



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:51 PM UTC

PDB ID : 2R93 / pdb_00002r93
Title : Elongation complex of RNA polymerase II with a hepatitis delta virus-derived RNA stem loop
Authors : Lehmann, E.; Brueckner, F.; Cramer, P.
Deposited on : 2007-09-12
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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

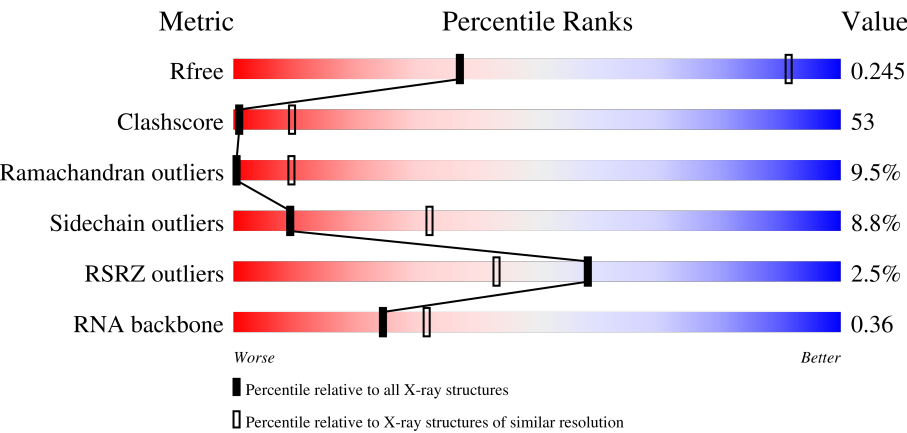
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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}	180053	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)
RNA backbone	3983	1017 (4.84-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	R	18	6% 28% 28% 22% 22%
2	A	1733	2% 26% 44% 11% • 18%
3	B	1224	2% 26% 50% 13% • 9%
4	C	318	23% 48% 12% • 16%

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Mol	Chain	Length	Quality of chain
5	D	221	2%30%37%12%19%
6	E	215	%31%58%10%
7	F	155	%18%31%7%43%
8	G	171	2%27%60%11%
9	H	146	7%25%53%14%8%
10	I	122	6%30%51%13%5%
11	J	70	%19%57%17%7%
12	K	120	%33%47%13%7%
13	L	70	4%16%34%14%34%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 31500 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 RNA chain called RNA (5'-R(*UP*GP*AP*UP*UP*CP*UP*CP*UP*AP*UP*CP*GP*GP*AP*AP*UP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	14	Total	C	N	O	P	0	0	0
			289	132	49	96	12			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	1422	Total	C	N	O	S	0	0	0
			11194	7054	1959	2119	62			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	1112	Total	C	N	O	S	0	0	0
			8841	5596	1550	1640	55			

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	267	Total	C	N	O	S	0	0	0
			2101	1320	349	419	13			

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	178	Total	C	N	O	S	0	0	0
			1434	887	257	288	2			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	F	88	Total	C	N	O	S	0	0	0
			712	455	120	134	3			

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	135	Total	C	N	O	S	0	0	0
			1084	683	183	214	4			

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	116	Total	C	N	O	S	0	0	0
			944	581	172	181	10			

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	112	Total	C	N	O	S	0	0	0
			904	580	154	168	2			

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	46	Total	C	N	O	S	0	0	0
			364	224	72	64	4			

- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

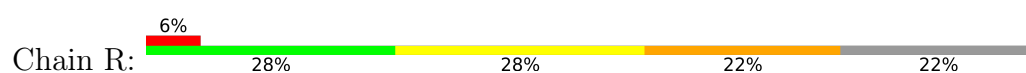
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

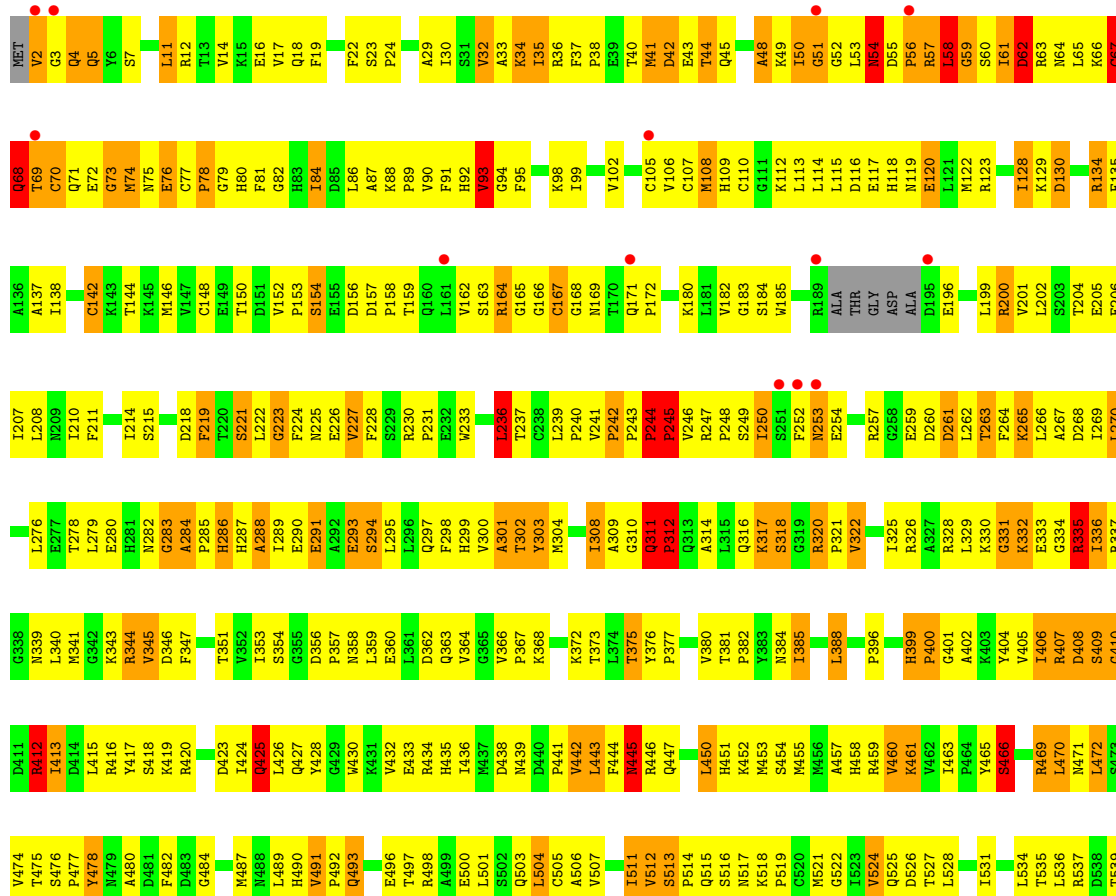
3 Residue-property plots

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

- Molecule 1: RNA (5'-R(*UP*GP*AP*UP*UP*CP*UP*CP*UP*AP*UP*CP*GP*GP*AP*AP*UP*C)-3')

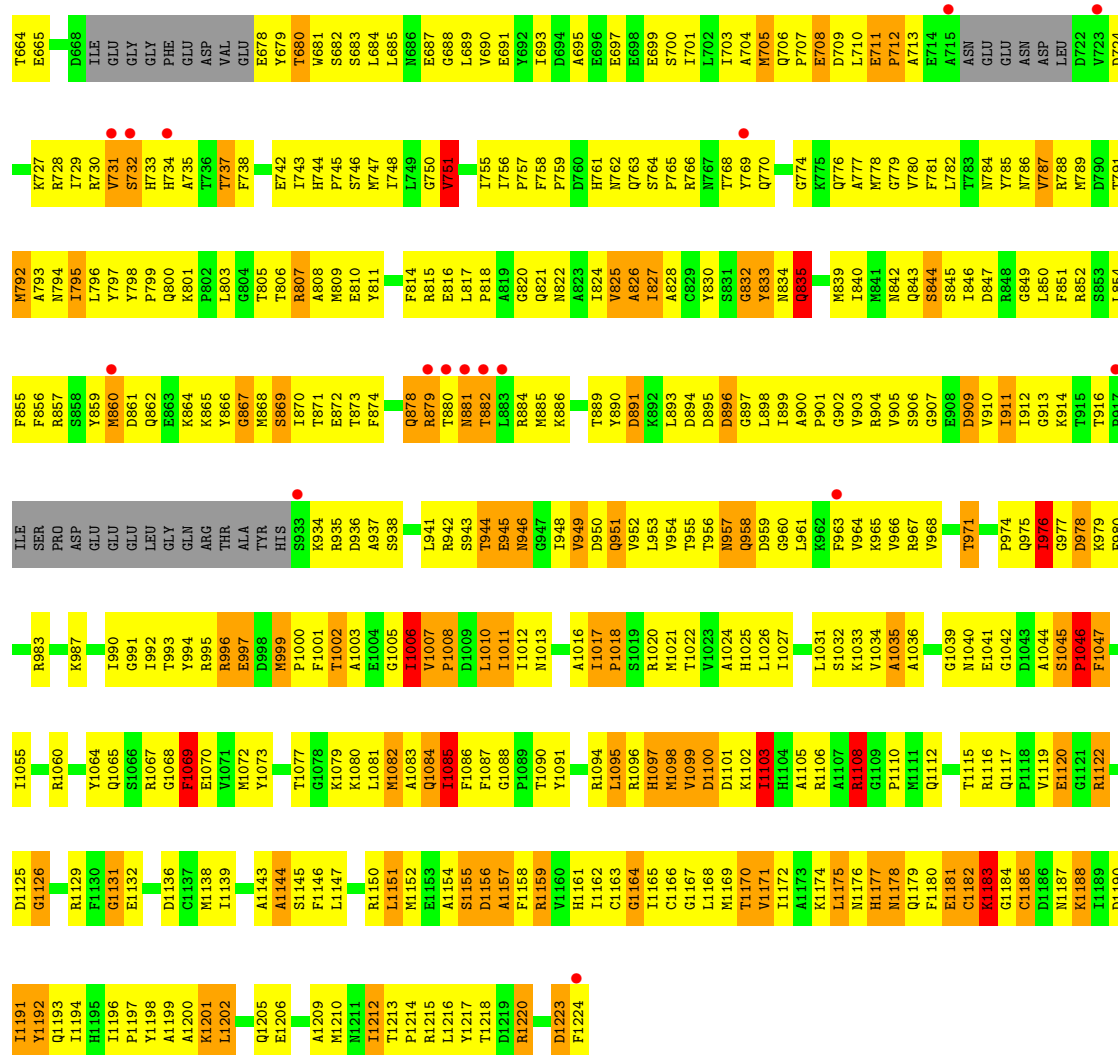


- Molecule 2: DNA-directed RNA polymerase II subunit RPB1



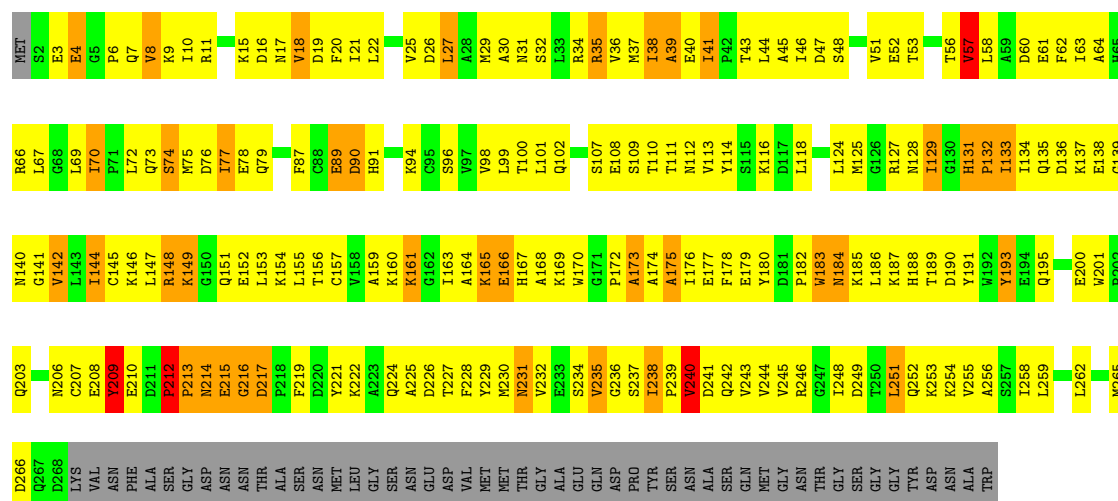
E1426	N1427	V1428	M1364	Y1365	L1429	L1430	G1431	Q1432	M1368	A1369	L1370	A1434	P1435	I1436	G1437	T1438	F1441	D1442	V1443	M1444	I1445	D1446	E1447	L1450	M1454	F1455	GLU	GLN	LYS	ILE	THR	GLU	ILE	ASP	GLY	GLN	S1401	F1402	E1403	E1404	VAL	THR	PRO	TYR	SER	ASN	GLU	SER	GLY	GLY	LEU	VAL	ASN	ALA	ASP	LEU	ASP	VAL	LYS	ASP	GLU		
D1359	M1364	Y1365	R1366	H1367	M1368	A1369	L1370	L1371	V1372	D1373	V1374	M1375	T1376	T1377	Q1378	G1379	L1381	T1385	R1386	H1387	G1388	F1389	S1392	M1393	T1394	G1395	A1396	L1397	M1398	R1399	G1400	S1401	F1402	E1403	E1404	I1405	V1406	E1407	T1408	L1409	F1410	E1411	E1412	E1413	A1416	A1417	L1418	D1419	D1420	R1421	G1422	V1423	V1424	E1425									
P1294	T1295	G1296	E1297	Y1298	V1299	K1300	E1301	P1302	E1303	W1304	V1305	L1306	E1307	T1308	D1309	G1310	V1311	N1312	L1313	S1314	E1315	V1316	M1317	V1318	V1319	P1320	D1323	P1324	T1325	R1326	I1327	Y1328	N1329	S1330	S1331	F1332	I1333	D1334	I1335	M1336	E1337	V1338	T1341	E1342	A1343	G1344	R1345	A1346	A1347	L1348	D1419	K1350	E1351	V1352	G1423	N1354	S1425						
W1228	S1229	E1230	D1231	N1232	D1233	L1236	I1237	L1238	R1239	G1240	R1241	V1242	V1243	R1244	P1245	LYS	SER	LEU	ASP	GLU	THR	GLU	A1254	E1255	E1256	D1257	H1258	M1259	L1260	K1261	I1262	I1263	N1264	T1266	M1267	L1268	I1271	T1272	M1209	G1210	Q1211	V1212	G1213	E1214	R1215	Q1218	T1219	F1220	K1221	M1284	N1278	I1279	E1280	R1281	V1282	L1283	Y1349	K1350	E1351	V1352	V1291	P1292	S1293
V1162	I1163	P1164	E1165	D1166	I1169	I1170	Q1171	L1172	H1173	F1174	S1175	L1176	L1177	ASP	GLU	GLY	ALA	GLU	GLN	SER	PHE	ASP	Q1187	Q1188	S1189	P1190	W1191	L1192	L1193	R1194	D1198	Q1128	Q1129	Q1130	A1131	K1132	L1133	I1134	T1138	T1141	K1144	S1145	V1146	T1147	I1148	A1149	S1150	I1151	I1152	Y1153	Y1154	D1155	P1156	S1160	T1161								
K1092	K1093	V1094	T1095	S1096	G1097	R1100	L1101	K1102	E1103	F1104	L1105	L1106	V1107	M1111	K1112	T1113	P1114	S1115	L1116	L1117	V1118	Y1119	L1120	E1121	P1122	G1123	H1124	D1127	Q1128	Q1129	Q1130	A1131	K1132	L1133	I1134	T1138	T1141	K1144	S1145	V1146	T1147	I1148	A1149	S1150	I1151	I1152	Y1153	Y1154	D1155	P1156	S1160	T1161											
A1027	T1028	R1029	R1030	V1031	L1032	Q1033	E1034	Y1035	R1036	L1037	T1038	K1039	Q1040	A1041	F1042	V1045	L1046	S1047	N1048	I1049	E1050	A1051	Q1052	S1056	V1057	M1058	H1059	P1060	G1061	E1062	M1063	V1064	G1065	V1066	L1067	A1068	A1069	Q1070	S1071	E1074	P1075	A1076	M1079	T1080	L1081	ASN	THR	PHE	HIS	PHE	ALA	GLY	VAL	ALA	SER								
R961	R962	T963	E964	Q965	R966	A967	Q968	Q969	T970	R971	H972	T973	D974	H975	T976	R977	Q978	R979	D980	L981	T982	T983	K984	D985	Y986	Y987	L988	L993	N996	L997	V998	V999	R1000	L1001	G1002	A1003	M1004	E1005	I1006	I1007	Q1008	N1009	A1010	Q1011	R1012	D1013	A1014	V1015	T1016	L1017	F1018	C1019	L1022	R1025	L1026								
L883	R886	G887	Q888	S889	D890	E894	R895	R896	H897	V898	K899	D900	L901	L902	N903	T904	L908	D909	P910	S911	K843	L912	L913	E914	Y919	D920	G921	D922	L923	Q926	V927	L928	L929	D930	E931	K938	D939	R940	K941	F942	L943	R944	Y868	E945	Y946	G950	K954	P955	L956	P957	Y958	R959	L960										
F815	H816	M817	R818	R821	L825	D826	T827	V828	V829	K830	E833	T834	G835	Y836	T837	Q838	R839	R840	L841	H842	K843	L844	E846	D847	T848	N849	V850	H851	D852	H853	N854	T855	T856	R857	N858	S859	L860	G861	N862	V863	F866	T867	Y868	C869	E870	D871	K872	N873	D874	L875	A876	H877	K878	F814									
W746	V747	M748	S751	K752	G753	S754	F755	T756	N757	T758	V759	K760	M761	S762	A763	G764	Y765	G766	Q767	Q768	R774	L775	A776	F777	G778	F779	D780	D781	R782	L783	L784	P785	H786	F787	S788	K789	P794	E795	S796	K797	G798	F799	V800	E801	N802	S803	Y804	L805	R806	G807	L808	D809	E812	F813	Q745								
E681	T682	A683	G684	E685	V686	K687	K688	K689	V690	V693	T694	K695	E696	A697	Q698	G699	T700	L701	L702	K705	H706	E636	K637	M708	T709	L710	Q640	V641	F646	K647	M648	T649	Q650	S579	V719	R720	F721	L722	N723	E724	A725	H659	R726	D727	K728	A729	G730	G665	R731	L732	N736	L737	D738	D739	L740	N741	H742	V743	K744	T690			
F540	I541	E542	L543	D544	G545	V546	L547	N548	M549	L550	Y551	W552	V553	T560	P561	T562	P563	A564	I565	I566	K567	P568	K569	P570	L571	W572	S573	G574	K575	Q576	L577	L578	S579	V580	H587	L588	Q589	R590	F591	D592	T595	T596	L597	L598	S599	P600	K601	D602	N603	G604	M605	L606	I607	L608	D609	G610							



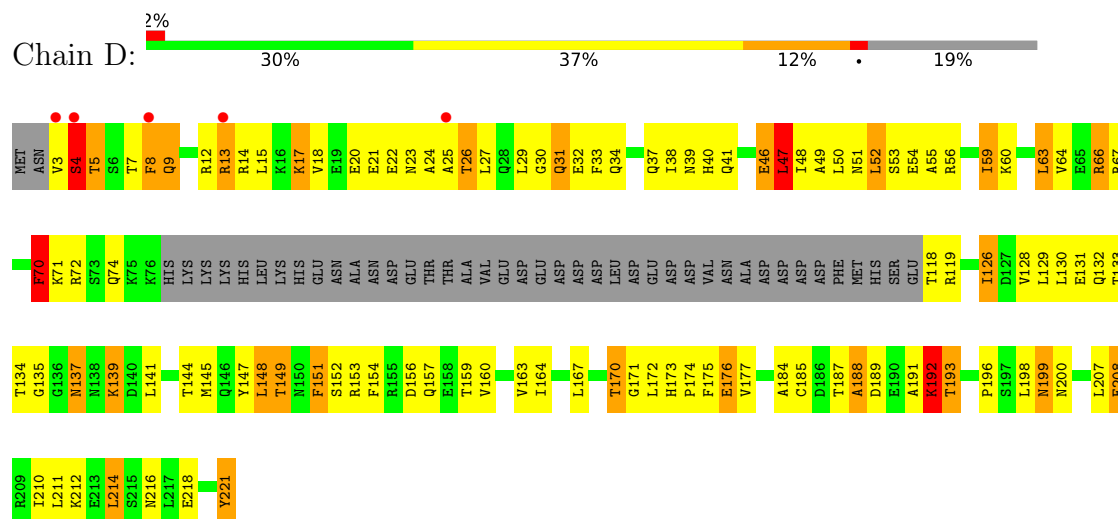


• Molecule 4: DNA-directed RNA polymerase II subunit RPB3

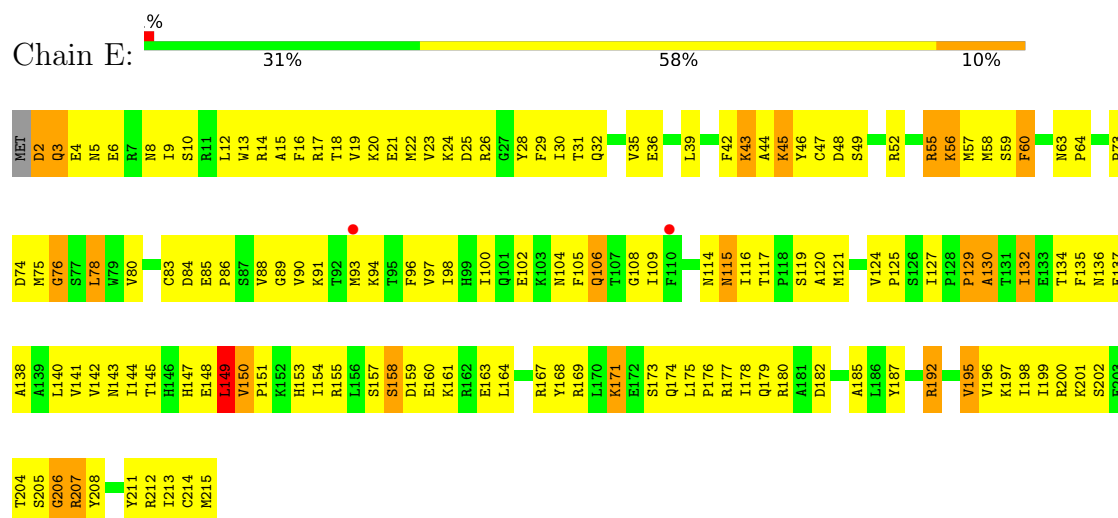
Chain C: 23% 48% 12% 16%



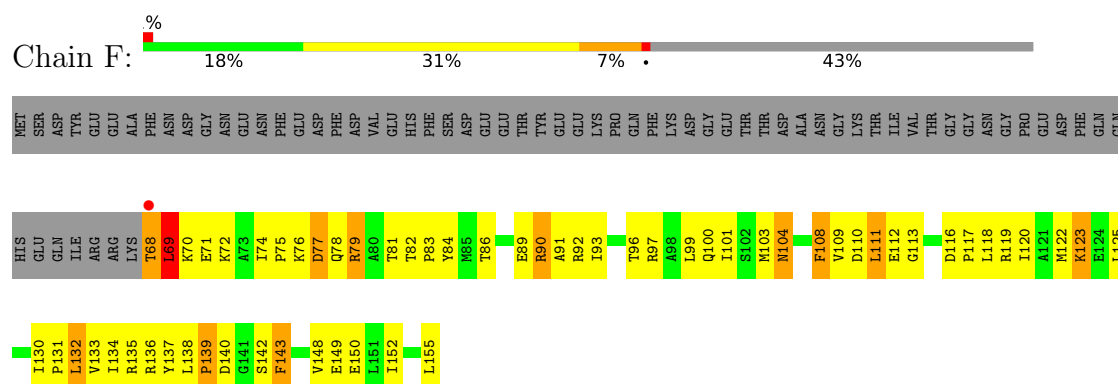
• Molecule 5: DNA-directed RNA polymerase II subunit RPB4



• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC1

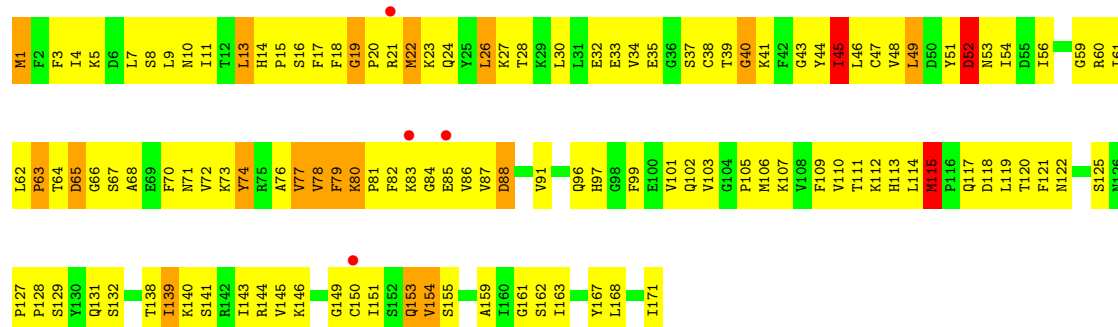


• Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC2

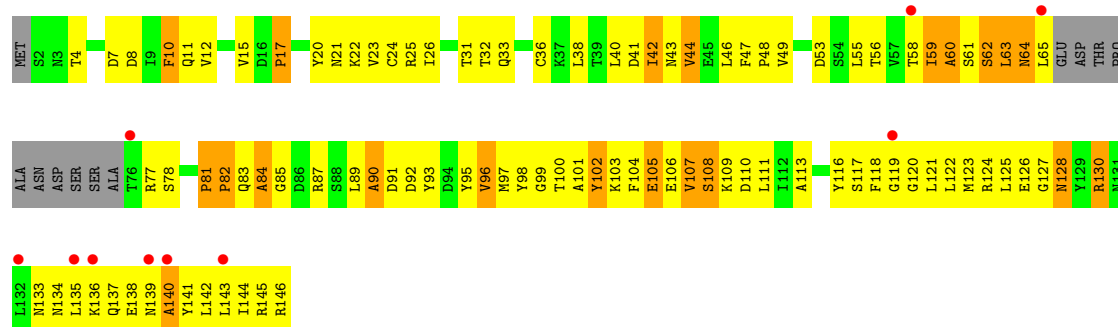


• Molecule 8: DNA-directed RNA polymerase II subunit RPB7

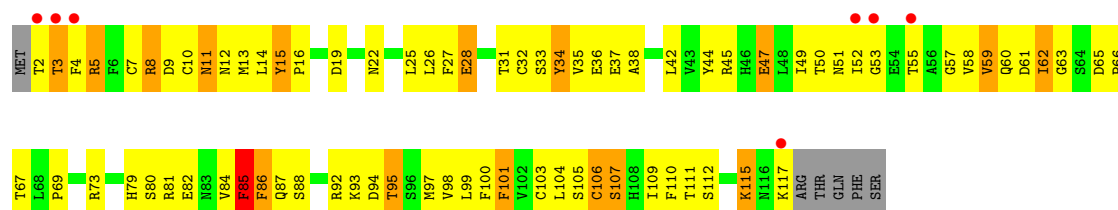




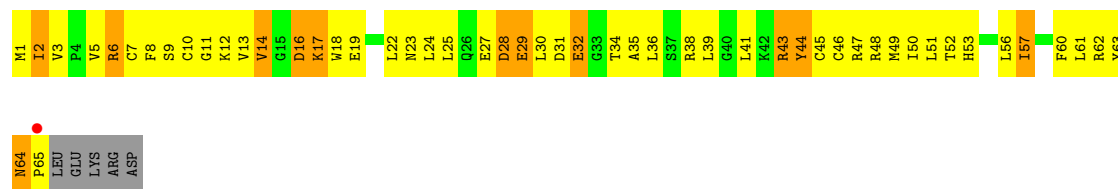
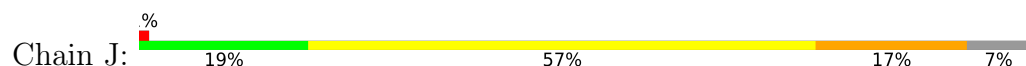
- Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC3



- Molecule 10: DNA-directed RNA polymerase II subunit RPB9

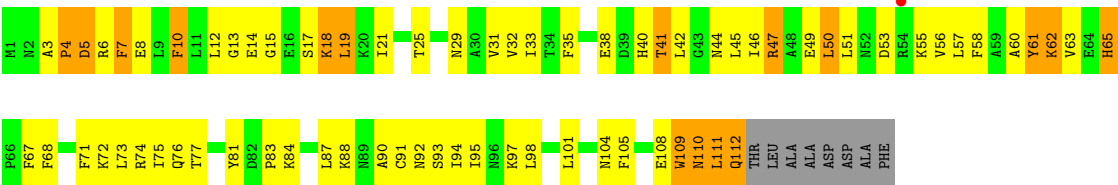


- Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC5

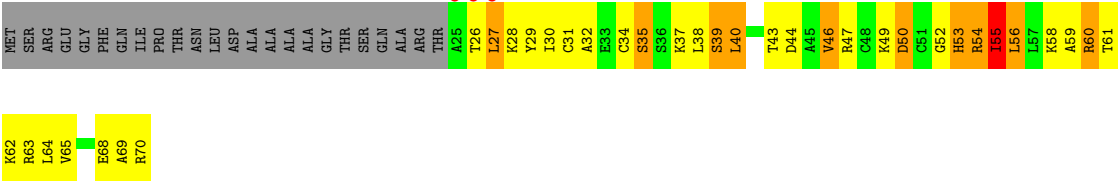


- Molecule 12: DNA-directed RNA polymerase II subunit RPB11





● Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC4



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	223.34Å 394.88Å 284.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 4.00 50.00 – 4.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-4.00) 97.1 (50.00-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.00 (at 4.00Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.216 , 0.241 0.224 , 0.245	Depositor DCC
R_{free} test set	2129 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å ²)	103.2	Xtriage
Anisotropy	0.674	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 61.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.011 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.010 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	31500	wwPDB-VP
Average B, all atoms (Å ²)	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	R	0.59	0/321	1.05	2/496 (0.4%)
2	A	0.52	1/11394 (0.0%)	1.10	91/15407 (0.6%)
3	B	0.50	0/9013	1.02	45/12152 (0.4%)
4	C	0.51	0/2139	1.10	16/2899 (0.6%)
5	D	0.47	0/1444	1.08	10/1935 (0.5%)
6	E	0.47	0/1788	1.04	12/2406 (0.5%)
7	F	0.64	0/723	1.36	5/974 (0.5%)
8	G	0.50	0/1368	1.13	13/1844 (0.7%)
9	H	0.48	0/1102	0.94	2/1492 (0.1%)
10	I	0.44	0/962	0.98	5/1295 (0.4%)
11	J	0.53	0/541	0.94	0/727
12	K	0.48	0/922	1.01	6/1244 (0.5%)
13	L	0.58	0/366	0.96	1/485 (0.2%)
All	All	0.51	1/32083 (0.0%)	1.06	208/43356 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	50	ILE	CA-CB	5.13	1.59	1.54

All (208) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	70	LYS	N-CA-C	-23.01	82.14	114.12
2	A	452	LYS	N-CA-C	-12.61	96.17	111.69
3	B	1185	CYS	N-CA-C	-11.44	99.43	113.50
5	D	26	THR	N-CA-C	-11.23	99.88	112.57
2	A	56	PRO	N-CA-C	-10.89	101.97	114.92
3	B	427	ASP	N-CA-C	-9.79	101.90	114.04
2	A	242	PRO	CA-C-N	9.71	130.39	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	242	PRO	C-N-CA	9.71	130.39	120.38
2	A	1176	LEU	N-CA-C	9.54	131.12	110.80
3	B	882	THR	N-CA-C	9.29	122.25	111.11
2	A	288	ALA	N-CA-C	-9.04	99.55	113.02
2	A	1261	LYS	N-CA-C	-8.88	103.56	114.75
5	D	171	GLY	N-CA-C	-8.84	102.81	115.27
2	A	266	LEU	N-CA-C	-8.44	102.02	111.14
2	A	1175	SER	N-CA-C	-8.31	101.11	111.75
8	G	62	LEU	CA-C-N	-8.21	109.58	119.84
8	G	62	LEU	C-N-CA	-8.21	109.58	119.84
2	A	425	GLN	N-CA-C	-8.06	96.61	109.59
2	A	293	GLU	N-CA-C	-7.97	103.16	113.12
2	A	982	THR	N-CA-C	-7.84	100.41	110.53
4	C	165	LYS	N-CA-C	-7.76	102.42	111.03
5	D	72	ARG	N-CA-C	-7.59	102.67	112.23
3	B	112	LEU	N-CA-C	7.55	121.46	110.28
2	A	311	GLN	N-CA-C	7.53	126.46	109.81
4	C	193	TYR	N-CA-C	7.50	117.87	108.19
2	A	134	ARG	N-CA-C	-7.37	101.74	111.24
3	B	1177	HIS	N-CA-C	-7.23	105.31	112.97
1	R	12	C	N1-C1'-C2'	7.21	122.82	112.00
2	A	344	ARG	N-CA-C	-7.17	98.92	110.32
2	A	710	LEU	N-CA-C	-7.15	103.49	111.71
2	A	1280	GLU	N-CA-C	7.12	114.61	108.78
8	G	40	GLY	N-CA-C	-7.08	105.88	114.66
8	G	52	ASP	N-CA-C	7.08	119.89	111.33
4	C	183	TRP	N-CA-C	-7.06	97.04	108.41
2	A	950	GLY	N-CA-C	-7.05	104.84	115.00
3	B	976	ILE	N-CA-C	7.02	117.16	110.42
2	A	291	GLU	N-CA-C	-6.98	104.79	113.38
13	L	68	GLU	N-CA-C	-6.98	100.15	110.48
4	C	39	ALA	N-CA-C	6.93	122.71	112.94
3	B	395	GLN	N-CA-C	-6.89	100.83	110.35
5	D	157	GLN	N-CA-C	-6.85	104.91	113.20
2	A	683	ILE	N-CA-C	-6.79	104.56	110.74
2	A	68	GLN	N-CA-C	-6.75	102.16	111.28
3	B	296	GLU	N-CA-C	-6.74	104.54	112.89
2	A	590	ARG	N-CA-C	6.70	118.75	108.30
3	B	66	ASP	N-CA-C	-6.70	103.42	112.26
3	B	628	THR	N-CA-C	-6.68	103.59	113.61
8	G	129	SER	N-CA-C	6.68	117.39	108.38
2	A	81	PHE	N-CA-C	6.66	119.67	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1104	ILE	N-CA-C	6.65	116.78	110.53
2	A	1291	VAL	CA-C-N	6.65	128.15	119.84
2	A	1291	VAL	C-N-CA	6.65	128.15	119.84
2	A	567	LYS	CA-C-N	-6.57	111.63	119.84
2	A	567	LYS	C-N-CA	-6.57	111.63	119.84
2	A	60	SER	N-CA-C	6.56	118.11	108.86
2	A	453	MET	N-CA-C	6.56	119.26	111.71
6	E	55	ARG	N-CA-C	6.52	118.47	111.36
2	A	938	LYS	N-CA-C	-6.49	104.25	111.71
7	F	77	ASP	N-CA-C	-6.46	101.22	110.59
3	B	732	SER	N-CA-C	6.43	116.72	108.24
2	A	301	ALA	N-CA-C	-6.39	102.84	112.04
2	A	120	GLU	N-CA-C	6.38	118.03	111.14
3	B	473	MET	N-CA-C	-6.37	102.00	111.81
3	B	1025	HIS	N-CA-C	-6.34	104.00	111.03
4	C	96	SER	N-CA-C	6.28	118.85	108.99
6	E	195	VAL	N-CA-C	6.26	116.88	108.11
2	A	78	PRO	N-CA-C	-6.21	102.52	111.22
2	A	860	LEU	N-CA-C	-6.21	104.76	112.90
2	A	682	THR	N-CA-C	-6.19	105.22	112.89
4	C	131	HIS	CA-C-N	6.17	127.55	119.84
4	C	131	HIS	C-N-CA	6.17	127.55	119.84
2	A	137	ALA	N-CA-C	-6.15	105.80	113.55
2	A	1403	GLU	N-CA-C	6.15	123.89	110.80
8	G	72	VAL	N-CA-C	6.14	116.34	108.12
2	A	1262	LYS	N-CA-C	-6.14	105.62	113.23
3	B	337	ARG	N-CA-C	6.12	118.92	111.82
12	K	75	ILE	N-CA-C	6.08	116.77	107.77
2	A	778	GLY	N-CA-C	-6.08	106.81	114.16
2	A	1263	ILE	N-CA-C	-6.07	105.75	113.22
3	B	297	ILE	N-CA-C	-6.07	104.38	111.00
12	K	65	HIS	CA-C-N	6.06	127.42	119.84
12	K	65	HIS	C-N-CA	6.06	127.42	119.84
2	A	236	LEU	N-CA-C	6.06	118.60	108.96
4	C	173	ALA	N-CA-C	6.06	118.41	111.02
5	D	38	ILE	N-CA-C	6.04	116.63	108.17
6	E	171	LYS	N-CA-C	-6.04	99.85	109.76
2	A	513	SER	N-CA-C	6.03	117.25	109.65
2	A	1138	ILE	CB-CA-C	-6.01	105.70	111.05
3	B	1085	ILE	N-CA-C	6.01	117.25	108.53
4	C	200	GLU	N-CA-C	6.01	119.72	112.38
7	F	108	PHE	N-CA-C	5.96	120.17	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	999	VAL	N-CA-C	-5.96	106.01	111.67
2	A	1039	LYS	N-CA-C	-5.94	104.38	111.69
2	A	636	GLU	N-CA-C	5.94	118.64	111.40
2	A	415	LEU	N-CA-C	5.93	119.34	111.75
2	A	466	SER	N-CA-C	5.93	123.43	110.80
3	B	937	ALA	N-CA-C	-5.92	104.92	113.21
3	B	774	GLY	N-CA-C	-5.92	106.42	113.99
5	D	188	ALA	N-CA-C	-5.92	105.91	113.01
7	F	69	LEU	CA-CB-CG	5.91	136.97	116.30
2	A	3	GLY	N-CA-C	-5.89	107.47	114.48
8	G	19	GLY	CA-C-N	5.89	127.20	119.84
8	G	19	GLY	C-N-CA	5.89	127.20	119.84
3	B	885	MET	CB-CA-C	-5.87	108.62	117.07
2	A	927	VAL	N-CA-C	-5.86	106.00	111.45
4	C	41	ILE	N-CA-C	5.82	113.63	107.76
2	A	294	SER	N-CA-C	-5.81	105.45	112.54
6	E	150	VAL	N-CA-C	5.80	113.62	107.76
3	B	911	ILE	N-CA-C	-5.79	107.86	113.53
8	G	45	ILE	N-CA-C	-5.78	99.99	108.54
2	A	244	PRO	N-CA-C	5.73	117.69	110.70
3	B	971	THR	N-CA-C	-5.71	102.06	110.52
2	A	62	ASP	N-CA-C	5.71	122.96	110.80
2	A	562	THR	CA-C-N	5.70	125.71	119.90
2	A	562	THR	C-N-CA	5.70	125.71	119.90
1	R	12	C	C4'-C3'-O3'	-5.66	104.51	113.00
6	E	173	SER	N-CA-C	5.64	119.43	112.54
10	I	31	THR	N-CA-C	-5.63	104.58	112.12
8	G	65	ASP	N-CA-C	-5.60	100.83	109.52
12	K	62	LYS	N-CA-C	5.59	117.02	108.52
6	E	150	VAL	CA-C-N	5.57	125.77	120.31
6	E	150	VAL	C-N-CA	5.57	125.77	120.31
2	A	413	ILE	CB-CA-C	-5.57	104.00	110.91
3	B	366	GLN	N-CA-C	-5.56	105.85	113.30
6	E	149	LEU	N-CA-C	5.54	118.25	111.82
2	A	888	GLY	N-CA-C	5.54	119.85	112.65
2	A	553	VAL	CA-C-N	5.53	125.89	119.47
2	A	553	VAL	C-N-CA	5.53	125.89	119.47
2	A	1445	ILE	CB-CA-C	-5.53	105.26	111.23
2	A	320	ARG	CA-C-N	5.52	126.74	119.84
2	A	320	ARG	C-N-CA	5.52	126.74	119.84
2	A	472	LEU	N-CA-C	5.52	116.98	110.97
2	A	227	VAL	CB-CA-C	-5.51	105.21	111.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	176	GLU	N-CA-C	-5.50	104.93	111.03
2	A	663	SER	N-CA-C	5.49	115.08	107.73
3	B	650	GLU	N-CA-C	5.44	116.79	108.52
9	H	42	ILE	N-CA-C	5.43	115.52	108.35
3	B	534	GLY	N-CA-C	-5.43	108.15	115.21
2	A	478	TYR	N-CA-C	-5.42	106.62	113.18
2	A	511	ILE	N-CA-C	5.42	116.15	110.62
3	B	1008	PRO	N-CA-C	5.42	119.83	111.21
10	I	28	GLU	N-CA-C	5.40	115.68	108.23
5	D	199	ASN	N-CA-C	5.39	122.29	110.80
2	A	1444	MET	N-CA-C	5.38	118.22	109.06
10	I	85	PHE	N-CA-C	5.38	118.05	110.14
5	D	70	PHE	N-CA-C	-5.38	106.39	113.17
3	B	835	GLN	N-CA-C	5.37	117.02	110.41
5	D	66	ARG	N-CA-C	-5.37	104.98	112.45
8	G	22	MET	N-CA-C	-5.36	104.78	112.13
3	B	949	VAL	N-CA-C	-5.35	101.32	109.78
10	I	5	ARG	N-CA-C	5.35	117.55	109.41
2	A	1311	VAL	N-CA-C	5.35	116.43	107.18
2	A	1399	ARG	N-CA-C	-5.34	105.56	111.71
3	B	1033	LYS	N-CA-C	-5.34	106.02	112.54
2	A	223	GLY	N-CA-C	5.32	125.80	113.18
12	K	18	LYS	N-CA-C	-5.32	104.89	111.33
2	A	998	LEU	N-CA-C	5.32	117.38	109.25
2	A	491	VAL	N-CA-C	5.31	113.72	107.77
4	C	27	LEU	N-CA-C	-5.30	104.75	111.11
4	C	135	GLN	N-CA-C	-5.28	104.50	112.99
4	C	57	VAL	N-CA-C	-5.27	106.74	112.80
2	A	412	ARG	N-CA-C	5.26	117.33	108.96
3	B	213	ILE	N-CA-C	5.26	116.55	108.71
2	A	1422	ARG	N-CA-C	-5.26	107.03	113.50
2	A	1155	ASP	CA-C-N	5.25	125.71	120.04
2	A	1155	ASP	C-N-CA	5.25	125.71	120.04
6	E	6	GLU	N-CA-C	-5.25	105.15	112.45
3	B	1007	VAL	CA-C-N	5.24	125.18	119.78
3	B	1007	VAL	C-N-CA	5.24	125.18	119.78
2	A	564	ALA	N-CA-C	-5.24	106.15	112.54
9	H	109	LYS	CB-CA-C	-5.24	110.55	116.63
2	A	158	PRO	N-CA-C	-5.23	107.92	114.20
2	A	1102	LYS	N-CA-C	-5.22	105.48	111.07
4	C	63	ILE	N-CA-C	-5.22	105.41	110.42
3	B	1201	LYS	N-CA-C	-5.22	105.02	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	833	GLU	N-CA-C	-5.21	105.66	112.23
4	C	225	ALA	N-CA-C	5.21	118.60	107.70
4	C	38	ILE	N-CA-C	5.21	115.42	110.42
8	G	77	VAL	N-CA-C	5.21	116.20	108.23
2	A	861	GLY	N-CA-C	-5.19	107.49	116.01
3	B	464	GLY	N-CA-C	-5.19	100.88	113.18
10	I	115	LYS	N-CA-C	-5.19	105.70	113.89
3	B	640	VAL	N-CA-C	5.16	119.05	113.43
2	A	82	GLY	N-CA-C	-5.15	103.51	112.06
3	B	885	MET	CA-C-O	5.14	120.92	117.94
3	B	805	THR	N-CA-C	5.14	116.62	108.96
2	A	142	CYS	N-CA-C	5.14	119.19	113.02
2	A	1032	LEU	N-CA-C	5.14	119.63	112.90
6	E	149	LEU	CA-C-N	-5.13	118.90	122.59
6	E	149	LEU	C-N-CA	-5.13	118.90	122.59
3	B	1164	GLY	N-CA-C	-5.12	109.04	114.67
12	K	19	LEU	N-CA-C	5.12	117.91	109.72
3	B	807	ARG	N-CA-C	-5.11	105.83	111.71
2	A	227	VAL	N-CA-C	5.11	116.20	111.81
7	F	70	LYS	CA-C-O	5.08	124.49	118.90
3	B	527	THR	CA-C-N	5.08	125.23	119.90
3	B	527	THR	C-N-CA	5.08	125.23	119.90
2	A	445	ASN	N-CA-C	5.07	115.84	108.14
2	A	436	ILE	N-CA-C	-5.06	102.97	109.30
2	A	983	ILE	N-CA-C	-5.06	104.77	111.09
3	B	573	GLN	N-CA-C	-5.05	105.96	111.82
2	A	539	THR	N-CA-C	5.04	116.96	109.25
3	B	340	ALA	N-CA-C	5.02	121.50	110.80
6	E	158	SER	N-CA-C	-5.02	107.21	113.19
3	B	292	ILE	N-CA-C	5.02	119.72	108.88
3	B	996	ARG	N-CA-C	5.02	116.75	111.28
3	B	896	ASP	N-CA-C	-5.01	107.00	113.01
8	G	63	PRO	N-CA-C	5.00	122.78	112.47

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	289	0	153	11	0
2	A	11194	0	11279	1259	0
3	B	8841	0	8875	1079	0
4	C	2101	0	2056	276	0
5	D	1434	0	1460	129	0
6	E	1752	0	1776	165	0
7	F	712	0	737	111	0
8	G	1340	0	1357	169	0
9	H	1084	0	1057	134	0
10	I	944	0	901	110	0
11	J	532	0	543	94	0
12	K	904	0	911	110	0
13	L	364	0	387	50	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	1	0	0	0	0
All	All	31500	0	31492	3359	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 53.

All (3359) 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:F:68:THR:HG21	7:F:69:LEU:N	1.59	1.16
7:F:69:LEU:HD23	7:F:71:GLU:CB	1.77	1.14
7:F:69:LEU:HD23	7:F:71:GLU:HB2	1.17	1.12
2:A:58:LEU:HD12	2:A:59:GLY:N	1.65	1.11
2:A:34:LYS:NZ	2:A:57:ARG:HH12	1.50	1.09
6:E:94:LYS:HE2	6:E:98:ILE:HD11	1.32	1.09
2:A:53:LEU:HD23	2:A:54:ASN:H	1.02	1.08
3:B:806:THR:HG22	3:B:808:ALA:H	1.10	1.08
9:H:100:THR:HG23	9:H:138:GLU:HA	1.30	1.08
3:B:510:LYS:HG2	3:B:511:PRO:HD3	1.36	1.08
7:F:68:THR:HB	7:F:69:LEU:CG	1.83	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:47:ARG:HB3	12:K:47:ARG:HH11	1.19	1.07
2:A:1161:THR:HG22	2:A:1163:ILE:H	1.17	1.07
2:A:41:MET:HB3	2:A:49:LYS:HA	1.32	1.07
2:A:58:LEU:HD12	2:A:59:GLY:H	0.88	1.05
5:D:40:HIS:HB3	8:G:73:LYS:HZ3	1.15	1.05
2:A:709:THR:HG22	2:A:711:ARG:H	1.23	1.04
10:I:34:TYR:HD2	10:I:35:VAL:N	1.54	1.04
3:B:343:ILE:HG23	3:B:347:LYS:HB2	1.34	1.04
2:A:225:ASN:HD22	2:A:228:PHE:H	1.04	1.02
5:D:40:HIS:HB3	8:G:73:LYS:NZ	1.72	1.02
2:A:1127:ASP:HB3	2:A:1130:GLN:HB3	1.33	1.02
7:F:68:THR:CB	7:F:69:LEU:HG	1.89	1.02
4:C:101:LEU:HD13	4:C:118:LEU:HD23	1.39	1.02
2:A:535:THR:HG21	2:A:616:VAL:HA	1.40	1.01
3:B:273:LEU:HB2	3:B:276:ILE:HD12	1.40	1.01
4:C:45:ALA:HA	4:C:72:LEU:HD12	1.43	1.01
2:A:114:LEU:HD13	2:A:171:GLN:HE22	1.26	1.00
4:C:47:ASP:HA	13:L:69:ALA:HB3	1.43	1.00
11:J:3:VAL:HG21	11:J:18:TRP:HB2	1.41	1.00
13:L:32:ALA:HB3	13:L:55:ILE:HD12	1.40	1.00
7:F:68:THR:HB	7:F:69:LEU:HG	1.42	1.00
2:A:567:LYS:HB3	9:H:96:VAL:H	1.22	1.00
3:B:364:ILE:HG12	3:B:585:VAL:HG13	1.42	0.99
3:B:515:HIS:H	3:B:518:HIS:HD2	1.06	0.99
8:G:15:PRO:HA	8:G:18:PHE:CD1	1.96	0.99
3:B:214:ALA:HB3	3:B:498:THR:HA	1.42	0.98
2:A:340:LEU:HD13	2:A:1429:ILE:HG23	1.44	0.98
9:H:4:THR:HA	9:H:60:ALA:HB2	1.41	0.97
7:F:68:THR:HB	7:F:69:LEU:CD1	1.94	0.97
8:G:138:THR:HG22	8:G:139:ILE:H	1.27	0.97
7:F:68:THR:CG2	7:F:69:LEU:N	2.27	0.97
4:C:43:THR:HG22	4:C:44:LEU:H	1.28	0.96
2:A:475:THR:HG23	2:A:476:SER:H	1.30	0.96
3:B:589:VAL:HG12	3:B:590:HIS:H	1.31	0.96
2:A:53:LEU:HD22	2:A:54:ASN:HD22	1.29	0.95
2:A:1174:PHE:HA	2:A:1176:LEU:HG	1.44	0.95
3:B:577:ALA:HB1	3:B:589:VAL:HG11	1.45	0.95
2:A:567:LYS:CD	2:A:568:PRO:HD2	1.97	0.95
2:A:567:LYS:CG	2:A:568:PRO:HD2	1.98	0.94
2:A:1373:ASP:HA	2:A:1376:THR:HG22	1.49	0.94
7:F:69:LEU:HD13	7:F:72:LYS:CG	1.98	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:882:THR:HG22	3:B:884:ARG:H	1.32	0.94
7:F:69:LEU:CD2	7:F:71:GLU:HB2	1.97	0.94
10:I:111:THR:HG22	10:I:112:SER:H	1.31	0.94
11:J:64:ASN:HB3	11:J:65:PRO:CD	1.97	0.94
4:C:57:VAL:HG11	11:J:60:PHE:HB3	1.51	0.93
4:C:32:SER:O	4:C:36:VAL:HG23	1.66	0.93
9:H:135:LEU:HD13	9:H:137:GLN:HE21	1.32	0.93
2:A:2:VAL:HG21	3:B:1157:ALA:HB1	1.47	0.93
2:A:567:LYS:HD2	2:A:568:PRO:HD2	1.49	0.92
2:A:855:THR:HG21	2:A:857:ARG:HE	1.34	0.92
3:B:583:ASN:HD21	3:B:628:THR:HG22	1.34	0.92
9:H:40:LEU:HD13	9:H:123:MET:HE3	1.48	0.92
9:H:130:ARG:HA	9:H:133:ASN:HD22	1.34	0.92
2:A:14:VAL:H	2:A:1432:GLN:HE22	1.13	0.92
2:A:779:PHE:HE1	2:A:785:PRO:HD3	1.32	0.92
8:G:23:LYS:HG3	8:G:56:ILE:HD11	1.50	0.92
8:G:127:PRO:HG2	8:G:138:THR:HG21	1.49	0.91
2:A:34:LYS:HZ1	2:A:57:ARG:HH12	0.96	0.91
5:D:144:THR:O	5:D:148:LEU:HB2	1.70	0.91
2:A:61:ILE:HG22	2:A:62:ASP:H	1.35	0.91
9:H:130:ARG:H	9:H:130:ARG:HD2	1.34	0.91
3:B:169:ARG:HB2	3:B:454:THR:HG23	1.53	0.91
3:B:25:ILE:HD11	3:B:653:VAL:O	1.69	0.91
7:F:68:THR:OG1	7:F:69:LEU:HG	1.71	0.91
2:A:1152:ILE:HG13	10:I:44:TYR:HB3	1.53	0.90
9:H:130:ARG:HB3	9:H:133:ASN:HB2	1.50	0.90
11:J:1:MET:H2	11:J:57:ILE:H	1.14	0.90
2:A:53:LEU:HD23	2:A:54:ASN:N	1.86	0.90
3:B:510:LYS:HG2	3:B:511:PRO:CD	2.01	0.90
3:B:1072:MET:HE3	3:B:1085:ILE:HB	1.54	0.90
2:A:1152:ILE:HD11	10:I:44:TYR:HD2	1.36	0.90
3:B:521:LEU:HD22	3:B:633:VAL:HG12	1.54	0.90
3:B:1097:HIS:H	3:B:1098:MET:HE2	1.34	0.89
8:G:34:VAL:HG12	8:G:45:ILE:HG21	1.54	0.89
11:J:44:TYR:HA	11:J:47:ARG:HB2	1.54	0.89
4:C:39:ALA:HA	4:C:164:ALA:HB3	1.54	0.89
8:G:13:LEU:HD21	8:G:17:PHE:HB2	1.55	0.89
2:A:269:ILE:HD13	2:A:300:VAL:HG22	1.55	0.89
2:A:34:LYS:HZ1	2:A:57:ARG:NH1	1.70	0.88
3:B:549:THR:HG22	3:B:550:ASP:H	1.38	0.88
5:D:17:LYS:HA	5:D:17:LYS:HE3	1.52	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:49:LYS:HZ1	2:A:61:ILE:HG13	1.37	0.88
3:B:622:LYS:HE2	10:I:59:VAL:HG22	1.55	0.88
3:B:1159:ARG:HD3	3:B:1193:GLN:HG3	1.54	0.88
2:A:1444:MET:HG2	8:G:60:ARG:HA	1.55	0.88
3:B:911:ILE:HD11	3:B:941:LEU:HD13	1.56	0.88
3:B:999:MET:HG3	3:B:1000:PRO:HD2	1.53	0.88
2:A:356:ASP:HB2	2:A:469:ARG:NH1	1.88	0.88
6:E:180:ARG:HH21	6:E:192:ARG:HB2	1.37	0.87
7:F:69:LEU:HB3	7:F:72:LYS:H	1.35	0.87
3:B:280:ILE:HB	3:B:285:ILE:HD11	1.55	0.87
3:B:65:GLU:HG3	3:B:66:ASP:H	1.39	0.87
2:A:1017:LEU:HB2	6:E:206:GLY:H	1.36	0.87
7:F:69:LEU:HB3	7:F:72:LYS:N	1.88	0.87
2:A:534:LEU:O	2:A:574:GLY:HA3	1.75	0.87
5:D:40:HIS:CB	8:G:73:LYS:HZ3	1.87	0.87
2:A:605:MET:HE2	2:A:607:ILE:HG12	1.55	0.86
2:A:563:PRO:HG3	2:A:572:TRP:CZ2	2.10	0.86
3:B:801:LYS:O	11:J:52:THR:HG23	1.73	0.86
2:A:34:LYS:HZ2	2:A:57:ARG:HH22	1.22	0.86
8:G:7:LEU:HB2	8:G:74:TYR:CE2	2.09	0.86
12:K:65:HIS:HD2	12:K:67:PHE:H	1.20	0.86
3:B:944:THR:HG21	3:B:1122:ARG:NH2	1.89	0.86
3:B:1002:THR:HG21	3:B:1006:ILE:HD12	1.58	0.86
8:G:18:PHE:HA	8:G:22:MET:HE3	1.58	0.85
10:I:115:LYS:HD3	10:I:117:LYS:HE3	1.55	0.85
2:A:763:ALA:O	2:A:803:SER:HB3	1.75	0.85
2:A:1017:LEU:HB2	6:E:206:GLY:N	1.90	0.85
2:A:1226:VAL:HG22	2:A:1240:CYS:HB3	1.58	0.85
2:A:34:LYS:HG2	2:A:36:ARG:HH21	1.40	0.85
4:C:174:ALA:HB2	4:C:235:VAL:HG22	1.57	0.85
11:J:5:VAL:HG12	11:J:6:ARG:HG3	1.57	0.85
2:A:399:HIS:HB3	2:A:400:PRO:HD3	1.56	0.85
3:B:515:HIS:H	3:B:518:HIS:CD2	1.92	0.85
2:A:58:LEU:CD1	2:A:59:GLY:H	1.84	0.85
2:A:225:ASN:ND2	2:A:228:PHE:H	1.74	0.85
6:E:198:ILE:HD11	6:E:212:ARG:HG3	1.58	0.85
8:G:1:MET:SD	8:G:79:PHE:HD1	1.99	0.85
3:B:766:ARG:HH22	3:B:1020:ARG:HH11	1.24	0.85
6:E:16:PHE:CZ	6:E:20:LYS:HE2	2.11	0.85
9:H:100:THR:OG1	9:H:138:GLU:HG3	1.77	0.85
4:C:45:ALA:HA	4:C:72:LEU:CD1	2.06	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:111:THR:HG22	8:G:113:HIS:H	1.42	0.84
2:A:901:LEU:H	2:A:926:GLN:NE2	1.75	0.84
2:A:903:ASN:HD22	2:A:904:THR:N	1.74	0.84
2:A:567:LYS:HB3	9:H:96:VAL:N	1.90	0.84
6:E:14:ARG:HH21	6:E:141:VAL:HG12	1.42	0.84
2:A:1336:MET:HE3	2:A:1381:LEU:HG	1.60	0.84
2:A:1116:LEU:HB2	2:A:1329:THR:OG1	1.78	0.83
4:C:36:VAL:HG21	4:C:251:LEU:HD22	1.57	0.83
8:G:49:LEU:HD21	8:G:77:VAL:HG23	1.59	0.83
3:B:806:THR:HG22	3:B:808:ALA:N	1.93	0.83
2:A:605:MET:HE3	2:A:606:LEU:H	1.43	0.83
2:A:1312:ASN:O	2:A:1316:VAL:HG23	1.78	0.83
2:A:598:LEU:HA	9:H:122:LEU:HD13	1.60	0.83
7:F:86:THR:OG1	7:F:89:GLU:HG3	1.78	0.83
3:B:340:ALA:HB2	3:B:343:ILE:HD12	1.60	0.83
3:B:1072:MET:CE	3:B:1085:ILE:HB	2.09	0.83
2:A:249:SER:O	2:A:250:ILE:HG13	1.79	0.83
3:B:343:ILE:CG2	3:B:347:LYS:HB2	2.07	0.83
2:A:567:LYS:NZ	9:H:46:LEU:HB2	1.94	0.83
9:H:93:TYR:HB3	9:H:144:ILE:O	1.79	0.82
1:R:12:C:H2'	1:R:13:G:C8	2.13	0.82
2:A:1189:SER:O	2:A:1241:ARG:HD3	1.79	0.82
2:A:1173:HIS:O	2:A:1176:LEU:HD23	1.77	0.82
3:B:594:ALA:HA	3:B:617:ARG:HH12	1.43	0.82
3:B:899:ILE:HD11	3:B:911:ILE:HA	1.59	0.82
2:A:779:PHE:CE1	2:A:785:PRO:HD3	2.14	0.82
2:A:899:VAL:HB	2:A:929:LEU:HD11	1.62	0.82
2:A:1332:PHE:H	2:A:1332:PHE:HD2	1.27	0.82
1:R:7:U:OP1	3:B:942:ARG:NH2	2.13	0.82
3:B:798:TYR:HE2	4:C:62:PHE:CE2	1.98	0.82
3:B:971:THR:OG1	4:C:61:GLU:HG3	1.80	0.82
9:H:100:THR:HG1	9:H:138:GLU:HG3	1.45	0.82
2:A:1227:ILE:HG22	2:A:1228:TRP:H	1.43	0.81
8:G:143:ILE:HG22	8:G:144:ARG:N	1.95	0.81
2:A:93:VAL:HG22	2:A:301:ALA:HA	1.62	0.81
2:A:353:ILE:HG21	2:A:487:MET:HE3	1.61	0.81
2:A:446:ARG:CD	2:A:480:ALA:HB2	2.11	0.81
2:A:1208:THR:HG22	2:A:1210:GLY:H	1.45	0.81
3:B:770:GLN:OE1	3:B:983:ARG:HA	1.80	0.81
7:F:116:ASP:HB3	7:F:119:ARG:HB2	1.63	0.81
4:C:7:GLN:HG2	12:K:104:ASN:HD22	1.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:541:ILE:HD13	2:A:549:MET:HE1	1.62	0.81
9:H:62:SER:HB2	9:H:64:ASN:HD22	1.45	0.81
2:A:768:GLN:HG2	2:A:816:HIS:HA	1.61	0.81
3:B:658:ILE:HG22	3:B:662:MET:HE2	1.61	0.81
2:A:84:ILE:HG22	2:A:239:LEU:HB3	1.63	0.80
10:I:34:TYR:CD2	10:I:35:VAL:N	2.45	0.80
7:F:69:LEU:HD13	7:F:72:LYS:HG3	1.61	0.80
2:A:215:SER:HB3	2:A:218:ASP:OD2	1.81	0.80
2:A:903:ASN:HD22	2:A:904:THR:H	1.27	0.80
2:A:537:ARG:HH12	9:H:122:LEU:HG	1.47	0.80
3:B:516:ASN:HD22	3:B:516:ASN:N	1.77	0.80
3:B:770:GLN:CD	3:B:983:ARG:HA	2.06	0.80
3:B:35:SER:HA	3:B:811:TYR:HE2	1.46	0.80
4:C:6:PRO:HB3	4:C:25:VAL:HG12	1.63	0.80
2:A:93:VAL:HG13	2:A:301:ALA:HB1	1.63	0.80
2:A:524:VAL:HG12	2:A:525:GLN:H	1.47	0.80
11:J:64:ASN:HB3	11:J:65:PRO:HD3	1.61	0.80
2:A:58:LEU:HD13	2:A:80:HIS:O	1.82	0.80
4:C:239:PRO:HB2	4:C:241:ASP:OD1	1.82	0.80
7:F:68:THR:CB	7:F:69:LEU:CG	2.52	0.80
2:A:34:LYS:CE	2:A:57:ARG:HH12	1.94	0.79
2:A:853:ASP:O	2:A:854:ASN:HB2	1.82	0.79
2:A:913:LEU:HD12	2:A:914:GLU:H	1.47	0.79
4:C:46:ILE:HG23	4:C:157:CYS:HB3	1.65	0.79
6:E:19:VAL:O	6:E:23:VAL:HG23	1.81	0.79
7:F:82:THR:HG22	7:F:84:TYR:H	1.45	0.79
3:B:830:TYR:CE2	3:B:1000:PRO:HD3	2.17	0.79
4:C:47:ASP:HA	13:L:69:ALA:CB	2.12	0.79
7:F:68:THR:HB	7:F:69:LEU:HD12	1.64	0.79
2:A:53:LEU:CD2	2:A:54:ASN:HD22	1.95	0.79
2:A:1445:ILE:H	2:A:1445:ILE:HD12	1.47	0.79
7:F:109:VAL:HG12	7:F:110:ASP:H	1.46	0.79
3:B:60:GLN:O	3:B:63:ILE:HG22	1.82	0.79
3:B:411:PRO:O	3:B:414:ALA:HB3	1.83	0.79
3:B:613:VAL:HG13	3:B:627:PHE:O	1.83	0.79
2:A:868:TYR:HD2	2:A:1058:VAL:HG21	1.48	0.79
2:A:1438:THR:HB	3:B:1144:ALA:HB3	1.65	0.79
7:F:109:VAL:HG12	7:F:110:ASP:N	1.97	0.79
7:F:130:ILE:O	7:F:148:VAL:HG21	1.83	0.79
8:G:143:ILE:HG22	8:G:144:ARG:H	1.47	0.79
11:J:14:VAL:HG12	11:J:50:ILE:HD11	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1114:PRO:HB2	2:A:1311:VAL:HG23	1.65	0.78
3:B:882:THR:CG2	3:B:884:ARG:HB2	2.13	0.78
3:B:245:GLU:O	3:B:246:LYS:HG3	1.81	0.78
8:G:138:THR:HG22	8:G:139:ILE:N	1.98	0.78
2:A:164:ARG:HG3	2:A:165:GLY:H	1.49	0.78
2:A:963:ILE:HD11	2:A:1048:ASN:HB3	1.65	0.78
4:C:166:GLU:HG3	12:K:10:PHE:HZ	1.48	0.78
9:H:12:VAL:HG13	9:H:26:ILE:HG23	1.64	0.78
3:B:953:LEU:HD21	3:B:965:LYS:HB2	1.63	0.78
3:B:710:LEU:HA	3:B:733:HIS:HB3	1.66	0.78
4:C:66:ARG:NH1	11:J:2:ILE:HG21	1.97	0.78
3:B:1095:LEU:H	3:B:1095:LEU:HD12	1.46	0.78
3:B:1197:PRO:HG2	3:B:1200:ALA:HB2	1.66	0.78
1:R:5:U:H2'	1:R:6:C:O4'	1.84	0.78
2:A:450:LEU:HB3	2:A:838:GLN:HE21	1.47	0.78
2:A:1161:THR:HG22	2:A:1163:ILE:N	1.97	0.78
2:A:1445:ILE:HD11	8:G:68:ALA:HB1	1.63	0.78
10:I:85:PHE:H	10:I:85:PHE:HD2	1.30	0.78
3:B:217:ARG:HE	3:B:405:ARG:HB2	1.50	0.77
3:B:579:ARG:HB2	3:B:586:TRP:NE1	1.99	0.77
5:D:47:LEU:HD11	8:G:3:PHE:CD2	2.19	0.77
3:B:167:ILE:HG22	3:B:453:ILE:HD12	1.66	0.77
3:B:828:ALA:HB2	3:B:1085:ILE:HG23	1.65	0.77
2:A:1373:ASP:HA	2:A:1376:THR:CG2	2.15	0.77
9:H:89:LEU:HB3	9:H:91:ASP:OD1	1.84	0.77
10:I:8:ARG:HG3	10:I:34:TYR:HE1	1.49	0.77
2:A:67:CYS:O	2:A:70:CYS:HB3	1.84	0.77
2:A:1329:THR:CG2	2:A:1331:SER:H	1.97	0.77
4:C:43:THR:HG22	4:C:44:LEU:N	1.99	0.77
2:A:1030:ARG:HG3	2:A:1034:GLU:OE2	1.85	0.77
3:B:825:VAL:CG1	3:B:826:ALA:N	2.47	0.77
13:L:32:ALA:HB3	13:L:55:ILE:CD1	2.15	0.77
2:A:783:THR:HG21	2:A:815:PHE:CZ	2.20	0.77
2:A:1424:VAL:HG13	2:A:1436:ILE:HD11	1.66	0.77
3:B:594:ALA:HA	3:B:617:ARG:NH1	1.98	0.77
3:B:1085:ILE:N	3:B:1085:ILE:HD12	2.00	0.77
2:A:70:CYS:O	2:A:72:GLU:HG2	1.85	0.76
3:B:593:PRO:HG2	3:B:617:ARG:NH2	1.99	0.76
3:B:758:PHE:HB3	3:B:761:HIS:HD2	1.50	0.76
9:H:4:THR:HA	9:H:60:ALA:CB	2.13	0.76
9:H:42:ILE:HG23	9:H:95:TYR:HE1	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:12:LYS:O	11:J:14:VAL:HG23	1.84	0.76
2:A:860:LEU:HD11	2:A:1393:ASN:HB2	1.67	0.76
3:B:637:LEU:HD12	3:B:693:ILE:HD12	1.67	0.76
4:C:46:ILE:HD12	4:C:67:LEU:HB3	1.66	0.76
3:B:96:TYR:HB2	3:B:129:PHE:HB2	1.66	0.76
12:K:49:GLU:HG3	12:K:94:ILE:HG12	1.66	0.76
2:A:40:THR:HG22	2:A:41:MET:HG3	1.66	0.76
7:F:90:ARG:HD3	7:F:155:LEU:HD12	1.66	0.76
9:H:100:THR:CG2	9:H:138:GLU:HA	2.14	0.76
4:C:254:LYS:O	4:C:258:ILE:HD13	1.85	0.76
2:A:351:THR:HB	3:B:1103:ILE:HD12	1.68	0.76
3:B:37:PHE:CE1	3:B:41:LYS:HG3	2.21	0.76
9:H:59:ILE:HG22	9:H:60:ALA:N	2.00	0.76
2:A:49:LYS:NZ	2:A:61:ILE:HG13	2.01	0.76
2:A:405:VAL:HG22	2:A:432:VAL:HG22	1.67	0.76
2:A:1420:ASP:HB3	2:A:1422:ARG:HG3	1.68	0.76
2:A:1121:GLU:HG2	2:A:1122:PRO:HD2	1.67	0.75
2:A:1152:ILE:HD11	10:I:44:TYR:CD2	2.18	0.75
3:B:378:LEU:O	3:B:382:ILE:HG13	1.86	0.75
2:A:629:LEU:O	2:A:633:VAL:HG23	1.86	0.75
4:C:186:LEU:HD21	4:C:224:GLN:O	1.87	0.75
2:A:58:LEU:HD11	2:A:244:PRO:HD2	1.66	0.75
2:A:774:ARG:NH2	2:A:797:LYS:HG3	2.00	0.75
3:B:273:LEU:CB	3:B:276:ILE:HD12	2.16	0.75
3:B:340:ALA:CB	3:B:343:ILE:HD12	2.16	0.75
2:A:34:LYS:NZ	2:A:57:ARG:NH1	2.28	0.75
2:A:351:THR:HG22	3:B:1103:ILE:HA	1.66	0.75
3:B:193:LYS:HZ2	13:L:32:ALA:HB1	1.51	0.75
6:E:22:MET:HE3	6:E:26:ARG:HE	1.52	0.75
3:B:980:PHE:HE1	3:B:990:ILE:HD11	1.51	0.75
3:B:1087:PHE:HD2	3:B:1088:GLY:N	1.84	0.75
2:A:608:ILE:HB	2:A:613:ILE:HD11	1.69	0.74
10:I:111:THR:HG22	10:I:112:SER:N	2.01	0.74
2:A:816:HIS:CD2	3:B:764:SER:HB2	2.21	0.74
3:B:1159:ARG:HB3	3:B:1159:ARG:HH11	1.52	0.74
3:B:1115:THR:O	3:B:1116:ARG:HB2	1.88	0.74
4:C:38:ILE:HA	4:C:173:ALA:HB2	1.69	0.74
2:A:657:LEU:O	2:A:657:LEU:HD12	1.85	0.74
3:B:616:ILE:HG13	3:B:697:GLU:HG3	1.68	0.74
2:A:283:GLY:O	2:A:285:PRO:HD3	1.87	0.74
2:A:500:GLU:OE2	2:A:1438:THR:HG21	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:172:PRO:O	4:C:235:VAL:HG23	1.88	0.74
12:K:45:LEU:HG	12:K:94:ILE:HD13	1.69	0.74
2:A:416:ARG:C	2:A:417:TYR:HD2	1.95	0.74
2:A:901:LEU:HB2	2:A:926:GLN:HG2	1.69	0.74
3:B:847:ASP:HB3	4:C:167:HIS:CD2	2.22	0.74
2:A:341:MET:HE3	2:A:843:LYS:NZ	2.01	0.74
4:C:73:GLN:HB3	4:C:131:HIS:H	1.52	0.74
9:H:102:TYR:OH	9:H:122:LEU:HD22	1.88	0.74
2:A:382:PRO:HB3	2:A:428:TYR:HE2	1.52	0.74
2:A:849:MET:CE	2:A:1061:GLY:HA2	2.18	0.74
3:B:193:LYS:NZ	13:L:32:ALA:HB1	2.02	0.74
2:A:475:THR:HG23	2:A:476:SER:N	2.03	0.74
3:B:847:ASP:HB3	4:C:167:HIS:NE2	2.02	0.74
2:A:24:PRO:HD2	2:A:233:TRP:HE1	1.50	0.73
2:A:590:ARG:HD3	2:A:604:GLY:HA2	1.70	0.73
2:A:981:LEU:CD2	2:A:1039:LYS:HA	2.18	0.73
2:A:1004:ASN:ND2	6:E:167:ARG:HD2	2.03	0.73
2:A:1152:ILE:HG22	2:A:1192:LEU:O	1.88	0.73
3:B:199:MET:HE2	3:B:492:LEU:HD23	1.70	0.73
3:B:583:ASN:ND2	3:B:628:THR:HG22	2.03	0.73
3:B:1065:GLN:HE21	3:B:1067:ARG:H	1.36	0.73
3:B:309:GLN:OE1	10:I:52:ILE:HD11	1.88	0.73
3:B:782:LEU:HD12	3:B:788:ARG:HH11	1.53	0.73
5:D:40:HIS:CB	8:G:73:LYS:NZ	2.47	0.73
11:J:23:ASN:C	11:J:25:LEU:H	1.95	0.73
12:K:47:ARG:HB3	12:K:47:ARG:NH1	1.99	0.73
2:A:55:ASP:N	2:A:56:PRO:HD3	2.04	0.73
2:A:751:SER:O	2:A:752:LYS:HG2	1.88	0.73
2:A:845:LEU:HD22	2:A:1374:VAL:HG21	1.71	0.73
2:A:1447:GLU:OE2	8:G:23:LYS:HB2	1.89	0.73
4:C:213:PRO:O	4:C:214:ASN:HB2	1.88	0.73
2:A:182:VAL:HG22	2:A:201:VAL:HA	1.69	0.73
3:B:217:ARG:NE	3:B:405:ARG:HB2	2.03	0.73
2:A:58:LEU:HD11	2:A:243:PRO:CB	2.19	0.73
2:A:738:LYS:HD2	2:A:740:LEU:HD21	1.69	0.73
2:A:1004:ASN:O	2:A:1008:GLN:HB2	1.89	0.73
3:B:37:PHE:HE1	3:B:41:LYS:HG3	1.52	0.73
12:K:65:HIS:CD2	12:K:67:PHE:H	2.07	0.73
13:L:39:SER:O	13:L:40:LEU:HG	1.88	0.73
3:B:313:MET:HE3	3:B:386:LEU:HD22	1.71	0.73
3:B:957:ASN:ND2	3:B:961:LEU:HD12	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:152:GLU:HG2	4:C:153:LEU:H	1.53	0.73
11:J:3:VAL:HG21	11:J:18:TRP:CB	2.19	0.73
3:B:1166:CYS:HB2	3:B:1215:ARG:NH1	2.04	0.72
7:F:111:LEU:HD12	7:F:111:LEU:H	1.53	0.72
3:B:906:SER:HA	3:B:946:ASN:HB2	1.71	0.72
4:C:262:LEU:HD11	12:K:87:LEU:HD23	1.71	0.72
2:A:22:PHE:CD1	3:B:1213:THR:HG22	2.24	0.72
3:B:1159:ARG:HB3	3:B:1159:ARG:NH1	2.03	0.72
2:A:230:ARG:H	2:A:233:TRP:HE3	1.35	0.72
2:A:477:PRO:HG2	2:A:521:MET:HG2	1.71	0.72
3:B:979:LYS:HG2	3:B:1095:LEU:HD13	1.69	0.72
4:C:43:THR:O	4:C:77:ILE:HG13	1.89	0.72
2:A:528:LEU:HD23	2:A:751:SER:HB3	1.70	0.72
3:B:365:THR:HG23	3:B:367:LEU:H	1.54	0.72
3:B:1220:ARG:NH1	3:B:1220:ARG:HB3	2.05	0.72
2:A:1198:ASP:HB3	2:A:1201:ALA:HB3	1.70	0.72
2:A:1279:ILE:HD11	2:A:1316:VAL:HG21	1.71	0.72
4:C:3:GLU:O	4:C:4:GLU:HB2	1.88	0.72
2:A:709:THR:HB	2:A:712:GLU:HG3	1.72	0.72
3:B:467:GLY:H	3:B:475:SER:HB3	1.55	0.72
3:B:708:GLU:O	3:B:710:LEU:N	2.22	0.72
3:B:825:VAL:HG12	3:B:826:ALA:N	2.03	0.72
4:C:251:LEU:O	4:C:251:LEU:HD12	1.89	0.72
10:I:25:LEU:HB3	10:I:38:ALA:HB2	1.69	0.72
2:A:12:ARG:O	3:B:1194:ILE:HG22	1.88	0.72
6:E:213:ILE:HG12	6:E:214:CYS:H	1.53	0.72
12:K:21:ILE:HG23	12:K:31:VAL:HG11	1.71	0.72
3:B:1006:ILE:HD13	11:J:44:TYR:CE2	2.25	0.72
3:B:1098:MET:HE3	3:B:1098:MET:H	1.55	0.72
8:G:96:GLN:HG3	8:G:97:HIS:HD2	1.53	0.72
2:A:24:PRO:HD2	2:A:233:TRP:NE1	2.05	0.72
3:B:100:PRO:HD2	3:B:180:TYR:HE1	1.53	0.72
3:B:363:HIS:O	3:B:364:ILE:HB	1.89	0.72
3:B:521:LEU:HB3	3:B:633:VAL:HG11	1.72	0.72
3:B:778:MET:HE1	3:B:1094:ARG:HD3	1.71	0.72
3:B:859:TYR:OH	3:B:941:LEU:HD12	1.90	0.72
2:A:1254:ALA:O	2:A:1255:GLU:HB2	1.90	0.71
3:B:39:ARG:NH2	3:B:665:GLU:HG2	2.06	0.71
2:A:798:GLY:HA2	2:A:815:PHE:CD1	2.25	0.71
3:B:862:GLN:HG2	3:B:963:PHE:HD1	1.54	0.71
9:H:127:GLY:O	9:H:128:ASN:HB2	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:134:THR:HG22	5:D:135:GLY:N	2.05	0.71
11:J:1:MET:HE2	11:J:56:LEU:HD12	1.71	0.71
2:A:567:LYS:HD3	9:H:95:TYR:CD2	2.26	0.71
3:B:756:ILE:O	3:B:759:PRO:HD3	1.90	0.71
3:B:1065:GLN:HE21	3:B:1067:ARG:N	1.87	0.71
3:B:1161:HIS:HB3	3:B:1171:VAL:HG11	1.72	0.71
3:B:1201:LYS:HE2	3:B:1205:GLN:OE1	1.90	0.71
6:E:15:ALA:O	6:E:19:VAL:HG23	1.91	0.71
12:K:111:LEU:HD12	12:K:112:GLN:NE2	2.05	0.71
2:A:849:MET:HE1	2:A:1061:GLY:HA2	1.73	0.71
3:B:746:SER:HB2	3:B:1046:PRO:HG2	1.73	0.71
7:F:89:GLU:O	7:F:93:ILE:HG13	1.91	0.71
3:B:53:GLN:HG2	3:B:547:VAL:HG22	1.71	0.71
3:B:312:GLU:O	3:B:315:LYS:HB2	1.91	0.71
3:B:955:THR:CG2	3:B:956:THR:N	2.53	0.71
6:E:207:ARG:HB2	6:E:207:ARG:HH11	1.55	0.71
2:A:23:SER:HA	2:A:233:TRP:NE1	2.06	0.71
2:A:53:LEU:CD2	2:A:54:ASN:H	1.93	0.71
3:B:589:VAL:HG12	3:B:590:HIS:N	2.04	0.71
3:B:681:TRP:HA	3:B:684:LEU:HD13	1.72	0.71
3:B:825:VAL:CG1	3:B:826:ALA:H	2.03	0.71
3:B:1069:PHE:H	3:B:1069:PHE:HD1	1.38	0.71
2:A:836:TYR:CE2	2:A:840:ARG:HD2	2.26	0.71
2:A:1329:THR:HG22	2:A:1331:SER:H	1.56	0.71
11:J:57:ILE:HA	11:J:60:PHE:HD2	1.54	0.71
2:A:49:LYS:HZ1	2:A:61:ILE:CG1	2.03	0.71
4:C:209:TYR:HD1	4:C:209:TYR:H	1.37	0.71
6:E:114:ASN:O	6:E:115:ASN:HB3	1.90	0.71
2:A:50:ILE:C	2:A:52:GLY:H	1.98	0.71
2:A:902:LEU:HG	2:A:926:GLN:HG3	1.71	0.71
2:A:1329:THR:HG22	2:A:1331:SER:N	2.06	0.71
2:A:1343:ALA:HB2	6:E:150:VAL:HG22	1.73	0.71
3:B:1182:CYS:O	3:B:1182:CYS:SG	2.48	0.71
7:F:79:ARG:NH2	7:F:150:GLU:OE1	2.22	0.71
2:A:339:ASN:HB3	3:B:1117:GLN:HE22	1.56	0.70
8:G:23:LYS:HG3	8:G:56:ILE:CD1	2.21	0.70
10:I:52:ILE:HG13	10:I:52:ILE:O	1.90	0.70
11:J:64:ASN:HD22	11:J:65:PRO:HD3	1.55	0.70
2:A:1324:PRO:HB2	6:E:142:VAL:HG11	1.72	0.70
3:B:233:PRO:HG2	3:B:234:ILE:HD12	1.73	0.70
2:A:858:ASN:C	2:A:858:ASN:HD22	1.97	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:216:GLU:OE1	3:B:537:LYS:HE2	1.91	0.70
3:B:287:ARG:HG2	3:B:292:ILE:HA	1.71	0.70
3:B:983:ARG:HH11	3:B:1091:TYR:HB3	1.55	0.70
4:C:66:ARG:NH2	11:J:3:VAL:O	2.24	0.70
6:E:135:PHE:HB3	6:E:140:LEU:HD11	1.73	0.70
2:A:69:THR:C	2:A:71:GLN:H	1.99	0.70
3:B:35:SER:O	3:B:39:ARG:HG3	1.91	0.70
2:A:1323:ASP:OD1	2:A:1325:THR:HB	1.91	0.70
3:B:905:VAL:HG23	3:B:941:LEU:HD22	1.74	0.70
4:C:40:GLU:HA	4:C:163:ILE:CG2	2.21	0.70
3:B:601:ARG:O	3:B:605:ARG:HG3	1.90	0.70
2:A:855:THR:CG2	2:A:857:ARG:HE	2.05	0.70
2:A:1115:SER:HB3	2:A:1330:ASN:HD21	1.57	0.70
3:B:351:TYR:O	3:B:355:ILE:HG13	1.91	0.70
7:F:119:ARG:HH11	7:F:119:ARG:HG3	1.56	0.70
8:G:15:PRO:HA	8:G:18:PHE:CE1	2.25	0.70
2:A:842:VAL:HG11	3:B:1136:ASP:OD2	1.92	0.70
6:E:23:VAL:O	6:E:28:TYR:HB2	1.92	0.70
6:E:85:GLU:HB2	6:E:88:VAL:HG22	1.74	0.70
5:D:56:ARG:HB2	5:D:148:LEU:HD22	1.72	0.70
4:C:203:GLN:HG2	4:C:207:CYS:SG	2.31	0.69
9:H:36:CYS:HA	9:H:126:GLU:O	1.92	0.69
2:A:34:LYS:HG2	2:A:36:ARG:NH2	2.05	0.69
2:A:63:ARG:HA	2:A:74:MET:CE	2.22	0.69
2:A:252:PHE:O	2:A:253:ASN:HB2	1.90	0.69
3:B:684:LEU:H	3:B:684:LEU:HD12	1.58	0.69
3:B:745:PRO:O	3:B:748:ILE:HG12	1.91	0.69
3:B:976:ILE:O	3:B:990:ILE:HB	1.92	0.69
2:A:92:HIS:O	2:A:94:GLY:N	2.26	0.69
2:A:567:LYS:CB	2:A:568:PRO:HD2	2.21	0.69
2:A:1420:ASP:O	2:A:1421:CYS:HB2	1.93	0.69
3:B:467:GLY:H	3:B:475:SER:CB	2.06	0.69
3:B:1147:LEU:O	3:B:1151:LEU:HD13	1.92	0.69
2:A:4:GLN:O	2:A:5:GLN:HB2	1.92	0.69
2:A:1211:GLN:O	2:A:1214:GLU:HB2	1.93	0.69
2:A:1348:LEU:HG	2:A:1372:VAL:HG23	1.74	0.69
2:A:679:ILE:HG12	2:A:732:LEU:HD12	1.75	0.69
2:A:1227:ILE:HG22	2:A:1228:TRP:N	2.07	0.69
2:A:1341:ILE:HD12	2:A:1379:GLY:O	1.92	0.69
3:B:39:ARG:HH21	3:B:665:GLU:CD	2.01	0.69
3:B:498:THR:CG2	3:B:537:LYS:HG3	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:153:HIS:HB3	6:E:196:VAL:CG1	2.22	0.69
2:A:42:ASP:HB3	2:A:45:GLN:H	1.57	0.69
2:A:53:LEU:HD22	2:A:54:ASN:ND2	2.04	0.69
3:B:642:ASP:HA	3:B:649:LYS:HA	1.75	0.69
2:A:526:ASP:HB2	3:B:835:GLN:OE1	1.92	0.69
3:B:294:ASP:O	3:B:296:GLU:N	2.24	0.69
2:A:311:GLN:O	2:A:312:PRO:C	2.35	0.69
2:A:728:LYS:O	2:A:732:LEU:HG	1.91	0.69
2:A:1074:GLU:C	2:A:1076:ALA:H	2.00	0.69
2:A:1313:LEU:HD23	2:A:1338:VAL:HG21	1.73	0.69
3:B:125:SER:HA	3:B:171:PRO:HA	1.73	0.69
10:I:7:CYS:HB2	10:I:34:TYR:CD1	2.28	0.69
3:B:579:ARG:HB2	3:B:586:TRP:HE1	1.56	0.69
4:C:98:VAL:O	4:C:99:LEU:HD22	1.93	0.69
9:H:89:LEU:C	9:H:91:ASP:H	2.00	0.69
2:A:345:VAL:HG23	2:A:346:ASP:O	1.92	0.69
2:A:903:ASN:ND2	2:A:904:THR:N	2.41	0.69
2:A:1153:TYR:CE1	10:I:42:LEU:HD13	2.28	0.69
2:A:1289:ARG:HD2	2:A:1303:GLU:OE2	1.93	0.69
2:A:1436:ILE:HD13	3:B:1139:ILE:HG23	1.75	0.69
3:B:654:ARG:HH11	3:B:654:ARG:HG3	1.58	0.69
6:E:179:GLN:HB2	6:E:182:ASP:HB2	1.75	0.69
9:H:15:VAL:HG22	9:H:26:ILE:HG12	1.75	0.69
9:H:38:LEU:HD12	9:H:124:ARG:O	1.93	0.69
10:I:101:PHE:HB2	10:I:110:PHE:CE2	2.28	0.69
1:R:3:A:H4'	2:A:447:GLN:NE2	2.07	0.68
2:A:14:VAL:N	2:A:1432:GLN:HE22	1.89	0.68
2:A:1174:PHE:CA	2:A:1176:LEU:HG	2.19	0.68
2:A:1445:ILE:HG12	8:G:18:PHE:HE2	1.57	0.68
3:B:637:LEU:O	3:B:690:VAL:HG13	1.92	0.68
4:C:166:GLU:HG3	12:K:10:PHE:CZ	2.26	0.68
4:C:212:PRO:HB3	4:C:213:PRO:HD2	1.74	0.68
3:B:424:LEU:O	3:B:428:ILE:HG13	1.93	0.68
8:G:117:GLN:C	8:G:119:LEU:H	2.01	0.68
2:A:457:ALA:HB3	2:A:506:ALA:HA	1.75	0.68
3:B:1097:HIS:N	3:B:1098:MET:HE2	2.07	0.68
6:E:202:SER:OG	6:E:204:THR:HG22	1.94	0.68
8:G:14:HIS:ND1	8:G:15:PRO:HD2	2.09	0.68
10:I:105:SER:O	10:I:106:CYS:HB3	1.94	0.68
3:B:393:LYS:HA	3:B:393:LYS:HE3	1.74	0.68
3:B:944:THR:HG21	3:B:1122:ARG:HH22	1.56	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:111:LEU:C	7:F:113:GLY:H	2.00	0.68
2:A:135:PHE:CD1	2:A:222:LEU:HD22	2.29	0.68
2:A:744:LYS:HG2	2:A:748:MET:HE2	1.75	0.68
2:A:855:THR:HG21	2:A:857:ARG:NE	2.09	0.68
2:A:1076:ALA:HA	2:A:1079:MET:CE	2.22	0.68
3:B:176:SER:O	3:B:182:SER:HB3	1.93	0.68
3:B:1087:PHE:CD2	3:B:1088:GLY:N	2.62	0.68
4:C:99:LEU:HD12	4:C:118:LEU:HB3	1.76	0.68
2:A:427:GLN:HG3	2:A:430:TRP:CZ2	2.29	0.68
2:A:1094:VAL:HG13	2:A:1113:THR:HG21	1.75	0.68
3:B:175:ARG:HG2	3:B:175:ARG:HH11	1.57	0.68
3:B:638:PHE:HB3	3:B:651:LEU:HD22	1.75	0.68
3:B:792:MET:HG3	3:B:855:PHE:HE1	1.59	0.68
4:C:148:ARG:HD3	4:C:149:LYS:HG3	1.75	0.68
8:G:96:GLN:HG3	8:G:97:HIS:CD2	2.28	0.68
3:B:172:ILE:HD13	3:B:178:ASN:HD22	1.58	0.68
2:A:1323:ASP:C	2:A:1325:THR:H	2.02	0.68
3:B:244:LEU:HD21	3:B:366:GLN:NE2	2.09	0.68
3:B:856:PHE:HD2	3:B:967:ARG:HD2	1.58	0.68
5:D:153:ARG:HB3	5:D:154:PHE:CE1	2.29	0.68
2:A:63:ARG:HA	2:A:74:MET:HE2	1.76	0.68
2:A:858:ASN:ND2	2:A:860:LEU:H	1.92	0.68
5:D:4:SER:O	5:D:5:THR:HB	1.92	0.68
2:A:61:ILE:HG22	2:A:62:ASP:N	2.08	0.67
2:A:93:VAL:HG23	2:A:304:MET:HE3	1.75	0.67
2:A:567:LYS:HB2	2:A:568:PRO:CD	2.24	0.67
3:B:975:GLN:O	3:B:990:ILE:HD12	1.93	0.67
3:B:1159:ARG:HE	3:B:1193:GLN:HE21	1.42	0.67
3:B:1162:ILE:HD11	3:B:1194:ILE:HD13	1.74	0.67
2:A:605:MET:HG2	2:A:621:THR:HG21	1.76	0.67
2:A:958:VAL:HG22	2:A:1052:GLN:HB3	1.77	0.67
3:B:361:LEU:HD21	3:B:377:PHE:CD2	2.28	0.67
2:A:1193:LEU:HB2	2:A:1260:LEU:HD11	1.76	0.67
3:B:39:ARG:HG2	3:B:39:ARG:HH11	1.59	0.67
3:B:563:MET:CE	3:B:580:VAL:HB	2.23	0.67
4:C:6:PRO:HB2	12:K:101:LEU:HD12	1.76	0.67
9:H:102:TYR:N	9:H:102:TYR:CD2	2.62	0.67
2:A:471:ASN:O	2:A:474:VAL:HG12	1.94	0.67
2:A:866:PHE:C	2:A:867:ILE:HD12	2.18	0.67
2:A:869:GLY:O	6:E:204:THR:HG21	1.94	0.67
3:B:23:ALA:HB1	3:B:24:PRO:HD2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:333:PHE:O	3:B:337:ARG:HG2	1.94	0.67
3:B:799:PRO:HB3	3:B:818:PRO:HG2	1.77	0.67
5:D:56:ARG:HD3	5:D:149:THR:HA	1.75	0.67
2:A:34:LYS:HD3	2:A:57:ARG:NH2	2.10	0.67
2:A:68:GLN:C	2:A:70:CYS:H	2.02	0.67
2:A:335:ARG:HA	2:A:339:ASN:HD22	1.59	0.67
2:A:1239:ARG:HH22	2:A:1241:ARG:NH2	1.92	0.67
3:B:810:GLU:HB2	3:B:815:ARG:HH22	1.59	0.67
4:C:40:GLU:HA	4:C:163:ILE:HG21	1.77	0.67
12:K:47:ARG:HH11	12:K:47:ARG:CB	2.02	0.67
2:A:552:TRP:HE1	12:K:62:LYS:HB2	1.59	0.67
3:B:1097:HIS:H	3:B:1098:MET:CE	2.04	0.67
2:A:172:PRO:HD3	2:A:185:TRP:NE1	2.09	0.67
2:A:528:LEU:O	2:A:531:ILE:HG22	1.95	0.67
2:A:547:LEU:HD22	12:K:58:PHE:CE1	2.30	0.67
2:A:828:ALA:CB	3:B:530:GLY:HA2	2.25	0.67
2:A:1015:VAL:HG12	2:A:1019:CYS:SG	2.35	0.67
2:A:1341:ILE:HG23	2:A:1342:GLU:N	2.10	0.67
3:B:798:TYR:HE2	4:C:62:PHE:CZ	2.13	0.67
4:C:46:ILE:CG2	4:C:157:CYS:HB3	2.24	0.67
9:H:62:SER:C	9:H:64:ASN:H	2.01	0.67
2:A:12:ARG:HD2	3:B:1218:THR:HB	1.77	0.67
2:A:605:MET:HE3	2:A:606:LEU:N	2.10	0.67
2:A:1291:VAL:HG13	2:A:1292:PRO:HD2	1.77	0.67
2:A:84:ILE:HD11	2:A:270:LEU:HD22	1.76	0.67
2:A:269:ILE:HD11	2:A:300:VAL:HA	1.77	0.67
2:A:899:VAL:HB	2:A:929:LEU:CD1	2.25	0.67
2:A:1450:LEU:O	2:A:1450:LEU:HG	1.95	0.67
3:B:778:MET:CE	3:B:1094:ARG:HD3	2.25	0.67
6:E:55:ARG:C	6:E:57:MET:H	2.02	0.67
2:A:984:LYS:O	2:A:988:LEU:HB2	1.95	0.66
3:B:57:TYR:N	3:B:57:TYR:HD1	1.93	0.66
3:B:181:LEU:HD22	3:B:189:LEU:HD22	1.77	0.66
3:B:1177:HIS:HB2	3:B:1179:GLN:HE21	1.59	0.66
3:B:100:PRO:HD2	3:B:180:TYR:CE1	2.29	0.66
3:B:1006:ILE:HD13	11:J:44:TYR:HE2	1.61	0.66
2:A:443:LEU:HD21	2:A:455:MET:HB3	1.77	0.66
3:B:121:ASN:HA	3:B:207:GLY:HA2	1.75	0.66
6:E:145:THR:HG21	6:E:187:TYR:CE2	2.29	0.66
11:J:14:VAL:HG12	11:J:14:VAL:O	1.94	0.66
2:A:114:LEU:HD13	2:A:171:GLN:NE2	2.05	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:164:ARG:HG3	2:A:165:GLY:N	2.11	0.66
2:A:463:ILE:HD11	2:A:469:ARG:HG3	1.77	0.66
5:D:189:ASP:O	5:D:193:THR:HB	1.95	0.66
2:A:7:SER:HB2	3:B:1175:LEU:HD22	1.77	0.66
2:A:1198:ASP:O	2:A:1202:MET:HG2	1.96	0.66
3:B:118:ARG:HG2	3:B:204:ILE:HD13	1.77	0.66
6:E:28:TYR:HE1	6:E:78:LEU:HD13	1.60	0.66
2:A:108:MET:HE3	2:A:210:ILE:CD1	2.25	0.66
3:B:199:MET:HE2	3:B:492:LEU:CD2	2.25	0.66
3:B:611:PRO:HB3	3:B:685:LEU:HD11	1.78	0.66
3:B:1197:PRO:HG2	3:B:1200:ALA:CB	2.24	0.66
6:E:177:ARG:HD3	6:E:215:MET:HG3	1.77	0.66
2:A:567:LYS:CB	9:H:95:TYR:HA	2.25	0.66
2:A:14:VAL:HG21	3:B:1216:LEU:HD12	1.78	0.66
2:A:262:LEU:HD12	2:A:328:ARG:NH2	2.10	0.66
3:B:1161:HIS:NE2	3:B:1175:LEU:HD21	2.11	0.66
7:F:69:LEU:HD23	7:F:71:GLU:HB3	1.74	0.66
8:G:79:PHE:HZ	8:G:106:MET:HE2	1.61	0.66
3:B:502:ILE:H	3:B:502:ILE:HD12	1.60	0.66
3:B:880:THR:O	3:B:881:ASN:HB2	1.94	0.66
6:E:153:HIS:HB3	6:E:196:VAL:HG11	1.76	0.66
2:A:37:PHE:HB2	2:A:52:GLY:HA3	1.78	0.66
2:A:152:VAL:CG1	2:A:153:PRO:HD2	2.26	0.66
2:A:472:LEU:O	2:A:475:THR:HG22	1.95	0.66
2:A:683:ILE:HG21	2:A:801:GLU:HG3	1.78	0.66
2:A:1319:VAL:HG13	2:A:1320:PRO:HD2	1.78	0.66
3:B:957:ASN:O	3:B:959:ASP:N	2.29	0.66
11:J:1:MET:N	11:J:56:LEU:N	2.43	0.66
2:A:58:LEU:CD1	2:A:59:GLY:N	2.53	0.65
2:A:134:ARG:O	2:A:138:ILE:HG13	1.96	0.65
2:A:202:LEU:HB3	2:A:207:ILE:HD11	1.79	0.65
2:A:356:ASP:HB2	2:A:469:ARG:HH11	1.59	0.65
2:A:567:LYS:HZ1	9:H:46:LEU:HB2	1.58	0.65
2:A:981:LEU:HD21	2:A:1038:THR:O	1.97	0.65
2:A:1116:LEU:N	2:A:1308:THR:HG22	2.11	0.65
3:B:98:THR:O	3:B:126:SER:HB2	1.97	0.65
3:B:825:VAL:HG13	3:B:826:ALA:H	1.61	0.65
2:A:90:VAL:CG1	2:A:297:GLN:HA	2.27	0.65
2:A:901:LEU:HD22	2:A:919:ILE:HG22	1.78	0.65
2:A:1116:LEU:HB3	2:A:1308:THR:HG21	1.78	0.65
3:B:882:THR:HG22	3:B:884:ARG:HB2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:642:ASP:HB3	3:B:649:LYS:CD	2.26	0.65
3:B:1187:ASN:O	3:B:1188:LYS:HB2	1.96	0.65
9:H:4:THR:CA	9:H:60:ALA:HB2	2.22	0.65
9:H:81:PRO:CB	9:H:82:PRO:HD2	2.26	0.65
2:A:913:LEU:HD12	2:A:914:GLU:N	2.10	0.65
3:B:526:GLU:HG2	3:B:538:ASN:HD22	1.61	0.65
3:B:828:ALA:HB2	3:B:1085:ILE:CG2	2.25	0.65
3:B:950:ASP:O	3:B:951:GLN:HB2	1.96	0.65
13:L:49:LYS:O	13:L:50:ASP:HB2	1.97	0.65
3:B:1159:ARG:NE	3:B:1193:GLN:HE21	1.95	0.65
5:D:48:ILE:HG21	8:G:4:ILE:HB	1.79	0.65
11:J:63:TYR:O	11:J:64:ASN:HB2	1.96	0.65
2:A:253:ASN:HB3	3:B:935:ARG:CZ	2.26	0.65
2:A:709:THR:HG22	2:A:711:ARG:N	2.03	0.65
2:A:1325:THR:O	6:E:148:GLU:HB2	1.96	0.65
3:B:579:ARG:HG2	3:B:579:ARG:HH11	1.62	0.65
3:B:821:GLN:NE2	3:B:851:PHE:HA	2.12	0.65
3:B:955:THR:HG22	3:B:956:THR:N	2.10	0.65
8:G:61:ILE:HG23	8:G:66:GLY:O	1.97	0.65
9:H:130:ARG:CB	9:H:133:ASN:HB2	2.26	0.65
2:A:41:MET:HB3	2:A:49:LYS:CA	2.20	0.65
2:A:353:ILE:HD13	2:A:487:MET:HE2	1.79	0.65
2:A:1370:LEU:O	2:A:1374:VAL:HG23	1.96	0.65
8:G:1:MET:HE1	8:G:80:LYS:H	1.60	0.65
8:G:1:MET:O	8:G:3:PHE:CE1	2.50	0.65
2:A:886:ILE:HG22	2:A:887:GLY:N	2.12	0.65
2:A:1209:MET:SD	2:A:1236:LEU:HD22	2.37	0.65
3:B:1096:ARG:O	3:B:1097:HIS:HB2	1.96	0.65
13:L:27:LEU:HD13	13:L:37:LYS:HE2	1.79	0.65
2:A:1348:LEU:O	2:A:1352:VAL:HG23	1.96	0.64
6:E:17:ARG:O	6:E:21:GLU:HG3	1.97	0.64
8:G:81:PRO:HG3	8:G:106:MET:SD	2.37	0.64
2:A:34:LYS:O	2:A:35:ILE:HB	1.97	0.64
2:A:560:ILE:HG13	9:H:78:SER:HB2	1.79	0.64
2:A:590:ARG:NH2	2:A:620:LYS:CB	2.60	0.64
9:H:113:ALA:HB2	9:H:126:GLU:HG3	1.78	0.64
2:A:69:THR:C	2:A:71:GLN:N	2.53	0.64
2:A:1166:ASP:OD2	2:A:1239:ARG:HD2	1.96	0.64
3:B:288:ALA:HA	3:B:331:LEU:HD12	1.79	0.64
3:B:464:GLY:HA2	3:B:479:VAL:O	1.97	0.64
5:D:33:PHE:HB3	5:D:47:LEU:HD21	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:48:ARG:HE	11:J:49:MET:HE2	1.60	0.64
12:K:93:SER:O	12:K:97:LYS:HG3	1.97	0.64
2:A:138:ILE:CD1	2:A:222:LEU:HD23	2.27	0.64
2:A:590:ARG:NH2	2:A:620:LYS:HB2	2.12	0.64
3:B:289:LEU:HD13	3:B:375:ALA:HB2	1.78	0.64
3:B:1084:GLN:NE2	3:B:1084:GLN:H	1.94	0.64
5:D:134:THR:HG22	5:D:135:GLY:H	1.60	0.64
6:E:24:LYS:HB3	6:E:30:ILE:HD12	1.79	0.64
11:J:1:MET:H1	11:J:56:LEU:N	1.95	0.64
11:J:44:TYR:HD2	11:J:44:TYR:N	1.95	0.64
2:A:808:LEU:HD23	2:A:813:PHE:HA	1.78	0.64
2:A:1332:PHE:N	2:A:1332:PHE:CD2	2.65	0.64
3:B:1065:GLN:HB2	4:C:201:TRP:CZ3	2.32	0.64
5:D:33:PHE:CE2	8:G:80:LYS:NZ	2.65	0.64
6:E:48:ASP:CG	6:E:49:SER:H	2.05	0.64
3:B:171:PRO:HD2	3:B:457:LEU:CD1	2.28	0.64
3:B:906:SER:O	3:B:941:LEU:HD23	1.98	0.64
4:C:67:LEU:HD11	4:C:155:LEU:CD1	2.28	0.64
6:E:124:VAL:HB	6:E:125:PRO:HD3	1.78	0.64
13:L:53:HIS:O	13:L:55:ILE:HG12	1.97	0.64
2:A:1445:ILE:HG12	8:G:18:PHE:CE2	2.32	0.64
3:B:563:MET:HE1	3:B:580:VAL:HB	1.80	0.64
3:B:840:ILE:HD13	3:B:994:TYR:HE1	1.61	0.64
4:C:107:SER:O	4:C:109:SER:N	2.30	0.64
5:D:119:ARG:HD3	5:D:221:TYR:CD2	2.33	0.64
8:G:128:PRO:O	8:G:138:THR:HG23	1.97	0.64
11:J:64:ASN:CB	11:J:65:PRO:CD	2.75	0.64
2:A:34:LYS:CG	2:A:36:ARG:HH21	2.11	0.64
2:A:35:ILE:HA	2:A:52:GLY:O	1.97	0.64
3:B:583:ASN:HD21	3:B:628:THR:CG2	2.08	0.64
3:B:995:ARG:HH12	4:C:165:LYS:HG2	1.62	0.64
4:C:17:ASN:N	4:C:240:VAL:HG11	2.12	0.64
8:G:145:VAL:HG12	8:G:146:LYS:N	2.11	0.64
9:H:59:ILE:HG22	9:H:60:ALA:H	1.62	0.64
3:B:23:ALA:H	3:B:654:ARG:HB3	1.63	0.64
4:C:36:VAL:HG21	4:C:251:LEU:HB2	1.79	0.64
4:C:66:ARG:HH21	11:J:5:VAL:H	1.46	0.64
2:A:12:ARG:NE	3:B:1192:TYR:HE2	1.96	0.64
2:A:144:THR:O	2:A:146:MET:HE2	1.97	0.64
2:A:351:THR:HB	3:B:1103:ILE:CD1	2.28	0.64
2:A:463:ILE:CD1	2:A:469:ARG:HG3	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:171:PRO:HD2	3:B:457:LEU:HD13	1.79	0.64
3:B:843:GLN:O	3:B:844:SER:C	2.40	0.64
4:C:100:THR:HG22	4:C:101:LEU:H	1.63	0.64
5:D:145:MET:O	5:D:149:THR:HB	1.98	0.64
6:E:180:ARG:NH2	6:E:192:ARG:HB2	2.12	0.64
8:G:143:ILE:CG2	8:G:144:ARG:H	2.11	0.64
12:K:53:ASP:OD1	12:K:55:LYS:HB2	1.98	0.64
2:A:445:ASN:HB2	2:A:454:SER:O	1.97	0.63
3:B:181:LEU:HD22	3:B:189:LEU:CD2	2.28	0.63
10:I:26:LEU:HD23	10:I:37:GLU:HA	1.80	0.63
2:A:981:LEU:HD23	2:A:1039:LYS:HA	1.79	0.63
8:G:122:ASN:ND2	8:G:125:SER:HB3	2.13	0.63
8:G:153:GLN:HG2	8:G:154:VAL:HG23	1.80	0.63
2:A:215:SER:HB3	2:A:218:ASP:CG	2.24	0.63
2:A:960:ILE:O	2:A:963:ILE:HG22	1.99	0.63
3:B:69:LEU:HD13	3:B:429:PHE:HD1	1.63	0.63
4:C:77:ILE:HA	4:C:129:ILE:HD11	1.79	0.63
4:C:244:VAL:O	4:C:248:ILE:HG13	1.96	0.63
6:E:169:ARG:HH12	7:F:74:ILE:HD11	1.63	0.63
9:H:100:THR:HG22	9:H:101:ALA:N	2.14	0.63
12:K:31:VAL:HG12	12:K:32:VAL:N	2.13	0.63
2:A:567:LYS:HB3	9:H:95:TYR:HA	1.81	0.63
2:A:694:THR:O	2:A:698:GLN:HG3	1.99	0.63
2:A:868:TYR:CE1	2:A:1064:VAL:HG11	2.33	0.63
3:B:313:MET:O	3:B:316:PRO:HD2	1.99	0.63
2:A:19:PHE:O	2:A:1416:ALA:HA	1.99	0.63
2:A:50:ILE:O	2:A:52:GLY:N	2.31	0.63
2:A:567:LYS:HB2	2:A:568:PRO:HD2	1.80	0.63
3:B:1163:CYS:SG	3:B:1165:ILE:HB	2.38	0.63
5:D:39:ASN:HD22	5:D:41:GLN:HB2	1.64	0.63
10:I:111:THR:CG2	10:I:112:SER:H	2.10	0.63
11:J:14:VAL:CG1	11:J:50:ILE:HD11	2.28	0.63
3:B:707:PRO:HG2	3:B:708:GLU:H	1.64	0.63
3:B:850:LEU:HD12	3:B:851:PHE:N	2.14	0.63
4:C:253:LYS:O	4:C:256:ALA:HB3	1.98	0.63
5:D:53:SER:H	5:D:148:LEU:CD2	2.12	0.63
7:F:125:LEU:HG	7:F:125:LEU:O	1.98	0.63
2:A:477:PRO:CG	2:A:521:MET:HG2	2.29	0.63
2:A:767:GLN:NE2	2:A:774:ARG:HB3	2.13	0.63
2:A:1006:ILE:CD1	6:E:163:GLU:HG3	2.29	0.63
2:A:1313:LEU:O	2:A:1315:GLU:N	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1332:PHE:HD2	2:A:1332:PHE:N	1.97	0.63
2:A:1333:ILE:HD13	2:A:1381:LEU:HD12	1.80	0.63
4:C:182:PRO:HG3	4:C:206:ASN:O	1.98	0.63
8:G:51:TYR:O	8:G:54:ILE:HG13	1.99	0.63
9:H:41:ASP:O	9:H:42:ILE:HG13	1.99	0.63
2:A:138:ILE:HD13	2:A:222:LEU:HD23	1.80	0.63
2:A:353:ILE:HG21	2:A:487:MET:CE	2.28	0.63
2:A:382:PRO:HD3	2:A:428:TYR:CD2	2.34	0.63
3:B:899:ILE:CD1	3:B:911:ILE:HA	2.29	0.63
8:G:45:ILE:HA	8:G:78:VAL:HG12	1.80	0.63
8:G:91:VAL:HA	8:G:101:VAL:HA	1.80	0.63
9:H:40:LEU:CD1	9:H:123:MET:HE3	2.25	0.63
9:H:89:LEU:O	9:H:91:ASP:N	2.28	0.63
2:A:248:PRO:O	2:A:260:ASP:HB2	1.99	0.63
2:A:284:ALA:C	2:A:286:HIS:H	2.06	0.63
2:A:302:THR:HG22	2:A:303:TYR:N	2.12	0.63
2:A:416:ARG:O	2:A:417:TYR:HD2	1.82	0.63
2:A:973:ILE:HG21	2:A:1036:ARG:O	1.98	0.63
3:B:112:LEU:HD12	3:B:113:TYR:H	1.63	0.63
2:A:971:PHE:HE2	2:A:1040:GLN:HG2	1.63	0.62
3:B:758:PHE:HB3	3:B:761:HIS:CD2	2.34	0.62
5:D:71:LYS:HA	5:D:74:GLN:HB2	1.80	0.62
2:A:605:MET:HE2	2:A:607:ILE:CG1	2.27	0.62
2:A:781:ASP:O	2:A:789:LYS:HA	1.99	0.62
2:A:852:TYR:CD2	2:A:1060:PRO:HB2	2.34	0.62
2:A:896:ARG:HD3	2:A:897:TYR:CE1	2.34	0.62
3:B:57:TYR:N	3:B:57:TYR:CD1	2.64	0.62
3:B:525:ALA:O	3:B:768:THR:HG23	1.99	0.62
4:C:107:SER:C	4:C:109:SER:H	2.06	0.62
5:D:47:LEU:HD11	8:G:3:PHE:CE2	2.34	0.62
7:F:97:ARG:O	7:F:101:ILE:HG13	1.99	0.62
11:J:44:TYR:N	11:J:44:TYR:CD2	2.66	0.62
12:K:90:ALA:O	12:K:94:ILE:HG13	1.99	0.62
2:A:269:ILE:CD1	2:A:300:VAL:HG22	2.27	0.62
2:A:647:GLY:O	2:A:651:LYS:HG3	2.00	0.62
3:B:886:LYS:HE2	3:B:936:ASP:OD1	1.98	0.62
3:B:999:MET:HG2	3:B:1007:VAL:HG22	1.81	0.62
3:B:1099:VAL:CG1	3:B:1100:ASP:N	2.62	0.62
3:B:1178:ASN:O	3:B:1180:PHE:CD1	2.52	0.62
2:A:2:VAL:HG21	3:B:1157:ALA:CB	2.24	0.62
2:A:446:ARG:HD3	2:A:480:ALA:HB2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:458:HIS:CE1	2:A:507:VAL:HG21	2.34	0.62
2:A:578:LEU:HD23	2:A:612:ILE:CD1	2.29	0.62
3:B:46:GLN:HG3	3:B:47:GLN:H	1.63	0.62
3:B:294:ASP:HB2	10:I:12:ASN:HA	1.81	0.62
3:B:997:GLU:CD	3:B:997:GLU:H	2.04	0.62
6:E:176:PRO:O	6:E:212:ARG:HA	1.99	0.62
2:A:798:GLY:HA2	2:A:815:PHE:HD1	1.65	0.62
2:A:1373:ASP:CA	2:A:1376:THR:HG22	2.25	0.62
3:B:387:LEU:O	3:B:392:ARG:HB2	2.00	0.62
6:E:28:TYR:CE1	6:E:78:LEU:HD13	2.34	0.62
7:F:69:LEU:HD13	7:F:72:LYS:CB	2.29	0.62
8:G:28:THR:O	8:G:32:GLU:HG3	1.99	0.62
2:A:33:ALA:HB1	2:A:56:PRO:HB2	1.81	0.62
2:A:115:LEU:HB2	2:A:122:MET:HE2	1.80	0.62
2:A:321:PRO:O	2:A:322:VAL:HB	1.99	0.62
2:A:401:GLY:C	2:A:435:HIS:HD2	2.06	0.62
2:A:471:ASN:OD1	2:A:472:LEU:N	2.33	0.62
2:A:993:LEU:HD23	2:A:1022:LEU:HD21	1.82	0.62
4:C:147:LEU:N	4:C:147:LEU:HD23	2.15	0.62
9:H:25:ARG:HA	9:H:41:ASP:HA	1.81	0.62
2:A:857:ARG:HD3	2:A:861:GLY:O	2.00	0.62
2:A:979:SER:OG	2:A:980:ASP:N	2.32	0.62
4:C:100:THR:HG22	4:C:101:LEU:N	2.15	0.62
5:D:63:LEU:HD12	5:D:129:LEU:HG	1.80	0.62
2:A:399:HIS:CB	2:A:400:PRO:HD3	2.28	0.62
2:A:446:ARG:HD2	2:A:480:ALA:HB2	1.81	0.62
2:A:470:LEU:HD22	2:A:487:MET:CE	2.29	0.62
2:A:1115:SER:O	2:A:1311:VAL:HG22	1.99	0.62
3:B:44:VAL:CG1	3:B:199:MET:HG2	2.30	0.62
6:E:46:TYR:CD2	6:E:58:MET:HG2	2.34	0.62
6:E:207:ARG:HH11	6:E:207:ARG:CB	2.13	0.62
8:G:138:THR:HG22	8:G:139:ILE:HG13	1.80	0.62
2:A:535:THR:CG2	2:A:616:VAL:HA	2.23	0.62
2:A:1445:ILE:H	2:A:1445:ILE:CD1	2.09	0.62
3:B:192:LEU:O	3:B:193:LYS:HB2	1.99	0.62
3:B:616:ILE:HD12	3:B:616:ILE:N	2.14	0.62
5:D:159:THR:O	5:D:163:VAL:HG23	1.98	0.62
6:E:178:ILE:HG22	6:E:213:ILE:O	1.99	0.62
2:A:34:LYS:HZ2	2:A:57:ARG:NH2	1.97	0.61
2:A:282:ASN:O	2:A:284:ALA:N	2.33	0.61
2:A:382:PRO:CB	2:A:428:TYR:HE2	2.13	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:278:GLN:HG2	3:B:279:ASP:H	1.65	0.61
3:B:615:MET:HB3	3:B:626:ILE:HG12	1.82	0.61
3:B:800:GLN:HB3	11:J:52:THR:HG21	1.80	0.61
3:B:821:GLN:HE22	3:B:851:PHE:HA	1.63	0.61
8:G:83:LYS:HG2	8:G:149:GLY:HA2	1.81	0.61
2:A:743:VAL:O	2:A:747:VAL:HG23	1.99	0.61
2:A:858:ASN:ND2	2:A:861:GLY:H	1.99	0.61
3:B:126:SER:O	3:B:169:ARG:HA	2.00	0.61
3:B:360:PHE:CD2	3:B:361:LEU:HB2	2.35	0.61
3:B:873:THR:O	3:B:914:LYS:HA	2.00	0.61
6:E:198:ILE:CD1	6:E:212:ARG:HG3	2.30	0.61
8:G:47:CYS:O	8:G:76:ALA:HB1	2.00	0.61
2:A:84:ILE:O	2:A:84:ILE:HG23	2.00	0.61
2:A:222:LEU:O	2:A:224:PHE:HD1	1.83	0.61
2:A:372:LYS:HA	2:A:435:HIS:ND1	2.14	0.61
2:A:1349:TYR:HB2	2:A:1372:VAL:HG21	1.80	0.61
3:B:1166:CYS:HB2	3:B:1215:ARG:HH12	1.63	0.61
6:E:169:ARG:HB3	7:F:140:ASP:OD2	2.00	0.61
8:G:26:LEU:HD12	8:G:56:ILE:HG21	1.82	0.61
11:J:57:ILE:HA	11:J:60:PHE:CD2	2.35	0.61
2:A:298:PHE:HZ	2:A:314:ALA:HB2	1.66	0.61
2:A:401:GLY:C	2:A:435:HIS:CD2	2.79	0.61
3:B:172:ILE:CD1	3:B:178:ASN:HD22	2.13	0.61
4:C:184:ASN:ND2	4:C:187:LYS:HA	2.15	0.61
6:E:213:ILE:HG12	6:E:214:CYS:N	2.15	0.61
8:G:119:LEU:HD12	8:G:131:GLN:O	2.00	0.61
2:A:1444:MET:HG2	8:G:60:ARG:CA	2.29	0.61
4:C:7:GLN:HG2	12:K:104:ASN:ND2	2.14	0.61
7:F:103:MET:O	7:F:104:ASN:HB2	1.98	0.61
12:K:42:LEU:HD21	12:K:46:ILE:HD11	1.82	0.61
4:C:11:ARG:NH2	4:C:229:TYR:HB3	2.15	0.61
8:G:14:HIS:CD2	8:G:16:SER:HB2	2.35	0.61
2:A:18:GLN:O	3:B:1215:ARG:HG2	2.01	0.61
2:A:24:PRO:HB3	2:A:237:THR:HB	1.82	0.61
2:A:458:HIS:HE2	2:A:478:TYR:HH	1.47	0.61
2:A:720:ARG:O	2:A:724:GLU:HB2	2.01	0.61
3:B:542:MET:HE2	3:B:743:ILE:HG13	1.82	0.61
3:B:797:TYR:O	11:J:1:MET:HG2	2.00	0.61
3:B:1084:GLN:NE2	3:B:1084:GLN:N	2.49	0.61
10:I:55:THR:HG23	10:I:86:PHE:HZ	1.65	0.61
2:A:450:LEU:H	2:A:450:LEU:HD12	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:567:LYS:CB	2:A:568:PRO:CD	2.78	0.61
2:A:596:THR:C	2:A:598:LEU:H	2.09	0.61
2:A:863:VAL:HG11	2:A:866:PHE:CE2	2.36	0.61
3:B:378:LEU:O	3:B:378:LEU:HD12	2.00	0.61
6:E:78:LEU:HD21	6:E:80:VAL:HG23	1.81	0.61
9:H:44:VAL:O	9:H:44:VAL:HG12	2.00	0.61
9:H:102:TYR:H	9:H:102:TYR:HD2	1.45	0.61
12:K:21:ILE:HG12	12:K:33:ILE:HG12	1.82	0.61
13:L:38:LEU:O	13:L:39:SER:HB3	2.00	0.61
2:A:16:GLU:HB3	2:A:1418:LEU:HD11	1.83	0.61
2:A:22:PHE:CE1	3:B:1213:THR:HG22	2.36	0.61
2:A:451:HIS:CD2	2:A:1074:GLU:HG3	2.36	0.61
2:A:596:THR:O	2:A:598:LEU:N	2.33	0.61
3:B:305:VAL:O	3:B:305:VAL:HG12	2.01	0.61
3:B:498:THR:HG21	3:B:537:LYS:HG3	1.81	0.61
2:A:458:HIS:NE2	2:A:478:TYR:OH	2.31	0.61
2:A:598:LEU:HD22	9:H:25:ARG:NH1	2.15	0.61
2:A:826:ASP:O	2:A:830:LYS:HB2	2.01	0.61
2:A:873:MET:HE3	2:A:957:PRO:HG3	1.82	0.61
3:B:220:GLY:O	3:B:222:ILE:HG13	2.01	0.61
3:B:842:ASN:ND2	3:B:845:SER:H	1.99	0.61
4:C:61:GLU:HA	4:C:64:ALA:HB3	1.83	0.61
4:C:73:GLN:NE2	4:C:75:MET:HB2	2.16	0.61
8:G:4:ILE:HG12	8:G:77:VAL:HG22	1.83	0.61
11:J:16:ASP:OD1	11:J:17:LYS:HD2	2.01	0.61
2:A:567:LYS:HD3	9:H:95:TYR:CG	2.35	0.60
2:A:622:VAL:O	2:A:622:VAL:HG13	2.01	0.60
4:C:191:TYR:HD2	4:C:201:TRP:CD1	2.19	0.60
2:A:58:LEU:HD11	2:A:243:PRO:HB3	1.82	0.60
2:A:105:CYS:O	2:A:114:LEU:HG	2.00	0.60
2:A:442:VAL:HB	2:A:489:LEU:HD11	1.83	0.60
2:A:567:LYS:CE	9:H:46:LEU:HB2	2.31	0.60
2:A:821:ARG:HB2	2:A:821:ARG:NH1	2.16	0.60
2:A:870:GLU:HG2	6:E:208:TYR:CG	2.36	0.60
2:A:1002:GLY:HA3	2:A:1007:ILE:HG21	1.82	0.60
2:A:1290:LYS:O	2:A:1291:VAL:HG23	2.01	0.60
3:B:102:VAL:CG2	3:B:112:LEU:HD22	2.31	0.60
3:B:180:TYR:HD1	3:B:180:TYR:H	1.49	0.60
3:B:215:GLN:OE1	3:B:479:VAL:HG22	2.01	0.60
3:B:1011:ILE:O	3:B:1011:ILE:HG22	2.00	0.60
2:A:779:PHE:O	2:A:780:VAL:C	2.44	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:653:VAL:CG2	3:B:689:LEU:HB3	2.31	0.60
11:J:7:CYS:SG	11:J:49:MET:HE3	2.42	0.60
2:A:239:LEU:HD12	2:A:240:PRO:HD2	1.83	0.60
2:A:317:LYS:O	2:A:318:SER:HB3	2.02	0.60
2:A:565:ILE:O	2:A:570:PRO:HA	2.01	0.60
2:A:1130:GLN:HA	2:A:1133:LEU:HD12	1.83	0.60
4:C:98:VAL:C	4:C:99:LEU:HD22	2.26	0.60
4:C:128:ASN:O	4:C:129:ILE:HG13	2.01	0.60
4:C:232:VAL:HG21	4:C:244:VAL:HG22	1.83	0.60
13:L:38:LEU:CD1	13:L:49:LYS:HE2	2.31	0.60
3:B:882:THR:HG21	3:B:884:ARG:HB2	1.84	0.60
3:B:1016:ALA:O	3:B:1020:ARG:HG3	2.01	0.60
4:C:34:ARG:O	4:C:38:ILE:HG13	2.02	0.60
5:D:24:ALA:C	5:D:26:THR:H	2.09	0.60
6:E:157:SER:C	6:E:159:ASP:H	2.08	0.60
3:B:190:TYR:CD2	11:J:62:ARG:HB3	2.37	0.60
3:B:282:ILE:HD12	3:B:382:ILE:HD13	1.84	0.60
3:B:859:TYR:CZ	3:B:941:LEU:HD12	2.37	0.60
4:C:43:THR:CG2	4:C:44:LEU:H	1.98	0.60
6:E:147:HIS:HD2	6:E:149:LEU:HB2	1.67	0.60
10:I:58:VAL:HG13	10:I:62:ILE:CD1	2.31	0.60
2:A:135:PHE:HD1	2:A:222:LEU:HD22	1.67	0.60
2:A:1063:MET:CG	2:A:1436:ILE:HG23	2.32	0.60
3:B:233:PRO:HG2	3:B:234:ILE:CD1	2.31	0.60
3:B:766:ARG:NH2	3:B:1020:ARG:HD3	2.16	0.60
4:C:18:VAL:CG2	4:C:240:VAL:HB	2.31	0.60
4:C:62:PHE:O	4:C:66:ARG:HG3	2.00	0.60
7:F:68:THR:HG21	7:F:69:LEU:CA	2.31	0.60
2:A:265:LYS:HD3	2:A:322:VAL:HG11	1.83	0.60
2:A:1017:LEU:HB3	6:E:205:SER:HA	1.83	0.60
3:B:826:ALA:HB2	3:B:1008:PRO:HB3	1.84	0.60
3:B:955:THR:HG22	3:B:956:THR:O	2.01	0.60
3:B:1180:PHE:O	3:B:1181:GLU:O	2.19	0.60
4:C:18:VAL:O	4:C:20:PHE:HD2	1.85	0.60
4:C:76:ASP:OD2	4:C:128:ASN:N	2.34	0.60
4:C:214:ASN:HB3	4:C:217:ASP:OD2	2.00	0.60
5:D:188:ALA:O	5:D:192:LYS:HG3	2.02	0.60
2:A:466:SER:O	3:B:1103:ILE:HD11	2.01	0.60
2:A:705:LYS:HB2	2:A:708:MET:HE3	1.83	0.60
2:A:857:ARG:NH1	7:F:139:PRO:HB2	2.16	0.60
2:A:863:VAL:HG11	2:A:866:PHE:CD2	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1428:VAL:HG13	3:B:1151:LEU:HD21	1.82	0.60
3:B:874:PHE:HA	3:B:913:GLY:O	2.02	0.60
6:E:22:MET:HE3	6:E:26:ARG:HH21	1.67	0.60
8:G:106:MET:HG2	8:G:107:LYS:N	2.17	0.60
2:A:340:LEU:HD13	2:A:1429:ILE:CG2	2.26	0.60
3:B:346:GLU:O	3:B:350:GLN:HB2	2.02	0.60
3:B:642:ASP:HB3	3:B:649:LYS:CG	2.32	0.60
5:D:40:HIS:CE1	5:D:41:GLN:HG3	2.37	0.60
6:E:84:ASP:O	6:E:86:PRO:HD3	2.02	0.60
2:A:504:LEU:HD11	7:F:91:ALA:HB1	1.83	0.59
2:A:1173:HIS:O	2:A:1176:LEU:CD2	2.48	0.59
2:A:1208:THR:HG22	2:A:1210:GLY:N	2.16	0.59
9:H:64:ASN:O	9:H:65:LEU:HB2	2.01	0.59
10:I:19:ASP:OD1	10:I:22:ASN:HB2	2.02	0.59
12:K:7:PHE:HA	12:K:10:PHE:CE2	2.37	0.59
12:K:55:LYS:HB3	12:K:81:TYR:CD1	2.37	0.59
2:A:166:GLY:O	2:A:167:CYS:SG	2.60	0.59
2:A:450:LEU:HB3	2:A:838:GLN:NE2	2.16	0.59
2:A:590:ARG:O	2:A:591:PHE:HB2	2.00	0.59
2:A:613:ILE:O	2:A:614:PHE:HB3	2.01	0.59
2:A:685:GLU:HG3	2:A:686:ALA:N	2.17	0.59
3:B:847:ASP:C	3:B:849:GLY:H	2.10	0.59
6:E:207:ARG:HB2	6:E:207:ARG:NH1	2.16	0.59
10:I:33:SER:O	10:I:35:VAL:HG23	2.01	0.59
11:J:9:SER:HB2	11:J:45:CYS:HB2	1.85	0.59
2:A:1369:ALA:O	2:A:1372:VAL:HG12	2.02	0.59
3:B:797:TYR:HB2	3:B:852:ARG:O	2.01	0.59
5:D:47:LEU:HD11	8:G:3:PHE:HD2	1.64	0.59
5:D:185:CYS:HB2	5:D:211:LEU:HD21	1.83	0.59
6:E:117:THR:HG22	6:E:119:SER:H	1.67	0.59
2:A:22:PHE:HE2	2:A:30:ILE:HD12	1.68	0.59
2:A:23:SER:HB3	2:A:233:TRP:CZ2	2.36	0.59
2:A:298:PHE:CZ	2:A:314:ALA:HB2	2.37	0.59
3:B:882:THR:HB	3:B:934:LYS:O	2.02	0.59
4:C:38:ILE:HA	4:C:173:ALA:CB	2.32	0.59
11:J:64:ASN:ND2	11:J:65:PRO:HD3	2.17	0.59
12:K:61:TYR:C	12:K:61:TYR:CD2	2.77	0.59
3:B:705:MET:H	3:B:710:LEU:CD1	2.15	0.59
4:C:187:LYS:HG3	4:C:219:PHE:CE1	2.38	0.59
10:I:50:THR:HG22	10:I:52:ILE:H	1.67	0.59
2:A:253:ASN:HB3	3:B:935:ARG:NH2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:399:HIS:O	2:A:401:GLY:N	2.36	0.59
2:A:650:GLN:O	2:A:654:ASN:ND2	2.36	0.59
2:A:1094:VAL:HG12	2:A:1095:THR:H	1.68	0.59
3:B:882:THR:HG22	3:B:884:ARG:N	2.12	0.59
3:B:1001:PHE:CE1	3:B:1073:TYR:HB2	2.38	0.59
4:C:39:ALA:CA	4:C:164:ALA:HB3	2.30	0.59
6:E:13:TRP:HB2	6:E:42:PHE:CE2	2.37	0.59
7:F:111:LEU:O	7:F:113:GLY:N	2.31	0.59
2:A:1115:SER:HB3	2:A:1330:ASN:ND2	2.16	0.59
3:B:653:VAL:HG22	3:B:689:LEU:HB3	1.84	0.59
3:B:761:HIS:HB2	3:B:1024:ALA:HB2	1.84	0.59
3:B:833:TYR:N	3:B:833:TYR:CD1	2.68	0.59
3:B:1085:ILE:HD12	3:B:1085:ILE:H	1.65	0.59
10:I:106:CYS:O	10:I:107:SER:HB2	2.03	0.59
2:A:442:VAL:HG21	2:A:460:VAL:HG23	1.84	0.59
2:A:475:THR:CG2	2:A:476:SER:H	2.12	0.59
2:A:929:LEU:HD23	2:A:983:ILE:HG21	1.85	0.59
2:A:1410:PHE:HA	3:B:1212:ILE:HD11	1.85	0.59
3:B:165:VAL:HG11	3:B:448:ILE:CD1	2.32	0.59
3:B:798:TYR:CE2	4:C:62:PHE:CE2	2.85	0.59
5:D:153:ARG:C	5:D:154:PHE:CD1	2.81	0.59
2:A:698:GLN:HA	10:I:97:MET:O	2.03	0.59
2:A:1130:GLN:HE21	2:A:1134:ILE:HD11	1.66	0.59
2:A:1329:THR:H	2:A:1335:ILE:HD11	1.66	0.59
3:B:39:ARG:HG2	3:B:39:ARG:NH1	2.17	0.59
3:B:365:THR:HG23	3:B:367:LEU:N	2.17	0.59
3:B:542:MET:HB3	3:B:636:PRO:HD2	1.85	0.59
3:B:1077:THR:HG22	12:K:44:ASN:ND2	2.17	0.59
4:C:8:VAL:HG12	4:C:9:LYS:H	1.68	0.59
5:D:29:LEU:HD13	8:G:82:PHE:CZ	2.38	0.59
2:A:55:ASP:CG	2:A:55:ASP:O	2.43	0.59
2:A:438:ASP:O	2:A:439:ASN:HB2	2.03	0.59
2:A:528:LEU:HD23	2:A:751:SER:CB	2.33	0.59
3:B:994:TYR:HB2	3:B:999:MET:CE	2.32	0.59
4:C:242:GLN:C	4:C:244:VAL:H	2.11	0.59
9:H:135:LEU:HD13	9:H:137:GLN:NE2	2.11	0.59
11:J:64:ASN:HB3	11:J:65:PRO:HD2	1.84	0.59
2:A:675:THR:OG1	2:A:736:ASN:ND2	2.36	0.58
2:A:1226:VAL:HG22	2:A:1240:CYS:CB	2.31	0.58
3:B:559:SER:HA	3:B:563:MET:HB3	1.85	0.58
3:B:693:ILE:HD13	3:B:701:ILE:HD13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:710:LEU:H	2:A:710:LEU:HD12	1.68	0.58
3:B:44:VAL:HG11	3:B:199:MET:HG2	1.84	0.58
3:B:360:PHE:CD2	3:B:360:PHE:C	2.80	0.58
3:B:463:THR:HB	3:B:465:ASN:H	1.68	0.58
3:B:1110:PRO:HG3	3:B:1125:ASP:HB3	1.85	0.58
4:C:164:ALA:HA	4:C:167:HIS:O	2.03	0.58
5:D:50:LEU:HD13	5:D:55:ALA:HA	1.84	0.58
3:B:65:GLU:HG3	3:B:66:ASP:N	2.16	0.58
3:B:121:ASN:HA	3:B:207:GLY:CA	2.33	0.58
3:B:744:HIS:HD2	3:B:746:SER:OG	1.85	0.58
4:C:66:ARG:NH2	11:J:5:VAL:HG23	2.16	0.58
7:F:119:ARG:HG3	7:F:119:ARG:NH1	2.18	0.58
7:F:130:ILE:O	7:F:148:VAL:CG2	2.51	0.58
13:L:55:ILE:O	13:L:56:LEU:HB2	2.02	0.58
2:A:93:VAL:CG2	2:A:301:ALA:HA	2.33	0.58
2:A:254:GLU:HB2	3:B:935:ARG:HH12	1.68	0.58
3:B:174:LEU:HD22	3:B:202:TYR:CE1	2.39	0.58
3:B:816:GLU:O	3:B:817:LEU:HD23	2.03	0.58
3:B:1072:MET:HE3	3:B:1085:ILE:HD13	1.85	0.58
3:B:1165:ILE:HG22	3:B:1166:CYS:N	2.17	0.58
4:C:187:LYS:C	4:C:189:THR:H	2.11	0.58
5:D:198:LEU:O	5:D:200:ASN:N	2.35	0.58
10:I:34:TYR:HD2	10:I:34:TYR:C	2.09	0.58
2:A:244:PRO:HB2	2:A:245:PRO:HD3	1.85	0.58
2:A:974:ASP:HB2	9:H:136:LYS:HZ2	1.68	0.58
3:B:54:PHE:CZ	3:B:59:LEU:HD13	2.37	0.58
3:B:258:LEU:HG	3:B:258:LEU:O	2.04	0.58
10:I:2:THR:O	10:I:3:THR:C	2.47	0.58
10:I:50:THR:HG22	10:I:51:ASN:H	1.68	0.58
11:J:2:ILE:HG22	11:J:3:VAL:O	2.03	0.58
12:K:57:LEU:HD12	12:K:77:THR:O	2.03	0.58
2:A:75:ASN:HA	3:B:1116:ARG:HH22	1.67	0.58
2:A:889:SER:HB3	2:A:1297:GLU:HG2	1.85	0.58
2:A:1127:ASP:CB	2:A:1130:GLN:HB3	2.22	0.58
2:A:1341:ILE:CG2	2:A:1342:GLU:N	2.66	0.58
3:B:706:GLN:HE22	3:B:730:ARG:NH1	2.01	0.58
7:F:116:ASP:HB3	7:F:119:ARG:CB	2.33	0.58
10:I:16:PRO:HB3	10:I:27:PHE:CD2	2.39	0.58
11:J:1:MET:H2	11:J:57:ILE:N	1.96	0.58
2:A:90:VAL:HG13	2:A:297:GLN:HA	1.86	0.58
2:A:325:ILE:HG22	3:B:1210:MET:HE2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:496:GLU:HG2	7:F:99:LEU:HD22	1.84	0.58
2:A:1101:LEU:HD11	2:A:1105:LEU:HD11	1.84	0.58
3:B:1096:ARG:O	3:B:1097:HIS:CB	2.51	0.58
4:C:56:THR:HG22	4:C:57:VAL:H	1.68	0.58
5:D:160:VAL:O	5:D:164:ILE:HG13	2.03	0.58
6:E:124:VAL:HG13	6:E:132:ILE:HD12	1.85	0.58
10:I:62:ILE:O	10:I:62:ILE:HG12	2.04	0.58
12:K:10:PHE:N	12:K:10:PHE:CD2	2.70	0.58
2:A:42:ASP:C	2:A:44:THR:H	2.11	0.58
2:A:853:ASP:OD1	2:A:855:THR:HG22	2.04	0.58
3:B:185:THR:O	3:B:186:GLU:C	2.47	0.58
3:B:766:ARG:NH2	3:B:1020:ARG:HH11	1.98	0.58
5:D:170:THR:HB	5:D:172:LEU:HG	1.85	0.58
6:E:157:SER:OG	6:E:160:GLU:HG3	2.04	0.58
2:A:381:THR:OG1	2:A:382:PRO:HD2	2.03	0.58
2:A:1127:ASP:HB3	2:A:1130:GLN:CB	2.23	0.58
2:A:1438:THR:O	7:F:92:ARG:HD2	2.03	0.58
3:B:833:TYR:N	3:B:833:TYR:HD1	2.01	0.58
4:C:89:GLU:O	4:C:90:ASP:HB3	2.02	0.58
4:C:124:LEU:O	4:C:125:MET:HB2	2.03	0.58
9:H:42:ILE:HG23	9:H:95:TYR:CE1	2.34	0.58
2:A:472:LEU:HD11	3:B:835:GLN:NE2	2.18	0.58
2:A:665:GLY:O	2:A:667:GLY:N	2.36	0.58
2:A:1350:LYS:O	2:A:1354:ASN:ND2	2.37	0.58
2:A:1430:LEU:O	3:B:1196:ILE:HG22	2.04	0.58
3:B:221:ASN:N	3:B:241:ARG:O	2.34	0.58
3:B:519:TRP:HE1	3:B:635:ARG:NH2	2.02	0.58
3:B:520:GLY:HA2	3:B:748:ILE:HG22	1.86	0.58
3:B:589:VAL:CG1	3:B:590:HIS:H	2.13	0.58
3:B:1156:ASP:HB3	3:B:1198:TYR:H	1.69	0.58
12:K:12:LEU:H	12:K:12:LEU:HD12	1.69	0.58
2:A:407:ARG:HB3	2:A:430:TRP:CE2	2.39	0.57
2:A:821:ARG:HB2	2:A:821:ARG:HH11	1.67	0.57
3:B:850:LEU:HD12	3:B:851:PHE:H	1.68	0.57
3:B:994:TYR:HB2	3:B:999:MET:HE1	1.84	0.57
8:G:14:HIS:HD2	8:G:16:SER:HB2	1.67	0.57
11:J:1:MET:H1	11:J:56:LEU:H	1.49	0.57
2:A:821:ARG:HD2	2:A:825:ILE:HD11	1.86	0.57
2:A:1441:PHE:CE2	7:F:89:GLU:HG2	2.40	0.57
3:B:807:ARG:HG2	3:B:1045:SER:OG	2.04	0.57
3:B:1001:PHE:CZ	3:B:1073:TYR:HB2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1181:GLU:OE1	3:B:1183:LYS:HG3	2.05	0.57
4:C:44:LEU:HB2	4:C:77:ILE:HD11	1.85	0.57
4:C:69:LEU:N	4:C:69:LEU:HD12	2.19	0.57
5:D:47:LEU:HD13	5:D:48:ILE:N	2.19	0.57
9:H:102:TYR:N	9:H:102:TYR:HD2	1.99	0.57
10:I:101:PHE:HE1	10:I:112:SER:HB2	1.70	0.57
12:K:21:ILE:HG23	12:K:31:VAL:CG1	2.35	0.57
3:B:324:ILE:HG12	3:B:329:THR:HG22	1.86	0.57
4:C:70:ILE:HG12	4:C:142:VAL:HG11	1.85	0.57
7:F:103:MET:HE1	8:G:65:ASP:HB2	1.86	0.57
8:G:51:TYR:C	8:G:51:TYR:CD2	2.82	0.57
2:A:308:ILE:HG22	2:A:309:ALA:H	1.68	0.57
2:A:340:LEU:HD21	3:B:1200:ALA:N	2.20	0.57
2:A:1074:GLU:C	2:A:1076:ALA:N	2.62	0.57
3:B:603:LEU:HB3	3:B:609:ILE:HG13	1.87	0.57
3:B:642:ASP:HB3	3:B:649:LYS:HG3	1.86	0.57
3:B:916:THR:O	3:B:935:ARG:HG3	2.04	0.57
3:B:1162:ILE:HD11	3:B:1194:ILE:CD1	2.34	0.57
7:F:68:THR:HG21	7:F:69:LEU:CB	2.34	0.57
9:H:105:GLU:HG2	9:H:106:GLU:N	2.20	0.57
10:I:14:LEU:HD22	10:I:28:GLU:O	2.05	0.57
10:I:34:TYR:CD2	10:I:34:TYR:C	2.80	0.57
2:A:605:MET:HE1	2:A:612:ILE:HG23	1.87	0.57
2:A:896:ARG:HD3	2:A:897:TYR:HE1	1.69	0.57
2:A:899:VAL:CB	2:A:929:LEU:HD11	2.32	0.57
2:A:1120:LEU:N	2:A:1120:LEU:CD1	2.68	0.57
2:A:1152:ILE:CD1	10:I:44:TYR:HD2	2.14	0.57
2:A:1444:MET:CE	7:F:135:ARG:HB2	2.35	0.57
3:B:190:TYR:HD2	11:J:62:ARG:O	1.85	0.57
4:C:18:VAL:HG23	4:C:240:VAL:HB	1.86	0.57
9:H:83:GLN:C	9:H:85:GLY:H	2.12	0.57
13:L:61:THR:HG22	13:L:62:LYS:N	2.19	0.57
2:A:360:GLU:HG2	2:A:363:GLN:OE1	2.04	0.57
2:A:1244:ARG:HB3	2:A:1245:PRO:HD2	1.84	0.57
2:A:1424:VAL:HG13	2:A:1436:ILE:CD1	2.35	0.57
3:B:1106:ARG:HD3	3:B:1126:GLY:O	2.03	0.57
4:C:238:ILE:HD11	4:C:246:ARG:NH1	2.18	0.57
5:D:33:PHE:CE1	8:G:80:LYS:HE3	2.40	0.57
8:G:154:VAL:HG12	8:G:155:SER:N	2.19	0.57
2:A:106:VAL:HG13	2:A:112:LYS:O	2.04	0.57
2:A:185:TRP:CZ3	2:A:200:ARG:HG2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:981:LEU:HD21	2:A:1039:LYS:HA	1.85	0.57
3:B:193:LYS:HD3	3:B:787:VAL:HG11	1.87	0.57
3:B:515:HIS:N	3:B:518:HIS:HD2	1.89	0.57
3:B:903:VAL:HG12	3:B:904:ARG:N	2.18	0.57
8:G:1:MET:HE3	8:G:80:LYS:O	2.04	0.57
2:A:920:LEU:HD23	2:A:921:GLY:N	2.20	0.57
2:A:1076:ALA:HA	2:A:1079:MET:HE3	1.86	0.57
3:B:309:GLN:CD	10:I:52:ILE:HD11	2.30	0.57
3:B:345:LYS:HA	3:B:348:ARG:HD2	1.85	0.57
10:I:8:ARG:HG3	10:I:34:TYR:CE1	2.36	0.57
2:A:19:PHE:HB3	2:A:1413:GLY:HA2	1.87	0.57
2:A:853:ASP:OD1	2:A:855:THR:N	2.38	0.57
4:C:147:LEU:HB2	4:C:151:GLN:HB2	1.87	0.57
11:J:23:ASN:C	11:J:25:LEU:N	2.61	0.57
13:L:30:ILE:O	13:L:56:LEU:HA	2.04	0.57
2:A:382:PRO:HB3	2:A:428:TYR:CE2	2.35	0.57
2:A:548:ASN:HA	12:K:60:ALA:HB1	1.87	0.57
2:A:946:VAL:HG22	6:E:201:LYS:HD2	1.85	0.57
2:A:1313:LEU:HD23	2:A:1338:VAL:CG2	2.34	0.57
2:A:1336:MET:CE	2:A:1381:LEU:HG	2.33	0.57
2:A:1418:LEU:HD12	2:A:1419:ASP:N	2.19	0.57
3:B:269:ILE:HG21	3:B:282:ILE:HD13	1.87	0.57
3:B:498:THR:HG22	3:B:537:LYS:HG3	1.87	0.57
3:B:516:ASN:N	3:B:516:ASN:ND2	2.46	0.57
4:C:148:ARG:CG	4:C:149:LYS:H	2.18	0.57
10:I:7:CYS:HB3	10:I:14:LEU:HD21	1.87	0.57
2:A:18:GLN:HB3	3:B:1215:ARG:HG3	1.87	0.56
2:A:332:LYS:HA	2:A:337:ARG:HD2	1.86	0.56
2:A:457:ALA:O	2:A:507:VAL:HG23	2.05	0.56
3:B:591:ARG:O	3:B:593:PRO:HD3	2.05	0.56
7:F:69:LEU:HD22	7:F:71:GLU:C	2.30	0.56
8:G:1:MET:SD	8:G:79:PHE:CD1	2.91	0.56
11:J:64:ASN:CB	11:J:65:PRO:HD3	2.33	0.56
13:L:52:GLY:O	13:L:53:HIS:C	2.47	0.56
2:A:490:HIS:HB3	3:B:1150:ARG:NH1	2.21	0.56
3:B:118:ARG:CG	3:B:204:ILE:HD13	2.35	0.56
3:B:308:TRP:HA	3:B:311:LEU:HD12	1.87	0.56
3:B:467:GLY:N	3:B:475:SER:HB3	2.18	0.56
3:B:641:GLU:C	3:B:643:ASP:H	2.12	0.56
3:B:955:THR:CG2	3:B:956:THR:H	2.16	0.56
5:D:47:LEU:HD13	5:D:48:ILE:H	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:35:ILE:HG22	2:A:35:ILE:O	2.06	0.56
2:A:310:GLY:O	2:A:312:PRO:HD2	2.04	0.56
2:A:373:THR:HG21	3:B:1105:ALA:HB3	1.87	0.56
2:A:504:LEU:HD12	2:A:504:LEU:N	2.20	0.56
2:A:675:THR:O	2:A:679:ILE:HG13	2.06	0.56
2:A:794:PRO:HG2	2:A:795:GLU:OE2	2.06	0.56
3:B:363:HIS:HD2	3:B:585:VAL:HG22	1.70	0.56
3:B:794:ASN:O	3:B:795:ILE:HD12	2.06	0.56
3:B:1095:LEU:HD12	3:B:1095:LEU:N	2.19	0.56
3:B:1181:GLU:HG3	3:B:1188:LYS:HE3	1.87	0.56
4:C:18:VAL:O	4:C:18:VAL:HG12	2.03	0.56
4:C:79:GLN:HE21	4:C:127:ARG:HD3	1.70	0.56
4:C:238:ILE:HG22	4:C:243:VAL:HG23	1.87	0.56
6:E:17:ARG:O	6:E:20:LYS:HB2	2.05	0.56
8:G:43:GLY:HA3	8:G:80:LYS:HB3	1.87	0.56
11:J:23:ASN:O	11:J:25:LEU:N	2.38	0.56
2:A:29:ALA:HB1	3:B:1184:GLY:CA	2.36	0.56
2:A:537:ARG:HD2	9:H:20:TYR:CE1	2.40	0.56
2:A:1155:ASP:OD2	2:A:1161:THR:HA	2.06	0.56
2:A:1385:THR:HG22	2:A:1386:ARG:H	1.69	0.56
3:B:401:PHE:HA	3:B:404:LYS:HG3	1.86	0.56
3:B:983:ARG:HD2	3:B:1091:TYR:HD2	1.69	0.56
4:C:234:SER:CB	4:C:240:VAL:HG13	2.36	0.56
5:D:144:THR:HG21	8:G:46:LEU:HD13	1.87	0.56
6:E:15:ALA:HA	6:E:140:LEU:O	2.06	0.56
7:F:69:LEU:HD13	7:F:72:LYS:CD	2.35	0.56
9:H:130:ARG:HD2	9:H:130:ARG:N	2.12	0.56
13:L:49:LYS:O	13:L:50:ASP:CB	2.54	0.56
2:A:87:ALA:HB3	2:A:276:LEU:HD23	1.88	0.56
2:A:106:VAL:HG12	2:A:107:CYS:N	2.20	0.56
2:A:606:LEU:HB3	2:A:614:PHE:CE2	2.40	0.56
2:A:828:ALA:HB1	3:B:530:GLY:HA2	1.86	0.56
2:A:868:TYR:CD2	2:A:1058:VAL:HG21	2.34	0.56
2:A:1030:ARG:NH1	2:A:1035:TYR:OH	2.39	0.56
3:B:580:VAL:HG13	3:B:624:LEU:HB3	1.88	0.56
3:B:758:PHE:CE1	3:B:1027:ILE:HG22	2.41	0.56
4:C:238:ILE:CG2	4:C:242:GLN:HB2	2.35	0.56
7:F:76:LYS:O	7:F:79:ARG:HD3	2.04	0.56
8:G:26:LEU:HD12	8:G:56:ILE:CG2	2.36	0.56
9:H:107:VAL:O	9:H:108:SER:O	2.22	0.56
2:A:590:ARG:HD3	2:A:604:GLY:CA	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:971:PHE:CE2	2:A:1040:GLN:HG2	2.39	0.56
3:B:94:LYS:HG2	3:B:95:ILE:N	2.20	0.56
3:B:313:MET:HE2	3:B:390:LEU:HD21	1.86	0.56
3:B:1007:VAL:CG2	3:B:1008:PRO:HD2	2.36	0.56
4:C:20:PHE:CE1	4:C:230:MET:HE3	2.41	0.56
5:D:4:SER:O	5:D:5:THR:CB	2.54	0.56
2:A:552:TRP:HE1	12:K:62:LYS:CB	2.17	0.56
2:A:600:PRO:HG2	2:A:601:LYS:H	1.69	0.56
2:A:714:PHE:CB	10:I:97:MET:HE1	2.36	0.56
2:A:1164:PRO:HG2	2:A:1165:GLU:H	1.70	0.56
2:A:1283:VAL:HG12	2:A:1284:MET:N	2.19	0.56
3:B:1007:VAL:HG22	3:B:1008:PRO:HD2	1.87	0.56
3:B:1178:ASN:O	3:B:1180:PHE:HD1	1.88	0.56
7:F:111:LEU:HD12	7:F:111:LEU:N	2.18	0.56
2:A:58:LEU:CD1	2:A:243:PRO:HB3	2.36	0.56
2:A:1444:MET:HE1	7:F:135:ARG:HB2	1.88	0.56
3:B:195:CYS:SG	3:B:196:PRO:HD2	2.46	0.56
3:B:640:VAL:O	3:B:640:VAL:HG12	2.05	0.56
3:B:978:ASP:OD2	3:B:1098:MET:HG2	2.06	0.56
10:I:80:SER:HB2	10:I:103:CYS:SG	2.45	0.56
2:A:93:VAL:CG2	2:A:304:MET:HE3	2.35	0.56
2:A:168:GLY:O	2:A:169:ASN:C	2.49	0.56
3:B:123:THR:OG1	3:B:458:LYS:HE2	2.06	0.56
3:B:685:LEU:C	3:B:687:GLU:H	2.12	0.56
6:E:22:MET:CE	6:E:26:ARG:HH21	2.19	0.56
7:F:103:MET:CE	8:G:65:ASP:HB2	2.36	0.56
8:G:48:VAL:HA	8:G:76:ALA:HB2	1.88	0.56
8:G:73:LYS:HE2	8:G:74:TYR:O	2.06	0.56
2:A:546:VAL:HG13	2:A:577:ILE:HG21	1.88	0.56
2:A:1349:TYR:HE1	2:A:1368:MET:HB2	1.71	0.56
3:B:53:GLN:HG2	3:B:547:VAL:CG2	2.36	0.56
3:B:168:GLY:H	3:B:450:ALA:HB1	1.70	0.56
3:B:809:MET:HE2	3:B:814:PHE:CD2	2.41	0.56
9:H:81:PRO:CB	9:H:82:PRO:CD	2.84	0.56
11:J:48:ARG:HD2	11:J:49:MET:N	2.21	0.56
13:L:28:LYS:O	13:L:29:TYR:HD2	1.89	0.56
2:A:18:GLN:H	3:B:1215:ARG:HB2	1.71	0.55
2:A:102:VAL:HG11	2:A:211:PHE:CE2	2.41	0.55
2:A:722:LEU:HD21	2:A:794:PRO:HB3	1.87	0.55
2:A:768:GLN:CG	2:A:816:HIS:HA	2.34	0.55
3:B:217:ARG:HD2	3:B:217:ARG:C	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:658:ILE:CG2	3:B:662:MET:HE2	2.35	0.55
3:B:704:ALA:HB2	3:B:738:PHE:CD2	2.41	0.55
4:C:52:GLU:HA	13:L:64:LEU:HD22	1.87	0.55
4:C:209:TYR:N	4:C:209:TYR:CD1	2.74	0.55
6:E:13:TRP:CE3	6:E:39:LEU:HD13	2.41	0.55
6:E:22:MET:HE3	6:E:26:ARG:NE	2.21	0.55
13:L:61:THR:HG21	13:L:63:ARG:HG2	1.87	0.55
3:B:361:LEU:HD21	3:B:377:PHE:HD2	1.71	0.55
3:B:640:VAL:O	3:B:641:GLU:C	2.49	0.55
3:B:796:LEU:HD12	3:B:852:ARG:O	2.06	0.55
3:B:957:ASN:HD22	3:B:961:LEU:HD12	1.70	0.55
4:C:189:THR:HG22	4:C:190:ASP:N	2.21	0.55
5:D:48:ILE:CG2	8:G:4:ILE:HB	2.36	0.55
7:F:111:LEU:C	7:F:113:GLY:N	2.64	0.55
7:F:143:PHE:C	7:F:143:PHE:CD1	2.84	0.55
8:G:114:LEU:HG	8:G:162:SER:HB3	1.89	0.55
10:I:34:TYR:HD2	10:I:35:VAL:H	1.49	0.55
12:K:47:ARG:C	12:K:47:ARG:HD2	2.30	0.55
2:A:546:VAL:HA	2:A:549:MET:HE3	1.89	0.55
2:A:663:SER:OG	2:A:664:THR:N	2.35	0.55
2:A:726:ARG:O	2:A:729:ALA:HB3	2.06	0.55
2:A:1115:SER:O	2:A:1116:LEU:HB3	2.06	0.55
3:B:295:GLY:O	3:B:299:GLU:HG2	2.06	0.55
3:B:1159:ARG:CD	3:B:1193:GLN:HE21	2.19	0.55
2:A:180:LYS:HZ1	2:A:294:SER:HB3	1.71	0.55
2:A:541:ILE:HG21	2:A:549:MET:HE1	1.88	0.55
8:G:106:MET:CG	8:G:107:LYS:N	2.70	0.55
2:A:260:ASP:OD1	2:A:261:ASP:N	2.39	0.55
2:A:367:PRO:HA	2:A:463:ILE:O	2.06	0.55
2:A:546:VAL:O	2:A:546:VAL:HG12	2.07	0.55
2:A:714:PHE:HB2	10:I:97:MET:HE1	1.89	0.55
2:A:1389:PHE:CD1	2:A:1389:PHE:C	2.83	0.55
3:B:953:LEU:CD2	3:B:965:LYS:HB2	2.34	0.55
3:B:1034:VAL:O	3:B:1036:ALA:N	2.39	0.55
5:D:52:LEU:HD21	5:D:147:TYR:HE2	1.72	0.55
6:E:55:ARG:HD2	6:E:83:CYS:O	2.06	0.55
8:G:7:LEU:CD1	8:G:45:ILE:HD11	2.37	0.55
2:A:963:ILE:HD11	2:A:1048:ASN:CB	2.35	0.55
2:A:1291:VAL:HG13	2:A:1292:PRO:CD	2.37	0.55
2:A:1305:VAL:HG12	2:A:1306:LEU:N	2.20	0.55
4:C:35:ARG:NH1	12:K:41:THR:N	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:90:ARG:HG3	7:F:91:ALA:N	2.18	0.55
8:G:18:PHE:HA	8:G:22:MET:CE	2.34	0.55
9:H:142:LEU:C	9:H:143:LEU:HD12	2.32	0.55
2:A:783:THR:HG21	2:A:815:PHE:CE2	2.41	0.55
2:A:886:ILE:HD11	2:A:943:LEU:HB3	1.89	0.55
2:A:954:TRP:HB3	2:A:955:PRO:HD2	1.89	0.55
2:A:1074:GLU:H	2:A:1075:PRO:HD2	1.72	0.55
2:A:1114:PRO:HB2	2:A:1311:VAL:CG2	2.34	0.55
3:B:1094:ARG:HH21	3:B:1098:MET:HG2	1.70	0.55
10:I:58:VAL:HG13	10:I:62:ILE:HD12	1.89	0.55
11:J:1:MET:N	11:J:57:ILE:H	1.96	0.55
2:A:325:ILE:HG21	3:B:1210:MET:HG3	1.89	0.55
2:A:591:PHE:HA	2:A:595:THR:HG21	1.88	0.55
2:A:1353:TYR:HD1	2:A:1368:MET:HE1	1.72	0.55
3:B:185:THR:H	3:B:188:ASP:HB2	1.70	0.55
3:B:637:LEU:HD21	3:B:742:GLU:OE2	2.07	0.55
3:B:642:ASP:HB3	3:B:649:LYS:HD2	1.89	0.55
3:B:871:THR:HG22	3:B:872:GLU:N	2.21	0.55
3:B:1202:LEU:HD23	3:B:1206:GLU:HG3	1.89	0.55
4:C:147:LEU:HD12	4:C:151:GLN:O	2.06	0.55
7:F:93:ILE:HD11	7:F:134:ILE:HD11	1.89	0.55
8:G:138:THR:CG2	8:G:139:ILE:H	1.99	0.55
9:H:40:LEU:HD22	9:H:123:MET:CE	2.37	0.55
12:K:110:ASN:O	12:K:111:LEU:CB	2.54	0.55
2:A:32:VAL:HG21	2:A:68:GLN:NE2	2.22	0.55
2:A:1076:ALA:HA	2:A:1079:MET:HE2	1.87	0.55
3:B:763:GLN:HG2	3:B:765:PRO:HD2	1.88	0.55
3:B:1102:LYS:O	3:B:1103:ILE:C	2.50	0.55
4:C:235:VAL:HG12	11:J:13:VAL:CG2	2.37	0.55
7:F:99:LEU:HD12	7:F:99:LEU:O	2.06	0.55
8:G:37:SER:OG	8:G:45:ILE:HB	2.07	0.55
2:A:34:LYS:CE	2:A:57:ARG:NH1	2.66	0.55
2:A:117:GLU:H	2:A:117:GLU:CD	2.15	0.55
2:A:261:ASP:OD1	2:A:322:VAL:HG13	2.07	0.55
2:A:1116:LEU:HB3	2:A:1308:THR:CG2	2.37	0.55
2:A:1401:SER:O	2:A:1402:PHE:HB2	2.07	0.55
3:B:190:TYR:CE2	11:J:62:ARG:HB3	2.42	0.55
5:D:39:ASN:ND2	5:D:41:GLN:HB2	2.22	0.55
9:H:64:ASN:O	9:H:65:LEU:CB	2.55	0.55
2:A:341:MET:HE3	2:A:843:LYS:HZ1	1.70	0.54
2:A:679:ILE:O	2:A:683:ILE:HG13	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1299:VAL:HG12	2:A:1300:LYS:N	2.22	0.54
4:C:226:ASP:O	4:C:227:THR:HB	2.07	0.54
5:D:172:LEU:HD22	5:D:176:GLU:OE1	2.07	0.54
8:G:153:GLN:CG	8:G:154:VAL:HG23	2.37	0.54
2:A:180:LYS:NZ	2:A:294:SER:HB3	2.22	0.54
2:A:406:ILE:HG22	2:A:412:ARG:HA	1.88	0.54
2:A:605:MET:HG2	2:A:621:THR:CG2	2.36	0.54
2:A:718:VAL:O	2:A:722:LEU:HD12	2.06	0.54
3:B:244:LEU:HD11	3:B:366:GLN:HE22	1.72	0.54
3:B:639:ILE:HG22	3:B:641:GLU:HG2	1.89	0.54
4:C:45:ALA:O	4:C:159:ALA:HA	2.07	0.54
7:F:68:THR:OG1	7:F:68:THR:O	2.23	0.54
8:G:1:MET:O	8:G:3:PHE:CD1	2.60	0.54
10:I:55:THR:HG22	10:I:58:VAL:CG2	2.38	0.54
10:I:85:PHE:CD1	10:I:99:LEU:HD13	2.42	0.54
2:A:69:THR:O	2:A:71:GLN:N	2.40	0.54
2:A:720:ARG:HB3	2:A:720:ARG:CZ	2.37	0.54
8:G:1:MET:SD	8:G:1:MET:C	2.90	0.54
8:G:143:ILE:CG2	8:G:144:ARG:N	2.63	0.54
2:A:18:GLN:HB2	3:B:1215:ARG:HB2	1.89	0.54
2:A:845:LEU:HB3	2:A:848:ILE:HD12	1.90	0.54
2:A:1041:ALA:O	2:A:1045:VAL:HG23	2.07	0.54
2:A:1063:MET:SD	2:A:1436:ILE:HG12	2.47	0.54
2:A:1293:SER:OG	2:A:1294:PRO:HD2	2.06	0.54
3:B:115:GLN:HG2	3:B:193:LYS:HB2	1.89	0.54
3:B:471:LYS:O	3:B:472:ALA:HB2	2.07	0.54
3:B:785:TYR:CD1	3:B:785:TYR:C	2.85	0.54
3:B:1117:GLN:HE21	3:B:1199:ALA:HB2	1.72	0.54
4:C:177:GLU:HB2	4:C:231:ASN:HB3	1.88	0.54
5:D:12:ARG:NE	5:D:14:ARG:HD2	2.22	0.54
6:E:10:SER:O	6:E:14:ARG:HG3	2.08	0.54
9:H:40:LEU:HD22	9:H:123:MET:HE3	1.89	0.54
10:I:69:PRO:HG2	10:I:85:PHE:CE2	2.42	0.54
12:K:6:ARG:O	12:K:8:GLU:N	2.41	0.54
2:A:17:VAL:HA	3:B:1215:ARG:O	2.08	0.54
2:A:358:ASN:O	2:A:359:LEU:HD23	2.07	0.54
2:A:382:PRO:HD3	2:A:428:TYR:HD2	1.71	0.54
2:A:1444:MET:HE1	7:F:135:ARG:NE	2.23	0.54
3:B:603:LEU:HD12	3:B:609:ILE:HG13	1.89	0.54
3:B:952:VAL:HG22	3:B:966:VAL:HG13	1.88	0.54
3:B:975:GLN:HG2	3:B:976:ILE:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:144:THR:O	2:A:146:MET:HG3	2.08	0.54
2:A:344:ARG:NH2	3:B:1120:GLU:HB2	2.22	0.54
2:A:577:ILE:O	2:A:580:VAL:HG23	2.07	0.54
2:A:1036:ARG:HG2	2:A:1036:ARG:HH11	1.72	0.54
3:B:234:ILE:HD12	3:B:234:ILE:N	2.23	0.54
3:B:479:VAL:O	3:B:480:SER:HB3	2.07	0.54
3:B:603:LEU:HD13	3:B:608:ASP:HB2	1.89	0.54
3:B:803:LEU:HB2	3:B:1032:SER:OG	2.06	0.54
3:B:1001:PHE:CD2	4:C:34:ARG:NH2	2.75	0.54
3:B:1201:LYS:HE2	3:B:1205:GLN:CD	2.33	0.54
6:E:145:THR:HG21	6:E:187:TYR:CD2	2.42	0.54
6:E:197:LYS:HE2	6:E:199:ILE:HD11	1.90	0.54
7:F:99:LEU:O	7:F:103:MET:HG2	2.08	0.54
9:H:139:ASN:O	9:H:140:ALA:HB2	2.08	0.54
10:I:14:LEU:HA	10:I:28:GLU:O	2.08	0.54
2:A:93:VAL:HG21	2:A:301:ALA:O	2.08	0.54
3:B:24:PRO:O	3:B:655:LYS:HB2	2.07	0.54
5:D:8:PHE:CE2	8:G:73:LYS:HD3	2.42	0.54
9:H:61:SER:O	9:H:62:SER:CB	2.56	0.54
12:K:111:LEU:HD12	12:K:111:LEU:O	2.08	0.54
2:A:75:ASN:O	2:A:76:GLU:CB	2.56	0.54
2:A:504:LEU:HD11	7:F:91:ALA:CB	2.37	0.54
2:A:1260:LEU:HD12	2:A:1260:LEU:O	2.07	0.54
2:A:1329:THR:HG23	2:A:1331:SER:H	1.69	0.54
3:B:661:LEU:HD23	3:B:679:TYR:O	2.08	0.54
3:B:1084:GLN:H	3:B:1084:GLN:HE21	1.54	0.54
4:C:165:LYS:O	12:K:6:ARG:NH1	2.40	0.54
8:G:88:ASP:HB3	8:G:144:ARG:HA	1.89	0.54
2:A:774:ARG:O	2:A:775:ILE:C	2.51	0.54
2:A:974:ASP:HB2	9:H:136:LYS:NZ	2.23	0.54
2:A:1038:THR:H	2:A:1041:ALA:HB3	1.72	0.54
2:A:1118:VAL:HG12	2:A:1327:ILE:HG13	1.89	0.54
2:A:1364:ASN:O	2:A:1365:TYR:C	2.51	0.54
3:B:102:VAL:HG23	3:B:112:LEU:HB2	1.89	0.54
3:B:344:LYS:O	3:B:346:GLU:N	2.41	0.54
3:B:549:THR:HB	3:B:628:THR:OG1	2.07	0.54
3:B:852:ARG:NH2	13:L:70:ARG:OXT	2.37	0.54
3:B:1182:CYS:O	3:B:1183:LYS:O	2.26	0.54
4:C:22:LEU:HD13	4:C:230:MET:HE1	1.89	0.54
4:C:142:VAL:H	11:J:16:ASP:HB3	1.72	0.54
13:L:61:THR:HG22	13:L:62:LYS:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:79:GLY:HA3	2:A:243:PRO:CG	2.38	0.54
2:A:351:THR:HG21	3:B:1103:ILE:HG13	1.90	0.54
2:A:399:HIS:HB3	2:A:400:PRO:CD	2.32	0.54
2:A:492:PRO:HB3	2:A:501:LEU:CD1	2.38	0.54
2:A:524:VAL:HG12	2:A:525:GLN:N	2.19	0.54
2:A:596:THR:C	2:A:598:LEU:N	2.66	0.54
2:A:1048:ASN:O	2:A:1049:ILE:C	2.51	0.54
3:B:265:SER:O	3:B:266:ALA:HB3	2.08	0.54
3:B:521:LEU:HB3	3:B:633:VAL:CG1	2.38	0.54
3:B:955:THR:HG23	3:B:956:THR:H	1.73	0.54
3:B:983:ARG:HD2	3:B:1091:TYR:CD2	2.43	0.54
3:B:1022:THR:HG23	3:B:1022:THR:O	2.08	0.54
2:A:1323:ASP:O	2:A:1325:THR:N	2.41	0.53
3:B:311:LEU:O	3:B:312:GLU:C	2.51	0.53
3:B:842:ASN:O	3:B:846:ILE:HG13	2.09	0.53
3:B:1005:GLY:HA2	4:C:176:ILE:O	2.07	0.53
10:I:13:MET:HE3	10:I:14:LEU:H	1.74	0.53
11:J:8:PHE:H	11:J:49:MET:HE3	1.73	0.53
2:A:50:ILE:C	2:A:52:GLY:N	2.62	0.53
2:A:84:ILE:O	2:A:84:ILE:CG2	2.56	0.53
2:A:541:ILE:HG21	2:A:549:MET:CE	2.39	0.53
2:A:551:TYR:CE2	12:K:62:LYS:HG2	2.44	0.53
2:A:1074:GLU:N	2:A:1075:PRO:HD2	2.23	0.53
2:A:1102:LYS:O	2:A:1106:ASN:ND2	2.41	0.53
2:A:1151:GLU:HA	10:I:44:TYR:O	2.08	0.53
3:B:254:LEU:HD23	3:B:381:MET:HE1	1.88	0.53
3:B:680:THR:O	3:B:684:LEU:CD1	2.57	0.53
3:B:737:THR:HG21	10:I:66:PRO:HA	1.88	0.53
4:C:221:TYR:CE1	4:C:222:LYS:HG3	2.43	0.53
7:F:69:LEU:CG	7:F:71:GLU:HB2	2.39	0.53
8:G:79:PHE:HE2	8:G:105:PRO:HG2	1.74	0.53
2:A:34:LYS:HB3	2:A:36:ARG:HE	1.73	0.53
2:A:152:VAL:HG13	2:A:153:PRO:HD2	1.91	0.53
2:A:265:LYS:N	2:A:265:LYS:HD2	2.23	0.53
2:A:482:PHE:C	2:A:484:GLY:H	2.16	0.53
2:A:503:GLN:C	2:A:504:LEU:HD12	2.33	0.53
2:A:567:LYS:CG	2:A:568:PRO:CD	2.81	0.53
3:B:36:ALA:HA	3:B:39:ARG:HD2	1.90	0.53
3:B:653:VAL:HG22	3:B:689:LEU:HD22	1.88	0.53
3:B:983:ARG:HH11	3:B:1091:TYR:CB	2.21	0.53
4:C:179:GLU:HG2	4:C:180:TYR:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:130:LEU:C	5:D:132:GLN:H	2.15	0.53
6:E:14:ARG:HH21	6:E:141:VAL:CG1	2.19	0.53
7:F:148:VAL:HG23	7:F:149:GLU:N	2.22	0.53
9:H:81:PRO:HB2	9:H:82:PRO:HD2	1.88	0.53
2:A:34:LYS:NZ	2:A:57:ARG:HH22	2.02	0.53
2:A:547:LEU:HD22	12:K:58:PHE:CD1	2.43	0.53
2:A:852:TYR:CE2	2:A:1060:PRO:HB2	2.43	0.53
2:A:1130:GLN:O	2:A:1134:ILE:HG13	2.08	0.53
2:A:1409:LEU:O	2:A:1412:ALA:HB3	2.09	0.53
3:B:446:LEU:O	3:B:447:ALA:HB3	2.07	0.53
6:E:124:VAL:HB	6:E:125:PRO:CD	2.38	0.53
7:F:109:VAL:CG1	7:F:110:ASP:N	2.68	0.53
7:F:131:PRO:C	7:F:132:LEU:HD23	2.33	0.53
8:G:88:ASP:OD2	8:G:88:ASP:N	2.40	0.53
10:I:98:VAL:HG12	10:I:99:LEU:N	2.24	0.53
2:A:567:LYS:HG3	2:A:568:PRO:HD2	1.88	0.53
2:A:567:LYS:HE3	9:H:46:LEU:HB2	1.91	0.53
2:A:1097:GLY:O	2:A:1100:ARG:HB3	2.08	0.53
3:B:44:VAL:O	3:B:45:SER:C	2.52	0.53
3:B:683:SER:O	3:B:687:GLU:HB2	2.09	0.53
3:B:992:ILE:HG12	3:B:993:THR:N	2.23	0.53
4:C:133:ILE:CD1	4:C:237:SER:HA	2.39	0.53
5:D:191:ALA:C	5:D:193:THR:H	2.16	0.53
7:F:69:LEU:HD13	7:F:72:LYS:HB2	1.90	0.53
2:A:38:PRO:HB3	2:A:270:LEU:HG	1.91	0.53
2:A:316:GLN:HB2	2:A:322:VAL:CG2	2.38	0.53
2:A:356:ASP:HB2	2:A:469:ARG:HH12	1.72	0.53
2:A:385:ILE:CD1	2:A:426:LEU:HB2	2.38	0.53
2:A:709:THR:CG2	2:A:711:ARG:HB2	2.39	0.53
2:A:786:HIS:CD2	3:B:703:ILE:HB	2.44	0.53
2:A:899:VAL:CG1	2:A:908:LEU:HD21	2.39	0.53
2:A:1141:THR:OG1	2:A:1205:LYS:HD3	2.08	0.53
2:A:1410:PHE:C	2:A:1412:ALA:H	2.16	0.53
3:B:912:ILE:O	3:B:938:SER:HB3	2.09	0.53
3:B:1129:ARG:HG2	3:B:1131:GLY:H	1.74	0.53
5:D:173:HIS:O	5:D:177:VAL:HG23	2.07	0.53
6:E:161:LYS:HD2	6:E:195:VAL:HG23	1.89	0.53
6:E:164:LEU:HD11	6:E:211:TYR:CE1	2.43	0.53
10:I:15:TYR:N	10:I:15:TYR:CD1	2.77	0.53
11:J:8:PHE:H	11:J:49:MET:CE	2.21	0.53
2:A:61:ILE:CG2	2:A:62:ASP:H	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:68:GLN:O	2:A:70:CYS:N	2.41	0.53
2:A:699:ALA:O	2:A:700:ASN:CB	2.57	0.53
3:B:25:ILE:HD11	3:B:653:VAL:C	2.34	0.53
3:B:38:PHE:HD1	3:B:811:TYR:CD2	2.27	0.53
3:B:797:TYR:HE1	3:B:854:LEU:CD2	2.21	0.53
3:B:911:ILE:HD11	3:B:941:LEU:CD1	2.34	0.53
3:B:1039:GLY:HA2	11:J:51:LEU:CD2	2.38	0.53
6:E:93:MET:HE2	6:E:120:ALA:HB1	1.90	0.53
8:G:30:LEU:O	8:G:34:VAL:HG23	2.09	0.53
9:H:89:LEU:C	9:H:91:ASP:N	2.65	0.53
2:A:899:VAL:HG13	2:A:908:LEU:HD21	1.91	0.53
2:A:1445:ILE:HD12	2:A:1445:ILE:N	2.20	0.53
3:B:516:ASN:ND2	3:B:516:ASN:H	2.06	0.53
3:B:563:MET:HE3	3:B:580:VAL:HB	1.91	0.53
9:H:116:TYR:HE2	9:H:140:ALA:CB	2.21	0.53
13:L:61:THR:CG2	13:L:63:ARG:HG2	2.39	0.53
3:B:295:GLY:H	3:B:298:LEU:HD23	1.73	0.53
3:B:570:VAL:CG2	3:B:573:GLN:HB3	2.38	0.53
3:B:601:ARG:HG2	3:B:615:MET:HE1	1.90	0.53
3:B:1174:LYS:O	3:B:1176:ASN:N	2.42	0.53
5:D:64:VAL:C	5:D:66:ARG:H	2.17	0.53
7:F:69:LEU:CD2	7:F:71:GLU:C	2.82	0.53
2:A:262:LEU:C	2:A:264:PHE:H	2.16	0.53
2:A:622:VAL:O	2:A:622:VAL:CG1	2.57	0.53
2:A:873:MET:C	2:A:1058:VAL:HG23	2.33	0.53
3:B:172:ILE:HD13	3:B:178:ASN:HB3	1.91	0.53
3:B:578:THR:C	3:B:589:VAL:HG13	2.33	0.53
4:C:241:ASP:O	4:C:245:VAL:HG23	2.09	0.53
5:D:167:LEU:O	5:D:170:THR:OG1	2.26	0.53
8:G:1:MET:O	8:G:1:MET:HE2	2.08	0.53
8:G:96:GLN:HB3	8:G:121:PHE:CE2	2.44	0.53
12:K:46:ILE:O	12:K:46:ILE:HG22	2.09	0.53
2:A:219:PHE:CE2	2:A:231:PRO:HD2	2.45	0.52
2:A:381:THR:HG22	2:A:384:ASN:ND2	2.24	0.52
2:A:427:GLN:HG3	2:A:430:TRP:CE2	2.44	0.52
2:A:1280:GLU:O	2:A:1281:ARG:C	2.52	0.52
3:B:129:PHE:HA	3:B:165:VAL:O	2.08	0.52
3:B:189:LEU:HA	3:B:192:LEU:HD12	1.91	0.52
3:B:460:ALA:C	3:B:462:ALA:H	2.17	0.52
3:B:542:MET:HE3	3:B:636:PRO:HG2	1.90	0.52
3:B:840:ILE:HG21	3:B:994:TYR:HD1	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:143:PHE:C	7:F:143:PHE:HD1	2.17	0.52
2:A:682:THR:HA	2:A:685:GLU:HG2	1.91	0.52
2:A:741:ASN:HD22	2:A:741:ASN:C	2.17	0.52
2:A:1121:GLU:CG	2:A:1122:PRO:HD2	2.35	0.52
4:C:242:GLN:C	4:C:244:VAL:N	2.66	0.52
1:R:6:C:O2	1:R:6:C:H2'	2.08	0.52
2:A:34:LYS:CB	2:A:36:ARG:HE	2.22	0.52
2:A:135:PHE:HA	2:A:138:ILE:HD12	1.91	0.52
2:A:629:LEU:HD22	2:A:633:VAL:CG2	2.39	0.52
2:A:1280:GLU:O	2:A:1282:VAL:HG23	2.09	0.52
3:B:979:LYS:HG2	3:B:1095:LEU:CD1	2.37	0.52
5:D:59:ILE:HG21	5:D:145:MET:SD	2.50	0.52
8:G:80:LYS:O	8:G:80:LYS:HG2	2.08	0.52
8:G:110:VAL:HG22	8:G:161:GLY:O	2.08	0.52
11:J:18:TRP:NE1	11:J:22:LEU:HD22	2.24	0.52
2:A:53:LEU:O	2:A:54:ASN:C	2.53	0.52
2:A:172:PRO:HB3	2:A:185:TRP:CD2	2.45	0.52
2:A:511:ILE:HA	2:A:521:MET:HE3	1.91	0.52
2:A:785:PRO:HG2	2:A:786:HIS:CD2	2.45	0.52
2:A:1313:LEU:C	2:A:1315:GLU:H	2.17	0.52
3:B:604:ARG:NH1	3:B:691:GLU:OE2	2.42	0.52
3:B:613:VAL:HG22	3:B:628:THR:HA	1.92	0.52
3:B:654:ARG:HG3	3:B:654:ARG:NH1	2.23	0.52
3:B:705:MET:HE2	3:B:745:PRO:HB3	1.91	0.52
4:C:56:THR:HG22	4:C:57:VAL:N	2.23	0.52
4:C:249:ASP:O	4:C:252:GLN:HB3	2.09	0.52
6:E:13:TRP:O	6:E:16:PHE:HB3	2.09	0.52
8:G:1:MET:HE1	8:G:80:LYS:N	2.23	0.52
8:G:7:LEU:HD11	8:G:45:ILE:HD11	1.92	0.52
2:A:58:LEU:O	2:A:59:GLY:O	2.28	0.52
2:A:337:ARG:HD3	3:B:1132:GLU:OE1	2.09	0.52
2:A:682:THR:HG23	2:A:728:LYS:HE3	1.92	0.52
2:A:1118:VAL:O	2:A:1305:VAL:HG13	2.10	0.52
3:B:31:TRP:CE3	3:B:34:ILE:HD12	2.45	0.52
3:B:684:LEU:O	3:B:689:LEU:HB2	2.10	0.52
3:B:996:ARG:HG2	3:B:1007:VAL:HG11	1.91	0.52
6:E:177:ARG:C	6:E:212:ARG:HD3	2.34	0.52
12:K:58:PHE:HE2	12:K:74:ARG:HE	1.53	0.52
2:A:22:PHE:CE2	2:A:30:ILE:HD12	2.45	0.52
2:A:56:PRO:O	2:A:57:ARG:HG3	2.09	0.52
2:A:332:LYS:HB2	2:A:337:ARG:NH1	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:848:ILE:HB	2:A:1065:GLY:HA3	1.91	0.52
2:A:870:GLU:HB2	6:E:204:THR:HG21	1.92	0.52
2:A:1006:ILE:HD11	6:E:163:GLU:HG3	1.91	0.52
2:A:1454:MET:O	2:A:1454:MET:HG3	2.09	0.52
3:B:129:PHE:HE2	3:B:166:PHE:HD1	1.58	0.52
3:B:957:ASN:O	3:B:958:GLN:C	2.51	0.52
3:B:1084:GLN:OE1	4:C:189:THR:CG2	2.58	0.52
3:B:1192:TYR:N	3:B:1192:TYR:CD1	2.77	0.52
4:C:239:PRO:O	4:C:241:ASP:N	2.43	0.52
8:G:15:PRO:HA	8:G:18:PHE:HD1	1.70	0.52
9:H:12:VAL:HG13	9:H:26:ILE:CG2	2.39	0.52
2:A:88:LYS:HE3	2:A:280:GLU:OE2	2.10	0.52
2:A:344:ARG:CZ	3:B:1120:GLU:HB2	2.40	0.52
2:A:384:ASN:OD1	2:A:388:LEU:HD12	2.09	0.52
2:A:442:VAL:CG2	2:A:460:VAL:HG23	2.40	0.52
2:A:590:ARG:HH22	2:A:620:LYS:HB3	1.74	0.52
2:A:844:ALA:C	2:A:845:LEU:HD23	2.35	0.52
3:B:363:HIS:CD2	3:B:585:VAL:HG22	2.44	0.52
3:B:558:LEU:O	3:B:560:GLU:N	2.43	0.52
3:B:579:ARG:CB	3:B:586:TRP:HE1	2.23	0.52
3:B:792:MET:HA	3:B:856:PHE:O	2.09	0.52
3:B:860:MET:HG2	3:B:861:ASP:N	2.25	0.52
3:B:944:THR:HG21	3:B:1122:ARG:CZ	2.40	0.52
6:E:30:ILE:HG22	6:E:31:THR:N	2.24	0.52
6:E:135:PHE:HD2	6:E:140:LEU:HD21	1.73	0.52
8:G:44:TYR:O	8:G:78:VAL:HG12	2.09	0.52
8:G:122:ASN:HD22	8:G:125:SER:HB3	1.74	0.52
10:I:55:THR:HG22	10:I:55:THR:O	2.10	0.52
2:A:757:ASN:OD1	3:B:1021:MET:HG3	2.10	0.52
2:A:1042:PHE:CE2	2:A:1046:LEU:HD11	2.45	0.52
2:A:1222:ASN:O	2:A:1223:ASP:HB3	2.10	0.52
2:A:1418:LEU:HD12	2:A:1419:ASP:H	1.75	0.52
3:B:22:SER:HA	3:B:654:ARG:CB	2.40	0.52
3:B:211:VAL:O	3:B:480:SER:HA	2.10	0.52
3:B:865:LYS:HE2	3:B:871:THR:OG1	2.09	0.52
6:E:157:SER:C	6:E:159:ASP:N	2.68	0.52
2:A:262:LEU:C	2:A:264:PHE:N	2.67	0.52
2:A:873:MET:HG3	2:A:1056:SER:O	2.10	0.52
2:A:899:VAL:HG22	2:A:1029:ARG:HG2	1.92	0.52
2:A:1059:HIS:ND1	7:F:86:THR:HA	2.24	0.52
3:B:172:ILE:HG22	3:B:173:MET:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:428:ILE:HG22	3:B:432:MET:HE2	1.91	0.52
3:B:1047:PHE:CD1	3:B:1047:PHE:N	2.77	0.52
3:B:1172:ILE:HG22	3:B:1172:ILE:O	2.09	0.52
4:C:35:ARG:NH1	12:K:41:THR:H	2.07	0.52
5:D:151:PHE:CD1	5:D:151:PHE:N	2.78	0.52
6:E:136:ASN:OD1	6:E:137:GLU:N	2.43	0.52
7:F:135:ARG:HG2	7:F:137:TYR:CE1	2.43	0.52
2:A:786:HIS:CD2	2:A:786:HIS:N	2.77	0.52
2:A:1005:GLU:O	2:A:1009:ASN:HB2	2.09	0.52
2:A:1144:LYS:HB2	2:A:1268:LEU:O	2.10	0.52
2:A:1293:SER:OG	2:A:1295:THR:HG23	2.10	0.52
2:A:1446:ASP:HB2	7:F:133:VAL:HG23	1.91	0.52
3:B:240:ILE:HG23	3:B:240:ILE:O	2.09	0.52
3:B:487:THR:CG2	3:B:488:TYR:N	2.72	0.52
4:C:3:GLU:O	4:C:4:GLU:CB	2.58	0.52
4:C:213:PRO:O	4:C:214:ASN:CB	2.56	0.52
7:F:109:VAL:CG1	7:F:110:ASP:H	2.17	0.52
2:A:75:ASN:O	2:A:76:GLU:HB3	2.10	0.51
2:A:1272:THR:C	2:A:1273:LEU:HD12	2.35	0.51
8:G:127:PRO:HG2	8:G:138:THR:CG2	2.32	0.51
9:H:11:GLN:HA	9:H:53:ASP:O	2.10	0.51
2:A:24:PRO:HD2	2:A:233:TRP:CD1	2.45	0.51
2:A:119:ASN:O	2:A:122:MET:HB3	2.10	0.51
2:A:218:ASP:O	2:A:219:PHE:C	2.52	0.51
2:A:285:PRO:HG2	2:A:288:ALA:HB3	1.92	0.51
2:A:372:LYS:HA	2:A:435:HIS:HD1	1.74	0.51
2:A:548:ASN:OD1	12:K:60:ALA:HB1	2.11	0.51
2:A:709:THR:HG21	10:I:93:LYS:O	2.11	0.51
2:A:1006:ILE:HD12	6:E:163:GLU:HG3	1.91	0.51
3:B:37:PHE:CD1	3:B:37:PHE:C	2.85	0.51
3:B:798:TYR:CE2	4:C:62:PHE:HE2	2.28	0.51
5:D:67:ARG:HB2	5:D:133:THR:HG21	1.91	0.51
6:E:116:ILE:O	6:E:121:MET:HE2	2.10	0.51
10:I:82:GLU:O	10:I:104:LEU:HG	2.09	0.51
2:A:152:VAL:HG12	2:A:153:PRO:HD2	1.92	0.51
2:A:262:LEU:O	2:A:264:PHE:N	2.44	0.51
2:A:618:GLU:OE1	2:A:620:LYS:HG3	2.10	0.51
2:A:965:GLN:O	2:A:968:GLN:HB2	2.10	0.51
2:A:1017:LEU:CB	6:E:206:GLY:H	2.18	0.51
3:B:95:ILE:HG13	3:B:130:VAL:HG22	1.91	0.51
3:B:102:VAL:HG12	3:B:104:GLU:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:36:VAL:CG2	4:C:251:LEU:HD22	2.33	0.51
4:C:248:ILE:HG23	12:K:98:LEU:HD22	1.92	0.51
7:F:111:LEU:H	7:F:111:LEU:CD1	2.23	0.51
9:H:100:THR:CG2	9:H:101:ALA:N	2.73	0.51
9:H:145:ARG:O	9:H:146:ARG:HB2	2.10	0.51
2:A:332:LYS:O	2:A:333:GLU:HB2	2.09	0.51
2:A:552:TRP:NE1	12:K:62:LYS:HB2	2.23	0.51
2:A:590:ARG:NH2	2:A:620:LYS:HB3	2.23	0.51
2:A:873:MET:HG2	2:A:957:PRO:HB3	1.93	0.51
3:B:542:MET:HG2	3:B:747:MET:HB3	1.92	0.51
3:B:622:LYS:HE2	10:I:59:VAL:CG2	2.35	0.51
4:C:234:SER:HB3	4:C:240:VAL:HG13	1.93	0.51
6:E:29:PHE:C	6:E:30:ILE:HG13	2.35	0.51
8:G:87:VAL:HG23	8:G:103:VAL:HG21	1.91	0.51
8:G:101:VAL:HG12	8:G:102:GLN:N	2.24	0.51
4:C:101:LEU:C	4:C:102:GLN:HG3	2.34	0.51
6:E:93:MET:HE3	6:E:120:ALA:O	2.11	0.51
7:F:69:LEU:CB	7:F:72:LYS:HB2	2.40	0.51
9:H:15:VAL:HG22	9:H:26:ILE:CD1	2.41	0.51
9:H:47:PHE:CD2	9:H:95:TYR:HD1	2.29	0.51
11:J:48:ARG:HE	11:J:49:MET:CE	2.23	0.51
1:R:7:U:P	3:B:942:ARG:HH22	2.34	0.51
2:A:438:ASP:OD1	2:A:461:LYS:HA	2.10	0.51
2:A:853:ASP:CG	2:A:855:THR:HG22	2.34	0.51
2:A:1242:VAL:HG12	2:A:1243:VAL:H	1.75	0.51
3:B:169:ARG:HD2	3:B:454:THR:HG21	1.92	0.51
3:B:893:LEU:HD11	3:B:910:VAL:HG11	1.92	0.51
3:B:1034:VAL:HG12	3:B:1035:ALA:N	2.23	0.51
2:A:90:VAL:HG11	2:A:297:GLN:HA	1.91	0.51
2:A:547:LEU:HD22	12:K:58:PHE:HE1	1.73	0.51
2:A:696:GLU:OE2	2:A:702:LEU:HD21	2.11	0.51
2:A:722:LEU:HD22	2:A:799:PHE:CD1	2.45	0.51
3:B:253:THR:HG22	3:B:254:LEU:N	2.26	0.51
3:B:641:GLU:HB3	3:B:643:ASP:OD2	2.11	0.51
2:A:334:GLY:O	2:A:336:ILE:N	2.43	0.51
2:A:512:VAL:O	2:A:512:VAL:HG12	2.11	0.51
2:A:669:THR:O	2:A:805:LEU:HD22	2.10	0.51
3:B:51:PHE:CD2	3:B:173:MET:HB3	2.46	0.51
3:B:100:PRO:CD	3:B:180:TYR:HE1	2.22	0.51
3:B:1081:LEU:O	3:B:1082:MET:C	2.52	0.51
12:K:41:THR:HG22	12:K:42:LEU:N	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:32:ALA:CB	13:L:55:ILE:HD12	2.26	0.51
2:A:87:ALA:CB	2:A:276:LEU:HD23	2.41	0.51
2:A:148:CYS:O	2:A:168:GLY:HA2	2.10	0.51
2:A:982:THR:O	2:A:985:ASP:HB2	2.11	0.51
2:A:1273:LEU:HD12	2:A:1273:LEU:N	2.26	0.51
3:B:244:LEU:HD21	3:B:366:GLN:HE21	1.76	0.51
3:B:299:GLU:OE2	3:B:572:HIS:HE1	1.93	0.51
3:B:570:VAL:HG23	3:B:573:GLN:HB3	1.92	0.51
3:B:878:GLN:O	3:B:879:ARG:C	2.52	0.51
3:B:1154:ALA:O	3:B:1155:SER:HB2	2.10	0.51
6:E:169:ARG:NH1	7:F:74:ILE:HD11	2.25	0.51
7:F:118:LEU:HD12	7:F:118:LEU:O	2.11	0.51
8:G:91:VAL:HG23	8:G:141:SER:O	2.10	0.51
9:H:83:GLN:O	9:H:85:GLY:N	2.41	0.51
2:A:343:LYS:HZ2	3:B:1151:LEU:HB3	1.76	0.51
2:A:782:ARG:NH2	3:B:699:GLU:O	2.42	0.51
3:B:781:PHE:HE2	3:B:793:ALA:HB1	1.75	0.51
3:B:1073:TYR:CE2	3:B:1080:LYS:HG2	2.45	0.51
4:C:10:ILE:CD1	12:K:108:GLU:HB3	2.41	0.51
5:D:23:ASN:O	8:G:83:LYS:HB2	2.11	0.51
5:D:208:GLU:O	5:D:212:LYS:HG3	2.11	0.51
10:I:50:THR:HG22	10:I:51:ASN:N	2.26	0.51
12:K:21:ILE:CG1	12:K:33:ILE:HG23	2.41	0.51
12:K:31:VAL:CG1	12:K:32:VAL:N	2.73	0.51
2:A:870:GLU:HG2	6:E:208:TYR:CD2	2.45	0.50
2:A:929:LEU:CD2	2:A:983:ILE:HG21	2.41	0.50
2:A:1265:ASN:C	2:A:1267:MET:N	2.67	0.50
3:B:288:ALA:O	3:B:331:LEU:HD11	2.10	0.50
3:B:547:VAL:HG13	3:B:548:GLY:N	2.26	0.50
3:B:562:GLY:HA3	3:B:590:HIS:CE1	2.46	0.50
3:B:755:ILE:HG23	3:B:809:MET:HE3	1.92	0.50
3:B:995:ARG:NH1	4:C:165:LYS:HG2	2.25	0.50
4:C:18:VAL:O	4:C:19:ASP:C	2.52	0.50
4:C:60:ASP:OD1	13:L:60:ARG:NH2	2.40	0.50
4:C:132:PRO:O	4:C:133:ILE:C	2.54	0.50
4:C:160:LYS:O	4:C:161:LYS:O	2.29	0.50
4:C:251:LEU:O	4:C:255:VAL:HG23	2.11	0.50
9:H:63:LEU:HB3	9:H:90:ALA:HB3	1.93	0.50
2:A:107:CYS:N	2:A:114:LEU:HD21	2.26	0.50
2:A:254:GLU:HB2	3:B:935:ARG:HH22	1.76	0.50
2:A:709:THR:HB	2:A:712:GLU:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:806:ARG:NH1	3:B:729:ILE:HG13	2.25	0.50
2:A:899:VAL:CG1	2:A:929:LEU:HD11	2.41	0.50
2:A:1236:LEU:C	2:A:1237:ILE:HG13	2.36	0.50
3:B:175:ARG:HG2	3:B:175:ARG:NH1	2.25	0.50
3:B:245:GLU:C	3:B:246:LYS:HG3	2.37	0.50
3:B:343:ILE:HG22	3:B:348:ARG:HG3	1.91	0.50
3:B:446:LEU:N	3:B:446:LEU:HD23	2.26	0.50
3:B:899:ILE:CG2	3:B:949:VAL:HG21	2.42	0.50
3:B:1010:LEU:O	3:B:1011:ILE:CG1	2.60	0.50
3:B:1034:VAL:C	3:B:1036:ALA:H	2.18	0.50
5:D:59:ILE:HG22	5:D:60:LYS:N	2.26	0.50
6:E:197:LYS:HG3	6:E:211:TYR:CE2	2.47	0.50
8:G:83:LYS:HE2	8:G:150:CYS:H	1.77	0.50
2:A:44:THR:O	2:A:45:GLN:HB2	2.10	0.50
2:A:528:LEU:HD23	2:A:751:SER:CA	2.41	0.50
2:A:588:LEU:O	2:A:606:LEU:HD12	2.11	0.50
2:A:1436:ILE:O	2:A:1437:GLY:C	2.53	0.50
3:B:29:ASP:O	3:B:30:SER:C	2.53	0.50
3:B:29:ASP:HB3	3:B:658:ILE:CD1	2.41	0.50
3:B:303:TYR:CD2	3:B:303:TYR:N	2.78	0.50
5:D:12:ARG:HG2	5:D:14:ARG:HG3	1.94	0.50
13:L:27:LEU:HD23	13:L:27:LEU:N	2.25	0.50
2:A:535:THR:O	2:A:575:LYS:HG3	2.12	0.50
2:A:683:ILE:HD13	2:A:801:GLU:HG3	1.94	0.50
2:A:836:TYR:CZ	2:A:840:ARG:HD2	2.46	0.50
2:A:1067:LEU:HD12	2:A:1367:HIS:CE1	2.46	0.50
3:B:129:PHE:HE2	3:B:166:PHE:CD1	2.29	0.50
3:B:611:PRO:CB	3:B:685:LEU:HD21	2.41	0.50
3:B:1045:SER:O	3:B:1046:PRO:O	2.29	0.50
5:D:8:PHE:CE2	5:D:40:HIS:HA	2.47	0.50
5:D:56:ARG:HA	5:D:148:LEU:HD13	1.94	0.50
6:E:39:LEU:O	6:E:42:PHE:HB3	2.10	0.50
6:E:202:SER:HB3	6:E:205:SER:O	2.12	0.50
8:G:149:GLY:O	8:G:159:ALA:HB1	2.11	0.50
2:A:12:ARG:CZ	3:B:1192:TYR:HE2	2.24	0.50
2:A:541:ILE:CD1	2:A:549:MET:HE1	2.38	0.50
2:A:1225:PHE:HE2	2:A:1227:ILE:HD11	1.76	0.50
2:A:1323:ASP:C	2:A:1325:THR:N	2.69	0.50
2:A:1445:ILE:HD11	8:G:68:ALA:CB	2.39	0.50
3:B:409:ALA:O	3:B:413:LEU:HG	2.11	0.50
3:B:449:ASN:C	3:B:451:LYS:H	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:117:GLN:C	8:G:119:LEU:N	2.69	0.50
11:J:47:ARG:HG2	11:J:47:ARG:HH11	1.77	0.50
2:A:49:LYS:HZ1	2:A:61:ILE:N	2.09	0.50
2:A:70:CYS:O	2:A:70:CYS:SG	2.70	0.50
2:A:207:ILE:HG22	2:A:211:PHE:CE1	2.47	0.50
2:A:785:PRO:HG2	2:A:786:HIS:HD2	1.77	0.50
2:A:921:GLY:O	2:A:922:ASP:C	2.54	0.50
2:A:1124:HIS:HB3	2:A:1130:GLN:HG2	1.94	0.50
2:A:1443:VAL:C	2:A:1444:MET:HG3	2.36	0.50
3:B:654:ARG:H	3:B:657:HIS:HD2	1.59	0.50
3:B:744:HIS:ND1	3:B:745:PRO:HD2	2.26	0.50
9:H:105:GLU:HG2	9:H:106:GLU:H	1.77	0.50
9:H:130:ARG:H	9:H:130:ARG:CD	2.10	0.50
2:A:89:PRO:C	2:A:204:THR:HG21	2.37	0.50
2:A:172:PRO:HG3	2:A:185:TRP:CZ2	2.46	0.50
2:A:325:ILE:CG2	3:B:1210:MET:HE2	2.41	0.50
2:A:339:ASN:HB3	3:B:1117:GLN:NE2	2.25	0.50
2:A:511:ILE:HG12	2:A:521:MET:HE3	1.94	0.50
3:B:166:PHE:C	3:B:167:ILE:HG13	2.36	0.50
3:B:705:MET:H	3:B:710:LEU:HD12	1.76	0.50
3:B:1081:LEU:HD12	3:B:1085:ILE:HD11	1.92	0.50
4:C:113:VAL:O	4:C:144:ILE:HB	2.12	0.50
5:D:51:ASN:O	5:D:52:LEU:C	2.55	0.50
2:A:49:LYS:HE2	2:A:61:ILE:HD12	1.93	0.50
2:A:89:PRO:O	2:A:204:THR:HG21	2.12	0.50
2:A:444:PHE:HB2	2:A:458:HIS:HD2	1.77	0.50
2:A:1242:VAL:HG12	2:A:1243:VAL:N	2.27	0.50
2:A:1259:MET:C	2:A:1261:LYS:H	2.20	0.50
2:A:1385:THR:HG22	2:A:1386:ARG:N	2.27	0.50
3:B:185:THR:O	3:B:188:ASP:N	2.45	0.50
3:B:286:PHE:CD1	3:B:297:ILE:HG23	2.47	0.50
3:B:388:CYS:C	3:B:390:LEU:H	2.19	0.50
3:B:582:VAL:HG23	3:B:626:ILE:HB	1.94	0.50
3:B:757:PRO:HD3	3:B:983:ARG:NH2	2.26	0.50
4:C:144:ILE:HG22	4:C:145:CYS:N	2.27	0.50
6:E:86:PRO:O	6:E:114:ASN:HB2	2.12	0.50
8:G:145:VAL:CG1	8:G:146:LYS:N	2.74	0.50
1:R:4:U:O2	1:R:16:A:H2	1.94	0.49
2:A:108:MET:HE3	2:A:210:ILE:HD13	1.94	0.49
2:A:399:HIS:CB	2:A:400:PRO:CD	2.90	0.49
2:A:899:VAL:CG2	2:A:1029:ARG:HG2	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:284:ILE:HG23	3:B:324:ILE:CD1	2.42	0.49
3:B:309:GLN:HG3	10:I:52:ILE:HD11	1.93	0.49
3:B:1034:VAL:HG21	3:B:1055:ILE:HG23	1.93	0.49
3:B:1065:GLN:HG3	3:B:1067:ARG:H	1.76	0.49
4:C:161:LYS:O	4:C:170:TRP:NE1	2.45	0.49
13:L:40:LEU:HD22	13:L:44:ASP:CB	2.41	0.49
2:A:92:HIS:O	2:A:95:PHE:N	2.45	0.49
2:A:224:PHE:CD2	2:A:231:PRO:HG3	2.46	0.49
2:A:385:ILE:HD11	2:A:426:LEU:HB2	1.92	0.49
2:A:1120:LEU:CD1	2:A:1120:LEU:H	2.25	0.49
2:A:1156:PRO:HA	2:A:1190:PRO:CB	2.42	0.49
3:B:39:ARG:NH2	3:B:665:GLU:CG	2.75	0.49
3:B:549:THR:HG22	3:B:550:ASP:N	2.18	0.49
3:B:893:LEU:HD11	3:B:910:VAL:CG1	2.42	0.49
3:B:896:ASP:OD2	13:L:58:LYS:HE3	2.12	0.49
6:E:192:ARG:HH11	6:E:192:ARG:HG3	1.77	0.49
2:A:335:ARG:CA	2:A:339:ASN:HD22	2.24	0.49
2:A:901:LEU:O	2:A:921:GLY:N	2.34	0.49
3:B:39:ARG:HH21	3:B:665:GLU:CG	2.25	0.49
3:B:211:VAL:HG23	3:B:483:LEU:HB2	1.94	0.49
3:B:281:PRO:HB3	3:B:320:ASP:OD2	2.12	0.49
3:B:345:LYS:O	3:B:348:ARG:HB2	2.12	0.49
3:B:453:ILE:O	3:B:457:LEU:HG	2.12	0.49
3:B:616:ILE:CG1	3:B:697:GLU:HA	2.42	0.49
3:B:784:ASN:HD21	3:B:788:ARG:HD2	1.76	0.49
3:B:832:GLY:O	3:B:835:GLN:NE2	2.44	0.49
3:B:865:LYS:NZ	3:B:869:SER:HA	2.27	0.49
3:B:872:GLU:CD	3:B:914:LYS:HE2	2.37	0.49
3:B:873:THR:CG2	3:B:874:PHE:N	2.76	0.49
3:B:945:GLU:O	3:B:946:ASN:HB3	2.13	0.49
4:C:251:LEU:HD11	12:K:45:LEU:CD2	2.43	0.49
9:H:61:SER:O	9:H:62:SER:HB3	2.12	0.49
11:J:27:GLU:C	11:J:29:GLU:H	2.20	0.49
12:K:13:GLY:O	12:K:14:GLU:C	2.53	0.49
2:A:29:ALA:HB1	3:B:1184:GLY:HA2	1.93	0.49
2:A:68:GLN:C	2:A:70:CYS:N	2.70	0.49
2:A:416:ARG:C	2:A:417:TYR:CD2	2.83	0.49
2:A:537:ARG:HD2	9:H:20:TYR:HE1	1.77	0.49
2:A:629:LEU:HD22	2:A:633:VAL:HG23	1.94	0.49
2:A:1220:PHE:O	2:A:1221:LYS:HB2	2.13	0.49
2:A:1444:MET:HE1	7:F:135:ARG:HE	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:54:PHE:HA	3:B:58:THR:HB	1.94	0.49
3:B:800:GLN:HB3	11:J:52:THR:CG2	2.42	0.49
3:B:890:TYR:CZ	3:B:910:VAL:HG21	2.48	0.49
3:B:1138:MET:HE3	3:B:1143:ALA:HB3	1.94	0.49
3:B:1156:ASP:O	3:B:1157:ALA:O	2.30	0.49
4:C:114:TYR:CD2	4:C:140:ASN:HB3	2.47	0.49
4:C:238:ILE:HG23	4:C:242:GLN:HB2	1.93	0.49
6:E:29:PHE:O	6:E:30:ILE:HG13	2.12	0.49
6:E:90:VAL:O	6:E:90:VAL:HG22	2.11	0.49
7:F:77:ASP:O	7:F:78:GLN:HB2	2.12	0.49
8:G:117:GLN:O	8:G:119:LEU:N	2.46	0.49
9:H:23:VAL:HG22	9:H:43:ASN:HA	1.93	0.49
10:I:55:THR:HG23	10:I:86:PHE:CZ	2.46	0.49
12:K:12:LEU:HD12	12:K:12:LEU:N	2.28	0.49
12:K:88:LYS:O	12:K:91:CYS:HB2	2.13	0.49
2:A:78:PRO:HA	3:B:1201:LYS:HZ2	1.77	0.49
2:A:108:MET:HE3	2:A:210:ILE:HD12	1.94	0.49
2:A:537:ARG:O	2:A:540:PHE:CE1	2.66	0.49
2:A:718:VAL:O	2:A:721:PHE:HB2	2.12	0.49
2:A:765:VAL:HG23	2:A:802:ASN:O	2.12	0.49
2:A:1037:LEU:HD12	2:A:1042:PHE:HD1	1.77	0.49
2:A:1410:PHE:HA	3:B:1212:ILE:CD1	2.41	0.49
3:B:290:GLY:C	3:B:291:ILE:HG13	2.37	0.49
3:B:327:ARG:HH22	3:B:371:GLU:HG2	1.77	0.49
3:B:562:GLY:C	3:B:590:HIS:HD1	2.16	0.49
3:B:825:VAL:O	3:B:826:ALA:HB2	2.13	0.49
9:H:113:ALA:HB1	9:H:125:LEU:O	2.11	0.49
11:J:28:ASP:O	11:J:29:GLU:C	2.56	0.49
1:R:4:U:H2'	1:R:5:U:C6	2.46	0.49
2:A:54:ASN:HB3	2:A:247:ARG:HH12	1.76	0.49
2:A:283:GLY:O	2:A:285:PRO:CD	2.58	0.49
2:A:868:TYR:CE1	2:A:1064:VAL:CG1	2.95	0.49
2:A:1410:PHE:HD2	3:B:1212:ILE:HD12	1.77	0.49
3:B:295:GLY:N	3:B:298:LEU:HD23	2.27	0.49
3:B:343:ILE:CG2	3:B:348:ARG:HG3	2.42	0.49
3:B:550:ASP:OD1	3:B:552:MET:HE3	2.12	0.49
3:B:582:VAL:HG12	3:B:587:HIS:NE2	2.28	0.49
3:B:654:ARG:C	3:B:656:GLY:H	2.19	0.49
4:C:236:GLY:C	4:C:238:ILE:N	2.70	0.49
6:E:55:ARG:C	6:E:57:MET:N	2.64	0.49
8:G:27:LYS:HD3	8:G:51:TYR:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:11:LEU:O	2:A:11:LEU:HD23	2.13	0.49
2:A:862:ASN:HA	6:E:174:GLN:HB3	1.93	0.49
2:A:1032:LEU:O	2:A:1036:ARG:HD3	2.12	0.49
2:A:1343:ALA:HB1	6:E:149:LEU:HB3	1.94	0.49
3:B:185:THR:O	3:B:188:ASP:HB2	2.12	0.49
3:B:314:LEU:O	3:B:317:CYS:HB3	2.13	0.49
3:B:569:TYR:CE1	3:B:589:VAL:HG21	2.48	0.49
3:B:735:ALA:O	3:B:738:PHE:HE1	1.96	0.49
3:B:778:MET:HE2	3:B:1094:ARG:HG2	1.95	0.49
7:F:89:GLU:OE2	7:F:134:ILE:HG21	2.13	0.49
2:A:90:VAL:HG12	2:A:297:GLN:NE2	2.28	0.49
2:A:457:ALA:HB3	2:A:506:ALA:CA	2.41	0.49
2:A:535:THR:HG23	2:A:575:LYS:HG2	1.95	0.49
2:A:1120:LEU:O	2:A:1323:ASP:N	2.46	0.49
2:A:1349:TYR:CA	2:A:1372:VAL:HG21	2.42	0.49
3:B:1151:LEU:N	3:B:1151:LEU:CD1	2.75	0.49
7:F:75:PRO:O	7:F:77:ASP:O	2.30	0.49
2:A:116:ASP:C	2:A:118:HIS:N	2.67	0.49
2:A:264:PHE:O	2:A:267:ALA:HB3	2.13	0.49
2:A:442:VAL:O	2:A:457:ALA:HA	2.13	0.49
2:A:513:SER:OG	2:A:515:GLN:HG2	2.13	0.49
2:A:569:LYS:O	2:A:571:LEU:HD13	2.12	0.49
2:A:600:PRO:C	2:A:602:ASP:H	2.20	0.49
3:B:33:VAL:HG21	3:B:638:PHE:HZ	1.76	0.49
3:B:234:ILE:HG12	3:B:257:LYS:HD3	1.94	0.49
3:B:604:ARG:C	3:B:606:LYS:H	2.21	0.49
3:B:616:ILE:HG23	3:B:700:SER:OG	2.12	0.49
3:B:766:ARG:HH22	3:B:1020:ARG:NH1	2.02	0.49
3:B:882:THR:HG22	3:B:884:ARG:CB	2.42	0.49
3:B:948:ILE:O	3:B:968:VAL:HG13	2.13	0.49
3:B:956:THR:CG2	3:B:960:GLY:HA2	2.43	0.49
3:B:1196:ILE:HB	3:B:1197:PRO:HD2	1.95	0.49
4:C:183:TRP:O	4:C:185:LYS:N	2.45	0.49
5:D:207:LEU:HD12	5:D:207:LEU:O	2.13	0.49
8:G:119:LEU:HD13	8:G:132:SER:HB2	1.94	0.49
10:I:101:PHE:CE1	10:I:112:SER:HB2	2.47	0.49
2:A:90:VAL:HG13	2:A:297:GLN:CD	2.38	0.49
2:A:108:MET:N	2:A:108:MET:SD	2.85	0.49
2:A:278:THR:O	2:A:278:THR:HG22	2.13	0.49
2:A:302:THR:CG2	2:A:303:TYR:N	2.76	0.49
2:A:353:ILE:HB	2:A:470:LEU:CD2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1213:GLY:O	2:A:1214:GLU:C	2.56	0.49
2:A:1226:VAL:HG13	2:A:1239:ARG:O	2.13	0.49
3:B:581:PHE:HA	3:B:585:VAL:O	2.12	0.49
3:B:980:PHE:CA	3:B:1095:LEU:HD11	2.43	0.49
4:C:76:ASP:O	4:C:79:GLN:HG2	2.13	0.49
4:C:107:SER:C	4:C:109:SER:N	2.70	0.49
4:C:116:LYS:HD3	4:C:140:ASN:HA	1.95	0.49
7:F:138:LEU:HB2	7:F:142:SER:O	2.13	0.49
9:H:62:SER:C	9:H:64:ASN:N	2.67	0.49
10:I:73:ARG:O	10:I:81:ARG:HA	2.12	0.49
12:K:55:LYS:HB3	12:K:81:TYR:HD1	1.77	0.49
2:A:418:SER:C	2:A:420:ARG:H	2.20	0.48
2:A:1329:THR:CG2	2:A:1331:SER:HB3	2.43	0.48
3:B:871:THR:HG22	3:B:872:GLU:O	2.13	0.48
4:C:20:PHE:HE1	4:C:22:LEU:HB2	1.77	0.48
4:C:235:VAL:HG11	11:J:6:ARG:NH2	2.28	0.48
5:D:51:ASN:OD1	5:D:54:GLU:HB3	2.12	0.48
6:E:46:TYR:CE2	6:E:58:MET:HA	2.48	0.48
6:E:136:ASN:OD1	6:E:138:ALA:N	2.46	0.48
9:H:101:ALA:HB2	9:H:116:TYR:CE1	2.48	0.48
10:I:61:ASP:C	10:I:63:GLY:H	2.21	0.48
12:K:6:ARG:C	12:K:8:GLU:H	2.20	0.48
2:A:527:THR:HG21	2:A:650:GLN:HA	1.95	0.48
2:A:1017:LEU:CB	6:E:205:SER:HA	2.43	0.48
2:A:1198:ASP:HB3	2:A:1201:ALA:CB	2.41	0.48
2:A:1227:ILE:CG2	2:A:1228:TRP:H	2.21	0.48
2:A:1428:VAL:HG13	3:B:1151:LEU:CD2	2.44	0.48
2:A:1446:ASP:HB2	7:F:133:VAL:CG2	2.43	0.48
3:B:236:HIS:CE1	3:B:389:ALA:HA	2.49	0.48
3:B:459:TYR:CZ	3:B:469:GLN:HG2	2.47	0.48
3:B:1180:PHE:HB3	3:B:1191:ILE:HD12	1.95	0.48
4:C:25:VAL:HG23	4:C:228:PHE:HE1	1.77	0.48
4:C:47:ASP:CA	13:L:69:ALA:CB	2.88	0.48
4:C:70:ILE:HD11	4:C:144:ILE:CG1	2.44	0.48
4:C:138:GLU:OE1	4:C:138:GLU:N	2.46	0.48
8:G:9:LEU:HD12	8:G:10:ASN:H	1.78	0.48
10:I:16:PRO:HB3	10:I:27:PHE:HD2	1.78	0.48
12:K:21:ILE:HG12	12:K:33:ILE:HG23	1.94	0.48
2:A:635:ARG:HH11	2:A:635:ARG:HA	1.78	0.48
2:A:964:ILE:O	2:A:967:ALA:HB3	2.12	0.48
2:A:1119:TYR:HA	2:A:1305:VAL:HG13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1134:ILE:O	2:A:1138:ILE:HG13	2.12	0.48
3:B:199:MET:SD	3:B:199:MET:N	2.83	0.48
3:B:705:MET:N	3:B:710:LEU:HD12	2.29	0.48
3:B:729:ILE:O	3:B:729:ILE:HG22	2.13	0.48
3:B:1223:ASP:HB3	3:B:1224:PHE:H	1.43	0.48
10:I:4:PHE:CD1	10:I:4:PHE:C	2.91	0.48
10:I:109:ILE:HG22	10:I:109:ILE:O	2.14	0.48
11:J:43:ARG:HG3	11:J:45:CYS:SG	2.53	0.48
2:A:1118:VAL:O	2:A:1118:VAL:HG23	2.13	0.48
3:B:48:LEU:O	3:B:49:ASP:C	2.56	0.48
3:B:309:GLN:HG3	10:I:52:ILE:CD1	2.44	0.48
3:B:579:ARG:HG2	3:B:579:ARG:NH1	2.26	0.48
3:B:582:VAL:HG12	3:B:582:VAL:O	2.12	0.48
3:B:1065:GLN:NE2	3:B:1067:ARG:H	2.08	0.48
4:C:91:HIS:ND1	4:C:91:HIS:O	2.47	0.48
8:G:125:SER:OG	8:G:128:PRO:HA	2.12	0.48
2:A:34:LYS:HE3	2:A:57:ARG:HH12	1.76	0.48
2:A:51:GLY:HA2	2:A:56:PRO:HA	1.96	0.48
2:A:206:GLU:O	2:A:210:ILE:HG13	2.13	0.48
2:A:608:ILE:HG13	2:A:613:ILE:HD12	1.95	0.48
2:A:971:PHE:O	2:A:972:HIS:C	2.56	0.48
3:B:40:GLU:OE1	3:B:682:SER:HB2	2.14	0.48
3:B:113:TYR:CD2	3:B:192:LEU:HD22	2.48	0.48
3:B:309:GLN:O	3:B:312:GLU:HB3	2.13	0.48
3:B:758:PHE:CE1	3:B:1027:ILE:CG2	2.96	0.48
3:B:873:THR:HG22	3:B:874:PHE:N	2.27	0.48
10:I:69:PRO:HG2	10:I:85:PHE:CD2	2.48	0.48
2:A:42:ASP:C	2:A:44:THR:N	2.70	0.48
2:A:518:LYS:HE2	2:A:624:SER:O	2.13	0.48
2:A:578:LEU:HD23	2:A:612:ILE:HD11	1.95	0.48
2:A:709:THR:HG21	2:A:711:ARG:HB2	1.96	0.48
2:A:718:VAL:HG12	2:A:722:LEU:HD11	1.95	0.48
2:A:1116:LEU:CB	2:A:1308:THR:HG21	2.43	0.48
2:A:1333:ILE:O	2:A:1337:GLU:HG3	2.14	0.48
3:B:114:PRO:HG2	3:B:115:GLN:H	1.78	0.48
3:B:287:ARG:NH1	3:B:324:ILE:O	2.46	0.48
3:B:997:GLU:HB3	4:C:35:ARG:HB3	1.95	0.48
4:C:21:ILE:HG12	4:C:229:TYR:HD2	1.78	0.48
5:D:134:THR:CG2	5:D:135:GLY:N	2.74	0.48
9:H:15:VAL:HG22	9:H:26:ILE:CG1	2.41	0.48
9:H:128:ASN:OD1	9:H:128:ASN:O	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:332:LYS:HG3	2:A:333:GLU:HG2	1.96	0.48
2:A:445:ASN:HB2	2:A:455:MET:HG2	1.95	0.48
2:A:1205:LYS:O	2:A:1206:ASP:C	2.57	0.48
3:B:361:LEU:N	3:B:362:PRO:CD	2.77	0.48
4:C:239:PRO:C	4:C:241:ASP:H	2.21	0.48
6:E:182:ASP:HB3	6:E:185:ALA:CB	2.44	0.48
13:L:43:THR:HG22	13:L:43:THR:O	2.13	0.48
2:A:896:ARG:NH2	2:A:1030:ARG:HH21	2.12	0.48
3:B:654:ARG:O	3:B:656:GLY:N	2.47	0.48
3:B:902:GLY:O	13:L:65:VAL:HG11	2.13	0.48
6:E:182:ASP:HB3	6:E:185:ALA:HB2	1.95	0.48
7:F:68:THR:HG21	7:F:69:LEU:HB2	1.96	0.48
8:G:80:LYS:N	8:G:80:LYS:HD3	2.29	0.48
9:H:58:THR:HG22	9:H:59:ILE:N	2.29	0.48
9:H:95:TYR:CE2	9:H:97:MET:HG3	2.49	0.48
2:A:541:ILE:HG22	2:A:546:VAL:HG23	1.95	0.48
2:A:547:LEU:HD13	12:K:58:PHE:CD1	2.48	0.48
2:A:860:LEU:CD1	2:A:1393:ASN:HB2	2.41	0.48
2:A:1224:LEU:HD12	2:A:1241:ARG:O	2.13	0.48
2:A:1349:TYR:CB	2:A:1372:VAL:HG21	2.44	0.48
3:B:1034:VAL:C	3:B:1036:ALA:N	2.70	0.48
3:B:1158:PHE:CD1	3:B:1159:ARG:N	2.81	0.48
4:C:36:VAL:HG21	4:C:251:LEU:CD2	2.38	0.48
4:C:66:ARG:NH1	11:J:2:ILE:CG2	2.72	0.48
4:C:114:TYR:CG	4:C:140:ASN:HB3	2.49	0.48
4:C:186:LEU:N	4:C:186:LEU:HD12	2.29	0.48
6:E:88:VAL:HG12	6:E:89:GLY:N	2.29	0.48
6:E:116:ILE:HG22	6:E:120:ALA:HB3	1.95	0.48
13:L:38:LEU:HD11	13:L:49:LYS:HE2	1.96	0.48
2:A:2:VAL:CG2	3:B:1157:ALA:HB1	2.33	0.48
2:A:62:ASP:HB3	2:A:64:ASN:ND2	2.28	0.48
2:A:451:HIS:NE2	2:A:1074:GLU:HG3	2.29	0.48
2:A:666:ILE:HD12	2:A:667:GLY:H	1.79	0.48
2:A:709:THR:HG23	10:I:94:ASP:HA	1.96	0.48
2:A:1376:THR:HG23	2:A:1377:THR:N	2.29	0.48
3:B:25:ILE:HG23	3:B:658:ILE:HD12	1.96	0.48
3:B:373:ARG:HG2	3:B:566:LEU:HD23	1.95	0.48
4:C:234:SER:HB2	4:C:240:VAL:HG13	1.96	0.48
5:D:27:LEU:HD22	5:D:173:HIS:CD2	2.49	0.48
5:D:29:LEU:HD22	8:G:82:PHE:CE2	2.48	0.48
5:D:153:ARG:HB3	5:D:154:PHE:CD1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:28:TYR:HE1	6:E:78:LEU:CD1	2.25	0.48
8:G:14:HIS:CE1	8:G:15:PRO:HD2	2.49	0.48
12:K:55:LYS:HB2	12:K:81:TYR:HE1	1.79	0.48
2:A:92:HIS:O	2:A:93:VAL:C	2.57	0.47
2:A:98:LYS:O	2:A:102:VAL:HG23	2.14	0.47
2:A:806:ARG:HH12	3:B:729:ILE:CD1	2.27	0.47
2:A:1120:LEU:N	2:A:1120:LEU:HD12	2.28	0.47
2:A:1120:LEU:H	2:A:1120:LEU:HD13	1.79	0.47
2:A:1289:ARG:NH1	2:A:1326:ARG:NH1	2.62	0.47
3:B:240:ILE:HD13	3:B:377:PHE:HE2	1.79	0.47
3:B:324:ILE:HD13	3:B:330:ALA:HA	1.95	0.47
3:B:824:ILE:HG22	3:B:824:ILE:O	2.13	0.47
3:B:1032:SER:O	3:B:1036:ALA:HB2	2.13	0.47
3:B:1147:LEU:C	3:B:1147:LEU:HD23	2.38	0.47
8:G:22:MET:O	8:G:23:LYS:C	2.56	0.47
10:I:15:TYR:HD1	10:I:15:TYR:H	1.61	0.47
10:I:34:TYR:HE2	10:I:36:GLU:HB3	1.78	0.47
13:L:34:CYS:O	13:L:34:CYS:SG	2.72	0.47
2:A:30:ILE:HD11	3:B:1168:LEU:HD13	1.96	0.47
2:A:37:PHE:N	2:A:37:PHE:CD1	2.82	0.47
2:A:347:PHE:CE2	2:A:375:THR:HG23	2.49	0.47
2:A:443:LEU:HD12	3:B:1146:PHE:CE2	2.49	0.47
2:A:754:SER:O	2:A:757:ASN:HB2	2.13	0.47
2:A:1265:ASN:ND2	3:B:265:SER:HB3	2.29	0.47
3:B:120:ARG:HG2	3:B:955:THR:HG21	1.96	0.47
3:B:558:LEU:O	3:B:561:TRP:N	2.47	0.47
3:B:558:LEU:C	3:B:560:GLU:N	2.72	0.47
3:B:806:THR:O	3:B:809:MET:HG3	2.14	0.47
3:B:1169:MET:O	3:B:1170:THR:C	2.58	0.47
3:B:129:PHE:CE2	3:B:166:PHE:HD1	2.32	0.47
3:B:172:ILE:HG21	3:B:178:ASN:HB3	1.95	0.47
3:B:388:CYS:C	3:B:390:LEU:N	2.72	0.47
3:B:575:PRO:HG2	3:B:576:ASP:H	1.80	0.47
3:B:846:ILE:HG23	3:B:974:PRO:HG2	1.96	0.47
4:C:75:MET:HE2	4:C:239:PRO:CD	2.45	0.47
5:D:17:LYS:HE3	5:D:17:LYS:CA	2.34	0.47
5:D:25:ALA:C	5:D:27:LEU:H	2.21	0.47
5:D:175:PHE:HE1	8:G:1:MET:HA	1.78	0.47
8:G:39:THR:HG22	8:G:41:LYS:H	1.78	0.47
9:H:62:SER:O	9:H:64:ASN:N	2.47	0.47
9:H:107:VAL:O	9:H:111:LEU:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:99:LEU:C	10:I:100:PHE:HD1	2.21	0.47
2:A:157:ASP:C	2:A:159:THR:H	2.21	0.47
2:A:284:ALA:C	2:A:286:HIS:N	2.73	0.47
2:A:295:LEU:O	2:A:298:PHE:HB3	2.14	0.47
2:A:527:THR:CG2	2:A:650:GLN:HA	2.45	0.47
2:A:590:ARG:HD3	2:A:604:GLY:C	2.40	0.47
2:A:1116:LEU:CB	2:A:1308:THR:CG2	2.93	0.47
2:A:1345:ARG:HG3	2:A:1376:THR:HG21	1.96	0.47
3:B:762:ASN:HD21	3:B:1024:ALA:HB3	1.80	0.47
4:C:125:MET:HB2	4:C:127:ARG:HE	1.79	0.47
4:C:242:GLN:HB3	4:C:246:ARG:HG3	1.96	0.47
6:E:19:VAL:HG11	6:E:80:VAL:HG11	1.95	0.47
10:I:101:PHE:N	10:I:101:PHE:CD1	2.82	0.47
2:A:208:LEU:HD23	2:A:208:LEU:C	2.39	0.47
2:A:224:PHE:CE2	2:A:231:PRO:HG3	2.49	0.47
3:B:847:ASP:C	3:B:849:GLY:N	2.72	0.47
3:B:903:VAL:CG1	3:B:904:ARG:N	2.78	0.47
3:B:1077:THR:HG22	12:K:44:ASN:HD21	1.78	0.47
3:B:1187:ASN:O	3:B:1188:LYS:CB	2.60	0.47
6:E:164:LEU:HD21	6:E:211:TYR:CG	2.49	0.47
7:F:84:TYR:CD2	7:F:152:ILE:HB	2.49	0.47
2:A:567:LYS:HB3	9:H:95:TYR:CA	2.44	0.47
2:A:711:ARG:O	2:A:714:PHE:HB3	2.15	0.47
2:A:1263:ILE:O	2:A:1267:MET:HG3	2.15	0.47
3:B:25:ILE:HG22	3:B:29:ASP:CB	2.45	0.47
3:B:94:LYS:HG2	3:B:95:ILE:H	1.79	0.47
3:B:376:PHE:HB3	3:B:586:TRP:CZ3	2.49	0.47
3:B:552:MET:C	3:B:554:ILE:H	2.22	0.47
3:B:610:ASN:O	3:B:612:GLU:N	2.48	0.47
3:B:827:ILE:HA	3:B:1012:ILE:O	2.14	0.47
3:B:1220:ARG:HB3	3:B:1220:ARG:HH11	1.79	0.47
5:D:18:VAL:O	5:D:18:VAL:HG22	2.13	0.47
5:D:175:PHE:HZ	8:G:85:GLU:HG3	1.78	0.47
9:H:127:GLY:N	9:H:130:ARG:HH22	2.12	0.47
13:L:28:LYS:C	13:L:29:TYR:HD2	2.22	0.47
2:A:61:ILE:O	2:A:63:ARG:N	2.48	0.47
2:A:384:ASN:CG	2:A:388:LEU:HD12	2.40	0.47
2:A:853:ASP:OD1	2:A:853:ASP:C	2.56	0.47
2:A:1068:ALA:HA	2:A:1367:HIS:ND1	2.30	0.47
2:A:1149:ALA:CB	10:I:47:GLU:HA	2.44	0.47
3:B:33:VAL:O	3:B:36:ALA:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:222:ILE:O	3:B:240:ILE:HA	2.15	0.47
3:B:360:PHE:CE2	3:B:361:LEU:HB2	2.49	0.47
3:B:364:ILE:HG12	3:B:585:VAL:CG1	2.30	0.47
3:B:582:VAL:O	3:B:582:VAL:CG1	2.63	0.47
3:B:706:GLN:NE2	3:B:730:ARG:NH1	2.62	0.47
3:B:745:PRO:C	3:B:747:MET:H	2.22	0.47
3:B:840:ILE:HG21	3:B:994:TYR:CD1	2.50	0.47
3:B:1103:ILE:O	3:B:1122:ARG:NH1	2.48	0.47
4:C:22:LEU:HD11	12:K:101:LEU:HD11	1.96	0.47
4:C:35:ARG:HH11	12:K:41:THR:N	2.11	0.47
4:C:89:GLU:O	4:C:90:ASP:CB	2.62	0.47
4:C:243:VAL:O	4:C:243:VAL:HG12	2.15	0.47
5:D:66:ARG:O	5:D:70:PHE:HB2	2.14	0.47
5:D:154:PHE:CE2	5:D:163:VAL:HG21	2.49	0.47
6:E:47:CYS:HA	6:E:52:ARG:O	2.14	0.47
6:E:153:HIS:HB3	6:E:196:VAL:HG13	1.96	0.47
7:F:69:LEU:HD22	7:F:72:LYS:N	2.30	0.47
8:G:15:PRO:CG	8:G:66:GLY:HA3	2.45	0.47
9:H:84:ALA:HA	9:H:87:ARG:HB2	1.95	0.47
13:L:55:ILE:O	13:L:56:LEU:CB	2.63	0.47
2:A:55:ASP:C	2:A:57:ARG:H	2.21	0.47
2:A:254:GLU:HB2	3:B:935:ARG:NH1	2.29	0.47
2:A:492:PRO:HB3	2:A:501:LEU:HD12	1.97	0.47
2:A:942:PHE:HD2	2:A:943:LEU:HD23	1.79	0.47
2:A:1225:PHE:CE2	2:A:1227:ILE:HD11	2.50	0.47
2:A:1279:ILE:HD11	2:A:1316:VAL:CG2	2.44	0.47
3:B:186:GLU:HG2	11:J:62:ARG:HH22	1.78	0.47
3:B:247:GLY:C	3:B:249:ARG:H	2.22	0.47
3:B:789:MET:HE2	3:B:953:LEU:HD22	1.97	0.47
3:B:1068:GLY:O	3:B:1069:PHE:O	2.33	0.47
3:B:1079:LYS:N	4:C:27:LEU:HD21	2.30	0.47
3:B:1162:ILE:HG23	3:B:1168:LEU:O	2.14	0.47
6:E:13:TRP:HB2	6:E:42:PHE:CD2	2.49	0.47
6:E:42:PHE:CZ	6:E:58:MET:HE3	2.49	0.47
6:E:100:ILE:HG23	6:E:105:PHE:CD1	2.49	0.47
8:G:99:PHE:CE2	8:G:115:MET:HE2	2.50	0.47
9:H:91:ASP:C	9:H:93:TYR:H	2.22	0.47
13:L:40:LEU:HD22	13:L:44:ASP:CG	2.40	0.47
2:A:84:ILE:CD1	2:A:270:LEU:HD22	2.43	0.47
2:A:673:GLY:O	2:A:676:MET:HB2	2.15	0.47
2:A:993:LEU:HD21	2:A:1049:ILE:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1156:PRO:HA	2:A:1190:PRO:HB3	1.96	0.47
2:A:1283:VAL:HG12	2:A:1284:MET:H	1.79	0.47
3:B:294:ASP:C	3:B:296:GLU:H	2.17	0.47
3:B:460:ALA:O	3:B:462:ALA:N	2.48	0.47
3:B:604:ARG:HH11	3:B:691:GLU:HG2	1.80	0.47
3:B:642:ASP:CA	3:B:649:LYS:HG3	2.44	0.47
3:B:889:THR:HG22	3:B:891:ASP:H	1.80	0.47
4:C:53:THR:O	4:C:153:LEU:HA	2.14	0.47
4:C:69:LEU:N	4:C:69:LEU:CD1	2.78	0.47
6:E:105:PHE:O	6:E:106:GLN:HB2	2.15	0.47
8:G:8:SER:HB3	8:G:73:LYS:HD2	1.95	0.47
12:K:111:LEU:O	12:K:112:GLN:CB	2.62	0.47
2:A:106:VAL:HG13	2:A:112:LYS:C	2.40	0.47
2:A:265:LYS:HD2	2:A:265:LYS:H	1.80	0.47
2:A:343:LYS:NZ	3:B:1151:LEU:HB3	2.30	0.47
2:A:590:ARG:HB3	2:A:605:MET:N	2.30	0.47
2:A:1265:ASN:C	2:A:1267:MET:H	2.23	0.47
3:B:35:SER:HA	3:B:811:TYR:CE2	2.37	0.47
3:B:361:LEU:O	3:B:363:HIS:O	2.33	0.47
3:B:785:TYR:CD1	3:B:786:ASN:N	2.83	0.47
3:B:905:VAL:CG2	3:B:941:LEU:HD22	2.41	0.47
3:B:1072:MET:HE1	3:B:1085:ILE:HB	1.94	0.47
3:B:1099:VAL:C	3:B:1101:ASP:H	2.23	0.47
3:B:1224:PHE:CE2	6:E:171:LYS:HG3	2.49	0.47
4:C:8:VAL:O	4:C:9:LYS:HG3	2.15	0.47
4:C:251:LEU:HD12	4:C:251:LEU:C	2.39	0.47
8:G:48:VAL:HG13	8:G:74:TYR:HD1	1.79	0.47
8:G:59:GLY:HA3	8:G:70:PHE:CD2	2.50	0.47
2:A:129:LYS:O	2:A:130:ASP:HB2	2.14	0.46
2:A:341:MET:HE3	2:A:843:LYS:HZ2	1.78	0.46
2:A:852:TYR:CD1	7:F:136:ARG:HB3	2.50	0.46
2:A:1187:GLN:NE2	2:A:1188:GLN:HE21	2.13	0.46
3:B:37:PHE:HD2	3:B:542:MET:SD	2.38	0.46
3:B:289:LEU:HD13	3:B:375:ALA:CB	2.45	0.46
3:B:603:LEU:HB3	3:B:609:ILE:CD1	2.44	0.46
3:B:840:ILE:HD13	3:B:994:TYR:CE1	2.47	0.46
3:B:1039:GLY:HA2	11:J:51:LEU:HD21	1.97	0.46
4:C:152:GLU:OE2	4:C:154:LYS:HE3	2.15	0.46
5:D:128:VAL:O	5:D:132:GLN:HG3	2.14	0.46
6:E:55:ARG:O	6:E:57:MET:N	2.47	0.46
11:J:35:ALA:O	11:J:39:LEU:HD12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:30:ILE:HG22	13:L:31:CYS:N	2.30	0.46
2:A:450:LEU:HD12	2:A:450:LEU:N	2.30	0.46
2:A:774:ARG:NH2	2:A:797:LYS:CG	2.76	0.46
2:A:1191:TRP:HB3	2:A:1260:LEU:HD23	1.97	0.46
3:B:123:THR:O	3:B:125:SER:N	2.46	0.46
3:B:205:ILE:N	3:B:205:ILE:HD12	2.31	0.46
3:B:282:ILE:CD1	3:B:382:ILE:HD13	2.46	0.46
3:B:424:LEU:CD2	3:B:453:ILE:HD11	2.45	0.46
3:B:942:ARG:O	3:B:944:THR:N	2.49	0.46
3:B:948:ILE:HG22	3:B:949:VAL:O	2.15	0.46
4:C:91:HIS:C	4:C:91:HIS:HD1	2.23	0.46
4:C:213:PRO:HG2	4:C:214:ASN:H	1.79	0.46
2:A:134:ARG:HD2	2:A:221:SER:O	2.16	0.46
2:A:356:ASP:OD2	12:K:65:HIS:HE1	1.99	0.46
2:A:1094:VAL:HG12	2:A:1095:THR:N	2.29	0.46
3:B:762:ASN:ND2	3:B:1024:ALA:HB3	2.30	0.46
3:B:777:ALA:HA	3:B:1095:LEU:HA	1.97	0.46
3:B:866:TYR:O	3:B:867:GLY:C	2.56	0.46
3:B:957:ASN:O	3:B:960:GLY:N	2.48	0.46
3:B:1099:VAL:HG12	3:B:1100:ASP:N	2.30	0.46
4:C:44:LEU:HD21	4:C:159:ALA:CB	2.45	0.46
6:E:43:LYS:O	6:E:45:LYS:N	2.47	0.46
11:J:19:GLU:O	11:J:23:ASN:HB2	2.15	0.46
11:J:45:CYS:O	11:J:48:ARG:HG3	2.16	0.46
12:K:10:PHE:N	12:K:10:PHE:HD2	2.14	0.46
12:K:110:ASN:O	12:K:111:LEU:HB3	2.14	0.46
2:A:474:VAL:HG22	2:A:478:TYR:HE1	1.80	0.46
2:A:571:LEU:HD22	9:H:46:LEU:HD11	1.98	0.46
2:A:720:ARG:HB3	2:A:720:ARG:NH1	2.30	0.46
3:B:461:LEU:N	3:B:461:LEU:HD12	2.30	0.46
3:B:1151:LEU:N	3:B:1151:LEU:HD12	2.31	0.46
5:D:71:LYS:HA	5:D:74:GLN:CB	2.45	0.46
6:E:24:LYS:HG3	6:E:25:ASP:N	2.30	0.46
6:E:108:GLY:HA3	6:E:132:ILE:HG23	1.96	0.46
7:F:96:THR:O	7:F:100:GLN:HG3	2.16	0.46
7:F:101:ILE:HD13	7:F:120:ILE:CG2	2.46	0.46
11:J:51:LEU:O	11:J:51:LEU:HD12	2.14	0.46
12:K:65:HIS:CD2	12:K:65:HIS:C	2.93	0.46
2:A:219:PHE:O	2:A:222:LEU:O	2.34	0.46
2:A:806:ARG:O	3:B:761:HIS:HE1	1.97	0.46
2:A:986:ILE:HD12	2:A:1032:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1027:ALA:O	2:A:1031:VAL:HG23	2.15	0.46
2:A:1030:ARG:HG3	2:A:1034:GLU:CD	2.41	0.46
2:A:1191:TRP:CE3	2:A:1191:TRP:HA	2.51	0.46
3:B:745:PRO:C	3:B:747:MET:N	2.73	0.46
3:B:1098:MET:H	3:B:1098:MET:CE	2.27	0.46
4:C:101:LEU:HD12	4:C:101:LEU:HA	1.80	0.46
5:D:126:ILE:HD13	5:D:145:MET:HE3	1.98	0.46
7:F:90:ARG:HD3	7:F:155:LEU:CD1	2.42	0.46
9:H:91:ASP:O	9:H:93:TYR:N	2.45	0.46
9:H:127:GLY:O	9:H:128:ASN:CB	2.60	0.46
11:J:31:ASP:O	11:J:32:GLU:C	2.58	0.46
2:A:335:ARG:NH1	3:B:1202:LEU:HD22	2.30	0.46
2:A:340:LEU:HD21	3:B:1200:ALA:CA	2.46	0.46
2:A:441:PRO:HD2	2:A:498:ARG:NH2	2.31	0.46
2:A:1193:LEU:HD12	2:A:1194:ARG:N	2.30	0.46
2:A:1244:ARG:HB3	2:A:1245:PRO:CD	2.45	0.46
3:B:37:PHE:C	3:B:37:PHE:HD1	2.22	0.46
3:B:373:ARG:CG	3:B:566:LEU:HD23	2.45	0.46
3:B:597:MET:HE2	3:B:601:ARG:HG3	1.98	0.46
3:B:758:PHE:CZ	3:B:1044:ALA:HA	2.50	0.46
3:B:1166:CYS:O	3:B:1168:LEU:N	2.42	0.46
4:C:152:GLU:HG2	4:C:153:LEU:N	2.26	0.46
4:C:183:TRP:CZ2	4:C:207:CYS:HB3	2.50	0.46
4:C:259:LEU:HD21	12:K:92:ASN:OD1	2.16	0.46
5:D:37:GLN:OE1	8:G:5:LYS:HD2	2.16	0.46
6:E:78:LEU:HD11	6:E:109:ILE:HD12	1.98	0.46
6:E:97:VAL:HG13	6:E:127:ILE:HD13	1.97	0.46
9:H:10:PHE:N	9:H:10:PHE:CD1	2.84	0.46
9:H:95:TYR:HB3	9:H:144:ILE:HB	1.98	0.46
11:J:44:TYR:HA	11:J:47:ARG:CB	2.35	0.46
2:A:116:ASP:OD2	2:A:164:ARG:HD2	2.16	0.46
2:A:172:PRO:HG3	2:A:185:TRP:CE2	2.51	0.46
2:A:563:PRO:HG3	2:A:572:TRP:CE2	2.48	0.46
2:A:588:LEU:O	2:A:606:LEU:HA	2.16	0.46
2:A:666:ILE:HD12	2:A:666:ILE:N	2.31	0.46
2:A:746:MET:HE3	3:B:1018:PRO:HG2	1.97	0.46
2:A:845:LEU:O	2:A:846:GLU:C	2.59	0.46
2:A:1224:LEU:HD11	2:A:1240:CYS:HB2	1.98	0.46
2:A:1341:ILE:CG2	2:A:1342:GLU:H	2.28	0.46
3:B:20:ASP:O	3:B:21:GLU:C	2.58	0.46
3:B:69:LEU:HD13	3:B:429:PHE:CD1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:542:MET:CE	3:B:743:ILE:HG13	2.46	0.46
3:B:563:MET:HE2	3:B:588:GLY:C	2.41	0.46
3:B:604:ARG:O	3:B:606:LYS:N	2.49	0.46
3:B:830:TYR:CD2	3:B:1000:PRO:HD3	2.51	0.46
3:B:1001:PHE:CE2	4:C:34:ARG:CZ	2.99	0.46
3:B:1125:ASP:O	3:B:1125:ASP:OD1	2.33	0.46
5:D:185:CYS:HB2	5:D:211:LEU:CD2	2.45	0.46
8:G:22:MET:C	8:G:24:GLN:N	2.73	0.46
11:J:48:ARG:HD2	11:J:48:ARG:C	2.41	0.46
12:K:46:ILE:O	12:K:50:LEU:HB2	2.16	0.46
2:A:18:GLN:CB	3:B:1215:ARG:HB2	2.46	0.46
2:A:184:SER:HB3	2:A:199:LEU:CD2	2.46	0.46
2:A:427:GLN:O	2:A:428:TYR:C	2.59	0.46
2:A:1169:ILE:HG22	2:A:1169:ILE:O	2.15	0.46
3:B:308:TRP:HZ3	10:I:45:ARG:HB3	1.79	0.46
3:B:552:MET:C	3:B:554:ILE:N	2.74	0.46
3:B:842:ASN:ND2	3:B:845:SER:OG	2.48	0.46
3:B:1138:MET:HE2	3:B:1146:PHE:HD2	1.81	0.46
4:C:212:PRO:CB	4:C:213:PRO:HD2	2.42	0.46
5:D:52:LEU:CD2	5:D:147:TYR:HE2	2.27	0.46
11:J:6:ARG:HG2	11:J:13:VAL:HA	1.98	0.46
12:K:58:PHE:HB3	12:K:76:GLN:HB3	1.96	0.46
2:A:244:PRO:CB	2:A:245:PRO:HD3	2.45	0.46
2:A:648:ASN:O	2:A:649:ILE:C	2.56	0.46
2:A:754:SER:O	2:A:755:PHE:C	2.58	0.46
2:A:1342:GLU:OE2	6:E:212:ARG:NH1	2.48	0.46
3:B:95:ILE:CG1	3:B:130:VAL:HG22	2.46	0.46
3:B:216:GLU:HA	3:B:406:LEU:HD23	1.97	0.46
3:B:899:ILE:HG21	3:B:949:VAL:HG21	1.98	0.46
3:B:1198:TYR:CD2	3:B:1198:TYR:O	2.69	0.46
6:E:31:THR:O	6:E:35:VAL:HG23	2.16	0.46
8:G:111:THR:HB	8:G:114:LEU:HB2	1.98	0.46
9:H:17:PRO:HB3	9:H:24:CYS:SG	2.55	0.46
9:H:81:PRO:HB3	9:H:82:PRO:HD2	1.97	0.46
9:H:123:MET:HE1	9:H:142:LEU:HD21	1.98	0.46
10:I:7:CYS:O	10:I:11:ASN:HA	2.16	0.46
10:I:85:PHE:CE1	10:I:99:LEU:HD13	2.50	0.46
11:J:48:ARG:HH21	11:J:49:MET:HE1	1.80	0.46
2:A:120:GLU:C	2:A:122:MET:N	2.72	0.46
2:A:497:THR:O	2:A:498:ARG:C	2.59	0.46
2:A:687:LYS:O	2:A:690:VAL:HB	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:783:THR:HG22	2:A:784:LEU:HG	1.98	0.46
2:A:1148:ILE:HG23	10:I:49:ILE:HB	1.97	0.46
3:B:99:LYS:HB3	3:B:100:PRO:HD2	1.98	0.46
3:B:327:ARG:NH2	3:B:371:GLU:HG2	2.30	0.46
3:B:648:HIS:CG	3:B:649:LYS:H	2.34	0.46
10:I:19:ASP:CG	10:I:22:ASN:HB2	2.41	0.46
10:I:85:PHE:CD2	10:I:85:PHE:N	2.77	0.46
2:A:90:VAL:HG12	2:A:91:PHE:N	2.31	0.45
2:A:514:PRO:CB	2:A:875:ALA:HB3	2.46	0.45
2:A:697:ALA:HB2	2:A:702:LEU:HD12	1.98	0.45
2:A:710:LEU:HD12	2:A:710:LEU:N	2.30	0.45
2:A:940:ARG:O	2:A:944:ARG:HG3	2.17	0.45
2:A:996:ASN:O	2:A:998:LEU:N	2.45	0.45
2:A:1174:PHE:C	2:A:1176:LEU:N	2.73	0.45
3:B:638:PHE:HB3	3:B:651:LEU:CD2	2.43	0.45
3:B:1110:PRO:O	3:B:1119:VAL:HG22	2.16	0.45
3:B:1159:ARG:HD2	3:B:1159:ARG:C	2.41	0.45
4:C:46:ILE:CD1	4:C:67:LEU:HB3	2.41	0.45
5:D:156:ASP:O	5:D:160:VAL:HG23	2.17	0.45
10:I:58:VAL:HG13	10:I:62:ILE:HD13	1.96	0.45
12:K:55:LYS:CB	12:K:81:TYR:CE1	2.99	0.45
2:A:63:ARG:HG2	2:A:74:MET:HE1	1.98	0.45
2:A:226:GLU:O	2:A:226:GLU:HG2	2.16	0.45
2:A:1010:ALA:O	2:A:1013:ASP:HB2	2.16	0.45
2:A:1011:GLN:O	2:A:1015:VAL:HG23	2.16	0.45
2:A:1068:ALA:HB3	2:A:1370:LEU:HD23	1.98	0.45
3:B:54:PHE:CE2	3:B:59:LEU:HD13	2.51	0.45
3:B:293:PRO:HG2	3:B:296:GLU:HB3	1.98	0.45
3:B:485:ARG:NH2	3:B:782:LEU:HD11	2.31	0.45
3:B:615:MET:HA	3:B:625:LYS:O	2.17	0.45
3:B:778:MET:CE	3:B:1094:ARG:CD	2.93	0.45
3:B:781:PHE:CE2	3:B:793:ALA:HB1	2.51	0.45
3:B:1182:CYS:O	3:B:1183:LYS:C	2.58	0.45
4:C:99:LEU:HB2	4:C:157:CYS:HB2	1.97	0.45
5:D:137:ASN:ND2	5:D:137:ASN:H	2.15	0.45
5:D:151:PHE:H	5:D:151:PHE:HD1	1.62	0.45
6:E:22:MET:HE3	6:E:26:ARG:NH2	2.30	0.45
8:G:38:CYS:SG	8:G:44:TYR:CE1	3.09	0.45
9:H:55:LEU:HD22	9:H:144:ILE:CG2	2.46	0.45
2:A:472:LEU:O	2:A:475:THR:CG2	2.63	0.45
2:A:802:ASN:ND2	2:A:812:GLU:OE1	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1208:THR:O	2:A:1212:VAL:HG23	2.16	0.45
3:B:274:PRO:HG3	3:B:359:GLU:O	2.16	0.45
3:B:664:THR:HG23	3:B:678:GLU:N	2.31	0.45
3:B:797:TYR:CE1	3:B:854:LEU:HD21	2.52	0.45
3:B:1156:ASP:HB3	3:B:1198:TYR:N	2.31	0.45
3:B:1198:TYR:CD2	3:B:1198:TYR:C	2.93	0.45
4:C:179:GLU:HG2	4:C:180:TYR:H	1.81	0.45
5:D:210:ILE:O	5:D:214:LEU:HG	2.15	0.45
12:K:19:LEU:HD21	12:K:35:PHE:CE2	2.51	0.45
2:A:98:LYS:O	2:A:99:ILE:C	2.59	0.45
2:A:405:VAL:O	2:A:413:ILE:HG13	2.16	0.45
2:A:767:GLN:OE1	2:A:799:PHE:HB2	2.16	0.45
2:A:818:MET:HA	3:B:514:LEU:HB3	1.98	0.45
2:A:1107:VAL:HG12	2:A:1107:VAL:O	2.17	0.45
2:A:1118:VAL:HG23	2:A:1306:LEU:HB2	1.98	0.45
2:A:1170:ILE:O	2:A:1174:PHE:HD1	1.99	0.45
3:B:405:ARG:HA	3:B:631:GLY:O	2.17	0.45
3:B:492:LEU:HB2	3:B:751:VAL:HG11	1.98	0.45
3:B:515:HIS:O	3:B:518:HIS:HB2	2.16	0.45
3:B:616:ILE:HG12	3:B:697:GLU:HA	1.98	0.45
3:B:1214:PRO:O	3:B:1214:PRO:HG2	2.16	0.45
4:C:37:MET:HA	4:C:41:ILE:HD11	1.98	0.45
5:D:24:ALA:C	5:D:26:THR:N	2.74	0.45
5:D:29:LEU:HD23	5:D:29:LEU:N	2.31	0.45
7:F:108:PHE:HE1	7:F:131:PRO:HG3	1.80	0.45
9:H:95:TYR:HE2	9:H:97:MET:CG	2.29	0.45
10:I:5:ARG:O	10:I:14:LEU:HG	2.16	0.45
11:J:36:LEU:HD22	11:J:41:LEU:HD12	1.98	0.45
2:A:182:VAL:CG1	2:A:183:GLY:N	2.80	0.45
2:A:219:PHE:CD2	2:A:231:PRO:HD2	2.52	0.45
2:A:254:GLU:CB	3:B:935:ARG:HH22	2.30	0.45
2:A:336:ILE:HG22	2:A:337:ARG:N	2.32	0.45
2:A:408:ASP:C	2:A:410:GLY:H	2.24	0.45
2:A:710:LEU:H	2:A:710:LEU:CD1	2.30	0.45
2:A:738:LYS:C	2:A:740:LEU:H	2.24	0.45
2:A:754:SER:H	2:A:757:ASN:HD22	1.64	0.45
2:A:852:TYR:CD2	2:A:1060:PRO:CB	3.00	0.45
2:A:855:THR:HG23	2:A:857:ARG:HG3	1.97	0.45
2:A:889:SER:HB3	2:A:1297:GLU:CG	2.47	0.45
2:A:920:LEU:HD23	2:A:920:LEU:C	2.41	0.45
3:B:211:VAL:CG2	3:B:483:LEU:HB2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:822:ASN:HD22	11:J:52:THR:HG21	1.80	0.45
4:C:15:LYS:O	4:C:240:VAL:HG22	2.16	0.45
4:C:235:VAL:HG12	11:J:13:VAL:HG23	1.99	0.45
6:E:135:PHE:CD2	6:E:140:LEU:HD21	2.50	0.45
7:F:89:GLU:HB3	7:F:134:ILE:CD1	2.47	0.45
2:A:14:VAL:HB	2:A:1430:LEU:HD13	1.99	0.45
2:A:48:ALA:O	2:A:49:LYS:HG2	2.17	0.45
2:A:261:ASP:O	2:A:264:PHE:HB2	2.16	0.45
2:A:335:ARG:N	2:A:339:ASN:HD22	2.15	0.45
2:A:1311:VAL:HG11	2:A:1329:THR:HG21	1.98	0.45
3:B:56:ASP:CB	3:B:57:TYR:HD1	2.30	0.45
3:B:100:PRO:HD3	3:B:172:ILE:HD12	1.98	0.45
3:B:258:LEU:O	3:B:258:LEU:CG	2.62	0.45
3:B:620:ARG:NH2	10:I:86:PHE:CD2	2.84	0.45
3:B:864:LYS:N	3:B:872:GLU:OE1	2.50	0.45
3:B:1090:THR:HG22	3:B:1091:TYR:N	2.30	0.45
4:C:31:ASN:O	4:C:32:SER:C	2.59	0.45
5:D:64:VAL:C	5:D:66:ARG:N	2.74	0.45
6:E:24:LYS:HB2	6:E:24:LYS:HE3	1.76	0.45
6:E:96:PHE:CE1	6:E:100:ILE:HD11	2.51	0.45
6:E:106:GLN:HA	6:E:130:ALA:CB	2.46	0.45
6:E:175:LEU:HD23	6:E:176:PRO:HD2	1.98	0.45
8:G:38:CYS:HB3	8:G:155:SER:HA	1.98	0.45
2:A:259:GLU:OE1	2:A:263:THR:HG21	2.16	0.45
2:A:334:GLY:O	2:A:335:ARG:C	2.60	0.45
2:A:567:LYS:CB	9:H:96:VAL:H	2.12	0.45
2:A:1405:THR:HB	2:A:1406:VAL:H	1.59	0.45
3:B:1060:ARG:HA	3:B:1060:ARG:HD2	1.61	0.45
4:C:31:ASN:O	4:C:34:ARG:HB3	2.16	0.45
4:C:146:LYS:C	4:C:147:LEU:HD23	2.42	0.45
4:C:255:VAL:O	4:C:255:VAL:HG12	2.17	0.45
12:K:56:VAL:HA	12:K:77:THR:HG22	1.99	0.45
1:R:3:A:H2'	1:R:4:U:C6	2.51	0.45
2:A:75:ASN:HA	3:B:1116:ARG:NH2	2.32	0.45
2:A:1100:ARG:HH21	2:A:1351:GLU:CD	2.25	0.45
2:A:1187:GLN:NE2	2:A:1188:GLN:NE2	2.64	0.45
2:A:1261:LYS:O	2:A:1264:GLU:HB3	2.17	0.45
3:B:402:GLY:HA2	3:B:695:ALA:HB3	1.99	0.45
3:B:731:VAL:HG12	3:B:732:SER:N	2.32	0.45
3:B:792:MET:HG3	3:B:855:PHE:CE1	2.45	0.45
3:B:843:GLN:O	3:B:846:ILE:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1183:LYS:N	3:B:1183:LYS:HE3	2.32	0.45
3:B:1220:ARG:HB3	3:B:1220:ARG:CZ	2.46	0.45
4:C:246:ARG:HA	4:C:249:ASP:HB3	1.98	0.45
7:F:118:LEU:O	7:F:122:MET:HG3	2.16	0.45
10:I:92:ARG:HG2	10:I:94:ASP:OD1	2.17	0.45
12:K:7:PHE:CD1	12:K:7:PHE:C	2.95	0.45
2:A:418:SER:C	2:A:420:ARG:N	2.75	0.45
2:A:562:THR:HA	2:A:563:PRO:HD3	1.85	0.45
2:A:788:SER:HB3	10:I:69:PRO:HB3	1.99	0.45
2:A:1015:VAL:O	2:A:1016:THR:C	2.59	0.45
3:B:557:PHE:C	3:B:557:PHE:CD2	2.94	0.45
3:B:980:PHE:CE1	3:B:990:ILE:HD11	2.41	0.45
3:B:1177:HIS:C	3:B:1179:GLN:H	2.25	0.45
4:C:8:VAL:HG21	12:K:105:PHE:HA	1.99	0.45
4:C:131:HIS:O	4:C:133:ILE:N	2.37	0.45
6:E:124:VAL:HA	6:E:132:ILE:HD12	1.99	0.45
8:G:45:ILE:HD13	8:G:78:VAL:HG13	1.98	0.45
9:H:104:PHE:CZ	9:H:136:LYS:HA	2.52	0.45
12:K:5:ASP:O	12:K:6:ARG:C	2.60	0.45
2:A:227:VAL:HG12	5:D:15:LEU:HD23	1.99	0.45
2:A:590:ARG:HH22	2:A:620:LYS:CB	2.28	0.45
2:A:974:ASP:C	2:A:976:THR:H	2.25	0.45
2:A:1149:ALA:HB2	10:I:47:GLU:HA	1.99	0.45
2:A:1214:GLU:O	2:A:1218:GLN:HG2	2.17	0.45
2:A:1230:GLU:C	2:A:1232:ASN:N	2.75	0.45
2:A:1332:PHE:CE1	2:A:1348:LEU:HD13	2.51	0.45
3:B:70:ILE:O	3:B:70:ILE:HG22	2.16	0.45
3:B:189:LEU:HD12	3:B:196:PRO:HA	1.97	0.45
3:B:424:LEU:HD22	3:B:453:ILE:HD11	1.98	0.45
3:B:549:THR:CG2	3:B:550:ASP:H	2.15	0.45
3:B:642:ASP:CA	3:B:649:LYS:HA	2.47	0.45
3:B:705:MET:HA	3:B:705:MET:HE3	1.99	0.45
3:B:811:TYR:N	3:B:811:TYR:CD1	2.85	0.45
3:B:889:THR:HG23	3:B:891:ASP:OD2	2.17	0.45
4:C:77:ILE:HA	4:C:77:ILE:HD13	1.69	0.45
6:E:177:ARG:O	6:E:212:ARG:CD	2.65	0.45
8:G:10:ASN:OD1	8:G:71:ASN:HA	2.15	0.45
9:H:107:VAL:HG21	9:H:126:GLU:OE2	2.16	0.45
13:L:40:LEU:HD22	13:L:44:ASP:HB3	1.99	0.45
2:A:396:PRO:HG3	2:A:416:ARG:HB3	1.98	0.44
2:A:927:VAL:O	2:A:931:GLU:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1011:GLN:NE2	2:A:1015:VAL:HG21	2.32	0.44
3:B:525:ALA:O	3:B:768:THR:HA	2.17	0.44
3:B:890:TYR:CE1	3:B:910:VAL:HG21	2.52	0.44
4:C:91:HIS:ND1	4:C:91:HIS:C	2.75	0.44
5:D:29:LEU:HB3	8:G:82:PHE:HE2	1.81	0.44
5:D:34:GLN:O	5:D:47:LEU:HD23	2.16	0.44
6:E:168:TYR:C	6:E:169:ARG:HG3	2.41	0.44
7:F:108:PHE:CE1	7:F:131:PRO:HG3	2.52	0.44
8:G:99:PHE:CD1	8:G:99:PHE:C	2.95	0.44
8:G:115:MET:HB3	8:G:163:ILE:HD11	1.99	0.44
11:J:10:CYS:SG	11:J:11:GLY:N	2.90	0.44
2:A:289:ILE:C	2:A:291:GLU:H	2.24	0.44
2:A:562:THR:HB	9:H:98:TYR:CD2	2.52	0.44
2:A:684:ALA:O	2:A:687:LYS:HB2	2.16	0.44
2:A:717:ASN:HA	2:A:720:ARG:HH12	1.82	0.44
2:A:898:ARG:O	2:A:1029:ARG:NH1	2.51	0.44
2:A:1120:LEU:CD1	2:A:1304:TRP:O	2.66	0.44
2:A:1193:LEU:HD12	2:A:1193:LEU:C	2.42	0.44
2:A:1394:THR:HG21	2:A:1398:MET:SD	2.58	0.44
2:A:1445:ILE:HD12	8:G:59:GLY:O	2.17	0.44
3:B:56:ASP:HB3	3:B:57:TYR:CD1	2.52	0.44
3:B:205:ILE:HG21	3:B:462:ALA:HB2	1.99	0.44
3:B:487:THR:O	3:B:490:SER:HB3	2.18	0.44
3:B:905:VAL:HG23	3:B:941:LEU:CD2	2.46	0.44
3:B:980:PHE:HE2	3:B:1094:ARG:HB2	1.81	0.44
3:B:1064:TYR:O	3:B:1065:GLN:C	2.60	0.44
3:B:1159:ARG:HD2	3:B:1159:ARG:O	2.17	0.44
3:B:1177:HIS:CB	3:B:1179:GLN:HE21	2.29	0.44
4:C:75:MET:HE2	4:C:239:PRO:HD3	1.99	0.44
4:C:166:GLU:OE1	13:L:70:ARG:NH2	2.43	0.44
8:G:66:GLY:O	8:G:67:SER:C	2.61	0.44
2:A:164:ARG:CG	2:A:165:GLY:N	2.75	0.44
2:A:472:LEU:HD11	3:B:835:GLN:CD	2.42	0.44
2:A:867:ILE:HD12	2:A:867:ILE:N	2.32	0.44
2:A:961:ARG:HH11	2:A:961:ARG:HG3	1.83	0.44
3:B:597:MET:HE2	3:B:601:ARG:HE	1.83	0.44
3:B:776:GLN:O	3:B:1095:LEU:HA	2.17	0.44
3:B:1065:GLN:NE2	3:B:1067:ARG:HG2	2.32	0.44
3:B:1151:LEU:CD1	3:B:1151:LEU:H	2.31	0.44
3:B:1202:LEU:O	3:B:1206:GLU:HG3	2.17	0.44
5:D:5:THR:O	5:D:5:THR:HG23	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:13:ARG:HB3	5:D:17:LYS:HZ3	1.82	0.44
5:D:31:GLN:O	5:D:34:GLN:HG3	2.17	0.44
8:G:39:THR:HG22	8:G:40:GLY:N	2.32	0.44
8:G:85:GLU:HG2	8:G:86:VAL:N	2.31	0.44
9:H:99:GLY:HA3	9:H:118:PHE:HA	1.99	0.44
13:L:58:LYS:O	13:L:58:LYS:HG2	2.16	0.44
2:A:102:VAL:HG11	2:A:211:PHE:HE2	1.82	0.44
2:A:114:LEU:O	2:A:115:LEU:HG	2.17	0.44
2:A:356:ASP:OD2	12:K:65:HIS:CE1	2.71	0.44
2:A:774:ARG:CZ	2:A:797:LYS:HG3	2.47	0.44
2:A:1152:ILE:CG1	10:I:44:TYR:HB3	2.36	0.44
2:A:1397:LEU:HB2	2:A:1426:GLU:OE1	2.17	0.44
2:A:1441:PHE:CZ	7:F:89:GLU:HA	2.52	0.44
3:B:215:GLN:HA	3:B:215:GLN:NE2	2.32	0.44
3:B:593:PRO:O	3:B:594:ALA:C	2.59	0.44
4:C:133:ILE:HD12	4:C:237:SER:HA	1.97	0.44
8:G:1:MET:HE2	8:G:3:PHE:HE1	1.82	0.44
12:K:68:PHE:N	12:K:68:PHE:CD2	2.83	0.44
2:A:332:LYS:H	2:A:337:ARG:HB3	1.82	0.44
2:A:843:LYS:HD3	2:A:846:GLU:OE2	2.17	0.44
2:A:1265:ASN:O	2:A:1267:MET:N	2.50	0.44
2:A:1305:VAL:CG1	2:A:1306:LEU:N	2.80	0.44
2:A:1450:LEU:HD21	8:G:18:PHE:O	2.18	0.44
3:B:168:GLY:N	3:B:450:ALA:HB1	2.31	0.44
3:B:1070:GLU:OE1	11:J:44:TYR:OH	2.34	0.44
3:B:1072:MET:CE	3:B:1087:PHE:HB2	2.48	0.44
4:C:94:LYS:HB2	4:C:94:LYS:HE3	1.80	0.44
7:F:68:THR:CB	7:F:69:LEU:CB	2.96	0.44
10:I:86:PHE:CE1	10:I:100:PHE:HB2	2.52	0.44
12:K:51:LEU:HD12	12:K:51:LEU:HA	1.82	0.44
2:A:357:PRO:HD2	3:B:833:TYR:CE1	2.52	0.44
2:A:1066:VAL:O	2:A:1069:ALA:HB3	2.18	0.44
2:A:1095:THR:O	2:A:1100:ARG:HB2	2.18	0.44
3:B:27:ALA:O	3:B:29:ASP:N	2.51	0.44
3:B:386:LEU:C	3:B:388:CYS:N	2.73	0.44
4:C:258:ILE:HD12	4:C:258:ILE:N	2.32	0.44
5:D:29:LEU:O	5:D:30:GLY:C	2.59	0.44
6:E:60:PHE:C	6:E:60:PHE:CD2	2.93	0.44
8:G:154:VAL:HG12	8:G:155:SER:H	1.83	0.44
9:H:58:THR:HG22	9:H:59:ILE:H	1.82	0.44
2:A:90:VAL:CG1	2:A:297:GLN:NE2	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:244:PRO:O	2:A:246:VAL:N	2.50	0.44
2:A:608:ILE:C	2:A:610:GLY:H	2.26	0.44
2:A:666:ILE:HD11	3:B:1067:ARG:O	2.17	0.44
2:A:825:ILE:HG22	2:A:826:ASP:N	2.32	0.44
2:A:1025:ARG:O	2:A:1026:LEU:HD23	2.17	0.44
2:A:1160:SER:HA	2:A:1170:ILE:CD1	2.48	0.44
2:A:1211:GLN:O	2:A:1212:VAL:C	2.61	0.44
3:B:259:TYR:HD1	3:B:259:TYR:H	1.66	0.44
3:B:487:THR:HG22	3:B:488:TYR:N	2.31	0.44
3:B:496:ARG:NH1	3:B:539:LEU:HB2	2.33	0.44
3:B:510:LYS:CG	3:B:511:PRO:HD3	2.26	0.44
3:B:642:ASP:CB	3:B:649:LYS:HG3	2.47	0.44
3:B:757:PRO:HD3	3:B:983:ARG:HH21	1.82	0.44
3:B:824:ILE:HG22	3:B:1008:PRO:HA	2.00	0.44
4:C:124:LEU:O	4:C:127:ARG:HG2	2.18	0.44
5:D:3:VAL:O	5:D:4:SER:CB	2.66	0.44
5:D:173:HIS:CD2	5:D:175:PHE:H	2.36	0.44
6:E:5:ASN:O	6:E:9:ILE:HG13	2.18	0.44
6:E:205:SER:O	6:E:206:GLY:C	2.61	0.44
10:I:53:GLY:C	10:I:55:THR:N	2.74	0.44
2:A:353:ILE:CD1	2:A:487:MET:HE2	2.45	0.44
2:A:577:ILE:C	2:A:579:SER:N	2.74	0.44
2:A:681:GLU:O	2:A:685:GLU:HG2	2.18	0.44
2:A:720:ARG:NH1	2:A:720:ARG:CB	2.81	0.44
2:A:1273:LEU:N	2:A:1273:LEU:CD1	2.81	0.44
3:B:458:LYS:O	3:B:459:TYR:C	2.60	0.44
3:B:606:LYS:HD2	3:B:608:ASP:OD2	2.18	0.44
3:B:654:ARG:C	3:B:656:GLY:N	2.76	0.44
3:B:681:TRP:C	3:B:683:SER:N	2.74	0.44
3:B:800:GLN:HB2	3:B:821:GLN:HA	1.99	0.44
3:B:1125:ASP:O	3:B:1126:GLY:O	2.36	0.44
3:B:1216:LEU:C	3:B:1217:TYR:HD1	2.26	0.44
4:C:133:ILE:HD13	4:C:236:GLY:C	2.43	0.44
7:F:75:PRO:HG3	7:F:78:GLN:OE1	2.18	0.44
9:H:82:PRO:C	9:H:84:ALA:H	2.24	0.44
13:L:47:ARG:HH21	13:L:54:ARG:NH2	2.14	0.44
2:A:56:PRO:O	2:A:57:ARG:NE	2.47	0.44
2:A:366:VAL:HG21	2:A:460:VAL:HG22	1.99	0.44
2:A:785:PRO:HG2	3:B:703:ILE:HD12	1.99	0.44
2:A:853:ASP:OD2	2:A:855:THR:HG22	2.18	0.44
2:A:1299:VAL:CG1	2:A:1300:LYS:N	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:224:GLN:O	3:B:238:ALA:HA	2.18	0.44
3:B:526:GLU:HG2	3:B:526:GLU:O	2.18	0.44
3:B:840:ILE:CG2	3:B:994:TYR:HD1	2.30	0.44
3:B:1164:GLY:HA3	3:B:1190:ASP:OD2	2.18	0.44
5:D:3:VAL:O	5:D:4:SER:HB3	2.18	0.44
5:D:37:GLN:OE1	8:G:5:LYS:NZ	2.35	0.44
5:D:148:LEU:O	5:D:152:SER:OG	2.33	0.44
7:F:125:LEU:O	7:F:125:LEU:CG	2.65	0.44
2:A:40:THR:CG2	2:A:41:MET:HG3	2.44	0.43
2:A:78:PRO:HA	3:B:1201:LYS:NZ	2.32	0.43
2:A:116:ASP:C	2:A:118:HIS:H	2.25	0.43
2:A:501:LEU:HA	2:A:505:CYS:HB2	2.00	0.43
2:A:599:SER:HA	2:A:600:PRO:HD2	1.89	0.43
2:A:665:GLY:O	2:A:666:ILE:C	2.61	0.43
2:A:923:LEU:O	2:A:927:VAL:HG23	2.18	0.43
2:A:964:ILE:O	2:A:967:ALA:N	2.51	0.43
2:A:1313:LEU:CD2	2:A:1338:VAL:HG21	2.45	0.43
3:B:22:SER:HA	3:B:654:ARG:HG3	2.00	0.43
3:B:309:GLN:CG	10:I:52:ILE:HD11	2.47	0.43
3:B:635:ARG:NH1	3:B:742:GLU:OE2	2.51	0.43
3:B:644:GLU:OE2	3:B:646:LEU:HB2	2.18	0.43
3:B:763:GLN:HG2	3:B:765:PRO:CG	2.47	0.43
3:B:1081:LEU:O	3:B:1083:ALA:N	2.50	0.43
3:B:1183:LYS:N	3:B:1183:LYS:CE	2.81	0.43
5:D:51:ASN:O	5:D:52:LEU:O	2.36	0.43
5:D:63:LEU:O	5:D:129:LEU:HD11	2.18	0.43
8:G:15:PRO:O	8:G:16:SER:C	2.61	0.43
2:A:630:ILE:HD13	2:A:646:PHE:CZ	2.53	0.43
2:A:719:VAL:C	2:A:721:PHE:N	2.75	0.43
2:A:719:VAL:C	2:A:721:PHE:H	2.26	0.43
2:A:809:THR:H	2:A:812:GLU:HB2	1.82	0.43
2:A:874:ASP:HA	2:A:1058:VAL:HG22	1.99	0.43
2:A:914:GLU:HB2	2:A:979:SER:O	2.17	0.43
2:A:1260:LEU:O	2:A:1260:LEU:CG	2.66	0.43
3:B:244:LEU:HD11	3:B:366:GLN:NE2	2.33	0.43
3:B:977:GLY:HA3	3:B:1099:VAL:CG2	2.48	0.43
4:C:44:LEU:HD21	4:C:159:ALA:HB1	1.98	0.43
4:C:174:ALA:O	4:C:175:ALA:HB2	2.18	0.43
10:I:8:ARG:HG3	10:I:8:ARG:H	1.61	0.43
10:I:10:CYS:O	10:I:11:ASN:C	2.61	0.43
10:I:87:GLN:O	10:I:88:SER:C	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:71:GLN:C	2:A:73:GLY:H	2.26	0.43
2:A:230:ARG:HB2	2:A:233:TRP:CE3	2.53	0.43
2:A:341:MET:HE2	2:A:1401:SER:OG	2.18	0.43
2:A:412:ARG:HH21	3:B:1108:ARG:NH1	2.16	0.43
2:A:818:MET:HE1	3:B:516:ASN:ND2	2.33	0.43
2:A:858:ASN:HD22	2:A:861:GLY:H	1.64	0.43
3:B:39:ARG:NH2	3:B:665:GLU:CD	2.72	0.43
3:B:205:ILE:O	3:B:206:ASN:C	2.60	0.43
3:B:360:PHE:C	3:B:360:PHE:HD2	2.25	0.43
3:B:469:GLN:HB2	3:B:470:LYS:H	1.54	0.43
3:B:530:GLY:O	3:B:531:GLN:C	2.61	0.43
3:B:603:LEU:HB3	3:B:609:ILE:CG1	2.48	0.43
3:B:797:TYR:HE1	3:B:854:LEU:HD21	1.83	0.43
6:E:78:LEU:HD23	6:E:78:LEU:C	2.43	0.43
6:E:153:HIS:CD2	6:E:198:ILE:HG12	2.54	0.43
2:A:43:GLU:O	2:A:44:THR:HB	2.19	0.43
2:A:146:MET:HB3	2:A:171:GLN:O	2.18	0.43
2:A:279:LEU:HD12	2:A:289:ILE:HG12	2.00	0.43
2:A:321:PRO:O	2:A:322:VAL:CB	2.66	0.43
2:A:343:LYS:NZ	3:B:1151:LEU:O	2.52	0.43
2:A:347:PHE:N	2:A:347:PHE:CD1	2.86	0.43
2:A:817:ALA:HA	3:B:764:SER:OG	2.18	0.43
3:B:269:ILE:HD11	3:B:386:LEU:HD21	1.99	0.43
3:B:552:MET:O	3:B:554:ILE:N	2.51	0.43
3:B:635:ARG:NH2	3:B:742:GLU:OE2	2.50	0.43
3:B:792:MET:HE2	3:B:857:ARG:NH2	2.34	0.43
3:B:1040:ASN:O	3:B:1042:GLY:N	2.51	0.43
4:C:10:ILE:HA	4:C:20:PHE:HB2	1.99	0.43
4:C:35:ARG:NH1	12:K:40:HIS:HB2	2.34	0.43
4:C:35:ARG:HH11	12:K:41:THR:CA	2.30	0.43
4:C:184:ASN:HD21	4:C:187:LYS:HA	1.79	0.43
4:C:187:LYS:HG3	4:C:219:PHE:HE1	1.82	0.43
6:E:75:MET:O	6:E:76:GLY:O	2.37	0.43
6:E:129:PRO:O	6:E:130:ALA:C	2.61	0.43
8:G:1:MET:HE2	8:G:3:PHE:CE1	2.54	0.43
8:G:14:HIS:HD2	8:G:16:SER:CB	2.30	0.43
8:G:45:ILE:HD13	8:G:78:VAL:CG1	2.48	0.43
8:G:115:MET:HA	8:G:163:ILE:HG13	2.00	0.43
9:H:118:PHE:O	9:H:120:GLY:N	2.52	0.43
13:L:70:ARG:HG2	13:L:70:ARG:HH11	1.84	0.43
2:A:34:LYS:O	2:A:35:ILE:CB	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:254:GLU:HG3	3:B:935:ARG:HH22	1.84	0.43
2:A:289:ILE:O	2:A:293:GLU:N	2.51	0.43
2:A:316:GLN:HG2	2:A:317:LYS:N	2.33	0.43
2:A:339:ASN:O	2:A:343:LYS:HG2	2.19	0.43
2:A:1116:LEU:CA	2:A:1308:THR:HG22	2.48	0.43
2:A:1215:ARG:HA	2:A:1218:GLN:HG2	1.99	0.43
3:B:210:LYS:HG3	3:B:461:LEU:O	2.17	0.43
3:B:685:LEU:C	3:B:687:GLU:N	2.77	0.43
3:B:1099:VAL:HG12	3:B:1100:ASP:H	1.82	0.43
4:C:26:ASP:O	4:C:27:LEU:C	2.62	0.43
4:C:73:GLN:CB	4:C:131:HIS:H	2.26	0.43
5:D:30:GLY:C	5:D:32:GLU:N	2.76	0.43
5:D:214:LEU:C	5:D:216:ASN:N	2.76	0.43
8:G:26:LEU:HD11	8:G:70:PHE:CD1	2.53	0.43
8:G:51:TYR:C	8:G:51:TYR:HD2	2.26	0.43
8:G:80:LYS:H	8:G:80:LYS:HD3	1.82	0.43
9:H:83:GLN:C	9:H:85:GLY:N	2.76	0.43
2:A:362:ASP:OD2	2:A:459:ARG:HD3	2.18	0.43
2:A:463:ILE:HD12	2:A:469:ARG:HD2	2.01	0.43
2:A:577:ILE:O	2:A:578:LEU:C	2.61	0.43
2:A:818:MET:HE1	3:B:516:ASN:HD21	1.83	0.43
2:A:894:GLU:O	2:A:898:ARG:HB3	2.19	0.43
2:A:976:THR:OG1	2:A:977:LYS:N	2.51	0.43
2:A:1118:VAL:CG2	2:A:1306:LEU:HB2	2.48	0.43
2:A:1202:MET:HE1	2:A:1212:VAL:HG21	2.00	0.43
2:A:1438:THR:HB	3:B:1144:ALA:CB	2.42	0.43
3:B:210:LYS:HD3	3:B:481:GLN:O	2.18	0.43
3:B:332:ASP:O	3:B:333:PHE:C	2.61	0.43
3:B:558:LEU:O	3:B:559:SER:C	2.62	0.43
3:B:684:LEU:HD12	3:B:684:LEU:N	2.30	0.43
5:D:185:CYS:O	5:D:211:LEU:HD22	2.19	0.43
12:K:53:ASP:HB3	12:K:56:VAL:HG23	2.00	0.43
2:A:17:VAL:HG23	2:A:1419:ASP:HB3	2.01	0.43
2:A:67:CYS:SG	2:A:77:CYS:SG	3.16	0.43
2:A:376:TYR:OH	2:A:498:ARG:HD2	2.19	0.43
2:A:713:SER:O	2:A:717:ASN:ND2	2.51	0.43
2:A:1004:ASN:HD21	6:E:167:ARG:HD2	1.81	0.43
2:A:1239:ARG:NH1	2:A:1239:ARG:HB3	2.33	0.43
2:A:1345:ARG:HD2	2:A:1373:ASP:OD1	2.19	0.43
2:A:1364:ASN:O	2:A:1366:ARG:N	2.52	0.43
3:B:230:ALA:HB3	3:B:231:PRO:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:658:ILE:HG22	3:B:659:ALA:N	2.33	0.43
3:B:834:ASN:O	3:B:1013:ASN:HB2	2.19	0.43
3:B:861:ASP:OD1	3:B:914:LYS:HD2	2.19	0.43
3:B:954:VAL:HG22	3:B:964:VAL:HG22	1.99	0.43
3:B:1215:ARG:C	3:B:1216:LEU:HD22	2.44	0.43
4:C:10:ILE:HA	4:C:20:PHE:CB	2.49	0.43
4:C:25:VAL:HG23	4:C:228:PHE:CE1	2.52	0.43
4:C:208:GLU:O	4:C:210:GLU:N	2.51	0.43
6:E:144:ILE:HG13	6:E:145:THR:N	2.32	0.43
8:G:87:VAL:CG2	8:G:103:VAL:HG21	2.49	0.43
11:J:3:VAL:HA	11:J:53:HIS:CE1	2.54	0.43
2:A:35:ILE:HD13	2:A:241:VAL:HG11	1.98	0.43
2:A:172:PRO:HD3	2:A:185:TRP:HE1	1.83	0.43
2:A:903:ASN:ND2	2:A:903:ASN:C	2.75	0.43
2:A:1100:ARG:NH2	2:A:1351:GLU:HG2	2.34	0.43
2:A:1219:THR:HG21	2:A:1271:ILE:CD1	2.49	0.43
3:B:37:PHE:HE1	3:B:41:LYS:CG	2.28	0.43
3:B:130:VAL:HB	3:B:167:ILE:CD1	2.49	0.43
3:B:308:TRP:CZ3	10:I:45:ARG:HB3	2.53	0.43
3:B:787:VAL:O	3:B:787:VAL:HG12	2.19	0.43
3:B:803:LEU:HD12	3:B:1032:SER:HB3	2.00	0.43
4:C:239:PRO:C	4:C:241:ASP:N	2.75	0.43
5:D:118:THR:O	5:D:118:THR:HG22	2.18	0.43
6:E:151:PRO:HB3	6:E:200:ARG:HB3	2.01	0.43
2:A:302:THR:O	2:A:304:MET:N	2.52	0.43
2:A:1220:PHE:CD1	2:A:1224:LEU:HD23	2.53	0.43
3:B:327:ARG:O	3:B:331:LEU:HD13	2.18	0.43
3:B:659:ALA:HA	3:B:662:MET:HE3	2.01	0.43
3:B:758:PHE:CE2	3:B:1044:ALA:HA	2.53	0.43
3:B:840:ILE:HB	3:B:1011:ILE:HB	2.01	0.43
3:B:1072:MET:HE2	3:B:1087:PHE:HB2	2.01	0.43
3:B:1099:VAL:HG13	3:B:1100:ASP:N	2.34	0.43
6:E:134:THR:C	6:E:135:PHE:HD1	2.26	0.43
9:H:118:PHE:N	9:H:118:PHE:CD1	2.87	0.43
10:I:94:ASP:O	10:I:95:THR:C	2.62	0.43
12:K:17:SER:O	12:K:18:LYS:C	2.61	0.43
2:A:108:MET:O	2:A:109:HIS:HB3	2.19	0.43
2:A:138:ILE:HD12	2:A:222:LEU:HD23	1.99	0.43
2:A:500:GLU:OE2	3:B:1145:SER:HB2	2.19	0.43
2:A:767:GLN:HB2	2:A:799:PHE:HD1	1.83	0.43
2:A:901:LEU:HD22	2:A:919:ILE:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1001:ARG:O	2:A:1002:GLY:O	2.37	0.43
2:A:1376:THR:O	2:A:1377:THR:C	2.61	0.43
3:B:483:LEU:HD12	3:B:484:ASN:N	2.34	0.43
3:B:527:THR:OG1	3:B:528:PRO:HD2	2.19	0.43
4:C:44:LEU:CD2	4:C:159:ALA:HB1	2.49	0.43
5:D:128:VAL:C	5:D:130:LEU:N	2.76	0.43
10:I:16:PRO:HB3	10:I:27:PHE:CE2	2.54	0.43
12:K:63:VAL:HG23	12:K:63:VAL:O	2.19	0.43
2:A:4:GLN:O	2:A:5:GLN:CB	2.65	0.42
2:A:14:VAL:CG2	3:B:1216:LEU:HD12	2.47	0.42
2:A:29:ALA:HB1	3:B:1184:GLY:HA3	2.00	0.42
2:A:72:GLU:OE2	3:B:1175:LEU:HD12	2.19	0.42
2:A:242:PRO:HD3	3:B:1209:ALA:CB	2.49	0.42
2:A:332:LYS:O	2:A:333:GLU:CB	2.67	0.42
2:A:688:LYS:C	2:A:690:VAL:N	2.76	0.42
2:A:765:VAL:HG12	2:A:766:GLY:N	2.33	0.42
2:A:1063:MET:HG3	2:A:1436:ILE:HG23	2.00	0.42
2:A:1206:ASP:HB3	2:A:1274:ARG:HH12	1.83	0.42
3:B:114:PRO:O	3:B:116:GLU:N	2.52	0.42
3:B:205:ILE:O	3:B:207:GLY:N	2.51	0.42
3:B:459:TYR:CE1	3:B:469:GLN:HG2	2.54	0.42
3:B:681:TRP:O	3:B:682:SER:C	2.62	0.42
3:B:687:GLU:O	3:B:688:GLY:C	2.62	0.42
3:B:710:LEU:CA	3:B:733:HIS:HB3	2.45	0.42
3:B:822:ASN:O	11:J:48:ARG:NH1	2.52	0.42
3:B:953:LEU:HB2	13:L:56:LEU:O	2.19	0.42
3:B:1182:CYS:C	3:B:1183:LYS:O	2.62	0.42
4:C:175:ALA:HB2	11:J:10:CYS:HB2	2.00	0.42
4:C:265:MET:HE1	12:K:19:LEU:O	2.19	0.42
5:D:29:LEU:HB3	8:G:82:PHE:CE2	2.54	0.42
6:E:12:LEU:HD12	6:E:12:LEU:O	2.19	0.42
6:E:13:TRP:CZ3	6:E:39:LEU:HB2	2.54	0.42
6:E:32:GLN:HG3	6:E:36:GLU:OE2	2.19	0.42
6:E:167:ARG:HD3	6:E:167:ARG:HA	1.75	0.42
7:F:69:LEU:HB2	7:F:72:LYS:HB2	2.01	0.42
2:A:58:LEU:CD1	2:A:244:PRO:HD2	2.42	0.42
2:A:331:GLY:O	2:A:332:LYS:O	2.37	0.42
2:A:779:PHE:CE2	3:B:517:THR:HG22	2.54	0.42
3:B:216:GLU:OE1	3:B:537:LYS:CE	2.63	0.42
3:B:244:LEU:HD13	3:B:247:GLY:O	2.19	0.42
3:B:653:VAL:CG2	3:B:689:LEU:HD22	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:770:GLN:OE1	3:B:983:ARG:CA	2.60	0.42
3:B:953:LEU:HD23	3:B:953:LEU:O	2.19	0.42
3:B:980:PHE:CE2	3:B:1094:ARG:HG3	2.53	0.42
4:C:16:ASP:O	4:C:17:ASN:CG	2.63	0.42
5:D:139:LYS:HE2	5:D:139:LYS:HB2	1.88	0.42
5:D:191:ALA:C	5:D:193:THR:N	2.77	0.42
7:F:138:LEU:HB3	7:F:139:PRO:HD2	2.01	0.42
9:H:7:ASP:O	9:H:8:ASP:HB2	2.19	0.42
9:H:56:THR:HB	9:H:145:ARG:HG2	2.00	0.42
2:A:34:LYS:HD3	2:A:57:ARG:HH22	1.80	0.42
2:A:353:ILE:HB	2:A:470:LEU:HD23	2.01	0.42
2:A:466:SER:HB3	3:B:1103:ILE:HG12	2.00	0.42
2:A:491:VAL:HG12	2:A:492:PRO:O	2.19	0.42
2:A:590:ARG:HG3	2:A:590:ARG:NH1	2.35	0.42
2:A:606:LEU:HD11	2:A:608:ILE:CG1	2.50	0.42
2:A:658:LEU:HG	2:A:659:HIS:ND1	2.34	0.42
2:A:722:LEU:O	2:A:725:ALA:HB3	2.19	0.42
2:A:1012:ARG:O	2:A:1016:THR:OG1	2.34	0.42
2:A:1036:ARG:HH11	2:A:1036:ARG:CG	2.32	0.42
2:A:1162:VAL:O	2:A:1162:VAL:HG12	2.18	0.42
2:A:1346:ALA:O	2:A:1350:LYS:HB2	2.20	0.42
3:B:746:SER:CB	3:B:1046:PRO:HG2	2.45	0.42
3:B:827:ILE:HD12	3:B:1086:PHE:HD2	1.84	0.42
3:B:911:ILE:O	3:B:911:ILE:HG22	2.20	0.42
4:C:44:LEU:HD23	4:C:44:LEU:C	2.44	0.42
5:D:30:GLY:O	5:D:32:GLU:N	2.52	0.42
5:D:141:LEU:HD12	5:D:141:LEU:HA	1.86	0.42
5:D:214:LEU:N	5:D:214:LEU:HD23	2.34	0.42
10:I:92:ARG:HB3	10:I:95:THR:OG1	2.19	0.42
2:A:86:LEU:HD12	2:A:236:LEU:O	2.19	0.42
2:A:166:GLY:O	2:A:167:CYS:CB	2.67	0.42
2:A:270:LEU:HD12	2:A:270:LEU:O	2.19	0.42
2:A:285:PRO:O	2:A:287:HIS:N	2.52	0.42
2:A:574:GLY:C	2:A:576:GLN:N	2.77	0.42
2:A:849:MET:CE	2:A:1061:GLY:CA	2.95	0.42
2:A:850:VAL:HG23	2:A:1064:VAL:HG21	2.02	0.42
2:A:1366:ARG:HG2	2:A:1366:ARG:HH11	1.82	0.42
3:B:31:TRP:CZ3	3:B:34:ILE:HD12	2.54	0.42
3:B:38:PHE:CD1	3:B:811:TYR:CD2	3.07	0.42
3:B:390:LEU:O	3:B:392:ARG:HG3	2.19	0.42
3:B:519:TRP:CD1	3:B:519:TRP:C	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:582:VAL:HA	3:B:626:ILE:O	2.19	0.42
3:B:610:ASN:C	3:B:612:GLU:H	2.27	0.42
3:B:658:ILE:C	3:B:660:LYS:N	2.77	0.42
3:B:744:HIS:CG	3:B:745:PRO:HD2	2.54	0.42
3:B:810:GLU:HA	3:B:815:ARG:HH12	1.84	0.42
3:B:1001:PHE:CD1	3:B:1001:PHE:C	2.97	0.42
4:C:48:SER:O	4:C:157:CYS:HA	2.19	0.42
4:C:176:ILE:HG22	4:C:177:GLU:O	2.19	0.42
4:C:236:GLY:O	4:C:237:SER:C	2.63	0.42
8:G:34:VAL:HG12	8:G:45:ILE:CG2	2.37	0.42
8:G:112:LYS:NZ	8:G:120:THR:HA	2.33	0.42
9:H:63:LEU:HD11	9:H:141:TYR:CD2	2.54	0.42
10:I:59:VAL:HG12	10:I:60:GLN:N	2.34	0.42
2:A:106:VAL:C	2:A:114:LEU:HD21	2.44	0.42
2:A:637:LYS:HB3	2:A:641:VAL:HG11	2.02	0.42
2:A:1019:CYS:O	2:A:1022:LEU:HB3	2.18	0.42
2:A:1315:GLU:C	2:A:1317:MET:N	2.74	0.42
3:B:69:LEU:HD22	3:B:429:PHE:CE1	2.54	0.42
3:B:128:LEU:HD11	3:B:170:LEU:CB	2.50	0.42
3:B:165:VAL:HG11	3:B:448:ILE:HD13	2.00	0.42
3:B:466:TRP:CE3	3:B:466:TRP:HA	2.53	0.42
3:B:763:GLN:O	3:B:764:SER:C	2.62	0.42
3:B:865:LYS:HZ3	3:B:869:SER:HA	1.85	0.42
4:C:99:LEU:HD13	4:C:99:LEU:HA	1.90	0.42
4:C:134:ILE:HG22	4:C:136:ASP:H	1.84	0.42
6:E:85:GLU:HB2	6:E:88:VAL:CG2	2.48	0.42
7:F:99:LEU:O	7:F:103:MET:CG	2.67	0.42
12:K:55:LYS:HB3	12:K:81:TYR:CE1	2.54	0.42
2:A:19:PHE:HE1	2:A:1396:ALA:HB3	1.84	0.42
2:A:210:ILE:O	2:A:214:ILE:HG13	2.20	0.42
2:A:608:ILE:C	2:A:610:GLY:N	2.76	0.42
2:A:851:HIS:CD2	2:A:857:ARG:HB2	2.54	0.42
2:A:1114:PRO:O	2:A:1115:SER:O	2.36	0.42
2:A:1332:PHE:O	2:A:1333:ILE:C	2.62	0.42
2:A:1434:ALA:O	2:A:1436:ILE:N	2.52	0.42
3:B:310:MET:O	3:B:313:MET:HB2	2.19	0.42
3:B:423:LYS:O	3:B:427:ASP:HB2	2.20	0.42
3:B:603:LEU:CD1	3:B:608:ASP:HB2	2.50	0.42
3:B:1010:LEU:O	3:B:1011:ILE:HG13	2.19	0.42
3:B:1181:GLU:O	3:B:1182:CYS:CB	2.68	0.42
4:C:248:ILE:HD13	12:K:101:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:119:ARG:HD3	5:D:221:TYR:CE2	2.54	0.42
6:E:102:GLU:C	6:E:104:ASN:N	2.77	0.42
7:F:109:VAL:HG11	7:F:123:LYS:HD3	2.00	0.42
7:F:138:LEU:O	7:F:140:ASP:N	2.52	0.42
10:I:84:VAL:HG13	10:I:84:VAL:O	2.19	0.42
2:A:418:SER:O	2:A:420:ARG:N	2.53	0.42
2:A:516:SER:O	2:A:517:ASN:C	2.62	0.42
3:B:170:LEU:HA	3:B:171:PRO:HD2	1.92	0.42
3:B:237:VAL:HG12	3:B:238:ALA:N	2.35	0.42
3:B:856:PHE:HD2	3:B:967:ARG:CD	2.30	0.42
4:C:6:PRO:HG2	12:K:101:LEU:HB2	2.01	0.42
4:C:112:ASN:HB2	4:C:114:TYR:CE1	2.55	0.42
5:D:175:PHE:CE1	8:G:1:MET:HA	2.55	0.42
6:E:116:ILE:CG2	6:E:120:ALA:HB3	2.50	0.42
8:G:52:ASP:C	8:G:53:ASN:HD22	2.27	0.42
12:K:58:PHE:HB3	12:K:76:GLN:HE21	1.83	0.42
2:A:64:ASN:O	2:A:65:LEU:C	2.62	0.42
2:A:128:ILE:O	2:A:128:ILE:HG22	2.20	0.42
2:A:347:PHE:CE2	2:A:493:GLN:OE1	2.73	0.42
2:A:973:ILE:HD11	2:A:1041:ALA:HB2	2.01	0.42
2:A:1334:ASP:C	2:A:1336:MET:N	2.76	0.42
3:B:37:PHE:CE2	3:B:542:MET:HA	2.54	0.42
3:B:212:LEU:HD12	3:B:409:ALA:HB1	2.01	0.42
3:B:234:ILE:HD12	3:B:234:ILE:H	1.85	0.42
3:B:448:ILE:O	3:B:450:ALA:N	2.52	0.42
3:B:900:ALA:O	3:B:902:GLY:N	2.53	0.42
6:E:18:THR:O	6:E:19:VAL:C	2.63	0.42
11:J:36:LEU:HD12	11:J:47:ARG:NH1	2.34	0.42
12:K:111:LEU:O	12:K:112:GLN:HB3	2.19	0.42
2:A:162:VAL:HG12	2:A:163:SER:N	2.35	0.42
2:A:207:ILE:CG2	2:A:211:PHE:CE1	3.03	0.42
2:A:444:PHE:CB	2:A:458:HIS:HD2	2.33	0.42
2:A:474:VAL:C	2:A:477:PRO:HD2	2.45	0.42
2:A:784:LEU:HD11	2:A:815:PHE:CE2	2.55	0.42
2:A:814:PHE:O	2:A:818:MET:HG3	2.20	0.42
2:A:1385:THR:C	2:A:1387:HIS:N	2.76	0.42
3:B:265:SER:O	3:B:266:ALA:CB	2.68	0.42
3:B:476:ARG:NH2	3:B:501:PRO:HG3	2.35	0.42
3:B:593:PRO:HG2	3:B:617:ARG:CZ	2.49	0.42
3:B:871:THR:CG2	3:B:872:GLU:N	2.82	0.42
3:B:1039:GLY:HA2	11:J:51:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:32:THR:HG22	9:H:33:GLN:OE1	2.19	0.42
12:K:83:PRO:O	12:K:84:LYS:C	2.61	0.42
2:A:412:ARG:NH2	3:B:1108:ARG:NH1	2.68	0.42
2:A:761:MET:HA	2:A:804:TYR:HB2	2.02	0.42
2:A:1009:ASN:HA	2:A:1012:ARG:NH1	2.35	0.42
2:A:1420:ASP:O	2:A:1421:CYS:CB	2.64	0.42
3:B:56:ASP:HB3	3:B:57:TYR:HD1	1.85	0.42
3:B:210:LYS:HA	3:B:481:GLN:O	2.20	0.42
3:B:216:GLU:HG2	3:B:217:ARG:N	2.35	0.42
3:B:262:GLU:O	3:B:262:GLU:HG2	2.19	0.42
3:B:895:ASP:C	3:B:897:GLY:N	2.78	0.42
3:B:1001:PHE:CE2	4:C:34:ARG:NE	2.88	0.42
5:D:25:ALA:HB2	8:G:84:GLY:O	2.19	0.42
8:G:140:LYS:H	8:G:140:LYS:HG2	1.68	0.42
9:H:103:LYS:HG2	9:H:104:PHE:N	2.35	0.42
10:I:53:GLY:C	10:I:55:THR:H	2.26	0.42
12:K:42:LEU:O	12:K:46:ILE:HG13	2.19	0.42
2:A:150:THR:HG22	2:A:150:THR:O	2.20	0.41
2:A:1230:GLU:C	2:A:1232:ASN:H	2.28	0.41
2:A:1410:PHE:HD2	3:B:1212:ILE:CD1	2.33	0.41
3:B:180:TYR:CD1	3:B:180:TYR:N	2.85	0.41
3:B:298:LEU:N	3:B:298:LEU:CD2	2.83	0.41
3:B:360:PHE:O	3:B:361:LEU:C	2.62	0.41
3:B:542:MET:HE3	3:B:636:PRO:CG	2.50	0.41
3:B:705:MET:HB3	3:B:706:GLN:H	1.71	0.41
4:C:25:VAL:CG2	4:C:228:PHE:HE1	2.33	0.41
6:E:4:GLU:O	6:E:8:ASN:HB2	2.19	0.41
8:G:45:ILE:HA	8:G:78:VAL:CG1	2.48	0.41
9:H:128:ASN:O	9:H:128:ASN:CG	2.61	0.41
13:L:53:HIS:HB3	13:L:55:ILE:CD1	2.50	0.41
2:A:7:SER:HB2	3:B:1175:LEU:CD2	2.49	0.41
2:A:7:SER:CB	3:B:1175:LEU:HD22	2.46	0.41
2:A:167:CYS:SG	2:A:167:CYS:O	2.78	0.41
2:A:289:ILE:C	2:A:291:GLU:N	2.77	0.41
2:A:364:VAL:O	2:A:364:VAL:HG13	2.18	0.41
2:A:896:ARG:NH2	2:A:1030:ARG:NH2	2.68	0.41
2:A:923:LEU:HD23	2:A:923:LEU:HA	1.90	0.41
2:A:1329:THR:HG21	2:A:1331:SER:HB3	2.01	0.41
3:B:273:LEU:O	3:B:276:ILE:HB	2.20	0.41
3:B:750:GLY:O	3:B:751:VAL:C	2.62	0.41
3:B:1002:THR:HG23	3:B:1006:ILE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:146:LYS:HB2	11:J:61:LEU:HD11	2.02	0.41
6:E:2:ASP:HB3	6:E:3:GLN:H	1.41	0.41
6:E:100:ILE:CG2	6:E:105:PHE:HB2	2.50	0.41
8:G:15:PRO:HG2	8:G:66:GLY:HA3	2.01	0.41
11:J:27:GLU:O	11:J:29:GLU:N	2.44	0.41
13:L:34:CYS:O	13:L:35:SER:C	2.63	0.41
2:A:852:TYR:HA	2:A:1060:PRO:HB3	2.02	0.41
2:A:1376:THR:HG23	2:A:1377:THR:H	1.84	0.41
2:A:1406:VAL:O	2:A:1407:GLU:C	2.63	0.41
3:B:171:PRO:HD2	3:B:457:LEU:HD12	2.00	0.41
3:B:621:GLU:O	3:B:621:GLU:HG3	2.20	0.41
4:C:35:ARG:HH12	12:K:40:HIS:HB2	1.84	0.41
4:C:152:GLU:CG	4:C:153:LEU:H	2.27	0.41
4:C:191:TYR:CD2	4:C:201:TRP:CD1	3.04	0.41
4:C:215:GLU:O	4:C:216:GLY:C	2.63	0.41
6:E:23:VAL:HB	6:E:30:ILE:HD11	2.01	0.41
6:E:48:ASP:CG	6:E:49:SER:N	2.73	0.41
12:K:3:ALA:O	12:K:4:PRO:O	2.39	0.41
1:R:12:C:H5'	2:A:320:ARG:NH2	2.34	0.41
2:A:182:VAL:HG12	2:A:183:GLY:N	2.35	0.41
2:A:290:GLU:HA	2:A:293:GLU:HB3	2.03	0.41
2:A:375:THR:OG1	2:A:376:TYR:N	2.52	0.41
2:A:1177:LEU:HD23	2:A:1177:LEU:HA	1.74	0.41
2:A:1206:ASP:O	2:A:1274:ARG:NH1	2.53	0.41
3:B:758:PHE:HZ	3:B:1031:LEU:HD22	1.86	0.41
3:B:781:PHE:O	3:B:782:LEU:HD23	2.19	0.41
3:B:828:ALA:O	3:B:834:ASN:ND2	2.53	0.41
3:B:898:LEU:HD13	3:B:952:VAL:HG11	2.02	0.41
3:B:976:ILE:HD13	3:B:991:GLY:O	2.21	0.41
3:B:1002:THR:O	3:B:1003:ALA:C	2.63	0.41
3:B:1003:ALA:HA	4:C:178:PHE:O	2.20	0.41
4:C:29:MET:HE2	12:K:98:LEU:CD2	2.50	0.41
5:D:8:PHE:O	5:D:9:GLN:HB2	2.21	0.41
5:D:130:LEU:O	5:D:132:GLN:N	2.48	0.41
8:G:91:VAL:HB	8:G:139:ILE:O	2.20	0.41
12:K:35:PHE:HE1	12:K:73:LEU:HB3	1.83	0.41
2:A:373:THR:HG21	3:B:1105:ALA:CB	2.50	0.41
2:A:723:ASN:O	2:A:724:GLU:C	2.62	0.41
2:A:756:ILE:O	2:A:759:ALA:HB3	2.21	0.41
2:A:816:HIS:CD2	3:B:764:SER:H	2.39	0.41
2:A:877:HIS:C	2:A:878:ILE:CG1	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1111:MET:H	2:A:1111:MET:HG2	1.59	0.41
2:A:1115:SER:OG	2:A:1116:LEU:N	2.53	0.41
2:A:1174:PHE:C	2:A:1176:LEU:HG	2.44	0.41
3:B:298:LEU:N	3:B:298:LEU:HD22	2.36	0.41
3:B:304:ASP:OD1	3:B:306:ASN:HB2	2.21	0.41
3:B:326:ASP:OD2	3:B:328:GLU:HB2	2.21	0.41
4:C:18:VAL:O	4:C:20:PHE:CD2	2.70	0.41
6:E:16:PHE:CE2	6:E:20:LYS:HE2	2.53	0.41
7:F:82:THR:HA	7:F:83:PRO:HD3	1.83	0.41
8:G:44:TYR:CD2	8:G:105:PRO:HB2	2.56	0.41
8:G:150:CYS:C	8:G:151:ILE:HG13	2.43	0.41
9:H:24:CYS:HB2	9:H:44:VAL:HG21	2.02	0.41
12:K:101:LEU:HD23	12:K:101:LEU:O	2.20	0.41
13:L:38:LEU:O	13:L:39:SER:CB	2.64	0.41
1:R:12:C:H2'	1:R:13:G:H8	1.79	0.41
2:A:41:MET:HA	2:A:50:ILE:H	1.86	0.41
2:A:409:SER:O	2:A:410:GLY:C	2.63	0.41
2:A:693:VAL:O	2:A:693:VAL:HG12	2.20	0.41
2:A:1427:ASN:HB3	2:A:1432:GLN:O	2.20	0.41
3:B:46:GLN:HE22	3:B:496:ARG:HA	1.86	0.41
3:B:284:ILE:HG12	3:B:324:ILE:HD12	2.02	0.41
3:B:288:ALA:N	3:B:330:ALA:HB1	2.35	0.41
3:B:303:TYR:N	3:B:303:TYR:HD2	2.18	0.41
3:B:681:TRP:O	3:B:683:SER:N	2.53	0.41
3:B:769:TYR:CD1	3:B:987:LYS:NZ	2.89	0.41
3:B:862:GLN:CG	3:B:963:PHE:HD1	2.28	0.41
3:B:899:ILE:CG2	3:B:903:VAL:HG21	2.51	0.41
3:B:1085:ILE:N	3:B:1085:ILE:CD1	2.69	0.41
3:B:1152:MET:C	3:B:1157:ALA:HB2	2.45	0.41
4:C:6:PRO:HB3	4:C:25:VAL:CG1	2.42	0.41
4:C:236:GLY:O	4:C:238:ILE:N	2.53	0.41
6:E:154:ILE:HG22	6:E:155:ARG:O	2.19	0.41
9:H:48:PRO:C	9:H:49:VAL:HG23	2.45	0.41
2:A:138:ILE:HD11	2:A:221:SER:O	2.21	0.41
2:A:404:TYR:HB2	2:A:433:GLU:HB2	2.02	0.41
2:A:974:ASP:OD2	2:A:976:THR:OG1	2.37	0.41
2:A:1074:GLU:O	2:A:1076:ALA:N	2.54	0.41
3:B:37:PHE:CD2	3:B:542:MET:SD	3.14	0.41
3:B:284:ILE:HG23	3:B:324:ILE:HD12	2.00	0.41
3:B:742:GLU:O	3:B:743:ILE:C	2.63	0.41
3:B:1099:VAL:O	3:B:1101:ASP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1115:THR:HG21	3:B:1117:GLN:HB2	2.03	0.41
3:B:1152:MET:O	3:B:1157:ALA:HB2	2.21	0.41
4:C:137:LYS:HB3	4:C:138:GLU:OE1	2.20	0.41
4:C:168:ALA:C	4:C:170:TRP:N	2.78	0.41
4:C:176:ILE:HG22	4:C:177:GLU:N	2.36	0.41
10:I:59:VAL:C	10:I:61:ASP:H	2.27	0.41
11:J:41:LEU:N	11:J:41:LEU:HD23	2.33	0.41
12:K:76:GLN:HB3	12:K:76:GLN:HE21	1.66	0.41
2:A:207:ILE:CG2	2:A:211:PHE:HE1	2.33	0.41
2:A:268:ASP:HB3	2:A:299:HIS:CE1	2.54	0.41
2:A:425:GLN:N	2:A:425:GLN:OE1	2.54	0.41
2:A:768:GLN:HG2	2:A:816:HIS:CA	2.42	0.41
2:A:809:THR:HG23	2:A:812:GLU:OE1	2.21	0.41
2:A:1334:ASP:O	2:A:1336:MET:N	2.53	0.41
2:A:1343:ALA:CB	6:E:150:VAL:HG22	2.45	0.41
3:B:324:ILE:CG2	3:B:325:GLN:N	2.84	0.41
3:B:339:THR:HB	3:B:351:TYR:CE2	2.55	0.41
3:B:377:PHE:C	3:B:379:GLY:N	2.75	0.41
3:B:711:GLU:HB2	3:B:712:PRO:CD	2.50	0.41
4:C:169:LYS:NZ	13:L:69:ALA:HB3	2.36	0.41
4:C:175:ALA:CB	11:J:43:ARG:HH12	2.34	0.41
4:C:252:GLN:O	4:C:253:LYS:C	2.63	0.41
5:D:53:SER:CB	5:D:152:SER:HB3	2.51	0.41
6:E:138:ALA:HA	6:E:141:VAL:HG23	2.03	0.41
6:E:157:SER:OG	6:E:159:ASP:HB2	2.21	0.41
10:I:32:CYS:SG	10:I:33:SER:N	2.93	0.41
10:I:65:ASP:OD1	10:I:67:THR:OG1	2.30	0.41
10:I:85:PHE:HD1	10:I:99:LEU:HD13	1.86	0.41
13:L:27:LEU:O	13:L:28:LYS:HG2	2.21	0.41
2:A:32:VAL:HG21	2:A:68:GLN:HE21	1.84	0.41
2:A:40:THR:HG21	2:A:41:MET:HE2	2.03	0.41
2:A:152:VAL:HG12	2:A:153:PRO:CD	2.50	0.41
2:A:222:LEU:O	2:A:224:PHE:N	2.53	0.41
2:A:254:GLU:HB2	3:B:935:ARG:NH2	2.35	0.41
2:A:351:THR:CG2	3:B:1103:ILE:HG13	2.50	0.41
2:A:444:PHE:CB	2:A:458:HIS:CD2	3.04	0.41
2:A:457:ALA:HB3	2:A:506:ALA:N	2.36	0.41
2:A:562:THR:HB	9:H:98:TYR:HD2	1.86	0.41
2:A:665:GLY:C	2:A:667:GLY:N	2.79	0.41
2:A:683:ILE:HD13	2:A:801:GLU:CG	2.50	0.41
2:A:730:GLY:C	2:A:732:LEU:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:857:ARG:HG2	2:A:863:VAL:HA	2.03	0.41
2:A:1129:GLU:C	2:A:1131:ALA:N	2.79	0.41
2:A:1219:THR:OG1	2:A:1271:ILE:HD11	2.21	0.41
2:A:1277:GLU:C	2:A:1279:ILE:H	2.28	0.41
2:A:1398:MET:HB2	2:A:1426:GLU:OE2	2.21	0.41
2:A:1443:VAL:O	2:A:1443:VAL:HG23	2.20	0.41
3:B:21:GLU:H	3:B:21:GLU:HG3	1.64	0.41
3:B:37:PHE:HE2	3:B:542:MET:HA	1.85	0.41
3:B:53:GLN:HB2	3:B:547:VAL:HG21	2.02	0.41
3:B:126:SER:OG	3:B:172:ILE:HD11	2.20	0.41
3:B:203:PHE:CD1	3:B:203:PHE:N	2.89	0.41
3:B:211:VAL:HG21	3:B:483:LEU:HD13	2.03	0.41
3:B:520:GLY:CA	3:B:748:ILE:HG22	2.50	0.41
3:B:557:PHE:CD2	3:B:557:PHE:O	2.74	0.41
3:B:611:PRO:HG2	3:B:685:LEU:HD21	2.03	0.41
3:B:641:GLU:C	3:B:643:ASP:N	2.77	0.41
3:B:778:MET:HE1	3:B:1094:ARG:CD	2.46	0.41
3:B:797:TYR:HE1	3:B:854:LEU:HD23	1.86	0.41
3:B:797:TYR:CE1	3:B:854:LEU:CD2	3.03	0.41
3:B:1079:LYS:CA	4:C:27:LEU:HD21	2.51	0.41
4:C:22:LEU:HD21	4:C:25:VAL:HG11	2.02	0.41
4:C:43:THR:CG2	4:C:44:LEU:N	2.66	0.41
4:C:74:SER:CB	4:C:77:ILE:HG12	2.51	0.41
4:C:98:VAL:HG12	4:C:99:LEU:N	2.35	0.41
4:C:259:LEU:CD1	12:K:88:LYS:HA	2.50	0.41
5:D:59:ILE:O	5:D:60:LYS:C	2.64	0.41
5:D:153:ARG:NH2	5:D:184:ALA:HA	2.36	0.41
5:D:188:ALA:O	5:D:192:LYS:CG	2.69	0.41
6:E:63:ASN:HA	6:E:64:PRO:HD3	1.88	0.41
7:F:68:THR:OG1	7:F:69:LEU:CG	2.55	0.41
7:F:117:PRO:C	7:F:119:ARG:H	2.29	0.41
8:G:101:VAL:CG1	8:G:102:GLN:N	2.84	0.41
8:G:144:ARG:HG2	8:G:168:LEU:HD23	2.03	0.41
9:H:31:THR:O	9:H:31:THR:HG22	2.21	0.41
9:H:99:GLY:HA3	9:H:117:SER:O	2.21	0.41
9:H:110:ASP:OD1	9:H:110:ASP:N	2.53	0.41
9:H:143:LEU:HD12	9:H:143:LEU:N	2.35	0.41
10:I:13:MET:C	10:I:14:LEU:HD23	2.46	0.41
10:I:15:TYR:O	10:I:28:GLU:HG2	2.21	0.41
10:I:106:CYS:O	10:I:107:SER:CB	2.68	0.41
11:J:32:GLU:CD	11:J:32:GLU:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:44:TYR:CA	11:J:47:ARG:HB2	2.37	0.41
12:K:19:LEU:HD22	12:K:33:ILE:CG2	2.51	0.41
13:L:28:LYS:C	13:L:29:TYR:CD2	2.99	0.41
2:A:172:PRO:HB3	2:A:185:TRP:CG	2.56	0.41
2:A:997:LEU:HD13	2:A:1018:PHE:CE2	2.55	0.41
2:A:1100:ARG:O	2:A:1103:GLU:HB3	2.21	0.41
2:A:1214:GLU:OE1	2:A:1214:GLU:HA	2.21	0.41
2:A:1220:PHE:CE2	2:A:1263:ILE:HG23	2.56	0.41
3:B:184:ALA:HB1	3:B:188:ASP:HB3	2.03	0.41
3:B:221:ASN:OD1	3:B:242:SER:HA	2.21	0.41
3:B:278:GLN:HG2	3:B:279:ASP:N	2.33	0.41
3:B:732:SER:HB2	3:B:734:HIS:CD2	2.57	0.41
3:B:779:GLY:O	3:B:795:ILE:HA	2.21	0.41
3:B:1220:ARG:HH11	3:B:1220:ARG:CB	2.34	0.41
4:C:22:LEU:CD2	4:C:25:VAL:HG11	2.51	0.41
4:C:100:THR:CG2	4:C:101:LEU:N	2.84	0.41
7:F:109:VAL:HG11	7:F:123:LYS:CD	2.51	0.41
12:K:38:GLU:HB3	12:K:71:PHE:HE2	1.86	0.41
2:A:24:PRO:CD	2:A:233:TRP:CD1	3.05	0.40
2:A:154:SER:C	2:A:156:ASP:H	2.29	0.40
2:A:207:ILE:O	2:A:208:LEU:C	2.64	0.40
2:A:230:ARG:O	2:A:231:PRO:C	2.64	0.40
2:A:300:VAL:O	2:A:300:VAL:HG12	2.21	0.40
2:A:443:LEU:HD12	3:B:1146:PHE:HE2	1.85	0.40
2:A:719:VAL:O	2:A:721:PHE:N	2.54	0.40
2:A:737:LEU:HD23	2:A:737:LEU:HA	1.88	0.40
2:A:741:ASN:C	2:A:741:ASN:ND2	2.80	0.40
2:A:962:ARG:O	2:A:964:ILE:N	2.54	0.40
2:A:1057:VAL:HG12	2:A:1058:VAL:N	2.37	0.40
2:A:1116:LEU:HB2	2:A:1329:THR:HG1	1.80	0.40
2:A:1349:TYR:N	2:A:1372:VAL:HG21	2.36	0.40
3:B:307:ASP:O	3:B:307:ASP:OD1	2.39	0.40
3:B:644:GLU:C	3:B:646:LEU:H	2.29	0.40
3:B:797:TYR:CE1	3:B:971:THR:HG23	2.56	0.40
4:C:56:THR:HG22	4:C:58:LEU:HD23	2.02	0.40
4:C:66:ARG:NH1	4:C:144:ILE:O	2.54	0.40
4:C:70:ILE:O	4:C:70:ILE:HG22	2.21	0.40
4:C:232:VAL:HG11	4:C:244:VAL:HG22	2.03	0.40
5:D:137:ASN:C	5:D:137:ASN:HD22	2.28	0.40
5:D:191:ALA:O	5:D:193:THR:N	2.54	0.40
6:E:91:LYS:C	6:E:93:MET:N	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:143:ASN:ND2	6:E:145:THR:OG1	2.54	0.40
6:E:161:LYS:C	6:E:163:GLU:N	2.78	0.40
8:G:48:VAL:HA	8:G:76:ALA:CB	2.50	0.40
8:G:144:ARG:O	8:G:168:LEU:HD22	2.21	0.40
11:J:30:LEU:HD11	11:J:38:ARG:HH12	1.86	0.40
12:K:61:TYR:HA	12:K:72:LYS:O	2.21	0.40
12:K:109:TRP:O	12:K:111:LEU:N	2.54	0.40
2:A:368:LYS:HE3	2:A:368:LYS:HB2	1.78	0.40
2:A:482:PHE:C	2:A:484:GLY:N	2.79	0.40
2:A:522:GLY:O	2:A:646:PHE:HE2	2.04	0.40
3:B:237:VAL:CG1	3:B:238:ALA:N	2.84	0.40
3:B:289:LEU:HD22	3:B:371:GLU:O	2.20	0.40
3:B:377:PHE:O	3:B:380:TYR:N	2.54	0.40
3:B:400:HIS:O	3:B:401:PHE:C	2.64	0.40
3:B:657:HIS:O	3:B:660:LYS:HB3	2.21	0.40
3:B:792:MET:H	3:B:857:ARG:HA	1.85	0.40
3:B:821:GLN:HE22	3:B:851:PHE:CA	2.32	0.40
3:B:868:MET:O	3:B:870:ILE:HG13	2.21	0.40
3:B:899:ILE:O	3:B:952:VAL:HG21	2.21	0.40
3:B:1087:PHE:CD2	3:B:1087:PHE:C	2.98	0.40
3:B:1095:LEU:H	3:B:1095:LEU:CD1	2.13	0.40
6:E:56:LYS:HE3	6:E:84:ASP:HB2	2.03	0.40
6:E:178:ILE:O	6:E:178:ILE:HG23	2.20	0.40
9:H:22:LYS:O	9:H:23:VAL:HG23	2.21	0.40
11:J:34:THR:O	11:J:35:ALA:C	2.64	0.40
12:K:42:LEU:CD2	12:K:46:ILE:HD11	2.50	0.40
12:K:62:LYS:O	12:K:71:PHE:HB2	2.21	0.40
13:L:46:VAL:O	13:L:46:VAL:HG12	2.20	0.40
2:A:34:LYS:CD	2:A:34:LYS:N	2.85	0.40
2:A:511:ILE:O	2:A:519:PRO:HA	2.21	0.40
2:A:524:VAL:CG1	2:A:525:GLN:H	2.26	0.40
2:A:666:ILE:HG23	3:B:1026:LEU:HB3	2.03	0.40
2:A:883:LEU:HD13	2:A:943:LEU:HD13	2.03	0.40
2:A:977:LYS:HB3	2:A:978:PRO:HD2	2.02	0.40
2:A:1308:THR:HG21	2:A:1310:GLY:O	2.22	0.40
3:B:213:ILE:HD12	3:B:497:ARG:HB3	2.03	0.40
3:B:460:ALA:C	3:B:462:ALA:N	2.77	0.40
3:B:463:THR:HB	3:B:464:GLY:H	1.71	0.40
3:B:728:ARG:HH12	3:B:1047:PHE:HB3	1.86	0.40
3:B:820:GLY:C	3:B:1091:TYR:CE1	2.99	0.40
3:B:872:GLU:OE2	3:B:914:LYS:HE2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:992:ILE:CG1	3:B:993:THR:N	2.84	0.40
3:B:1181:GLU:O	3:B:1182:CYS:HB2	2.21	0.40
4:C:77:ILE:C	4:C:79:GLN:H	2.29	0.40
4:C:252:GLN:NE2	12:K:95:ILE:HG23	2.36	0.40
5:D:46:GLU:O	5:D:47:LEU:C	2.65	0.40
5:D:52:LEU:O	5:D:53:SER:OG	2.31	0.40
7:F:135:ARG:HD3	7:F:143:PHE:CD2	2.56	0.40
9:H:38:LEU:HD13	9:H:125:LEU:HD13	2.03	0.40
2:A:23:SER:HA	2:A:233:TRP:CD1	2.56	0.40
2:A:57:ARG:O	2:A:68:GLN:HG3	2.22	0.40
2:A:122:MET:O	2:A:123:ARG:C	2.64	0.40
2:A:184:SER:HB3	2:A:199:LEU:HD23	2.04	0.40
2:A:402:ALA:HB1	2:A:433:GLU:O	2.22	0.40
2:A:628:GLY:O	2:A:632:VAL:HG23	2.22	0.40
2:A:714:PHE:CG	10:I:97:MET:HE1	2.57	0.40
2:A:777:PHE:CD1	2:A:781:ASP:HA	2.56	0.40
2:A:839:ARG:O	2:A:840:ARG:C	2.65	0.40
2:A:1001:ARG:NE	7:F:83:PRO:HD3	2.36	0.40
2:A:1148:ILE:HD11	2:A:1198:ASP:HA	2.03	0.40
2:A:1227:ILE:CG2	2:A:1228:TRP:N	2.78	0.40
2:A:1239:ARG:HH22	2:A:1241:ARG:HH22	1.68	0.40
2:A:1297:GLU:H	2:A:1297:GLU:HG3	1.60	0.40
2:A:1402:PHE:CE1	2:A:1403:GLU:HG3	2.57	0.40
2:A:1447:GLU:OE1	2:A:1447:GLU:O	2.40	0.40
3:B:240:ILE:CG2	3:B:254:LEU:HB3	2.51	0.40
3:B:388:CYS:O	3:B:391:ASP:N	2.51	0.40
3:B:502:ILE:HD12	3:B:502:ILE:N	2.34	0.40
3:B:822:ASN:ND2	11:J:52:THR:HG21	2.35	0.40
3:B:824:ILE:CG2	3:B:1087:PHE:CE2	3.04	0.40
3:B:895:ASP:C	3:B:897:GLY:H	2.29	0.40
3:B:1010:LEU:HD12	3:B:1010:LEU:HA	1.79	0.40
4:C:111:THR:C	4:C:112:ASN:HD22	2.29	0.40
4:C:186:LEU:N	4:C:186:LEU:CD1	2.84	0.40
4:C:262:LEU:HA	4:C:262:LEU:HD23	1.88	0.40
5:D:49:ALA:CB	5:D:174:PRO:O	2.69	0.40
5:D:154:PHE:CD1	5:D:154:PHE:N	2.90	0.40
7:F:140:ASP:OD1	7:F:140:ASP:C	2.65	0.40
8:G:99:PHE:O	8:G:109:PHE:HD1	2.05	0.40
10:I:100:PHE:CD1	10:I:100:PHE:N	2.89	0.40
2:A:79:GLY:HA3	2:A:243:PRO:HG3	2.02	0.40
2:A:157:ASP:C	2:A:159:THR:N	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:329:LEU:O	2:A:330:LYS:C	2.64	0.40
2:A:377:PRO:HD3	2:A:493:GLN:OE1	2.22	0.40
2:A:417:TYR:CD2	2:A:417:TYR:N	2.90	0.40
2:A:683:ILE:HG21	2:A:801:GLU:CG	2.49	0.40
2:A:909:ASP:C	2:A:911:SER:H	2.29	0.40
2:A:1120:LEU:HD23	2:A:1124:HIS:O	2.22	0.40
2:A:1319:VAL:CG1	2:A:1320:PRO:HD2	2.49	0.40
3:B:34:ILE:O	3:B:35:SER:C	2.65	0.40
3:B:63:ILE:HD12	3:B:63:ILE:HA	1.95	0.40
3:B:100:PRO:HD3	3:B:172:ILE:CD1	2.51	0.40
3:B:227:LYS:HB2	3:B:395:GLN:OE1	2.22	0.40
3:B:236:HIS:HB2	3:B:258:LEU:HD23	2.04	0.40
3:B:276:ILE:HA	3:B:338:GLY:HA2	2.02	0.40
3:B:570:VAL:HA	3:B:571:PRO:HD2	1.75	0.40
3:B:763:GLN:HG2	3:B:765:PRO:CD	2.51	0.40
3:B:834:ASN:ND2	3:B:1013:ASN:HA	2.36	0.40
3:B:952:VAL:HG12	3:B:953:LEU:N	2.35	0.40
4:C:6:PRO:CG	12:K:101:LEU:HB2	2.51	0.40
4:C:10:ILE:H	4:C:10:ILE:HG13	1.58	0.40
4:C:11:ARG:HH21	4:C:229:TYR:HB3	1.85	0.40
4:C:27:LEU:O	4:C:30:ALA:HB3	2.21	0.40
5:D:4:SER:OG	5:D:5:THR:N	2.49	0.40
8:G:21:ARG:HA	8:G:21:ARG:HD3	1.85	0.40
8:G:145:VAL:HG12	8:G:146:LYS:H	1.86	0.40
9:H:118:PHE:HD1	9:H:121:LEU:O	2.05	0.40
11:J:1:MET:O	11:J:2:ILE:HB	2.21	0.40
12:K:47:ARG:HD2	12:K:47:ARG:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	1412/1733 (82%)	1032 (73%)	252 (18%)	128 (9%)	0	10
3	B	1096/1224 (90%)	781 (71%)	206 (19%)	109 (10%)	0	8
4	C	265/318 (83%)	169 (64%)	66 (25%)	30 (11%)	0	5
5	D	174/221 (79%)	133 (76%)	27 (16%)	14 (8%)	1	12
6	E	212/215 (99%)	166 (78%)	32 (15%)	14 (7%)	1	15
7	F	85/155 (55%)	70 (82%)	11 (13%)	4 (5%)	2	19
8	G	169/171 (99%)	128 (76%)	32 (19%)	9 (5%)	1	18
9	H	131/146 (90%)	78 (60%)	33 (25%)	20 (15%)	0	3
10	I	114/122 (93%)	76 (67%)	26 (23%)	12 (10%)	0	7
11	J	63/70 (90%)	37 (59%)	16 (25%)	10 (16%)	0	3
12	K	110/120 (92%)	88 (80%)	15 (14%)	7 (6%)	1	15
13	L	44/70 (63%)	20 (46%)	12 (27%)	12 (27%)	0	0
All	All	3875/4565 (85%)	2778 (72%)	728 (19%)	369 (10%)	0	9

All (369) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	42	ASP
2	A	48	ALA
2	A	54	ASN
2	A	57	ARG
2	A	62	ASP
2	A	69	THR
2	A	93	VAL
2	A	130	ASP
2	A	154	SER
2	A	167	CYS
2	A	223	GLY
2	A	250	ILE
2	A	253	ASN
2	A	286	HIS
2	A	311	GLN
2	A	312	PRO
2	A	318	SER
2	A	332	LYS
2	A	335	ARG
2	A	536	LEU
2	A	567	LYS
2	A	597	LEU

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Mol	Chain	Res	Type
2	A	666	ILE
2	A	765	VAL
2	A	780	VAL
2	A	968	GLN
2	A	969	GLN
2	A	1002	GLY
2	A	1115	SER
2	A	1116	LEU
2	A	1120	LEU
2	A	1124	HIS
2	A	1212	VAL
2	A	1223	ASP
2	A	1255	GLU
2	A	1314	SER
2	A	1365	TYR
3	B	20	ASP
3	B	45	SER
3	B	108	VAL
3	B	186	GLU
3	B	206	ASN
3	B	266	ALA
3	B	340	ALA
3	B	345	LYS
3	B	367	LEU
3	B	401	PHE
3	B	470	LYS
3	B	708	GLU
3	B	709	ASP
3	B	731	VAL
3	B	751	VAL
3	B	825	VAL
3	B	826	ALA
3	B	881	ASN
3	B	909	ASP
3	B	943	SER
3	B	958	GLN
3	B	1011	ILE
3	B	1041	GLU
3	B	1046	PRO
3	B	1069	PHE
3	B	1097	HIS
3	B	1155	SER

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Mol	Chain	Res	Type
3	B	1156	ASP
3	B	1157	ALA
3	B	1171	VAL
3	B	1175	LEU
3	B	1181	GLU
3	B	1182	CYS
3	B	1183	LYS
3	B	1188	LYS
4	C	4	GLU
4	C	133	ILE
4	C	149	LYS
4	C	161	LYS
4	C	184	ASN
4	C	212	PRO
4	C	214	ASN
4	C	215	GLU
5	D	4	SER
5	D	5	THR
5	D	20	GLU
5	D	199	ASN
6	E	59	SER
6	E	106	GLN
8	G	63	PRO
8	G	139	ILE
9	H	62	SER
9	H	64	ASN
9	H	108	SER
9	H	128	ASN
9	H	140	ALA
10	I	79	HIS
10	I	106	CYS
11	J	6	ARG
11	J	32	GLU
11	J	64	ASN
12	K	7	PHE
12	K	110	ASN
12	K	111	LEU
13	L	35	SER
13	L	50	ASP
13	L	53	HIS
13	L	59	ALA
13	L	60	ARG

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Mol	Chain	Res	Type
2	A	4	GLN
2	A	44	THR
2	A	59	GLY
2	A	67	CYS
2	A	73	GLY
2	A	74	MET
2	A	76	GLU
2	A	283	GLY
2	A	303	TYR
2	A	331	GLY
2	A	336	ILE
2	A	380	VAL
2	A	410	GLY
2	A	543	LEU
2	A	661	GLY
2	A	753	GLY
2	A	755	PHE
2	A	789	LYS
2	A	846	GLU
2	A	854	ASN
2	A	871	ASP
2	A	986	ILE
2	A	1016	THR
2	A	1036	ARG
2	A	1127	ASP
2	A	1221	LYS
2	A	1378	GLN
2	A	1402	PHE
2	A	1405	THR
3	B	22	SER
3	B	28	GLU
3	B	65	GLU
3	B	184	ALA
3	B	259	TYR
3	B	260	GLY
3	B	295	GLY
3	B	365	THR
3	B	394	ASP
3	B	460	ALA
3	B	461	LEU
3	B	467	GLY
3	B	559	SER

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Mol	Chain	Res	Type
3	B	591	ARG
3	B	605	ARG
3	B	643	ASP
3	B	655	LYS
3	B	827	ILE
3	B	867	GLY
3	B	879	ARG
3	B	907	GLY
3	B	951	GLN
3	B	978	ASP
3	B	1035	ALA
3	B	1100	ASP
3	B	1108	ARG
3	B	1126	GLY
3	B	1131	GLY
4	C	51	VAL
4	C	87	PHE
4	C	90	ASP
4	C	108	GLU
4	C	110	THR
4	C	132	PRO
4	C	213	PRO
4	C	217	ASP
4	C	231	ASN
4	C	240	VAL
5	D	9	GLN
5	D	21	GLU
5	D	52	LEU
5	D	192	LYS
5	D	218	GLU
6	E	44	ALA
6	E	45	LYS
6	E	73	PRO
6	E	76	GLY
6	E	130	ALA
6	E	192	ARG
7	F	81	THR
7	F	112	GLU
8	G	19	GLY
8	G	118	ASP
8	G	167	TYR
9	H	21	ASN

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Mol	Chain	Res	Type
9	H	59	ILE
9	H	63	LEU
9	H	81	PRO
9	H	82	PRO
9	H	84	ALA
9	H	90	ALA
10	I	3	THR
10	I	11	ASN
10	I	47	GLU
10	I	57	GLY
10	I	95	THR
11	J	2	ILE
11	J	24	LEU
11	J	28	ASP
11	J	29	GLU
12	K	15	GLY
12	K	109	TRP
13	L	54	ARG
2	A	35	ILE
2	A	58	LEU
2	A	113	LEU
2	A	263	THR
2	A	322	VAL
2	A	399	HIS
2	A	423	ASP
2	A	465	TYR
2	A	591	PHE
2	A	592	ASP
2	A	738	LYS
2	A	847	ASP
2	A	1122	PRO
2	A	1233	ASP
2	A	1281	ARG
2	A	1377	THR
3	B	115	GLN
3	B	258	LEU
3	B	308	TRP
3	B	369	GLY
3	B	450	ALA
3	B	531	GLN
3	B	641	GLU
3	B	642	ASP

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Mol	Chain	Res	Type
3	B	711	GLU
3	B	712	PRO
3	B	727	LYS
3	B	792	MET
3	B	891	ASP
3	B	901	PRO
3	B	1006	ILE
3	B	1082	MET
3	B	1167	GLY
3	B	1178	ASN
4	C	141	GLY
4	C	142	VAL
4	C	148	ARG
4	C	156	THR
4	C	209	TYR
5	D	31	GLN
5	D	131	GLU
6	E	115	ASN
9	H	17	PRO
9	H	77	ARG
10	I	8	ARG
10	I	107	SER
12	K	29	ASN
13	L	26	THR
2	A	5	GLN
2	A	66	LYS
2	A	400	PRO
2	A	409	SER
2	A	419	LYS
2	A	424	ILE
2	A	544	ASP
2	A	619	LYS
2	A	706	HIS
2	A	739	ASP
2	A	958	VAL
2	A	1266	THR
2	A	1366	ARG
2	A	1392	SER
3	B	46	GLN
3	B	58	THR
3	B	368	GLU
3	B	571	PRO

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Mol	Chain	Res	Type
3	B	575	PRO
3	B	613	VAL
3	B	680	THR
3	B	705	MET
3	B	869	SER
3	B	945	GLU
4	C	78	GLU
4	C	139	GLY
4	C	188	HIS
5	D	196	PRO
6	E	3	GLN
6	E	43	LYS
6	E	56	LYS
6	E	206	GLY
8	G	20	PRO
8	G	35	GLU
8	G	154	VAL
9	H	119	GLY
11	J	17	LYS
11	J	57	ILE
2	A	70	CYS
2	A	84	ILE
2	A	164	ARG
2	A	245	PRO
2	A	257	ARG
2	A	1176	LEU
2	A	1231	ASP
3	B	124	TYR
3	B	267	ARG
3	B	474	SER
3	B	832	GLY
3	B	946	ASN
4	C	18	VAL
4	C	175	ALA
7	F	104	ASN
9	H	60	ALA
9	H	92	ASP
9	H	105	GLU
10	I	9	ASP
12	K	4	PRO
13	L	40	LEU
2	A	61	ILE

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Mol	Chain	Res	Type
2	A	219	PHE
2	A	317	LYS
2	A	700	ASN
2	A	720	ARG
2	A	868	TYR
2	A	910	PRO
2	A	1071	SER
2	A	1114	PRO
2	A	1324	PRO
2	A	1437	GLY
3	B	291	ILE
3	B	611	PRO
3	B	713	ALA
3	B	1017	ILE
3	B	1018	PRO
3	B	1112	GLN
3	B	1144	ALA
5	D	47	LEU
11	J	14	VAL
13	L	39	SER
13	L	55	ILE
13	L	56	LEU
2	A	51	GLY
2	A	284	ALA
2	A	639	PRO
2	A	673	GLY
2	A	963	ILE
2	A	1094	VAL
3	B	305	VAL
3	B	1045	SER
2	A	600	PRO
2	A	1395	GLY
3	B	1103	ILE
5	D	59	ILE
9	H	44	VAL
10	I	59	VAL
2	A	128	ILE
2	A	244	PRO
2	A	1335	ILE
3	B	282	ILE
3	B	362	PRO
6	E	129	PRO

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Mol	Chain	Res	Type
7	F	139	PRO
8	G	115	MET
10	I	62	ILE
2	A	196	GLU
2	A	1435	PRO
3	B	478	GLY
4	C	70	ILE
4	C	216	GLY
9	H	107	VAL
2	A	756	ILE
13	L	46	VAL

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	
2	A	1245/1520 (82%)	1126 (90%)	119 (10%)	8	28
3	B	964/1061 (91%)	877 (91%)	87 (9%)	9	31
4	C	235/274 (86%)	217 (92%)	18 (8%)	12	35
5	D	160/200 (80%)	137 (86%)	23 (14%)	3	17
6	E	196/197 (100%)	188 (96%)	8 (4%)	27	49
7	F	78/137 (57%)	70 (90%)	8 (10%)	7	25
8	G	152/152 (100%)	135 (89%)	17 (11%)	6	22
9	H	119/128 (93%)	114 (96%)	5 (4%)	26	49
10	I	110/116 (95%)	105 (96%)	5 (4%)	24	47
11	J	60/65 (92%)	56 (93%)	4 (7%)	15	39
12	K	97/102 (95%)	89 (92%)	8 (8%)	10	34
13	L	40/57 (70%)	38 (95%)	2 (5%)	22	45
All	All	3456/4009 (86%)	3152 (91%)	304 (9%)	9	32

All (304) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	2	VAL
2	A	11	LEU
2	A	32	VAL
2	A	34	LYS
2	A	41	MET
2	A	54	ASN
2	A	58	LEU
2	A	62	ASP
2	A	67	CYS
2	A	68	GLN
2	A	93	VAL
2	A	108	MET
2	A	110	CYS
2	A	142	CYS
2	A	200	ARG
2	A	205	GLU
2	A	221	SER
2	A	236	LEU
2	A	245	PRO
2	A	261	ASP
2	A	265	LYS
2	A	270	LEU
2	A	302	THR
2	A	308	ILE
2	A	312	PRO
2	A	326	ARG
2	A	335	ARG
2	A	345	VAL
2	A	354	SER
2	A	375	THR
2	A	385	ILE
2	A	388	LEU
2	A	406	ILE
2	A	407	ARG
2	A	408	ASP
2	A	412	ARG
2	A	425	GLN
2	A	434	ARG
2	A	442	VAL
2	A	443	LEU
2	A	445	ASN
2	A	450	LEU
2	A	460	VAL

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Mol	Chain	Res	Type
2	A	461	LYS
2	A	466	SER
2	A	469	ARG
2	A	470	LEU
2	A	493	GLN
2	A	504	LEU
2	A	512	VAL
2	A	524	VAL
2	A	560	ILE
2	A	562	THR
2	A	566	ILE
2	A	576	GLN
2	A	616	VAL
2	A	618	GLU
2	A	622	VAL
2	A	629	LEU
2	A	635	ARG
2	A	657	LEU
2	A	658	LEU
2	A	664	THR
2	A	666	ILE
2	A	720	ARG
2	A	739	ASP
2	A	741	ASN
2	A	758	ILE
2	A	768	GLN
2	A	779	PHE
2	A	821	ARG
2	A	827	THR
2	A	834	THR
2	A	858	ASN
2	A	886	ILE
2	A	890	ASP
2	A	919	ILE
2	A	929	LEU
2	A	939	ASP
2	A	941	LYS
2	A	969	GLN
2	A	1001	ARG
2	A	1017	LEU
2	A	1029	ARG
2	A	1035	TYR

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Mol	Chain	Res	Type
2	A	1050	GLU
2	A	1052	GLN
2	A	1067	LEU
2	A	1111	MET
2	A	1116	LEU
2	A	1120	LEU
2	A	1122	PRO
2	A	1127	ASP
2	A	1138	ILE
2	A	1146	VAL
2	A	1152	ILE
2	A	1175	SER
2	A	1187	GLN
2	A	1206	ASP
2	A	1240	CYS
2	A	1260	LEU
2	A	1264	GLU
2	A	1271	ILE
2	A	1291	VAL
2	A	1295	THR
2	A	1297	GLU
2	A	1325	THR
2	A	1329	THR
2	A	1332	PHE
2	A	1333	ILE
2	A	1359	ASP
2	A	1372	VAL
2	A	1389	PHE
2	A	1394	THR
2	A	1404	GLU
2	A	1405	THR
2	A	1408	ILE
2	A	1442	ASP
2	A	1445	ILE
3	B	57	TYR
3	B	104	GLU
3	B	106	ASP
3	B	175	ARG
3	B	178	ASN
3	B	199	MET
3	B	250	PHE
3	B	258	LEU

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Mol	Chain	Res	Type
3	B	268	THR
3	B	283	VAL
3	B	286	PHE
3	B	303	TYR
3	B	365	THR
3	B	371	GLU
3	B	378	LEU
3	B	393	LYS
3	B	408	LEU
3	B	416	LEU
3	B	427	ASP
3	B	429	PHE
3	B	463	THR
3	B	466	TRP
3	B	473	MET
3	B	482	VAL
3	B	485	ARG
3	B	496	ARG
3	B	498	THR
3	B	502	ILE
3	B	513	GLN
3	B	516	ASN
3	B	537	LYS
3	B	539	LEU
3	B	582	VAL
3	B	591	ARG
3	B	593	PRO
3	B	603	LEU
3	B	615	MET
3	B	616	ILE
3	B	635	ARG
3	B	644	GLU
3	B	724	ASP
3	B	737	THR
3	B	751	VAL
3	B	780	VAL
3	B	787	VAL
3	B	791	THR
3	B	795	ILE
3	B	833	TYR
3	B	835	GLN
3	B	839	MET

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Mol	Chain	Res	Type
3	B	844	SER
3	B	860	MET
3	B	878	GLN
3	B	894	ASP
3	B	909	ASP
3	B	944	THR
3	B	957	ASN
3	B	976	ILE
3	B	997	GLU
3	B	999	MET
3	B	1002	THR
3	B	1006	ILE
3	B	1010	LEU
3	B	1017	ILE
3	B	1046	PRO
3	B	1047	PHE
3	B	1069	PHE
3	B	1084	GLN
3	B	1085	ILE
3	B	1095	LEU
3	B	1098	MET
3	B	1099	VAL
3	B	1103	ILE
3	B	1108	ARG
3	B	1120	GLU
3	B	1122	ARG
3	B	1151	LEU
3	B	1159	ARG
3	B	1170	THR
3	B	1183	LYS
3	B	1185	CYS
3	B	1191	ILE
3	B	1192	TYR
3	B	1202	LEU
3	B	1212	ILE
3	B	1220	ARG
3	B	1223	ASP
4	C	8	VAL
4	C	35	ARG
4	C	57	VAL
4	C	74	SER
4	C	77	ILE

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Mol	Chain	Res	Type
4	C	89	GLU
4	C	129	ILE
4	C	144	ILE
4	C	166	GLU
4	C	193	TYR
4	C	195	GLN
4	C	209	TYR
4	C	212	PRO
4	C	235	VAL
4	C	238	ILE
4	C	240	VAL
4	C	251	LEU
4	C	266	ASP
5	D	4	SER
5	D	7	THR
5	D	8	PHE
5	D	13	ARG
5	D	17	LYS
5	D	22	GLU
5	D	46	GLU
5	D	47	LEU
5	D	63	LEU
5	D	70	PHE
5	D	126	ILE
5	D	137	ASN
5	D	139	LYS
5	D	148	LEU
5	D	149	THR
5	D	151	PHE
5	D	170	THR
5	D	187	THR
5	D	192	LYS
5	D	193	THR
5	D	208	GLU
5	D	214	LEU
5	D	221	TYR
6	E	2	ASP
6	E	60	PHE
6	E	74	ASP
6	E	78	LEU
6	E	132	ILE
6	E	149	LEU

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Mol	Chain	Res	Type
6	E	158	SER
6	E	207	ARG
7	F	68	THR
7	F	69	LEU
7	F	79	ARG
7	F	90	ARG
7	F	111	LEU
7	F	123	LYS
7	F	132	LEU
7	F	143	PHE
8	G	1	MET
8	G	11	ILE
8	G	13	LEU
8	G	26	LEU
8	G	33	GLU
8	G	45	ILE
8	G	49	LEU
8	G	52	ASP
8	G	64	THR
8	G	74	TYR
8	G	78	VAL
8	G	79	PHE
8	G	80	LYS
8	G	88	ASP
8	G	115	MET
8	G	153	GLN
8	G	171	ILE
9	H	10	PHE
9	H	96	VAL
9	H	102	TYR
9	H	130	ARG
9	H	134	ASN
10	I	15	TYR
10	I	34	TYR
10	I	85	PHE
10	I	86	PHE
10	I	101	PHE
11	J	16	ASP
11	J	43	ARG
11	J	44	TYR
11	J	46	CYS
12	K	5	ASP

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Mol	Chain	Res	Type
12	K	10	PHE
12	K	25	THR
12	K	41	THR
12	K	47	ARG
12	K	50	LEU
12	K	61	TYR
12	K	112	GLN
13	L	27	LEU
13	L	55	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (121) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	54	ASN
2	A	64	ASN
2	A	71	GLN
2	A	75	ASN
2	A	80	HIS
2	A	92	HIS
2	A	109	HIS
2	A	160	GLN
2	A	171	GLN
2	A	225	ASN
2	A	256	GLN
2	A	299	HIS
2	A	316	GLN
2	A	339	ASN
2	A	435	HIS
2	A	447	GLN
2	A	515	GLN
2	A	587	HIS
2	A	611	GLN
2	A	660	ASN
2	A	717	ASN
2	A	736	ASN
2	A	741	ASN
2	A	767	GLN
2	A	768	GLN
2	A	786	HIS
2	A	858	ASN
2	A	903	ASN
2	A	926	GLN

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Mol	Chain	Res	Type
2	A	969	GLN
2	A	994	GLN
2	A	1070	GLN
2	A	1106	ASN
2	A	1124	HIS
2	A	1128	GLN
2	A	1130	GLN
2	A	1140	HIS
2	A	1187	GLN
2	A	1188	GLN
2	A	1203	ASN
2	A	1211	GLN
2	A	1232	ASN
2	A	1265	ASN
2	A	1354	ASN
2	A	1432	GLN
3	B	46	GLN
3	B	53	GLN
3	B	60	GLN
3	B	178	ASN
3	B	236	HIS
3	B	255	GLN
3	B	363	HIS
3	B	366	GLN
3	B	465	ASN
3	B	499	ASN
3	B	513	GLN
3	B	515	HIS
3	B	516	ASN
3	B	518	HIS
3	B	538	ASN
3	B	587	HIS
3	B	706	GLN
3	B	734	HIS
3	B	744	HIS
3	B	763	GLN
3	B	786	ASN
3	B	794	ASN
3	B	821	GLN
3	B	842	ASN
3	B	957	ASN
3	B	975	GLN

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Mol	Chain	Res	Type
3	B	1015	HIS
3	B	1062	HIS
3	B	1065	GLN
3	B	1084	GLN
3	B	1117	GLN
3	B	1179	GLN
3	B	1193	GLN
3	B	1195	HIS
4	C	73	GLN
4	C	79	GLN
4	C	112	ASN
4	C	131	HIS
4	C	140	ASN
4	C	151	GLN
4	C	167	HIS
4	C	184	ASN
4	C	203	GLN
4	C	231	ASN
5	D	39	ASN
5	D	137	ASN
5	D	173	HIS
5	D	216	ASN
6	E	8	ASN
6	E	101	GLN
6	E	104	ASN
6	E	114	ASN
6	E	143	ASN
6	E	147	HIS
7	F	104	ASN
8	G	14	HIS
8	G	53	ASN
8	G	97	HIS
8	G	122	ASN
8	G	126	ASN
9	H	64	ASN
9	H	133	ASN
9	H	134	ASN
9	H	137	GLN
10	I	11	ASN
10	I	12	ASN
10	I	83	ASN
10	I	90	GLN

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Mol	Chain	Res	Type
11	J	53	HIS
11	J	64	ASN
12	K	29	ASN
12	K	44	ASN
12	K	65	HIS
12	K	76	GLN
12	K	104	ASN
12	K	112	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	12/18 (66%)	4 (33%)	0

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	6	C
1	R	7	U
1	R	13	G
1	R	17	U

There are no RNA pucker outliers to report.

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 oligosaccharides 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
7	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	68:THR	C	69:LEU	N	4.50

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	R	14/18 (77%)	0.56	1 (7%) 22 21	128, 147, 176, 188	0
2	A	1422/1733 (82%)	0.06	33 (2%) 61 45	57, 116, 171, 200	0
3	B	1112/1224 (90%)	0.18	30 (2%) 56 41	61, 126, 184, 200	0
4	C	267/318 (83%)	0.04	0 100 100	73, 111, 159, 176	0
5	D	178/221 (80%)	0.28	5 (2%) 55 40	88, 133, 179, 192	0
6	E	214/215 (99%)	0.18	2 (0%) 81 64	93, 154, 191, 199	0
7	F	88/155 (56%)	-0.16	1 (1%) 78 60	61, 93, 130, 153	0
8	G	171/171 (100%)	0.10	4 (2%) 61 45	88, 116, 155, 163	0
9	H	135/146 (92%)	0.67	10 (7%) 20 20	131, 161, 187, 196	0
10	I	116/122 (95%)	0.50	7 (6%) 27 24	110, 161, 191, 196	0
11	J	65/70 (92%)	-0.00	1 (1%) 72 54	79, 109, 145, 149	0
12	K	112/120 (93%)	-0.10	1 (0%) 81 64	76, 115, 140, 158	0
13	L	46/70 (65%)	0.77	3 (6%) 25 23	107, 170, 191, 193	0
All	All	3940/4583 (85%)	0.14	98 (2%) 58 43	57, 122, 182, 200	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	1081	LEU	7.0
5	D	3	VAL	6.8
10	I	2	THR	4.9
2	A	69	THR	4.2
3	B	883	LEU	4.1
9	H	65	LEU	4.1
13	L	27	LEU	3.8
3	B	715	ALA	3.8
2	A	975	HIS	3.7

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Mol	Chain	Res	Type	RSRZ
5	D	25	ALA	3.7
9	H	136	LYS	3.5
3	B	446	LEU	3.4
3	B	734	HIS	3.4
3	B	860	MET	3.3
3	B	246	LYS	3.2
3	B	882	THR	3.2
3	B	963	PHE	3.2
2	A	2	VAL	3.1
10	I	3	THR	3.1
2	A	1080	THR	3.0
2	A	1254	ALA	3.0
13	L	25	ALA	3.0
9	H	132	LEU	2.9
2	A	56	PRO	2.9
8	G	21	ARG	2.9
10	I	52	ILE	2.9
13	L	26	THR	2.8
3	B	250	PHE	2.8
2	A	3	GLY	2.7
3	B	917	PRO	2.7
11	J	65	PRO	2.7
2	A	1172	LEU	2.7
5	D	8	PHE	2.7
9	H	140	ALA	2.7
2	A	171	GLN	2.7
3	B	251	ILE	2.7
10	I	117	LYS	2.6
9	H	76	THR	2.6
1	R	12	C	2.6
8	G	83	LYS	2.6
9	H	119	GLY	2.5
2	A	189	ARG	2.5
7	F	68	THR	2.5
2	A	195	ASP	2.5
5	D	13	ARG	2.4
2	A	253	ASN	2.4
2	A	105	CYS	2.4
3	B	262	GLU	2.4
3	B	879	ARG	2.4
2	A	51	GLY	2.4
2	A	1302	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
2	A	1092	LYS	2.4
9	H	143	LEU	2.4
3	B	1224	PHE	2.4
6	E	110	PHE	2.4
2	A	1176	LEU	2.4
2	A	1455	PRO	2.3
2	A	252	PHE	2.3
2	A	251	SER	2.3
10	I	4	PHE	2.3
3	B	266	ALA	2.3
9	H	135	LEU	2.3
2	A	1093	LYS	2.3
3	B	164	LYS	2.3
10	I	53	GLY	2.3
3	B	881	ASN	2.3
3	B	435	THR	2.2
3	B	880	THR	2.2
3	B	641	GLU	2.2
6	E	93	MET	2.2
10	I	55	THR	2.2
8	G	150	CYS	2.2
2	A	1187	GLN	2.2
2	A	1177	LEU	2.2
3	B	561	TRP	2.2
2	A	904	THR	2.2
3	B	345	LYS	2.2
3	B	471	LYS	2.2
2	A	1257	ASP	2.2
9	H	139	ASN	2.2
2	A	1175	SER	2.2
5	D	4	SER	2.2
3	B	769	TYR	2.2
8	G	85	GLU	2.2
2	A	1154	TYR	2.1
2	A	587	HIS	2.1
3	B	732	SER	2.1
2	A	1245	PRO	2.1
3	B	476	ARG	2.1
12	K	54	ARG	2.1
3	B	245	GLU	2.1
2	A	969	GLN	2.1
3	B	731	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	A	161	LEU	2.1
9	H	58	THR	2.1
3	B	933	SER	2.1
2	A	1387	HIS	2.0
3	B	723	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	ZN	I	204	1/1	0.96	0.09	190,190,190,190	0
15	MG	A	1	1/1	0.98	0.08	68,68,68,68	0
14	ZN	L	105	1/1	0.99	0.04	156,156,156,156	0
14	ZN	A	1506	1/1	0.99	0.05	119,119,119,119	0
14	ZN	I	203	1/1	1.00	0.08	113,113,113,113	0
14	ZN	A	1508	1/1	1.00	0.06	79,79,79,79	0
14	ZN	J	101	1/1	1.00	0.04	86,86,86,86	0
14	ZN	B	1307	1/1	1.00	0.06	78,78,78,78	0
14	ZN	C	302	1/1	1.00	0.07	71,71,71,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.