



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 10:23 pm BST

PDB ID : 1BR2
Title : SMOOTH MUSCLE MYOSIN MOTOR DOMAIN COMPLEXED WITH
MGADP.OLF4
Authors : Dominguez, R.; Trybus, K.M.; Cohen, C.
Deposited on : 1998-08-26
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

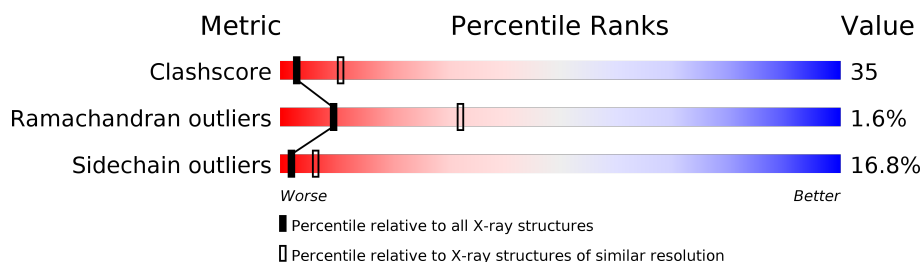
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	791	
1	B	791	
1	C	791	
1	D	791	
1	E	791	
1	F	791	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ALF	D	999	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 31830 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

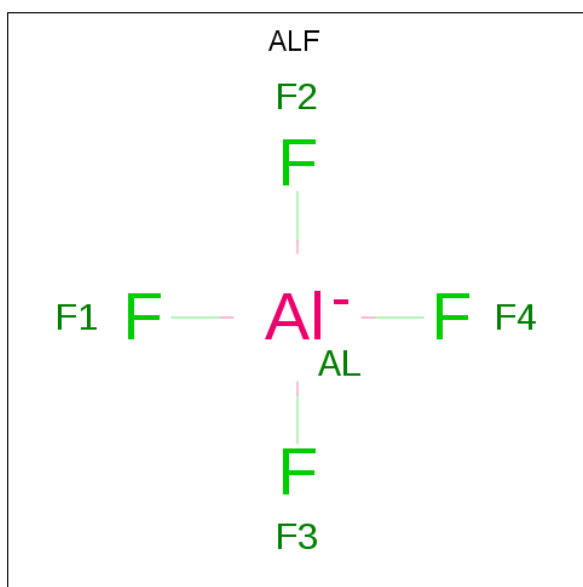
- Molecule 1 is a protein called MYOSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	673	Total	C	N	O	S	0	0	0
			5270	3360	900	982	28			
1	B	673	Total	C	N	O	S	0	0	0
			5270	3360	900	982	28			
1	C	673	Total	C	N	O	S	0	0	0
			5270	3360	900	982	28			
1	D	673	Total	C	N	O	S	0	0	0
			5270	3360	900	982	28			
1	E	673	Total	C	N	O	S	0	0	0
			5270	3360	900	982	28			
1	F	673	Total	C	N	O	S	0	0	0
			5270	3360	900	982	28			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

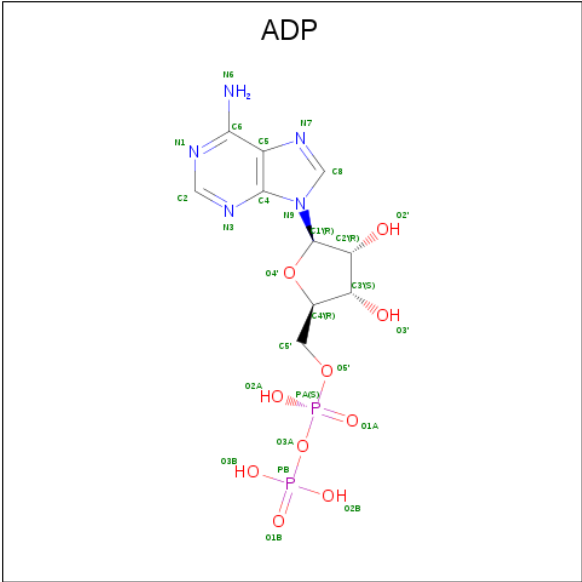
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Mg	0	0
			1	1		
2	E	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	F	1	Total	Mg	0	0
			1	1		

- Molecule 3 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Al	F	0	0
			5	1	4		
3	B	1	Total	Al	F	0	0
			5	1	4		
3	C	1	Total	Al	F	0	0
			5	1	4		
3	D	1	Total	Al	F	0	0
			5	1	4		
3	E	1	Total	Al	F	0	0
			5	1	4		
3	F	1	Total	Al	F	0	0
			5	1	4		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is water.

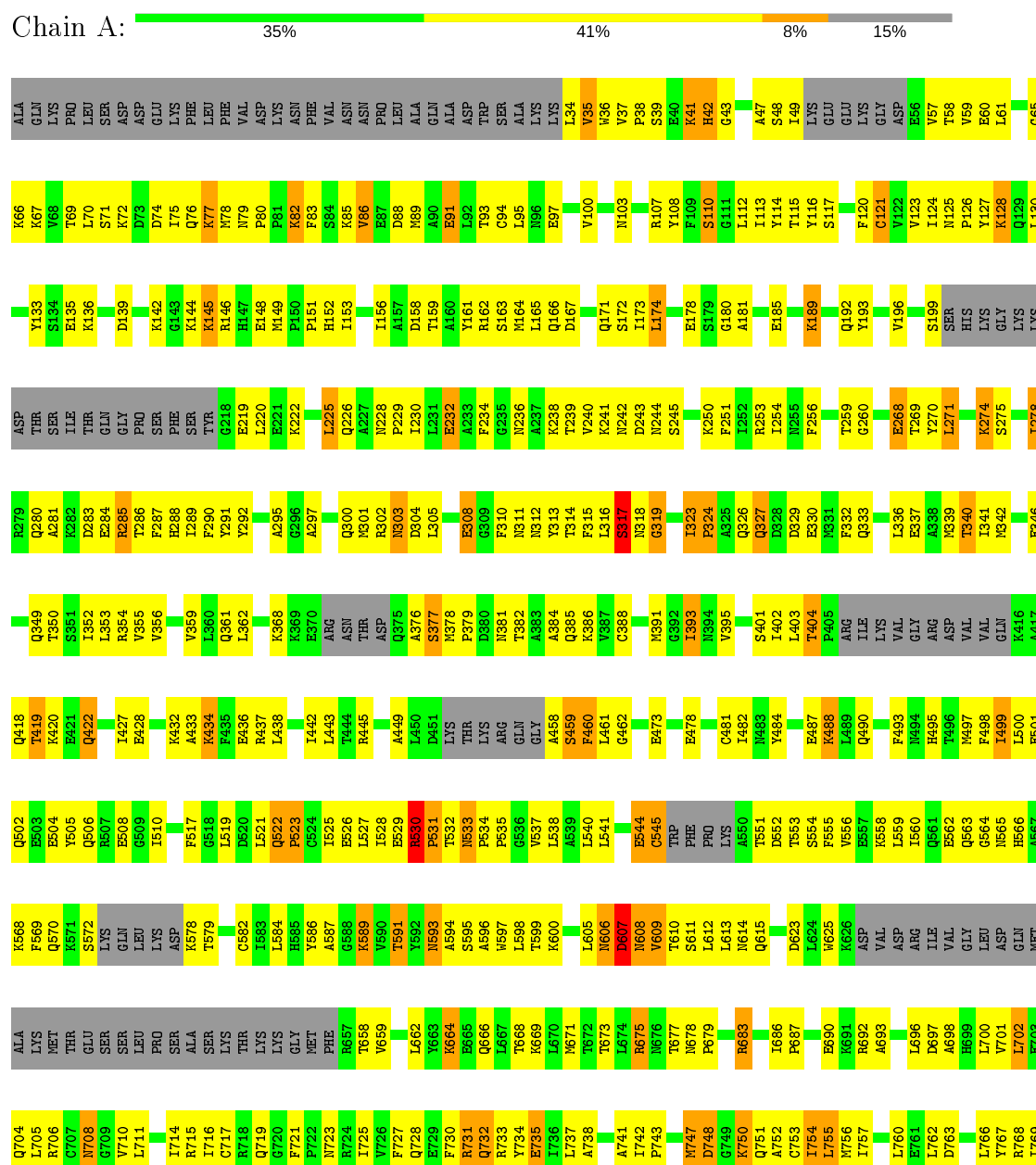
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	O	0	0
			2	2		
5	B	2	Total	O	0	0
			2	2		
5	C	2	Total	O	0	0
			2	2		
5	D	2	Total	O	0	0
			2	2		
5	E	2	Total	O	0	0
			2	2		
5	F	2	Total	O	0	0
			2	2		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

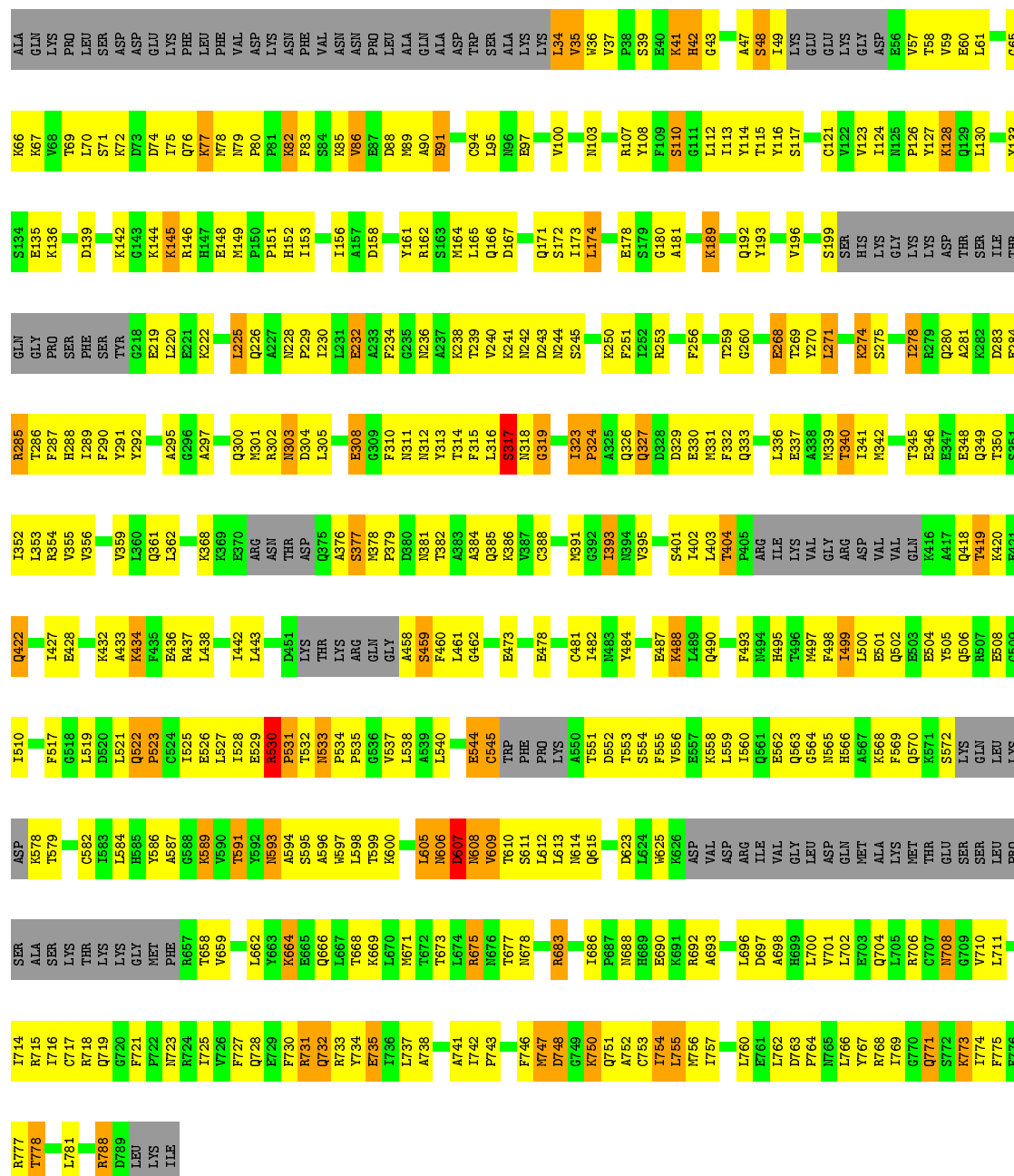
• Molecule 1: MYOSIN





- Molecule 1: MYOSIN

Chain B:

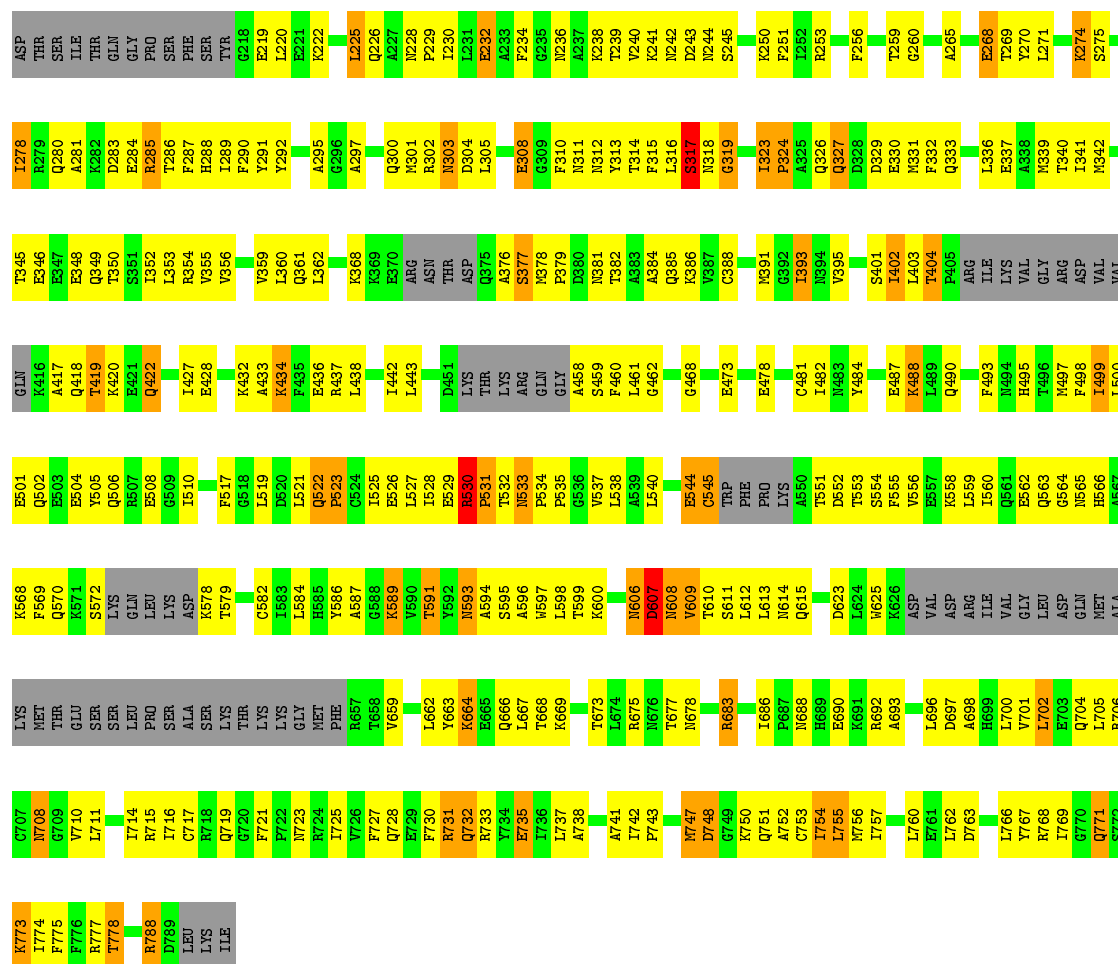


- Molecule 1: MYOSIN

Chain C:

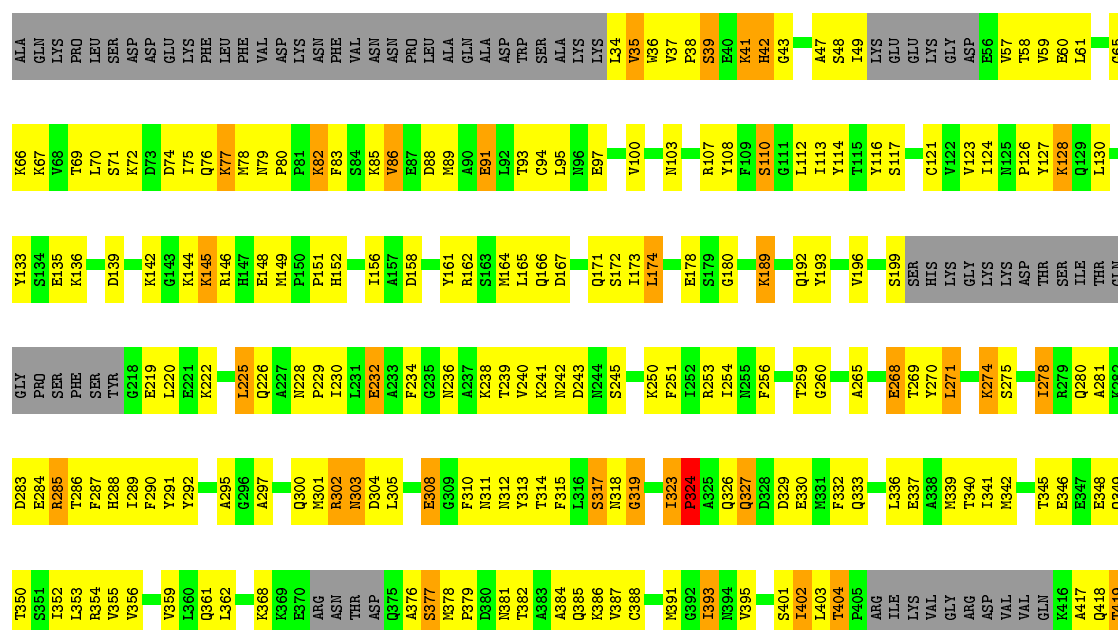


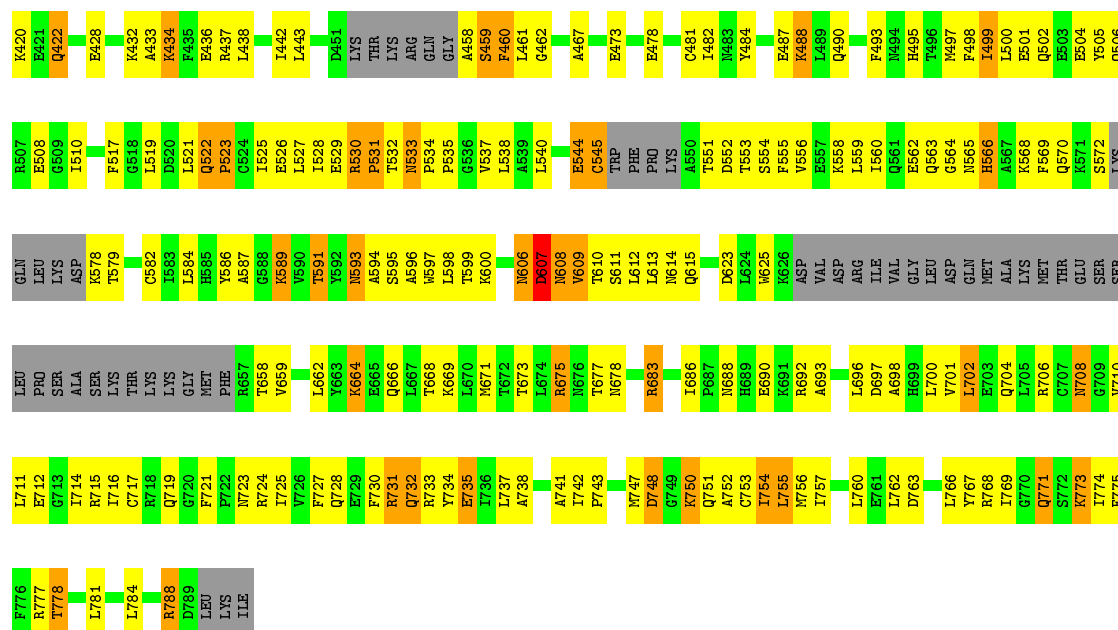
ALA	GLN	LYS	PRO	LEU	SER	ASP	ASP	GLU	LYS	PHE	LEU	PHE	VAL	ASP	LYS	ASP	LYS	ASP	GLN	GLY	PRO	SER	PHE	SER	TYR	G218	E219	L220	Q76	K77	M78	M79	P80	P81	K82	F83	S84	K85	V86	E87	D88	M89	ALA	GLN	ALA	ASP	TRP	C94	L95	N96	E97	V100	N103	R107	Y108	F109	S110	G111	L112	I113	Y114	T115	Y116	S117	V123	I124	M125	P126	Y127	K128	Q129	L130	Y133	S134	L61	E60	V69	T58	V57	E56	ASP	GLY	LYS	GLU	LYS	LYS	ASP	E56	E66	G65																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
K66	K67	V68	T69	L70	S71	K72	D73	D74	I75	Q76	K77	M78	M79	P80	P81	K82	F83	S84	K85	V86	E87	D88	M89	ALA	GLN	ALA	ASP	TRP	C94	L95	N96	E97	V100	N103	R107	Y108	F109	S110	G111	L112	I113	Y114	T115	Y116	S117	V123	I124	M125	P126	Y127	K128	Q129	L130	Y133	S134	L61	E60	V69	T58	V57	E56	ASP	GLY	LYS	GLU	LYS	LYS	ASP	E56	E66	G65																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
K136	D139	K142	K143	K144	K145	R146	E148	M149	P150	F151	H152	I156	A157	D158	Y161	R162	S163	M164	L165	Q166	D167	C94	L95	N96	E97	V100	N103	R107	Y108	F109	S110	G111	L112	I113	Y114	T115	Y116	S117	V123	I124	M125	P126	Y127	K128	Q129	L130	Y133	S134	L61	E60	V69	T58	V57	E56	ASP	GLY	LYS	GLU	LYS	LYS	ASP	E56	E66	G65																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
GLN	GLY	PRO	SER	PHE	SER	TYR	G218	E219	L220	Q76	K77	M78	M79	P80	P81	K82	F83	S84	K85	V86	E87	D88	M89	ALA	GLN	ALA	ASP	TRP	C94	L95	N96	E97	V100	N103	R107	Y108	F109	S110	G111	L112	I113	Y114	T115	Y116	S117	V123	I124	M125	P126	Y127	K128	Q129	L130	Y133	S134	L61	E60	V69	T58	V57	E56	ASP	GLY	LYS	GLU	LYS	LYS	ASP	E56	E66	G65																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
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L353	R354	V355	V356	V359	L360	Q361	I365	K368	E370	ARG	ASN	THR	ASP	THR	A376	S377	M378	P379	D380	N381	T382	A383	L461	Q462	E473	E478	C481	I482	N483	Y484	E487	K488	L489	Q490	F493	M494	H495	T496	M497	F498	I499	L500	E501	Q502	VAL	GLN	K416	A417	Q418	T419	K420																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
E491	Q492	I497	E498	K499	A433	K434	F435	E436	R437	L438	T442	L443	D451	LYS	THR	LYS	ARG	GLN	GLY	A458	S459	F460	Q462	E473	E478	C481	I482	N483	Y484	E487	K488	L489	Q490	F493	M494	H495	T496	M497	F498	I499	L500	E501	Q502	VAL	GLN	K416	A417	Q418	T419	K420																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
G509	I510	F517	G518	L519	P520	L521	Q522	P523	C524	R437	E526	L527	E528	E529	R530	P531	T532	N533	P534	P535	G536	V537	L538	A539	L540	E544	C545	TRP	PHE	PRO	LYS	A550	T551	D552	T553	S554	F555	V556	E557	Q561	E562	Q563	G564	N565	A566	A567	K568	F569	LYS	MET	LYS	GLU	THR	K571	S572	LYS	GLN	LEU																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
LYS	ASP	R578	T579	C582	T583	L584	H585	F586	A587	G588	K589	T590	T591	F592	M593	A594	S595	A596	A597	L598	T599	K600	L605	M606	D607	N608	V609	T610	S611	L612	M614	Q615	D623	L624	M625	R626	ASP	VAL	ASP	ANG	ILE	VAL	GLY	LEU	ASP	GLN	MET	ALA	LYS	MET	LYS	THR	GLU	SER	LYS	LEU																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
PRO	SER	ALA	SER	LYS	THR	LYS	LYS	GLY	PHE	R657	T658	V659	L662	V663	K664	R665	Q666	L667	T668	R669	L670	M671	T672	T673	L674	R675	N676	T677	N678	R683	L686	E690	R691	R692	A693	L696	D697	A698	H699	L700	V701	L702	E703	Q704	L705	R706	C707	N708	I714	L715	L716	L717	L718	L719	L720	L721	L722	L723	L724	L725	L726	L727	L728	L729	L730	L731	L732	L733	L734	L735	L736	L737	L738	L739	L740	L741	L742	L743	L744	L745	L746	L747	L748	L749	L750	L751	L752	L753	L754	L755	L756	L757	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768	L769	L770	L771	L772	L773	L774	L775	L776	L777	L778	L779	L780	L781	L782	L783	L784	L785	L786	L787	L788	L789	L790	L791	L792	L793	L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811	L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	L1000	L1001	L1002	L1003	L1004	L1005	L1006	L1007	L1008	L1009	L1010	L1011	L1012	L1013	L1014	L1015	L1016	L1017	L1018	L1019	L1020	L1021	L1022	L1023	L1024	L1025	L1026	L1027	L1028	L1029	L1030	L1031	L1032	L1033	L1034	L1035	L1036	L1037	L1038	L1039	L1040	L1041	L1042	L1043	L1044	L1045	L1046	L1047	L1048	L1049	L1050	L1051	L1052	L1053	L1054	L1055	L1056	L1057	L1058	L1059	L1060	L1061	L1062	L1063	L1064	L1065	L1066	L1067	L1068	L1069	L1070	L1071	L1072	L1073	L1074	L1075	L1076	L1077	L1078	L1079	L1080	L1081	L1082	L1083	L1084	L1085	L1086	L1087	L1088	L1089	L1090	L1091	L1092	L1093	L1094	L1095	L1096	L1097	L1098	L1099	L1100	L1101	L1102	L1103	L1104	L1105	L1106	L1107	L1108	L1109	L1110	L1111	L1112	L1113	L1114	L1115	L1116	L1117	L1118	L1119	L1120	L1121	L1122	L1123	L1124	L1125	L1126	L1127	L1128	L1129	L1130	L1131	L1132	L1133	L1134	L1135	L1136	L1137	L1138	L1139	L1140	L1141	L1142	L1143	L1144	L1145	L1146	L1147	L1148	L1149	L1150	L1151	L1152	L1153	L1154	L1155	L1156	L1157	L1158	L1159	L1160	L1161	L1162	L1163	L1164	L1165	L1166	L1167	L1168	L1169	L1170	L1171	L1172	L1173	L1174	L1175	L1176	L1177	L1178	L1179	L1180	L1181	L1182	L1183	L1184	L1185	L1186	L1187	L1188	L1189	L1190	L1191	L1192	L1193	L1194	L1195	L1196	L1197	L1198	L1199	L1200	L1201	L1202	L1203	L1204	L1205	L1206	L1207	L1208	L1209	L1210	L1211	L1212	L1213	L1214	L1215	L1216	L1217	L1218	L1219	L1220	L1221	L1222	L1223	L1224	L1225	L1226	L1227	L1228	L1229	L1230	L1231	L1232	L1233	L1234	L1235	L1236	L1237	L1238	L1239	L1240	L1241	L1242	L1243	L1244	L1245	L1246	L1247	L1248	L1249	L1250	L1251	L1252	L1253	L1254	L1255	L1256	L1257	L1258	L1259	L1260	L1261	L1262	L1263	L1264	L1265	L1266	L1267	L1268	L1269	L1270	L1271	L1272	L1273	L1274	L1275	L1276	L1277	L1278	L1279	L1280	L1281	L1282	L1283	L1284	L1285	L1286	L1287	L1288	L1289	L1290	L1291	L1292	L1293	L1294	L1295	L1296	L1297	L1298	L1299	L1300	L1301	L1302	L1303	L1304	L1305	L1306	L1307	L1308	L1309	L1310	L1311	L1312	L1313	L1314	L1315	L1316	L1317	L1318	L1319	L1320	L1321	L1322	L1323	L1324	L1325	L1326	L1327	L1328	L1329	L1330	L1331	L1332	L1333	L1334	L1335	L1336	L1337	L1338	L1339	L1340	L1341	L1342	L1343	L1344	L1345	L1346	L1347	L1348	L1349	L1350	L1351	L1352	L1353	L1354	L1355	L1356	L1357	L1358	L1359	L1360	L1361	L1362	L1363	L1364	L1365	L1366	L1367	L1368	L1369	L1370	L1371	L1372	L1373	L1374	L1375	L1376	L1377	L1378	L1379	L1380	L1381	L1382	L1383	L1384	L1385	L1386	L1387	L1388	L1389	L1390	L1391	L1392	L1393	L1394	L1395	L1396	L1397	L1398	L1399	L1400	L1401	L1402	L1403	L1404	L1405	L1406	L1407	L1408	L1409	L1410	L1411	L1412	L1413	L1414	L1415	L1416	L1417	L1418	L1419	L1420	L1421	L1422	L1423	L1424	L1425	L1426	L1427	L1428	L1429	L1430	L1431	L1432	L1433	L1434	L1435	L1436	L1437	L1438	L1439	L1440	L1441	L1442	L1443	L1444	L1445	L1446	L1447	L1448	L1449	L1450	L1451	L1452	L1453	L1454	L1455	L1456	L1457	L1458	L1459	L1460	L1461	L1462	L1463	L1464	L1465	L1466	L1467	L1468	L1469	L1470	L1471	L1472	L1473	L1474	L1475	L1476	L1477	L1478	L1479	L1480	L1481	L1482	L1483	L1484	L1485	L1486	L1487	L1488	L1489	L1490	L1491	L1492	L1493	L1494	L1495	L1496	L1497	L1498	L1499	L1500	L1501	L1502	L1503	L1504	L1505	L1506	L1507	L1508	L1509	L1510	L1511	L1512	L1513	L1514	L1515	L1516	L1517	L1518	L1519	L1520	L1521	L1522	L1523	L1524	L1525	L1526	L1527	L1528	L1529	L1530	L1531	L1532	L1533	L1534	L1535	L1536	L1537	L1538	L1539	L1540	L1541	L1542	L1543	L1544	L1545	L1546	L1547	L1548	L1549	L1550	L1551	L1552	L1553	L1554	L1555	L1556	L1557	L1558	L1559	L1560	L1561	L1562	L1563	L1564	L1565	L1566	L1567	L1568	L1569	L1570	L1571	L1572	L1573	L1574	L1575



• Molecule 1: MYOSIN

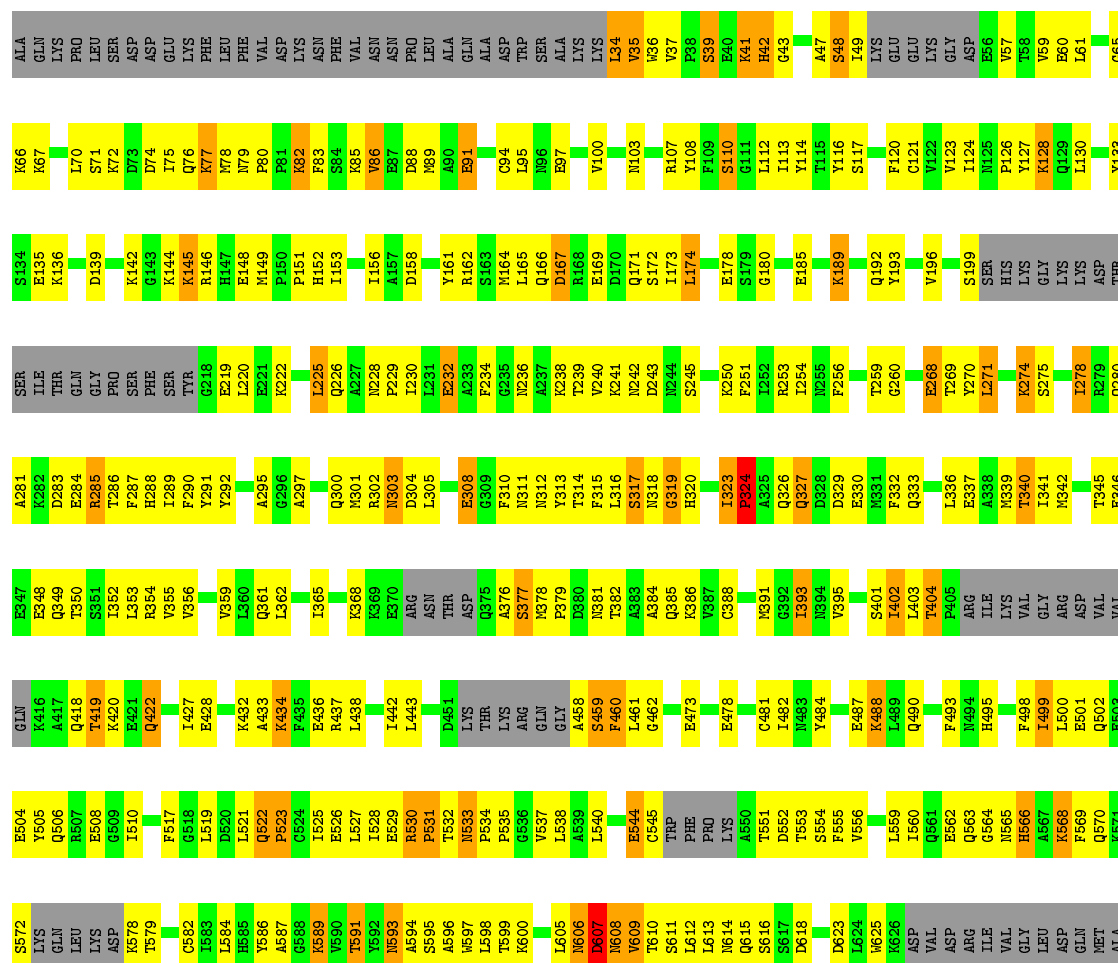
Chain E:

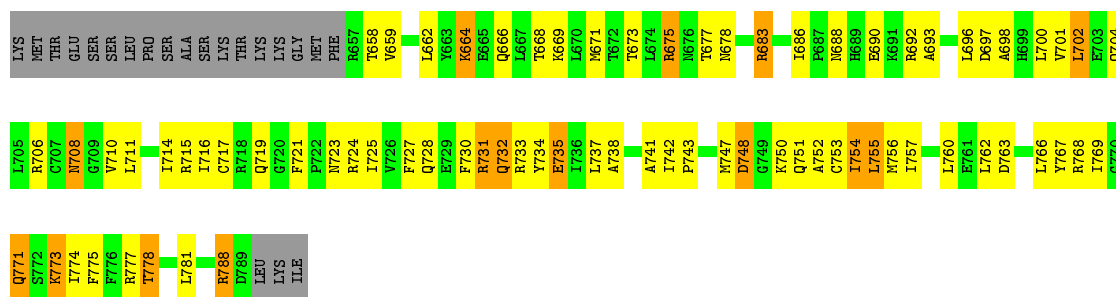




● Molecule 1: MYOSIN

Chain F: 37% 39% 9% 15%





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	134.01Å 107.67Å 188.31Å 90.00° 90.66° 90.00°	Depositor
Resolution (Å)	10.00 – 2.90	Depositor
% Data completeness (in resolution range)	83.1 (10.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.232 , 0.291	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	31830	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.49	1/5364 (0.0%)	0.65	2/7253 (0.0%)
1	B	0.48	0/5364	0.65	2/7253 (0.0%)
1	C	0.49	0/5364	0.65	2/7253 (0.0%)
1	D	0.50	0/5364	0.66	2/7253 (0.0%)
1	E	0.46	0/5364	0.61	0/7253
1	F	0.45	0/5364	0.61	0/7253
All	All	0.48	1/32184 (0.0%)	0.64	8/43518 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	121	CYS	CB-SG	-5.00	1.73	1.81

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	530	ARG	NE-CZ-NH2	7.39	124.00	120.30
1	C	530	ARG	NE-CZ-NH2	7.30	123.95	120.30
1	A	530	ARG	NE-CZ-NH2	7.27	123.93	120.30
1	D	530	ARG	NE-CZ-NH2	7.16	123.88	120.30
1	A	747	MET	CG-SD-CE	6.17	110.06	100.20
1	C	747	MET	CG-SD-CE	6.16	110.06	100.20
1	B	747	MET	CG-SD-CE	6.13	110.02	100.20
1	D	747	MET	CG-SD-CE	6.12	109.99	100.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5270	0	5145	373	0
1	B	5270	0	5145	365	0
1	C	5270	0	5145	369	0
1	D	5270	0	5145	354	0
1	E	5270	0	5145	363	0
1	F	5270	0	5145	356	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	5	0	0	1	0
3	B	5	0	0	1	0
3	C	5	0	0	1	0
3	D	5	0	0	2	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
4	A	27	0	12	1	0
4	B	27	0	12	1	0
4	C	27	0	12	1	0
4	D	27	0	12	1	0
4	E	27	0	12	0	0
4	F	27	0	12	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
5	E	2	0	0	0	0
5	F	2	0	0	0	0
All	All	31830	0	30942	2173	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 35.

All (2173) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:529:GLU:O	1:D:531:PRO:HD3	1.30	1.27
1:A:529:GLU:O	1:A:531:PRO:HD3	1.30	1.24
1:C:529:GLU:O	1:C:531:PRO:HD3	1.30	1.24
1:B:529:GLU:O	1:B:531:PRO:HD3	1.30	1.23
1:D:323:ILE:CG2	1:D:324:PRO:HD2	1.68	1.23
1:B:323:ILE:CG2	1:B:324:PRO:HD2	1.68	1.23
1:C:323:ILE:CG2	1:C:324:PRO:HD2	1.68	1.22
1:A:323:ILE:CG2	1:A:324:PRO:HD2	1.68	1.21
1:D:323:ILE:HG23	1:D:324:PRO:HD2	1.15	1.15
1:D:533:ASN:HB2	1:D:534:PRO:HD2	1.24	1.14
1:B:533:ASN:HB2	1:B:534:PRO:HD2	1.24	1.14
1:F:323:ILE:HG23	1:F:324:PRO:HD2	1.18	1.13
1:A:533:ASN:CB	1:A:534:PRO:CD	2.27	1.12
1:B:533:ASN:CB	1:B:534:PRO:CD	2.27	1.12
1:D:533:ASN:CB	1:D:534:PRO:CD	2.27	1.12
1:A:533:ASN:HB2	1:A:534:PRO:HD2	1.24	1.12
1:F:529:GLU:O	1:F:531:PRO:HD3	1.47	1.12
1:B:323:ILE:HG23	1:B:324:PRO:HD2	1.15	1.12
1:C:323:ILE:HG23	1:C:324:PRO:HD2	1.15	1.11
1:C:533:ASN:CB	1:C:534:PRO:CD	2.27	1.11
1:E:323:ILE:HG23	1:E:324:PRO:HD2	1.19	1.10
1:E:529:GLU:O	1:E:531:PRO:HD3	1.50	1.09
1:C:533:ASN:HB2	1:C:534:PRO:HD2	1.24	1.09
1:A:323:ILE:HG23	1:A:324:PRO:HD2	1.15	1.08
1:E:323:ILE:CG2	1:E:324:PRO:HD2	1.86	1.05
1:E:533:ASN:HB2	1:E:534:PRO:HD2	1.40	1.03
1:F:323:ILE:CG2	1:F:324:PRO:HD2	1.87	1.03
1:F:533:ASN:HB2	1:F:534:PRO:HD2	1.41	1.01
1:D:533:ASN:HB3	1:D:534:PRO:HD3	1.43	1.01
1:C:533:ASN:HB3	1:C:534:PRO:HD3	1.43	1.01
1:B:533:ASN:HB3	1:B:534:PRO:HD3	1.43	1.01
1:B:533:ASN:CB	1:B:534:PRO:HD2	1.89	1.00
1:A:533:ASN:HB3	1:A:534:PRO:HD3	1.43	1.00
1:D:533:ASN:CB	1:D:534:PRO:HD2	1.89	0.98
1:E:533:ASN:CB	1:E:534:PRO:CD	2.41	0.98
1:A:533:ASN:CB	1:A:534:PRO:HD2	1.89	0.97
1:C:533:ASN:CB	1:C:534:PRO:HD2	1.89	0.97
1:A:533:ASN:HB2	1:A:534:PRO:CD	1.94	0.96
1:F:533:ASN:CB	1:F:534:PRO:CD	2.42	0.96
1:C:533:ASN:HB3	1:C:534:PRO:CD	1.94	0.95
1:C:533:ASN:HB2	1:C:534:PRO:CD	1.94	0.95
1:C:544:GLU:HB3	1:C:598:LEU:HD21	1.49	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:544:GLU:HB3	1:F:598:LEU:HD21	1.49	0.94
1:B:568:LYS:HA	1:B:584:LEU:HD12	1.49	0.93
1:A:533:ASN:HB3	1:A:534:PRO:CD	1.94	0.92
1:E:568:LYS:HA	1:E:584:LEU:HD12	1.51	0.92
1:F:533:ASN:CB	1:F:534:PRO:HD2	1.99	0.92
1:A:568:LYS:HA	1:A:584:LEU:HD12	1.51	0.92
1:A:696:LEU:HD21	1:A:701:VAL:HG21	1.50	0.91
1:D:544:GLU:HB3	1:D:598:LEU:HD21	1.50	0.91
1:A:584:LEU:HD23	1:A:589:LYS:HG3	1.51	0.91
1:E:544:GLU:HB3	1:E:598:LEU:HD21	1.49	0.91
1:A:544:GLU:HB3	1:A:598:LEU:HD21	1.53	0.91
1:B:529:GLU:O	1:B:531:PRO:CD	2.19	0.91
1:C:568:LYS:HA	1:C:584:LEU:HD12	1.53	0.91
1:B:696:LEU:HD21	1:B:701:VAL:HG21	1.54	0.90
1:F:696:LEU:HD21	1:F:701:VAL:HG21	1.52	0.90
1:E:584:LEU:HD23	1:E:589:LYS:HG3	1.51	0.90
1:D:748:ASP:OD1	1:D:751:GLN:N	2.05	0.90
1:B:544:GLU:HB3	1:B:598:LEU:HD21	1.53	0.90
1:C:606:ASN:ND2	1:C:608:ASN:HB2	1.87	0.90
1:C:584:LEU:HD23	1:C:589:LYS:HG3	1.52	0.90
1:A:748:ASP:OD1	1:A:751:GLN:N	2.05	0.89
1:C:529:GLU:O	1:C:531:PRO:CD	2.19	0.89
1:B:748:ASP:OD1	1:B:751:GLN:N	2.05	0.89
1:B:323:ILE:CG2	1:B:324:PRO:CD	2.51	0.89
1:B:533:ASN:HB3	1:B:534:PRO:CD	1.94	0.89
1:A:323:ILE:CG2	1:A:324:PRO:CD	2.51	0.89
1:C:748:ASP:OD1	1:C:751:GLN:N	2.05	0.89
1:D:584:LEU:HD23	1:D:589:LYS:HG3	1.55	0.89
1:A:529:GLU:O	1:A:531:PRO:CD	2.19	0.89
1:D:568:LYS:HA	1:D:584:LEU:HD12	1.55	0.89
1:E:533:ASN:CB	1:E:534:PRO:HD2	1.99	0.89
1:E:696:LEU:HD21	1:E:701:VAL:HG21	1.53	0.89
1:B:584:LEU:HD23	1:B:589:LYS:HG3	1.55	0.88
1:D:323:ILE:CG2	1:D:324:PRO:CD	2.51	0.88
1:F:568:LYS:HA	1:F:584:LEU:HD12	1.52	0.88
1:D:533:ASN:HB3	1:D:534:PRO:CD	1.94	0.88
1:A:606:ASN:ND2	1:A:608:ASN:HB2	1.88	0.88
1:D:696:LEU:HD21	1:D:701:VAL:HG21	1.54	0.87
1:E:533:ASN:HB3	1:E:534:PRO:CD	2.03	0.87
1:F:584:LEU:HD23	1:F:589:LYS:HG3	1.54	0.87
1:F:533:ASN:HB3	1:F:534:PRO:CD	2.04	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:606:ASN:HD21	1:C:608:ASN:HB2	1.40	0.87
1:B:323:ILE:HG23	1:B:324:PRO:CD	2.04	0.86
1:D:323:ILE:HG23	1:D:324:PRO:CD	2.04	0.86
1:A:751:GLN:NE2	1:C:692:ARG:HH22	1.73	0.86
1:C:323:ILE:CG2	1:C:324:PRO:CD	2.51	0.86
1:A:742:ILE:HD11	1:A:752:ALA:O	1.75	0.86
1:B:742:ILE:HD11	1:B:752:ALA:O	1.75	0.86
1:B:606:ASN:ND2	1:B:608:ASN:HB2	1.91	0.85
1:F:606:ASN:ND2	1:F:608:ASN:HB2	1.90	0.85
1:D:529:GLU:O	1:D:531:PRO:CD	2.19	0.85
1:F:742:ILE:HD11	1:F:752:ALA:O	1.76	0.85
1:A:323:ILE:HG23	1:A:324:PRO:CD	2.04	0.84
1:D:606:ASN:ND2	1:D:608:ASN:HB2	1.92	0.84
1:B:145:LYS:HB2	1:B:148:GLU:HG3	1.59	0.84
1:C:544:GLU:HG3	1:C:555:PHE:HB2	1.59	0.84
1:A:606:ASN:HD21	1:A:608:ASN:HB2	1.42	0.84
1:A:751:GLN:CD	1:C:692:ARG:HH22	1.81	0.84
1:C:145:LYS:HB2	1:C:148:GLU:HG3	1.58	0.84
1:D:145:LYS:HB2	1:D:148:GLU:HG3	1.60	0.83
1:C:696:LEU:HD21	1:C:701:VAL:HG21	1.57	0.83
1:E:742:ILE:HD11	1:E:752:ALA:O	1.79	0.83
1:F:145:LYS:HB2	1:F:148:GLU:HG3	1.61	0.83
1:A:323:ILE:HG22	1:A:324:PRO:HD2	1.61	0.82
1:F:606:ASN:HD21	1:F:608:ASN:HB2	1.43	0.82
1:A:544:GLU:HG3	1:A:555:PHE:HB2	1.62	0.82
1:A:145:LYS:HB2	1:A:148:GLU:HG3	1.59	0.82
1:E:533:ASN:HB3	1:E:534:PRO:HD3	1.61	0.82
1:B:606:ASN:HD21	1:B:608:ASN:HB2	1.45	0.82
1:E:606:ASN:ND2	1:E:608:ASN:HB2	1.95	0.82
1:C:323:ILE:HG23	1:C:324:PRO:CD	2.04	0.81
1:D:419:THR:H	1:D:422:GLN:HG3	1.45	0.81
1:E:43:GLY:H	1:E:698:ALA:HB1	1.44	0.81
1:A:378:MET:HE2	1:A:381:ASN:HA	1.63	0.81
1:F:544:GLU:HG3	1:F:555:PHE:HB2	1.62	0.81
1:C:742:ILE:HD11	1:C:752:ALA:O	1.79	0.81
1:E:49:ILE:HA	1:E:59:VAL:HG12	1.63	0.81
1:F:49:ILE:HA	1:F:59:VAL:HG12	1.63	0.81
1:D:544:GLU:HG3	1:D:555:PHE:HB2	1.61	0.81
1:D:742:ILE:HD11	1:D:752:ALA:O	1.80	0.81
1:E:419:THR:H	1:E:422:GLN:HG3	1.46	0.81
1:B:156:ILE:HG22	1:B:173:ILE:HD13	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:ILE:HG22	1:C:324:PRO:HD2	1.61	0.81
1:C:593:ASN:HD22	1:C:595:SER:H	1.28	0.81
1:E:715:ARG:HG3	1:E:715:ARG:HH11	1.45	0.81
1:B:419:THR:H	1:B:422:GLN:HG3	1.44	0.80
1:E:145:LYS:HB2	1:E:148:GLU:HG3	1.62	0.80
1:E:544:GLU:HG3	1:E:555:PHE:HB2	1.63	0.80
1:B:593:ASN:HD22	1:B:595:SER:H	1.29	0.80
1:A:49:ILE:HA	1:A:59:VAL:HG12	1.64	0.80
1:D:606:ASN:HD21	1:D:608:ASN:HB2	1.46	0.80
1:E:391:MET:HG2	1:E:434:LYS:HZ1	1.47	0.80
1:F:43:GLY:H	1:F:698:ALA:HB1	1.47	0.80
1:B:715:ARG:HG3	1:B:715:ARG:HH11	1.47	0.80
1:B:43:GLY:H	1:B:698:ALA:HB1	1.47	0.80
1:A:128:LYS:HD3	1:A:693:ALA:HB1	1.63	0.80
1:D:323:ILE:HG22	1:D:324:PRO:HD2	1.62	0.80
1:B:323:ILE:HG22	1:B:324:PRO:HD2	1.61	0.79
1:C:49:ILE:HA	1:C:59:VAL:HG12	1.63	0.79
1:A:85:LYS:HB3	1:A:107:ARG:HG2	1.64	0.79
1:B:49:ILE:HA	1:B:59:VAL:HG12	1.63	0.79
1:F:533:ASN:HB3	1:F:534:PRO:HD3	1.64	0.79
1:D:715:ARG:HG3	1:D:715:ARG:HH11	1.47	0.79
1:A:593:ASN:HD22	1:A:595:SER:H	1.29	0.79
1:D:49:ILE:HA	1:D:59:VAL:HG12	1.65	0.79
1:E:593:ASN:HD22	1:E:595:SER:H	1.30	0.79
1:A:751:GLN:HE22	1:C:692:ARG:NH2	1.80	0.79
1:C:715:ARG:HH11	1:C:715:ARG:HG3	1.48	0.79
1:D:43:GLY:H	1:D:698:ALA:HB1	1.46	0.79
1:D:85:LYS:HB3	1:D:107:ARG:HG2	1.64	0.79
1:F:715:ARG:HH11	1:F:715:ARG:HG3	1.47	0.78
1:E:737:LEU:HD21	1:E:788:ARG:HA	1.65	0.78
1:F:85:LYS:HB3	1:F:107:ARG:HG2	1.63	0.78
1:A:743:PRO:HG2	1:A:747:MET:SD	2.24	0.78
1:C:85:LYS:HB3	1:C:107:ARG:HG2	1.64	0.78
1:A:419:THR:H	1:A:422:GLN:HG3	1.48	0.78
1:D:593:ASN:HD22	1:D:595:SER:H	1.27	0.78
1:F:128:LYS:HD3	1:F:693:ALA:HB1	1.66	0.78
1:B:544:GLU:HG3	1:B:555:PHE:HB2	1.64	0.78
1:F:743:PRO:HG2	1:F:747:MET:SD	2.23	0.78
1:B:743:PRO:HG2	1:B:747:MET:SD	2.24	0.78
1:C:498:PHE:O	1:C:502:GLN:HG3	1.84	0.78
1:E:128:LYS:HD3	1:E:693:ALA:HB1	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:748:ASP:OD1	1:E:751:GLN:N	2.16	0.78
1:F:156:ILE:HG22	1:F:173:ILE:HD13	1.65	0.78
1:B:128:LYS:HD3	1:B:693:ALA:HB1	1.65	0.78
1:D:391:MET:HG2	1:D:434:LYS:HZ1	1.48	0.78
1:A:751:GLN:OE1	1:C:692:ARG:NH2	2.16	0.78
1:C:743:PRO:HG2	1:C:747:MET:SD	2.24	0.78
1:A:419:THR:HG23	1:A:422:GLN:NE2	1.99	0.77
1:E:606:ASN:HD21	1:E:608:ASN:HB2	1.49	0.77
1:F:593:ASN:HD22	1:F:595:SER:H	1.32	0.77
1:C:128:LYS:HD3	1:C:693:ALA:HB1	1.66	0.77
1:D:743:PRO:HG2	1:D:747:MET:SD	2.24	0.77
1:B:378:MET:HE1	1:B:384:ALA:HB2	1.67	0.77
1:A:715:ARG:HG3	1:A:715:ARG:HH11	1.48	0.77
1:D:378:MET:HE1	1:D:384:ALA:HB2	1.66	0.77
1:A:43:GLY:H	1:A:698:ALA:HB1	1.49	0.77
1:B:498:PHE:O	1:B:502:GLN:HG3	1.85	0.77
1:F:419:THR:H	1:F:422:GLN:HG3	1.49	0.77
1:E:85:LYS:HB3	1:E:107:ARG:HG2	1.67	0.77
1:D:419:THR:HG23	1:D:422:GLN:NE2	2.00	0.76
1:D:742:ILE:HG13	1:D:747:MET:HG2	1.67	0.76
1:B:742:ILE:HG13	1:B:747:MET:HG2	1.67	0.76
1:D:128:LYS:HD3	1:D:693:ALA:HB1	1.67	0.76
1:B:391:MET:HG2	1:B:434:LYS:HZ1	1.51	0.76
1:E:156:ILE:HG22	1:E:173:ILE:HD13	1.67	0.76
1:C:156:ILE:HG22	1:C:173:ILE:HD13	1.65	0.76
1:F:498:PHE:O	1:F:502:GLN:HG3	1.86	0.76
1:F:378:MET:HE1	1:F:384:ALA:HB2	1.68	0.76
1:C:742:ILE:HG13	1:C:747:MET:HG2	1.67	0.76
1:C:419:THR:HG23	1:C:422:GLN:NE2	2.00	0.76
1:C:419:THR:H	1:C:422:GLN:HG3	1.48	0.75
1:C:43:GLY:H	1:C:698:ALA:HB1	1.48	0.75
1:D:156:ILE:HG22	1:D:173:ILE:HD13	1.68	0.75
1:F:391:MET:HG2	1:F:434:LYS:HZ1	1.51	0.75
1:A:419:THR:H	1:A:422:GLN:HE21	1.34	0.75
1:B:85:LYS:HB3	1:B:107:ARG:HG2	1.67	0.75
1:F:529:GLU:O	1:F:531:PRO:CD	2.32	0.75
1:D:582:CYS:SG	1:D:591:THR:HB	2.27	0.75
1:F:737:LEU:HD21	1:F:788:ARG:HA	1.68	0.75
1:E:743:PRO:HG2	1:E:747:MET:SD	2.27	0.75
1:A:742:ILE:HG13	1:A:747:MET:HG2	1.67	0.74
1:E:527:LEU:HD12	1:E:527:LEU:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:737:LEU:HD21	1:B:788:ARG:HA	1.69	0.74
1:F:323:ILE:CG2	1:F:324:PRO:CD	2.66	0.74
1:E:742:ILE:HG13	1:E:747:MET:HG2	1.70	0.74
1:F:748:ASP:OD1	1:F:751:GLN:N	2.20	0.74
1:E:323:ILE:CG2	1:E:324:PRO:CD	2.65	0.74
1:A:156:ILE:HG22	1:A:173:ILE:HD13	1.67	0.74
1:D:737:LEU:HD21	1:D:788:ARG:HA	1.70	0.74
1:E:738:ALA:HB1	1:E:741:ALA:HB2	1.69	0.74
1:A:737:LEU:HD21	1:A:788:ARG:HA	1.68	0.74
1:D:419:THR:H	1:D:422:GLN:HE21	1.36	0.74
1:C:540:LEU:HD13	1:C:559:LEU:HA	1.70	0.73
1:F:743:PRO:CG	1:F:747:MET:SD	2.76	0.73
1:E:498:PHE:O	1:E:502:GLN:HG3	1.89	0.73
1:B:419:THR:HG23	1:B:422:GLN:NE2	2.03	0.73
1:E:529:GLU:O	1:E:531:PRO:CD	2.35	0.73
1:E:419:THR:HG23	1:E:422:GLN:NE2	2.03	0.73
1:B:540:LEU:HD13	1:B:559:LEU:HA	1.69	0.73
1:A:527:LEU:O	1:A:527:LEU:HD12	1.87	0.73
1:A:540:LEU:HD13	1:A:559:LEU:HA	1.70	0.73
1:C:391:MET:HG2	1:C:434:LYS:HZ1	1.54	0.73
1:A:498:PHE:O	1:A:502:GLN:HG3	1.88	0.73
1:C:737:LEU:HD21	1:C:788:ARG:HA	1.69	0.73
1:F:280:GLN:OE1	1:F:317:SER:HB2	1.88	0.73
1:C:419:THR:H	1:C:422:GLN:HE21	1.35	0.73
1:E:508:GLU:HG2	1:E:775:PHE:HE1	1.54	0.73
1:C:401:SER:HB3	1:C:608:ASN:HB3	1.71	0.72
1:E:378:MET:HE1	1:E:384:ALA:HB2	1.70	0.72
1:A:391:MET:HG2	1:A:434:LYS:HZ1	1.53	0.72
1:A:535:PRO:O	1:A:563:GLN:NE2	2.22	0.72
1:C:743:PRO:CG	1:C:747:MET:SD	2.77	0.72
1:C:535:PRO:O	1:C:563:GLN:NE2	2.22	0.72
1:D:743:PRO:CG	1:D:747:MET:SD	2.77	0.72
1:F:419:THR:HG23	1:F:422:GLN:NE2	2.04	0.72
1:D:535:PRO:O	1:D:563:GLN:NE2	2.22	0.72
1:A:743:PRO:CG	1:A:747:MET:SD	2.77	0.72
1:A:738:ALA:HB1	1:A:741:ALA:HB2	1.71	0.72
1:B:535:PRO:O	1:B:563:GLN:NE2	2.22	0.72
1:B:508:GLU:HG2	1:B:775:PHE:HE1	1.55	0.72
1:D:498:PHE:O	1:D:502:GLN:HG3	1.90	0.72
1:D:738:ALA:HB1	1:D:741:ALA:HB2	1.71	0.72
1:B:419:THR:H	1:B:422:GLN:HE21	1.35	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:743:PRO:CG	1:B:747:MET:SD	2.77	0.71
1:F:540:LEU:HD13	1:F:559:LEU:HA	1.71	0.71
1:D:508:GLU:HG2	1:D:775:PHE:HE1	1.54	0.71
1:E:419:THR:H	1:E:422:GLN:HE21	1.37	0.71
1:F:419:THR:H	1:F:422:GLN:HE21	1.36	0.71
1:B:419:THR:N	1:B:422:GLN:HE21	1.89	0.71
1:B:738:ALA:HB1	1:B:741:ALA:HB2	1.71	0.71
1:C:738:ALA:HB1	1:C:741:ALA:HB2	1.71	0.71
1:D:527:LEU:O	1:D:527:LEU:HD12	1.91	0.71
1:A:378:MET:HE1	1:A:384:ALA:HB2	1.72	0.71
1:A:242:ASN:HB3	1:A:245:SER:HB2	1.72	0.71
1:C:378:MET:HE1	1:C:384:ALA:HB2	1.71	0.71
1:C:242:ASN:HB3	1:C:245:SER:HB2	1.72	0.71
1:A:401:SER:HB3	1:A:608:ASN:HB3	1.73	0.71
1:B:527:LEU:O	1:B:527:LEU:HD12	1.91	0.71
1:D:731:ARG:HH21	1:D:742:ILE:HG21	1.55	0.71
1:F:569:PHE:CD1	1:F:570:GLN:N	2.59	0.71
1:E:540:LEU:HD13	1:E:559:LEU:HA	1.71	0.70
1:D:731:ARG:HH11	1:D:731:ARG:HG3	1.57	0.70
1:F:742:ILE:HG13	1:F:747:MET:HG2	1.72	0.70
1:B:526:GLU:O	1:B:530:ARG:HB2	1.92	0.70
1:C:280:GLN:OE1	1:C:317:SER:HB2	1.90	0.70
1:E:569:PHE:CD1	1:E:570:GLN:N	2.60	0.70
1:A:731:ARG:HG3	1:A:731:ARG:HH11	1.57	0.70
1:F:527:LEU:HD12	1:F:527:LEU:O	1.90	0.70
1:A:731:ARG:NH2	1:A:742:ILE:HG21	2.07	0.70
1:C:527:LEU:HD12	1:C:527:LEU:O	1.91	0.70
1:E:378:MET:HE2	1:E:381:ASN:HA	1.74	0.70
1:B:533:ASN:HB2	1:B:534:PRO:CD	1.94	0.70
1:C:731:ARG:HH21	1:C:742:ILE:HG21	1.57	0.70
1:D:731:ARG:NH2	1:D:742:ILE:HG21	2.07	0.70
1:B:401:SER:HB3	1:B:608:ASN:HB3	1.74	0.69
1:E:419:THR:N	1:E:422:GLN:HE21	1.90	0.69
1:F:533:ASN:HB2	1:F:534:PRO:CD	2.13	0.69
1:F:731:ARG:HH21	1:F:742:ILE:HG21	1.55	0.69
1:E:346:GLU:O	1:E:350:THR:HG23	1.93	0.69
1:F:508:GLU:HG2	1:F:775:PHE:HE1	1.56	0.69
1:F:346:GLU:O	1:F:350:THR:HG23	1.92	0.69
1:D:540:LEU:HD13	1:D:559:LEU:HA	1.75	0.69
1:A:419:THR:N	1:A:422:GLN:HE21	1.89	0.69
1:E:743:PRO:CG	1:E:747:MET:SD	2.81	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:731:ARG:NH2	1:C:742:ILE:HG21	2.08	0.69
1:D:72:LYS:HA	1:D:75:ILE:HD12	1.73	0.69
1:A:569:PHE:CD1	1:A:570:GLN:N	2.61	0.69
1:A:731:ARG:HH21	1:A:742:ILE:HG21	1.57	0.69
1:A:751:GLN:OE1	1:C:692:ARG:NH1	2.26	0.69
1:A:72:LYS:HA	1:A:75:ILE:HD12	1.74	0.69
1:D:526:GLU:O	1:D:530:ARG:HB2	1.93	0.69
1:A:537:VAL:HG22	1:A:559:LEU:HD11	1.74	0.69
1:C:419:THR:N	1:C:422:GLN:HE21	1.91	0.69
1:C:569:PHE:CD1	1:C:570:GLN:N	2.61	0.69
1:A:274:LYS:HG2	1:A:436:GLU:HB2	1.75	0.69
1:B:280:GLN:OE1	1:B:317:SER:HB2	1.92	0.69
1:E:582:CYS:SG	1:E:591:THR:HB	2.33	0.69
1:F:731:ARG:NH2	1:F:742:ILE:HG21	2.07	0.69
1:C:607:ASP:HA	1:C:610:THR:HB	1.75	0.68
1:D:419:THR:N	1:D:422:GLN:HE21	1.89	0.68
1:E:526:GLU:O	1:E:530:ARG:HB2	1.93	0.68
1:E:72:LYS:HA	1:E:75:ILE:HD12	1.74	0.68
1:F:323:ILE:HG23	1:F:324:PRO:CD	2.11	0.68
1:E:537:VAL:HG22	1:E:559:LEU:HD11	1.75	0.68
1:E:418:GLN:HA	1:E:422:GLN:NE2	2.08	0.68
1:B:708:ASN:N	1:B:708:ASN:HD22	1.91	0.68
1:C:274:LYS:HG2	1:C:436:GLU:HB2	1.75	0.68
1:C:537:VAL:HG22	1:C:559:LEU:HD11	1.74	0.68
1:A:728:GLN:O	1:A:732:GLN:HG2	1.94	0.68
1:D:401:SER:HB3	1:D:608:ASN:HB3	1.76	0.68
1:E:280:GLN:OE1	1:E:317:SER:HB2	1.93	0.68
1:A:582:CYS:SG	1:A:591:THR:HB	2.34	0.68
1:B:537:VAL:HG22	1:B:559:LEU:HD11	1.74	0.68
1:B:731:ARG:HH21	1:B:742:ILE:HG21	1.59	0.68
1:C:72:LYS:HA	1:C:75:ILE:HD12	1.75	0.68
1:D:242:ASN:HB3	1:D:245:SER:HB2	1.74	0.68
1:C:731:ARG:HH11	1:C:731:ARG:HG3	1.59	0.68
1:D:569:PHE:CD1	1:D:570:GLN:N	2.62	0.68
1:B:72:LYS:HA	1:B:75:ILE:HD12	1.74	0.68
1:D:196:VAL:HG12	1:D:196:VAL:O	1.94	0.68
1:F:72:LYS:HA	1:F:75:ILE:HD12	1.75	0.68
1:D:274:LYS:HG2	1:D:436:GLU:HB2	1.75	0.67
1:E:116:TYR:CZ	1:E:151:PRO:HA	2.29	0.67
1:F:401:SER:HB3	1:F:608:ASN:HB3	1.75	0.67
1:A:508:GLU:HG2	1:A:775:PHE:HE1	1.57	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:527:LEU:CD1	1:B:563:GLN:HG3	2.25	0.67
1:F:281:ALA:O	1:F:284:GLU:HB2	1.95	0.67
1:A:596:ALA:O	1:A:600:LYS:HG3	1.94	0.67
1:F:332:PHE:CE2	1:F:336:LEU:HD11	2.29	0.67
1:F:535:PRO:O	1:F:563:GLN:NE2	2.27	0.67
1:F:686:ILE:HG22	1:F:704:GLN:NE2	2.10	0.67
1:A:116:TYR:CZ	1:A:151:PRO:HA	2.29	0.67
1:A:280:GLN:OE1	1:A:317:SER:HB2	1.95	0.67
1:B:232:GLU:O	1:B:236:ASN:HB2	1.95	0.67
1:C:508:GLU:HG2	1:C:775:PHE:HE1	1.57	0.67
1:F:79:ASN:ND2	1:F:94:CYS:HB2	2.10	0.67
1:E:401:SER:HB3	1:E:608:ASN:HB3	1.74	0.67
1:F:274:LYS:HB3	1:F:432:LYS:HB3	1.76	0.67
1:D:332:PHE:CE2	1:D:336:LEU:HD11	2.30	0.67
1:D:418:GLN:HA	1:D:422:GLN:NE2	2.10	0.67
1:E:535:PRO:O	1:E:563:GLN:NE2	2.28	0.67
1:B:274:LYS:HB3	1:B:432:LYS:HB3	1.76	0.67
1:C:526:GLU:O	1:C:530:ARG:HB2	1.94	0.67
1:D:116:TYR:CZ	1:D:151:PRO:HA	2.30	0.67
1:F:419:THR:N	1:F:422:GLN:HE21	1.92	0.67
1:A:332:PHE:CE2	1:A:336:LEU:HD11	2.30	0.67
1:B:274:LYS:HG2	1:B:436:GLU:HB2	1.77	0.67
1:B:731:ARG:NH2	1:B:742:ILE:HG21	2.09	0.67
1:D:725:ILE:HD11	1:D:730:PHE:HD1	1.60	0.67
1:B:116:TYR:CZ	1:B:151:PRO:HA	2.30	0.67
1:B:418:GLN:HA	1:B:422:GLN:NE2	2.09	0.67
1:C:232:GLU:O	1:C:236:ASN:HB2	1.94	0.67
1:D:280:GLN:OE1	1:D:317:SER:HB2	1.94	0.67
1:B:569:PHE:CD1	1:B:570:GLN:N	2.63	0.67
1:C:79:ASN:ND2	1:C:94:CYS:HB2	2.10	0.66
1:F:537:VAL:HG22	1:F:559:LEU:HD11	1.76	0.66
1:B:725:ILE:HD11	1:B:730:PHE:HD1	1.60	0.66
1:D:537:VAL:HG22	1:D:559:LEU:HD11	1.77	0.66
1:E:332:PHE:CE2	1:E:336:LEU:HD11	2.31	0.66
1:E:731:ARG:HH21	1:E:742:ILE:HG21	1.60	0.66
1:B:242:ASN:HB3	1:B:245:SER:HB2	1.76	0.66
1:B:540:LEU:CD1	1:B:559:LEU:HA	2.26	0.66
1:D:281:ALA:O	1:D:284:GLU:HB2	1.95	0.66
1:D:433:ALA:O	1:D:437:ARG:HG3	1.96	0.66
1:A:526:GLU:O	1:A:530:ARG:HB2	1.94	0.66
1:B:107:ARG:HB3	1:B:112:LEU:HB2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:ASN:O	1:B:107:ARG:HG3	1.95	0.66
1:B:728:GLN:O	1:B:732:GLN:HG2	1.96	0.66
1:C:582:CYS:SG	1:C:591:THR:HB	2.35	0.66
1:C:686:ILE:HG22	1:C:704:GLN:NE2	2.09	0.66
1:E:731:ARG:HG3	1:E:731:ARG:HH11	1.60	0.66
1:E:731:ARG:NH2	1:E:742:ILE:HG21	2.11	0.66
1:F:728:GLN:O	1:F:732:GLN:HG2	1.95	0.66
1:C:274:LYS:HB3	1:C:432:LYS:HB3	1.76	0.66
1:C:596:ALA:O	1:C:600:LYS:HG3	1.96	0.66
1:E:274:LYS:HB3	1:E:432:LYS:HB3	1.77	0.66
1:A:308:GLU:HB3	1:A:312:ASN:HB2	1.77	0.66
1:D:308:GLU:HB3	1:D:312:ASN:HB2	1.77	0.66
1:D:527:LEU:CD1	1:D:563:GLN:HG3	2.26	0.66
1:A:708:ASN:HD22	1:A:708:ASN:N	1.93	0.66
1:B:346:GLU:O	1:B:350:THR:HG23	1.95	0.66
1:C:346:GLU:O	1:C:350:THR:HG23	1.95	0.66
1:C:708:ASN:HD22	1:C:708:ASN:N	1.94	0.66
1:E:433:ALA:O	1:E:437:ARG:HG3	1.95	0.66
1:E:232:GLU:O	1:E:236:ASN:HB2	1.96	0.66
1:B:378:MET:HE2	1:B:381:ASN:HA	1.78	0.66
1:F:607:ASP:HA	1:F:610:THR:HB	1.77	0.66
1:A:607:ASP:HA	1:A:610:THR:HB	1.78	0.65
1:A:79:ASN:ND2	1:A:94:CYS:HB2	2.12	0.65
1:C:418:GLN:HA	1:C:422:GLN:NE2	2.11	0.65
1:C:769:ILE:HD13	1:C:774:ILE:HG23	1.78	0.65
1:E:596:ALA:O	1:E:600:LYS:HG3	1.96	0.65
1:A:725:ILE:HD11	1:A:730:PHE:HD1	1.61	0.65
1:C:728:GLN:O	1:C:732:GLN:HG2	1.96	0.65
1:B:433:ALA:O	1:B:437:ARG:HG3	1.96	0.65
1:B:731:ARG:HG3	1:B:731:ARG:HH11	1.61	0.65
1:B:79:ASN:ND2	1:B:94:CYS:HB2	2.11	0.65
1:D:346:GLU:O	1:D:350:THR:HG23	1.95	0.65
1:C:116:TYR:CZ	1:C:151:PRO:HA	2.31	0.65
1:C:281:ALA:O	1:C:284:GLU:HB2	1.97	0.65
1:E:725:ILE:HD11	1:E:730:PHE:HD1	1.60	0.65
1:F:242:ASN:HB3	1:F:245:SER:HB2	1.76	0.65
1:B:281:ALA:O	1:B:284:GLU:HB2	1.96	0.65
1:C:433:ALA:O	1:C:437:ARG:HG3	1.96	0.65
1:D:686:ILE:HG22	1:D:704:GLN:NE2	2.11	0.65
1:A:433:ALA:O	1:A:437:ARG:HG3	1.96	0.65
1:A:77:LYS:CE	1:A:77:LYS:H	2.09	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:540:LEU:CD1	1:C:559:LEU:HA	2.27	0.65
1:B:332:PHE:CE2	1:B:336:LEU:HD11	2.31	0.65
1:D:596:ALA:O	1:D:600:LYS:HG3	1.97	0.65
1:D:731:ARG:NH1	1:D:731:ARG:HG3	2.11	0.65
1:F:433:ALA:O	1:F:437:ARG:HG3	1.97	0.65
1:A:696:LEU:CD2	1:A:701:VAL:HG21	2.27	0.65
1:B:305:LEU:HD22	1:B:354:ARG:HA	1.79	0.65
1:D:103:ASN:O	1:D:107:ARG:HG3	1.96	0.65
1:E:715:ARG:HG3	1:E:715:ARG:NH1	2.12	0.65
1:F:378:MET:HE2	1:F:381:ASN:HA	1.79	0.65
1:F:582:CYS:SG	1:F:591:THR:HB	2.36	0.65
1:F:731:ARG:HG3	1:F:731:ARG:HH11	1.60	0.65
1:F:769:ILE:HD13	1:F:774:ILE:HG23	1.79	0.65
1:E:607:ASP:HA	1:E:610:THR:HB	1.78	0.65
1:F:596:ALA:O	1:F:600:LYS:HG3	1.97	0.65
1:C:488:LYS:HE2	1:C:529:GLU:OE1	1.97	0.65
1:D:232:GLU:O	1:D:236:ASN:HB2	1.96	0.65
1:D:488:LYS:HE2	1:D:529:GLU:OE1	1.96	0.65
1:E:708:ASN:HD22	1:E:708:ASN:N	1.94	0.65
1:F:526:GLU:O	1:F:530:ARG:HB2	1.96	0.65
1:A:145:LYS:HB2	1:A:148:GLU:CG	2.27	0.64
1:A:540:LEU:CD1	1:A:559:LEU:HA	2.26	0.64
1:D:769:ILE:HD13	1:D:774:ILE:HG23	1.79	0.64
1:E:242:ASN:HB3	1:E:245:SER:HB2	1.80	0.64
1:F:738:ALA:HB1	1:F:741:ALA:HB2	1.78	0.64
1:D:728:GLN:O	1:D:732:GLN:HG2	1.96	0.64
1:E:274:LYS:HG2	1:E:436:GLU:HB2	1.78	0.64
1:F:540:LEU:CD1	1:F:559:LEU:HA	2.27	0.64
1:A:232:GLU:O	1:A:236:ASN:HB2	1.97	0.64
1:B:582:CYS:SG	1:B:591:THR:HB	2.37	0.64
1:B:57:VAL:HB	1:B:75:ILE:HD11	1.80	0.64
1:C:332:PHE:CE2	1:C:336:LEU:HD11	2.32	0.64
1:D:607:ASP:HA	1:D:610:THR:HB	1.79	0.64
1:E:728:GLN:O	1:E:732:GLN:HG2	1.97	0.64
1:A:305:LEU:HD22	1:A:354:ARG:HA	1.80	0.64
1:F:376:ALA:HB2	1:F:420:LYS:N	2.13	0.64
1:A:103:ASN:O	1:A:107:ARG:HG3	1.97	0.64
1:A:281:ALA:O	1:A:284:GLU:HB2	1.96	0.64
1:A:418:GLN:HA	1:A:422:GLN:NE2	2.12	0.64
1:A:527:LEU:CD1	1:A:563:GLN:HG3	2.27	0.64
1:B:596:ALA:O	1:B:600:LYS:HG3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:LYS:HB2	1:C:148:GLU:CG	2.25	0.64
1:E:281:ALA:O	1:E:284:GLU:HB2	1.97	0.64
1:E:79:ASN:ND2	1:E:94:CYS:HB2	2.11	0.64
1:F:274:LYS:HG2	1:F:436:GLU:HB2	1.78	0.64
1:B:715:ARG:NH1	1:B:715:ARG:HG3	2.13	0.64
1:D:274:LYS:HB3	1:D:432:LYS:HB3	1.79	0.64
1:D:79:ASN:ND2	1:D:94:CYS:HB2	2.12	0.64
1:B:607:ASP:HA	1:B:610:THR:HB	1.77	0.64
1:D:593:ASN:ND2	1:D:595:SER:H	1.95	0.64
1:C:527:LEU:CD1	1:C:563:GLN:HG3	2.28	0.64
1:A:196:VAL:HG12	1:A:196:VAL:O	1.98	0.64
1:C:725:ILE:HD11	1:C:730:PHE:HD1	1.63	0.64
1:F:107:ARG:HB3	1:F:112:LEU:HB2	1.80	0.64
1:F:725:ILE:HD11	1:F:730:PHE:HD1	1.63	0.64
1:C:731:ARG:HG2	1:C:756:MET:HE2	1.79	0.63
1:A:346:GLU:O	1:A:350:THR:HG23	1.97	0.63
1:A:673:THR:O	1:A:677:THR:HG23	1.98	0.63
1:F:308:GLU:HB3	1:F:312:ASN:HB2	1.81	0.63
1:A:715:ARG:HG3	1:A:715:ARG:NH1	2.13	0.63
1:F:708:ASN:N	1:F:708:ASN:HD22	1.94	0.63
1:A:488:LYS:HE2	1:A:529:GLU:OE1	1.98	0.63
1:C:103:ASN:O	1:C:107:ARG:HG3	1.99	0.63
1:D:742:ILE:HG23	1:D:743:PRO:HD2	1.81	0.63
1:B:517:PHE:CE2	1:B:716:ILE:HD13	2.34	0.63
1:C:196:VAL:HG12	1:C:196:VAL:O	1.97	0.63
1:D:107:ARG:HB3	1:D:112:LEU:HB2	1.79	0.63
1:E:103:ASN:O	1:E:107:ARG:HG3	1.99	0.63
1:C:305:LEU:HD22	1:C:354:ARG:HA	1.79	0.63
1:E:145:LYS:HB2	1:E:148:GLU:CG	2.27	0.63
1:A:742:ILE:HG23	1:A:743:PRO:HD2	1.81	0.63
1:B:145:LYS:HB2	1:B:148:GLU:CG	2.27	0.63
1:C:308:GLU:HB3	1:C:312:ASN:HB2	1.79	0.63
1:C:57:VAL:HB	1:C:75:ILE:HD11	1.80	0.63
1:D:305:LEU:HD22	1:D:354:ARG:HA	1.81	0.63
1:D:708:ASN:HD22	1:D:708:ASN:N	1.95	0.63
1:E:308:GLU:HB3	1:E:312:ASN:HB2	1.80	0.63
1:F:116:TYR:CZ	1:F:151:PRO:HA	2.34	0.63
1:F:271:LEU:HD23	1:F:482:ILE:HG13	1.81	0.63
1:C:107:ARG:HB3	1:C:112:LEU:HB2	1.79	0.63
1:D:174:LEU:N	1:D:174:LEU:HD23	2.13	0.63
1:F:174:LEU:N	1:F:174:LEU:HD23	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:305:LEU:HD22	1:F:354:ARG:HA	1.81	0.63
1:C:742:ILE:HG23	1:C:743:PRO:HD2	1.81	0.63
1:D:517:PHE:CE2	1:D:716:ILE:HD13	2.33	0.63
1:F:715:ARG:HG3	1:F:715:ARG:NH1	2.12	0.63
1:B:308:GLU:HB3	1:B:312:ASN:HB2	1.80	0.62
1:D:378:MET:HE2	1:D:381:ASN:HA	1.80	0.62
1:A:748:ASP:OD1	1:A:748:ASP:O	2.18	0.62
1:E:107:ARG:HB3	1:E:112:LEU:HB2	1.80	0.62
1:E:517:PHE:CE2	1:E:716:ILE:HD13	2.34	0.62
1:C:391:MET:HE2	1:C:434:LYS:HE3	1.81	0.62
1:A:107:ARG:HB3	1:A:112:LEU:HB2	1.80	0.62
1:A:274:LYS:HB3	1:A:432:LYS:HB3	1.82	0.62
1:A:686:ILE:HG22	1:A:704:GLN:NE2	2.15	0.62
1:B:488:LYS:HE2	1:B:529:GLU:OE1	1.99	0.62
1:B:673:THR:O	1:B:677:THR:HG23	1.99	0.62
1:B:748:ASP:O	1:B:748:ASP:OD1	2.17	0.62
1:C:715:ARG:NH1	1:C:715:ARG:HG3	2.13	0.62
1:D:748:ASP:O	1:D:748:ASP:OD1	2.18	0.62
1:F:145:LYS:HB2	1:F:148:GLU:CG	2.28	0.62
1:F:418:GLN:HA	1:F:422:GLN:NE2	2.13	0.62
1:A:174:LEU:N	1:A:174:LEU:HD23	2.14	0.62
1:B:174:LEU:N	1:B:174:LEU:HD23	2.15	0.62
1:B:731:ARG:NH1	1:B:731:ARG:HG3	2.15	0.62
1:C:731:ARG:NH1	1:C:731:ARG:HG3	2.13	0.62
1:F:673:THR:O	1:F:677:THR:HG23	1.98	0.62
1:A:377:SER:O	1:A:379:PRO:HD3	2.00	0.62
1:C:419:THR:HG23	1:C:422:GLN:CD	2.20	0.62
1:D:715:ARG:HG3	1:D:715:ARG:NH1	2.13	0.62
1:F:527:LEU:CD1	1:F:563:GLN:HG3	2.30	0.62
1:B:377:SER:O	1:B:379:PRO:HD3	2.00	0.62
1:C:748:ASP:OD1	1:C:748:ASP:O	2.18	0.62
1:E:731:ARG:NH1	1:E:731:ARG:HG3	2.14	0.62
1:C:376:ALA:HB2	1:C:420:LYS:N	2.14	0.61
1:E:540:LEU:CD1	1:E:559:LEU:HA	2.30	0.61
1:A:271:LEU:HD23	1:A:482:ILE:HG13	1.81	0.61
1:B:196:VAL:HG12	1:B:196:VAL:O	1.99	0.61
1:B:271:LEU:HD23	1:B:482:ILE:HG13	1.83	0.61
1:B:552:ASP:O	1:B:555:PHE:HB3	2.00	0.61
1:C:517:PHE:CE2	1:C:716:ILE:HD13	2.35	0.61
1:F:232:GLU:O	1:F:236:ASN:HB2	2.00	0.61
1:A:288:HIS:HB3	1:A:292:TYR:CZ	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:508:GLU:HG3	1:C:771:GLN:H	1.65	0.61
1:E:488:LYS:HE2	1:E:529:GLU:OE1	2.00	0.61
1:F:225:LEU:N	1:F:225:LEU:HD23	2.15	0.61
1:A:57:VAL:HB	1:A:75:ILE:HD11	1.82	0.61
1:B:742:ILE:HG23	1:B:743:PRO:HD2	1.81	0.61
1:C:271:LEU:HD23	1:C:482:ILE:HG13	1.81	0.61
1:C:673:THR:O	1:C:677:THR:HG23	2.00	0.61
1:F:757:ILE:HA	1:F:760:LEU:HD12	1.82	0.61
1:D:145:LYS:HB2	1:D:148:GLU:CG	2.28	0.61
1:E:552:ASP:O	1:E:555:PHE:HB3	2.01	0.61
1:F:103:ASN:O	1:F:107:ARG:HG3	2.00	0.61
1:A:234:PHE:CE2	1:A:289:ILE:HG12	2.36	0.61
1:F:295:ALA:HB2	1:F:310:PHE:HZ	1.65	0.61
1:E:686:ILE:HG22	1:E:704:GLN:NE2	2.16	0.61
1:F:196:VAL:O	1:F:196:VAL:HG12	2.00	0.61
1:F:731:ARG:HG3	1:F:731:ARG:NH1	2.14	0.61
1:A:133:TYR:CD1	1:A:189:LYS:HD2	2.36	0.61
1:A:769:ILE:HD13	1:A:774:ILE:HG23	1.83	0.61
1:D:673:THR:O	1:D:677:THR:HG23	2.01	0.61
1:A:419:THR:HG23	1:A:422:GLN:CD	2.20	0.61
1:B:593:ASN:ND2	1:B:595:SER:H	1.98	0.61
1:D:77:LYS:CE	1:D:77:LYS:H	2.13	0.61
1:F:57:VAL:HB	1:F:75:ILE:HD11	1.83	0.61
1:A:731:ARG:NH1	1:A:731:ARG:HG3	2.10	0.60
1:C:593:ASN:ND2	1:C:595:SER:H	1.97	0.60
1:D:271:LEU:HD23	1:D:482:ILE:HG13	1.82	0.60
1:B:323:ILE:HG22	1:B:324:PRO:CD	2.26	0.60
1:B:522:GLN:N	1:B:523:PRO:HD2	2.15	0.60
1:C:174:LEU:N	1:C:174:LEU:HD23	2.16	0.60
1:D:388:CYS:SG	1:D:393:ILE:HG22	2.41	0.60
1:D:757:ILE:HA	1:D:760:LEU:HD12	1.84	0.60
1:E:742:ILE:HG23	1:E:743:PRO:HD2	1.83	0.60
1:B:89:MET:CE	1:B:100:VAL:HG13	2.32	0.60
1:C:522:GLN:N	1:C:523:PRO:HD2	2.16	0.60
1:E:174:LEU:HD23	1:E:174:LEU:N	2.16	0.60
1:E:664:LYS:O	1:E:668:THR:HG23	2.00	0.60
1:E:731:ARG:HG2	1:E:756:MET:HE2	1.82	0.60
1:E:769:ILE:HD13	1:E:774:ILE:HG23	1.82	0.60
1:A:323:ILE:HG22	1:A:324:PRO:CD	2.26	0.60
1:A:593:ASN:ND2	1:A:595:SER:H	1.98	0.60
1:B:288:HIS:HB3	1:B:292:TYR:CZ	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:391:MET:HG2	1:D:434:LYS:NZ	2.16	0.60
1:E:225:LEU:N	1:E:225:LEU:HD23	2.16	0.60
1:E:673:THR:O	1:E:677:THR:HG23	2.01	0.60
1:A:522:GLN:N	1:A:523:PRO:HD2	2.15	0.60
1:C:664:LYS:O	1:C:668:THR:HG23	2.02	0.60
1:A:376:ALA:HB2	1:A:420:LYS:N	2.16	0.60
1:D:225:LEU:N	1:D:225:LEU:HD23	2.15	0.60
1:A:382:THR:O	1:A:385:GLN:HB2	2.02	0.60
1:B:418:GLN:HA	1:B:422:GLN:HE21	1.66	0.60
1:B:686:ILE:HG22	1:B:704:GLN:NE2	2.16	0.60
1:E:288:HIS:HB3	1:E:292:TYR:CZ	2.36	0.60
1:E:305:LEU:HD22	1:E:354:ARG:HA	1.82	0.60
1:E:377:SER:O	1:E:379:PRO:HD3	2.01	0.60
1:E:57:VAL:HB	1:E:75:ILE:HD11	1.83	0.60
1:E:757:ILE:HA	1:E:760:LEU:HD12	1.84	0.60
1:F:133:TYR:CD1	1:F:189:LYS:HD2	2.36	0.60
1:A:285:ARG:HB2	1:A:291:TYR:CZ	2.37	0.60
1:B:419:THR:HG23	1:B:422:GLN:CD	2.22	0.60
1:B:376:ALA:HB2	1:B:420:LYS:N	2.17	0.60
1:D:664:LYS:O	1:D:668:THR:HG23	2.02	0.60
1:F:696:LEU:CD2	1:F:701:VAL:HG21	2.28	0.60
1:B:77:LYS:CE	1:B:77:LYS:H	2.15	0.60
1:C:77:LYS:CE	1:C:77:LYS:H	2.14	0.60
1:E:593:ASN:ND2	1:E:595:SER:H	1.98	0.60
1:F:664:LYS:O	1:F:668:THR:HG23	2.02	0.60
1:C:288:HIS:HB3	1:C:292:TYR:CZ	2.36	0.60
1:C:391:MET:HG2	1:C:434:LYS:NZ	2.16	0.60
1:D:234:PHE:CE2	1:D:289:ILE:HG12	2.37	0.60
1:D:419:THR:HG23	1:D:422:GLN:CD	2.22	0.60
1:D:593:ASN:C	1:D:593:ASN:HD22	2.04	0.60
1:E:527:LEU:CD1	1:E:563:GLN:HG3	2.31	0.60
1:E:80:PRO:HD2	1:E:83:PHE:CE2	2.37	0.60
1:F:171:GLN:OE1	1:F:678:ASN:HB3	2.02	0.60
1:A:751:GLN:OE1	1:C:692:ARG:CZ	2.50	0.59
1:B:225:LEU:HD23	1:B:225:LEU:N	2.16	0.59
1:E:391:MET:HG2	1:E:434:LYS:NZ	2.17	0.59
1:A:508:GLU:HG3	1:A:771:GLN:H	1.66	0.59
1:B:664:LYS:O	1:B:668:THR:HG23	2.02	0.59
1:F:144:LYS:HG3	1:F:149:MET:HG3	1.83	0.59
1:F:517:PHE:CE1	1:F:716:ILE:HD13	2.37	0.59
1:A:731:ARG:HG2	1:A:756:MET:HE2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ASP:O	1:A:91:GLU:HB2	2.02	0.59
1:F:403:LEU:O	1:F:404:THR:HG23	2.02	0.59
1:F:77:LYS:H	1:F:77:LYS:CE	2.14	0.59
1:B:382:THR:O	1:B:385:GLN:HB2	2.02	0.59
1:F:508:GLU:HG3	1:F:771:GLN:H	1.68	0.59
1:D:288:HIS:HB3	1:D:292:TYR:CZ	2.38	0.59
1:A:552:ASP:O	1:A:555:PHE:HB3	2.02	0.59
1:B:234:PHE:CE2	1:B:289:ILE:HG12	2.38	0.59
1:B:696:LEU:CD2	1:B:701:VAL:HG21	2.30	0.59
1:B:767:TYR:O	1:B:768:ARG:NH1	2.35	0.59
1:C:285:ARG:HB2	1:C:291:TYR:CZ	2.37	0.59
1:C:323:ILE:HG22	1:C:324:PRO:CD	2.26	0.59
1:D:696:LEU:CD2	1:D:701:VAL:HG21	2.30	0.59
1:F:488:LYS:HE2	1:F:529:GLU:OE1	2.03	0.59
1:F:767:TYR:O	1:F:768:ARG:NH1	2.36	0.59
1:A:136:LYS:O	1:A:139:ASP:HB2	2.03	0.59
1:A:757:ILE:HG12	1:A:762:LEU:HD12	1.85	0.59
1:C:378:MET:HE2	1:C:381:ASN:HA	1.83	0.59
1:D:171:GLN:OE1	1:D:678:ASN:HB3	2.02	0.59
1:D:377:SER:O	1:D:379:PRO:HD3	2.02	0.59
1:E:271:LEU:HD23	1:E:482:ILE:HG13	1.83	0.59
1:F:552:ASP:O	1:F:555:PHE:HB3	2.02	0.59
1:D:522:GLN:N	1:D:523:PRO:HD2	2.17	0.59
1:E:535:PRO:HB2	1:E:540:LEU:HD21	1.84	0.59
1:E:80:PRO:HD2	1:E:83:PHE:CD2	2.38	0.59
1:C:710:VAL:O	1:C:714:ILE:HG13	2.03	0.59
1:E:376:ALA:HB2	1:E:420:LYS:N	2.18	0.59
1:C:133:TYR:CD1	1:C:189:LYS:HD2	2.37	0.59
1:C:377:SER:O	1:C:379:PRO:HD3	2.02	0.59
1:C:593:ASN:HD22	1:C:593:ASN:C	2.05	0.59
1:E:61:LEU:O	1:E:65:GLY:HA2	2.03	0.59
1:E:77:LYS:H	1:E:77:LYS:CE	2.15	0.59
1:F:593:ASN:ND2	1:F:595:SER:H	2.00	0.59
1:B:419:THR:N	1:B:422:GLN:HG3	2.18	0.58
1:B:606:ASN:HB3	1:B:609:VAL:CG1	2.33	0.58
1:B:80:PRO:HD2	1:B:83:PHE:CD2	2.38	0.58
1:D:535:PRO:HB2	1:D:540:LEU:HD21	1.84	0.58
1:D:540:LEU:CD1	1:D:559:LEU:HA	2.33	0.58
1:E:136:LYS:O	1:E:139:ASP:HB2	2.04	0.58
1:C:225:LEU:N	1:C:225:LEU:HD23	2.17	0.58
1:D:152:HIS:O	1:D:156:ILE:HD12	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:368:LYS:O	1:F:376:ALA:HA	2.03	0.58
1:B:757:ILE:HA	1:B:760:LEU:HD12	1.86	0.58
1:C:89:MET:CE	1:C:100:VAL:HG13	2.33	0.58
1:C:544:GLU:HG3	1:C:555:PHE:CB	2.31	0.58
1:E:522:GLN:N	1:E:523:PRO:HD2	2.18	0.58
1:B:757:ILE:HG12	1:B:762:LEU:HD12	1.85	0.58
1:E:144:LYS:HG3	1:E:149:MET:HG3	1.85	0.58
1:A:225:LEU:N	1:A:225:LEU:HD23	2.17	0.58
1:A:606:ASN:HB3	1:A:609:VAL:CG1	2.32	0.58
1:D:349:GLN:O	1:D:353:LEU:HG	2.03	0.58
1:E:696:LEU:CD2	1:E:701:VAL:HG21	2.29	0.58
1:A:403:LEU:O	1:A:404:THR:HG23	2.03	0.58
1:A:391:MET:HG2	1:A:434:LYS:NZ	2.17	0.58
1:D:382:THR:O	1:D:385:GLN:HB2	2.03	0.58
1:A:77:LYS:HZ2	1:A:77:LYS:H	1.52	0.58
1:B:769:ILE:HD13	1:B:774:ILE:HG23	1.85	0.58
1:B:508:GLU:HG3	1:B:771:GLN:H	1.69	0.58
1:C:757:ILE:HA	1:C:760:LEU:HD12	1.85	0.58
1:F:288:HIS:HB3	1:F:292:TYR:CZ	2.39	0.58
1:F:593:ASN:HD22	1:F:593:ASN:C	2.06	0.58
1:A:593:ASN:C	1:A:593:ASN:HD22	2.06	0.58
1:E:133:TYR:CD1	1:E:189:LYS:HD2	2.38	0.58
1:E:285:ARG:HB2	1:E:291:TYR:CZ	2.39	0.58
1:F:61:LEU:O	1:F:65:GLY:HA2	2.04	0.58
1:A:368:LYS:O	1:A:376:ALA:HA	2.04	0.58
1:B:538:LEU:HD12	1:B:664:LYS:HD2	1.85	0.58
1:C:368:LYS:O	1:C:376:ALA:HA	2.04	0.58
1:D:295:ALA:HB2	1:D:310:PHE:HZ	1.69	0.58
1:E:196:VAL:O	1:E:196:VAL:HG12	2.02	0.58
1:F:544:GLU:HG3	1:F:555:PHE:CB	2.33	0.58
1:F:88:ASP:O	1:F:91:GLU:HB2	2.04	0.58
1:A:517:PHE:CE2	1:A:716:ILE:HD13	2.39	0.58
1:B:133:TYR:CD1	1:B:189:LYS:HD2	2.39	0.58
1:D:376:ALA:HB2	1:D:420:LYS:N	2.17	0.58
1:D:418:GLN:HA	1:D:422:GLN:HE21	1.68	0.58
1:E:234:PHE:CE2	1:E:289:ILE:HG12	2.39	0.58
1:E:418:GLN:HA	1:E:422:GLN:HE21	1.68	0.58
1:E:593:ASN:C	1:E:593:ASN:HD22	2.07	0.58
1:A:80:PRO:HD2	1:A:83:PHE:CD2	2.39	0.57
1:C:144:LYS:HG3	1:C:149:MET:HG3	1.86	0.57
1:D:88:ASP:O	1:D:91:GLU:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:606:ASN:HB3	1:E:609:VAL:CG1	2.33	0.57
1:F:391:MET:HG2	1:F:434:LYS:NZ	2.19	0.57
1:A:295:ALA:HB2	1:A:310:PHE:HZ	1.68	0.57
1:A:538:LEU:HD12	1:A:664:LYS:HD2	1.86	0.57
1:A:544:GLU:HG3	1:A:555:PHE:CB	2.32	0.57
1:B:80:PRO:HD2	1:B:83:PHE:CE2	2.39	0.57
1:C:382:THR:O	1:C:385:GLN:HB2	2.04	0.57
1:C:80:PRO:HD2	1:C:83:PHE:CD2	2.39	0.57
1:E:594:ALA:HA	1:E:597:TRP:CD1	2.39	0.57
1:F:606:ASN:HB3	1:F:609:VAL:CG1	2.34	0.57
1:B:288:HIS:HB3	1:B:292:TYR:CE1	2.39	0.57
1:B:171:GLN:OE1	1:B:678:ASN:HB3	2.04	0.57
1:C:418:GLN:HA	1:C:422:GLN:HE21	1.68	0.57
1:D:144:LYS:HG3	1:D:149:MET:HG3	1.86	0.57
1:D:57:VAL:HB	1:D:75:ILE:HD11	1.83	0.57
1:A:144:LYS:HG3	1:A:149:MET:HG3	1.84	0.57
1:B:725:ILE:HD11	1:B:730:PHE:CD1	2.39	0.57
1:B:88:ASP:O	1:B:91:GLU:HB2	2.04	0.57
1:D:391:MET:HE2	1:D:434:LYS:HE3	1.86	0.57
1:D:606:ASN:HB3	1:D:609:VAL:CG1	2.35	0.57
1:E:702:LEU:O	1:E:706:ARG:HG3	2.05	0.57
1:A:80:PRO:HD2	1:A:83:PHE:CE2	2.38	0.57
1:C:295:ALA:HB2	1:C:310:PHE:HZ	1.68	0.57
1:C:552:ASP:O	1:C:555:PHE:HB3	2.04	0.57
1:D:41:LYS:HB2	1:D:42:HIS:CE1	2.39	0.57
1:F:377:SER:O	1:F:379:PRO:HD3	2.04	0.57
1:E:295:ALA:HB2	1:E:310:PHE:HZ	1.70	0.57
1:E:178:GLU:OE2	1:E:686:ILE:HG21	2.05	0.57
1:A:288:HIS:HB3	1:A:292:TYR:CE1	2.40	0.57
1:D:725:ILE:HD11	1:D:730:PHE:CD1	2.40	0.57
1:D:767:TYR:O	1:D:768:ARG:NH1	2.37	0.57
1:F:80:PRO:HD2	1:F:83:PHE:CD2	2.40	0.57
1:B:540:LEU:HD12	1:B:559:LEU:HD12	1.87	0.57
1:B:710:VAL:O	1:B:714:ILE:HG13	2.04	0.57
1:C:61:LEU:O	1:C:65:GLY:HA2	2.05	0.57
1:C:79:ASN:HD21	1:C:94:CYS:HB2	1.70	0.57
1:E:368:LYS:O	1:E:376:ALA:HA	2.05	0.57
1:E:544:GLU:HG3	1:E:555:PHE:CB	2.34	0.57
1:B:368:LYS:O	1:B:376:ALA:HA	2.05	0.57
1:B:61:LEU:O	1:B:65:GLY:HA2	2.04	0.57
1:D:552:ASP:O	1:D:555:PHE:HB3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:738:ALA:O	1:D:741:ALA:CB	2.53	0.57
1:F:418:GLN:HA	1:F:422:GLN:HE21	1.70	0.57
1:F:522:GLN:N	1:F:523:PRO:HD2	2.19	0.57
1:A:361:GLN:HG2	1:A:386:LYS:HB2	1.87	0.57
1:D:86:VAL:HG23	1:D:103:ASN:ND2	2.20	0.57
1:E:419:THR:HG23	1:E:422:GLN:CD	2.25	0.57
1:E:538:LEU:HD12	1:E:664:LYS:HD2	1.87	0.57
1:E:79:ASN:HD21	1:E:94:CYS:HB2	1.70	0.57
1:F:89:MET:CE	1:F:100:VAL:HG13	2.35	0.57
1:F:382:THR:O	1:F:385:GLN:HB2	2.04	0.57
1:A:171:GLN:OE1	1:A:678:ASN:HB3	2.05	0.56
1:B:391:MET:HG2	1:B:434:LYS:NZ	2.18	0.56
1:C:403:LEU:O	1:C:404:THR:HG23	2.05	0.56
1:E:376:ALA:O	1:E:403:LEU:HD22	2.05	0.56
1:E:278:ILE:HD13	1:E:432:LYS:HD3	1.87	0.56
1:E:743:PRO:HD2	1:E:747:MET:HG2	1.87	0.56
1:E:767:TYR:O	1:E:768:ARG:NH1	2.36	0.56
1:F:742:ILE:HG23	1:F:743:PRO:HD2	1.86	0.56
1:A:767:TYR:O	1:A:768:ARG:NH1	2.36	0.56
1:C:738:ALA:O	1:C:741:ALA:CB	2.53	0.56
1:D:288:HIS:HB3	1:D:292:TYR:CE1	2.40	0.56
1:D:80:PRO:HD2	1:D:83:PHE:CD2	2.40	0.56
1:E:403:LEU:O	1:E:404:THR:HG23	2.05	0.56
1:E:725:ILE:HD11	1:E:730:PHE:CD1	2.39	0.56
1:E:508:GLU:HG3	1:E:771:GLN:H	1.70	0.56
1:F:757:ILE:HG23	1:F:762:LEU:HB2	1.87	0.56
1:A:256:PHE:O	1:A:458:ALA:HB3	2.05	0.56
1:C:136:LYS:O	1:C:139:ASP:HB2	2.05	0.56
1:E:323:ILE:HG23	1:E:324:PRO:CD	2.12	0.56
1:C:686:ILE:HG22	1:C:704:GLN:HE22	1.71	0.56
1:C:77:LYS:HZ2	1:C:77:LYS:H	1.53	0.56
1:D:133:TYR:CD1	1:D:189:LYS:HD2	2.40	0.56
1:D:323:ILE:HG22	1:D:324:PRO:CD	2.26	0.56
1:D:731:ARG:HG2	1:D:756:MET:HE2	1.87	0.56
1:E:70:LEU:HD12	1:E:71:SER:O	2.06	0.56
1:A:738:ALA:O	1:A:741:ALA:CB	2.53	0.56
1:B:144:LYS:HG3	1:B:149:MET:HG3	1.88	0.56
1:B:295:ALA:HB2	1:B:310:PHE:HZ	1.69	0.56
1:B:391:MET:HE2	1:B:434:LYS:HE3	1.87	0.56
1:B:41:LYS:HB2	1:B:42:HIS:CE1	2.41	0.56
1:C:540:LEU:HD12	1:C:559:LEU:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:540:LEU:HD21	1:C:562:GLU:HG3	1.87	0.56
1:B:738:ALA:O	1:B:741:ALA:CB	2.53	0.56
1:A:540:LEU:HD21	1:A:562:GLU:HG3	1.87	0.56
1:B:361:GLN:HG2	1:B:386:LYS:HB2	1.87	0.56
1:B:731:ARG:HG2	1:B:756:MET:HE2	1.86	0.56
1:C:88:ASP:O	1:C:91:GLU:HB2	2.05	0.56
1:D:710:VAL:O	1:D:714:ILE:HG13	2.06	0.56
1:E:288:HIS:HB3	1:E:292:TYR:CE1	2.41	0.56
1:F:308:GLU:HB2	1:F:313:TYR:CZ	2.41	0.56
1:A:89:MET:CE	1:A:100:VAL:HG13	2.36	0.56
1:A:108:TYR:CD2	1:A:696:LEU:HD12	2.40	0.56
1:B:278:ILE:HD13	1:B:432:LYS:HD3	1.87	0.56
1:D:256:PHE:O	1:D:458:ALA:HB3	2.04	0.56
1:D:544:GLU:HG3	1:D:555:PHE:CB	2.33	0.56
1:E:382:THR:O	1:E:385:GLN:HB2	2.04	0.56
1:E:88:ASP:O	1:E:91:GLU:HB2	2.06	0.56
1:F:748:ASP:O	1:F:748:ASP:OD1	2.24	0.56
1:F:80:PRO:HD2	1:F:83:PHE:CE2	2.40	0.56
1:A:41:LYS:HB2	1:A:42:HIS:CE1	2.40	0.56
1:B:403:LEU:O	1:B:404:THR:HG23	2.05	0.56
1:D:361:GLN:HG2	1:D:386:LYS:HB2	1.88	0.56
1:F:285:ARG:HB2	1:F:291:TYR:CZ	2.41	0.56
1:F:77:LYS:H	1:F:77:LYS:HZ2	1.54	0.56
1:A:664:LYS:O	1:A:668:THR:HG23	2.05	0.56
1:A:70:LEU:HD12	1:A:71:SER:O	2.06	0.56
1:C:80:PRO:HD2	1:C:83:PHE:CE2	2.40	0.56
1:E:41:LYS:HB2	1:E:42:HIS:CE1	2.41	0.56
1:C:278:ILE:HD13	1:C:432:LYS:HD3	1.88	0.56
1:E:308:GLU:HB2	1:E:313:TYR:CZ	2.41	0.56
1:E:563:GLN:O	1:E:565:ASN:N	2.39	0.56
1:E:171:GLN:OE1	1:E:678:ASN:HB3	2.05	0.56
1:F:41:LYS:HB2	1:F:42:HIS:CE1	2.41	0.56
1:A:308:GLU:HB2	1:A:313:TYR:CZ	2.41	0.55
1:A:710:VAL:O	1:A:714:ILE:HG13	2.05	0.55
1:A:757:ILE:HA	1:A:760:LEU:HD12	1.88	0.55
1:C:725:ILE:HD11	1:C:730:PHE:CD1	2.42	0.55
1:D:80:PRO:HD2	1:D:83:PHE:CE2	2.42	0.55
1:F:419:THR:HG23	1:F:422:GLN:CD	2.26	0.55
1:F:594:ALA:HA	1:F:597:TRP:CD1	2.42	0.55
1:F:743:PRO:CD	1:F:747:MET:SD	2.95	0.55
1:B:301:MET:HA	1:B:304:ASP:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:517:PHE:CZ	1:B:716:ILE:HD13	2.41	0.55
1:E:361:GLN:HG2	1:E:386:LYS:HB2	1.88	0.55
1:E:757:ILE:HG12	1:E:762:LEU:HD12	1.87	0.55
1:A:61:LEU:O	1:A:65:GLY:HA2	2.06	0.55
1:C:41:LYS:HB2	1:C:42:HIS:CE1	2.42	0.55
1:D:301:MET:HA	1:D:304:ASP:HB3	1.89	0.55
1:D:61:LEU:O	1:D:65:GLY:HA2	2.07	0.55
1:E:89:MET:CE	1:E:100:VAL:HG13	2.37	0.55
1:F:540:LEU:HD21	1:F:562:GLU:HG3	1.88	0.55
1:F:690:GLU:HG2	1:F:692:ARG:NH2	2.22	0.55
1:A:349:GLN:O	1:A:353:LEU:HG	2.06	0.55
1:B:79:ASN:HD21	1:B:94:CYS:HB2	1.71	0.55
1:D:97:GLU:HA	1:D:711:LEU:HD11	1.88	0.55
1:E:349:GLN:O	1:E:353:LEU:HG	2.06	0.55
1:B:327:GLN:O	1:B:330:GLU:HB2	2.07	0.55
1:C:152:HIS:O	1:C:156:ILE:HD12	2.07	0.55
1:C:308:GLU:HB2	1:C:313:TYR:CZ	2.42	0.55
1:C:696:LEU:CD2	1:C:701:VAL:HG21	2.33	0.55
1:A:70:LEU:HD13	1:A:74:ASP:HB2	1.88	0.55
1:B:544:GLU:HG3	1:B:555:PHE:CB	2.34	0.55
1:C:757:ILE:HG12	1:C:762:LEU:HD12	1.87	0.55
1:D:419:THR:N	1:D:422:GLN:HG3	2.19	0.55
1:A:86:VAL:HG23	1:A:103:ASN:ND2	2.22	0.55
1:B:285:ARG:HB2	1:B:291:TYR:CZ	2.42	0.55
1:B:95:LEU:HD11	1:B:714:ILE:HG21	1.89	0.55
1:C:234:PHE:CE2	1:C:289:ILE:HG12	2.42	0.55
1:C:594:ALA:HA	1:C:597:TRP:CD1	2.41	0.55
1:D:285:ARG:HB2	1:D:291:TYR:CZ	2.41	0.55
1:F:70:LEU:HD12	1:F:71:SER:O	2.06	0.55
1:F:79:ASN:HD21	1:F:94:CYS:HB2	1.70	0.55
1:B:108:TYR:CD2	1:B:696:LEU:HD12	2.42	0.55
1:D:178:GLU:OE2	1:D:686:ILE:HG21	2.07	0.55
1:D:403:LEU:O	1:D:404:THR:HG23	2.07	0.55
1:A:278:ILE:HD13	1:A:432:LYS:HD3	1.89	0.55
1:B:594:ALA:HA	1:B:597:TRP:CD1	2.42	0.55
1:C:702:LEU:O	1:C:706:ARG:HG3	2.07	0.55
1:F:535:PRO:HB2	1:F:540:LEU:HD21	1.88	0.55
1:F:540:LEU:HD12	1:F:559:LEU:HD12	1.89	0.55
1:A:702:LEU:O	1:A:706:ARG:HG3	2.06	0.55
1:B:376:ALA:O	1:B:403:LEU:HD22	2.07	0.55
1:C:171:GLN:OE1	1:C:678:ASN:HB3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:757:ILE:HG23	1:E:762:LEU:HB2	1.88	0.55
1:F:349:GLN:O	1:F:353:LEU:HG	2.08	0.55
1:A:418:GLN:HA	1:A:422:GLN:HE21	1.70	0.54
1:A:725:ILE:HD11	1:A:730:PHE:CD1	2.40	0.54
1:B:308:GLU:HB2	1:B:313:TYR:CZ	2.42	0.54
1:B:540:LEU:HD21	1:B:562:GLU:HG3	1.88	0.54
1:B:77:LYS:HZ2	1:B:77:LYS:H	1.53	0.54
1:B:593:ASN:C	1:B:593:ASN:HD22	2.10	0.54
1:C:538:LEU:HD12	1:C:664:LYS:HD2	1.89	0.54
1:D:243:ASP:OD2	1:D:324:PRO:HG3	2.07	0.54
1:F:136:LYS:O	1:F:139:ASP:HB2	2.07	0.54
1:F:731:ARG:HG2	1:F:756:MET:HE2	1.89	0.54
1:F:757:ILE:HG12	1:F:762:LEU:HD12	1.88	0.54
1:B:136:LYS:O	1:B:139:ASP:HB2	2.07	0.54
1:C:301:MET:HA	1:C:304:ASP:HB3	1.89	0.54
1:E:725:ILE:O	1:E:773:LYS:HB2	2.07	0.54
1:D:368:LYS:O	1:D:376:ALA:HA	2.08	0.54
1:D:757:ILE:HG12	1:D:762:LEU:HD12	1.89	0.54
1:F:710:VAL:O	1:F:714:ILE:HG13	2.06	0.54
1:A:97:GLU:HA	1:A:711:LEU:HD11	1.89	0.54
1:B:349:GLN:O	1:B:353:LEU:HG	2.06	0.54
1:C:535:PRO:HB2	1:C:540:LEU:HD21	1.89	0.54
1:C:97:GLU:HA	1:C:711:LEU:HD11	1.89	0.54
1:D:136:LYS:O	1:D:139:ASP:HB2	2.07	0.54
1:D:508:GLU:HG3	1:D:771:GLN:H	1.71	0.54
1:E:86:VAL:HG23	1:E:103:ASN:ND2	2.22	0.54
1:E:70:LEU:HD13	1:E:74:ASP:HB2	1.90	0.54
1:A:37:VAL:HG11	1:A:59:VAL:HG21	1.90	0.54
1:B:286:THR:OG1	1:B:287:PHE:N	2.40	0.54
1:D:308:GLU:HB2	1:D:313:TYR:CZ	2.42	0.54
1:E:243:ASP:OD2	1:E:324:PRO:HG3	2.08	0.54
1:F:391:MET:HE2	1:F:434:LYS:HE3	1.89	0.54
1:F:117:SER:HB2	1:F:714:ILE:HD11	1.89	0.54
1:B:535:PRO:HB2	1:B:540:LEU:HD21	1.89	0.54
1:B:757:ILE:HG23	1:B:762:LEU:HB2	1.88	0.54
1:C:286:THR:OG1	1:C:287:PHE:N	2.40	0.54
1:C:606:ASN:HB3	1:C:609:VAL:CG1	2.38	0.54
1:D:77:LYS:H	1:D:77:LYS:HZ2	1.54	0.54
1:F:702:LEU:O	1:F:706:ARG:HG3	2.07	0.54
1:A:152:HIS:O	1:A:156:ILE:HD12	2.07	0.54
1:B:256:PHE:O	1:B:458:ALA:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:LEU:HD13	1:B:74:ASP:HB2	1.89	0.54
1:B:748:ASP:C	1:B:748:ASP:OD1	2.46	0.54
1:C:391:MET:HE2	1:C:434:LYS:CE	2.38	0.54
1:D:89:MET:CE	1:D:100:VAL:HG13	2.37	0.54
1:E:517:PHE:CZ	1:E:716:ILE:HD13	2.43	0.54
1:E:743:PRO:HD2	1:E:747:MET:CG	2.38	0.54
1:F:278:ILE:HD13	1:F:432:LYS:HD3	1.88	0.54
1:F:686:ILE:HG22	1:F:704:GLN:HE22	1.72	0.54
1:B:742:ILE:HD11	1:B:752:ALA:C	2.28	0.54
1:D:79:ASN:HD21	1:D:94:CYS:HB2	1.72	0.54
1:E:499:ILE:HG22	1:E:500:LEU:N	2.22	0.54
1:F:301:MET:HA	1:F:304:ASP:HB3	1.90	0.54
1:A:757:ILE:HG23	1:A:762:LEU:HB2	1.90	0.54
1:C:269:THR:HG23	1:C:443:LEU:HD22	1.90	0.54
1:C:767:TYR:O	1:C:768:ARG:NH1	2.38	0.54
1:D:378:MET:CE	1:D:381:ASN:HA	2.38	0.54
1:E:180:GLY:C	1:E:686:ILE:HD12	2.27	0.54
1:A:594:ALA:HA	1:A:597:TRP:CD1	2.43	0.53
1:A:751:GLN:NE2	1:C:692:ARG:NH2	2.40	0.53
1:D:748:ASP:C	1:D:748:ASP:OD1	2.46	0.53
1:E:540:LEU:HD12	1:E:559:LEU:HD12	1.88	0.53
1:F:85:LYS:HE2	1:F:110:SER:OG	2.07	0.53
1:A:540:LEU:HD12	1:A:559:LEU:HD12	1.90	0.53
1:D:278:ILE:HD13	1:D:432:LYS:HD3	1.89	0.53
1:E:535:PRO:HB2	1:E:540:LEU:CD2	2.39	0.53
1:F:86:VAL:HG23	1:F:103:ASN:ND2	2.23	0.53
1:F:725:ILE:HD11	1:F:730:PHE:CD1	2.42	0.53
1:A:79:ASN:HD21	1:A:94:CYS:HB2	1.71	0.53
1:B:97:GLU:HA	1:B:711:LEU:HD11	1.90	0.53
1:B:743:PRO:HD2	1:B:747:MET:HG2	1.90	0.53
1:C:563:GLN:O	1:C:565:ASN:N	2.41	0.53
1:C:108:TYR:CD2	1:C:696:LEU:HD12	2.43	0.53
1:C:748:ASP:OD1	1:C:748:ASP:C	2.46	0.53
1:D:72:LYS:HA	1:D:75:ILE:CD1	2.38	0.53
1:E:419:THR:N	1:E:422:GLN:HG3	2.20	0.53
1:F:361:GLN:HG2	1:F:386:LYS:HB2	1.90	0.53
1:F:563:GLN:O	1:F:565:ASN:N	2.41	0.53
1:F:538:LEU:HD12	1:F:664:LYS:HD2	1.90	0.53
1:F:748:ASP:OD1	1:F:748:ASP:C	2.47	0.53
1:A:563:GLN:O	1:A:565:ASN:N	2.41	0.53
1:B:70:LEU:HD12	1:B:71:SER:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:VAL:HG22	1:C:36:TRP:H	1.74	0.53
1:C:70:LEU:HD12	1:C:71:SER:O	2.08	0.53
1:D:173:ILE:C	1:D:174:LEU:HD23	2.28	0.53
1:D:563:GLN:O	1:D:565:ASN:N	2.41	0.53
1:F:256:PHE:O	1:F:458:ALA:HB3	2.07	0.53
1:F:97:GLU:HA	1:F:711:LEU:HD11	1.90	0.53
1:A:743:PRO:HD2	1:A:747:MET:HG2	1.90	0.53
1:A:77:LYS:NZ	1:A:77:LYS:H	2.06	0.53
1:B:37:VAL:HG11	1:B:59:VAL:HG21	1.90	0.53
1:C:86:VAL:HG23	1:C:103:ASN:ND2	2.24	0.53
1:C:349:GLN:O	1:C:353:LEU:HG	2.08	0.53
1:C:419:THR:HG23	1:C:422:GLN:CG	2.39	0.53
1:D:510:ILE:HD12	1:D:768:ARG:HB3	1.89	0.53
1:D:517:PHE:CZ	1:D:716:ILE:HD13	2.43	0.53
1:D:725:ILE:O	1:D:773:LYS:HB2	2.08	0.53
1:E:97:GLU:HA	1:E:711:LEU:HD11	1.90	0.53
1:E:738:ALA:O	1:E:741:ALA:CB	2.57	0.53
1:F:173:ILE:C	1:F:174:LEU:HD23	2.28	0.53
1:F:35:VAL:HG22	1:F:36:TRP:H	1.73	0.53
1:A:72:LYS:HA	1:A:75:ILE:CD1	2.39	0.53
1:E:391:MET:HE2	1:E:434:LYS:HE3	1.89	0.53
1:E:748:ASP:OD1	1:E:748:ASP:O	2.26	0.53
1:F:152:HIS:O	1:F:156:ILE:HD12	2.09	0.53
1:A:419:THR:N	1:A:422:GLN:HG3	2.21	0.53
1:A:180:GLY:C	1:A:686:ILE:HD12	2.28	0.53
1:B:303:ASN:HD22	1:B:304:ASP:N	2.07	0.53
1:C:743:PRO:CD	1:C:747:MET:SD	2.97	0.53
1:C:36:TRP:CE2	1:C:78:MET:HG2	2.44	0.53
1:D:281:ALA:O	1:D:318:ASN:ND2	2.41	0.53
1:D:743:PRO:CD	1:D:747:MET:SD	2.97	0.53
1:E:556:VAL:HG21	1:E:579:THR:CA	2.39	0.53
1:F:376:ALA:O	1:F:403:LEU:HD22	2.09	0.53
1:F:419:THR:N	1:F:422:GLN:HG3	2.23	0.53
1:A:743:PRO:CD	1:A:747:MET:SD	2.97	0.53
1:B:743:PRO:CD	1:B:747:MET:SD	2.97	0.53
1:B:86:VAL:HG23	1:B:103:ASN:ND2	2.24	0.53
1:C:361:GLN:HG2	1:C:386:LYS:HB2	1.91	0.53
1:D:196:VAL:O	1:D:196:VAL:CG1	2.57	0.53
1:F:295:ALA:HB2	1:F:310:PHE:CZ	2.44	0.53
1:F:499:ILE:HG22	1:F:500:LEU:N	2.23	0.53
1:A:243:ASP:OD2	1:A:324:PRO:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:748:ASP:C	1:A:748:ASP:OD1	2.46	0.53
1:B:178:GLU:OE2	1:B:686:ILE:HG21	2.09	0.53
1:C:85:LYS:HE2	1:C:110:SER:OG	2.08	0.53
1:C:180:GLY:C	1:C:686:ILE:HD12	2.30	0.53
1:C:226:GLN:HB2	1:C:342:MET:HE2	1.90	0.53
1:C:288:HIS:HB3	1:C:292:TYR:CE1	2.44	0.53
1:C:303:ASN:HD22	1:C:304:ASP:N	2.07	0.53
1:C:376:ALA:O	1:C:403:LEU:HD22	2.08	0.53
1:C:743:PRO:HD2	1:C:747:MET:HG2	1.90	0.53
1:D:743:PRO:HD2	1:D:747:MET:HG2	1.90	0.53
1:E:152:HIS:O	1:E:156:ILE:HD12	2.09	0.53
1:E:502:GLN:O	1:E:505:TYR:HB2	2.09	0.53
1:E:556:VAL:HG21	1:E:579:THR:HA	1.91	0.53
1:F:725:ILE:O	1:F:773:LYS:HB2	2.09	0.53
1:A:742:ILE:HD11	1:A:752:ALA:C	2.29	0.52
1:D:565:ASN:O	1:D:566:HIS:C	2.48	0.52
1:B:419:THR:H	1:B:422:GLN:NE2	2.06	0.52
1:B:563:GLN:O	1:B:565:ASN:N	2.41	0.52
1:B:702:LEU:O	1:B:706:ARG:HG3	2.10	0.52
1:B:738:ALA:CB	1:B:741:ALA:HB2	2.39	0.52
1:F:742:ILE:HD11	1:F:752:ALA:C	2.29	0.52
1:A:303:ASN:HD22	1:A:304:ASP:N	2.07	0.52
1:A:419:THR:HG23	1:A:422:GLN:CG	2.39	0.52
1:A:391:MET:HE2	1:A:434:LYS:HE3	1.91	0.52
1:D:738:ALA:CB	1:D:741:ALA:HB2	2.39	0.52
1:F:238:LYS:NZ	1:F:283:ASP:O	2.42	0.52
1:F:108:TYR:CD2	1:F:696:LEU:HD12	2.44	0.52
1:F:743:PRO:HD2	1:F:747:MET:CG	2.40	0.52
1:A:161:TYR:O	1:A:164:MET:HB3	2.09	0.52
1:A:499:ILE:HG22	1:A:500:LEU:N	2.25	0.52
1:B:85:LYS:HE2	1:B:110:SER:OG	2.10	0.52
1:B:180:GLY:C	1:B:686:ILE:HD12	2.29	0.52
1:C:243:ASP:OD2	1:C:324:PRO:HG3	2.09	0.52
1:F:288:HIS:HB3	1:F:292:TYR:CE1	2.44	0.52
1:B:565:ASN:O	1:B:566:HIS:C	2.48	0.52
1:D:540:LEU:HD21	1:D:562:GLU:HG3	1.92	0.52
1:F:161:TYR:O	1:F:164:MET:HB3	2.09	0.52
1:A:376:ALA:O	1:A:403:LEU:HD22	2.10	0.52
1:B:746:PHE:HD1	1:C:389:HIS:CD2	2.28	0.52
1:C:565:ASN:O	1:C:566:HIS:C	2.48	0.52
1:D:70:LEU:HD12	1:D:71:SER:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:378:MET:CE	1:E:381:ASN:HA	2.39	0.52
1:F:517:PHE:CZ	1:F:716:ILE:HD13	2.44	0.52
1:A:327:GLN:O	1:A:330:GLU:HB2	2.10	0.52
1:A:725:ILE:O	1:A:773:LYS:HB2	2.10	0.52
1:C:158:ASP:O	1:C:162:ARG:HG2	2.10	0.52
1:C:256:PHE:O	1:C:458:ALA:HB3	2.09	0.52
1:D:85:LYS:HE2	1:D:110:SER:OG	2.10	0.52
1:A:565:ASN:O	1:A:566:HIS:C	2.48	0.52
1:B:230:ILE:HD11	1:B:342:MET:HB2	1.92	0.52
1:C:690:GLU:HG2	1:C:692:ARG:NH2	2.25	0.52
1:D:540:LEU:HD12	1:D:559:LEU:HD12	1.92	0.52
1:D:594:ALA:HA	1:D:597:TRP:CD1	2.45	0.52
1:F:70:LEU:HD13	1:F:74:ASP:HB2	1.90	0.52
1:A:158:ASP:O	1:A:162:ARG:HG2	2.10	0.52
1:A:508:GLU:HG3	1:A:508:GLU:O	2.10	0.52
1:A:535:PRO:HB2	1:A:540:LEU:HD21	1.90	0.52
1:B:510:ILE:HD12	1:B:768:ARG:HB3	1.90	0.52
1:B:556:VAL:HG21	1:B:579:THR:CA	2.40	0.52
1:C:743:PRO:HD2	1:C:747:MET:CG	2.40	0.52
1:E:540:LEU:HD21	1:E:562:GLU:HG3	1.92	0.52
1:B:318:ASN:O	1:B:319:GLY:C	2.49	0.52
1:C:487:GLU:HG3	1:C:521:LEU:HD13	1.92	0.52
1:C:499:ILE:HG22	1:C:500:LEU:N	2.24	0.52
1:D:43:GLY:H	1:D:698:ALA:CB	2.21	0.52
1:D:535:PRO:HB2	1:D:540:LEU:CD2	2.39	0.52
1:D:686:ILE:HG22	1:D:704:GLN:HE22	1.73	0.52
1:D:702:LEU:O	1:D:706:ARG:HG3	2.10	0.52
1:E:161:TYR:O	1:E:164:MET:HB3	2.09	0.52
1:F:743:PRO:HD2	1:F:747:MET:HG2	1.92	0.52
1:A:510:ILE:HD12	1:A:768:ARG:HB3	1.92	0.51
1:B:243:ASP:OD2	1:B:324:PRO:HG3	2.11	0.51
1:C:742:ILE:HD11	1:C:752:ALA:C	2.30	0.51
1:A:173:ILE:C	1:A:174:LEU:HD23	2.31	0.51
1:A:117:SER:HB2	1:A:714:ILE:HD11	1.92	0.51
1:B:690:GLU:HG2	1:B:692:ARG:NH2	2.26	0.51
1:B:77:LYS:NZ	1:B:77:LYS:H	2.08	0.51
1:D:742:ILE:HD11	1:D:752:ALA:C	2.30	0.51
1:D:743:PRO:HD2	1:D:747:MET:CG	2.40	0.51
1:F:378:MET:HG3	1:F:378:MET:O	2.10	0.51
1:F:535:PRO:HB2	1:F:540:LEU:CD2	2.40	0.51
1:A:690:GLU:HG2	1:A:692:ARG:NH2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:THR:HG23	1:B:422:GLN:CG	2.40	0.51
1:D:303:ASN:HD22	1:D:304:ASP:N	2.07	0.51
1:B:161:TYR:O	1:B:164:MET:HB3	2.10	0.51
1:C:556:VAL:HG21	1:C:579:THR:CA	2.41	0.51
1:D:586:TYR:CG	1:D:587:ALA:N	2.78	0.51
1:E:301:MET:HA	1:E:304:ASP:HB3	1.93	0.51
1:B:327:GLN:O	1:B:330:GLU:N	2.44	0.51
1:B:43:GLY:H	1:B:698:ALA:CB	2.22	0.51
1:B:499:ILE:HG22	1:B:500:LEU:N	2.24	0.51
1:C:77:LYS:NZ	1:C:77:LYS:H	2.09	0.51
1:D:286:THR:OG1	1:D:287:PHE:N	2.44	0.51
1:D:70:LEU:HD13	1:D:74:ASP:HB2	1.92	0.51
1:E:419:THR:H	1:E:422:GLN:NE2	2.07	0.51
1:E:586:TYR:CG	1:E:587:ALA:N	2.78	0.51
1:A:301:MET:HA	1:A:304:ASP:HB3	1.91	0.51
1:C:327:GLN:O	1:C:330:GLU:N	2.44	0.51
1:D:161:TYR:O	1:D:164:MET:HB3	2.10	0.51
1:D:238:LYS:NZ	1:D:283:ASP:O	2.44	0.51
1:D:37:VAL:HG11	1:D:59:VAL:HG21	1.92	0.51
1:E:690:GLU:HG2	1:E:692:ARG:NH2	2.26	0.51
1:F:234:PHE:CE2	1:F:289:ILE:HG12	2.45	0.51
1:B:152:HIS:O	1:B:156:ILE:HD12	2.10	0.51
1:B:578:LYS:C	1:B:579:THR:HG23	2.31	0.51
1:B:743:PRO:HD2	1:B:747:MET:CG	2.40	0.51
1:C:527:LEU:HD22	1:C:566:HIS:CD2	2.46	0.51
1:D:108:TYR:CD2	1:D:696:LEU:HD12	2.45	0.51
1:D:318:ASN:O	1:D:319:GLY:C	2.49	0.51
1:D:36:TRP:CE2	1:D:78:MET:HG2	2.45	0.51
1:D:499:ILE:HG22	1:D:500:LEU:N	2.25	0.51
1:F:158:ASP:O	1:F:162:ARG:HG2	2.11	0.51
1:F:36:TRP:CE2	1:F:78:MET:HG2	2.46	0.51
1:F:766:LEU:HA	1:F:777:ARG:HG3	1.93	0.51
1:A:743:PRO:HD2	1:A:747:MET:CG	2.40	0.51
1:C:388:CYS:SG	1:C:393:ILE:HG22	2.51	0.51
1:C:757:ILE:HG23	1:C:762:LEU:HB2	1.92	0.51
1:D:757:ILE:HG23	1:D:762:LEU:HB2	1.92	0.51
1:F:39:SER:HG	1:F:42:HIS:H	1.59	0.51
1:B:35:VAL:HG22	1:B:36:TRP:H	1.76	0.51
1:B:95:LEU:CD1	1:B:714:ILE:HG21	2.40	0.51
1:C:37:VAL:HG11	1:C:59:VAL:HG21	1.93	0.51
1:C:70:LEU:HD13	1:C:74:ASP:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:327:GLN:O	1:D:330:GLU:N	2.43	0.51
1:D:180:GLY:C	1:D:686:ILE:HD12	2.31	0.51
1:E:269:THR:HG23	1:E:443:LEU:HD22	1.92	0.51
1:E:286:THR:OG1	1:E:287:PHE:N	2.43	0.51
1:E:37:VAL:HG11	1:E:59:VAL:HG21	1.92	0.51
1:E:35:VAL:HG12	1:E:47:ALA:O	2.11	0.51
1:E:72:LYS:HA	1:E:75:ILE:CD1	2.40	0.51
1:A:36:TRP:CE2	1:A:78:MET:HG2	2.45	0.51
1:C:318:ASN:O	1:C:319:GLY:C	2.49	0.51
1:D:376:ALA:O	1:D:403:LEU:HD22	2.11	0.51
1:E:578:LYS:C	1:E:579:THR:HG23	2.31	0.51
1:E:743:PRO:CD	1:E:747:MET:SD	2.99	0.51
1:F:158:ASP:O	1:F:161:TYR:HB3	2.11	0.51
1:A:556:VAL:HG21	1:A:579:THR:HA	1.93	0.50
1:A:766:LEU:HA	1:A:777:ARG:HG3	1.92	0.50
1:B:527:LEU:HD22	1:B:566:HIS:CD2	2.46	0.50
1:C:327:GLN:O	1:C:330:GLU:HB2	2.10	0.50
1:D:578:LYS:C	1:D:579:THR:HG23	2.31	0.50
1:E:85:LYS:HE2	1:E:110:SER:OG	2.10	0.50
1:F:419:THR:H	1:F:422:GLN:NE2	2.08	0.50
1:F:490:GLN:O	1:F:493:PHE:HB3	2.11	0.50
1:A:556:VAL:HG21	1:A:579:THR:CA	2.41	0.50
1:C:173:ILE:C	1:C:174:LEU:HD23	2.32	0.50
1:C:117:SER:HB2	1:C:714:ILE:HD11	1.93	0.50
1:E:281:ALA:O	1:E:318:ASN:ND2	2.45	0.50
1:E:303:ASN:HD22	1:E:304:ASP:N	2.09	0.50
1:E:710:VAL:O	1:E:714:ILE:HG13	2.11	0.50
1:E:77:LYS:H	1:E:77:LYS:HZ2	1.58	0.50
1:A:460:PHE:CD1	1:A:460:PHE:C	2.85	0.50
1:C:378:MET:HG3	1:C:378:MET:O	2.12	0.50
1:C:517:PHE:CZ	1:C:716:ILE:HD13	2.46	0.50
1:D:327:GLN:O	1:D:330:GLU:HB2	2.11	0.50
1:D:77:LYS:H	1:D:77:LYS:NZ	2.10	0.50
1:F:243:ASP:OD2	1:F:324:PRO:HG3	2.12	0.50
1:A:527:LEU:HD22	1:A:566:HIS:CD2	2.46	0.50
1:B:434:LYS:HG2	1:B:625:TRP:HZ2	1.76	0.50
1:B:725:ILE:O	1:B:773:LYS:HB2	2.11	0.50
1:B:72:LYS:HA	1:B:75:ILE:CD1	2.41	0.50
1:C:378:MET:CE	1:C:381:ASN:HA	2.41	0.50
1:D:60:GLU:HA	1:D:67:LYS:HA	1.93	0.50
1:F:487:GLU:HG3	1:F:521:LEU:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ILE:HD11	1:A:342:MET:HB2	1.93	0.50
1:A:318:ASN:O	1:A:319:GLY:C	2.49	0.50
1:B:269:THR:HG23	1:B:443:LEU:HD22	1.94	0.50
1:B:586:TYR:CG	1:B:587:ALA:N	2.80	0.50
1:D:35:VAL:HG12	1:D:47:ALA:O	2.11	0.50
1:E:117:SER:HB2	1:E:714:ILE:HD11	1.92	0.50
1:E:510:ILE:HD12	1:E:768:ARG:HB3	1.92	0.50
1:F:72:LYS:HA	1:F:75:ILE:CD1	2.42	0.50
1:B:766:LEU:HA	1:B:777:ARG:HG3	1.93	0.50
1:D:165:LEU:HD21	1:D:260:GLY:HA2	1.94	0.50
1:E:742:ILE:HD11	1:E:752:ALA:C	2.31	0.50
1:F:37:VAL:HG11	1:F:59:VAL:HG21	1.92	0.50
1:A:178:GLU:OE2	1:A:686:ILE:HG21	2.11	0.50
1:A:165:LEU:HD21	1:A:260:GLY:HA2	1.94	0.50
1:B:556:VAL:HG21	1:B:579:THR:HA	1.92	0.50
1:B:611:SER:O	1:B:614:ASN:HB3	2.10	0.50
1:C:43:GLY:H	1:C:698:ALA:CB	2.22	0.50
1:C:438:LEU:O	1:C:442:ILE:HG13	2.12	0.50
1:C:738:ALA:CB	1:C:741:ALA:HB2	2.39	0.50
1:E:388:CYS:SG	1:E:393:ILE:HG22	2.52	0.50
1:E:748:ASP:C	1:E:748:ASP:OD1	2.50	0.50
1:F:556:VAL:HG21	1:F:579:THR:CA	2.41	0.50
1:A:355:VAL:O	1:A:359:VAL:HG23	2.12	0.50
1:A:60:GLU:HA	1:A:67:LYS:HA	1.94	0.50
1:B:158:ASP:O	1:B:161:TYR:HB3	2.12	0.50
1:B:238:LYS:NZ	1:B:283:ASP:O	2.44	0.50
1:C:434:LYS:HG2	1:C:625:TRP:HZ2	1.77	0.50
1:D:690:GLU:HG2	1:D:692:ARG:NH2	2.27	0.50
1:E:230:ILE:HD11	1:E:342:MET:HB2	1.94	0.50
1:B:754:ILE:HD13	1:F:692:ARG:NH2	2.27	0.50
1:F:688:ASN:ND2	1:F:692:ARG:O	2.33	0.50
1:A:526:GLU:OE1	1:A:526:GLU:HA	2.12	0.50
1:B:173:ILE:C	1:B:174:LEU:HD23	2.32	0.50
1:D:36:TRP:NE1	1:D:78:MET:HG2	2.27	0.50
1:E:256:PHE:O	1:E:458:ALA:HB3	2.12	0.50
1:E:337:GLU:O	1:E:341:ILE:HG13	2.12	0.50
1:F:43:GLY:H	1:F:698:ALA:CB	2.21	0.50
1:F:77:LYS:H	1:F:77:LYS:NZ	2.09	0.50
1:A:278:ILE:HD12	1:A:428:GLU:HG2	1.93	0.49
1:B:117:SER:HB2	1:B:714:ILE:HD11	1.92	0.49
1:C:281:ALA:O	1:C:318:ASN:ND2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:611:SER:O	1:C:614:ASN:HB3	2.12	0.49
1:C:510:ILE:HD12	1:C:768:ARG:HB3	1.94	0.49
1:C:36:TRP:NE1	1:C:78:MET:HG2	2.27	0.49
1:D:659:VAL:HA	1:D:662:LEU:HD12	1.95	0.49
1:E:108:TYR:CD2	1:E:696:LEU:HD12	2.47	0.49
1:E:738:ALA:CB	1:E:741:ALA:HB2	2.39	0.49
1:E:754:ILE:HG22	1:E:755:LEU:HD23	1.94	0.49
1:F:556:VAL:HG21	1:F:579:THR:HA	1.94	0.49
1:F:60:GLU:HA	1:F:67:LYS:HA	1.94	0.49
1:A:490:GLN:O	1:A:493:PHE:HB3	2.12	0.49
1:B:498:PHE:CE2	1:B:519:LEU:HD13	2.48	0.49
1:E:165:LEU:HD21	1:E:260:GLY:HA2	1.93	0.49
1:F:303:ASN:HD22	1:F:304:ASP:N	2.09	0.49
1:F:566:HIS:CD2	1:F:568:LYS:H	2.30	0.49
1:A:586:TYR:CG	1:A:587:ALA:N	2.80	0.49
1:B:158:ASP:O	1:B:162:ARG:HG2	2.11	0.49
1:B:36:TRP:CE2	1:B:78:MET:HG2	2.47	0.49
1:B:538:LEU:CD1	1:B:664:LYS:HD2	2.42	0.49
1:C:238:LYS:NZ	1:C:283:ASP:O	2.44	0.49
1:D:230:ILE:HD11	1:D:342:MET:HB2	1.94	0.49
1:F:578:LYS:C	1:F:579:THR:HG23	2.33	0.49
1:A:327:GLN:O	1:A:330:GLU:N	2.45	0.49
1:A:738:ALA:CB	1:A:741:ALA:HB2	2.39	0.49
1:B:35:VAL:HG12	1:B:47:ALA:O	2.12	0.49
1:B:535:PRO:HB2	1:B:540:LEU:CD2	2.43	0.49
1:C:538:LEU:CD1	1:C:664:LYS:HD2	2.43	0.49
1:D:487:GLU:HG3	1:D:521:LEU:HD13	1.93	0.49
1:E:36:TRP:CE2	1:E:78:MET:HG2	2.47	0.49
1:E:419:THR:HG23	1:E:422:GLN:CG	2.43	0.49
1:F:89:MET:HE1	1:F:100:VAL:HG13	1.94	0.49
1:F:565:ASN:O	1:F:566:HIS:C	2.50	0.49
1:B:391:MET:HE2	1:B:434:LYS:CE	2.43	0.49
1:C:161:TYR:O	1:C:164:MET:HB3	2.11	0.49
1:D:117:SER:HB2	1:D:714:ILE:HD11	1.94	0.49
1:D:556:VAL:HG21	1:D:579:THR:CA	2.41	0.49
1:D:606:ASN:HB3	1:D:609:VAL:HG13	1.94	0.49
1:F:290:PHE:CE1	1:F:356:VAL:HG13	2.47	0.49
1:F:586:TYR:CG	1:F:587:ALA:N	2.80	0.49
1:A:35:VAL:HG22	1:A:36:TRP:H	1.76	0.49
1:B:526:GLU:OE1	1:B:526:GLU:HA	2.12	0.49
1:B:767:TYR:O	1:B:768:ARG:HG2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:ALA:HB1	1:C:301:MET:HG2	1.94	0.49
1:C:725:ILE:O	1:C:773:LYS:HB2	2.12	0.49
1:D:337:GLU:O	1:D:341:ILE:HG13	2.13	0.49
1:D:566:HIS:CD2	1:D:568:LYS:H	2.31	0.49
1:E:173:ILE:C	1:E:174:LEU:HD23	2.33	0.49
1:E:60:GLU:HA	1:E:67:LYS:HA	1.93	0.49
1:F:226:GLN:HB2	1:F:342:MET:HE2	1.95	0.49
1:F:240:VAL:HG23	1:F:241:LYS:HG2	1.95	0.49
1:A:578:LYS:C	1:A:579:THR:HG23	2.32	0.49
1:A:434:LYS:HG2	1:A:625:TRP:HZ2	1.78	0.49
1:A:697:ASP:HB3	1:A:700:LEU:HB3	1.94	0.49
1:C:165:LEU:HD21	1:C:260:GLY:HA2	1.94	0.49
1:C:578:LYS:C	1:C:579:THR:HG23	2.32	0.49
1:D:271:LEU:HG	1:D:271:LEU:O	2.12	0.49
1:D:295:ALA:HB2	1:D:310:PHE:CZ	2.48	0.49
1:D:611:SER:O	1:D:614:ASN:HB3	2.13	0.49
1:D:434:LYS:HG2	1:D:625:TRP:HZ2	1.78	0.49
1:E:763:ASP:HB3	1:E:766:LEU:HG	1.95	0.49
1:F:508:GLU:O	1:F:508:GLU:HG3	2.12	0.49
1:A:226:GLN:HB2	1:A:342:MET:HE2	1.95	0.49
1:A:297:ALA:HB1	1:A:301:MET:HG2	1.95	0.49
1:B:337:GLU:O	1:B:341:ILE:HG13	2.12	0.49
1:B:393:ILE:HG13	1:B:612:LEU:HB3	1.94	0.49
1:C:508:GLU:HG3	1:C:508:GLU:O	2.13	0.49
1:D:419:THR:H	1:D:422:GLN:NE2	2.06	0.49
1:E:39:SER:HG	1:E:42:HIS:H	1.60	0.49
1:E:688:ASN:ND2	1:E:692:ARG:O	2.34	0.49
1:E:727:PHE:HA	1:E:753:CYS:SG	2.53	0.49
1:F:278:ILE:HD12	1:F:428:GLU:HG2	1.93	0.49
1:A:566:HIS:CD2	1:A:568:LYS:H	2.31	0.49
1:B:281:ALA:O	1:B:318:ASN:ND2	2.46	0.49
1:B:478:GLU:OE2	1:B:600:LYS:HE2	2.13	0.49
1:D:89:MET:HE1	1:D:100:VAL:HG13	1.94	0.49
1:D:113:ILE:O	1:D:123:VAL:HA	2.12	0.49
1:D:419:THR:HG23	1:D:422:GLN:CG	2.43	0.49
1:E:565:ASN:O	1:E:566:HIS:C	2.50	0.49
1:F:327:GLN:O	1:F:330:GLU:HB2	2.13	0.49
1:F:95:LEU:HD11	1:F:714:ILE:HG21	1.93	0.49
1:C:158:ASP:O	1:C:161:TYR:HB3	2.12	0.49
1:C:271:LEU:O	1:C:271:LEU:HG	2.12	0.49
1:C:178:GLU:OE2	1:C:686:ILE:HG21	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:606:ASN:HB3	1:E:609:VAL:HG13	1.94	0.49
1:E:434:LYS:HG2	1:E:625:TRP:HZ2	1.78	0.49
1:E:36:TRP:NE1	1:E:78:MET:HG2	2.28	0.49
1:F:393:ILE:HD11	1:F:613:LEU:HA	1.95	0.49
1:F:180:GLY:C	1:F:686:ILE:HD12	2.32	0.49
1:A:337:GLU:O	1:A:341:ILE:HG13	2.13	0.48
1:A:419:THR:H	1:A:422:GLN:NE2	2.05	0.48
1:A:35:VAL:HG12	1:A:47:ALA:O	2.13	0.48
1:E:327:GLN:O	1:E:330:GLU:HB2	2.13	0.48
1:E:290:PHE:CE1	1:E:356:VAL:HG13	2.48	0.48
1:F:165:LEU:HD21	1:F:260:GLY:HA2	1.94	0.48
1:F:286:THR:OG1	1:F:287:PHE:N	2.45	0.48
1:F:35:VAL:HG22	1:F:76:GLN:O	2.13	0.48
1:A:196:VAL:CG1	1:A:196:VAL:O	2.60	0.48
1:A:295:ALA:HB2	1:A:310:PHE:CZ	2.47	0.48
1:A:606:ASN:HB3	1:A:609:VAL:HG13	1.94	0.48
1:A:80:PRO:HB2	1:A:82:LYS:HG2	1.96	0.48
1:B:196:VAL:CG1	1:B:196:VAL:O	2.61	0.48
1:B:219:GLU:O	1:B:220:LEU:C	2.52	0.48
1:B:508:GLU:O	1:B:508:GLU:HG3	2.14	0.48
1:B:606:ASN:HB3	1:B:609:VAL:HG13	1.94	0.48
1:C:196:VAL:CG1	1:C:196:VAL:O	2.60	0.48
1:C:295:ALA:HB2	1:C:310:PHE:CZ	2.47	0.48
1:C:278:ILE:HB	1:C:315:PHE:CE1	2.48	0.48
1:C:60:GLU:HA	1:C:67:LYS:HA	1.94	0.48
1:D:556:VAL:HG21	1:D:579:THR:HA	1.94	0.48
1:F:460:PHE:C	1:F:460:PHE:CD1	2.86	0.48
1:C:556:VAL:HG21	1:C:579:THR:HA	1.93	0.48
1:E:318:ASN:O	1:E:319:GLY:C	2.51	0.48
1:F:606:ASN:HB3	1:F:609:VAL:HG13	1.94	0.48
1:A:686:ILE:HG22	1:A:704:GLN:HE22	1.77	0.48
1:B:60:GLU:HA	1:B:67:LYS:HA	1.94	0.48
1:C:219:GLU:O	1:C:222:LYS:N	2.46	0.48
1:C:419:THR:H	1:C:422:GLN:NE2	2.07	0.48
1:C:478:GLU:OE2	1:C:600:LYS:HE2	2.14	0.48
1:D:158:ASP:O	1:D:162:ARG:HG2	2.14	0.48
1:E:158:ASP:O	1:E:161:TYR:HB3	2.13	0.48
1:E:43:GLY:H	1:E:698:ALA:CB	2.20	0.48
1:E:540:LEU:HD11	1:E:562:GLU:HB2	1.95	0.48
1:F:337:GLU:O	1:F:341:ILE:HG13	2.13	0.48
1:F:611:SER:O	1:F:614:ASN:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:LYS:NZ	1:A:283:ASP:O	2.46	0.48
1:B:355:VAL:O	1:B:359:VAL:HG23	2.14	0.48
1:C:95:LEU:HD11	1:C:714:ILE:HG21	1.96	0.48
1:C:766:LEU:HA	1:C:777:ARG:HG3	1.95	0.48
1:D:490:GLN:O	1:D:493:PHE:HB3	2.14	0.48
1:E:526:GLU:HA	1:E:526:GLU:OE1	2.13	0.48
1:F:754:ILE:HG22	1:F:755:LEU:HD23	1.94	0.48
1:F:510:ILE:HD12	1:F:768:ARG:HB3	1.94	0.48
1:F:95:LEU:CD1	1:F:714:ILE:HG21	2.44	0.48
1:A:271:LEU:O	1:A:271:LEU:HG	2.13	0.48
1:A:290:PHE:CE1	1:A:356:VAL:HG13	2.49	0.48
1:B:295:ALA:HB2	1:B:310:PHE:CZ	2.48	0.48
1:B:754:ILE:HG22	1:B:755:LEU:HD23	1.96	0.48
1:C:526:GLU:HA	1:C:526:GLU:OE1	2.14	0.48
1:C:586:TYR:CG	1:C:587:ALA:N	2.82	0.48
1:E:478:GLU:OE2	1:E:600:LYS:HE2	2.14	0.48
1:E:766:LEU:HA	1:E:777:ARG:HG3	1.95	0.48
1:F:178:GLU:OE2	1:F:686:ILE:HG21	2.13	0.48
1:A:487:GLU:HG3	1:A:521:LEU:HD13	1.95	0.48
1:A:535:PRO:HB2	1:A:540:LEU:CD2	2.43	0.48
1:C:107:ARG:NH1	1:C:114:TYR:O	2.46	0.48
1:D:219:GLU:O	1:D:220:LEU:C	2.52	0.48
1:E:731:ARG:HG2	1:E:756:MET:CE	2.44	0.48
1:A:85:LYS:HE2	1:A:110:SER:OG	2.13	0.48
1:C:498:PHE:CE2	1:C:519:LEU:HD13	2.49	0.48
1:F:540:LEU:HD11	1:F:562:GLU:HB2	1.96	0.48
1:F:697:ASP:HB3	1:F:700:LEU:HB3	1.96	0.48
1:F:763:ASP:HB3	1:F:766:LEU:HG	1.96	0.48
1:F:36:TRP:NE1	1:F:78:MET:HG2	2.28	0.48
1:A:77:LYS:HZ2	1:A:77:LYS:N	2.11	0.48
1:C:566:HIS:CD2	1:C:568:LYS:H	2.31	0.48
1:D:508:GLU:HG3	1:D:508:GLU:O	2.13	0.48
1:D:697:ASP:HB3	1:D:700:LEU:HB3	1.96	0.48
1:D:766:LEU:HA	1:D:777:ARG:HG3	1.95	0.48
1:E:487:GLU:HG3	1:E:521:LEU:HD13	1.96	0.48
1:F:742:ILE:HG12	1:F:752:ALA:HB1	1.96	0.48
1:A:538:LEU:CD1	1:A:664:LYS:HD2	2.43	0.48
1:A:517:PHE:CZ	1:A:716:ILE:HD13	2.47	0.48
1:B:226:GLN:HB2	1:B:342:MET:HE2	1.96	0.48
1:B:35:VAL:HG21	1:B:75:ILE:HG22	1.96	0.48
1:B:566:HIS:CD2	1:B:568:LYS:H	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:77:LYS:NZ	1:E:77:LYS:H	2.11	0.48
1:F:158:ASP:HB2	1:F:193:TYR:CZ	2.49	0.48
1:F:196:VAL:O	1:F:196:VAL:CG1	2.62	0.48
1:F:378:MET:CE	1:F:381:ASN:HA	2.43	0.48
1:A:611:SER:O	1:A:614:ASN:HB3	2.14	0.47
1:A:36:TRP:NE1	1:A:78:MET:HG2	2.29	0.47
1:B:165:LEU:HD21	1:B:260:GLY:HA2	1.95	0.47
1:C:228:ASN:HB2	1:C:229:PRO:HD3	1.96	0.47
1:C:460:PHE:C	1:C:460:PHE:CD1	2.86	0.47
1:C:535:PRO:HB2	1:C:540:LEU:CD2	2.43	0.47
1:D:228:ASN:HB2	1:D:229:PRO:HD3	1.96	0.47
1:D:502:GLN:O	1:D:505:TYR:HB2	2.14	0.47
1:E:327:GLN:O	1:E:330:GLU:N	2.47	0.47
1:E:611:SER:O	1:E:614:ASN:HB3	2.13	0.47
1:A:393:ILE:HG13	1:A:612:LEU:HB3	1.96	0.47
1:A:545:CYS:SG	1:A:598:LEU:HD23	2.53	0.47
1:C:490:GLN:O	1:C:493:PHE:HB3	2.14	0.47
1:F:434:LYS:HG2	1:F:625:TRP:HZ2	1.78	0.47
1:B:378:MET:CE	1:B:381:ASN:HA	2.42	0.47
1:C:89:MET:HE1	1:C:100:VAL:HG13	1.95	0.47
1:D:763:ASP:HB3	1:D:766:LEU:HG	1.96	0.47
1:F:753:CYS:HA	1:F:756:MET:HE3	1.95	0.47
1:A:219:GLU:O	1:A:220:LEU:C	2.53	0.47
1:B:686:ILE:HG22	1:B:704:GLN:HE22	1.78	0.47
1:C:393:ILE:HG13	1:C:612:LEU:HB3	1.95	0.47
1:C:754:ILE:HG22	1:C:755:LEU:HD23	1.97	0.47
1:E:268:GLU:HG2	1:E:270:TYR:OH	2.14	0.47
1:E:538:LEU:CD1	1:E:664:LYS:HD2	2.44	0.47
1:A:158:ASP:HB2	1:A:193:TYR:CZ	2.49	0.47
1:A:540:LEU:HD11	1:A:562:GLU:HB2	1.96	0.47
1:B:35:VAL:HG22	1:B:76:GLN:O	2.14	0.47
1:B:659:VAL:HA	1:B:662:LEU:HD12	1.97	0.47
1:D:727:PHE:HA	1:D:753:CYS:SG	2.55	0.47
1:F:269:THR:HG23	1:F:443:LEU:HD22	1.95	0.47
1:A:158:ASP:O	1:A:161:TYR:HB3	2.14	0.47
1:B:271:LEU:HG	1:B:271:LEU:O	2.14	0.47
1:B:278:ILE:HB	1:B:315:PHE:CE1	2.50	0.47
1:B:666:GLN:HA	1:B:669:LYS:HD3	1.96	0.47
1:B:697:ASP:HB3	1:B:700:LEU:HB3	1.96	0.47
1:C:419:THR:N	1:C:422:GLN:HG3	2.21	0.47
1:D:278:ILE:HB	1:D:315:PHE:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:219:GLU:O	1:F:220:LEU:C	2.53	0.47
1:F:339:MET:CE	1:F:352:ILE:HD13	2.45	0.47
1:F:35:VAL:HG21	1:F:75:ILE:HG22	1.97	0.47
1:A:754:ILE:HG22	1:A:755:LEU:HD23	1.96	0.47
1:B:419:THR:H	1:B:422:GLN:CG	2.22	0.47
1:B:742:ILE:HG22	1:B:743:PRO:O	2.15	0.47
1:C:219:GLU:O	1:C:220:LEU:C	2.51	0.47
1:C:337:GLU:O	1:C:341:ILE:HG13	2.15	0.47
1:C:551:THR:CB	1:C:553:THR:HG22	2.45	0.47
1:C:763:ASP:HB3	1:C:766:LEU:HG	1.96	0.47
1:D:35:VAL:HG22	1:D:36:TRP:H	1.80	0.47
1:E:238:LYS:NZ	1:E:283:ASP:O	2.47	0.47
1:E:490:GLN:O	1:E:493:PHE:HB3	2.15	0.47
1:F:164:MET:SD	1:F:459:SER:HB2	2.55	0.47
1:A:731:ARG:HG2	1:A:756:MET:CE	2.44	0.47
1:A:767:TYR:O	1:A:768:ARG:HG2	2.15	0.47
1:B:487:GLU:HG3	1:B:521:LEU:HD13	1.95	0.47
1:D:460:PHE:C	1:D:460:PHE:CD1	2.88	0.47
1:E:113:ILE:O	1:E:123:VAL:HA	2.15	0.47
1:E:278:ILE:HB	1:E:315:PHE:CE1	2.49	0.47
1:F:116:TYR:CZ	1:F:146:ARG:HG2	2.50	0.47
1:F:230:ILE:HD11	1:F:342:MET:HB2	1.97	0.47
1:F:402:ILE:HG22	1:F:403:LEU:N	2.30	0.47
1:A:734:TYR:OH	1:A:781:LEU:HD22	2.15	0.47
1:B:240:VAL:HG23	1:B:241:LYS:HG2	1.97	0.47
1:B:327:GLN:HB2	1:B:330:GLU:CD	2.35	0.47
1:B:731:ARG:HG2	1:B:756:MET:CE	2.43	0.47
1:D:297:ALA:HB1	1:D:301:MET:HG2	1.96	0.47
1:D:393:ILE:HG13	1:D:612:LEU:HB3	1.97	0.47
1:F:251:PHE:CZ	1:F:462:GLY:HA3	2.50	0.47
1:F:271:LEU:HG	1:F:271:LEU:O	2.15	0.47
1:F:419:THR:HG23	1:F:422:GLN:CG	2.44	0.47
1:A:89:MET:HE1	1:A:100:VAL:HG13	1.97	0.47
1:A:607:ASP:CA	1:A:610:THR:HB	2.45	0.47
1:A:666:GLN:HA	1:A:669:LYS:HD3	1.96	0.47
1:B:734:TYR:OH	1:B:781:LEU:HD22	2.14	0.47
1:E:158:ASP:O	1:E:162:ARG:HG2	2.14	0.47
1:E:228:ASN:HB2	1:E:229:PRO:HD3	1.97	0.47
1:E:271:LEU:O	1:E:271:LEU:HG	2.14	0.47
1:E:566:HIS:CD2	1:E:568:LYS:H	2.32	0.47
1:E:43:GLY:HA3	1:E:702:LEU:CD1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:43:GLY:HA3	1:F:702:LEU:CD1	2.45	0.47
1:A:107:ARG:NH1	1:A:114:TYR:O	2.48	0.47
1:A:278:ILE:HB	1:A:315:PHE:CE1	2.49	0.47
1:A:742:ILE:HG22	1:A:743:PRO:O	2.15	0.47
1:B:460:PHE:C	1:B:460:PHE:CD1	2.88	0.47
1:C:61:LEU:HG	1:C:66:LYS:O	2.15	0.47
1:C:711:LEU:O	1:C:715:ARG:HG2	2.15	0.47
1:D:339:MET:CE	1:D:352:ILE:HD13	2.45	0.47
1:E:297:ALA:HB1	1:E:301:MET:HG2	1.97	0.47
1:E:419:THR:H	1:E:422:GLN:CG	2.24	0.47
1:E:502:GLN:HA	1:E:505:TYR:CD2	2.50	0.47
1:E:658:THR:O	1:E:662:LEU:HD12	2.15	0.47
1:F:253:ARG:HG3	1:F:460:PHE:CD1	2.50	0.47
1:F:281:ALA:O	1:F:318:ASN:ND2	2.48	0.47
1:C:540:LEU:HD11	1:C:562:GLU:HB2	1.97	0.46
1:D:538:LEU:HD12	1:D:664:LYS:HD2	1.96	0.46
1:D:742:ILE:HG22	1:D:743:PRO:O	2.15	0.46
1:E:219:GLU:O	1:E:220:LEU:C	2.52	0.46
1:E:666:GLN:HA	1:E:669:LYS:HD3	1.96	0.46
1:E:686:ILE:HG22	1:E:704:GLN:HE22	1.80	0.46
1:F:527:LEU:HD22	1:F:566:HIS:CD2	2.49	0.46
1:F:731:ARG:O	1:F:735:GLU:HB2	2.15	0.46
1:A:236:ASN:ND2	1:A:244:ASN:O	2.49	0.46
1:A:286:THR:OG1	1:A:287:PHE:N	2.46	0.46
1:A:391:MET:HE2	1:A:434:LYS:CE	2.45	0.46
1:A:57:VAL:HG12	1:A:59:VAL:HG13	1.98	0.46
1:B:228:ASN:HB2	1:B:229:PRO:HD3	1.97	0.46
1:C:158:ASP:HB2	1:C:193:TYR:CZ	2.50	0.46
1:D:495:HIS:CD2	1:D:500:LEU:HG	2.50	0.46
1:D:393:ILE:HD11	1:D:613:LEU:HA	1.97	0.46
1:A:269:THR:HG23	1:A:443:LEU:HD22	1.96	0.46
1:A:551:THR:CB	1:A:553:THR:HG22	2.45	0.46
1:B:57:VAL:HG12	1:B:59:VAL:HG13	1.97	0.46
1:D:278:ILE:HD12	1:D:428:GLU:HG2	1.98	0.46
1:F:731:ARG:HG2	1:F:756:MET:CE	2.45	0.46
1:A:717:CYS:O	1:A:778:THR:HG22	2.15	0.46
1:C:253:ARG:HG3	1:C:460:PHE:CD1	2.50	0.46
1:C:57:VAL:HG12	1:C:59:VAL:HG13	1.98	0.46
1:D:240:VAL:HG23	1:D:241:LYS:HG2	1.96	0.46
1:D:566:HIS:HD2	1:D:568:LYS:H	1.64	0.46
1:D:754:ILE:HG22	1:D:755:LEU:HD23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:607:ASP:CA	1:E:610:THR:HB	2.46	0.46
1:E:697:ASP:HB3	1:E:700:LEU:HB3	1.97	0.46
1:F:532:THR:OG1	1:F:533:ASN:ND2	2.48	0.46
1:C:607:ASP:CA	1:C:610:THR:HB	2.43	0.46
1:E:323:ILE:HG22	1:E:324:PRO:CD	2.45	0.46
1:E:498:PHE:CE2	1:E:519:LEU:HD13	2.50	0.46
1:F:297:ALA:HB1	1:F:301:MET:HG2	1.97	0.46
1:B:427:ILE:HA	1:B:427:ILE:HD13	1.78	0.46
1:B:77:LYS:HZ2	1:B:77:LYS:N	2.14	0.46
1:B:36:TRP:NE1	1:B:78:MET:HG2	2.31	0.46
1:C:172:SER:HA	1:C:462:GLY:O	2.15	0.46
1:C:290:PHE:CE1	1:C:356:VAL:HG13	2.49	0.46
1:C:72:LYS:HA	1:C:75:ILE:CD1	2.43	0.46
1:C:731:ARG:O	1:C:735:GLU:HB2	2.16	0.46
1:C:742:ILE:HG22	1:C:743:PRO:O	2.15	0.46
1:D:540:LEU:HD11	1:D:562:GLU:HB2	1.98	0.46
1:E:251:PHE:CZ	1:E:462:GLY:HA3	2.51	0.46
1:E:508:GLU:HG3	1:E:508:GLU:O	2.16	0.46
1:F:659:VAL:HA	1:F:662:LEU:HD12	1.98	0.46
1:A:738:ALA:O	1:A:741:ALA:HB2	2.16	0.46
1:B:121:CYS:O	1:B:683:ARG:HG2	2.16	0.46
1:B:43:GLY:HA3	1:B:702:LEU:CD1	2.46	0.46
1:B:727:PHE:HA	1:B:753:CYS:SG	2.55	0.46
1:C:659:VAL:HA	1:C:662:LEU:HD12	1.97	0.46
1:D:36:TRP:HB2	1:D:76:GLN:O	2.16	0.46
1:E:532:THR:OG1	1:E:533:ASN:ND2	2.49	0.46
1:E:527:LEU:HD22	1:E:566:HIS:CD2	2.50	0.46
1:E:584:LEU:HD23	1:E:589:LYS:CG	2.36	0.46
1:E:712:GLU:OE1	1:E:712:GLU:N	2.43	0.46
1:F:607:ASP:CA	1:F:610:THR:HB	2.45	0.46
1:A:532:THR:OG1	1:A:533:ASN:ND2	2.49	0.46
1:B:226:GLN:C	1:B:229:PRO:HD2	2.35	0.46
1:B:278:ILE:HD12	1:B:428:GLU:HG2	1.97	0.46
1:C:39:SER:HG	1:C:42:HIS:H	1.62	0.46
1:C:606:ASN:HB3	1:C:609:VAL:HG13	1.98	0.46
1:C:77:LYS:N	1:C:77:LYS:HZ2	2.14	0.46
1:D:378:MET:HE1	1:D:384:ALA:CB	2.42	0.46
1:D:666:GLN:HA	1:D:669:LYS:HD3	1.98	0.46
1:D:77:LYS:HZ2	1:D:77:LYS:N	2.13	0.46
1:E:295:ALA:HB2	1:E:310:PHE:CZ	2.49	0.46
1:E:495:HIS:CD2	1:E:500:LEU:HG	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:738:ALA:O	1:F:741:ALA:CB	2.64	0.46
1:F:727:PHE:HA	1:F:753:CYS:SG	2.56	0.46
1:B:339:MET:CE	1:B:352:ILE:HD13	2.45	0.46
1:B:607:ASP:CA	1:B:610:THR:HB	2.46	0.46
1:C:697:ASP:HB3	1:C:700:LEU:HB3	1.98	0.46
1:D:34:LEU:HD12	1:D:34:LEU:HA	1.74	0.46
1:E:57:VAL:HG12	1:E:59:VAL:HG13	1.97	0.46
1:F:381:ASN:O	1:F:382:THR:C	2.54	0.46
1:F:478:GLU:OE2	1:F:600:LYS:HE2	2.15	0.46
1:A:35:VAL:HG22	1:A:76:GLN:O	2.16	0.46
1:B:251:PHE:CZ	1:B:462:GLY:HA3	2.51	0.46
1:B:738:ALA:O	1:B:741:ALA:HB2	2.16	0.46
1:C:35:VAL:HG22	1:C:76:GLN:O	2.15	0.46
1:C:508:GLU:HG3	1:C:771:GLN:N	2.29	0.46
1:C:35:VAL:HG21	1:C:75:ILE:HG22	1.98	0.46
1:D:419:THR:H	1:D:422:GLN:CG	2.23	0.46
1:D:502:GLN:HA	1:D:505:TYR:CD2	2.51	0.46
1:D:532:THR:OG1	1:D:533:ASN:ND2	2.49	0.46
1:E:460:PHE:CD1	1:E:460:PHE:C	2.89	0.46
1:E:563:GLN:OE1	1:E:563:GLN:HA	2.16	0.46
1:F:239:THR:HG23	1:F:245:SER:HB3	1.98	0.46
1:A:300:GLN:O	1:A:304:ASP:HB2	2.17	0.45
1:A:173:ILE:HG13	1:A:461:LEU:HD21	1.99	0.45
1:B:290:PHE:CE1	1:B:356:VAL:HG13	2.51	0.45
1:B:508:GLU:HG3	1:B:771:GLN:N	2.31	0.45
1:B:532:THR:OG1	1:B:533:ASN:ND2	2.49	0.45
1:B:540:LEU:HD11	1:B:562:GLU:HB2	1.97	0.45
1:B:566:HIS:HD2	1:B:568:LYS:H	1.64	0.45
1:D:268:GLU:HG2	1:D:270:TYR:OH	2.16	0.45
1:D:526:GLU:OE1	1:D:526:GLU:HA	2.16	0.45
1:E:226:GLN:HB2	1:E:342:MET:HE2	1.98	0.45
1:E:659:VAL:HA	1:E:662:LEU:HD12	1.97	0.45
1:F:327:GLN:O	1:F:330:GLU:N	2.48	0.45
1:F:393:ILE:HG13	1:F:612:LEU:HB3	1.99	0.45
1:F:502:GLN:HA	1:F:505:TYR:CD2	2.51	0.45
1:F:743:PRO:HD2	1:F:747:MET:SD	2.56	0.45
1:A:498:PHE:CE2	1:A:519:LEU:HD13	2.51	0.45
1:A:563:GLN:OE1	1:A:563:GLN:HA	2.17	0.45
1:A:478:GLU:OE2	1:A:600:LYS:HE2	2.17	0.45
1:A:393:ILE:HD11	1:A:613:LEU:HA	1.98	0.45
1:B:508:GLU:HG2	1:B:775:PHE:CE1	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:999:ALF:F4	4:B:998:ADP:PB	2.65	0.45
1:C:271:LEU:HD22	1:C:481:CYS:HB2	1.98	0.45
1:D:41:LYS:H	1:D:41:LYS:HG2	1.44	0.45
1:D:607:ASP:CA	1:D:610:THR:HB	2.45	0.45
1:E:196:VAL:O	1:E:196:VAL:CG1	2.64	0.45
1:E:35:VAL:HG22	1:E:76:GLN:O	2.16	0.45
1:E:35:VAL:HG22	1:E:36:TRP:H	1.82	0.45
1:C:126:PRO:HB3	1:C:130:LEU:HD11	1.98	0.45
1:F:228:ASN:HB2	1:F:229:PRO:HD3	1.98	0.45
1:F:35:VAL:HG13	1:F:36:TRP:N	2.30	0.45
1:F:498:PHE:CE2	1:F:519:LEU:HD13	2.51	0.45
1:F:711:LEU:O	1:F:715:ARG:HG2	2.16	0.45
1:A:251:PHE:CZ	1:A:462:GLY:HA3	2.51	0.45
1:A:659:VAL:HA	1:A:662:LEU:HD12	1.96	0.45
1:A:43:GLY:HA3	1:A:702:LEU:CD1	2.46	0.45
1:A:97:GLU:HG2	1:A:711:LEU:CD1	2.47	0.45
1:C:173:ILE:HG13	1:C:461:LEU:HD21	1.99	0.45
1:C:95:LEU:CD1	1:C:714:ILE:HG21	2.45	0.45
1:D:551:THR:CB	1:D:553:THR:HG22	2.47	0.45
1:E:253:ARG:HG3	1:E:460:PHE:CD1	2.52	0.45
1:F:318:ASN:O	1:F:319:GLY:C	2.54	0.45
1:A:228:ASN:HB2	1:A:229:PRO:HD3	1.99	0.45
1:A:281:ALA:O	1:A:318:ASN:ND2	2.47	0.45
1:C:532:THR:OG1	1:C:533:ASN:ND2	2.49	0.45
1:E:738:ALA:O	1:E:741:ALA:HB3	2.16	0.45
1:F:538:LEU:CD1	1:F:664:LYS:HD2	2.46	0.45
1:A:316:LEU:O	1:A:317:SER:C	2.55	0.45
1:A:43:GLY:H	1:A:698:ALA:CB	2.24	0.45
1:B:35:VAL:HG11	1:B:75:ILE:CG2	2.47	0.45
1:C:240:VAL:HG23	1:C:241:LYS:HG2	1.97	0.45
1:C:35:VAL:HG11	1:C:75:ILE:CG2	2.46	0.45
1:C:545:CYS:SG	1:C:598:LEU:HD23	2.56	0.45
1:C:731:ARG:HG2	1:C:756:MET:CE	2.45	0.45
1:D:391:MET:HE2	1:D:434:LYS:CE	2.47	0.45
1:D:738:ALA:O	1:D:741:ALA:HB2	2.16	0.45
1:E:393:ILE:HG13	1:E:612:LEU:HB3	1.97	0.45
1:E:731:ARG:O	1:E:735:GLU:HB2	2.17	0.45
1:E:80:PRO:HB2	1:E:82:LYS:HG2	1.99	0.45
1:F:438:LEU:O	1:F:442:ILE:HG13	2.15	0.45
1:A:271:LEU:HD22	1:A:481:CYS:HB2	1.97	0.45
1:A:711:LEU:O	1:A:715:ARG:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:999:ALF:F4	4:A:998:ADP:PB	2.65	0.45
1:B:381:ASN:O	1:B:382:THR:C	2.55	0.45
1:B:552:ASP:HA	1:B:598:LEU:HD12	1.99	0.45
1:C:502:GLN:HA	1:C:505:TYR:CD2	2.51	0.45
1:D:478:GLU:OE2	1:D:600:LYS:HE2	2.17	0.45
1:D:717:CYS:O	1:D:778:THR:HG22	2.17	0.45
1:F:323:ILE:HG22	1:F:324:PRO:CD	2.47	0.45
1:F:566:HIS:HD2	1:F:568:LYS:H	1.64	0.45
1:F:666:GLN:HA	1:F:669:LYS:HD3	1.98	0.45
1:A:268:GLU:HG2	1:A:270:TYR:OH	2.17	0.45
1:A:525:ILE:O	1:A:529:GLU:HG2	2.17	0.45
1:A:658:THR:O	1:A:662:LEU:HD12	2.17	0.45
1:B:238:LYS:HB3	1:B:285:ARG:HG2	1.98	0.45
1:B:525:ILE:O	1:B:529:GLU:HG2	2.17	0.45
1:B:80:PRO:HB2	1:B:82:LYS:HG2	1.98	0.45
1:C:34:LEU:HD12	1:C:34:LEU:HA	1.74	0.45
1:C:381:ASN:O	1:C:382:THR:C	2.55	0.45
1:C:35:VAL:HG12	1:C:47:ALA:O	2.17	0.45
1:C:566:HIS:HD2	1:C:568:LYS:H	1.63	0.45
1:D:239:THR:HG23	1:D:245:SER:HB3	1.99	0.45
1:D:242:ASN:OD1	1:D:243:ASP:N	2.49	0.45
1:D:711:LEU:O	1:D:715:ARG:HG2	2.17	0.45
1:A:219:GLU:O	1:A:222:LYS:N	2.50	0.45
1:A:566:HIS:HD2	1:A:568:LYS:H	1.64	0.45
1:A:95:LEU:HD11	1:A:714:ILE:HG21	1.98	0.45
1:B:490:GLN:O	1:B:493:PHE:HB3	2.16	0.45
1:B:731:ARG:CG	1:B:731:ARG:HH11	2.30	0.45
1:C:268:GLU:HG2	1:C:270:TYR:OH	2.16	0.45
1:D:158:ASP:O	1:D:161:TYR:HB3	2.15	0.45
1:D:538:LEU:CD1	1:D:664:LYS:HD2	2.47	0.45
1:E:242:ASN:OD1	1:E:243:ASP:N	2.50	0.45
1:E:551:THR:CB	1:E:553:THR:HG22	2.47	0.45
1:F:327:GLN:HB2	1:F:330:GLU:CD	2.38	0.45
1:F:502:GLN:O	1:F:505:TYR:HB2	2.16	0.45
1:F:35:VAL:HG11	1:F:75:ILE:CG2	2.46	0.45
1:A:114:TYR:CE1	1:A:153:ILE:HB	2.52	0.45
1:A:226:GLN:C	1:A:229:PRO:HD2	2.37	0.45
1:A:508:GLU:HG3	1:A:771:GLN:N	2.31	0.45
1:B:438:LEU:O	1:B:442:ILE:HG13	2.16	0.45
1:D:427:ILE:HA	1:D:427:ILE:HD13	1.76	0.45
1:D:527:LEU:HD22	1:D:566:HIS:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:LEU:CD1	1:D:714:ILE:HG21	2.47	0.45
1:A:508:GLU:HG2	1:A:775:PHE:CE1	2.46	0.44
1:A:721:PHE:HB2	1:A:775:PHE:HB3	1.98	0.44
1:A:95:LEU:CD1	1:A:714:ILE:HG21	2.47	0.44
1:B:116:TYR:CZ	1:B:146:ARG:HG2	2.52	0.44
1:C:230:ILE:HD11	1:C:342:MET:HB2	1.99	0.44
1:D:355:VAL:O	1:D:359:VAL:HG23	2.17	0.44
3:D:999:ALF:F4	4:D:998:ADP:PB	2.65	0.44
1:E:271:LEU:HD22	1:E:481:CYS:HB2	1.99	0.44
1:E:734:TYR:OH	1:E:781:LEU:HD22	2.17	0.44
1:F:219:GLU:O	1:F:222:LYS:N	2.50	0.44
1:F:271:LEU:HD22	1:F:481:CYS:HB2	1.99	0.44
1:A:41:LYS:HG2	1:A:41:LYS:H	1.46	0.44
1:A:738:ALA:O	1:A:741:ALA:HB3	2.17	0.44
1:B:297:ALA:HB1	1:B:301:MET:HG2	1.98	0.44
1:B:378:MET:HG3	1:B:378:MET:O	2.16	0.44
1:C:738:ALA:O	1:C:741:ALA:HB3	2.17	0.44
1:C:756:MET:HE3	1:C:756:MET:HB2	1.55	0.44
1:E:742:ILE:HG12	1:E:752:ALA:HB1	1.99	0.44
1:A:388:CYS:SG	1:A:393:ILE:HG22	2.57	0.44
1:A:502:GLN:HA	1:A:505:TYR:CD2	2.52	0.44
1:B:746:PHE:CG	1:C:306:LEU:HD11	2.52	0.44
1:C:239:THR:HG23	1:C:245:SER:HB3	1.99	0.44
1:C:402:ILE:HG22	1:C:403:LEU:N	2.33	0.44
1:C:563:GLN:OE1	1:C:563:GLN:HA	2.16	0.44
1:D:114:TYR:CE1	1:D:153:ILE:HB	2.53	0.44
1:D:269:THR:HG23	1:D:443:LEU:HD22	2.00	0.44
1:E:355:VAL:O	1:E:359:VAL:HG23	2.17	0.44
1:E:711:LEU:O	1:E:715:ARG:HG2	2.18	0.44
1:F:551:THR:CB	1:F:553:THR:HG22	2.48	0.44
1:F:61:LEU:HG	1:F:66:LYS:O	2.18	0.44
1:F:80:PRO:HB2	1:F:82:LYS:HG2	1.99	0.44
1:A:164:MET:SD	1:A:459:SER:HB2	2.57	0.44
1:B:219:GLU:O	1:B:222:LYS:N	2.51	0.44
1:C:316:LEU:O	1:C:317:SER:C	2.55	0.44
1:C:666:GLN:HA	1:C:669:LYS:HD3	1.98	0.44
1:C:767:TYR:CD1	1:C:767:TYR:C	2.90	0.44
1:D:526:GLU:OE1	1:D:530:ARG:HD3	2.17	0.44
1:D:552:ASP:HA	1:D:598:LEU:HD12	1.99	0.44
1:D:393:ILE:HD11	1:D:612:LEU:O	2.17	0.44
1:D:731:ARG:HG2	1:D:756:MET:CE	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:35:VAL:HG12	1:F:47:ALA:O	2.17	0.44
1:F:584:LEU:HD23	1:F:589:LYS:CG	2.37	0.44
1:B:158:ASP:HB2	1:B:193:TYR:CZ	2.53	0.44
1:B:97:GLU:HG2	1:B:711:LEU:CD1	2.48	0.44
1:D:107:ARG:NH1	1:D:114:TYR:O	2.50	0.44
1:D:300:GLN:O	1:D:304:ASP:HB2	2.17	0.44
1:D:327:GLN:HB2	1:D:330:GLU:CD	2.38	0.44
1:D:42:HIS:O	1:D:43:GLY:C	2.55	0.44
1:D:438:LEU:O	1:D:442:ILE:HG13	2.18	0.44
1:D:97:GLU:HG2	1:D:711:LEU:CD1	2.48	0.44
1:E:238:LYS:HB3	1:E:285:ARG:HG2	2.00	0.44
1:E:566:HIS:HD2	1:E:568:LYS:H	1.65	0.44
1:F:388:CYS:SG	1:F:393:ILE:HG22	2.57	0.44
1:F:385:GLN:HA	1:F:395:VAL:HG22	2.00	0.44
1:F:508:GLU:HG3	1:F:771:GLN:N	2.30	0.44
1:B:268:GLU:HG2	1:B:270:TYR:OH	2.18	0.44
1:B:747:MET:CE	1:B:751:GLN:HB3	2.47	0.44
1:C:327:GLN:HB2	1:C:330:GLU:CD	2.38	0.44
1:C:393:ILE:HD11	1:C:613:LEU:HA	1.98	0.44
1:C:434:LYS:HG2	1:C:625:TRP:CZ2	2.53	0.44
1:D:116:TYR:CZ	1:D:146:ARG:HG2	2.53	0.44
1:D:563:GLN:OE1	1:D:563:GLN:HA	2.17	0.44
1:E:756:MET:HB2	1:E:756:MET:HE3	1.56	0.44
1:A:584:LEU:HD23	1:A:589:LYS:CG	2.35	0.44
1:B:242:ASN:OD1	1:B:243:ASP:N	2.51	0.44
1:B:551:THR:CB	1:B:553:THR:HG22	2.47	0.44
1:C:278:ILE:HD12	1:C:428:GLU:HG2	1.99	0.44
3:C:999:ALF:F4	4:C:998:ADP:PB	2.65	0.44
1:D:493:PHE:CZ	1:D:497:MET:HG3	2.52	0.44
1:D:688:ASN:ND2	1:D:692:ARG:O	2.35	0.44
1:E:158:ASP:HB2	1:E:193:TYR:CZ	2.52	0.44
1:E:240:VAL:HG23	1:E:241:LYS:HG2	1.99	0.44
1:E:742:ILE:HG23	1:E:743:PRO:CD	2.47	0.44
1:F:340:THR:HG22	1:F:341:ILE:N	2.33	0.44
1:F:173:ILE:HG13	1:F:461:LEU:HD21	1.99	0.44
1:A:222:LYS:O	1:A:226:GLN:HG2	2.18	0.44
1:A:240:VAL:HG23	1:A:241:LYS:HG2	1.99	0.44
1:B:393:ILE:HD11	1:B:613:LEU:HA	1.99	0.44
1:B:42:HIS:O	1:B:43:GLY:C	2.56	0.44
1:D:251:PHE:CZ	1:D:462:GLY:HA3	2.53	0.44
1:D:545:CYS:SG	1:D:598:LEU:HD23	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:508:GLU:HG3	1:E:771:GLN:N	2.32	0.44
1:E:751:GLN:O	1:E:755:LEU:HG	2.18	0.44
1:E:95:LEU:HD11	1:E:714:ILE:HG21	2.00	0.44
1:F:36:TRP:HB2	1:F:76:GLN:O	2.18	0.44
1:F:427:ILE:HD13	1:F:427:ILE:HA	1.80	0.44
1:F:77:LYS:N	1:F:77:LYS:HZ2	2.14	0.44
1:C:251:PHE:CZ	1:C:462:GLY:HA3	2.53	0.44
1:C:164:MET:SD	1:C:459:SER:HB2	2.58	0.44
1:C:97:GLU:HG2	1:C:711:LEU:CD1	2.48	0.44
1:C:738:ALA:O	1:C:741:ALA:HB2	2.16	0.44
1:D:225:LEU:CD2	1:D:225:LEU:N	2.81	0.44
1:D:738:ALA:O	1:D:741:ALA:HB3	2.17	0.44
1:D:751:GLN:O	1:D:755:LEU:HG	2.18	0.44
1:E:558:LYS:O	1:E:562:GLU:HG2	2.18	0.44
1:E:89:MET:HE1	1:E:100:VAL:HG13	1.98	0.44
1:F:113:ILE:O	1:F:123:VAL:HA	2.18	0.44
1:F:126:PRO:HB3	1:F:130:LEU:HD11	1.99	0.44
1:A:378:MET:HG3	1:A:378:MET:O	2.18	0.43
1:B:495:HIS:CD2	1:B:500:LEU:HG	2.53	0.43
1:C:751:GLN:O	1:C:755:LEU:HG	2.18	0.43
1:E:41:LYS:HG2	1:E:41:LYS:H	1.47	0.43
1:E:508:GLU:HG2	1:E:775:PHE:CE1	2.43	0.43
1:F:116:TYR:CE2	1:F:146:ARG:HG2	2.53	0.43
1:F:355:VAL:O	1:F:359:VAL:HG23	2.17	0.43
1:A:116:TYR:CZ	1:A:146:ARG:HG2	2.53	0.43
1:A:323:ILE:HG22	1:A:324:PRO:N	2.34	0.43
1:A:495:HIS:CD2	1:A:500:LEU:HG	2.54	0.43
1:A:742:ILE:HG23	1:A:743:PRO:CD	2.47	0.43
1:B:289:ILE:HD12	1:B:289:ILE:HA	1.85	0.43
1:B:558:LYS:O	1:B:562:GLU:HG2	2.18	0.43
1:C:35:VAL:HG13	1:C:36:TRP:N	2.32	0.43
1:C:734:TYR:OH	1:C:781:LEU:HD22	2.18	0.43
1:D:508:GLU:HG3	1:D:771:GLN:N	2.33	0.43
1:D:558:LYS:O	1:D:562:GLU:HG2	2.18	0.43
1:D:742:ILE:HG23	1:D:743:PRO:CD	2.47	0.43
1:D:747:MET:CE	1:D:751:GLN:HB3	2.48	0.43
1:E:95:LEU:CD1	1:E:714:ILE:HG21	2.48	0.43
1:F:121:CYS:O	1:F:683:ARG:HG2	2.18	0.43
1:F:717:CYS:O	1:F:778:THR:HG22	2.17	0.43
1:A:727:PHE:HA	1:A:753:CYS:SG	2.57	0.43
1:A:756:MET:HE3	1:A:756:MET:HB2	1.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:VAL:HG11	1:A:75:ILE:CG2	2.49	0.43
1:B:316:LEU:O	1:B:317:SER:C	2.55	0.43
1:B:253:ARG:HG3	1:B:460:PHE:CD1	2.54	0.43
1:B:563:GLN:OE1	1:B:563:GLN:HA	2.16	0.43
1:B:717:CYS:O	1:B:778:THR:HG22	2.18	0.43
1:B:731:ARG:O	1:B:735:GLU:HB2	2.18	0.43
1:C:43:GLY:HA3	1:C:702:LEU:CD1	2.47	0.43
1:D:158:ASP:HB2	1:D:193:TYR:CZ	2.53	0.43
1:D:316:LEU:O	1:D:317:SER:C	2.55	0.43
1:D:381:ASN:O	1:D:382:THR:C	2.57	0.43
1:D:498:PHE:CE2	1:D:519:LEU:HD13	2.52	0.43
1:E:323:ILE:HG22	1:E:324:PRO:HD2	1.90	0.43
1:E:42:HIS:O	1:E:43:GLY:C	2.56	0.43
1:F:42:HIS:O	1:F:43:GLY:C	2.56	0.43
1:F:721:PHE:HB2	1:F:775:PHE:HB3	2.00	0.43
1:A:327:GLN:HB2	1:A:330:GLU:CD	2.39	0.43
1:B:721:PHE:HB2	1:B:775:PHE:HB3	1.99	0.43
1:C:323:ILE:HG22	1:C:324:PRO:N	2.33	0.43
1:D:35:VAL:N	1:D:47:ALA:O	2.51	0.43
1:E:393:ILE:HD11	1:E:613:LEU:HA	1.98	0.43
1:F:391:MET:HE2	1:F:434:LYS:CE	2.48	0.43
1:F:751:GLN:O	1:F:755:LEU:HG	2.19	0.43
1:A:239:THR:HG23	1:A:245:SER:HB3	1.99	0.43
1:A:242:ASN:OD1	1:A:243:ASP:N	2.51	0.43
1:B:181:ALA:N	1:B:686:ILE:HD12	2.32	0.43
1:C:225:LEU:N	1:C:225:LEU:CD2	2.82	0.43
1:C:48:SER:O	1:C:59:VAL:HB	2.19	0.43
1:D:95:LEU:HD11	1:D:714:ILE:HG21	2.00	0.43
1:E:107:ARG:NH1	1:E:114:TYR:O	2.51	0.43
1:E:126:PRO:HB3	1:E:130:LEU:HD11	2.00	0.43
1:E:345:THR:HG23	1:E:348:GLU:OE1	2.19	0.43
1:E:767:TYR:O	1:E:768:ARG:HG2	2.18	0.43
1:F:35:VAL:HG21	1:F:75:ILE:CG2	2.48	0.43
1:A:362:LEU:HA	1:A:362:LEU:HD23	1.88	0.43
1:C:116:TYR:CZ	1:C:146:ARG:HG2	2.54	0.43
1:C:242:ASN:OD1	1:C:243:ASP:N	2.51	0.43
1:C:250:LYS:HD2	1:C:252:ILE:HD11	2.01	0.43
1:C:181:ALA:N	1:C:686:ILE:HD12	2.33	0.43
1:D:35:VAL:HG21	1:D:75:ILE:HG22	2.01	0.43
1:E:228:ASN:O	1:E:229:PRO:C	2.56	0.43
1:E:526:GLU:OE1	1:E:530:ARG:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:717:CYS:O	1:E:778:THR:HG22	2.19	0.43
1:F:242:ASN:OD1	1:F:243:ASP:N	2.51	0.43
1:F:268:GLU:HG2	1:F:270:TYR:OH	2.19	0.43
1:F:278:ILE:HB	1:F:315:PHE:CE1	2.54	0.43
1:A:35:VAL:HG21	1:A:75:ILE:HG22	1.99	0.43
1:A:528:ILE:HG23	1:A:538:LEU:HG	2.00	0.43
1:B:658:THR:O	1:B:662:LEU:HD12	2.19	0.43
1:C:238:LYS:HB3	1:C:285:ARG:HG2	2.01	0.43
1:D:57:VAL:HG12	1:D:59:VAL:HG13	1.99	0.43
1:D:767:TYR:CD1	1:D:767:TYR:C	2.92	0.43
1:D:468:GLY:N	3:D:999:ALF:F1	2.40	0.43
1:E:525:ILE:O	1:E:529:GLU:HG2	2.19	0.43
1:F:225:LEU:N	1:F:225:LEU:CD2	2.80	0.43
1:F:526:GLU:OE1	1:F:530:ARG:HD3	2.19	0.43
1:A:126:PRO:HB3	1:A:130:LEU:HD11	2.01	0.43
1:A:333:GLN:O	1:A:337:GLU:HB2	2.19	0.43
1:A:381:ASN:O	1:A:382:THR:C	2.55	0.43
1:A:493:PHE:CZ	1:A:497:MET:HG3	2.54	0.43
1:A:747:MET:CE	1:A:751:GLN:HB3	2.48	0.43
1:B:300:GLN:O	1:B:304:ASP:HB2	2.18	0.43
1:B:271:LEU:HD22	1:B:481:CYS:HB2	2.00	0.43
1:C:300:GLN:O	1:C:304:ASP:HB2	2.18	0.43
1:C:526:GLU:OE1	1:C:530:ARG:HD3	2.19	0.43
1:D:378:MET:O	1:D:378:MET:HG3	2.19	0.43
1:D:721:PHE:HB2	1:D:775:PHE:HB3	2.00	0.43
1:E:192:GLN:O	1:E:196:VAL:HG23	2.19	0.43
1:E:219:GLU:O	1:E:222:LYS:N	2.52	0.43
1:E:333:GLN:O	1:E:337:GLU:HB2	2.18	0.43
1:F:365:ILE:HG23	1:F:378:MET:HE3	2.01	0.43
1:F:747:MET:CE	1:F:751:GLN:HB3	2.49	0.43
1:A:327:GLN:HE21	1:A:327:GLN:HB3	1.73	0.43
1:B:35:VAL:HG13	1:B:36:TRP:N	2.34	0.43
1:B:493:PHE:CZ	1:B:497:MET:HG3	2.54	0.43
1:B:61:LEU:HG	1:B:66:LYS:O	2.18	0.43
1:B:763:ASP:HB3	1:B:766:LEU:HG	2.01	0.43
1:E:528:ILE:HG23	1:E:538:LEU:HG	2.01	0.43
1:E:708:ASN:ND2	1:E:708:ASN:N	2.65	0.43
1:E:750:LYS:HE3	1:E:769:ILE:HG22	2.01	0.43
1:E:79:ASN:OD1	1:E:93:THR:HB	2.19	0.43
1:F:300:GLN:O	1:F:304:ASP:HB2	2.19	0.43
1:F:528:ILE:HG23	1:F:538:LEU:HG	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:48:SER:O	1:F:59:VAL:HB	2.19	0.43
1:F:57:VAL:HG12	1:F:59:VAL:HG13	2.00	0.43
1:B:172:SER:HA	1:B:462:GLY:O	2.18	0.43
1:B:688:ASN:ND2	1:B:692:ARG:O	2.36	0.43
1:C:493:PHE:CZ	1:C:497:MET:HG3	2.54	0.43
1:C:605:LEU:HD12	1:C:605:LEU:HA	1.85	0.43
1:D:323:ILE:HG22	1:D:324:PRO:N	2.34	0.43
1:F:767:TYR:O	1:F:768:ARG:HG2	2.18	0.43
1:A:113:ILE:O	1:A:123:VAL:HA	2.19	0.42
1:A:419:THR:H	1:A:422:GLN:CG	2.26	0.42
1:A:274:LYS:CG	1:A:436:GLU:HB2	2.46	0.42
1:A:767:TYR:C	1:A:767:TYR:CD1	2.91	0.42
1:B:339:MET:HE2	1:B:352:ILE:HD13	2.01	0.42
1:C:528:ILE:HG23	1:C:538:LEU:HG	2.01	0.42
1:E:747:MET:HE3	1:E:751:GLN:HB3	2.01	0.42
1:F:172:SER:HA	1:F:462:GLY:O	2.19	0.42
1:F:495:HIS:CD2	1:F:500:LEU:HG	2.54	0.42
1:F:731:ARG:CG	1:F:731:ARG:HH11	2.30	0.42
1:A:172:SER:HA	1:A:462:GLY:O	2.19	0.42
1:B:323:ILE:HG22	1:B:324:PRO:N	2.33	0.42
1:B:48:SER:O	1:B:59:VAL:HB	2.19	0.42
1:C:355:VAL:O	1:C:359:VAL:HG23	2.19	0.42
1:E:544:GLU:HA	1:E:544:GLU:OE1	2.20	0.42
1:E:721:PHE:HB2	1:E:775:PHE:HB3	2.01	0.42
1:F:526:GLU:HA	1:F:526:GLU:OE1	2.18	0.42
1:A:731:ARG:O	1:A:735:GLU:HB2	2.20	0.42
1:B:126:PRO:HB3	1:B:130:LEU:HD11	2.01	0.42
1:B:225:LEU:CD2	1:B:225:LEU:N	2.82	0.42
1:B:164:MET:SD	1:B:459:SER:HB2	2.59	0.42
1:C:291:TYR:HA	1:C:310:PHE:HE1	1.84	0.42
1:B:746:PHE:CD1	1:C:306:LEU:HD11	2.54	0.42
1:C:58:THR:HA	1:C:69:THR:HA	2.01	0.42
1:C:747:MET:CE	1:C:751:GLN:HB3	2.49	0.42
1:D:345:THR:HG23	1:D:348:GLU:OE1	2.19	0.42
1:D:271:LEU:HD22	1:D:481:CYS:HB2	2.02	0.42
1:D:731:ARG:O	1:D:735:GLU:HB2	2.19	0.42
1:D:80:PRO:HB2	1:D:82:LYS:HG2	2.01	0.42
1:E:116:TYR:CZ	1:E:146:ARG:HG2	2.55	0.42
1:E:756:MET:O	1:E:760:LEU:HG	2.19	0.42
1:E:36:TRP:HB2	1:E:76:GLN:O	2.19	0.42
1:F:192:GLN:O	1:F:196:VAL:HG23	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:508:GLU:HG2	1:F:775:PHE:CE1	2.45	0.42
1:F:527:LEU:HB2	1:F:566:HIS:CE1	2.55	0.42
1:F:563:GLN:HA	1:F:563:GLN:OE1	2.19	0.42
1:A:537:VAL:HG22	1:A:559:LEU:CD1	2.47	0.42
1:A:750:LYS:HE3	1:A:769:ILE:HG22	2.01	0.42
1:B:173:ILE:HG13	1:B:461:LEU:HD21	2.00	0.42
1:B:239:THR:HG23	1:B:245:SER:HB3	2.00	0.42
1:B:525:ILE:O	1:B:529:GLU:CG	2.67	0.42
1:C:525:ILE:O	1:C:529:GLU:HG2	2.19	0.42
1:D:162:ARG:HG2	1:D:162:ARG:H	1.68	0.42
1:D:290:PHE:CE1	1:D:356:VAL:HG13	2.54	0.42
1:D:401:SER:HB3	1:D:608:ASN:CB	2.48	0.42
1:D:61:LEU:HG	1:D:66:LYS:O	2.19	0.42
1:E:381:ASN:O	1:E:382:THR:C	2.56	0.42
1:A:117:SER:OG	1:A:120:PHE:CE2	2.73	0.42
1:A:339:MET:CE	1:A:352:ILE:HD13	2.49	0.42
1:A:605:LEU:HA	1:A:605:LEU:HD12	1.88	0.42
1:B:35:VAL:HG21	1:B:75:ILE:CG2	2.49	0.42
1:C:271:LEU:HD22	1:C:481:CYS:CB	2.49	0.42
1:C:495:HIS:CD2	1:C:500:LEU:HG	2.55	0.42
1:E:724:ARG:HG3	1:E:724:ARG:O	2.20	0.42
1:E:747:MET:CE	1:E:751:GLN:HB3	2.48	0.42
1:F:525:ILE:O	1:F:529:GLU:HG2	2.20	0.42
1:F:738:ALA:CB	1:F:741:ALA:HB2	2.47	0.42
1:A:253:ARG:HG3	1:A:460:PHE:CD1	2.54	0.42
1:B:292:TYR:CE2	1:B:331:MET:HB3	2.54	0.42
1:B:528:ILE:HG23	1:B:538:LEU:HG	2.01	0.42
1:B:690:GLU:C	1:B:692:ARG:N	2.70	0.42
1:B:711:LEU:O	1:B:715:ARG:HG2	2.20	0.42
1:C:333:GLN:O	1:C:337:GLU:HB2	2.19	0.42
1:C:36:TRP:HB2	1:C:76:GLN:O	2.20	0.42
1:C:385:GLN:HA	1:C:395:VAL:HG22	2.00	0.42
1:C:558:LYS:O	1:C:562:GLU:HG2	2.19	0.42
1:C:750:LYS:HE3	1:C:769:ILE:HG22	2.01	0.42
1:D:219:GLU:O	1:D:222:LYS:N	2.52	0.42
1:D:236:ASN:ND2	1:D:244:ASN:O	2.52	0.42
1:D:172:SER:HA	1:D:462:GLY:O	2.20	0.42
1:E:173:ILE:HG13	1:E:461:LEU:HD21	2.00	0.42
1:E:225:LEU:CD2	1:E:225:LEU:N	2.82	0.42
1:E:327:GLN:HB2	1:E:330:GLU:CD	2.40	0.42
1:E:339:MET:CE	1:E:352:ILE:HD13	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:391:MET:HE2	1:E:434:LYS:CE	2.48	0.42
1:E:545:CYS:SG	1:E:598:LEU:HD23	2.60	0.42
1:F:254:ILE:O	1:F:460:PHE:HA	2.20	0.42
1:F:724:ARG:HG3	1:F:724:ARG:O	2.20	0.42
1:F:767:TYR:C	1:F:767:TYR:CD1	2.92	0.42
1:F:97:GLU:HG2	1:F:711:LEU:CD1	2.49	0.42
1:A:192:GLN:O	1:A:196:VAL:HG23	2.19	0.42
1:A:61:LEU:HG	1:A:66:LYS:O	2.20	0.42
1:A:763:ASP:HB3	1:A:766:LEU:HG	2.01	0.42
1:B:333:GLN:O	1:B:337:GLU:HB2	2.19	0.42
1:B:393:ILE:HD11	1:B:612:LEU:O	2.19	0.42
1:B:41:LYS:HG2	1:B:41:LYS:H	1.44	0.42
1:B:502:GLN:HA	1:B:505:TYR:CD2	2.54	0.42
1:B:750:LYS:HE3	1:B:769:ILE:HG22	2.02	0.42
1:C:427:ILE:HA	1:C:427:ILE:HD13	1.75	0.42
1:C:742:ILE:HG12	1:C:752:ALA:HB1	2.00	0.42
1:D:291:TYR:HA	1:D:310:PHE:HE1	1.84	0.42
1:D:253:ARG:HG3	1:D:460:PHE:CD1	2.54	0.42
1:D:743:PRO:HD2	1:D:747:MET:SD	2.60	0.42
1:E:278:ILE:HD12	1:E:428:GLU:HG2	2.00	0.42
1:F:34:LEU:HA	1:F:34:LEU:HD12	1.75	0.42
1:F:434:LYS:HG2	1:F:625:TRP:CZ2	2.55	0.42
1:F:756:MET:HB2	1:F:756:MET:HE3	1.57	0.42
1:A:308:GLU:HB3	1:A:312:ASN:CB	2.48	0.42
1:A:401:SER:HB3	1:A:608:ASN:CB	2.47	0.42
1:A:393:ILE:HD11	1:A:612:LEU:O	2.20	0.42
1:A:671:MET:O	1:A:675:ARG:HD2	2.20	0.42
1:A:743:PRO:HD2	1:A:747:MET:SD	2.60	0.42
1:B:340:THR:HG22	1:B:341:ILE:N	2.35	0.42
1:B:388:CYS:SG	1:B:393:ILE:HG22	2.60	0.42
1:B:526:GLU:OE1	1:B:530:ARG:HD3	2.19	0.42
1:B:545:CYS:SG	1:B:598:LEU:HD23	2.59	0.42
1:B:742:ILE:HG12	1:B:752:ALA:HB1	2.02	0.42
1:C:540:LEU:HD12	1:C:559:LEU:CD1	2.50	0.42
1:C:717:CYS:O	1:C:778:THR:HG22	2.19	0.42
1:C:80:PRO:HB2	1:C:82:LYS:HG2	2.01	0.42
1:D:117:SER:OG	1:D:120:PHE:CE2	2.72	0.42
1:E:671:MET:O	1:E:675:ARG:HD2	2.20	0.42
1:E:690:GLU:C	1:E:692:ARG:N	2.73	0.42
1:A:107:ARG:HD3	1:A:115:THR:OG1	2.20	0.42
1:A:271:LEU:HD22	1:A:481:CYS:CB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:690:GLU:C	1:A:692:ARG:N	2.72	0.42
1:B:385:GLN:HA	1:B:395:VAL:HG22	2.02	0.42
1:B:58:THR:OG1	1:B:69:THR:HG23	2.20	0.42
1:C:222:LYS:O	1:C:226:GLN:HG2	2.19	0.42
1:C:274:LYS:CG	1:C:436:GLU:HB2	2.47	0.42
1:D:385:GLN:HA	1:D:395:VAL:HG22	2.02	0.42
1:D:402:ILE:HG22	1:D:403:LEU:N	2.33	0.42
1:E:162:ARG:HG2	1:E:162:ARG:H	1.64	0.42
1:E:401:SER:HB3	1:E:608:ASN:CB	2.45	0.42
1:E:417:ALA:C	1:E:418:GLN:HE21	2.22	0.42
1:E:747:MET:HE3	1:E:751:GLN:CB	2.50	0.42
1:E:97:GLU:HG2	1:E:711:LEU:CD1	2.49	0.42
1:F:226:GLN:C	1:F:229:PRO:HD2	2.40	0.42
1:F:228:ASN:O	1:F:229:PRO:C	2.56	0.42
1:A:42:HIS:O	1:A:43:GLY:C	2.58	0.42
1:B:274:LYS:CG	1:B:436:GLU:HB2	2.48	0.42
1:B:671:MET:O	1:B:675:ARG:HD2	2.19	0.42
1:D:290:PHE:HD1	1:D:360:LEU:HD11	1.85	0.42
1:D:121:CYS:O	1:D:683:ARG:HG2	2.20	0.42
1:E:385:GLN:HA	1:E:395:VAL:HG22	2.01	0.42
1:E:402:ILE:HD13	1:E:402:ILE:HA	1.93	0.42
1:E:61:LEU:O	1:E:65:GLY:CA	2.68	0.42
1:A:527:LEU:HB2	1:A:566:HIS:CE1	2.54	0.41
1:B:113:ILE:O	1:B:123:VAL:HA	2.20	0.41
1:B:58:THR:HA	1:B:69:THR:HA	2.02	0.41
1:B:742:ILE:HG23	1:B:743:PRO:CD	2.47	0.41
1:B:753:CYS:HA	1:B:756:MET:HE3	2.01	0.41
1:C:593:ASN:C	1:C:593:ASN:ND2	2.73	0.41
1:C:743:PRO:HD2	1:C:747:MET:SD	2.60	0.41
1:D:173:ILE:HG13	1:D:461:LEU:HD21	2.02	0.41
1:D:43:GLY:HA3	1:D:702:LEU:CD1	2.49	0.41
1:D:72:LYS:O	1:D:75:ILE:HD12	2.20	0.41
1:E:38:PRO:HD3	1:E:74:ASP:O	2.20	0.41
1:E:271:LEU:HD22	1:E:481:CYS:CB	2.50	0.41
1:A:185:GLU:O	1:A:189:LYS:HG2	2.20	0.41
1:A:438:LEU:O	1:A:442:ILE:HG13	2.20	0.41
1:A:721:PHE:CB	1:A:775:PHE:HB3	2.50	0.41
1:A:784:LEU:HA	1:A:784:LEU:HD23	1.89	0.41
1:B:107:ARG:NH1	1:B:114:TYR:O	2.54	0.41
1:B:291:TYR:HA	1:B:310:PHE:HE1	1.85	0.41
1:D:226:GLN:HB2	1:D:342:MET:HE2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:525:ILE:O	1:D:529:GLU:HG2	2.20	0.41
1:D:58:THR:OG1	1:D:69:THR:HG23	2.20	0.41
1:E:323:ILE:HG22	1:E:324:PRO:N	2.34	0.41
1:E:362:LEU:HD23	1:E:387:VAL:HG21	2.01	0.41
1:E:606:ASN:O	1:E:609:VAL:HG13	2.21	0.41
1:E:77:LYS:N	1:E:77:LYS:HZ2	2.18	0.41
1:F:362:LEU:HA	1:F:362:LEU:HD23	1.90	0.41
1:F:609:VAL:O	1:F:612:LEU:HB2	2.19	0.41
1:F:742:ILE:HG23	1:F:743:PRO:CD	2.51	0.41
1:A:181:ALA:N	1:A:686:ILE:HD12	2.34	0.41
1:A:385:GLN:HA	1:A:395:VAL:HG22	2.02	0.41
1:A:38:PRO:HD3	1:A:74:ASP:O	2.21	0.41
1:A:525:ILE:O	1:A:529:GLU:CG	2.68	0.41
1:A:558:LYS:O	1:A:562:GLU:HG2	2.20	0.41
1:A:77:LYS:H	1:A:77:LYS:CD	2.32	0.41
1:B:192:GLN:O	1:B:196:VAL:HG23	2.20	0.41
1:B:605:LEU:HA	1:B:605:LEU:HD12	1.85	0.41
1:B:35:VAL:CG2	1:B:75:ILE:HG22	2.51	0.41
1:C:340:THR:HG22	1:C:341:ILE:N	2.36	0.41
1:C:727:PHE:HA	1:C:753:CYS:SG	2.59	0.41
1:D:333:GLN:O	1:D:337:GLU:HB2	2.20	0.41
1:D:362:LEU:HD23	1:D:362:LEU:HA	1.87	0.41
1:D:690:GLU:C	1:D:692:ARG:N	2.72	0.41
1:E:172:SER:HA	1:E:462:GLY:O	2.20	0.41
1:E:434:LYS:HG2	1:E:625:TRP:CZ2	2.54	0.41
1:E:467:ALA:HB3	1:E:482:ILE:HG12	2.02	0.41
1:F:715:ARG:CG	1:F:715:ARG:NH1	2.81	0.41
1:B:738:ALA:O	1:B:741:ALA:HB3	2.17	0.41
1:D:300:GLN:O	1:D:303:ASN:ND2	2.53	0.41
1:D:183:LYS:HZ1	1:D:468:GLY:HA3	1.86	0.41
1:D:508:GLU:HG2	1:D:775:PHE:CE1	2.43	0.41
1:E:88:ASP:HA	1:E:116:TYR:O	2.20	0.41
1:F:303:ASN:C	1:F:303:ASN:HD22	2.24	0.41
1:F:671:MET:O	1:F:675:ARG:HD2	2.20	0.41
1:F:721:PHE:CB	1:F:775:PHE:HB3	2.51	0.41
1:B:345:THR:HG23	1:B:348:GLU:OE1	2.21	0.41
1:B:721:PHE:CB	1:B:775:PHE:HB3	2.51	0.41
1:C:527:LEU:HB2	1:C:566:HIS:CE1	2.55	0.41
1:C:393:ILE:HD11	1:C:612:LEU:O	2.20	0.41
1:E:527:LEU:HB2	1:E:566:HIS:CE1	2.55	0.41
1:F:616:SER:C	1:F:618:ASP:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:THR:HA	1:A:69:THR:HA	2.02	0.41
1:B:114:TYR:CE1	1:B:153:ILE:HB	2.55	0.41
1:B:271:LEU:HD22	1:B:481:CYS:CB	2.50	0.41
1:B:238:LYS:HB3	1:B:285:ARG:HD3	2.03	0.41
1:B:756:MET:HE3	1:B:756:MET:HB2	1.55	0.41
1:C:192:GLN:O	1:C:196:VAL:HG23	2.20	0.41
1:D:116:TYR:CE2	1:D:146:ARG:HG2	2.55	0.41
1:D:192:GLN:O	1:D:196:VAL:HG23	2.20	0.41
1:D:327:GLN:HE21	1:D:327:GLN:HB3	1.73	0.41
1:D:35:VAL:HG22	1:D:76:GLN:O	2.19	0.41
1:E:300:GLN:O	1:E:304:ASP:HB2	2.20	0.41
1:E:340:THR:HG22	1:E:341:ILE:N	2.35	0.41
1:E:438:LEU:O	1:E:442:ILE:HG13	2.20	0.41
1:E:743:PRO:HD2	1:E:747:MET:SD	2.61	0.41
1:E:781:LEU:HD23	1:E:784:LEU:HD12	2.01	0.41
1:F:289:ILE:HA	1:F:289:ILE:HD12	1.81	0.41
1:F:658:THR:O	1:F:662:LEU:HD12	2.21	0.41
1:A:254:ILE:O	1:A:460:PHE:HA	2.21	0.41
1:C:82:LYS:HB3	1:C:82:LYS:HE2	1.90	0.41
1:D:226:GLN:C	1:D:229:PRO:HD2	2.40	0.41
1:D:292:TYR:CE2	1:D:331:MET:HB3	2.56	0.41
1:D:417:ALA:C	1:D:418:GLN:HE21	2.24	0.41
1:D:528:ILE:HG23	1:D:538:LEU:HG	2.02	0.41
1:D:701:VAL:O	1:D:705:LEU:HG	2.19	0.41
1:E:254:ILE:O	1:E:460:PHE:HA	2.20	0.41
1:E:61:LEU:HG	1:E:66:LYS:O	2.20	0.41
1:E:121:CYS:O	1:E:683:ARG:HG2	2.21	0.41
1:B:362:LEU:HD23	1:B:362:LEU:HA	1.86	0.41
1:B:566:HIS:O	1:B:569:PHE:N	2.53	0.41
1:D:434:LYS:HG2	1:D:625:TRP:CZ2	2.56	0.41
1:E:222:LYS:O	1:E:226:GLN:HG2	2.21	0.41
1:E:540:LEU:HD12	1:E:559:LEU:CD1	2.51	0.41
1:A:419:THR:O	1:A:420:LYS:C	2.59	0.41
1:A:677:THR:O	1:A:679:PRO:HD3	2.21	0.41
1:A:742:ILE:HG12	1:A:752:ALA:HB1	2.03	0.41
1:B:107:ARG:HD3	1:B:115:THR:OG1	2.21	0.41
1:B:34:LEU:HA	1:B:34:LEU:HD12	1.74	0.41
1:C:671:MET:O	1:C:675:ARG:HD2	2.21	0.41
1:D:419:THR:O	1:D:420:LYS:C	2.58	0.41
1:D:663:TYR:CE2	1:D:667:LEU:HD22	2.56	0.41
1:E:291:TYR:HA	1:E:310:PHE:HE1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:297:ALA:HB3	1:E:302:ARG:HD2	2.03	0.41
1:E:731:ARG:CG	1:E:731:ARG:HH11	2.29	0.41
1:F:107:ARG:NH1	1:F:114:TYR:O	2.54	0.41
1:F:117:SER:OG	1:F:120:PHE:CE2	2.72	0.41
1:A:159:THR:O	1:A:163:SER:HB2	2.21	0.41
1:A:35:VAL:HG21	1:A:75:ILE:CG2	2.51	0.41
1:A:427:ILE:HD13	1:A:427:ILE:HA	1.75	0.41
1:B:527:LEU:HB2	1:B:566:HIS:CE1	2.56	0.41
1:C:113:ILE:O	1:C:123:VAL:HA	2.21	0.41
1:C:41:LYS:HG2	1:C:41:LYS:H	1.46	0.41
1:F:114:TYR:CE1	1:F:153:ILE:HB	2.56	0.41
1:F:310:PHE:CE1	1:F:320:HIS:HD2	2.39	0.41
1:F:731:ARG:HA	1:F:756:MET:HE1	2.03	0.41
1:A:225:LEU:N	1:A:225:LEU:CD2	2.82	0.41
1:A:552:ASP:HA	1:A:598:LEU:HD12	2.03	0.41
1:A:121:CYS:O	1:A:683:ARG:HG2	2.21	0.41
1:B:434:LYS:HG2	1:B:625:TRP:CZ2	2.53	0.41
1:B:743:PRO:HD2	1:B:747:MET:SD	2.60	0.41
1:B:36:TRP:HB2	1:B:76:GLN:O	2.21	0.41
1:B:90:ALA:O	1:B:718:ARG:NH1	2.53	0.41
1:C:184:THR:HG22	1:C:188:LYS:HE3	2.02	0.41
1:C:365:ILE:HG23	1:C:378:MET:HE3	2.03	0.41
1:C:403:LEU:HD23	1:C:403:LEU:HA	1.94	0.41
1:C:38:PRO:HD3	1:C:74:ASP:O	2.21	0.41
1:C:781:LEU:HD23	1:C:784:LEU:HD12	2.02	0.41
1:E:239:THR:HG23	1:E:245:SER:HB3	2.03	0.41
1:E:35:VAL:HG21	1:E:75:ILE:HG22	2.02	0.41
1:E:164:MET:SD	1:E:459:SER:HB2	2.61	0.41
1:F:393:ILE:HD11	1:F:612:LEU:O	2.21	0.41
1:A:721:PHE:CD1	1:A:721:PHE:N	2.89	0.40
1:A:79:ASN:OD1	1:A:93:THR:HB	2.21	0.40
1:B:763:ASP:OD1	1:B:764:PRO:HD2	2.21	0.40
1:C:226:GLN:C	1:C:229:PRO:HD2	2.41	0.40
1:C:419:THR:H	1:C:422:GLN:CG	2.26	0.40
1:D:145:LYS:CB	1:D:148:GLU:HG3	2.43	0.40
1:D:58:THR:HA	1:D:69:THR:HA	2.02	0.40
1:F:291:TYR:HA	1:F:310:PHE:HE1	1.85	0.40
1:F:690:GLU:C	1:F:692:ARG:N	2.72	0.40
1:A:340:THR:HG22	1:A:341:ILE:N	2.36	0.40
1:A:606:ASN:O	1:A:609:VAL:HG13	2.21	0.40
1:A:125:ASN:O	1:A:687:PRO:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:747:MET:CE	1:A:751:GLN:CB	3.00	0.40
1:C:35:VAL:HG21	1:C:75:ILE:CG2	2.51	0.40
1:C:690:GLU:C	1:C:692:ARG:N	2.73	0.40
1:C:747:MET:HG3	1:C:752:ALA:HB2	2.03	0.40
1:C:721:PHE:HB2	1:C:775:PHE:HB3	2.02	0.40
1:D:184:THR:HG22	1:D:188:LYS:HE3	2.03	0.40
1:E:402:ILE:HG22	1:E:403:LEU:N	2.36	0.40
1:E:35:VAL:N	1:E:47:ALA:O	2.51	0.40
1:F:167:ASP:HB2	1:F:169:GLU:HG2	2.03	0.40
1:F:323:ILE:HG22	1:F:324:PRO:N	2.35	0.40
1:F:345:THR:HG23	1:F:348:GLU:OE1	2.21	0.40
1:F:734:TYR:OH	1:F:781:LEU:HD22	2.21	0.40
1:A:445:ARG:HH12	1:A:449:ALA:HB2	1.86	0.40
1:A:541:LEU:O	1:A:544:GLU:N	2.54	0.40
1:C:107:ARG:HD3	1:C:115:THR:OG1	2.21	0.40
1:C:228:ASN:O	1:C:229:PRO:C	2.59	0.40
1:C:35:VAL:N	1:C:47:ALA:O	2.55	0.40
1:C:61:LEU:O	1:C:65:GLY:CA	2.70	0.40
1:C:742:ILE:HG23	1:C:743:PRO:CD	2.47	0.40
1:D:126:PRO:HB3	1:D:130:LEU:HD11	2.03	0.40
1:D:185:GLU:O	1:D:189:LYS:HG2	2.22	0.40
1:D:38:PRO:HD3	1:D:74:ASP:O	2.22	0.40
1:E:493:PHE:CZ	1:E:497:MET:HG3	2.56	0.40
1:E:721:PHE:CB	1:E:775:PHE:HB3	2.50	0.40
1:F:185:GLU:O	1:F:189:LYS:HG2	2.21	0.40
1:F:333:GLN:O	1:F:337:GLU:HB2	2.20	0.40
1:A:228:ASN:O	1:A:229:PRO:C	2.60	0.40
1:C:285:ARG:HB2	1:C:291:TYR:CE2	2.56	0.40
1:C:525:ILE:O	1:C:529:GLU:CG	2.70	0.40
1:E:35:VAL:HG11	1:E:75:ILE:CG2	2.51	0.40
1:E:378:MET:O	1:E:378:MET:HG3	2.22	0.40
1:A:526:GLU:OE1	1:A:530:ARG:HD3	2.22	0.40
1:A:701:VAL:O	1:A:705:LEU:HG	2.21	0.40
1:B:236:ASN:ND2	1:B:244:ASN:O	2.55	0.40
1:C:339:MET:CE	1:C:352:ILE:HD13	2.52	0.40
1:C:378:MET:HE1	1:C:384:ALA:CB	2.48	0.40
1:E:278:ILE:CD1	1:E:432:LYS:HD3	2.52	0.40
1:E:58:THR:HA	1:E:69:THR:HA	2.04	0.40
1:F:316:LEU:O	1:F:317:SER:C	2.60	0.40
1:F:544:GLU:HA	1:F:544:GLU:OE1	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	655/791 (83%)	582 (89%)	63 (10%)	10 (2%)	10	34
1	B	655/791 (83%)	586 (90%)	59 (9%)	10 (2%)	10	34
1	C	655/791 (83%)	583 (89%)	63 (10%)	9 (1%)	11	36
1	D	655/791 (83%)	583 (89%)	62 (10%)	10 (2%)	10	34
1	E	655/791 (83%)	581 (89%)	62 (10%)	12 (2%)	8	29
1	F	655/791 (83%)	585 (89%)	59 (9%)	11 (2%)	9	31
All	All	3930/4746 (83%)	3500 (89%)	368 (9%)	62 (2%)	9	32

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	317	SER
1	A	324	PRO
1	A	533	ASN
1	A	564	GLY
1	B	317	SER
1	B	324	PRO
1	B	533	ASN
1	B	564	GLY
1	C	317	SER
1	C	324	PRO
1	C	533	ASN
1	C	564	GLY
1	D	317	SER
1	D	324	PRO
1	D	533	ASN
1	D	564	GLY
1	E	317	SER
1	E	533	ASN
1	E	564	GLY
1	F	317	SER

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Mol	Chain	Res	Type
1	F	324	PRO
1	F	533	ASN
1	F	564	GLY
1	A	319	GLY
1	A	530	ARG
1	A	607	ASP
1	B	319	GLY
1	B	530	ARG
1	B	607	ASP
1	C	319	GLY
1	C	530	ARG
1	C	607	ASP
1	D	319	GLY
1	D	530	ARG
1	E	319	GLY
1	E	324	PRO
1	E	607	ASP
1	F	319	GLY
1	F	607	ASP
1	D	607	ASP
1	E	531	PRO
1	F	531	PRO
1	A	531	PRO
1	B	531	PRO
1	C	531	PRO
1	D	531	PRO
1	E	530	ARG
1	F	530	ARG
1	A	523	PRO
1	B	523	PRO
1	C	523	PRO
1	D	265	ALA
1	D	523	PRO
1	E	265	ALA
1	E	523	PRO
1	F	271	LEU
1	F	523	PRO
1	A	271	LEU
1	B	271	LEU
1	E	271	LEU
1	E	566	HIS
1	F	566	HIS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	555/696 (80%)	462 (83%)	93 (17%)	2	6
1	B	555/696 (80%)	463 (83%)	92 (17%)	2	7
1	C	555/696 (80%)	461 (83%)	94 (17%)	2	6
1	D	555/696 (80%)	463 (83%)	92 (17%)	2	7
1	E	555/696 (80%)	463 (83%)	92 (17%)	2	7
1	F	555/696 (80%)	460 (83%)	95 (17%)	2	6
All	All	3330/4176 (80%)	2772 (83%)	558 (17%)	2	6

All (558) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	35	VAL
1	A	39	SER
1	A	41	LYS
1	A	42	HIS
1	A	48	SER
1	A	77	LYS
1	A	82	LYS
1	A	86	VAL
1	A	91	GLU
1	A	110	SER
1	A	124	ILE
1	A	127	TYR
1	A	128	LYS
1	A	135	GLU
1	A	142	LYS
1	A	145	LYS
1	A	166	GLN
1	A	167	ASP
1	A	174	LEU
1	A	189	LYS
1	A	199	SER

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Mol	Chain	Res	Type
1	A	225	LEU
1	A	232	GLU
1	A	250	LYS
1	A	259	THR
1	A	268	GLU
1	A	274	LYS
1	A	275	SER
1	A	278	ILE
1	A	285	ARG
1	A	302	ARG
1	A	303	ASN
1	A	308	GLU
1	A	311	ASN
1	A	314	THR
1	A	317	SER
1	A	323	ILE
1	A	326	GLN
1	A	327	GLN
1	A	329	ASP
1	A	340	THR
1	A	377	SER
1	A	393	ILE
1	A	402	ILE
1	A	404	THR
1	A	419	THR
1	A	422	GLN
1	A	434	LYS
1	A	459	SER
1	A	460	PHE
1	A	473	GLU
1	A	484	TYR
1	A	488	LYS
1	A	499	ILE
1	A	501	GLU
1	A	504	GLU
1	A	506	GLN
1	A	522	GLN
1	A	544	GLU
1	A	545	CYS
1	A	554	SER
1	A	560	ILE
1	A	572	SER

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Mol	Chain	Res	Type
1	A	589	LYS
1	A	591	THR
1	A	593	ASN
1	A	599	THR
1	A	606	ASN
1	A	607	ASP
1	A	608	ASN
1	A	609	VAL
1	A	615	GLN
1	A	623	ASP
1	A	664	LYS
1	A	675	ARG
1	A	683	ARG
1	A	702	LEU
1	A	708	ASN
1	A	719	GLN
1	A	723	ASN
1	A	731	ARG
1	A	732	GLN
1	A	733	ARG
1	A	735	GLU
1	A	748	ASP
1	A	750	LYS
1	A	754	ILE
1	A	755	LEU
1	A	771	GLN
1	A	773	LYS
1	A	778	THR
1	A	788	ARG
1	B	34	LEU
1	B	35	VAL
1	B	39	SER
1	B	41	LYS
1	B	42	HIS
1	B	48	SER
1	B	77	LYS
1	B	82	LYS
1	B	86	VAL
1	B	91	GLU
1	B	110	SER
1	B	124	ILE
1	B	127	TYR

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Mol	Chain	Res	Type
1	B	128	LYS
1	B	135	GLU
1	B	142	LYS
1	B	145	LYS
1	B	166	GLN
1	B	167	ASP
1	B	174	LEU
1	B	189	LYS
1	B	199	SER
1	B	225	LEU
1	B	232	GLU
1	B	250	LYS
1	B	259	THR
1	B	268	GLU
1	B	274	LYS
1	B	275	SER
1	B	278	ILE
1	B	285	ARG
1	B	302	ARG
1	B	303	ASN
1	B	308	GLU
1	B	311	ASN
1	B	314	THR
1	B	317	SER
1	B	323	ILE
1	B	326	GLN
1	B	327	GLN
1	B	329	ASP
1	B	340	THR
1	B	377	SER
1	B	393	ILE
1	B	402	ILE
1	B	404	THR
1	B	419	THR
1	B	422	GLN
1	B	434	LYS
1	B	459	SER
1	B	473	GLU
1	B	484	TYR
1	B	488	LYS
1	B	499	ILE
1	B	501	GLU

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Mol	Chain	Res	Type
1	B	504	GLU
1	B	506	GLN
1	B	522	GLN
1	B	544	GLU
1	B	545	CYS
1	B	554	SER
1	B	560	ILE
1	B	572	SER
1	B	589	LYS
1	B	591	THR
1	B	593	ASN
1	B	599	THR
1	B	605	LEU
1	B	606	ASN
1	B	607	ASP
1	B	608	ASN
1	B	609	VAL
1	B	615	GLN
1	B	623	ASP
1	B	664	LYS
1	B	675	ARG
1	B	683	ARG
1	B	708	ASN
1	B	719	GLN
1	B	723	ASN
1	B	731	ARG
1	B	732	GLN
1	B	733	ARG
1	B	735	GLU
1	B	748	ASP
1	B	750	LYS
1	B	754	ILE
1	B	755	LEU
1	B	771	GLN
1	B	773	LYS
1	B	778	THR
1	B	788	ARG
1	C	34	LEU
1	C	35	VAL
1	C	39	SER
1	C	41	LYS
1	C	42	HIS

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Mol	Chain	Res	Type
1	C	48	SER
1	C	77	LYS
1	C	82	LYS
1	C	86	VAL
1	C	91	GLU
1	C	110	SER
1	C	124	ILE
1	C	127	TYR
1	C	128	LYS
1	C	135	GLU
1	C	142	LYS
1	C	145	LYS
1	C	166	GLN
1	C	167	ASP
1	C	174	LEU
1	C	189	LYS
1	C	199	SER
1	C	225	LEU
1	C	232	GLU
1	C	250	LYS
1	C	259	THR
1	C	268	GLU
1	C	274	LYS
1	C	275	SER
1	C	278	ILE
1	C	285	ARG
1	C	302	ARG
1	C	303	ASN
1	C	308	GLU
1	C	311	ASN
1	C	314	THR
1	C	317	SER
1	C	323	ILE
1	C	326	GLN
1	C	327	GLN
1	C	329	ASP
1	C	340	THR
1	C	377	SER
1	C	393	ILE
1	C	402	ILE
1	C	404	THR
1	C	419	THR

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Mol	Chain	Res	Type
1	C	422	GLN
1	C	434	LYS
1	C	459	SER
1	C	460	PHE
1	C	473	GLU
1	C	484	TYR
1	C	488	LYS
1	C	499	ILE
1	C	501	GLU
1	C	504	GLU
1	C	506	GLN
1	C	522	GLN
1	C	544	GLU
1	C	545	CYS
1	C	554	SER
1	C	560	ILE
1	C	572	SER
1	C	589	LYS
1	C	591	THR
1	C	593	ASN
1	C	599	THR
1	C	605	LEU
1	C	606	ASN
1	C	607	ASP
1	C	608	ASN
1	C	609	VAL
1	C	615	GLN
1	C	623	ASP
1	C	664	LYS
1	C	675	ARG
1	C	683	ARG
1	C	702	LEU
1	C	708	ASN
1	C	719	GLN
1	C	723	ASN
1	C	731	ARG
1	C	732	GLN
1	C	733	ARG
1	C	735	GLU
1	C	748	ASP
1	C	750	LYS
1	C	754	ILE

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Mol	Chain	Res	Type
1	C	755	LEU
1	C	771	GLN
1	C	773	LYS
1	C	778	THR
1	C	788	ARG
1	D	34	LEU
1	D	35	VAL
1	D	39	SER
1	D	41	LYS
1	D	42	HIS
1	D	48	SER
1	D	77	LYS
1	D	82	LYS
1	D	86	VAL
1	D	91	GLU
1	D	110	SER
1	D	124	ILE
1	D	127	TYR
1	D	128	LYS
1	D	135	GLU
1	D	142	LYS
1	D	145	LYS
1	D	166	GLN
1	D	167	ASP
1	D	174	LEU
1	D	189	LYS
1	D	199	SER
1	D	225	LEU
1	D	232	GLU
1	D	250	LYS
1	D	259	THR
1	D	268	GLU
1	D	274	LYS
1	D	275	SER
1	D	278	ILE
1	D	285	ARG
1	D	302	ARG
1	D	303	ASN
1	D	308	GLU
1	D	311	ASN
1	D	314	THR
1	D	317	SER

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Mol	Chain	Res	Type
1	D	323	ILE
1	D	326	GLN
1	D	327	GLN
1	D	329	ASP
1	D	340	THR
1	D	377	SER
1	D	393	ILE
1	D	402	ILE
1	D	404	THR
1	D	419	THR
1	D	422	GLN
1	D	434	LYS
1	D	459	SER
1	D	473	GLU
1	D	484	TYR
1	D	488	LYS
1	D	499	ILE
1	D	501	GLU
1	D	504	GLU
1	D	506	GLN
1	D	522	GLN
1	D	544	GLU
1	D	545	CYS
1	D	554	SER
1	D	560	ILE
1	D	572	SER
1	D	589	LYS
1	D	591	THR
1	D	593	ASN
1	D	599	THR
1	D	606	ASN
1	D	607	ASP
1	D	608	ASN
1	D	609	VAL
1	D	615	GLN
1	D	623	ASP
1	D	664	LYS
1	D	675	ARG
1	D	683	ARG
1	D	702	LEU
1	D	708	ASN
1	D	719	GLN

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Mol	Chain	Res	Type
1	D	723	ASN
1	D	731	ARG
1	D	732	GLN
1	D	733	ARG
1	D	735	GLU
1	D	748	ASP
1	D	750	LYS
1	D	754	ILE
1	D	755	LEU
1	D	771	GLN
1	D	773	LYS
1	D	778	THR
1	D	788	ARG
1	E	34	LEU
1	E	35	VAL
1	E	39	SER
1	E	41	LYS
1	E	42	HIS
1	E	48	SER
1	E	77	LYS
1	E	82	LYS
1	E	86	VAL
1	E	91	GLU
1	E	110	SER
1	E	124	ILE
1	E	127	TYR
1	E	128	LYS
1	E	135	GLU
1	E	142	LYS
1	E	145	LYS
1	E	166	GLN
1	E	167	ASP
1	E	174	LEU
1	E	189	LYS
1	E	199	SER
1	E	225	LEU
1	E	232	GLU
1	E	250	LYS
1	E	259	THR
1	E	268	GLU
1	E	274	LYS
1	E	275	SER

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Mol	Chain	Res	Type
1	E	278	ILE
1	E	285	ARG
1	E	302	ARG
1	E	303	ASN
1	E	308	GLU
1	E	311	ASN
1	E	314	THR
1	E	323	ILE
1	E	324	PRO
1	E	326	GLN
1	E	327	GLN
1	E	329	ASP
1	E	377	SER
1	E	393	ILE
1	E	402	ILE
1	E	404	THR
1	E	419	THR
1	E	422	GLN
1	E	434	LYS
1	E	459	SER
1	E	460	PHE
1	E	473	GLU
1	E	484	TYR
1	E	488	LYS
1	E	499	ILE
1	E	501	GLU
1	E	504	GLU
1	E	506	GLN
1	E	522	GLN
1	E	544	GLU
1	E	545	CYS
1	E	554	SER
1	E	560	ILE
1	E	572	SER
1	E	589	LYS
1	E	591	THR
1	E	593	ASN
1	E	599	THR
1	E	606	ASN
1	E	607	ASP
1	E	608	ASN
1	E	609	VAL

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Mol	Chain	Res	Type
1	E	615	GLN
1	E	623	ASP
1	E	664	LYS
1	E	675	ARG
1	E	683	ARG
1	E	702	LEU
1	E	708	ASN
1	E	719	GLN
1	E	723	ASN
1	E	731	ARG
1	E	732	GLN
1	E	733	ARG
1	E	735	GLU
1	E	748	ASP
1	E	750	LYS
1	E	754	ILE
1	E	755	LEU
1	E	771	GLN
1	E	773	LYS
1	E	778	THR
1	E	788	ARG
1	F	34	LEU
1	F	35	VAL
1	F	39	SER
1	F	41	LYS
1	F	42	HIS
1	F	48	SER
1	F	77	LYS
1	F	82	LYS
1	F	86	VAL
1	F	91	GLU
1	F	110	SER
1	F	124	ILE
1	F	127	TYR
1	F	128	LYS
1	F	135	GLU
1	F	142	LYS
1	F	145	LYS
1	F	166	GLN
1	F	167	ASP
1	F	174	LEU
1	F	189	LYS

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Mol	Chain	Res	Type
1	F	199	SER
1	F	225	LEU
1	F	232	GLU
1	F	250	LYS
1	F	259	THR
1	F	268	GLU
1	F	274	LYS
1	F	275	SER
1	F	278	ILE
1	F	285	ARG
1	F	302	ARG
1	F	303	ASN
1	F	308	GLU
1	F	311	ASN
1	F	314	THR
1	F	323	ILE
1	F	324	PRO
1	F	326	GLN
1	F	327	GLN
1	F	329	ASP
1	F	340	THR
1	F	377	SER
1	F	393	ILE
1	F	402	ILE
1	F	404	THR
1	F	419	THR
1	F	422	GLN
1	F	434	LYS
1	F	459	SER
1	F	460	PHE
1	F	473	GLU
1	F	484	TYR
1	F	488	LYS
1	F	499	ILE
1	F	501	GLU
1	F	504	GLU
1	F	506	GLN
1	F	522	GLN
1	F	544	GLU
1	F	545	CYS
1	F	554	SER
1	F	560	ILE

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Mol	Chain	Res	Type
1	F	568	LYS
1	F	572	SER
1	F	589	LYS
1	F	591	THR
1	F	593	ASN
1	F	599	THR
1	F	605	LEU
1	F	606	ASN
1	F	607	ASP
1	F	608	ASN
1	F	609	VAL
1	F	615	GLN
1	F	623	ASP
1	F	664	LYS
1	F	675	ARG
1	F	683	ARG
1	F	702	LEU
1	F	708	ASN
1	F	719	GLN
1	F	723	ASN
1	F	731	ARG
1	F	732	GLN
1	F	733	ARG
1	F	735	GLU
1	F	748	ASP
1	F	750	LYS
1	F	754	ILE
1	F	755	LEU
1	F	771	GLN
1	F	773	LYS
1	F	778	THR
1	F	788	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	236	ASN
1	A	303	ASN
1	A	327	GLN
1	A	333	GLN
1	A	418	GLN
1	A	422	GLN

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Mol	Chain	Res	Type
1	A	533	ASN
1	A	566	HIS
1	A	593	ASN
1	A	606	ASN
1	A	614	ASN
1	A	666	GLN
1	A	699	HIS
1	A	708	ASN
1	A	719	GLN
1	B	236	ASN
1	B	303	ASN
1	B	327	GLN
1	B	333	GLN
1	B	418	GLN
1	B	422	GLN
1	B	533	ASN
1	B	566	HIS
1	B	593	ASN
1	B	606	ASN
1	B	614	ASN
1	B	666	GLN
1	B	699	HIS
1	B	708	ASN
1	B	719	GLN
1	C	303	ASN
1	C	327	GLN
1	C	333	GLN
1	C	418	GLN
1	C	422	GLN
1	C	533	ASN
1	C	566	HIS
1	C	593	ASN
1	C	606	ASN
1	C	614	ASN
1	C	666	GLN
1	C	699	HIS
1	C	708	ASN
1	C	719	GLN
1	C	751	GLN
1	D	236	ASN
1	D	303	ASN
1	D	327	GLN

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Mol	Chain	Res	Type
1	D	333	GLN
1	D	418	GLN
1	D	422	GLN
1	D	533	ASN
1	D	566	HIS
1	D	593	ASN
1	D	606	ASN
1	D	614	ASN
1	D	666	GLN
1	D	699	HIS
1	D	708	ASN
1	D	719	GLN
1	D	751	GLN
1	E	236	ASN
1	E	303	ASN
1	E	327	GLN
1	E	333	GLN
1	E	418	GLN
1	E	422	GLN
1	E	533	ASN
1	E	566	HIS
1	E	593	ASN
1	E	606	ASN
1	E	614	ASN
1	E	666	GLN
1	E	699	HIS
1	E	708	ASN
1	E	719	GLN
1	E	751	GLN
1	F	303	ASN
1	F	327	GLN
1	F	333	GLN
1	F	418	GLN
1	F	422	GLN
1	F	533	ASN
1	F	566	HIS
1	F	593	ASN
1	F	606	ASN
1	F	614	ASN
1	F	666	GLN
1	F	699	HIS
1	F	708	ASN

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Mol	Chain	Res	Type
1	F	719	GLN
1	F	751	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	ADP	E	998	3,2	24,29,29	0.94	1 (4%)	29,45,45	1.08	1 (3%)
3	ALF	A	999	2,5,4	0,4,4	0.00	-	-		
3	ALF	C	999	2,5,4	0,4,4	0.00	-	-		
3	ALF	B	999	1,2,5,4	0,4,4	0.00	-	-		
4	ADP	C	998	3,2	24,29,29	0.78	0	29,45,45	1.24	3 (10%)
4	ADP	B	998	3,2	24,29,29	0.78	0	29,45,45	1.24	3 (10%)
3	ALF	D	999	1,2,5,4	0,4,4	0.00	-	-		
3	ALF	F	999	1,2,4	0,4,4	0.00	-	-		
4	ADP	F	998	3,2	24,29,29	1.06	2 (8%)	29,45,45	1.12	3 (10%)
4	ADP	D	998	3,2	24,29,29	0.77	0	29,45,45	1.25	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ADP	A	998	3,2	24,29,29	0.77	0	29,45,45	1.25	3 (10%)
3	ALF	E	999	2,4	0,4,4	0.00	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	E	998	3,2	-	5/12/32/32	0/3/3/3
4	ADP	C	998	3,2	-	5/12/32/32	0/3/3/3
4	ADP	B	998	3,2	-	5/12/32/32	0/3/3/3
4	ADP	F	998	3,2	-	5/12/32/32	0/3/3/3
4	ADP	D	998	3,2	-	5/12/32/32	0/3/3/3
4	ADP	A	998	3,2	-	5/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	998	ADP	PB-O3B	-2.23	1.46	1.54
4	E	998	ADP	O4'-C1'	-2.22	1.38	1.41
4	F	998	ADP	C2-N3	2.08	1.35	1.32

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	998	ADP	C5-C6-N6	2.90	124.77	120.35
4	C	998	ADP	C5-C6-N6	2.86	124.69	120.35
4	B	998	ADP	C5-C6-N6	2.84	124.67	120.35
4	A	998	ADP	C5-C6-N6	2.84	124.66	120.35
4	F	998	ADP	C5-C6-N6	2.46	124.08	120.35
4	A	998	ADP	O3'-C3'-C2'	2.44	119.72	111.82
4	D	998	ADP	O3'-C3'-C2'	2.43	119.69	111.82
4	B	998	ADP	O3'-C3'-C2'	2.42	119.66	111.82
4	C	998	ADP	O3'-C3'-C2'	2.41	119.63	111.82
4	F	998	ADP	O3'-C3'-C2'	2.30	119.27	111.82
4	C	998	ADP	O2B-PB-O3A	2.26	112.23	104.64
4	B	998	ADP	O2B-PB-O3A	2.26	112.20	104.64
4	D	998	ADP	O2B-PB-O3A	2.26	112.20	104.64
4	A	998	ADP	O2B-PB-O3A	2.25	112.17	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	998	ADP	C5'-C6-N6	2.19	123.68	120.35
4	F	998	ADP	C1'-N9-C4	-2.00	123.12	126.64

There are no chirality outliers.

All (30) torsion outliers are listed below:

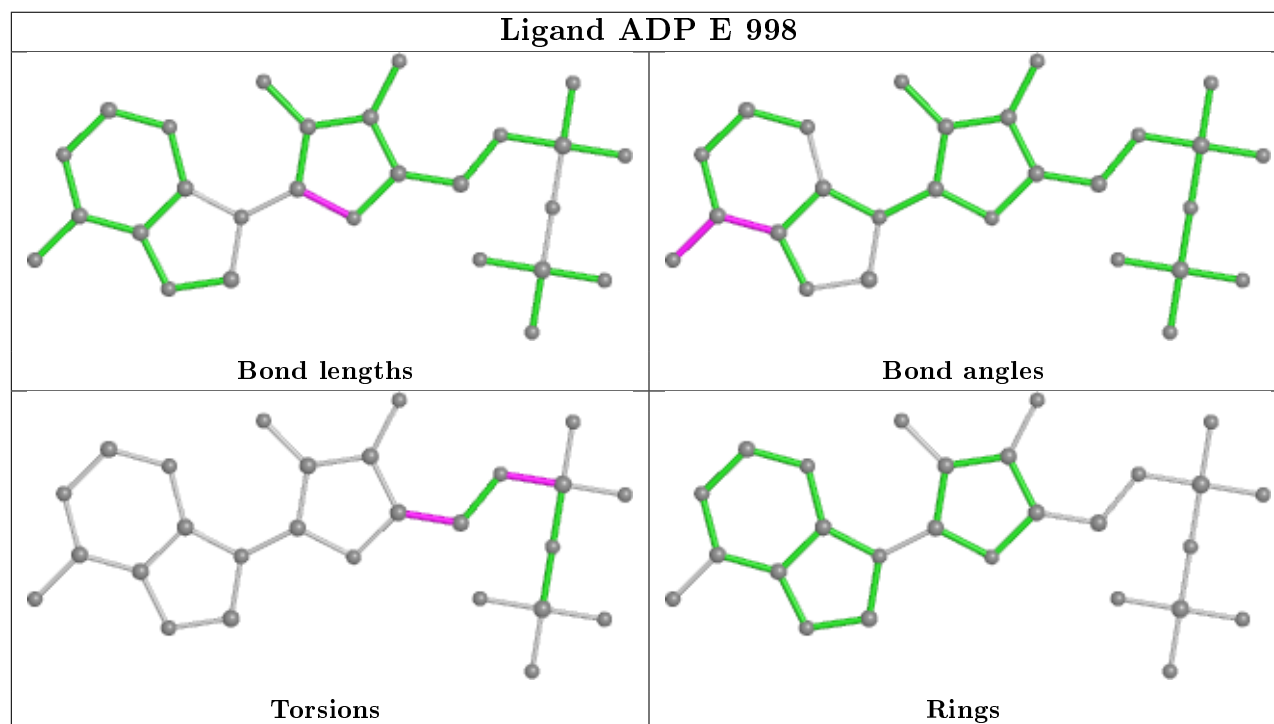
Mol	Chain	Res	Type	Atoms
4	E	998	ADP	C5'-O5'-PA-O1A
4	E	998	ADP	C5'-O5'-PA-O2A
4	C	998	ADP	C5'-O5'-PA-O1A
4	C	998	ADP	C5'-O5'-PA-O2A
4	B	998	ADP	C5'-O5'-PA-O1A
4	B	998	ADP	C5'-O5'-PA-O2A
4	D	998	ADP	C5'-O5'-PA-O1A
4	D	998	ADP	C5'-O5'-PA-O2A
4	F	998	ADP	C5'-O5'-PA-O1A
4	F	998	ADP	C5'-O5'-PA-O2A
4	A	998	ADP	C5'-O5'-PA-O1A
4	A	998	ADP	C5'-O5'-PA-O2A
4	C	998	ADP	O4'-C4'-C5'-O5'
4	C	998	ADP	C3'-C4'-C5'-O5'
4	B	998	ADP	O4'-C4'-C5'-O5'
4	B	998	ADP	C3'-C4'-C5'-O5'
4	D	998	ADP	O4'-C4'-C5'-O5'
4	D	998	ADP	C3'-C4'-C5'-O5'
4	A	998	ADP	O4'-C4'-C5'-O5'
4	A	998	ADP	C3'-C4'-C5'-O5'
4	E	998	ADP	C3'-C4'-C5'-O5'
4	F	998	ADP	C3'-C4'-C5'-O5'
4	E	998	ADP	O4'-C4'-C5'-O5'
4	F	998	ADP	O4'-C4'-C5'-O5'
4	E	998	ADP	C5'-O5'-PA-O3A
4	C	998	ADP	C5'-O5'-PA-O3A
4	B	998	ADP	C5'-O5'-PA-O3A
4	D	998	ADP	C5'-O5'-PA-O3A
4	F	998	ADP	C5'-O5'-PA-O3A
4	A	998	ADP	C5'-O5'-PA-O3A

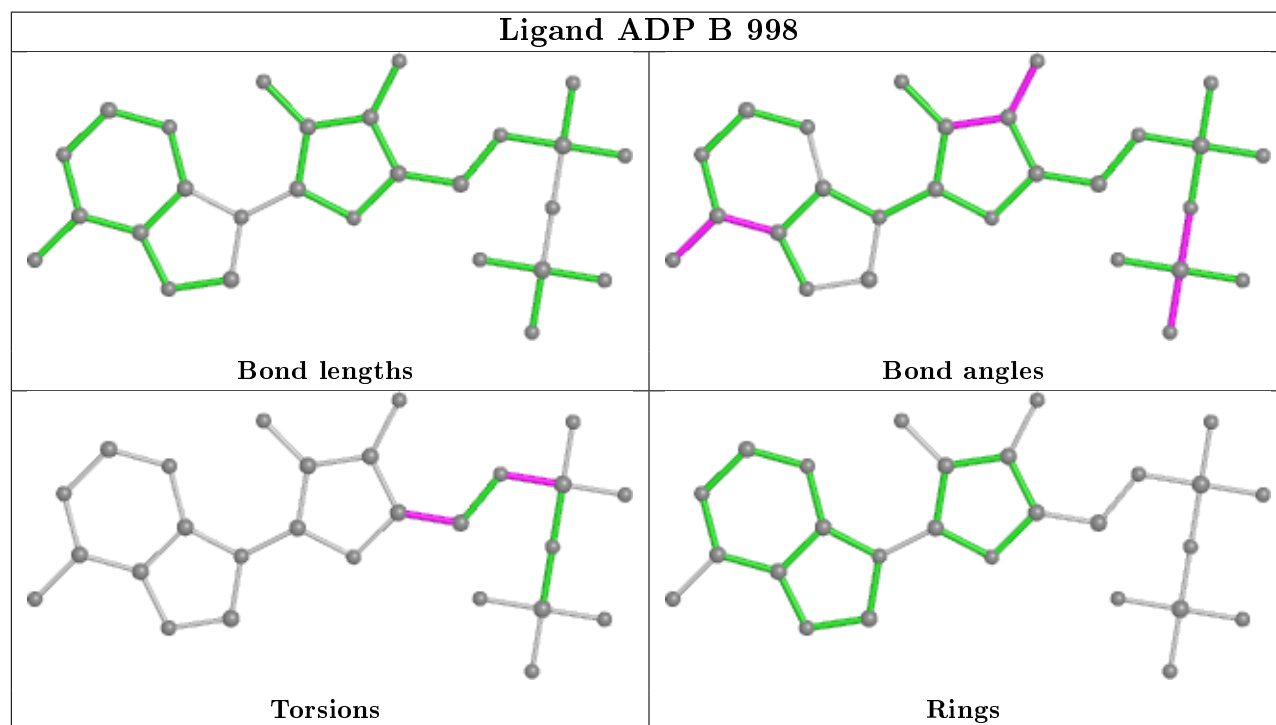
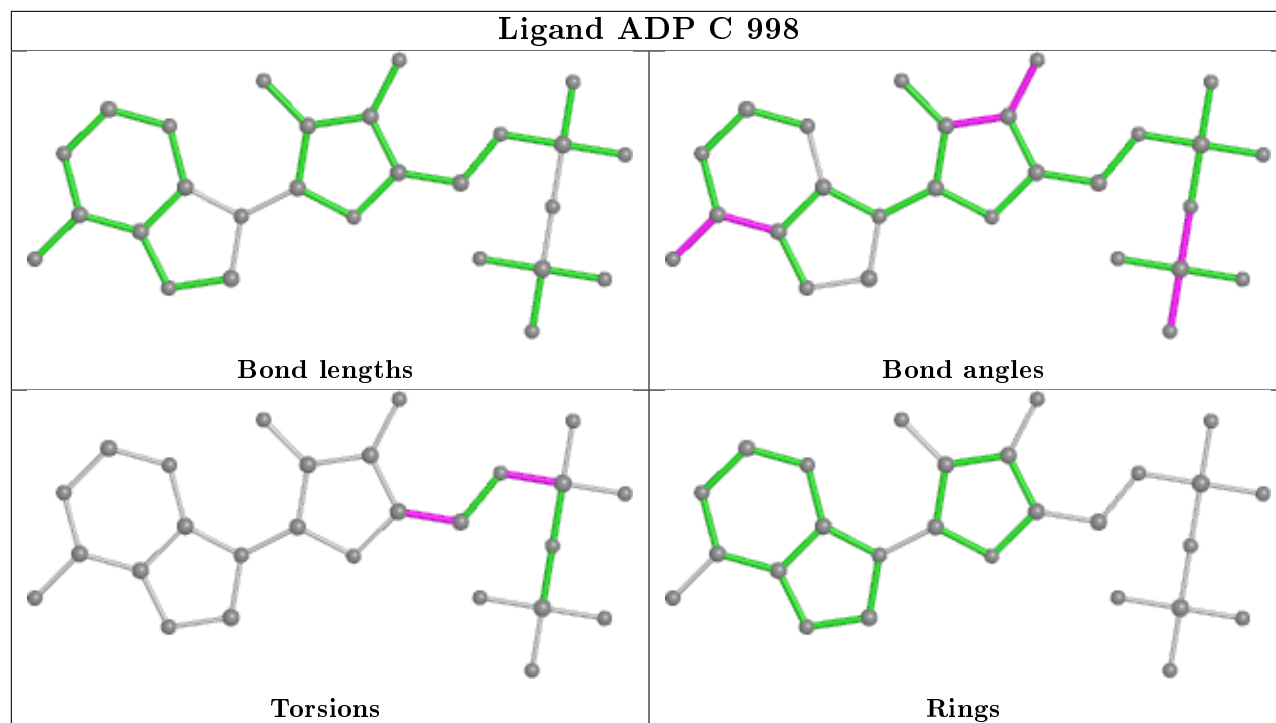
There are no ring outliers.

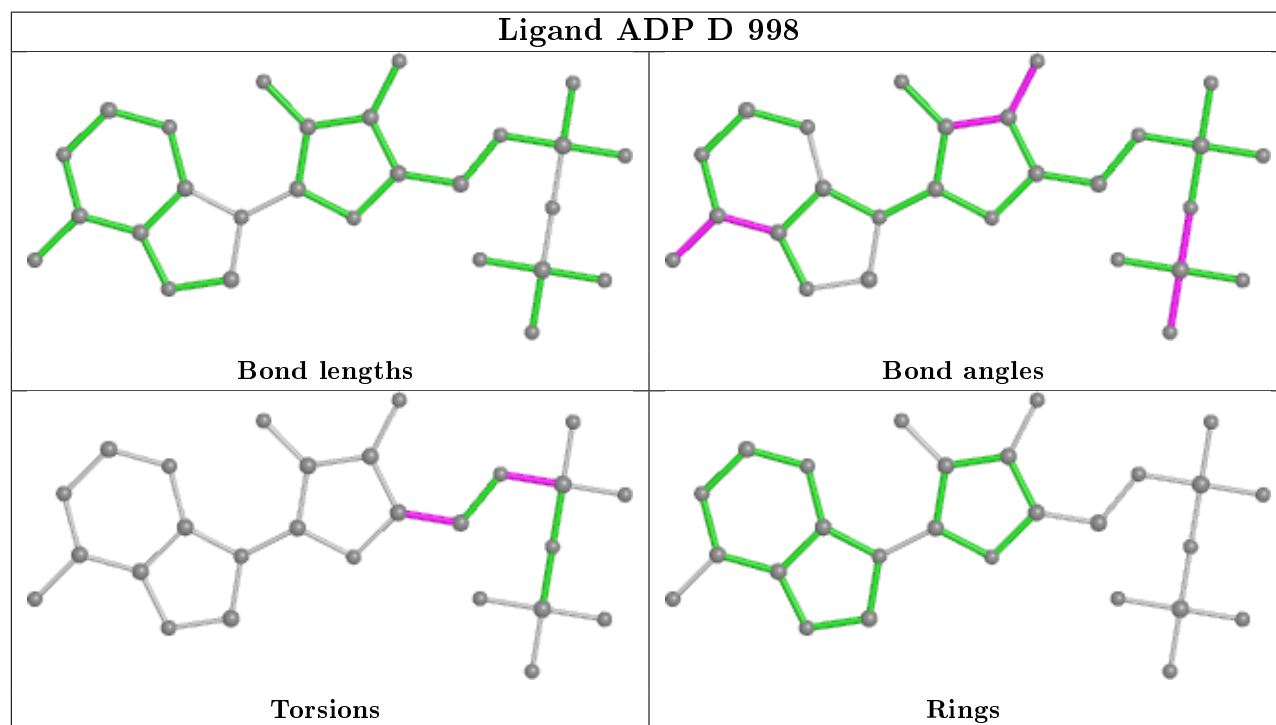
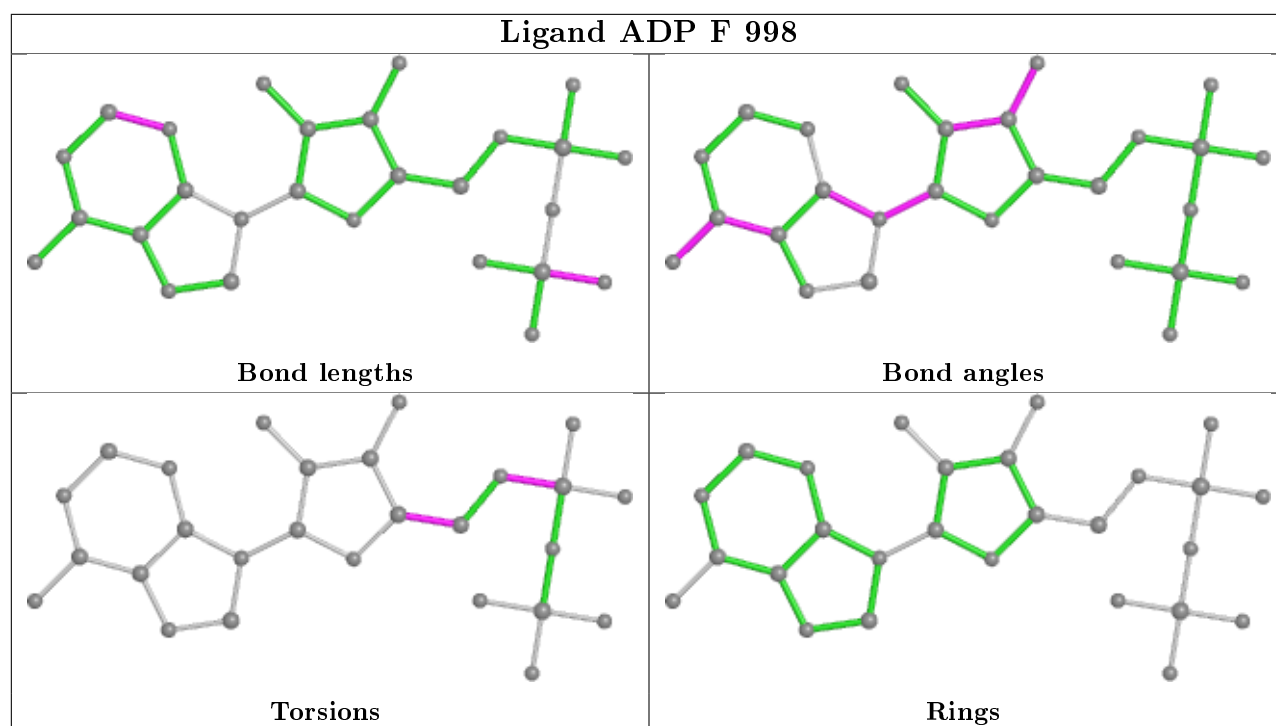
8 monomers are involved in 5 short contacts:

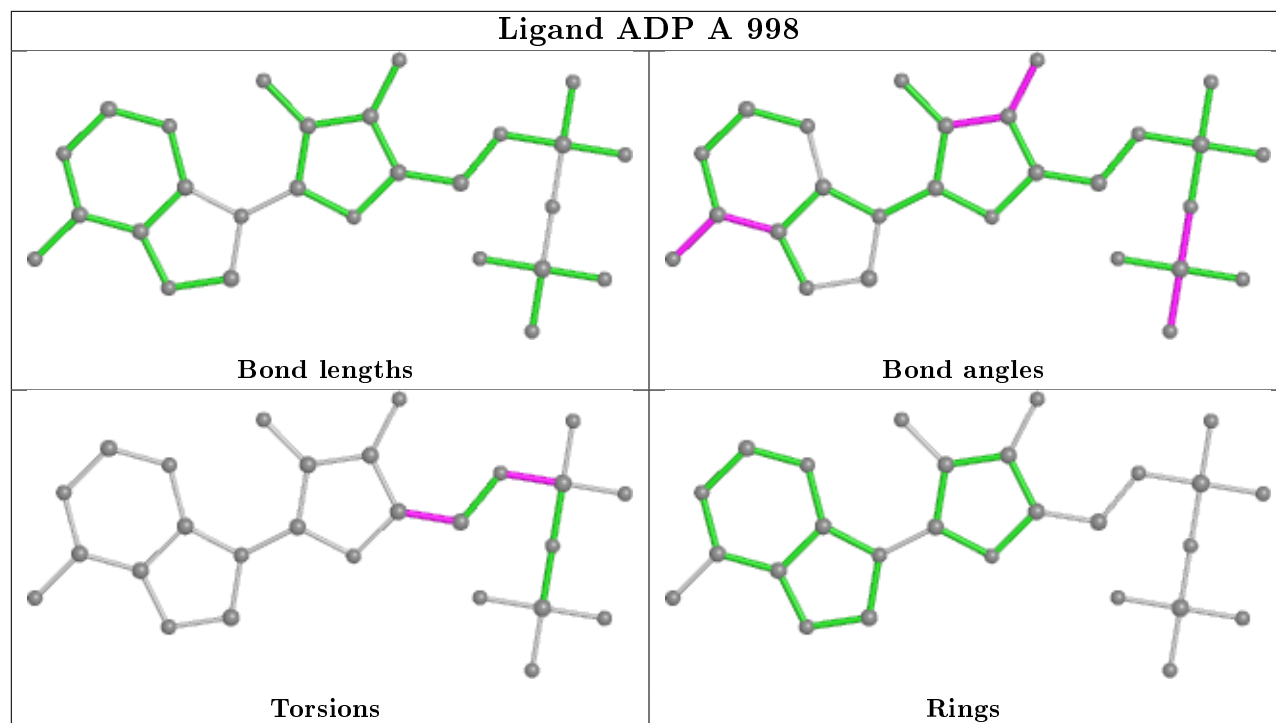
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	ALF	1	0
3	C	999	ALF	1	0
3	B	999	ALF	1	0
4	C	998	ADP	1	0
4	B	998	ADP	1	0
3	D	999	ALF	2	0
4	D	998	ADP	1	0
4	A	998	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.