:877:ALA:N	2.10	0.67
1:B:116:VAL:HG13	1:B:645:LYS:CG	2.16	0.67
1:B:32:ASN:HD22	1:B:643:THR:HG23	1.60	0.67
1:B:264:VAL:HG13	1:B:331:LEU:HD23	1.76	0.67
1:B:848:ALA:HB3	1:B:895:VAL:CG2	2.24	0.67
1:B:1161:VAL:HG12	1:B:1163:SER:H	1.59	0.67
1:B:1564:GLU:O	1:B:1565:ASN:HB2	1.94	0.67
1:A:74:THR:HG22	1:A:86:VAL:HG23	1.76	0.66
1:B:157:PRO:HB3	1:B:808:LEU:HD21	1.77	0.66
1:B:66:LYS:HZ3	1:B:94:LYS:HG2	1.60	0.66
1:A:271:ILE:CG2	1:A:287:LEU:HD22	2.24	0.66
1:A:561:LEU:HA	1:A:584:GLU:O	1.95	0.66
1:A:701:MET:HE1	1:A:1458:SER:H	1.60	0.66
1:B:808:LEU:HD12	1:B:814:ILE:HD11	1.76	0.66
1:A:848:ALA:O	1:A:895:VAL:HG22	1.95	0.66
1:B:864:GLU:OE2	1:B:880:ARG:HD3	1.96	0.66
1:B:1563:ILE:HD12	1:B:1563:ILE:N	2.11	0.66
1:B:436:THR:HG22	1:B:437:ARG:N	2.10	0.66
1:A:610:THR:HG22	1:A:613:LYS:CG	2.26	0.66
1:A:558:MET:HB3	1:A:812:LYS:NZ	2.10	0.66
1:A:1297:ILE:HB	1:A:1306:VAL:HG13	1.78	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1391:TYR:CG	1:A:1397:ALA:HB2	2.31	0.66
1:B:208:TYR:HB3	1:B:216:VAL:HG13	1.78	0.66
1:B:1566:ILE:HG13	1:B:1576:VAL:HG13	1.78	0.66
1:B:104:PHE:CE1	1:B:656:ALA:HB2	2.31	0.66
1:B:863:VAL:HG12	1:B:913:ALA:HB2	1.77	0.66
1:B:781:ASP:OD2	1:B:783:ASN:HB3	1.96	0.66
1:A:1368:PRO:HA	1:A:1383:MET:HG2	1.76	0.66
1:B:377:ASN:HB2	1:B:381:SER:OG	1.96	0.65
1:B:330:ILE:HD11	1:B:750:ASP:OD1	1.96	0.65
1:A:1547:LEU:HA	1:A:1561:MET:HG3	1.78	0.65
1:B:323:ILE:HG13	1:B:347:ILE:HD11	1.77	0.65
1:A:637:PHE:CE1	1:A:644:LEU:HD11	2.31	0.65
1:A:318:LEU:HA	1:A:321:LYS:HD3	1.78	0.65
1:A:1213:ALA:HB2	1:A:1219:TRP:CE2	2.32	0.65
1:B:846:ILE:HD13	1:B:897:TYR:O	1.96	0.65
1:B:400:GLN:HG2	1:B:401:ASP:N	2.11	0.65
1:A:331:LEU:HD22	1:A:333:SER:OG	1.96	0.65
1:B:198:VAL:HG22	1:B:199:ASN:N	2.11	0.65
1:A:829:PHE:CD2	1:A:853:TYR:HE2	2.12	0.65
1:A:396:GLN:HG3	1:A:397:SER:H	1.61	0.65
1:B:272:PHE:CD1	1:B:325:VAL:HG21	2.22	0.65
1:B:701:MET:CE	1:B:1420:LEU:HD21	2.26	0.65
1:B:270:VAL:O	1:B:287:LEU:HA	1.97	0.65
1:A:106:THR:HG22	1:A:119:VAL:HG13	1.77	0.65
1:A:58:THR:HA	1:A:70:SER:O	1.95	0.65
1:B:406:LYS:HD2	1:B:460:ARG:HG2	1.78	0.65
1:B:1415:GLU:OE1	1:B:1418:LYS:CE	2.44	0.65
1:B:32:ASN:ND2	1:B:643:THR:HG23	2.12	0.65
1:A:852:ASN:HB3	1:A:887:ILE:CG2	2.26	0.65
1:B:1201:LEU:HD23	1:B:1242:ARG:HD3	1.79	0.65
1:B:1003:ILE:HD12	1:B:1268:THR:HA	1.77	0.65
1:A:1554:ASP:C	1:A:1586:ILE:HD11	2.17	0.65
1:A:44:LEU:HD13	1:A:55:VAL:CG1	2.20	0.65
1:A:354:ILE:O	1:A:437:ARG:HG3	1.97	0.65
1:B:1502:LYS:HE2	1:B:1590:GLU:HG3	1.79	0.65
1:B:128:TYR:HB2	1:B:151:VAL:HG12	1.79	0.65
1:B:350:SER:HB2	1:B:433:ARG:O	1.97	0.65
1:A:490:TYR:CE2	1:A:515:LEU:HD22	2.31	0.65
1:B:287:LEU:HD23	1:B:287:LEU:H	1.62	0.65
1:A:314:ARG:HA	1:A:314:ARG:NE	2.11	0.65
1:B:566:GLY:HA3	1:B:580:THR:HG23	1.79	0.65
1:A:398:LEU:HD11	1:A:403:GLY:C	2.17	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1397:ALA:HB3	1:A:1449:VAL:HB	1.77	0.65
1:B:117:GLU:C	1:B:118:LYS:HG2	2.15	0.65
1:B:1128:MET:HE3	1:B:1142:LEU:HB2	1.79	0.65
1:B:272:PHE:CD2	1:B:301:LEU:HG	2.31	0.64
1:A:605:LYS:O	1:A:608:LYS:HG2	1.97	0.64
1:A:558:MET:C	1:A:812:LYS:NZ	2.49	0.64
1:A:348:VAL:CG1	1:A:350:SER:C	2.65	0.64
1:A:895:VAL:O	1:A:895:VAL:HG23	1.98	0.64
1:B:689:ARG:O	1:B:693:GLU:HG3	1.97	0.64
1:A:1010:GLY:HA3	1:A:1067:ALA:HA	1.79	0.64
1:B:377:ASN:HD21	1:B:383:ALA:HA	1.62	0.64
1:B:1397:ALA:HB3	1:B:1449:VAL:HB	1.79	0.64
1:B:149:PHE:HD1	1:B:187:ILE:HG12	1.63	0.64
1:A:323:ILE:O	1:A:345:ILE:HB	1.98	0.64
1:B:446:THR:HG21	1:B:450:SER:O	1.98	0.64
1:A:76:LEU:HB3	1:A:82:TYR:HB3	1.80	0.64
1:B:839:VAL:HG13	1:B:842:GLU:CD	2.18	0.64
1:B:1270:ALA:O	1:B:1274:VAL:HG12	1.97	0.64
1:A:1223:ASN:O	1:A:1224:GLN:HG2	1.96	0.64
1:B:323:ILE:HD11	1:B:347:ILE:HD11	1.79	0.64
1:A:554:LYS:O	1:A:556:SER:N	2.31	0.64
1:B:840:ARG:NH2	1:B:972:ASP:HB3	2.13	0.64
1:A:176:ARG:HE	1:A:1093:ALA:HB1	1.62	0.64
1:B:1573:GLU:HG2	1:B:1580:ARG:NH2	2.12	0.64
1:A:605:LYS:CE	1:A:605:LYS:H	2.10	0.64
1:A:362:PHE:HA	1:A:442:LEU:O	1.98	0.64
1:B:171:GLY:O	1:B:172:ILE:HB	1.98	0.64
1:B:729:ILE:HA	1:B:732:LEU:HB3	1.80	0.64
1:B:290:VAL:HG11	1:B:298:GLU:H	1.62	0.64
1:B:389:VAL:HG12	1:B:390:THR:H	1.62	0.64
1:A:1504:CYS:HB2	1:A:1508:THR:OG1	1.98	0.64
1:B:429:ILE:HG21	1:B:433:ARG:HD2	1.79	0.64
1:B:1012:GLN:HG2	1:B:1480:TYR:CZ	2.32	0.64
1:B:778:LYS:HG3	1:B:779:GLN:HG2	1.80	0.64
1:B:227:VAL:HG12	1:B:229:PRO:CD	2.20	0.63
1:A:290:VAL:HG21	1:A:298:GLU:O	1.98	0.63
1:B:228:LEU:O	1:B:228:LEU:CD2	2.45	0.63
1:A:977:THR:HB	1:A:1345:THR:HB	1.79	0.63
1:B:1493:PRO:CB	1:B:1497:ASP:OD2	2.43	0.63
1:B:57:VAL:HG21	1:B:86:VAL:HG21	1.79	0.63
1:B:303:ARG:HA	1:B:306:LEU:HB2	1.81	0.63
1:A:1369:ALA:HB1	1:A:1370:PRO:HD2	1.80	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:128:TYR:CE2	1:B:617:VAL:HG12	2.33	0.63
1:A:615:TRP:O	1:A:617:VAL:N	2.31	0.63
1:B:610:THR:HG23	1:B:613:LYS:H	1.63	0.63
1:A:530:VAL:HG21	1:A:642:LEU:HD11	1.81	0.63
1:B:1265:TYR:HB2	1:B:1271:THR:OG1	1.99	0.63
1:A:134:ASP:HB3	1:A:138:TYR:OH	1.98	0.63
1:A:240:LYS:O	1:A:240:LYS:HG3	1.99	0.63
1:A:834:LEU:HD22	1:A:846:ILE:HG21	1.78	0.63
1:A:885:ILE:HD12	1:A:893:VAL:HG11	1.80	0.63
2:A:2001:NAG:H61	2:A:2002:NAG:O7	1.98	0.63
1:A:610:THR:HG23	1:A:613:LYS:H	1.64	0.63
1:A:645:LYS:O	1:A:646:THR:HB	1.98	0.63
1:B:389:VAL:HG12	1:B:390:THR:N	2.14	0.63
1:B:1116:ILE:HG23	1:B:1139:ASP:HB3	1.80	0.63
1:B:454:LEU:HB2	1:B:533:TYR:HE2	1.62	0.63
1:A:489:THR:HG22	1:A:503:ARG:NE	2.13	0.63
1:A:605:LYS:N	1:A:605:LYS:HE2	2.14	0.63
1:A:838:VAL:HA	1:A:1408:THR:HG21	1.81	0.63
1:B:458:VAL:HG11	1:B:469:LEU:HD21	1.80	0.62
1:B:359:THR:HG22	1:B:360:PRO:CD	2.29	0.62
1:A:995:ASP:HB3	1:A:998:ARG:HB2	1.81	0.62
1:A:287:LEU:H	1:A:287:LEU:HD23	1.63	0.62
1:A:354:ILE:O	1:A:354:ILE:HD12	1.99	0.62
1:A:61:ASP:CB	1:A:63:PRO:HD2	2.21	0.62
1:B:134:ASP:OD2	1:B:768:SER:HB2	1.99	0.62
1:B:1391:TYR:CG	1:B:1397:ALA:HB2	2.34	0.62
1:B:135:LYS:HB3	1:B:600:VAL:HG11	1.82	0.62
1:B:997:GLU:OE2	2:B:2003:BMA:H4	1.99	0.62
1:B:36:LEU:HD12	1:B:124:LEU:HD13	1.80	0.62
1:A:653:GLN:HB3	1:A:655:ARG:HG2	1.80	0.62
1:A:362:PHE:CE2	1:A:631:ARG:NH1	2.67	0.62
1:B:268:ALA:HB2	1:B:329:VAL:HG22	1.81	0.62
1:B:319:VAL:C	1:B:321:LYS:H	2.03	0.62
1:A:633:TYR:O	1:A:637:PHE:HD2	1.83	0.62
1:B:272:PHE:CZ	1:B:301:LEU:HB2	2.34	0.62
1:A:674:MET:CG	1:A:751:ASP:HA	2.30	0.62
1:B:274:VAL:HG23	1:B:283:LEU:HD11	1.79	0.62
1:A:239:GLU:HB3	1:A:241:PHE:CZ	2.35	0.62
1:A:1012:GLN:HG2	1:A:1480:TYR:CZ	2.34	0.62
1:A:1545:THR:CG2	1:A:1563:ILE:HG23	2.29	0.62
1:B:448:GLY:O	1:B:450:SER:N	2.33	0.62
1:B:904:ILE:CG2	1:B:905:GLY:N	2.61	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:35:ARG:HB3	1:B:38:SER:OG	2.00	0.62
1:A:451:ASN:HB2	1:A:478:ASP:OD2	2.00	0.62
1:B:460:ARG:HH21	1:B:462:GLU:HB2	1.64	0.62
1:A:348:VAL:HG11	1:A:350:SER:O	2.00	0.62
1:B:44:LEU:HD12	1:B:84:SER:O	2.00	0.62
1:B:839:VAL:HG13	1:B:842:GLU:OE1	2.00	0.62
1:B:316:ASP:O	1:B:318:LEU:N	2.32	0.62
1:A:1549:GLN:HB3	1:A:1560:ILE:HD12	1.81	0.62
1:A:574:ARG:HH12	1:A:920:ILE:HB	1.62	0.62
1:B:269:PHE:CE1	1:B:289:ARG:HD3	2.34	0.62
1:A:348:VAL:CG1	1:A:350:SER:O	2.48	0.62
1:A:800:THR:CG2	1:A:823:THR:HG22	2.27	0.61
1:B:241:PHE:CD2	1:B:378:PRO:HG3	2.35	0.61
1:B:673:LEU:HG	1:B:674:MET:N	2.14	0.61
1:A:97:LYS:HE2	1:A:124:LEU:HD21	1.81	0.61
1:A:354:ILE:HG22	1:A:375:VAL:HG22	1.82	0.61
1:B:290:VAL:HG21	1:B:298:GLU:O	2.00	0.61
1:A:62:PHE:N	1:A:63:PRO:CD	2.63	0.61
1:A:1022:ILE:HD11	1:A:1275:PHE:CG	2.35	0.61
1:B:396:GLN:NE2	1:B:407:LEU:HA	2.08	0.61
1:B:32:ASN:HB2	1:B:641:GLY:HA2	1.81	0.61
1:A:1543:TYR:HB3	1:A:1563:ILE:CG2	2.31	0.61
1:A:476:ARG:CB	1:A:476:ARG:HH11	2.12	0.61
1:A:846:ILE:HD13	1:A:897:TYR:O	2.00	0.61
1:B:876:THR:HB	1:B:879:LYS:HG3	1.82	0.61
1:A:311:GLN:HB3	1:A:312:PRO:HD3	1.83	0.61
1:A:848:ALA:HB3	1:A:895:VAL:HG21	1.82	0.61
1:B:116:VAL:HG11	1:B:645:LYS:HG2	1.79	0.61
1:A:347:ILE:HG22	1:A:347:ILE:O	1.99	0.61
1:A:270:VAL:O	1:A:287:LEU:HA	2.00	0.61
1:A:287:LEU:HD21	1:A:678:MET:SD	2.40	0.61
1:A:152:ASP:HB3	1:A:158:VAL:CG2	2.31	0.61
1:A:306:LEU:C	1:A:308:ASN:H	2.03	0.61
1:A:420:ILE:CD1	1:A:439:MET:HB3	2.30	0.61
1:B:319:VAL:O	1:B:321:LYS:N	2.34	0.61
1:A:794:LEU:HD21	1:A:824:VAL:HG22	1.81	0.61
1:A:611:GLN:OE1	1:A:614:ILE:HD11	2.00	0.61
1:A:829:PHE:HD2	1:A:853:TYR:CE2	2.14	0.61
1:B:309:GLY:O	1:B:311:GLN:N	2.34	0.61
1:B:56:SER:O	1:B:109:ALA:HA	1.99	0.61
1:A:575:PRO:C	1:A:577:GLN:H	2.04	0.61
1:B:436:THR:HG22	1:B:437:ARG:H	1.66	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:798:ILE:HG21	1:B:829:PHE:HZ	1.64	0.61
1:A:610:THR:CG2	1:A:613:LYS:CG	2.79	0.61
1:A:34:LEU:HD22	1:A:40:GLU:HG3	1.83	0.61
1:B:906:LEU:N	1:B:906:LEU:HD23	2.14	0.61
1:A:729:ILE:O	1:A:733:ARG:HB2	2.01	0.61
1:A:268:ALA:HB2	1:A:329:VAL:HG22	1.82	0.61
1:B:407:LEU:CD2	1:B:408:SER:H	2.14	0.60
1:A:1563:ILE:HD12	1:A:1578:GLN:O	2.02	0.60
1:A:1289:LYS:HD3	1:A:1289:LYS:N	2.12	0.60
1:B:1575:GLN:HB3	1:B:1578:GLN:CD	2.21	0.60
1:B:373:VAL:HG11	1:B:388:VAL:CG1	2.31	0.60
1:A:111:PHE:CD1	1:A:111:PHE:C	2.75	0.60
1:B:129:LEU:HB2	1:B:217:PHE:HD2	1.63	0.60
1:B:269:PHE:O	1:B:327:ALA:HB1	2.01	0.60
1:B:430:PRO:C	1:B:432:GLY:H	2.04	0.60
1:B:1545:THR:HB	1:B:1561:MET:HG2	1.84	0.60
1:B:904:ILE:HD13	1:B:932:PRO:HB3	1.84	0.60
1:A:871:PHE:CZ	1:A:909:VAL:HG22	2.36	0.60
1:B:128:TYR:OH	1:B:618:VAL:HA	2.02	0.60
1:A:359:THR:O	1:A:627:PRO:HG2	2.00	0.60
1:A:171:GLY:O	1:A:172:ILE:HB	2.01	0.60
1:A:252:VAL:HG23	1:A:252:VAL:O	2.01	0.60
1:B:1297:ILE:HB	1:B:1306:VAL:HG13	1.84	0.60
1:A:575:PRO:O	1:A:577:GLN:N	2.33	0.60
1:A:615:TRP:C	1:A:617:VAL:N	2.54	0.60
1:B:562:VAL:HG12	1:B:563:VAL:N	2.17	0.60
1:A:612:ARG:HH11	1:A:612:ARG:HG2	1.65	0.60
1:B:323:ILE:CD1	1:B:347:ILE:HD11	2.31	0.60
1:A:653:GLN:O	1:A:654:GLN:HG2	2.02	0.60
1:B:389:VAL:HG21	1:B:425:LYS:HD2	1.83	0.60
1:A:876:THR:HB	1:A:879:LYS:CG	2.30	0.60
1:B:781:ASP:C	1:B:783:ASN:N	2.55	0.60
1:A:1112:LYS:HB3	1:A:1113:PRO:HD2	1.84	0.60
1:B:859:LEU:N	1:B:859:LEU:HD22	2.17	0.60
1:B:1377:GLN:N	1:B:1377:GLN:CD	2.54	0.60
1:B:398:LEU:CD1	1:B:405:ALA:H	2.12	0.60
1:B:872:CYS:HB2	1:B:900:VAL:HB	1.84	0.60
1:B:107:VAL:O	1:B:117:GLU:HA	2.00	0.60
1:A:116:VAL:HG11	1:A:645:LYS:HB3	1.84	0.60
1:B:1563:ILE:HD13	1:B:1578:GLN:H	1.66	0.60
1:B:994:ILE:HG23	1:B:1044:SER:HB3	1.84	0.60
1:B:653:GLN:H	1:B:653:GLN:NE2	1.99	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:137:ILE:HB	1:A:603:LEU:HD23	1.84	0.60
1:A:407:LEU:HD22	1:A:409:ILE:HG23	1.84	0.60
1:A:830:ILE:O	1:A:830:ILE:HG23	2.02	0.60
1:A:147:ARG:HE	1:A:189:THR:HG22	1.66	0.60
1:A:1496:GLU:O	1:A:1498:GLY:N	2.34	0.60
1:B:931:VAL:HG13	1:B:932:PRO:HD2	1.84	0.59
1:B:1237:LEU:HD21	1:B:1277:ALA:HA	1.82	0.59
1:A:530:VAL:HG12	1:A:548:SER:CB	2.32	0.59
1:B:580:THR:HA	1:B:791:ASN:HA	1.84	0.59
1:A:272:PHE:CD2	1:A:301:LEU:HG	2.37	0.59
1:A:250:LEU:HD12	1:A:250:LEU:H	1.65	0.59
1:A:712:ILE:HG21	1:A:719:VAL:HG22	1.85	0.59
1:A:58:THR:OG1	1:A:108:VAL:HB	2.02	0.59
1:B:1045:LEU:O	1:B:1049:ARG:HG3	2.02	0.59
1:A:530:VAL:HG12	1:A:548:SER:HB3	1.84	0.59
1:B:852:ASN:O	1:B:852:ASN:CG	2.40	0.59
1:B:843:GLN:HG3	1:B:900:VAL:HG22	1.83	0.59
1:A:507:GLU:OE1	1:A:508:PRO:HD2	2.01	0.59
1:B:323:ILE:HG22	1:B:324:TYR:N	2.16	0.59
1:A:1545:THR:HG22	1:A:1563:ILE:HG23	1.84	0.59
1:B:272:PHE:CD1	1:B:325:VAL:CG2	2.80	0.59
1:A:1654:MET:HA	1:A:1657:PHE:HB3	1.84	0.59
1:A:566:GLY:HA3	1:A:580:THR:HG23	1.84	0.59
1:A:271:ILE:HG23	1:A:287:LEU:CD2	2.32	0.59
1:A:1354:LYS:HA	1:A:1489:ARG:HH21	1.65	0.59
1:A:1270:ALA:O	1:A:1274:VAL:HG12	2.03	0.59
1:A:1542:VAL:HG22	1:A:1603:TRP:HB2	1.82	0.59
1:A:1544:LYS:HB3	1:A:1565:ASN:HB3	1.84	0.59
1:A:83:LEU:C	1:A:83:LEU:CD1	2.56	0.59
1:B:347:ILE:O	1:B:347:ILE:HG22	2.03	0.59
1:A:311:GLN:HB3	1:A:312:PRO:CD	2.32	0.59
1:B:121:LEU:O	1:B:122:ILE:HD13	2.02	0.59
1:B:977:THR:HB	1:B:1345:THR:CB	2.31	0.59
1:B:850:LEU:HD11	1:B:863:VAL:HG11	1.84	0.59
1:A:1242:ARG:O	1:A:1243:LYS:HB2	2.03	0.59
1:B:218:SER:O	1:B:219:ALA:HB2	2.03	0.59
1:B:273:GLY:O	1:B:324:TYR:CD2	2.56	0.59
1:B:72:GLU:HG3	1:B:86:VAL:HG13	1.85	0.59
1:A:737:SER:O	1:B:1222:PRO:HB3	2.02	0.59
1:B:958:ARG:HG3	1:B:1332:LYS:HG2	1.85	0.59
1:A:843:GLN:HG2	1:A:900:VAL:HG22	1.85	0.59
1:A:590:ARG:NH1	1:A:775:GLU:O	2.36	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:837:SER:HA	1:A:929:LYS:HB2	1.85	0.59
1:A:100:LYS:HD3	1:A:100:LYS:H	1.67	0.59
1:B:66:LYS:HZ1	1:B:94:LYS:HG2	1.64	0.59
1:B:561:LEU:CD1	1:B:807:SER:HB3	2.33	0.59
1:A:670:SER:HA	1:A:673:LEU:HD11	1.84	0.59
1:A:852:ASN:ND2	1:A:888:PRO:O	2.36	0.59
1:B:148:VAL:HG12	1:B:188:LEU:HB2	1.84	0.59
1:A:1014:MET:HG3	1:A:1080:TYR:CE2	2.38	0.59
1:A:541:GLN:HA	1:A:541:GLN:HE21	1.68	0.59
1:A:852:ASN:HB3	1:A:887:ILE:HG21	1.83	0.59
1:B:1498:GLY:C	1:B:1500:LEU:H	2.07	0.59
1:A:1528:GLU:HA	1:A:1531:LEU:HB2	1.85	0.59
1:B:362:PHE:CD1	1:B:631:ARG:HG3	2.38	0.58
1:A:1289:LYS:H	1:A:1289:LYS:CD	2.14	0.58
1:B:1437:SER:O	1:B:1438:ASN:C	2.41	0.58
1:A:1469:LEU:N	1:A:1499:MET:O	2.36	0.58
1:B:802:GLU:O	1:B:804:LEU:HD13	2.03	0.58
1:B:38:SER:O	1:B:39:GLU:HG2	2.03	0.58
1:B:164:ILE:HD13	1:B:190:LEU:HD11	1.85	0.58
1:B:852:ASN:HB2	1:B:859:LEU:HD23	1.85	0.58
1:A:1147:LEU:CD1	1:A:1168:ILE:HG23	2.32	0.58
1:A:169:PRO:HD3	1:A:203:TRP:CD1	2.38	0.58
1:A:575:PRO:CB	1:A:796:ASP:HA	2.33	0.58
1:B:102:HIS:O	1:B:103:LYS:HG3	2.03	0.58
1:A:250:LEU:CD1	1:A:250:LEU:H	2.16	0.58
1:A:584:GLU:HG2	1:A:787:THR:HG22	1.85	0.58
1:A:1014:MET:HG3	1:A:1080:TYR:HE2	1.67	0.58
1:B:564:LYS:HG2	1:B:565:ASN:N	2.18	0.58
1:A:1437:SER:O	1:A:1438:ASN:C	2.41	0.58
1:A:1204:ASP:HA	1:A:1207:THR:CG2	2.33	0.58
1:A:876:THR:CG2	1:A:877:ALA:N	2.67	0.58
1:B:850:LEU:HD12	1:B:885:ILE:HD11	1.85	0.58
1:B:460:ARG:HH12	1:B:552:ASP:H	1.50	0.58
1:B:384:ARG:HA	1:B:400:GLN:CB	2.33	0.58
1:B:439:MET:HG2	1:B:440:GLN:N	2.18	0.58
1:A:344:GLY:O	1:A:346:PRO:HD3	2.04	0.58
1:B:1601:LEU:HB3	1:B:1627:GLU:HB2	1.86	0.58
1:A:832:LEU:HD21	1:A:909:VAL:HG12	1.86	0.58
1:A:58:THR:HG22	1:A:71:ASN:HD22	1.67	0.58
1:A:931:VAL:HG11	1:A:1438:ASN:HB3	1.85	0.58
1:B:61:ASP:C	1:B:63:PRO:HD2	2.24	0.58
1:A:854:ARG:CZ	1:A:859:LEU:HD11	2.33	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:570:GLU:C	1:B:572:HIS:H	2.07	0.58
1:A:1184:ARG:HH11	1:A:1184:ARG:HG2	1.67	0.58
1:A:825:MET:HG3	1:A:826:GLN:N	2.18	0.58
1:A:824:VAL:O	1:A:824:VAL:HG12	2.04	0.58
1:B:377:ASN:O	1:B:379:ASP:N	2.32	0.58
1:B:642:LEU:O	1:B:643:THR:CG2	2.52	0.58
1:A:34:LEU:HB2	1:A:121:LEU:O	2.04	0.58
1:A:1138:LYS:HE3	1:A:1139:ASP:OD2	2.04	0.58
1:B:524:ILE:O	1:B:553:VAL:HG22	2.03	0.57
1:A:854:ARG:HD2	1:A:857:GLU:HB2	1.85	0.57
1:B:236:GLU:OE1	1:B:237:PRO:HD2	2.04	0.57
1:B:1600:TYR:HD2	1:B:1628:LEU:HA	1.69	0.57
1:B:1298:GLN:HG2	1:B:1305:ALA:HB2	1.86	0.57
1:B:398:LEU:HA	1:B:405:ALA:CB	2.32	0.57
1:B:1206:LEU:O	1:B:1206:LEU:HD22	2.04	0.57
1:A:529:LEU:HD12	1:A:530:VAL:N	2.19	0.57
1:B:881:HIS:HE1	1:B:897:TYR:HE2	1.51	0.57
1:B:72:GLU:CG	1:B:86:VAL:HG13	2.34	0.57
1:B:348:VAL:HG12	1:B:349:THR:N	2.18	0.57
1:B:348:VAL:HG12	1:B:350:SER:H	1.68	0.57
1:B:163:PHE:HB2	1:B:208:TYR:CE1	2.39	0.57
1:B:1600:TYR:CD2	1:B:1628:LEU:HA	2.40	0.57
1:B:1582:PHE:HB3	1:B:1620:ILE:HD11	1.85	0.57
1:A:41:THR:HB	1:A:87:THR:HG22	1.86	0.57
1:A:1579:GLU:O	1:A:1580:ARG:NH1	2.37	0.57
1:B:74:THR:CG2	1:B:84:SER:HB2	2.33	0.57
1:A:302:LYS:HD2	1:A:304:GLN:OE1	2.03	0.57
1:B:985:PRO:CB	1:B:1256:ASN:ND2	2.68	0.57
1:B:825:MET:CG	1:B:826:GLN:N	2.68	0.57
1:A:149:PHE:HD1	1:A:187:ILE:HG12	1.70	0.57
1:A:384:ARG:HD2	1:A:400:GLN:HB2	1.87	0.57
1:B:839:VAL:HA	1:B:931:VAL:O	2.03	0.57
1:A:235:LEU:HD12	1:A:340:ALA:HB1	1.87	0.57
1:A:1259:ARG:NH1	1:A:1340:THR:HG21	2.19	0.57
1:B:524:ILE:HA	1:B:553:VAL:HG21	1.85	0.57
1:A:615:TRP:C	1:A:617:VAL:H	2.06	0.57
1:A:295:GLY:C	1:A:296:ASN:HD22	2.08	0.57
1:A:611:GLN:NE2	1:A:815:CYS:HA	2.19	0.57
1:B:457:SER:HB3	1:B:472:ASN:HB2	1.86	0.57
1:A:866:LEU:HD11	1:A:910:GLU:OE2	2.04	0.57
1:A:933:GLU:HG2	1:A:970:VAL:HG11	1.86	0.57
1:A:1136:ARG:HD3	1:A:1181:GLU:HB3	1.86	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:55:VAL:HG13	1:B:111:PHE:HB3	1.87	0.57
1:B:272:PHE:HA	1:B:325:VAL:HG22	1.86	0.57
1:A:577:GLN:O	1:A:794:LEU:HB2	2.05	0.57
1:B:60:HIS:O	1:B:105:VAL:HG22	2.04	0.57
1:A:105:VAL:HB	1:A:122:ILE:HD11	1.86	0.57
1:B:904:ILE:CD1	1:B:932:PRO:HB3	2.35	0.57
1:A:885:ILE:CD1	1:A:893:VAL:HG11	2.35	0.57
1:A:473:PHE:HB2	1:A:513:VAL:HG12	1.85	0.57
1:B:269:PHE:HE1	1:B:289:ARG:HD3	1.70	0.57
1:A:159:GLY:HA2	1:A:181:SER:OG	2.05	0.57
1:A:969:GLN:HA	1:A:1348:HIS:O	2.05	0.57
1:B:463:LEU:HD13	1:B:467:GLU:HG2	1.87	0.56
1:A:281:ILE:O	1:A:281:ILE:HG23	2.04	0.56
1:B:35:ARG:CZ	1:B:153:HIS:HB2	2.35	0.56
1:A:235:LEU:HD12	1:A:340:ALA:CB	2.34	0.56
1:B:1022:ILE:HD11	1:B:1275:PHE:CD1	2.39	0.56
1:B:129:LEU:HD23	1:B:150:THR:HA	1.87	0.56
1:A:830:ILE:HD11	1:A:911:VAL:CG1	2.34	0.56
1:A:1268:THR:HB	1:A:1272:PHE:CE2	2.40	0.56
1:A:129:LEU:HG	1:A:209:TYR:CE1	2.40	0.56
1:A:504:GLN:HE21	1:A:504:GLN:HA	1.69	0.56
1:A:613:LYS:O	1:A:617:VAL:HG23	2.05	0.56
1:B:1575:GLN:O	1:B:1578:GLN:HG3	2.04	0.56
1:A:290:VAL:HG11	1:A:298:GLU:N	2.17	0.56
1:B:592:GLY:O	1:B:805:ALA:HA	2.05	0.56
1:B:611:GLN:HE21	1:B:816:VAL:N	2.03	0.56
1:B:876:THR:HG22	1:B:877:ALA:N	2.21	0.56
1:A:198:VAL:HG22	1:A:199:ASN:N	2.21	0.56
1:A:137:ILE:HD12	1:A:603:LEU:HD21	1.86	0.56
1:A:1500:LEU:O	1:A:1500:LEU:HD12	2.05	0.56
1:B:1247:THR:O	1:B:1247:THR:HG22	2.05	0.56
1:A:163:PHE:HE1	1:A:178:SER:HG	1.52	0.56
1:A:525:PRO:O	1:A:526:SER:O	2.24	0.56
1:A:852:ASN:C	1:A:852:ASN:OD1	2.43	0.56
1:B:445:ASN:HB2	1:B:632:ASN:HD21	1.71	0.56
1:B:876:THR:CG2	1:B:877:ALA:N	2.69	0.56
1:A:1593:LYS:HE2	1:A:1595:LYS:NZ	2.20	0.56
1:B:1147:LEU:CD1	1:B:1168:ILE:HG23	2.35	0.56
1:A:1564:GLU:O	1:A:1565:ASN:HB2	2.05	0.56
1:B:506:ARG:NE	1:B:510:GLN:O	2.38	0.56
1:B:946:LEU:O	1:B:1338:GLN:HA	2.05	0.56
1:B:559:GLY:HA3	1:B:812:LYS:HD2	1.87	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:490:TYR:HB2	1:A:529:LEU:HD11	1.86	0.56
1:A:1415:GLU:O	1:A:1419:THR:HG23	2.04	0.56
1:B:1406:MET:SD	1:B:1412:PRO:HD3	2.46	0.56
1:A:994:ILE:HG23	1:A:1044:SER:HB3	1.86	0.56
1:B:396:GLN:HG2	1:B:406:LYS:O	2.05	0.56
1:B:150:THR:HG22	1:B:162:VAL:HG21	1.87	0.56
1:A:827:ASP:HB3	1:A:854:ARG:HB3	1.88	0.56
1:B:168:THR:HG23	1:B:172:ILE:O	2.06	0.56
1:A:779:GLN:O	1:A:781:ASP:N	2.36	0.56
1:A:83:LEU:O	1:A:83:LEU:CD1	2.54	0.56
1:A:321:LYS:O	1:A:347:ILE:N	2.33	0.56
1:B:573:HIS:CE1	1:B:579:ILE:HD11	2.41	0.56
1:B:754:ILE:CG2	1:B:755:PRO:HD2	2.35	0.56
1:A:32:ASN:HB2	1:A:641:GLY:CA	2.35	0.56
1:B:1527:LEU:HG	1:B:1646:ASP:HB3	1.88	0.56
1:A:701:MET:CE	1:A:1458:SER:H	2.19	0.56
1:B:701:MET:HE1	1:B:1420:LEU:HD21	1.88	0.56
1:B:825:MET:HG3	1:B:826:GLN:N	2.20	0.56
1:B:398:LEU:CA	1:B:405:ALA:HB2	2.32	0.55
1:A:1568:LYS:HG3	1:A:1569:SER:N	2.21	0.55
1:B:835:PRO:HG3	1:B:844:VAL:HG11	1.89	0.55
1:A:83:LEU:HD12	1:A:84:SER:N	2.21	0.55
1:B:334:GLY:O	1:B:335:SER:HB2	2.07	0.55
1:B:808:LEU:CB	1:B:814:ILE:HG12	2.30	0.55
1:A:887:ILE:HD12	1:A:887:ILE:N	2.21	0.55
1:A:492:ILE:HD13	1:A:529:LEU:HD13	1.88	0.55
1:A:910:GLU:CG	1:A:925:LYS:HB3	2.36	0.55
1:B:155:LEU:O	1:B:813:GLY:HA2	2.06	0.55
1:A:814:ILE:O	1:A:814:ILE:HG22	2.05	0.55
1:A:400:GLN:HG2	1:A:401:ASP:N	2.20	0.55
1:A:361:LYS:HD3	1:A:362:PHE:CZ	2.40	0.55
1:A:593:LEU:HD12	1:A:772:THR:CG2	2.36	0.55
1:B:306:LEU:C	1:B:308:ASN:N	2.59	0.55
1:A:1190:ILE:O	1:A:1190:ILE:HD13	2.05	0.55
1:A:1300:PRO:HG2	1:A:1301:SER:H	1.71	0.55
1:B:525:PRO:HG2	1:B:526:SER:H	1.71	0.55
1:A:575:PRO:HB2	1:A:796:ASP:HA	1.87	0.55
1:B:578:GLN:OE1	1:B:791:ASN:HB3	2.06	0.55
1:B:915:VAL:CB	1:B:920:ILE:HB	2.35	0.55
1:B:354:ILE:HD12	1:B:355:HIS:N	2.22	0.55
1:A:231:PHE:CE1	1:A:338:VAL:HB	2.42	0.55
1:A:55:VAL:HG13	1:A:111:PHE:CB	2.26	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1569:SER:O	1:B:1571:SER:N	2.39	0.55
1:B:1576:VAL:O	1:B:1578:GLN:HG2	2.07	0.55
1:B:475:LEU:HB2	1:B:488:TYR:OH	2.06	0.55
1:A:366:ALA:HB2	1:A:413:ASN:CG	2.27	0.55
1:A:1502:LYS:O	1:A:1503:LEU:C	2.44	0.55
1:B:489:THR:HB	1:B:532:TYR:CE2	2.41	0.55
1:A:137:ILE:HD12	1:A:603:LEU:CD2	2.37	0.55
1:B:769:TRP:CD1	1:B:769:TRP:N	2.75	0.55
1:B:785:ILE:HG22	1:B:787:THR:HG22	1.88	0.55
1:A:112:GLY:O	1:A:114:VAL:HG22	2.06	0.55
1:B:1461:VAL:O	1:B:1461:VAL:HG23	2.06	0.55
1:B:1494:ASP:C	1:B:1496:GLU:H	2.10	0.55
1:A:149:PHE:CZ	1:A:806:VAL:CG1	2.89	0.55
1:A:1285:VAL:O	1:A:1285:VAL:HG12	2.07	0.55
1:B:1577:LYS:CE	1:B:1577:LYS:HA	2.37	0.55
1:B:560:THR:O	1:B:561:LEU:HD23	2.06	0.55
1:A:798:ILE:HG21	1:A:829:PHE:CZ	2.42	0.55
1:B:1494:ASP:O	1:B:1496:GLU:N	2.39	0.55
1:A:334:GLY:O	1:A:335:SER:HB2	2.07	0.55
1:B:634:ALA:HA	1:B:652:THR:HG22	1.88	0.55
1:B:68:VAL:O	1:B:68:VAL:HG13	2.06	0.55
1:B:642:LEU:C	1:B:643:THR:HG23	2.28	0.55
1:A:242:TYR:CG	1:A:250:LEU:HD11	2.42	0.55
1:B:1501:SER:O	1:B:1502:LYS:C	2.44	0.55
1:A:561:LEU:HD13	1:A:807:SER:HB3	1.89	0.55
1:B:1568:LYS:HG3	1:B:1569:SER:N	2.22	0.55
1:B:458:VAL:HG13	1:B:459:PRO:HD2	1.89	0.55
1:B:754:ILE:N	1:B:754:ILE:HD12	2.22	0.55
1:A:1547:LEU:HB3	1:A:1596:GLU:HA	1.89	0.55
1:A:1265:TYR:HB2	1:A:1271:THR:OG1	2.07	0.55
1:B:487:TYR:HB3	1:B:505:TYR:CD1	2.41	0.55
1:B:1284:ASP:C	1:B:1286:PRO:HD3	2.27	0.54
1:B:1405:SER:CB	1:B:1441:THR:HG22	2.37	0.54
1:B:1622:LYS:HG3	1:B:1623:ASP:OD1	2.07	0.54
1:B:701:MET:HE3	1:B:1420:LEU:HD21	1.89	0.54
1:B:577:GLN:HG2	1:B:578:GLN:O	2.07	0.54
1:B:581:LEU:N	1:B:790:MET:O	2.35	0.54
1:A:829:PHE:CD2	1:A:853:TYR:CE2	2.91	0.54
1:A:1566:ILE:HD12	1:A:1576:VAL:HG23	1.89	0.54
1:B:423:ARG:HG2	1:B:434:GLN:HE22	1.72	0.54
1:B:369:PHE:O	1:B:408:SER:HA	2.07	0.54
1:A:578:GLN:HB2	1:A:793:PHE:CD1	2.42	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:156:LEU:HD22	1:B:811:LYS:HA	1.88	0.54
1:B:360:PRO:CB	1:B:628:GLY:HA2	2.38	0.54
1:A:1287:ASP:HA	1:A:1289:LYS:HE2	1.87	0.54
1:B:74:THR:HG21	1:B:84:SER:HB2	1.88	0.54
1:B:1184:ARG:NH1	1:B:1221:GLU:OE1	2.40	0.54
1:A:904:ILE:HG23	1:A:930:VAL:O	2.07	0.54
1:A:1579:GLU:O	1:A:1580:ARG:CG	2.54	0.54
1:A:714:GLN:NE2	1:A:1424:VAL:HG13	2.21	0.54
1:A:487:TYR:HA	1:A:505:TYR:HA	1.88	0.54
1:A:429:ILE:HB	1:A:433:ARG:HB3	1.88	0.54
1:B:578:GLN:HG2	1:B:579:ILE:N	2.22	0.54
1:A:612:ARG:HG2	1:A:612:ARG:NH1	2.22	0.54
1:A:136:THR:OG1	1:A:604:ASN:HB3	2.07	0.54
1:B:105:VAL:O	1:B:120:VAL:HG23	2.06	0.54
1:A:164:ILE:HG23	1:A:207:ALA:HB2	1.90	0.54
1:A:1249:PRO:HB2	1:A:1250:PRO:HD3	1.90	0.54
1:A:861:VAL:HG12	1:A:862:ARG:N	2.23	0.54
1:A:1575:GLN:O	1:A:1578:GLN:HG2	2.07	0.54
1:B:104:PHE:HE1	1:B:656:ALA:HB2	1.72	0.54
1:A:250:LEU:N	1:A:250:LEU:CD1	2.71	0.54
1:B:336:ASP:OD1	1:B:1377:GLN:NE2	2.41	0.54
1:B:478:ASP:O	1:B:481:GLU:HG2	2.08	0.54
1:B:885:ILE:HD12	1:B:893:VAL:HG11	1.88	0.54
1:B:653:GLN:C	1:B:655:ARG:H	2.11	0.54
1:A:83:LEU:O	1:A:83:LEU:HD12	2.08	0.54
1:B:377:ASN:HB2	1:B:381:SER:HG	1.71	0.54
1:B:1545:THR:CG2	1:B:1563:ILE:HG23	2.37	0.54
1:A:1622:LYS:HG3	1:A:1623:ASP:OD1	2.08	0.54
1:B:726:CYS:O	1:B:729:ILE:HD12	2.07	0.54
1:A:541:GLN:CA	1:A:541:GLN:HE21	2.21	0.54
1:B:825:MET:CG	1:B:826:GLN:H	2.21	0.54
1:A:1078:THR:O	1:A:1082:VAL:HG23	2.08	0.54
1:B:1549:GLN:HB2	1:B:1560:ILE:HB	1.90	0.54
1:B:225:GLU:O	1:B:227:VAL:HG23	2.07	0.54
1:B:270:VAL:HG22	1:B:327:ALA:CB	2.37	0.54
1:B:593:LEU:HD12	1:B:772:THR:HG23	1.90	0.54
1:B:79:ASN:C	1:B:79:ASN:ND2	2.61	0.54
1:A:573:HIS:HB2	1:A:824:VAL:HA	1.90	0.53
1:A:592:GLY:O	1:A:805:ALA:HA	2.08	0.53
1:A:58:THR:HG22	1:A:71:ASN:ND2	2.23	0.53
1:A:1136:ARG:O	1:A:1137:GLU:HB2	2.08	0.53
1:A:504:GLN:O	1:A:504:GLN:HG3	2.09	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:2001:NAG:H61	2:B:2002:NAG:C7	2.38	0.53
1:A:215:GLN:OE1	1:A:215:GLN:N	2.42	0.53
1:A:80:ASN:HD22	1:A:83:LEU:H	1.56	0.53
1:A:524:ILE:HD11	1:A:556:SER:HB3	1.89	0.53
1:A:829:PHE:HB2	1:A:851:TYR:HB2	1.90	0.53
1:A:336:ASP:OD2	1:A:1377:GLN:NE2	2.42	0.53
1:B:605:LYS:HB3	1:B:608:LYS:HE2	1.89	0.53
1:A:70:SER:OG	1:A:88:ILE:HD13	2.09	0.53
1:B:610:THR:HG22	1:B:613:LYS:HD2	1.88	0.53
1:B:876:THR:HB	1:B:879:LYS:CG	2.37	0.53
1:B:45:GLU:HG2	1:B:82:TYR:HB2	1.89	0.53
1:A:906:LEU:HD23	1:A:906:LEU:N	2.23	0.53
1:B:585:ALA:HB3	1:B:777:LEU:HD13	1.89	0.53
1:A:574:ARG:HH11	1:A:918:HIS:CE1	2.26	0.53
1:A:805:ALA:O	1:A:806:VAL:HG23	2.08	0.53
1:A:559:GLY:HA3	1:A:812:LYS:HE3	1.91	0.53
1:A:674:MET:HG2	1:A:751:ASP:HA	1.91	0.53
1:A:977:THR:HA	1:A:1345:THR:HA	1.91	0.53
1:A:735:GLN:HA	1:A:738:ARG:HG2	1.88	0.53
1:B:1543:TYR:HB2	1:B:1545:THR:HG23	1.89	0.53
1:B:575:PRO:HB2	1:B:796:ASP:HB2	1.89	0.53
1:A:348:VAL:HG21	1:A:378:PRO:HB3	1.91	0.53
1:A:1610:TRP:O	1:A:1616:ILE:HG23	2.09	0.53
1:A:208:TYR:HB3	1:A:216:VAL:HG13	1.90	0.53
1:A:1300:PRO:HG3	1:A:1327:GLU:HB3	1.90	0.53
1:A:326:SER:HA	1:A:341:GLU:HA	1.90	0.53
1:A:1366:ILE:HD12	1:A:1385:LEU:HD13	1.91	0.53
1:A:1193:TYR:HA	1:A:1238:ALA:HB2	1.91	0.53
1:B:1039:GLU:H	1:B:1039:GLU:CD	2.12	0.53
1:A:650:LEU:HD12	1:A:651:GLU:O	2.08	0.53
1:B:977:THR:HB	1:B:1345:THR:CG2	2.39	0.53
1:A:1573:GLU:OE2	1:A:1580:ARG:NH2	2.41	0.53
1:A:138:TYR:CZ	1:A:144:VAL:HG22	2.43	0.53
1:A:161:THR:HG22	1:A:180:SER:HB2	1.90	0.53
1:B:1004:GLN:OE1	1:B:1261:TYR:HB3	2.08	0.53
1:A:323:ILE:N	1:A:345:ILE:O	2.42	0.53
1:A:118:LYS:HZ2	1:A:645:LYS:HD2	1.71	0.53
1:B:97:LYS:HA	1:B:103:LYS:NZ	2.23	0.53
1:A:346:PRO:CB	1:A:348:VAL:HG23	2.34	0.53
1:A:303:ARG:HA	1:A:306:LEU:HB2	1.90	0.53
1:B:1128:MET:HE3	1:B:1142:LEU:CA	2.39	0.53
1:A:438:THR:HG22	1:A:439:MET:H	1.73	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:396:GLN:CG	1:B:407:LEU:HG	2.36	0.53
1:A:272:PHE:CD1	1:A:325:VAL:CG2	2.88	0.53
1:B:672:GLN:HG2	1:B:673:LEU:N	2.23	0.53
1:B:593:LEU:HD11	1:B:774:ILE:CD1	2.35	0.53
1:B:1507:ASP:HA	1:B:1510:ARG:HB3	1.91	0.53
1:B:468:THR:HG22	1:B:518:THR:HG22	1.90	0.53
1:B:1382:SER:HB3	1:B:1462:HIS:ND1	2.24	0.53
1:A:580:THR:HA	1:A:791:ASN:HA	1.91	0.53
1:A:1472:PRO:HB3	1:A:1492:HIS:CD2	2.43	0.53
1:A:839:VAL:HA	1:A:931:VAL:O	2.09	0.53
1:B:32:ASN:ND2	1:B:643:THR:CG2	2.72	0.53
1:B:574:ARG:O	1:B:577:GLN:HB3	2.09	0.53
1:A:284:THR:O	1:A:287:LEU:HD23	2.08	0.53
1:B:374:TYR:CE2	1:B:376:THR:HG23	2.35	0.53
1:A:846:ILE:HD11	1:A:899:ILE:HD12	1.89	0.53
1:A:1010:GLY:HA3	1:A:1077:LEU:HD11	1.91	0.53
1:A:731:GLN:HG3	1:A:732:LEU:N	2.23	0.53
1:B:131:ILE:HG12	1:B:148:VAL:HG23	1.90	0.53
1:A:618:VAL:HG12	1:A:622:ASP:OD1	2.09	0.53
1:A:55:VAL:HG12	1:A:56:SER:H	1.74	0.53
1:A:1575:GLN:HB3	1:A:1578:GLN:HE22	1.71	0.53
1:B:574:ARG:HG3	1:B:575:PRO:HD2	1.91	0.53
1:A:85:THR:HG21	1:A:501:VAL:HG21	1.90	0.53
1:A:1217:ASN:HD22	1:A:1217:ASN:H	1.57	0.53
1:B:1285:VAL:N	1:B:1286:PRO:CD	2.69	0.53
1:B:904:ILE:CG2	1:B:905:GLY:H	2.20	0.53
1:B:1289:LYS:N	1:B:1289:LYS:HE2	2.24	0.53
1:A:1077:LEU:O	1:A:1081:VAL:HG23	2.07	0.53
1:B:283:LEU:HB2	1:B:286:SER:OG	2.08	0.53
1:A:420:ILE:HD12	1:A:439:MET:HB3	1.89	0.53
1:A:199:ASN:HD21	1:A:1056:LEU:HB3	1.73	0.53
1:A:1255:LEU:HD22	1:A:1274:VAL:HG23	1.91	0.53
1:B:838:VAL:HG21	1:B:928:LEU:HD11	1.90	0.53
1:A:1545:THR:HG22	1:A:1563:ILE:HA	1.91	0.53
1:A:1470:ILE:CG2	1:A:1499:MET:CG	2.87	0.53
1:A:834:LEU:CD2	1:A:846:ILE:HG21	2.39	0.52
1:A:399:THR:OG1	1:A:402:ASP:HB2	2.09	0.52
1:A:1517:PHE:HE2	1:A:1592:LEU:HD22	1.73	0.52
1:B:41:THR:OG1	1:B:498:LEU:HD13	2.09	0.52
1:A:272:PHE:CD1	1:A:325:VAL:HG21	2.22	0.52
1:A:454:LEU:HD12	1:A:455:HIS:H	1.74	0.52
1:A:272:PHE:HD2	1:A:286:SER:HB3	1.74	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:524:ILE:CG2	1:A:525:PRO:HD3	2.33	0.52
1:A:1289:LYS:HA	1:A:1312:TRP:CD1	2.44	0.52
1:B:530:VAL:HG21	1:B:642:LEU:CD1	2.32	0.52
1:B:105:VAL:O	1:B:120:VAL:N	2.40	0.52
1:A:862:ARG:NH1	1:A:884:THR:OG1	2.43	0.52
1:B:800:THR:HG23	1:B:823:THR:HG22	1.90	0.52
1:A:1227:TYR:CE2	1:A:1482:ASN:HB2	2.45	0.52
1:A:578:GLN:HB2	1:A:793:PHE:CE1	2.45	0.52
1:A:580:THR:HB	1:A:791:ASN:HD21	1.75	0.52
1:A:384:ARG:HA	1:A:400:GLN:HB2	1.91	0.52
1:B:549:VAL:HG12	1:B:550:TRP:N	2.25	0.52
1:A:285:HIS:HB2	1:A:305:VAL:HG13	1.90	0.52
1:B:229:PRO:HG3	1:B:762:ARG:HB2	1.90	0.52
1:A:421:THR:HG22	1:A:438:THR:OG1	2.10	0.52
1:A:164:ILE:HD12	1:A:164:ILE:H	1.73	0.52
1:B:976:GLU:OE2	1:B:1322:GLU:HG2	2.10	0.52
1:B:721:ALA:O	1:B:724:ASP:HB3	2.09	0.52
1:A:1039:GLU:CD	1:A:1039:GLU:H	2.10	0.52
1:A:611:GLN:HE21	1:A:816:VAL:H	1.57	0.52
1:A:852:ASN:CB	1:A:859:LEU:HD23	2.38	0.52
1:A:1362:LEU:O	1:A:1489:ARG:HD3	2.09	0.52
1:A:179:LYS:HD2	1:A:190:LEU:HD21	1.92	0.52
1:B:1570:GLY:O	1:B:1572:ASP:N	2.43	0.52
1:A:374:TYR:CD1	1:A:404:VAL:HG22	2.44	0.52
1:A:385:HIS:HA	1:A:398:LEU:O	2.10	0.52
1:B:336:ASP:CG	1:B:1377:GLN:NE2	2.62	0.52
1:A:712:ILE:HG12	1:A:1424:VAL:HG12	1.92	0.52
1:B:1614:PRO:HG2	1:B:1615:LYS:H	1.75	0.52
1:A:306:LEU:C	1:A:308:ASN:N	2.63	0.52
1:B:1041:ARG:O	1:B:1045:LEU:HD23	2.10	0.52
1:B:1041:ARG:NH1	1:B:1045:LEU:HD21	2.25	0.52
1:B:1533:LYS:HA	1:B:1536:GLU:HG3	1.91	0.52
1:A:637:PHE:HB3	1:A:642:LEU:HB2	1.92	0.52
1:A:321:LYS:HB3	1:A:347:ILE:HB	1.91	0.52
1:B:308:ASN:O	1:B:309:GLY:C	2.48	0.52
1:B:482:GLN:HG2	1:B:506:ARG:HH22	1.75	0.52
1:A:285:HIS:HB2	1:A:305:VAL:CG1	2.40	0.52
1:A:1308:HIS:ND1	1:A:1319:ARG:HD2	2.24	0.52
1:A:62:PHE:HB3	1:A:104:PHE:O	2.08	0.52
1:B:371:LEU:HD23	1:B:371:LEU:N	2.15	0.52
1:A:558:MET:HB3	1:A:812:LYS:HZ3	1.73	0.52
1:A:854:ARG:HD3	1:A:857:GLU:OE1	2.10	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:198:VAL:CG2	1:B:199:ASN:N	2.73	0.52
1:B:1213:ALA:HB2	1:B:1219:TRP:CZ2	2.45	0.52
1:B:762:ARG:HG2	1:B:762:ARG:HH11	1.75	0.52
1:A:931:VAL:HG21	1:A:1438:ASN:HB3	1.92	0.52
1:B:977:THR:HA	1:B:1345:THR:HA	1.92	0.52
1:A:673:LEU:CD1	1:A:674:MET:H	2.23	0.52
1:B:843:GLN:OE1	1:B:1502:LYS:HA	2.10	0.52
1:A:140:PRO:HD3	1:A:224:LYS:O	2.10	0.52
1:A:1017:MET:O	1:A:1021:VAL:HG23	2.10	0.52
1:A:637:PHE:CG	1:A:650:LEU:HD22	2.45	0.51
1:B:158:VAL:HG12	1:B:160:GLN:HG3	1.92	0.51
1:B:852:ASN:CG	1:B:887:ILE:CG2	2.79	0.51
1:A:399:THR:O	1:A:403:GLY:HA2	2.09	0.51
1:B:871:PHE:CZ	1:B:909:VAL:HG22	2.45	0.51
1:B:445:ASN:HB2	1:B:632:ASN:ND2	2.25	0.51
1:A:30:THR:HG22	1:A:42:VAL:HG22	1.91	0.51
1:A:562:VAL:HG12	1:A:563:VAL:N	2.25	0.51
1:B:794:LEU:HD13	1:B:824:VAL:HG22	1.93	0.51
1:B:1280:GLN:HG2	1:B:1283:LYS:HD2	1.90	0.51
1:B:642:LEU:O	1:B:643:THR:HG23	2.09	0.51
1:B:843:GLN:CG	1:B:900:VAL:HG22	2.40	0.51
1:B:358:LYS:HD2	1:B:550:TRP:CH2	2.44	0.51
1:A:176:ARG:HE	1:A:1093:ALA:CB	2.23	0.51
1:A:933:GLU:HG3	1:A:1556:PHE:HE1	1.76	0.51
1:A:800:THR:HA	1:A:823:THR:HA	1.93	0.51
1:B:234:GLN:NE2	1:B:257:ARG:NH2	2.49	0.51
1:B:1498:GLY:O	1:B:1501:SER:N	2.43	0.51
1:B:849:ILE:HA	1:B:893:VAL:O	2.09	0.51
1:A:971:PRO:HD3	1:A:1350:LYS:HE2	1.92	0.51
1:B:808:LEU:O	1:B:808:LEU:HD23	2.10	0.51
1:B:591:VAL:HG13	1:B:807:SER:HB2	1.93	0.51
1:B:670:SER:O	1:B:672:GLN:N	2.44	0.51
1:B:375:VAL:HG12	1:B:376:THR:N	2.26	0.51
1:B:1289:LYS:H	1:B:1289:LYS:HE2	1.75	0.51
1:B:876:THR:HG22	1:B:878:LYS:H	1.76	0.51
1:B:276:ASP:CB	1:B:279:ARG:HB2	2.34	0.51
1:A:362:PHE:CE1	1:A:631:ARG:HD2	2.46	0.51
1:B:492:ILE:HD11	1:B:529:LEU:HD12	1.93	0.51
1:B:885:ILE:CD1	1:B:893:VAL:HG11	2.41	0.51
1:A:390:THR:HG22	1:A:422:VAL:HG13	1.92	0.51
1:A:204:LYS:HA	1:A:220:GLU:HA	1.93	0.51
1:B:119:VAL:HB	1:B:654:GLN:HG3	1.93	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:827:ASP:CB	1:A:854:ARG:HH21	2.22	0.51
1:A:334:GLY:O	1:A:335:SER:CB	2.57	0.51
1:B:1061:LYS:CE	1:B:1061:LYS:H	2.23	0.51
1:B:30:THR:N	1:B:644:LEU:HD21	2.26	0.51
1:A:494:ASN:O	1:A:495:LYS:HB2	2.10	0.51
1:B:350:SER:OG	1:B:435:ALA:HB2	2.11	0.51
1:B:762:ARG:NH1	1:B:764:GLN:O	2.43	0.51
1:A:1147:LEU:HD11	1:A:1168:ILE:HG23	1.93	0.51
1:A:1288:HIS:HB3	1:A:1312:TRP:CE3	2.45	0.51
1:B:421:THR:HG22	1:B:438:THR:CB	2.32	0.51
1:A:1406:MET:SD	1:A:1412:PRO:HD3	2.51	0.51
1:B:132:GLN:O	1:B:146:TYR:HA	2.10	0.51
1:A:1161:VAL:HG12	1:A:1163:SER:H	1.75	0.51
1:B:1366:ILE:HD12	1:B:1385:LEU:HD13	1.92	0.51
1:B:271:ILE:HG23	1:B:287:LEU:HD22	1.92	0.51
1:B:985:PRO:HB3	1:B:1256:ASN:ND2	2.26	0.51
1:B:1184:ARG:HH12	1:B:1221:GLU:CD	2.14	0.51
1:B:175:LYS:HD2	1:B:192:TRP:CD1	2.46	0.51
1:A:80:ASN:HD22	1:A:82:TYR:N	2.09	0.51
1:A:839:VAL:HG21	1:A:1471:GLN:HG3	1.93	0.51
1:A:645:LYS:HG2	1:A:646:THR:H	1.75	0.51
1:B:852:ASN:ND2	1:B:888:PRO:O	2.40	0.51
1:A:284:THR:O	1:A:287:LEU:CD2	2.59	0.51
1:B:623:ILE:HG23	1:B:625:CYS:H	1.76	0.51
1:B:365:PRO:HG2	1:B:453:TYR:CE1	2.46	0.51
1:A:1041:ARG:HH11	1:A:1045:LEU:HD11	1.74	0.51
1:B:276:ASP:HB2	1:B:279:ARG:CB	2.33	0.51
1:A:456:LEU:HD21	1:A:473:PHE:CD1	2.46	0.51
1:A:633:TYR:CD1	1:A:634:ALA:N	2.79	0.51
1:B:852:ASN:HB2	1:B:859:LEU:CD2	2.41	0.51
1:A:290:VAL:CG1	1:A:298:GLU:H	2.18	0.51
1:A:384:ARG:O	1:A:386:ILE:HG13	2.11	0.51
1:B:905:GLY:C	1:B:906:LEU:HD23	2.30	0.51
1:A:442:LEU:HB2	1:A:631:ARG:NH2	2.26	0.51
1:B:1606:SER:O	1:B:1609:LEU:HB2	2.10	0.51
1:B:732:LEU:HD13	1:B:732:LEU:O	2.10	0.51
1:B:798:ILE:CG2	1:B:829:PHE:HZ	2.24	0.51
1:B:801:TRP:O	1:B:802:GLU:HG2	2.11	0.51
1:B:638:THR:CG2	1:B:652:THR:HB	2.41	0.51
1:A:472:ASN:HA	1:A:514:VAL:HG22	1.93	0.51
1:B:658:PRO:HG2	1:B:659:GLN:H	1.75	0.51
1:B:461:VAL:O	1:B:463:LEU:HG	2.11	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1415:GLU:OE1	1:B:1415:GLU:CA	2.50	0.50
1:B:699:ASN:O	1:B:702:LYS:HD2	2.11	0.50
1:B:805:ALA:O	1:B:806:VAL:HG23	2.11	0.50
1:A:377:ASN:ND2	1:A:383:ALA:HA	2.24	0.50
1:B:848:ALA:HB3	1:B:895:VAL:HG22	1.93	0.50
1:A:971:PRO:HD3	1:A:1350:LYS:CE	2.42	0.50
1:A:982:GLN:O	1:A:1339:GLY:HA3	2.11	0.50
1:B:573:HIS:CE1	1:B:579:ILE:CD1	2.94	0.50
1:B:590:ARG:O	1:B:807:SER:OG	2.22	0.50
1:A:1353:GLY:O	1:A:1354:LYS:HB2	2.12	0.50
1:B:1526:THR:O	1:B:1530:ARG:HG2	2.11	0.50
1:A:1505:HIS:O	1:A:1506:LYS:C	2.49	0.50
1:A:458:VAL:CG2	1:A:471:VAL:HG13	2.42	0.50
1:B:374:TYR:HE2	1:B:376:THR:CG2	2.21	0.50
1:B:138:TYR:CZ	1:B:144:VAL:HG22	2.47	0.50
1:B:275:GLN:HB3	1:B:322:SER:O	2.11	0.50
1:A:268:ALA:CB	1:A:329:VAL:HG22	2.41	0.50
1:A:1534:ALA:O	1:A:1539:VAL:HG21	2.11	0.50
1:A:274:VAL:HB	1:A:281:ILE:CG2	2.42	0.50
1:A:62:PHE:N	1:A:63:PRO:HD2	2.27	0.50
1:A:574:ARG:NH1	1:A:918:HIS:ND1	2.60	0.50
1:B:887:ILE:HD12	1:B:887:ILE:N	2.26	0.50
1:A:1288:HIS:O	1:A:1312:TRP:HB2	2.12	0.50
1:A:454:LEU:HD23	1:A:546:ALA:HA	1.93	0.50
1:A:854:ARG:NH1	1:A:859:LEU:CD1	2.74	0.50
1:B:147:ARG:HG3	1:B:771:TRP:CH2	2.47	0.50
1:B:1259:ARG:HH11	1:B:1340:THR:HG21	1.76	0.50
1:B:553:VAL:HG23	1:B:554:LYS:N	2.26	0.50
1:A:315:ALA:O	1:A:319:VAL:HG23	2.11	0.50
1:A:323:ILE:CD1	1:A:347:ILE:HD11	2.39	0.50
1:A:793:PHE:O	1:A:794:LEU:O	2.29	0.50
1:A:454:LEU:HD12	1:A:455:HIS:N	2.27	0.50
1:A:507:GLU:HB3	1:A:510:GLN:HE22	1.76	0.50
1:A:1156:ILE:N	1:A:1156:ILE:HD12	2.24	0.50
1:B:1249:PRO:HB2	1:B:1250:PRO:HD3	1.93	0.50
1:A:358:LYS:HB3	1:A:550:TRP:CZ3	2.47	0.50
1:B:866:LEU:HD21	1:B:912:LYS:NZ	2.26	0.50
1:A:512:LEU:O	1:A:512:LEU:HG	2.12	0.50
1:A:77:ASN:O	1:A:80:ASN:ND2	2.43	0.50
1:B:62:PHE:CG	1:B:63:PRO:HD3	2.46	0.50
1:A:852:ASN:HB3	1:A:887:ILE:HG22	1.92	0.50
1:A:374:TYR:HD1	1:A:404:VAL:HG22	1.76	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:373:VAL:O	1:B:373:VAL:HG12	2.11	0.50
1:A:423:ARG:HD2	1:A:425:LYS:NZ	2.26	0.50
1:B:268:ALA:CB	1:B:329:VAL:HG22	2.41	0.50
1:A:262:GLU:OE2	1:A:891:SER:HA	2.11	0.50
1:B:1552:LEU:HD12	1:B:1552:LEU:H	1.77	0.50
1:B:386:ILE:HB	1:B:398:LEU:HB3	1.94	0.50
1:A:798:ILE:HG21	1:A:829:PHE:HZ	1.76	0.50
1:A:593:LEU:HD11	1:A:774:ILE:HD11	1.93	0.50
1:B:274:VAL:HG12	1:B:275:GLN:N	2.27	0.50
1:A:1540:ASP:OD2	1:A:1571:SER:HB3	2.12	0.50
1:A:236:GLU:OE1	1:A:237:PRO:HD2	2.12	0.50
1:A:251:LYS:CD	1:A:300:ILE:HG12	2.41	0.50
1:A:794:LEU:HD21	1:A:824:VAL:HG21	1.94	0.50
1:B:371:LEU:CD2	1:B:371:LEU:H	2.15	0.50
1:A:290:VAL:HG11	1:A:298:GLU:O	2.11	0.50
1:A:1576:VAL:HG12	1:A:1577:LYS:N	2.27	0.50
1:B:1003:ILE:HG22	1:B:1005:THR:H	1.76	0.50
1:B:597:ASP:OD2	1:B:599:GLY:N	2.45	0.50
1:B:800:THR:HA	1:B:823:THR:HA	1.93	0.50
1:B:1359:LYS:HB3	1:B:1485:GLU:HB3	1.93	0.50
1:A:55:VAL:HG21	1:A:76:LEU:HG	1.94	0.49
1:B:227:VAL:CG1	1:B:762:ARG:HA	2.42	0.49
1:B:580:THR:HA	1:B:790:MET:O	2.11	0.49
1:A:1237:LEU:CD2	1:A:1277:ALA:HA	2.40	0.49
1:A:719:VAL:HG12	1:A:723:LEU:CD2	2.42	0.49
1:A:331:LEU:HD13	1:A:1377:GLN:HE21	1.76	0.49
1:B:1600:TYR:HA	1:B:1629:TRP:H	1.78	0.49
1:B:585:ALA:HB3	1:B:777:LEU:CD1	2.42	0.49
1:A:1592:LEU:HB3	1:A:1594:LEU:HG	1.93	0.49
1:B:1552:LEU:HD23	1:B:1589:ARG:NE	2.27	0.49
1:A:670:SER:N	1:A:673:LEU:HD21	2.27	0.49
1:B:1377:GLN:H	1:B:1377:GLN:CD	2.15	0.49
1:A:362:PHE:HD1	1:A:630:GLY:C	2.15	0.49
1:B:1289:LYS:H	1:B:1289:LYS:CE	2.24	0.49
1:B:1358:LYS:O	1:B:1359:LYS:HB2	2.10	0.49
1:A:485:ILE:HG13	1:A:506:ARG:HH21	1.76	0.49
1:B:117:GLU:O	1:B:118:LYS:CD	2.60	0.49
1:B:156:LEU:O	1:B:158:VAL:HG23	2.13	0.49
1:A:557:CYS:SG	1:A:611:GLN:HG3	2.52	0.49
1:A:117:GLU:O	1:A:118:LYS:HD2	2.12	0.49
1:B:992:ASP:HB2	1:B:998:ARG:CB	2.37	0.49
1:A:1573:GLU:OE2	1:A:1580:ARG:NE	2.45	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:712:ILE:CG2	1:A:719:VAL:HG22	2.42	0.49
1:B:31:PRO:HA	1:B:641:GLY:O	2.12	0.49
1:B:561:LEU:HD12	1:B:815:CYS:HB3	1.95	0.49
1:B:1588:CYS:O	1:B:1592:LEU:HB2	2.13	0.49
1:B:1609:LEU:HG	1:B:1616:ILE:HG21	1.95	0.49
1:B:1156:ILE:HD12	1:B:1156:ILE:N	2.26	0.49
1:B:765:PHE:O	1:B:766:PRO:C	2.51	0.49
1:A:421:THR:HG22	1:A:438:THR:HG23	1.94	0.49
1:B:439:MET:HG2	1:B:440:GLN:H	1.77	0.49
1:B:838:VAL:HA	1:B:1408:THR:HG21	1.93	0.49
1:B:1060:GLN:HB3	1:B:1061:LYS:HE3	1.93	0.49
1:B:862:ARG:HB2	1:B:916:TYR:HE1	1.77	0.49
1:A:1391:TYR:CD1	1:A:1397:ALA:HB2	2.46	0.49
1:B:1363:ARG:NH2	1:B:1454:GLU:OE1	2.45	0.49
1:A:229:PRO:O	1:A:259:LEU:HD11	2.13	0.49
1:B:325:VAL:O	1:B:342:ARG:N	2.44	0.49
1:B:32:ASN:N	1:B:641:GLY:O	2.46	0.49
1:B:895:VAL:O	1:B:895:VAL:CG2	2.58	0.49
1:B:528:ARG:HA	1:B:549:VAL:O	2.13	0.49
1:B:830:ILE:HG13	1:B:850:LEU:CD2	2.43	0.49
1:A:1022:ILE:HD12	1:A:1276:GLN:HA	1.95	0.49
1:B:260:TYR:HE1	1:B:798:ILE:HG12	1.77	0.49
1:A:1111:GLN:HB2	1:A:1117:PHE:CE2	2.47	0.49
1:B:302:LYS:HD2	1:B:304:GLN:OE1	2.12	0.49
1:A:574:ARG:O	1:A:575:PRO:C	2.49	0.49
1:B:1541:TYR:O	1:B:1603:TRP:HA	2.12	0.49
1:B:459:PRO:HD2	1:B:469:LEU:HD11	1.94	0.49
1:B:904:ILE:HG23	1:B:930:VAL:O	2.12	0.49
1:B:848:ALA:HB3	1:B:895:VAL:HG21	1.94	0.49
1:B:798:ILE:HG21	1:B:829:PHE:CZ	2.46	0.49
1:B:1531:LEU:HD22	1:B:1654:MET:SD	2.53	0.49
1:A:642:LEU:O	1:A:643:THR:HG23	2.11	0.49
1:A:904:ILE:CD1	1:A:932:PRO:HB3	2.43	0.49
1:A:116:VAL:HG13	1:A:645:LYS:NZ	2.28	0.49
1:B:104:PHE:CZ	1:B:656:ALA:HB2	2.48	0.49
1:A:798:ILE:HG12	1:A:829:PHE:HZ	1.78	0.49
1:A:852:ASN:CG	1:A:859:LEU:CD2	2.81	0.49
1:A:561:LEU:CD1	1:A:807:SER:CB	2.90	0.49
1:A:864:GLU:OE2	1:A:880:ARG:HD3	2.12	0.49
1:B:319:VAL:C	1:B:321:LYS:N	2.66	0.49
1:B:250:LEU:O	1:B:251:LYS:C	2.50	0.49
1:B:1217:ASN:HD21	1:B:1218:ARG:CD	2.22	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:375:VAL:HB	1:A:398:LEU:CD2	2.43	0.49
1:A:863:VAL:HG12	1:A:913:ALA:HB2	1.95	0.49
1:B:342:ARG:HH21	1:B:345:ILE:HG12	1.78	0.49
1:B:359:THR:CG2	1:B:360:PRO:CD	2.88	0.49
1:B:852:ASN:CG	1:B:887:ILE:HG22	2.33	0.49
1:B:110:THR:HB	1:B:115:GLN:CB	2.37	0.49
1:B:580:THR:HB	1:B:791:ASN:ND2	2.28	0.49
1:A:121:LEU:HD23	1:A:122:ILE:H	1.78	0.49
1:B:1003:ILE:CD1	1:B:1268:THR:HA	2.43	0.49
1:A:1496:GLU:HG2	1:B:1204:ASP:OD1	2.13	0.49
1:A:934:GLY:HA3	1:A:970:VAL:HG21	1.93	0.49
1:B:1351:LEU:HD23	1:B:1351:LEU:N	2.28	0.49
1:B:1024:VAL:HG13	1:B:1033:TRP:HH2	1.77	0.49
1:A:118:LYS:HA	1:A:118:LYS:CE	2.34	0.48
1:B:1576:VAL:HG12	1:B:1577:LYS:H	1.78	0.48
1:A:355:HIS:HB3	1:A:437:ARG:NH1	2.28	0.48
1:B:303:ARG:CA	1:B:306:LEU:HB2	2.43	0.48
1:A:159:GLY:HA3	1:A:182:GLN:HG3	1.94	0.48
1:A:1045:LEU:O	1:A:1049:ARG:HG3	2.13	0.48
1:A:864:GLU:OE2	1:A:880:ARG:HB2	2.13	0.48
1:B:1541:TYR:HB2	1:B:1543:TYR:CE1	2.48	0.48
1:B:633:TYR:OH	1:B:650:LEU:HA	2.12	0.48
1:B:110:THR:CB	1:B:115:GLN:HB3	2.38	0.48
1:B:436:THR:CG2	1:B:437:ARG:N	2.77	0.48
1:A:1555:ASP:N	1:A:1586:ILE:HD11	2.28	0.48
1:B:159:GLY:HA2	1:B:181:SER:OG	2.13	0.48
1:A:950:HIS:O	1:A:951:LEU:HD23	2.13	0.48
1:A:60:HIS:CG	1:A:65:LYS:HB2	2.48	0.48
1:A:986:VAL:HG22	1:A:990:THR:HG23	1.95	0.48
1:A:529:LEU:O	1:A:548:SER:HA	2.14	0.48
1:A:634:ALA:O	1:A:638:THR:HG23	2.13	0.48
1:B:1575:GLN:HB3	1:B:1578:GLN:NE2	2.28	0.48
1:B:566:GLY:HA3	1:B:580:THR:CG2	2.43	0.48
1:B:915:VAL:CG2	1:B:920:ILE:HB	2.42	0.48
1:B:623:ILE:HG12	1:B:624:GLY:H	1.78	0.48
1:B:729:ILE:O	1:B:733:ARG:HB2	2.13	0.48
1:A:1530:ARG:HG3	1:A:1650:PHE:HZ	1.79	0.48
1:A:358:LYS:HB2	1:A:372:MET:CE	2.44	0.48
1:B:350:SER:HA	1:B:433:ARG:HB2	1.95	0.48
1:A:490:TYR:HB3	1:A:531:ALA:HB2	1.95	0.48
1:B:1605:VAL:HG12	1:B:1606:SER:N	2.26	0.48
1:B:990:THR:O	1:B:994:ILE:HG13	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1128:MET:HE3	1:B:1142:LEU:CB	2.44	0.48
1:B:1279:ALA:O	1:B:1283:LYS:HB2	2.13	0.48
1:A:1099:LEU:O	1:A:1102:THR:HB	2.13	0.48
1:B:464:LYS:HZ2	1:B:554:LYS:HE2	1.78	0.48
1:A:72:GLU:HG3	1:A:73:ASN:N	2.27	0.48
1:A:281:ILE:HD13	1:A:310:VAL:CG2	2.28	0.48
1:B:62:PHE:N	1:B:63:PRO:CD	2.76	0.48
1:B:611:GLN:O	1:B:614:ILE:HG12	2.13	0.48
1:A:751:ASP:C	1:A:753:ILE:H	2.17	0.48
1:A:673:LEU:HD22	1:A:751:ASP:OD2	2.13	0.48
1:B:44:LEU:HD11	1:B:86:VAL:CG2	2.39	0.48
1:A:910:GLU:OE1	1:A:925:LYS:HD3	2.13	0.48
1:A:1156:ILE:CD1	1:A:1156:ILE:H	2.25	0.48
1:B:994:ILE:HG22	1:B:1040:LYS:HE2	1.95	0.48
1:B:610:THR:CG2	1:B:613:LYS:HG3	2.43	0.48
1:A:843:GLN:CG	1:A:900:VAL:HG22	2.43	0.48
1:A:1328:ARG:NH2	1:A:1330:THR:HG23	2.28	0.48
1:B:396:GLN:HA	1:B:396:GLN:OE1	2.13	0.48
1:A:644:LEU:H	1:A:650:LEU:CD2	2.26	0.48
1:B:120:VAL:HG12	1:B:121:LEU:H	1.77	0.48
1:B:79:ASN:C	1:B:79:ASN:HD22	2.16	0.48
1:B:1157:CYS:HB2	1:B:1164:LEU:HD12	1.96	0.48
1:A:149:PHE:CD1	1:A:187:ILE:HG12	2.47	0.48
1:B:1542:VAL:HA	1:B:1602:VAL:O	2.14	0.48
1:B:712:ILE:HG21	1:B:719:VAL:HG22	1.96	0.48
1:B:130:PHE:HE1	1:B:617:VAL:HG21	1.79	0.48
1:B:940:THR:HA	1:B:1344:VAL:HG22	1.95	0.48
1:B:1213:ALA:HB2	1:B:1219:TRP:CE2	2.49	0.48
1:A:389:VAL:HG12	1:A:390:THR:N	2.27	0.48
1:B:1024:VAL:HG11	1:B:1091:LEU:HD13	1.96	0.48
1:A:1244:ASP:O	1:A:1246:ASP:N	2.47	0.48
1:B:1509:CYS:O	1:B:1513:GLU:HG2	2.13	0.48
1:A:388:VAL:HG21	1:A:405:ALA:HB2	1.94	0.48
1:A:318:LEU:HD13	1:A:321:LYS:HZ2	1.79	0.48
1:B:362:PHE:HD1	1:B:630:GLY:CA	2.27	0.48
1:B:834:LEU:CD2	1:B:846:ILE:HG21	2.43	0.48
1:A:129:LEU:HB2	1:A:217:PHE:CD2	2.49	0.48
1:B:1227:TYR:CE2	1:B:1482:ASN:HB2	2.49	0.48
1:A:515:LEU:HD12	1:A:516:PRO:HD2	1.96	0.48
1:A:187:ILE:H	1:A:808:LEU:HD13	1.78	0.48
1:A:398:LEU:HG	1:A:399:THR:O	2.14	0.48
1:B:843:GLN:O	1:B:1467:VAL:HG13	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:481:GLU:OE2	1:B:538:ALA:HB2	2.14	0.48
1:B:863:VAL:HG12	1:B:913:ALA:CB	2.43	0.48
1:A:574:ARG:O	1:A:577:GLN:CB	2.62	0.48
1:B:1566:ILE:HD11	1:B:1576:VAL:HG22	1.93	0.48
1:A:382:PRO:CB	1:A:403:GLY:HA3	2.40	0.48
1:B:1204:ASP:HA	1:B:1207:THR:HG23	1.96	0.48
1:B:487:TYR:HB3	1:B:505:TYR:HD1	1.77	0.48
1:B:468:THR:CG2	1:B:518:THR:HG22	2.44	0.48
1:A:534:THR:O	1:A:534:THR:HG22	2.13	0.48
1:A:672:GLN:O	1:A:675:GLU:HB3	2.13	0.48
1:A:617:VAL:O	1:A:621:ALA:HB3	2.14	0.47
1:A:977:THR:HB	1:A:1345:THR:CB	2.42	0.47
1:A:1018:THR:O	1:A:1022:ILE:HG23	2.14	0.47
1:A:519:ILE:HG22	1:A:519:ILE:O	2.13	0.47
1:A:319:VAL:C	1:A:321:LYS:H	2.18	0.47
1:B:359:THR:HG23	1:B:371:LEU:HA	1.97	0.47
1:A:271:ILE:CD1	1:A:753:ILE:HD13	2.43	0.47
1:B:271:ILE:CG2	1:B:287:LEU:HD22	2.44	0.47
1:A:402:ASP:HB3	1:A:404:VAL:HG23	1.95	0.47
1:A:1275:PHE:O	1:A:1276:GLN:C	2.53	0.47
1:B:423:ARG:HG2	1:B:434:GLN:NE2	2.30	0.47
1:B:493:MET:HB2	1:B:528:ARG:HB3	1.96	0.47
1:B:138:TYR:CE2	1:B:144:VAL:HG22	2.49	0.47
1:B:731:GLN:HG3	1:B:732:LEU:N	2.28	0.47
1:A:41:THR:HA	1:A:87:THR:HA	1.95	0.47
1:B:818:ASP:OD1	1:B:819:PRO:HD2	2.13	0.47
1:B:1369:ALA:HB1	1:B:1370:PRO:HD2	1.96	0.47
1:B:368:PRO:HA	1:B:409:ILE:O	2.14	0.47
1:B:566:GLY:CA	1:B:580:THR:HG23	2.44	0.47
1:A:798:ILE:HG12	1:A:829:PHE:CZ	2.49	0.47
1:B:1217:ASN:H	1:B:1217:ASN:HD22	1.62	0.47
1:A:1203:GLY:O	1:A:1207:THR:HG22	2.14	0.47
1:B:330:ILE:O	1:B:330:ILE:HG13	2.14	0.47
1:A:158:VAL:HG12	1:A:160:GLN:HG3	1.95	0.47
1:B:840:ARG:HH22	1:B:972:ASP:HB3	1.79	0.47
1:A:173:PRO:HG3	1:A:176:ARG:NH2	2.28	0.47
2:A:2001:NAG:H61	2:A:2002:NAG:C7	2.44	0.47
1:A:1548:ILE:HG22	1:A:1560:ILE:O	2.14	0.47
1:B:88:ILE:HG22	1:B:89:LYS:N	2.29	0.47
1:B:1404:ILE:HG23	1:B:1475:VAL:HG22	1.96	0.47
1:A:1285:VAL:N	1:A:1286:PRO:CD	2.78	0.47
1:A:270:VAL:HA	1:A:327:ALA:HB2	1.95	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:520:THR:HG22	1:B:521:SER:N	2.28	0.47
1:B:36:LEU:HA	1:B:90:ILE:O	2.15	0.47
1:B:99:ASP:HB2	1:B:100:LYS:NZ	2.30	0.47
1:B:361:LYS:HB3	1:B:361:LYS:NZ	2.30	0.47
1:B:305:VAL:O	1:B:305:VAL:HG12	2.14	0.47
1:B:238:GLU:HB3	1:B:251:LYS:O	2.14	0.47
1:B:362:PHE:HD1	1:B:630:GLY:HA2	1.79	0.47
1:B:60:HIS:CD2	1:B:65:LYS:HD3	2.49	0.47
1:B:1468:GLY:HA3	1:B:1501:SER:O	2.14	0.47
1:B:800:THR:CG2	1:B:823:THR:HG22	2.44	0.47
1:A:944:ARG:HG3	1:A:944:ARG:HH11	1.79	0.47
1:A:944:ARG:NH1	1:A:959:GLU:HB3	2.28	0.47
1:A:44:LEU:CD1	1:A:55:VAL:HG11	2.25	0.47
1:A:650:LEU:HD12	1:A:651:GLU:C	2.35	0.47
1:A:104:PHE:CE1	1:A:656:ALA:HB2	2.48	0.47
1:A:354:ILE:C	1:A:354:ILE:HD12	2.34	0.47
1:A:712:ILE:HD11	1:A:722:PHE:CG	2.50	0.47
1:B:528:ARG:HH22	1:B:623:ILE:HD11	1.79	0.47
1:B:528:ARG:CZ	1:B:623:ILE:HD11	2.45	0.47
1:A:601:PHE:CD2	1:A:802:GLU:HG3	2.46	0.47
1:B:1546:ARG:HD2	1:B:1599:HIS:CE1	2.50	0.47
1:A:1136:ARG:HH11	1:A:1183:ARG:NH1	2.12	0.47
1:A:426:LYS:HB3	1:A:429:ILE:HG12	1.97	0.47
1:A:324:TYR:HB2	1:A:342:ARG:O	2.15	0.47
1:B:98:SER:HB2	1:B:100:LYS:HE2	1.96	0.47
1:B:51:GLY:O	1:B:78:SER:HB3	2.13	0.47
1:A:699:ASN:O	1:A:702:LYS:N	2.42	0.47
1:A:528:ARG:HH12	1:A:624:GLY:HA3	1.80	0.47
1:A:780:ALA:HB3	1:A:786:SER:HA	1.97	0.47
1:B:464:LYS:HB3	1:B:465:PRO:HD2	1.95	0.47
1:A:56:SER:HA	1:A:73:ASN:HB2	1.96	0.47
1:B:272:PHE:HZ	1:B:299:ALA:O	1.97	0.47
1:A:577:GLN:HG2	1:A:578:GLN:O	2.15	0.47
1:B:104:PHE:CD1	1:B:121:LEU:HG	2.50	0.47
1:A:348:VAL:HG12	1:A:350:SER:C	2.35	0.47
1:B:451:ASN:HD22	1:B:476:ARG:HH12	1.63	0.47
1:A:561:LEU:HD13	1:A:807:SER:CB	2.45	0.47
1:A:168:THR:O	1:A:170:ASP:N	2.43	0.47
1:B:1362:LEU:O	1:B:1489:ARG:HD3	2.15	0.47
1:B:1109:GLU:O	1:B:1110:LYS:HD3	2.14	0.47
1:B:1318:LEU:O	1:B:1319:ARG:HG2	2.15	0.47
1:A:799:THR:OG1	1:A:800:THR:N	2.48	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1545:THR:HB	1:B:1561:MET:CG	2.44	0.47
1:B:904:ILE:HG22	1:B:905:GLY:H	1.75	0.47
1:B:431:GLU:O	1:B:434:GLN:HG2	2.14	0.47
1:A:998:ARG:HH11	1:A:998:ARG:HG3	1.80	0.47
1:A:1401:ILE:HD12	1:A:1480:TYR:HD1	1.79	0.47
1:A:1587:LYS:HG3	1:A:1588:CYS:N	2.30	0.47
1:A:459:PRO:HD2	1:A:469:LEU:HD11	1.95	0.47
1:B:119:VAL:HB	1:B:654:GLN:HE21	1.80	0.47
1:B:1502:LYS:CE	1:B:1590:GLU:HG3	2.43	0.47
1:A:227:VAL:HG12	1:A:229:PRO:HD3	1.96	0.47
1:B:1131:GLY:O	1:B:1134:ASP:HB2	2.15	0.47
1:B:1347:TYR:CE1	1:B:1349:ALA:HB2	2.50	0.47
1:B:118:LYS:HD3	1:B:645:LYS:CE	2.29	0.46
1:B:852:ASN:C	1:B:854:ARG:H	2.18	0.46
1:B:673:LEU:HD21	1:B:751:ASP:CG	2.36	0.46
1:A:242:TYR:CE1	1:A:246:ASP:OD1	2.68	0.46
1:B:128:TYR:CB	1:B:151:VAL:HG12	2.44	0.46
1:A:423:ARG:HA	1:A:435:ALA:O	2.14	0.46
1:A:1502:LYS:O	1:A:1504:CYS:N	2.48	0.46
1:A:978:LYS:HD2	2:A:2001:NAG:H62	1.97	0.46
1:B:866:LEU:HD21	1:B:912:LYS:HZ3	1.80	0.46
1:A:251:LYS:NZ	1:A:300:ILE:HG12	2.30	0.46
1:A:1030:THR:CB	1:A:1032:GLN:HE21	2.28	0.46
1:B:797:SER:O	1:B:799:THR:HG22	2.15	0.46
1:A:1269:GLN:O	1:A:1273:MET:HB2	2.15	0.46
1:A:689:ARG:O	1:A:693:GLU:HG3	2.15	0.46
1:A:1601:LEU:HD12	1:A:1627:GLU:HG3	1.98	0.46
1:B:62:PHE:HB3	1:B:104:PHE:HB2	1.94	0.46
1:B:63:PRO:CG	1:B:64:ALA:H	2.25	0.46
1:A:242:TYR:CD1	1:A:250:LEU:CD1	2.94	0.46
1:A:859:LEU:H	1:A:859:LEU:CD2	2.21	0.46
1:B:264:VAL:CG1	1:B:265:ASP:N	2.78	0.46
1:A:445:ASN:O	1:A:632:ASN:OD1	2.32	0.46
1:B:1288:HIS:H	1:B:1289:LYS:HZ1	1.62	0.46
1:A:1092:ILE:HG22	1:A:1093:ALA:N	2.30	0.46
1:A:1253:ARG:O	1:A:1256:ASN:HB3	2.14	0.46
1:A:452:ASN:O	1:A:545:VAL:HG21	2.15	0.46
1:A:80:ASN:HB2	1:A:83:LEU:HG	1.98	0.46
1:B:250:LEU:HD12	1:B:301:LEU:HB3	1.96	0.46
1:B:1566:ILE:HD13	1:B:1574:VAL:HG12	1.97	0.46
1:A:1576:VAL:CG1	1:A:1577:LYS:N	2.78	0.46
1:B:446:THR:OG1	1:B:450:SER:HB3	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:537:ASN:HD22	1:A:538:ALA:H	1.63	0.46
1:A:1470:ILE:CG2	1:A:1499:MET:HG2	2.42	0.46
1:A:1415:GLU:HA	1:A:1415:GLU:OE1	2.15	0.46
1:B:468:THR:HG22	1:B:518:THR:CG2	2.45	0.46
1:A:156:LEU:HD22	1:A:811:LYS:HA	1.96	0.46
1:B:1078:THR:O	1:B:1082:VAL:HG23	2.16	0.46
1:B:719:VAL:HG12	1:B:723:LEU:HD23	1.96	0.46
1:A:909:VAL:O	1:A:925:LYS:HA	2.16	0.46
1:B:326:SER:HA	1:B:341:GLU:HA	1.97	0.46
1:B:183:ASN:HB3	1:B:184:GLN:NE2	2.30	0.46
1:A:110:THR:O	1:A:110:THR:OG1	2.33	0.46
1:A:74:THR:HG22	1:A:86:VAL:CG2	2.44	0.46
1:A:644:LEU:H	1:A:650:LEU:HD21	1.80	0.46
1:B:1564:GLU:HG3	1:B:1599:HIS:CD2	2.51	0.46
1:A:151:VAL:H	1:A:209:TYR:HH	1.62	0.46
1:A:60:HIS:CD2	1:A:65:LYS:HD2	2.50	0.46
1:A:475:LEU:HB2	1:A:488:TYR:OH	2.16	0.46
1:A:54:GLN:HA	1:A:75:GLN:HB3	1.97	0.46
1:A:769:TRP:CH2	1:A:794:LEU:HD12	2.50	0.46
1:A:931:VAL:HG13	1:A:932:PRO:HD2	1.96	0.46
1:B:701:MET:O	1:B:702:LYS:CB	2.60	0.46
1:B:833:ARG:O	1:B:846:ILE:HB	2.15	0.46
1:A:355:HIS:N	1:A:355:HIS:ND1	2.64	0.46
1:A:1003:ILE:HD13	1:A:1015:ILE:HD12	1.98	0.46
1:B:147:ARG:HG3	1:B:771:TRP:CZ2	2.51	0.46
1:A:1574:VAL:N	1:A:1575:GLN:OE1	2.48	0.46
1:A:633:TYR:N	1:A:633:TYR:CD1	2.82	0.46
1:A:314:ARG:NE	1:A:314:ARG:CA	2.74	0.46
1:B:386:ILE:HB	1:B:398:LEU:CD2	2.45	0.46
1:B:475:LEU:HG	1:B:476:ARG:N	2.31	0.46
1:A:631:ARG:O	1:A:632:ASN:HB2	2.16	0.46
1:B:1077:LEU:O	1:B:1081:VAL:HG23	2.15	0.46
1:A:50:GLN:HG3	1:A:51:GLY:H	1.81	0.46
1:B:282:SER:O	1:B:284:THR:N	2.49	0.46
1:A:756:GLU:O	1:A:758:ASP:N	2.48	0.46
1:B:485:ILE:HD12	1:B:485:ILE:H	1.80	0.46
1:B:396:GLN:HG3	1:B:397:SER:H	1.81	0.46
1:B:348:VAL:HG12	1:B:349:THR:H	1.81	0.46
1:A:1437:SER:O	1:A:1439:LYS:N	2.49	0.46
1:A:610:THR:HG23	1:A:613:LYS:N	2.29	0.46
1:B:271:ILE:HG23	1:B:287:LEU:CD2	2.46	0.46
1:A:97:LYS:HE2	1:A:124:LEU:CD2	2.45	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1363:ARG:NH2	1:A:1454:GLU:OE1	2.48	0.46
1:B:1086:ALA:HB2	1:B:1153:ALA:HB2	1.97	0.46
1:A:1563:ILE:CD1	1:A:1578:GLN:O	2.63	0.46
1:A:575:PRO:C	1:A:577:GLN:N	2.70	0.46
1:A:491:MET:HG3	1:A:501:VAL:CG1	2.43	0.46
1:A:827:ASP:HB2	1:A:854:ARG:NH2	2.26	0.46
1:B:1288:HIS:HB3	1:B:1312:TRP:CE3	2.51	0.46
1:A:308:ASN:N	1:A:308:ASN:HD22	2.11	0.46
1:B:1351:LEU:HD13	1:B:1490:PHE:CD2	2.51	0.46
1:B:707:ARG:NE	1:B:710:GLN:OE1	2.49	0.46
1:B:1147:LEU:HD11	1:B:1168:ILE:HG23	1.98	0.46
1:B:1288:HIS:N	1:B:1289:LYS:HE2	2.31	0.46
1:B:1156:ILE:CD1	1:B:1156:ILE:H	2.28	0.46
1:B:260:TYR:CE1	1:B:798:ILE:HG12	2.51	0.46
1:A:825:MET:CG	1:A:826:GLN:N	2.79	0.46
1:A:960:GLU:HG2	1:A:1330:THR:HG22	1.98	0.46
1:B:961:VAL:HG11	1:B:1343:VAL:HG21	1.98	0.46
1:B:1659:CYS:C	1:B:1661:ASN:H	2.18	0.46
1:B:654:GLN:O	1:B:654:GLN:HG2	2.16	0.45
1:A:59:VAL:HG11	1:A:90:ILE:HG23	1.98	0.45
1:A:164:ILE:HD13	1:A:190:LEU:HD11	1.98	0.45
1:A:280:ARG:HG2	1:A:324:TYR:CE2	2.51	0.45
1:A:468:THR:HA	1:A:517:LEU:O	2.16	0.45
1:A:202:VAL:HG12	1:A:202:VAL:O	2.16	0.45
1:A:867:TYR:HB2	1:A:875:ALA:O	2.17	0.45
1:B:117:GLU:O	1:B:645:LYS:HE3	2.16	0.45
1:B:1563:ILE:HD12	1:B:1578:GLN:O	2.15	0.45
1:A:124:LEU:N	1:A:124:LEU:HD23	2.31	0.45
1:A:346:PRO:HG3	1:A:378:PRO:HB2	1.97	0.45
1:B:1587:LYS:HG3	1:B:1588:CYS:SG	2.57	0.45
1:A:1267:SER:OG	1:A:1268:THR:N	2.48	0.45
1:B:1289:LYS:HG2	1:B:1290:GLU:OE2	2.16	0.45
1:A:59:VAL:HG11	1:A:90:ILE:CG2	2.46	0.45
1:A:90:ILE:HA	1:A:91:PRO:HD2	1.41	0.45
1:B:260:TYR:OH	1:B:798:ILE:HD11	2.16	0.45
1:B:860:LYS:HB3	1:B:916:TYR:HB2	1.96	0.45
1:A:76:LEU:HD22	1:A:82:TYR:O	2.15	0.45
1:B:430:PRO:C	1:B:432:GLY:N	2.69	0.45
1:A:272:PHE:CD2	1:A:286:SER:HB3	2.51	0.45
1:A:318:LEU:HD22	1:A:321:LYS:HZ2	1.81	0.45
1:A:989:MET:HB3	1:A:1275:PHE:CE1	2.51	0.45
1:B:562:VAL:CG1	1:B:563:VAL:N	2.79	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1100:CYS:SG	1:A:1160:GLN:HG3	2.56	0.45
1:A:1097:LYS:HE2	1:A:1101:GLU:CG	2.45	0.45
1:B:1558:GLU:HG2	1:B:1583:ILE:HD12	1.98	0.45
1:B:1551:LYS:NZ	1:B:1581:LYS:HE2	2.30	0.45
1:A:80:ASN:ND2	1:A:82:TYR:N	2.64	0.45
1:A:852:ASN:ND2	1:A:859:LEU:HD23	2.31	0.45
1:A:382:PRO:HB3	1:A:403:GLY:CA	2.40	0.45
1:B:1401:ILE:HD12	1:B:1480:TYR:CD1	2.44	0.45
1:A:843:GLN:O	1:A:1467:VAL:HG13	2.17	0.45
1:B:181:SER:HB3	1:B:188:LEU:HD21	1.97	0.45
1:A:1530:ARG:HH12	1:A:1647:LEU:HD21	1.81	0.45
1:A:578:GLN:HG2	1:A:579:ILE:N	2.30	0.45
1:B:156:LEU:HA	1:B:157:PRO:HD2	1.71	0.45
1:B:32:ASN:CB	1:B:641:GLY:HA2	2.46	0.45
1:A:374:TYR:HA	1:A:404:VAL:HG13	1.99	0.45
1:B:1600:TYR:CE2	1:B:1628:LEU:HG	2.52	0.45
1:B:1405:SER:HA	1:B:1441:THR:HA	1.98	0.45
1:A:527:PHE:CE1	1:A:551:VAL:HB	2.52	0.45
1:A:1140:VAL:HG21	1:A:1182:LEU:HD21	1.98	0.45
1:B:534:THR:HG22	1:B:542:ARG:HG2	1.98	0.45
1:A:205:ILE:HG22	1:A:206:LYS:H	1.82	0.45
1:B:1258:GLN:HE21	1:B:1258:GLN:HB3	1.49	0.45
1:B:464:LYS:NZ	1:B:554:LYS:HE2	2.32	0.45
1:A:701:MET:HE2	1:A:1458:SER:HB3	1.98	0.45
1:A:116:VAL:CG1	1:A:645:LYS:HB3	2.46	0.45
1:A:375:VAL:HB	1:A:398:LEU:HD22	1.99	0.45
1:B:57:VAL:CG2	1:B:86:VAL:HG21	2.45	0.45
1:A:507:GLU:HB3	1:A:510:GLN:HE21	1.80	0.45
1:B:492:ILE:HG21	1:B:499:LEU:HD23	1.98	0.45
1:B:600:VAL:CG2	1:B:765:PHE:CG	2.99	0.45
1:A:562:VAL:CG1	1:A:563:VAL:N	2.79	0.45
1:B:1558:GLU:HG2	1:B:1583:ILE:CD1	2.47	0.45
1:A:1254:TRP:CZ2	1:A:1258:GLN:HG3	2.51	0.45
1:A:1382:SER:CB	1:A:1462:HIS:ND1	2.79	0.45
1:A:582:LYS:HD2	1:A:789:LEU:HD21	1.99	0.45
1:B:117:GLU:O	1:B:645:LYS:CE	2.65	0.45
1:A:244:ILE:CD1	1:A:349:THR:CG2	2.95	0.45
1:A:314:ARG:HE	1:A:315:ALA:H	1.64	0.45
1:B:754:ILE:HG23	1:B:755:PRO:HD2	1.97	0.45
1:A:384:ARG:O	1:A:398:LEU:HD23	2.17	0.45
1:B:1501:SER:O	1:B:1503:LEU:N	2.50	0.45
1:B:330:ILE:HD11	1:B:750:ASP:CG	2.35	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:863:VAL:HG12	1:A:913:ALA:CB	2.47	0.45
1:B:1288:HIS:O	1:B:1312:TRP:HB2	2.17	0.45
1:B:1544:LYS:HB3	1:B:1565:ASN:HB3	1.98	0.45
1:A:1012:GLN:HG2	1:A:1480:TYR:CE2	2.52	0.45
1:B:1298:GLN:HG2	1:B:1305:ALA:CB	2.46	0.45
1:A:1608:ASP:HB2	1:A:1619:ILE:O	2.16	0.45
1:B:1375:LYS:HD3	1:B:1375:LYS:O	2.17	0.45
1:A:244:ILE:CD1	1:A:349:THR:HG21	2.46	0.45
1:A:904:ILE:HD13	1:A:932:PRO:HB3	1.99	0.45
1:A:611:GLN:O	1:A:614:ILE:HG12	2.17	0.45
1:B:360:PRO:HB3	1:B:628:GLY:HA2	1.98	0.45
1:A:718:CYS:SG	1:A:1424:VAL:HG11	2.56	0.45
1:A:600:VAL:HG22	1:A:765:PHE:CB	2.47	0.45
1:B:480:GLY:O	1:B:482:GLN:N	2.49	0.45
1:A:154:LYS:HB2	1:A:156:LEU:HG	1.99	0.45
1:A:931:VAL:CG1	1:A:1438:ASN:HB3	2.47	0.45
1:B:458:VAL:CG1	1:B:469:LEU:HD21	2.46	0.45
1:B:840:ARG:CZ	1:B:972:ASP:HB3	2.46	0.45
1:A:487:TYR:HB3	1:A:505:TYR:CD1	2.52	0.45
1:A:1570:GLY:O	1:A:1571:SER:C	2.56	0.45
1:B:1134:ASP:C	1:B:1136:ARG:H	2.19	0.45
1:B:933:GLU:CD	1:B:933:GLU:H	2.20	0.45
1:A:566:GLY:HA3	1:A:580:THR:CG2	2.47	0.45
1:B:852:ASN:CB	1:B:859:LEU:HD23	2.46	0.45
1:A:368:PRO:CA	1:A:410:ASN:HA	2.40	0.45
1:B:712:ILE:HG23	1:B:1424:VAL:CG1	2.47	0.45
1:B:356:PHE:HE1	1:B:437:ARG:HG3	1.82	0.45
1:A:1531:LEU:HG	1:A:1650:PHE:CZ	2.52	0.45
1:B:242:TYR:CE1	1:B:246:ASP:HB2	2.51	0.45
1:B:173:PRO:HG3	1:B:176:ARG:NH2	2.32	0.45
1:B:1190:ILE:HD13	1:B:1190:ILE:O	2.17	0.45
1:A:633:TYR:N	1:A:633:TYR:HD1	2.15	0.44
1:B:573:HIS:ND1	1:B:579:ILE:CD1	2.73	0.44
1:B:834:LEU:HD22	1:B:846:ILE:HG21	1.97	0.44
1:A:887:ILE:CD1	1:A:887:ILE:N	2.79	0.44
1:A:386:ILE:O	1:A:398:LEU:N	2.50	0.44
1:B:919:PHE:O	1:B:920:ILE:HD13	2.17	0.44
1:A:910:GLU:CB	1:A:925:LYS:HB3	2.47	0.44
1:A:134:ASP:OD2	1:A:145:LEU:HD12	2.17	0.44
1:B:1064:ALA:HB1	1:B:1073:PRO:HB3	1.99	0.44
1:A:1585:HIS:HD2	1:A:1587:LYS:H	1.65	0.44
1:B:1092:ILE:HG22	1:B:1093:ALA:N	2.32	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:74:THR:OG1	1:A:75:GLN:N	2.50	0.44
1:B:1415:GLU:O	1:B:1419:THR:HG23	2.17	0.44
1:A:673:LEU:HD13	1:A:674:MET:HG3	1.98	0.44
1:A:1508:THR:O	1:A:1511:CYS:HB3	2.18	0.44
1:A:147:ARG:NE	1:A:189:THR:HG22	2.29	0.44
1:A:769:TRP:CD1	1:A:769:TRP:N	2.85	0.44
1:B:156:LEU:CD2	1:B:811:LYS:HA	2.47	0.44
1:A:904:ILE:CG2	1:A:905:GLY:N	2.66	0.44
1:B:1498:GLY:C	1:B:1500:LEU:N	2.69	0.44
1:A:134:ASP:OD1	1:A:135:LYS:HG2	2.17	0.44
1:A:561:LEU:CD1	1:A:807:SER:HB3	2.47	0.44
1:A:1256:ASN:ND2	1:A:1259:ARG:HH12	2.16	0.44
1:B:1362:LEU:CD1	1:B:1489:ARG:HB2	2.48	0.44
1:A:1600:TYR:CD2	1:A:1628:LEU:HA	2.52	0.44
1:B:1488:ILE:O	1:B:1488:ILE:HG23	2.17	0.44
1:B:1554:ASP:O	1:B:1586:ILE:HD11	2.18	0.44
1:B:386:ILE:HB	1:B:398:LEU:HD23	1.99	0.44
1:A:355:HIS:HB3	1:A:437:ARG:CZ	2.47	0.44
1:A:366:ALA:HB2	1:A:413:ASN:ND2	2.32	0.44
1:B:520:THR:CG2	1:B:521:SER:H	2.22	0.44
1:B:829:PHE:HB2	1:B:851:TYR:HD2	1.83	0.44
1:B:1646:ASP:HA	1:B:1649:ASN:ND2	2.32	0.44
1:B:146:TYR:CD1	1:B:205:ILE:HD13	2.52	0.44
1:B:861:VAL:HG12	1:B:862:ARG:N	2.33	0.44
1:A:597:ASP:OD2	1:A:599:GLY:N	2.50	0.44
1:B:1019:PRO:HD3	1:B:1272:PHE:CE1	2.52	0.44
1:A:1103:VAL:O	1:A:1107:ILE:HG12	2.17	0.44
1:B:430:PRO:O	1:B:432:GLY:N	2.49	0.44
1:A:63:PRO:HG2	1:A:64:ALA:H	1.82	0.44
1:A:645:LYS:O	1:A:646:THR:CB	2.63	0.44
1:A:269:PHE:O	1:A:327:ALA:HB1	2.17	0.44
1:B:451:ASN:HB2	1:B:478:ASP:OD1	2.17	0.44
1:A:1010:GLY:CA	1:A:1067:ALA:HA	2.46	0.44
1:B:283:LEU:O	1:B:286:SER:HB2	2.18	0.44
1:B:334:GLY:O	1:B:335:SER:CB	2.66	0.44
1:B:227:VAL:HG11	1:B:761:SER:O	2.18	0.44
1:B:97:LYS:HA	1:B:103:LYS:HZ2	1.82	0.44
1:B:387:PRO:HG3	1:B:425:LYS:O	2.17	0.44
1:B:1289:LYS:H	1:B:1289:LYS:CD	2.30	0.44
1:A:765:PHE:O	1:A:766:PRO:C	2.54	0.44
1:A:561:LEU:CD1	1:A:807:SER:HB2	2.47	0.44
1:B:610:THR:HG22	1:B:613:LYS:CD	2.46	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:438:THR:HG22	1:A:439:MET:N	2.32	0.44
1:B:526:SER:HA	1:B:552:ASP:HA	2.00	0.44
1:A:62:PHE:CE2	1:A:103:LYS:HD3	2.52	0.44
1:B:398:LEU:HD11	1:B:403:GLY:C	2.36	0.44
1:A:362:PHE:CZ	1:A:631:ARG:HD2	2.52	0.44
1:B:492:ILE:HD13	1:B:492:ILE:HA	1.89	0.44
1:A:482:GLN:O	1:A:484:LYS:N	2.51	0.44
1:B:281:ILE:O	1:B:283:LEU:N	2.51	0.44
1:A:781:ASP:HB3	1:A:785:ILE:O	2.18	0.44
1:B:1434:ASN:HB3	1:B:1441:THR:OG1	2.18	0.44
1:A:1041:ARG:NH1	1:A:1045:LEU:HD11	2.33	0.44
1:B:346:PRO:HG3	1:B:378:PRO:HB2	2.00	0.44
1:B:359:THR:HG23	1:B:372:MET:H	1.83	0.44
1:A:106:THR:HG22	1:A:119:VAL:CG2	2.44	0.44
1:B:1585:HIS:HD2	1:B:1587:LYS:H	1.66	0.44
1:B:446:THR:HG21	1:B:450:SER:C	2.38	0.44
1:B:848:ALA:O	1:B:895:VAL:HG22	2.18	0.44
1:B:830:ILE:O	1:B:830:ILE:HG23	2.17	0.44
1:A:1549:GLN:CB	1:A:1560:ILE:HD12	2.48	0.44
1:A:1510:ARG:HA	1:A:1513:GLU:HG3	2.00	0.44
1:B:870:ALA:HB1	1:B:907:HIS:CD2	2.52	0.44
1:A:370:ASP:HB3	1:A:460:ARG:HE	1.83	0.44
1:A:1105:TRP:CD1	1:A:1109:GLU:HG3	2.53	0.44
1:A:754:ILE:N	1:A:755:PRO:CD	2.81	0.44
1:B:461:VAL:O	1:B:462:GLU:C	2.56	0.44
1:A:1545:THR:HG23	1:A:1563:ILE:HG23	1.98	0.44
1:B:859:LEU:CD2	1:B:859:LEU:N	2.80	0.44
1:A:491:MET:N	1:A:491:MET:SD	2.90	0.44
1:A:753:ILE:HG23	1:A:753:ILE:O	2.18	0.44
1:A:31:PRO:HG2	1:A:34:LEU:HD21	2.00	0.44
1:A:695:GLY:HA2	1:A:722:PHE:CE2	2.53	0.44
1:B:354:ILE:HD11	1:B:437:ARG:HB3	1.99	0.44
1:B:794:LEU:HD13	1:B:824:VAL:CG2	2.47	0.44
1:A:943:VAL:O	1:A:944:ARG:HD3	2.18	0.44
1:A:1453:VAL:HG23	1:A:1454:GLU:N	2.31	0.44
1:B:214:GLN:O	1:B:215:GLN:C	2.57	0.44
1:A:1286:PRO:HB2	1:A:1289:LYS:HZ3	1.82	0.43
1:B:1566:ILE:CG2	1:B:1568:LYS:O	2.66	0.43
1:B:1003:ILE:HG12	1:B:1015:ILE:HD12	1.99	0.43
1:A:47:HIS:HD2	1:A:534:THR:OG1	2.01	0.43
1:A:1461:VAL:O	1:A:1461:VAL:HG23	2.18	0.43
1:A:577:GLN:O	1:A:794:LEU:CB	2.66	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:577:GLN:HG2	1:A:578:GLN:N	2.32	0.43
1:B:62:PHE:HE2	1:B:103:LYS:HG2	1.83	0.43
1:B:561:LEU:CD1	1:B:815:CYS:HB3	2.48	0.43
1:A:270:VAL:O	1:A:287:LEU:CA	2.65	0.43
1:B:271:ILE:HD12	1:B:755:PRO:HG3	1.99	0.43
1:A:1003:ILE:HG23	1:A:1005:THR:H	1.83	0.43
1:A:1500:LEU:C	1:A:1500:LEU:HD12	2.38	0.43
1:B:1494:ASP:C	1:B:1496:GLU:N	2.71	0.43
1:B:1136:ARG:C	1:B:1138:LYS:H	2.22	0.43
1:B:326:SER:HB2	1:B:340:ALA:O	2.18	0.43
1:A:370:ASP:CB	1:A:460:ARG:HE	2.32	0.43
1:B:415:ARG:O	1:B:443:PRO:HG3	2.18	0.43
1:B:263:GLN:HE21	1:B:295:GLY:HA3	1.83	0.43
1:A:318:LEU:CD1	1:A:321:LYS:HZ2	2.31	0.43
1:B:377:ASN:HB3	1:B:378:PRO:HD2	2.00	0.43
1:A:270:VAL:HG13	1:A:327:ALA:HB2	1.99	0.43
1:B:450:SER:OG	1:B:451:ASN:N	2.50	0.43
1:A:364:LYS:HA	1:A:365:PRO:HD2	1.68	0.43
1:B:1609:LEU:HG	1:B:1616:ILE:CG2	2.48	0.43
1:B:145:LEU:HA	1:B:145:LEU:HD23	1.84	0.43
1:A:762:ARG:HG3	1:A:765:PHE:CZ	2.54	0.43
1:B:354:ILE:HD12	1:B:354:ILE:C	2.39	0.43
1:A:1213:ALA:HB2	1:A:1219:TRP:CZ2	2.53	0.43
1:B:1128:MET:HE3	1:B:1142:LEU:HA	2.00	0.43
1:B:306:LEU:HA	1:B:306:LEU:HD23	1.67	0.43
1:A:137:ILE:HG23	1:A:224:LYS:HG3	1.99	0.43
1:B:1184:ARG:HG2	1:B:1184:ARG:HH11	1.83	0.43
1:A:35:ARG:NH1	1:A:153:HIS:HB3	2.33	0.43
1:B:169:PRO:HD3	1:B:203:TRP:CE2	2.53	0.43
1:A:130:PHE:HE1	1:A:617:VAL:HG21	1.84	0.43
1:B:1568:LYS:HG3	1:B:1569:SER:H	1.82	0.43
1:A:96:LEU:O	1:A:97:LYS:C	2.56	0.43
1:A:379:ASP:N	1:A:379:ASP:OD1	2.52	0.43
1:A:31:PRO:HA	1:A:641:GLY:O	2.18	0.43
1:B:264:VAL:HG12	1:B:265:ASP:N	2.32	0.43
1:A:148:VAL:O	1:A:188:LEU:HB2	2.18	0.43
1:A:1470:ILE:HG21	1:A:1499:MET:CG	2.46	0.43
1:A:396:GLN:HG3	1:A:397:SER:N	2.32	0.43
1:B:533:TYR:CE2	1:B:545:VAL:HB	2.53	0.43
1:A:420:ILE:HD12	1:A:420:ILE:O	2.18	0.43
1:A:421:THR:CG2	1:A:438:THR:HG23	2.49	0.43
1:B:258:PHE:C	1:B:260:TYR:H	2.21	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1193:TYR:CE1	1:B:1237:LEU:HB3	2.52	0.43
1:B:1319:ARG:HG2	1:B:1319:ARG:HH11	1.82	0.43
1:A:102:HIS:ND1	1:A:102:HIS:N	2.67	0.43
1:A:968:ASP:OD2	1:A:1349:ALA:HB1	2.18	0.43
1:B:524:ILE:HG21	1:B:558:MET:HG2	1.99	0.43
1:A:359:THR:HG23	1:A:371:LEU:CA	2.44	0.43
1:A:574:ARG:O	1:A:577:GLN:HB3	2.18	0.43
1:B:561:LEU:HA	1:B:584:GLU:O	2.19	0.43
1:A:407:LEU:CD2	1:A:408:SER:H	2.20	0.43
1:A:270:VAL:HG21	1:A:299:ALA:CB	2.47	0.43
1:B:537:ASN:ND2	1:B:538:ALA:N	2.60	0.43
1:A:832:LEU:HD21	1:A:909:VAL:CG1	2.49	0.43
1:A:481:GLU:O	1:A:482:GLN:C	2.57	0.43
1:A:100:LYS:HD3	1:A:100:LYS:N	2.34	0.43
1:B:1405:SER:HB3	1:B:1441:THR:HG22	1.98	0.43
1:B:657:ASP:HB3	1:B:659:GLN:O	2.18	0.43
1:B:989:MET:O	1:B:993:ALA:HB2	2.19	0.43
1:B:1633:GLU:HG3	1:B:1634:GLU:HG3	2.01	0.43
1:B:420:ILE:O	1:B:420:ILE:HD12	2.19	0.43
1:A:244:ILE:HD12	1:A:349:THR:HG21	2.00	0.43
1:A:1493:PRO:HB2	1:A:1494:ASP:H	1.61	0.43
1:B:701:MET:HG2	1:B:701:MET:H	1.44	0.43
1:B:642:LEU:C	1:B:643:THR:CG2	2.87	0.43
1:B:532:TYR:HA	1:B:545:VAL:O	2.18	0.43
1:A:487:TYR:CD1	1:A:503:ARG:HD2	2.54	0.43
1:A:1259:ARG:HH11	1:A:1340:THR:HG21	1.82	0.43
1:B:365:PRO:HG2	1:B:453:TYR:HE1	1.84	0.43
1:B:326:SER:HB3	1:B:341:GLU:CB	2.49	0.43
1:A:870:ALA:HB1	1:A:907:HIS:CD2	2.54	0.43
1:B:465:PRO:O	1:B:519:ILE:O	2.37	0.43
1:B:362:PHE:CE2	1:B:631:ARG:NE	2.86	0.43
1:B:1542:VAL:HG22	1:B:1603:TRP:HB2	2.01	0.43
1:B:1563:ILE:H	1:B:1563:ILE:CD1	2.20	0.43
1:A:346:PRO:CG	1:A:348:VAL:HG23	2.49	0.43
1:A:364:LYS:HB2	1:A:364:LYS:HE3	1.83	0.43
1:B:850:LEU:CD1	1:B:885:ILE:HD11	2.48	0.43
1:B:415:ARG:HB3	1:B:443:PRO:HG3	2.01	0.43
1:A:1186:TYR:C	1:A:1186:TYR:CD2	2.92	0.43
1:B:447:GLN:HG3	1:B:447:GLN:O	2.19	0.43
1:A:653:GLN:HB3	1:A:655:ARG:CG	2.48	0.43
1:B:574:ARG:O	1:B:577:GLN:CB	2.67	0.43
1:B:1605:VAL:HB	1:B:1608:ASP:OD1	2.19	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1470:ILE:CG2	1:A:1499:MET:HG3	2.49	0.43
1:B:172:ILE:HD11	1:B:1098:ASP:OD1	2.19	0.43
1:A:1344:VAL:HG12	1:A:1345:THR:N	2.34	0.43
1:A:729:ILE:HD12	1:A:730:THR:N	2.33	0.43
1:B:1405:SER:HA	1:B:1441:THR:HG22	2.00	0.43
1:A:274:VAL:HG11	1:A:321:LYS:HZ3	1.84	0.43
1:B:630:GLY:CA	1:B:636:VAL:HG22	2.49	0.43
1:A:458:VAL:HG11	1:A:469:LEU:HD21	2.01	0.43
1:B:1545:THR:CB	1:B:1561:MET:HG2	2.48	0.43
1:B:701:MET:CE	1:B:1458:SER:H	2.32	0.43
1:B:977:THR:HB	1:B:1345:THR:HG22	2.01	0.43
1:B:458:VAL:HG23	1:B:471:VAL:HG13	2.01	0.43
1:B:197:LEU:HD21	1:B:1058:PHE:CZ	2.54	0.43
1:B:533:TYR:CZ	1:B:545:VAL:HB	2.53	0.43
1:B:785:ILE:HG22	1:B:787:THR:CG2	2.49	0.43
1:B:1190:ILE:CG2	1:B:1191:ALA:N	2.82	0.43
1:A:274:VAL:HG11	1:A:321:LYS:NZ	2.34	0.43
1:B:251:LYS:HG3	1:B:300:ILE:HG23	1.99	0.43
1:B:852:ASN:HB3	1:B:887:ILE:HG21	2.01	0.43
1:A:559:GLY:N	1:A:812:LYS:NZ	2.66	0.43
1:B:1233:SER:OG	1:B:1274:VAL:HA	2.19	0.43
1:A:59:VAL:HG23	1:A:70:SER:OG	2.18	0.43
1:A:998:ARG:NH1	1:A:998:ARG:HG3	2.34	0.43
1:B:1410:PHE:CE1	1:B:1463:GLN:HB2	2.54	0.43
1:B:460:ARG:HH21	1:B:462:GLU:CB	2.32	0.42
1:A:644:LEU:N	1:A:650:LEU:HD21	2.34	0.42
1:B:345:ILE:O	1:B:345:ILE:HG22	2.19	0.42
1:A:674:MET:O	1:A:678:MET:HG3	2.19	0.42
1:A:377:ASN:O	1:A:379:ASP:N	2.52	0.42
1:A:413:ASN:O	1:A:414:LYS:HG2	2.19	0.42
1:B:612:ARG:HH11	1:B:612:ARG:HG2	1.84	0.42
1:A:59:VAL:HB	1:A:69:LEU:HB2	2.00	0.42
1:A:1554:ASP:HA	1:A:1586:ILE:HD11	2.01	0.42
1:A:1012:GLN:HG3	1:A:1012:GLN:H	1.49	0.42
1:A:172:ILE:HG21	1:A:1056:LEU:HD21	2.00	0.42
1:B:1275:PHE:CD2	1:B:1275:PHE:C	2.92	0.42
1:A:352:TYR:HE2	1:A:429:ILE:HD13	1.82	0.42
1:A:1042:GLN:HA	1:A:1045:LEU:HD12	2.00	0.42
1:A:1026:TYR:CE1	1:A:1030:THR:HG21	2.54	0.42
1:A:1351:LEU:HD13	1:A:1490:PHE:CD2	2.54	0.42
1:A:53:ILE:HB	1:A:76:LEU:HB2	2.01	0.42
1:A:62:PHE:CG	1:A:63:PRO:HD3	2.54	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:398:LEU:HG	1:B:399:THR:O	2.19	0.42
1:A:558:MET:CB	1:A:812:LYS:NZ	2.82	0.42
1:B:712:ILE:HD11	1:B:722:PHE:CG	2.53	0.42
1:A:137:ILE:HA	1:A:222:GLU:O	2.19	0.42
1:A:429:ILE:HG22	1:A:433:ARG:HD2	2.01	0.42
1:A:944:ARG:NH1	1:A:944:ARG:HG3	2.33	0.42
1:B:910:GLU:HG3	1:B:925:LYS:HB3	2.00	0.42
1:A:570:GLU:HG2	1:A:571:LYS:H	1.82	0.42
1:B:323:ILE:CG2	1:B:324:TYR:N	2.80	0.42
1:A:391:GLN:OE1	1:A:420:ILE:HA	2.18	0.42
1:A:44:LEU:O	1:A:45:GLU:HG3	2.19	0.42
1:B:243:TYR:HH	1:B:245:ASP:HB2	1.78	0.42
1:A:574:ARG:NH1	1:A:918:HIS:CE1	2.87	0.42
1:B:359:THR:O	1:B:627:PRO:HG2	2.19	0.42
1:A:812:LYS:C	1:A:812:LYS:HD3	2.38	0.42
1:A:1362:LEU:CD1	1:A:1489:ARG:HB2	2.50	0.42
1:A:303:ARG:O	1:A:307:LEU:HG	2.18	0.42
1:A:1541:TYR:O	1:A:1603:TRP:HA	2.19	0.42
1:A:1184:ARG:O	1:A:1188:VAL:HG23	2.19	0.42
1:B:166:ILE:HD12	1:B:175:LYS:HD3	2.02	0.42
1:A:990:THR:HG21	1:A:1026:TYR:CD2	2.54	0.42
1:A:778:LYS:C	1:A:780:ALA:H	2.22	0.42
1:B:1396:ASP:HA	1:B:1451:HIS:HB3	2.00	0.42
1:A:55:VAL:CG2	1:A:76:LEU:HG	2.49	0.42
1:A:530:VAL:HG12	1:A:548:SER:HB2	2.01	0.42
1:A:637:PHE:CE1	1:A:644:LEU:CD1	3.00	0.42
1:A:615:TRP:CE3	1:A:615:TRP:HA	2.54	0.42
1:A:673:LEU:CD1	1:A:674:MET:HG3	2.49	0.42
1:A:854:ARG:NH1	1:A:859:LEU:HD11	2.33	0.42
1:A:354:ILE:CG2	1:A:375:VAL:HG22	2.48	0.42
1:B:134:ASP:HB3	1:B:138:TYR:OH	2.19	0.42
1:B:830:ILE:HD11	1:B:911:VAL:HG12	2.02	0.42
1:B:514:VAL:CG1	1:B:515:LEU:N	2.83	0.42
1:B:355:HIS:N	1:B:355:HIS:ND1	2.66	0.42
1:B:149:PHE:CD1	1:B:187:ILE:HG12	2.50	0.42
1:A:163:PHE:HD2	1:A:208:TYR:CE2	2.37	0.42
1:A:358:LYS:HB2	1:A:372:MET:HE2	2.00	0.42
1:A:143:THR:HB	1:A:193:ASN:ND2	2.34	0.42
1:A:881:HIS:ND1	1:A:881:HIS:O	2.52	0.42
1:A:556:SER:OG	1:A:557:CYS:N	2.51	0.42
1:B:271:ILE:CD1	1:B:755:PRO:HG3	2.50	0.42
1:B:528:ARG:HH12	1:B:623:ILE:HG12	1.85	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:244:ILE:HD11	1:A:319:VAL:CG2	2.26	0.42
1:A:918:HIS:ND1	1:A:918:HIS:O	2.53	0.42
1:B:846:ILE:CD1	1:B:899:ILE:HD12	2.40	0.42
1:B:148:VAL:CG1	1:B:188:LEU:HD12	2.50	0.42
1:A:1116:ILE:HG23	1:A:1139:ASP:HB3	2.01	0.42
1:B:1505:HIS:ND1	1:B:1506:LYS:N	2.57	0.42
1:B:1499:MET:C	1:B:1501:SER:H	2.18	0.42
1:A:876:THR:CG2	1:A:877:ALA:H	2.32	0.42
1:B:504:GLN:HG3	1:B:515:LEU:HD13	2.02	0.42
1:A:1499:MET:C	1:A:1501:SER:H	2.23	0.42
1:A:1265:TYR:CD2	1:A:1274:VAL:HG11	2.55	0.42
1:B:53:ILE:HG22	1:B:111:PHE:HB2	2.01	0.42
1:A:1314:SER:HB2	1:A:1319:ARG:HH22	1.85	0.42
1:B:1650:PHE:O	1:B:1654:MET:HB2	2.20	0.42
1:A:1600:TYR:HE2	1:A:1628:LEU:HG	1.84	0.42
1:B:680:LYS:HD2	1:B:683:GLN:NE2	2.35	0.42
1:A:175:LYS:HD2	1:A:192:TRP:CD1	2.54	0.42
1:A:310:VAL:HG12	1:A:311:GLN:N	2.35	0.42
1:A:578:GLN:OE1	1:A:791:ASN:HB3	2.20	0.42
1:B:888:PRO:CB	1:B:891:SER:HB2	2.43	0.42
1:A:1435:ARG:HG3	1:A:1435:ARG:H	1.36	0.42
1:B:269:PHE:CE1	1:B:289:ARG:CD	3.02	0.42
1:B:287:LEU:HD12	1:B:674:MET:HE2	2.02	0.42
1:A:124:LEU:H	1:A:124:LEU:HD23	1.84	0.42
1:B:1469:LEU:N	1:B:1499:MET:O	2.51	0.42
1:B:1590:GLU:C	1:B:1592:LEU:H	2.23	0.42
1:B:931:VAL:CG1	1:B:932:PRO:HD2	2.49	0.42
1:B:612:ARG:NH1	1:B:616:ASP:OD2	2.53	0.42
1:A:1503:LEU:HD12	1:A:1503:LEU:HA	1.75	0.42
1:B:707:ARG:HD2	1:B:707:ARG:HA	1.93	0.42
1:B:363:PHE:CD1	1:B:364:LYS:N	2.88	0.42
1:B:611:GLN:HG2	1:B:816:VAL:CB	2.46	0.42
1:B:74:THR:HG23	1:B:84:SER:HB2	2.01	0.42
1:A:1204:ASP:HA	1:A:1207:THR:HG22	2.02	0.42
1:B:197:LEU:O	1:B:198:VAL:HB	2.19	0.42
1:B:445:ASN:H	1:B:632:ASN:ND2	2.17	0.42
1:A:215:GLN:O	1:A:215:GLN:HG2	2.20	0.42
1:A:1539:VAL:HG12	1:A:1540:ASP:H	1.85	0.42
1:A:699:ASN:O	1:A:702:LYS:HE2	2.20	0.42
1:A:468:THR:CG2	1:A:518:THR:HG22	2.50	0.42
1:A:570:GLU:C	1:A:572:HIS:H	2.23	0.42
1:A:1527:LEU:HG	1:A:1646:ASP:CB	2.50	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:981:LEU:HD13	1:A:1295:VAL:HG11	2.01	0.42
1:B:1214:LYS:HD3	1:B:1214:LYS:HA	1.94	0.42
1:A:290:VAL:CG2	1:A:298:GLU:O	2.68	0.41
1:A:36:LEU:HD12	1:A:124:LEU:CB	2.40	0.41
1:B:1607:SER:C	1:B:1609:LEU:H	2.22	0.41
1:A:765:PHE:N	1:A:765:PHE:CD1	2.88	0.41
1:A:1265:TYR:CE2	1:A:1274:VAL:HG21	2.55	0.41
1:A:236:GLU:OE2	1:A:342:ARG:HD3	2.20	0.41
1:A:229:PRO:O	1:A:259:LEU:CD1	2.68	0.41
1:B:413:ASN:O	1:B:414:LYS:HG3	2.20	0.41
1:B:1107:ILE:HD12	1:B:1167:SER:CB	2.49	0.41
1:A:283:LEU:O	1:A:286:SER:HB2	2.20	0.41
1:B:629:SER:O	1:B:636:VAL:HG22	2.19	0.41
1:B:852:ASN:CG	1:B:887:ILE:HG21	2.40	0.41
1:A:270:VAL:O	1:A:287:LEU:CB	2.68	0.41
1:B:998:ARG:HA	1:B:998:ARG:NE	2.35	0.41
1:A:895:VAL:O	1:A:895:VAL:CG2	2.67	0.41
1:A:1466:ASN:O	1:A:1503:LEU:CD2	2.68	0.41
1:A:489:THR:HG22	1:A:503:ARG:CD	2.50	0.41
1:A:1599:HIS:O	1:A:1629:TRP:HB3	2.19	0.41
1:A:1138:LYS:O	1:A:1139:ASP:HB2	2.20	0.41
1:A:351:PRO:HG2	1:A:352:TYR:CD2	2.55	0.41
1:B:1061:LYS:HE2	1:B:1061:LYS:H	1.84	0.41
1:B:169:PRO:HD3	1:B:203:TRP:NE1	2.35	0.41
1:A:536:ILE:HG22	1:A:542:ARG:HA	2.03	0.41
1:B:104:PHE:HB3	1:B:119:VAL:HG12	2.02	0.41
1:B:60:HIS:CG	1:B:65:LYS:HD3	2.55	0.41
1:B:1112:LYS:HB3	1:B:1113:PRO:CD	2.42	0.41
1:A:386:ILE:N	1:A:398:LEU:HB3	2.31	0.41
1:B:986:VAL:HB	1:B:1282:GLN:HE22	1.85	0.41
1:A:729:ILE:HA	1:A:732:LEU:HB3	2.02	0.41
1:A:1629:TRP:CE3	1:A:1647:LEU:HD13	2.55	0.41
1:B:769:TRP:HB3	1:B:795:LYS:HE3	2.03	0.41
1:B:1060:GLN:OE1	1:B:1073:PRO:HG3	2.20	0.41
1:A:465:PRO:HA	1:A:519:ILE:HG22	2.02	0.41
1:A:708:ARG:HD2	1:A:1427:TYR:OH	2.20	0.41
1:A:940:THR:HG22	1:A:1262:GLY:H	1.85	0.41
1:A:1225:LYS:HG3	1:A:1484:ASP:CG	2.41	0.41
1:B:154:LYS:HB2	1:B:156:LEU:HG	2.01	0.41
1:B:1563:ILE:CD1	1:B:1578:GLN:H	2.33	0.41
1:A:398:LEU:HD11	1:A:403:GLY:O	2.21	0.41
1:A:850:LEU:HD11	1:A:863:VAL:HG11	2.01	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:311:GLN:HA	1:B:312:PRO:HD3	1.56	0.41
1:A:872:CYS:HB2	1:A:900:VAL:HB	2.02	0.41
1:A:233:VAL:HG12	1:A:340:ALA:HB2	2.02	0.41
1:B:634:ALA:O	1:B:638:THR:HG23	2.19	0.41
1:B:1436:ASP:HB2	2:B:2002:NAG:O6	2.20	0.41
1:A:390:THR:CG2	1:A:422:VAL:HG13	2.50	0.41
1:A:457:SER:OG	1:A:472:ASN:HB2	2.20	0.41
1:A:1585:HIS:CD2	1:A:1587:LYS:H	2.38	0.41
1:A:1068:PHE:CD1	1:A:1429:SER:HB3	2.56	0.41
1:B:559:GLY:CA	1:B:812:LYS:HD2	2.50	0.41
1:B:319:VAL:HG11	1:B:349:THR:HG23	2.01	0.41
1:B:106:THR:HA	1:B:119:VAL:HA	2.02	0.41
1:B:457:SER:O	1:B:458:VAL:HG23	2.20	0.41
1:B:270:VAL:HG22	1:B:327:ALA:HB2	2.01	0.41
1:A:754:ILE:O	1:A:754:ILE:HG22	2.20	0.41
1:B:140:PRO:HD3	1:B:224:LYS:O	2.20	0.41
1:A:274:VAL:HG11	1:A:321:LYS:HE2	2.03	0.41
1:A:274:VAL:HG23	1:A:283:LEU:CD1	2.45	0.41
1:A:272:PHE:CA	1:A:325:VAL:HG22	2.43	0.41
1:B:32:ASN:HD22	1:B:32:ASN:HA	1.55	0.41
1:A:409:ILE:HD12	1:A:409:ILE:C	2.41	0.41
1:A:128:TYR:HB2	1:A:151:VAL:HG12	2.03	0.41
1:A:1226:LEU:HD12	1:A:1482:ASN:HA	2.03	0.41
1:B:1481:TYR:O	1:B:1482:ASN:HB2	2.21	0.41
1:A:143:THR:HA	1:A:193:ASN:HA	2.03	0.41
1:A:1374:LYS:HG2	1:A:1374:LYS:H	1.56	0.41
1:A:473:PHE:HE2	1:A:515:LEU:HB3	1.86	0.41
1:A:313:SER:O	1:A:314:ARG:HB2	2.21	0.41
1:A:318:LEU:CD2	1:A:321:LYS:HZ2	2.34	0.41
1:A:615:TRP:O	1:A:616:ASP:C	2.58	0.41
1:B:712:ILE:HG23	1:B:1424:VAL:HG12	2.03	0.41
1:A:365:PRO:HB3	1:A:414:LYS:O	2.20	0.41
1:B:171:GLY:O	1:B:172:ILE:CB	2.68	0.41
1:B:131:ILE:CG1	1:B:148:VAL:HG23	2.50	0.41
1:A:163:PHE:O	1:A:207:ALA:HA	2.21	0.41
1:B:1474:ALA:HB2	1:B:1490:PHE:CD1	2.56	0.41
1:B:173:PRO:HD2	1:B:1095:ASP:OD2	2.21	0.41
1:A:1028:ASP:OD1	1:A:1033:TRP:CZ3	2.73	0.41
1:B:525:PRO:HB3	1:B:615:TRP:CE3	2.55	0.41
1:B:646:THR:OG1	1:B:650:LEU:HB2	2.20	0.41
1:B:673:LEU:HG	1:B:674:MET:H	1.82	0.41
1:B:714:GLN:HB2	1:B:718:CYS:SG	2.60	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:537:ASN:HB3	1:B:541:GLN:H	1.86	0.41
1:A:866:LEU:HD21	1:A:912:LYS:NZ	2.35	0.41
1:B:281:ILE:HG21	1:B:310:VAL:HG21	2.02	0.41
1:A:726:CYS:O	1:A:729:ILE:HD12	2.20	0.41
1:B:769:TRP:O	1:B:770:LEU:HB3	2.20	0.41
1:A:205:ILE:HG22	1:A:206:LYS:N	2.34	0.41
1:A:1509:CYS:O	1:A:1513:GLU:HG2	2.20	0.41
1:A:1527:LEU:HG	1:A:1646:ASP:CG	2.41	0.41
1:A:1079:ALA:HB2	1:A:1146:VAL:HG22	2.02	0.41
1:B:553:VAL:O	1:B:554:LYS:C	2.59	0.41
1:B:524:ILE:HG22	1:B:525:PRO:CD	2.45	0.41
1:A:1543:TYR:O	1:A:1601:LEU:HD23	2.20	0.41
1:A:456:LEU:HA	1:A:456:LEU:HD23	1.76	0.41
1:A:654:GLN:HE21	1:A:654:GLN:HB3	1.63	0.41
1:A:490:TYR:HB2	1:A:529:LEU:CD1	2.50	0.41
1:A:274:VAL:HG13	1:A:321:LYS:HG3	2.02	0.41
1:A:314:ARG:HE	1:A:315:ALA:N	2.17	0.41
1:B:583:ILE:HD13	1:B:774:ILE:HD11	2.03	0.41
1:B:1500:LEU:HG	1:B:1500:LEU:O	2.21	0.41
1:B:537:ASN:HB2	1:B:541:GLN:O	2.20	0.41
1:A:564:LYS:HG2	1:A:565:ASN:H	1.83	0.41
1:B:528:ARG:HD3	1:B:640:ALA:CB	2.51	0.41
1:A:1554:ASP:CA	1:A:1586:ILE:HD11	2.51	0.41
1:B:303:ARG:O	1:B:307:LEU:N	2.33	0.41
1:B:309:GLY:O	1:B:310:VAL:C	2.58	0.41
1:A:241:PHE:C	1:A:241:PHE:CD1	2.95	0.41
1:B:35:ARG:CG	1:B:38:SER:HB3	2.51	0.41
1:A:733:ARG:C	1:A:735:GLN:H	2.24	0.41
1:B:148:VAL:CG1	1:B:148:VAL:O	2.68	0.41
1:B:1600:TYR:CD2	1:B:1628:LEU:HG	2.55	0.41
1:B:482:GLN:HG2	1:B:482:GLN:O	2.21	0.41
1:B:285:HIS:HB2	1:B:305:VAL:HG13	2.03	0.41
1:B:1393:GLY:C	1:B:1395:GLN:H	2.23	0.41
1:B:730:THR:HG22	1:B:734:GLN:HE22	1.86	0.41
1:A:1457:LEU:HD12	1:A:1457:LEU:HA	1.77	0.41
1:B:1215:GLU:O	1:B:1216:LYS:HB2	2.21	0.41
1:B:808:LEU:HA	1:B:814:ILE:HA	2.03	0.41
1:B:714:GLN:N	1:B:714:GLN:CD	2.74	0.41
1:A:421:THR:HG22	1:A:438:THR:CG2	2.51	0.41
1:A:541:GLN:C	1:A:543:GLU:H	2.25	0.41
1:A:1256:ASN:ND2	1:A:1259:ARG:NH1	2.68	0.41
1:A:30:THR:CG2	1:A:42:VAL:HG13	2.51	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:205:ILE:O	1:A:206:LYS:HB2	2.20	0.41
1:A:1225:LYS:HG3	1:A:1484:ASP:OD2	2.21	0.41
1:B:922:ASP:OD1	1:B:923:GLY:N	2.54	0.41
1:A:874:LEU:HA	1:A:874:LEU:HD23	1.84	0.41
1:B:381:SER:O	1:B:382:PRO:C	2.59	0.40
1:B:398:LEU:HD12	1:B:405:ALA:HB2	2.04	0.40
1:B:637:PHE:HB3	1:B:642:LEU:HB2	2.03	0.40
1:B:597:ASP:HB2	1:B:766:PRO:HG2	2.02	0.40
1:B:36:LEU:HB2	1:B:124:LEU:HD13	2.03	0.40
1:A:1567:ILE:HG23	1:A:1654:MET:CB	2.51	0.40
1:B:1551:LYS:HZ3	1:B:1581:LYS:HE2	1.86	0.40
1:B:1637:ASP:O	1:B:1641:GLN:HB2	2.21	0.40
1:B:708:ARG:HG2	1:B:708:ARG:H	1.70	0.40
1:B:1034:GLU:HG3	1:B:1035:LYS:N	2.35	0.40
1:B:276:ASP:OD2	1:B:321:LYS:NZ	2.50	0.40
1:A:1543:TYR:HB3	1:A:1563:ILE:HG23	2.02	0.40
1:A:312:PRO:O	1:A:317:ALA:HB3	2.20	0.40
1:A:806:VAL:HG22	1:A:816:VAL:HG13	2.01	0.40
1:A:750:ASP:O	1:A:751:ASP:C	2.59	0.40
1:A:507:GLU:CG	1:A:508:PRO:HD2	2.51	0.40
1:A:1362:LEU:HD23	1:A:1389:THR:HB	2.03	0.40
1:A:933:GLU:HG2	1:A:970:VAL:CG1	2.50	0.40
1:B:785:ILE:HG22	1:B:785:ILE:O	2.21	0.40
1:A:549:VAL:HG12	1:A:550:TRP:N	2.35	0.40
1:B:1308:HIS:ND1	1:B:1319:ARG:HD2	2.36	0.40
1:B:1505:HIS:CE1	1:B:1506:LYS:HG3	2.56	0.40
1:B:136:THR:CG2	1:B:607:ASN:HB2	2.51	0.40
1:B:847:ARG:HH11	1:B:847:ARG:HG2	1.86	0.40
1:A:319:VAL:HG12	1:A:320:GLY:N	2.36	0.40
1:A:1311:LEU:O	1:A:1312:TRP:C	2.60	0.40
1:B:633:TYR:O	1:B:637:PHE:CD2	2.53	0.40
1:B:832:LEU:HD21	1:B:909:VAL:HG12	2.03	0.40
1:B:1437:SER:O	1:B:1439:LYS:N	2.54	0.40
1:A:131:ILE:HB	1:A:219:ALA:HB2	2.04	0.40
1:B:1265:TYR:CZ	1:B:1274:VAL:HG21	2.57	0.40
1:B:434:GLN:HG3	1:B:434:GLN:O	2.22	0.40
1:B:358:LYS:HB3	1:B:550:TRP:CZ3	2.56	0.40
1:A:1091:LEU:O	1:A:1092:ILE:HD13	2.22	0.40
1:A:478:ASP:O	1:A:479:PRO:C	2.59	0.40
1:B:148:VAL:O	1:B:148:VAL:HG13	2.20	0.40
1:B:1024:VAL:HG13	1:B:1033:TRP:CH2	2.56	0.40
1:B:534:THR:HG21	1:B:542:ARG:HE	1.86	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1407:MET:HB2	1:B:1410:PHE:CD2	2.56	0.40
1:B:704:PRO:O	1:B:705:CYS:C	2.60	0.40
1:B:1278:LEU:HA	1:B:1278:LEU:HD23	1.88	0.40
1:B:629:SER:O	1:B:636:VAL:HA	2.21	0.40
1:B:712:ILE:CG2	1:B:719:VAL:HG22	2.52	0.40
1:B:128:TYR:CE1	1:B:618:VAL:HG13	2.57	0.40
1:A:1567:ILE:HG23	1:A:1654:MET:HB2	2.03	0.40
1:B:985:PRO:HB2	1:B:1256:ASN:ND2	2.37	0.40
1:B:756:GLU:O	1:B:757:GLU:C	2.59	0.40
1:A:804:LEU:HD22	1:A:804:LEU:N	2.36	0.40
1:A:574:ARG:O	1:A:575:PRO:O	2.39	0.40
1:B:852:ASN:C	1:B:854:ARG:N	2.75	0.40
1:A:269:PHE:N	1:A:269:PHE:CD2	2.90	0.40
1:A:270:VAL:O	1:A:287:LEU:HB3	2.21	0.40
1:B:481:GLU:O	1:B:483:ALA:N	2.55	0.40
1:A:481:GLU:OE2	1:A:538:ALA:HB2	2.21	0.40
1:B:1448:LYS:HD2	1:B:1449:VAL:N	2.36	0.40
1:A:1184:ARG:NH1	1:A:1184:ARG:HG2	2.36	0.40
1:A:1232:THR:O	1:A:1235:ALA:HB3	2.21	0.40
1:B:982:GLN:O	1:B:1339:GLY:HA3	2.21	0.40
1:B:1140:VAL:HG21	1:B:1182:LEU:HD21	2.04	0.40
1:A:609:LEU:HA	1:A:609:LEU:HD23	1.88	0.40
1:A:1352:LYS:HG3	1:A:1352:LYS:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1602/1661 (96%)	1285 (80%)	213 (13%)	104 (6%)	2	11
1	B	1602/1661 (96%)	1268 (79%)	239 (15%)	95 (6%)	2	14
All	All	3204/3322 (96%)	2553 (80%)	452 (14%)	199 (6%)	2	13

All (199) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	PRO
1	A	91	PRO
1	A	187	ILE
1	A	212	SER
1	A	244	ILE
1	A	313	SER
1	A	384	ARG
1	A	482	GLN
1	A	526	SER
1	A	537	ASN
1	A	554	LYS
1	A	555	ASP
1	A	646	THR
1	A	757	GLU
1	A	778	LYS
1	A	780	ALA
1	A	794	LEU
1	A	817	ALA
1	A	888	PRO
1	A	971	PRO
1	A	1225	LYS
1	A	1245	TYR
1	A	1314	SER
1	A	1497	ASP
1	A	1506	LYS
1	A	1579	GLU
1	A	1613	LYS
1	A	1632	ALA
1	B	63	PRO
1	B	78	SER
1	B	140	PRO
1	B	219	ALA
1	B	302	LYS
1	B	310	VAL
1	B	312	PRO
1	B	317	ALA
1	B	427	ASP
1	B	449	ASN
1	B	479	PRO
1	B	481	GLU
1	B	482	GLN
1	B	537	ASN
1	B	622	ASP

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Mol	Chain	Res	Type
1	B	623	ILE
1	B	626	THR
1	B	653	GLN
1	B	716	ASP
1	B	757	GLU
1	B	785	ILE
1	B	798	ILE
1	B	817	ALA
1	B	1132	PHE
1	B	1225	LYS
1	B	1571	SER
1	B	1572	ASP
1	B	1632	ALA
1	A	78	SER
1	A	120	VAL
1	A	125	GLN
1	A	282	SER
1	A	309	GLY
1	A	483	ALA
1	A	543	GLU
1	A	576	GLY
1	A	616	ASP
1	A	629	SER
1	A	671	VAL
1	A	751	ASP
1	A	756	GLU
1	A	762	ARG
1	A	1010	GLY
1	A	1127	GLU
1	A	1350	LYS
1	A	1483	LEU
1	A	1493	PRO
1	A	1502	LYS
1	A	1570	GLY
1	A	1580	ARG
1	B	215	GLN
1	B	244	ILE
1	B	248	ASP
1	B	282	SER
1	B	320	GLY
1	B	462	GLU
1	B	603	LEU

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Mol	Chain	Res	Type
1	B	655	ARG
1	B	780	ALA
1	B	1010	GLY
1	B	1095	ASP
1	B	1266	GLY
1	B	1314	SER
1	B	1495	LYS
1	B	1570	GLY
1	B	1628	LEU
1	A	93	SER
1	A	219	ALA
1	A	250	LEU
1	A	283	LEU
1	A	335	SER
1	A	365	PRO
1	A	382	PRO
1	A	385	HIS
1	A	449	ASN
1	A	451	ASN
1	A	512	LEU
1	A	560	THR
1	A	603	LEU
1	A	752	ASP
1	A	889	ALA
1	A	918	HIS
1	A	1353	GLY
1	A	1372	THR
1	A	1438	ASN
1	A	1482	ASN
1	A	1653	ASN
1	B	82	TYR
1	B	126	SER
1	B	134	ASP
1	B	157	PRO
1	B	174	VAL
1	B	283	LEU
1	B	525	PRO
1	B	571	LYS
1	B	687	ASP
1	B	755	PRO
1	B	812	LYS
1	B	987	ALA

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Mol	Chain	Res	Type
1	B	1482	ASN
1	B	1613	LYS
1	B	1614	PRO
1	A	50	GLN
1	A	140	PRO
1	A	378	PRO
1	A	570	GLU
1	A	675	GLU
1	A	972	ASP
1	A	1435	ARG
1	A	1436	ASP
1	A	1657	PHE
1	B	47	HIS
1	B	185	PHE
1	B	251	LYS
1	B	378	PRO
1	B	384	ARG
1	B	464	LYS
1	B	540	GLY
1	B	671	VAL
1	B	702	LYS
1	B	971	PRO
1	B	1040	LYS
1	B	1372	THR
1	B	1438	ASN
1	B	1483	LEU
1	A	172	ILE
1	A	479	PRO
1	A	516	PRO
1	A	535	LEU
1	A	904	ILE
1	A	1555	ASP
1	A	1565	ASN
1	B	237	PRO
1	B	448	GLY
1	B	657	ASP
1	B	724	ASP
1	B	840	ARG
1	B	1223	ASN
1	B	1565	ASN
1	B	1637	ASP
1	A	174	VAL

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Mol	Chain	Res	Type
1	A	759	ILE
1	A	806	VAL
1	A	1540	ASP
1	B	172	ILE
1	B	334	GLY
1	B	577	GLN
1	B	661	PRO
1	B	822	VAL
1	B	1137	GLU
1	B	1597	GLY
1	A	360	PRO
1	A	466	GLY
1	A	575	PRO
1	A	623	ILE
1	A	657	ASP
1	A	1266	GLY
1	B	360	PRO
1	B	508	PRO
1	A	169	PRO
1	B	246	ASP
1	A	252	VAL
1	A	311	GLN
1	A	1538	GLY
1	B	373	VAL
1	B	461	VAL
1	B	806	VAL
1	A	766	PRO
1	A	658	PRO
1	A	1658	GLY
1	B	766	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	1420/1465 (97%)	1238 (87%)	182 (13%)	6	27
1	B	1420/1465 (97%)	1234 (87%)	186 (13%)	6	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2840/2930 (97%)	2472 (87%)	368 (13%)	6 26

All (368) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	SER
1	A	41	THR
1	A	58	THR
1	A	61	ASP
1	A	75	GLN
1	A	80	ASN
1	A	83	LEU
1	A	95	GLU
1	A	98	SER
1	A	100	LYS
1	A	107	VAL
1	A	110	THR
1	A	113	ASN
1	A	114	VAL
1	A	118	LYS
1	A	120	VAL
1	A	121	LEU
1	A	125	GLN
1	A	128	TYR
1	A	135	LYS
1	A	139	THR
1	A	140	PRO
1	A	143	THR
1	A	146	TYR
1	A	151	VAL
1	A	164	ILE
1	A	174	VAL
1	A	200	MET
1	A	218	SER
1	A	228	LEU
1	A	235	LEU
1	A	254	ILE
1	A	265	ASP
1	A	267	THR
1	A	270	VAL
1	A	278	ASP
1	A	287	LEU

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Mol	Chain	Res	Type
1	A	288	THR
1	A	294	ASP
1	A	314	ARG
1	A	316	ASP
1	A	318	LEU
1	A	321	LYS
1	A	322	SER
1	A	328	THR
1	A	330	ILE
1	A	336	ASP
1	A	346	PRO
1	A	356	PHE
1	A	358	LYS
1	A	359	THR
1	A	361	LYS
1	A	399	THR
1	A	400	GLN
1	A	404	VAL
1	A	407	LEU
1	A	410	ASN
1	A	412	GLN
1	A	422	VAL
1	A	427	ASP
1	A	434	GLN
1	A	442	LEU
1	A	463	LEU
1	A	467	GLU
1	A	468	THR
1	A	471	VAL
1	A	476	ARG
1	A	479	PRO
1	A	484	LYS
1	A	491	MET
1	A	501	VAL
1	A	504	GLN
1	A	513	VAL
1	A	535	LEU
1	A	537	ASN
1	A	541	GLN
1	A	555	ASP
1	A	565	ASN
1	A	600	VAL

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Mol	Chain	Res	Type
1	A	601	PHE
1	A	605	LYS
1	A	618	VAL
1	A	631	ARG
1	A	633	TYR
1	A	650	LEU
1	A	654	GLN
1	A	658	PRO
1	A	673	LEU
1	A	677	ARG
1	A	687	ASP
1	A	692	CYS
1	A	701	MET
1	A	702	LYS
1	A	707	ARG
1	A	714	GLN
1	A	723	LEU
1	A	729	ILE
1	A	750	ASP
1	A	751	ASP
1	A	752	ASP
1	A	756	GLU
1	A	776	ASP
1	A	796	ASP
1	A	798	ILE
1	A	804	LEU
1	A	808	LEU
1	A	814	ILE
1	A	846	ILE
1	A	852	ASN
1	A	854	ARG
1	A	855	GLU
1	A	859	LEU
1	A	867	TYR
1	A	871	PHE
1	A	881	HIS
1	A	906	LEU
1	A	927	THR
1	A	928	LEU
1	A	940	THR
1	A	945	THR
1	A	958	ARG

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Mol	Chain	Res	Type
1	A	962	PRO
1	A	971	PRO
1	A	977	THR
1	A	978	LYS
1	A	988	GLN
1	A	999	LEU
1	A	1009	CYS
1	A	1012	GLN
1	A	1033	TRP
1	A	1039	GLU
1	A	1056	LEU
1	A	1077	LEU
1	A	1133	ARG
1	A	1134	ASP
1	A	1135	THR
1	A	1164	LEU
1	A	1190	ILE
1	A	1205	ARG
1	A	1207	THR
1	A	1217	ASN
1	A	1223	ASN
1	A	1244	ASP
1	A	1249	PRO
1	A	1257	GLU
1	A	1260	TYR
1	A	1275	PHE
1	A	1282	GLN
1	A	1289	LYS
1	A	1299	LEU
1	A	1306	VAL
1	A	1323	THR
1	A	1328	ARG
1	A	1341	LEU
1	A	1345	THR
1	A	1351	LEU
1	A	1357	CYS
1	A	1358	LYS
1	A	1371	GLU
1	A	1375	LYS
1	A	1377	GLN
1	A	1380	LYS
1	A	1389	THR

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Mol	Chain	Res	Type
1	A	1396	ASP
1	A	1422	THR
1	A	1435	ARG
1	A	1447	ASP
1	A	1448	LYS
1	A	1452	THR
1	A	1457	LEU
1	A	1489	ARG
1	A	1492	HIS
1	A	1496	GLU
1	A	1497	ASP
1	A	1527	LEU
1	A	1547	LEU
1	A	1549	GLN
1	A	1561	MET
1	A	1562	VAL
1	A	1563	ILE
1	A	1569	SER
1	A	1601	LEU
1	B	30	THR
1	B	32	ASN
1	B	44	LEU
1	B	50	GLN
1	B	54	GLN
1	B	55	VAL
1	B	58	THR
1	B	65	LYS
1	B	69	LEU
1	B	75	GLN
1	B	79	ASN
1	B	82	TYR
1	B	100	LYS
1	B	105	VAL
1	B	110	THR
1	B	113	ASN
1	B	117	GLU
1	B	120	VAL
1	B	121	LEU
1	B	123	SER
1	B	140	PRO
1	B	143	THR
1	B	146	TYR

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Mol	Chain	Res	Type
1	B	151	VAL
1	B	152	ASP
1	B	168	THR
1	B	182	GLN
1	B	183	ASN
1	B	184	GLN
1	B	200	MET
1	B	218	SER
1	B	243	TYR
1	B	246	ASP
1	B	278	ASP
1	B	288	THR
1	B	294	ASP
1	B	296	ASN
1	B	316	ASP
1	B	328	THR
1	B	350	SER
1	B	352	TYR
1	B	354	ILE
1	B	355	HIS
1	B	360	PRO
1	B	361	LYS
1	B	364	LYS
1	B	374	TYR
1	B	376	THR
1	B	382	PRO
1	B	400	GLN
1	B	407	LEU
1	B	408	SER
1	B	409	ILE
1	B	410	ASN
1	B	416	ASP
1	B	422	VAL
1	B	423	ARG
1	B	429	ILE
1	B	433	ARG
1	B	438	THR
1	B	446	THR
1	B	455	HIS
1	B	478	ASP
1	B	479	PRO
1	B	486	ARG

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Mol	Chain	Res	Type
1	B	487	TYR
1	B	491	MET
1	B	503	ARG
1	B	508	PRO
1	B	515	LEU
1	B	524	ILE
1	B	535	LEU
1	B	537	ASN
1	B	551	VAL
1	B	553	VAL
1	B	557	CYS
1	B	558	MET
1	B	565	ASN
1	B	570	GLU
1	B	618	VAL
1	B	626	THR
1	B	627	PRO
1	B	645	LYS
1	B	653	GLN
1	B	654	GLN
1	B	672	GLN
1	B	673	LEU
1	B	675	GLU
1	B	677	ARG
1	B	687	ASP
1	B	697	ARG
1	B	701	MET
1	B	708	ARG
1	B	718	CYS
1	B	750	ASP
1	B	798	ILE
1	B	799	THR
1	B	804	LEU
1	B	808	LEU
1	B	812	LYS
1	B	818	ASP
1	B	830	ILE
1	B	839	VAL
1	B	846	ILE
1	B	859	LEU
1	B	867	TYR
1	B	881	HIS

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Mol	Chain	Res	Type
1	B	918	HIS
1	B	927	THR
1	B	928	LEU
1	B	940	THR
1	B	945	THR
1	B	962	PRO
1	B	971	PRO
1	B	977	THR
1	B	986	VAL
1	B	988	GLN
1	B	997	GLU
1	B	999	LEU
1	B	1009	CYS
1	B	1012	GLN
1	B	1018	THR
1	B	1028	ASP
1	B	1033	TRP
1	B	1039	GLU
1	B	1040	LYS
1	B	1042	GLN
1	B	1056	LEU
1	B	1061	LYS
1	B	1129	ILE
1	B	1133	ARG
1	B	1134	ASP
1	B	1135	THR
1	B	1139	ASP
1	B	1160	GLN
1	B	1164	LEU
1	B	1190	ILE
1	B	1205	ARG
1	B	1206	LEU
1	B	1207	THR
1	B	1217	ASN
1	B	1218	ARG
1	B	1223	ASN
1	B	1244	ASP
1	B	1258	GLN
1	B	1259	ARG
1	B	1260	TYR
1	B	1275	PHE
1	B	1280	GLN

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Mol	Chain	Res	Type
1	B	1289	LYS
1	B	1298	GLN
1	B	1303	ASN
1	B	1306	VAL
1	B	1311	LEU
1	B	1328	ARG
1	B	1341	LEU
1	B	1345	THR
1	B	1346	VAL
1	B	1351	LEU
1	B	1357	CYS
1	B	1358	LYS
1	B	1375	LYS
1	B	1377	GLN
1	B	1396	ASP
1	B	1415	GLU
1	B	1422	THR
1	B	1445	TYR
1	B	1447	ASP
1	B	1448	LYS
1	B	1452	THR
1	B	1456	CYS
1	B	1484	ASP
1	B	1489	ARG
1	B	1535	CYS
1	B	1549	GLN
1	B	1561	MET
1	B	1563	ILE
1	B	1575	GLN
1	B	1577	LYS
1	B	1593	LYS
1	B	1603	TRP
1	B	1610	TRP
1	B	1612	GLU
1	B	1634	GLU
1	B	1635	CYS
1	B	1653	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS

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Mol	Chain	Res	Type
1	A	54	GLN
1	A	71	ASN
1	A	80	ASN
1	A	183	ASN
1	A	193	ASN
1	A	199	ASN
1	A	296	ASN
1	A	308	ASN
1	A	353	GLN
1	A	377	ASN
1	A	440	GLN
1	A	494	ASN
1	A	510	GLN
1	A	537	ASN
1	A	541	GLN
1	A	653	GLN
1	A	654	GLN
1	A	841	ASN
1	A	883	GLN
1	A	1032	GLN
1	A	1054	GLN
1	A	1090	ASN
1	A	1160	GLN
1	A	1217	ASN
1	A	1223	ASN
1	A	1256	ASN
1	A	1282	GLN
1	A	1377	GLN
1	A	1434	ASN
1	A	1578	GLN
1	A	1585	HIS
1	A	1636	GLN
1	A	1641	GLN
1	A	1643	GLN
1	A	1649	ASN
1	B	32	ASN
1	B	54	GLN
1	B	71	ASN
1	B	79	ASN
1	B	113	ASN
1	B	182	GLN
1	B	183	ASN

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Mol	Chain	Res	Type
1	B	184	GLN
1	B	193	ASN
1	B	234	GLN
1	B	263	GLN
1	B	296	ASN
1	B	377	ASN
1	B	396	GLN
1	B	413	ASN
1	B	434	GLN
1	B	451	ASN
1	B	474	HIS
1	B	494	ASN
1	B	537	ASN
1	B	611	GLN
1	B	632	ASN
1	B	653	GLN
1	B	654	GLN
1	B	714	GLN
1	B	734	GLN
1	B	791	ASN
1	B	852	ASN
1	B	881	HIS
1	B	883	GLN
1	B	917	ASN
1	B	1013	ASN
1	B	1032	GLN
1	B	1042	GLN
1	B	1054	GLN
1	B	1069	GLN
1	B	1090	ASN
1	B	1160	GLN
1	B	1217	ASN
1	B	1223	ASN
1	B	1258	GLN
1	B	1282	GLN
1	B	1298	GLN
1	B	1434	ASN
1	B	1585	HIS
1	B	1641	GLN
1	B	1643	GLN
1	B	1649	ASN
1	B	1653	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

6 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	A	2001	1,2	12,14,15	0.59	0	15,19,21	1.12	1 (6%)
2	NAG	A	2002	2	12,14,15	0.64	0	15,19,21	1.02	2 (13%)
2	BMA	A	2003	2	10,11,12	0.43	0	11,15,17	0.79	1 (9%)
2	NAG	B	2001	1,2	12,14,15	0.60	0	15,19,21	1.35	2 (13%)
2	NAG	B	2002	2	12,14,15	0.61	0	15,19,21	1.36	2 (13%)
2	BMA	B	2003	2	10,11,12	0.43	0	11,15,17	0.84	1 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	2001	1,2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	2002	2	-	0/6/23/26	0/1/1/1
2	BMA	A	2003	2	-	0/2/19/22	0/1/1/1
2	NAG	B	2001	1,2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	B	2002	2	-	0/6/23/26	0/1/1/1
2	BMA	B	2003	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2002	NAG	O5-C5-C6	3.28	110.42	106.98
2	A	2001	NAG	O5-C5-C6	3.17	110.31	106.98
2	B	2001	NAG	O5-C5-C6	3.15	110.28	106.98
2	B	2001	NAG	O5-C5-C4	2.74	114.13	110.65
2	B	2002	NAG	C3-C2-N2	-2.57	107.85	111.76
2	A	2002	NAG	C3-C4-C5	-2.32	106.06	110.20
2	A	2003	BMA	O5-C5-C6	2.23	109.32	106.98
2	B	2003	BMA	O5-C5-C6	2.22	109.31	106.98
2	A	2002	NAG	C3-C2-N2	-2.13	108.51	111.76

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	2001	NAG	C1
2	B	2001	NAG	C1

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1610/1661 (96%)	-0.11	11 (0%) 84 28	15, 101, 169, 200	0
1	B	1610/1661 (96%)	-0.13	7 (0%) 90 41	17, 96, 169, 200	0
All	All	3220/3322 (96%)	-0.12	18 (0%) 86 32	15, 99, 169, 200	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	742	LEU	3.4
1	A	348	VAL	3.1
1	B	1654	MET	3.0
1	A	741	ALA	3.0
1	A	349	THR	2.6
1	B	671	VAL	2.5
1	A	276	ASP	2.4
1	B	741	ALA	2.3
1	A	100	LYS	2.3
1	A	125	GLN	2.3
1	A	352	TYR	2.3
1	B	1659	CYS	2.2
1	A	431	GLU	2.2
1	A	279	ARG	2.2
1	A	1133	ARG	2.2
1	B	425	LYS	2.0
1	B	92	ALA	2.0
1	B	415	ARG	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 ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NAG	A	2002	14/15	0.32	2.71	80,81,82,82	0
2	NAG	A	2001	14/15	0.24	1.15	74,80,81,82	0
2	NAG	B	2002	14/15	0.26	0.74	80,80,81,82	0
2	BMA	B	2003	11/12	0.23	0.69	80,81,81,82	0
2	NAG	B	2001	14/15	0.14	-1.10	73,80,81,82	0
2	BMA	A	2003	11/12	0.40	-	81,81,82,82	0

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.