



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:43 PM GMT

PDB ID : 1Y1W
Title : Complete RNA Polymerase II elongation complex
Authors : Cramer, P.; Kettenberger, H.; Armache, K.-J.
Deposited on : 2004-11-19
Resolution : 4.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

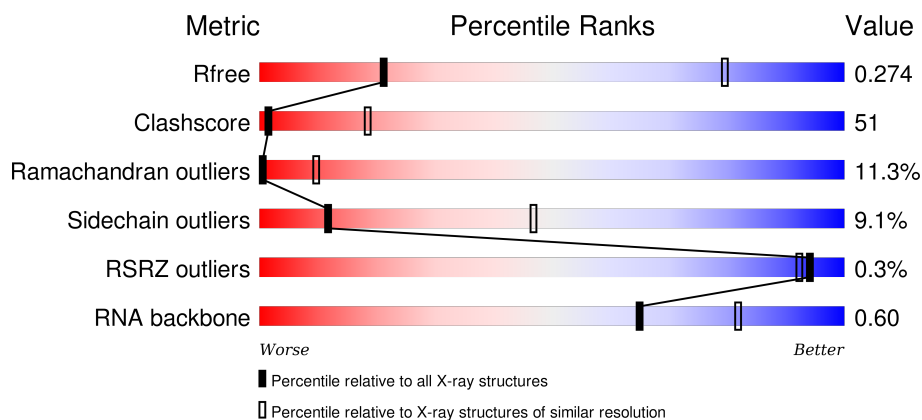
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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}	91344	1010 (4.42-3.56)
Clashscore	102246	1052 (4.40-3.60)
Ramachandran outliers	100387	1005 (4.40-3.60)
Sidechain outliers	100360	1013 (4.42-3.58)
RSRZ outliers	91569	1013 (4.42-3.56)
RNA backbone	2183	1079 (5.04-2.80)

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

Mol	Chain	Length	Quality of chain
1	T	19	<div> <div>5%</div> <div> <div>32%</div> <div>68%</div> </div> </div>
2	N	7	<div> <div>14%</div> <div> <div>14%</div> <div>71%</div> <div>14%</div> </div> </div>
3	P	10	<div> <div>80%</div> <div>20%</div> </div>
4	A	1733	<div> <div>25%</div> <div> <div>45%</div> <div>10%</div> <div>18%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
5	B	1224	
6	C	318	
7	D	221	
8	E	215	
9	F	155	
10	G	171	
11	H	146	
12	I	122	
13	J	70	
14	K	120	
15	L	70	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 31802 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a DNA chain called 5'-D(P*AP*GP*TP*AP*CP*TP*TP*AP*CP*GP*CP*CP*TP*GP*GP*TP*CP*AP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	19	Total	C	N	O	P	21	0	0
			387	185	67	116	19			

- Molecule 2 is a DNA chain called 5'-D(*AP*AP*GP*TP*AP*CP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	7	Total	C	N	O	P	20	0	0
			141	69	27	39	6			

- Molecule 3 is a RNA chain called 5'-R(*AP*AP*GP*AP*CP*CP*AP*GP*GP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	10	Total	C	N	O	P	0	0	0
			214	97	44	64	9			

- Molecule 4 is a protein called DNA-directed RNA polymerase II largest subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1416	Total	C	N	O	S	0	0	0
			11140	7021	1946	2111	62			

- Molecule 5 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	1112	Total	C	N	O	S	0	0	0
			8836	5594	1548	1639	55			

- Molecule 6 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 7 is a protein called DNA-directed RNA polymerase II 32 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	D	177	Total	C	N	O	S	0	0	0
			1356	840	241	273	2			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 10 is a protein called DNA-directed RNA polymerase II 19 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 13 is a protein called DNA-directed RNA polymerases I/II/III subunit 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 14 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 15 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	J	1	Total	Zn	0	0
			1	1		
16	B	1	Total	Zn	0	0
			1	1		
16	I	2	Total	Zn	0	0
			2	2		
16	C	1	Total	Zn	0	0
			1	1		
16	A	2	Total	Zn	0	0
			2	2		
16	L	1	Total	Zn	0	0
			1	1		

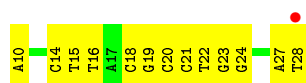
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Mg	0	0
			1	1		

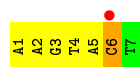
3 Residue-property plots [i](#)

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.

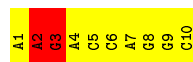
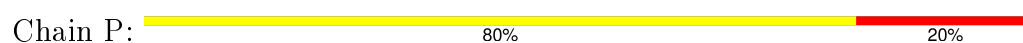
- Molecule 1: 5'-D(P*AP*GP*TP*AP*CP*TP*TP*AP*CP*GP*CP*CP*TP*GP*GP*TP*CP*AP*T)-3'



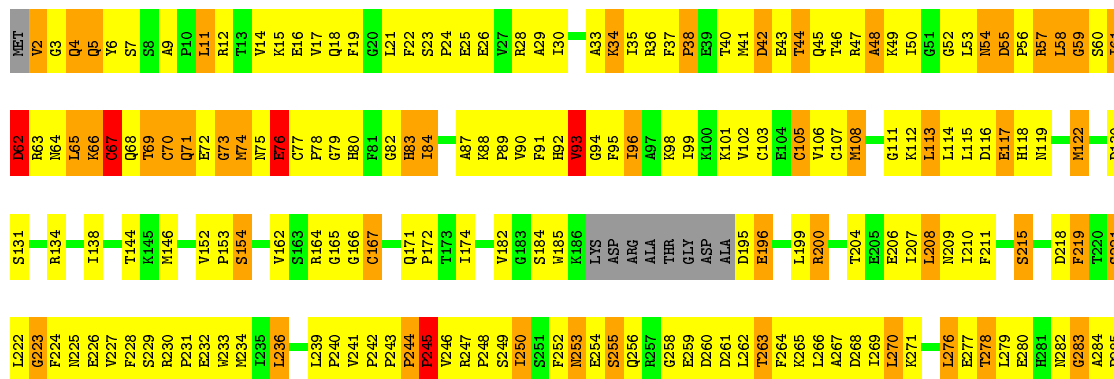
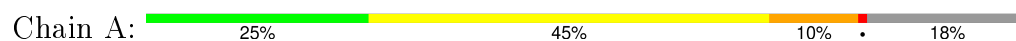
- Molecule 2: 5'-D(*AP*AP*GP*TP*AP*CP*T)-3'



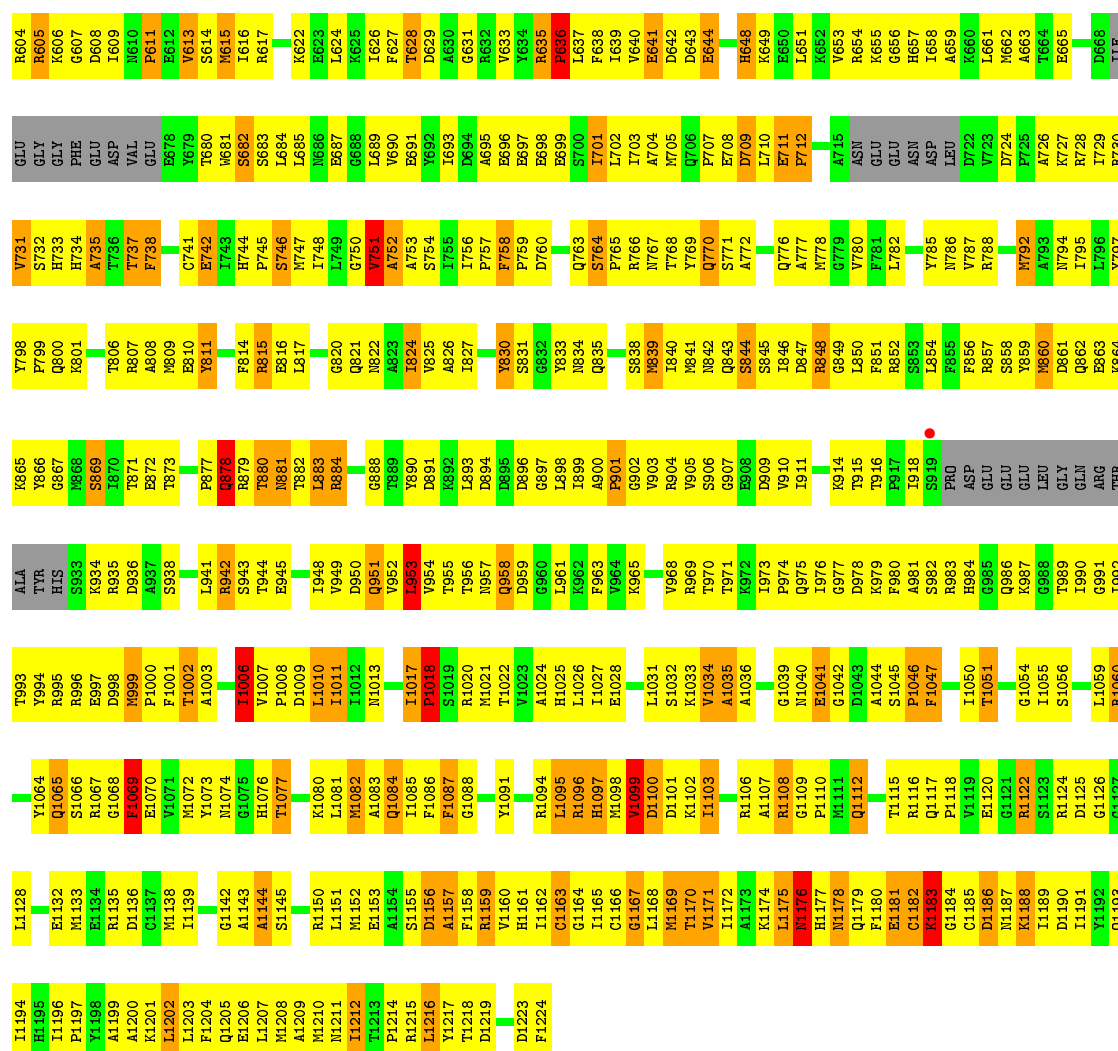
- Molecule 3: 5'-R(*AP*AP*GP*AP*CP*CP*AP*GP*GP*C)-3'



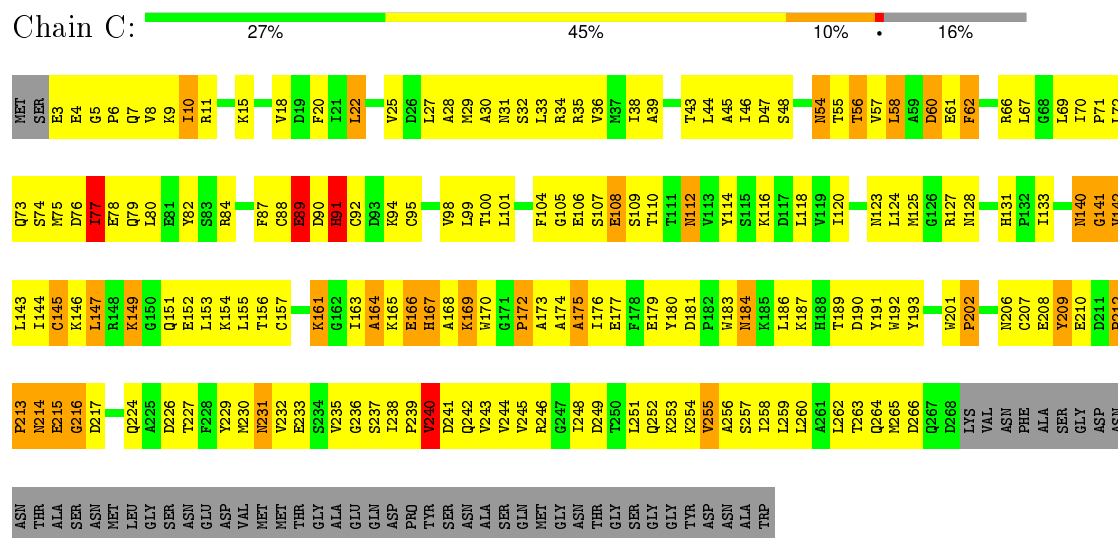
- Molecule 4: DNA-directed RNA polymerase II largest subunit



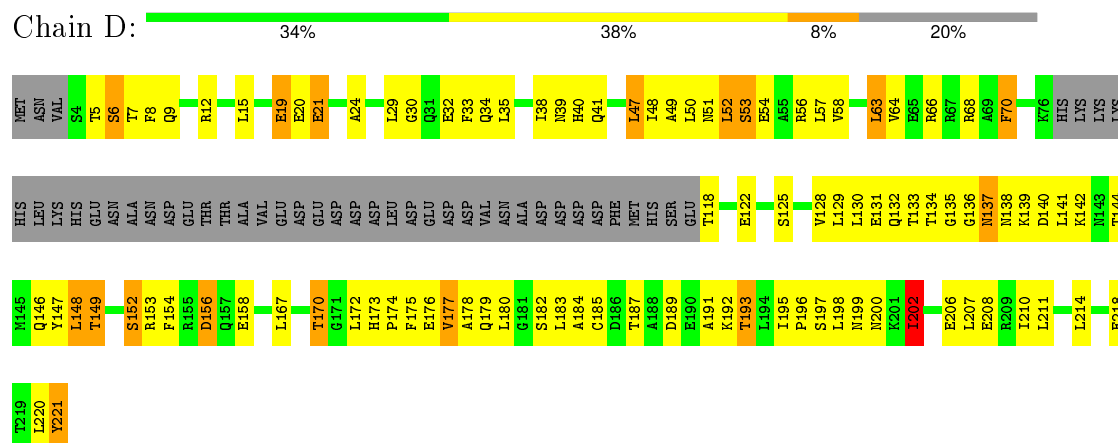
V1299	D1223	T1161	K1092	A1027	R961	G887	E822	I756	A684	G615	V551	G484	D423	F347	H286
K1300	L1224	V1162	K1093	T1028	R962	G888	G823	I757	E585	V616	H552	D485	I424	S348	H287
E1301		I1163	V1094	R1029	I963	S889	L324	I758	A687	E617	H553	E486	Q425	A349	A288
P1302	I1227	P1164	T1095	R1030	I964	D890	I825		K687	E618	H554	N487	Q427	R350	I289
K1303	M1228	E1165	S1096	V1031	Q965	A891	D826	M761	V690	K619	H555	N488	Y428	T351	E291
V1305		D1166	G1097	L1032	N966	R896	T827	T762	L691	K620	H556	N489	G428	V352	K291
L1306	D1231	E1167	V1098	Q1033	A967	R897	A828	I763	L692	T821	H557	H490	K430	I353	K292
E1307		I1168	P1099	E1034	Q968	R898	V829	C764	D693	G622	H558	E491	N430	S354	E293
T1308	L1236	I1169	R1100	Y1035	Q969	R899	K330	T765	V693	G623	H559	P492	K431	G355	S294
D1309	I1237	Q1170	T1070	L1037	F971	V899	T831	T766	K695	S624	H560	Q493	V432	G356	L295
V1310	I1238	Q1171	K1102	L1036	F972	D900	A832	T767	K696	S625	H561		E433	P357	L296
G1311	L1172	H1173	L1105	T1038	H972	L901	E833	T768	E596	K626	H562	T487	R434	N358	D297
N1312	H1174	H1175	N1106	L1039	I973	L902	T834	T769	A697	G627	H563	R498	H435		P298
L1313	S1175	L1176	V1107	Q1040	S979	N903	G835	V770	Q698	G628	H564	A499		V864	H299
S1314	V1242	L1177		A1041	D980	T904	I837	R774	N700	L629	H566	E500	D438	G365	V300
V1316	ARG	LEU	M1110	W1044	L981	H906	Q838	I775	L701	I630	H567		N439	V366	A301
K1317	PRO	ASP	M1111	V1045	T907	R907	R839	F779	T709	L645	H568		D440	S369	T302
L1318	LVS	GLU	K1112		L908	L908	R840	T780	L710	G637	H570		P441	K372	K304
V1319	SER	GLU	T1113	N1048	D909	D909	L841	I781	R711		H571		V442		D305
P1320	LEU	ALA	P1114	I1049	P910	P910	L842	T782	E712		H572		L443	Y376	D307
	ASP	GLU	S1115	E1050	S911	S911	K943	T783	S713	C642	H573		N445		I308
	ALA	GLN	L1116	A1051	L912	L912	A844	T784	F714		H574		R446		K308
	SER	SER	T1117	Q1052	L913	L913	L845	L785	E715	L646	H575		Q447	T381	A309
	THR	ASP	V1118	F1053	E914	E914	E846	T786		G647	H577		P448	P382	G310
P1323	GLU	ASP	V1119	L1054	D982	I919	I848	F787	V718		H578		S449	N383	Q311
P1324					L993	L993	R849	T788	E719	N648	H579		L450	N384	P312
T1325	A1284	Q1187	E1120	R1055	L994	L920	N849	F789	V719	K649	H580		H451	R385	Q313
R1326	E1285	Q1188	E1121	S1056	G994	G921		T790	R720	Q650	H581		K452	D386	A314
V1328	E1286	P1189	S1189	P1057	R995	R995		T791	F721	K651	H582		N453	K387	L315
		G1123	G1123	V1058	N996	D922	H852		L722	G652	H584		K454	L388	K316
N1330	L1260	H1124	H1124	H1059	L987	Q926	D853		E723		H585		P455		K317
S1331	K1261	L1192		P1060	L988	Q926	N854		N723		H586		N456	V392	S318
F1332		L1193	D127	G1061	P999	I920	T855	F794	E724		H587		A457		G319
I1333	E1264	R1194	Q1130	E1062	L1000	L929	T856	T795	A725	N654	H588		H458	P396	R320
D1334	L1195	L1195		M1063	R1001	D930	R857	T796	R726		H589		V524		P321
I1335	T1266	A1196	L1133	V1064	K1002	Y933	N858	K797	D727	L658	H589		R459	H399	V322
M1336	L1267	L1197	I1134	G1065	K1003	Y934	L860	T798	K728	H659	H590		V460	P400	K323
E1337	L1268	D1198		V1066	N1004	Q935	G861	T799	A729	H660	H591		D526	G401	S324
V1339		R1199		L1067	E1005	Q935	N862	R800	G730	H661	H592		T527	A402	I325
					I1006	L936		E801	R731	F662	H593		L528	K403	K326
I1340	I1271		E1139	A1068	I1007	L936	V863	N802	L732		H594			Y404	A327
K1341	R1274	M1202	H1140	A1069	I1007	D939	I864	S803	N736	T664	H595			Y405	R328
E1342	G1275	K1205	T1141	Q1070	Q1008	D939	I864	S804	L737		H596		S466	I406	
A1343		D1206	T1142	S1071	N1009	R940	Q865	T804	K738	H665	H597		T467	R407	G331
G1344	I1279	L1267	L1143	I1072	A1010	K941	P866	L805	D739	H666	H598		F468	D408	K332
R1345	E1280	T1208		G1073	Q1011	F942	I867	R806	L740	H668	H599		R469	S409	E333
A1346		M1209	T1147	P1075	R1012	L943	G869	G807	N741	T669	H600		L470	G410	G334
V1347	V1282	G1210	I1148	E1074	A1014	V946	E870	T809	N742	I670	H601		N471	G410	
L1348	A1347	Q1211	A1149	A1076	V1015	F947	D871	P810	V743	A671	D602		L472	D411	K335
V1349	M1284	V1212	S1150		T1016	V943	G872	Q811	V743	D672	H603		S473	R412	I336
K1350		G1213	E1151	L1081	T1017	D949	N873	E812	K744	G673	H604		V474	I413	R337
E1351	R1289	E1214	I1152	ASN	L1017	D949	D874	F813	Q745	G674	H605		T475	D143	G338
V1352	K1290	R1215	Y1153	THR	P1018	N953	A875	F814	N746	T675	H606		S476	L415	I339
				PHE	C1019	N954		F815	L607	M676	H607		P477	R416	L340
	V1291	I1216	Y1154	HIS	C1020	N954		F816	V747		H608			Y417	N341
V1355	P1292	K1217	D1155	PHE	L1021	P955	Q881	H816			H609		N478	S418	K342
I1356	S1293	Q1218	P1156	ALA	L1022	I956	S882	A817	S751	I679	H610		N479	K419	K343
	P1294	T1219	D1157	GLY	A1023	P957	L883	N818	K752	T680	H611		A480	K419	
		F1220	P1158	VAL	S1024	P958	E884	G819	G753	E681	H612		D481	R420	R344
D1359			R1159	ALA	L1025	N959	T885	G820	S754	H613	H613		F482	A421	V345
		K1221		SER	L1026	I960	I886	R821	F755	I683	H614		D483	G422	



- Molecule 6: DNA-directed RNA polymerase II 45 kDa polypeptide



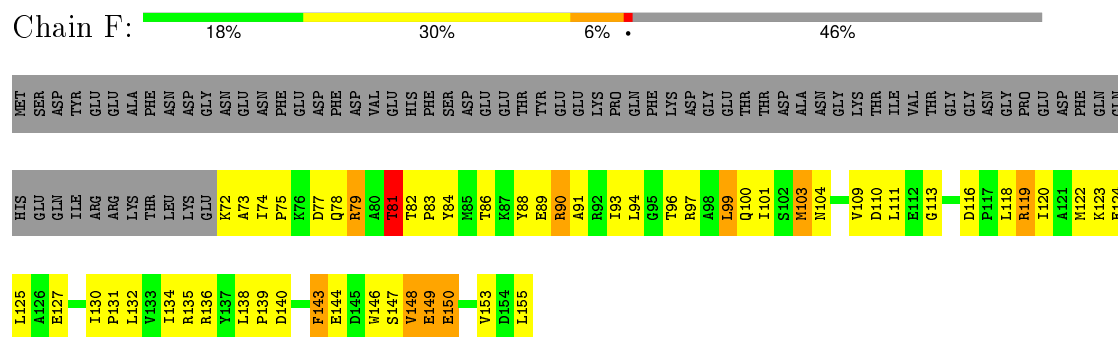
- Molecule 7: DNA-directed RNA polymerase II 32 kDa polypeptide



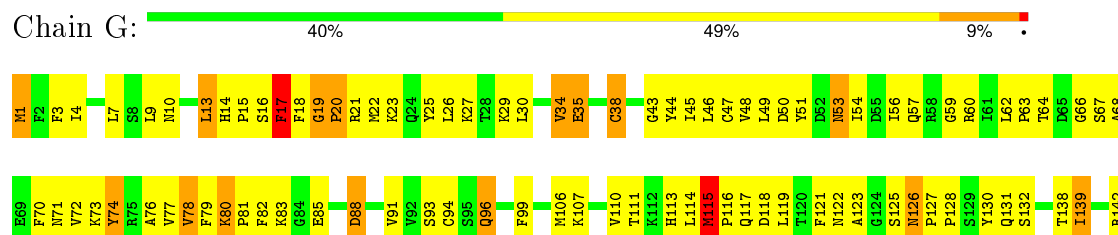
- Molecule 8: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide



- Molecule 9: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide



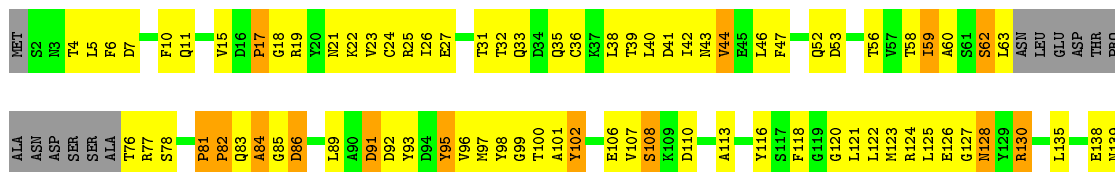
- Molecule 10: DNA-directed RNA polymerase II 19 kDa polypeptide





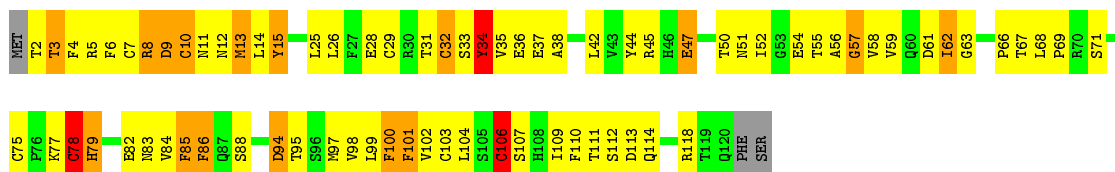
- Molecule 11: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide

Chain H:



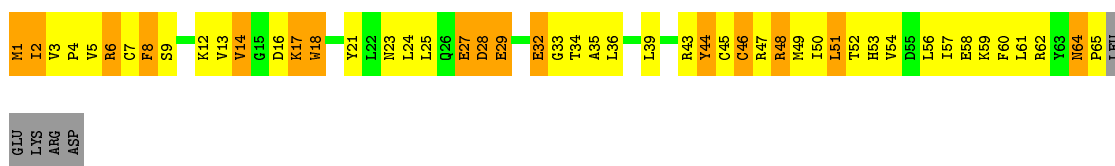
- Molecule 12: DNA-directed RNA polymerase II subunit 9

Chain I:



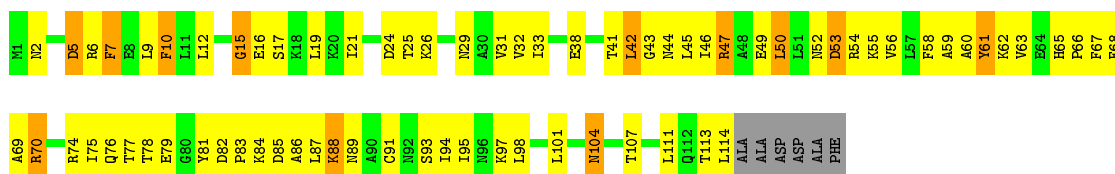
- Molecule 13: DNA-directed RNA polymerases I/II/III subunit 10

Chain J:



- Molecule 14: DNA-directed RNA polymerase II 13.6 kDa polypeptide

Chain K:



- Molecule 15: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide

Chain L:





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	221.37Å 392.50Å 283.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 4.00 48.83 – 3.78	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-4.00) 94.4 (48.83-3.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.10 (at 4.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.253 , 0.276 0.260 , 0.274	Depositor DCC
R_{free} test set	2054 reflections (2.01%)	DCC
Wilson B-factor (Å ²)	76.9	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.18 , -11.4	EDS
Estimated twinning fraction	0.210 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.209 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.28$, $\langle L^2 \rangle = 0.11$	Xtriage
Outliers	0 of 101979 reflections	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	31802	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	T	1.15	1/432 (0.2%)	1.03	1/664 (0.2%)
2	N	1.74	1/158 (0.6%)	0.91	1/242 (0.4%)
3	P	1.17	2/240 (0.8%)	1.06	3/373 (0.8%)
4	A	0.50	0/11339	0.75	5/15334 (0.0%)
5	B	0.51	1/9008 (0.0%)	0.74	5/12146 (0.0%)
6	C	0.56	0/2133	0.76	0/2891
7	D	0.46	0/1365	0.71	0/1837
8	E	0.45	0/1788	0.64	0/2406
9	F	0.56	0/691	0.80	0/933
10	G	0.55	0/1368	0.76	0/1844
11	H	0.40	0/1086	0.65	0/1470
12	I	0.49	1/989 (0.1%)	0.72	0/1331
13	J	0.52	0/541	0.80	0/727
14	K	0.52	0/937	0.70	0/1265
15	L	0.47	0/365	0.74	0/485
All	All	0.54	6/32440 (0.0%)	0.75	15/43948 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	B	0	1
6	C	0	1
All	All	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	10	DA	O3'-P	-9.11	1.50	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	6	DC	O3'-P	7.11	1.69	1.61
12	I	78	CYS	CB-SG	-6.30	1.71	1.82
3	P	3	G	P-OP1	-6.03	1.38	1.49
5	B	503	GLY	CA-C	6.02	1.61	1.51
3	P	3	G	C2-N2	5.18	1.39	1.34

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	10	DA	OP1-P-O3'	7.38	121.44	105.20
3	P	3	G	O5'-P-OP1	-7.04	99.36	105.70
3	P	2	A	C2'-C3'-O3'	6.95	124.82	113.70
2	N	6	DC	P-O3'-C3'	6.32	127.28	119.70
5	B	1185	CYS	N-CA-C	-6.23	94.17	111.00
5	B	504	ARG	NE-CZ-NH2	-6.21	117.19	120.30
4	A	567	LYS	C-N-CD	5.73	140.42	128.40
5	B	503	GLY	C-N-CA	5.63	135.77	121.70
5	B	505	ASP	CB-CG-OD2	-5.58	113.28	118.30
4	A	452	LYS	N-CA-C	-5.58	95.94	111.00
3	P	3	G	N9-C1'-C2'	5.24	120.81	114.00
4	A	425	GLN	N-CA-C	-5.18	97.02	111.00
4	A	76	GLU	CB-CA-C	-5.18	100.05	110.40
5	B	508	LEU	CA-CB-CG	-5.16	103.43	115.30
4	A	466	SER	N-CA-C	5.09	124.75	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	B	503	GLY	Mainchain
6	C	82	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	T	387	0	216	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	141	0	81	8	0
3	P	214	0	111	13	0
4	A	11140	0	11217	1300	0
5	B	8836	0	8871	1003	0
6	C	2095	0	2051	255	0
7	D	1356	0	1319	117	0
8	E	1752	0	1776	148	0
9	F	679	0	701	86	0
10	G	1340	0	1357	157	0
11	H	1068	0	1040	110	0
12	I	971	0	930	105	0
13	J	532	0	542	94	0
14	K	919	0	929	93	0
15	L	363	0	387	45	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
17	A	1	0	0	0	0
All	All	31802	0	31528	3238	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 51.

All (3238) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:40:HIS:HB3	10:G:73:LYS:NZ	1.61	1.14
14:K:47:ARG:HH11	14:K:47:ARG:HB3	1.00	1.14
4:A:53:LEU:HD23	4:A:54:ASN:H	1.08	1.12
4:A:76:GLU:O	4:A:76:GLU:HG3	1.53	1.08
4:A:53:LEU:HD23	4:A:54:ASN:N	1.70	1.07
7:D:48:ILE:HG21	10:G:4:ILE:HB	1.33	1.07
5:B:273:LEU:HB2	5:B:276:ILE:HD12	1.33	1.06
5:B:467:GLY:H	5:B:475:SER:HB3	1.18	1.06
5:B:824:ILE:HG22	5:B:1087:PHE:HE2	1.21	1.05
4:A:56:PRO:O	4:A:57:ARG:HG3	1.55	1.05
1:T:20:DC:H4'	4:A:447:GLN:NE2	1.70	1.05
6:C:43:THR:HG22	6:C:44:LEU:H	1.18	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:779:PHE:HE1	4:A:785:PRO:HD3	1.21	1.04
5:B:217:ARG:HE	5:B:405:ARG:HB2	1.20	1.04
4:A:1094:VAL:HG13	4:A:1113:THR:HG21	1.34	1.03
5:B:1072:MET:HE3	5:B:1085:ILE:HB	1.37	1.03
4:A:399:HIS:HB3	4:A:400:PRO:HD3	1.35	1.03
11:H:100:THR:HG23	11:H:138:GLU:HA	1.41	1.02
5:B:23:ALA:HB1	5:B:24:PRO:HD2	1.40	1.02
4:A:1017:LEU:HB2	8:E:206:GLY:H	1.25	1.01
4:A:1161:THR:HG22	4:A:1163:ILE:H	1.23	1.01
4:A:855:THR:HG21	4:A:857:ARG:HE	1.22	1.00
6:C:142:VAL:H	13:J:16:ASP:HB3	1.28	0.99
4:A:963:ILE:HD11	4:A:1048:ASN:HB3	1.43	0.99
12:I:85:PHE:HD2	12:I:85:PHE:H	1.06	0.99
4:A:1424:VAL:HG13	4:A:1436:ILE:HD11	1.44	0.98
7:D:40:HIS:HB3	10:G:73:LYS:HZ3	1.13	0.97
5:B:467:GLY:N	5:B:475:SER:HB3	1.78	0.97
4:A:901:LEU:H	4:A:926:GLN:NE2	1.63	0.97
5:B:589:VAL:HG12	5:B:590:HIS:H	1.25	0.97
14:K:47:ARG:NH1	14:K:47:ARG:HB3	1.80	0.96
8:E:19:VAL:O	8:E:23:VAL:HG23	1.66	0.96
4:A:84:ILE:HD11	4:A:270:LEU:HD13	1.47	0.96
11:H:4:THR:HA	11:H:60:ALA:HB2	1.45	0.96
4:A:40:THR:HG22	4:A:41:MET:HG3	1.48	0.96
13:J:5:VAL:HG12	13:J:6:ARG:HG3	1.47	0.96
1:T:22:DT:H2"	1:T:23:DG:H5"	1.48	0.95
7:D:47:LEU:HD13	7:D:48:ILE:H	1.30	0.95
6:C:166:GLU:HG3	14:K:10:PHE:HZ	1.31	0.95
10:G:15:PRO:HA	10:G:18:PHE:CD1	2.01	0.95
4:A:1329:THR:H	4:A:1335:ILE:HD11	1.30	0.95
10:G:1:MET:SD	10:G:79:PHE:HD1	1.89	0.95
6:C:39:ALA:HA	6:C:164:ALA:HB3	1.49	0.94
5:B:1065:GLN:HE21	5:B:1067:ARG:H	1.08	0.94
4:A:563:PRO:HG3	4:A:572:TRP:CZ2	2.02	0.94
4:A:244:PRO:HB2	4:A:245:PRO:HD3	1.48	0.94
5:B:1072:MET:CE	5:B:1085:ILE:HB	1.98	0.94
6:C:45:ALA:HA	6:C:72:LEU:HD12	1.50	0.93
4:A:535:THR:HG21	4:A:616:VAL:HA	1.50	0.93
14:K:65:HIS:HD2	14:K:67:PHE:H	1.17	0.93
5:B:778:MET:HE1	5:B:1094:ARG:HD3	1.49	0.93
5:B:847:ASP:HB3	6:C:167:HIS:NE2	1.84	0.93
5:B:65:GLU:HG3	5:B:66:ASP:H	1.33	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:754:SER:H	4:A:757:ASN:HD22	1.08	0.92
14:K:47:ARG:CB	14:K:47:ARG:HH11	1.82	0.92
4:A:829:VAL:HG21	5:B:508:LEU:HD13	1.50	0.92
5:B:189:LEU:HA	5:B:192:LEU:HD12	1.52	0.92
5:B:46:GLN:HG3	5:B:47:GLN:H	1.33	0.92
4:A:768:GLN:HG2	4:A:816:HIS:HA	1.51	0.92
10:G:138:THR:HG22	10:G:139:ILE:H	1.32	0.92
4:A:779:PHE:CE1	4:A:785:PRO:HD3	2.05	0.91
8:E:198:ILE:HD11	8:E:212:ARG:HG3	1.52	0.91
6:C:262:LEU:HD11	14:K:87:LEU:HD23	1.53	0.91
5:B:1224:PHE:HE2	8:E:171:LYS:HG3	1.33	0.91
5:B:1065:GLN:HE21	5:B:1067:ARG:N	1.68	0.91
4:A:1445:ILE:H	4:A:1445:ILE:HD12	1.36	0.90
4:A:903:ASN:ND2	4:A:905:ASP:H	1.68	0.90
5:B:999:MET:HG3	5:B:1000:PRO:HD2	1.54	0.90
3:P:2:A:H2'	3:P:3:G:C8	2.05	0.90
6:C:57:VAL:HG11	13:J:60:PHE:HB3	1.52	0.90
4:A:567:LYS:CG	4:A:568:PRO:HD2	2.02	0.89
8:E:180:ARG:HH21	8:E:192:ARG:HB2	1.34	0.89
6:C:47:ASP:HA	15:L:69:ALA:HB3	1.50	0.89
10:G:1:MET:SD	10:G:79:PHE:CD1	2.66	0.89
13:J:64:ASN:HB3	13:J:65:PRO:CD	2.03	0.89
8:E:94:LYS:HE2	8:E:98:ILE:HD11	1.54	0.89
13:J:36:LEU:HD12	13:J:47:ARG:NH1	1.88	0.89
5:B:918:ILE:HB	5:B:935:ARG:HD2	1.54	0.88
5:B:1007:VAL:HG22	5:B:1008:PRO:HD2	1.53	0.88
5:B:778:MET:CE	5:B:1094:ARG:HD3	2.03	0.88
3:P:2:A:H2'	3:P:3:G:H8	1.37	0.88
6:C:44:LEU:HB2	6:C:77:ILE:HD11	1.54	0.88
5:B:579:ARG:HB2	5:B:586:TRP:HE1	1.39	0.88
4:A:858:ASN:ND2	4:A:860:LEU:H	1.72	0.88
10:G:23:LYS:HG3	10:G:56:ILE:HD11	1.54	0.88
4:A:1189:SER:O	4:A:1241:ARG:HD3	1.74	0.88
4:A:1409:LEU:HD13	5:B:1207:LEU:HD21	1.52	0.88
4:A:335:ARG:NH1	5:B:1202:LEU:HD13	1.89	0.87
4:A:901:LEU:HG	4:A:926:GLN:HE21	1.40	0.87
4:A:356:ASP:HB2	4:A:469:ARG:NH1	1.90	0.87
7:D:144:THR:O	7:D:148:LEU:HB2	1.75	0.87
4:A:392:VAL:HG13	4:A:415:LEU:HD11	1.56	0.86
5:B:847:ASP:HB3	6:C:167:HIS:HE2	1.34	0.86
4:A:541:ILE:HG22	4:A:546:VAL:HG23	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:211:VAL:O	5:B:480:SER:HA	1.75	0.86
5:B:579:ARG:HB2	5:B:586:TRP:NE1	1.91	0.86
4:A:353:ILE:HG21	4:A:487:MET:HE3	1.56	0.86
1:T:20:DC:H4'	4:A:447:GLN:HE22	1.40	0.86
10:G:7:LEU:HB2	10:G:74:TYR:CE2	2.10	0.86
6:C:43:THR:HG22	6:C:44:LEU:N	1.88	0.86
4:A:709:THR:HG23	12:I:94:ASP:HA	1.57	0.86
5:B:549:THR:HG22	5:B:550:ASP:H	1.40	0.86
4:A:1341:ILE:HG23	4:A:1342:GLU:N	1.90	0.85
5:B:466:TRP:O	5:B:468:GLU:N	2.08	0.85
4:A:825:ILE:HG22	5:B:508:LEU:HD11	1.59	0.85
4:A:709:THR:HG22	4:A:711:ARG:H	1.38	0.85
6:C:32:SER:O	6:C:36:VAL:HG23	1.76	0.85
4:A:1329:THR:HG22	4:A:1331:SER:H	1.41	0.85
4:A:1444:MET:HE1	9:F:135:ARG:HB2	1.58	0.85
9:F:93:ILE:HD11	9:F:134:ILE:HD11	1.58	0.85
4:A:1312:ASN:O	4:A:1316:VAL:HG23	1.77	0.85
5:B:1197:PRO:HG2	5:B:1200:ALA:HB2	1.59	0.84
7:D:153:ARG:NH2	7:D:184:ALA:HA	1.92	0.84
11:H:81:PRO:HB2	11:H:82:PRO:HD2	1.58	0.84
5:B:800:GLN:HB3	13:J:52:THR:HG21	1.55	0.84
4:A:503:GLN:HE21	9:F:90:ARG:HH21	1.21	0.84
6:C:213:PRO:O	6:C:214:ASN:HB2	1.77	0.84
12:I:8:ARG:HG3	12:I:34:TYR:HE1	1.40	0.84
4:A:1329:THR:CG2	4:A:1331:SER:H	1.90	0.84
4:A:1242:VAL:HG12	4:A:1243:VAL:H	1.41	0.84
6:C:241:ASP:O	6:C:245:VAL:HG23	1.77	0.83
4:A:828:ALA:CB	5:B:530:GLY:HA2	2.08	0.83
5:B:168:GLY:H	5:B:450:ALA:HB1	1.40	0.83
4:A:528:LEU:O	4:A:531:ILE:HG22	1.78	0.83
4:A:567:LYS:HG3	4:A:568:PRO:HD2	1.57	0.83
6:C:56:THR:HG22	6:C:57:VAL:H	1.43	0.83
5:B:521:LEU:HB3	5:B:633:VAL:HG11	1.60	0.83
4:A:808:LEU:HD23	4:A:813:PHE:HA	1.60	0.83
4:A:340:LEU:HD13	4:A:1429:ILE:HG23	1.61	0.83
8:E:213:ILE:HG12	8:E:214:CYS:H	1.44	0.83
6:C:47:ASP:HA	15:L:69:ALA:CB	2.07	0.83
4:A:442:VAL:HB	4:A:489:LEU:HD11	1.61	0.83
5:B:882:THR:HG22	5:B:884:ARG:H	1.41	0.82
4:A:741:ASN:HD22	4:A:744:LYS:H	1.27	0.82
5:B:25:ILE:HD11	5:B:653:VAL:O	1.77	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:J:57:ILE:HA	13:J:60:PHE:HD2	1.44	0.82
5:B:507:LYS:O	5:B:512:ARG:NE	2.10	0.82
5:B:806:THR:HG22	5:B:808:ALA:H	1.42	0.82
5:B:1096:ARG:O	5:B:1097:HIS:HB2	1.77	0.82
12:I:8:ARG:HG3	12:I:34:TYR:CE1	2.13	0.82
5:B:770:GLN:OE1	5:B:983:ARG:HA	1.80	0.82
4:A:475:THR:HG23	4:A:476:SER:H	1.42	0.82
6:C:232:VAL:HG21	6:C:244:VAL:HG22	1.60	0.82
4:A:351:THR:HB	5:B:1103:ILE:HD12	1.62	0.82
5:B:217:ARG:NE	5:B:405:ARG:HB2	1.94	0.82
13:J:16:ASP:OD1	13:J:17:LYS:HD2	1.80	0.82
4:A:55:ASP:C	4:A:57:ARG:H	1.78	0.82
4:A:1329:THR:HG22	4:A:1331:SER:N	1.94	0.82
5:B:955:THR:HG22	5:B:956:THR:H	1.44	0.82
5:B:172:ILE:HD13	5:B:178:ASN:HB3	1.60	0.82
4:A:1444:MET:CE	9:F:135:ARG:HB2	2.08	0.82
5:B:955:THR:HG22	5:B:956:THR:N	1.95	0.82
11:H:102:TYR:OH	11:H:122:LEU:HD22	1.78	0.81
8:E:175:LEU:HD23	8:E:176:PRO:HD2	1.60	0.81
4:A:794:PRO:HG2	4:A:795:GLU:OE2	1.80	0.81
13:J:3:VAL:HG21	13:J:18:TRP:HB2	1.61	0.81
5:B:467:GLY:O	5:B:468:GLU:HB2	1.81	0.81
4:A:1341:ILE:HG23	4:A:1342:GLU:H	1.45	0.81
4:A:1420:ASP:HB3	4:A:1422:ARG:HG3	1.62	0.81
4:A:560:ILE:HG13	11:H:78:SER:HB2	1.62	0.81
5:B:521:LEU:HD22	5:B:633:VAL:HG12	1.63	0.81
5:B:955:THR:HG23	15:L:54:ARG:O	1.80	0.81
4:A:567:LYS:HB3	11:H:96:VAL:H	1.46	0.81
13:J:64:ASN:HB3	13:J:65:PRO:HD3	1.60	0.81
6:C:244:VAL:O	6:C:248:ILE:HG13	1.79	0.81
5:B:1065:GLN:NE2	5:B:1067:ARG:H	1.78	0.81
8:E:2:ASP:O	8:E:3:GLN:HG2	1.81	0.81
4:A:70:CYS:O	4:A:72:GLU:HG2	1.80	0.81
4:A:475:THR:HG23	4:A:476:SER:N	1.96	0.81
4:A:829:VAL:C	4:A:831:THR:H	1.82	0.80
5:B:899:ILE:HD11	5:B:911:ILE:HA	1.61	0.80
5:B:516:ASN:N	5:B:516:ASN:HD22	1.76	0.80
4:A:106:VAL:HG13	4:A:112:LYS:O	1.81	0.80
5:B:515:HIS:HD2	5:B:517:THR:H	1.29	0.80
8:E:16:PHE:CZ	8:E:20:LYS:HE2	2.17	0.80
5:B:233:PRO:HG2	5:B:234:ILE:HD12	1.61	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:78:PRO:HB3	5:B:1201:LYS:HE3	1.62	0.80
5:B:98:THR:O	5:B:126:SER:HB2	1.81	0.80
6:C:184:ASN:ND2	6:C:187:LYS:HA	1.97	0.80
4:A:567:LYS:NZ	11:H:46:LEU:HB2	1.97	0.80
4:A:868:TYR:CE1	4:A:1064:VAL:HG11	2.17	0.80
5:B:1159:ARG:HB3	5:B:1159:ARG:HH11	1.47	0.80
4:A:310:GLY:O	4:A:312:PRO:HD2	1.81	0.80
5:B:952:VAL:HG12	5:B:953:LEU:H	1.46	0.80
12:I:71:SER:OG	12:I:83:ASN:HB2	1.82	0.80
5:B:824:ILE:HG22	5:B:1087:PHE:CE2	2.13	0.80
4:A:768:GLN:CG	4:A:816:HIS:HA	2.11	0.80
9:F:86:THR:HG23	9:F:89:GLU:OE1	1.82	0.79
14:K:21:ILE:HG12	14:K:33:ILE:HG12	1.65	0.79
12:I:26:LEU:HD23	12:I:37:GLU:HA	1.62	0.79
5:B:1099:VAL:O	5:B:1101:ASP:N	2.16	0.79
11:H:59:ILE:HG22	11:H:60:ALA:N	1.97	0.79
13:J:12:LYS:O	13:J:14:VAL:HG23	1.83	0.79
6:C:186:LEU:HD21	6:C:224:GLN:O	1.82	0.79
5:B:705:MET:H	5:B:710:LEU:HD12	1.47	0.79
4:A:76:GLU:O	4:A:76:GLU:CG	2.29	0.79
14:K:113:THR:O	14:K:114:LEU:HB2	1.81	0.79
10:G:13:LEU:HD21	10:G:17:PHE:HB2	1.61	0.79
4:A:903:ASN:C	4:A:903:ASN:HD22	1.86	0.79
11:H:4:THR:HA	11:H:60:ALA:CB	2.13	0.79
11:H:93:TYR:HB3	11:H:144:ILE:O	1.83	0.79
4:A:253:ASN:HB3	5:B:935:ARG:NH2	1.98	0.79
10:G:34:VAL:HG12	10:G:45:ILE:HG21	1.64	0.78
6:C:212:PRO:HB3	6:C:213:PRO:HD2	1.63	0.78
5:B:37:PHE:HE2	5:B:542:MET:HA	1.47	0.78
10:G:128:PRO:O	10:G:138:THR:HG23	1.83	0.78
5:B:508:LEU:O	5:B:509:ALA:HB2	1.82	0.78
5:B:401:PHE:HA	5:B:404:LYS:HG3	1.65	0.78
11:H:23:VAL:HG22	11:H:43:ASN:HA	1.66	0.78
4:A:35:ILE:HG22	4:A:35:ILE:O	1.84	0.78
5:B:1183:LYS:HE3	5:B:1183:LYS:N	1.99	0.77
5:B:953:LEU:HD21	5:B:965:LYS:HB2	1.65	0.77
5:B:863:GLU:OE2	5:B:873:THR:HA	1.84	0.77
6:C:166:GLU:HG3	14:K:10:PHE:CZ	2.19	0.77
4:A:524:VAL:HG12	4:A:525:GLN:H	1.49	0.77
4:A:798:GLY:HA2	4:A:815:PHE:CD1	2.19	0.77
4:A:588:LEU:O	4:A:606:LEU:HA	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:483:LEU:HD11	5:B:491:THR:HG23	1.67	0.77
8:E:117:THR:HG22	8:E:119:SER:H	1.47	0.77
4:A:1424:VAL:HG11	5:B:1139:ILE:HD13	1.66	0.77
4:A:754:SER:H	4:A:757:ASN:ND2	1.83	0.77
5:B:1159:ARG:HD3	5:B:1193:GLN:CG	2.13	0.77
6:C:70:ILE:HG12	6:C:142:VAL:HG11	1.66	0.77
4:A:321:PRO:O	4:A:322:VAL:HB	1.85	0.77
5:B:1162:ILE:HG22	5:B:1163:CYS:H	1.49	0.77
4:A:590:ARG:NH2	4:A:620:LYS:HB3	1.99	0.77
14:K:65:HIS:CD2	14:K:67:PHE:H	2.02	0.77
4:A:567:LYS:HB3	11:H:95:TYR:HA	1.67	0.77
4:A:1116:LEU:HB2	4:A:1329:THR:OG1	1.83	0.77
4:A:836:TYR:CE2	4:A:840:ARG:HD2	2.19	0.77
5:B:859:TYR:OH	5:B:941:LEU:HD12	1.85	0.76
5:B:102:VAL:HG23	5:B:112:LEU:HB2	1.66	0.76
5:B:1201:LYS:HE2	5:B:1205:GLN:OE1	1.85	0.76
4:A:399:HIS:CB	4:A:400:PRO:HD3	2.15	0.76
5:B:503:GLY:HA3	5:B:507:LYS:HE3	1.67	0.76
8:E:22:MET:HE3	8:E:26:ARG:HE	1.50	0.76
8:E:29:PHE:O	8:E:30:ILE:HG13	1.85	0.76
6:C:43:THR:CG2	6:C:44:LEU:H	1.96	0.76
5:B:39:ARG:NH2	5:B:665:GLU:HG2	2.01	0.76
5:B:1034:VAL:HG12	5:B:1035:ALA:N	1.99	0.76
5:B:53:GLN:HG2	5:B:547:VAL:HG22	1.66	0.76
4:A:886:ILE:HD11	4:A:943:LEU:HB3	1.66	0.76
11:H:42:ILE:HG23	11:H:95:TYR:HE1	1.50	0.76
4:A:1291:VAL:HG13	4:A:1292:PRO:HD2	1.66	0.76
7:D:48:ILE:CG2	10:G:4:ILE:HB	2.12	0.76
5:B:798:TYR:HE2	6:C:62:PHE:CE2	2.03	0.76
12:I:8:ARG:CG	12:I:34:TYR:HE1	1.99	0.76
5:B:363:HIS:O	5:B:364:ILE:HB	1.85	0.75
4:A:534:LEU:O	4:A:574:GLY:HA3	1.85	0.75
4:A:87:ALA:HB3	4:A:276:LEU:HD23	1.67	0.75
5:B:1007:VAL:CG2	5:B:1008:PRO:HD2	2.16	0.75
5:B:1159:ARG:NH1	5:B:1159:ARG:HB3	2.01	0.75
4:A:152:VAL:CG1	4:A:153:PRO:HD2	2.17	0.75
6:C:179:GLU:HG2	6:C:180:TYR:N	1.99	0.75
4:A:225:ASN:HD22	4:A:228:PHE:H	1.32	0.75
4:A:1424:VAL:HG13	4:A:1436:ILE:CD1	2.15	0.75
5:B:200:GLY:HA2	5:B:202:TYR:CE2	2.22	0.75
7:D:40:HIS:CB	10:G:73:LYS:NZ	2.46	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1343:ALA:HB2	8:E:150:VAL:HG22	1.66	0.75
4:A:590:ARG:NH1	4:A:590:ARG:HG3	2.02	0.75
5:B:37:PHE:CD1	5:B:41:LYS:HG3	2.22	0.75
5:B:995:ARG:HH12	6:C:165:LYS:HG2	1.52	0.75
4:A:855:THR:CG2	4:A:857:ARG:HE	1.99	0.75
5:B:577:ALA:HB1	5:B:589:VAL:HG11	1.68	0.75
5:B:613:VAL:HG13	5:B:627:PHE:O	1.87	0.75
5:B:351:TYR:CE1	5:B:355:ILE:HD11	2.21	0.75
7:D:170:THR:CG2	7:D:172:LEU:HG	2.17	0.75
5:B:37:PHE:CE1	5:B:41:LYS:HG3	2.22	0.75
4:A:899:VAL:HB	4:A:929:LEU:CD1	2.17	0.75
1:T:15:DT:H5"	4:A:1407:GLU:OE2	1.87	0.75
4:A:388:LEU:O	4:A:392:VAL:HG23	1.87	0.74
4:A:741:ASN:HD21	4:A:743:VAL:HB	1.50	0.74
4:A:92:HIS:O	4:A:94:GLY:N	2.19	0.74
4:A:1004:ASN:ND2	8:E:167:ARG:HD2	2.02	0.74
4:A:670:ILE:HG23	4:A:805:LEU:HD21	1.68	0.74
4:A:1116:LEU:N	4:A:1308:THR:HG22	2.02	0.74
4:A:993:LEU:HD23	4:A:1022:LEU:HD21	1.70	0.74
6:C:66:ARG:NH2	13:J:5:VAL:HG23	2.01	0.74
4:A:93:VAL:HG13	4:A:301:ALA:HB1	1.67	0.74
5:B:604:ARG:NH2	5:B:613:VAL:O	2.20	0.74
5:B:1099:VAL:CG1	5:B:1100:ASP:N	2.50	0.74
4:A:438:ASP:O	4:A:439:ASN:HB2	1.87	0.74
4:A:49:LYS:NZ	4:A:61:ILE:HG13	2.03	0.74
4:A:1332:PHE:HD2	4:A:1332:PHE:N	1.85	0.74
4:A:87:ALA:CB	4:A:276:LEU:HD23	2.18	0.74
5:B:359:GLU:O	5:B:362:PRO:HD3	1.87	0.74
5:B:378:LEU:HD12	5:B:378:LEU:O	1.86	0.74
4:A:1161:THR:HG22	4:A:1163:ILE:N	2.02	0.74
5:B:801:LYS:O	13:J:52:THR:HG23	1.88	0.74
5:B:223:VAL:HG11	5:B:381:MET:HG2	1.68	0.74
5:B:642:ASP:O	5:B:644:GLU:N	2.20	0.74
9:F:81:THR:HG21	9:F:136:ARG:HD3	1.70	0.74
4:A:858:ASN:HD22	4:A:858:ASN:C	1.89	0.74
5:B:996:ARG:NH1	6:C:38:ILE:HG23	2.01	0.74
4:A:107:CYS:SG	4:A:171:GLN:HG2	2.28	0.74
4:A:646:PHE:O	4:A:650:GLN:HG3	1.88	0.74
4:A:69:THR:O	4:A:71:GLN:N	2.21	0.73
5:B:902:GLY:O	15:L:65:VAL:HG11	1.87	0.73
14:K:12:LEU:H	14:K:12:LEU:HD12	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:80:LYS:HD3	10:G:80:LYS:N	2.03	0.73
4:A:335:ARG:HA	4:A:339:ASN:HB2	1.68	0.73
4:A:248:PRO:O	4:A:260:ASP:HB2	1.87	0.73
7:D:40:HIS:HB3	10:G:73:LYS:HZ2	1.51	0.73
5:B:1224:PHE:CE2	8:E:171:LYS:HG3	2.20	0.73
5:B:906:SER:O	5:B:941:LEU:HD23	1.87	0.73
4:A:239:LEU:HD12	4:A:240:PRO:HD2	1.69	0.73
14:K:45:LEU:HG	14:K:94:ILE:HD13	1.69	0.73
4:A:1121:GLU:HG2	4:A:1122:PRO:HD2	1.68	0.73
4:A:783:THR:HG21	4:A:815:PHE:CZ	2.23	0.73
4:A:384:ASN:OD1	4:A:388:LEU:HD12	1.89	0.73
4:A:164:ARG:HG3	4:A:165:GLY:N	2.02	0.73
5:B:370:PHE:HE2	5:B:373:ARG:HH11	1.36	0.73
4:A:855:THR:HG21	4:A:857:ARG:NE	2.01	0.73
4:A:1422:ARG:HH22	5:B:1224:PHE:C	1.91	0.73
7:D:138:ASN:OD1	7:D:141:LEU:HB2	1.89	0.73
12:I:7:CYS:HB3	12:I:14:LEU:HD21	1.71	0.73
10:G:23:LYS:HG3	10:G:56:ILE:CD1	2.18	0.73
4:A:856:THR:HB	4:A:865:GLN:HB2	1.69	0.73
4:A:1348:LEU:HG	4:A:1372:VAL:CG2	2.18	0.73
5:B:295:GLY:H	5:B:298:LEU:HD23	1.53	0.73
7:D:29:LEU:HD22	10:G:82:PHE:CE2	2.24	0.72
5:B:615:MET:HB3	5:B:626:ILE:HG12	1.71	0.72
5:B:975:GLN:O	5:B:990:ILE:HD12	1.89	0.72
4:A:903:ASN:HD22	4:A:904:THR:N	1.87	0.72
4:A:382:PRO:HB3	4:A:428:TYR:HE2	1.53	0.72
4:A:302:THR:HA	4:A:305:ASP:O	1.89	0.72
4:A:567:LYS:CD	4:A:568:PRO:HD2	2.19	0.72
5:B:507:LYS:H	5:B:512:ARG:HH21	1.35	0.72
5:B:1017:ILE:HB	5:B:1018:PRO:HD3	1.71	0.72
5:B:603:LEU:HD13	5:B:608:ASP:HB2	1.71	0.72
6:C:165:LYS:O	14:K:6:ARG:NH1	2.22	0.72
4:A:347:PHE:H	5:B:1107:ALA:HA	1.55	0.72
5:B:171:PRO:HD2	5:B:457:LEU:HD13	1.71	0.72
9:F:119:ARG:HG3	9:F:119:ARG:HH11	1.53	0.72
7:D:176:GLU:O	7:D:178:ALA:N	2.18	0.72
4:A:1239:ARG:HH22	4:A:1241:ARG:NH2	1.87	0.72
5:B:879:ARG:HH11	5:B:883:LEU:HD22	1.54	0.72
5:B:1001:PHE:CE1	5:B:1073:TYR:HB2	2.24	0.72
5:B:281:PRO:HG2	5:B:284:ILE:HG13	1.69	0.72
10:G:74:TYR:HD2	10:G:74:TYR:H	1.35	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:365:THR:HG23	5:B:367:LEU:H	1.55	0.72
5:B:502:ILE:HG12	5:B:535:LEU:HD13	1.71	0.72
5:B:361:LEU:HD21	5:B:377:PHE:CD2	2.24	0.72
5:B:594:ALA:HA	5:B:617:ARG:NH1	2.05	0.72
15:L:30:ILE:O	15:L:56:LEU:HA	1.88	0.72
7:D:134:THR:HG22	7:D:136:GLY:H	1.52	0.72
5:B:589:VAL:HG12	5:B:590:HIS:N	2.04	0.72
5:B:112:LEU:HD12	5:B:113:TYR:H	1.54	0.72
5:B:953:LEU:O	5:B:953:LEU:HD23	1.89	0.72
4:A:67:CYS:O	4:A:70:CYS:HB3	1.90	0.72
11:H:40:LEU:HD13	11:H:123:MET:HB2	1.70	0.72
5:B:847:ASP:HB3	6:C:167:HIS:CD2	2.24	0.72
5:B:1095:LEU:HD12	5:B:1095:LEU:H	1.54	0.72
6:C:98:VAL:C	6:C:99:LEU:HD23	2.09	0.72
7:D:33:PHE:CE1	10:G:80:LYS:HE3	2.24	0.71
12:I:50:THR:HG22	12:I:52:ILE:H	1.55	0.71
5:B:1099:VAL:HG12	5:B:1100:ASP:H	1.53	0.71
5:B:223:VAL:CG1	5:B:381:MET:HG2	2.19	0.71
5:B:601:ARG:O	5:B:605:ARG:HG3	1.89	0.71
4:A:567:LYS:HZ1	11:H:46:LEU:HB2	1.53	0.71
5:B:23:ALA:HB1	5:B:24:PRO:CD	2.19	0.71
4:A:1437:GLY:O	4:A:1439:GLY:N	2.23	0.71
6:C:45:ALA:HA	6:C:72:LEU:CD1	2.19	0.71
5:B:562:GLY:HA3	5:B:590:HIS:CE1	2.26	0.71
4:A:897:TYR:HD2	4:A:936:LEU:HD13	1.55	0.71
5:B:800:GLN:HB3	13:J:52:THR:CG2	2.20	0.71
5:B:411:PRO:O	5:B:414:ALA:HB3	1.89	0.71
4:A:590:ARG:HB3	4:A:605:MET:N	2.05	0.71
13:J:14:VAL:CG1	13:J:50:ILE:HD11	2.20	0.71
6:C:183:TRP:CZ2	6:C:207:CYS:HB3	2.25	0.71
4:A:598:LEU:HA	11:H:122:LEU:HD13	1.71	0.71
5:B:364:ILE:HG12	5:B:585:VAL:HG13	1.72	0.71
4:A:164:ARG:HG3	4:A:165:GLY:H	1.52	0.71
4:A:800:VAL:HG22	4:A:812:GLU:HB3	1.73	0.71
10:G:119:LEU:HD12	10:G:131:GLN:O	1.91	0.71
4:A:1239:ARG:HH22	4:A:1241:ARG:HH22	1.39	0.71
5:B:1085:ILE:HD12	5:B:1085:ILE:N	2.06	0.71
4:A:1094:VAL:HG13	4:A:1113:THR:CG2	2.16	0.71
10:G:30:LEU:HD13	10:G:72:VAL:HG11	1.72	0.71
5:B:1069:PHE:HD1	5:B:1069:PHE:H	1.37	0.71
5:B:35:SER:HA	5:B:811:TYR:HE2	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:K:7:PHE:HA	14:K:10:PHE:CE2	2.26	0.71
12:I:34:TYR:CD2	12:I:35:VAL:N	2.59	0.71
5:B:728:ARG:HH12	5:B:1047:PHE:HB3	1.56	0.71
5:B:737:THR:HG21	12:I:66:PRO:HA	1.73	0.71
5:B:710:LEU:HA	5:B:733:HIS:HB3	1.74	0.70
4:A:1006:ILE:HD12	8:E:163:GLU:HG3	1.73	0.70
5:B:882:THR:HG22	5:B:884:ARG:N	2.05	0.70
12:I:111:THR:HG22	12:I:112:SER:N	2.06	0.70
4:A:1151:GLU:OE2	12:I:45:ARG:HD2	1.90	0.70
4:A:1191:TRP:CD1	4:A:1256:GLU:HB2	2.27	0.70
8:E:124:VAL:HG13	8:E:132:ILE:HB	1.71	0.70
4:A:250:ILE:O	4:A:258:GLY:HA3	1.91	0.70
5:B:871:THR:HG22	5:B:872:GLU:O	1.90	0.70
11:H:81:PRO:CB	11:H:82:PRO:HD2	2.20	0.70
4:A:1332:PHE:N	4:A:1332:PHE:CD2	2.58	0.70
5:B:794:ASN:C	5:B:795:ILE:HD12	2.11	0.70
4:A:244:PRO:HB2	4:A:245:PRO:CD	2.20	0.70
5:B:1163:CYS:SG	5:B:1165:ILE:HB	2.30	0.70
4:A:63:ARG:HA	4:A:74:MET:SD	2.32	0.70
11:H:36:CYS:HA	11:H:126:GLU:O	1.91	0.70
5:B:365:THR:HG23	5:B:367:LEU:HG	1.74	0.70
8:E:213:ILE:HG12	8:E:214:CYS:N	2.06	0.70
5:B:827:ILE:HD12	5:B:1086:PHE:HD2	1.55	0.70
5:B:615:MET:C	5:B:616:ILE:HD12	2.11	0.70
5:B:1073:TYR:CE2	5:B:1080:LYS:HG2	2.27	0.70
6:C:20:PHE:HE1	6:C:22:LEU:HD12	1.56	0.70
4:A:903:ASN:HD22	4:A:905:ASP:H	1.37	0.70
4:A:346:ASP:HB3	5:B:1108:ARG:H	1.56	0.70
6:C:66:ARG:NH1	13:J:2:ILE:HG21	2.07	0.70
9:F:103:MET:O	9:F:104:ASN:HB2	1.91	0.70
4:A:382:PRO:HD3	4:A:428:TYR:CD2	2.26	0.70
7:D:130:LEU:C	7:D:132:GLN:H	1.95	0.70
14:K:50:LEU:HD11	14:K:75:ILE:HD13	1.72	0.70
4:A:1155:ASP:OD2	4:A:1161:THR:HG23	1.91	0.70
10:G:15:PRO:HA	10:G:18:PHE:CE1	2.27	0.70
4:A:1341:ILE:CG2	4:A:1342:GLU:H	2.04	0.70
13:J:8:PHE:H	13:J:49:MET:CE	2.05	0.70
4:A:1394:THR:HG21	4:A:1398:MET:SD	2.32	0.70
15:L:48:CYS:HB3	15:L:51:CYS:O	1.91	0.69
7:D:66:ARG:HD2	7:D:133:THR:HB	1.74	0.69
4:A:56:PRO:O	4:A:57:ARG:CG	2.38	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1450:LEU:HG	4:A:1450:LEU:O	1.92	0.69
6:C:177:GLU:HB2	6:C:231:ASN:HB3	1.74	0.69
14:K:31:VAL:HG12	14:K:32:VAL:N	2.07	0.69
5:B:1002:THR:HG21	5:B:1006:ILE:HD12	1.74	0.69
4:A:254:GLU:HB2	5:B:935:ARG:HH12	1.56	0.69
5:B:847:ASP:C	5:B:849:GLY:H	1.93	0.69
4:A:79:GLY:HA3	4:A:243:PRO:CG	2.21	0.69
5:B:948:ILE:HG22	5:B:949:VAL:O	1.92	0.69
9:F:125:LEU:O	9:F:125:LEU:HG	1.91	0.69
4:A:816:HIS:CD2	5:B:764:SER:HB2	2.27	0.69
4:A:722:LEU:O	4:A:725:ALA:HB3	1.91	0.69
5:B:708:GLU:O	5:B:710:LEU:N	2.26	0.69
8:E:135:PHE:HD2	8:E:140:LEU:HD21	1.55	0.69
4:A:450:LEU:N	4:A:450:LEU:HD12	2.07	0.69
11:H:59:ILE:HG22	11:H:60:ALA:H	1.58	0.69
4:A:49:LYS:HE2	4:A:61:ILE:HD12	1.73	0.69
4:A:427:GLN:HG3	4:A:430:TRP:CZ2	2.27	0.69
5:B:701:ILE:HD11	5:B:703:ILE:HD11	1.74	0.69
5:B:1099:VAL:HG12	5:B:1100:ASP:N	2.07	0.69
13:J:48:ARG:HD2	13:J:49:MET:N	2.08	0.69
4:A:1293:SER:OG	4:A:1294:PRO:HD2	1.93	0.69
7:D:47:LEU:HD13	7:D:48:ILE:N	2.05	0.69
7:D:34:GLN:O	7:D:47:LEU:HD23	1.92	0.69
4:A:665:GLY:O	4:A:667:GLY:N	2.26	0.69
4:A:463:ILE:HB	4:A:464:PRO:HD2	1.75	0.69
4:A:107:CYS:N	4:A:114:LEU:HD21	2.08	0.69
8:E:22:MET:HE3	8:E:26:ARG:NE	2.07	0.69
15:L:58:LYS:HG2	15:L:58:LYS:O	1.92	0.69
4:A:1030:ARG:HG3	4:A:1034:GLU:OE2	1.92	0.69
15:L:38:LEU:O	15:L:39:SER:HB3	1.91	0.69
4:A:154:SER:HB3	4:A:162:VAL:HG21	1.74	0.69
5:B:496:ARG:HB3	5:B:496:ARG:HH11	1.57	0.69
4:A:55:ASP:C	4:A:57:ARG:N	2.47	0.69
4:A:853:ASP:OD1	4:A:855:THR:N	2.26	0.69
4:A:857:ARG:HD3	4:A:861:GLY:O	1.92	0.69
4:A:901:LEU:HG	4:A:926:GLN:NE2	2.08	0.69
6:C:239:PRO:HB2	6:C:241:ASP:OD1	1.92	0.69
8:E:135:PHE:HB3	8:E:140:LEU:HD11	1.75	0.69
6:C:263:THR:C	6:C:265:MET:H	1.96	0.69
3:P:10:C:H4'	4:A:485:ASP:OD1	1.92	0.69
6:C:5:GLY:O	6:C:7:GLN:HG3	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:503:GLN:HE21	9:F:90:ARG:NH2	1.91	0.69
4:A:886:ILE:HG22	4:A:887:GLY:N	2.08	0.69
4:A:694:THR:O	4:A:698:GLN:HG3	1.90	0.69
5:B:831:SER:HB3	5:B:994:TYR:OH	1.93	0.68
4:A:107:CYS:H	4:A:114:LEU:HD21	1.56	0.68
14:K:46:ILE:O	14:K:50:LEU:HB2	1.92	0.68
7:D:52:LEU:HD21	7:D:147:TYR:HE2	1.57	0.68
10:G:7:LEU:HD11	10:G:45:ILE:HD11	1.76	0.68
4:A:853:ASP:O	4:A:854:ASN:HB2	1.92	0.68
5:B:806:THR:HG22	5:B:808:ALA:N	2.08	0.68
1:T:15:DT:H1'	4:A:1386:ARG:NH1	2.09	0.68
4:A:88:LYS:HE3	4:A:280:GLU:OE2	1.94	0.68
5:B:1115:THR:O	5:B:1116:ARG:HB2	1.92	0.68
4:A:591:PHE:HA	4:A:595:THR:HG21	1.76	0.68
4:A:866:PHE:O	4:A:867:ILE:HG13	1.94	0.68
5:B:1165:ILE:HG22	5:B:1166:CYS:N	2.07	0.68
4:A:1332:PHE:H	4:A:1332:PHE:HD2	1.40	0.68
5:B:282:ILE:HD12	5:B:382:ILE:HD13	1.75	0.68
4:A:672:ASP:HB2	4:A:736:ASN:OD1	1.92	0.68
4:A:285:PRO:HG2	4:A:288:ALA:HB3	1.74	0.68
4:A:885:THR:O	4:A:940:ARG:HD2	1.92	0.68
4:A:567:LYS:HD3	11:H:95:TYR:CD2	2.28	0.68
4:A:666:ILE:HD12	4:A:667:GLY:H	1.57	0.68
5:B:1180:PHE:HB3	5:B:1191:ILE:HD12	1.76	0.68
11:H:99:GLY:HA3	11:H:118:PHE:HA	1.75	0.68
5:B:1223:ASP:O	5:B:1224:PHE:HB2	1.92	0.68
9:F:82:THR:HG22	9:F:84:TYR:H	1.56	0.68
4:A:547:LEU:HD22	14:K:58:PHE:CD1	2.29	0.68
5:B:824:ILE:CG2	5:B:1087:PHE:HE2	2.03	0.68
6:C:167:HIS:CE1	15:L:70:ARG:HB3	2.29	0.68
4:A:1348:LEU:HG	4:A:1372:VAL:HG23	1.74	0.68
5:B:293:PRO:HG2	5:B:296:GLU:HB3	1.75	0.68
6:C:114:TYR:HB3	6:C:140:ASN:O	1.93	0.68
3:P:1:A:H2'	3:P:2:A:C8	2.28	0.68
13:J:44:TYR:HA	13:J:47:ARG:HB2	1.74	0.68
4:A:325:ILE:HG21	5:B:1210:MET:HG3	1.76	0.68
4:A:1152:ILE:HG13	12:I:44:TYR:HB3	1.76	0.68
4:A:763:ALA:O	4:A:803:SER:HB3	1.93	0.68
6:C:56:THR:HG22	6:C:57:VAL:N	2.09	0.68
15:L:40:LEU:HD13	15:L:44:ASP:HB3	1.76	0.68
8:E:198:ILE:CD1	8:E:212:ARG:HG3	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:152:VAL:HG12	4:A:153:PRO:HD2	1.75	0.68
5:B:502:ILE:HG22	5:B:507:LYS:HD2	1.76	0.68
5:B:745:PRO:O	5:B:748:ILE:HG12	1.94	0.68
9:F:130:ILE:O	9:F:148:VAL:HG21	1.93	0.68
4:A:1445:ILE:N	4:A:1445:ILE:HD12	2.06	0.67
6:C:73:GLN:NE2	6:C:74:SER:H	1.92	0.67
4:A:475:THR:CG2	4:A:476:SER:H	2.07	0.67
4:A:800:VAL:HG13	4:A:812:GLU:OE1	1.94	0.67
6:C:253:LYS:O	6:C:256:ALA:HB3	1.95	0.67
4:A:567:LYS:CE	11:H:46:LEU:HB2	2.25	0.67
9:F:90:ARG:HG3	9:F:91:ALA:N	2.09	0.67
6:C:179:GLU:HG2	6:C:180:TYR:H	1.59	0.67
5:B:1208:MET:O	5:B:1211:ASN:N	2.23	0.67
5:B:653:VAL:CG2	5:B:689:LEU:HB3	2.24	0.67
4:A:1341:ILE:CG2	4:A:1342:GLU:N	2.57	0.67
4:A:503:GLN:NE2	9:F:90:ARG:HH21	1.92	0.67
7:D:170:THR:HG21	7:D:172:LEU:HG	1.75	0.67
4:A:69:THR:C	4:A:71:GLN:H	1.95	0.67
4:A:458:HIS:CE1	4:A:507:VAL:HG21	2.30	0.67
4:A:3:GLY:O	4:A:4:GLN:HB2	1.94	0.67
2:N:3:DG:H2''	2:N:4:DT:OP2	1.93	0.67
4:A:55:ASP:CG	4:A:55:ASP:O	2.31	0.67
1:T:23:DG:H2'	1:T:24:DG:C8	2.29	0.67
13:J:44:TYR:HA	13:J:47:ARG:CB	2.24	0.67
7:D:198:LEU:O	7:D:200:ASN:N	2.27	0.67
5:B:393:LYS:HA	5:B:393:LYS:HE3	1.77	0.67
4:A:356:ASP:HB2	4:A:469:ARG:HH11	1.56	0.67
10:G:138:THR:HG22	10:G:139:ILE:N	2.09	0.67
5:B:1045:SER:O	5:B:1046:PRO:O	2.12	0.67
7:D:40:HIS:CB	10:G:73:LYS:HZ2	2.07	0.67
4:A:399:HIS:HB3	4:A:400:PRO:CD	2.17	0.67
4:A:590:ARG:HH11	4:A:590:ARG:HG3	1.59	0.67
4:A:1017:LEU:HB2	8:E:206:GLY:N	2.06	0.67
4:A:869:GLY:O	8:E:204:THR:HG21	1.94	0.67
4:A:79:GLY:HA3	4:A:243:PRO:HG2	1.77	0.67
4:A:844:ALA:C	4:A:845:LEU:HD23	2.15	0.67
5:B:955:THR:CG2	5:B:956:THR:H	2.08	0.67
5:B:746:SER:HB2	5:B:1046:PRO:HG2	1.76	0.67
8:E:90:VAL:HG23	8:E:120:ALA:HA	1.76	0.67
5:B:108:VAL:HG12	5:B:109:THR:H	1.58	0.67
8:E:48:ASP:CG	8:E:49:SER:H	1.99	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:758:PHE:CE1	5:B:1027:ILE:HG22	2.29	0.67
12:I:55:THR:CG2	12:I:58:VAL:HG21	2.25	0.67
5:B:860:MET:HG2	5:B:861:ASP:N	2.10	0.67
4:A:450:LEU:H	4:A:450:LEU:HD12	1.60	0.67
8:E:157:SER:OG	8:E:160:GLU:HG3	1.94	0.67
4:A:874:ASP:N	4:A:1058:VAL:HG22	2.10	0.66
5:B:192:LEU:O	5:B:193:LYS:HB2	1.95	0.66
4:A:1336:MET:CE	4:A:1381:LEU:HG	2.26	0.66
4:A:19:PHE:O	4:A:1416:ALA:HA	1.95	0.66
5:B:244:LEU:HD21	5:B:366:GLN:NE2	2.09	0.66
5:B:563:MET:HE3	5:B:580:VAL:HB	1.76	0.66
5:B:1065:GLN:NE2	5:B:1066:SER:N	2.42	0.66
5:B:515:HIS:CD2	5:B:517:THR:H	2.12	0.66
5:B:125:SER:HA	5:B:171:PRO:HA	1.77	0.66
4:A:351:THR:HG22	5:B:1103:ILE:HA	1.76	0.66
4:A:1261:LYS:O	4:A:1264:GLU:HB3	1.95	0.66
5:B:975:GLN:HG2	5:B:976:ILE:H	1.60	0.66
5:B:899:ILE:CD1	5:B:911:ILE:HA	2.26	0.66
5:B:95:ILE:HG13	5:B:130:VAL:HG22	1.77	0.66
11:H:17:PRO:HB3	11:H:24:CYS:SG	2.35	0.66
4:A:567:LYS:HE3	11:H:46:LEU:HB2	1.78	0.66
5:B:376:PHE:CE2	5:B:569:TYR:HD2	2.12	0.66
5:B:508:LEU:O	5:B:509:ALA:CB	2.43	0.66
4:A:1444:MET:HG2	10:G:60:ARG:HA	1.75	0.66
4:A:503:GLN:C	4:A:504:LEU:HD12	2.16	0.66
4:A:12:ARG:HD2	5:B:1218:THR:HB	1.76	0.66
10:G:143:ILE:HG22	10:G:144:ARG:N	2.10	0.66
6:C:39:ALA:CA	6:C:164:ALA:HB3	2.22	0.66
4:A:335:ARG:HH12	5:B:1202:LEU:HD13	1.58	0.66
5:B:516:ASN:ND2	5:B:516:ASN:N	2.43	0.66
5:B:642:ASP:HB3	5:B:649:LYS:CD	2.26	0.66
11:H:126:GLU:C	11:H:130:ARG:HH22	1.98	0.66
6:C:66:ARG:HH21	13:J:5:VAL:HG23	1.61	0.66
5:B:852:ARG:HH22	15:L:70:ARG:C	1.99	0.66
4:A:899:VAL:HB	4:A:929:LEU:HD11	1.77	0.66
4:A:666:ILE:HD11	5:B:1067:ARG:O	1.95	0.66
12:I:32:CYS:SG	12:I:33:SER:N	2.69	0.66
5:B:503:GLY:HA3	5:B:507:LYS:CE	2.25	0.66
5:B:952:VAL:HG12	5:B:953:LEU:N	2.11	0.66
1:T:20:DC:H4'	4:A:447:GLN:CD	2.16	0.66
5:B:859:TYR:CZ	5:B:941:LEU:HD12	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:23:SER:HA	4:A:233:TRP:CD1	2.31	0.66
4:A:1291:VAL:HG13	4:A:1292:PRO:CD	2.26	0.66
4:A:701:LEU:HD21	12:I:114:GLN:HB2	1.78	0.66
4:A:590:ARG:HH21	4:A:620:LYS:HB3	1.60	0.66
5:B:357:GLN:O	5:B:366:GLN:HA	1.96	0.66
11:H:81:PRO:CB	11:H:82:PRO:CD	2.73	0.66
5:B:39:ARG:HH21	5:B:665:GLU:HG2	1.60	0.66
5:B:229:ALA:HB1	5:B:231:PRO:HD2	1.77	0.66
10:G:43:GLY:HA3	10:G:80:LYS:HB3	1.76	0.65
4:A:868:TYR:HD2	4:A:1058:VAL:HG21	1.59	0.65
5:B:46:GLN:HG3	5:B:47:GLN:N	2.10	0.65
5:B:1182:CYS:SG	5:B:1182:CYS:O	2.54	0.65
8:E:153:HIS:HB3	8:E:196:VAL:HG11	1.78	0.65
4:A:567:LYS:CB	11:H:95:TYR:HA	2.25	0.65
4:A:535:THR:CG2	4:A:616:VAL:HA	2.26	0.65
7:D:56:ARG:HD3	7:D:149:THR:HA	1.77	0.65
4:A:269:ILE:HD13	4:A:300:VAL:HG22	1.78	0.65
4:A:1120:LEU:O	4:A:1323:ASP:HB2	1.96	0.65
6:C:147:LEU:HB2	6:C:151:GLN:HB2	1.78	0.65
10:G:59:GLY:HA3	10:G:70:PHE:CD2	2.32	0.65
9:F:79:ARG:HG3	9:F:144:GLU:OE1	1.96	0.65
5:B:821:GLN:HE22	5:B:851:PHE:HA	1.60	0.65
11:H:100:THR:OG1	11:H:138:GLU:HG3	1.97	0.65
5:B:995:ARG:NH1	6:C:165:LYS:HG2	2.10	0.65
5:B:616:ILE:N	5:B:616:ILE:HD12	2.11	0.65
4:A:548:ASN:OD1	14:K:60:ALA:HB1	1.97	0.65
4:A:2:VAL:HG21	5:B:1157:ALA:C	2.17	0.65
5:B:978:ASP:OD2	5:B:1098:MET:HG2	1.95	0.65
4:A:108:MET:SD	4:A:108:MET:N	2.69	0.65
4:A:1115:SER:O	4:A:1116:LEU:HB3	1.94	0.65
5:B:179:CYS:SG	5:B:181:LEU:HB2	2.37	0.65
6:C:177:GLU:HG3	6:C:231:ASN:HD22	1.62	0.65
5:B:465:ASN:HD22	5:B:465:ASN:N	1.95	0.65
4:A:907:THR:CG2	4:A:908:LEU:N	2.58	0.65
7:D:134:THR:HG22	7:D:135:GLY:N	2.12	0.65
8:E:202:SER:OG	8:E:204:THR:HG22	1.97	0.65
8:E:176:PRO:O	8:E:212:ARG:HA	1.96	0.65
5:B:121:ASN:HA	5:B:207:GLY:HA2	1.79	0.65
5:B:766:ARG:HH22	5:B:1020:ARG:HH11	1.42	0.65
5:B:172:ILE:HD13	5:B:178:ASN:CB	2.27	0.65
5:B:642:ASP:HA	5:B:649:LYS:HA	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:56:THR:HB	11:H:145:ARG:HG2	1.79	0.65
5:B:557:PHE:CD2	5:B:557:PHE:C	2.69	0.65
4:A:1224:LEU:HD12	4:A:1241:ARG:O	1.97	0.65
4:A:385:ILE:HG22	4:A:386:ASP:N	2.11	0.65
6:C:252:GLN:HG3	14:K:95:ILE:HG23	1.79	0.65
5:B:840:ILE:HB	5:B:1011:ILE:HB	1.77	0.65
4:A:18:GLN:HB2	5:B:1215:ARG:HB2	1.80	0.65
6:C:77:ILE:HG23	6:C:161:LYS:HE3	1.79	0.64
5:B:190:TYR:CE2	13:J:62:ARG:HB3	2.31	0.64
7:D:130:LEU:O	7:D:132:GLN:N	2.29	0.64
2:N:1:DA:H1'	2:N:2:DA:O5'	1.96	0.64
3:P:9:G:H5''	5:B:776:GLN:HE22	1.62	0.64
6:C:80:LEU:HD11	6:C:95:CYS:CA	2.28	0.64
7:D:202:ILE:HG21	7:D:207:LEU:HB2	1.78	0.64
7:D:5:THR:O	7:D:6:SER:O	2.15	0.64
4:A:1438:THR:HB	5:B:1144:ALA:HB3	1.80	0.64
4:A:332:LYS:HG3	4:A:333:GLU:HG2	1.77	0.64
4:A:618:GLU:O	4:A:620:LYS:N	2.30	0.64
5:B:604:ARG:HH22	5:B:614:SER:HA	1.63	0.64
4:A:630:ILE:HD13	4:A:646:PHE:CZ	2.32	0.64
8:E:84:ASP:O	8:E:86:PRO:HD3	1.97	0.64
4:A:68:GLN:C	4:A:70:CYS:H	2.00	0.64
10:G:81:PRO:HG3	10:G:106:MET:SD	2.36	0.64
10:G:1:MET:HE3	10:G:80:LYS:C	2.17	0.64
11:H:4:THR:CA	11:H:60:ALA:HB2	2.22	0.64
4:A:901:LEU:CG	4:A:926:GLN:HE21	2.10	0.64
5:B:515:HIS:O	5:B:518:HIS:HB2	1.97	0.64
4:A:1402:PHE:CE1	4:A:1403:GLU:HG3	2.33	0.64
4:A:979:SER:OG	4:A:980:ASP:N	2.30	0.64
4:A:33:ALA:O	4:A:83:HIS:HD2	1.81	0.64
10:G:34:VAL:CG1	10:G:45:ILE:HG21	2.26	0.64
5:B:999:MET:HE3	5:B:999:MET:HA	1.77	0.64
6:C:238:ILE:CG2	6:C:242:GLN:HB2	2.27	0.64
8:E:179:GLN:HB2	8:E:182:ASP:HB2	1.78	0.64
4:A:1206:ASP:HB3	4:A:1274:ARG:HH12	1.61	0.64
4:A:798:GLY:HA2	4:A:815:PHE:HD1	1.60	0.64
5:B:705:MET:H	5:B:710:LEU:CD1	2.11	0.64
5:B:295:GLY:N	5:B:298:LEU:HD23	2.13	0.64
8:E:93:MET:SD	8:E:97:VAL:HG23	2.37	0.64
11:H:99:GLY:N	11:H:118:PHE:HD2	1.96	0.64
8:E:192:ARG:HH11	8:E:192:ARG:HG3	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:777:ALA:HA	5:B:1095:LEU:HA	1.78	0.64
12:I:6:PHE:HB3	12:I:12:ASN:O	1.97	0.64
4:A:1428:VAL:HG13	5:B:1151:LEU:CD2	2.27	0.64
4:A:901:LEU:O	4:A:921:GLY:N	2.30	0.64
8:E:15:ALA:O	8:E:19:VAL:HG23	1.98	0.64
7:D:122:GLU:HA	7:D:125:SER:OG	1.98	0.64
4:A:863:VAL:HG11	4:A:866:PHE:CD2	2.33	0.64
6:C:172:PRO:O	6:C:235:VAL:HG23	1.97	0.64
5:B:911:ILE:HD11	5:B:941:LEU:HD13	1.78	0.64
10:G:88:ASP:HB3	10:G:144:ARG:HA	1.80	0.64
4:A:1072:ILE:O	4:A:1075:PRO:HD2	1.98	0.64
4:A:1166:ASP:OD2	4:A:1239:ARG:HD2	1.97	0.63
4:A:1116:LEU:HD11	4:A:1118:VAL:HG13	1.80	0.63
13:J:36:LEU:HD12	13:J:47:ARG:HH12	1.61	0.63
4:A:1107:VAL:HG12	4:A:1107:VAL:O	1.98	0.63
7:D:56:ARG:HB2	7:D:148:LEU:HD22	1.79	0.63
5:B:1183:LYS:N	5:B:1183:LYS:CE	2.61	0.63
4:A:518:LYS:HE2	4:A:624:SER:O	1.97	0.63
10:G:9:LEU:HD12	10:G:10:ASN:H	1.62	0.63
8:E:14:ARG:HH21	8:E:141:VAL:CG1	2.11	0.63
4:A:467:THR:O	4:A:469:ARG:HG3	1.99	0.63
6:C:22:LEU:HD13	6:C:230:MET:CE	2.28	0.63
5:B:635:ARG:NH2	5:B:742:GLU:OE2	2.32	0.63
4:A:547:LEU:HB3	14:K:58:PHE:HE1	1.63	0.63
6:C:191:TYR:HD2	6:C:201:TRP:CD1	2.16	0.63
5:B:880:THR:O	5:B:881:ASN:HB2	1.97	0.63
4:A:1323:ASP:OD1	4:A:1325:THR:HB	1.98	0.63
5:B:798:TYR:HE2	6:C:62:PHE:CZ	2.17	0.63
4:A:901:LEU:HD22	4:A:919:ILE:CG2	2.28	0.63
4:A:902:LEU:HG	4:A:926:GLN:HG3	1.81	0.63
4:A:541:ILE:HD13	4:A:549:MET:CE	2.29	0.63
4:A:1341:ILE:HD12	4:A:1379:GLY:O	1.98	0.63
5:B:212:LEU:HD23	5:B:480:SER:HB2	1.80	0.63
5:B:1087:PHE:HD2	5:B:1088:GLY:N	1.97	0.63
5:B:549:THR:H	5:B:628:THR:HG23	1.63	0.63
4:A:1325:THR:O	8:E:148:GLU:HB2	1.98	0.63
4:A:84:ILE:HG23	4:A:84:ILE:O	1.97	0.63
7:D:173:HIS:O	7:D:177:VAL:HG23	1.98	0.63
5:B:121:ASN:HA	5:B:207:GLY:CA	2.28	0.63
5:B:622:LYS:HE2	12:I:59:VAL:HG22	1.79	0.63
10:G:1:MET:O	10:G:1:MET:SD	2.56	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:567:LYS:HB3	11:H:96:VAL:N	2.12	0.63
4:A:265:LYS:NZ	4:A:322:VAL:HG22	2.14	0.63
13:J:44:TYR:HD2	13:J:44:TYR:H	1.47	0.63
4:A:265:LYS:HE2	4:A:322:VAL:CG1	2.29	0.63
4:A:18:GLN:O	5:B:1215:ARG:HG2	1.98	0.63
4:A:728:LYS:O	4:A:732:LEU:HG	1.97	0.63
5:B:857:ARG:HD2	5:B:945:GLU:OE1	1.97	0.63
6:C:164:ALA:HA	6:C:167:HIS:O	1.98	0.63
4:A:504:LEU:HD11	9:F:91:ALA:HB1	1.79	0.63
4:A:828:ALA:HB2	5:B:530:GLY:HA2	1.79	0.63
4:A:613:ILE:O	4:A:614:PHE:HB3	1.97	0.63
5:B:284:ILE:HD13	5:B:333:PHE:HD2	1.63	0.63
4:A:552:TRP:HE3	4:A:651:LYS:HB3	1.64	0.63
6:C:73:GLN:HB3	6:C:131:HIS:H	1.62	0.62
5:B:65:GLU:HG3	5:B:66:ASP:N	2.11	0.62
5:B:604:ARG:NH1	5:B:691:GLU:OE2	2.31	0.62
7:D:176:GLU:C	7:D:178:ALA:H	2.02	0.62
5:B:237:VAL:HG22	5:B:257:LYS:HA	1.81	0.62
4:A:782:ARG:NH2	5:B:699:GLU:O	2.31	0.62
6:C:73:GLN:HE21	6:C:74:SER:H	1.45	0.62
4:A:853:ASP:OD1	4:A:855:THR:HG22	1.98	0.62
10:G:18:PHE:HA	10:G:22:MET:CE	2.28	0.62
15:L:53:HIS:O	15:L:55:ILE:HG12	1.99	0.62
4:A:404:TYR:HB2	4:A:433:GLU:HB2	1.80	0.62
4:A:720:ARG:O	4:A:724:GLU:HB2	1.98	0.62
4:A:606:LEU:HB3	4:A:614:PHE:CE2	2.33	0.62
5:B:1034:VAL:HG23	5:B:1059:LEU:HD13	1.81	0.62
8:E:157:SER:C	8:E:159:ASP:H	2.03	0.62
5:B:205:ILE:O	5:B:207:GLY:N	2.33	0.62
4:A:665:GLY:HA2	5:B:1026:LEU:HD21	1.79	0.62
5:B:1159:ARG:HD3	5:B:1193:GLN:HG3	1.79	0.62
5:B:642:ASP:HB3	5:B:649:LYS:HG3	1.80	0.62
4:A:809:THR:OG1	4:A:812:GLU:HG3	1.98	0.62
4:A:75:ASN:O	4:A:76:GLU:HB3	1.98	0.62
4:A:901:LEU:N	4:A:926:GLN:NE2	2.41	0.62
14:K:10:PHE:CD2	14:K:10:PHE:N	2.68	0.62
4:A:767:GLN:OE1	4:A:799:PHE:HB2	2.00	0.62
5:B:233:PRO:HG2	5:B:234:ILE:CD1	2.28	0.62
4:A:71:GLN:C	4:A:73:GLY:H	2.02	0.62
5:B:293:PRO:HG2	5:B:296:GLU:CB	2.30	0.62
5:B:827:ILE:HD12	5:B:1086:PHE:CD2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:93:VAL:HG22	4:A:301:ALA:HA	1.82	0.62
5:B:36:ALA:HA	5:B:39:ARG:HD2	1.81	0.62
6:C:152:GLU:OE2	6:C:154:LYS:HE3	1.99	0.62
4:A:1214:GLU:O	4:A:1218:GLN:HG2	1.99	0.62
6:C:133:ILE:CD1	6:C:237:SER:HA	2.30	0.62
5:B:1082:MET:O	6:C:189:THR:HG23	1.99	0.62
12:I:62:ILE:HG12	12:I:62:ILE:O	2.00	0.62
4:A:783:THR:HG21	4:A:815:PHE:CE2	2.35	0.62
4:A:541:ILE:HD13	4:A:549:MET:HE1	1.81	0.62
4:A:14:VAL:H	4:A:1432:GLN:HE22	1.48	0.62
4:A:23:SER:HB3	4:A:233:TRP:CE2	2.35	0.62
4:A:899:VAL:HB	4:A:929:LEU:HD12	1.82	0.62
4:A:1019:CYS:O	4:A:1022:LEU:N	2.32	0.62
5:B:1107:ALA:O	5:B:1108:ARG:HG2	1.99	0.62
5:B:758:PHE:CE2	5:B:1044:ALA:HA	2.35	0.62
4:A:699:ALA:HB3	4:A:701:LEU:HG	1.81	0.62
4:A:714:PHE:O	4:A:718:VAL:HG23	2.00	0.62
4:A:590:ARG:HB2	4:A:605:MET:HB3	1.81	0.62
4:A:855:THR:HG23	4:A:857:ARG:HG3	1.80	0.62
5:B:515:HIS:H	5:B:518:HIS:HD2	1.47	0.62
4:A:308:ILE:HG22	4:A:309:ALA:H	1.64	0.62
8:E:207:ARG:CB	8:E:207:ARG:HH11	2.12	0.62
13:J:2:ILE:H	13:J:57:ILE:CG2	2.13	0.62
4:A:897:TYR:CD2	4:A:936:LEU:HD13	2.35	0.62
11:H:113:ALA:HB2	11:H:126:GLU:HG3	1.81	0.62
4:A:675:THR:O	4:A:679:ILE:HG13	1.98	0.62
4:A:1209:MET:HE1	4:A:1236:LEU:HB3	1.82	0.62
4:A:1017:LEU:HB3	8:E:205:SER:HA	1.80	0.62
7:D:53:SER:HB3	7:D:152:SER:CA	2.30	0.62
5:B:43:LEU:HD11	5:B:811:TYR:O	2.00	0.62
4:A:1063:MET:CG	4:A:1436:ILE:HG23	2.30	0.62
4:A:262:LEU:O	4:A:264:PHE:N	2.33	0.62
7:D:134:THR:CG2	7:D:135:GLY:N	2.62	0.62
5:B:737:THR:CG2	12:I:66:PRO:HA	2.30	0.62
4:A:1120:LEU:HD13	4:A:1304:TRP:O	2.00	0.62
5:B:611:PRO:HB3	5:B:685:LEU:HD11	1.80	0.62
11:H:44:VAL:HG12	11:H:44:VAL:O	1.99	0.62
4:A:1057:VAL:HG12	4:A:1058:VAL:H	1.64	0.61
13:J:57:ILE:HA	13:J:60:PHE:CD2	2.32	0.61
5:B:189:LEU:O	5:B:192:LEU:N	2.29	0.61
4:A:384:ASN:CG	4:A:388:LEU:HD12	2.21	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:53:SER:HB3	7:D:152:SER:HA	1.82	0.61
6:C:212:PRO:CB	6:C:213:PRO:HD2	2.30	0.61
5:B:1162:ILE:HD11	5:B:1194:ILE:HD13	1.82	0.61
4:A:1007:ILE:C	4:A:1009:ASN:H	2.03	0.61
4:A:1227:ILE:HG22	4:A:1228:TRP:N	2.14	0.61
8:E:23:VAL:HG13	8:E:78:LEU:HD13	1.82	0.61
4:A:463:ILE:HD12	4:A:469:ARG:HD2	1.82	0.61
4:A:825:ILE:CG2	5:B:508:LEU:HD11	2.30	0.61
5:B:1169:MET:HE1	5:B:1201:LYS:HA	1.81	0.61
4:A:340:LEU:HD21	5:B:1200:ALA:N	2.15	0.61
13:J:14:VAL:HG12	13:J:14:VAL:O	2.00	0.61
5:B:842:ASN:ND2	5:B:845:SER:H	1.98	0.61
7:D:47:LEU:HD11	10:G:3:PHE:CD2	2.35	0.61
4:A:319:GLY:HA3	5:B:471:LYS:HA	1.82	0.61
11:H:89:LEU:C	11:H:91:ASP:H	2.04	0.61
4:A:1155:ASP:OD1	4:A:1161:THR:HA	2.00	0.61
5:B:1065:GLN:HE21	5:B:1066:SER:N	1.97	0.61
5:B:770:GLN:CD	5:B:983:ARG:HA	2.20	0.61
4:A:349:ALA:C	5:B:1128:LEU:HD11	2.20	0.61
4:A:738:LYS:HB2	4:A:740:LEU:HG	1.83	0.61
4:A:471:ASN:OD1	4:A:472:LEU:N	2.34	0.61
4:A:765:VAL:HG12	4:A:766:GLY:N	2.15	0.61
4:A:263:THR:HG22	4:A:263:THR:O	2.00	0.61
10:G:1:MET:HG3	10:G:85:GLU:OE2	2.01	0.61
5:B:763:GLN:HG2	5:B:765:PRO:HD2	1.82	0.61
5:B:865:LYS:HE2	5:B:871:THR:OG1	2.01	0.61
4:A:1305:VAL:HG12	4:A:1306:LEU:N	2.16	0.61
4:A:337:ARG:HD3	5:B:1132:GLU:OE1	2.01	0.61
5:B:705:MET:N	5:B:710:LEU:HD12	2.13	0.61
6:C:98:VAL:O	6:C:99:LEU:HD23	2.00	0.61
4:A:1127:ASP:HB3	4:A:1130:GLN:CB	2.30	0.61
4:A:40:THR:HG22	4:A:41:MET:CG	2.28	0.61
14:K:65:HIS:HD2	14:K:67:PHE:N	1.94	0.61
9:F:89:GLU:OE2	9:F:134:ILE:HG21	2.01	0.61
5:B:496:ARG:NH1	5:B:539:LEU:HB2	2.16	0.61
4:A:730:GLY:O	4:A:732:LEU:N	2.34	0.61
5:B:825:VAL:CG1	5:B:826:ALA:N	2.63	0.61
5:B:569:TYR:CE1	5:B:589:VAL:HG21	2.35	0.61
4:A:666:ILE:CD1	4:A:667:GLY:H	2.14	0.61
5:B:114:PRO:HG2	5:B:115:GLN:H	1.65	0.61
5:B:1006:ILE:HD13	13:J:44:TYR:CE2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:49:LYS:HZ1	4:A:61:ILE:N	1.97	0.61
5:B:227:LYS:HB2	5:B:395:GLN:OE1	2.00	0.61
8:E:180:ARG:HH21	8:E:192:ARG:CB	2.10	0.61
4:A:244:PRO:O	4:A:246:VAL:N	2.33	0.61
4:A:321:PRO:O	4:A:322:VAL:CB	2.49	0.61
4:A:351:THR:HB	5:B:1103:ILE:CD1	2.30	0.61
4:A:981:LEU:CD2	4:A:1039:LYS:HA	2.31	0.61
9:F:101:ILE:HD11	9:F:124:GLU:OE1	2.01	0.61
5:B:496:ARG:NH1	5:B:496:ARG:HB3	2.15	0.61
4:A:1410:PHE:HA	5:B:1212:ILE:HD11	1.83	0.61
3:P:8:G:O2'	3:P:9:G:H5'	2.00	0.61
6:C:76:ASP:OD2	6:C:128:ASN:N	2.34	0.61
4:A:1114:PRO:O	4:A:1115:SER:O	2.19	0.61
4:A:1149:ALA:HB2	12:I:47:GLU:HA	1.83	0.61
4:A:1198:ASP:O	4:A:1202:MET:HG2	2.01	0.61
4:A:50:ILE:O	4:A:52:GLY:N	2.31	0.60
5:B:999:MET:CE	5:B:999:MET:HA	2.31	0.60
3:P:9:G:H5''	5:B:776:GLN:NE2	2.16	0.60
4:A:1002:GLY:HA3	4:A:1007:ILE:HG21	1.82	0.60
9:F:111:LEU:C	9:F:113:GLY:H	2.04	0.60
12:I:101:PHE:CD1	12:I:101:PHE:N	2.67	0.60
10:G:1:MET:C	10:G:1:MET:SD	2.80	0.60
4:A:598:LEU:HD22	11:H:25:ARG:NH1	2.16	0.60
10:G:14:HIS:ND1	10:G:15:PRO:HD2	2.16	0.60
4:A:384:ASN:O	4:A:385:ILE:C	2.40	0.60
9:F:135:ARG:HD3	9:F:143:PHE:CD2	2.36	0.60
4:A:466:SER:O	5:B:1103:ILE:HD11	2.01	0.60
5:B:955:THR:CG2	5:B:956:THR:N	2.63	0.60
4:A:746:MET:HE3	5:B:1018:PRO:HG2	1.83	0.60
5:B:794:ASN:O	5:B:795:ILE:HD12	2.00	0.60
5:B:822:ASN:O	13:J:48:ARG:NH1	2.34	0.60
4:A:481:ASP:OD1	4:A:485:ASP:OD2	2.19	0.60
5:B:846:ILE:HG23	5:B:974:PRO:HG2	1.83	0.60
4:A:1313:LEU:O	4:A:1315:GLU:N	2.34	0.60
4:A:1057:VAL:HG12	4:A:1058:VAL:N	2.16	0.60
4:A:265:LYS:HD2	4:A:265:LYS:N	2.16	0.60
5:B:1197:PRO:HG2	5:B:1200:ALA:CB	2.29	0.60
4:A:504:LEU:HD11	9:F:91:ALA:CB	2.31	0.60
6:C:112:ASN:HB2	6:C:114:TYR:CE1	2.36	0.60
5:B:744:HIS:CG	5:B:745:PRO:HD2	2.36	0.60
5:B:230:ALA:N	5:B:231:PRO:HD2	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:850:LEU:HD12	5:B:851:PHE:N	2.16	0.60
5:B:213:ILE:HD12	5:B:497:ARG:HB3	1.83	0.60
6:C:124:LEU:O	6:C:127:ARG:HG2	2.02	0.60
11:H:89:LEU:HB3	11:H:91:ASP:OD1	2.02	0.60
6:C:66:ARG:NH2	13:J:3:VAL:O	2.34	0.60
4:A:341:MET:HE1	4:A:843:LYS:NZ	2.17	0.60
4:A:114:LEU:HD13	4:A:171:GLN:OE1	2.02	0.60
4:A:979:SER:OG	4:A:981:LEU:HG	2.01	0.60
4:A:1097:GLY:O	4:A:1100:ARG:HB3	2.01	0.60
4:A:1364:ASN:HD22	4:A:1365:TYR:N	1.99	0.60
4:A:475:THR:CG2	4:A:476:SER:N	2.64	0.60
4:A:366:VAL:HG21	4:A:460:VAL:HG22	1.84	0.60
1:T:18:DC:H5'	4:A:832:ALA:O	2.02	0.60
4:A:818:MET:HA	5:B:514:LEU:HB3	1.84	0.60
4:A:108:MET:SD	4:A:210:ILE:HD13	2.41	0.60
6:C:80:LEU:CD1	6:C:95:CYS:HA	2.32	0.60
5:B:696:GLU:O	5:B:699:GLU:HB2	2.00	0.60
6:C:67:LEU:HD11	6:C:155:LEU:CD1	2.32	0.60
14:K:49:GLU:HG3	14:K:94:ILE:CG1	2.32	0.60
4:A:783:THR:HG22	4:A:784:LEU:HG	1.82	0.60
5:B:225:VAL:HG11	5:B:385:LEU:HA	1.84	0.60
4:A:1362:TYR:CD1	4:A:1363:VAL:N	2.70	0.60
5:B:118:ARG:HH22	5:B:194:GLU:CD	2.05	0.60
4:A:1373:ASP:HA	4:A:1376:THR:HG22	1.82	0.60
4:A:1121:GLU:CG	4:A:1122:PRO:HD2	2.31	0.60
12:I:13:MET:HG3	12:I:14:LEU:N	2.16	0.60
4:A:90:VAL:HG13	4:A:297:GLN:HA	1.82	0.60
4:A:965:GLN:O	4:A:968:GLN:HB2	2.02	0.60
6:C:69:LEU:HD12	6:C:69:LEU:N	2.16	0.59
4:A:998:LEU:H	4:A:998:LEU:HD12	1.66	0.59
9:F:96:THR:O	9:F:99:LEU:HB3	2.02	0.59
4:A:265:LYS:HE2	4:A:322:VAL:HG13	1.83	0.59
6:C:18:VAL:O	6:C:18:VAL:HG12	2.02	0.59
5:B:515:HIS:H	5:B:518:HIS:CD2	2.19	0.59
5:B:637:LEU:HD12	5:B:693:ILE:HD12	1.84	0.59
5:B:1166:CYS:O	5:B:1166:CYS:SG	2.59	0.59
5:B:378:LEU:O	5:B:382:ILE:HG13	2.00	0.59
12:I:111:THR:HG22	12:I:112:SER:H	1.67	0.59
14:K:61:TYR:C	14:K:61:TYR:CD2	2.76	0.59
4:A:289:ILE:C	4:A:291:GLU:H	2.05	0.59
5:B:816:GLU:O	5:B:817:LEU:HD23	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:I:52:ILE:HG13	12:I:52:ILE:O	2.01	0.59
4:A:741:ASN:ND2	4:A:743:VAL:HB	2.18	0.59
4:A:230:ARG:H	4:A:233:TRP:HE3	1.42	0.59
4:A:49:LYS:HZ3	4:A:61:ILE:HG13	1.66	0.59
5:B:642:ASP:HB3	5:B:649:LYS:CG	2.33	0.59
7:D:54:GLU:O	7:D:58:VAL:HG23	2.01	0.59
4:A:834:THR:HG22	4:A:835:GLY:N	2.17	0.59
4:A:262:LEU:C	4:A:264:PHE:H	2.05	0.59
5:B:834:ASN:HA	5:B:838:SER:O	2.01	0.59
6:C:35:ARG:NH1	14:K:41:THR:OG1	2.34	0.59
5:B:1162:ILE:HG22	5:B:1163:CYS:N	2.16	0.59
5:B:616:ILE:HG13	5:B:697:GLU:HG3	1.84	0.59
6:C:18:VAL:CG2	6:C:240:VAL:HB	2.32	0.59
5:B:521:LEU:HB3	5:B:633:VAL:CG1	2.31	0.59
4:A:1336:MET:HE3	4:A:1381:LEU:HG	1.84	0.59
4:A:1299:VAL:HG12	4:A:1300:LYS:N	2.16	0.59
4:A:663:SER:OG	4:A:664:THR:N	2.34	0.59
5:B:46:GLN:CG	5:B:47:GLN:H	2.11	0.59
4:A:78:PRO:CB	5:B:1201:LYS:HE3	2.32	0.59
6:C:18:VAL:HG23	6:C:240:VAL:HB	1.84	0.59
5:B:446:LEU:O	5:B:447:ALA:HB3	2.03	0.59
4:A:785:PRO:HG2	4:A:786:HIS:HD2	1.67	0.59
11:H:27:GLU:HA	11:H:38:LEU:O	2.03	0.59
4:A:971:PHE:CE2	4:A:1040:GLN:HG2	2.37	0.59
4:A:264:PHE:O	4:A:267:ALA:HB3	2.01	0.59
1:T:24:DG:OP1	5:B:857:ARG:NH2	2.35	0.59
13:J:47:ARG:HH11	13:J:47:ARG:HG2	1.66	0.59
9:F:86:THR:OG1	9:F:89:GLU:HG3	2.03	0.59
11:H:81:PRO:HB2	11:H:82:PRO:CD	2.31	0.59
4:A:69:THR:C	4:A:71:GLN:N	2.55	0.59
5:B:287:ARG:HG2	5:B:292:ILE:HA	1.83	0.59
5:B:552:MET:HA	5:B:555:ILE:HB	1.84	0.59
12:I:82:GLU:HB3	12:I:104:LEU:HD12	1.84	0.59
12:I:99:LEU:C	12:I:100:PHE:HD1	2.06	0.59
4:A:47:ARG:HH12	4:A:254:GLU:HG2	1.68	0.59
4:A:23:SER:HB3	4:A:233:TRP:CZ2	2.38	0.59
13:J:7:CYS:HB2	13:J:46:CYS:HB3	1.84	0.59
5:B:408:LEU:HG	5:B:409:ALA:H	1.66	0.59
5:B:376:PHE:HE2	5:B:569:TYR:HD2	1.50	0.59
6:C:166:GLU:O	6:C:167:HIS:HB2	2.02	0.59
4:A:829:VAL:O	4:A:831:THR:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1001:PHE:CE2	6:C:34:ARG:CZ	2.85	0.59
4:A:61:ILE:HG22	4:A:62:ASP:H	1.68	0.59
5:B:294:ASP:O	5:B:296:GLU:N	2.32	0.59
4:A:407:ARG:HG2	4:A:430:TRP:CH2	2.37	0.59
7:D:51:ASN:O	7:D:54:GLU:HB3	2.03	0.59
6:C:254:LYS:O	6:C:256:ALA:N	2.35	0.59
4:A:408:ASP:O	4:A:410:GLY:N	2.34	0.59
5:B:1084:GLN:NE2	5:B:1084:GLN:N	2.51	0.59
11:H:91:ASP:C	11:H:93:TYR:H	2.06	0.59
4:A:852:TYR:CE2	4:A:1060:PRO:HB2	2.38	0.59
5:B:114:PRO:HG3	5:B:181:LEU:HD11	1.85	0.59
8:E:178:ILE:HG22	8:E:213:ILE:O	2.02	0.59
5:B:850:LEU:HD12	5:B:851:PHE:H	1.67	0.59
14:K:69:ALA:O	14:K:70:ARG:HB3	2.03	0.59
5:B:522:VAL:HG11	5:B:537:LYS:HB3	1.85	0.59
11:H:143:LEU:N	11:H:143:LEU:HD12	2.18	0.58
6:C:18:VAL:O	6:C:20:PHE:HD2	1.85	0.58
6:C:238:ILE:HG23	6:C:242:GLN:HB2	1.85	0.58
5:B:1162:ILE:O	5:B:1171:VAL:HG21	2.03	0.58
4:A:1010:ALA:HA	4:A:1013:ASP:OD2	2.02	0.58
4:A:537:ARG:NH1	11:H:120:GLY:O	2.36	0.58
4:A:364:VAL:O	4:A:364:VAL:HG13	2.03	0.58
7:D:47:LEU:HD11	10:G:3:PHE:HD2	1.68	0.58
13:J:21:TYR:HB2	13:J:39:LEU:HD13	1.85	0.58
4:A:1444:MET:HE1	9:F:135:ARG:CB	2.32	0.58
4:A:224:PHE:CE2	4:A:231:PRO:HG3	2.37	0.58
8:E:90:VAL:HA	8:E:120:ALA:HB2	1.84	0.58
4:A:746:MET:CE	5:B:1018:PRO:HG2	2.34	0.58
5:B:731:VAL:HG12	5:B:732:SER:N	2.18	0.58
8:E:169:ARG:HH12	9:F:74:ILE:HD11	1.68	0.58
10:G:1:MET:O	10:G:3:PHE:CE1	2.57	0.58
4:A:567:LYS:CG	4:A:568:PRO:CD	2.79	0.58
11:H:100:THR:HG22	11:H:101:ALA:N	2.18	0.58
4:A:225:ASN:ND2	4:A:228:PHE:H	2.00	0.58
4:A:1070:GLN:O	4:A:1072:ILE:N	2.37	0.58
4:A:119:ASN:O	4:A:122:MET:HB3	2.03	0.58
4:A:218:ASP:HA	4:A:221:SER:OG	2.03	0.58
4:A:269:ILE:HD11	4:A:300:VAL:HA	1.86	0.58
5:B:842:ASN:HD22	5:B:845:SER:CB	2.16	0.58
4:A:1299:VAL:HG12	4:A:1300:LYS:H	1.69	0.58
4:A:1454:MET:O	4:A:1454:MET:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1364:ASN:O	4:A:1365:TYR:C	2.42	0.58
7:D:51:ASN:O	7:D:52:LEU:O	2.22	0.58
9:F:77:ASP:C	9:F:79:ARG:H	2.05	0.58
11:H:18:GLY:O	11:H:19:ARG:HB2	2.04	0.58
4:A:1435:PRO:O	4:A:1436:ILE:HG13	2.03	0.58
4:A:843:LYS:HD3	4:A:846:GLU:OE2	2.04	0.58
7:D:56:ARG:NH2	7:D:57:LEU:HD21	2.18	0.58
9:F:73:ALA:HA	9:F:143:PHE:CE1	2.38	0.58
7:D:47:LEU:CD1	7:D:48:ILE:H	2.11	0.58
4:A:1445:ILE:HG12	10:G:18:PHE:CE2	2.38	0.58
10:G:17:PHE:CD2	10:G:17:PHE:N	2.69	0.58
9:F:90:ARG:HD3	9:F:155:LEU:CD1	2.33	0.58
4:A:1035:TYR:O	4:A:1037:LEU:N	2.36	0.58
4:A:35:ILE:HD12	4:A:241:VAL:HG21	1.86	0.58
4:A:50:ILE:C	4:A:52:GLY:H	2.06	0.58
4:A:382:PRO:HD3	4:A:428:TYR:HD2	1.67	0.58
5:B:606:LYS:HD2	5:B:608:ASP:OD2	2.04	0.58
4:A:982:THR:HB	4:A:985:ASP:H	1.68	0.58
5:B:1051:THR:HB	5:B:1054:GLY:H	1.68	0.58
4:A:658:LEU:HD23	4:A:659:HIS:CE1	2.38	0.58
5:B:57:TYR:CD1	5:B:57:TYR:N	2.70	0.58
5:B:798:TYR:CE2	6:C:62:PHE:CE2	2.90	0.58
4:A:541:ILE:CG2	4:A:546:VAL:HG23	2.32	0.58
15:L:40:LEU:HD22	15:L:44:ASP:CG	2.24	0.58
5:B:118:ARG:HH11	5:B:204:ILE:HD11	1.68	0.58
7:D:175:PHE:HZ	10:G:85:GLU:HG3	1.69	0.58
10:G:1:MET:HE1	10:G:80:LYS:H	1.67	0.58
11:H:38:LEU:HD12	11:H:124:ARG:O	2.04	0.58
5:B:653:VAL:HG22	5:B:689:LEU:HB3	1.85	0.58
6:C:36:VAL:HG21	6:C:251:LEU:HD22	1.85	0.58
4:A:408:ASP:C	4:A:410:GLY:H	2.07	0.58
7:D:7:THR:O	7:D:9:GLN:N	2.37	0.58
5:B:797:TYR:HE1	5:B:854:LEU:CD2	2.17	0.58
4:A:774:ARG:NH2	4:A:797:LYS:HB2	2.18	0.57
4:A:23:SER:HA	4:A:233:TRP:NE1	2.18	0.57
5:B:707:PRO:O	5:B:711:GLU:HG3	2.04	0.57
5:B:377:PHE:O	5:B:380:TYR:N	2.37	0.57
5:B:990:ILE:HG22	5:B:991:GLY:N	2.19	0.57
5:B:1099:VAL:C	5:B:1101:ASP:H	2.06	0.57
4:A:299:HIS:O	4:A:301:ALA:N	2.37	0.57
1:T:16:DT:H4'	4:A:1403:GLU:OE2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:112:ASN:HD22	6:C:112:ASN:N	2.02	0.57
6:C:100:THR:HG22	6:C:101:LEU:N	2.18	0.57
5:B:981:ALA:HB2	5:B:987:LYS:HA	1.86	0.57
8:E:114:ASN:O	8:E:115:ASN:HB3	2.03	0.57
6:C:66:ARG:NH2	13:J:5:VAL:CG2	2.68	0.57
4:A:254:GLU:O	4:A:256:GLN:N	2.37	0.57
5:B:1215:ARG:C	5:B:1216:LEU:HD23	2.24	0.57
7:D:35:LEU:HD23	7:D:174:PRO:HD2	1.86	0.57
4:A:500:GLU:OE2	5:B:1145:SER:HB2	2.04	0.57
4:A:1434:ALA:HB3	4:A:1436:ILE:HD12	1.86	0.57
5:B:879:ARG:NH1	5:B:883:LEU:HD22	2.18	0.57
5:B:351:TYR:O	5:B:355:ILE:HG13	2.04	0.57
4:A:670:ILE:HG23	4:A:805:LEU:CD2	2.35	0.57
5:B:862:GLN:HG2	5:B:963:PHE:HD1	1.70	0.57
5:B:1102:LYS:O	5:B:1103:ILE:C	2.41	0.57
13:J:1:MET:N	13:J:56:LEU:N	2.53	0.57
4:A:836:TYR:O	4:A:839:ARG:N	2.38	0.57
5:B:731:VAL:HG12	5:B:732:SER:H	1.69	0.57
5:B:63:ILE:O	5:B:67:SER:HB3	2.04	0.57
5:B:957:ASN:O	5:B:959:ASP:N	2.38	0.57
5:B:838:SER:HB2	5:B:989:THR:O	2.04	0.57
4:A:1242:VAL:HG12	4:A:1243:VAL:N	2.18	0.57
4:A:743:VAL:O	4:A:747:VAL:HG23	2.04	0.57
5:B:1040:ASN:O	5:B:1041:GLU:C	2.43	0.57
4:A:185:TRP:CZ3	4:A:200:ARG:HG2	2.39	0.57
4:A:1365:TYR:O	4:A:1367:HIS:N	2.38	0.57
4:A:1164:PRO:HG2	4:A:1165:GLU:H	1.68	0.57
4:A:42:ASP:HB3	4:A:45:GLN:H	1.68	0.57
4:A:244:PRO:CB	4:A:245:PRO:CD	2.83	0.57
4:A:469:ARG:NH2	5:B:991:GLY:O	2.38	0.57
5:B:1011:ILE:O	5:B:1011:ILE:HG22	2.04	0.57
5:B:999:MET:HB3	5:B:1007:VAL:HG21	1.87	0.57
4:A:1242:VAL:O	4:A:1243:VAL:HB	2.05	0.57
5:B:953:LEU:CD2	5:B:965:LYS:HB2	2.35	0.57
5:B:1107:ALA:O	5:B:1108:ARG:O	2.23	0.57
5:B:1115:THR:HG22	5:B:1117:GLN:HG3	1.87	0.57
5:B:321:GLY:O	5:B:323:VAL:N	2.37	0.57
5:B:167:ILE:HG22	5:B:453:ILE:HD12	1.86	0.57
4:A:55:ASP:N	4:A:56:PRO:HD3	2.20	0.57
10:G:18:PHE:HA	10:G:22:MET:HE2	1.85	0.57
4:A:982:THR:O	4:A:985:ASP:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:782:LEU:HD12	5:B:788:ARG:HH11	1.70	0.57
4:A:1441:PHE:CZ	9:F:89:GLU:HA	2.40	0.57
6:C:22:LEU:HD23	6:C:25:VAL:HG21	1.85	0.57
5:B:234:ILE:N	5:B:234:ILE:HD12	2.20	0.57
4:A:63:ARG:HA	4:A:74:MET:CE	2.34	0.57
5:B:821:GLN:NE2	5:B:851:PHE:HA	2.19	0.57
4:A:730:GLY:C	4:A:732:LEU:H	2.08	0.57
5:B:310:MET:O	5:B:313:MET:HB2	2.04	0.57
14:K:31:VAL:CG1	14:K:32:VAL:N	2.68	0.56
11:H:116:TYR:HB2	11:H:123:MET:HB3	1.85	0.56
8:E:94:LYS:CE	8:E:98:ILE:HD11	2.30	0.56
5:B:806:THR:N	5:B:809:MET:HE3	2.20	0.56
5:B:39:ARG:HG2	5:B:39:ARG:HH11	1.70	0.56
14:K:6:ARG:O	14:K:9:LEU:HG	2.05	0.56
5:B:950:ASP:O	5:B:951:GLN:HB2	2.05	0.56
6:C:258:ILE:N	6:C:258:ILE:HD12	2.19	0.56
10:G:51:TYR:C	10:G:51:TYR:CD2	2.79	0.56
4:A:1308:THR:HG23	4:A:1309:ASP:N	2.19	0.56
1:T:27:DA:C2	3:P:3:G:N2	2.74	0.56
7:D:153:ARG:HH22	7:D:184:ALA:HA	1.67	0.56
13:J:14:VAL:HG12	13:J:50:ILE:HD11	1.85	0.56
12:I:111:THR:HG22	12:I:113:ASP:N	2.20	0.56
4:A:1199:ARG:O	4:A:1202:MET:HB2	2.05	0.56
11:H:15:VAL:HG22	11:H:26:ILE:HD11	1.86	0.56
4:A:540:PHE:HB3	4:A:571:LEU:HD23	1.87	0.56
10:G:1:MET:CE	10:G:1:MET:O	2.53	0.56
5:B:654:ARG:H	5:B:657:HIS:HD2	1.52	0.56
4:A:874:ASP:CA	4:A:1058:VAL:HG22	2.36	0.56
5:B:582:VAL:HG23	5:B:626:ILE:HB	1.87	0.56
4:A:35:ILE:CD1	4:A:241:VAL:HG21	2.35	0.56
4:A:47:ARG:HH12	4:A:254:GLU:CG	2.18	0.56
5:B:980:PHE:HE2	5:B:1094:ARG:HG3	1.70	0.56
4:A:858:ASN:ND2	4:A:858:ASN:C	2.55	0.56
4:A:265:LYS:HD2	4:A:265:LYS:H	1.71	0.56
5:B:1152:MET:SD	5:B:1197:PRO:HD3	2.45	0.56
4:A:416:ARG:C	4:A:417:TYR:HD2	2.09	0.56
12:I:34:TYR:HD2	12:I:35:VAL:N	2.03	0.56
4:A:311:GLN:O	4:A:312:PRO:C	2.44	0.56
4:A:789:LYS:HE3	12:I:67:THR:CB	2.35	0.56
5:B:315:LYS:N	5:B:316:PRO:HD2	2.21	0.56
5:B:27:ALA:O	5:B:29:ASP:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:39:LEU:O	8:E:42:PHE:HB3	2.05	0.56
6:C:123:ASN:HD22	6:C:125:MET:HG2	1.68	0.56
6:C:3:GLU:HB3	14:K:104:ASN:HD21	1.70	0.56
4:A:331:GLY:O	4:A:332:LYS:HB3	2.04	0.56
6:C:38:ILE:HA	6:C:173:ALA:HB2	1.88	0.56
5:B:811:TYR:N	5:B:811:TYR:CD1	2.72	0.56
4:A:49:LYS:HZ1	4:A:61:ILE:HG13	1.70	0.56
13:J:43:ARG:HG3	13:J:45:CYS:SG	2.45	0.56
4:A:590:ARG:HH11	4:A:590:ARG:CG	2.18	0.56
4:A:901:LEU:H	4:A:926:GLN:HE21	1.48	0.56
6:C:22:LEU:HD13	6:C:230:MET:HE1	1.88	0.56
4:A:299:HIS:C	4:A:301:ALA:H	2.09	0.56
9:F:75:PRO:HG2	9:F:78:GLN:HB2	1.87	0.56
5:B:195:CYS:SG	5:B:197:PHE:HB2	2.46	0.56
4:A:909:ASP:O	4:A:911:SER:N	2.39	0.56
15:L:43:THR:O	15:L:43:THR:HG22	2.04	0.56
4:A:1364:ASN:HD22	4:A:1364:ASN:C	2.09	0.56
13:J:2:ILE:H	13:J:57:ILE:HG22	1.70	0.56
4:A:466:SER:HB2	5:B:1099:VAL:HG11	1.87	0.56
4:A:1007:ILE:O	4:A:1009:ASN:N	2.38	0.56
4:A:1319:VAL:HG13	4:A:1320:PRO:HD2	1.88	0.56
5:B:526:GLU:HG2	5:B:538:ASN:HD22	1.70	0.56
4:A:68:GLN:O	4:A:70:CYS:N	2.38	0.56
5:B:217:ARG:C	5:B:217:ARG:HD2	2.26	0.56
4:A:567:LYS:HD3	11:H:95:TYR:CG	2.40	0.56
4:A:1335:ILE:HG23	4:A:1339:LEU:HD12	1.87	0.56
4:A:384:ASN:O	4:A:386:ASP:N	2.38	0.56
4:A:230:ARG:N	4:A:233:TRP:CE3	2.64	0.56
9:F:109:VAL:HG21	9:F:124:GLU:HA	1.88	0.56
4:A:852:TYR:CD2	4:A:1060:PRO:HB2	2.41	0.56
4:A:871:ASP:OD1	4:A:1366:ARG:NH2	2.39	0.56
4:A:382:PRO:HD3	4:A:428:TYR:CE2	2.41	0.56
4:A:499:ALA:O	4:A:503:GLN:HB2	2.05	0.56
7:D:63:LEU:HD13	7:D:133:THR:OG1	2.05	0.56
5:B:842:ASN:HD22	5:B:845:SER:HB3	1.71	0.56
5:B:63:ILE:HD12	5:B:421:PHE:CE2	2.40	0.56
5:B:265:SER:O	5:B:266:ALA:HB3	2.05	0.56
4:A:547:LEU:HD22	14:K:58:PHE:HD1	1.70	0.56
4:A:75:ASN:O	4:A:76:GLU:CB	2.53	0.56
10:G:80:LYS:HG2	10:G:80:LYS:O	2.05	0.56
5:B:309:GLN:HG3	12:I:52:ILE:CD1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:78:LEU:HD23	8:E:79:TRP:N	2.20	0.56
4:A:1343:ALA:HB2	8:E:150:VAL:CG2	2.35	0.56
4:A:548:ASN:HA	14:K:60:ALA:HB1	1.87	0.56
5:B:980:PHE:CD2	5:B:1094:ARG:HA	2.41	0.56
5:B:197:PHE:HZ	5:B:816:GLU:HG2	1.71	0.56
6:C:226:ASP:O	6:C:227:THR:HB	2.06	0.56
14:K:15:GLY:O	14:K:16:GLU:HG3	2.06	0.56
5:B:217:ARG:HE	5:B:405:ARG:CB	2.07	0.56
4:A:907:THR:HG22	4:A:908:LEU:N	2.18	0.56
4:A:1441:PHE:HB2	9:F:135:ARG:O	2.05	0.56
4:A:1015:VAL:HG12	4:A:1019:CYS:SG	2.45	0.56
4:A:1283:VAL:HG12	4:A:1284:MET:H	1.71	0.56
2:N:5:DA:H2"	2:N:6:DC:OP2	2.05	0.56
14:K:63:VAL:O	14:K:63:VAL:HG23	2.06	0.56
12:I:100:PHE:N	12:I:100:PHE:CD1	2.74	0.55
4:A:913:LEU:HD12	4:A:914:GLU:N	2.21	0.55
4:A:546:VAL:O	4:A:550:LEU:HG	2.06	0.55
4:A:754:SER:N	4:A:757:ASN:HD22	1.92	0.55
4:A:757:ASN:HA	5:B:1021:MET:SD	2.46	0.55
4:A:1369:ALA:O	4:A:1372:VAL:HG12	2.06	0.55
13:J:48:ARG:HE	13:J:49:MET:HE2	1.70	0.55
6:C:252:GLN:CG	14:K:95:ILE:HG23	2.36	0.55
4:A:649:ILE:O	4:A:653:VAL:HG23	2.06	0.55
12:I:2:THR:O	12:I:3:THR:C	2.43	0.55
4:A:1220:PHE:O	4:A:1221:LYS:HB2	2.05	0.55
14:K:49:GLU:HG3	14:K:94:ILE:HG12	1.88	0.55
4:A:1436:ILE:O	4:A:1437:GLY:C	2.42	0.55
5:B:358:LYS:HA	5:B:366:GLN:HB3	1.89	0.55
5:B:830:TYR:CE2	5:B:1000:PRO:HD3	2.42	0.55
4:A:306:ASN:HB2	4:A:324:SER:HB3	1.88	0.55
4:A:1430:LEU:HB2	4:A:1432:GLN:HG3	1.88	0.55
4:A:115:LEU:O	4:A:122:MET:HE2	2.07	0.55
5:B:1034:VAL:CG1	5:B:1035:ALA:N	2.69	0.55
4:A:929:LEU:CD2	4:A:983:ILE:HG21	2.36	0.55
5:B:197:PHE:CZ	5:B:816:GLU:HG2	2.41	0.55
5:B:523:CYS:SG	5:B:524:PRO:HD2	2.46	0.55
4:A:1283:VAL:HG12	4:A:1284:MET:N	2.21	0.55
8:E:35:VAL:C	8:E:37:LEU:H	2.10	0.55
6:C:48:SER:O	6:C:157:CYS:HA	2.06	0.55
4:A:356:ASP:O	4:A:358:ASN:N	2.39	0.55
10:G:91:VAL:HB	10:G:139:ILE:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1444:MET:HE3	9:F:135:ARG:HB2	1.87	0.55
5:B:542:MET:HG2	5:B:747:MET:HB3	1.88	0.55
5:B:702:LEU:HD12	5:B:703:ILE:H	1.71	0.55
4:A:673:GLY:O	4:A:676:MET:HB2	2.05	0.55
4:A:1007:ILE:C	4:A:1009:ASN:N	2.59	0.55
4:A:567:LYS:HZ2	11:H:47:PHE:HB2	1.71	0.55
5:B:980:PHE:CE2	5:B:1094:ARG:HG3	2.41	0.55
4:A:628:GLY:O	4:A:632:VAL:HG23	2.06	0.55
10:G:20:PRO:HG2	10:G:21:ARG:H	1.70	0.55
10:G:79:PHE:CZ	10:G:106:MET:HE1	2.41	0.55
5:B:579:ARG:HG2	5:B:579:ARG:HH11	1.71	0.55
4:A:43:GLU:O	4:A:44:THR:HB	2.07	0.55
4:A:1372:VAL:O	4:A:1376:THR:HG22	2.07	0.55
4:A:24:PRO:HD2	4:A:233:TRP:CD1	2.40	0.55
5:B:108:VAL:HG12	5:B:109:THR:N	2.22	0.55
5:B:57:TYR:HD1	5:B:57:TYR:N	2.04	0.55
5:B:240:ILE:CG2	5:B:254:LEU:HB3	2.36	0.55
4:A:685:GLU:HG3	4:A:686:ALA:N	2.20	0.55
12:I:106:CYS:O	12:I:107:SER:HB2	2.06	0.55
4:A:598:LEU:O	4:A:599:SER:C	2.45	0.55
5:B:918:ILE:HD12	5:B:935:ARG:HD3	1.89	0.55
5:B:1095:LEU:H	5:B:1095:LEU:CD1	2.14	0.55
5:B:1159:ARG:HD3	5:B:1193:GLN:HG2	1.87	0.55
4:A:1290:LYS:O	4:A:1291:VAL:HG23	2.06	0.55
14:K:46:ILE:O	14:K:46:ILE:HG22	2.07	0.55
4:A:1428:VAL:HG13	5:B:1151:LEU:HD21	1.88	0.55
13:J:23:ASN:C	13:J:25:LEU:H	2.10	0.55
4:A:445:ASN:HB2	4:A:455:MET:HG2	1.89	0.55
5:B:763:GLN:C	5:B:765:PRO:HD2	2.27	0.55
8:E:23:VAL:O	8:E:28:TYR:HB2	2.07	0.55
4:A:667:GLY:HA3	6:C:192:TRP:CH2	2.41	0.55
4:A:1377:THR:O	4:A:1379:GLY:N	2.40	0.55
8:E:177:ARG:HD3	8:E:215:MET:HG3	1.89	0.55
4:A:341:MET:HE1	4:A:843:LYS:HZ3	1.71	0.55
4:A:828:ALA:HB1	5:B:530:GLY:HA2	1.85	0.55
14:K:58:PHE:HB3	14:K:76:GLN:HB3	1.89	0.55
12:I:100:PHE:N	12:I:100:PHE:HD1	2.04	0.55
4:A:35:ILE:HG22	4:A:84:ILE:HD12	1.88	0.55
4:A:1345:ARG:NH1	4:A:1373:ASP:OD1	2.36	0.55
6:C:31:ASN:O	6:C:32:SER:C	2.42	0.55
5:B:502:ILE:HG12	5:B:535:LEU:CD1	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1180:PHE:O	5:B:1181:GLU:O	2.24	0.55
5:B:214:ALA:HB3	5:B:498:THR:HA	1.89	0.55
4:A:881:GLN:NE2	4:A:958:VAL:O	2.35	0.55
4:A:207:ILE:O	4:A:208:LEU:C	2.45	0.55
4:A:524:VAL:HG12	4:A:525:GLN:N	2.19	0.55
4:A:528:LEU:HD23	4:A:751:SER:HA	1.89	0.55
4:A:224:PHE:HD2	4:A:229:SER:O	1.90	0.55
4:A:1209:MET:CE	4:A:1236:LEU:HB3	2.36	0.55
5:B:843:GLN:O	5:B:844:SER:C	2.45	0.55
5:B:973:ILE:HG23	5:B:974:PRO:HD2	1.89	0.55
10:G:51:TYR:O	10:G:54:ILE:HG13	2.06	0.55
4:A:870:GLU:HG2	8:E:208:TYR:CD2	2.42	0.55
5:B:847:ASP:C	5:B:849:GLY:N	2.60	0.55
10:G:15:PRO:O	10:G:16:SER:C	2.46	0.55
4:A:414:ASP:OD1	4:A:416:ARG:HG3	2.07	0.55
5:B:520:GLY:HA2	5:B:748:ILE:HG22	1.89	0.55
9:F:130:ILE:O	9:F:148:VAL:CG2	2.55	0.55
4:A:1027:ALA:O	4:A:1028:THR:C	2.43	0.55
12:I:56:ALA:O	12:I:57:GLY:O	2.25	0.55
5:B:880:THR:HB	5:B:934:LYS:HD2	1.88	0.54
4:A:1279:ILE:HD11	4:A:1316:VAL:HG21	1.89	0.54
5:B:1197:PRO:O	5:B:1200:ALA:HB3	2.07	0.54
12:I:34:TYR:HE2	12:I:36:GLU:HB3	1.71	0.54
4:A:1385:THR:HG22	4:A:1386:ARG:N	2.22	0.54
7:D:130:LEU:C	7:D:132:GLN:N	2.61	0.54
11:H:127:GLY:O	11:H:128:ASN:HB2	2.07	0.54
8:E:157:SER:C	8:E:159:ASP:N	2.61	0.54
4:A:679:ILE:O	4:A:682:THR:N	2.40	0.54
4:A:789:LYS:HE3	12:I:67:THR:HB	1.89	0.54
4:A:90:VAL:HG12	4:A:91:PHE:N	2.21	0.54
10:G:106:MET:CG	10:G:107:LYS:N	2.70	0.54
10:G:56:ILE:O	10:G:57:GLN:HB2	2.06	0.54
15:L:32:ALA:HB3	15:L:55:ILE:HD12	1.88	0.54
4:A:418:SER:O	4:A:420:ARG:N	2.40	0.54
4:A:446:ARG:HB2	4:A:487:MET:SD	2.48	0.54
7:D:53:SER:CB	7:D:153:ARG:H	2.19	0.54
7:D:53:SER:HB3	7:D:152:SER:CB	2.37	0.54
8:E:14:ARG:HH21	8:E:141:VAL:HG12	1.72	0.54
4:A:366:VAL:CG2	4:A:460:VAL:HG22	2.37	0.54
5:B:472:ALA:HB1	5:B:474:SER:HB3	1.88	0.54
6:C:145:CYS:HA	13:J:2:ILE:HD11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:13:LEU:HD22	10:G:14:HIS:O	2.07	0.54
5:B:1002:THR:HG23	5:B:1006:ILE:HG13	1.88	0.54
9:F:81:THR:HB	9:F:136:ARG:NH1	2.23	0.54
8:E:124:VAL:HG13	8:E:132:ILE:HD12	1.88	0.54
5:B:1031:LEU:HD13	5:B:1055:ILE:HD11	1.89	0.54
4:A:1032:LEU:O	4:A:1036:ARG:HD3	2.07	0.54
5:B:769:TYR:O	5:B:771:SER:N	2.40	0.54
4:A:1161:THR:OG1	4:A:1239:ARG:NH2	2.41	0.54
13:J:1:MET:H2	13:J:56:LEU:N	2.04	0.54
5:B:830:TYR:O	5:B:831:SER:C	2.44	0.54
4:A:146:MET:HA	4:A:171:GLN:HB2	1.90	0.54
5:B:39:ARG:HG2	5:B:39:ARG:NH1	2.23	0.54
5:B:1166:CYS:O	5:B:1168:LEU:N	2.39	0.54
8:E:22:MET:HE1	8:E:26:ARG:HH21	1.71	0.54
8:E:207:ARG:HB3	8:E:207:ARG:HH11	1.72	0.54
4:A:1127:ASP:HB3	4:A:1130:GLN:HB3	1.87	0.54
4:A:1100:ARG:HH21	4:A:1351:GLU:CG	2.21	0.54
4:A:1208:THR:HG22	4:A:1210:GLY:H	1.73	0.54
5:B:278:GLN:HG2	5:B:279:ASP:H	1.72	0.54
5:B:997:GLU:H	5:B:997:GLU:CD	2.11	0.54
4:A:590:ARG:HD2	4:A:605:MET:HB3	1.89	0.54
4:A:1118:VAL:O	4:A:1305:VAL:HG13	2.07	0.54
4:A:365:GLY:O	4:A:468:PHE:HA	2.08	0.54
6:C:242:GLN:C	6:C:244:VAL:H	2.09	0.54
5:B:1034:VAL:C	5:B:1036:ALA:H	2.09	0.54
7:D:170:THR:HB	7:D:172:LEU:H	1.73	0.54
8:E:161:LYS:HD2	8:E:195:VAL:HG23	1.88	0.54
10:G:145:VAL:HG12	10:G:146:LYS:N	2.23	0.54
11:H:4:THR:O	11:H:5:LEU:HD23	2.08	0.54
5:B:710:LEU:O	5:B:711:GLU:HG2	2.07	0.54
5:B:35:SER:O	5:B:39:ARG:HG3	2.07	0.54
4:A:61:ILE:O	4:A:63:ARG:N	2.41	0.54
15:L:39:SER:O	15:L:40:LEU:HG	2.08	0.54
6:C:120:ILE:HD13	6:C:124:LEU:HD21	1.90	0.54
4:A:742:ASN:O	4:A:745:GLN:HB2	2.07	0.54
10:G:7:LEU:O	10:G:73:LYS:HD2	2.08	0.54
14:K:21:ILE:HG23	14:K:31:VAL:CG1	2.38	0.54
4:A:341:MET:CE	4:A:843:LYS:NZ	2.71	0.54
4:A:1401:SER:O	4:A:1402:PHE:HB2	2.07	0.54
6:C:263:THR:C	6:C:265:MET:N	2.61	0.54
4:A:986:ILE:HG22	4:A:987:VAL:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:224:GLN:O	5:B:238:ALA:HA	2.08	0.54
4:A:252:PHE:O	4:A:256:GLN:NE2	2.40	0.54
10:G:122:ASN:ND2	10:G:125:SER:HB3	2.23	0.54
6:C:174:ALA:O	6:C:175:ALA:HB2	2.07	0.54
6:C:147:LEU:HD12	6:C:151:GLN:O	2.07	0.54
4:A:981:LEU:HD21	4:A:1038:THR:C	2.28	0.54
4:A:1017:LEU:CB	8:E:205:SER:HA	2.38	0.54
13:J:21:TYR:HB2	13:J:39:LEU:CD1	2.38	0.54
6:C:214:ASN:HB3	6:C:217:ASP:OD2	2.08	0.54
6:C:239:PRO:O	6:C:241:ASP:N	2.41	0.54
4:A:105:CYS:O	4:A:114:LEU:HG	2.07	0.54
5:B:604:ARG:NH2	5:B:614:SER:HA	2.22	0.54
7:D:52:LEU:O	7:D:54:GLU:N	2.40	0.54
4:A:1127:ASP:HB3	4:A:1130:GLN:HB2	1.90	0.54
6:C:107:SER:C	6:C:109:SER:H	2.10	0.54
15:L:60:ARG:HG2	15:L:61:THR:H	1.73	0.54
11:H:139:ASN:O	11:H:140:ALA:HB2	2.08	0.54
4:A:244:PRO:CB	4:A:245:PRO:HD3	2.29	0.54
8:E:29:PHE:O	8:E:30:ILE:CG1	2.55	0.54
5:B:1106:ARG:NH1	5:B:1110:PRO:HD2	2.23	0.54
6:C:80:LEU:HD11	6:C:95:CYS:C	2.28	0.54
4:A:134:ARG:O	4:A:138:ILE:HG13	2.07	0.54
4:A:696:GLU:O	4:A:696:GLU:HG2	2.08	0.54
5:B:309:GLN:HG3	12:I:52:ILE:HD11	1.89	0.53
4:A:666:ILE:N	4:A:666:ILE:HD12	2.22	0.53
4:A:844:ALA:O	4:A:845:LEU:HD23	2.08	0.53
4:A:774:ARG:O	4:A:775:ILE:C	2.46	0.53
5:B:1159:ARG:HE	5:B:1193:GLN:HE21	1.56	0.53
12:I:14:LEU:HA	12:I:28:GLU:O	2.08	0.53
12:I:111:THR:HG22	12:I:113:ASP:H	1.73	0.53
6:C:256:ALA:O	6:C:259:LEU:N	2.41	0.53
10:G:88:ASP:OD2	10:G:88:ASP:N	2.40	0.53
4:A:21:LEU:HG	4:A:1413:GLY:O	2.08	0.53
14:K:58:PHE:HE2	14:K:74:ARG:HE	1.53	0.53
5:B:466:TRP:C	5:B:468:GLU:H	2.09	0.53
4:A:42:ASP:HB3	4:A:45:GLN:HA	1.90	0.53
4:A:836:TYR:CD2	4:A:840:ARG:HD2	2.44	0.53
8:E:3:GLN:HG3	8:E:4:GLU:N	2.22	0.53
5:B:53:GLN:HG2	5:B:547:VAL:CG2	2.36	0.53
9:F:119:ARG:NH1	9:F:119:ARG:HG3	2.21	0.53
13:J:8:PHE:H	13:J:49:MET:HE3	1.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:758:PHE:CE1	5:B:1027:ILE:CG2	2.91	0.53
9:F:109:VAL:HG11	9:F:123:LYS:HG2	1.90	0.53
4:A:1156:PRO:HA	4:A:1190:PRO:CB	2.38	0.53
4:A:868:TYR:CE1	4:A:1064:VAL:CG1	2.88	0.53
5:B:980:PHE:HD2	5:B:1094:ARG:HA	1.72	0.53
5:B:521:LEU:HD13	5:B:633:VAL:HB	1.90	0.53
7:D:35:LEU:H	7:D:35:LEU:HD12	1.72	0.53
7:D:49:ALA:HB2	7:D:174:PRO:HB3	1.90	0.53
10:G:110:VAL:HG22	10:G:161:GLY:O	2.08	0.53
4:A:761:MET:HA	4:A:804:TYR:HB2	1.89	0.53
5:B:1022:THR:HG23	5:B:1022:THR:O	2.08	0.53
10:G:7:LEU:CD1	10:G:45:ILE:HD11	2.38	0.53
11:H:116:TYR:O	11:H:122:LEU:HA	2.08	0.53
5:B:798:TYR:CE2	6:C:62:PHE:HE2	2.24	0.53
4:A:913:LEU:HD12	4:A:914:GLU:H	1.73	0.53
5:B:65:GLU:CG	5:B:66:ASP:H	2.16	0.53
4:A:265:LYS:HZ3	4:A:322:VAL:HG22	1.73	0.53
4:A:417:TYR:CD2	4:A:417:TYR:N	2.75	0.53
5:B:952:VAL:O	5:B:953:LEU:HB3	2.08	0.53
11:H:113:ALA:HB1	11:H:125:LEU:O	2.09	0.53
5:B:205:ILE:HD12	5:B:205:ILE:N	2.23	0.53
4:A:1001:ARG:O	4:A:1002:GLY:O	2.26	0.53
5:B:196:PRO:HG2	5:B:197:PHE:H	1.73	0.53
6:C:89:GLU:O	6:C:89:GLU:HG2	2.07	0.53
4:A:195:ASP:O	4:A:196:GLU:HB3	2.08	0.53
4:A:586:ILE:HG22	4:A:587:HIS:N	2.24	0.53
5:B:986:GLN:HA	5:B:986:GLN:OE1	2.08	0.53
4:A:399:HIS:O	4:A:401:GLY:N	2.41	0.53
6:C:39:ALA:HA	6:C:164:ALA:CB	2.29	0.53
5:B:168:GLY:N	5:B:450:ALA:HB1	2.18	0.53
5:B:225:VAL:HA	5:B:237:VAL:O	2.09	0.53
6:C:189:THR:HG22	6:C:190:ASP:N	2.23	0.53
5:B:640:VAL:O	5:B:641:GLU:C	2.47	0.53
5:B:942:ARG:O	5:B:944:THR:N	2.42	0.53
5:B:1219:ASP:O	5:B:1219:ASP:OD1	2.27	0.53
12:I:50:THR:CG2	12:I:52:ILE:HG12	2.39	0.53
4:A:1116:LEU:HD12	4:A:1116:LEU:C	2.29	0.53
4:A:534:LEU:HG	4:A:534:LEU:O	2.08	0.53
4:A:903:ASN:C	4:A:903:ASN:ND2	2.58	0.53
4:A:847:ASP:OD1	4:A:848:ILE:HG13	2.08	0.53
5:B:1001:PHE:CD2	6:C:34:ARG:NH2	2.77	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:95:PHE:CD1	4:A:234:MET:HG2	2.44	0.53
4:A:1410:PHE:HA	5:B:1212:ILE:CD1	2.39	0.53
5:B:750:GLY:O	5:B:751:VAL:C	2.46	0.53
4:A:401:GLY:C	4:A:435:HIS:HD2	2.12	0.53
4:A:1118:VAL:CG2	4:A:1306:LEU:HB2	2.39	0.53
4:A:829:VAL:C	4:A:831:THR:N	2.50	0.53
5:B:479:VAL:O	5:B:480:SER:HB3	2.09	0.53
4:A:218:ASP:HA	4:A:221:SER:HG	1.74	0.53
4:A:1151:GLU:HA	12:I:44:TYR:O	2.09	0.53
11:H:83:GLN:C	11:H:85:GLY:H	2.12	0.53
5:B:872:GLU:HA	5:B:915:THR:O	2.09	0.53
6:C:168:ALA:O	6:C:170:TRP:N	2.42	0.53
10:G:14:HIS:CE1	10:G:15:PRO:HD2	2.43	0.53
9:F:103:MET:CE	10:G:66:GLY:H	2.22	0.53
4:A:665:GLY:C	4:A:666:ILE:HD12	2.29	0.53
4:A:152:VAL:HG12	4:A:153:PRO:CD	2.37	0.53
4:A:71:GLN:O	4:A:73:GLY:N	2.37	0.53
4:A:427:GLN:HB2	4:A:430:TRP:CD1	2.44	0.53
5:B:1050:ILE:HG22	5:B:1051:THR:N	2.24	0.53
7:D:40:HIS:CE1	7:D:41:GLN:HG3	2.43	0.53
4:A:401:GLY:C	4:A:435:HIS:CD2	2.82	0.53
4:A:1434:ALA:CB	4:A:1436:ILE:HD12	2.39	0.53
10:G:14:HIS:CD2	10:G:16:SER:H	2.27	0.53
6:C:184:ASN:HD21	6:C:187:LYS:HA	1.69	0.53
5:B:637:LEU:O	5:B:690:VAL:HG13	2.09	0.53
4:A:1030:ARG:NH1	4:A:1035:TYR:OH	2.41	0.53
5:B:843:GLN:O	5:B:846:ILE:HB	2.09	0.53
4:A:497:THR:HG22	4:A:498:ARG:N	2.24	0.53
9:F:140:ASP:C	9:F:140:ASP:OD1	2.48	0.53
10:G:1:MET:O	10:G:3:PHE:CD1	2.62	0.53
10:G:3:PHE:CE1	10:G:80:LYS:HE2	2.44	0.53
4:A:601:LYS:HB2	4:A:603:ASN:ND2	2.24	0.53
4:A:241:VAL:HG13	4:A:266:LEU:HD13	1.90	0.53
6:C:175:ALA:O	6:C:176:ILE:HG13	2.09	0.53
7:D:185:CYS:HB2	7:D:211:LEU:HD22	1.89	0.53
6:C:20:PHE:CE1	6:C:22:LEU:HD12	2.42	0.53
5:B:118:ARG:HG2	5:B:204:ILE:HD13	1.91	0.53
11:H:95:TYR:HB3	11:H:144:ILE:HB	1.91	0.52
4:A:18:GLN:O	5:B:1215:ARG:CG	2.57	0.52
5:B:1216:LEU:N	5:B:1216:LEU:HD23	2.24	0.52
8:E:29:PHE:C	8:E:30:ILE:HG13	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:900:ALA:HB3	15:L:61:THR:OG1	2.09	0.52
5:B:216:GLU:HA	5:B:406:LEU:HD23	1.91	0.52
10:G:49:LEU:HD21	10:G:77:VAL:HG23	1.89	0.52
5:B:1189:ILE:HG22	5:B:1190:ASP:N	2.23	0.52
10:G:111:THR:HB	10:G:114:LEU:HB2	1.91	0.52
5:B:558:LEU:C	5:B:560:GLU:H	2.13	0.52
7:D:33:PHE:CZ	10:G:80:LYS:HE3	2.44	0.52
10:G:80:LYS:HD3	10:G:80:LYS:H	1.73	0.52
5:B:467:GLY:O	5:B:468:GLU:CB	2.56	0.52
5:B:918:ILE:HG21	5:B:935:ARG:NH1	2.25	0.52
15:L:52:GLY:O	15:L:53:HIS:C	2.48	0.52
10:G:138:THR:CG2	10:G:139:ILE:H	2.13	0.52
5:B:1160:VAL:HG12	5:B:1161:HIS:H	1.72	0.52
4:A:382:PRO:CB	4:A:428:TYR:HE2	2.22	0.52
6:C:235:VAL:HG13	13:J:13:VAL:CG2	2.40	0.52
6:C:263:THR:O	6:C:265:MET:N	2.42	0.52
4:A:90:VAL:CG1	4:A:297:GLN:HA	2.39	0.52
10:G:34:VAL:HG12	10:G:45:ILE:CG2	2.35	0.52
6:C:73:GLN:HE21	6:C:74:SER:N	2.07	0.52
4:A:35:ILE:CG2	4:A:84:ILE:HD12	2.40	0.52
5:B:113:TYR:HB3	5:B:114:PRO:HD2	1.91	0.52
1:T:27:DA:H2"	1:T:28:DT:OP2	2.08	0.52
4:A:249:SER:O	4:A:250:ILE:HG13	2.09	0.52
5:B:1115:THR:HG21	5:B:1117:GLN:NE2	2.23	0.52
5:B:758:PHE:HE1	5:B:1027:ILE:HG22	1.73	0.52
6:C:133:ILE:HD11	6:C:237:SER:HA	1.92	0.52
4:A:1101:LEU:HB2	4:A:1355:VAL:HG11	1.91	0.52
11:H:31:THR:O	11:H:31:THR:HG22	2.10	0.52
4:A:399:HIS:CB	4:A:400:PRO:CD	2.79	0.52
4:A:567:LYS:HB3	11:H:95:TYR:CA	2.38	0.52
5:B:980:PHE:HE2	5:B:1094:ARG:CG	2.21	0.52
4:A:1345:ARG:HG3	4:A:1376:THR:HG21	1.90	0.52
5:B:1202:LEU:O	5:B:1206:GLU:HG3	2.09	0.52
5:B:745:PRO:C	5:B:747:MET:H	2.12	0.52
4:A:152:VAL:HG13	4:A:153:PRO:HD2	1.89	0.52
4:A:765:VAL:HG23	4:A:802:ASN:O	2.10	0.52
10:G:47:CYS:O	10:G:76:ALA:HB1	2.08	0.52
4:A:946:VAL:HG22	8:E:201:LYS:HD2	1.90	0.52
10:G:26:LEU:O	10:G:27:LYS:C	2.47	0.52
5:B:831:SER:CB	5:B:994:TYR:OH	2.58	0.52
4:A:825:ILE:HG22	5:B:508:LEU:CD1	2.36	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:31:ASN:O	6:C:34:ARG:N	2.42	0.52
4:A:1004:ASN:O	4:A:1008:GLN:HB2	2.10	0.52
9:F:147:SER:OG	9:F:150:GLU:HG3	2.09	0.52
4:A:621:THR:O	4:A:629:LEU:HB2	2.09	0.52
10:G:96:GLN:HA	10:G:121:PHE:CE2	2.45	0.52
12:I:61:ASP:C	12:I:63:GLY:H	2.13	0.52
8:E:55:ARG:HD2	8:E:83:CYS:O	2.09	0.52
4:A:1153:TYR:CE1	12:I:42:LEU:HD13	2.45	0.52
6:C:66:ARG:NH1	6:C:144:ILE:O	2.43	0.52
5:B:579:ARG:CB	5:B:586:TRP:HE1	2.16	0.52
5:B:563:MET:HE1	5:B:587:HIS:HB2	1.92	0.52
6:C:8:VAL:HG12	6:C:9:LYS:H	1.74	0.52
4:A:1336:MET:HE2	4:A:1381:LEU:HG	1.92	0.52
5:B:758:PHE:N	5:B:759:PRO:CD	2.73	0.52
4:A:647:GLY:O	4:A:651:LYS:HG3	2.09	0.52
5:B:842:ASN:O	5:B:846:ILE:HG13	2.10	0.52
5:B:288:ALA:HA	5:B:331:LEU:HD12	1.92	0.52
5:B:429:PHE:HA	5:B:432:MET:HE3	1.92	0.52
4:A:35:ILE:HA	4:A:52:GLY:O	2.10	0.52
4:A:341:MET:CE	5:B:1135:ARG:NH1	2.73	0.52
7:D:153:ARG:HB3	7:D:154:PHE:CE1	2.45	0.52
6:C:22:LEU:HD13	6:C:230:MET:HE3	1.92	0.52
4:A:95:PHE:O	4:A:96:ILE:C	2.48	0.52
8:E:90:VAL:HG22	8:E:90:VAL:O	2.09	0.52
4:A:92:HIS:HB2	4:A:236:LEU:HD21	1.90	0.52
5:B:282:ILE:CD1	5:B:382:ILE:HD13	2.40	0.52
13:J:45:CYS:O	13:J:48:ARG:HG3	2.08	0.52
12:I:55:THR:HG22	12:I:58:VAL:HG21	1.91	0.52
5:B:225:VAL:O	5:B:226:PHE:CD2	2.63	0.52
4:A:91:PHE:HB2	4:A:297:GLN:HE22	1.74	0.52
15:L:61:THR:CG2	15:L:63:ARG:HG2	2.39	0.52
10:G:115:MET:CB	10:G:116:PRO:HD2	2.40	0.52
8:E:78:LEU:C	8:E:78:LEU:HD23	2.29	0.52
5:B:847:ASP:O	5:B:849:GLY:N	2.43	0.52
5:B:44:VAL:O	5:B:45:SER:C	2.48	0.52
3:P:3:G:H2'	3:P:4:A:C8	2.45	0.52
4:A:17:VAL:HA	5:B:1215:ARG:O	2.10	0.52
4:A:840:ARG:NH2	4:A:1106:ASN:OD1	2.42	0.52
5:B:1132:GLU:O	5:B:1135:ARG:HB3	2.09	0.52
7:D:56:ARG:HD2	7:D:149:THR:OG1	2.09	0.52
4:A:381:THR:CG2	4:A:383:TYR:H	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:353:ILE:HD12	4:A:487:MET:HE2	1.91	0.52
12:I:13:MET:O	12:I:14:LEU:HD23	2.10	0.52
4:A:698:GLN:HA	12:I:97:MET:O	2.08	0.52
6:C:80:LEU:HD11	6:C:95:CYS:HA	1.91	0.52
4:A:730:GLY:C	4:A:732:LEU:N	2.62	0.52
4:A:91:PHE:HB2	4:A:297:GLN:NE2	2.24	0.52
4:A:316:GLN:O	4:A:317:LYS:C	2.48	0.52
5:B:954:VAL:O	15:L:55:ILE:O	2.27	0.52
8:E:198:ILE:HD11	8:E:212:ARG:CG	2.33	0.52
4:A:337:ARG:NH2	4:A:839:ARG:HH12	2.08	0.52
4:A:840:ARG:O	4:A:841:LEU:C	2.48	0.52
12:I:55:THR:HG21	12:I:109:ILE:HD13	1.92	0.52
6:C:146:LYS:C	6:C:147:LEU:HD23	2.29	0.52
5:B:557:PHE:HD2	5:B:557:PHE:C	2.12	0.52
6:C:206:ASN:OD1	6:C:229:TYR:CD2	2.63	0.52
4:A:47:ARG:O	4:A:48:ALA:HB2	2.10	0.52
4:A:535:THR:HG23	4:A:575:LYS:HE2	1.91	0.52
6:C:6:PRO:HB3	6:C:25:VAL:HG12	1.92	0.52
5:B:400:HIS:ND1	5:B:517:THR:HG21	2.25	0.52
4:A:1193:LEU:HD12	4:A:1194:ARG:N	2.24	0.52
12:I:55:THR:O	12:I:55:THR:HG22	2.10	0.52
6:C:60:ASP:OD2	15:L:60:ARG:NH2	2.42	0.52
15:L:61:THR:HG22	15:L:63:ARG:HG2	1.91	0.52
4:A:1066:VAL:O	4:A:1069:ALA:HB3	2.09	0.52
4:A:166:GLY:O	4:A:167:CYS:SG	2.68	0.52
4:A:567:LYS:CB	4:A:568:PRO:CD	2.87	0.51
4:A:41:MET:O	4:A:50:ILE:HG13	2.11	0.51
5:B:549:THR:HG22	5:B:550:ASP:N	2.17	0.51
6:C:215:GLU:O	6:C:216:GLY:C	2.48	0.51
4:A:427:GLN:HG3	4:A:430:TRP:CE2	2.44	0.51
4:A:788:SER:O	4:A:789:LYS:O	2.29	0.51
5:B:324:ILE:HD13	5:B:330:ALA:HA	1.92	0.51
4:A:1156:PRO:O	4:A:1158:PRO:HD3	2.10	0.51
14:K:53:ASP:OD1	14:K:55:LYS:HB2	2.10	0.51
14:K:21:ILE:HG23	14:K:31:VAL:HG11	1.92	0.51
4:A:1063:MET:SD	4:A:1436:ILE:HG12	2.50	0.51
4:A:244:PRO:O	4:A:247:ARG:N	2.38	0.51
5:B:503:GLY:H	5:B:507:LYS:HD2	1.76	0.51
5:B:896:ASP:CG	15:L:58:LYS:HZ2	2.14	0.51
4:A:444:PHE:CB	4:A:458:HIS:HD2	2.24	0.51
8:E:153:HIS:HB3	8:E:196:VAL:CG1	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:890:TYR:OH	5:B:936:ASP:OD2	2.27	0.51
5:B:661:LEU:C	5:B:663:ALA:H	2.13	0.51
7:D:50:LEU:HD11	10:G:4:ILE:HD11	1.93	0.51
4:A:356:ASP:HB2	4:A:469:ARG:HH12	1.73	0.51
7:D:56:ARG:HA	7:D:148:LEU:HD13	1.93	0.51
4:A:93:VAL:CG2	4:A:301:ALA:HA	2.40	0.51
5:B:603:LEU:HD13	5:B:608:ASP:CB	2.38	0.51
4:A:896:ARG:NH2	4:A:1030:ARG:NH2	2.58	0.51
13:J:7:CYS:CB	13:J:46:CYS:HB3	2.41	0.51
5:B:205:ILE:O	5:B:206:ASN:C	2.49	0.51
4:A:648:ASN:O	4:A:649:ILE:C	2.48	0.51
4:A:167:CYS:O	4:A:167:CYS:SG	2.69	0.51
7:D:47:LEU:CD1	7:D:48:ILE:N	2.71	0.51
11:H:102:TYR:N	11:H:102:TYR:CD2	2.78	0.51
4:A:1115:SER:C	4:A:1308:THR:HG22	2.31	0.51
8:E:13:TRP:O	8:E:16:PHE:HB3	2.09	0.51
6:C:254:LYS:O	6:C:258:ILE:HD13	2.11	0.51
4:A:1197:LEU:HD12	4:A:1209:MET:HE1	1.93	0.51
9:F:111:LEU:H	9:F:111:LEU:HD12	1.75	0.51
5:B:20:ASP:O	5:B:22:SER:N	2.42	0.51
10:G:80:LYS:O	10:G:82:PHE:CE1	2.64	0.51
5:B:469:GLN:O	5:B:470:LYS:HB2	2.10	0.51
4:A:1279:ILE:HG23	4:A:1308:THR:OG1	2.11	0.51
3:P:5:C:H2'	3:P:6:C:C6	2.45	0.51
6:C:35:ARG:NH1	14:K:41:THR:H	2.08	0.51
4:A:98:LYS:O	4:A:99:ILE:C	2.49	0.51
5:B:603:LEU:HB3	5:B:609:ILE:CD1	2.41	0.51
6:C:116:LYS:HD3	6:C:140:ASN:HB3	1.93	0.51
5:B:785:TYR:C	5:B:785:TYR:CD1	2.83	0.51
5:B:1172:ILE:O	5:B:1172:ILE:HG22	2.11	0.51
4:A:567:LYS:HD2	4:A:568:PRO:HD2	1.90	0.51
4:A:600:PRO:C	4:A:602:ASP:H	2.12	0.51
5:B:999:MET:HE2	5:B:1000:PRO:HD2	1.92	0.51
5:B:193:LYS:NZ	15:L:32:ALA:HB1	2.25	0.51
15:L:46:VAL:O	15:L:46:VAL:HG12	2.11	0.51
15:L:27:LEU:HD13	15:L:37:LYS:HE2	1.92	0.51
5:B:230:ALA:N	5:B:231:PRO:CD	2.73	0.51
4:A:1144:LYS:HB2	4:A:1268:LEU:O	2.10	0.51
5:B:1084:GLN:NE2	5:B:1084:GLN:H	2.07	0.51
4:A:1327:ILE:HG22	8:E:147:HIS:CE1	2.45	0.51
5:B:115:GLN:HG2	5:B:193:LYS:CB	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:243:VAL:HG12	6:C:243:VAL:O	2.10	0.51
5:B:757:PRO:HD3	5:B:983:ARG:NH2	2.26	0.51
4:A:1438:THR:HB	5:B:1144:ALA:CB	2.40	0.51
4:A:357:PRO:HD2	5:B:833:TYR:CE1	2.46	0.51
4:A:37:PHE:N	4:A:37:PHE:CD1	2.79	0.51
13:J:2:ILE:HG12	13:J:57:ILE:HD12	1.93	0.51
12:I:50:THR:HG22	12:I:51:ASN:N	2.26	0.51
4:A:1116:LEU:HG	4:A:1308:THR:HB	1.92	0.51
13:J:64:ASN:CB	13:J:65:PRO:CD	2.85	0.51
4:A:102:VAL:O	4:A:105:CYS:HB2	2.11	0.51
9:F:99:LEU:HD21	10:G:64:THR:O	2.10	0.51
10:G:49:LEU:HD23	10:G:49:LEU:N	2.26	0.51
12:I:25:LEU:HB3	12:I:38:ALA:HB2	1.93	0.51
4:A:89:PRO:HB2	4:A:204:THR:HG22	1.92	0.51
10:G:74:TYR:CD2	10:G:74:TYR:N	2.79	0.51
6:C:76:ASP:O	6:C:79:GLN:HG2	2.11	0.51
4:A:1063:MET:HG3	4:A:1436:ILE:HG23	1.92	0.51
4:A:82:GLY:O	4:A:241:VAL:N	2.38	0.51
8:E:22:MET:HE1	8:E:26:ARG:NH2	2.26	0.51
5:B:298:LEU:N	5:B:298:LEU:CD2	2.74	0.51
10:G:119:LEU:HD13	10:G:132:SER:HB2	1.93	0.51
7:D:52:LEU:C	7:D:54:GLU:H	2.14	0.51
4:A:278:THR:O	4:A:282:ASN:HB2	2.11	0.51
14:K:24:ASP:OD2	14:K:74:ARG:NH1	2.43	0.51
4:A:1094:VAL:HG12	4:A:1095:THR:N	2.26	0.51
5:B:361:LEU:N	5:B:362:PRO:CD	2.73	0.51
7:D:52:LEU:CD2	7:D:147:TYR:HE2	2.23	0.51
2:N:2:DA:H2"	2:N:3:DG:OP2	2.10	0.51
4:A:1101:LEU:O	4:A:1101:LEU:HD12	2.10	0.51
5:B:410:GLY:O	5:B:412:LEU:N	2.44	0.51
4:A:29:ALA:HB1	5:B:1184:GLY:HA2	1.91	0.51
12:I:98:VAL:C	12:I:99:LEU:HD23	2.31	0.50
4:A:44:THR:O	4:A:45:GLN:HB2	2.12	0.50
4:A:84:ILE:HD11	4:A:270:LEU:CD1	2.29	0.50
5:B:872:GLU:CD	5:B:914:LYS:HE2	2.32	0.50
9:F:103:MET:HE2	10:G:66:GLY:H	1.76	0.50
4:A:666:ILE:H	5:B:1026:LEU:HD22	1.76	0.50
4:A:71:GLN:C	4:A:73:GLY:N	2.65	0.50
4:A:1333:ILE:HG22	4:A:1334:ASP:N	2.26	0.50
14:K:56:VAL:HA	14:K:77:THR:HG22	1.93	0.50
5:B:221:ASN:N	5:B:241:ARG:O	2.33	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:61:GLN:HG2	8:E:62:ALA:N	2.26	0.50
4:A:817:ALA:HA	5:B:764:SER:OG	2.11	0.50
13:J:1:MET:HE2	13:J:60:PHE:CE2	2.47	0.50
5:B:580:VAL:HG22	5:B:624:LEU:HB3	1.93	0.50
5:B:882:THR:CG2	5:B:884:ARG:HB2	2.40	0.50
4:A:353:ILE:CD1	4:A:487:MET:HE2	2.41	0.50
9:F:81:THR:HG21	9:F:136:ARG:CD	2.41	0.50
4:A:809:THR:H	4:A:812:GLU:HB2	1.76	0.50
5:B:841:MET:SD	5:B:846:ILE:HD11	2.51	0.50
1:T:18:DC:H3'	1:T:18:DC:OP1	2.11	0.50
4:A:1451:VAL:O	4:A:1454:MET:HG2	2.11	0.50
4:A:632:VAL:O	4:A:633:VAL:C	2.49	0.50
5:B:48:LEU:O	5:B:51:PHE:N	2.42	0.50
4:A:873:MET:HG2	4:A:957:PRO:HB3	1.92	0.50
5:B:1056:SER:HB3	5:B:1066:SER:HB2	1.94	0.50
13:J:44:TYR:N	13:J:44:TYR:CD2	2.79	0.50
13:J:7:CYS:HA	13:J:49:MET:HE3	1.92	0.50
10:G:99:PHE:HZ	10:G:163:ILE:HD13	1.76	0.50
4:A:512:VAL:HA	4:A:519:PRO:HA	1.94	0.50
9:F:116:ASP:C	9:F:116:ASP:OD1	2.49	0.50
14:K:58:PHE:HB3	14:K:76:GLN:HE21	1.76	0.50
12:I:85:PHE:HD1	12:I:99:LEU:HD13	1.77	0.50
4:A:79:GLY:HA3	4:A:243:PRO:HG3	1.93	0.50
12:I:34:TYR:CE2	12:I:36:GLU:HB3	2.45	0.50
5:B:770:GLN:OE1	5:B:983:ARG:CA	2.56	0.50
5:B:1177:HIS:O	5:B:1179:GLN:N	2.45	0.50
7:D:156:ASP:C	7:D:158:GLU:H	2.13	0.50
7:D:156:ASP:C	7:D:158:GLU:N	2.65	0.50
13:J:27:GLU:C	13:J:29:GLU:H	2.14	0.50
4:A:784:LEU:HB3	4:A:785:PRO:HD2	1.94	0.50
4:A:590:ARG:HD3	4:A:604:GLY:C	2.32	0.50
11:H:123:MET:HG2	11:H:124:ARG:N	2.26	0.50
4:A:446:ARG:HB2	4:A:487:MET:HG2	1.94	0.50
12:I:33:SER:O	12:I:35:VAL:HG23	2.11	0.50
12:I:5:ARG:HD3	12:I:36:GLU:OE2	2.12	0.50
4:A:326:ARG:HH22	4:A:1407:GLU:HG3	1.76	0.50
12:I:111:THR:CG2	12:I:112:SER:N	2.74	0.50
5:B:825:VAL:HG12	5:B:826:ALA:N	2.26	0.50
5:B:658:ILE:HG22	5:B:659:ALA:N	2.27	0.50
6:C:55:THR:O	6:C:55:THR:HG22	2.11	0.50
7:D:33:PHE:CZ	10:G:80:LYS:CE	2.95	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:817:ALA:O	4:A:819:GLY:N	2.45	0.50
11:H:123:MET:HE1	11:H:142:LEU:HD11	1.93	0.50
12:I:85:PHE:N	12:I:85:PHE:HD2	1.89	0.50
5:B:1095:LEU:HD12	5:B:1095:LEU:N	2.22	0.50
4:A:1430:LEU:O	5:B:1197:PRO:HD2	2.11	0.50
5:B:745:PRO:O	5:B:747:MET:N	2.44	0.50
4:A:326:ARG:NH2	4:A:1407:GLU:HG3	2.26	0.50
4:A:412:ARG:NH2	5:B:1108:ARG:NH1	2.60	0.50
8:E:124:VAL:CG1	8:E:132:ILE:HB	2.39	0.50
5:B:205:ILE:CD1	5:B:205:ILE:N	2.74	0.50
5:B:1072:MET:HE1	5:B:1085:ILE:HB	1.90	0.50
4:A:768:GLN:HG2	4:A:816:HIS:CA	2.31	0.50
4:A:779:PHE:O	4:A:780:VAL:C	2.50	0.50
11:H:27:GLU:HG2	11:H:39:THR:HG23	1.93	0.50
9:F:138:LEU:HB3	9:F:139:PRO:HD2	1.94	0.50
6:C:70:ILE:HD11	6:C:144:ILE:HG12	1.94	0.50
4:A:1041:ALA:O	4:A:1044:TRP:HB3	2.12	0.50
4:A:963:ILE:HD11	4:A:1048:ASN:CB	2.28	0.50
4:A:608:ILE:HD12	4:A:613:ILE:CD1	2.42	0.50
4:A:886:ILE:HG13	4:A:943:LEU:CD1	2.42	0.50
10:G:9:LEU:HG	10:G:10:ASN:N	2.27	0.50
13:J:53:HIS:C	13:J:53:HIS:CD2	2.84	0.50
7:D:220:LEU:O	7:D:221:TYR:HD1	1.94	0.50
4:A:573:SER:OG	4:A:576:GLN:HB2	2.11	0.50
7:D:33:PHE:CE2	10:G:80:LYS:NZ	2.61	0.50
5:B:681:TRP:O	5:B:683:SER:N	2.45	0.50
12:I:69:PRO:HG2	12:I:85:PHE:CD2	2.47	0.50
5:B:882:THR:O	5:B:883:LEU:HB2	2.11	0.50
4:A:464:PRO:HG2	4:A:465:TYR:HD1	1.77	0.50
4:A:420:ARG:O	4:A:421:ALA:C	2.50	0.50
8:E:22:MET:CE	8:E:26:ARG:HH21	2.25	0.50
4:A:1334:ASP:O	4:A:1336:MET:N	2.45	0.50
4:A:1410:PHE:HD2	5:B:1212:ILE:HD12	1.77	0.50
6:C:101:LEU:HD13	6:C:118:LEU:HD23	1.94	0.50
5:B:26:THR:O	5:B:29:ASP:HB2	2.11	0.50
6:C:105:GLY:HA3	6:C:149:LYS:O	2.11	0.50
4:A:942:PHE:C	4:A:942:PHE:CD2	2.85	0.50
4:A:547:LEU:HB3	14:K:58:PHE:CE1	2.44	0.50
6:C:69:LEU:CD1	6:C:69:LEU:N	2.74	0.50
5:B:865:LYS:NZ	5:B:869:SER:HA	2.27	0.50
6:C:35:ARG:NH1	14:K:41:THR:N	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:238:ILE:HG22	6:C:243:VAL:HG23	1.94	0.50
4:A:65:LEU:O	4:A:66:LYS:O	2.30	0.50
4:A:552:TRP:O	4:A:554:PRO:HD3	2.12	0.50
5:B:734:HIS:O	5:B:735:ALA:HB2	2.12	0.50
4:A:658:LEU:HD23	4:A:659:HIS:HE1	1.76	0.50
6:C:208:GLU:O	6:C:210:GLU:N	2.45	0.50
10:G:3:PHE:CD1	10:G:80:LYS:NZ	2.77	0.49
5:B:525:ALA:O	5:B:768:THR:HA	2.11	0.49
5:B:115:GLN:HG2	5:B:193:LYS:HB2	1.93	0.49
4:A:18:GLN:H	5:B:1215:ARG:HB2	1.76	0.49
6:C:8:VAL:HG12	6:C:9:LYS:N	2.26	0.49
4:A:442:VAL:CB	4:A:489:LEU:HD11	2.37	0.49
4:A:268:ASP:O	4:A:269:ILE:C	2.50	0.49
5:B:171:PRO:HD2	5:B:457:LEU:CD1	2.39	0.49
15:L:40:LEU:HD22	15:L:44:ASP:CB	2.42	0.49
4:A:1120:LEU:HD12	4:A:1120:LEU:N	2.26	0.49
6:C:249:ASP:O	6:C:252:GLN:HB3	2.12	0.49
4:A:500:GLU:OE1	5:B:1143:ALA:C	2.50	0.49
4:A:30:ILE:HG23	5:B:1170:THR:HG23	1.94	0.49
5:B:175:ARG:HG2	5:B:175:ARG:HH11	1.77	0.49
7:D:33:PHE:CZ	10:G:80:LYS:NZ	2.79	0.49
5:B:766:ARG:NH2	5:B:1020:ARG:HH11	2.10	0.49
6:C:66:ARG:CZ	13:J:2:ILE:HG21	2.42	0.49
5:B:309:GLN:OE1	12:I:52:ILE:HD11	2.12	0.49
4:A:266:LEU:O	4:A:267:ALA:C	2.49	0.49
6:C:34:ARG:O	6:C:38:ILE:HG13	2.11	0.49
4:A:808:LEU:HD23	4:A:813:PHE:CA	2.37	0.49
4:A:1394:THR:O	4:A:1395:GLY:O	2.30	0.49
9:F:77:ASP:C	9:F:79:ARG:N	2.66	0.49
4:A:2:VAL:HG21	5:B:1158:PHE:N	2.27	0.49
4:A:1124:HIS:HB3	4:A:1130:GLN:HG2	1.93	0.49
8:E:35:VAL:O	8:E:37:LEU:N	2.44	0.49
4:A:842:VAL:HG11	5:B:1136:ASP:OD2	2.12	0.49
4:A:947:PHE:CD2	4:A:954:TRP:CZ2	3.00	0.49
7:D:29:LEU:HD22	10:G:82:PHE:CD2	2.47	0.49
11:H:41:ASP:O	11:H:42:ILE:HG13	2.13	0.49
4:A:901:LEU:HA	4:A:907:THR:OG1	2.13	0.49
4:A:262:LEU:C	4:A:264:PHE:N	2.65	0.49
6:C:167:HIS:HD2	6:C:168:ALA:H	1.60	0.49
10:G:13:LEU:O	10:G:67:SER:HA	2.12	0.49
4:A:1059:HIS:O	4:A:1061:GLY:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:90:ARG:HD3	9:F:155:LEU:HD11	1.94	0.49
4:A:489:LEU:HD12	4:A:490:HIS:N	2.26	0.49
5:B:32:ALA:O	5:B:35:SER:HB2	2.11	0.49
4:A:608:ILE:C	4:A:610:GLY:N	2.64	0.49
5:B:642:ASP:HB3	5:B:649:LYS:HD2	1.93	0.49
5:B:1106:ARG:NH1	5:B:1110:PRO:CD	2.76	0.49
13:J:45:CYS:SG	13:J:46:CYS:N	2.85	0.49
4:A:283:GLY:O	4:A:285:PRO:HD3	2.12	0.49
10:G:143:ILE:HG22	10:G:144:ARG:H	1.76	0.49
4:A:909:ASP:C	4:A:911:SER:H	2.16	0.49
4:A:317:LYS:O	4:A:318:SER:CB	2.60	0.49
10:G:94:CYS:SG	10:G:99:PHE:HB3	2.51	0.49
5:B:487:THR:O	5:B:490:SER:HB3	2.12	0.49
4:A:567:LYS:HB2	4:A:568:PRO:CD	2.43	0.49
11:H:142:LEU:C	11:H:143:LEU:HD12	2.32	0.49
4:A:863:VAL:HG11	4:A:866:PHE:CE2	2.48	0.49
4:A:541:ILE:HG21	4:A:549:MET:HE3	1.93	0.49
4:A:1369:ALA:O	4:A:1370:LEU:C	2.49	0.49
4:A:1019:CYS:O	4:A:1020:CYS:C	2.50	0.49
6:C:91:HIS:HD2	6:C:91:HIS:O	1.94	0.49
5:B:1084:GLN:C	5:B:1085:ILE:HD12	2.33	0.49
5:B:765:PRO:O	5:B:768:THR:N	2.45	0.49
5:B:860:MET:HG2	5:B:861:ASP:H	1.77	0.49
4:A:1329:THR:HG23	4:A:1331:SER:H	1.75	0.49
7:D:144:THR:HG21	10:G:46:LEU:HD13	1.95	0.49
4:A:381:THR:HG21	4:A:383:TYR:CD1	2.48	0.49
6:C:31:ASN:ND2	6:C:35:ARG:HD2	2.28	0.49
4:A:113:LEU:O	4:A:114:LEU:HD23	2.13	0.49
4:A:219:PHE:CE2	4:A:231:PRO:HD2	2.47	0.49
5:B:744:HIS:HD2	5:B:746:SER:OG	1.94	0.49
4:A:64:ASN:O	4:A:65:LEU:C	2.50	0.49
4:A:1149:ALA:CB	12:I:47:GLU:HA	2.43	0.49
5:B:810:GLU:CB	5:B:815:ARG:HH22	2.26	0.49
5:B:327:ARG:O	5:B:331:LEU:HD13	2.12	0.49
4:A:166:GLY:O	4:A:167:CYS:CB	2.61	0.49
14:K:53:ASP:HB3	14:K:56:VAL:HG23	1.93	0.49
4:A:457:ALA:HB3	4:A:506:ALA:HA	1.94	0.49
4:A:984:LYS:O	4:A:988:LEU:HB2	2.11	0.49
5:B:235:SER:O	5:B:236:HIS:HD2	1.94	0.49
5:B:96:TYR:HB2	5:B:129:PHE:HB2	1.94	0.49
4:A:898:ARG:HB2	4:A:933:TYR:CE1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:595:THR:O	4:A:596:THR:HG23	2.12	0.49
4:A:870:GLU:HG2	8:E:208:TYR:CG	2.47	0.49
5:B:579:ARG:N	5:B:589:VAL:HG13	2.28	0.49
4:A:794:PRO:C	4:A:796:SER:H	2.14	0.49
4:A:298:PHE:HD2	4:A:299:HIS:CD2	2.31	0.49
5:B:281:PRO:O	5:B:283:VAL:N	2.45	0.49
5:B:728:ARG:NH1	5:B:1047:PHE:HB3	2.25	0.49
4:A:4:GLN:O	4:A:5:GLN:O	2.31	0.49
4:A:1130:GLN:O	4:A:1134:ILE:HG13	2.12	0.49
10:G:145:VAL:CG1	10:G:146:LYS:N	2.76	0.49
8:E:55:ARG:C	8:E:57:MET:H	2.14	0.49
5:B:1039:GLY:HA2	13:J:51:LEU:CD2	2.42	0.49
14:K:107:THR:O	14:K:111:LEU:HG	2.12	0.49
4:A:866:PHE:C	4:A:867:ILE:HG13	2.30	0.49
13:J:3:VAL:HG21	13:J:18:TRP:CB	2.38	0.49
4:A:913:LEU:CD2	4:A:919:ILE:HD12	2.41	0.49
5:B:1065:GLN:NE2	5:B:1067:ARG:N	2.45	0.49
4:A:1389:PHE:CD1	4:A:1389:PHE:C	2.85	0.49
4:A:1431:GLY:HA3	5:B:1152:MET:SD	2.53	0.49
4:A:381:THR:HG23	4:A:382:PRO:HD2	1.95	0.49
4:A:608:ILE:C	4:A:610:GLY:H	2.16	0.49
5:B:1106:ARG:HH12	5:B:1110:PRO:HG2	1.78	0.49
15:L:49:LYS:O	15:L:50:ASP:CB	2.60	0.49
5:B:465:ASN:ND2	5:B:465:ASN:N	2.61	0.49
5:B:622:LYS:CE	12:I:59:VAL:HG22	2.43	0.49
5:B:498:THR:HB	5:B:537:LYS:O	2.12	0.49
4:A:958:VAL:O	4:A:958:VAL:HG12	2.12	0.49
5:B:640:VAL:O	5:B:640:VAL:HG12	2.11	0.49
8:E:43:LYS:O	8:E:45:LYS:N	2.44	0.49
14:K:31:VAL:CG1	14:K:32:VAL:H	2.26	0.49
5:B:879:ARG:O	5:B:880:THR:HB	2.12	0.49
6:C:242:GLN:C	6:C:244:VAL:N	2.65	0.49
4:A:215:SER:HB3	4:A:218:ASP:OD2	2.12	0.49
4:A:295:LEU:O	4:A:298:PHE:HB3	2.12	0.49
4:A:606:LEU:HB3	4:A:614:PHE:CD2	2.47	0.49
5:B:205:ILE:HG22	5:B:206:ASN:N	2.28	0.49
10:G:115:MET:HB3	10:G:116:PRO:HD2	1.94	0.49
13:J:34:THR:O	13:J:35:ALA:C	2.51	0.49
10:G:74:TYR:HD2	10:G:74:TYR:N	2.07	0.49
5:B:460:ALA:HB1	5:B:466:TRP:CZ3	2.48	0.49
5:B:763:GLN:O	5:B:765:PRO:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:372:LYS:HA	4:A:435:HIS:ND1	2.28	0.49
5:B:307:ASP:O	5:B:309:GLN:N	2.46	0.49
4:A:1349:TYR:CE1	4:A:1368:MET:HE3	2.48	0.49
5:B:1196:ILE:HG13	5:B:1196:ILE:O	2.11	0.49
6:C:10:ILE:HA	6:C:20:PHE:HB2	1.93	0.49
5:B:1032:SER:O	5:B:1036:ALA:HB2	2.12	0.49
7:D:134:THR:CG2	7:D:135:GLY:H	2.26	0.49
4:A:1036:ARG:HH11	4:A:1036:ARG:HG2	1.77	0.49
5:B:575:PRO:HG2	5:B:576:ASP:H	1.78	0.49
4:A:1280:GLU:O	4:A:1281:ARG:O	2.30	0.49
4:A:590:ARG:HH21	4:A:620:LYS:CB	2.24	0.49
13:J:57:ILE:O	13:J:60:PHE:HB2	2.13	0.49
4:A:535:THR:CG2	4:A:575:LYS:HE2	2.42	0.49
5:B:102:VAL:CG2	5:B:112:LEU:HD22	2.43	0.49
8:E:175:LEU:HD23	8:E:176:PRO:CD	2.39	0.49
4:A:341:MET:HE3	5:B:1135:ARG:NH1	2.28	0.49
4:A:231:PRO:C	4:A:233:TRP:H	2.16	0.49
4:A:299:HIS:C	4:A:301:ALA:N	2.66	0.49
14:K:12:LEU:CD1	14:K:12:LEU:H	2.24	0.49
13:J:48:ARG:HE	13:J:49:MET:CE	2.26	0.49
8:E:134:THR:C	8:E:135:PHE:HD1	2.16	0.49
6:C:254:LYS:C	6:C:256:ALA:H	2.16	0.49
4:A:253:ASN:HB3	5:B:935:ARG:CZ	2.42	0.48
4:A:18:GLN:HB3	5:B:1215:ARG:HG3	1.94	0.48
7:D:167:LEU:HB3	7:D:177:VAL:HG13	1.95	0.48
6:C:154:LYS:O	6:C:155:LEU:HD23	2.12	0.48
8:E:46:TYR:CD2	8:E:58:MET:HG2	2.48	0.48
5:B:318:VAL:O	5:B:320:ASP:N	2.46	0.48
10:G:44:TYR:O	10:G:78:VAL:HA	2.13	0.48
5:B:203:PHE:N	5:B:203:PHE:CD1	2.81	0.48
5:B:371:GLU:H	5:B:371:GLU:CD	2.17	0.48
12:I:85:PHE:N	12:I:85:PHE:CD2	2.61	0.48
14:K:65:HIS:CD2	14:K:67:PHE:HB2	2.48	0.48
10:G:123:ALA:C	10:G:125:SER:H	2.16	0.48
14:K:82:ASP:OD1	14:K:84:LYS:N	2.45	0.48
4:A:18:GLN:CB	5:B:1215:ARG:HB2	2.42	0.48
5:B:996:ARG:HH12	6:C:38:ILE:HG23	1.77	0.48
4:A:608:ILE:HB	4:A:613:ILE:HD11	1.94	0.48
4:A:164:ARG:CG	4:A:165:GLY:H	2.20	0.48
9:F:75:PRO:O	9:F:77:ASP:O	2.31	0.48
5:B:844:SER:HB3	5:B:848:ARG:HH12	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1187:ASN:O	5:B:1188:LYS:CB	2.61	0.48
13:J:53:HIS:CD2	13:J:54:VAL:N	2.81	0.48
7:D:189:ASP:O	7:D:193:THR:HB	2.13	0.48
11:H:99:GLY:N	11:H:118:PHE:CD2	2.80	0.48
4:A:382:PRO:HB3	4:A:428:TYR:CE2	2.41	0.48
4:A:1191:TRP:HB3	4:A:1260:LEU:HD23	1.96	0.48
6:C:258:ILE:CD1	6:C:258:ILE:N	2.75	0.48
4:A:1213:GLY:O	4:A:1216:ILE:N	2.46	0.48
5:B:240:ILE:O	5:B:240:ILE:HG23	2.13	0.48
8:E:55:ARG:C	8:E:57:MET:N	2.67	0.48
4:A:1195:LEU:HD11	4:A:1267:MET:CE	2.44	0.48
5:B:595:ARG:O	5:B:596:LEU:C	2.51	0.48
4:A:532:ARG:O	4:A:535:THR:HB	2.13	0.48
4:A:577:ILE:C	4:A:579:SER:N	2.64	0.48
4:A:1373:ASP:HA	4:A:1376:THR:CG2	2.43	0.48
4:A:1102:LYS:HG2	4:A:1106:ASN:HD21	1.77	0.48
4:A:668:ASP:HB3	4:A:743:VAL:HG23	1.94	0.48
5:B:910:VAL:HG12	5:B:911:ILE:N	2.28	0.48
4:A:115:LEU:HB2	4:A:122:MET:CE	2.43	0.48
4:A:809:THR:HG23	4:A:812:GLU:HG3	1.95	0.48
13:J:8:PHE:H	13:J:49:MET:HE1	1.79	0.48
10:G:88:ASP:HA	10:G:144:ARG:HA	1.96	0.48
4:A:1162:VAL:HG12	4:A:1162:VAL:O	2.13	0.48
5:B:470:LYS:C	5:B:472:ALA:H	2.15	0.48
11:H:23:VAL:HG13	11:H:42:ILE:O	2.14	0.48
6:C:69:LEU:H	6:C:69:LEU:CD1	2.27	0.48
4:A:971:PHE:HE2	4:A:1040:GLN:HG2	1.79	0.48
4:A:1279:ILE:HD11	4:A:1316:VAL:CG2	2.42	0.48
4:A:14:VAL:HG21	5:B:1216:LEU:HD13	1.95	0.48
4:A:466:SER:HB3	5:B:1103:ILE:HG12	1.94	0.48
4:A:1291:VAL:HG13	4:A:1292:PRO:N	2.29	0.48
5:B:370:PHE:HE2	5:B:373:ARG:NH1	2.06	0.48
8:E:124:VAL:HG13	8:E:132:ILE:CB	2.40	0.48
6:C:259:LEU:HD13	14:K:91:CYS:HB2	1.95	0.48
5:B:810:GLU:HB2	5:B:815:ARG:HH22	1.79	0.48
10:G:20:PRO:HG2	10:G:21:ARG:N	2.28	0.48
5:B:897:GLY:O	5:B:898:LEU:HD23	2.14	0.48
4:A:1168:GLU:O	4:A:1172:LEU:HG	2.13	0.48
5:B:1084:GLN:HG2	6:C:201:TRP:CZ2	2.48	0.48
4:A:381:THR:HG23	4:A:383:TYR:H	1.79	0.48
5:B:120:ARG:HG2	5:B:955:THR:HG21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:117:THR:O	8:E:120:ALA:N	2.45	0.48
4:A:407:ARG:HB3	4:A:430:TRP:CE2	2.49	0.48
9:F:131:PRO:C	9:F:132:LEU:HD23	2.34	0.48
6:C:255:VAL:HG12	14:K:91:CYS:HB3	1.94	0.48
5:B:815:ARG:HD3	5:B:1041:GLU:OE2	2.14	0.48
5:B:558:LEU:O	5:B:560:GLU:N	2.46	0.48
4:A:683:ILE:HD13	4:A:801:GLU:HG3	1.96	0.48
4:A:313:GLN:O	4:A:314:ALA:HB3	2.13	0.48
4:A:1116:LEU:CD1	4:A:1118:VAL:HG13	2.43	0.48
5:B:834:ASN:HB3	5:B:840:ILE:HG13	1.95	0.48
4:A:335:ARG:CA	4:A:339:ASN:HB2	2.41	0.48
7:D:53:SER:HB3	7:D:153:ARG:H	1.79	0.48
12:I:34:TYR:O	12:I:35:VAL:HG23	2.13	0.48
4:A:775:ILE:HB	4:A:797:LYS:O	2.14	0.48
5:B:333:PHE:O	5:B:334:ILE:HG13	2.14	0.48
6:C:254:LYS:C	6:C:256:ALA:N	2.64	0.48
5:B:1039:GLY:HA2	13:J:51:LEU:HD21	1.95	0.48
5:B:345:LYS:O	5:B:347:LYS:HG2	2.13	0.48
4:A:770:VAL:HA	4:A:822:GLU:OE1	2.14	0.48
8:E:96:PHE:CZ	8:E:100:ILE:HD11	2.49	0.48
3:P:5:C:H2'	3:P:6:C:H6	1.78	0.48
6:C:215:GLU:O	6:C:217:ASP:N	2.46	0.48
1:T:15:DT:H1'	4:A:1386:ARG:HH12	1.77	0.48
15:L:36:SER:O	15:L:37:LYS:C	2.51	0.48
10:G:143:ILE:CG2	10:G:144:ARG:N	2.77	0.48
10:G:10:ASN:OD1	10:G:71:ASN:HA	2.13	0.48
5:B:29:ASP:HB3	5:B:658:ILE:CD1	2.44	0.48
10:G:20:PRO:CG	10:G:21:ARG:H	2.26	0.48
13:J:23:ASN:C	13:J:25:LEU:N	2.66	0.48
5:B:129:PHE:HA	5:B:165:VAL:O	2.14	0.48
5:B:877:PRO:C	5:B:878:GLN:HG3	2.34	0.48
5:B:180:TYR:H	5:B:180:TYR:HD1	1.61	0.48
7:D:19:GLU:O	7:D:21:GLU:N	2.47	0.48
4:A:596:THR:C	4:A:598:LEU:N	2.67	0.48
11:H:100:THR:HG22	11:H:101:ALA:H	1.79	0.48
4:A:388:LEU:HD22	4:A:432:VAL:HG21	1.96	0.48
4:A:1441:PHE:CE2	9:F:89:GLU:HG2	2.49	0.48
4:A:95:PHE:O	4:A:98:LYS:N	2.40	0.48
5:B:360:PHE:O	5:B:361:LEU:C	2.52	0.48
4:A:1396:ALA:O	4:A:1398:MET:N	2.47	0.48
4:A:1450:LEU:HD21	10:G:19:GLY:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:407:ARG:HG2	4:A:430:TRP:CZ3	2.49	0.48
8:E:154:ILE:H	8:E:196:VAL:HG12	1.79	0.48
5:B:992:ILE:HD11	14:K:66:PRO:HB2	1.95	0.48
4:A:626:ASN:O	4:A:631:HIS:CD2	2.67	0.48
5:B:1187:ASN:O	5:B:1188:LYS:HB2	2.13	0.48
10:G:150:CYS:C	10:G:151:ILE:HG13	2.33	0.48
5:B:1077:THR:HG22	14:K:44:ASN:HD21	1.78	0.48
4:A:565:ILE:O	4:A:570:PRO:HA	2.14	0.48
4:A:545:GLN:O	4:A:548:ASN:N	2.47	0.48
4:A:1341:ILE:O	4:A:1344:GLY:N	2.47	0.48
5:B:1033:LYS:NZ	5:B:1070:GLU:OE1	2.45	0.48
5:B:642:ASP:CB	5:B:649:LYS:HG3	2.43	0.48
5:B:758:PHE:HB2	5:B:1024:ALA:HB1	1.96	0.48
6:C:3:GLU:HG2	6:C:4:GLU:N	2.29	0.48
5:B:661:LEU:C	5:B:663:ALA:N	2.67	0.48
11:H:62:SER:O	11:H:63:LEU:C	2.50	0.48
5:B:1065:GLN:HG3	5:B:1067:ARG:H	1.78	0.47
4:A:577:ILE:O	4:A:580:VAL:HG23	2.14	0.47
10:G:125:SER:OG	10:G:128:PRO:HA	2.14	0.47
4:A:381:THR:O	4:A:384:ASN:N	2.43	0.47
4:A:608:ILE:HG13	4:A:613:ILE:HD12	1.95	0.47
5:B:95:ILE:CG1	5:B:130:VAL:HG22	2.41	0.47
5:B:205:ILE:CG2	5:B:206:ASN:N	2.76	0.47
5:B:63:ILE:HA	5:B:421:PHE:CE2	2.49	0.47
4:A:53:LEU:CD2	4:A:54:ASN:N	2.60	0.47
6:C:74:SER:HB2	6:C:77:ILE:HG12	1.94	0.47
4:A:853:ASP:O	4:A:854:ASN:CB	2.60	0.47
13:J:56:LEU:O	13:J:59:LYS:N	2.47	0.47
4:A:265:LYS:CE	4:A:322:VAL:HG13	2.44	0.47
5:B:401:PHE:HD2	5:B:521:LEU:HD12	1.79	0.47
5:B:97:VAL:HG12	5:B:178:ASN:HD21	1.77	0.47
4:A:1013:ASP:O	4:A:1015:VAL:N	2.46	0.47
9:F:81:THR:HG1	9:F:146:TRP:HE1	1.63	0.47
4:A:856:THR:HG22	4:A:864:ILE:HB	1.95	0.47
15:L:40:LEU:HD13	15:L:44:ASP:CB	2.43	0.47
4:A:172:PRO:HG3	4:A:185:TRP:CZ2	2.49	0.47
11:H:106:GLU:O	11:H:108:SER:N	2.46	0.47
11:H:116:TYR:HE2	11:H:140:ALA:CB	2.27	0.47
11:H:91:ASP:O	11:H:93:TYR:N	2.47	0.47
4:A:873:MET:C	4:A:1058:VAL:CG2	2.82	0.47
4:A:666:ILE:CD1	4:A:667:GLY:N	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:184:ALA:O	7:D:185:CYS:SG	2.69	0.47
5:B:1165:ILE:CG2	5:B:1166:CYS:N	2.76	0.47
9:F:75:PRO:HG3	9:F:78:GLN:OE1	2.14	0.47
3:P:7:A:H2'	3:P:8:G:O4'	2.14	0.47
5:B:446:LEU:HD23	5:B:446:LEU:N	2.29	0.47
5:B:522:VAL:HG12	5:B:523:CYS:N	2.27	0.47
4:A:172:PRO:HB3	4:A:185:TRP:CE2	2.49	0.47
4:A:369:SER:HB3	14:K:2:ASN:HD21	1.78	0.47
4:A:1025:ARG:O	4:A:1026:LEU:HD23	2.14	0.47
4:A:872:GLY:O	4:A:1058:VAL:HG23	2.14	0.47
5:B:615:MET:CB	5:B:626:ILE:HG12	2.43	0.47
10:G:26:LEU:O	10:G:29:LYS:N	2.47	0.47
5:B:102:VAL:CG2	5:B:112:LEU:HB2	2.41	0.47
6:C:36:VAL:HG21	6:C:251:LEU:HB2	1.94	0.47
5:B:258:LEU:O	5:B:259:TYR:O	2.33	0.47
5:B:1040:ASN:O	5:B:1042:GLY:N	2.47	0.47
5:B:386:LEU:O	5:B:388:CYS:N	2.48	0.47
6:C:91:HIS:CD2	6:C:91:HIS:C	2.88	0.47
5:B:435:THR:CG2	5:B:437:GLU:HB2	2.44	0.47
5:B:1081:LEU:O	5:B:1083:ALA:O	2.33	0.47
4:A:67:CYS:O	4:A:68:GLN:HB2	2.14	0.47
5:B:1084:GLN:HE21	5:B:1084:GLN:H	1.62	0.47
4:A:817:ALA:O	4:A:818:MET:C	2.53	0.47
4:A:1445:ILE:HG12	10:G:18:PHE:HE2	1.77	0.47
11:H:82:PRO:C	11:H:84:ALA:H	2.13	0.47
5:B:903:VAL:HG12	5:B:904:ARG:N	2.28	0.47
5:B:360:PHE:C	5:B:360:PHE:CD2	2.88	0.47
5:B:756:ILE:O	5:B:759:PRO:HD3	2.14	0.47
4:A:277:GLU:C	4:A:279:LEU:H	2.18	0.47
11:H:11:GLN:HA	11:H:53:ASP:O	2.15	0.47
4:A:1105:LEU:HD22	4:A:1384:VAL:HG21	1.97	0.47
5:B:1214:PRO:O	5:B:1214:PRO:HG2	2.14	0.47
4:A:58:LEU:O	4:A:59:GLY:O	2.32	0.47
10:G:27:LYS:O	10:G:30:LEU:HB3	2.14	0.47
10:G:66:GLY:O	10:G:67:SER:C	2.52	0.47
4:A:1115:SER:OG	4:A:1116:LEU:N	2.47	0.47
5:B:1216:LEU:O	5:B:1217:TYR:HD1	1.96	0.47
4:A:1059:HIS:ND1	9:F:86:THR:HA	2.30	0.47
5:B:820:GLY:N	5:B:1091:TYR:OH	2.48	0.47
15:L:58:LYS:O	15:L:59:ALA:O	2.31	0.47
6:C:183:TRP:CE2	6:C:207:CYS:HB3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:277:GLU:O	4:A:279:LEU:N	2.47	0.47
5:B:969:ARG:NH1	6:C:61:GLU:OE1	2.48	0.47
5:B:54:PHE:HA	5:B:58:THR:HB	1.95	0.47
5:B:1085:ILE:CD1	5:B:1085:ILE:N	2.75	0.47
6:C:76:ASP:O	6:C:77:ILE:C	2.52	0.47
4:A:567:LYS:HD2	4:A:568:PRO:CD	2.45	0.47
4:A:852:TYR:HA	4:A:1060:PRO:HB3	1.96	0.47
13:J:56:LEU:O	13:J:57:ILE:C	2.53	0.47
4:A:1437:GLY:HA3	9:F:88:TYR:CD2	2.50	0.47
8:E:78:LEU:HD21	8:E:80:VAL:HG23	1.97	0.47
4:A:43:GLU:O	4:A:44:THR:CB	2.63	0.47
5:B:916:THR:O	5:B:935:ARG:HG3	2.14	0.47
10:G:14:HIS:HD2	10:G:16:SER:CB	2.27	0.47
4:A:545:GLN:O	4:A:546:VAL:C	2.52	0.47
5:B:1070:GLU:OE1	13:J:44:TYR:OH	2.33	0.47
13:J:36:LEU:O	13:J:39:LEU:N	2.48	0.47
6:C:236:GLY:C	6:C:238:ILE:N	2.68	0.47
5:B:711:GLU:H	5:B:712:PRO:HD2	1.79	0.47
5:B:1183:LYS:HA	5:B:1186:ASP:HA	1.96	0.47
7:D:176:GLU:C	7:D:178:ALA:N	2.64	0.47
4:A:1213:GLY:O	4:A:1214:GLU:C	2.52	0.47
4:A:726:ARG:HD2	4:A:765:VAL:O	2.15	0.47
4:A:471:ASN:O	4:A:474:VAL:HG12	2.15	0.47
4:A:533:LYS:HE3	4:A:745:GLN:HE22	1.79	0.47
4:A:1265:ASN:O	4:A:1268:LEU:N	2.41	0.47
10:G:99:PHE:C	10:G:99:PHE:CD1	2.88	0.47
6:C:27:LEU:O	6:C:28:ALA:C	2.52	0.47
5:B:787:VAL:O	5:B:787:VAL:HG12	2.15	0.47
4:A:259:GLU:OE1	4:A:259:GLU:HA	2.14	0.47
8:E:168:TYR:HB2	8:E:170:LEU:HG	1.97	0.47
7:D:195:ILE:O	7:D:197:SER:N	2.47	0.47
10:G:149:GLY:O	10:G:159:ALA:HB1	2.15	0.47
7:D:24:ALA:HA	10:G:83:LYS:O	2.15	0.47
12:I:51:ASN:O	12:I:54:GLU:HG3	2.15	0.47
1:T:23:DG:H2'	1:T:24:DG:H8	1.78	0.47
6:C:46:ILE:HG13	6:C:72:LEU:HD11	1.97	0.47
4:A:836:TYR:CZ	4:A:840:ARG:HD2	2.50	0.47
4:A:60:SER:C	4:A:61:ILE:HG13	2.35	0.47
5:B:593:PRO:HG2	5:B:617:ARG:NH2	2.29	0.47
4:A:343:LYS:HE2	5:B:1156:ASP:OD2	2.15	0.47
6:C:89:GLU:O	6:C:90:ASP:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:492:PRO:HB2	4:A:497:THR:HG22	1.96	0.47
5:B:1174:LYS:O	5:B:1176:ASN:HB2	2.14	0.47
11:H:138:GLU:O	11:H:139:ASN:C	2.52	0.47
5:B:798:TYR:HE2	6:C:62:PHE:HE2	1.52	0.47
4:A:1305:VAL:CG1	4:A:1306:LEU:N	2.77	0.47
6:C:46:ILE:HG23	6:C:157:CYS:HB3	1.97	0.47
5:B:838:SER:HA	5:B:989:THR:O	2.15	0.47
4:A:1342:GLU:CG	8:E:198:ILE:HD13	2.45	0.47
4:A:300:VAL:O	4:A:300:VAL:HG12	2.13	0.47
5:B:948:ILE:O	5:B:968:VAL:HG13	2.15	0.47
15:L:40:LEU:CD1	15:L:44:ASP:HB3	2.45	0.47
4:A:1323:ASP:C	4:A:1325:THR:H	2.17	0.47
4:A:1453:TYR:O	4:A:1454:MET:HB3	2.15	0.47
12:I:25:LEU:O	12:I:38:ALA:HB2	2.15	0.47
7:D:206:GLU:C	7:D:208:GLU:N	2.66	0.47
4:A:350:ARG:HH11	4:A:350:ARG:HG3	1.80	0.47
5:B:366:GLN:O	5:B:367:LEU:O	2.33	0.47
5:B:582:VAL:HA	5:B:626:ILE:O	2.15	0.47
5:B:1069:PHE:CD1	5:B:1069:PHE:N	2.80	0.47
4:A:352:VAL:O	4:A:467:THR:HB	2.15	0.47
5:B:45:SER:O	5:B:46:GLN:C	2.53	0.47
5:B:1001:PHE:HE2	6:C:34:ARG:CZ	2.27	0.47
5:B:899:ILE:HD12	5:B:911:ILE:HG23	1.96	0.47
5:B:39:ARG:HH21	5:B:665:GLU:CG	2.25	0.47
4:A:630:ILE:HD13	4:A:646:PHE:HZ	1.79	0.47
11:H:127:GLY:HA3	11:H:130:ARG:NH2	2.29	0.47
4:A:996:ASN:O	4:A:998:LEU:HD12	2.15	0.47
5:B:552:MET:C	5:B:554:ILE:H	2.17	0.47
4:A:89:PRO:HB2	4:A:204:THR:CG2	2.45	0.47
5:B:487:THR:CG2	5:B:488:TYR:N	2.78	0.47
5:B:1174:LYS:O	5:B:1176:ASN:N	2.47	0.47
4:A:1018:PHE:O	4:A:1021:LEU:HB3	2.15	0.47
5:B:984:HIS:CG	5:B:1025:HIS:HB2	2.50	0.47
4:A:406:ILE:HG13	4:A:431:LYS:HB2	1.97	0.47
14:K:49:GLU:HG3	14:K:94:ILE:HG13	1.97	0.46
11:H:58:THR:HG22	11:H:59:ILE:N	2.30	0.46
5:B:834:ASN:ND2	5:B:1013:ASN:HA	2.30	0.46
5:B:839:MET:HE1	5:B:980:PHE:HB3	1.96	0.46
8:E:192:ARG:NH1	8:E:192:ARG:HG3	2.28	0.46
13:J:13:VAL:C	13:J:14:VAL:HG23	2.35	0.46
4:A:231:PRO:O	4:A:233:TRP:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:231:PRO:HA	4:A:234:MET:HE2	1.98	0.46
5:B:1034:VAL:O	5:B:1036:ALA:N	2.48	0.46
4:A:939:ASP:OD1	4:A:1023:ARG:NH1	2.48	0.46
7:D:51:ASN:C	7:D:52:LEU:O	2.52	0.46
6:C:140:ASN:O	6:C:141:GLY:O	2.32	0.46
9:F:132:LEU:O	9:F:148:VAL:HG22	2.15	0.46
5:B:94:LYS:HG2	5:B:95:ILE:N	2.30	0.46
5:B:225:VAL:CG1	5:B:385:LEU:HA	2.44	0.46
4:A:308:ILE:HG22	4:A:309:ALA:N	2.29	0.46
4:A:1451:VAL:C	4:A:1453:TYR:H	2.18	0.46
6:C:229:TYR:CD1	6:C:229:TYR:N	2.83	0.46
5:B:570:VAL:HA	5:B:571:PRO:HD2	1.73	0.46
14:K:59:ALA:HA	14:K:74:ARG:O	2.15	0.46
4:A:57:ARG:HB3	4:A:68:GLN:HG2	1.97	0.46
1:T:20:DC:H2''	1:T:21:DC:O5'	2.15	0.46
8:E:94:LYS:HG3	8:E:98:ILE:CD1	2.45	0.46
4:A:549:MET:SD	4:A:577:ILE:HD11	2.55	0.46
5:B:838:SER:CA	5:B:989:THR:O	2.62	0.46
4:A:337:ARG:CZ	4:A:839:ARG:HH12	2.28	0.46
4:A:844:ALA:HB2	4:A:1389:PHE:CE2	2.49	0.46
7:D:141:LEU:O	7:D:142:LYS:C	2.54	0.46
5:B:293:PRO:C	5:B:294:ASP:O	2.52	0.46
15:L:46:VAL:CG1	15:L:56:LEU:HD12	2.45	0.46
4:A:427:GLN:HB2	4:A:430:TRP:NE1	2.30	0.46
7:D:51:ASN:OD1	7:D:52:LEU:O	2.33	0.46
13:J:32:GLU:O	13:J:34:THR:N	2.48	0.46
5:B:970:THR:HG22	5:B:971:THR:N	2.30	0.46
12:I:77:LYS:O	12:I:79:HIS:N	2.48	0.46
14:K:68:PHE:CD2	14:K:68:PHE:N	2.80	0.46
14:K:47:ARG:HD3	14:K:59:ALA:O	2.15	0.46
11:H:116:TYR:HE2	11:H:140:ALA:HB1	1.81	0.46
5:B:589:VAL:CG1	5:B:590:HIS:H	2.00	0.46
4:A:270:LEU:O	4:A:271:LYS:C	2.53	0.46
4:A:1447:GLU:OE2	10:G:23:LYS:HB2	2.15	0.46
11:H:98:TYR:C	11:H:118:PHE:HD2	2.18	0.46
4:A:574:GLY:O	4:A:575:LYS:C	2.53	0.46
4:A:1348:LEU:HG	4:A:1372:VAL:HG22	1.94	0.46
4:A:1102:LYS:O	4:A:1106:ASN:ND2	2.48	0.46
4:A:1405:THR:HB	4:A:1406:VAL:H	1.47	0.46
5:B:108:VAL:CG1	5:B:109:THR:H	2.19	0.46
4:A:996:ASN:HB3	4:A:1050:GLU:OE2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:226:ASP:O	6:C:227:THR:CB	2.63	0.46
4:A:693:VAL:HA	4:A:696:GLU:HB3	1.97	0.46
4:A:883:LEU:CD2	4:A:1021:LEU:HB2	2.45	0.46
14:K:93:SER:O	14:K:97:LYS:HG3	2.16	0.46
13:J:1:MET:N	13:J:56:LEU:H	2.13	0.46
12:I:99:LEU:C	12:I:100:PHE:CD1	2.89	0.46
5:B:364:ILE:HG22	5:B:365:THR:N	2.31	0.46
4:A:562:THR:HA	4:A:563:PRO:HD3	1.83	0.46
4:A:356:ASP:OD2	14:K:65:HIS:HE1	1.99	0.46
5:B:189:LEU:HD23	5:B:192:LEU:HD12	1.97	0.46
4:A:846:GLU:OE1	4:A:1425:SER:OG	2.33	0.46
6:C:15:LYS:O	6:C:240:VAL:HG22	2.16	0.46
4:A:722:LEU:HD22	4:A:799:PHE:CD1	2.51	0.46
12:I:83:ASN:HA	12:I:102:VAL:O	2.16	0.46
5:B:1034:VAL:C	5:B:1036:ALA:N	2.69	0.46
12:I:111:THR:CG2	12:I:112:SER:H	2.29	0.46
4:A:500:GLU:OE2	4:A:1438:THR:HG21	2.15	0.46
5:B:424:LEU:O	5:B:428:ILE:HG13	2.16	0.46
4:A:785:PRO:HG2	4:A:786:HIS:CD2	2.47	0.46
4:A:42:ASP:HB3	4:A:45:GLN:CA	2.46	0.46
5:B:38:PHE:CD1	5:B:811:TYR:CD2	3.04	0.46
5:B:638:PHE:HD2	5:B:690:VAL:HG22	1.80	0.46
2:N:3:DG:OP2	2:N:3:DG:H2'	2.16	0.46
4:A:500:GLU:OE2	5:B:1145:SER:CB	2.64	0.46
9:F:109:VAL:HG12	9:F:110:ASP:N	2.30	0.46
10:G:115:MET:CB	10:G:116:PRO:CD	2.94	0.46
5:B:1177:HIS:C	5:B:1179:GLN:H	2.19	0.46
5:B:695:ALA:O	5:B:698:GLU:HB3	2.16	0.46
4:A:116:ASP:O	4:A:118:HIS:N	2.48	0.46
5:B:405:ARG:HA	5:B:631:GLY:O	2.16	0.46
13:J:1:MET:HE2	13:J:60:PHE:HE2	1.81	0.46
4:A:490:HIS:HB3	5:B:1150:ARG:NH1	2.31	0.46
7:D:35:LEU:HD21	7:D:173:HIS:HB3	1.97	0.46
5:B:758:PHE:HZ	5:B:1031:LEU:HD22	1.81	0.46
8:E:54:GLN:O	8:E:57:MET:HB3	2.16	0.46
5:B:329:THR:O	5:B:332:ASP:HB3	2.16	0.46
4:A:1446:ASP:HB3	4:A:1449:SER:OG	2.16	0.46
4:A:1289:ARG:HD2	4:A:1303:GLU:OE2	2.16	0.46
14:K:31:VAL:HG12	14:K:32:VAL:H	1.80	0.46
5:B:1072:MET:CE	5:B:1087:PHE:HD1	2.28	0.46
12:I:98:VAL:HG12	12:I:99:LEU:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:168:ALA:C	6:C:170:TRP:N	2.69	0.46
6:C:248:ILE:HD13	14:K:101:LEU:HD22	1.98	0.46
5:B:780:VAL:HG12	5:B:782:LEU:O	2.16	0.46
5:B:310:MET:HG3	5:B:386:LEU:CD1	2.46	0.46
4:A:1028:THR:O	4:A:1032:LEU:HD12	2.16	0.46
8:E:46:TYR:CE2	8:E:58:MET:HA	2.51	0.46
4:A:684:ALA:O	4:A:687:LYS:HB2	2.15	0.46
5:B:455:SER:O	5:B:456:GLY:C	2.53	0.46
10:G:53:ASN:HD22	10:G:53:ASN:N	2.13	0.46
4:A:130:ASP:O	4:A:131:SER:C	2.54	0.46
11:H:22:LYS:O	11:H:23:VAL:HG23	2.15	0.46
4:A:1153:TYR:CD2	4:A:1163:ILE:HD11	2.51	0.46
6:C:70:ILE:HG22	6:C:70:ILE:O	2.16	0.46
5:B:562:GLY:HA3	5:B:590:HIS:ND1	2.31	0.46
4:A:41:MET:O	4:A:42:ASP:C	2.54	0.46
4:A:1327:ILE:HG22	8:E:147:HIS:HE1	1.81	0.46
5:B:999:MET:HG2	5:B:1007:VAL:HG22	1.98	0.46
4:A:849:MET:HE1	4:A:1061:GLY:HA2	1.98	0.46
4:A:715:GLU:OE2	4:A:774:ARG:NH1	2.49	0.46
4:A:11:LEU:HB2	5:B:1193:GLN:OE1	2.16	0.46
5:B:1183:LYS:HE3	5:B:1183:LYS:O	2.15	0.46
6:C:163:ILE:O	6:C:165:LYS:N	2.48	0.46
7:D:35:LEU:CD2	7:D:174:PRO:HD2	2.45	0.46
6:C:99:LEU:HD23	6:C:99:LEU:N	2.31	0.46
9:F:109:VAL:HG13	9:F:127:GLU:OE1	2.16	0.46
12:I:82:GLU:O	12:I:104:LEU:HG	2.16	0.46
4:A:626:ASN:C	4:A:628:GLY:H	2.19	0.46
4:A:551:TYR:CE2	14:K:62:LYS:HE2	2.50	0.46
4:A:920:LEU:HD23	4:A:920:LEU:C	2.35	0.46
4:A:913:LEU:HD23	4:A:919:ILE:HD12	1.97	0.46
4:A:404:TYR:CE2	4:A:414:ASP:HA	2.50	0.46
4:A:446:ARG:NH1	4:A:479:ASN:O	2.49	0.46
4:A:470:LEU:HD22	4:A:487:MET:CE	2.46	0.46
12:I:8:ARG:O	12:I:10:CYS:N	2.49	0.46
6:C:9:LYS:O	6:C:10:ILE:C	2.54	0.46
5:B:1096:ARG:O	5:B:1097:HIS:CB	2.54	0.46
1:T:15:DT:H2''	1:T:16:DT:H5'	1.97	0.46
9:F:81:THR:HB	9:F:136:ARG:HH11	1.80	0.46
6:C:75:MET:O	6:C:246:ARG:NH2	2.48	0.46
4:A:1237:ILE:HG22	4:A:1238:ILE:N	2.31	0.46
5:B:814:PHE:O	5:B:816:GLU:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:626:ASN:O	4:A:628:GLY:N	2.46	0.46
4:A:1265:ASN:C	4:A:1267:MET:N	2.68	0.46
5:B:210:LYS:HG3	5:B:461:LEU:O	2.15	0.46
5:B:303:TYR:N	5:B:303:TYR:CD2	2.82	0.46
4:A:596:THR:O	4:A:598:LEU:N	2.49	0.46
11:H:93:TYR:CD1	11:H:93:TYR:N	2.83	0.46
4:A:874:ASP:N	4:A:1058:VAL:CG2	2.79	0.46
6:C:70:ILE:HD11	6:C:144:ILE:CG1	2.46	0.46
4:A:340:LEU:CD2	5:B:1199:ALA:HB3	2.45	0.46
9:F:143:PHE:C	9:F:143:PHE:CD1	2.90	0.46
8:E:17:ARG:O	8:E:20:LYS:HB2	2.16	0.46
5:B:1182:CYS:O	5:B:1183:LYS:O	2.34	0.46
5:B:377:PHE:C	5:B:379:GLY:N	2.67	0.46
4:A:630:ILE:HG23	4:A:642:CYS:SG	2.56	0.46
5:B:283:VAL:O	5:B:286:PHE:N	2.49	0.46
14:K:42:LEU:HD21	14:K:46:ILE:HD11	1.98	0.46
4:A:1001:ARG:HG2	4:A:1001:ARG:HH11	1.81	0.46
9:F:111:LEU:N	9:F:111:LEU:HD12	2.29	0.46
4:A:1451:VAL:C	4:A:1453:TYR:N	2.68	0.46
5:B:29:ASP:HB3	5:B:658:ILE:HD13	1.96	0.46
10:G:121:PHE:HB2	10:G:130:TYR:CE2	2.51	0.46
5:B:48:LEU:O	5:B:49:ASP:C	2.52	0.46
5:B:1060:ARG:HD2	5:B:1060:ARG:HA	1.48	0.46
4:A:1222:ASN:O	4:A:1223:ASP:HB3	2.15	0.46
11:H:58:THR:HB	11:H:143:LEU:HD13	1.98	0.45
4:A:854:ASN:HB3	4:A:1000:LEU:HD21	1.98	0.45
5:B:882:THR:HB	5:B:934:LYS:O	2.15	0.45
5:B:1065:GLN:NE2	5:B:1067:ARG:HG2	2.31	0.45
4:A:563:PRO:HG3	4:A:572:TRP:CE2	2.50	0.45
8:E:177:ARG:C	8:E:212:ARG:HD3	2.36	0.45
4:A:774:ARG:O	4:A:775:ILE:O	2.34	0.45
4:A:103:CYS:O	4:A:106:VAL:O	2.34	0.45
6:C:181:ASP:OD2	6:C:184:ASN:HA	2.14	0.45
5:B:745:PRO:C	5:B:747:MET:N	2.70	0.45
4:A:856:THR:HG22	4:A:856:THR:O	2.15	0.45
8:E:161:LYS:C	8:E:163:GLU:H	2.19	0.45
5:B:842:ASN:ND2	5:B:845:SER:CB	2.78	0.45
14:K:43:GLY:HA3	14:K:61:TYR:CE1	2.50	0.45
4:A:1045:VAL:O	4:A:1049:ILE:HG13	2.16	0.45
4:A:1435:PRO:HA	4:A:1439:GLY:O	2.16	0.45
5:B:581:PHE:N	5:B:624:LEU:O	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:114:PRO:O	5:B:116:GLU:N	2.49	0.45
4:A:1409:LEU:CD1	5:B:1207:LEU:HD21	2.36	0.45
4:A:337:ARG:CZ	4:A:839:ARG:NH1	2.79	0.45
4:A:418:SER:C	4:A:420:ARG:H	2.18	0.45
4:A:418:SER:C	4:A:420:ARG:N	2.68	0.45
11:H:84:ALA:C	11:H:86:ASP:N	2.69	0.45
6:C:241:ASP:OD1	6:C:242:GLN:N	2.48	0.45
5:B:38:PHE:HD1	5:B:811:TYR:CD2	2.34	0.45
6:C:179:GLU:CG	6:C:180:TYR:N	2.74	0.45
4:A:1011:GLN:NE2	4:A:1015:VAL:HG21	2.32	0.45
12:I:13:MET:HG3	12:I:14:LEU:H	1.80	0.45
7:D:137:ASN:C	7:D:137:ASN:HD22	2.19	0.45
7:D:64:VAL:C	7:D:66:ARG:H	2.19	0.45
7:D:52:LEU:C	7:D:54:GLU:N	2.69	0.45
4:A:58:LEU:HD22	4:A:80:HIS:O	2.16	0.45
4:A:907:THR:HG23	4:A:908:LEU:H	1.81	0.45
10:G:13:LEU:CD2	10:G:17:PHE:HB2	2.39	0.45
5:B:1007:VAL:HG22	5:B:1008:PRO:CD	2.35	0.45
4:A:1342:GLU:OE2	8:E:212:ARG:NH1	2.49	0.45
4:A:324:SER:O	4:A:325:ILE:C	2.53	0.45
4:A:415:LEU:HD23	4:A:415:LEU:HA	1.69	0.45
7:D:153:ARG:C	7:D:154:PHE:CD1	2.89	0.45
6:C:10:ILE:HA	6:C:20:PHE:CB	2.46	0.45
5:B:1115:THR:CG2	5:B:1117:GLN:HG3	2.46	0.45
4:A:1072:ILE:C	4:A:1075:PRO:HD2	2.36	0.45
4:A:1147:THR:HA	4:A:1197:LEU:HD23	1.98	0.45
8:E:114:ASN:O	8:E:115:ASN:CB	2.64	0.45
5:B:769:TYR:O	5:B:772:ALA:N	2.49	0.45
4:A:1280:GLU:O	4:A:1281:ARG:C	2.54	0.45
4:A:1289:ARG:NH1	4:A:1326:ARG:NH1	2.63	0.45
7:D:68:ARG:C	7:D:70:PHE:H	2.20	0.45
5:B:765:PRO:O	5:B:766:ARG:C	2.53	0.45
4:A:590:ARG:O	4:A:591:PHE:HB2	2.15	0.45
4:A:590:ARG:HD2	4:A:605:MET:CB	2.46	0.45
5:B:864:LYS:N	5:B:872:GLU:OE1	2.48	0.45
5:B:918:ILE:HG21	5:B:935:ARG:HH11	1.81	0.45
4:A:1118:VAL:O	4:A:1118:VAL:HG23	2.15	0.45
4:A:808:LEU:CD2	4:A:813:PHE:HA	2.38	0.45
5:B:1182:CYS:C	5:B:1183:LYS:HE3	2.35	0.45
7:D:64:VAL:C	7:D:66:ARG:N	2.68	0.45
5:B:69:LEU:HD22	5:B:429:PHE:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:235:SER:C	5:B:236:HIS:HD2	2.19	0.45
5:B:199:MET:N	5:B:199:MET:SD	2.83	0.45
4:A:816:HIS:HE2	5:B:764:SER:H	1.64	0.45
10:G:23:LYS:HG2	10:G:27:LYS:HE3	1.98	0.45
4:A:526:ASP:OD1	5:B:1013:ASN:ND2	2.49	0.45
5:B:113:TYR:CD2	5:B:192:LEU:HD22	2.51	0.45
15:L:32:ALA:HB3	15:L:55:ILE:CD1	2.47	0.45
4:A:836:TYR:O	4:A:837:ILE:C	2.55	0.45
11:H:84:ALA:C	11:H:86:ASP:H	2.19	0.45
13:J:50:ILE:O	13:J:52:THR:N	2.49	0.45
9:F:90:ARG:HD3	9:F:155:LEU:HD12	1.97	0.45
4:A:438:ASP:OD1	4:A:462:VAL:HG23	2.16	0.45
8:E:134:THR:C	8:E:135:PHE:CD1	2.89	0.45
8:E:157:SER:O	8:E:159:ASP:N	2.49	0.45
4:A:185:TRP:HZ3	4:A:200:ARG:HG2	1.82	0.45
6:C:88:CYS:SG	6:C:91:HIS:C	2.95	0.45
4:A:511:ILE:O	4:A:519:PRO:HA	2.16	0.45
13:J:27:GLU:O	13:J:29:GLU:N	2.49	0.45
5:B:570:VAL:HG23	5:B:573:GLN:HB3	1.97	0.45
4:A:477:PRO:CG	4:A:521:MET:HG2	2.47	0.45
4:A:622:VAL:HG22	4:A:622:VAL:O	2.17	0.45
4:A:784:LEU:HD11	4:A:815:PHE:CE2	2.51	0.45
12:I:69:PRO:HG2	12:I:85:PHE:CE2	2.52	0.45
5:B:918:ILE:HD12	5:B:935:ARG:CD	2.47	0.45
4:A:575:LYS:NZ	4:A:615:GLY:H	2.15	0.45
5:B:979:LYS:O	5:B:980:PHE:CD2	2.70	0.45
4:A:1370:LEU:O	4:A:1373:ASP:N	2.48	0.45
4:A:1102:LYS:HG2	4:A:1106:ASN:ND2	2.30	0.45
4:A:1106:ASN:O	4:A:1107:VAL:HB	2.17	0.45
4:A:841:LEU:O	4:A:845:LEU:HG	2.17	0.45
4:A:709:THR:HB	4:A:712:GLU:HG3	1.99	0.45
5:B:1103:ILE:O	5:B:1122:ARG:NH1	2.49	0.45
7:D:35:LEU:HD12	7:D:35:LEU:N	2.32	0.45
1:T:16:DT:C5'	4:A:1386:ARG:NH1	2.80	0.45
7:D:146:GLN:O	7:D:147:TYR:C	2.54	0.45
4:A:289:ILE:C	4:A:291:GLU:N	2.70	0.45
5:B:195:CYS:SG	5:B:196:PRO:HD2	2.56	0.45
12:I:61:ASP:O	12:I:63:GLY:N	2.49	0.45
5:B:221:ASN:OD1	5:B:242:SER:HA	2.15	0.45
4:A:344:ARG:HD2	5:B:1118:PRO:O	2.17	0.45
5:B:766:ARG:NH2	5:B:1020:ARG:HD3	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:763:GLN:O	5:B:764:SER:C	2.55	0.45
5:B:839:MET:HE3	5:B:1010:LEU:HD21	1.98	0.45
4:A:479:ASN:O	4:A:479:ASN:OD1	2.34	0.45
4:A:774:ARG:H	4:A:774:ARG:HG2	1.62	0.45
12:I:26:LEU:CD2	12:I:37:GLU:HA	2.41	0.45
5:B:637:LEU:HD23	5:B:742:GLU:HA	1.97	0.45
14:K:5:ASP:O	14:K:6:ARG:C	2.55	0.45
4:A:1074:GLU:HB3	4:A:1075:PRO:CD	2.46	0.45
5:B:732:SER:HB2	5:B:734:HIS:CD2	2.51	0.45
5:B:797:TYR:HE1	5:B:854:LEU:HD21	1.81	0.45
10:G:20:PRO:CG	10:G:21:ARG:N	2.80	0.45
4:A:492:PRO:O	4:A:493:GLN:NE2	2.50	0.45
10:G:111:THR:HG22	10:G:113:HIS:H	1.82	0.45
4:A:282:ASN:O	4:A:284:ALA:N	2.50	0.45
4:A:1142:THR:O	4:A:1143:LEU:C	2.54	0.45
8:E:136:ASN:OD1	8:E:138:ALA:N	2.50	0.45
6:C:58:LEU:CD2	6:C:58:LEU:N	2.80	0.45
5:B:863:GLU:O	5:B:961:LEU:HD22	2.16	0.45
10:G:14:HIS:HD2	10:G:16:SER:HB2	1.82	0.45
4:A:1348:LEU:O	4:A:1352:VAL:HG23	2.17	0.45
14:K:88:LYS:O	14:K:89:ASN:C	2.55	0.45
4:A:341:MET:CE	4:A:843:LYS:HZ1	2.29	0.45
9:F:148:VAL:O	9:F:149:GLU:C	2.54	0.45
6:C:133:ILE:HD12	6:C:237:SER:HA	1.99	0.45
4:A:1265:ASN:O	4:A:1267:MET:N	2.50	0.45
5:B:596:LEU:O	5:B:600:LEU:HG	2.16	0.45
8:E:129:PRO:O	8:E:130:ALA:O	2.34	0.45
4:A:566:ILE:O	4:A:567:LYS:O	2.34	0.45
4:A:590:ARG:NH2	4:A:620:LYS:CB	2.75	0.45
5:B:980:PHE:HE2	5:B:1094:ARG:CB	2.30	0.45
4:A:446:ARG:CD	4:A:480:ALA:HB2	2.47	0.45
5:B:1001:PHE:HD2	6:C:34:ARG:NH2	2.15	0.45
4:A:7:SER:C	4:A:9:ALA:H	2.20	0.45
4:A:7:SER:OG	5:B:1193:GLN:NE2	2.50	0.45
4:A:1004:ASN:OD1	4:A:1005:GLU:N	2.50	0.45
5:B:594:ALA:HA	5:B:617:ARG:HH12	1.79	0.45
5:B:737:THR:O	5:B:738:PHE:C	2.55	0.45
4:A:1006:ILE:HD12	8:E:163:GLU:CG	2.46	0.45
8:E:48:ASP:CG	8:E:49:SER:N	2.68	0.45
4:A:1206:ASP:HB3	4:A:1274:ARG:NH1	2.31	0.45
4:A:1100:ARG:NH2	4:A:1351:GLU:HG2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:318:VAL:C	5:B:320:ASP:N	2.71	0.45
4:A:477:PRO:HG2	4:A:521:MET:HG2	1.98	0.45
4:A:1148:ILE:HB	4:A:1196:GLU:O	2.17	0.45
4:A:57:ARG:O	4:A:68:GLN:NE2	2.49	0.45
5:B:25:ILE:HD11	5:B:653:VAL:C	2.37	0.45
8:E:202:SER:HB3	8:E:205:SER:O	2.15	0.45
13:J:2:ILE:HG22	13:J:3:VAL:O	2.17	0.45
4:A:1118:VAL:HG12	4:A:1327:ILE:HG13	1.99	0.45
5:B:189:LEU:O	5:B:190:TYR:C	2.55	0.45
4:A:846:GLU:HB2	4:A:847:ASP:H	1.64	0.45
4:A:416:ARG:C	4:A:417:TYR:CD2	2.89	0.45
13:J:13:VAL:O	13:J:14:VAL:CG2	2.65	0.45
4:A:218:ASP:O	4:A:219:PHE:C	2.56	0.45
5:B:708:GLU:O	5:B:709:ASP:C	2.56	0.45
5:B:1208:MET:HA	5:B:1212:ILE:O	2.17	0.45
7:D:202:ILE:CG2	7:D:207:LEU:HB2	2.44	0.45
4:A:682:THR:HG23	4:A:728:LYS:HE3	1.99	0.45
4:A:1111:MET:H	4:A:1111:MET:HG2	1.52	0.45
4:A:960:ILE:O	4:A:961:ARG:C	2.55	0.45
4:A:871:ASP:HB3	8:E:204:THR:HG23	2.00	0.44
4:A:1164:PRO:O	4:A:1166:ASP:N	2.50	0.44
4:A:42:ASP:HB3	4:A:45:GLN:N	2.30	0.44
4:A:577:ILE:O	4:A:578:LEU:C	2.51	0.44
4:A:839:ARG:O	4:A:840:ARG:C	2.54	0.44
5:B:1200:ALA:O	5:B:1203:LEU:HB3	2.17	0.44
4:A:504:LEU:HD12	4:A:504:LEU:N	2.31	0.44
5:B:351:TYR:CD1	5:B:355:ILE:HD11	2.52	0.44
4:A:65:LEU:O	4:A:66:LYS:C	2.55	0.44
9:F:119:ARG:CG	9:F:119:ARG:NH1	2.80	0.44
8:E:124:VAL:HA	8:E:132:ILE:HD12	1.99	0.44
15:L:28:LYS:HB2	15:L:39:SER:HA	1.98	0.44
5:B:1115:THR:HG21	5:B:1117:GLN:CD	2.38	0.44
6:C:112:ASN:CB	6:C:114:TYR:CE1	2.99	0.44
5:B:843:GLN:HB2	5:B:993:THR:HB	1.98	0.44
5:B:785:TYR:CD1	5:B:786:ASN:N	2.85	0.44
11:H:33:GLN:C	11:H:35:GLN:H	2.21	0.44
11:H:42:ILE:HG23	11:H:95:TYR:CE1	2.41	0.44
5:B:653:VAL:HG23	5:B:689:LEU:HB3	1.96	0.44
5:B:687:GLU:O	5:B:689:LEU:HG	2.18	0.44
8:E:98:ILE:O	8:E:100:ILE:N	2.50	0.44
5:B:181:LEU:HD22	5:B:189:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1349:TYR:CA	4:A:1372:VAL:HG21	2.46	0.44
4:A:353:ILE:HB	4:A:470:LEU:CD2	2.48	0.44
4:A:144:THR:O	4:A:146:MET:HG3	2.18	0.44
4:A:268:ASP:HB3	4:A:299:HIS:CE1	2.52	0.44
4:A:7:SER:HB2	5:B:1175:LEU:HD22	1.99	0.44
5:B:1106:ARG:NH2	5:B:1109:GLY:H	2.14	0.44
4:A:1191:TRP:HD1	4:A:1256:GLU:HB2	1.81	0.44
4:A:3:GLY:O	4:A:4:GLN:CB	2.64	0.44
9:F:111:LEU:C	9:F:113:GLY:N	2.70	0.44
2:N:5:DA:H1'	2:N:6:DC:O5'	2.18	0.44
5:B:833:TYR:N	5:B:833:TYR:CD1	2.84	0.44
5:B:436:VAL:HG12	5:B:436:VAL:O	2.17	0.44
4:A:901:LEU:HD22	4:A:919:ILE:HG22	2.00	0.44
4:A:823:GLY:O	4:A:825:ILE:N	2.50	0.44
14:K:82:ASP:O	14:K:85:ASP:HB2	2.17	0.44
6:C:35:ARG:HH11	14:K:41:THR:CA	2.30	0.44
4:A:298:PHE:O	4:A:301:ALA:HB3	2.16	0.44
4:A:225:ASN:ND2	4:A:227:VAL:H	2.14	0.44
8:E:161:LYS:C	8:E:163:GLU:N	2.71	0.44
15:L:27:LEU:HD23	15:L:27:LEU:N	2.31	0.44
4:A:289:ILE:O	4:A:291:GLU:N	2.50	0.44
12:I:68:LEU:HB3	12:I:84:VAL:HG23	1.98	0.44
5:B:591:ARG:O	5:B:592:ASN:C	2.55	0.44
4:A:807:GLY:HA2	5:B:760:ASP:O	2.17	0.44
6:C:92:CYS:C	6:C:94:LYS:N	2.71	0.44
4:A:1098:VAL:N	4:A:1099:PRO:HD2	2.33	0.44
6:C:74:SER:HB2	6:C:77:ILE:CG1	2.47	0.44
5:B:217:ARG:HG3	5:B:405:ARG:O	2.18	0.44
4:A:1239:ARG:HB3	4:A:1239:ARG:NH1	2.32	0.44
4:A:901:LEU:HD22	4:A:919:ILE:HG21	2.00	0.44
4:A:50:ILE:C	4:A:52:GLY:N	2.67	0.44
4:A:84:ILE:O	4:A:84:ILE:CG2	2.64	0.44
5:B:882:THR:HG21	5:B:935:ARG:HA	1.98	0.44
4:A:666:ILE:HD12	4:A:667:GLY:N	2.31	0.44
10:G:127:PRO:HG2	10:G:138:THR:HG21	1.99	0.44
8:E:116:ILE:HG22	8:E:117:THR:N	2.32	0.44
12:I:6:PHE:HA	12:I:14:LEU:HG	1.98	0.44
5:B:603:LEU:HB3	5:B:609:ILE:HD11	1.99	0.44
5:B:1106:ARG:HD2	5:B:1125:ASP:O	2.18	0.44
4:A:1450:LEU:O	4:A:1450:LEU:CG	2.64	0.44
4:A:1070:GLN:O	4:A:1071:SER:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:673:GLY:N	4:A:674:PRO:HD2	2.32	0.44
6:C:123:ASN:ND2	6:C:125:MET:SD	2.90	0.44
4:A:441:PRO:HD2	4:A:498:ARG:NH2	2.33	0.44
10:G:49:LEU:HG	10:G:76:ALA:HA	2.00	0.44
4:A:1215:ARG:HA	4:A:1215:ARG:HD2	1.73	0.44
4:A:871:ASP:C	4:A:871:ASP:OD1	2.56	0.44
4:A:921:GLY:O	4:A:922:ASP:C	2.54	0.44
5:B:376:PHE:O	5:B:586:TRP:HZ3	2.00	0.44
6:C:31:ASN:OD1	6:C:34:ARG:NH1	2.51	0.44
12:I:34:TYR:O	12:I:35:VAL:CG2	2.66	0.44
5:B:507:LYS:N	5:B:512:ARG:HH21	2.11	0.44
4:A:723:ASN:C	4:A:725:ALA:N	2.68	0.44
4:A:608:ILE:O	4:A:610:GLY:N	2.50	0.44
4:A:61:ILE:HG22	4:A:62:ASP:N	2.32	0.44
14:K:12:LEU:N	14:K:12:LEU:HD12	2.26	0.44
5:B:1031:LEU:HA	5:B:1055:ILE:HD13	2.00	0.44
5:B:753:ALA:O	5:B:756:ILE:HG13	2.17	0.44
5:B:842:ASN:ND2	5:B:845:SER:OG	2.50	0.44
4:A:652:VAL:O	4:A:653:VAL:C	2.56	0.44
14:K:55:LYS:HB3	14:K:81:TYR:CD1	2.53	0.44
10:G:38:CYS:SG	10:G:44:TYR:CE1	3.11	0.44
8:E:129:PRO:O	8:E:130:ALA:C	2.56	0.44
5:B:680:THR:O	5:B:684:LEU:HD12	2.18	0.44
4:A:547:LEU:HD22	14:K:58:PHE:CE1	2.52	0.44
4:A:853:ASP:OD1	4:A:855:THR:CG2	2.63	0.44
12:I:85:PHE:CD1	12:I:99:LEU:HD13	2.53	0.44
5:B:1065:GLN:NE2	5:B:1066:SER:H	2.14	0.44
4:A:1356:ILE:HD12	4:A:1368:MET:SD	2.58	0.44
4:A:1430:LEU:O	5:B:1196:ILE:HG22	2.18	0.44
5:B:983:ARG:HD2	5:B:1091:TYR:HD2	1.83	0.44
4:A:93:VAL:HG21	4:A:301:ALA:O	2.17	0.44
4:A:650:GLN:O	4:A:654:ASN:ND2	2.51	0.44
11:H:110:ASP:O	11:H:128:ASN:ND2	2.49	0.44
4:A:853:ASP:OD1	4:A:855:THR:CB	2.66	0.44
5:B:616:ILE:HG13	5:B:697:GLU:HA	2.00	0.44
4:A:255:SER:OG	5:B:918:ILE:HG23	2.17	0.44
4:A:336:ILE:HG22	4:A:337:ARG:N	2.32	0.44
4:A:668:ASP:HA	4:A:741:ASN:OD1	2.18	0.44
4:A:224:PHE:CZ	4:A:231:PRO:HG3	2.52	0.44
5:B:603:LEU:HB3	5:B:609:ILE:HG13	1.98	0.44
13:J:8:PHE:N	13:J:49:MET:HE3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:699:ALA:O	4:A:700:ASN:HB3	2.18	0.44
5:B:893:LEU:HD22	5:B:897:GLY:C	2.38	0.44
14:K:52:ASN:O	14:K:54:ARG:N	2.51	0.44
12:I:86:PHE:CE1	12:I:100:PHE:HB2	2.52	0.44
5:B:882:THR:O	5:B:883:LEU:CB	2.64	0.44
10:G:14:HIS:CD2	10:G:16:SER:HB2	2.53	0.44
4:A:1420:ASP:O	4:A:1421:CYS:HB2	2.18	0.44
5:B:1223:ASP:HB3	5:B:1224:PHE:H	1.68	0.44
5:B:1204:PHE:O	5:B:1207:LEU:HB2	2.18	0.44
4:A:340:LEU:HD21	5:B:1199:ALA:HB3	2.00	0.44
4:A:711:ARG:NH1	12:I:95:THR:HB	2.33	0.44
4:A:23:SER:O	4:A:26:GLU:N	2.50	0.44
7:D:35:LEU:HD23	7:D:174:PRO:CD	2.47	0.44
5:B:368:GLU:O	5:B:370:PHE:N	2.49	0.44
7:D:130:LEU:HD22	7:D:134:THR:OG1	2.18	0.44
4:A:896:ARG:NH2	4:A:1030:ARG:HH21	2.16	0.44
4:A:1227:ILE:CG2	4:A:1228:TRP:N	2.81	0.44
9:F:101:ILE:HD13	9:F:120:ILE:CG2	2.47	0.44
5:B:29:ASP:OD1	5:B:658:ILE:HD13	2.18	0.44
4:A:376:TYR:OH	4:A:498:ARG:HD2	2.18	0.44
4:A:1053:PHE:C	4:A:1055:ARG:H	2.21	0.44
4:A:1141:THR:OG1	4:A:1205:LYS:HD3	2.17	0.44
4:A:1170:ILE:HG13	4:A:1170:ILE:H	1.61	0.44
11:H:10:PHE:CD1	11:H:10:PHE:N	2.85	0.44
8:E:82:PHE:N	8:E:82:PHE:CD1	2.86	0.44
4:A:68:GLN:C	4:A:70:CYS:N	2.70	0.44
10:G:4:ILE:O	10:G:4:ILE:HG22	2.18	0.44
5:B:763:GLN:HG2	5:B:765:PRO:CD	2.47	0.44
4:A:567:LYS:HZ2	11:H:47:PHE:CB	2.31	0.44
14:K:87:LEU:O	14:K:88:LYS:C	2.56	0.44
4:A:858:ASN:HD21	4:A:860:LEU:H	1.60	0.44
5:B:1202:LEU:O	5:B:1203:LEU:C	2.56	0.44
4:A:442:VAL:HB	4:A:489:LEU:CD1	2.42	0.44
4:A:774:ARG:CZ	4:A:797:LYS:CB	2.96	0.44
5:B:639:ILE:HD11	5:B:691:GLU:HB2	2.00	0.44
1:T:15:DT:H1'	1:T:16:DT:H5'	2.00	0.44
8:E:124:VAL:N	8:E:125:PRO:HD2	2.33	0.44
15:L:27:LEU:O	15:L:28:LYS:HG2	2.18	0.44
2:N:1:DA:C1'	2:N:2:DA:O5'	2.66	0.44
8:E:207:ARG:CB	8:E:207:ARG:NH1	2.80	0.44
5:B:726:ALA:HB1	5:B:1051:THR:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:1:MET:SD	10:G:79:PHE:CE1	3.10	0.43
4:A:399:HIS:CG	4:A:400:PRO:N	2.82	0.43
4:A:567:LYS:HG3	4:A:568:PRO:CD	2.38	0.43
4:A:1058:VAL:O	4:A:1060:PRO:HD3	2.18	0.43
4:A:242:PRO:HD3	5:B:1209:ALA:CB	2.48	0.43
5:B:879:ARG:HH11	5:B:883:LEU:CD2	2.27	0.43
4:A:15:LYS:O	4:A:1421:CYS:HB2	2.18	0.43
4:A:845:LEU:O	4:A:846:GLU:C	2.54	0.43
7:D:211:LEU:HD23	7:D:214:LEU:HD12	1.99	0.43
4:A:311:GLN:HB3	4:A:312:PRO:HD3	2.00	0.43
5:B:1163:CYS:SG	5:B:1166:CYS:N	2.83	0.43
10:G:117:GLN:O	10:G:119:LEU:N	2.51	0.43
6:C:91:HIS:CD2	6:C:91:HIS:O	2.70	0.43
4:A:508:PRO:O	4:A:511:ILE:HG13	2.18	0.43
8:E:168:TYR:CB	8:E:170:LEU:HG	2.47	0.43
1:T:19:DG:H2''	1:T:20:DC:O5'	2.18	0.43
11:H:5:LEU:O	11:H:6:PHE:HB2	2.16	0.43
11:H:59:ILE:CG2	11:H:60:ALA:N	2.68	0.43
4:A:871:ASP:OD2	4:A:873:MET:HB2	2.18	0.43
5:B:579:ARG:HG2	5:B:579:ARG:NH1	2.32	0.43
4:A:254:GLU:HG3	5:B:935:ARG:HH22	1.82	0.43
4:A:42:ASP:OD1	4:A:45:GLN:O	2.36	0.43
5:B:112:LEU:HD12	5:B:113:TYR:N	2.29	0.43
4:A:1344:GLY:O	4:A:1345:ARG:C	2.56	0.43
6:C:232:VAL:HG21	6:C:244:VAL:CG2	2.41	0.43
6:C:6:PRO:HB3	6:C:25:VAL:CG1	2.49	0.43
4:A:230:ARG:N	4:A:233:TRP:CZ3	2.80	0.43
6:C:186:LEU:N	6:C:186:LEU:HD12	2.33	0.43
5:B:34:ILE:O	5:B:35:SER:C	2.57	0.43
5:B:1050:ILE:CG2	5:B:1051:THR:N	2.81	0.43
11:H:15:VAL:HG22	11:H:26:ILE:CG1	2.48	0.43
5:B:558:LEU:C	5:B:560:GLU:N	2.72	0.43
8:E:101:GLN:NE2	8:E:127:ILE:HG21	2.33	0.43
5:B:527:THR:OG1	5:B:528:PRO:HD2	2.18	0.43
5:B:484:ASN:ND2	5:B:486:TYR:CE1	2.86	0.43
4:A:779:PHE:CE1	4:A:785:PRO:CD	2.90	0.43
6:C:56:THR:HG22	6:C:58:LEU:HD23	2.00	0.43
5:B:1135:ARG:O	5:B:1138:MET:N	2.51	0.43
4:A:114:LEU:O	4:A:115:LEU:HG	2.18	0.43
1:T:14:DC:C6	1:T:15:DT:H73	2.53	0.43
6:C:116:LYS:HD3	6:C:140:ASN:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:157:SER:HG	8:E:160:GLU:HG3	1.82	0.43
5:B:421:PHE:O	5:B:424:LEU:HB3	2.18	0.43
4:A:493:GLN:H	4:A:497:THR:HG21	1.82	0.43
5:B:20:ASP:C	5:B:22:SER:H	2.22	0.43
4:A:34:LYS:HD3	4:A:34:LYS:N	2.33	0.43
4:A:852:TYR:CD2	4:A:1060:PRO:CB	3.02	0.43
5:B:464:GLY:HA2	5:B:479:VAL:O	2.19	0.43
4:A:1385:THR:O	4:A:1387:HIS:N	2.51	0.43
5:B:642:ASP:CA	5:B:649:LYS:HG3	2.47	0.43
8:E:133:GLU:HB3	8:E:135:PHE:HE1	1.84	0.43
10:G:9:LEU:CG	10:G:10:ASN:N	2.82	0.43
8:E:35:VAL:C	8:E:37:LEU:N	2.71	0.43
4:A:34:LYS:HB3	4:A:36:ARG:HE	1.83	0.43
5:B:91:SER:OG	5:B:133:LYS:HB2	2.19	0.43
5:B:792:MET:HA	5:B:856:PHE:O	2.17	0.43
4:A:184:SER:HB3	4:A:199:LEU:CD2	2.49	0.43
4:A:660:ASN:O	4:A:661:GLY:O	2.36	0.43
4:A:77:CYS:SG	4:A:77:CYS:O	2.76	0.43
4:A:786:HIS:CD2	4:A:786:HIS:N	2.86	0.43
4:A:1239:ARG:HH11	4:A:1239:ARG:CB	2.32	0.43
5:B:957:ASN:O	5:B:958:GLN:C	2.57	0.43
14:K:10:PHE:HD2	14:K:10:PHE:N	2.16	0.43
4:A:243:PRO:O	4:A:244:PRO:C	2.57	0.43
4:A:535:THR:O	4:A:575:LYS:HG3	2.19	0.43
14:K:85:ASP:O	14:K:88:LYS:HB2	2.19	0.43
4:A:1430:LEU:C	5:B:1197:PRO:HD2	2.39	0.43
5:B:859:TYR:CE1	5:B:941:LEU:HD12	2.53	0.43
4:A:113:LEU:HG	4:A:218:ASP:OD1	2.18	0.43
10:G:88:ASP:CB	10:G:144:ARG:HA	2.47	0.43
13:J:28:ASP:O	13:J:29:GLU:C	2.57	0.43
4:A:1211:GLN:O	4:A:1212:VAL:C	2.57	0.43
4:A:174:ILE:HG23	4:A:182:VAL:O	2.18	0.43
12:I:15:TYR:N	12:I:15:TYR:CD1	2.86	0.43
4:A:784:LEU:C	4:A:786:HIS:H	2.21	0.43
11:H:123:MET:HE3	11:H:142:LEU:HD21	2.00	0.43
4:A:857:ARG:CZ	9:F:139:PRO:HG3	2.48	0.43
4:A:264:PHE:O	4:A:267:ALA:N	2.51	0.43
4:A:41:MET:HB3	4:A:48:ALA:O	2.18	0.43
4:A:42:ASP:HA	4:A:46:THR:O	2.19	0.43
14:K:83:PRO:O	14:K:84:LYS:C	2.56	0.43
13:J:44:TYR:HA	13:J:47:ARG:HB3	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:335:ARG:HB3	4:A:336:ILE:H	1.70	0.43
11:H:82:PRO:O	11:H:84:ALA:N	2.35	0.43
5:B:521:LEU:HD13	5:B:633:VAL:CG1	2.48	0.43
5:B:104:GLU:OE1	15:L:54:ARG:NH2	2.52	0.43
4:A:7:SER:CB	5:B:1175:LEU:HD22	2.49	0.43
5:B:710:LEU:C	5:B:711:GLU:HG2	2.39	0.43
4:A:650:GLN:HB3	4:A:654:ASN:HD21	1.83	0.43
5:B:769:TYR:C	5:B:771:SER:N	2.69	0.43
10:G:35:GLU:OE2	10:G:48:VAL:HG23	2.19	0.43
5:B:299:GLU:OE1	5:B:571:PRO:HG2	2.19	0.43
5:B:399:ASP:OD2	5:B:510:LYS:HB2	2.17	0.43
5:B:23:ALA:O	5:B:654:ARG:HD2	2.18	0.43
5:B:653:VAL:O	5:B:654:ARG:HD3	2.19	0.43
6:C:69:LEU:HB3	13:J:6:ARG:HD3	2.01	0.43
5:B:1142:GLY:HA3	9:F:88:TYR:HE2	1.84	0.43
4:A:907:THR:CG2	4:A:908:LEU:H	2.29	0.43
4:A:667:GLY:HA3	6:C:192:TRP:HH2	1.83	0.43
4:A:562:THR:HB	11:H:98:TYR:CD2	2.54	0.43
5:B:1001:PHE:CD1	5:B:1001:PHE:C	2.92	0.43
7:D:210:ILE:O	7:D:214:LEU:HG	2.18	0.43
4:A:106:VAL:HA	4:A:114:LEU:HD21	2.00	0.43
5:B:520:GLY:H	5:B:748:ILE:HG22	1.82	0.43
5:B:1162:ILE:C	5:B:1171:VAL:HG21	2.38	0.43
5:B:294:ASP:N	5:B:294:ASP:OD2	2.48	0.43
8:E:124:VAL:HG13	8:E:132:ILE:CG1	2.48	0.43
13:J:43:ARG:HG2	13:J:43:ARG:H	1.70	0.43
9:F:132:LEU:N	9:F:132:LEU:HD23	2.34	0.43
8:E:93:MET:SD	8:E:97:VAL:CG2	3.06	0.43
4:A:474:VAL:HG13	4:A:474:VAL:O	2.18	0.43
9:F:99:LEU:C	9:F:99:LEU:HD12	2.38	0.43
4:A:1156:PRO:HA	4:A:1190:PRO:HB3	2.00	0.43
12:I:84:VAL:HG13	12:I:84:VAL:O	2.19	0.43
4:A:871:ASP:HB3	8:E:204:THR:CG2	2.48	0.43
12:I:50:THR:HG22	12:I:52:ILE:N	2.30	0.43
5:B:616:ILE:CG1	5:B:697:GLU:HA	2.49	0.43
10:G:18:PHE:HA	10:G:22:MET:HE3	1.99	0.43
5:B:1064:TYR:O	5:B:1065:GLN:C	2.57	0.43
4:A:535:THR:HG21	4:A:616:VAL:CA	2.35	0.43
4:A:16:GLU:HB3	4:A:1418:LEU:HD11	1.99	0.43
5:B:1001:PHE:CE2	6:C:34:ARG:NE	2.86	0.43
5:B:97:VAL:HG12	5:B:178:ASN:ND2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:911:ILE:O	5:B:911:ILE:HG22	2.19	0.43
4:A:23:SER:O	4:A:25:GLU:N	2.51	0.43
5:B:31:TRP:CE3	5:B:34:ILE:HD12	2.54	0.43
5:B:34:ILE:O	5:B:37:PHE:HB3	2.19	0.43
4:A:1074:GLU:HB3	4:A:1075:PRO:HD3	2.00	0.43
5:B:797:TYR:O	5:B:799:PRO:HD3	2.19	0.43
4:A:21:LEU:HD11	4:A:1414:ALA:HA	2.00	0.43
5:B:936:ASP:OD1	5:B:938:SER:N	2.45	0.43
4:A:988:LEU:HD23	4:A:988:LEU:HA	1.91	0.43
4:A:933:TYR:C	4:A:935:GLN:H	2.21	0.43
14:K:19:LEU:HD22	14:K:33:ILE:CG2	2.49	0.43
5:B:563:MET:HA	5:B:589:VAL:O	2.19	0.43
5:B:959:ASP:HB2	5:B:961:LEU:HG	2.01	0.43
4:A:562:THR:HB	11:H:98:TYR:CE2	2.54	0.43
4:A:79:GLY:CA	4:A:243:PRO:CG	2.96	0.43
7:D:51:ASN:ND2	7:D:54:GLU:OE2	2.51	0.43
4:A:1261:LYS:HA	4:A:1264:GLU:HB3	2.00	0.43
4:A:1199:ARG:O	4:A:1202:MET:N	2.48	0.43
5:B:310:MET:HG3	5:B:386:LEU:HD13	2.01	0.43
5:B:371:GLU:N	5:B:371:GLU:CD	2.70	0.43
8:E:131:THR:HG21	8:E:191:LYS:NZ	2.33	0.43
4:A:1139:GLU:O	4:A:1275:GLY:HA3	2.18	0.43
4:A:966:ASN:O	4:A:967:ALA:C	2.57	0.43
13:J:5:VAL:HG12	13:J:6:ARG:CG	2.33	0.43
4:A:356:ASP:C	4:A:358:ASN:H	2.22	0.43
5:B:179:CYS:SG	5:B:181:LEU:CB	3.06	0.43
14:K:83:PRO:O	14:K:86:ALA:N	2.52	0.43
5:B:1201:LYS:O	5:B:1204:PHE:HB2	2.19	0.43
4:A:503:GLN:NE2	9:F:90:ARG:NH2	2.62	0.43
4:A:767:GLN:NE2	4:A:774:ARG:CB	2.82	0.43
5:B:33:VAL:HG21	5:B:638:PHE:HZ	1.84	0.43
15:L:30:ILE:HD11	15:L:59:ALA:HB2	2.00	0.43
5:B:949:VAL:HG12	5:B:950:ASP:N	2.34	0.43
10:G:77:VAL:O	10:G:77:VAL:HG12	2.19	0.43
4:A:350:ARG:HG3	4:A:350:ARG:NH1	2.34	0.43
5:B:251:ILE:O	5:B:251:ILE:HG22	2.19	0.43
4:A:55:ASP:N	4:A:56:PRO:CD	2.82	0.42
6:C:39:ALA:O	6:C:164:ALA:HB3	2.19	0.42
4:A:365:GLY:HA3	4:A:463:ILE:HD13	2.01	0.42
15:L:55:ILE:H	15:L:55:ILE:HG12	1.46	0.42
4:A:1431:GLY:HA3	5:B:1197:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:392:VAL:CG1	4:A:415:LEU:HD11	2.39	0.42
6:C:173:ALA:O	6:C:174:ALA:HB3	2.19	0.42
6:C:179:GLU:CG	6:C:180:TYR:H	2.31	0.42
4:A:939:ASP:OD2	4:A:1020:CYS:HA	2.19	0.42
4:A:62:ASP:HB3	4:A:64:ASN:ND2	2.34	0.42
5:B:593:PRO:O	5:B:594:ALA:C	2.57	0.42
10:G:117:GLN:C	10:G:119:LEU:H	2.22	0.42
11:H:128:ASN:CG	11:H:128:ASN:O	2.57	0.42
5:B:1115:THR:CG2	5:B:1117:GLN:NE2	2.82	0.42
8:E:14:ARG:HH21	8:E:141:VAL:HG11	1.81	0.42
5:B:259:TYR:HD1	5:B:259:TYR:H	1.67	0.42
4:A:556:TRP:CZ2	4:A:558:GLY:HA2	2.54	0.42
4:A:825:ILE:CG2	5:B:508:LEU:CD1	2.95	0.42
4:A:306:ASN:ND2	4:A:322:VAL:HB	2.34	0.42
4:A:325:ILE:HG21	5:B:1210:MET:CG	2.46	0.42
4:A:767:GLN:HE21	4:A:774:ARG:HB3	1.84	0.42
9:F:77:ASP:O	9:F:79:ARG:N	2.53	0.42
4:A:1362:TYR:HD1	4:A:1363:VAL:N	2.16	0.42
6:C:88:CYS:SG	6:C:91:HIS:CA	3.07	0.42
10:G:126:ASN:HD22	10:G:126:ASN:HA	1.59	0.42
12:I:103:CYS:HB3	12:I:106:CYS:SG	2.59	0.42
4:A:332:LYS:O	4:A:334:GLY:N	2.52	0.42
5:B:681:TRP:C	5:B:683:SER:N	2.73	0.42
12:I:54:GLU:HB3	12:I:100:PHE:CE2	2.54	0.42
4:A:1434:ALA:HA	4:A:1435:PRO:HD3	1.88	0.42
6:C:248:ILE:H	6:C:248:ILE:HG13	1.55	0.42
4:A:1406:VAL:O	4:A:1407:GLU:C	2.58	0.42
5:B:1180:PHE:HB3	5:B:1191:ILE:CD1	2.48	0.42
2:N:2:DA:H1'	2:N:3:DG:O5'	2.19	0.42
5:B:552:MET:C	5:B:554:ILE:N	2.71	0.42
6:C:90:ASP:O	6:C:91:HIS:CB	2.67	0.42
4:A:355:GLY:N	4:A:482:PHE:CE1	2.87	0.42
9:F:118:LEU:O	9:F:118:LEU:HD12	2.19	0.42
5:B:273:LEU:HD12	5:B:280:ILE:HD12	2.01	0.42
5:B:470:LYS:HB3	5:B:471:LYS:H	1.65	0.42
4:A:600:PRO:HG2	4:A:601:LYS:H	1.84	0.42
4:A:1365:TYR:O	4:A:1366:ARG:C	2.57	0.42
4:A:870:GLU:HB2	8:E:204:THR:HG21	2.01	0.42
4:A:857:ARG:HG2	4:A:863:VAL:HA	2.02	0.42
6:C:70:ILE:HA	6:C:71:PRO:HD2	1.83	0.42
13:J:1:MET:HA	13:J:57:ILE:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1343:ALA:O	4:A:1346:ALA:HB3	2.19	0.42
4:A:525:GLN:O	4:A:526:ASP:C	2.58	0.42
5:B:999:MET:HE2	5:B:1000:PRO:CD	2.49	0.42
5:B:102:VAL:HG22	5:B:112:LEU:HD22	2.01	0.42
3:P:4:A:O2'	3:P:5:C:H5'	2.18	0.42
4:A:1409:LEU:HD13	5:B:1207:LEU:CD2	2.37	0.42
4:A:774:ARG:CZ	4:A:797:LYS:HG3	2.49	0.42
5:B:33:VAL:O	5:B:34:ILE:C	2.58	0.42
6:C:143:LEU:HD21	6:C:146:LYS:CE	2.48	0.42
5:B:862:GLN:HG2	5:B:963:PHE:CD1	2.51	0.42
5:B:1143:ALA:O	5:B:1144:ALA:C	2.58	0.42
4:A:90:VAL:HG13	4:A:297:GLN:CD	2.39	0.42
10:G:44:TYR:O	10:G:78:VAL:HG12	2.20	0.42
5:B:455:SER:O	5:B:458:LYS:N	2.52	0.42
4:A:1053:PHE:C	4:A:1055:ARG:N	2.73	0.42
13:J:58:GLU:HA	13:J:61:LEU:HD12	2.02	0.42
4:A:755:PHE:O	4:A:756:ILE:C	2.58	0.42
5:B:305:VAL:O	5:B:305:VAL:HG12	2.19	0.42
7:D:38:ILE:HG22	7:D:39:ASN:O	2.19	0.42
1:T:19:DG:H4'	5:B:1133:MET:SD	2.58	0.42
11:H:101:ALA:HB2	11:H:116:TYR:CE1	2.54	0.42
5:B:581:PHE:HA	5:B:585:VAL:O	2.19	0.42
4:A:261:ASP:O	4:A:264:PHE:HB2	2.20	0.42
12:I:29:CYS:SG	12:I:32:CYS:SG	3.17	0.42
4:A:223:GLY:O	4:A:224:PHE:CD1	2.73	0.42
4:A:93:VAL:CG1	4:A:301:ALA:HB1	2.42	0.42
5:B:496:ARG:HH12	5:B:539:LEU:HB2	1.82	0.42
14:K:95:ILE:O	14:K:98:LEU:HB2	2.19	0.42
10:G:9:LEU:HD12	10:G:10:ASN:N	2.32	0.42
4:A:789:LYS:HE3	12:I:67:THR:OG1	2.19	0.42
6:C:90:ASP:CG	6:C:90:ASP:O	2.58	0.42
4:A:1066:VAL:O	4:A:1067:LEU:C	2.58	0.42
5:B:1136:ASP:N	5:B:1136:ASP:OD1	2.52	0.42
5:B:984:HIS:CD2	5:B:1025:HIS:HB2	2.54	0.42
6:C:30:ALA:O	6:C:33:LEU:HB3	2.19	0.42
4:A:117:GLU:H	4:A:117:GLU:CD	2.22	0.42
11:H:123:MET:HE3	11:H:142:LEU:CD2	2.49	0.42
10:G:18:PHE:HZ	10:G:68:ALA:HB2	1.85	0.42
10:G:25:TYR:O	10:G:26:LEU:C	2.58	0.42
4:A:1118:VAL:HG23	4:A:1306:LEU:HB2	2.00	0.42
5:B:975:GLN:HG2	5:B:976:ILE:N	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:72:LYS:O	9:F:73:ALA:HB3	2.19	0.42
6:C:240:VAL:O	6:C:244:VAL:HG23	2.19	0.42
5:B:806:THR:CG2	5:B:808:ALA:HB3	2.49	0.42
14:K:113:THR:O	14:K:114:LEU:CB	2.62	0.42
5:B:361:LEU:HD21	5:B:377:PHE:HD2	1.79	0.42
5:B:1106:ARG:NH1	5:B:1110:PRO:HG2	2.33	0.42
10:G:88:ASP:HB3	10:G:144:ARG:CA	2.49	0.42
6:C:80:LEU:HD12	6:C:95:CYS:HA	2.02	0.42
5:B:259:TYR:HB2	5:B:268:THR:HG23	2.01	0.42
11:H:15:VAL:HG22	11:H:26:ILE:CD1	2.49	0.42
10:G:47:CYS:SG	10:G:48:VAL:N	2.92	0.42
7:D:191:ALA:C	7:D:193:THR:H	2.23	0.42
12:I:77:LYS:C	12:I:79:HIS:H	2.23	0.42
4:A:889:SER:C	4:A:891:ALA:N	2.69	0.42
4:A:67:CYS:O	4:A:68:GLN:CB	2.68	0.42
5:B:763:GLN:HG2	5:B:765:PRO:CG	2.50	0.42
5:B:872:GLU:HG2	5:B:916:THR:OG1	2.20	0.42
4:A:1329:THR:O	4:A:1335:ILE:HD12	2.20	0.42
4:A:78:PRO:HG3	5:B:1160:VAL:HG13	2.00	0.42
5:B:1160:VAL:HG11	5:B:1169:MET:SD	2.59	0.42
5:B:1156:ASP:O	5:B:1157:ALA:O	2.37	0.42
4:A:1438:THR:HG22	4:A:1438:THR:O	2.18	0.42
9:F:99:LEU:HD12	9:F:99:LEU:O	2.19	0.42
8:E:114:ASN:HA	8:E:114:ASN:HD22	1.63	0.42
4:A:881:GLN:O	4:A:953:ASN:HA	2.19	0.42
5:B:235:SER:C	5:B:236:HIS:CD2	2.93	0.42
12:I:110:PHE:CD2	12:I:110:PHE:N	2.88	0.42
4:A:737:LEU:HD23	4:A:737:LEU:HA	1.75	0.42
4:A:1368:MET:O	4:A:1372:VAL:HB	2.19	0.42
4:A:860:LEU:HD11	4:A:1393:ASN:HB2	2.02	0.42
4:A:1423:GLY:H	4:A:1426:GLU:HG3	1.85	0.42
4:A:1444:MET:HG2	10:G:60:ARG:CA	2.48	0.42
5:B:520:GLY:CA	5:B:748:ILE:HG22	2.50	0.42
5:B:1163:CYS:SG	5:B:1165:ILE:CB	3.04	0.42
4:A:1333:ILE:O	4:A:1337:GLU:HG3	2.19	0.42
7:D:135:GLY:C	7:D:137:ASN:H	2.22	0.42
4:A:896:ARG:HD3	4:A:897:TYR:HE1	1.84	0.42
4:A:810:PRO:HA	5:B:1047:PHE:CE2	2.54	0.42
4:A:1193:LEU:HD22	4:A:1260:LEU:HD11	2.02	0.42
5:B:758:PHE:CZ	5:B:1031:LEU:HD22	2.54	0.42
5:B:287:ARG:NH1	5:B:324:ILE:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:128:PRO:HA	8:E:129:PRO:C	2.40	0.42
5:B:311:LEU:O	5:B:312:GLU:C	2.58	0.42
4:A:514:PRO:HB2	4:A:875:ALA:HB3	2.01	0.42
11:H:76:THR:HG22	11:H:76:THR:O	2.19	0.42
1:T:19:DG:OP2	4:A:332:LYS:NZ	2.42	0.42
4:A:971:PHE:O	4:A:972:HIS:C	2.58	0.42
4:A:241:VAL:O	4:A:242:PRO:C	2.58	0.42
4:A:1115:SER:C	4:A:1308:THR:CG2	2.88	0.42
4:A:1426:GLU:H	4:A:1426:GLU:HG2	1.56	0.42
4:A:767:GLN:HE21	4:A:774:ARG:CB	2.33	0.42
1:T:16:DT:H5"	4:A:1386:ARG:NH1	2.35	0.42
7:D:128:VAL:O	7:D:132:GLN:HG3	2.20	0.42
13:J:7:CYS:CA	13:J:49:MET:HE3	2.50	0.42
5:B:1031:LEU:HD23	5:B:1044:ALA:HB2	2.02	0.42
4:A:33:ALA:O	4:A:83:HIS:CD2	2.67	0.42
9:F:109:VAL:HG11	9:F:123:LYS:CG	2.50	0.42
4:A:1315:GLU:C	4:A:1317:MET:N	2.72	0.42
4:A:445:ASN:HB2	4:A:455:MET:HA	2.01	0.42
5:B:1178:ASN:O	5:B:1179:GLN:C	2.58	0.42
4:A:1157:ASP:C	4:A:1159:ARG:H	2.23	0.42
4:A:332:LYS:HG3	4:A:333:GLU:N	2.35	0.42
11:H:143:LEU:C	11:H:144:ILE:HG13	2.40	0.42
6:C:56:THR:HG22	6:C:58:LEU:H	1.85	0.42
5:B:365:THR:HG23	5:B:367:LEU:N	2.31	0.42
4:A:219:PHE:O	4:A:222:LEU:O	2.36	0.42
8:E:90:VAL:CA	8:E:120:ALA:HB2	2.47	0.42
4:A:1381:LEU:HA	4:A:1381:LEU:HD23	1.88	0.42
6:C:259:LEU:CD1	14:K:91:CYS:HB2	2.50	0.42
5:B:314:LEU:O	5:B:317:CYS:HB3	2.20	0.42
5:B:510:LYS:N	5:B:511:PRO:HD3	2.35	0.42
10:G:142:ARG:O	10:G:171:ILE:HG13	2.20	0.42
5:B:566:LEU:O	5:B:567:GLU:C	2.58	0.42
4:A:584:ASN:O	4:A:637:LYS:HE3	2.20	0.42
5:B:766:ARG:HD3	5:B:766:ARG:HA	1.77	0.41
5:B:683:SER:O	5:B:687:GLU:HB2	2.20	0.41
4:A:1048:ASN:O	4:A:1049:ILE:C	2.58	0.41
4:A:1424:VAL:CG1	5:B:1139:ILE:HD13	2.45	0.41
5:B:563:MET:CE	5:B:580:VAL:HB	2.45	0.41
5:B:1065:GLN:HG3	5:B:1068:GLY:H	1.84	0.41
6:C:213:PRO:HG2	6:C:214:ASN:H	1.85	0.41
4:A:794:PRO:O	4:A:796:SER:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:910:VAL:CG1	5:B:911:ILE:N	2.82	0.41
4:A:218:ASP:O	4:A:219:PHE:O	2.38	0.41
7:D:167:LEU:O	7:D:170:THR:OG1	2.31	0.41
4:A:1332:PHE:O	4:A:1333:ILE:C	2.57	0.41
4:A:782:ARG:HB3	4:A:789:LYS:HA	2.02	0.41
12:I:101:PHE:HD1	12:I:101:PHE:N	2.18	0.41
5:B:324:ILE:CG2	5:B:325:GLN:N	2.82	0.41
4:A:909:ASP:C	4:A:911:SER:N	2.73	0.41
7:D:191:ALA:O	7:D:193:THR:N	2.53	0.41
4:A:964:ILE:O	4:A:967:ALA:HB3	2.19	0.41
9:F:97:ARG:HA	9:F:97:ARG:HD2	1.76	0.41
4:A:814:PHE:O	4:A:817:ALA:HB3	2.20	0.41
6:C:62:PHE:O	6:C:66:ARG:HG3	2.20	0.41
4:A:40:THR:CG2	4:A:41:MET:HG3	2.33	0.41
6:C:262:LEU:HA	6:C:262:LEU:HD23	1.80	0.41
4:A:417:TYR:O	4:A:418:SER:O	2.37	0.41
5:B:859:TYR:OH	5:B:941:LEU:CD1	2.62	0.41
15:L:38:LEU:O	15:L:39:SER:CB	2.61	0.41
6:C:107:SER:C	6:C:109:SER:N	2.74	0.41
4:A:898:ARG:NH1	4:A:930:ASP:OD1	2.50	0.41
5:B:971:THR:OG1	6:C:61:GLU:HG3	2.20	0.41
4:A:1073:GLY:O	4:A:1076:ALA:HB3	2.20	0.41
5:B:998:ASP:HB3	5:B:1076:HIS:HE1	1.85	0.41
5:B:765:PRO:O	5:B:767:ASN:N	2.53	0.41
5:B:654:ARG:O	5:B:656:GLY:N	2.53	0.41
4:A:868:TYR:CD2	4:A:1058:VAL:HG21	2.48	0.41
8:E:18:THR:O	8:E:19:VAL:C	2.57	0.41
10:G:22:MET:O	10:G:23:LYS:C	2.58	0.41
5:B:990:ILE:CG2	5:B:991:GLY:N	2.83	0.41
4:A:18:GLN:HG2	4:A:1418:LEU:HD13	2.01	0.41
4:A:381:THR:HG23	4:A:382:PRO:CD	2.50	0.41
4:A:1242:VAL:O	4:A:1243:VAL:CB	2.66	0.41
8:E:16:PHE:CE2	8:E:20:LYS:HE2	2.53	0.41
5:B:651:LEU:HD11	5:B:707:PRO:CB	2.50	0.41
5:B:125:SER:CA	5:B:171:PRO:HA	2.49	0.41
12:I:55:THR:HG23	12:I:58:VAL:HG21	2.01	0.41
5:B:258:LEU:O	5:B:258:LEU:HG	2.19	0.41
5:B:526:GLU:OE2	5:B:752:ALA:HB2	2.20	0.41
13:J:23:ASN:O	13:J:25:LEU:N	2.52	0.41
5:B:1164:GLY:HA3	5:B:1190:ASP:OD2	2.20	0.41
4:A:29:ALA:HB1	5:B:1184:GLY:CA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:933:TYR:C	4:A:935:GLN:N	2.74	0.41
4:A:1111:MET:CE	4:A:1330:ASN:OD1	2.68	0.41
4:A:452:LYS:HE2	4:A:452:LYS:HB3	1.85	0.41
10:G:106:MET:HG2	10:G:107:LYS:N	2.36	0.41
5:B:468:GLU:HB3	5:B:469:GLN:H	1.49	0.41
5:B:376:PHE:HB3	5:B:586:TRP:CZ3	2.55	0.41
4:A:254:GLU:HB2	5:B:935:ARG:NH1	2.29	0.41
5:B:834:ASN:CA	5:B:838:SER:O	2.69	0.41
10:G:138:THR:HG22	10:G:139:ILE:HG13	2.02	0.41
4:A:1409:LEU:O	4:A:1412:ALA:HB3	2.21	0.41
4:A:341:MET:HE1	5:B:1135:ARG:NH1	2.35	0.41
11:H:82:PRO:C	11:H:84:ALA:N	2.74	0.41
5:B:34:ILE:O	5:B:37:PHE:N	2.53	0.41
5:B:170:LEU:HA	5:B:171:PRO:HD2	1.82	0.41
5:B:121:ASN:OD1	5:B:963:PHE:HZ	2.04	0.41
4:A:676:MET:O	4:A:679:ILE:HB	2.21	0.41
4:A:1227:ILE:HG22	4:A:1228:TRP:H	1.80	0.41
4:A:629:LEU:O	4:A:633:VAL:HG23	2.21	0.41
5:B:278:GLN:HG2	5:B:279:ASP:N	2.35	0.41
5:B:429:PHE:HA	5:B:432:MET:CE	2.49	0.41
4:A:278:THR:HG22	4:A:278:THR:O	2.19	0.41
4:A:279:LEU:O	4:A:284:ALA:HB2	2.20	0.41
7:D:179:GLN:O	7:D:183:LEU:HB2	2.20	0.41
11:H:95:TYR:CE2	11:H:97:MET:CG	3.04	0.41
4:A:853:ASP:C	4:A:853:ASP:OD1	2.59	0.41
5:B:365:THR:CG2	5:B:366:GLN:N	2.81	0.41
6:C:168:ALA:C	6:C:170:TRP:H	2.24	0.41
5:B:1068:GLY:O	5:B:1069:PHE:O	2.39	0.41
4:A:463:ILE:HB	4:A:464:PRO:CD	2.49	0.41
5:B:980:PHE:CA	5:B:1095:LEU:HD11	2.50	0.41
4:A:404:TYR:CD2	4:A:414:ASP:HA	2.55	0.41
4:A:106:VAL:HG13	4:A:112:LYS:C	2.37	0.41
8:E:22:MET:CE	8:E:26:ARG:NH2	2.82	0.41
12:I:4:PHE:HE1	12:I:6:PHE:HE2	1.69	0.41
7:D:63:LEU:HA	7:D:63:LEU:HD22	1.91	0.41
5:B:758:PHE:N	5:B:759:PRO:HD2	2.35	0.41
6:C:154:LYS:C	6:C:155:LEU:HD23	2.40	0.41
5:B:842:ASN:HB3	5:B:1009:ASP:HA	2.03	0.41
5:B:769:TYR:C	5:B:771:SER:H	2.24	0.41
5:B:1187:ASN:OD1	5:B:1188:LYS:N	2.45	0.41
12:I:61:ASP:C	12:I:63:GLY:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:402:ALA:CB	4:A:434:ARG:HA	2.51	0.41
4:A:970:THR:O	4:A:970:THR:HG22	2.20	0.41
14:K:45:LEU:C	14:K:47:ARG:H	2.23	0.41
6:C:191:TYR:CD2	6:C:201:TRP:CD1	3.03	0.41
4:A:604:GLY:O	4:A:605:MET:HB2	2.21	0.41
6:C:66:ARG:NH1	13:J:2:ILE:CG2	2.82	0.41
5:B:861:ASP:OD1	5:B:914:LYS:HD2	2.21	0.41
4:A:115:LEU:HB2	4:A:122:MET:HE2	2.02	0.41
4:A:115:LEU:CB	4:A:122:MET:HE2	2.50	0.41
5:B:744:HIS:CD2	5:B:745:PRO:HD2	2.55	0.41
8:E:30:ILE:HG22	8:E:31:THR:N	2.35	0.41
4:A:1334:ASP:C	4:A:1336:MET:N	2.74	0.41
12:I:4:PHE:HE1	12:I:6:PHE:CE2	2.39	0.41
9:F:123:LYS:O	9:F:124:GLU:C	2.57	0.41
4:A:207:ILE:CG2	4:A:211:PHE:CE1	3.03	0.41
4:A:690:VAL:O	4:A:691:LEU:C	2.59	0.41
4:A:277:GLU:C	4:A:279:LEU:N	2.74	0.41
4:A:947:PHE:CD2	4:A:954:TRP:CE2	3.08	0.41
4:A:116:ASP:C	4:A:118:HIS:N	2.74	0.41
4:A:482:PHE:C	4:A:484:GLY:H	2.24	0.41
4:A:680:THR:HG23	5:B:729:ILE:CD1	2.51	0.41
4:A:1388:GLY:O	4:A:1390:ASN:N	2.53	0.41
5:B:578:THR:O	5:B:578:THR:HG22	2.21	0.41
4:A:768:GLN:HG3	4:A:816:HIS:HA	2.01	0.41
4:A:262:LEU:HD12	4:A:328:ARG:NH2	2.35	0.41
5:B:1065:GLN:HE21	5:B:1066:SER:CA	2.33	0.41
6:C:31:ASN:O	6:C:34:ARG:HB3	2.20	0.41
6:C:239:PRO:O	6:C:240:VAL:C	2.58	0.41
4:A:527:THR:O	4:A:531:ILE:HB	2.21	0.41
4:A:723:ASN:O	4:A:724:GLU:C	2.59	0.41
7:D:138:ASN:C	7:D:140:ASP:N	2.72	0.41
5:B:333:PHE:C	5:B:334:ILE:HG13	2.41	0.41
6:C:260:LEU:O	6:C:263:THR:HB	2.20	0.41
9:F:147:SER:O	9:F:148:VAL:C	2.59	0.41
6:C:147:LEU:HD23	6:C:147:LEU:N	2.36	0.41
4:A:349:ALA:CA	5:B:1128:LEU:HD11	2.51	0.41
12:I:101:PHE:HD1	12:I:101:PHE:H	1.67	0.41
4:A:206:GLU:O	4:A:207:ILE:C	2.59	0.41
14:K:53:ASP:C	14:K:55:LYS:H	2.24	0.41
9:F:97:ARG:NH1	9:F:100:GLN:OE1	2.53	0.41
6:C:11:ARG:HD3	6:C:209:TYR:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:K:38:GLU:HA	14:K:38:GLU:OE1	2.20	0.41
14:K:31:VAL:O	14:K:74:ARG:HA	2.21	0.41
12:I:98:VAL:HG12	12:I:99:LEU:N	2.36	0.41
4:A:574:GLY:O	4:A:577:ILE:N	2.51	0.41
4:A:1373:ASP:CA	4:A:1376:THR:HG22	2.50	0.41
13:J:44:TYR:HD2	13:J:44:TYR:N	2.13	0.41
4:A:306:ASN:HD22	4:A:322:VAL:HG12	1.86	0.41
4:A:304:MET:HG2	5:B:1210:MET:HG2	2.03	0.41
4:A:1425:SER:O	4:A:1426:GLU:C	2.59	0.41
4:A:403:LYS:O	4:A:404:TYR:CD2	2.74	0.41
4:A:146:MET:CA	4:A:171:GLN:HB2	2.50	0.41
4:A:608:ILE:CG1	4:A:613:ILE:HD12	2.51	0.41
5:B:604:ARG:O	5:B:607:GLY:N	2.54	0.41
15:L:38:LEU:CD1	15:L:49:LYS:HE2	2.50	0.41
4:A:343:LYS:NZ	5:B:1151:LEU:O	2.43	0.41
4:A:408:ASP:C	4:A:410:GLY:N	2.72	0.41
5:B:730:ARG:O	5:B:731:VAL:O	2.39	0.41
5:B:388:CYS:O	5:B:391:ASP:N	2.50	0.41
5:B:314:LEU:O	5:B:315:LYS:C	2.59	0.41
10:G:21:ARG:HD3	10:G:21:ARG:HA	1.85	0.41
7:D:206:GLU:C	7:D:208:GLU:H	2.24	0.41
4:A:964:ILE:O	4:A:967:ALA:N	2.54	0.41
7:D:180:LEU:HD23	7:D:180:LEU:HA	1.87	0.41
6:C:54:ASN:HB2	6:C:153:LEU:HD12	2.03	0.41
4:A:590:ARG:HD3	4:A:604:GLY:O	2.20	0.41
11:H:59:ILE:O	11:H:60:ALA:HB3	2.20	0.41
11:H:25:ARG:HA	11:H:41:ASP:HA	2.03	0.41
13:J:3:VAL:HA	13:J:4:PRO:HD3	1.84	0.41
4:A:1041:ALA:O	4:A:1045:VAL:HG23	2.20	0.41
12:I:54:GLU:OE2	12:I:118:ARG:NH1	2.53	0.41
8:E:78:LEU:HA	8:E:107:THR:HB	2.02	0.41
5:B:865:LYS:C	5:B:866:TYR:CD1	2.95	0.41
5:B:873:THR:O	5:B:914:LYS:HA	2.20	0.41
4:A:1445:ILE:H	4:A:1445:ILE:CD1	2.19	0.41
5:B:840:ILE:CG2	5:B:994:TYR:HD1	2.34	0.41
4:A:1349:TYR:O	4:A:1350:LYS:C	2.59	0.41
5:B:464:GLY:CA	5:B:479:VAL:O	2.68	0.41
6:C:18:VAL:O	6:C:20:PHE:CD2	2.71	0.41
4:A:722:LEU:HD21	4:A:794:PRO:HB3	2.03	0.41
5:B:899:ILE:CG2	5:B:903:VAL:HG21	2.50	0.41
5:B:516:ASN:ND2	5:B:516:ASN:H	2.16	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:93:VAL:HA	4:A:96:ILE:CD1	2.51	0.41
6:C:181:ASP:OD1	6:C:186:LEU:HD13	2.21	0.41
5:B:953:LEU:HD23	5:B:965:LYS:H	1.86	0.41
4:A:993:LEU:O	4:A:994:GLN:C	2.59	0.41
4:A:61:ILE:CG2	4:A:62:ASP:H	2.29	0.41
4:A:73:GLY:O	4:A:74:MET:C	2.59	0.41
5:B:298:LEU:N	5:B:298:LEU:HD22	2.35	0.41
5:B:1110:PRO:HG3	5:B:1124:ARG:O	2.21	0.41
4:A:973:ILE:HD13	4:A:1037:LEU:HA	2.03	0.41
10:G:88:ASP:HB3	10:G:144:ARG:CB	2.51	0.41
4:A:1070:GLN:C	4:A:1072:ILE:N	2.74	0.41
8:E:14:ARG:NH2	8:E:141:VAL:HG12	2.34	0.41
6:C:67:LEU:HD11	6:C:155:LEU:HD12	2.01	0.41
5:B:992:ILE:HG12	5:B:993:THR:N	2.36	0.41
4:A:1127:ASP:O	4:A:1130:GLN:HB3	2.20	0.41
6:C:100:THR:CG2	6:C:101:LEU:N	2.84	0.41
5:B:60:GLN:O	5:B:63:ILE:HG22	2.21	0.41
5:B:492:LEU:HB2	5:B:751:VAL:HG11	2.03	0.41
10:G:49:LEU:O	10:G:50:ASP:C	2.59	0.41
5:B:285:ILE:O	5:B:288:ALA:HB3	2.21	0.41
4:A:954:TRP:HB3	4:A:955:PRO:HD2	2.02	0.41
5:B:129:PHE:CD2	5:B:166:PHE:HA	2.56	0.41
13:J:32:GLU:O	13:J:35:ALA:N	2.54	0.41
11:H:62:SER:OG	11:H:63:LEU:N	2.53	0.41
8:E:191:LYS:O	8:E:193:GLY:N	2.54	0.41
5:B:261:ARG:HB3	5:B:261:ARG:NH1	2.35	0.41
5:B:704:ALA:HB3	5:B:741:CYS:SG	2.61	0.41
5:B:62:ILE:HG23	5:B:418:LYS:HG2	2.03	0.41
7:D:118:THR:O	7:D:118:THR:HG22	2.20	0.41
4:A:817:ALA:O	4:A:820:GLY:N	2.54	0.41
4:A:1062:GLU:OE2	9:F:88:TYR:OH	2.36	0.41
8:E:94:LYS:HG3	8:E:98:ILE:HD11	2.01	0.41
4:A:414:ASP:OD1	4:A:416:ARG:CG	2.69	0.41
5:B:807:ARG:HG2	5:B:1045:SER:OG	2.21	0.41
5:B:1186:ASP:C	5:B:1186:ASP:OD1	2.59	0.41
7:D:63:LEU:HD12	7:D:129:LEU:HG	2.03	0.41
5:B:949:VAL:HG12	5:B:950:ASP:H	1.86	0.41
5:B:1187:ASN:OD1	5:B:1189:ILE:N	2.53	0.41
5:B:1074:ASN:HB2	5:B:1081:LEU:HD21	2.03	0.41
4:A:1364:ASN:O	4:A:1366:ARG:HG3	2.21	0.40
14:K:7:PHE:HA	14:K:10:PHE:HE2	1.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:79:GLY:CA	4:A:243:PRO:HG3	2.51	0.40
4:A:231:PRO:C	4:A:233:TRP:N	2.74	0.40
4:A:23:SER:O	4:A:24:PRO:C	2.59	0.40
5:B:33:VAL:O	5:B:36:ALA:N	2.55	0.40
5:B:1106:ARG:HG3	5:B:1107:ALA:N	2.35	0.40
5:B:753:ALA:HA	5:B:756:ILE:CD1	2.51	0.40
4:A:1236:LEU:C	4:A:1237:ILE:HG13	2.42	0.40
4:A:690:VAL:O	4:A:693:VAL:N	2.54	0.40
6:C:90:ASP:O	6:C:91:HIS:HB3	2.20	0.40
13:J:51:LEU:O	13:J:51:LEU:HD12	2.21	0.40
4:A:791:ASP:OD1	4:A:791:ASP:C	2.59	0.40
5:B:546:SER:OG	5:B:631:GLY:N	2.42	0.40
11:H:40:LEU:CD1	11:H:123:MET:HB2	2.45	0.40
11:H:59:ILE:CG2	11:H:60:ALA:H	2.27	0.40
8:E:205:SER:O	8:E:206:GLY:C	2.60	0.40
4:A:857:ARG:NH1	9:F:139:PRO:HB2	2.36	0.40
13:J:1:MET:HE2	13:J:56:LEU:HD12	2.03	0.40
4:A:241:VAL:HA	4:A:242:PRO:HD2	1.93	0.40
4:A:1339:LEU:O	8:E:150:VAL:HG21	2.21	0.40
4:A:577:ILE:O	4:A:579:SER:N	2.55	0.40
4:A:1377:THR:O	4:A:1378:GLN:C	2.60	0.40
4:A:1409:LEU:HD23	4:A:1409:LEU:HA	1.85	0.40
4:A:265:LYS:HZ3	4:A:322:VAL:HG13	1.87	0.40
12:I:88:SER:HB3	12:I:95:THR:HG21	2.02	0.40
5:B:977:GLY:HA3	5:B:1099:VAL:CG2	2.52	0.40
4:A:767:GLN:NE2	4:A:774:ARG:HB2	2.36	0.40
4:A:6:TYR:CD1	4:A:7:SER:N	2.89	0.40
4:A:886:ILE:HD11	4:A:943:LEU:CB	2.45	0.40
4:A:239:LEU:CD1	4:A:240:PRO:HD2	2.46	0.40
5:B:901:PRO:HD2	15:L:59:ALA:O	2.21	0.40
6:C:246:ARG:HA	6:C:249:ASP:HB3	2.02	0.40
5:B:257:LYS:O	5:B:258:LEU:HB2	2.21	0.40
5:B:446:LEU:O	5:B:447:ALA:CB	2.67	0.40
4:A:1219:THR:HG21	4:A:1271:ILE:HG13	2.02	0.40
10:G:45:ILE:HD13	10:G:45:ILE:HA	1.94	0.40
4:A:59:GLY:HA2	4:A:67:CYS:SG	2.62	0.40
4:A:1040:GLN:O	4:A:1041:ALA:C	2.59	0.40
8:E:79:TRP:CD1	8:E:96:PHE:HE1	2.38	0.40
9:F:103:MET:O	9:F:104:ASN:CB	2.61	0.40
4:A:1339:LEU:HD13	8:E:147:HIS:CD2	2.56	0.40
4:A:524:VAL:HG12	4:A:525:GLN:HE21	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:J:47:ARG:HH11	13:J:47:ARG:CG	2.34	0.40
7:D:56:ARG:HH22	7:D:57:LEU:HD21	1.83	0.40
4:A:432:VAL:O	4:A:433:GLU:C	2.59	0.40
6:C:174:ALA:O	6:C:175:ALA:CB	2.69	0.40
12:I:8:ARG:H	12:I:8:ARG:HG3	1.72	0.40
5:B:899:ILE:HD13	5:B:905:VAL:HG11	2.03	0.40
5:B:635:ARG:HB2	5:B:636:PRO:HD2	2.03	0.40
5:B:662:MET:HA	5:B:665:GLU:HB2	2.02	0.40
8:E:31:THR:OG1	8:E:34:GLU:N	2.50	0.40
7:D:177:VAL:H	7:D:177:VAL:HG23	1.67	0.40
4:A:49:LYS:NZ	4:A:61:ILE:CG1	2.79	0.40
5:B:648:HIS:CG	5:B:649:LYS:N	2.89	0.40
4:A:645:LEU:O	4:A:646:PHE:C	2.58	0.40
5:B:1047:PHE:N	5:B:1047:PHE:CD1	2.81	0.40
7:D:64:VAL:O	7:D:66:ARG:N	2.55	0.40
6:C:177:GLU:CB	6:C:231:ASN:HB3	2.48	0.40
4:A:1072:ILE:O	4:A:1075:PRO:CD	2.69	0.40
4:A:833:GLU:O	4:A:834:THR:C	2.59	0.40
4:A:28:ARG:O	4:A:29:ALA:C	2.60	0.40
4:A:755:PHE:O	4:A:758:ILE:N	2.55	0.40
5:B:729:ILE:O	5:B:729:ILE:HG22	2.21	0.40
4:A:543:LEU:HD12	4:A:547:LEU:HG	2.03	0.40
4:A:54:ASN:HA	4:A:58:LEU:HD12	2.04	0.40
4:A:815:PHE:O	4:A:816:HIS:C	2.60	0.40
4:A:1437:GLY:CA	9:F:88:TYR:CD2	3.04	0.40
5:B:582:VAL:HG12	5:B:587:HIS:NE2	2.37	0.40
5:B:979:LYS:HG2	5:B:1095:LEU:CD1	2.51	0.40
5:B:1207:LEU:O	5:B:1210:MET:HB2	2.21	0.40
5:B:1167:GLY:O	5:B:1215:ARG:HA	2.22	0.40
5:B:550:ASP:OD1	5:B:551:PRO:HD2	2.22	0.40
5:B:168:GLY:HA2	5:B:454:THR:OG1	2.21	0.40
4:A:1013:ASP:C	4:A:1015:VAL:N	2.75	0.40
4:A:809:THR:CG2	4:A:812:GLU:HG3	2.52	0.40
4:A:809:THR:O	4:A:810:PRO:C	2.60	0.40
5:B:386:LEU:C	5:B:388:CYS:N	2.74	0.40
5:B:27:ALA:O	5:B:30:SER:OG	2.36	0.40
4:A:350:ARG:NH1	4:A:488:ASN:OD1	2.49	0.40
5:B:461:LEU:HD12	5:B:461:LEU:N	2.35	0.40
14:K:24:ASP:OD1	14:K:26:LYS:N	2.54	0.40
4:A:596:THR:C	4:A:598:LEU:H	2.24	0.40
4:A:599:SER:HA	4:A:600:PRO:HD2	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:41:ASP:HB2	11:H:121:LEU:HB3	2.02	0.40
11:H:58:THR:HG22	11:H:59:ILE:H	1.86	0.40
6:C:58:LEU:N	6:C:58:LEU:HD22	2.37	0.40
5:B:376:PHE:CE2	5:B:569:TYR:CD2	3.02	0.40
8:E:98:ILE:C	8:E:100:ILE:N	2.74	0.40
4:A:1115:SER:O	4:A:1311:VAL:CG2	2.70	0.40
4:A:1335:ILE:CG2	4:A:1335:ILE:O	2.69	0.40
5:B:1008:PRO:HB2	5:B:1010:LEU:O	2.21	0.40
8:E:177:ARG:O	8:E:212:ARG:CD	2.70	0.40
6:C:169:LYS:NZ	15:L:69:ALA:HB3	2.37	0.40
4:A:353:ILE:HD13	4:A:487:MET:HG3	2.04	0.40
4:A:709:THR:HG22	4:A:710:LEU:N	2.37	0.40
6:C:22:LEU:CD2	6:C:25:VAL:HG21	2.50	0.40
4:A:794:PRO:C	4:A:796:SER:N	2.75	0.40
8:E:17:ARG:O	8:E:21:GLU:HG3	2.22	0.40
5:B:35:SER:HA	5:B:811:TYR:CE2	2.46	0.40
5:B:637:LEU:CD2	5:B:742:GLU:HA	2.51	0.40
4:A:886:ILE:HG13	4:A:943:LEU:HD13	2.03	0.40
4:A:650:GLN:C	4:A:654:ASN:ND2	2.75	0.40
5:B:294:ASP:OD1	12:I:12:ASN:HB3	2.21	0.40
9:F:82:THR:HA	9:F:83:PRO:HD3	1.81	0.40
5:B:1027:ILE:O	5:B:1028:GLU:C	2.60	0.40
4:A:1206:ASP:O	4:A:1274:ARG:NH1	2.52	0.40
5:B:814:PHE:C	5:B:816:GLU:N	2.75	0.40
5:B:371:GLU:N	5:B:371:GLU:OE1	2.55	0.40
5:B:180:TYR:CD1	5:B:180:TYR:N	2.90	0.40
5:B:564:GLU:HA	5:B:565:PRO:HD2	1.91	0.40
9:F:94:LEU:HD21	9:F:122:MET:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	1406/1733 (81%)	936 (67%)	311 (22%)	159 (11%)	0	10
5	B	1096/1224 (90%)	740 (68%)	215 (20%)	141 (13%)	0	7
6	C	264/318 (83%)	166 (63%)	64 (24%)	34 (13%)	0	7
7	D	173/221 (78%)	118 (68%)	38 (22%)	17 (10%)	1	14
8	E	212/215 (99%)	154 (73%)	44 (21%)	14 (7%)	1	25
9	F	82/155 (53%)	63 (77%)	16 (20%)	3 (4%)	4	40
10	G	169/171 (99%)	133 (79%)	24 (14%)	12 (7%)	1	23
11	H	129/146 (88%)	85 (66%)	28 (22%)	16 (12%)	0	8
12	I	117/122 (96%)	79 (68%)	27 (23%)	11 (9%)	1	16
13	J	63/70 (90%)	34 (54%)	15 (24%)	14 (22%)	0	1
14	K	112/120 (93%)	87 (78%)	17 (15%)	8 (7%)	1	23
15	L	44/70 (63%)	17 (39%)	18 (41%)	9 (20%)	0	2
All	All	3867/4565 (85%)	2612 (68%)	817 (21%)	438 (11%)	0	10

All (438) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	5	GLN
4	A	48	ALA
4	A	54	ASN
4	A	55	ASP
4	A	57	ARG
4	A	62	ASP
4	A	65	LEU
4	A	66	LYS
4	A	70	CYS
4	A	74	MET
4	A	76	GLU
4	A	93	VAL
4	A	154	SER
4	A	167	CYS
4	A	244	PRO
4	A	255	SER
4	A	286	HIS
4	A	311	GLN
4	A	318	SER
4	A	322	VAL
4	A	335	ARG
4	A	385	ILE

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Mol	Chain	Res	Type
4	A	409	SER
4	A	418	SER
4	A	423	ASP
4	A	536	LEU
4	A	567	LYS
4	A	619	LYS
4	A	626	ASN
4	A	666	ILE
4	A	765	VAL
4	A	775	ILE
4	A	780	VAL
4	A	789	LYS
4	A	847	ASP
4	A	968	GLN
4	A	1002	GLY
4	A	1016	THR
4	A	1036	ARG
4	A	1115	SER
4	A	1116	LEU
4	A	1122	PRO
4	A	1212	VAL
4	A	1223	ASP
4	A	1281	ARG
4	A	1314	SER
4	A	1341	ILE
4	A	1365	TYR
4	A	1366	ARG
4	A	1378	GLN
4	A	1403	GLU
4	A	1438	THR
5	B	28	GLU
5	B	45	SER
5	B	108	VAL
5	B	206	ASN
5	B	258	LEU
5	B	259	TYR
5	B	308	TRP
5	B	367	LEU
5	B	467	GLY
5	B	474	SER
5	B	504	ARG
5	B	509	ALA

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Mol	Chain	Res	Type
5	B	511	PRO
5	B	629	ASP
5	B	643	ASP
5	B	709	ASP
5	B	731	VAL
5	B	751	VAL
5	B	881	ASN
5	B	907	GLY
5	B	943	SER
5	B	958	GLN
5	B	1046	PRO
5	B	1100	ASP
5	B	1108	ARG
5	B	1157	ALA
5	B	1171	VAL
5	B	1175	LEU
5	B	1181	GLU
5	B	1182	CYS
5	B	1186	ASP
5	B	1188	LYS
6	C	91	HIS
6	C	110	THR
6	C	141	GLY
6	C	149	LYS
6	C	156	THR
6	C	161	LYS
6	C	184	ASN
6	C	213	PRO
6	C	214	ASN
6	C	215	GLU
6	C	231	ASN
7	D	6	SER
7	D	8	PHE
7	D	19	GLU
7	D	20	GLU
7	D	21	GLU
7	D	52	LEU
7	D	131	GLU
7	D	177	VAL
7	D	199	ASN
8	E	106	GLN
8	E	130	ALA

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Mol	Chain	Res	Type
9	F	81	THR
10	G	63	PRO
10	G	139	ILE
11	H	81	PRO
11	H	128	ASN
11	H	140	ALA
12	I	3	THR
12	I	9	ASP
12	I	57	GLY
12	I	79	HIS
13	J	2	ILE
13	J	6	ARG
13	J	32	GLU
13	J	64	ASN
15	L	50	ASP
15	L	53	HIS
15	L	59	ALA
4	A	42	ASP
4	A	44	THR
4	A	59	GLY
4	A	111	GLY
4	A	113	LEU
4	A	117	GLU
4	A	219	PHE
4	A	226	GLU
4	A	232	GLU
4	A	263	THR
4	A	278	THR
4	A	290	GLU
4	A	300	VAL
4	A	312	PRO
4	A	364	VAL
4	A	399	HIS
4	A	421	ALA
4	A	424	ILE
4	A	661	GLY
4	A	731	ARG
4	A	753	GLY
4	A	795	GLU
4	A	830	LYS
4	A	846	GLU
4	A	986	ILE

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Mol	Chain	Res	Type
4	A	1014	ALA
4	A	1071	SER
4	A	1165	GLU
4	A	1221	LYS
4	A	1386	ARG
4	A	1395	GLY
4	A	1397	LEU
4	A	1405	THR
5	B	21	GLU
5	B	27	ALA
5	B	46	GLN
5	B	114	PRO
5	B	115	GLN
5	B	186	GLU
5	B	229	ALA
5	B	257	LYS
5	B	260	GLY
5	B	282	ILE
5	B	322	PHE
5	B	334	ILE
5	B	369	GLY
5	B	468	GLU
5	B	470	LYS
5	B	513	GLN
5	B	540	SER
5	B	559	SER
5	B	682	SER
5	B	746	SER
5	B	770	GLN
5	B	848	ARG
5	B	869	SER
5	B	891	ASP
5	B	1006	ILE
5	B	1041	GLU
5	B	1069	PHE
5	B	1126	GLY
5	B	1156	ASP
5	B	1167	GLY
5	B	1178	ASN
5	B	1183	LYS
6	C	78	GLU
6	C	164	ALA

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Mol	Chain	Res	Type
6	C	167	HIS
6	C	175	ALA
6	C	202	PRO
6	C	209	TYR
6	C	216	GLY
6	C	240	VAL
6	C	264	GLN
7	D	12	ARG
7	D	53	SER
7	D	192	LYS
8	E	36	GLU
8	E	44	ALA
8	E	59	SER
8	E	73	PRO
8	E	74	ASP
8	E	192	ARG
8	E	206	GLY
10	G	35	GLU
10	G	53	ASN
10	G	154	VAL
11	H	21	ASN
11	H	32	THR
11	H	59	ILE
11	H	82	PRO
11	H	84	ALA
11	H	92	ASP
11	H	108	SER
12	I	78	CYS
12	I	106	CYS
13	J	8	PHE
13	J	14	VAL
13	J	18	TRP
13	J	28	ASP
13	J	29	GLU
13	J	33	GLY
13	J	51	LEU
14	K	7	PHE
14	K	15	GLY
14	K	29	ASN
14	K	53	ASP
14	K	88	LYS
4	A	4	GLN

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Mol	Chain	Res	Type
4	A	61	ILE
4	A	67	CYS
4	A	69	THR
4	A	71	GLN
4	A	223	GLY
4	A	245	PRO
4	A	253	ASN
4	A	317	LYS
4	A	357	PRO
4	A	419	LYS
4	A	439	ASN
4	A	517	ASN
4	A	525	GLN
4	A	534	LEU
4	A	817	ALA
4	A	818	MET
4	A	824	LEU
4	A	829	VAL
4	A	1008	GLN
4	A	1028	THR
4	A	1067	LEU
4	A	1114	PRO
4	A	1127	ASP
4	A	1133	LEU
4	A	1240	CYS
4	A	1242	VAL
4	A	1335	ILE
4	A	1389	PHE
5	B	48	LEU
5	B	58	THR
5	B	100	PRO
5	B	266	ALA
5	B	319	GLU
5	B	387	LEU
5	B	591	ARG
5	B	605	ARG
5	B	636	PRO
5	B	641	GLU
5	B	648	HIS
5	B	655	LYS
5	B	711	GLU
5	B	867	GLY

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Mol	Chain	Res	Type
5	B	878	GLN
5	B	951	GLN
5	B	1003	ALA
5	B	1017	ILE
5	B	1035	ALA
5	B	1097	HIS
5	B	1112	GLN
5	B	1144	ALA
5	B	1153	GLU
5	B	1155	SER
6	C	87	PHE
6	C	169	LYS
6	C	255	VAL
7	D	15	LEU
7	D	218	GLU
8	E	115	ASN
8	E	138	ALA
9	F	150	GLU
10	G	62	LEU
10	G	118	ASP
11	H	17	PRO
11	H	44	VAL
11	H	77	ARG
11	H	107	VAL
12	I	47	GLU
12	I	62	ILE
13	J	17	LYS
15	L	35	SER
15	L	40	LEU
15	L	43	THR
15	L	54	ARG
15	L	56	LEU
4	A	58	LEU
4	A	250	ILE
4	A	283	GLY
4	A	333	GLU
4	A	336	ILE
4	A	400	PRO
4	A	465	TYR
4	A	526	ASP
4	A	592	ASP
4	A	605	MET

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Mol	Chain	Res	Type
4	A	648	ASN
4	A	652	VAL
4	A	910	PRO
4	A	958	VAL
4	A	1231	ASP
4	A	1266	THR
4	A	1302	PRO
5	B	49	ASP
5	B	67	SER
5	B	364	ILE
5	B	418	LYS
5	B	466	TRP
5	B	590	HIS
5	B	727	LYS
5	B	735	ALA
5	B	738	PHE
5	B	752	ALA
5	B	754	SER
5	B	764	SER
5	B	792	MET
5	B	815	ARG
5	B	883	LEU
5	B	884	ARG
5	B	888	GLY
5	B	953	LEU
5	B	982	SER
5	B	1065	GLN
5	B	1103	ILE
5	B	1176	ASN
6	C	60	ASP
6	C	108	GLU
6	C	142	VAL
6	C	212	PRO
6	C	257	SER
7	D	30	GLY
8	E	45	LYS
8	E	99	HIS
10	G	115	MET
11	H	52	GLN
12	I	11	ASN
12	I	34	TYR
14	K	70	ARG

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Mol	Chain	Res	Type
14	K	79	GLU
14	K	104	ASN
4	A	101	LYS
4	A	386	ASP
4	A	599	SER
4	A	920	LEU
4	A	1120	LEU
4	A	1164	PRO
4	A	1370	LEU
5	B	30	SER
5	B	65	GLU
5	B	94	LYS
5	B	309	GLN
5	B	383	ASN
5	B	401	PHE
5	B	411	PRO
5	B	414	ALA
5	B	510	LYS
5	B	571	PRO
5	B	880	THR
5	B	942	ARG
5	B	1011	ILE
6	C	56	THR
6	C	84	ARG
7	D	196	PRO
9	F	149	GLU
10	G	17	PHE
10	G	20	PRO
11	H	135	LEU
13	J	24	LEU
13	J	27	GLU
4	A	276	LEU
4	A	492	PRO
4	A	598	LEU
4	A	649	ILE
4	A	756	ILE
4	A	1006	ILE
4	A	1057	VAL
4	A	1377	THR
5	B	261	ARG
5	B	844	SER
5	B	1082	MET

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Mol	Chain	Res	Type
6	C	89	GLU
10	G	34	VAL
12	I	32	CYS
4	A	38	PRO
4	A	96	ILE
5	B	23	ALA
5	B	295	GLY
5	B	410	GLY
5	B	478	GLY
5	B	520	GLY
5	B	551	PRO
5	B	1018	PRO
5	B	1099	VAL
6	C	77	ILE
4	A	84	ILE
4	A	196	GLU
4	A	1158	PRO
5	B	575	PRO
5	B	613	VAL
6	C	10	ILE
4	A	396	PRO
4	A	653	VAL
4	A	1384	VAL
4	A	1454	MET
5	B	283	VAL
5	B	712	PRO
5	B	824	ILE
6	C	172	PRO
10	G	19	GLY
15	L	46	VAL
4	A	1060	PRO
7	D	202	ILE
4	A	73	GLY
4	A	321	PRO
4	A	1406	VAL
5	B	611	PRO
5	B	758	PHE
8	E	129	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	
4	A	1239/1520 (82%)	1125 (91%)	114 (9%)	11	46
5	B	964/1061 (91%)	873 (91%)	91 (9%)	11	45
6	C	234/274 (85%)	213 (91%)	21 (9%)	12	47
7	D	140/200 (70%)	124 (89%)	16 (11%)	7	36
8	E	196/197 (100%)	188 (96%)	8 (4%)	37	73
9	F	74/137 (54%)	65 (88%)	9 (12%)	6	33
10	G	152/152 (100%)	139 (91%)	13 (9%)	13	50
11	H	117/128 (91%)	109 (93%)	8 (7%)	20	59
12	I	113/116 (97%)	98 (87%)	15 (13%)	5	30
13	J	60/65 (92%)	55 (92%)	5 (8%)	14	51
14	K	99/102 (97%)	90 (91%)	9 (9%)	12	47
15	L	40/57 (70%)	37 (92%)	3 (8%)	17	56
All	All	3428/4009 (86%)	3116 (91%)	312 (9%)	12	47

All (312) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	2	VAL
4	A	11	LEU
4	A	22	PHE
4	A	34	LYS
4	A	38	PRO
4	A	62	ASP
4	A	67	CYS
4	A	83	HIS
4	A	93	VAL
4	A	105	CYS
4	A	108	MET
4	A	122	MET
4	A	200	ARG
4	A	208	LEU

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Mol	Chain	Res	Type
4	A	209	ASN
4	A	215	SER
4	A	221	SER
4	A	236	LEU
4	A	245	PRO
4	A	270	LEU
4	A	293	GLU
4	A	302	THR
4	A	312	PRO
4	A	320	ARG
4	A	321	PRO
4	A	335	ARG
4	A	350	ARG
4	A	354	SER
4	A	381	THR
4	A	396	PRO
4	A	404	TYR
4	A	406	ILE
4	A	407	ARG
4	A	408	ASP
4	A	418	SER
4	A	425	GLN
4	A	443	LEU
4	A	445	ASN
4	A	449	SER
4	A	450	LEU
4	A	451	HIS
4	A	454	SER
4	A	462	VAL
4	A	470	LEU
4	A	481	ASP
4	A	493	GLN
4	A	497	THR
4	A	498	ARG
4	A	503	GLN
4	A	515	GLN
4	A	545	GLN
4	A	560	ILE
4	A	562	THR
4	A	598	LEU
4	A	618	GLU
4	A	626	ASN

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Mol	Chain	Res	Type
4	A	666	ILE
4	A	670	ILE
4	A	711	ARG
4	A	739	ASP
4	A	768	GLN
4	A	774	ARG
4	A	779	PHE
4	A	821	ARG
4	A	827	THR
4	A	831	THR
4	A	834	THR
4	A	845	LEU
4	A	858	ASN
4	A	871	ASP
4	A	890	ASP
4	A	903	ASN
4	A	929	LEU
4	A	940	ARG
4	A	949	ASP
4	A	992	ASP
4	A	1016	THR
4	A	1029	ARG
4	A	1030	ARG
4	A	1035	TYR
4	A	1052	GLN
4	A	1067	LEU
4	A	1110	ASN
4	A	1111	MET
4	A	1116	LEU
4	A	1122	PRO
4	A	1127	ASP
4	A	1152	ILE
4	A	1155	ASP
4	A	1170	ILE
4	A	1173	HIS
4	A	1193	LEU
4	A	1264	GLU
4	A	1271	ILE
4	A	1291	VAL
4	A	1295	THR
4	A	1298	TYR
4	A	1309	ASP

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Mol	Chain	Res	Type
4	A	1329	THR
4	A	1332	PHE
4	A	1333	ILE
4	A	1359	ASP
4	A	1364	ASN
4	A	1366	ARG
4	A	1372	VAL
4	A	1386	ARG
4	A	1389	PHE
4	A	1394	THR
4	A	1405	THR
4	A	1432	GLN
4	A	1442	ASP
4	A	1443	VAL
4	A	1445	ILE
4	A	1447	GLU
5	B	30	SER
5	B	44	VAL
5	B	57	TYR
5	B	61	ASP
5	B	175	ARG
5	B	188	ASP
5	B	194	GLU
5	B	199	MET
5	B	217	ARG
5	B	223	VAL
5	B	225	VAL
5	B	261	ARG
5	B	268	THR
5	B	286	PHE
5	B	294	ASP
5	B	298	LEU
5	B	365	THR
5	B	371	GLU
5	B	378	LEU
5	B	393	LYS
5	B	396	ASP
5	B	399	ASP
5	B	401	PHE
5	B	411	PRO
5	B	417	PHE
5	B	427	ASP

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Mol	Chain	Res	Type
5	B	429	PHE
5	B	463	THR
5	B	465	ASN
5	B	466	TRP
5	B	476	ARG
5	B	485	ARG
5	B	496	ARG
5	B	498	THR
5	B	502	ILE
5	B	516	ASN
5	B	557	PHE
5	B	570	VAL
5	B	582	VAL
5	B	593	PRO
5	B	603	LEU
5	B	615	MET
5	B	628	THR
5	B	635	ARG
5	B	636	PRO
5	B	644	GLU
5	B	682	SER
5	B	701	ILE
5	B	724	ASP
5	B	737	THR
5	B	742	GLU
5	B	751	VAL
5	B	811	TYR
5	B	830	TYR
5	B	835	GLN
5	B	839	MET
5	B	858	SER
5	B	860	MET
5	B	878	GLN
5	B	894	ASP
5	B	901	PRO
5	B	909	ASP
5	B	953	LEU
5	B	999	MET
5	B	1002	THR
5	B	1006	ILE
5	B	1010	LEU
5	B	1018	PRO

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Mol	Chain	Res	Type
5	B	1034	VAL
5	B	1047	PHE
5	B	1051	THR
5	B	1060	ARG
5	B	1069	PHE
5	B	1077	THR
5	B	1084	GLN
5	B	1087	PHE
5	B	1095	LEU
5	B	1096	ARG
5	B	1099	VAL
5	B	1112	GLN
5	B	1120	GLU
5	B	1122	ARG
5	B	1159	ARG
5	B	1163	CYS
5	B	1169	MET
5	B	1170	THR
5	B	1176	ASN
5	B	1183	LYS
5	B	1202	LEU
5	B	1212	ILE
5	B	1216	LEU
6	C	22	LEU
6	C	29	MET
6	C	54	ASN
6	C	58	LEU
6	C	62	PHE
6	C	77	ILE
6	C	89	GLU
6	C	91	HIS
6	C	104	PHE
6	C	106	GLU
6	C	108	GLU
6	C	112	ASN
6	C	140	ASN
6	C	145	CYS
6	C	147	LEU
6	C	166	GLU
6	C	193	TYR
6	C	202	PRO
6	C	233	GLU

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Mol	Chain	Res	Type
6	C	240	VAL
6	C	266	ASP
7	D	32	GLU
7	D	47	LEU
7	D	63	LEU
7	D	70	PHE
7	D	137	ASN
7	D	139	LYS
7	D	148	LEU
7	D	149	THR
7	D	152	SER
7	D	156	ASP
7	D	170	THR
7	D	182	SER
7	D	187	THR
7	D	193	THR
7	D	202	ILE
7	D	221	TYR
8	E	60	PHE
8	E	74	ASP
8	E	82	PHE
8	E	104	ASN
8	E	114	ASN
8	E	183	PRO
8	E	207	ARG
8	E	215	MET
9	F	79	ARG
9	F	81	THR
9	F	90	ARG
9	F	99	LEU
9	F	103	MET
9	F	119	ARG
9	F	143	PHE
9	F	148	VAL
9	F	153	VAL
10	G	1	MET
10	G	13	LEU
10	G	17	PHE
10	G	38	CYS
10	G	74	TYR
10	G	78	VAL
10	G	80	LYS

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Mol	Chain	Res	Type
10	G	88	ASP
10	G	93	SER
10	G	96	GLN
10	G	115	MET
10	G	126	ASN
10	G	171	ILE
11	H	7	ASP
11	H	62	SER
11	H	86	ASP
11	H	91	ASP
11	H	95	TYR
11	H	102	TYR
11	H	130	ARG
11	H	143	LEU
12	I	8	ARG
12	I	9	ASP
12	I	10	CYS
12	I	13	MET
12	I	15	TYR
12	I	31	THR
12	I	34	TYR
12	I	75	CYS
12	I	78	CYS
12	I	85	PHE
12	I	86	PHE
12	I	94	ASP
12	I	100	PHE
12	I	101	PHE
12	I	106	CYS
13	J	1	MET
13	J	9	SER
13	J	44	TYR
13	J	46	CYS
13	J	48	ARG
14	K	5	ASP
14	K	10	PHE
14	K	17	SER
14	K	25	THR
14	K	42	LEU
14	K	47	ARG
14	K	50	LEU
14	K	61	TYR

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Mol	Chain	Res	Type
14	K	78	THR
15	L	55	ILE
15	L	68	GLU
15	L	70	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	83	HIS
4	A	92	HIS
4	A	225	ASN
4	A	256	GLN
4	A	282	ASN
4	A	299	HIS
4	A	306	ASN
4	A	339	ASN
4	A	435	HIS
4	A	479	ASN
4	A	493	GLN
4	A	503	GLN
4	A	517	ASN
4	A	525	GLN
4	A	603	ASN
4	A	611	GLN
4	A	654	ASN
4	A	741	ASN
4	A	757	ASN
4	A	767	GLN
4	A	768	GLN
4	A	786	HIS
4	A	858	ASN
4	A	903	ASN
4	A	926	GLN
4	A	1130	GLN
4	A	1265	ASN
4	A	1364	ASN
4	A	1432	GLN
5	B	178	ASN
5	B	215	GLN
5	B	236	HIS
5	B	350	GLN
5	B	363	HIS

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Mol	Chain	Res	Type
5	B	366	GLN
5	B	383	ASN
5	B	465	ASN
5	B	484	ASN
5	B	515	HIS
5	B	516	ASN
5	B	518	HIS
5	B	538	ASN
5	B	734	HIS
5	B	744	HIS
5	B	776	GLN
5	B	821	GLN
5	B	842	ASN
5	B	975	GLN
5	B	1015	HIS
5	B	1025	HIS
5	B	1065	GLN
5	B	1076	HIS
5	B	1084	GLN
5	B	1097	HIS
5	B	1117	GLN
5	B	1179	GLN
5	B	1193	GLN
6	C	24	ASN
6	C	73	GLN
6	C	91	HIS
6	C	112	ASN
6	C	123	ASN
6	C	231	ASN
6	C	252	GLN
7	D	40	HIS
7	D	137	ASN
7	D	179	GLN
8	E	8	ASN
8	E	101	GLN
8	E	104	ASN
8	E	114	ASN
8	E	147	HIS
10	G	14	HIS
10	G	53	ASN
10	G	97	HIS
10	G	122	ASN

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Mol	Chain	Res	Type
10	G	126	ASN
11	H	131	ASN
12	I	12	ASN
12	I	60	GLN
12	I	89	GLN
14	K	44	ASN
14	K	65	HIS
14	K	76	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	P	9/10 (90%)	1 (11%)	1 (11%)

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	P	3	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	P	2	A

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	T	18/19 (94%)	0.43	1 (5%) 28 20	69, 103, 131, 137	0
2	N	6/7 (85%)	1.00	1 (16%) 2 3	97, 99, 108, 108	0
3	P	10/10 (100%)	0.34	0 100 100	80, 94, 125, 127	0
4	A	1416/1733 (81%)	-0.75	4 (0%) 94 92	21, 75, 151, 195	0
5	B	1112/1224 (90%)	-0.69	4 (0%) 93 90	20, 87, 156, 186	0
6	C	266/318 (83%)	-0.78	0 100 100	34, 71, 130, 150	0
7	D	177/221 (80%)	-0.55	0 100 100	43, 99, 137, 155	0
8	E	214/215 (99%)	-0.54	0 100 100	47, 132, 177, 181	0
9	F	84/155 (54%)	-0.92	0 100 100	21, 49, 93, 113	0
10	G	171/171 (100%)	-0.76	0 100 100	47, 76, 106, 122	0
11	H	133/146 (91%)	-0.32	0 100 100	91, 130, 165, 175	0
12	I	119/122 (97%)	-0.37	0 100 100	63, 122, 153, 191	0
13	J	65/70 (92%)	-0.87	0 100 100	37, 69, 113, 118	0
14	K	114/120 (95%)	-0.79	0 100 100	37, 75, 104, 118	0
15	L	46/70 (65%)	-0.33	0 100 100	73, 127, 160, 168	0
All	All	3951/4601 (85%)	-0.68	10 (0%) 94 92	20, 84, 156, 195	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	1176	LEU	5.0
5	B	471	LYS	3.3
4	A	1175	SER	2.6
1	T	28	DT	2.5
5	B	470	LYS	2.3
4	A	1455	PRO	2.3
5	B	504	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
4	A	1092	LYS	2.1
5	B	919	SER	2.0
2	N	6	DC	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
16	ZN	C	319	1/1	0.99	0.09	-0.80	28,28,28,28	0
16	ZN	A	1734	1/1	0.98	0.09	-0.99	73,73,73,73	0
16	ZN	I	204	1/1	0.98	0.10	-1.19	141,141,141,141	0
16	ZN	L	105	1/1	0.99	0.10	-1.41	90,90,90,90	0
16	ZN	B	1307	1/1	1.00	0.08	-1.50	31,31,31,31	0
16	ZN	A	1735	1/1	0.99	0.05	-1.78	36,36,36,36	0
16	ZN	J	101	1/1	0.99	0.06	-2.14	45,45,45,45	0
16	ZN	I	203	1/1	0.99	0.08	-2.40	80,80,80,80	0
17	MG	A	1736	1/1	0.99	0.07	-	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.