



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:16 PM UTC

PDB ID : 1EA0 / pdb_00001ea0
Title : Alpha subunit of A. brasilense glutamate synthase
Authors : Binda, C.; Bossi, R.T.; Vanoni, M.A.; Mattevi, A.
Deposited on : 2000-11-02
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

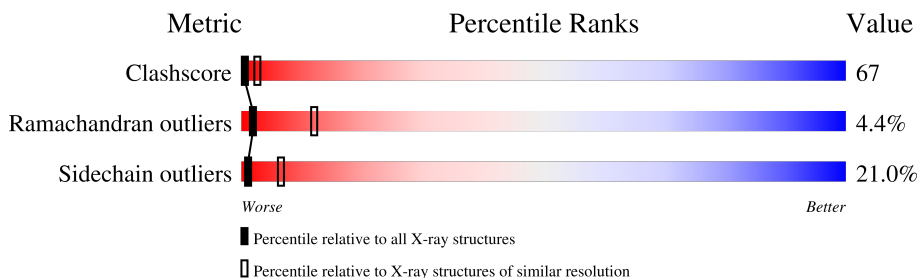
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1479	20% 47% 25% 6% •
1	B	1479	23% 45% 24% 5% •

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
2	OMT	A	2473	-	X	-	-
2	OMT	B	2473	-	X	-	-
5	F3S	A	2476	-	-	X	-
5	F3S	B	2476	-	-	X	-

2 Entry composition [i](#)

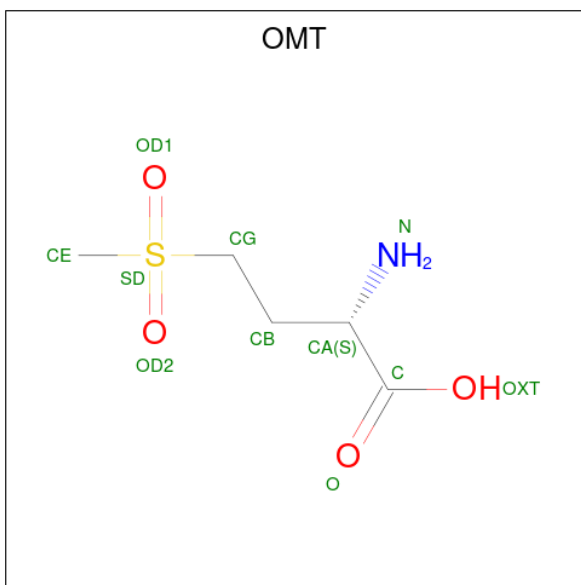
There are 5 unique types of molecules in this entry. The entry contains 22478 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GLUTAMATE SYNTHASE [NADPH] LARGE CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1452	Total 11180	C 7018	N 2005	O 2098	S 59	0	0	0
1	B	1452	Total 11180	C 7018	N 2005	O 2098	S 59	0	0	0

- Molecule 2 is S-DIOXYMETHIONINE (CCD ID: OMT) (formula: C₅H₁₁NO₄S).



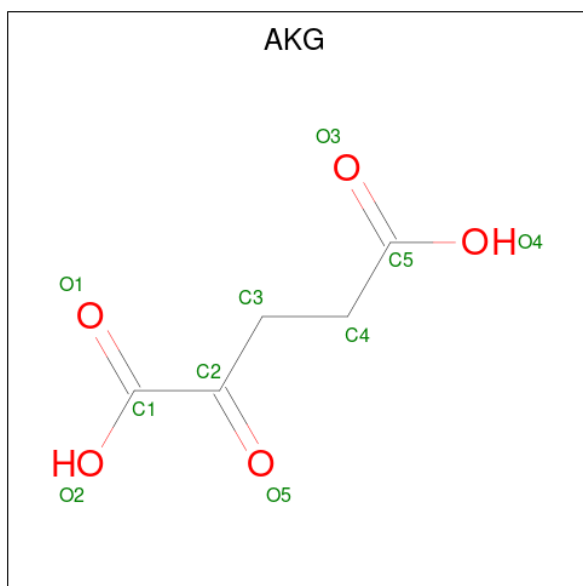
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	Total 11	C 5	N 1	O 4	S 1	0	0
2	B	1	Total 11	C 5	N 1	O 4	S 1	0	0

- Molecule 3 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).



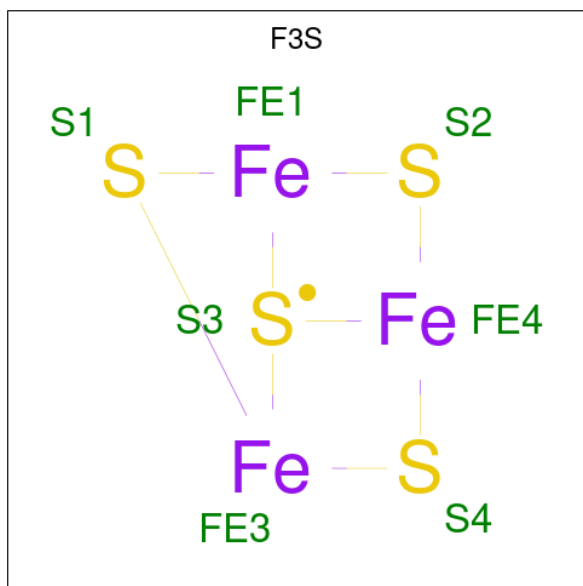
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 4 is 2-OXOGLUTARIC ACID (CCD ID: AKG) (formula: $C_5H_6O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	5	5		
4	B	1	Total	C	O	0	0
			10	5	5		

- Molecule 5 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).




Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Fe	S	0	0
			7	3	4		
5	B	1	Total	Fe	S	0	0
			7	3	4		

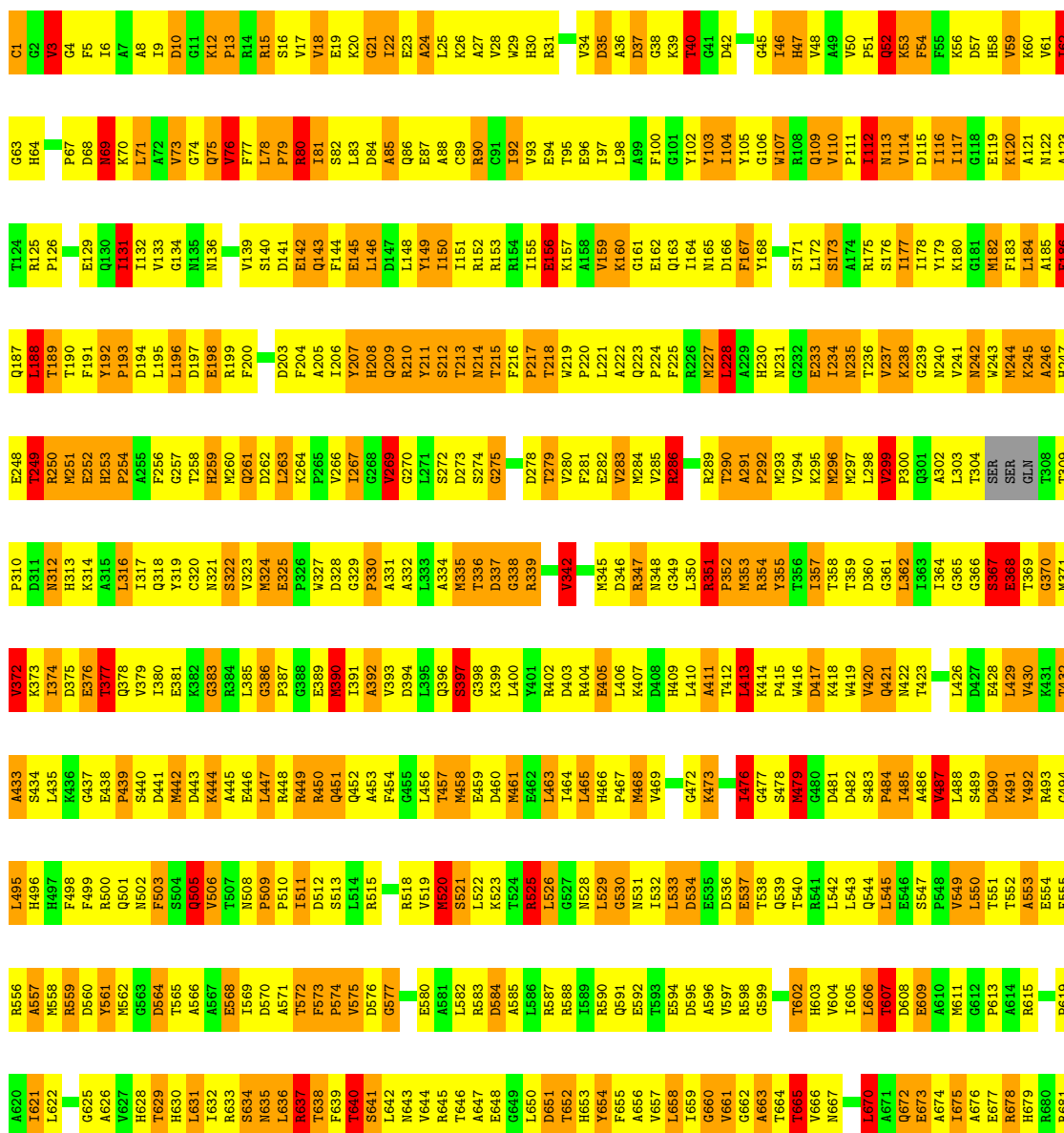
3 Residue-property plots

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

Chain A: 



G682	V743	S814	F886	H952	A1018	M1084	G1152	D1212	G1277	E1344	D1407	E1467
L883	S744	E815	G887	H953	D1019	M1086	L1153	A1213	V1281	E1348	E1408	V1468
F694	R745	Q816	G888	L956	I1020	L1086	F1155	R1214	G1282	V1348	E1409	P1469
M687	I746	K819	E889	L956	I1021	G1086	G1154	R1214	Q1282	R1349	S1409	V1470
P688	G748	R820	P891	H958	I1022	A1088	R1156	V1216	G1283	I1411	F1412	H1471
L689	G748	P821	P891	S959	I1023	E1088	S1157	A1219	K1285	M1350	F1412	L1472
E890	G753	P822	A892	S959	I1024	E1089	L1158	A1219	K1285	S1351	Q1413	P80
K691	I754	P823	A892	S959	G1025	F1090	M1159	R1220	L1286	T1354	R1414	L1414
M692	Q755	M823	P894	P961	S1027	I1092	E1160	I1222	E1287	V1355	E1416	A1416
M693	Q756	L825	D897	V963	I1030	G1093	I1162	F1223	M1289	V1356	V1417	G1117
A694	K757	K826	K898	N964	T1030	I1094	G1163	E1224	G1290	V1357	G1418	SER
M695	V758	R826	K899	N965	S1033	A1095	R1164	E1225	D1291	E1358	H1419	ALA
Y696	L759	L829	N899	I966	S1033	S1086	T1165	G1226	A1292	G1359	Y1420	GLU
K697	E760	E830	N902	S967	P1034	G1101	D1166	E1227	M1293	C1360	E1421	E1421
K698	Q761	L831	W903	P968	Q1035	Q1035	L1167	K1228	D1294	G1361	S1422	S1422
A699	H762	R832	N904	P969	T1036	C1102	L1168	M1229	E1295	S1362	Q1423	Q1423
I700	H763	S833	S905	P970	S1037	I1103	H1169	Q1230	V1296	M1363	L1424	L1424
D701	T764	T834	A906	I977	I1038	K1104	R1170	L1231	G1297	E1366	K1425	K1425
D702	A765	K835	I907	D973	K1039	V1105	V1171	R1240	K1298	E1366	H1426	H1426
G703	Y766	A836	K908	I974	F1040	R1106	SER	A1235	G1299	Y1367	L1427	L1427
L704	E767	P837	Q909	Y975	A1041	Q1107	ARG	R1236	L1300	M1368	T1428	T1428
K705	E768	V838	V910	S976	G1042	C1108	GLY	N1237	S1301	T1369	E1429	E1429
K706	E769	P839	A911	I977	L1043	H1109	ALA	Q1238	G1302	G1370	E1430	E1430
I707	V770	V840	S912	I978	P1044	S1110	GLU	Q1239	G1303	G1371	H1431	H1431
M708	L771	D841	G913	D979	M1045	M1111	HIS	R1240	T1304	T1372	V1432	V1432
S709	L773	E842	R914	L980	M1046	T1112	LEU	G1243	I1305	A1373	E1433	E1433
K710	Q774	V843	F915	A981	M1047	C1113	ASP	G1244	V1306	V1374	E1434	E1434
M711	V775	E844	G916	Q982	G1048	P1114	D1180	R1244	V1307	L1375	Q1436	Q1436
G712	Q776	S845	V917	L983	L1049	V1115	L1181	R1245	R1308	L1376	Q1436	Q1436
I713	G777	L846	T918	I984	S1050	V1116	D1182	L1246	F1309	G1377	S1437	S1437
S714	V778	T847	A919	Y985	E1051	V1117	L1183	S1247	T1310	R1376	R1438	R1438
V715	Y779	A848	E920	D986	M1052	C1118	M184	S1248	V1311	V1379	F1439	F1439
I716	R782	I849	R850	L987	H1053	V1119	P1185	M1249	S1312	A1440	A1440	A1440
S717	K783	R851	N923	Q988	Q1054	Q1120	R1186	V1250	S1313	D1381	A1441	A1441
S718	S784	R852	Q924	Q989	V1055	D1121	L1187	T1251	P1314	E1442	E1442	E1442
R720	G785	F853	Q925	I990	L1056	R1122	A1188	K1252	L1315	F1383	I1443	I1443
G721	D786	I894	E929	P992	T1057	K1123	Q1189	K1253	E1316	L1444	L1444	L1444
G722	R787	T855	E929	P992	L1058	L1124	V1190	F1254	T1317	M1445	D1446	D1446
G723	H788	P856	R931	V998	R1059	L1125	D1191	G1255	M1318	G1386	V1447	V1447
F725	E791	G857	K931	K999	R1060	Q1126	G1193	F1257	K1319	T1387	A1448	A1448
E726	G792	S859	A933	L1000	L1061	T1131	GLU	Q1260	T1321	G1389	E1449	E1449
A727	G793	M860	Q934	V1001	H1063	P1132	ASN	P1261	I1322	G1390	E1450	E1450
I728	V794	G861	Q935	S1002	R1064	E1133	ALA	G1262	H1323	A1392	V1451	V1451
G729	I795	A862	A936	R1003	R1066	K1134	TYR	H1263	T1326	V1393	K1453	K1453
L730	R730	L863	K937	S1004	L1067	V1136	CYS	I1265	V1327	V1395	V1455	V1455
R732	Q799	S864	G939	I1006	R1068	THR	LEU	I1266	Y1329	D1396	Q1456	Q1456
A733	Q800	G869	E940	G1007	T1069	F1139	GLN	R1267	L1397	L1397	V1457	V1457
L734	A801	T870	E941	G1008	D1070	T1141	G1203	L1268	A1333	D1398	V1458	V1458
V735	V802	T870	G942	I1009	G1071	L1142	F1141	R1269	G1334	D1399	P1459	P1459
A736	T803	L871	G942	I1009	K1074	A1143	M1205	G1270	K1335	S1400	K1460	K1460
E737	N804	N872	Q943	A1010	K1074	E1144	E1144	T1271	L1336	L401	E1461	E1461
H738	D805	K875	L944	A1011	T1075	E1145	Y1207	A1272	F1337	P1402	S1462	S1462
F739	S806	K875	K948	A1014	R1077	E1145	P1208	G1273	A1338	L1403	L1463	L1463
P740	K812	D883	V949	K1015	D1078	T1149	I1149	Q1274	A1339	Y1404	M1464	M1464
A741	P740	S884	T950	A1016	L1150	L1150	T1209	S1275	G1340	E1405	R1465	R1465
M742	Y813	G885	E951	M1017	V1080	A1151	L1211	L1276	Q1341	L1406	L1466	L1466

• Molecule 1: GLUTAMATE SYNTHASE [NADPH] LARGE CHAIN



C1	V34	I46	V49	V50	P51	K53	F54	K56	V59	V61	I62	G63	H64	D68	L71	A72
G2	D35	H47	V49	V50	P51	K53	F54	K56	V59	V61	I62	G63	H64	D68	L71	A72
V3	A36	K39	G41	D42	L46	H47	V49	V50	P51	K53	F54	K56	V59	V61	I62	G63
G4	D37	C38	T40	D42	L46	H47	V49	V50	P51	K53	F54	K56	V59	V61	I62	G63
F5	D37	C38	T40	D42	L46	H47	V49	V50	P51	K53	F54	K56	V59	V61	I62	G63
A8	C38	K39	G41	D42	L46	H47	V49	V50	P51	K53	F54	K56	V59	V61	I62	G63
I9	C38	K39	G41	D42	L46	H47	V49	V50	P51	K53	F54	K56	V59	V61	I62	G63
D10	C38	K39	G41	D42	L46	H47	V49	V50	P51	K53	F54	K56	V59	V61	I62	G63
K11	C38	K39	G41	D42	L46	H47	V49	V50	P51	K53	F54	K56	V59	V61	I62	G63
G12	C38	K39	G41	D42	L46	H47	V49	V50	P51	K53	F54	K56	V59	V61	I62	G63
P13	C38	K39	G41	D42	L46	H47	V49	V50	P51	K53	F54	K56	V59	V61	I62	G63
S16	C38	K39	G41	D42	L46	H47	V49	V50	P51	K53	F54	K56	V59	V61	I62	G63
V17	C38	K39	G41	D42	L46	H47	V49	V50	P51	K53	F54	K56	V59	V61	I62	G63
I22	C38	K39	G41	D42	L46	H47	V49	V50	P51	K53	F54	K56	V59	V61	I62	G63
E23	C38	K39	G41	D42	L46	H47	V49	V50	P51	K53	F54	K56	V59	V61	I62	G63
A24	C38	K39	G41	D42	L46	H47	V49	V50	P51	K53	F54	K56	V59	V61	I62	G63
L25	C38	K39	G41	D42	L46	H47	V49	V50	P51	K53	F54	K56	V59	V61	I62	G63
K26	C38	K39	G41	D42	L46	H47	V49	V50	P51	K53	F54	K56	V59	V61	I62	G63
A27	C38	K39	G41	D42	L46	H47	V49	V50	P51	K53	F54	K56	V59	V61	I62	G63
V28	C38	K39	G41	D42	L46	H47	V49	V50	P51	K53	F54	K56	V59	V61	I62	G63
W29	C38	K39	G41	D42	L46	H47	V49	V50	P51	K53	F54	K56	V59	V61	I62	G63
H30	C38	K39	G41	D42	L46	H47	V49	V50	P51	K53	F54	K56	V59	V61	I62	G63
R31	C38	K39	G41	D42	L46	H47	V49	V50	P51	K53	F54	K56	V59	V61	I62	G63

P1034	P969	P837	G776	S714	I589	H528	H466	K399	A331	I267	Y207	D141	V73
Q1035	P970	V838	G777	V715	E592	L529	P467	R402	M335	G268	H208	E142	G74
S1036	Q909	P839	F78	I716	E593	Q530	M468	D403	T336	V269	Q209	Q143	Q75
T1037	Y910	P840	Y779	S717	E594	M531	V469	E404	D377	G270	R210	F144	V76
I1038	A911	D841	R780	S718	D595	L532	G472	R405	G338	L271	Y211	E145	F77
K1039	S912	E842	F781	Y719	D596	D534	K473	E406	G338	S272	S212	L146	L78
L1040	G913	U843	R782	R720	A596	D535	K474	L406	R339	D773	T213	D147	P79
M1041	A914	E844	K783	G721	V597	E536	E475	K407	R339	S274	M214	L148	R80
N1042	F915	S845	S784	G722	R598	D536	A475	Q408	V342	S274	T215	Y149	I81
O1043	G916	I846	G785	G723	T602	L542	D481	R414	M348	D278	T216	I150	S82
P1044	Y917	T847	D786	F725	H603	L543	D482	P415	G343	Q279	F216	I151	L83
Q1045	R918	A848	R787	A663	H604	Q544	S483	W416	M345	D280	P217	R152	D84
R1046	A919	E849	H788	E726	V604	L545	P484	D417	R281	V280	T218	R153	A85
S1047	E920	R850	G789	A727	L605	E546	A486	K418	F281	W281	W219	R154	Q86
T1048	Y921	I851	F789	I728	M611	S547	A486	W419	R387	E282	P220	R154	Q86
U1049	L922	F853	W790	G729	P548	V487	V487	W419	M348	V283	L221	I155	E87
V1050	R925	I854	E791	L730	L543	L543	D482	R414	M348	V283	L221	I155	E87
W1051	G925	T855	G792	S731	D608	Q544	S483	W416	G344	Q279	F216	I150	S82
X1052	R926	P856	R793	R732	E609	L545	P484	D417	M345	D280	P217	R152	L83
Y1053	Q927	G857	W794	A733	E610	E546	A486	K418	R281	V280	T218	R153	A85
Z1054	L928	H858	I795	L734	M611	S547	A486	W419	F281	W281	W219	R153	A85
A1055	R929	S859	H796	V735	G612	P548	V487	W419	R387	E282	P220	R154	Q86
B1056	E929	T859	T797	A736	H612	V549	L488	Q421	M348	V283	L221	I155	E87
C1057	R930	K860	L798	E737	A614	L550	S489	N422	G344	Q279	F216	I150	S82
D1058	G931	C861	H798	H738	R615	T551	D490	T423	M345	D280	P217	R152	L83
E1059	R932	A862	W799	H739	A616	T552	K491	W426	R281	V280	T218	R153	A85
F1060	G933	C863	R800	P740	L617	A553	Y492	L426	R387	E282	P220	R154	Q86
G1061	A934	S864	T803	R741	P618	E554	R493	D427	M348	V283	L221	I155	E87
H1062	G935	R865	N804	M742	P619	F555	G494	R428	L363	M297	L228	E162	E94
I1063	E936	E866	D805	V743	A620	R556	L495	L429	L364	M297	L228	E162	E94
J1064	R937	A867	S806	S744	R621	A557	H496	V430	G365	V299	M235	S171	Y105
K1065	P938	H868	Y807	R745	S682	M558	H497	G366	G366	V237	V237	S173	G106
L1066	G939	C869	T808	I746	L683	R559	F498	G437	S367	K238	K238	A174	I107
M1067	E940	T870	R809	S747	T624	D560	F499	E438	E368	G239	G239	R175	R108
N1068	G941	L871	F810	G748	Y661	M625	R500	P439	E368	M240	M240	R175	Q109
O1069	E942	N872	X811	G748	A626	M662	Q501	S440	G370	N241	N241	S176	V110
P1070	G943	H873	K812	R752	V627	G563	M502	D441	M371	SER	M242	I177	P111
Q1071	R944	A874	Y813	W752	H628	D564	F503	M442	GLN	M243	M243	I178	P111
R1072	P945	H875	S814	G753	T629	T565	S504	D443	I374	M244	M244	M182	M113
S1073	G946	K876	E815	I754	L689	A566	S504	K444	D375	M244	M244	F183	V114
T1074	F947	R877	R816	Q755	E590	A567	V506	K444	E376	M244	M244	L184	D115
U1075	K948	L878	W817	K756	L631	A567	V506	K444	E376	M244	M244	L184	D115
V1076	Y949	N818	N818	H757	R633	I569	T507	E446	T377	M244	M244	L184	D115
W1077	R950	K883	K819	V758	R634	I569	P509	R448	Q378	M244	M244	L184	D115
X1078	E951	S884	R820	L759	M635	A571	P510	R449	V379	M244	M244	L184	D115
Y1079	R952	G885	P821	E760	L636	T572	I511	R450	E381	M244	M244	L184	D115
Z1080	E953	E886	R822	Q761	R637	F573	D512	Q451	L385	M244	M244	L184	D115
A1081	R954	G887	M823	H762	T638	P574	S513	Q452	I317	M244	M244	L184	D115
B1082	G955	G888	K824	A763	F639	P574	S513	Q452	Q318	M244	M244	L184	D115
C1083	L956	E889	R825	T764	T640	D576	R515	G455	Y319	M244	M244	L184	D115
D1084	R957	D890	L825	A765	S641	G577	R518	G455	C320	M244	M244	L184	D115
E1085	E958	F891	S826	Y765	D701	D577	R518	G455	M321	M244	M244	L184	D115
F1086	S959	R892	D827	Y766	D702	L642	R518	G455	R389	M244	M244	L184	D115
G1087	T960	L828	L828	Y767	G703	M643	V519	T457	M389	M244	M244	L184	D115
H1088	R961	R893	L829	E768	L704	V644	M520	M458	I391	M244	M244	L184	D115
I1089	F894	E894	E830	E769	L705	R645	S521	E459	A392	M244	M244	L184	D115
J1090	G963	L831	R831	V770	K706	T646	R583	D460	E325	M244	M244	L184	D115
K1091	D897	H832	H832	V771	I707	A647	K593	M461	D394	M244	M244	L184	D115
L1092	K896	S833	S833	H772	E648	A585	T524	E462	L385	M244	M244	L184	D115
M1093	N899	T834	T834	P774	G949	L586	R525	L463	Q396	M244	M244	L184	D115
N1094	P968	R835	R835	L773	L650	R587	L526	I464	S397	M244	M244	L184	D115
O1095	A906	A836	A836	V775	D651	R588	G527	L465	G398	M244	M244	L184	D115

D1446	W1447	A1448	R1449	E1450	V1451	T1452	K1453	F1454	W1455	P1459	K1460	E1461	M1462	L1463	N1464	R1465	L1466	E1467	V1468	P1469	V1470	H1471	L1472	PRO	LYS	ALA	ILE	SER	ALA	GLU																												
V1379	G1380	D1381	M1382	F1383	A1384	A1385	G1386	M1387	T1388	G1389	G1390	Y1393	V1394	Y1395	D1396	L1397	D1398	D1399	S1400	L1401	P1402	I1405	M1406	D1407	E1408	S1409	V1410	I1411	F1412	Q1413	R1414	V1417	G1418	H1419	Y1420	E1421	S1422	Q1423	L1424	K1425	H1426	L1427	I1428	E1429	E1430	H1431	V1432	T1433	E1434	T1435	Q1436	S1437	R1438	F1439	A1440	A1441		
S1301	G1302	R1308	F1309	T1310	T1311	E1316	T1317	M1318	I1322	I1323	G1324	M1325	T1326	V1327	L1328	Y1329	G1334	K1335	L1336	F1337	A1338	A1339	G1340	Q1341	A1342	G1343	E1344	F1345	R1346	A1347	V1348	R1349	M1350	T1354	V1355	V1356	V1357	E1358	G1359	C1360	E1366	Y1367	M1368	T1369	G1370	G1371	T1372	A1373	V1374	I1375	L1376	K1298						
B1218	A1219	R1220	P1221	L1222	R1229	Y1233	R1236	N1237	T1238	Q1239	R1240	G1243	T1244	R1245	L1246	S1247	S1248	M1249	V1250	T1251	R1252	K1253	M1256	F1257	G1258	L1259	Q1260	P1261	I1264	T1265	L1268	R1269	G1270	T1271	Q1274	G1277	A1278	F1279	A1280	V1281	Q1282	M1289	D1291	A1292	N1293	D1294	K1298											
S1096	L1097	I1098	A1099	M1100	G1101	C1102	I1103	M1104	V1105	R1106	Q1107	C1108	H1109	S1110	M1111	T1112	C1113	P1114	V1115	G1116	V1117	C1118	V1119	Q1120	D1121	D1122	M1123	L1124	R1125	Q1126	K1127	F1128	V1129	G1130	T1131	P1132	E1133	K1134	V1135	V1136	M1137	L1138	F1139	T1140	F1141	L1142	A1143	E1144	E1145	V1146	R1147	E1148	A1151	G1152	L1153	G1154	F1155	R1156
S1157	L1158	M1159	E1160	V1161	I1162	G1163	R1164	T1165	D1166	L1167	L1168	H1169	Q1170	V1171	SER	ARG	GLY	ALA	GLU	HIS	LEU	ASP	D1180	L1181	D1182	L1183	M1184	P1185	R1186	L1187	V1190	F1191	P1192	G1193	GLU	ASN	ALA	ARG	TYR	CYS	THR	LEU	GLN	G1203	R1204	N1205	E1206	V1207	P1208	D1209	T1210	L1211	D1212	A1213	R1214	I1215	V1216	A1217

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	233.61Å 233.61Å 305.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.00	Depositor
% Data completeness (in resolution range)	98.6 (20.00-3.00)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.256 , 0.287	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	22478	wwPDB-VP
Average B, all atoms (Å ²)	57.0	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: AKG, FMN, F3S, OMT

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	1.44	81/11383 (0.7%)	2.01	407/15390 (2.6%)
1	B	1.49	93/11383 (0.8%)	1.99	404/15390 (2.6%)
All	All	1.47	174/22766 (0.8%)	2.00	811/30780 (2.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	2
1	B	0	2
All	All	1	4

All (174) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	838	VAL	CA-CB	-18.76	1.38	1.55
1	A	746	ILE	CA-CB	-12.96	1.37	1.54
1	A	848	ALA	CA-CB	-9.35	1.38	1.53
1	A	849	ILE	CA-CB	-9.22	1.43	1.54
1	B	1289	MET	SD-CE	9.03	2.02	1.79
1	B	713	ILE	CA-CB	-8.81	1.43	1.54
1	B	132	ILE	CA-CB	-8.64	1.44	1.54
1	B	500	ARG	C-O	-8.21	1.13	1.23
1	A	1104	MET	SD-CE	-8.10	1.59	1.79
1	B	963	VAL	CA-CB	-7.91	1.44	1.54
1	A	910	VAL	CA-CB	-7.89	1.43	1.54
1	A	741	ALA	CA-CB	-7.76	1.42	1.53
1	B	1136	VAL	CA-CB	-7.75	1.44	1.54
1	B	1055	VAL	CA-CB	-7.42	1.44	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	838	VAL	CA-CB	-7.28	1.44	1.54
1	B	222	ALA	CA-CB	-7.28	1.41	1.53
1	B	862	ALA	CA-CB	-7.26	1.42	1.53
1	B	227	MET	SD-CE	-7.17	1.61	1.79
1	A	3	VAL	CA-CB	-7.16	1.42	1.54
1	B	8	ALA	CA-CB	-7.15	1.43	1.53
1	B	996	VAL	CA-CB	-7.12	1.45	1.54
1	A	1047	MET	SD-CE	-7.11	1.61	1.79
1	B	1256	MET	SD-CE	-7.10	1.61	1.79
1	A	1162	ILE	CA-CB	-7.09	1.47	1.54
1	A	795	ILE	CA-CB	-6.96	1.45	1.54
1	B	291	ALA	CA-CB	-6.96	1.44	1.53
1	A	1087	ALA	CA-CB	-6.94	1.42	1.53
1	A	728	ILE	C-O	-6.93	1.16	1.24
1	B	1117	VAL	CA-CB	-6.90	1.45	1.54
1	B	849	ILE	CA-CB	-6.87	1.46	1.54
1	B	1293	ASN	C-O	-6.84	1.15	1.24
1	A	1136	VAL	CA-CB	-6.81	1.46	1.54
1	A	269	VAL	CA-CB	-6.76	1.47	1.54
1	A	222	ALA	CA-CB	-6.74	1.42	1.53
1	A	713	ILE	CA-CB	-6.66	1.46	1.54
1	A	838	VAL	N-CA	-6.65	1.40	1.46
1	B	848	ALA	CA-CB	-6.65	1.42	1.53
1	B	1342	ALA	CA-CB	-6.63	1.43	1.53
1	A	1151	ALA	CA-CB	-6.61	1.43	1.53
1	B	1087	ALA	CA-CB	-6.59	1.42	1.53
1	B	506	VAL	CA-CB	-6.57	1.46	1.54
1	B	605	ILE	CA-CB	-6.54	1.46	1.54
1	A	132	ILE	CA-CB	-6.53	1.46	1.54
1	B	17	VAL	CA-CB	-6.53	1.46	1.54
1	B	283	VAL	CA-CB	-6.49	1.46	1.54
1	B	917	VAL	CA-CB	-6.48	1.46	1.53
1	A	981	ALA	CA-CB	-6.46	1.43	1.53
1	A	875	MET	SD-CE	-6.43	1.63	1.79
1	B	746	ILE	CA-CB	-6.43	1.45	1.54
1	B	728	ILE	CA-CB	-6.42	1.46	1.54
1	B	158	ALA	CA-CB	-6.42	1.43	1.53
1	B	155	ILE	CA-CB	-6.42	1.46	1.54
1	A	300	PRO	CA-C	-6.42	1.45	1.52
1	B	390	MET	SD-CE	-6.41	1.63	1.79
1	B	1374	VAL	CA-CB	-6.41	1.46	1.54
1	A	917	VAL	CA-CB	-6.40	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	131	ILE	CA-CB	-6.38	1.46	1.54
1	A	1117	VAL	CA-CB	-6.37	1.45	1.54
1	B	468	MET	SD-CE	6.34	1.95	1.79
1	B	27	ALA	CA-CB	-6.34	1.42	1.53
1	A	390	MET	SD-CE	-6.32	1.63	1.79
1	A	334	ALA	CA-CB	-6.32	1.43	1.53
1	B	700	ILE	CA-CB	-6.31	1.45	1.54
1	B	116	ILE	CA-CB	-6.29	1.45	1.54
1	A	801	ALA	CA-CB	-6.28	1.43	1.53
1	A	1010	ALA	CA-CB	-6.28	1.43	1.53
1	A	1021	ILE	CA-CB	-6.25	1.46	1.54
1	A	1188	ALA	CA-CB	-6.20	1.42	1.53
1	B	85	ALA	CA-CB	-6.18	1.43	1.53
1	A	267	ILE	CA-CB	-6.18	1.46	1.53
1	A	391	ILE	CA-CB	-6.13	1.46	1.55
1	A	1008	THR	CA-CB	-6.09	1.44	1.53
1	A	1170	GLN	C-O	-6.02	1.16	1.24
1	A	117	ILE	CA-CB	-6.01	1.45	1.54
1	B	139	VAL	CA-CB	-6.00	1.46	1.54
1	A	1055	VAL	CA-CB	-5.99	1.46	1.54
1	B	374	ILE	CA-CB	-5.97	1.46	1.54
1	B	252	GLU	N-CA	-5.96	1.39	1.46
1	B	1016	ALA	CA-CB	-5.95	1.44	1.53
1	B	1080	VAL	CA-CB	-5.92	1.47	1.54
1	B	1009	ILE	CA-CB	-5.91	1.46	1.54
1	B	663	ALA	CA-CB	-5.91	1.43	1.53
1	B	604	VAL	CA-CB	-5.88	1.47	1.54
1	B	1213	ALA	CA-CB	-5.87	1.43	1.53
1	A	991	ASN	C-O	-5.83	1.19	1.24
1	A	1011	ALA	CA-CB	-5.83	1.44	1.53
1	B	693	MET	SD-CE	-5.80	1.65	1.79
1	A	950	THR	CA-CB	-5.78	1.43	1.53
1	B	671	ALA	CA-C	-5.77	1.45	1.52
1	A	700	ILE	CA-CB	-5.75	1.46	1.54
1	B	927	GLU	C-O	-5.74	1.16	1.23
1	B	1387	MET	SD-CE	-5.74	1.65	1.79
1	B	567	ALA	CA-CB	-5.73	1.44	1.53
1	B	1018	ALA	C-O	-5.71	1.17	1.23
1	A	1213	ALA	CA-CB	-5.70	1.44	1.53
1	B	353	MET	SD-CE	-5.69	1.65	1.79
1	B	391	ILE	CA-C	-5.69	1.45	1.52
1	B	155	ILE	CA-C	-5.68	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1162	ILE	CA-CB	-5.66	1.47	1.54
1	B	910	VAL	CA-CB	-5.66	1.47	1.54
1	B	1237	ASN	C-O	-5.65	1.16	1.24
1	B	92	ILE	CA-CB	-5.64	1.47	1.54
1	B	906	ALA	CA-CB	-5.64	1.43	1.53
1	A	754	ILE	CA-CB	-5.59	1.46	1.54
1	A	1219	ALA	CA-CB	-5.59	1.45	1.53
1	B	99	ALA	CA-CB	-5.59	1.43	1.53
1	B	279	THR	CA-CB	-5.56	1.44	1.53
1	B	22	ILE	CA-CB	-5.54	1.48	1.54
1	B	757	LYS	C-O	-5.54	1.17	1.24
1	A	1062	ARG	CA-C	-5.54	1.45	1.52
1	A	1168	LEU	C-O	-5.53	1.16	1.24
1	A	843	VAL	CA-C	-5.51	1.47	1.53
1	A	1071	GLY	C-O	-5.51	1.16	1.23
1	A	116	ILE	CA-CB	-5.48	1.47	1.54
1	A	131	ILE	CA-CB	-5.43	1.47	1.54
1	A	476	ILE	CA-CB	-5.43	1.46	1.55
1	A	17	VAL	CA-CB	-5.39	1.47	1.54
1	A	324	MET	SD-CE	5.38	1.93	1.79
1	B	1170	GLN	CA-C	-5.37	1.46	1.52
1	A	299	VAL	CA-CB	-5.37	1.47	1.54
1	A	1016	ALA	CA-CB	-5.36	1.45	1.53
1	A	22	ILE	CA-CB	-5.36	1.47	1.54
1	B	73	VAL	CA-CB	-5.36	1.47	1.54
1	A	1357	VAL	CA-CB	-5.36	1.50	1.55
1	A	468	MET	SD-CE	5.35	1.93	1.79
1	B	1059	ASN	CA-C	-5.34	1.46	1.52
1	A	573	PHE	C-O	-5.34	1.18	1.24
1	A	150	ILE	CA-CB	-5.33	1.47	1.54
1	A	73	VAL	CA-CB	-5.33	1.47	1.54
1	B	1428	ILE	CA-CB	-5.32	1.47	1.54
1	A	325	GLU	CA-C	-5.31	1.45	1.52
1	A	675	ILE	CA-CB	-5.29	1.48	1.54
1	B	1022	LEU	CA-C	-5.29	1.46	1.52
1	B	1039	LYS	CA-C	-5.28	1.45	1.52
1	A	1065	VAL	N-CA	-5.27	1.40	1.46
1	A	13	PRO	CA-C	-5.27	1.46	1.52
1	B	507	THR	CA-CB	-5.27	1.45	1.53
1	B	1451	VAL	CA-CB	-5.27	1.48	1.54
1	B	794	VAL	CA-CB	-5.26	1.48	1.54
1	A	1038	ILE	CA-CB	-5.22	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	795	ILE	CA-CB	-5.21	1.48	1.54
1	A	1457	VAL	CA-CB	-5.21	1.47	1.54
1	A	505	GLN	CA-C	-5.20	1.49	1.52
1	A	1428	ILE	CA-CB	-5.19	1.47	1.54
1	A	799	GLN	C-O	5.19	1.30	1.24
1	B	1104	MET	SD-CE	-5.18	1.66	1.79
1	A	948	LYS	CA-C	-5.17	1.45	1.52
1	B	668	ALA	CA-CB	-5.17	1.46	1.52
1	B	837	PRO	CA-C	-5.17	1.46	1.52
1	B	159	VAL	CA-CB	-5.17	1.48	1.54
1	B	176	SER	CA-C	-5.16	1.46	1.52
1	B	170	CYS	C-O	-5.16	1.17	1.24
1	B	913	GLY	CA-C	-5.16	1.47	1.51
1	B	1222	LEU	C-O	-5.15	1.18	1.24
1	B	371	MET	SD-CE	-5.14	1.66	1.79
1	B	355	TYR	C-O	-5.14	1.17	1.23
1	A	1126	GLN	CA-C	-5.14	1.45	1.52
1	A	374	ILE	CA-CB	-5.10	1.47	1.54
1	A	1417	VAL	CA-CB	-5.10	1.47	1.54
1	B	991	ASN	CA-C	-5.08	1.47	1.52
1	A	383	GLY	C-O	5.08	1.28	1.24
1	B	230	HIS	CA-C	-5.07	1.46	1.52
1	B	1322	ILE	CA-CB	-5.06	1.47	1.54
1	B	754	ILE	CA-CB	-5.06	1.47	1.54
1	B	875	MET	SD-CE	-5.06	1.67	1.79
1	A	291	ALA	CA-CB	-5.05	1.47	1.53
1	B	1095	ALA	CA-CB	-5.05	1.45	1.53
1	A	1292	ALA	CA-CB	-5.05	1.45	1.54
1	A	660	GLY	C-O	-5.05	1.17	1.23
1	A	1039	LYS	CA-C	-5.03	1.46	1.52
1	A	511	ILE	CA-C	-5.02	1.48	1.52
1	B	1035	GLN	CA-C	-5.02	1.45	1.52
1	B	733	ALA	CA-CB	-5.01	1.45	1.53
1	A	85	ALA	CA-CB	-5.01	1.45	1.53

All (811) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	888	GLY	N-CA-C	-18.23	83.89	110.88
1	B	671	ALA	N-CA-C	-15.81	96.60	114.62
1	A	672	GLN	N-CA-C	-15.18	94.81	111.36
1	B	337	ASP	N-CA-C	-14.54	88.66	109.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	505	GLN	CA-C-N	-14.14	104.75	121.71
1	A	505	GLN	C-N-CA	-14.14	104.75	121.71
1	B	915	PHE	CA-C-O	-13.76	105.94	121.07
1	A	681	ARG	N-CA-C	-13.54	92.87	111.56
1	B	607	THR	N-CA-C	13.35	129.36	109.07
1	B	672	GLN	N-CA-C	-12.79	97.42	111.36
1	B	1390	GLY	N-CA-C	-12.51	92.52	111.42
1	B	505	GLN	CA-C-N	-12.38	107.85	121.84
1	B	505	GLN	C-N-CA	-12.38	107.85	121.84
1	B	915	PHE	CA-CB-CG	-12.28	101.52	113.80
1	B	940	GLU	N-CA-C	12.25	136.89	110.80
1	A	106	GLY	N-CA-C	11.84	128.75	112.17
1	A	940	GLU	N-CA-C	11.71	135.74	110.80
1	A	575	VAL	N-CA-C	-11.03	101.93	112.96
1	A	785	GLY	N-CA-C	10.96	125.76	112.49
1	A	838	VAL	N-CA-CB	-10.82	104.36	111.83
1	A	337	ASP	N-CA-C	-10.63	93.38	109.86
1	A	948	LYS	N-CA-C	-10.56	98.58	114.64
1	B	767	ASN	N-CA-C	-10.52	100.68	112.57
1	A	107	TRP	N-CA-C	10.51	124.19	110.43
1	A	843	VAL	CB-CA-C	-10.49	100.06	111.59
1	B	106	GLY	N-CA-C	10.20	122.38	112.08
1	A	262	ASP	N-CA-C	-10.17	100.28	112.89
1	B	726	GLU	N-CA-C	-9.99	93.37	108.46
1	A	963	VAL	CB-CA-C	-9.94	98.58	110.91
1	B	948	LYS	N-CA-C	-9.92	98.71	114.09
1	B	182	MET	CB-CA-C	-9.86	97.97	111.88
1	B	963	VAL	CB-CA-C	-9.83	98.06	111.63
1	B	1113	CYS	CA-C-O	9.78	125.65	119.29
1	B	1465	ARG	CA-C-N	-9.62	108.90	123.14
1	B	1465	ARG	C-N-CA	-9.62	108.90	123.14
1	B	1355	VAL	CB-CA-C	-9.59	93.92	111.18
1	A	1355	VAL	CB-CA-C	-9.50	94.25	110.30
1	B	50	VAL	CB-CA-C	-9.47	99.79	110.68
1	A	342	VAL	N-CA-C	9.45	122.54	108.46
1	B	782	ARG	N-CA-C	-9.42	95.08	109.96
1	A	1465	ARG	CA-C-N	-9.41	109.77	122.85
1	A	1465	ARG	C-N-CA	-9.41	109.77	122.85
1	B	938	PRO	CA-C-N	-9.40	102.99	121.41
1	B	938	PRO	C-N-CA	-9.40	102.99	121.41
1	A	977	ILE	N-CA-C	9.35	120.16	110.62
1	A	283	VAL	CB-CA-C	-9.27	100.11	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	702	ASP	N-CA-C	-9.24	101.27	112.54
1	B	100	PHE	N-CA-C	-9.19	101.59	113.17
1	A	104	ILE	N-CA-C	9.18	120.84	106.88
1	A	64	HIS	N-CA-C	-9.17	96.74	109.95
1	A	738	HIS	N-CA-C	9.15	125.56	113.30
1	B	849	ILE	N-CA-C	9.08	119.89	110.36
1	B	952	MET	N-CA-C	-9.07	101.36	111.07
1	A	1409	SER	CA-C-N	-8.99	110.80	123.03
1	A	1409	SER	C-N-CA	-8.99	110.80	123.03
1	A	372	VAL	CB-CA-C	-8.98	96.55	111.29
1	A	1207	VAL	N-CA-C	8.94	116.52	109.19
1	A	925	CYS	N-CA-C	8.93	120.47	107.88
1	A	607	THR	N-CA-C	8.92	122.85	108.76
1	B	684	PHE	N-CA-C	-8.91	94.65	109.80
1	A	738	HIS	CA-C-N	-8.89	111.16	123.96
1	A	738	HIS	C-N-CA	-8.89	111.16	123.96
1	B	79	PRO	N-CA-C	-8.88	97.10	111.21
1	B	978	GLU	N-CA-C	-8.88	101.57	111.07
1	B	812	LYS	N-CA-C	-8.87	102.97	113.88
1	B	478	SER	N-CA-C	8.86	121.61	108.14
1	A	490	ASP	N-CA-CB	-8.81	97.40	110.53
1	B	783	LYS	N-CA-C	-8.75	99.62	110.65
1	A	100	PHE	N-CA-C	-8.70	102.58	113.02
1	B	968	PRO	N-CA-C	-8.68	100.12	110.70
1	B	459	GLU	N-CA-C	-8.56	100.97	111.33
1	B	107	TRP	N-CA-C	8.55	122.10	110.55
1	B	226	ARG	N-CA-C	8.54	120.59	111.28
1	A	1093	GLY	N-CA-C	8.53	117.97	110.21
1	A	1075	THR	N-CA-C	8.50	122.07	109.24
1	B	369	THR	CA-C-N	-8.42	104.90	121.41
1	B	369	THR	C-N-CA	-8.42	104.90	121.41
1	B	738	HIS	N-CA-C	8.41	123.67	113.41
1	B	40	THR	N-CA-C	8.40	121.25	109.15
1	B	283	VAL	CB-CA-C	-8.39	100.81	112.14
1	B	464	ILE	N-CA-CB	-8.38	104.76	111.64
1	B	1334	GLY	N-CA-C	-8.32	103.68	112.08
1	A	1466	LEU	N-CA-C	8.29	123.16	107.75
1	B	743	VAL	CB-CA-C	-8.27	102.49	111.59
1	A	906	ALA	N-CA-C	8.25	121.39	111.82
1	A	795	ILE	N-CA-C	8.24	119.03	110.62
1	B	368	GLU	N-CA-CB	8.22	123.09	110.60
1	A	159	VAL	CB-CA-C	-8.21	101.28	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	259	HIS	N-CA-C	8.16	121.28	111.82
1	A	849	ILE	N-CA-C	8.15	118.24	110.42
1	A	90	ARG	N-CA-C	8.13	121.06	111.71
1	B	1379	VAL	CA-C-N	-8.09	113.97	122.30
1	B	1379	VAL	C-N-CA	-8.09	113.97	122.30
1	A	228	LEU	N-CA-C	8.07	122.64	109.72
1	B	1063	HIS	N-CA-C	-8.07	100.99	113.02
1	A	641	SER	N-CA-C	-8.04	97.23	110.17
1	B	832	ARG	N-CA-C	-8.01	97.72	110.14
1	A	794	VAL	CB-CA-C	8.00	122.21	111.97
1	B	474	GLU	N-CA-C	8.00	121.94	108.90
1	A	36	ALA	N-CA-C	-8.00	102.78	112.54
1	B	913	GLY	N-CA-C	-7.99	95.60	111.34
1	A	1350	ASN	CA-C-N	-7.98	111.28	123.17
1	A	1350	ASN	C-N-CA	-7.98	111.28	123.17
1	B	391	ILE	N-CA-C	-7.95	97.85	108.35
1	B	782	ARG	CA-C-N	-7.94	110.65	122.24
1	B	782	ARG	C-N-CA	-7.94	110.65	122.24
1	B	1093	GLY	N-CA-C	7.92	117.42	110.21
1	A	915	PHE	N-CA-C	7.90	127.64	110.80
1	A	511	ILE	CB-CA-C	-7.89	99.80	112.03
1	B	640	THR	CB-CA-C	-7.88	95.42	110.24
1	A	337	ASP	CA-C-N	-7.87	110.30	120.14
1	A	337	ASP	C-N-CA	-7.87	110.30	120.14
1	B	704	LEU	N-CA-CB	-7.85	97.23	110.49
1	A	1063	HIS	N-CA-C	-7.84	101.34	113.02
1	B	727	ALA	CA-C-N	-7.83	109.98	122.50
1	B	727	ALA	C-N-CA	-7.83	109.98	122.50
1	A	783	LYS	N-CA-C	-7.81	104.18	112.93
1	A	1390	GLY	N-CA-C	-7.77	94.78	113.18
1	A	487	VAL	CB-CA-C	-7.76	101.88	112.04
1	B	1374	VAL	CB-CA-C	-7.75	100.13	111.68
1	A	805	ASP	CB-CA-C	-7.75	101.48	111.86
1	B	90	ARG	N-CA-C	7.74	119.72	111.28
1	A	391	ILE	N-CA-C	-7.67	97.45	108.42
1	B	64	HIS	N-CA-C	-7.66	98.92	109.95
1	A	812	LYS	N-CA-C	-7.66	102.87	112.90
1	B	1062	ARG	NE-CZ-NH1	-7.63	113.87	121.50
1	A	1244	THR	CA-C-N	-7.62	110.07	120.28
1	A	1244	THR	C-N-CA	-7.62	110.07	120.28
1	A	457	THR	N-CA-C	7.56	119.17	108.74
1	B	519	VAL	CB-CA-C	-7.56	99.84	112.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	860	MET	N-CA-C	-7.55	98.28	109.15
1	A	1106	ARG	N-CA-C	7.53	121.90	111.74
1	A	3	VAL	N-CA-C	-7.51	96.55	108.95
1	B	228	LEU	N-CA-C	7.48	120.53	109.24
1	B	915	PHE	CA-C-N	-7.46	106.78	121.41
1	B	915	PHE	C-N-CA	-7.46	106.78	121.41
1	B	618	ILE	CB-CA-C	-7.45	104.02	110.94
1	B	863	LEU	N-CA-C	7.44	121.58	109.59
1	B	686	SER	N-CA-C	-7.44	104.24	112.72
1	B	368	GLU	CA-CB-CG	7.41	128.93	114.10
1	B	1053	HIS	CB-CA-C	-7.41	98.09	110.68
1	B	237	VAL	N-CA-C	7.38	118.17	110.72
1	B	702	ASP	N-CA-C	-7.37	104.17	113.01
1	B	791	GLU	N-CA-C	-7.37	97.86	109.50
1	A	715	VAL	CB-CA-C	-7.37	99.21	111.29
1	A	978	GLU	CA-CB-CG	-7.32	99.46	114.10
1	A	3	VAL	CB-CA-C	-7.32	99.42	110.55
1	A	915	PHE	CA-C-N	-7.32	107.07	121.41
1	A	915	PHE	C-N-CA	-7.32	107.07	121.41
1	A	687	MET	N-CA-C	7.31	120.09	109.71
1	B	262	ASP	N-CA-C	-7.29	103.36	111.82
1	B	1075	THR	N-CA-C	7.28	120.13	109.07
1	A	237	VAL	N-CA-C	7.24	118.01	110.62
1	A	442	MET	CA-C-N	-7.23	111.99	122.19
1	A	442	MET	C-N-CA	-7.23	111.99	122.19
1	B	1468	VAL	CB-CA-C	-7.23	102.56	110.95
1	A	503	PHE	CA-C-N	-7.22	111.47	122.81
1	A	503	PHE	C-N-CA	-7.22	111.47	122.81
1	B	511	ILE	CB-CA-C	-7.20	101.91	111.70
1	A	549	VAL	N-CA-C	7.20	118.95	108.58
1	A	1126	GLN	N-CA-C	-7.20	103.66	113.30
1	A	1017	ASN	N-CA-C	7.16	121.31	112.58
1	A	182	MET	CB-CA-C	-7.15	101.04	111.91
1	B	843	VAL	CB-CA-C	-7.15	102.06	111.13
1	A	801	ALA	N-CA-C	7.14	119.69	111.11
1	B	250	ARG	CB-CA-C	-7.11	98.36	109.80
1	A	980	LEU	CB-CA-C	-7.05	99.03	110.74
1	B	74	GLY	N-CA-C	-7.05	98.15	110.71
1	A	952	MET	N-CA-C	-7.05	103.53	111.07
1	B	773	LEU	N-CA-C	-7.04	100.88	109.83
1	A	1149	ILE	CB-CA-C	-7.02	102.53	112.22
1	B	3	VAL	N-CA-C	-7.02	97.25	108.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	727	ALA	CA-C-N	-7.01	114.09	122.93
1	A	727	ALA	C-N-CA	-7.01	114.09	122.93
1	A	613	PRO	N-CD-CG	-7.00	92.70	103.20
1	B	807	TYR	N-CA-C	-6.99	103.71	111.82
1	A	163	GLN	CA-C-N	-6.98	114.13	122.93
1	A	163	GLN	C-N-CA	-6.98	114.13	122.93
1	A	10	ASP	N-CA-C	6.96	121.36	113.01
1	B	978	GLU	CA-CB-CG	-6.96	100.18	114.10
1	A	502	ASN	N-CA-C	-6.94	100.52	110.59
1	A	609	GLU	CA-C-N	-6.91	108.33	121.54
1	A	609	GLU	C-N-CA	-6.91	108.33	121.54
1	A	1091	GLY	CA-C-N	-6.91	114.33	123.17
1	A	1091	GLY	C-N-CA	-6.91	114.33	123.17
1	A	1208	PRO	CB-CA-C	-6.91	102.55	111.46
1	A	837	PRO	N-CD-CG	-6.90	92.86	103.20
1	A	729	GLY	N-CA-C	6.89	123.21	114.25
1	B	925	CYS	N-CA-C	6.89	117.59	107.88
1	B	1268	LEU	CB-CA-C	-6.88	100.24	110.62
1	B	263	LEU	N-CA-C	6.87	119.64	111.33
1	A	782	ARG	CA-C-N	-6.85	111.28	122.65
1	A	782	ARG	C-N-CA	-6.85	111.28	122.65
1	B	1114	PRO	CB-CA-C	-6.84	100.27	111.56
1	B	618	ILE	N-CA-C	-6.84	102.75	108.63
1	B	738	HIS	CA-C-N	-6.84	111.43	124.01
1	B	738	HIS	C-N-CA	-6.84	111.43	124.01
1	B	1350	ASN	CA-C-N	-6.84	112.30	122.83
1	B	1350	ASN	C-N-CA	-6.84	112.30	122.83
1	B	90	ARG	N-CA-CB	6.83	120.16	110.12
1	A	1036	THR	N-CA-C	-6.82	103.30	111.69
1	A	485	ILE	N-CA-C	-6.81	98.52	108.87
1	B	714	SER	CB-CA-C	-6.81	99.21	110.72
1	A	300	PRO	CA-C-O	-6.80	113.69	122.12
1	A	178	ILE	N-CA-C	6.79	117.68	108.17
1	A	887	GLY	N-CA-C	6.79	129.28	113.18
1	B	489	SER	CA-C-N	6.79	130.63	120.31
1	B	489	SER	C-N-CA	6.79	130.63	120.31
1	B	457	THR	N-CA-C	6.79	117.00	108.45
1	B	716	ILE	N-CA-C	6.77	120.51	111.44
1	B	746	ILE	N-CA-CB	6.76	121.13	112.34
1	B	651	ASP	CB-CA-C	-6.76	98.76	110.45
1	A	651	ASP	N-CA-C	6.75	120.38	110.59
1	A	1074	LYS	CB-CA-C	-6.75	98.21	109.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	325	GLU	CB-CA-C	-6.75	102.16	109.85
1	A	290	THR	CB-CA-C	-6.74	97.00	110.42
1	A	907	ILE	N-CA-CB	-6.74	103.41	111.90
1	A	1118	CYS	N-CA-C	6.72	119.19	109.71
1	B	464	ILE	N-CA-C	6.72	116.93	111.62
1	A	70	LYS	N-CA-C	-6.71	99.36	110.17
1	A	392	ALA	N-CA-C	6.71	118.40	108.60
1	B	1217	ALA	N-CA-C	-6.71	103.44	111.69
1	A	1420	TYR	N-CA-C	-6.70	103.45	111.69
1	B	186	GLU	N-CA-C	-6.70	104.21	112.38
1	A	479	MET	CG-SD-CE	6.70	115.63	100.90
1	A	964	MET	CB-CA-C	-6.69	97.81	109.64
1	B	575	VAL	N-CA-C	-6.68	106.06	111.81
1	B	159	VAL	N-CA-C	-6.67	103.81	110.62
1	B	1146	VAL	N-CA-C	-6.65	104.28	110.53
1	A	1388	THR	N-CA-C	6.64	124.95	110.80
1	A	690	GLU	N-CA-C	-6.64	102.67	111.24
1	A	192	TYR	CB-CA-C	-6.63	101.86	111.01
1	A	800	GLN	N-CA-C	-6.63	102.94	111.02
1	A	855	THR	N-CA-C	-6.62	98.09	109.15
1	B	1092	ILE	N-CA-C	6.62	117.25	106.72
1	A	1292	ALA	N-CA-C	6.61	119.46	109.41
1	A	1117	VAL	CA-C-N	-6.61	112.87	122.06
1	A	1117	VAL	C-N-CA	-6.61	112.87	122.06
1	A	822	PRO	CA-C-O	-6.61	113.38	121.31
1	A	1005	GLY	N-CA-C	-6.61	105.93	114.85
1	B	1099	ALA	N-CA-C	-6.59	104.18	111.82
1	A	351	ARG	NE-CZ-NH2	6.55	125.10	119.20
1	A	574	PRO	CB-CA-C	-6.55	102.67	111.12
1	A	272	SER	N-CA-C	-6.54	102.09	110.53
1	B	608	ASP	N-CA-CB	-6.54	100.51	110.26
1	B	836	ALA	N-CA-C	-6.53	101.84	110.40
1	A	1034	PRO	CA-C-O	-6.53	113.99	121.56
1	A	1306	VAL	CB-CA-C	-6.53	100.45	110.50
1	B	907	ILE	N-CA-CB	-6.52	103.68	111.90
1	A	1356	VAL	N-CA-C	-6.52	99.75	108.35
1	A	253	HIS	N-CA-C	-6.50	100.71	108.25
1	A	1367	TYR	CB-CA-C	-6.49	101.47	111.66
1	A	149	TYR	CA-C-N	-6.49	110.30	121.97
1	A	149	TYR	C-N-CA	-6.49	110.30	121.97
1	B	1246	LEU	N-CA-C	-6.49	103.90	110.97
1	A	793	GLY	CA-C-O	6.48	127.73	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	938	PRO	CA-C-N	-6.47	108.72	121.41
1	A	938	PRO	C-N-CA	-6.47	108.72	121.41
1	B	639	PHE	N-CA-C	6.46	121.37	112.90
1	B	654	TYR	CA-C-N	-6.46	112.04	120.44
1	B	654	TYR	C-N-CA	-6.46	112.04	120.44
1	B	915	PHE	N-CA-C	6.45	118.89	111.02
1	A	746	ILE	CB-CA-C	-6.43	100.11	110.28
1	A	1157	SER	N-CA-C	6.43	118.29	108.07
1	A	1071	GLY	CA-C-N	-6.42	113.78	122.63
1	A	1071	GLY	C-N-CA	-6.42	113.78	122.63
1	A	52	GLN	N-CA-C	6.40	119.07	111.71
1	A	724	ASN	N-CA-C	6.39	120.61	110.70
1	B	804	ASN	N-CA-C	-6.39	104.75	112.54
1	A	62	ILE	N-CA-C	-6.38	104.39	113.07
1	A	1464	ASN	CA-C-N	-6.38	112.01	122.54
1	A	1464	ASN	C-N-CA	-6.38	112.01	122.54
1	A	1065	VAL	N-CA-CB	-6.37	100.01	111.92
1	A	110	VAL	N-CA-C	6.36	114.10	108.63
1	A	12	LYS	CA-C-N	6.36	126.38	119.89
1	A	12	LYS	C-N-CA	6.36	126.38	119.89
1	A	520	MET	CB-CG-SD	-6.35	93.64	112.70
1	B	1101	GLY	N-CA-C	6.35	123.91	114.95
1	B	1409	SER	CA-C-N	-6.35	110.54	121.97
1	B	1409	SER	C-N-CA	-6.35	110.54	121.97
1	B	448	ARG	CA-C-N	-6.34	109.91	120.68
1	B	448	ARG	C-N-CA	-6.34	109.91	120.68
1	B	890	ASP	CA-C-O	6.34	125.76	119.49
1	B	1338	ALA	N-CA-C	6.33	118.75	107.80
1	B	1451	VAL	CB-CA-C	-6.32	103.76	112.04
1	B	323	VAL	N-CA-C	6.31	116.46	110.53
1	A	173	SER	CA-C-N	-6.31	112.13	122.54
1	A	173	SER	C-N-CA	-6.31	112.13	122.54
1	A	367	SER	N-CA-C	-6.31	104.29	112.68
1	B	228	LEU	CB-CA-C	-6.31	96.19	110.07
1	B	1419	HIS	N-CA-C	-6.31	104.48	111.36
1	A	188	LEU	N-CA-C	-6.30	104.49	111.36
1	A	76	VAL	N-CA-C	6.29	117.83	108.46
1	A	836	ALA	CA-C-N	6.29	126.26	120.03
1	A	836	ALA	C-N-CA	6.29	126.26	120.03
1	B	887	GLY	N-CA-C	6.28	128.07	113.18
1	A	79	PRO	N-CA-C	-6.27	101.24	111.15
1	A	368	GLU	N-CA-CB	6.27	120.92	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	978	GLU	N-CA-C	-6.27	104.45	111.28
1	A	940	GLU	O-C-N	-6.26	114.26	122.59
1	A	338	GLY	N-CA-C	6.26	121.44	113.24
1	B	1064	ARG	N-CA-C	-6.26	105.80	113.50
1	B	935	GLY	CA-C-O	6.25	126.83	120.45
1	B	888	GLY	CA-C-O	-6.25	115.45	121.83
1	A	716	ILE	N-CA-C	6.25	118.86	111.05
1	B	182	MET	CG-SD-CE	-6.25	87.16	100.90
1	A	1302	GLY	CA-C-N	-6.25	115.87	122.30
1	A	1302	GLY	C-N-CA	-6.25	115.87	122.30
1	A	71	LEU	N-CA-CB	-6.24	100.77	110.57
1	A	1053	HIS	CB-CA-C	-6.24	100.83	110.81
1	B	573	PHE	N-CA-C	6.24	118.28	108.55
1	B	938	PRO	CA-C-O	6.24	129.91	120.05
1	A	339	ARG	N-CA-CB	-6.24	101.36	110.40
1	A	1450	GLU	N-CA-C	6.23	117.87	111.14
1	A	1274	GLN	N-CA-C	6.23	118.34	110.24
1	B	683	LEU	CB-CG-CD2	-6.23	92.00	110.70
1	B	53	LYS	N-CA-C	-6.23	104.18	110.97
1	B	369	THR	O-C-N	-6.23	114.95	122.48
1	B	117	ILE	N-CA-CB	-6.22	101.98	112.44
1	B	1437	SER	N-CA-C	6.22	118.43	108.41
1	B	863	LEU	CB-CA-C	6.22	120.58	109.38
1	B	918	THR	N-CA-CB	-6.22	99.96	111.53
1	A	892	ALA	N-CA-C	-6.22	103.81	111.33
1	A	1003	ARG	CA-C-N	-6.21	112.25	120.95
1	A	1003	ARG	C-N-CA	-6.21	112.25	120.95
1	A	1465	ARG	N-CA-C	-6.21	105.34	113.17
1	A	1338	ALA	N-CA-C	6.21	120.23	107.37
1	B	490	ASP	N-CA-CB	-6.21	100.65	110.28
1	A	238	LYS	N-CA-C	-6.21	105.56	113.01
1	A	665	THR	N-CA-CB	-6.21	100.02	111.13
1	A	291	ALA	O-C-N	6.20	124.55	120.27
1	B	157	LYS	N-CA-C	6.20	118.83	111.33
1	A	186	GLU	CA-CB-CG	-6.20	101.71	114.10
1	A	1410	VAL	N-CA-CB	-6.20	103.12	112.35
1	A	109	GLN	CA-C-N	-6.19	112.69	121.23
1	A	109	GLN	C-N-CA	-6.19	112.69	121.23
1	B	228	LEU	N-CA-CB	-6.19	100.93	111.69
1	B	269	VAL	CB-CA-C	-6.18	103.10	111.63
1	B	1020	ILE	CA-C-N	-6.18	114.53	123.06
1	B	1020	ILE	C-N-CA	-6.18	114.53	123.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	469	VAL	CB-CA-C	-6.17	103.81	112.14
1	B	342	VAL	N-CA-C	6.17	117.65	108.46
1	B	486	ALA	CA-C-N	-6.16	111.84	120.53
1	B	486	ALA	C-N-CA	-6.16	111.84	120.53
1	B	633	ARG	CA-C-N	-6.15	114.00	123.17
1	B	633	ARG	C-N-CA	-6.15	114.00	123.17
1	A	376	GLU	N-CA-C	-6.15	103.73	111.11
1	B	187	GLN	N-CA-C	6.14	119.72	112.72
1	A	736	ALA	N-CA-C	-6.14	103.32	111.24
1	A	782	ARG	N-CA-C	-6.14	100.85	109.69
1	A	1228	LYS	N-CA-C	-6.13	100.63	110.14
1	B	703	GLY	CA-C-N	6.13	133.25	121.54
1	B	703	GLY	C-N-CA	6.13	133.25	121.54
1	A	292	PRO	CA-C-N	-6.13	112.06	120.28
1	A	292	PRO	C-N-CA	-6.13	112.06	120.28
1	A	250	ARG	CB-CA-C	-6.12	100.05	109.29
1	A	491	LYS	N-CA-C	6.12	118.38	108.34
1	B	279	THR	N-CA-CB	-6.12	100.52	109.82
1	A	413	LEU	N-CA-C	6.12	117.95	111.28
1	A	228	LEU	CB-CA-C	-6.11	97.29	109.33
1	B	3	VAL	CB-CA-C	-6.11	99.98	110.30
1	B	956	LEU	CB-CA-C	-6.11	101.29	110.88
1	B	1037	SER	CA-C-O	6.11	126.89	119.38
1	A	1307	VAL	CB-CA-C	-6.10	101.82	110.12
1	A	850	ARG	CA-CB-CG	6.10	126.31	114.10
1	A	1062	ARG	NE-CZ-NH2	6.10	124.69	119.20
1	A	746	ILE	CG1-CB-CG2	6.09	128.97	110.70
1	B	1110	SER	N-CA-C	6.09	120.44	112.89
1	A	1300	LEU	CA-C-N	-6.08	114.11	122.87
1	A	1300	LEU	C-N-CA	-6.08	114.11	122.87
1	A	836	ALA	N-CA-C	-6.08	101.27	110.39
1	B	350	LEU	N-CA-C	6.08	120.69	113.28
1	B	182	MET	N-CA-CB	-6.07	102.80	110.45
1	A	50	VAL	CB-CA-C	-6.05	100.34	111.36
1	A	448	ARG	CB-CA-C	6.05	120.96	110.68
1	B	626	ALA	CA-C-N	-6.04	112.18	120.46
1	B	626	ALA	C-N-CA	-6.04	112.18	120.46
1	B	192	TYR	CB-CA-C	-6.04	101.78	111.02
1	B	1214	ARG	N-CA-C	-6.04	105.82	113.43
1	A	602	THR	N-CA-CB	-6.04	102.25	110.95
1	A	296	MET	CA-C-N	-6.04	111.57	120.38
1	A	296	MET	C-N-CA	-6.04	111.57	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	487	VAL	N-CA-CB	6.04	118.01	110.47
1	A	942	GLY	N-CA-C	6.03	120.26	112.54
1	B	816	GLN	N-CA-C	-6.03	104.04	111.33
1	B	848	ALA	CA-C-N	-6.03	112.83	120.60
1	B	848	ALA	C-N-CA	-6.03	112.83	120.60
1	B	645	ARG	N-CA-C	-6.02	98.59	108.41
1	B	917	VAL	CB-CA-C	6.02	117.73	111.23
1	A	1064	ARG	NE-CZ-NH1	-6.01	115.49	121.50
1	A	1156	ARG	N-CA-C	-6.01	105.26	112.59
1	B	91	CYS	CA-CB-SG	-6.00	100.59	114.40
1	B	859	SER	N-CA-C	6.00	119.16	110.28
1	A	46	ILE	N-CA-C	-5.99	100.06	108.27
1	A	918	THR	N-CA-CB	-5.99	100.39	111.53
1	A	1377	GLY	N-CA-C	5.99	118.65	110.69
1	B	836	ALA	CA-C-N	5.98	125.92	119.76
1	B	836	ALA	C-N-CA	5.98	125.92	119.76
1	B	1311	THR	N-CA-C	-5.98	105.08	112.38
1	B	487	VAL	CB-CA-C	-5.98	104.21	112.04
1	A	1434	GLU	N-CA-C	5.97	117.87	111.36
1	B	1405	ILE	N-CA-C	5.97	117.75	109.45
1	A	1294	ASP	N-CA-C	5.96	118.24	110.43
1	B	624	THR	OG1-CB-CG2	-5.96	97.37	109.30
1	A	577	GLY	N-CA-C	5.96	127.29	113.18
1	A	275	GLY	N-CA-C	-5.95	105.59	112.50
1	B	531	ASN	N-CA-C	5.94	118.80	107.75
1	B	937	LYS	CA-C-N	5.94	125.42	119.24
1	B	937	LYS	C-N-CA	5.94	125.42	119.24
1	A	478	SER	N-CA-C	5.94	117.27	108.60
1	A	1062	ARG	NE-CZ-NH1	-5.93	115.56	121.50
1	B	1252	ARG	N-CA-C	5.93	119.34	111.75
1	A	1468	VAL	CB-CA-C	-5.92	100.59	111.36
1	B	71	LEU	N-CA-CB	-5.92	101.33	110.56
1	B	650	LEU	N-CA-C	5.92	120.05	112.12
1	A	300	PRO	N-CA-C	-5.91	102.59	111.57
1	A	738	HIS	CB-CA-C	-5.91	100.19	110.17
1	B	236	THR	N-CA-CB	-5.90	101.58	110.91
1	A	1113	CYS	CA-C-O	5.89	123.68	119.32
1	B	1056	LEU	CB-CG-CD1	-5.89	93.03	110.70
1	A	164	ILE	N-CA-C	5.89	116.78	108.36
1	B	392	ALA	N-CA-C	5.88	118.23	108.99
1	B	732	ARG	CG-CD-NE	-5.87	99.08	112.00
1	B	948	LYS	CB-CG-CD	-5.87	97.80	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1369	THR	N-CA-CB	-5.87	101.75	111.49
1	B	377	THR	N-CA-CB	-5.87	100.58	110.49
1	B	202	SER	N-CA-C	5.86	117.43	108.52
1	B	36	ALA	N-CA-C	-5.86	105.02	111.82
1	A	193	PRO	N-CD-CG	-5.86	94.41	103.20
1	B	941	GLY	N-CA-C	5.86	127.06	113.18
1	A	331	ALA	N-CA-C	5.85	117.14	107.20
1	A	775	VAL	CB-CA-C	-5.85	104.36	112.02
1	A	386	GLY	N-CA-C	-5.84	100.42	112.34
1	B	938	PRO	CB-CA-C	-5.84	103.33	113.20
1	A	575	VAL	CB-CA-C	-5.84	105.92	111.06
1	B	1168	LEU	CB-CA-C	-5.84	100.80	110.14
1	B	1112	THR	CA-C-N	-5.83	114.04	121.74
1	B	1112	THR	C-N-CA	-5.83	114.04	121.74
1	A	869	GLY	CA-C-N	-5.83	112.86	120.44
1	A	869	GLY	C-N-CA	-5.83	112.86	120.44
1	B	1381	ASP	N-CA-C	5.82	123.21	110.80
1	A	1264	ILE	N-CA-C	-5.82	99.11	107.78
1	A	269	VAL	N-CA-C	5.82	118.97	109.78
1	B	647	ALA	N-CA-C	-5.82	103.66	112.04
1	B	214	ASN	CB-CA-C	-5.82	97.89	111.09
1	B	1074	LYS	CB-CA-C	-5.81	99.87	109.99
1	B	264	LYS	N-CA-C	5.81	117.94	110.39
1	B	1407	ASP	CB-CA-C	-5.81	98.86	110.42
1	B	774	PRO	CA-C-N	-5.81	113.80	120.88
1	B	774	PRO	C-N-CA	-5.81	113.80	120.88
1	A	1118	CYS	CB-CA-C	5.79	120.64	112.07
1	B	1466	LEU	CB-CG-CD1	-5.79	93.33	110.70
1	A	1321	THR	OG1-CB-CG2	-5.79	97.72	109.30
1	A	640	THR	CB-CA-C	-5.79	97.77	110.67
1	A	661	VAL	N-CA-C	-5.77	97.34	109.34
1	B	764	THR	CA-C-N	-5.77	113.60	122.60
1	B	764	THR	C-N-CA	-5.77	113.60	122.60
1	B	828	LEU	CA-C-N	-5.77	114.86	122.99
1	B	828	LEU	C-N-CA	-5.77	114.86	122.99
1	B	1075	THR	N-CA-CB	-5.76	102.04	111.66
1	B	994	ALA	N-CA-C	5.76	119.00	110.48
1	A	1254	PHE	N-CA-C	-5.75	106.06	114.39
1	B	1031	GLY	N-CA-C	-5.74	107.54	114.66
1	B	463	LEU	N-CA-C	5.73	117.53	111.28
1	A	145	GLU	CA-C-N	-5.73	112.80	120.54
1	A	145	GLU	C-N-CA	-5.73	112.80	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	862	ALA	N-CA-C	-5.73	104.39	111.33
1	B	1061	LEU	CA-C-O	5.72	125.19	118.90
1	B	456	LEU	CB-CG-CD2	-5.72	93.54	110.70
1	A	545	LEU	CA-CB-CG	-5.72	96.29	116.30
1	B	339	ARG	N-CA-CB	-5.71	103.00	110.59
1	B	1091	GLY	CA-C-N	-5.70	115.34	123.10
1	B	1091	GLY	C-N-CA	-5.70	115.34	123.10
1	B	441	ASP	CA-C-N	-5.70	113.87	122.81
1	B	441	ASP	C-N-CA	-5.70	113.87	122.81
1	A	1037	SER	CA-C-N	-5.70	112.40	121.34
1	A	1037	SER	C-N-CA	-5.70	112.40	121.34
1	B	933	ALA	N-CA-C	5.70	117.13	108.07
1	A	957	ARG	N-CA-C	5.69	120.09	113.20
1	B	1184	ASN	O-C-N	5.69	124.19	120.27
1	B	838	VAL	CB-CA-C	-5.69	101.01	111.36
1	B	549	VAL	N-CA-C	5.68	116.48	108.36
1	A	917	VAL	N-CA-C	5.68	116.56	107.98
1	A	858	MET	N-CA-C	-5.67	98.84	108.26
1	B	413	LEU	N-CA-C	5.67	117.54	111.36
1	A	739	PHE	N-CA-C	-5.67	98.96	109.06
1	A	110	VAL	CB-CA-C	-5.67	105.67	110.94
1	A	354	ARG	CG-CD-NE	-5.66	99.54	112.00
1	B	746	ILE	CG1-CB-CG2	5.66	127.69	110.70
1	B	826	ARG	N-CA-C	-5.66	105.20	111.71
1	A	1443	ILE	N-CA-C	-5.66	104.02	111.09
1	A	13	PRO	CB-CA-C	-5.66	104.15	111.39
1	B	12	LYS	CA-C-N	5.66	125.61	119.78
1	B	12	LYS	C-N-CA	5.66	125.61	119.78
1	B	1383	PHE	CA-C-N	-5.66	116.44	126.45
1	B	1383	PHE	C-N-CA	-5.66	116.44	126.45
1	A	40	THR	N-CA-C	5.65	118.75	109.76
1	B	602	THR	N-CA-CB	-5.65	102.34	110.65
1	B	1434	GLU	CA-C-N	5.65	129.64	120.60
1	B	1434	GLU	C-N-CA	5.65	129.64	120.60
1	B	1164	ARG	NE-CZ-NH1	-5.65	115.85	121.50
1	B	700	ILE	CB-CA-C	5.65	119.05	111.94
1	B	1354	THR	N-CA-C	-5.64	100.20	109.40
1	A	761	GLN	N-CA-C	-5.64	105.14	111.28
1	B	992	PRO	N-CD-CG	-5.63	94.75	103.20
1	B	233	GLU	CA-C-N	-5.63	115.22	123.10
1	B	233	GLU	C-N-CA	-5.63	115.22	123.10
1	B	344	GLY	N-CA-C	5.63	119.35	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1303	GLY	N-CA-C	-5.63	103.69	112.58
1	B	945	PRO	N-CD-CG	-5.62	94.76	103.20
1	B	1059	ASN	N-CA-C	-5.62	105.10	112.41
1	A	132	ILE	N-CA-C	5.62	116.20	107.99
1	B	156	GLU	N-CA-C	-5.62	104.17	111.02
1	B	1417	VAL	CB-CA-C	-5.62	102.83	111.08
1	A	75	GLN	CA-C-N	-5.61	115.14	122.94
1	A	75	GLN	C-N-CA	-5.61	115.14	122.94
1	B	1466	LEU	N-CA-C	5.61	118.68	107.62
1	A	1272	ALA	CA-C-N	-5.61	116.52	122.30
1	A	1272	ALA	C-N-CA	-5.61	116.52	122.30
1	A	73	VAL	CB-CA-C	-5.60	101.02	110.71
1	B	397	SER	CA-CB-OG	-5.60	99.90	111.10
1	B	1461	GLU	CA-C-N	-5.60	113.36	122.26
1	B	1461	GLU	C-N-CA	-5.60	113.36	122.26
1	B	376	GLU	N-CA-C	-5.60	105.18	111.28
1	A	156	GLU	CA-CB-CG	5.59	125.29	114.10
1	A	1108	CYS	CB-CA-C	5.59	121.41	110.67
1	A	1357	VAL	N-CA-CB	-5.59	102.83	111.05
1	A	373	LYS	N-CA-C	5.59	118.12	110.24
1	A	21	GLY	CA-C-N	-5.58	111.92	121.97
1	A	21	GLY	C-N-CA	-5.58	111.92	121.97
1	A	530	GLY	CA-C-N	-5.58	114.46	123.23
1	A	530	GLY	C-N-CA	-5.58	114.46	123.23
1	B	1257	PHE	N-CA-C	5.58	120.81	112.94
1	A	251	MET	CB-CG-SD	-5.58	95.95	112.70
1	B	1427	LEU	N-CA-C	-5.58	104.89	110.97
1	B	244	MET	N-CA-C	-5.58	104.70	112.45
1	B	80	ARG	CA-C-N	-5.58	113.74	121.77
1	B	80	ARG	C-N-CA	-5.58	113.74	121.77
1	A	18	VAL	CA-C-N	-5.58	112.74	120.38
1	A	18	VAL	C-N-CA	-5.58	112.74	120.38
1	A	505	GLN	N-CA-C	5.57	119.49	111.02
1	B	973	ASP	N-CA-C	-5.56	103.76	110.88
1	A	1122	ASP	CA-C-N	-5.56	112.39	120.29
1	A	1122	ASP	C-N-CA	-5.56	112.39	120.29
1	B	992	PRO	CA-C-N	-5.56	112.30	121.92
1	B	992	PRO	C-N-CA	-5.56	112.30	121.92
1	A	550	LEU	N-CA-C	5.56	118.15	108.76
1	B	159	VAL	CB-CA-C	-5.56	104.64	112.14
1	B	736	ALA	N-CA-C	-5.55	104.87	111.03
1	B	940	GLU	CA-C-N	-5.53	110.57	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	940	GLU	C-N-CA	-5.53	110.57	121.41
1	A	92	ILE	CA-C-N	-5.53	112.88	120.46
1	A	92	ILE	C-N-CA	-5.53	112.88	120.46
1	B	259	HIS	N-CA-C	5.53	119.28	112.54
1	A	117	ILE	N-CA-CB	-5.52	102.27	112.43
1	B	155	ILE	CA-C-N	5.52	128.47	120.79
1	B	155	ILE	C-N-CA	5.52	128.47	120.79
1	B	1400	SER	N-CA-C	-5.52	106.45	114.12
1	A	564	ASP	N-CA-C	-5.51	105.37	111.71
1	B	1310	THR	CA-C-N	5.51	129.42	120.60
1	B	1310	THR	C-N-CA	5.51	129.42	120.60
1	A	233	GLU	CA-C-N	-5.51	115.61	123.10
1	A	233	GLU	C-N-CA	-5.51	115.61	123.10
1	B	964	MET	N-CA-C	5.51	118.43	110.28
1	A	1407	ASP	CB-CA-C	-5.51	99.46	110.42
1	B	331	ALA	N-CA-C	5.50	117.07	107.49
1	B	1157	SER	N-CA-C	5.50	116.88	108.52
1	B	296	MET	CA-CB-CG	-5.50	103.10	114.10
1	A	840	VAL	N-CA-C	5.50	116.13	110.36
1	B	1071	GLY	CA-C-N	-5.50	112.18	121.85
1	B	1071	GLY	C-N-CA	-5.50	112.18	121.85
1	B	1342	ALA	N-CA-C	-5.49	102.06	110.14
1	A	533	LEU	N-CA-C	5.49	119.15	112.23
1	B	328	ASP	N-CA-C	5.49	118.93	110.42
1	A	351	ARG	NE-CZ-NH1	-5.49	116.01	121.50
1	A	950	THR	N-CA-CB	-5.49	101.22	110.49
1	A	651	ASP	CB-CA-C	-5.48	100.15	110.51
1	A	330	PRO	N-CA-C	-5.48	102.59	111.14
1	B	290	THR	N-CA-CB	-5.47	101.24	110.49
1	A	637	ARG	CA-C-N	-5.47	111.58	120.72
1	A	637	ARG	C-N-CA	-5.47	111.58	120.72
1	B	1311	THR	N-CA-CB	-5.47	101.02	110.32
1	A	1286	LEU	CA-C-N	-5.46	115.50	122.77
1	A	1286	LEU	C-N-CA	-5.46	115.50	122.77
1	A	670	LEU	N-CA-C	-5.46	106.81	112.93
1	A	439	PRO	CB-CA-C	-5.45	101.91	110.96
1	A	992	PRO	N-CD-CG	-5.45	95.03	103.20
1	A	228	LEU	N-CA-CB	-5.45	101.76	111.08
1	A	597	VAL	N-CA-C	5.45	116.18	110.62
1	B	92	ILE	CA-C-N	-5.45	113.70	120.56
1	B	92	ILE	C-N-CA	-5.45	113.70	120.56
1	B	240	ASN	N-CA-C	-5.44	105.26	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1135	VAL	CA-C-N	-5.44	112.18	121.97
1	B	1135	VAL	C-N-CA	-5.44	112.18	121.97
1	B	747	SER	N-CA-C	-5.43	99.23	110.80
1	B	481	ASP	N-CA-C	-5.43	98.38	107.99
1	B	260	MET	CA-C-N	-5.43	111.89	120.63
1	B	260	MET	C-N-CA	-5.43	111.89	120.63
1	A	1408	GLU	N-CA-C	5.42	122.35	110.80
1	B	1052	VAL	CA-C-N	-5.42	112.96	120.38
1	B	1052	VAL	C-N-CA	-5.42	112.96	120.38
1	A	234	ILE	N-CA-CB	-5.42	105.60	112.15
1	A	824	GLN	N-CA-CB	-5.41	102.27	111.69
1	B	622	LEU	CA-C-N	-5.41	112.60	120.29
1	B	622	LEU	C-N-CA	-5.41	112.60	120.29
1	B	700	ILE	N-CA-C	-5.41	105.84	111.58
1	A	1027	SER	CA-C-N	-5.40	113.82	121.54
1	A	1027	SER	C-N-CA	-5.40	113.82	121.54
1	B	420	VAL	N-CA-C	-5.40	105.11	111.00
1	B	968	PRO	N-CD-CG	-5.40	95.10	103.20
1	B	272	SER	N-CA-C	-5.40	102.90	110.35
1	A	28	VAL	CA-C-N	-5.39	112.11	120.31
1	A	28	VAL	C-N-CA	-5.39	112.11	120.31
1	A	568	GLU	CA-C-N	-5.39	116.14	123.10
1	A	568	GLU	C-N-CA	-5.39	116.14	123.10
1	B	1349	ARG	NE-CZ-NH1	-5.39	116.11	121.50
1	B	713	ILE	N-CA-CB	-5.39	103.68	110.31
1	A	484	PRO	CB-CA-C	-5.39	103.11	111.40
1	B	1229	MET	N-CA-C	5.38	117.86	109.52
1	B	861	GLY	N-CA-C	-5.38	100.43	113.18
1	B	627	VAL	N-CA-C	5.37	116.10	110.62
1	A	746	ILE	CA-CB-CG2	-5.37	101.37	110.50
1	A	69	ASN	CB-CA-C	-5.36	99.75	110.42
1	B	1003	ARG	CA-C-N	-5.36	113.76	121.42
1	B	1003	ARG	C-N-CA	-5.36	113.76	121.42
1	A	1143	ALA	CA-C-N	-5.36	113.04	120.38
1	A	1143	ALA	C-N-CA	-5.36	113.04	120.38
1	B	1044	PRO	CB-CA-C	-5.36	104.53	111.39
1	B	347	ARG	N-CA-C	5.35	119.43	113.01
1	B	1128	PHE	N-CA-C	5.35	117.98	109.96
1	A	473	LYS	CA-C-N	-5.34	113.55	122.64
1	A	473	LYS	C-N-CA	-5.34	113.55	122.64
1	A	1382	ASN	CA-C-O	-5.34	115.78	122.03
1	A	109	GLN	N-CA-CB	5.33	117.80	109.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212	SER	O-C-N	5.33	128.74	123.46
1	B	126	PRO	CA-C-O	-5.33	114.06	121.90
1	A	823	MET	N-CA-CB	-5.33	103.91	111.00
1	B	875	MET	CA-C-N	-5.33	112.05	120.63
1	B	875	MET	C-N-CA	-5.33	112.05	120.63
1	B	795	ILE	CB-CA-C	-5.33	105.06	111.88
1	B	155	ILE	N-CA-C	-5.32	105.53	110.53
1	B	149	TYR	N-CA-C	-5.32	105.17	110.97
1	B	356	THR	OG1-CB-CG2	-5.32	98.66	109.30
1	B	1085	LEU	N-CA-C	-5.32	106.63	113.01
1	A	211	TYR	CB-CA-C	-5.32	100.48	111.22
1	B	1106	ARG	N-CA-C	5.31	118.72	111.39
1	A	683	LEU	CA-C-N	-5.31	113.78	122.54
1	A	683	LEU	C-N-CA	-5.31	113.78	122.54
1	A	1038	ILE	CA-C-N	-5.31	113.71	121.99
1	A	1038	ILE	C-N-CA	-5.31	113.71	121.99
1	A	574	PRO	CA-C-O	-5.30	115.32	121.95
1	A	506	VAL	CA-C-O	5.30	124.44	118.98
1	A	379	VAL	CA-C-N	-5.29	114.03	121.55
1	A	379	VAL	C-N-CA	-5.29	114.03	121.55
1	A	871	LEU	CA-C-N	-5.28	112.15	120.60
1	A	871	LEU	C-N-CA	-5.28	112.15	120.60
1	A	182	MET	CA-C-O	-5.28	115.36	122.44
1	A	888	GLY	O-C-N	5.28	129.01	122.78
1	A	1071	GLY	O-C-N	-5.28	115.84	122.70
1	B	90	ARG	CA-C-N	-5.27	113.59	120.44
1	B	90	ARG	C-N-CA	-5.27	113.59	120.44
1	B	1371	GLY	N-CA-C	-5.27	103.87	112.83
1	A	1027	SER	N-CA-C	5.27	122.02	110.80
1	A	782	ARG	CA-CB-CG	-5.26	103.57	114.10
1	B	603	HIS	CA-C-N	-5.26	115.67	122.99
1	B	603	HIS	C-N-CA	-5.26	115.67	122.99
1	A	861	GLY	N-CA-C	-5.26	100.72	113.18
1	A	863	LEU	N-CA-C	5.26	118.29	110.14
1	B	575	VAL	CB-CA-C	-5.26	105.50	111.55
1	A	103	TYR	N-CA-C	5.26	117.64	108.76
1	B	230	HIS	N-CA-CB	-5.25	102.21	110.77
1	B	520	MET	CB-CG-SD	-5.25	96.94	112.70
1	A	1445	ASN	N-CA-C	5.25	119.16	112.34
1	B	976	SER	O-C-N	-5.25	118.69	123.41
1	A	773	LEU	N-CA-C	-5.24	102.65	110.20
1	B	16	SER	N-CA-C	5.24	117.00	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	213	THR	N-CA-CB	-5.24	101.63	110.49
1	B	1168	LEU	N-CA-C	5.24	116.94	108.34
1	A	1376	LEU	CA-CB-CG	-5.24	97.96	116.30
1	A	598	ARG	N-CA-C	-5.24	105.26	110.97
1	A	726	GLU	N-CA-C	-5.24	99.91	108.76
1	A	1318	ASN	CA-C-N	-5.22	114.36	122.67
1	A	1318	ASN	C-N-CA	-5.22	114.36	122.67
1	A	1295	TYR	N-CA-C	5.22	118.95	112.58
1	B	266	VAL	CA-C-N	-5.22	116.13	123.13
1	B	266	VAL	C-N-CA	-5.22	116.13	123.13
1	B	1081	ILE	CB-CA-C	-5.22	105.20	112.04
1	A	525	ARG	CA-C-N	-5.22	115.80	123.00
1	A	525	ARG	C-N-CA	-5.22	115.80	123.00
1	A	652	THR	N-CA-C	5.22	117.37	111.11
1	A	1096	SER	N-CA-CB	5.22	118.37	110.28
1	B	330	PRO	N-CA-C	-5.21	103.01	111.14
1	A	1059	ASN	N-CA-C	-5.21	105.21	112.30
1	B	824	GLN	N-CA-CB	-5.21	101.83	111.52
1	A	713	ILE	N-CA-C	5.21	116.25	108.54
1	B	691	LYS	CA-C-N	-5.21	114.28	120.00
1	B	691	LYS	C-N-CA	-5.21	114.28	120.00
1	B	977	ILE	N-CA-C	5.21	117.56	111.05
1	A	1435	THR	N-CA-CB	-5.20	103.00	110.65
1	B	826	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	A	114	VAL	CB-CA-C	-5.20	102.76	111.29
1	A	110	VAL	CA-CB-CG1	-5.20	101.56	110.40
1	B	689	LEU	CA-CB-CG	-5.20	98.12	116.30
1	A	1339	ALA	CA-C-N	-5.19	113.74	120.91
1	A	1339	ALA	C-N-CA	-5.19	113.74	120.91
1	A	215	THR	N-CA-C	-5.19	107.61	114.31
1	B	1465	ARG	N-CA-C	-5.19	106.54	112.92
1	B	442	MET	CA-C-N	-5.18	115.57	122.72
1	B	442	MET	C-N-CA	-5.18	115.57	122.72
1	A	214	ASN	CB-CA-C	-5.18	99.33	111.09
1	A	934	GLN	CB-CA-C	-5.18	99.48	109.37
1	B	469	VAL	CB-CA-C	-5.18	105.07	112.22
1	A	487	VAL	N-CA-CB	5.17	116.94	110.47
1	A	502	ASN	CA-C-O	-5.17	115.84	121.89
1	B	1006	ILE	N-CA-C	-5.17	105.34	110.62
1	A	823	MET	N-CA-C	-5.17	107.99	114.56
1	A	75	GLN	CA-CB-CG	-5.17	103.76	114.10
1	A	1257	PHE	N-CA-C	5.17	119.13	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	213	THR	OG1-CB-CG2	-5.17	98.97	109.30
1	A	728	ILE	O-C-N	-5.17	117.29	123.03
1	B	230	HIS	CB-CA-C	-5.16	102.19	110.14
1	B	1017	ASN	N-CA-C	5.16	118.88	112.58
1	A	397	SER	CA-CB-OG	-5.16	100.78	111.10
1	B	507	THR	N-CA-CB	-5.16	102.53	110.01
1	B	846	ILE	CB-CA-C	-5.16	105.10	112.22
1	B	1393	TYR	N-CA-C	-5.15	102.16	110.14
1	B	651	ASP	N-CA-C	5.15	118.08	110.46
1	B	678	ARG	NE-CZ-NH1	-5.15	116.35	121.50
1	A	1308	ARG	CA-C-O	5.15	125.24	120.50
1	B	1108	CYS	CB-CA-C	5.15	119.60	110.85
1	B	1468	VAL	N-CA-C	5.15	112.25	107.56
1	B	1027	SER	CB-CA-C	-5.15	100.84	110.36
1	A	286	ARG	NE-CZ-NH1	-5.14	116.36	121.50
1	A	1037	SER	CA-C-O	5.14	125.88	119.97
1	B	692	GLY	N-CA-C	-5.14	106.19	112.77
1	B	512	ASP	CB-CA-C	-5.13	102.69	111.31
1	B	1062	ARG	NE-CZ-NH2	5.13	123.82	119.20
1	B	1244	THR	CA-C-N	-5.13	112.50	120.31
1	B	1244	THR	C-N-CA	-5.13	112.50	120.31
1	A	168	TYR	CA-C-N	-5.13	116.59	122.95
1	A	168	TYR	C-N-CA	-5.13	116.59	122.95
1	A	791	GLU	N-CA-C	-5.13	101.57	109.52
1	A	1374	VAL	CB-CA-C	-5.12	102.89	111.29
1	B	855	THR	N-CA-C	-5.12	101.26	109.04
1	A	635	ASN	N-CA-CB	-5.12	104.12	111.70
1	B	178	ILE	N-CA-C	5.12	115.34	107.77
1	B	547	SER	O-C-N	-5.12	118.27	121.85
1	A	160	LYS	CA-C-N	-5.11	113.69	120.13
1	A	160	LYS	C-N-CA	-5.11	113.69	120.13
1	A	1064	ARG	CD-NE-CZ	-5.11	117.25	124.40
1	B	337	ASP	CA-C-N	-5.11	107.81	122.06
1	B	337	ASP	C-N-CA	-5.11	107.81	122.06
1	A	1223	PHE	CA-C-N	-5.11	112.73	122.53
1	A	1223	PHE	C-N-CA	-5.11	112.73	122.53
1	B	821	PRO	N-CA-C	-5.11	104.47	110.70
1	B	1042	GLY	N-CA-C	5.10	125.28	113.18
1	B	544	GLN	N-CA-C	5.10	117.38	108.76
1	B	148	LEU	CA-C-N	5.10	127.38	120.65
1	B	148	LEU	C-N-CA	5.10	127.38	120.65
1	B	686	SER	CA-C-N	5.10	127.58	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	686	SER	C-N-CA	5.10	127.58	120.65
1	B	17	VAL	CB-CA-C	-5.10	105.36	112.04
1	A	576	ASP	N-CA-C	-5.09	106.76	112.87
1	A	90	ARG	N-CA-CB	5.09	118.06	110.22
1	A	907	ILE	CB-CA-C	-5.09	104.37	110.99
1	A	15	ARG	N-CA-C	-5.09	105.44	111.69
1	B	8	ALA	N-CA-C	-5.09	100.87	108.96
1	B	1030	THR	N-CA-C	-5.08	100.79	108.52
1	B	564	ASP	N-CA-C	-5.08	105.87	111.71
1	B	1258	GLY	CA-C-N	-5.08	115.56	122.93
1	B	1258	GLY	C-N-CA	-5.08	115.56	122.93
1	B	1466	LEU	CA-CB-CG	5.08	134.08	116.30
1	B	1464	ASN	CA-C-N	-5.07	114.53	122.65
1	B	1464	ASN	C-N-CA	-5.07	114.53	122.65
1	A	1059	ASN	CB-CA-C	-5.07	102.53	110.85
1	B	68	ASP	N-CA-C	-5.07	106.26	112.90
1	A	167	PHE	N-CA-C	-5.07	102.01	110.17
1	A	352	PRO	CB-CA-C	-5.07	104.58	111.12
1	A	835	LYS	CD-CE-NZ	5.07	128.11	111.90
1	B	490	ASP	CB-CA-C	-5.07	100.94	110.67
1	A	731	SER	N-CA-C	5.06	117.77	110.28
1	B	46	ILE	N-CA-C	-5.06	100.61	108.86
1	A	936	ALA	N-CA-C	-5.06	105.47	111.69
1	A	830	GLU	CA-C-N	-5.06	115.93	123.11
1	A	830	GLU	C-N-CA	-5.06	115.93	123.11
1	A	1283	GLY	N-CA-C	-5.06	108.46	114.48
1	B	826	ARG	NE-CZ-NH1	-5.06	116.44	121.50
1	A	246	ALA	N-CA-C	-5.05	107.07	113.43
1	B	326	PRO	N-CA-C	5.04	122.86	112.47
1	B	665	THR	N-CA-CB	-5.04	102.01	111.13
1	B	1069	THR	N-CA-C	5.04	116.84	109.24
1	B	76	VAL	N-CA-C	5.03	117.07	108.86
1	A	182	MET	CA-CB-CG	-5.03	104.04	114.10
1	A	411	ALA	N-CA-C	-5.03	105.88	111.36
1	A	80	ARG	CA-C-N	-5.02	115.88	121.85
1	A	80	ARG	C-N-CA	-5.02	115.88	121.85
1	B	342	VAL	CB-CA-C	-5.02	102.77	110.50
1	B	602	THR	OG1-CB-CG2	-5.02	99.26	109.30
1	B	546	GLU	N-CA-C	-5.01	107.15	114.12
1	B	1269	ARG	CG-CD-NE	-5.01	100.97	112.00
1	A	342	VAL	CB-CA-C	-5.01	102.78	110.50
1	A	112	ILE	CA-C-N	-5.01	115.57	123.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	ILE	C-N-CA	-5.01	115.57	123.13
1	B	661	VAL	N-CA-C	-5.01	98.92	109.34
1	A	557	ALA	CA-C-N	5.01	127.26	120.65
1	A	557	ALA	C-N-CA	5.01	127.26	120.65
1	A	1289	MET	CB-CA-C	-5.01	102.59	111.05
1	A	1049	LEU	CA-C-N	-5.00	113.94	120.44
1	A	1049	LEU	C-N-CA	-5.00	113.94	120.44
1	A	157	LYS	N-CA-C	5.00	116.81	111.36
1	B	155	ILE	O-C-N	5.00	127.10	121.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	915	PHE	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1002	SER	Mainchain
1	A	325	GLU	Mainchain
1	B	1168	LEU	Mainchain
1	B	725	PHE	Mainchain

5.2 Too-close contacts [i](#)

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	11180	0	11210	1601	0
1	B	11180	0	11212	1396	0
2	A	11	0	10	3	0
2	B	11	0	10	2	0
3	A	31	0	19	5	0
3	B	31	0	19	7	0
4	A	10	0	4	0	0
4	B	10	0	4	3	0
5	A	7	0	0	2	0
5	B	7	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	22478	0	22488	2997	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 67.

All (2997) 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:B:182:MET:CE	1:B:217:PRO:HB2	1.30	1.59
1:A:875:MET:HE1	1:A:1139:PHE:CE2	1.35	1.58
1:B:1449:ARG:HH11	1:B:1449:ARG:CB	0.97	1.56
1:A:182:MET:HE3	1:A:217:PRO:CB	1.18	1.54
1:B:182:MET:HE3	1:B:217:PRO:CB	1.01	1.49
1:A:182:MET:CE	1:A:217:PRO:HB2	1.45	1.47
1:B:1289:MET:CE	1:B:1289:MET:SD	2.02	1.47
1:A:253:HIS:ND1	1:A:254:PRO:HD2	1.17	1.46
1:A:1449:ARG:HB2	1:A:1449:ARG:NH1	1.18	1.45
1:A:522:LEU:HD21	1:A:705:LEU:CD2	1.47	1.44
1:A:825:LEU:CD1	1:A:1186:ARG:HH12	1.32	1.43
1:A:1449:ARG:HH11	1:A:1449:ARG:CB	1.32	1.43
1:B:182:MET:CE	1:B:217:PRO:CB	1.89	1.39
1:A:825:LEU:HD13	1:A:1186:ARG:NH1	1.35	1.36
1:A:505:GLN:NE2	1:A:1001:VAL:H	1.23	1.34
1:B:430:VAL:HG13	1:B:554:GLU:CB	1.59	1.33
1:B:253:HIS:CG	1:B:254:PRO:HD2	1.62	1.32
1:A:290:THR:CG2	1:A:292:PRO:HD2	1.57	1.31
1:B:729:GLY:O	1:B:748:GLY:HA3	1.31	1.29
1:A:1391:MET:HE2	1:A:1458:VAL:CG2	1.61	1.28
1:A:253:HIS:CG	1:A:254:PRO:HD2	1.67	1.28
1:B:825:LEU:CD1	1:B:1186:ARG:HH12	1.46	1.28
1:A:253:HIS:ND1	1:A:254:PRO:CD	1.94	1.27
1:B:825:LEU:HD13	1:B:1186:ARG:NH1	1.46	1.27
1:A:430:VAL:HG13	1:A:554:GLU:CB	1.64	1.25
1:B:1449:ARG:HB2	1:B:1449:ARG:NH1	0.93	1.25
1:A:875:MET:CE	1:A:1139:PHE:CE2	2.22	1.23
1:B:452:GLN:HE21	1:B:764:THR:CG2	1.50	1.23
1:B:1047:MET:HG2	1:B:1186:ARG:CZ	1.69	1.22
1:B:746:ILE:CG2	1:B:1182:ASP:H	1.54	1.21
1:A:59:VAL:HG21	1:A:105:TYR:CD2	1.77	1.20
1:A:375:ASP:OD2	1:A:377:THR:HB	1.35	1.18
1:B:1047:MET:SD	1:B:1186:ARG:NH2	2.16	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:ARG:HD2	1:A:1367:TYR:CE1	1.80	1.17
1:A:838:VAL:HG13	1:A:839:PRO:HD2	1.23	1.17
1:A:479:MET:HG3	1:A:1104:MET:HE1	1.28	1.16
1:B:253:HIS:ND1	1:B:254:PRO:HD2	1.57	1.16
1:A:778:PHE:CE2	1:A:1039:LYS:HD2	1.80	1.16
1:B:710:LYS:HG2	1:B:939:GLY:HA3	1.25	1.16
1:A:139:VAL:HG12	1:A:140:SER:H	1.01	1.15
1:B:139:VAL:HG12	1:B:140:SER:N	1.60	1.15
1:A:746:ILE:CG2	1:A:1182:ASP:H	1.58	1.15
1:B:1111:ASN:OD1	1:B:1119:VAL:HG23	1.45	1.14
1:A:1111:ASN:OD1	1:A:1119:VAL:HG23	1.44	1.14
1:B:999:LYS:CG	1:B:1022:LEU:HD23	1.78	1.14
1:B:1401:LEU:HD12	1:B:1401:LEU:O	1.45	1.13
1:A:526:LEU:HD12	1:A:526:LEU:N	1.63	1.13
1:A:381:GLU:OE1	1:A:402:ARG:NH1	1.81	1.13
1:B:1115:VAL:O	1:B:1115:VAL:HG12	1.49	1.13
1:A:825:LEU:CD1	1:A:1186:ARG:NH1	1.98	1.12
1:A:1212:ASP:O	1:A:1216:VAL:HG23	1.47	1.12
1:B:1047:MET:HE2	1:B:1186:ARG:HH22	1.11	1.12
1:A:515:ARG:CD	1:A:1367:TYR:CE1	2.30	1.12
1:B:452:GLN:HE21	1:B:764:THR:HG21	0.98	1.12
1:A:253:HIS:CE1	1:A:254:PRO:HD2	1.85	1.12
1:B:30:HIS:CD2	1:B:31:ARG:HG3	1.85	1.10
1:A:387:PRO:HD3	1:A:1344:GLU:OE2	1.51	1.10
1:B:290:THR:HG23	1:B:292:PRO:HD2	1.27	1.09
1:B:405:GLU:OE1	1:B:405:GLU:N	1.86	1.09
1:A:182:MET:CE	1:A:217:PRO:CB	2.13	1.09
1:A:715:VAL:O	1:A:715:VAL:HG12	1.44	1.09
1:A:1221:PRO:HB2	1:A:1229:MET:HE2	1.29	1.09
1:B:999:LYS:HG3	1:B:1022:LEU:HD23	1.19	1.09
1:B:430:VAL:HG13	1:B:554:GLU:HB3	1.31	1.09
1:B:430:VAL:CG1	1:B:554:GLU:HB2	1.82	1.09
1:A:59:VAL:CG2	1:A:105:TYR:CD2	2.34	1.08
1:B:746:ILE:HG23	1:B:1182:ASP:HB3	1.32	1.08
1:A:452:GLN:HE21	1:A:764:THR:CG2	1.66	1.08
1:A:522:LEU:HD21	1:A:705:LEU:HD21	1.22	1.08
1:A:672:GLN:HG3	1:A:693:MET:HE2	1.24	1.08
1:A:1391:MET:CE	1:A:1458:VAL:HG22	1.83	1.08
1:B:238:LYS:O	1:B:242:ASN:ND2	1.86	1.08
1:B:728:ILE:HD12	1:B:1047:MET:CE	1.82	1.08
1:A:522:LEU:CD2	1:A:705:LEU:HD21	1.83	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:746:ILE:HG21	1:B:1182:ASP:N	1.69	1.08
1:A:826:ARG:HH11	1:A:826:ARG:HG2	1.18	1.08
1:A:1376:LEU:N	1:A:1376:LEU:HD23	1.62	1.08
1:B:1349:ARG:HG2	1:B:1349:ARG:HH11	0.97	1.08
1:A:452:GLN:HE21	1:A:764:THR:HG23	1.13	1.07
1:A:960:THR:HG22	1:A:963:VAL:HG23	1.32	1.07
1:B:515:ARG:HD2	1:B:1367:TYR:CE2	1.86	1.07
1:B:430:VAL:CG1	1:B:554:GLU:CB	2.32	1.07
1:A:236:THR:HG21	1:A:328:ASP:H	1.00	1.07
1:A:746:ILE:HG21	1:A:1182:ASP:H	1.12	1.07
1:B:236:THR:HG21	1:B:328:ASP:H	1.17	1.07
1:A:430:VAL:HG13	1:A:554:GLU:HB3	1.17	1.07
1:A:113:ASN:C	1:A:113:ASN:HD22	1.59	1.06
1:A:345:MET:HG3	1:A:346:ASP:H	1.18	1.06
1:B:227:MET:HE3	1:B:282:GLU:HA	1.37	1.06
1:A:522:LEU:HD21	1:A:705:LEU:HD23	1.33	1.06
1:A:236:THR:CG2	1:A:328:ASP:H	1.69	1.06
1:B:417:ASP:O	1:B:419:TRP:N	1.89	1.06
1:A:290:THR:HG22	1:A:292:PRO:HD2	1.29	1.05
1:B:139:VAL:HG11	1:B:143:GLN:HB3	1.36	1.05
1:B:515:ARG:CD	1:B:1367:TYR:CE2	2.39	1.05
1:A:182:MET:HE3	1:A:217:PRO:HB3	1.38	1.05
1:B:505:GLN:NE2	1:B:1000:LEU:HB3	1.72	1.05
1:A:235:ASN:HD22	1:A:236:THR:N	1.52	1.05
1:A:974:ILE:HD11	1:A:983:LEU:HD12	1.34	1.05
1:B:113:ASN:ND2	1:B:115:ASP:H	1.54	1.04
1:B:182:MET:HE1	1:B:217:PRO:C	1.82	1.04
1:A:1115:VAL:O	1:A:1115:VAL:HG12	1.55	1.04
1:B:1047:MET:CE	1:B:1186:ARG:HH22	1.70	1.04
1:B:299:VAL:HG12	1:B:299:VAL:O	1.53	1.04
1:B:912:SER:HB2	1:B:968:PRO:HD2	1.39	1.04
1:B:999:LYS:HG3	1:B:1022:LEU:CD2	1.87	1.04
1:B:1062:ARG:HG3	1:B:1062:ARG:O	1.58	1.04
1:B:1317:THR:HG22	1:B:1318:ASN:N	1.71	1.04
1:A:295:LYS:NZ	1:A:299:VAL:O	1.90	1.03
1:B:746:ILE:HG21	1:B:1182:ASP:H	0.87	1.03
1:B:1221:PRO:HD2	1:B:1229:MET:HE1	1.39	1.03
1:B:1401:LEU:HD12	1:B:1401:LEU:C	1.74	1.03
1:B:236:THR:CG2	1:B:328:ASP:H	1.70	1.03
1:A:113:ASN:ND2	1:A:115:ASP:H	1.56	1.03
1:A:238:LYS:O	1:A:242:ASN:ND2	1.91	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:GLN:NE2	1:A:1001:VAL:N	2.06	1.03
1:B:825:LEU:HD13	1:B:1186:ARG:HH12	1.04	1.03
1:A:1210:THR:HG22	1:A:1211:LEU:H	0.91	1.02
1:B:182:MET:HE3	1:B:217:PRO:HB3	1.05	1.02
1:A:405:GLU:OE1	1:A:405:GLU:N	1.92	1.02
1:A:522:LEU:CD2	1:A:705:LEU:CD2	2.37	1.02
1:B:1076:GLY:HA3	1:B:1145:GLU:HG2	1.36	1.02
1:A:102:TYR:CE2	1:A:144:PHE:CE1	2.48	1.02
1:B:1131:THR:HG23	1:B:1133:GLU:OE1	1.57	1.02
1:A:1184:ASN:HB3	1:A:1185:PRO:HD3	1.39	1.01
1:B:464:ILE:HD11	1:B:779:TYR:CE2	1.93	1.01
1:A:1210:THR:HG22	1:A:1211:LEU:N	1.74	1.01
1:A:1008:THR:HG22	1:A:1009:ILE:N	1.74	1.01
1:B:499:PHE:HE1	1:B:742:MET:HE1	1.25	1.01
1:A:1317:THR:CG2	1:A:1358:GLU:OE1	2.08	1.00
1:A:145:GLU:OE1	1:A:173:SER:HB2	1.57	1.00
1:B:100:PHE:O	1:B:137:LYS:HE3	1.60	1.00
1:A:182:MET:HE1	1:A:217:PRO:C	1.87	1.00
1:A:672:GLN:HG3	1:A:693:MET:CE	1.91	1.00
1:A:290:THR:HG22	1:A:292:PRO:CD	1.90	1.00
1:B:290:THR:CG2	1:B:292:PRO:HD2	1.92	1.00
1:B:1449:ARG:HH11	1:B:1449:ARG:HB3	1.26	1.00
1:A:430:VAL:CG1	1:A:554:GLU:HB3	1.92	0.99
1:B:1349:ARG:HG2	1:B:1349:ARG:NH1	1.71	0.99
1:A:1393:TYR:O	1:A:1394:VAL:HG23	1.62	0.99
1:B:963:VAL:HG12	1:B:964:MET:N	1.76	0.99
1:A:295:LYS:NZ	1:A:299:VAL:HG12	1.78	0.99
1:A:251:MET:HE3	1:A:533:LEU:HD11	1.45	0.99
1:A:310:PRO:HG3	1:A:404:ARG:NH2	1.75	0.99
1:A:958:HIS:O	1:A:1369:THR:HG22	1.62	0.99
1:A:1210:THR:CG2	1:A:1211:LEU:H	1.76	0.99
1:A:248:GLU:HA	1:A:251:MET:HG2	1.41	0.99
1:B:787:ARG:HH12	1:B:821:PRO:HG2	1.25	0.99
1:B:389:GLU:HB3	1:B:403:ASP:OD2	1.61	0.98
1:B:381:GLU:OE1	1:B:402:ARG:NH1	1.96	0.98
1:B:501:GLN:HE21	1:B:653:HIS:CD2	1.81	0.98
1:B:913:GLY:HA2	1:B:1349:ARG:HD3	1.44	0.98
1:A:430:VAL:CG1	1:A:554:GLU:CB	2.42	0.98
1:A:139:VAL:HG12	1:A:140:SER:N	1.76	0.98
1:B:1184:ASN:HB3	1:B:1185:PRO:HD3	1.42	0.98
1:A:1387:MET:HG2	1:A:1387:MET:O	1.64	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:603:HIS:HA	1:B:640:THR:HG22	1.44	0.97
1:B:1210:THR:HG22	1:B:1211:LEU:H	1.28	0.97
1:B:139:VAL:HG12	1:B:140:SER:H	1.19	0.96
1:A:778:PHE:CZ	1:A:1039:LYS:HD2	1.99	0.96
1:B:353:MET:HE2	1:B:366:GLY:O	1.64	0.96
1:A:505:GLN:HE22	1:A:1001:VAL:N	1.62	0.96
1:A:1449:ARG:O	1:A:1452:THR:HB	1.66	0.96
1:B:513:SER:HB3	1:B:520:MET:CE	1.95	0.96
1:B:920:GLU:HB3	1:B:1256:MET:HE2	1.47	0.96
1:B:1039:LYS:O	1:B:1040:PHE:CD1	2.19	0.96
1:B:1317:THR:CG2	1:B:1358:GLU:OE1	2.13	0.96
1:A:959:SER:HA	1:A:1369:THR:CG2	1.94	0.96
1:B:317:ILE:O	1:B:321:ASN:ND2	1.99	0.96
1:B:652:THR:HG22	1:B:703:GLY:HA3	1.47	0.96
1:A:266:VAL:HG12	1:A:279:THR:CG2	1.96	0.95
1:A:1447:TRP:CE2	1:A:1451:VAL:HG22	1.99	0.95
1:A:447:LEU:HD21	1:A:674:ALA:HA	1.46	0.95
1:B:565:THR:HG22	1:B:602:THR:HB	1.44	0.95
1:B:430:VAL:HG13	1:B:554:GLU:HB2	1.36	0.95
1:B:603:HIS:CA	1:B:640:THR:HG22	1.95	0.95
1:B:1349:ARG:HH11	1:B:1349:ARG:CG	1.72	0.95
1:B:746:ILE:O	1:B:747:SER:O	1.85	0.95
1:B:652:THR:CG2	1:B:703:GLY:HA3	1.97	0.95
1:B:387:PRO:HD3	1:B:1344:GLU:OE2	1.67	0.95
1:B:734:LEU:CD1	1:B:738:HIS:HD2	1.80	0.95
1:A:345:MET:HG3	1:A:346:ASP:N	1.72	0.95
1:B:30:HIS:ND1	1:B:1238:THR:HA	1.82	0.95
1:A:734:LEU:CD1	1:A:738:HIS:HD2	1.79	0.94
1:B:452:GLN:NE2	1:B:764:THR:HG21	1.82	0.94
1:A:52:GLN:HE22	1:A:71:LEU:H	1.16	0.94
1:A:291:ALA:HB3	1:A:292:PRO:HD3	1.46	0.94
1:B:728:ILE:HD12	1:B:1047:MET:HE3	1.49	0.94
1:B:950:THR:HG22	1:B:951:GLU:N	1.78	0.94
1:B:959:SER:HA	1:B:1369:THR:CG2	1.96	0.94
1:B:310:PRO:HG3	1:B:404:ARG:NH2	1.82	0.94
1:B:242:ASN:H	1:B:242:ASN:HD22	1.10	0.94
1:A:426:LEU:HD22	1:A:543:LEU:HB3	1.47	0.94
1:A:999:LYS:HG3	1:A:1022:LEU:HD23	1.49	0.94
1:B:531:ASN:HB3	1:B:534:ASP:HB2	1.49	0.93
1:B:447:LEU:HD12	1:B:451:GLN:HG3	1.50	0.93
1:B:1008:THR:HG22	1:B:1009:ILE:N	1.83	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ASN:O	1:A:1015:LYS:HE2	1.67	0.93
1:B:145:GLU:OE1	1:B:173:SER:HB2	1.68	0.93
1:B:1170:GLN:O	1:B:1170:GLN:HG2	1.68	0.93
1:A:958:HIS:O	1:A:1369:THR:CG2	2.17	0.93
1:A:1366:GLU:HG2	1:A:1367:TYR:CD2	2.04	0.93
1:B:253:HIS:CG	1:B:254:PRO:CD	2.51	0.93
1:A:875:MET:HE1	1:A:1139:PHE:HE2	1.17	0.93
1:A:510:PRO:HD2	1:A:970:PRO:HB3	1.52	0.92
1:A:838:VAL:CG1	1:A:839:PRO:HD2	2.00	0.92
1:B:950:THR:HG22	1:B:952:MET:H	1.32	0.92
1:B:1449:ARG:HB2	1:B:1449:ARG:CZ	1.98	0.92
1:A:1076:GLY:HA3	1:A:1145:GLU:HG2	1.51	0.92
1:B:464:ILE:HD11	1:B:779:TYR:CZ	2.05	0.92
3:B:2474:FMN:H1'2	3:B:2474:FMN:O4'	1.69	0.92
1:A:464:ILE:HD11	1:A:779:TYR:CE1	2.05	0.91
1:B:452:GLN:NE2	1:B:764:THR:CG2	2.33	0.91
1:A:404:ARG:HB3	1:A:405:GLU:OE1	1.69	0.91
1:B:464:ILE:CD1	1:B:779:TYR:CE2	2.54	0.91
1:B:313:HIS:O	1:B:317:ILE:HG13	1.68	0.91
1:A:218:THR:HG23	1:A:220:PRO:HD2	1.52	0.91
1:A:950:THR:HG22	1:A:951:GLU:N	1.83	0.91
1:B:1366:GLU:HG2	1:B:1367:TYR:CD1	2.05	0.91
1:B:706:LYS:NZ	1:B:940:GLU:OE1	2.01	0.91
1:B:950:THR:CG2	1:B:951:GLU:N	2.32	0.91
1:A:59:VAL:CG2	1:A:105:TYR:HD2	1.82	0.91
1:B:568:GLU:C	1:B:569:ILE:HD13	1.97	0.91
1:A:299:VAL:O	1:A:299:VAL:HG12	1.69	0.90
1:B:254:PRO:HG2	1:B:255:ALA:H	1.36	0.90
1:B:1317:THR:HG21	1:B:1358:GLU:OE1	1.69	0.90
1:A:826:ARG:HG2	1:A:826:ARG:NH1	1.83	0.90
1:B:825:LEU:CD1	1:B:1186:ARG:NH1	2.17	0.90
1:A:153:ARG:NH2	1:A:263:LEU:O	2.04	0.90
1:A:266:VAL:O	1:A:279:THR:HG21	1.71	0.90
1:B:704:LEU:O	1:B:706:LYS:N	2.04	0.90
1:A:266:VAL:HG12	1:A:279:THR:HG23	1.51	0.90
1:A:113:ASN:C	1:A:113:ASN:ND2	2.27	0.90
1:A:505:GLN:HE22	1:A:1001:VAL:H	0.93	0.90
1:A:499:PHE:HE2	1:A:742:MET:HE1	1.34	0.90
1:B:155:ILE:O	1:B:159:VAL:HG23	1.71	0.90
1:B:513:SER:HB3	1:B:520:MET:HE2	1.54	0.90
1:B:838:VAL:HG13	1:B:839:PRO:HD2	1.54	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:826:ARG:HG2	1:B:826:ARG:HH11	1.35	0.90
1:A:584:ASP:OD1	1:A:584:ASP:N	2.04	0.90
1:B:213:THR:HB	1:B:1008:THR:HG23	1.52	0.90
1:B:417:ASP:O	1:B:418:LYS:C	2.12	0.90
1:B:588:ARG:O	1:B:592:GLU:HG3	1.72	0.89
1:A:102:TYR:CE2	1:A:144:PHE:HE1	1.88	0.89
1:A:582:LEU:H	1:A:755:GLN:HE22	1.17	0.89
1:B:526:LEU:N	1:B:526:LEU:HD12	1.88	0.89
1:A:403:ASP:OD1	1:A:407:LYS:NZ	2.05	0.89
1:B:652:THR:HG21	1:B:703:GLY:CA	2.03	0.89
1:A:290:THR:CG2	1:A:292:PRO:CD	2.46	0.89
1:A:710:LYS:HG2	1:A:939:GLY:HA3	1.55	0.89
1:B:950:THR:HG22	1:B:952:MET:N	1.88	0.89
1:A:387:PRO:CD	1:A:1344:GLU:OE2	2.20	0.89
1:A:950:THR:CG2	1:A:951:GLU:N	2.35	0.89
1:A:52:GLN:NE2	1:A:71:LEU:H	1.70	0.88
1:B:570:ASP:OD1	1:B:572:THR:HB	1.73	0.88
1:B:768:GLU:HG2	1:B:769:GLU:H	1.34	0.88
1:B:139:VAL:HG11	1:B:143:GLN:CB	2.03	0.88
1:B:437:GLY:HA2	1:B:690:GLU:OE2	1.73	0.88
1:B:731:SER:HA	1:B:748:GLY:H	1.37	0.88
1:A:295:LYS:HZ3	1:A:299:VAL:HG12	1.38	0.88
1:A:862:ALA:O	1:A:1118:CYS:HB2	1.71	0.88
1:B:499:PHE:CE1	1:B:742:MET:HE1	2.07	0.88
1:B:734:LEU:CD1	1:B:738:HIS:CD2	2.57	0.88
1:A:235:ASN:HD22	1:A:235:ASN:C	1.80	0.88
1:A:511:ILE:HG22	1:A:512:ASP:N	1.86	0.88
1:A:960:THR:HG22	1:A:963:VAL:CG2	2.03	0.88
1:B:218:THR:HG23	1:B:220:PRO:HD2	1.55	0.88
1:B:218:THR:HG21	1:B:221:LEU:HG	1.56	0.88
1:B:501:GLN:HE21	1:B:653:HIS:HD2	0.90	0.88
1:B:515:ARG:HH22	1:B:966:ILE:HB	1.37	0.88
1:A:142:GLU:H	1:A:142:GLU:CD	1.80	0.88
1:A:1221:PRO:CG	1:A:1229:MET:HE1	2.03	0.88
1:A:236:THR:HG21	1:A:328:ASP:N	1.86	0.88
1:A:562:MET:HE3	1:A:566:ALA:HB2	1.55	0.88
1:A:353:MET:CE	1:A:366:GLY:O	2.22	0.88
1:A:392:ALA:O	1:A:400:LEU:HD12	1.74	0.88
1:A:838:VAL:HG13	1:A:839:PRO:CD	2.03	0.87
1:A:1401:LEU:O	1:A:1401:LEU:HD12	1.74	0.87
1:A:582:LEU:H	1:A:755:GLN:NE2	1.71	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:HIS:ND1	1:B:254:PRO:CD	2.37	0.87
1:B:918:THR:HG22	1:B:921:TYR:H	1.38	0.87
1:A:146:LEU:HD12	1:A:146:LEU:O	1.75	0.87
1:A:372:VAL:HG12	1:A:372:VAL:O	1.74	0.87
1:B:139:VAL:CG1	1:B:140:SER:H	1.87	0.87
1:B:426:LEU:CD2	1:B:543:LEU:HB3	2.04	0.87
1:B:430:VAL:CG1	1:B:554:GLU:HB3	2.02	0.87
1:B:139:VAL:CG1	1:B:140:SER:N	2.35	0.87
1:B:501:GLN:NE2	1:B:653:HIS:HD2	1.73	0.87
1:A:52:GLN:HE22	1:A:71:LEU:N	1.73	0.87
1:A:227:MET:HE2	1:A:282:GLU:HG2	1.56	0.87
1:A:825:LEU:HD11	1:A:1186:ARG:HH12	1.41	0.86
1:B:746:ILE:C	1:B:747:SER:O	2.16	0.86
1:A:724:ASN:ND2	1:A:724:ASN:H	1.73	0.86
1:A:825:LEU:HD13	1:A:1186:ARG:HH11	1.38	0.86
1:B:30:HIS:HD2	1:B:31:ARG:HG3	1.38	0.86
1:B:113:ASN:C	1:B:113:ASN:HD22	1.78	0.86
1:B:253:HIS:H	1:B:260:MET:HE1	1.39	0.86
1:B:182:MET:HE2	1:B:217:PRO:HB2	1.54	0.86
1:A:405:GLU:H	1:A:405:GLU:CD	1.81	0.86
1:B:377:THR:HG22	1:B:378:GLN:HG3	1.56	0.86
1:A:290:THR:HG23	1:A:292:PRO:HD2	1.56	0.86
1:A:479:MET:HG3	1:A:1104:MET:CE	2.05	0.86
1:A:1221:PRO:HG2	1:A:1229:MET:HE1	1.57	0.86
1:B:505:GLN:HE22	1:B:1000:LEU:HB3	1.36	0.86
1:B:734:LEU:HD11	1:B:738:HIS:CD2	2.10	0.86
1:A:430:VAL:HG13	1:A:554:GLU:HB2	1.56	0.86
1:A:6:ILE:HG12	1:A:364:ILE:HG23	1.57	0.86
1:B:1047:MET:HG2	1:B:1186:ARG:NH2	1.91	0.86
1:A:353:MET:HE2	1:A:366:GLY:O	1.76	0.85
1:A:734:LEU:CD1	1:A:738:HIS:CD2	2.58	0.85
1:B:875:MET:HE1	1:B:1139:PHE:CE2	2.10	0.85
1:B:652:THR:HG21	1:B:703:GLY:HA2	1.59	0.85
1:A:482:ASP:OD1	1:A:788:HIS:HD2	1.59	0.85
1:A:843:VAL:HG12	1:A:844:GLU:N	1.89	0.85
1:A:1338:ALA:O	1:A:1340:GLY:N	2.08	0.85
1:B:659:ILE:HA	1:B:663:ALA:HB3	1.54	0.85
1:B:1047:MET:CG	1:B:1186:ARG:NH2	2.38	0.85
1:B:1128:PHE:CZ	1:B:1130:GLY:HA3	2.11	0.85
1:A:724:ASN:H	1:A:724:ASN:HD22	1.25	0.85
1:B:746:ILE:HG23	1:B:1182:ASP:CB	2.05	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1311:THR:HG23	1:A:1312:SER:N	1.89	0.85
1:A:704:LEU:O	1:A:706:LYS:N	2.10	0.85
1:A:513:SER:HB3	1:A:520:MET:CE	2.06	0.85
1:A:838:VAL:HG12	1:A:839:PRO:N	1.92	0.85
1:B:52:GLN:HE22	1:B:71:LEU:HB2	1.42	0.85
1:B:253:HIS:CE1	1:B:254:PRO:HD2	2.11	0.85
1:A:746:ILE:HG23	1:A:1182:ASP:HB3	1.58	0.84
1:A:1391:MET:HE2	1:A:1458:VAL:HG22	0.88	0.84
1:A:1425:LYS:HD3	1:A:1447:TRP:CE2	2.12	0.84
1:A:588:ARG:O	1:A:592:GLU:HG3	1.78	0.84
1:A:875:MET:CE	1:A:1139:PHE:HE2	1.73	0.84
1:B:52:GLN:HE22	1:B:71:LEU:H	1.24	0.84
1:A:482:ASP:OD1	1:A:788:HIS:CD2	2.29	0.84
1:A:604:VAL:HG23	1:A:640:THR:HG21	1.58	0.84
1:A:875:MET:HE1	1:A:1139:PHE:CD2	2.12	0.84
1:A:937:LYS:HE3	1:A:1033:SER:HB2	1.59	0.84
1:A:1401:LEU:HD12	1:A:1401:LEU:C	2.03	0.84
1:B:843:VAL:HG12	1:B:844:GLU:N	1.92	0.84
1:A:409:HIS:O	1:A:412:THR:HB	1.76	0.84
1:A:659:ILE:HG21	1:A:716:ILE:HD11	1.59	0.84
1:B:555:PHE:CD1	1:B:555:PHE:C	2.55	0.84
1:A:704:LEU:O	1:A:705:LEU:C	2.20	0.84
1:A:1115:VAL:O	1:A:1115:VAL:CG1	2.24	0.84
1:B:777:GLY:O	1:B:788:HIS:HE1	1.60	0.84
1:A:364:ILE:HD12	1:A:374:ILE:HD11	1.60	0.83
1:A:729:GLY:O	1:A:748:GLY:HA3	1.78	0.83
1:A:731:SER:HA	1:A:748:GLY:H	1.42	0.83
1:B:734:LEU:HD12	1:B:738:HIS:HD2	1.43	0.83
1:B:787:ARG:NH1	1:B:821:PRO:HG2	1.94	0.83
1:B:1062:ARG:O	1:B:1062:ARG:CG	2.26	0.83
1:A:526:LEU:N	1:A:526:LEU:CD1	2.40	0.83
1:A:838:VAL:CG1	1:A:839:PRO:CD	2.56	0.83
1:A:1062:ARG:NH2	1:A:1088:GLU:OE2	2.12	0.83
1:A:430:VAL:CG1	1:A:554:GLU:HB2	2.08	0.83
1:A:515:ARG:HH22	1:A:966:ILE:HB	1.42	0.83
1:A:1388:THR:CG2	1:A:1388:THR:O	2.27	0.83
1:A:434:SER:OG	1:A:438:GLU:OE2	1.97	0.83
1:A:950:THR:HG22	1:A:952:MET:H	1.42	0.83
1:A:734:LEU:HD11	1:A:738:HIS:CD2	2.12	0.83
1:A:1221:PRO:HB2	1:A:1229:MET:CE	2.09	0.83
1:A:982:GLN:HE22	1:A:1240:ARG:HD2	1.43	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1115:VAL:O	1:B:1115:VAL:CG1	2.22	0.82
1:A:227:MET:HE3	1:A:282:GLU:HA	1.59	0.82
1:A:266:VAL:O	1:A:279:THR:CG2	2.28	0.82
1:A:670:LEU:O	1:A:670:LEU:HD22	1.78	0.82
1:A:426:LEU:CD2	1:A:543:LEU:HB3	2.09	0.82
1:A:459:GLU:O	1:A:463:LEU:HB2	1.78	0.82
1:A:912:SER:HB2	1:A:968:PRO:HD2	1.62	0.82
1:B:1349:ARG:NH1	1:B:1349:ARG:CG	2.34	0.82
1:A:59:VAL:HG22	1:A:105:TYR:HD2	1.44	0.82
1:A:1447:TRP:CE2	1:A:1451:VAL:CG2	2.61	0.82
1:B:1370:GLY:N	1:B:1389:GLY:O	2.12	0.82
1:A:464:ILE:HD11	1:A:779:TYR:CZ	2.13	0.82
1:A:526:LEU:HD12	1:A:526:LEU:H	1.45	0.82
1:A:397:SER:HB2	1:A:399:LYS:HG3	1.61	0.82
1:A:746:ILE:HG21	1:A:1182:ASP:N	1.94	0.82
1:B:253:HIS:CD2	1:B:254:PRO:HD2	2.14	0.82
1:B:959:SER:HA	1:B:1369:THR:HG21	1.61	0.82
1:B:1471:HIS:O	1:B:1472:LEU:HB2	1.80	0.82
1:B:430:VAL:HG11	1:B:554:GLU:HB2	1.61	0.82
1:B:299:VAL:O	1:B:299:VAL:CG1	2.28	0.82
1:B:1039:LYS:O	1:B:1040:PHE:HD1	1.63	0.82
1:B:1216:VAL:HG11	1:B:1249:MET:HE2	1.61	0.82
1:B:1184:ASN:HB3	1:B:1185:PRO:CD	2.10	0.81
1:A:452:GLN:NE2	1:A:764:THR:CG2	2.42	0.81
1:A:950:THR:HG22	1:A:952:MET:N	1.95	0.81
1:B:240:ASN:HD21	1:B:327:TRP:HA	1.45	0.81
1:B:815:GLU:OE1	1:B:815:GLU:HA	1.80	0.81
1:A:513:SER:HB3	1:A:520:MET:HE2	1.61	0.81
1:A:932:VAL:O	1:A:933:ALA:HB2	1.78	0.81
1:B:866:GLU:OE2	1:B:1125:ARG:NH2	2.14	0.81
1:A:253:HIS:CG	1:A:254:PRO:CD	2.52	0.81
1:B:242:ASN:ND2	1:B:242:ASN:H	1.79	0.81
1:A:531:ASN:OD1	1:A:533:LEU:HB2	1.81	0.81
1:A:1376:LEU:HB3	1:A:1439:PHE:HE2	1.45	0.81
1:B:973:ASP:OD2	1:B:1298:LYS:HE3	1.79	0.81
1:A:342:VAL:HG11	1:A:390:MET:HE2	1.61	0.81
1:A:515:ARG:HD2	1:A:1367:TYR:HE1	1.46	0.81
1:B:182:MET:CE	1:B:217:PRO:CA	2.58	0.81
1:A:447:LEU:HD12	1:A:451:GLN:HG3	1.62	0.80
1:B:426:LEU:HD11	1:B:558:MET:HG3	1.62	0.80
1:B:824:GLN:O	1:B:827:ASP:HB2	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:THR:HG22	1:A:291:ALA:N	1.95	0.80
1:A:513:SER:CB	1:A:520:MET:HE2	2.11	0.80
1:A:454:PHE:CG	1:A:648:GLU:HB2	2.17	0.80
1:A:746:ILE:CG2	1:A:1182:ASP:N	2.43	0.80
1:B:302:ALA:HA	1:B:347:ARG:HH12	1.46	0.80
1:B:417:ASP:C	1:B:419:TRP:N	2.38	0.80
1:B:479:MET:HG3	1:B:1104:MET:HE1	1.61	0.80
1:A:182:MET:CE	1:A:217:PRO:C	2.54	0.80
1:B:1080:VAL:CG1	1:B:1084:MET:HE3	2.12	0.80
1:B:310:PRO:HG3	1:B:404:ARG:HH22	1.45	0.80
1:A:734:LEU:HD11	1:A:738:HIS:HD2	1.46	0.80
1:A:1184:ASN:HB3	1:A:1185:PRO:CD	2.11	0.80
1:A:1290:GLY:O	1:A:1291:ASP:HB3	1.82	0.80
1:B:963:VAL:CG1	1:B:964:MET:N	2.45	0.80
1:B:582:LEU:H	1:B:755:GLN:NE2	1.80	0.80
1:B:710:LYS:CG	1:B:939:GLY:HA3	2.10	0.80
1:A:787:ARG:HH12	1:A:821:PRO:HB2	1.47	0.79
1:B:652:THR:CG2	1:B:703:GLY:CA	2.59	0.79
1:A:1322:ILE:HG23	1:A:1323:ILE:HG23	1.64	0.79
1:B:1047:MET:HG2	1:B:1186:ARG:NH1	1.97	0.79
1:A:974:ILE:HD11	1:A:983:LEU:CD1	2.13	0.79
1:B:778:PHE:CZ	1:B:1039:LYS:HD2	2.18	0.79
1:B:1131:THR:HB	1:B:1134:LYS:HG3	1.64	0.79
1:B:1388:THR:CG2	1:B:1388:THR:O	2.29	0.79
1:A:47:HIS:CE1	1:A:176:SER:HB3	2.18	0.79
1:A:317:ILE:HG22	1:A:321:ASN:HD21	1.47	0.79
1:B:235:ASN:HD22	1:B:236:THR:N	1.80	0.79
1:B:447:LEU:HD21	1:B:674:ALA:HA	1.64	0.79
1:B:536:ASP:C	1:B:536:ASP:OD1	2.25	0.79
1:A:501:GLN:HE21	1:A:653:HIS:HD2	1.30	0.79
1:A:595:ASP:O	1:A:596:ALA:C	2.21	0.79
1:B:466:HIS:CE1	1:B:684:PHE:CE1	2.70	0.79
1:B:974:ILE:HD11	1:B:983:LEU:HD12	1.62	0.79
1:A:973:ASP:OD2	1:A:1298:LYS:HE3	1.81	0.79
1:B:746:ILE:O	1:B:747:SER:C	2.22	0.79
1:A:90:ARG:NH1	1:A:129:GLU:OE1	2.16	0.79
1:B:1047:MET:CG	1:B:1186:ARG:CZ	2.56	0.79
1:B:1121:ASP:OD2	1:B:1124:LEU:HB2	1.82	0.79
1:B:602:THR:C	1:B:640:THR:CG2	2.56	0.79
1:B:37:ASP:OD2	1:B:40:THR:HB	1.82	0.79
1:A:230:HIS:HE1	1:A:234:ILE:HG13	1.45	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:TYR:C	1:A:355:TYR:CD1	2.61	0.78
1:A:536:ASP:C	1:A:536:ASP:OD1	2.25	0.78
1:A:580:GLU:O	1:A:584:ASP:OD1	2.01	0.78
1:A:447:LEU:HD21	1:A:674:ALA:CA	2.14	0.78
1:B:693:MET:HA	1:B:693:MET:HE3	1.63	0.78
1:B:1318:ASN:HD22	1:B:1318:ASN:H	1.30	0.78
1:A:375:ASP:OD2	1:A:377:THR:CB	2.26	0.78
1:A:1043:LEU:HD23	1:A:1044:PRO:HD2	1.66	0.78
1:A:959:SER:HA	1:A:1369:THR:HG23	1.63	0.78
1:B:1317:THR:CG2	1:B:1318:ASN:N	2.44	0.78
1:A:450:ARG:O	1:A:452:GLN:N	2.17	0.78
1:A:728:ILE:HD12	1:A:1047:MET:HE3	1.63	0.78
1:A:1401:LEU:CD1	1:A:1405:ILE:HB	2.13	0.78
1:B:266:VAL:HG12	1:B:279:THR:CG2	2.14	0.78
1:B:565:THR:CG2	1:B:602:THR:HB	2.13	0.78
1:A:139:VAL:CG1	1:A:140:SER:H	1.90	0.78
1:A:24:ALA:HB1	1:A:207:TYR:CE2	2.19	0.78
1:A:177:ILE:HD13	1:A:179:TYR:HE1	1.49	0.78
1:A:213:THR:HB	1:A:1008:THR:HG23	1.66	0.78
1:A:227:MET:HE2	1:A:282:GLU:CG	2.13	0.78
1:B:950:THR:CG2	1:B:952:MET:H	1.96	0.78
1:A:310:PRO:HG3	1:A:404:ARG:HH22	1.43	0.77
1:A:465:LEU:C	1:A:465:LEU:HD12	2.08	0.77
1:B:260:MET:O	1:B:263:LEU:HB2	1.84	0.77
1:B:218:THR:O	1:B:218:THR:HG22	1.82	0.77
1:A:236:THR:CG2	1:A:328:ASP:N	2.45	0.77
1:B:405:GLU:H	1:B:405:GLU:CD	1.90	0.77
1:B:522:LEU:HD21	1:B:705:LEU:CD2	2.14	0.77
1:B:531:ASN:OD1	1:B:533:LEU:HB2	1.83	0.77
1:B:746:ILE:CG2	1:B:1182:ASP:N	2.37	0.77
1:A:182:MET:HE3	1:A:217:PRO:CA	2.11	0.77
1:A:930:ILE:HD13	1:A:983:LEU:HD13	1.65	0.77
1:A:1395:TYR:CE1	1:A:1397:LEU:HD21	2.20	0.77
1:B:249:THR:HG22	1:B:250:ARG:HG2	1.67	0.77
1:A:551:THR:OG1	1:A:554:GLU:HG2	1.84	0.77
1:B:580:GLU:O	1:B:584:ASP:OD1	2.03	0.77
1:B:1131:THR:HG22	1:B:1134:LYS:H	1.49	0.77
1:B:826:ARG:NH1	1:B:1046:GLU:OE2	2.18	0.77
1:A:1008:THR:CG2	1:A:1009:ILE:N	2.44	0.77
1:B:505:GLN:NE2	1:B:1001:VAL:H	1.83	0.77
1:B:515:ARG:HD2	1:B:1367:TYR:HE2	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:562:MET:HE3	1:B:566:ALA:HB2	1.66	0.77
1:B:551:THR:OG1	1:B:554:GLU:HG2	1.85	0.77
1:B:731:SER:CA	1:B:748:GLY:H	1.98	0.77
1:B:1449:ARG:CB	1:B:1449:ARG:NH1	1.80	0.77
1:A:113:ASN:HD21	1:A:115:ASP:H	1.31	0.76
1:A:1356:VAL:HG22	1:A:1374:VAL:HG21	1.67	0.76
1:B:572:THR:CG2	1:B:573:PHE:N	2.47	0.76
1:B:985:TYR:HE1	1:B:1207:VAL:HG13	1.50	0.76
1:B:1216:VAL:CG1	1:B:1249:MET:HE2	2.14	0.76
1:A:528:ASN:HB3	1:A:542:LEU:HD22	1.66	0.76
1:B:658:LEU:HD23	1:B:666:VAL:HG21	1.67	0.76
1:B:1369:THR:C	1:B:1389:GLY:O	2.28	0.76
1:A:890:ASP:O	1:A:893:ARG:HB2	1.84	0.76
1:A:959:SER:HA	1:A:1369:THR:HG21	1.67	0.76
1:A:413:LEU:O	1:A:414:LYS:HD2	1.85	0.76
1:B:826:ARG:HG2	1:B:826:ARG:NH1	1.99	0.76
1:B:1043:LEU:HD23	1:B:1044:PRO:HD2	1.67	0.76
1:A:447:LEU:HD13	1:A:670:LEU:HD21	1.65	0.76
1:A:450:ARG:O	1:A:453:ALA:N	2.19	0.76
1:B:153:ARG:NH2	1:B:263:LEU:O	2.18	0.76
1:B:295:LYS:HD2	1:B:390:MET:HE3	1.67	0.76
1:B:582:LEU:H	1:B:755:GLN:HE22	1.30	0.76
1:B:875:MET:HE1	1:B:1139:PHE:CD2	2.20	0.76
1:B:1084:MET:SD	1:B:1168:LEU:HD21	2.25	0.76
1:A:1131:THR:HB	1:A:1134:LYS:HG3	1.68	0.76
1:B:982:GLN:HE22	1:B:1240:ARG:HD2	1.49	0.76
1:A:1220:ARG:HG3	1:A:1224:GLU:HG3	1.67	0.76
1:A:1471:HIS:O	1:A:1472:LEU:HB2	1.85	0.76
1:B:704:LEU:O	1:B:705:LEU:C	2.25	0.76
1:A:643:ASN:HB3	1:A:665:THR:HG22	1.68	0.76
1:A:260:MET:O	1:A:263:LEU:N	2.19	0.76
1:B:426:LEU:CD1	1:B:558:MET:HG3	2.16	0.76
1:B:522:LEU:HD21	1:B:705:LEU:HD21	1.68	0.76
1:A:829:LEU:HD13	1:A:1168:LEU:HD13	1.67	0.75
1:A:1374:VAL:O	1:A:1375:ILE:CG1	2.34	0.75
1:A:826:ARG:NH1	1:A:1046:GLU:OE2	2.19	0.75
1:B:1401:LEU:C	1:B:1401:LEU:CD1	2.55	0.75
1:A:1221:PRO:CB	1:A:1229:MET:HE2	2.11	0.75
1:A:999:LYS:HG3	1:A:1022:LEU:CD2	2.17	0.75
1:B:438:GLU:OE1	1:B:672:GLN:NE2	2.20	0.75
1:B:452:GLN:CG	1:B:765:ALA:HB2	2.17	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:LEU:HD23	1:A:324:MET:HG2	1.68	0.75
1:A:452:GLN:CG	1:A:765:ALA:HB2	2.16	0.75
1:B:175:ARG:HH11	1:B:175:ARG:HG3	1.52	0.75
1:B:820:ARG:HB3	1:B:821:PRO:CD	2.16	0.75
1:A:536:ASP:OD1	1:A:536:ASP:O	2.05	0.75
1:B:317:ILE:HG22	1:B:321:ASN:HD21	1.52	0.75
1:B:584:ASP:OD1	1:B:584:ASP:N	2.14	0.75
1:B:1039:LYS:C	1:B:1040:PHE:CD1	2.65	0.75
1:A:207:TYR:N	1:A:207:TYR:CD1	2.54	0.75
1:A:513:SER:CB	1:A:520:MET:CE	2.64	0.75
1:A:643:ASN:HB3	1:A:665:THR:CG2	2.16	0.75
1:A:950:THR:CG2	1:A:951:GLU:H	1.98	0.75
1:A:1317:THR:HG22	1:A:1318:ASN:N	2.00	0.75
1:A:1394:VAL:O	1:A:1394:VAL:HG12	1.87	0.75
1:A:443:ASP:O	1:A:445:ALA:N	2.20	0.74
1:A:536:ASP:OD1	1:A:538:THR:HG22	1.85	0.74
1:A:1413:GLN:HG3	1:A:1414:ARG:O	1.87	0.74
1:B:375:ASP:OD2	1:B:377:THR:HB	1.87	0.74
1:A:60:LYS:O	1:A:63:GLY:N	2.19	0.74
1:A:139:VAL:HG11	1:A:143:GLN:CB	2.17	0.74
1:B:59:VAL:CG2	1:B:105:TYR:CD2	2.70	0.74
1:A:643:ASN:HD22	1:A:665:THR:CB	2.01	0.74
1:B:1084:MET:SD	1:B:1168:LEU:CD2	2.75	0.74
1:B:465:LEU:C	1:B:465:LEU:HD12	2.12	0.74
1:B:139:VAL:CG1	1:B:143:GLN:CB	2.66	0.74
1:B:450:ARG:O	1:B:453:ALA:N	2.20	0.74
1:B:731:SER:HA	1:B:747:SER:CA	2.17	0.74
1:A:528:ASN:CB	1:A:542:LEU:HD22	2.17	0.74
1:A:824:GLN:HE21	1:A:824:GLN:CA	1.99	0.74
1:B:753:GLY:O	1:B:754:ILE:C	2.25	0.74
1:A:342:VAL:HG13	1:A:392:ALA:HB2	1.69	0.74
1:A:537:GLU:HG3	1:A:538:THR:N	1.92	0.74
1:A:1131:THR:HG22	1:A:1133:GLU:N	2.02	0.74
1:A:515:ARG:HD2	1:A:1367:TYR:CZ	2.22	0.74
1:A:862:ALA:O	1:A:1118:CYS:CB	2.35	0.74
1:B:1131:THR:HG22	1:B:1133:GLU:N	2.03	0.74
1:A:102:TYR:CD2	1:A:144:PHE:HE1	2.06	0.73
1:A:731:SER:CA	1:A:748:GLY:H	2.01	0.73
1:B:1289:MET:CE	1:B:1289:MET:HB2	2.17	0.73
1:A:609:GLU:OE2	1:A:645:ARG:HD3	1.88	0.73
1:B:295:LYS:NZ	1:B:299:VAL:O	2.17	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:724:ASN:ND2	1:A:724:ASN:N	2.36	0.73
1:A:1394:VAL:HG11	1:A:1401:LEU:CD2	2.17	0.73
1:B:528:ASN:C	1:B:529:LEU:HD23	2.13	0.73
1:B:891:PRO:HA	1:B:894:PHE:CE2	2.24	0.73
1:A:727:ALA:HB3	1:A:744:SER:HB2	1.69	0.73
1:A:728:ILE:HD12	1:A:1047:MET:CE	2.17	0.73
1:A:824:GLN:HA	1:A:824:GLN:NE2	2.01	0.73
1:A:1289:MET:HE3	1:A:1289:MET:H	1.52	0.73
1:B:146:LEU:HD12	1:B:146:LEU:O	1.88	0.73
1:B:746:ILE:HG22	1:B:747:SER:O	1.88	0.73
1:A:290:THR:CG2	1:A:291:ALA:N	2.51	0.73
1:A:295:LYS:CE	1:A:299:VAL:HG12	2.18	0.73
1:A:1401:LEU:HD11	1:A:1405:ILE:HB	1.71	0.73
1:B:295:LYS:HD2	1:B:390:MET:CE	2.19	0.73
1:B:465:LEU:HD12	1:B:465:LEU:O	1.89	0.73
1:A:573:PHE:HB2	1:A:574:PRO:HD2	1.71	0.73
1:B:214:ASN:O	1:B:1015:LYS:HE2	1.88	0.73
1:B:665:THR:HG22	1:B:665:THR:O	1.89	0.73
1:A:464:ILE:CD1	1:A:779:TYR:CE1	2.71	0.73
1:A:1460:LYS:O	1:A:1462:MET:N	2.21	0.73
1:B:1113:CYS:O	1:B:1115:VAL:N	2.22	0.73
1:B:511:ILE:HG22	1:B:512:ASP:N	2.03	0.73
1:B:602:THR:C	1:B:640:THR:HG22	2.14	0.73
1:A:1391:MET:CE	1:A:1458:VAL:CG2	2.56	0.73
1:B:787:ARG:HH12	1:B:821:PRO:CG	2.00	0.73
1:A:1062:ARG:HG3	1:A:1062:ARG:O	1.89	0.72
1:A:1425:LYS:HD3	1:A:1447:TRP:NE1	2.03	0.72
1:A:1447:TRP:CZ2	1:A:1451:VAL:HG22	2.24	0.72
1:B:731:SER:HA	1:B:747:SER:HA	1.71	0.72
1:A:324:MET:HE2	1:A:327:TRP:HE1	1.54	0.72
1:A:387:PRO:HD3	1:A:1344:GLU:CD	2.15	0.72
1:B:290:THR:CG2	1:B:292:PRO:CD	2.68	0.72
1:B:780:ARG:HH21	1:B:1105:VAL:HG23	1.53	0.72
1:B:829:LEU:HD13	1:B:1168:LEU:HD13	1.70	0.72
1:B:838:VAL:HG12	1:B:839:PRO:N	2.02	0.72
1:A:850:ARG:HH11	1:A:850:ARG:HG3	1.53	0.72
1:B:52:GLN:NE2	1:B:71:LEU:H	1.87	0.72
1:B:838:VAL:CG1	1:B:839:PRO:HD2	2.19	0.72
1:A:918:THR:HG23	1:A:1256:MET:SD	2.30	0.72
1:A:1221:PRO:CD	1:A:1229:MET:HE1	2.19	0.72
1:B:223:GLN:HB3	1:B:224:PRO:HA	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:THR:HG21	1:B:328:ASP:N	2.00	0.72
1:B:820:ARG:CB	1:B:821:PRO:CD	2.67	0.72
1:A:976:SER:OG	1:A:978:GLU:HG3	1.90	0.72
1:A:189:THR:HG22	1:A:190:THR:N	2.04	0.72
1:B:781:PHE:CE2	1:B:791:GLU:HB3	2.25	0.72
1:A:290:THR:HG22	1:A:292:PRO:N	2.05	0.72
1:A:1356:VAL:HG11	1:A:1431:HIS:HB2	1.71	0.72
1:B:493:ARG:NH2	1:B:786:ASP:OD1	2.21	0.72
1:B:1076:GLY:CA	1:B:1145:GLU:HG2	2.18	0.72
1:B:1184:ASN:O	1:B:1187:LEU:N	2.22	0.72
1:B:1369:THR:HG22	1:B:1369:THR:O	1.89	0.72
1:B:3:VAL:HG22	1:B:231:ASN:HB2	1.72	0.72
1:B:1417:VAL:HG12	1:B:1419:HIS:H	1.54	0.72
1:B:959:SER:HA	1:B:1369:THR:HG23	1.69	0.72
1:A:985:TYR:HE1	1:A:1207:VAL:HG13	1.53	0.71
1:B:218:THR:CG2	1:B:221:LEU:HG	2.20	0.71
1:B:731:SER:HA	1:B:748:GLY:N	2.04	0.71
1:B:780:ARG:NH2	1:B:1105:VAL:HG23	2.04	0.71
1:A:515:ARG:CD	1:A:1367:TYR:HE1	1.96	0.71
1:A:1230:GLN:NE2	1:A:1267:ARG:HD3	2.05	0.71
1:B:1164:ARG:NH1	1:B:1166:ASP:OD2	2.23	0.71
1:A:447:LEU:HD12	1:A:447:LEU:C	2.14	0.71
1:B:182:MET:HE3	1:B:217:PRO:HB2	0.79	0.71
1:B:525:ARG:HG2	1:B:542:LEU:HD13	1.71	0.71
1:B:603:HIS:N	1:B:640:THR:HG22	2.05	0.71
1:A:1289:MET:H	1:A:1289:MET:CE	2.03	0.71
1:B:242:ASN:ND2	1:B:242:ASN:N	2.37	0.71
1:A:1466:LEU:O	1:A:1467:GLU:C	2.33	0.71
1:B:88:ALA:O	1:B:92:ILE:HG13	1.91	0.71
1:A:454:PHE:HE2	1:A:647:ALA:CB	2.03	0.71
1:A:1216:VAL:CG1	1:A:1249:MET:HE2	2.21	0.71
1:A:1317:THR:HG23	1:A:1358:GLU:OE1	1.88	0.71
1:B:500:ARG:NH2	1:B:1040:PHE:HA	2.05	0.71
1:B:704:LEU:C	1:B:706:LYS:N	2.49	0.71
1:B:875:MET:CE	1:B:1139:PHE:CE2	2.73	0.71
1:A:479:MET:CG	1:A:1104:MET:HE1	2.15	0.71
1:A:746:ILE:HG23	1:A:1182:ASP:H	1.54	0.71
1:B:588:ARG:O	1:B:592:GLU:CG	2.38	0.71
1:B:842:GLU:HB3	1:B:1156:ARG:HD3	1.72	0.71
1:A:312:ASN:OD1	1:A:312:ASN:N	2.22	0.71
1:A:1131:THR:HG23	1:A:1133:GLU:OE1	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:593:THR:O	1:B:597:VAL:HG23	1.91	0.71
1:A:1396:ASP:C	1:A:1396:ASP:OD1	2.34	0.71
1:B:295:LYS:NZ	1:B:299:VAL:HG12	2.06	0.71
1:B:907:ILE:HG23	1:B:927:GLU:HG2	1.73	0.71
1:B:1047:MET:CE	1:B:1186:ARG:NH2	2.44	0.71
1:B:417:ASP:C	1:B:419:TRP:H	1.96	0.71
1:B:426:LEU:HD22	1:B:543:LEU:HB3	1.73	0.70
1:A:381:GLU:CD	1:A:402:ARG:NH1	2.48	0.70
1:A:1222:LEU:C	1:A:1222:LEU:HD12	2.16	0.70
1:B:59:VAL:HG21	1:B:105:TYR:CD2	2.26	0.70
1:B:210:ARG:HA	2:B:2473:OMT:HE3	1.72	0.70
1:B:295:LYS:CB	1:B:390:MET:HE1	2.20	0.70
1:B:513:SER:CB	1:B:520:MET:HE2	2.20	0.70
1:B:1289:MET:HB2	1:B:1289:MET:HE3	1.71	0.70
1:B:266:VAL:O	1:B:279:THR:CG2	2.39	0.70
1:B:459:GLU:O	1:B:463:LEU:HB2	1.91	0.70
1:B:958:HIS:O	1:B:1369:THR:HG22	1.90	0.70
1:A:96:GLU:HA	1:A:96:GLU:OE1	1.89	0.70
1:B:454:PHE:CE2	1:B:647:ALA:HB3	2.26	0.70
1:B:1053:HIS:ND1	1:B:1062:ARG:NH1	2.39	0.70
1:B:1053:HIS:CE1	1:B:1062:ARG:HH11	2.08	0.70
1:B:1253:LYS:HG3	1:B:1253:LYS:O	1.91	0.70
1:A:140:SER:O	1:A:143:GLN:N	2.24	0.70
1:A:183:PHE:CE1	1:A:188:LEU:HA	2.26	0.70
1:A:177:ILE:HD13	1:A:179:TYR:CE1	2.26	0.70
1:A:838:VAL:CG1	1:A:839:PRO:N	2.54	0.70
1:A:734:LEU:HD12	1:A:738:HIS:HD2	1.54	0.70
1:A:997:THR:HG22	1:A:998:VAL:N	2.05	0.70
1:B:450:ARG:O	1:B:451:GLN:C	2.35	0.70
1:B:739:PHE:O	1:B:740:PRO:O	2.10	0.70
1:B:1121:ASP:OD1	1:B:1122:ASP:N	2.25	0.70
1:B:1212:ASP:O	1:B:1216:VAL:HG23	1.90	0.70
1:B:1394:VAL:O	1:B:1394:VAL:HG12	1.91	0.70
1:A:113:ASN:HD22	1:A:114:VAL:N	1.89	0.70
1:A:1076:GLY:HA3	1:A:1145:GLU:CG	2.22	0.70
1:A:1311:THR:CG2	1:A:1312:SER:N	2.55	0.70
1:B:602:THR:C	1:B:640:THR:HG23	2.17	0.70
1:B:1076:GLY:HA3	1:B:1145:GLU:CG	2.17	0.70
1:A:461:MET:HE1	1:A:465:LEU:HD23	1.74	0.70
1:A:1221:PRO:CG	1:A:1229:MET:CE	2.70	0.70
1:B:802:VAL:HG23	1:B:1137:ASN:HB2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:985:TYR:CE1	1:B:1207:VAL:CG1	2.75	0.70
1:A:218:THR:HG21	1:A:221:LEU:HG	1.73	0.69
1:A:345:MET:HE1	1:A:385:LEU:HB2	1.73	0.69
1:A:413:LEU:O	1:A:414:LYS:CD	2.40	0.69
1:B:353:MET:HG2	1:B:385:LEU:HD23	1.72	0.69
1:B:447:LEU:HD12	1:B:451:GLN:CG	2.22	0.69
1:B:603:HIS:N	1:B:640:THR:CG2	2.54	0.69
1:B:1102:CYS:HG	5:B:2476:F3S:FE1	1.09	0.69
1:B:1414:ARG:NH2	1:B:1455:TRP:CZ2	2.60	0.69
1:A:491:LYS:O	1:A:492:TYR:C	2.35	0.69
1:A:501:GLN:HE21	1:A:653:HIS:CD2	2.10	0.69
1:A:1019:ASP:OD2	1:A:1204:ARG:HB2	1.93	0.69
1:A:1121:ASP:OD2	1:A:1124:LEU:HB2	1.92	0.69
1:B:447:LEU:CD1	1:B:451:GLN:HG3	2.22	0.69
1:B:419:TRP:O	1:B:540:THR:HG21	1.92	0.69
1:B:1053:HIS:CE1	1:B:1062:ARG:NH1	2.60	0.69
1:B:1105:VAL:HG13	1:B:1107:GLN:HG3	1.74	0.69
1:B:242:ASN:HD22	1:B:242:ASN:N	1.87	0.69
1:B:1054:GLN:O	1:B:1057:THR:N	2.26	0.69
1:B:657:VAL:O	1:B:658:LEU:C	2.32	0.69
1:A:143:GLN:C	1:A:143:GLN:HE21	2.01	0.69
1:B:728:ILE:HD12	1:B:1047:MET:HE1	1.74	0.69
1:A:59:VAL:HG21	1:A:105:TYR:CE2	2.27	0.69
1:A:454:PHE:CD2	1:A:648:GLU:HB2	2.28	0.69
1:A:1291:ASP:C	1:A:1291:ASP:OD1	2.35	0.69
1:B:985:TYR:CE1	1:B:1207:VAL:HG13	2.27	0.69
1:A:52:GLN:CD	1:A:71:LEU:H	2.01	0.69
1:A:182:MET:HE3	1:A:217:PRO:HB2	0.70	0.69
1:A:313:HIS:O	1:A:317:ILE:HG13	1.93	0.69
1:A:496:HIS:O	1:A:653:HIS:HE1	1.76	0.69
1:A:515:ARG:NE	1:A:1367:TYR:CE1	2.60	0.69
1:B:113:ASN:ND2	1:B:113:ASN:C	2.49	0.69
1:B:122:ASN:OD1	1:B:125:ARG:NH1	2.26	0.69
1:B:309:THR:HB	1:B:314:LYS:HE3	1.74	0.69
1:B:1090:PHE:CD1	1:B:1090:PHE:N	2.60	0.69
1:A:875:MET:HE1	1:A:1139:PHE:CZ	2.20	0.69
1:A:1221:PRO:HG2	1:A:1229:MET:CE	2.23	0.69
1:B:1447:TRP:CE2	1:B:1451:VAL:HG22	2.28	0.69
1:B:107:TRP:N	1:B:107:TRP:CD1	2.59	0.69
1:B:302:ALA:HB2	1:B:347:ARG:NH1	2.07	0.69
1:A:208:HIS:CD2	1:A:209:GLN:O	2.46	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ASN:HD21	1:A:327:TRP:HA	1.58	0.68
1:B:236:THR:CG2	1:B:328:ASP:N	2.52	0.68
1:A:9:ILE:HG13	1:A:361:GLY:O	1.93	0.68
1:A:1415:ILE:HG21	1:A:1421:GLU:HB2	1.75	0.68
1:A:358:THR:HB	1:A:360:ASP:OD1	1.92	0.68
1:B:386:GLY:O	1:B:389:GLU:HG3	1.93	0.68
1:A:208:HIS:CE1	1:A:223:GLN:OE1	2.45	0.68
1:A:353:MET:HE3	1:A:366:GLY:O	1.94	0.68
1:A:426:LEU:HD23	1:A:426:LEU:H	1.59	0.68
1:A:1276:LEU:HD12	1:A:1277:GLY:N	2.08	0.68
1:A:1362:SER:HA	1:A:1380:GLY:HA3	1.74	0.68
1:A:1375:ILE:C	1:A:1376:LEU:HD23	2.19	0.68
1:B:1348:VAL:O	1:B:1348:VAL:HG13	1.91	0.68
1:A:37:ASP:C	1:A:37:ASP:OD1	2.33	0.68
1:A:52:GLN:HE22	1:A:71:LEU:HB2	1.59	0.68
1:A:732:ARG:H	1:A:747:SER:CB	2.07	0.68
1:A:913:GLY:HA2	1:A:1349:ARG:HD3	1.76	0.68
1:A:1338:ALA:HB3	1:A:1357:VAL:HG22	1.74	0.68
1:B:37:ASP:C	1:B:37:ASP:OD1	2.37	0.68
1:B:211:TYR:HD1	1:B:212:SER:H	1.42	0.68
1:B:296:MET:O	1:B:297:MET:C	2.33	0.68
1:B:604:VAL:HG23	1:B:640:THR:HG21	1.73	0.68
1:B:826:ARG:HG2	1:B:1046:GLU:OE2	1.93	0.68
1:B:932:VAL:O	1:B:933:ALA:HB2	1.92	0.68
1:B:1449:ARG:O	1:B:1452:THR:HB	1.93	0.68
1:A:295:LYS:HD3	1:A:295:LYS:C	2.19	0.68
1:A:414:LYS:HB3	1:A:415:PRO:CD	2.23	0.68
1:A:1317:THR:HG21	1:A:1358:GLU:OE1	1.92	0.68
1:B:794:VAL:HG12	1:B:795:ILE:N	2.06	0.68
1:B:885:GLY:C	1:B:887:GLY:H	2.01	0.68
1:A:152:ARG:O	1:A:156:GLU:HB2	1.94	0.68
1:B:250:ARG:O	1:B:531:ASN:ND2	2.27	0.68
1:B:732:ARG:H	1:B:747:SER:HB3	1.57	0.68
1:B:1170:GLN:O	1:B:1170:GLN:CG	2.39	0.68
1:A:248:GLU:HA	1:A:251:MET:CG	2.22	0.68
1:A:447:LEU:CD1	1:A:451:GLN:HG3	2.23	0.68
1:A:985:TYR:CE1	1:A:1207:VAL:HG13	2.28	0.68
1:A:359:THR:HG23	1:A:378:GLN:O	1.94	0.68
1:A:446:GLU:O	1:A:447:LEU:C	2.36	0.68
1:A:505:GLN:HE21	1:A:1001:VAL:H	1.33	0.68
1:B:389:GLU:CB	1:B:403:ASP:OD2	2.40	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:MET:HG3	1:B:673:GLU:OE2	1.92	0.68
1:B:999:LYS:HG2	1:B:1022:LEU:HD23	1.72	0.68
1:A:8:ALA:HA	1:A:362:LEU:HD12	1.75	0.67
1:B:522:LEU:CD2	1:B:705:LEU:HD21	2.24	0.67
1:A:146:LEU:HD12	1:A:146:LEU:C	2.16	0.67
1:A:310:PRO:CG	1:A:404:ARG:NH2	2.56	0.67
1:A:394:ASP:C	1:A:394:ASP:OD1	2.37	0.67
1:A:461:MET:CE	1:A:465:LEU:HD23	2.24	0.67
1:A:918:THR:HG22	1:A:920:GLU:H	1.59	0.67
1:B:1466:LEU:O	1:B:1467:GLU:C	2.37	0.67
1:A:4:GLY:HA3	1:A:207:TYR:CZ	2.29	0.67
1:A:289:ARG:NH2	1:A:532:ILE:O	2.27	0.67
1:A:506:VAL:HG11	1:A:980:LEU:HD22	1.75	0.67
1:A:850:ARG:HH11	1:A:850:ARG:CG	2.08	0.67
1:A:1388:THR:O	1:A:1388:THR:HG22	1.93	0.67
1:A:1412:PHE:HA	1:A:1456:GLN:O	1.94	0.67
1:B:266:VAL:HG12	1:B:279:THR:HG23	1.76	0.67
1:A:777:GLY:O	1:A:788:HIS:HE1	1.77	0.67
1:A:1220:ARG:N	1:A:1221:PRO:HD2	2.10	0.67
1:A:1221:PRO:HD2	1:A:1229:MET:HE1	1.76	0.67
1:B:843:VAL:CG1	1:B:844:GLU:N	2.58	0.67
1:A:336:THR:OG1	1:A:337:ASP:O	2.13	0.67
1:A:454:PHE:HE2	1:A:647:ALA:HB3	1.58	0.67
1:B:731:SER:O	1:B:735:VAL:HG23	1.93	0.67
1:A:960:THR:CG2	1:A:963:VAL:CG2	2.73	0.67
1:B:98:LEU:O	1:B:101:GLY:N	2.25	0.67
1:B:113:ASN:HD22	1:B:114:VAL:N	1.92	0.67
1:B:1388:THR:O	1:B:1388:THR:HG22	1.94	0.67
1:A:746:ILE:O	1:A:747:SER:O	2.13	0.67
1:B:394:ASP:C	1:B:394:ASP:OD1	2.38	0.67
1:B:838:VAL:CG1	1:B:839:PRO:CD	2.73	0.67
1:A:403:ASP:CG	1:A:407:LYS:HZ3	2.02	0.67
1:B:559:ARG:HD2	1:B:605:ILE:CD1	2.25	0.67
1:A:139:VAL:HG11	1:A:143:GLN:HB3	1.77	0.67
1:B:113:ASN:HD22	1:B:115:ASP:H	1.41	0.67
1:B:454:PHE:HE2	1:B:647:ALA:HB3	1.58	0.67
1:B:746:ILE:HD11	1:B:1186:ARG:NH2	2.10	0.67
1:B:1059:ASN:N	1:B:1059:ASN:HD22	1.91	0.67
1:A:746:ILE:HG22	1:A:747:SER:N	2.09	0.66
1:A:1458:VAL:HG13	1:A:1459:PRO:HD2	1.76	0.66
1:B:496:HIS:ND1	1:B:654:TYR:HD1	1.93	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:732:ARG:H	1:B:747:SER:CB	2.07	0.66
1:A:525:ARG:C	1:A:526:LEU:HD12	2.21	0.66
1:A:661:VAL:HG12	1:A:661:VAL:O	1.94	0.66
1:B:302:ALA:CA	1:B:347:ARG:HH12	2.08	0.66
1:B:146:LEU:HD12	1:B:146:LEU:C	2.19	0.66
1:A:354:ARG:NH2	1:A:1292:ALA:O	2.29	0.66
1:A:746:ILE:C	1:A:747:SER:O	2.35	0.66
1:B:355:TYR:CD1	1:B:355:TYR:C	2.72	0.66
1:A:122:ASN:OD1	1:A:125:ARG:NH1	2.25	0.66
1:A:414:LYS:HB3	1:A:415:PRO:HD3	1.76	0.66
1:B:289:ARG:NH2	1:B:532:ILE:O	2.28	0.66
1:B:559:ARG:HD2	1:B:605:ILE:HD13	1.78	0.66
1:B:1102:CYS:SG	5:B:2476:F3S:S2	2.93	0.66
1:A:1003:ARG:HG3	1:A:1003:ARG:HH11	1.61	0.66
1:B:515:ARG:HD2	1:B:1367:TYR:CZ	2.31	0.66
1:A:454:PHE:CE2	1:A:647:ALA:HB3	2.30	0.66
1:A:629:THR:O	1:A:630:HIS:C	2.37	0.66
1:B:478:SER:O	1:B:1106:ARG:NH1	2.28	0.66
1:B:1212:ASP:CG	1:B:1243:GLY:H	2.04	0.66
1:A:355:TYR:C	1:A:355:TYR:HD1	2.03	0.66
1:A:731:SER:HA	1:A:748:GLY:N	2.11	0.66
1:A:1230:GLN:NE2	1:A:1267:ARG:CD	2.59	0.66
1:B:461:MET:CE	1:B:465:LEU:HD23	2.26	0.66
1:B:780:ARG:NH2	1:B:1105:VAL:CG2	2.59	0.66
1:A:172:LEU:HG	1:A:172:LEU:O	1.94	0.66
1:A:1144:GLU:HG3	1:A:1144:GLU:O	1.95	0.66
1:B:908:LYS:HD2	1:B:921:TYR:CD1	2.31	0.66
1:A:442:MET:HE1	1:A:447:LEU:HA	1.76	0.66
1:B:107:TRP:CD1	1:B:107:TRP:H	2.12	0.66
1:B:1413:GLN:HG3	1:B:1414:ARG:O	1.96	0.66
1:A:420:VAL:HA	1:A:540:THR:HG21	1.78	0.65
1:A:1394:VAL:HG11	1:A:1401:LEU:HD22	1.76	0.65
1:B:603:HIS:CA	1:B:640:THR:CG2	2.71	0.65
1:B:1135:VAL:O	1:B:1136:VAL:C	2.33	0.65
1:B:1274:GLN:HE21	1:B:1293:ASN:HB3	1.61	0.65
1:A:452:GLN:HG3	1:A:765:ALA:HB2	1.77	0.65
1:A:491:LYS:NZ	1:A:785:GLY:HA3	2.11	0.65
1:B:909:GLN:NE2	1:B:929:GLU:OE1	2.28	0.65
1:B:1164:ARG:HD2	1:B:1166:ASP:OD1	1.96	0.65
1:A:102:TYR:CD2	1:A:144:PHE:CE1	2.82	0.65
1:A:1105:VAL:HG13	1:A:1107:GLN:HG3	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1297:GLY:O	1:A:1328:LEU:HA	1.95	0.65
1:B:139:VAL:CG1	1:B:143:GLN:HB2	2.25	0.65
1:B:142:GLU:H	1:B:142:GLU:CD	2.05	0.65
1:B:182:MET:HE1	1:B:217:PRO:CA	2.23	0.65
1:B:447:LEU:HD12	1:B:447:LEU:C	2.22	0.65
1:B:454:PHE:HE2	1:B:647:ALA:CB	2.09	0.65
1:B:734:LEU:HD11	1:B:738:HIS:HD2	1.51	0.65
1:A:94:GLU:O	1:A:95:THR:C	2.35	0.65
1:A:251:MET:HB2	1:A:533:LEU:HD12	1.78	0.65
1:A:450:ARG:O	1:A:451:GLN:C	2.37	0.65
1:A:1050:SER:O	1:A:1054:GLN:HG3	1.97	0.65
1:B:295:LYS:HB3	1:B:390:MET:HE1	1.78	0.65
1:B:572:THR:HG21	1:B:615:ARG:HB3	1.78	0.65
1:A:1207:VAL:HG13	1:A:1208:PRO:HD2	1.77	0.65
1:A:62:ILE:O	1:A:62:ILE:HG22	1.96	0.65
1:A:208:HIS:CD2	1:A:208:HIS:C	2.74	0.65
1:B:56:LYS:HG2	1:B:71:LEU:HD22	1.79	0.65
1:B:218:THR:HG22	1:B:221:LEU:H	1.62	0.65
1:B:666:VAL:CG1	1:B:667:ASN:N	2.58	0.65
1:A:107:TRP:CD1	1:A:107:TRP:H	2.15	0.65
1:A:621:ILE:HG13	1:A:658:LEU:HD13	1.79	0.65
1:A:1311:THR:HG23	1:A:1312:SER:H	1.60	0.65
1:B:734:LEU:HD12	1:B:738:HIS:CD2	2.25	0.65
1:B:960:THR:HG22	1:B:963:VAL:HG23	1.77	0.65
1:B:1058:LEU:O	1:B:1058:LEU:HD22	1.95	0.65
1:A:297:MET:HE1	1:A:323:VAL:HG11	1.78	0.65
1:A:403:ASP:CG	1:A:407:LYS:NZ	2.54	0.65
1:A:746:ILE:HG22	1:A:747:SER:O	1.97	0.65
1:A:1431:HIS:O	1:A:1435:THR:HG22	1.95	0.65
1:B:1131:THR:HB	1:B:1134:LYS:CG	2.26	0.65
1:B:1131:THR:CG2	1:B:1133:GLU:OE1	2.42	0.65
1:A:208:HIS:CE1	1:A:223:GLN:CD	2.75	0.65
1:A:531:ASN:O	1:A:532:ILE:C	2.38	0.65
1:A:704:LEU:C	1:A:706:LYS:N	2.55	0.65
1:A:443:ASP:O	1:A:444:LYS:C	2.39	0.64
1:A:734:LEU:HD12	1:A:734:LEU:C	2.21	0.64
1:A:958:HIS:ND1	1:A:958:HIS:N	2.45	0.64
1:A:317:ILE:HG22	1:A:321:ASN:ND2	2.11	0.64
1:A:453:ALA:O	1:A:761:GLN:HG3	1.98	0.64
1:A:824:GLN:CA	1:A:824:GLN:NE2	2.57	0.64
1:A:1395:TYR:CE1	1:A:1397:LEU:CD2	2.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:GLU:O	1:B:120:LYS:C	2.38	0.64
1:B:625:GLY:O	1:B:626:ALA:C	2.39	0.64
1:B:950:THR:CG2	1:B:951:GLU:H	2.07	0.64
1:A:253:HIS:CE1	1:A:254:PRO:CD	2.62	0.64
1:A:426:LEU:CD1	1:A:558:MET:HG3	2.28	0.64
1:B:990:ILE:HG13	1:B:990:ILE:O	1.97	0.64
1:B:1401:LEU:N	1:B:1402:PRO:CD	2.59	0.64
1:A:253:HIS:ND1	1:A:254:PRO:N	2.45	0.64
1:A:370:GLY:HA3	1:A:1237:ASN:HB3	1.80	0.64
1:B:938:PRO:O	1:B:939:GLY:C	2.35	0.64
1:A:74:GLY:CA	1:A:172:LEU:HD13	2.27	0.64
1:A:974:ILE:CD1	1:A:983:LEU:HD12	2.19	0.64
1:B:569:ILE:HD13	1:B:569:ILE:N	2.12	0.64
1:B:1164:ARG:HB3	1:B:1167:LEU:HD12	1.80	0.64
1:A:209:GLN:HG3	1:A:210:ARG:N	2.13	0.64
1:A:216:PHE:CZ	1:B:81:ILE:HD13	2.32	0.64
1:A:512:ASP:OD2	1:A:1367:TYR:OH	2.12	0.64
1:A:985:TYR:CE1	1:A:1207:VAL:CG1	2.80	0.64
1:A:1449:ARG:HB2	1:A:1449:ARG:CZ	2.19	0.64
1:B:1131:THR:HG22	1:B:1134:LYS:N	2.12	0.64
1:A:52:GLN:HE22	1:A:71:LEU:CB	2.11	0.64
1:B:452:GLN:HG3	1:B:765:ALA:HB2	1.78	0.64
1:A:182:MET:CE	1:A:217:PRO:CA	2.72	0.64
1:A:302:ALA:HA	1:A:347:ARG:HH12	1.62	0.64
1:A:643:ASN:HD22	1:A:665:THR:CG2	2.10	0.64
1:A:1435:THR:HG23	1:A:1437:SER:H	1.63	0.64
1:B:555:PHE:HD1	1:B:556:ARG:N	1.96	0.64
1:A:227:MET:CE	1:A:282:GLU:HG2	2.28	0.63
1:A:359:THR:HG23	1:A:378:GLN:HB3	1.79	0.63
1:A:426:LEU:HD11	1:A:558:MET:HG3	1.79	0.63
1:A:891:PRO:HB3	1:A:894:PHE:CE2	2.34	0.63
1:A:1349:ARG:HG2	1:A:1349:ARG:HH11	1.62	0.63
1:A:1447:TRP:CD2	1:A:1451:VAL:HG22	2.33	0.63
1:B:446:GLU:O	1:B:447:LEU:C	2.40	0.63
1:B:482:ASP:OD1	1:B:788:HIS:HD2	1.81	0.63
1:A:386:GLY:O	1:A:389:GLU:HG3	1.98	0.63
1:A:1112:THR:O	1:A:1114:PRO:HD3	1.97	0.63
1:A:1282:GLN:HA	1:A:1302:GLY:O	1.99	0.63
1:B:193:PRO:O	1:B:194:ASP:C	2.40	0.63
1:B:442:MET:HE3	1:B:446:GLU:HB3	1.81	0.63
1:B:443:ASP:OD2	1:B:445:ALA:HB3	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:820:ARG:HB3	1:B:821:PRO:HD2	1.78	0.63
1:B:947:PHE:O	1:B:947:PHE:HD1	1.80	0.63
1:A:248:GLU:O	1:A:250:ARG:N	2.31	0.63
1:A:259:HIS:O	1:A:260:MET:C	2.39	0.63
1:A:452:GLN:HG3	1:A:764:THR:HG22	1.79	0.63
1:A:815:GLU:HA	1:A:815:GLU:OE1	1.98	0.63
1:B:52:GLN:HE22	1:B:71:LEU:CB	2.09	0.63
1:B:319:TYR:O	1:B:322:SER:OG	2.09	0.63
1:B:1369:THR:CG2	1:B:1369:THR:O	2.46	0.63
1:A:958:HIS:O	1:A:1369:THR:HG21	1.99	0.63
1:A:1395:TYR:CZ	1:A:1397:LEU:HD21	2.34	0.63
1:B:339:ARG:HG3	1:B:396:GLN:HG3	1.80	0.63
1:B:490:ASP:CG	1:B:787:ARG:HH21	2.06	0.63
1:A:547:SER:C	1:A:549:VAL:H	2.05	0.63
1:A:693:MET:O	1:A:694:ALA:C	2.37	0.63
1:A:1164:ARG:NH1	1:A:1166:ASP:OD2	2.31	0.63
1:A:1220:ARG:HB3	1:A:1221:PRO:HD3	1.81	0.63
1:B:351:ARG:HA	1:B:351:ARG:HE	1.64	0.63
1:B:409:HIS:O	1:B:412:THR:HB	1.98	0.63
1:B:609:GLU:O	1:B:611:MET:N	2.30	0.63
1:A:116:ILE:HD13	1:A:190:THR:CG2	2.29	0.63
1:A:182:MET:HE1	1:A:217:PRO:O	1.97	0.63
1:A:1007:GLY:O	1:A:1010:ALA:HB3	1.99	0.63
1:B:492:TYR:OH	1:B:648:GLU:OE2	2.14	0.63
1:A:56:LYS:O	1:A:57:ASP:C	2.42	0.63
1:A:57:ASP:O	1:A:58:HIS:C	2.41	0.63
1:A:145:GLU:O	1:A:146:LEU:C	2.41	0.63
1:A:843:VAL:CG1	1:A:844:GLU:N	2.59	0.63
1:A:978:GLU:O	1:A:981:ALA:HB3	1.99	0.63
1:A:1417:VAL:HG12	1:A:1419:HIS:H	1.64	0.63
1:B:152:ARG:O	1:B:156:GLU:HB2	1.99	0.63
1:B:453:ALA:O	1:B:761:GLN:HG3	1.97	0.63
1:B:528:ASN:CB	1:B:542:LEU:HD22	2.29	0.63
1:B:653:HIS:O	1:B:654:TYR:C	2.39	0.63
1:B:1131:THR:CG2	1:B:1133:GLU:HB2	2.29	0.63
1:B:1389:GLY:HA2	1:B:1459:PRO:HG2	1.81	0.63
1:A:369:THR:HG22	1:A:1293:ASN:HD21	1.62	0.63
1:A:938:PRO:HG2	1:A:1041:ALA:HB1	1.81	0.63
1:B:643:ASN:HB3	1:B:665:THR:CG2	2.29	0.63
1:B:1112:THR:O	1:B:1114:PRO:HD3	1.99	0.63
1:B:1121:ASP:OD1	1:B:1121:ASP:C	2.42	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1290:GLY:O	1:B:1291:ASP:HB3	1.99	0.63
1:A:403:ASP:OD2	1:A:407:LYS:NZ	2.32	0.63
1:A:1300:LEU:HD12	1:A:1301:SER:H	1.64	0.63
1:A:1376:LEU:HB3	1:A:1439:PHE:CE2	2.32	0.63
1:B:52:GLN:HE22	1:B:71:LEU:N	1.96	0.63
1:B:266:VAL:O	1:B:279:THR:HG23	1.98	0.63
1:B:602:THR:O	1:B:640:THR:HG22	1.99	0.63
1:B:1447:TRP:O	1:B:1451:VAL:HG23	1.98	0.63
1:A:30:HIS:HE1	1:A:368:GLU:OE1	1.81	0.62
1:A:662:GLY:O	1:A:720:ARG:HD3	1.98	0.62
1:A:1450:GLU:OE1	1:A:1453:LYS:NZ	2.24	0.62
1:B:1009:ILE:O	1:B:1010:ALA:C	2.37	0.62
1:B:1159:ASN:O	1:B:1161:VAL:N	2.32	0.62
1:A:57:ASP:O	1:A:60:LYS:N	2.32	0.62
1:A:606:LEU:C	1:A:607:THR:HG22	2.24	0.62
1:A:695:ASN:O	1:A:696:TYR:C	2.37	0.62
1:A:731:SER:HA	1:A:747:SER:HB2	1.80	0.62
1:A:746:ILE:HG23	1:A:1182:ASP:CB	2.29	0.62
1:A:1221:PRO:CB	1:A:1229:MET:CE	2.73	0.62
1:A:1449:ARG:NH1	1:A:1449:ARG:CB	2.14	0.62
1:B:59:VAL:HG22	1:B:105:TYR:CD2	2.33	0.62
1:B:423:THR:OG1	1:B:540:THR:HG22	2.00	0.62
1:B:918:THR:O	1:B:919:ALA:C	2.42	0.62
1:A:24:ALA:CB	1:A:207:TYR:CE2	2.82	0.62
1:A:317:ILE:O	1:A:321:ASN:ND2	2.29	0.62
1:A:345:MET:CE	1:A:385:LEU:HB2	2.28	0.62
1:A:465:LEU:HD12	1:A:465:LEU:O	1.98	0.62
1:A:643:ASN:HD22	1:A:665:THR:HG21	1.65	0.62
1:B:538:THR:O	1:B:538:THR:HG23	1.97	0.62
1:A:643:ASN:HD22	1:A:665:THR:HB	1.64	0.62
1:B:510:PRO:HD2	1:B:970:PRO:HB3	1.81	0.62
1:A:515:ARG:NH2	1:A:966:ILE:HB	2.13	0.62
1:A:603:HIS:HA	1:A:640:THR:HG22	1.81	0.62
1:B:518:ARG:NH2	1:B:1382:ASN:HD22	1.98	0.62
1:A:80:ARG:HD3	1:A:125:ARG:O	1.98	0.62
1:B:513:SER:HB3	1:B:520:MET:HE1	1.79	0.62
1:B:1291:ASP:C	1:B:1291:ASP:OD1	2.42	0.62
1:A:675:ILE:O	1:A:678:ARG:HB2	1.98	0.62
1:A:1356:VAL:HG22	1:A:1374:VAL:CG2	2.30	0.62
1:B:745:ARG:O	1:B:746:ILE:HG13	1.98	0.62
1:B:806:SER:OG	1:B:809:THR:N	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:864:SER:HG	1:B:867:ALA:H	1.48	0.62
1:A:513:SER:HB3	1:A:520:MET:HE1	1.81	0.62
1:A:908:LYS:HE2	1:A:924:GLN:O	2.00	0.62
1:A:970:PRO:HG2	1:A:970:PRO:O	2.00	0.62
1:B:171:SER:OG	1:B:177:ILE:HA	2.00	0.62
1:B:739:PHE:C	1:B:740:PRO:O	2.43	0.62
1:B:920:GLU:CB	1:B:1256:MET:HE2	2.27	0.62
1:B:1394:VAL:HG11	1:B:1401:LEU:HD22	1.79	0.62
1:A:364:ILE:CD1	1:A:374:ILE:HD11	2.30	0.62
1:B:260:MET:O	1:B:263:LEU:N	2.31	0.62
1:B:1052:VAL:O	1:B:1053:HIS:C	2.38	0.62
1:A:29:TRP:CD1	1:A:29:TRP:H	2.16	0.62
1:A:299:VAL:O	1:A:299:VAL:CG1	2.43	0.61
1:A:466:HIS:ND1	1:A:678:ARG:NH1	2.46	0.61
1:A:732:ARG:NH1	1:B:94:GLU:OE2	2.28	0.61
1:B:243:TRP:HA	1:B:243:TRP:CE3	2.35	0.61
1:B:353:MET:HG2	1:B:385:LEU:CD2	2.29	0.61
1:B:521:SER:OG	1:B:522:LEU:N	2.33	0.61
1:A:1062:ARG:O	1:A:1062:ARG:CG	2.43	0.61
1:B:249:THR:HG23	1:B:249:THR:O	1.98	0.61
1:B:794:VAL:HG21	1:B:817:VAL:HG23	1.82	0.61
1:A:555:PHE:C	1:A:555:PHE:CD1	2.78	0.61
1:A:1348:VAL:O	1:A:1348:VAL:HG13	1.99	0.61
1:A:1374:VAL:O	1:A:1375:ILE:HG13	1.98	0.61
1:B:74:GLY:CA	1:B:172:LEU:HD13	2.30	0.61
1:B:439:PRO:HG2	1:B:439:PRO:O	1.99	0.61
1:A:295:LYS:HD3	1:A:295:LYS:O	2.01	0.61
1:A:423:THR:OG1	1:A:540:THR:HG22	2.00	0.61
1:B:450:ARG:O	1:B:452:GLN:N	2.34	0.61
1:B:515:ARG:NE	1:B:1367:TYR:CE2	2.68	0.61
1:A:102:TYR:HE2	1:A:144:PHE:CE1	2.13	0.61
1:B:482:ASP:OD1	1:B:788:HIS:CD2	2.53	0.61
1:B:918:THR:HG22	1:B:921:TYR:N	2.13	0.61
1:B:976:SER:OG	1:B:978:GLU:HG3	2.00	0.61
1:B:1401:LEU:N	1:B:1402:PRO:HD2	2.16	0.61
1:A:107:TRP:CD1	1:A:107:TRP:N	2.69	0.61
1:B:526:LEU:HD12	1:B:526:LEU:H	1.66	0.61
1:B:1383:PHE:O	1:B:1384:ALA:HB3	2.00	0.61
1:A:1212:ASP:CG	1:A:1243:GLY:H	2.07	0.61
1:A:1401:LEU:C	1:A:1401:LEU:CD1	2.74	0.61
1:B:279:THR:HG22	1:B:280:VAL:N	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1169:HIS:ND1	1:B:1169:HIS:N	2.49	0.61
1:A:355:TYR:CD1	1:A:355:TYR:O	2.54	0.61
1:B:529:LEU:HD23	1:B:529:LEU:N	1.92	0.61
1:A:45:GLY:HA2	1:A:180:LYS:HA	1.81	0.61
1:A:511:ILE:HG22	1:A:512:ASP:H	1.61	0.61
1:A:531:ASN:HB3	1:A:534:ASP:HB2	1.83	0.61
1:A:1395:TYR:CE2	1:A:1443:ILE:HD13	2.35	0.61
1:B:235:ASN:HD21	1:B:328:ASP:HB3	1.64	0.61
1:B:658:LEU:HD23	1:B:666:VAL:CG2	2.29	0.61
1:B:1121:ASP:OD1	1:B:1123:LYS:N	2.33	0.61
1:B:1210:THR:HG22	1:B:1211:LEU:N	2.09	0.61
1:A:143:GLN:HE21	1:A:143:GLN:CA	2.14	0.61
1:A:320:CYS:O	1:A:323:VAL:N	2.33	0.61
1:B:521:SER:C	1:B:522:LEU:HD23	2.26	0.61
1:B:691:LYS:O	1:B:691:LYS:HG3	2.00	0.61
1:A:531:ASN:C	1:A:533:LEU:N	2.57	0.60
1:A:743:VAL:CG1	1:A:745:ARG:HG3	2.31	0.60
1:A:897:ASP:C	1:A:897:ASP:OD1	2.42	0.60
1:A:1374:VAL:O	1:A:1375:ILE:HG12	2.01	0.60
1:A:1446:ASP:O	1:A:1447:TRP:C	2.42	0.60
1:B:24:ALA:O	1:B:26:LYS:N	2.34	0.60
1:B:515:ARG:CD	1:B:1367:TYR:HE2	2.04	0.60
1:B:594:GLU:OE1	1:B:598:ARG:NH2	2.34	0.60
1:B:908:LYS:HD2	1:B:921:TYR:CE1	2.36	0.60
1:B:930:ILE:HD13	1:B:983:LEU:HD13	1.83	0.60
1:B:1084:MET:SD	1:B:1168:LEU:HD23	2.41	0.60
1:A:140:SER:O	1:A:141:ASP:C	2.44	0.60
1:A:293:MET:HG2	1:A:410:LEU:HD23	1.82	0.60
1:A:493:ARG:NH2	1:A:786:ASP:OD1	2.32	0.60
1:A:572:THR:CG2	1:A:615:ARG:HB3	2.31	0.60
1:B:102:TYR:CE1	1:B:144:PHE:CE1	2.89	0.60
1:B:353:MET:HE2	1:B:366:GLY:C	2.26	0.60
1:B:505:GLN:NE2	1:B:1000:LEU:CB	2.59	0.60
1:B:913:GLY:HA2	1:B:1349:ARG:CD	2.27	0.60
1:A:18:VAL:O	1:A:19:GLU:C	2.42	0.60
1:A:706:LYS:O	1:A:707:ILE:C	2.43	0.60
1:B:183:PHE:CE1	1:B:188:LEU:HA	2.37	0.60
1:B:1159:ASN:C	1:B:1161:VAL:H	2.09	0.60
1:A:246:ALA:O	1:A:247:HIS:C	2.42	0.60
1:A:295:LYS:HE2	1:A:299:VAL:CG1	2.31	0.60
1:A:481:ASP:C	1:A:481:ASP:OD1	2.44	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1315:LEU:HB3	1:A:1320:ASN:HD22	1.67	0.60
1:A:677:GLU:C	1:A:677:GLU:OE1	2.44	0.60
1:A:1026:ASN:CG	1:A:1027:SER:N	2.60	0.60
1:A:1170:GLN:OE1	1:A:1183:LEU:HB2	2.01	0.60
1:A:1432:VAL:HG22	1:A:1440:ALA:HB3	1.84	0.60
1:B:266:VAL:O	1:B:279:THR:HG21	2.01	0.60
1:B:342:VAL:HG11	1:B:390:MET:HE2	1.82	0.60
1:B:447:LEU:HD21	1:B:674:ALA:CA	2.29	0.60
1:B:957:ARG:HH11	1:B:965:LEU:HD12	1.65	0.60
1:B:1047:MET:HE2	1:B:1186:ARG:NH2	1.97	0.60
1:A:47:HIS:HE1	1:A:176:SER:HB3	1.63	0.60
1:A:731:SER:N	1:A:748:GLY:H	2.00	0.60
1:A:823:MET:C	1:A:824:GLN:HE21	2.10	0.60
1:A:1388:THR:O	1:A:1388:THR:HG23	2.01	0.60
1:A:1400:SER:O	1:A:1401:LEU:C	2.44	0.60
1:A:260:MET:O	1:A:263:LEU:HB2	2.02	0.60
1:A:479:MET:HG3	1:A:1104:MET:SD	2.42	0.60
1:A:565:THR:CG2	1:A:602:THR:HB	2.31	0.60
1:A:652:THR:HG21	1:A:703:GLY:HA3	1.84	0.60
1:A:950:THR:HG23	1:A:951:GLU:H	1.66	0.60
1:A:1311:THR:CG2	1:A:1312:SER:H	2.14	0.60
1:A:1391:MET:HE2	1:A:1458:VAL:HG21	1.76	0.60
1:B:481:ASP:C	1:B:481:ASP:OD1	2.44	0.60
1:B:670:LEU:O	1:B:670:LEU:HD22	2.01	0.60
1:B:1432:VAL:O	1:B:1433:THR:C	2.45	0.60
1:A:249:THR:CG2	1:A:250:ARG:HG2	2.31	0.60
1:A:575:VAL:HG13	1:A:759:LEU:HD22	1.84	0.60
1:A:1090:PHE:N	1:A:1090:PHE:CD1	2.69	0.60
1:A:1171:VAL:O	1:A:1171:VAL:HG12	2.00	0.60
1:B:312:ASN:HB2	1:B:411:ALA:HB1	1.83	0.60
1:B:390:MET:HG3	1:B:406:LEU:HD23	1.84	0.60
1:B:570:ASP:O	1:B:588:ARG:NH2	2.34	0.60
1:A:369:THR:HG23	1:A:370:GLY:N	2.17	0.60
1:A:494:GLY:O	1:A:495:LEU:C	2.42	0.60
1:A:1038:ILE:O	1:A:1038:ILE:HG22	2.02	0.60
1:A:1401:LEU:HD11	1:A:1405:ILE:HD12	1.82	0.60
1:A:1412:PHE:N	1:A:1412:PHE:CD1	2.70	0.60
1:B:572:THR:HG23	1:B:573:PHE:N	2.17	0.60
1:A:149:TYR:O	1:A:150:ILE:C	2.42	0.60
1:A:351:ARG:HA	1:A:351:ARG:HE	1.66	0.60
1:A:1393:TYR:O	1:A:1394:VAL:CG2	2.44	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:GLU:HA	1:B:251:MET:HG2	1.84	0.60
1:B:417:ASP:O	1:B:420:VAL:N	2.33	0.60
1:B:508:ASN:HB2	1:B:509:PRO:HD2	1.84	0.60
1:B:1045:TRP:O	1:B:1046:GLU:C	2.44	0.60
1:A:731:SER:O	1:A:735:VAL:HG23	2.02	0.59
1:A:732:ARG:H	1:A:747:SER:HB3	1.65	0.59
1:A:761:GLN:O	1:A:764:THR:HB	2.02	0.59
1:A:1424:LEU:HD23	1:A:1428:ILE:HG13	1.83	0.59
1:B:464:ILE:CD1	1:B:779:TYR:CZ	2.81	0.59
1:A:312:ASN:HB2	1:A:411:ALA:HB1	1.83	0.59
1:A:75:GLN:C	1:A:76:VAL:HG12	2.27	0.59
1:A:253:HIS:CE1	1:A:254:PRO:CG	2.85	0.59
1:B:560:ASP:O	1:B:562:MET:N	2.36	0.59
1:B:989:GLN:O	1:B:1245:ARG:HD3	2.01	0.59
1:A:377:THR:HG22	1:A:378:GLN:HG3	1.84	0.59
1:A:515:ARG:NE	1:A:1367:TYR:HE1	1.99	0.59
1:B:479:MET:HG3	1:B:1104:MET:CE	2.30	0.59
1:B:572:THR:HG22	1:B:573:PHE:N	2.16	0.59
1:B:1093:GLY:O	1:B:1094:THR:C	2.45	0.59
1:A:193:PRO:O	1:A:194:ASP:C	2.43	0.59
1:A:223:GLN:HB3	1:A:224:PRO:HA	1.85	0.59
1:A:296:MET:O	1:A:297:MET:C	2.40	0.59
1:A:466:HIS:CE1	1:A:684:PHE:CE1	2.91	0.59
1:A:607:THR:HB	1:A:645:ARG:HB2	1.84	0.59
1:A:918:THR:CG2	1:A:1256:MET:SD	2.90	0.59
1:B:149:TYR:CD2	1:B:286:ARG:HG3	2.37	0.59
1:B:559:ARG:NH1	1:B:568:GLU:OE2	2.35	0.59
1:B:1420:TYR:O	1:B:1422:SER:N	2.36	0.59
1:A:842:GLU:HB3	1:A:1156:ARG:HD3	1.84	0.59
1:A:1131:THR:HB	1:A:1134:LYS:CG	2.32	0.59
1:A:1356:VAL:HG11	1:A:1431:HIS:CG	2.38	0.59
1:B:857:GLY:O	3:B:2474:FMN:C4A	2.50	0.59
1:A:1212:ASP:OD2	1:A:1243:GLY:C	2.44	0.59
1:A:1316:GLU:O	1:A:1317:THR:C	2.45	0.59
1:B:120:LYS:CA	1:B:120:LYS:HE2	2.31	0.59
1:B:225:PHE:HB3	1:B:278:ASP:OD2	2.02	0.59
1:B:244:MET:HE2	1:B:244:MET:HA	1.84	0.59
1:B:676:ALA:O	1:B:677:GLU:C	2.45	0.59
1:B:1171:VAL:O	1:B:1171:VAL:HG12	2.02	0.59
1:B:1420:TYR:OH	1:B:1466:LEU:HD22	2.02	0.59
1:A:208:HIS:ND1	1:A:223:GLN:OE1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:603:HIS:CA	1:A:640:THR:HG22	2.32	0.59
1:A:826:ARG:NH1	1:A:826:ARG:CG	2.58	0.59
1:A:846:ILE:O	1:A:847:THR:C	2.45	0.59
1:B:947:PHE:O	1:B:947:PHE:CD1	2.56	0.59
1:B:1077:ARG:O	1:B:1078:ASP:C	2.45	0.59
1:A:89:CYS:O	1:A:93:VAL:HG23	2.03	0.59
1:A:1425:LYS:CD	1:A:1447:TRP:CE2	2.86	0.59
1:B:447:LEU:CD1	1:B:451:GLN:CG	2.80	0.59
1:B:684:PHE:HB3	1:B:687:MET:HE3	1.85	0.59
1:B:938:PRO:O	1:B:940:GLU:N	2.36	0.59
1:B:1055:VAL:O	1:B:1056:LEU:C	2.41	0.59
1:B:1109:HIS:ND1	1:B:1109:HIS:N	2.44	0.59
1:B:1131:THR:HG21	1:B:1133:GLU:HB2	1.83	0.59
3:B:2474:FMN:O4'	3:B:2474:FMN:C1'	2.10	0.59
1:A:515:ARG:HD3	1:A:1367:TYR:CE1	2.31	0.59
1:B:1132:PRO:O	1:B:1136:VAL:HG23	2.02	0.59
1:A:139:VAL:CG1	1:A:143:GLN:CB	2.81	0.58
1:A:249:THR:HG22	1:A:250:ARG:HG2	1.85	0.58
1:A:316:LEU:O	1:A:319:TYR:HB3	2.02	0.58
1:A:1369:THR:C	1:A:1389:GLY:O	2.46	0.58
1:B:397:SER:HB2	1:B:399:LYS:HG3	1.84	0.58
1:B:551:THR:O	1:B:554:GLU:HG2	2.03	0.58
1:B:589:ILE:HD12	1:B:627:VAL:HG23	1.85	0.58
1:A:92:ILE:O	1:A:93:VAL:C	2.45	0.58
1:A:139:VAL:CG1	1:A:143:GLN:HB2	2.32	0.58
1:A:330:PRO:HA	1:A:350:LEU:HB2	1.84	0.58
1:A:345:MET:CE	1:A:385:LEU:CB	2.81	0.58
1:A:884:SER:OG	1:A:885:GLY:N	2.33	0.58
1:A:1008:THR:HG22	1:A:1009:ILE:H	1.64	0.58
1:B:657:VAL:HG12	1:B:658:LEU:N	2.14	0.58
1:B:720:ARG:C	1:B:722:GLY:H	2.11	0.58
1:B:869:GLY:O	1:B:873:VAL:HG23	2.03	0.58
1:A:1320:ASN:C	1:A:1341:GLN:HG3	2.28	0.58
1:B:897:ASP:C	1:B:897:ASP:OD1	2.45	0.58
1:B:913:GLY:CA	1:B:1349:ARG:HD3	2.27	0.58
1:B:1438:ARG:O	1:B:1439:PHE:C	2.45	0.58
1:A:24:ALA:O	1:A:26:LYS:N	2.36	0.58
1:A:359:THR:HG23	1:A:378:GLN:CA	2.33	0.58
1:A:1375:ILE:O	1:A:1375:ILE:HG22	2.02	0.58
1:B:31:ARG:NH1	1:B:368:GLU:OE1	2.37	0.58
1:A:511:ILE:CG2	1:A:512:ASP:N	2.59	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:MET:O	1:A:560:ASP:N	2.36	0.58
1:A:746:ILE:O	1:A:747:SER:C	2.43	0.58
1:B:4:GLY:HA3	1:B:207:TYR:CZ	2.39	0.58
1:B:1222:LEU:C	1:B:1222:LEU:HD12	2.24	0.58
1:A:825:LEU:HD12	1:A:1186:ARG:NH1	2.13	0.58
1:A:1307:VAL:HG12	1:A:1322:ILE:CD1	2.33	0.58
1:A:1425:LYS:HE2	1:A:1447:TRP:CD1	2.38	0.58
1:B:303:LEU:HD11	1:B:314:LYS:HG2	1.85	0.58
1:B:322:SER:O	1:B:528:ASN:ND2	2.35	0.58
1:B:1274:GLN:NE2	1:B:1293:ASN:HB3	2.17	0.58
1:A:236:THR:HG23	1:A:240:ASN:HD21	1.69	0.58
1:A:531:ASN:O	1:A:533:LEU:N	2.36	0.58
1:A:1216:VAL:HG13	1:A:1249:MET:HE2	1.86	0.58
1:B:324:MET:HE2	1:B:327:TRP:HE1	1.67	0.58
1:B:997:THR:HG22	1:B:998:VAL:N	2.19	0.58
1:A:5:PHE:O	1:A:365:GLY:N	2.34	0.58
1:A:76:VAL:HG13	1:A:129:GLU:O	2.04	0.58
1:A:102:TYR:HA	1:A:136:ASN:OD1	2.04	0.58
1:A:291:ALA:HB3	1:A:292:PRO:CD	2.27	0.58
1:A:570:ASP:OD1	1:A:572:THR:HB	2.04	0.58
1:A:914:ARG:NH2	1:A:973:ASP:OD1	2.35	0.58
1:A:1251:THR:OG1	1:A:1281:VAL:HG11	2.04	0.58
1:B:573:PHE:HB2	1:B:574:PRO:HD2	1.85	0.58
1:B:838:VAL:CG1	1:B:839:PRO:N	2.66	0.58
1:B:838:VAL:O	1:B:1151:ALA:HB1	2.04	0.58
1:B:850:ARG:O	1:B:853:PHE:HB2	2.03	0.58
1:B:958:HIS:O	1:B:1369:THR:CG2	2.51	0.58
1:A:150:ILE:HG22	1:A:150:ILE:O	2.02	0.58
1:A:1285:LYS:HA	1:A:1304:THR:O	2.04	0.58
1:B:78:LEU:HB3	1:B:79:PRO:HD2	1.86	0.58
1:B:1336:LEU:HB3	1:B:1355:VAL:HG13	1.84	0.58
1:A:22:ILE:O	1:A:23:GLU:C	2.45	0.58
1:A:582:LEU:O	1:A:585:ALA:HB3	2.03	0.58
1:A:663:ALA:O	1:A:720:ARG:NE	2.35	0.58
1:A:734:LEU:HD12	1:A:734:LEU:O	2.04	0.58
1:B:528:ASN:HB2	1:B:542:LEU:HD22	1.86	0.58
1:B:643:ASN:HB3	1:B:665:THR:HG21	1.85	0.58
1:B:1222:LEU:H	1:B:1229:MET:HE2	1.67	0.58
1:A:244:MET:O	1:A:246:ALA:N	2.36	0.57
1:A:547:SER:C	1:A:549:VAL:N	2.58	0.57
1:A:1438:ARG:O	1:A:1439:PHE:C	2.45	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:484:PRO:HG3	1:B:823:MET:HG3	1.85	0.57
1:A:119:GLU:O	1:A:120:LYS:C	2.47	0.57
1:A:582:LEU:HB3	1:A:755:GLN:HE21	1.69	0.57
1:A:957:ARG:HD2	1:A:965:LEU:HD12	1.87	0.57
1:A:1374:VAL:C	1:A:1375:ILE:HG13	2.28	0.57
1:A:1447:TRP:CD2	1:A:1451:VAL:CG2	2.87	0.57
1:B:607:THR:HB	1:B:645:ARG:HB2	1.86	0.57
1:B:1316:GLU:O	1:B:1317:THR:C	2.46	0.57
1:A:236:THR:HG23	1:A:240:ASN:ND2	2.19	0.57
1:A:457:THR:O	1:A:460:ASP:HB2	2.04	0.57
1:A:823:MET:O	1:A:824:GLN:NE2	2.36	0.57
1:B:211:TYR:O	1:B:212:SER:HB3	2.05	0.57
1:B:461:MET:HE1	1:B:465:LEU:HD23	1.84	0.57
1:B:515:ARG:NH2	1:B:966:ILE:HB	2.16	0.57
1:B:845:SER:O	1:B:848:ALA:HB3	2.04	0.57
1:A:893:ARG:HG2	1:A:903:TRP:HB2	1.85	0.57
1:B:693:MET:O	1:B:694:ALA:C	2.44	0.57
1:B:1051:GLU:O	1:B:1052:VAL:C	2.46	0.57
1:A:218:THR:HG22	1:A:221:LEU:H	1.69	0.57
1:A:625:GLY:O	1:A:626:ALA:C	2.42	0.57
1:A:982:GLN:NE2	1:A:1240:ARG:HD2	2.16	0.57
1:B:295:LYS:HE2	1:B:299:VAL:CG1	2.35	0.57
1:B:731:SER:N	1:B:748:GLY:H	2.02	0.57
1:B:1368:MET:HB3	1:B:1387:MET:HG3	1.86	0.57
1:A:447:LEU:HD12	1:A:447:LEU:O	2.04	0.57
1:A:894:PHE:CD2	1:A:924:GLN:HG3	2.39	0.57
1:A:1077:ARG:O	1:A:1078:ASP:C	2.44	0.57
1:A:1282:GLN:CA	1:A:1302:GLY:O	2.52	0.57
1:A:1335:LYS:HA	1:A:1354:THR:O	2.05	0.57
1:B:100:PHE:O	1:B:137:LYS:CE	2.46	0.57
1:B:648:GLU:CG	1:B:648:GLU:O	2.51	0.57
1:B:768:GLU:HG2	1:B:769:GLU:N	2.09	0.57
1:B:1318:ASN:H	1:B:1318:ASN:ND2	2.01	0.57
1:A:447:LEU:CD2	1:A:674:ALA:HA	2.30	0.57
1:A:570:ASP:O	1:A:572:THR:N	2.37	0.57
1:A:753:GLY:O	1:A:754:ILE:C	2.45	0.57
1:B:136:ASN:OD1	1:B:136:ASN:N	2.38	0.57
1:B:312:ASN:OD1	1:B:312:ASN:N	2.25	0.57
1:B:1050:SER:O	1:B:1051:GLU:C	2.46	0.57
1:A:419:TRP:O	1:A:422:ASN:HB2	2.05	0.57
1:A:913:GLY:O	1:A:915:PHE:N	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:GLN:NE2	1:B:71:LEU:HB2	2.17	0.57
1:B:295:LYS:HZ3	1:B:299:VAL:HG12	1.68	0.57
1:B:777:GLY:O	1:B:788:HIS:CE1	2.51	0.57
1:A:45:GLY:HA3	1:A:224:PRO:HD2	1.85	0.57
1:A:61:VAL:O	1:A:61:VAL:CG1	2.51	0.57
1:A:139:VAL:HG12	1:A:143:GLN:HB2	1.87	0.57
1:A:260:MET:O	1:A:263:LEU:CB	2.52	0.57
1:A:447:LEU:HD13	1:A:670:LEU:CD2	2.33	0.57
1:A:560:ASP:O	1:A:562:MET:N	2.38	0.57
1:A:857:GLY:HA2	1:A:883:ASP:O	2.05	0.57
1:B:950:THR:HG23	1:B:951:GLU:H	1.69	0.57
1:A:551:THR:HG23	1:A:554:GLU:OE2	2.05	0.57
1:B:248:GLU:O	1:B:250:ARG:N	2.37	0.57
1:B:494:GLY:O	1:B:495:LEU:C	2.48	0.57
1:A:894:PHE:CE2	1:A:924:GLN:HG3	2.40	0.56
1:B:37:ASP:OD1	1:B:38:GLY:N	2.38	0.56
1:B:40:THR:O	1:B:40:THR:HG22	2.04	0.56
1:B:235:ASN:ND2	1:B:328:ASP:O	2.38	0.56
1:B:403:ASP:C	1:B:403:ASP:OD1	2.46	0.56
1:B:1220:ARG:N	1:B:1221:PRO:CD	2.67	0.56
1:B:1396:ASP:C	1:B:1396:ASP:OD1	2.45	0.56
3:B:2474:FMN:O4'	3:B:2474:FMN:H9	2.05	0.56
1:A:102:TYR:CE2	1:A:144:PHE:CD1	2.93	0.56
1:A:251:MET:SD	1:A:532:ILE:HD11	2.44	0.56
1:A:294:VAL:O	1:A:295:LYS:C	2.47	0.56
1:A:560:ASP:O	1:A:561:TYR:C	2.46	0.56
1:A:1076:GLY:CA	1:A:1145:GLU:HG2	2.29	0.56
1:B:80:ARG:HD3	1:B:125:ARG:O	2.05	0.56
1:B:823:MET:O	1:B:824:GLN:NE2	2.37	0.56
1:B:857:GLY:HA2	1:B:883:ASP:O	2.06	0.56
1:A:15:ARG:HD2	1:A:200:PHE:O	2.06	0.56
1:A:386:GLY:H	1:A:389:GLU:HG3	1.71	0.56
1:A:969:PRO:HD2	1:A:970:PRO:HD2	1.88	0.56
1:A:1010:ALA:HB2	1:A:1052:VAL:HG22	1.88	0.56
1:A:1075:THR:CG2	1:A:1076:GLY:N	2.66	0.56
1:A:1288:VAL:O	1:A:1288:VAL:HG12	2.05	0.56
1:A:1398:ASP:O	1:A:1399:ASP:C	2.47	0.56
1:B:236:THR:HG22	1:B:328:ASP:H	1.62	0.56
1:B:239:GLY:O	1:B:243:TRP:CD1	2.59	0.56
1:B:466:HIS:ND1	1:B:678:ARG:NH1	2.53	0.56
1:B:660:GLY:HA2	1:B:721:GLY:H	1.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1247:SER:OG	1:B:1280:ALA:HA	2.04	0.56
1:A:248:GLU:C	1:A:250:ARG:H	2.13	0.56
1:A:250:ARG:NH1	1:A:530:GLY:HA2	2.20	0.56
1:A:621:ILE:HG12	1:A:657:VAL:CG1	2.36	0.56
1:A:732:ARG:HD2	1:B:94:GLU:OE1	2.06	0.56
1:B:1:CYS:SG	1:B:211:TYR:HB2	2.45	0.56
1:B:437:GLY:O	1:B:438:GLU:C	2.48	0.56
1:B:1122:ASP:O	1:B:1126:GLN:HG3	2.04	0.56
1:B:1251:THR:OG1	1:B:1281:VAL:HG11	2.05	0.56
1:B:1348:VAL:O	1:B:1348:VAL:CG1	2.53	0.56
1:A:252:GLU:HA	1:A:260:MET:HE3	1.87	0.56
1:A:293:MET:HG2	1:A:410:LEU:CD2	2.35	0.56
1:A:409:HIS:O	1:A:413:LEU:HD23	2.06	0.56
1:A:652:THR:CG2	1:A:703:GLY:HA3	2.35	0.56
1:A:729:GLY:C	1:A:748:GLY:HA3	2.29	0.56
1:A:782:ARG:C	1:A:784:SER:H	2.12	0.56
1:B:3:VAL:CG2	1:B:231:ASN:HB2	2.36	0.56
1:B:227:MET:HE2	1:B:282:GLU:HG2	1.86	0.56
1:B:466:HIS:HB3	1:B:467:PRO:HD3	1.87	0.56
1:B:628:HIS:O	1:B:629:THR:C	2.47	0.56
1:B:797:THR:HG21	1:B:812:LYS:HG2	1.86	0.56
1:A:711:MET:O	1:A:713:ILE:N	2.39	0.56
1:B:209:GLN:HG3	1:B:210:ARG:N	2.20	0.56
1:B:1366:GLU:CG	1:B:1367:TYR:CD1	2.84	0.56
1:B:116:ILE:HD13	1:B:190:THR:CG2	2.35	0.56
1:B:570:ASP:OD1	1:B:572:THR:N	2.38	0.56
1:B:1366:GLU:HG2	1:B:1367:TYR:CE1	2.41	0.56
1:B:1393:TYR:CD2	1:B:1424:LEU:HD12	2.41	0.56
1:A:1135:VAL:O	1:A:1136:VAL:C	2.45	0.56
1:B:485:ILE:O	1:B:486:ALA:C	2.48	0.56
1:B:1075:THR:HG23	1:B:1145:GLU:OE2	2.06	0.56
1:A:961:PRO:O	1:A:963:VAL:N	2.39	0.56
1:A:1226:GLY:O	1:A:1227:GLU:O	2.23	0.56
1:B:116:ILE:HD13	1:B:190:THR:HG22	1.88	0.56
1:B:162:GLU:HB3	1:B:164:ILE:HD12	1.88	0.56
1:B:449:ARG:HD3	1:B:765:ALA:O	2.06	0.56
1:B:918:THR:HG23	1:B:1256:MET:CE	2.36	0.56
1:A:711:MET:O	1:A:713:ILE:HG13	2.06	0.56
1:A:1163:GLY:O	1:A:1165:THR:N	2.39	0.56
1:A:175:ARG:HH22	1:A:203:ASP:CG	2.14	0.55
1:A:813:TYR:O	1:A:816:GLN:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:704:LEU:C	1:B:706:LYS:H	2.14	0.55
1:B:763:ALA:O	1:B:764:THR:C	2.48	0.55
1:B:985:TYR:CD1	1:B:1207:VAL:HG11	2.42	0.55
1:B:1326:THR:HG22	1:B:1329:TYR:HB2	1.89	0.55
1:A:51:PRO:HG3	1:A:200:PHE:CE2	2.41	0.55
1:A:230:HIS:CE1	1:A:234:ILE:HG13	2.35	0.55
1:A:244:MET:O	1:A:245:LYS:C	2.44	0.55
1:A:670:LEU:O	1:A:670:LEU:CD2	2.53	0.55
1:A:1054:GLN:O	1:A:1057:THR:N	2.39	0.55
1:A:1222:LEU:HD12	1:A:1222:LEU:O	2.07	0.55
1:B:387:PRO:CD	1:B:1344:GLU:OE2	2.47	0.55
1:B:938:PRO:HG2	1:B:1041:ALA:HB1	1.88	0.55
1:A:392:ALA:O	1:A:400:LEU:CD1	2.53	0.55
1:A:1053:HIS:CE1	1:A:1062:ARG:HH11	2.24	0.55
1:B:254:PRO:HG2	1:B:255:ALA:N	2.10	0.55
1:A:37:ASP:OD2	1:A:40:THR:HB	2.06	0.55
1:A:177:ILE:CD1	1:A:179:TYR:HE1	2.17	0.55
1:A:556:ARG:O	1:A:557:ALA:C	2.44	0.55
1:A:1111:ASN:OD1	1:A:1119:VAL:CG2	2.37	0.55
1:A:1305:ILE:O	1:A:1336:LEU:HD12	2.06	0.55
1:B:571:ALA:HB2	1:B:606:LEU:CD2	2.37	0.55
1:B:675:ILE:O	1:B:678:ARG:HB2	2.07	0.55
1:A:96:GLU:OE1	1:A:96:GLU:CA	2.54	0.55
1:A:932:VAL:O	1:A:933:ALA:CB	2.45	0.55
1:B:235:ASN:HB3	1:B:508:ASN:ND2	2.22	0.55
1:B:846:ILE:O	1:B:847:THR:C	2.48	0.55
1:A:155:ILE:O	1:A:159:VAL:HG23	2.07	0.55
1:A:171:SER:OG	1:A:177:ILE:HA	2.06	0.55
1:A:938:PRO:O	1:A:940:GLU:N	2.40	0.55
1:A:1230:GLN:O	1:A:1231:LEU:HD23	2.06	0.55
1:B:148:LEU:HD22	1:B:172:LEU:HG	1.87	0.55
1:B:227:MET:HE2	1:B:282:GLU:CG	2.37	0.55
1:B:666:VAL:HG12	1:B:667:ASN:N	2.18	0.55
1:B:1058:LEU:C	1:B:1059:ASN:HD22	2.15	0.55
1:B:1093:GLY:O	1:B:1096:SER:N	2.39	0.55
1:A:269:VAL:HG23	1:A:270:GLY:N	2.22	0.55
1:B:556:ARG:O	1:B:557:ALA:C	2.48	0.55
1:B:612:GLY:O	1:B:762:HIS:CE1	2.60	0.55
1:B:979:ASP:O	1:B:980:LEU:C	2.49	0.55
1:B:1406:ASN:C	1:B:1406:ASN:OD1	2.48	0.55
1:A:235:ASN:ND2	1:A:236:THR:N	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:GLU:O	1:A:595:ASP:C	2.48	0.55
1:A:657:VAL:O	1:A:658:LEU:C	2.48	0.55
1:B:337:ASP:C	1:B:337:ASP:OD1	2.49	0.55
1:B:351:ARG:HH12	1:B:978:GLU:CD	2.14	0.55
1:B:710:LYS:HG2	1:B:939:GLY:CA	2.18	0.55
1:B:867:ALA:HB1	1:B:1100:MET:HE1	1.88	0.55
1:A:24:ALA:C	1:A:26:LYS:N	2.65	0.55
1:A:973:ASP:OD2	1:A:1298:LYS:CE	2.54	0.55
1:B:621:ILE:HG13	1:B:658:LEU:CD1	2.37	0.55
1:B:670:LEU:HD22	1:B:670:LEU:C	2.31	0.55
1:B:776:GLY:O	1:B:782:ARG:HD2	2.07	0.55
1:B:1236:ARG:C	1:B:1238:THR:H	2.15	0.55
1:A:244:MET:C	1:A:246:ALA:N	2.65	0.55
1:A:359:THR:HG23	1:A:378:GLN:C	2.32	0.55
1:A:1424:LEU:O	1:A:1425:LYS:C	2.49	0.55
1:B:1322:ILE:HG23	1:B:1323:ILE:HG23	1.88	0.55
1:A:149:TYR:HE1	1:A:282:GLU:OE1	1.91	0.54
1:A:248:GLU:C	1:A:250:ARG:N	2.64	0.54
1:A:430:VAL:HG11	1:A:554:GLU:HB2	1.88	0.54
1:A:1054:GLN:O	1:A:1055:VAL:C	2.49	0.54
1:A:1131:THR:CG2	1:A:1133:GLU:OE1	2.54	0.54
1:B:60:LYS:O	1:B:63:GLY:N	2.39	0.54
1:B:223:GLN:HB3	1:B:224:PRO:CA	2.37	0.54
1:B:515:ARG:CZ	1:B:1367:TYR:HE2	2.20	0.54
1:B:820:ARG:CB	1:B:821:PRO:HD2	2.37	0.54
1:B:953:ILE:O	1:B:954:ALA:C	2.50	0.54
1:B:1008:THR:HG22	1:B:1009:ILE:H	1.70	0.54
1:A:631:LEU:HD13	1:A:636:LEU:HB3	1.90	0.54
1:A:824:GLN:HE21	1:A:824:GLN:HA	1.65	0.54
1:B:61:VAL:O	1:B:61:VAL:HG12	2.08	0.54
1:B:744:SER:O	1:B:746:ILE:N	2.40	0.54
1:A:240:ASN:HB3	1:A:327:TRP:CZ2	2.41	0.54
1:A:313:HIS:H	1:A:313:HIS:CD2	2.24	0.54
1:A:452:GLN:NE2	1:A:764:THR:HG21	2.21	0.54
1:A:468:MET:HG2	1:A:699:ALA:CB	2.38	0.54
1:A:826:ARG:HH11	1:A:826:ARG:CG	1.97	0.54
1:A:1219:ALA:O	1:A:1220:ARG:C	2.47	0.54
1:A:1243:GLY:O	1:A:1244:THR:C	2.49	0.54
1:A:1300:LEU:HD12	1:A:1301:SER:N	2.22	0.54
1:B:953:ILE:HG22	1:B:954:ALA:N	2.22	0.54
1:A:572:THR:HG23	1:A:615:ARG:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:629:THR:O	1:A:632:ILE:N	2.39	0.54
1:A:950:THR:CG2	1:A:952:MET:H	2.15	0.54
1:A:1302:GLY:HA2	1:A:1334:GLY:N	2.23	0.54
1:A:1356:VAL:HG11	1:A:1431:HIS:CB	2.36	0.54
1:B:295:LYS:CE	1:B:299:VAL:HG12	2.37	0.54
1:A:1143:ALA:O	1:A:1144:GLU:C	2.45	0.54
1:B:875:MET:O	1:B:876:ASN:C	2.47	0.54
1:A:67:PRO:HG3	1:A:105:TYR:OH	2.08	0.54
1:A:249:THR:OG1	1:A:635:ASN:HB3	2.07	0.54
1:A:442:MET:HG2	1:A:446:GLU:HG2	1.88	0.54
1:A:1110:SER:C	1:A:1112:THR:HG23	2.32	0.54
1:A:1304:THR:HG23	1:A:1335:LYS:HB2	1.89	0.54
1:A:1336:LEU:HB3	1:A:1355:VAL:HG13	1.88	0.54
1:A:1394:VAL:O	1:A:1394:VAL:CG1	2.55	0.54
1:B:911:ALA:O	1:B:912:SER:C	2.49	0.54
1:B:1121:ASP:O	1:B:1125:ARG:HG3	2.07	0.54
1:A:35:ASP:HB3	1:A:37:ASP:H	1.71	0.54
1:A:518:ARG:NH2	1:A:1382:ASN:HD22	2.06	0.54
1:A:636:LEU:O	1:A:637:ARG:C	2.50	0.54
1:A:643:ASN:ND2	1:A:665:THR:HB	2.23	0.54
1:A:1075:THR:O	1:A:1076:GLY:C	2.50	0.54
1:A:1222:LEU:H	1:A:1229:MET:CE	2.20	0.54
1:A:1290:GLY:O	1:A:1291:ASP:CB	2.53	0.54
1:B:47:HIS:CE1	1:B:176:SER:HB3	2.42	0.54
1:B:529:LEU:HB3	1:B:638:THR:OG1	2.08	0.54
1:B:949:VAL:C	1:B:950:THR:O	2.48	0.54
1:B:1054:GLN:O	1:B:1057:THR:HB	2.08	0.54
1:A:561:TYR:CD1	1:A:561:TYR:O	2.61	0.54
1:A:664:THR:HA	1:A:720:ARG:NE	2.22	0.54
1:A:937:LYS:HE3	1:A:1033:SER:CB	2.34	0.54
1:A:937:LYS:HB2	1:A:940:GLU:HG3	1.89	0.54
1:B:62:ILE:HG22	1:B:62:ILE:O	2.08	0.54
1:B:824:GLN:CA	1:B:824:GLN:HE21	2.20	0.54
1:B:1131:THR:O	1:B:1134:LYS:N	2.41	0.54
1:A:236:THR:OG1	1:A:718:SER:HB3	2.07	0.54
1:A:481:ASP:HB2	1:A:1038:ILE:O	2.08	0.54
1:A:787:ARG:HH12	1:A:821:PRO:CB	2.17	0.54
1:A:853:PHE:CE1	1:A:1079:ILE:HD13	2.42	0.54
1:A:1093:GLY:O	1:A:1096:SER:N	2.41	0.54
1:B:24:ALA:C	1:B:26:LYS:N	2.65	0.54
1:B:111:PRO:C	1:B:112:ILE:HG23	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:THR:OG1	1:B:635:ASN:HB3	2.08	0.54
1:B:743:VAL:CG1	1:B:745:ARG:HG3	2.38	0.54
1:B:991:ASN:C	1:B:991:ASN:OD1	2.51	0.54
1:A:573:PHE:HB2	1:A:574:PRO:CD	2.36	0.54
1:A:1061:LEU:O	1:A:1064:ARG:HB2	2.08	0.54
1:B:260:MET:O	1:B:263:LEU:CB	2.56	0.54
1:B:690:GLU:H	1:B:690:GLU:CD	2.15	0.54
1:A:61:VAL:O	1:A:61:VAL:HG12	2.07	0.53
1:A:302:ALA:HA	1:A:347:ARG:NH1	2.23	0.53
1:A:492:TYR:C	1:A:492:TYR:CD1	2.86	0.53
1:A:515:ARG:CZ	1:A:1367:TYR:HE1	2.20	0.53
1:A:537:GLU:C	1:A:539:GLN:H	2.15	0.53
1:A:676:ALA:O	1:A:677:GLU:C	2.50	0.53
1:A:1427:LEU:O	1:A:1430:GLU:N	2.41	0.53
1:B:1146:VAL:O	1:B:1147:ARG:C	2.46	0.53
1:B:1388:THR:O	1:B:1388:THR:HG23	2.06	0.53
1:B:1470:VAL:O	1:B:1470:VAL:CG1	2.55	0.53
1:A:653:HIS:O	1:A:654:TYR:C	2.51	0.53
1:A:708:MET:O	1:A:710:LYS:N	2.41	0.53
1:A:976:SER:O	1:A:979:ASP:HB2	2.08	0.53
1:B:731:SER:HB2	1:B:747:SER:HB2	1.89	0.53
1:B:746:ILE:HG12	1:B:1182:ASP:O	2.08	0.53
1:B:1424:LEU:HD21	1:B:1428:ILE:HD11	1.89	0.53
1:A:1216:VAL:HG11	1:A:1249:MET:HE2	1.90	0.53
1:B:443:ASP:O	1:B:446:GLU:N	2.40	0.53
1:B:823:MET:C	1:B:824:GLN:HE21	2.17	0.53
1:A:253:HIS:CE1	1:A:254:PRO:HG2	2.44	0.53
1:A:1016:ALA:O	1:A:1017:ASN:HB2	2.08	0.53
1:A:1121:ASP:OD1	1:A:1122:ASP:N	2.42	0.53
1:A:85:ALA:O	1:A:86:GLN:C	2.48	0.53
1:A:565:THR:HG22	1:A:602:THR:HB	1.89	0.53
1:A:571:ALA:HB2	1:A:606:LEU:CD2	2.39	0.53
1:A:1057:THR:HG22	1:A:1190:VAL:HG11	1.91	0.53
1:A:1435:THR:HG23	1:A:1437:SER:N	2.23	0.53
1:B:443:ASP:O	1:B:445:ALA:N	2.41	0.53
1:B:891:PRO:HA	1:B:894:PHE:CD2	2.43	0.53
1:B:917:VAL:HG13	1:B:922:LEU:HD21	1.90	0.53
1:B:1159:ASN:C	1:B:1161:VAL:N	2.66	0.53
1:B:1420:TYR:O	1:B:1421:GLU:C	2.46	0.53
1:A:53:LYS:O	1:A:54:PHE:C	2.50	0.53
1:A:369:THR:HG22	1:A:1293:ASN:ND2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:THR:CG2	1:A:615:ARG:NE	2.72	0.53
1:A:843:VAL:HG12	1:A:844:GLU:H	1.70	0.53
1:A:1219:ALA:C	1:A:1221:PRO:HD2	2.34	0.53
1:B:40:THR:O	1:B:40:THR:CG2	2.57	0.53
1:B:348:ASN:HB2	1:B:350:LEU:HG	1.89	0.53
1:B:857:GLY:O	3:B:2474:FMN:C10	2.56	0.53
1:B:1468:VAL:O	1:B:1468:VAL:HG12	2.07	0.53
1:A:838:VAL:HG12	1:A:839:PRO:CD	2.32	0.53
1:A:1220:ARG:N	1:A:1221:PRO:CD	2.71	0.53
1:B:978:GLU:HG3	1:B:979:ASP:H	1.73	0.53
1:A:83:LEU:O	1:A:84:ASP:C	2.50	0.53
1:A:608:ASP:OD2	1:A:646:THR:HA	2.09	0.53
1:A:826:ARG:HG2	1:A:1046:GLU:OE2	2.07	0.53
1:B:240:ASN:ND2	1:B:327:TRP:CD2	2.77	0.53
1:B:615:ARG:HG2	1:B:615:ARG:HH11	1.73	0.53
1:B:1407:ASP:O	1:B:1408:GLU:C	2.50	0.53
1:A:160:LYS:O	1:A:161:GLY:C	2.50	0.53
1:A:660:GLY:HA2	1:A:721:GLY:H	1.74	0.53
1:A:1091:GLY:C	1:A:1092:ILE:HG13	2.34	0.53
1:A:1274:GLN:HE21	1:A:1293:ASN:HB3	1.74	0.53
1:A:1385:ALA:HB2	1:A:1406:ASN:HD22	1.74	0.53
1:B:474:GLU:O	1:B:475:ALA:C	2.52	0.53
1:B:1161:VAL:O	1:B:1161:VAL:CG1	2.57	0.53
1:B:1401:LEU:HB3	1:B:1402:PRO:HD3	1.91	0.53
1:A:31:ARG:NH1	1:A:368:GLU:OE2	2.42	0.53
1:A:317:ILE:CG2	1:A:321:ASN:HD21	2.19	0.53
1:A:754:ILE:O	1:A:755:GLN:C	2.48	0.53
1:A:1080:VAL:CG1	1:A:1084:MET:HE3	2.39	0.53
1:A:1307:VAL:HG12	1:A:1322:ILE:HD13	1.89	0.53
1:B:256:PHE:O	1:B:259:HIS:HB2	2.08	0.53
1:B:447:LEU:HD11	1:B:451:GLN:NE2	2.23	0.53
1:B:595:ASP:O	1:B:596:ALA:C	2.51	0.53
1:B:602:THR:O	1:B:640:THR:CG2	2.57	0.53
1:B:830:GLU:HG2	1:B:831:LEU:N	2.24	0.53
1:A:250:ARG:O	1:A:531:ASN:ND2	2.42	0.52
1:B:281:PHE:O	1:B:285:VAL:HG23	2.09	0.52
1:B:602:THR:O	1:B:640:THR:HA	2.09	0.52
1:B:1058:LEU:O	1:B:1058:LEU:CD2	2.57	0.52
1:B:1452:THR:HG22	1:B:1453:LYS:HG3	1.91	0.52
1:A:389:GLU:HA	1:A:403:ASP:OD2	2.09	0.52
1:A:491:LYS:HZ1	1:A:785:GLY:HA3	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:587:ARG:O	1:A:590:ARG:HB2	2.09	0.52
1:A:1316:GLU:O	1:A:1318:ASN:N	2.42	0.52
1:B:500:ARG:HD2	1:B:728:ILE:CG2	2.39	0.52
1:B:549:VAL:O	1:B:697:LYS:HE3	2.10	0.52
1:B:1233:TYR:O	1:B:1268:LEU:HA	2.09	0.52
1:B:1323:ILE:HD12	1:B:1327:VAL:HG21	1.91	0.52
1:A:561:TYR:C	1:A:561:TYR:CD1	2.86	0.52
1:A:1375:ILE:HB	1:A:1394:VAL:HG22	1.91	0.52
1:B:1432:VAL:O	1:B:1436:GLN:N	2.40	0.52
1:A:659:ILE:HA	1:A:663:ALA:HB3	1.91	0.52
1:A:731:SER:CA	1:A:747:SER:HB2	2.40	0.52
1:A:804:ASN:O	1:A:805:ASP:HB3	2.08	0.52
1:A:1070:ASP:C	1:A:1070:ASP:OD1	2.52	0.52
1:A:1420:TYR:OH	1:A:1466:LEU:HD22	2.09	0.52
1:B:574:PRO:HD3	1:B:615:ARG:HH12	1.74	0.52
1:B:1075:THR:CG2	1:B:1076:GLY:N	2.73	0.52
1:B:1326:THR:HG22	1:B:1326:THR:O	2.10	0.52
1:B:1338:ALA:O	1:B:1340:GLY:N	2.43	0.52
1:A:9:ILE:HG13	1:A:361:GLY:C	2.35	0.52
1:A:73:VAL:O	1:A:172:LEU:HA	2.09	0.52
1:A:143:GLN:O	1:A:143:GLN:NE2	2.41	0.52
1:A:520:MET:HE3	1:A:705:LEU:HD13	1.91	0.52
1:A:1061:LEU:O	1:A:1063:HIS:N	2.43	0.52
1:A:1113:CYS:O	1:A:1115:VAL:N	2.43	0.52
1:A:1122:ASP:O	1:A:1126:GLN:HG3	2.09	0.52
1:A:1374:VAL:C	1:A:1375:ILE:CG1	2.82	0.52
1:B:349:GLY:HA3	1:B:387:PRO:HG3	1.91	0.52
1:B:484:PRO:HG3	1:B:823:MET:CG	2.40	0.52
1:B:575:VAL:HG23	1:B:614:ALA:O	2.08	0.52
1:B:630:HIS:O	1:B:631:LEU:C	2.49	0.52
1:B:763:ALA:O	1:B:765:ALA:N	2.42	0.52
1:B:855:THR:HG22	1:B:855:THR:O	2.09	0.52
1:B:1470:VAL:O	1:B:1470:VAL:HG13	2.08	0.52
1:A:528:ASN:C	1:A:529:LEU:HD23	2.35	0.52
1:A:531:ASN:C	1:A:533:LEU:H	2.18	0.52
1:A:672:GLN:O	1:A:673:GLU:C	2.52	0.52
1:A:845:SER:O	1:A:848:ALA:HB3	2.09	0.52
1:A:1011:ALA:O	1:A:1014:ALA:HB3	2.09	0.52
1:A:1030:THR:N	3:A:2474:FMN:HM82	2.24	0.52
1:B:1030:THR:OG1	4:B:2475:AKG:O1	2.24	0.52
1:B:1113:CYS:O	1:B:1114:PRO:C	2.48	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1221:PRO:HB2	1:B:1229:MET:HE2	1.91	0.52
1:B:1088:GLU:HG2	1:B:1162:ILE:HD13	1.92	0.52
1:B:1428:ILE:HG22	1:B:1428:ILE:O	2.10	0.52
1:A:319:TYR:O	1:A:322:SER:OG	2.17	0.52
1:A:353:MET:CE	1:A:366:GLY:C	2.82	0.52
1:A:432:THR:O	1:A:434:SER:N	2.43	0.52
1:A:651:ASP:OD1	1:A:651:ASP:N	2.43	0.52
1:B:236:THR:HG22	1:B:328:ASP:N	2.24	0.52
1:B:419:TRP:O	1:B:540:THR:CB	2.58	0.52
1:B:629:THR:O	1:B:632:ILE:N	2.42	0.52
1:B:1394:VAL:HG11	1:B:1401:LEU:CD2	2.40	0.52
1:A:317:ILE:C	1:A:321:ASN:HD22	2.18	0.52
1:A:1007:GLY:N	1:A:1051:GLU:OE2	2.41	0.52
1:B:295:LYS:HE2	1:B:299:VAL:HG12	1.92	0.52
1:B:342:VAL:HG12	1:B:343:GLY:N	2.24	0.52
1:B:672:GLN:HG3	1:B:693:MET:SD	2.50	0.52
1:A:175:ARG:NH2	1:A:203:ASP:OD2	2.42	0.52
1:A:251:MET:HE3	1:A:533:LEU:CD1	2.28	0.52
1:A:281:PHE:O	1:A:285:VAL:HG23	2.11	0.52
1:A:528:ASN:HB2	1:A:542:LEU:HD22	1.90	0.52
1:A:1155:PHE:N	1:A:1155:PHE:CD1	2.77	0.52
1:A:1354:THR:HA	1:A:1372:THR:O	2.10	0.52
1:B:1075:THR:O	1:B:1076:GLY:C	2.50	0.52
1:A:105:TYR:H	1:A:105:TYR:HD1	1.57	0.51
1:A:414:LYS:CB	1:A:415:PRO:CD	2.87	0.51
1:A:572:THR:CG2	1:A:573:PHE:N	2.73	0.51
1:A:1207:VAL:HG13	1:A:1208:PRO:CD	2.39	0.51
1:A:1438:ARG:O	1:A:1440:ALA:N	2.42	0.51
1:B:621:ILE:HG12	1:B:657:VAL:CG1	2.40	0.51
1:A:266:VAL:O	1:A:279:THR:HG23	2.08	0.51
1:A:1375:ILE:O	1:A:1377:GLY:N	2.39	0.51
1:A:250:ARG:NE	1:A:639:PHE:CE1	2.73	0.51
1:A:295:LYS:C	1:A:295:LYS:CD	2.83	0.51
1:A:442:MET:HE3	1:A:447:LEU:N	2.24	0.51
1:A:606:LEU:C	1:A:607:THR:CG2	2.83	0.51
1:A:672:GLN:CG	1:A:693:MET:CE	2.79	0.51
1:A:997:THR:CG2	1:A:998:VAL:N	2.73	0.51
1:A:1250:VAL:HG13	1:A:1254:PHE:HD2	1.75	0.51
1:B:5:PHE:CE2	1:B:365:GLY:HA3	2.45	0.51
1:B:302:ALA:CA	1:B:347:ARG:NH1	2.72	0.51
1:B:555:PHE:CD1	1:B:556:ARG:N	2.77	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1018:ALA:O	1:B:1065:VAL:HG23	2.11	0.51
1:B:182:MET:CE	1:B:217:PRO:HB3	1.95	0.51
1:B:446:GLU:O	1:B:449:ARG:N	2.43	0.51
1:B:511:ILE:CG2	1:B:512:ASP:N	2.73	0.51
1:B:528:ASN:HB3	1:B:542:LEU:HD22	1.92	0.51
1:B:1047:MET:O	1:B:1048:GLY:C	2.53	0.51
1:A:87:GLU:O	1:A:88:ALA:C	2.53	0.51
1:A:133:VAL:CG1	1:A:134:GLY:N	2.74	0.51
1:A:417:ASP:O	1:A:418:LYS:C	2.52	0.51
1:A:1184:ASN:O	1:A:1187:LEU:N	2.44	0.51
1:B:61:VAL:O	1:B:61:VAL:CG1	2.58	0.51
1:B:85:ALA:O	1:B:86:GLN:C	2.53	0.51
1:B:447:LEU:CD1	1:B:451:GLN:CD	2.83	0.51
1:B:720:ARG:C	1:B:722:GLY:N	2.69	0.51
1:B:1077:ARG:HG2	1:B:1078:ASP:N	2.26	0.51
1:B:1245:ARG:HG3	1:B:1245:ARG:O	2.10	0.51
1:B:1424:LEU:O	1:B:1425:LYS:C	2.53	0.51
1:A:449:ARG:O	1:A:450:ARG:O	2.28	0.51
1:A:522:LEU:CG	1:A:705:LEU:HD21	2.38	0.51
1:A:673:GLU:O	1:A:674:ALA:C	2.53	0.51
1:A:705:LEU:HD23	1:A:705:LEU:N	2.26	0.51
1:A:776:GLY:O	1:A:782:ARG:HD2	2.10	0.51
1:A:949:VAL:C	1:A:950:THR:O	2.50	0.51
1:B:634:SER:O	1:B:635:ASN:C	2.52	0.51
1:B:868:HIS:O	1:B:869:GLY:C	2.49	0.51
1:B:1092:ILE:HG22	1:B:1092:ILE:O	2.10	0.51
1:A:706:LYS:NZ	1:A:940:GLU:OE1	2.40	0.51
1:A:731:SER:HA	1:A:747:SER:CA	2.40	0.51
1:A:1222:LEU:H	1:A:1229:MET:HE2	1.75	0.51
1:B:537:GLU:HG3	1:B:538:THR:N	2.08	0.51
1:B:985:TYR:CE1	1:B:1207:VAL:HG11	2.44	0.51
1:A:342:VAL:HG11	1:A:390:MET:CE	2.37	0.51
1:A:602:THR:C	1:A:640:THR:CG2	2.83	0.51
1:A:710:LYS:CG	1:A:939:GLY:HA3	2.34	0.51
1:A:871:LEU:O	1:A:872:ASN:C	2.52	0.51
1:A:957:ARG:HD2	1:A:965:LEU:CD1	2.41	0.51
1:B:677:GLU:C	1:B:677:GLU:OE1	2.54	0.51
1:B:1289:MET:CE	1:B:1289:MET:CB	2.87	0.51
1:B:1438:ARG:O	1:B:1441:ALA:N	2.43	0.51
1:B:1447:TRP:CD2	1:B:1451:VAL:HG22	2.45	0.51
1:A:1:CYS:HB3	2:A:2473:OMT:HE1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:VAL:HG21	1:A:167:PHE:CD2	2.46	0.51
1:A:316:LEU:C	1:A:316:LEU:HD12	2.36	0.51
1:A:791:GLU:O	1:A:795:ILE:HG13	2.11	0.51
1:A:855:THR:O	1:A:855:THR:HG22	2.10	0.51
1:A:893:ARG:HG2	1:A:903:TRP:CB	2.40	0.51
1:A:1401:LEU:N	1:A:1402:PRO:HD2	2.26	0.51
1:A:1432:VAL:O	1:A:1433:THR:C	2.53	0.51
1:B:24:ALA:C	1:B:26:LYS:H	2.19	0.51
1:B:74:GLY:HA2	1:B:172:LEU:HD13	1.92	0.51
1:B:131:ILE:HG23	1:B:131:ILE:O	2.09	0.51
1:B:1141:PHE:O	1:B:1142:LEU:C	2.54	0.51
1:A:1132:PRO:O	1:A:1133:GLU:C	2.52	0.51
1:A:1220:ARG:HG3	1:A:1224:GLU:CG	2.38	0.51
1:A:1415:ILE:CG2	1:A:1421:GLU:HB2	2.41	0.51
1:B:496:HIS:O	1:B:653:HIS:HE1	1.94	0.51
1:B:503:PHE:N	1:B:503:PHE:CD1	2.79	0.51
1:B:746:ILE:CG2	1:B:1182:ASP:HB3	2.22	0.51
1:A:209:GLN:HG3	1:A:210:ARG:H	1.76	0.50
1:A:244:MET:HA	1:A:247:HIS:HB2	1.92	0.50
1:A:1214:ARG:O	1:A:1215:ILE:C	2.53	0.50
1:A:1253:LYS:HG3	1:A:1253:LYS:O	2.11	0.50
1:B:335:MET:HE3	1:B:342:VAL:HB	1.93	0.50
1:B:447:LEU:HD11	1:B:451:GLN:CD	2.36	0.50
1:B:447:LEU:O	1:B:451:GLN:HG3	2.11	0.50
1:B:673:GLU:O	1:B:674:ALA:C	2.54	0.50
1:B:1376:LEU:HB3	1:B:1439:PHE:HE2	1.75	0.50
1:A:1:CYS:HB3	2:A:2473:OMT:CE	2.41	0.50
1:A:359:THR:HG23	1:A:378:GLN:CB	2.41	0.50
1:A:547:SER:OG	1:A:549:VAL:HB	2.11	0.50
1:A:707:ILE:HA	1:A:710:LYS:HD2	1.92	0.50
1:A:1236:ARG:C	1:A:1238:THR:H	2.17	0.50
1:B:302:ALA:CB	1:B:347:ARG:NH1	2.73	0.50
1:B:679:HIS:NE2	1:B:687:MET:O	2.42	0.50
1:B:1080:VAL:HG12	1:B:1084:MET:HE3	1.90	0.50
1:B:1440:ALA:O	1:B:1441:ALA:C	2.53	0.50
1:A:94:GLU:HG2	1:A:104:ILE:HD13	1.92	0.50
1:A:1359:GLY:O	1:A:1360:CYS:CB	2.58	0.50
1:B:485:ILE:O	1:B:488:LEU:N	2.43	0.50
1:B:536:ASP:OD1	1:B:536:ASP:O	2.28	0.50
1:B:1183:LEU:O	1:B:1187:LEU:HG	2.11	0.50
1:A:235:ASN:ND2	1:A:236:THR:HB	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:ASP:C	1:A:445:ALA:N	2.70	0.50
1:A:509:PRO:HB3	1:A:975:TYR:HD1	1.77	0.50
1:A:763:ALA:O	1:A:767:ASN:HB2	2.11	0.50
1:B:402:ARG:O	1:B:403:ASP:C	2.51	0.50
1:B:447:LEU:CD1	1:B:447:LEU:C	2.84	0.50
1:A:228:LEU:HD22	1:A:278:ASP:HA	1.94	0.50
1:A:309:THR:CG2	1:A:314:LYS:HG3	2.42	0.50
1:B:243:TRP:CD1	1:B:325:GLU:OE1	2.65	0.50
1:B:558:MET:C	1:B:560:ASP:N	2.69	0.50
1:B:1204:ARG:O	1:B:1205:ASN:C	2.51	0.50
1:A:62:ILE:O	1:A:62:ILE:CG2	2.60	0.50
1:A:105:TYR:N	1:A:105:TYR:CD1	2.80	0.50
1:A:369:THR:O	1:A:371:MET:N	2.43	0.50
1:A:394:ASP:OD1	1:A:396:GLN:N	2.43	0.50
1:A:404:ARG:CB	1:A:405:GLU:OE1	2.51	0.50
1:A:643:ASN:HB3	1:A:665:THR:HG21	1.93	0.50
1:A:676:ALA:O	1:A:679:HIS:N	2.45	0.50
1:A:731:SER:HA	1:A:747:SER:CB	2.42	0.50
1:A:746:ILE:HG23	1:A:1182:ASP:N	2.21	0.50
1:B:197:ASP:OD1	1:B:199:ARG:HB2	2.11	0.50
1:B:476:ILE:HA	1:B:1034:PRO:HA	1.94	0.50
1:B:720:ARG:O	1:B:722:GLY:N	2.45	0.50
1:B:1002:SER:HB2	1:B:1048:GLY:HA3	1.93	0.50
1:B:1068:ARG:NE	1:B:1089:GLU:OE1	2.38	0.50
1:B:1131:THR:CG2	1:B:1133:GLU:N	2.72	0.50
1:B:1221:PRO:HD2	1:B:1229:MET:CE	2.26	0.50
1:A:1:CYS:SG	1:A:211:TYR:HD2	2.35	0.50
1:A:54:PHE:HA	1:A:199:ARG:HD2	1.94	0.50
1:A:484:PRO:HG3	1:A:823:MET:HG3	1.94	0.50
1:A:1023:ILE:HD12	1:A:1023:ILE:N	2.27	0.50
1:B:520:MET:HE1	1:B:705:LEU:O	2.12	0.50
1:B:702:ASP:O	1:B:703:GLY:C	2.55	0.50
1:B:797:THR:HG23	1:B:812:LYS:HE2	1.94	0.50
1:B:1460:LYS:O	1:B:1462:MET:N	2.44	0.50
1:A:80:ARG:HG3	1:A:80:ARG:O	2.12	0.50
1:A:970:PRO:O	1:A:970:PRO:CG	2.60	0.50
1:A:1236:ARG:C	1:A:1238:THR:N	2.67	0.50
1:A:1421:GLU:HG3	1:A:1451:VAL:HG11	1.94	0.50
1:B:451:GLN:OE1	1:B:773:LEU:HD11	2.11	0.50
1:B:505:GLN:NE2	1:B:1001:VAL:N	2.55	0.50
1:B:629:THR:O	1:B:630:HIS:C	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:689:LEU:O	1:B:690:GLU:C	2.55	0.50
1:B:746:ILE:CG2	1:B:1182:ASP:CB	2.86	0.50
1:B:766:TYR:C	1:B:768:GLU:H	2.18	0.50
1:B:1080:VAL:O	1:B:1081:ILE:C	2.54	0.50
1:A:30:HIS:ND1	1:A:1238:THR:HA	2.26	0.50
1:A:52:GLN:NE2	1:A:71:LEU:HB2	2.27	0.50
1:A:312:ASN:HB2	1:A:411:ALA:CB	2.41	0.50
1:A:443:ASP:O	1:A:446:GLU:N	2.28	0.50
1:A:466:HIS:HB3	1:A:467:PRO:HD3	1.94	0.50
1:A:652:THR:HG21	1:A:703:GLY:CA	2.41	0.50
1:A:731:SER:HB2	1:A:747:SER:HB2	1.94	0.50
1:A:798:LEU:O	1:A:802:VAL:HG22	2.12	0.50
1:A:1108:CYS:SG	5:A:2476:F3S:S4	2.94	0.50
1:A:1245:ARG:O	1:A:1246:LEU:C	2.55	0.50
1:A:1318:ASN:H	1:A:1318:ASN:HD22	1.60	0.50
1:B:236:THR:OG1	1:B:718:SER:HB3	2.12	0.50
1:B:355:TYR:CD1	1:B:355:TYR:O	2.65	0.50
1:B:569:ILE:HG22	1:B:589:ILE:HG22	1.93	0.50
1:B:883:ASP:O	1:B:884:SER:C	2.55	0.50
1:B:1207:VAL:HG13	1:B:1208:PRO:HD2	1.92	0.50
1:B:1435:THR:HG23	1:B:1437:SER:CB	2.42	0.50
1:A:225:PHE:HB3	1:A:278:ASP:OD2	2.12	0.49
1:A:351:ARG:HH12	1:A:978:GLU:CD	2.19	0.49
1:A:353:MET:O	1:A:353:MET:HG3	2.12	0.49
1:A:621:ILE:HG12	1:A:657:VAL:HG12	1.93	0.49
1:A:704:LEU:C	1:A:706:LYS:H	2.20	0.49
1:A:782:ARG:C	1:A:784:SER:N	2.70	0.49
1:A:860:MET:HE1	1:A:893:ARG:NH1	2.27	0.49
1:B:486:ALA:O	1:B:487:VAL:C	2.51	0.49
1:B:739:PHE:O	1:B:740:PRO:C	2.55	0.49
1:B:792:GLY:O	1:B:793:GLY:C	2.51	0.49
1:B:1204:ARG:O	1:B:1206:GLU:N	2.45	0.49
1:A:24:ALA:O	1:A:27:ALA:N	2.27	0.49
1:A:339:ARG:HG3	1:A:396:GLN:HG3	1.93	0.49
1:A:359:THR:CG2	1:A:378:GLN:HA	2.42	0.49
1:A:442:MET:CE	1:A:447:LEU:HA	2.41	0.49
1:A:461:MET:HA	1:A:461:MET:HE3	1.94	0.49
1:A:1417:VAL:CG1	1:A:1418:GLY:N	2.73	0.49
1:B:419:TRP:O	1:B:540:THR:CG2	2.59	0.49
1:B:443:ASP:O	1:B:444:LYS:C	2.54	0.49
1:B:696:TYR:CZ	1:B:700:ILE:CD1	2.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1003:ARG:HG3	1:B:1004:SER:N	2.24	0.49
1:A:90:ARG:HB3	1:A:107:TRP:CH2	2.48	0.49
1:A:508:ASN:HB2	1:A:509:PRO:HD2	1.95	0.49
1:A:1052:VAL:O	1:A:1053:HIS:C	2.51	0.49
1:A:1400:SER:O	1:A:1403:LEU:N	2.27	0.49
1:B:381:GLU:CD	1:B:402:ARG:NH1	2.67	0.49
1:B:479:MET:HG3	1:B:1104:MET:SD	2.52	0.49
1:A:47:HIS:HE1	1:A:176:SER:CB	2.25	0.49
1:A:51:PRO:HG3	1:A:200:PHE:CD2	2.48	0.49
1:A:227:MET:HE2	1:A:282:GLU:HG3	1.93	0.49
1:A:236:THR:HG22	1:A:328:ASP:N	2.26	0.49
1:A:492:TYR:CG	1:A:761:GLN:HG2	2.47	0.49
1:B:113:ASN:HD21	1:B:115:ASP:H	1.47	0.49
1:B:290:THR:CG2	1:B:291:ALA:N	2.75	0.49
1:B:354:ARG:NH2	1:B:1292:ALA:O	2.46	0.49
1:B:515:ARG:HD3	1:B:1367:TYR:CE2	2.40	0.49
1:B:1059:ASN:O	1:B:1060:ARG:HB2	2.12	0.49
1:B:1113:CYS:C	1:B:1115:VAL:N	2.69	0.49
1:A:21:GLY:O	1:A:22:ILE:C	2.49	0.49
1:A:213:THR:O	1:A:214:ASN:ND2	2.43	0.49
1:A:291:ALA:CB	1:A:292:PRO:HD3	2.31	0.49
1:A:316:LEU:O	1:A:317:ILE:C	2.53	0.49
1:A:560:ASP:C	1:A:562:MET:N	2.70	0.49
1:A:960:THR:CG2	1:A:963:VAL:HG21	2.42	0.49
1:A:961:PRO:C	1:A:963:VAL:H	2.20	0.49
1:A:979:ASP:O	1:A:980:LEU:C	2.55	0.49
1:A:1054:GLN:O	1:A:1057:THR:HB	2.12	0.49
1:A:1244:THR:O	1:A:1245:ARG:C	2.51	0.49
1:A:1368:MET:HB3	1:A:1387:MET:HG3	1.94	0.49
1:B:30:HIS:HD2	1:B:31:ARG:N	2.10	0.49
1:B:621:ILE:HG13	1:B:658:LEU:HD12	1.93	0.49
1:A:110:VAL:O	1:A:112:ILE:HG23	2.13	0.49
1:A:353:MET:HE2	1:A:366:GLY:C	2.36	0.49
1:A:805:ASP:CG	1:A:805:ASP:O	2.49	0.49
1:A:1349:ARG:CG	1:A:1349:ARG:NH1	2.75	0.49
1:A:1393:TYR:C	1:A:1394:VAL:HG23	2.34	0.49
1:B:302:ALA:HB2	1:B:347:ARG:HH11	1.77	0.49
1:B:495:LEU:HD12	1:B:495:LEU:HA	1.36	0.49
1:B:561:TYR:CD1	1:B:561:TYR:C	2.90	0.49
1:B:693:MET:HE3	1:B:693:MET:CA	2.39	0.49
1:B:1184:ASN:O	1:B:1186:ARG:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1211:LEU:HG	1:B:1215:ILE:HD11	1.94	0.49
1:B:1260:GLN:O	1:B:1261:PRO:C	2.56	0.49
1:B:1400:SER:C	1:B:1402:PRO:HD2	2.38	0.49
1:A:235:ASN:C	1:A:235:ASN:ND2	2.52	0.49
1:A:243:TRP:HA	1:A:243:TRP:CE3	2.47	0.49
1:A:664:THR:HA	1:A:720:ARG:HE	1.77	0.49
1:A:689:LEU:HG	1:A:689:LEU:O	2.11	0.49
1:A:1460:LYS:O	1:A:1461:GLU:C	2.55	0.49
1:B:253:HIS:CE1	1:B:254:PRO:CD	2.88	0.49
1:B:838:VAL:HG12	1:B:839:PRO:CD	2.40	0.49
1:B:850:ARG:HD2	1:B:878:ILE:HD12	1.94	0.49
1:B:871:LEU:O	1:B:872:ASN:C	2.54	0.49
1:B:1070:ASP:C	1:B:1070:ASP:OD1	2.55	0.49
1:B:1310:THR:HG22	1:B:1311:THR:HG22	1.95	0.49
1:B:1400:SER:O	1:B:1401:LEU:C	2.56	0.49
1:A:15:ARG:O	1:A:16:SER:C	2.53	0.49
1:A:266:VAL:CG1	1:A:279:THR:HG23	2.33	0.49
1:A:428:GLU:O	1:A:429:LEU:C	2.52	0.49
1:A:485:ILE:HG12	1:A:488:LEU:HD12	1.95	0.49
1:A:969:PRO:HD2	1:A:970:PRO:CD	2.42	0.49
1:A:1401:LEU:O	1:A:1401:LEU:CD1	2.53	0.49
1:B:242:ASN:HA	1:B:245:LYS:HG3	1.94	0.49
1:B:698:LYS:O	1:B:698:LYS:HG2	2.13	0.49
1:B:1068:ARG:NH2	1:B:1089:GLU:OE1	2.46	0.49
1:A:918:THR:O	1:A:919:ALA:C	2.51	0.49
1:A:1038:ILE:O	1:A:1038:ILE:CG2	2.61	0.49
1:A:1281:VAL:HA	1:A:1301:SER:O	2.13	0.49
1:B:452:GLN:HG3	1:B:764:THR:HG22	1.94	0.49
1:B:582:LEU:CB	1:B:755:GLN:HE21	2.26	0.49
1:A:116:ILE:HD13	1:A:190:THR:HG21	1.94	0.49
1:A:197:ASP:OD1	1:A:199:ARG:N	2.37	0.49
1:A:369:THR:C	1:A:371:MET:H	2.20	0.49
1:A:736:ALA:O	1:A:737:GLU:C	2.53	0.49
1:A:1447:TRP:HA	1:A:1447:TRP:CE3	2.48	0.49
1:B:290:THR:O	1:B:294:VAL:HG23	2.12	0.49
1:B:417:ASP:HA	1:B:420:VAL:HG12	1.95	0.49
1:B:428:GLU:O	1:B:429:LEU:C	2.51	0.49
1:B:1417:VAL:HG12	1:B:1419:HIS:N	2.26	0.49
1:A:253:HIS:ND1	1:A:254:PRO:CG	2.71	0.48
1:A:1395:TYR:CD2	1:A:1443:ILE:HD13	2.48	0.48
1:B:251:MET:HE3	1:B:533:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1401:LEU:HD11	1:B:1405:ILE:HB	1.94	0.48
1:A:191:PHE:CE1	1:A:192:TYR:CE1	3.01	0.48
1:A:482:ASP:OD1	1:A:788:HIS:HB3	2.13	0.48
1:A:918:THR:HG22	1:A:920:GLU:N	2.26	0.48
1:A:1030:THR:HG21	1:A:1033:SER:HB3	1.95	0.48
1:A:1045:TRP:O	1:A:1046:GLU:C	2.54	0.48
1:A:1440:ALA:O	1:A:1443:ILE:N	2.42	0.48
1:B:211:TYR:HD1	1:B:212:SER:N	2.08	0.48
1:B:254:PRO:O	1:B:257:GLY:N	2.37	0.48
1:B:1236:ARG:C	1:B:1238:THR:N	2.70	0.48
1:A:248:GLU:O	1:A:249:THR:C	2.56	0.48
1:A:661:VAL:O	1:A:661:VAL:CG1	2.61	0.48
1:A:1326:THR:HG22	1:A:1329:TYR:HB2	1.95	0.48
1:A:1376:LEU:CB	1:A:1439:PHE:HE2	2.19	0.48
1:A:1417:VAL:HG12	1:A:1418:GLY:N	2.27	0.48
1:A:1441:ALA:O	1:A:1444:LEU:HB2	2.13	0.48
1:B:389:GLU:CA	1:B:403:ASP:OD2	2.61	0.48
1:B:810:PHE:O	1:B:813:TYR:HB3	2.13	0.48
1:B:869:GLY:O	1:B:870:THR:C	2.52	0.48
1:B:1278:ALA:O	1:B:1279:PHE:HB2	2.12	0.48
1:A:74:GLY:HA2	1:A:172:LEU:HD13	1.96	0.48
1:A:87:GLU:O	1:A:90:ARG:N	2.47	0.48
1:A:97:ILE:HD13	1:A:133:VAL:HG21	1.95	0.48
1:A:430:VAL:HG22	1:A:557:ALA:HB3	1.95	0.48
1:A:454:PHE:CD2	1:A:648:GLU:HA	2.48	0.48
1:A:521:SER:C	1:A:522:LEU:HD23	2.38	0.48
1:A:909:GLN:NE2	1:A:929:GLU:OE1	2.46	0.48
1:A:1359:GLY:O	1:A:1360:CYS:HB3	2.12	0.48
1:A:1366:GLU:HG2	1:A:1367:TYR:CE2	2.47	0.48
1:B:110:VAL:CG2	1:B:130:GLN:HG3	2.43	0.48
1:B:175:ARG:HG3	1:B:175:ARG:NH1	2.23	0.48
1:B:572:THR:CG2	1:B:615:ARG:HB3	2.42	0.48
1:B:594:GLU:O	1:B:597:VAL:N	2.45	0.48
1:B:1163:GLY:O	1:B:1165:THR:N	2.45	0.48
1:B:1164:ARG:HH11	1:B:1166:ASP:CG	2.21	0.48
1:B:1190:VAL:C	1:B:1192:PRO:HD3	2.38	0.48
1:B:1407:ASP:O	1:B:1409:SER:N	2.46	0.48
1:A:369:THR:CG2	1:A:370:GLY:N	2.76	0.48
1:A:538:THR:O	1:A:538:THR:HG23	2.13	0.48
1:A:1184:ASN:O	1:A:1186:ARG:N	2.46	0.48
1:B:562:MET:HE2	1:B:605:ILE:HD11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:580:GLU:O	1:B:581:ALA:C	2.56	0.48
1:B:1212:ASP:OD1	1:B:1243:GLY:N	2.34	0.48
1:B:1427:LEU:O	1:B:1430:GLU:N	2.46	0.48
1:A:15:ARG:HG3	1:A:19:GLU:HG3	1.94	0.48
1:A:1068:ARG:NE	1:A:1089:GLU:OE1	2.39	0.48
1:A:1428:ILE:O	1:A:1428:ILE:HG22	2.14	0.48
1:B:252:GLU:HA	1:B:260:MET:HE3	1.95	0.48
1:B:700:ILE:C	1:B:703:GLY:H	2.22	0.48
1:B:848:ALA:O	1:B:849:ILE:C	2.54	0.48
1:B:1008:THR:O	1:B:1011:ALA:HB3	2.14	0.48
1:A:3:VAL:HG22	1:A:231:ASN:HB2	1.96	0.48
1:A:345:MET:HG2	1:A:349:GLY:HA2	1.95	0.48
1:A:602:THR:C	1:A:640:THR:HG22	2.38	0.48
1:A:858:MET:HA	3:A:2474:FMN:N5	2.29	0.48
1:A:1141:PHE:O	1:A:1142:LEU:C	2.55	0.48
1:B:146:LEU:C	1:B:146:LEU:CD1	2.87	0.48
1:B:731:SER:HA	1:B:747:SER:CB	2.43	0.48
1:B:978:GLU:O	1:B:981:ALA:HB3	2.12	0.48
1:B:1184:ASN:C	1:B:1186:ARG:N	2.71	0.48
1:A:496:HIS:O	1:A:653:HIS:CE1	2.61	0.48
1:A:1047:MET:O	1:A:1048:GLY:C	2.56	0.48
1:A:1210:THR:CG2	1:A:1211:LEU:N	2.47	0.48
1:A:1228:LYS:C	1:A:1229:MET:HG2	2.39	0.48
1:A:1230:GLN:HE21	1:A:1267:ARG:HD3	1.76	0.48
1:B:701:ASP:C	1:B:703:GLY:N	2.69	0.48
1:B:763:ALA:C	1:B:765:ALA:N	2.72	0.48
1:B:1131:THR:CG2	1:B:1133:GLU:H	2.27	0.48
1:B:1221:PRO:CD	1:B:1229:MET:HE1	2.27	0.48
3:B:2474:FMN:HM71	3:B:2474:FMN:HM83	1.53	0.48
1:B:208:HIS:CD2	1:B:208:HIS:C	2.92	0.48
1:B:317:ILE:C	1:B:321:ASN:HD22	2.18	0.48
1:B:393:VAL:HG12	1:B:394:ASP:N	2.29	0.48
1:B:582:LEU:HB2	1:B:755:GLN:HE21	1.79	0.48
1:B:856:PRO:HB3	3:B:2474:FMN:H3'	1.95	0.48
1:B:1424:LEU:HD23	1:B:1428:ILE:HG13	1.96	0.48
1:A:1276:LEU:HD12	1:A:1276:LEU:C	2.36	0.48
1:A:1396:ASP:OD1	1:A:1396:ASP:O	2.30	0.48
1:B:105:TYR:N	1:B:105:TYR:CD1	2.81	0.48
1:B:430:VAL:HG22	1:B:557:ALA:HB3	1.94	0.48
1:B:513:SER:HA	1:B:520:MET:HE2	1.96	0.48
1:B:1077:ARG:CG	1:B:1078:ASP:N	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1427:LEU:O	1:B:1428:ILE:C	2.56	0.48
1:A:12:LYS:HA	1:A:13:PRO:HD3	1.72	0.47
1:B:162:GLU:CB	1:B:164:ILE:HD12	2.44	0.47
1:B:452:GLN:CG	1:B:764:THR:HG22	2.43	0.47
1:B:472:GLY:O	1:B:473:LYS:HG3	2.14	0.47
1:B:1105:VAL:HG22	1:B:1105:VAL:O	2.14	0.47
1:B:1396:ASP:OD1	1:B:1396:ASP:O	2.32	0.47
1:A:513:SER:HB2	1:A:520:MET:CE	2.43	0.47
1:A:552:THR:HG22	1:A:552:THR:O	2.14	0.47
1:A:631:LEU:N	1:A:631:LEU:HD23	2.29	0.47
1:A:869:GLY:O	1:A:870:THR:C	2.54	0.47
1:A:1412:PHE:HD2	1:A:1455:TRP:CZ3	2.33	0.47
1:A:1447:TRP:O	1:A:1451:VAL:HG23	2.14	0.47
1:B:235:ASN:HB3	1:B:508:ASN:HD21	1.79	0.47
1:B:501:GLN:OE1	1:B:710:LYS:NZ	2.43	0.47
1:B:550:LEU:HB3	1:B:554:GLU:HG3	1.96	0.47
1:B:609:GLU:C	1:B:611:MET:H	2.22	0.47
1:B:986:ASP:O	1:B:987:LEU:C	2.55	0.47
1:B:1057:THR:HG22	1:B:1058:LEU:N	2.22	0.47
1:A:203:ASP:OD1	1:A:203:ASP:N	2.44	0.47
1:A:246:ALA:C	1:A:248:GLU:N	2.70	0.47
1:A:990:ILE:HG23	1:A:991:ASN:N	2.29	0.47
1:A:1396:ASP:OD1	1:A:1399:ASP:N	2.47	0.47
1:A:1425:LYS:CE	1:A:1447:TRP:CD1	2.97	0.47
1:B:182:MET:CE	1:B:217:PRO:C	2.62	0.47
1:B:269:VAL:HG23	1:B:270:GLY:N	2.21	0.47
1:B:727:ALA:HB3	1:B:744:SER:HB2	1.95	0.47
1:B:953:ILE:O	1:B:955:ARG:N	2.47	0.47
1:B:1424:LEU:HD23	1:B:1424:LEU:C	2.39	0.47
1:A:31:ARG:HD2	1:A:368:GLU:OE2	2.15	0.47
1:A:242:ASN:HD22	1:A:242:ASN:H	1.61	0.47
1:A:429:LEU:HG	1:A:429:LEU:O	2.14	0.47
1:A:636:LEU:C	1:A:638:THR:N	2.68	0.47
1:A:683:LEU:HA	1:A:683:LEU:HD23	1.55	0.47
1:A:1117:VAL:HG12	1:A:1118:CYS:N	2.29	0.47
1:A:1124:LEU:HA	1:A:1124:LEU:HD12	1.28	0.47
1:A:1369:THR:HG22	1:A:1369:THR:O	2.13	0.47
1:B:465:LEU:HD21	1:B:675:ILE:HG13	1.95	0.47
1:B:515:ARG:NE	1:B:1367:TYR:HE2	2.09	0.47
1:B:963:VAL:CG1	1:B:964:MET:H	2.25	0.47
1:A:218:THR:CG2	1:A:221:LEU:H	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:MET:CE	1:A:282:GLU:CG	2.88	0.47
1:A:442:MET:CE	1:A:447:LEU:CA	2.92	0.47
1:A:745:ARG:C	1:A:746:ILE:HG13	2.40	0.47
1:A:1369:THR:CG2	1:A:1369:THR:O	2.63	0.47
1:B:37:ASP:OD1	1:B:39:LYS:N	2.34	0.47
1:B:227:MET:HE3	1:B:282:GLU:CA	2.27	0.47
1:B:704:LEU:O	1:B:707:ILE:N	2.48	0.47
1:B:756:LYS:O	1:B:757:LYS:C	2.58	0.47
1:B:1170:GLN:HB2	1:B:1183:LEU:HD12	1.96	0.47
1:A:78:LEU:HD12	1:A:129:GLU:HG3	1.97	0.47
1:A:253:HIS:CD2	1:A:254:PRO:HD2	2.40	0.47
1:A:337:ASP:O	1:A:338:GLY:C	2.56	0.47
1:A:1159:ASN:C	1:A:1161:VAL:H	2.22	0.47
1:A:1424:LEU:HD21	1:A:1428:ILE:HD11	1.97	0.47
1:B:139:VAL:HG12	1:B:143:GLN:HB2	1.97	0.47
1:B:189:THR:O	1:B:189:THR:HG23	2.14	0.47
1:B:693:MET:HA	1:B:693:MET:CE	2.27	0.47
1:B:826:ARG:HD2	1:B:1078:ASP:OD1	2.14	0.47
1:B:1131:THR:O	1:B:1132:PRO:C	2.58	0.47
1:A:136:ASN:OD1	1:A:136:ASN:N	2.47	0.47
1:A:420:VAL:C	1:A:422:ASN:H	2.23	0.47
1:A:509:PRO:O	1:A:509:PRO:HG2	2.14	0.47
1:A:526:LEU:HB3	1:A:641:SER:HB3	1.97	0.47
1:A:550:LEU:HD13	1:A:555:PHE:HA	1.95	0.47
1:A:657:VAL:HG12	1:A:658:LEU:N	2.30	0.47
1:A:823:MET:HB2	1:A:823:MET:HE3	1.61	0.47
1:A:917:VAL:HG13	1:A:922:LEU:HD21	1.95	0.47
1:A:953:ILE:O	1:A:956:LEU:HB2	2.15	0.47
1:A:1149:ILE:O	1:A:1149:ILE:CG2	2.59	0.47
1:A:1212:ASP:HB3	1:A:1245:ARG:HB3	1.96	0.47
1:A:1414:ARG:NH2	1:A:1455:TRP:CZ2	2.82	0.47
1:A:1430:GLU:O	1:A:1431:HIS:C	2.58	0.47
1:A:1450:GLU:O	1:A:1451:VAL:C	2.57	0.47
1:B:53:LYS:O	1:B:54:PHE:C	2.58	0.47
1:B:227:MET:CE	1:B:282:GLU:HG2	2.44	0.47
1:B:260:MET:O	1:B:261:GLN:C	2.48	0.47
1:B:290:THR:HG22	1:B:293:MET:H	1.78	0.47
1:B:560:ASP:O	1:B:561:TYR:C	2.58	0.47
1:B:589:ILE:O	1:B:593:THR:OG1	2.28	0.47
1:B:743:VAL:HG12	1:B:744:SER:N	2.30	0.47
1:B:824:GLN:NE2	1:B:824:GLN:CA	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:840:VAL:O	1:B:841:ASP:C	2.56	0.47
1:B:908:LYS:HB3	1:B:921:TYR:CZ	2.49	0.47
1:B:1420:TYR:C	1:B:1422:SER:N	2.69	0.47
1:A:231:ASN:HB3	1:A:332:ALA:HB3	1.96	0.47
1:A:240:ASN:O	1:A:241:VAL:C	2.58	0.47
1:A:281:PHE:CZ	1:A:335:MET:HG2	2.50	0.47
1:A:454:PHE:CD2	1:A:648:GLU:CA	2.98	0.47
1:A:559:ARG:NH1	1:A:568:GLU:OE2	2.48	0.47
1:A:603:HIS:N	1:A:640:THR:HG22	2.30	0.47
1:A:863:LEU:HB3	1:A:1118:CYS:HB3	1.97	0.47
1:A:938:PRO:O	1:A:939:GLY:C	2.53	0.47
1:A:1222:LEU:N	1:A:1229:MET:HE2	2.30	0.47
1:A:1243:GLY:O	1:A:1246:LEU:N	2.47	0.47
1:A:1458:VAL:HG13	1:A:1459:PRO:CD	2.42	0.47
1:B:147:ASP:O	1:B:151:ILE:HG13	2.15	0.47
1:B:150:ILE:HG21	1:B:259:HIS:CG	2.50	0.47
1:B:227:MET:CE	1:B:282:GLU:CG	2.93	0.47
1:B:286:ARG:HD3	1:B:286:ARG:HA	1.55	0.47
1:B:347:ARG:HH11	1:B:347:ARG:HB2	1.79	0.47
1:B:477:GLY:O	1:B:478:SER:HB3	2.15	0.47
1:B:525:ARG:HG3	1:B:544:GLN:HG3	1.97	0.47
1:A:110:VAL:HG12	1:A:111:PRO:N	2.28	0.47
1:A:253:HIS:H	1:A:260:MET:HE1	1.79	0.47
1:A:468:MET:HG2	1:A:699:ALA:HB1	1.97	0.47
1:A:499:PHE:CE2	1:A:742:MET:HE1	2.27	0.47
1:A:1075:THR:HG22	1:A:1077:ARG:N	2.30	0.47
1:B:25:LEU:HD21	1:B:207:TYR:HB2	1.97	0.47
1:B:248:GLU:C	1:B:250:ARG:N	2.73	0.47
1:B:621:ILE:HG12	1:B:657:VAL:HG11	1.97	0.47
1:B:948:LYS:C	1:B:950:THR:H	2.23	0.47
1:B:1219:ALA:HA	1:B:1229:MET:CE	2.45	0.47
1:B:1431:HIS:O	1:B:1432:VAL:C	2.54	0.47
1:A:47:HIS:HB3	1:A:206:ILE:HB	1.96	0.47
1:A:218:THR:HG22	1:A:218:THR:O	2.08	0.47
1:A:297:MET:HE2	1:A:297:MET:HB3	1.53	0.47
1:A:446:GLU:O	1:A:449:ARG:N	2.48	0.47
1:A:894:PHE:HD1	1:A:904:ASN:ND2	2.13	0.47
1:A:911:ALA:O	1:A:912:SER:C	2.57	0.47
1:A:1383:PHE:O	1:A:1384:ALA:HB3	2.15	0.47
1:B:244:MET:O	1:B:245:LYS:C	2.57	0.47
1:B:547:SER:C	1:B:549:VAL:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:558:MET:C	1:B:560:ASP:H	2.23	0.47
1:B:571:ALA:C	1:B:618:ILE:HD12	2.40	0.47
1:B:912:SER:CB	1:B:968:PRO:O	2.62	0.47
1:A:250:ARG:NH2	1:A:639:PHE:CE1	2.79	0.46
1:A:313:HIS:CD2	1:A:313:HIS:N	2.83	0.46
1:A:935:GLY:HA3	1:A:1025:GLY:O	2.15	0.46
1:A:1212:ASP:OD1	1:A:1243:GLY:N	2.24	0.46
1:A:1326:THR:HG22	1:A:1326:THR:O	2.15	0.46
1:A:1424:LEU:HD23	1:A:1424:LEU:C	2.40	0.46
1:B:30:HIS:CE1	1:B:368:GLU:OE2	2.68	0.46
1:B:1184:ASN:N	1:B:1185:PRO:HD2	2.30	0.46
1:B:1325:ASN:O	1:B:1326:THR:HB	2.14	0.46
1:A:191:PHE:HE1	1:A:192:TYR:CE1	2.33	0.46
1:A:207:TYR:N	1:A:207:TYR:HD1	2.08	0.46
1:A:284:MET:HB3	1:A:284:MET:HE3	1.72	0.46
1:A:348:ASN:HB2	1:A:350:LEU:HG	1.96	0.46
1:A:376:GLU:O	1:A:378:GLN:N	2.49	0.46
1:A:498:PHE:CD1	1:A:498:PHE:N	2.82	0.46
1:A:1001:VAL:O	1:A:1002:SER:C	2.55	0.46
1:A:1412:PHE:HD2	1:A:1455:TRP:CE3	2.33	0.46
1:B:12:LYS:HA	1:B:13:PRO:HD3	1.75	0.46
1:B:24:ALA:O	1:B:25:LEU:C	2.57	0.46
1:B:496:HIS:CD2	1:B:497:HIS:HD2	2.33	0.46
1:B:520:MET:HA	1:B:714:SER:O	2.15	0.46
1:B:1401:LEU:O	1:B:1401:LEU:CD1	2.38	0.46
1:B:1463:LEU:HD23	1:B:1463:LEU:HA	1.71	0.46
1:A:57:ASP:O	1:A:60:LYS:HB2	2.15	0.46
1:A:98:LEU:HD23	1:A:98:LEU:HA	1.82	0.46
1:A:256:PHE:O	1:A:257:GLY:C	2.56	0.46
1:A:280:VAL:O	1:A:281:PHE:C	2.58	0.46
1:A:558:MET:C	1:A:560:ASP:N	2.72	0.46
1:A:603:HIS:N	1:A:640:THR:CG2	2.78	0.46
1:A:724:ASN:HD22	1:A:724:ASN:N	2.02	0.46
1:A:1005:GLY:O	1:A:1009:ILE:HD12	2.16	0.46
1:B:30:HIS:CE1	1:B:1237:ASN:O	2.68	0.46
1:B:656:ALA:O	1:B:657:VAL:C	2.58	0.46
1:B:745:ARG:C	1:B:746:ILE:HG13	2.40	0.46
1:B:839:PRO:HG2	1:B:842:GLU:OE1	2.15	0.46
1:B:1061:LEU:O	1:B:1064:ARG:HB2	2.15	0.46
1:A:5:PHE:CE2	1:A:365:GLY:HA3	2.50	0.46
1:B:209:GLN:HG3	1:B:210:ARG:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:820:ARG:HB3	1:B:821:PRO:HD3	1.94	0.46
1:B:824:GLN:NE2	1:B:824:GLN:HA	2.30	0.46
1:B:1131:THR:HG22	1:B:1133:GLU:CA	2.46	0.46
1:B:1468:VAL:O	1:B:1469:PRO:C	2.57	0.46
1:A:9:ILE:O	1:A:398:GLY:HA2	2.15	0.46
1:A:345:MET:CE	1:A:385:LEU:HB3	2.45	0.46
1:A:345:MET:CG	1:A:346:ASP:N	2.55	0.46
1:A:572:THR:HG22	1:A:615:ARG:NE	2.30	0.46
1:A:583:ARG:CZ	1:A:587:ARG:HH12	2.27	0.46
1:A:787:ARG:NH1	1:A:821:PRO:HB2	2.24	0.46
1:A:850:ARG:O	1:A:853:PHE:HB2	2.15	0.46
1:A:940:GLU:O	1:A:969:PRO:HA	2.15	0.46
1:A:1101:GLY:O	1:A:1102:CYS:C	2.57	0.46
1:B:336:THR:C	1:B:337:ASP:O	2.50	0.46
1:B:389:GLU:HA	1:B:403:ASP:OD2	2.15	0.46
1:B:457:THR:O	1:B:461:MET:HG2	2.15	0.46
1:B:842:GLU:HB3	1:B:1156:ARG:CD	2.43	0.46
1:A:52:GLN:O	1:A:56:LYS:HB2	2.16	0.46
1:A:111:PRO:C	1:A:112:ILE:HG23	2.40	0.46
1:A:335:MET:HB2	1:A:335:MET:HE3	1.56	0.46
1:A:521:SER:OG	1:A:522:LEU:N	2.44	0.46
1:A:572:THR:HG21	1:A:615:ARG:NE	2.30	0.46
1:A:969:PRO:CD	1:A:970:PRO:HD2	2.46	0.46
1:A:1009:ILE:O	1:A:1010:ALA:C	2.59	0.46
1:A:1226:GLY:O	1:A:1227:GLU:C	2.59	0.46
1:A:1376:LEU:N	1:A:1376:LEU:CD2	2.33	0.46
1:B:615:ARG:HG2	1:B:615:ARG:NH1	2.30	0.46
1:B:695:ASN:O	1:B:696:TYR:C	2.57	0.46
1:B:1143:ALA:O	1:B:1146:VAL:N	2.47	0.46
1:B:1210:THR:CG2	1:B:1211:LEU:H	2.07	0.46
1:B:1357:VAL:CG1	1:B:1359:GLY:O	2.63	0.46
1:A:81:ILE:HD13	1:B:216:PHE:CE1	2.50	0.46
1:A:260:MET:HA	1:A:263:LEU:HB2	1.98	0.46
1:A:456:LEU:HD23	1:A:456:LEU:HA	1.65	0.46
1:A:472:GLY:O	1:A:473:LYS:HG3	2.16	0.46
1:A:536:ASP:OD1	1:A:538:THR:N	2.49	0.46
1:A:565:THR:HG22	1:A:565:THR:O	2.15	0.46
1:A:833:SER:OG	1:A:834:THR:N	2.49	0.46
1:B:89:CYS:O	1:B:93:VAL:HG23	2.16	0.46
1:B:125:ARG:HG3	1:B:219:TRP:CZ2	2.51	0.46
1:B:430:VAL:HG13	1:B:554:GLU:CA	2.37	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:732:ARG:O	1:B:733:ALA:C	2.59	0.46
1:B:787:ARG:O	1:B:788:HIS:ND1	2.49	0.46
1:B:1076:GLY:N	1:B:1145:GLU:OE2	2.49	0.46
1:B:1347:ALA:O	1:B:1348:VAL:C	2.54	0.46
1:A:965:LEU:HD23	1:A:965:LEU:HA	1.33	0.46
1:A:1230:GLN:C	1:A:1231:LEU:HD23	2.41	0.46
1:A:1249:MET:HE3	1:A:1249:MET:HB3	1.78	0.46
1:B:290:THR:HG22	1:B:292:PRO:N	2.31	0.46
1:B:1114:PRO:HB2	1:B:1115:VAL:HG23	1.97	0.46
1:B:1212:ASP:OD2	1:B:1243:GLY:CA	2.63	0.46
1:B:1424:LEU:CD2	1:B:1428:ILE:HD11	2.46	0.46
1:A:353:MET:HG2	1:A:385:LEU:HD23	1.97	0.46
1:A:393:VAL:CG1	1:A:394:ASP:N	2.77	0.46
1:A:856:PRO:C	1:A:883:ASP:HB3	2.41	0.46
1:A:1102:CYS:SG	1:A:1104:MET:N	2.89	0.46
1:B:304:THR:CG2	1:B:518:ARG:HD2	2.46	0.46
1:B:355:TYR:C	1:B:355:TYR:HD1	2.20	0.46
1:B:416:TRP:O	1:B:419:TRP:HB2	2.16	0.46
1:B:419:TRP:O	1:B:540:THR:OG1	2.27	0.46
1:B:629:THR:O	1:B:632:ILE:HB	2.16	0.46
1:B:878:ILE:HG21	1:B:1136:VAL:HG13	1.97	0.46
1:B:1010:ALA:HB2	1:B:1052:VAL:HG22	1.97	0.46
1:B:1057:THR:HG22	1:B:1190:VAL:HG11	1.98	0.46
1:B:1077:ARG:O	1:B:1079:ILE:N	2.48	0.46
1:A:237:VAL:C	1:A:239:GLY:N	2.73	0.46
1:A:805:ASP:O	1:A:805:ASP:OD1	2.33	0.46
1:B:29:TRP:CD1	1:B:29:TRP:H	2.34	0.46
1:B:359:THR:HG23	1:B:378:GLN:O	2.16	0.46
1:B:417:ASP:HA	1:B:420:VAL:CG1	2.46	0.46
1:B:608:ASP:OD2	1:B:647:ALA:N	2.42	0.46
1:B:632:ILE:HD12	1:B:632:ILE:HG23	1.66	0.46
1:B:833:SER:OG	1:B:834:THR:N	2.48	0.46
1:A:357:ILE:HD11	1:A:400:LEU:HD21	1.98	0.45
1:A:833:SER:HB3	1:A:1153:LEU:HD22	1.98	0.45
1:A:842:GLU:HG2	1:A:1156:ARG:HH11	1.80	0.45
1:A:1264:ILE:HG22	1:A:1284:ILE:HA	1.98	0.45
1:B:107:TRP:H	1:B:107:TRP:HD1	1.60	0.45
1:B:570:ASP:OD1	1:B:570:ASP:C	2.59	0.45
1:A:248:GLU:OE2	1:A:266:VAL:N	2.44	0.45
1:A:329:GLY:O	1:A:330:PRO:C	2.56	0.45
1:A:914:ARG:HH22	1:A:973:ASP:CG	2.23	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1113:CYS:C	1:A:1115:VAL:N	2.71	0.45
1:A:1397:LEU:HD22	1:A:1453:LYS:HD2	1.97	0.45
1:B:1:CYS:HB3	2:B:2473:OMT:HE1	1.97	0.45
1:B:266:VAL:HG12	1:B:266:VAL:O	2.15	0.45
1:B:1043:LEU:O	1:B:1044:PRO:C	2.58	0.45
1:B:1113:CYS:C	1:B:1115:VAL:H	2.23	0.45
1:B:1424:LEU:HD22	1:B:1447:TRP:HH2	1.80	0.45
1:A:370:GLY:CA	1:A:1237:ASN:HB3	2.45	0.45
1:A:555:PHE:HD1	1:A:556:ARG:N	2.14	0.45
1:A:1310:THR:O	1:A:1313:SER:N	2.33	0.45
1:A:1315:LEU:HB3	1:A:1320:ASN:ND2	2.31	0.45
1:A:1438:ARG:O	1:A:1441:ALA:N	2.49	0.45
1:B:211:TYR:CD1	1:B:212:SER:N	2.80	0.45
1:B:487:VAL:HG13	1:B:498:PHE:HE2	1.81	0.45
1:B:572:THR:HG23	1:B:616:ALA:O	2.15	0.45
1:B:757:LYS:O	1:B:758:VAL:C	2.53	0.45
1:B:798:LEU:O	1:B:801:ALA:HB3	2.16	0.45
1:B:815:GLU:O	1:B:816:GLN:C	2.59	0.45
1:A:498:PHE:H	1:A:498:PHE:HD1	1.64	0.45
1:A:582:LEU:CB	1:A:755:GLN:HE21	2.30	0.45
1:A:974:ILE:O	1:A:974:ILE:HG22	2.16	0.45
1:A:1049:LEU:HD21	1:A:1087:ALA:HB2	1.98	0.45
1:A:1231:LEU:O	1:A:1266:ILE:HA	2.16	0.45
1:B:700:ILE:O	1:B:703:GLY:N	2.49	0.45
1:B:875:MET:CE	1:B:1139:PHE:HE2	2.25	0.45
1:B:1207:VAL:HG13	1:B:1208:PRO:CD	2.46	0.45
1:B:1468:VAL:HG12	1:B:1469:PRO:O	2.17	0.45
1:A:260:MET:HE2	1:A:260:MET:HB2	1.54	0.45
1:A:348:ASN:O	1:A:349:GLY:C	2.59	0.45
1:A:1401:LEU:N	1:A:1402:PRO:CD	2.79	0.45
1:A:1416:GLU:OE1	1:A:1471:HIS:CD2	2.70	0.45
1:B:143:GLN:HE21	1:B:143:GLN:C	2.24	0.45
1:B:731:SER:HA	1:B:747:SER:HB2	1.99	0.45
1:A:24:ALA:C	1:A:26:LYS:H	2.23	0.45
1:A:179:TYR:HD2	1:A:192:TYR:CD2	2.34	0.45
1:A:251:MET:HB2	1:A:533:LEU:CD1	2.43	0.45
1:A:397:SER:O	1:A:398:GLY:C	2.58	0.45
1:A:510:PRO:CD	1:A:970:PRO:HB3	2.37	0.45
1:A:608:ASP:O	1:A:611:MET:N	2.44	0.45
1:B:102:TYR:HA	1:B:136:ASN:OD1	2.16	0.45
1:B:806:SER:OG	1:B:809:THR:CB	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:991:ASN:HA	1:B:992:PRO:HD2	1.83	0.45
1:B:1054:GLN:O	1:B:1055:VAL:C	2.60	0.45
1:B:1432:VAL:HG12	1:B:1433:THR:N	2.31	0.45
1:A:103:TYR:HD2	1:A:105:TYR:CE1	2.35	0.45
1:A:359:THR:CG2	1:A:378:GLN:CA	2.95	0.45
1:A:520:MET:HE3	1:A:705:LEU:CD1	2.47	0.45
1:A:554:GLU:OE2	1:A:697:LYS:HE3	2.17	0.45
1:A:701:ASP:C	1:A:703:GLY:N	2.71	0.45
1:A:1274:GLN:NE2	1:A:1293:ASN:HB3	2.30	0.45
1:A:1440:ALA:O	1:A:1441:ALA:C	2.58	0.45
1:B:345:MET:HE2	1:B:345:MET:HB2	1.29	0.45
1:B:413:LEU:O	1:B:414:LYS:HD2	2.16	0.45
1:B:414:LYS:HB3	1:B:415:PRO:CD	2.47	0.45
1:B:790:TRP:CZ2	1:B:1074:LYS:HG2	2.51	0.45
1:B:806:SER:HG	1:B:809:THR:H	1.57	0.45
1:B:1026:ASN:HB3	1:B:1043:LEU:N	2.31	0.45
1:B:1080:VAL:HG11	1:B:1084:MET:HE3	1.95	0.45
1:A:102:TYR:HE2	1:A:144:PHE:CD1	2.34	0.45
1:A:131:ILE:HG23	1:A:131:ILE:O	2.16	0.45
1:A:228:LEU:HA	1:A:228:LEU:HD12	1.29	0.45
1:A:386:GLY:N	1:A:389:GLU:OE2	2.48	0.45
1:A:449:ARG:HD3	1:A:765:ALA:O	2.17	0.45
1:A:459:GLU:O	1:A:463:LEU:CB	2.59	0.45
1:A:1084:MET:SD	1:A:1168:LEU:HD21	2.57	0.45
1:B:266:VAL:HG12	1:B:279:THR:HG22	1.97	0.45
1:B:426:LEU:HD23	1:B:543:LEU:HB3	1.93	0.45
1:B:612:GLY:O	1:B:762:HIS:HE1	1.99	0.45
1:B:671:ALA:O	1:B:675:ILE:HD12	2.17	0.45
1:B:696:TYR:CZ	1:B:700:ILE:HD11	2.52	0.45
1:A:110:VAL:HG12	1:A:111:PRO:O	2.17	0.45
1:A:266:VAL:HG12	1:A:266:VAL:O	2.16	0.45
1:A:375:ASP:O	1:A:376:GLU:C	2.60	0.45
1:A:734:LEU:HD12	1:A:738:HIS:CD2	2.41	0.45
1:A:1062:ARG:HH11	1:A:1062:ARG:HD3	1.53	0.45
1:A:1084:MET:SD	1:A:1168:LEU:CD2	3.05	0.45
1:A:1109:HIS:ND1	1:A:1109:HIS:N	2.45	0.45
1:B:230:HIS:HE1	1:B:234:ILE:HG13	1.82	0.45
1:B:242:ASN:C	1:B:244:MET:N	2.72	0.45
1:B:263:LEU:HA	1:B:263:LEU:HD12	1.11	0.45
1:B:513:SER:CA	1:B:520:MET:HE2	2.47	0.45
1:B:984:ILE:O	1:B:988:LYS:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1094:THR:O	1:B:1097:LEU:HB2	2.17	0.45
1:B:1170:GLN:OE1	1:B:1183:LEU:HB2	2.17	0.45
1:B:1210:THR:CG2	1:B:1211:LEU:N	2.75	0.45
1:A:393:VAL:HG12	1:A:394:ASP:N	2.23	0.45
1:A:495:LEU:HD12	1:A:495:LEU:HA	1.53	0.45
1:A:500:ARG:NH2	1:A:1041:ALA:O	2.48	0.45
1:A:857:GLY:N	1:A:883:ASP:HB3	2.31	0.45
1:A:1260:GLN:O	1:A:1261:PRO:C	2.60	0.45
1:B:165:ASN:O	1:B:166:ASP:CB	2.65	0.45
1:B:175:ARG:NH1	1:B:175:ARG:CG	2.79	0.45
1:A:56:LYS:HE2	1:A:67:PRO:O	2.17	0.44
1:A:225:PHE:HB3	1:A:278:ASP:CG	2.42	0.44
1:A:458:MET:HE3	1:A:458:MET:HB2	1.76	0.44
1:A:510:PRO:HD2	1:A:970:PRO:CB	2.34	0.44
1:A:537:GLU:C	1:A:539:GLN:N	2.74	0.44
1:A:660:GLY:HA2	1:A:721:GLY:N	2.32	0.44
1:A:992:PRO:HA	1:A:1204:ARG:NH2	2.32	0.44
1:A:1057:THR:HG22	1:A:1058:LEU:N	2.27	0.44
1:B:30:HIS:HD2	1:B:31:ARG:H	1.65	0.44
1:B:304:THR:HG21	1:B:518:ARG:HD2	1.98	0.44
1:B:918:THR:HG23	1:B:1256:MET:SD	2.56	0.44
1:B:1374:VAL:HG12	1:B:1375:ILE:N	2.32	0.44
1:B:1435:THR:HG23	1:B:1437:SER:HB2	1.98	0.44
1:A:10:ASP:C	1:A:10:ASP:OD1	2.59	0.44
1:A:184:LEU:HB3	1:A:186:GLU:HG3	1.99	0.44
1:A:386:GLY:O	1:A:387:PRO:C	2.60	0.44
1:A:572:THR:HG21	1:A:615:ARG:HE	1.82	0.44
1:A:636:LEU:HD12	1:A:636:LEU:HA	1.60	0.44
1:A:1302:GLY:H	1:A:1333:ALA:C	2.24	0.44
1:B:211:TYR:O	1:B:212:SER:CB	2.58	0.44
1:B:317:ILE:HG22	1:B:321:ASN:ND2	2.27	0.44
1:B:440:SER:O	1:B:441:ASP:OD1	2.36	0.44
1:B:443:ASP:C	1:B:445:ALA:N	2.75	0.44
1:B:819:LYS:HD3	1:B:819:LYS:HA	1.60	0.44
1:B:1075:THR:HG22	1:B:1076:GLY:N	2.31	0.44
1:B:1099:ALA:C	1:B:1101:GLY:H	2.26	0.44
1:B:1102:CYS:SG	5:B:2476:F3S:S1	3.06	0.44
1:A:216:PHE:HA	1:A:217:PRO:HD3	1.73	0.44
1:A:316:LEU:O	1:A:319:TYR:N	2.50	0.44
1:A:526:LEU:CD1	1:A:526:LEU:H	2.17	0.44
1:A:989:GLN:O	1:A:1245:ARG:HD3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1360:CYS:O	1:A:1361:GLY:O	2.35	0.44
1:A:1415:ILE:HG21	1:A:1421:GLU:CB	2.44	0.44
1:B:30:HIS:CD2	1:B:31:ARG:N	2.86	0.44
1:B:78:LEU:HB3	1:B:79:PRO:CD	2.48	0.44
1:B:92:ILE:O	1:B:93:VAL:C	2.59	0.44
1:B:312:ASN:HB2	1:B:411:ALA:CB	2.46	0.44
1:B:622:LEU:HD12	1:B:622:LEU:HA	1.59	0.44
1:B:689:LEU:O	1:B:689:LEU:HD12	2.18	0.44
1:B:728:ILE:CD1	1:B:1047:MET:CE	2.74	0.44
1:B:957:ARG:HD2	1:B:965:LEU:CD1	2.48	0.44
1:B:964:MET:O	1:B:965:LEU:HD23	2.18	0.44
1:B:985:TYR:O	1:B:988:LYS:N	2.50	0.44
1:B:1016:ALA:O	1:B:1017:ASN:HB2	2.17	0.44
1:A:197:ASP:OD2	1:A:199:ARG:NH2	2.50	0.44
1:A:309:THR:HG22	1:A:310:PRO:O	2.17	0.44
1:A:485:ILE:O	1:A:486:ALA:C	2.60	0.44
1:A:551:THR:O	1:A:552:THR:C	2.61	0.44
1:A:918:THR:O	1:A:921:TYR:N	2.51	0.44
1:B:196:LEU:HA	1:B:196:LEU:HD23	1.55	0.44
1:B:303:LEU:HG	1:B:303:LEU:O	2.17	0.44
1:B:456:LEU:HD23	1:B:456:LEU:HA	1.11	0.44
1:B:736:ALA:O	1:B:737:GLU:C	2.58	0.44
1:A:52:GLN:NE2	1:A:71:LEU:N	2.44	0.44
1:A:81:ILE:HD13	1:B:216:PHE:CZ	2.53	0.44
1:A:353:MET:HA	1:A:366:GLY:O	2.18	0.44
1:A:489:SER:OG	1:A:490:ASP:N	2.48	0.44
1:A:636:LEU:O	1:A:638:THR:N	2.51	0.44
1:A:648:GLU:HG2	1:A:654:TYR:CE2	2.53	0.44
1:A:819:LYS:HD3	1:A:819:LYS:HA	1.73	0.44
1:A:908:LYS:HD2	1:A:921:TYR:CD1	2.53	0.44
1:A:1170:GLN:O	1:A:1170:GLN:HG2	2.16	0.44
1:B:228:LEU:HD22	1:B:278:ASP:HA	1.98	0.44
1:B:528:ASN:O	1:B:529:LEU:HD23	2.17	0.44
1:B:582:LEU:O	1:B:585:ALA:HB3	2.17	0.44
1:B:670:LEU:HD23	1:B:670:LEU:HA	1.48	0.44
1:A:30:HIS:N	1:A:30:HIS:CD2	2.85	0.44
1:A:357:ILE:HD11	1:A:400:LEU:CD2	2.47	0.44
1:A:420:VAL:O	1:A:422:ASN:N	2.50	0.44
1:A:520:MET:HE1	1:A:705:LEU:O	2.17	0.44
1:A:991:ASN:HA	1:A:992:PRO:HD2	1.84	0.44
1:A:1210:THR:O	1:A:1211:LEU:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1435:THR:HG23	1:A:1437:SER:CB	2.47	0.44
1:A:1447:TRP:CE2	1:A:1451:VAL:HG21	2.52	0.44
1:B:293:MET:HG2	1:B:410:LEU:HD23	2.00	0.44
1:B:1003:ARG:NH1	1:B:1004:SER:O	2.50	0.44
1:B:1184:ASN:CB	1:B:1185:PRO:CD	2.80	0.44
1:B:1329:TYR:HD1	1:B:1348:VAL:HG13	1.82	0.44
1:B:1366:GLU:CG	1:B:1367:TYR:CE1	3.00	0.44
1:A:6:ILE:HD13	1:A:20:LYS:HB2	1.99	0.44
1:A:345:MET:HB2	1:A:345:MET:HE2	1.15	0.44
1:A:419:TRP:CE2	1:A:537:GLU:HB3	2.53	0.44
1:A:763:ALA:O	1:A:764:THR:C	2.58	0.44
1:A:839:PRO:HG2	1:A:842:GLU:HB2	1.99	0.44
1:A:964:MET:O	1:A:965:LEU:HD23	2.18	0.44
1:A:1053:HIS:ND1	1:A:1062:ARG:HD3	2.33	0.44
1:B:8:ALA:HA	1:B:362:LEU:HD12	2.00	0.44
1:B:249:THR:O	1:B:249:THR:CG2	2.55	0.44
1:B:1006:ILE:HG23	1:B:1007:GLY:N	2.32	0.44
1:B:1050:SER:O	1:B:1051:GLU:O	2.36	0.44
1:B:1277:GLY:O	1:B:1278:ALA:C	2.60	0.44
1:A:125:ARG:HG3	1:A:219:TRP:CZ2	2.53	0.44
1:A:292:PRO:O	1:A:293:MET:C	2.55	0.44
1:A:420:VAL:CG1	1:A:421:GLN:N	2.81	0.44
1:A:442:MET:CE	1:A:447:LEU:N	2.81	0.44
1:A:559:ARG:HD2	1:A:605:ILE:CD1	2.48	0.44
1:A:732:ARG:O	1:A:733:ALA:C	2.59	0.44
1:A:1113:CYS:C	1:A:1115:VAL:H	2.25	0.44
1:B:165:ASN:O	1:B:166:ASP:HB2	2.18	0.44
1:B:485:ILE:HD13	1:B:485:ILE:HG21	1.68	0.44
1:B:492:TYR:CD1	1:B:492:TYR:C	2.94	0.44
1:B:606:LEU:C	1:B:607:THR:HG22	2.43	0.44
1:B:643:ASN:HB3	1:B:665:THR:HG22	1.98	0.44
1:B:860:MET:HB2	1:B:860:MET:HE2	1.39	0.44
1:B:985:TYR:O	1:B:986:ASP:C	2.61	0.44
1:B:1420:TYR:OH	1:B:1466:LEU:CD2	2.65	0.44
1:B:1447:TRP:O	1:B:1450:GLU:N	2.51	0.44
1:A:59:VAL:HG12	1:A:60:LYS:N	2.32	0.44
1:A:230:HIS:C	1:A:230:HIS:CD2	2.94	0.44
1:A:274:SER:O	1:A:275:GLY:C	2.60	0.44
1:A:479:MET:HB3	1:A:1106:ARG:NH1	2.31	0.44
1:A:634:SER:O	1:A:635:ASN:HB2	2.16	0.44
1:B:508:ASN:HB2	1:B:509:PRO:CD	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:622:LEU:HD13	1:B:739:PHE:HZ	1.82	0.44
1:B:643:ASN:HD22	1:B:665:THR:HG21	1.83	0.44
1:B:1132:PRO:O	1:B:1133:GLU:C	2.56	0.44
1:B:1244:THR:OG1	1:B:1278:ALA:HB3	2.18	0.44
1:A:454:PHE:N	1:A:454:PHE:CD1	2.81	0.43
1:A:463:LEU:HA	1:A:463:LEU:HD23	1.48	0.43
1:A:731:SER:O	1:A:734:LEU:HB3	2.18	0.43
1:A:944:LEU:HA	1:A:944:LEU:HD12	1.72	0.43
1:A:1149:ILE:O	1:A:1149:ILE:HG22	2.12	0.43
1:A:1219:ALA:HA	1:A:1229:MET:HE3	2.00	0.43
1:B:59:VAL:HG22	1:B:105:TYR:HD2	1.78	0.43
1:B:98:LEU:HD23	1:B:98:LEU:HA	1.62	0.43
1:B:111:PRO:C	1:B:112:ILE:CG2	2.91	0.43
1:B:175:ARG:HH11	1:B:175:ARG:CG	2.19	0.43
1:B:515:ARG:H	1:B:515:ARG:HG3	1.63	0.43
1:B:571:ALA:HB2	1:B:606:LEU:HD22	1.98	0.43
1:A:295:LYS:HE2	1:A:299:VAL:HG11	1.98	0.43
1:A:360:ASP:OD1	1:A:360:ASP:N	2.49	0.43
1:A:858:MET:HA	3:A:2474:FMN:C5A	2.48	0.43
1:A:987:LEU:HD23	1:A:987:LEU:HA	1.70	0.43
1:A:1394:VAL:HG11	1:A:1401:LEU:HD23	1.98	0.43
1:B:244:MET:HE2	1:B:244:MET:CA	2.43	0.43
1:B:289:ARG:NH1	1:B:535:GLU:HB2	2.33	0.43
1:B:310:PRO:CG	1:B:404:ARG:NH2	2.66	0.43
1:B:364:ILE:HD12	1:B:374:ILE:HD11	2.00	0.43
1:B:463:LEU:HD23	1:B:463:LEU:HA	1.20	0.43
1:B:511:ILE:HG21	1:B:511:ILE:HD13	1.76	0.43
1:B:823:MET:HB2	1:B:823:MET:HE3	1.50	0.43
1:B:843:VAL:HG11	1:B:1147:ARG:HB3	2.00	0.43
1:B:934:GLN:HE21	1:B:934:GLN:HB2	1.58	0.43
1:B:1164:ARG:HB3	1:B:1167:LEU:CD1	2.47	0.43
1:B:1184:ASN:O	1:B:1185:PRO:C	2.61	0.43
1:A:438:GLU:OE1	1:A:553:ALA:HB2	2.18	0.43
1:A:850:ARG:CG	1:A:850:ARG:NH1	2.76	0.43
1:A:875:MET:CE	1:A:1139:PHE:CZ	2.90	0.43
1:A:937:LYS:CE	1:A:1033:SER:HB2	2.40	0.43
1:A:1159:ASN:O	1:A:1161:VAL:N	2.50	0.43
1:A:1212:ASP:OD2	1:A:1243:GLY:CA	2.67	0.43
1:A:1425:LYS:CD	1:A:1447:TRP:CD1	3.02	0.43
1:A:1468:VAL:HG12	1:A:1469:PRO:O	2.18	0.43
1:B:219:TRP:N	1:B:220:PRO:CD	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:HIS:CD2	1:B:313:HIS:H	2.34	0.43
1:B:500:ARG:NH2	1:B:1039:LYS:O	2.50	0.43
1:B:520:MET:HE3	1:B:705:LEU:HB3	2.00	0.43
1:B:558:MET:O	1:B:560:ASP:N	2.51	0.43
1:B:825:LEU:O	1:B:826:ARG:C	2.59	0.43
1:B:958:HIS:N	1:B:958:HIS:HD1	2.16	0.43
1:B:1068:ARG:HA	1:B:1089:GLU:O	2.17	0.43
1:A:16:SER:O	1:A:20:LYS:CG	2.66	0.43
1:A:452:GLN:NE2	1:A:764:THR:HG23	1.99	0.43
1:A:509:PRO:HB3	1:A:975:TYR:CD1	2.53	0.43
1:A:826:ARG:NH1	1:A:1046:GLU:CD	2.76	0.43
1:A:871:LEU:HA	1:A:871:LEU:HD23	1.68	0.43
1:A:902:ASN:C	1:A:902:ASN:OD1	2.60	0.43
1:A:990:ILE:O	1:A:990:ILE:HG13	2.19	0.43
1:A:1026:ASN:ND2	1:A:1027:SER:N	2.66	0.43
1:A:1156:ARG:HE	1:A:1156:ARG:HB2	1.72	0.43
1:A:1438:ARG:C	1:A:1440:ALA:N	2.76	0.43
1:B:207:TYR:CD1	1:B:207:TYR:N	2.85	0.43
1:B:943:GLN:HE21	1:B:1033:SER:HA	1.83	0.43
1:B:978:GLU:H	1:B:978:GLU:HG2	1.21	0.43
1:B:1336:LEU:HD23	1:B:1355:VAL:CG1	2.48	0.43
1:A:120:LYS:O	1:A:123:ALA:HB3	2.18	0.43
1:A:191:PHE:O	1:A:191:PHE:CD1	2.72	0.43
1:A:208:HIS:CD2	1:A:209:GLN:C	2.96	0.43
1:A:385:LEU:HD12	1:A:389:GLU:C	2.44	0.43
1:A:387:PRO:HD2	1:A:1344:GLU:OE2	2.14	0.43
1:A:572:THR:CG2	1:A:615:ARG:HE	2.32	0.43
1:A:602:THR:C	1:A:640:THR:HG23	2.43	0.43
1:A:611:MET:HE3	1:A:611:MET:HB3	1.88	0.43
1:A:633:ARG:NH2	1:A:737:GLU:O	2.38	0.43
1:A:1026:ASN:ND2	1:A:1026:ASN:C	2.77	0.43
1:A:1301:SER:O	1:A:1301:SER:OG	2.37	0.43
1:A:1395:TYR:HE1	1:A:1397:LEU:HG	1.82	0.43
1:B:82:SER:O	1:B:83:LEU:C	2.60	0.43
1:B:284:MET:HE2	1:B:294:VAL:HG13	2.01	0.43
1:B:303:LEU:O	1:B:304:THR:C	2.61	0.43
1:B:677:GLU:OE2	1:B:681:ARG:NH1	2.52	0.43
1:B:694:ALA:O	1:B:695:ASN:C	2.58	0.43
1:B:1212:ASP:OD2	1:B:1243:GLY:C	2.61	0.43
1:B:1467:GLU:O	1:B:1469:PRO:HD3	2.18	0.43
1:A:121:ALA:C	1:A:123:ALA:N	2.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:MET:CE	1:A:217:PRO:O	2.62	0.43
1:A:261:GLN:HE21	1:A:264:LYS:HD2	1.83	0.43
1:A:309:THR:HB	1:A:314:LYS:HE3	1.99	0.43
1:A:852:ARG:NH1	1:A:1088:GLU:O	2.50	0.43
1:A:861:GLY:O	1:A:862:ALA:C	2.61	0.43
1:A:897:ASP:OD1	1:A:899:ASN:N	2.50	0.43
1:A:983:LEU:HD22	1:A:987:LEU:HG	2.01	0.43
1:A:1003:ARG:HH11	1:A:1003:ARG:CG	2.29	0.43
1:A:1050:SER:O	1:A:1051:GLU:C	2.60	0.43
1:A:1407:ASP:O	1:A:1408:GLU:C	2.61	0.43
1:B:254:PRO:CG	1:B:255:ALA:H	2.21	0.43
1:B:308:THR:O	1:B:308:THR:CG2	2.67	0.43
1:B:850:ARG:NH1	1:B:878:ILE:HB	2.33	0.43
1:B:873:VAL:O	1:B:874:ALA:C	2.60	0.43
1:B:1133:GLU:H	1:B:1133:GLU:CD	2.27	0.43
1:A:114:VAL:HG11	1:A:125:ARG:NH1	2.33	0.43
1:A:142:GLU:CD	1:A:142:GLU:N	2.58	0.43
1:A:302:ALA:CA	1:A:347:ARG:NH1	2.81	0.43
1:A:536:ASP:CG	1:A:538:THR:HG22	2.44	0.43
1:A:545:LEU:HA	1:A:545:LEU:HD23	1.19	0.43
1:A:551:THR:H	1:A:554:GLU:CG	2.32	0.43
1:A:575:VAL:HG13	1:A:759:LEU:CD2	2.47	0.43
1:A:621:ILE:HG12	1:A:657:VAL:HG11	2.00	0.43
1:A:1011:ALA:O	1:A:1014:ALA:N	2.52	0.43
1:A:1058:LEU:HA	1:A:1058:LEU:HD23	1.88	0.43
1:A:1131:THR:HG22	1:A:1133:GLU:H	1.81	0.43
1:A:1139:PHE:N	1:A:1139:PHE:CD1	2.86	0.43
1:A:1315:LEU:HD13	1:A:1320:ASN:ND2	2.33	0.43
1:A:1363:ASN:HD22	1:A:1363:ASN:HA	1.60	0.43
1:A:1395:TYR:CE2	1:A:1443:ILE:CD1	3.01	0.43
1:B:49:ALA:O	1:B:50:VAL:C	2.58	0.43
1:B:251:MET:CE	1:B:533:LEU:HD11	2.49	0.43
1:B:345:MET:HG3	1:B:346:ASP:N	2.32	0.43
1:B:647:ALA:HB2	1:B:669:TYR:OH	2.19	0.43
1:B:706:LYS:O	1:B:707:ILE:C	2.59	0.43
1:B:897:ASP:OD1	1:B:899:ASN:N	2.52	0.43
1:B:913:GLY:CA	1:B:1349:ARG:CD	2.94	0.43
1:B:1032:ALA:O	1:B:1033:SER:HB2	2.19	0.43
1:B:1124:LEU:HA	1:B:1124:LEU:HD12	1.30	0.43
1:A:558:MET:C	1:A:560:ASP:H	2.24	0.43
1:A:666:VAL:HG12	1:A:667:ASN:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1113:CYS:O	1:A:1114:PRO:C	2.61	0.43
1:B:390:MET:HG3	1:B:406:LEU:CD2	2.48	0.43
1:B:1044:PRO:HG2	1:B:1047:MET:HE3	2.01	0.43
1:B:1129:VAL:O	1:B:1129:VAL:HG23	2.19	0.43
1:A:558:MET:O	1:A:559:ARG:C	2.60	0.43
1:A:1351:SER:OG	1:A:1369:THR:HB	2.18	0.43
1:B:228:LEU:HA	1:B:228:LEU:HD12	1.88	0.43
1:B:235:ASN:HD22	1:B:236:THR:H	1.61	0.43
1:B:454:PHE:CG	1:B:648:GLU:HB2	2.53	0.43
1:B:794:VAL:CG2	1:B:817:VAL:HG23	2.49	0.43
1:B:802:VAL:CG2	1:B:1137:ASN:HB2	2.46	0.43
1:B:1077:ARG:C	1:B:1079:ILE:N	2.75	0.43
1:B:1097:LEU:HD23	1:B:1097:LEU:HA	1.69	0.43
1:B:1366:GLU:OE2	1:B:1367:TYR:CE1	2.71	0.43
1:A:52:GLN:NE2	1:A:71:LEU:CB	2.78	0.43
1:A:56:LYS:CG	1:A:71:LEU:HD22	2.49	0.43
1:A:216:PHE:CE1	1:B:81:ILE:HD13	2.54	0.43
1:A:293:MET:HB3	1:A:293:MET:HE3	1.72	0.43
1:A:432:THR:O	1:A:433:ALA:C	2.61	0.43
1:A:805:ASP:OD1	1:A:805:ASP:C	2.58	0.43
1:A:992:PRO:HA	1:A:1204:ARG:HH22	1.84	0.43
1:A:1113:CYS:HB3	1:A:1119:VAL:CG1	2.49	0.43
1:A:1139:PHE:N	1:A:1139:PHE:HD1	2.15	0.43
1:A:1348:VAL:O	1:A:1348:VAL:CG1	2.65	0.43
1:A:1458:VAL:CG1	1:A:1459:PRO:CD	2.97	0.43
1:B:513:SER:CB	1:B:520:MET:CE	2.79	0.43
1:B:562:MET:CE	1:B:605:ILE:HD11	2.49	0.43
1:B:660:GLY:HA2	1:B:721:GLY:N	2.33	0.43
1:B:814:SER:O	1:B:818:ASN:N	2.47	0.43
1:A:29:TRP:C	1:A:31:ARG:N	2.75	0.42
1:A:204:PHE:CD2	1:A:204:PHE:C	2.94	0.42
1:A:330:PRO:HB3	1:A:350:LEU:HB3	2.01	0.42
1:A:353:MET:O	1:A:353:MET:CG	2.67	0.42
1:A:565:THR:HG22	1:A:603:HIS:HD2	1.83	0.42
1:A:690:GLU:O	1:A:691:LYS:C	2.62	0.42
1:A:929:GLU:HA	1:A:997:THR:HB	2.01	0.42
1:A:1339:ALA:HB2	1:A:1435:THR:OG1	2.19	0.42
1:A:1420:TYR:OH	1:A:1466:LEU:CD2	2.66	0.42
1:B:81:ILE:O	1:B:81:ILE:CG2	2.67	0.42
1:B:175:ARG:HH22	1:B:203:ASP:CG	2.27	0.42
1:B:290:THR:HG22	1:B:292:PRO:CD	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:743:VAL:HG11	1:B:745:ARG:HG3	2.00	0.42
1:B:824:GLN:O	1:B:827:ASP:CB	2.58	0.42
1:A:46:ILE:HG12	1:A:48:VAL:HG13	2.01	0.42
1:A:90:ARG:HB3	1:A:107:TRP:CZ2	2.54	0.42
1:A:415:PRO:O	1:A:416:TRP:C	2.61	0.42
1:A:605:ILE:HA	1:A:643:ASN:O	2.20	0.42
1:A:622:LEU:HD13	1:A:739:PHE:HZ	1.84	0.42
1:A:1156:ARG:O	1:A:1157:SER:HB3	2.17	0.42
1:A:1158:LEU:HA	1:A:1158:LEU:HD12	1.62	0.42
1:A:1184:ASN:C	1:A:1186:ARG:N	2.76	0.42
1:A:1264:ILE:HG22	1:A:1283:GLY:O	2.19	0.42
1:B:403:ASP:OD1	1:B:407:LYS:HG3	2.18	0.42
1:B:550:LEU:HA	1:B:554:GLU:OE2	2.19	0.42
1:B:651:ASP:OD1	1:B:651:ASP:N	2.38	0.42
1:B:928:LEU:HA	1:B:928:LEU:HD23	1.65	0.42
1:B:1011:ALA:O	1:B:1014:ALA:N	2.52	0.42
1:B:1047:MET:HB2	1:B:1048:GLY:H	1.77	0.42
1:B:1139:PHE:O	1:B:1140:THR:C	2.59	0.42
1:B:1398:ASP:O	1:B:1399:ASP:C	2.61	0.42
1:A:195:LEU:HA	1:A:195:LEU:HD23	1.57	0.42
1:A:515:ARG:HH22	1:A:966:ILE:CB	2.23	0.42
1:A:522:LEU:HA	1:A:716:ILE:HG22	2.01	0.42
1:A:840:VAL:O	1:A:841:ASP:C	2.61	0.42
1:A:1221:PRO:O	1:A:1222:LEU:C	2.63	0.42
1:A:1425:LYS:HD2	1:A:1447:TRP:CD2	2.54	0.42
1:A:1447:TRP:NE1	1:A:1451:VAL:HG21	2.34	0.42
1:B:116:ILE:HD11	1:B:191:PHE:HB2	2.01	0.42
1:B:252:GLU:HA	1:B:260:MET:CE	2.50	0.42
1:B:442:MET:HB2	1:B:673:GLU:HG2	2.01	0.42
1:B:586:LEU:HD23	1:B:586:LEU:HA	1.85	0.42
1:B:1384:ALA:O	1:B:1385:ALA:C	2.60	0.42
1:A:82:SER:O	1:A:83:LEU:C	2.62	0.42
1:A:133:VAL:HG12	1:A:134:GLY:N	2.34	0.42
1:A:194:ASP:HB3	1:A:200:PHE:CE1	2.54	0.42
1:A:210:ARG:HA	2:A:2473:OMT:HE3	2.01	0.42
1:A:1156:ARG:O	1:A:1157:SER:CB	2.62	0.42
1:A:1161:VAL:O	1:A:1161:VAL:HG13	2.18	0.42
1:A:1190:VAL:C	1:A:1192:PRO:HD3	2.44	0.42
1:A:1416:GLU:O	1:A:1417:VAL:C	2.61	0.42
1:B:409:HIS:O	1:B:413:LEU:HD23	2.18	0.42
1:B:420:VAL:HA	1:B:540:THR:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:540:THR:O	1:B:542:LEU:HG	2.20	0.42
1:B:732:ARG:H	1:B:747:SER:HA	1.85	0.42
1:B:965:LEU:HD23	1:B:965:LEU:HA	1.69	0.42
1:B:1346:PHE:O	1:B:1347:ALA:HB3	2.17	0.42
1:B:1435:THR:HG23	1:B:1437:SER:N	2.34	0.42
1:A:260:MET:O	1:A:261:GLN:C	2.61	0.42
1:A:295:LYS:CE	1:A:299:VAL:CG1	2.89	0.42
1:A:515:ARG:H	1:A:515:ARG:HG3	1.52	0.42
1:A:820:ARG:CB	1:A:821:PRO:CD	2.96	0.42
1:A:991:ASN:OD1	1:A:991:ASN:C	2.60	0.42
1:A:1463:LEU:HA	1:A:1463:LEU:HD23	1.66	0.42
1:B:204:PHE:CD2	1:B:204:PHE:C	2.97	0.42
1:B:248:GLU:C	1:B:250:ARG:H	2.27	0.42
1:B:533:LEU:HA	1:B:533:LEU:HD23	1.42	0.42
1:B:1076:GLY:O	1:B:1077:ARG:C	2.62	0.42
1:B:1281:VAL:HA	1:B:1301:SER:O	2.20	0.42
1:A:185:ALA:O	1:A:186:GLU:C	2.58	0.42
1:A:335:MET:HE3	1:A:342:VAL:HB	2.01	0.42
1:A:420:VAL:C	1:A:422:ASN:N	2.76	0.42
1:A:486:ALA:O	1:A:487:VAL:C	2.59	0.42
1:A:591:GLN:O	1:A:594:GLU:N	2.52	0.42
1:A:893:ARG:O	1:A:904:ASN:HB2	2.20	0.42
1:A:903:TRP:CD1	1:A:903:TRP:N	2.86	0.42
1:A:917:VAL:CG1	1:A:922:LEU:HD21	2.50	0.42
1:A:1121:ASP:OD1	1:A:1121:ASP:C	2.62	0.42
3:A:2474:FMN:H9	3:A:2474:FMN:H1'2	1.70	0.42
1:B:51:PRO:HD2	1:B:55:PHE:HD2	1.84	0.42
1:B:216:PHE:HA	1:B:217:PRO:HD3	1.76	0.42
1:B:254:PRO:CG	1:B:255:ALA:N	2.81	0.42
1:B:267:ILE:HG12	1:B:279:THR:HG21	2.01	0.42
1:B:375:ASP:OD2	1:B:377:THR:CB	2.61	0.42
1:B:376:GLU:O	1:B:377:THR:C	2.61	0.42
1:B:828:LEU:HD23	1:B:828:LEU:HA	1.79	0.42
1:B:885:GLY:O	1:B:887:GLY:N	2.52	0.42
1:B:1430:GLU:O	1:B:1431:HIS:C	2.62	0.42
1:A:47:HIS:ND1	1:A:47:HIS:C	2.77	0.42
1:A:143:GLN:CA	1:A:143:GLN:NE2	2.78	0.42
1:A:309:THR:HG21	1:A:314:LYS:HG3	2.02	0.42
1:A:688:PRO:C	1:A:690:GLU:N	2.77	0.42
1:A:691:LYS:O	1:A:691:LYS:HG3	2.20	0.42
1:A:952:MET:O	1:A:953:ILE:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:969:PRO:N	1:A:970:PRO:HD2	2.35	0.42
1:A:1394:VAL:CG1	1:A:1401:LEU:HD23	2.49	0.42
1:B:159:VAL:O	1:B:160:LYS:C	2.62	0.42
1:B:193:PRO:C	1:B:195:LEU:N	2.75	0.42
1:B:550:LEU:HD13	1:B:555:PHE:HA	2.01	0.42
1:B:787:ARG:H	1:B:787:ARG:HG3	1.23	0.42
1:B:1007:GLY:O	1:B:1008:THR:C	2.62	0.42
1:A:111:PRO:C	1:A:112:ILE:CG2	2.93	0.42
1:A:112:ILE:HA	1:A:191:PHE:O	2.20	0.42
1:A:447:LEU:CD1	1:A:451:GLN:CG	2.96	0.42
1:A:464:ILE:C	1:A:467:PRO:HD2	2.45	0.42
1:A:949:VAL:O	1:A:950:THR:O	2.37	0.42
1:A:985:TYR:CE1	1:A:1207:VAL:HG11	2.52	0.42
1:A:985:TYR:CD1	1:A:1207:VAL:HG11	2.54	0.42
1:A:1460:LYS:C	1:A:1462:MET:N	2.77	0.42
1:B:172:LEU:C	1:B:172:LEU:HD12	2.43	0.42
1:B:366:GLY:HA3	1:B:371:MET:HE2	2.01	0.42
1:B:730:LEU:C	1:B:748:GLY:N	2.78	0.42
1:B:826:ARG:NH1	1:B:826:ARG:CG	2.67	0.42
1:B:868:HIS:O	1:B:870:THR:N	2.53	0.42
1:B:878:ILE:HG21	1:B:878:ILE:HD13	1.66	0.42
1:B:1066:ARG:NH1	1:B:1089:GLU:OE2	2.53	0.42
1:B:1143:ALA:O	1:B:1144:GLU:C	2.58	0.42
1:B:1155:PHE:CZ	1:B:1167:LEU:HD21	2.54	0.42
1:B:1274:GLN:NE2	1:B:1294:ASP:H	2.18	0.42
1:B:1282:GLN:HA	1:B:1302:GLY:O	2.20	0.42
1:B:1417:VAL:CG1	1:B:1419:HIS:H	2.28	0.42
1:A:165:ASN:O	1:A:166:ASP:HB2	2.20	0.42
1:A:284:MET:CE	1:A:294:VAL:HG13	2.50	0.42
1:A:352:PRO:HB2	1:A:367:SER:O	2.20	0.42
1:A:386:GLY:H	1:A:389:GLU:CG	2.33	0.42
1:A:419:TRP:CE3	1:A:537:GLU:HA	2.55	0.42
1:A:653:HIS:O	1:A:655:PHE:N	2.53	0.42
1:A:770:VAL:O	1:A:770:VAL:HG12	2.19	0.42
1:A:1131:THR:HG21	1:A:1133:GLU:HB2	2.01	0.42
1:B:438:GLU:HG3	1:B:693:MET:CG	2.50	0.42
1:B:447:LEU:HD12	1:B:451:GLN:CD	2.45	0.42
1:B:505:GLN:HE22	1:B:1001:VAL:N	2.17	0.42
1:B:652:THR:O	1:B:653:HIS:C	2.63	0.42
1:A:37:ASP:OD1	1:A:38:GLY:N	2.53	0.42
1:A:376:GLU:HG3	1:A:1310:THR:OG1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:VAL:HG12	1:A:421:GLN:N	2.35	0.42
1:A:505:GLN:NE2	1:A:1000:LEU:HB3	2.35	0.42
1:A:583:ARG:NE	1:A:587:ARG:NH1	2.68	0.42
1:A:842:GLU:OE1	1:A:1156:ARG:NH1	2.52	0.42
1:A:990:ILE:O	1:A:1248:SER:OG	2.36	0.42
1:A:1022:LEU:HA	1:A:1068:ARG:O	2.19	0.42
1:A:1159:ASN:C	1:A:1161:VAL:N	2.76	0.42
1:A:1274:GLN:H	1:A:1274:GLN:HG2	1.35	0.42
1:A:1349:ARG:NH1	1:A:1367:TYR:O	2.52	0.42
1:A:1370:GLY:N	1:A:1389:GLY:O	2.53	0.42
1:B:105:TYR:HD1	1:B:105:TYR:H	1.68	0.42
1:B:253:HIS:CE1	1:B:254:PRO:CG	3.03	0.42
1:B:404:ARG:HB3	1:B:405:GLU:OE1	2.20	0.42
1:B:457:THR:HA	1:B:773:LEU:HB3	2.02	0.42
1:B:574:PRO:HG2	1:B:574:PRO:O	2.19	0.42
1:B:608:ASP:OD2	1:B:646:THR:HA	2.20	0.42
1:B:1358:GLU:HA	1:B:1376:LEU:HB2	2.02	0.42
1:A:250:ARG:HH21	1:A:639:PHE:HE1	1.62	0.41
1:A:468:MET:O	1:A:472:GLY:N	2.51	0.41
1:A:629:THR:O	1:A:631:LEU:N	2.53	0.41
1:A:656:ALA:O	1:A:657:VAL:C	2.61	0.41
1:A:696:TYR:CZ	1:A:700:ILE:HD11	2.55	0.41
1:A:821:PRO:HA	1:A:822:PRO:HD3	1.84	0.41
1:A:894:PHE:CD1	1:A:904:ASN:ND2	2.88	0.41
1:A:1246:LEU:O	1:A:1249:MET:HB2	2.20	0.41
1:A:1407:ASP:O	1:A:1409:SER:N	2.53	0.41
3:A:2474:FMN:HM71	3:A:2474:FMN:HM83	1.69	0.41
1:B:232:GLY:HA3	1:B:330:PRO:O	2.20	0.41
1:B:253:HIS:N	1:B:260:MET:HE1	2.19	0.41
1:B:319:TYR:O	1:B:320:CYS:C	2.61	0.41
1:B:420:VAL:C	1:B:422:ASN:H	2.28	0.41
1:B:632:ILE:HD13	1:B:632:ILE:HA	1.92	0.41
1:B:957:ARG:HD2	1:B:965:LEU:HD12	2.02	0.41
1:A:565:THR:CG2	1:A:603:HIS:HD2	2.33	0.41
1:A:608:ASP:O	1:A:609:GLU:C	2.62	0.41
1:A:1039:LYS:O	1:A:1040:PHE:CD1	2.73	0.41
1:A:1170:GLN:HB2	1:A:1183:LEU:HD12	2.02	0.41
1:A:1236:ARG:O	1:A:1238:THR:N	2.53	0.41
1:A:1349:ARG:HH11	1:A:1349:ARG:CG	2.22	0.41
1:A:1356:VAL:CG1	1:A:1431:HIS:CG	3.03	0.41
1:B:5:PHE:CZ	1:B:365:GLY:HA3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:ASP:HB2	1:B:210:ARG:O	2.20	0.41
1:B:250:ARG:NE	1:B:639:PHE:CE1	2.83	0.41
1:B:444:LYS:HE3	1:B:681:ARG:HH12	1.85	0.41
1:B:689:LEU:HD12	1:B:689:LEU:C	2.18	0.41
1:B:751:LEU:HA	1:B:751:LEU:HD23	1.49	0.41
1:A:139:VAL:CG1	1:A:140:SER:N	2.54	0.41
1:A:286:ARG:HA	1:A:286:ARG:HD3	1.60	0.41
1:A:435:LEU:C	1:A:437:GLY:N	2.77	0.41
1:A:631:LEU:HA	1:A:631:LEU:HD22	1.39	0.41
1:A:708:MET:O	1:A:709:SER:C	2.63	0.41
1:A:757:LYS:O	1:A:758:VAL:C	2.59	0.41
1:A:1061:LEU:C	1:A:1063:HIS:H	2.28	0.41
1:B:218:THR:CG2	1:B:221:LEU:H	2.30	0.41
1:B:244:MET:C	1:B:246:ALA:N	2.78	0.41
1:B:500:ARG:HD2	1:B:728:ILE:HG21	2.02	0.41
1:B:559:ARG:O	1:B:559:ARG:HG3	2.17	0.41
1:B:631:LEU:HD22	1:B:631:LEU:HA	1.74	0.41
1:B:970:PRO:O	1:B:970:PRO:HG2	2.19	0.41
1:B:987:LEU:HD23	1:B:987:LEU:HA	1.80	0.41
1:B:1222:LEU:N	1:B:1229:MET:HE2	2.32	0.41
1:A:78:LEU:HB3	1:A:79:PRO:HD2	2.00	0.41
1:A:253:HIS:H	1:A:260:MET:CE	2.34	0.41
1:A:273:ASP:N	1:A:273:ASP:OD1	2.54	0.41
1:A:358:THR:CB	1:A:360:ASP:OD1	2.65	0.41
1:A:447:LEU:CD1	1:A:670:LEU:HD21	2.44	0.41
1:A:855:THR:O	1:A:855:THR:CG2	2.69	0.41
1:A:978:GLU:HG3	1:A:979:ASP:H	1.86	0.41
1:A:1273:GLY:O	1:A:1274:GLN:C	2.63	0.41
1:A:1375:ILE:HD13	1:A:1375:ILE:HG21	1.75	0.41
1:A:1384:ALA:O	1:A:1385:ALA:C	2.57	0.41
1:B:87:GLU:O	1:B:90:ARG:N	2.54	0.41
1:B:552:THR:O	1:B:552:THR:HG22	2.19	0.41
1:B:588:ARG:HH11	1:B:588:ARG:HD3	1.68	0.41
1:B:677:GLU:O	1:B:678:ARG:C	2.62	0.41
1:B:807:TYR:O	1:B:810:PHE:HB3	2.19	0.41
1:B:856:PRO:HG2	1:B:1093:GLY:HA3	2.02	0.41
1:B:957:ARG:NH2	4:B:2475:AKG:O4	2.40	0.41
1:B:1252:ARG:HH11	1:B:1252:ARG:HD3	1.68	0.41
1:A:87:GLU:C	1:A:89:CYS:N	2.74	0.41
1:A:97:ILE:HA	1:A:151:ILE:HD13	2.01	0.41
1:A:282:GLU:O	1:A:283:VAL:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:THR:HG21	1:A:518:ARG:HD2	2.03	0.41
1:A:476:ILE:CG2	1:A:477:GLY:N	2.83	0.41
1:A:695:ASN:O	1:A:698:LYS:N	2.53	0.41
1:A:890:ASP:HA	1:A:891:PRO:HD3	1.85	0.41
1:A:956:LEU:HA	1:A:956:LEU:HD23	1.70	0.41
1:A:1354:THR:HG23	1:A:1372:THR:HB	2.01	0.41
1:B:175:ARG:NH2	1:B:203:ASP:OD2	2.54	0.41
1:B:292:PRO:O	1:B:293:MET:C	2.60	0.41
1:B:481:ASP:HB2	1:B:1038:ILE:HG22	2.02	0.41
1:B:504:SER:HB2	1:B:508:ASN:OD1	2.21	0.41
1:B:661:VAL:O	1:B:661:VAL:HG12	2.21	0.41
1:B:666:VAL:HG13	1:B:667:ASN:N	2.34	0.41
1:B:875:MET:SD	1:B:1139:PHE:CE2	3.14	0.41
1:B:1135:VAL:O	1:B:1138:LEU:N	2.54	0.41
1:B:1146:VAL:C	1:B:1148:GLU:N	2.77	0.41
1:B:1359:GLY:O	1:B:1360:CYS:HB3	2.20	0.41
1:B:1412:PHE:CD1	1:B:1412:PHE:N	2.88	0.41
1:B:1447:TRP:O	1:B:1448:ALA:C	2.63	0.41
1:A:189:THR:CG2	1:A:190:THR:N	2.63	0.41
1:A:443:ASP:OD2	1:A:445:ALA:HB3	2.21	0.41
1:A:555:PHE:CD1	1:A:556:ARG:N	2.89	0.41
1:A:742:MET:HE3	1:A:742:MET:HB2	1.84	0.41
1:A:1057:THR:CG2	1:A:1190:VAL:HG11	2.50	0.41
1:A:1162:ILE:C	1:A:1164:ARG:H	2.27	0.41
1:A:1349:ARG:HG2	1:A:1349:ARG:NH1	2.31	0.41
1:B:860:MET:HE1	1:B:893:ARG:NH1	2.35	0.41
1:B:1161:VAL:O	1:B:1161:VAL:HG12	2.21	0.41
1:B:1216:VAL:HG13	1:B:1249:MET:HE2	1.96	0.41
1:A:193:PRO:O	1:A:196:LEU:N	2.52	0.41
1:A:198:GLU:H	1:A:198:GLU:HG3	1.72	0.41
1:A:309:THR:HB	1:A:314:LYS:CE	2.51	0.41
1:A:447:LEU:HD11	1:A:451:GLN:CD	2.46	0.41
1:A:522:LEU:O	1:A:523:LYS:C	2.63	0.41
1:A:1235:ALA:HA	1:A:1239:GLN:OE1	2.21	0.41
1:B:325:GLU:HA	1:B:326:PRO:HD3	1.92	0.41
1:B:526:LEU:N	1:B:526:LEU:CD1	2.64	0.41
1:B:739:PHE:HB3	1:B:740:PRO:HD2	2.03	0.41
1:B:919:ALA:CB	1:B:1281:VAL:CG1	2.98	0.41
1:B:986:ASP:OD2	1:B:1298:LYS:NZ	2.48	0.41
1:B:1058:LEU:HA	1:B:1058:LEU:HD23	1.64	0.41
1:B:1219:ALA:HA	1:B:1229:MET:HE3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1317:THR:HG22	1:B:1318:ASN:CA	2.46	0.41
1:A:324:MET:HE2	1:A:327:TRP:NE1	2.31	0.41
1:A:406:LEU:O	1:A:409:HIS:HB3	2.21	0.41
1:A:501:GLN:OE1	1:A:710:LYS:NZ	2.47	0.41
1:A:672:GLN:HG3	1:A:693:MET:SD	2.60	0.41
1:A:720:ARG:C	1:A:722:GLY:H	2.29	0.41
1:A:728:ILE:HD12	1:A:1047:MET:HE1	2.00	0.41
1:A:864:SER:HB3	1:A:1116:GLY:O	2.21	0.41
1:B:30:HIS:HE2	1:B:31:ARG:HD2	1.86	0.41
1:B:802:VAL:CG2	1:B:1134:LYS:O	2.69	0.41
1:A:52:GLN:HE21	1:A:52:GLN:HB3	1.56	0.41
1:A:77:PHE:HB3	1:A:126:PRO:CB	2.50	0.41
1:A:149:TYR:HE2	1:A:263:LEU:HD21	1.86	0.41
1:A:173:SER:HG	1:A:176:SER:H	1.65	0.41
1:A:303:LEU:HD11	1:A:314:LYS:HG2	2.01	0.41
1:A:350:LEU:HD23	1:A:350:LEU:HA	1.55	0.41
1:A:452:GLN:CG	1:A:764:THR:HG22	2.48	0.41
1:A:454:PHE:CD2	1:A:648:GLU:CB	3.00	0.41
1:A:562:MET:HE3	1:A:566:ALA:CB	2.38	0.41
1:A:575:VAL:C	1:A:577:GLY:N	2.77	0.41
1:A:706:LYS:NZ	1:A:1034:PRO:HG2	2.36	0.41
1:A:784:SER:HB3	1:A:785:GLY:H	1.66	0.41
1:A:842:GLU:O	1:A:1156:ARG:HG2	2.21	0.41
1:A:843:VAL:CG1	1:A:844:GLU:H	2.31	0.41
1:A:862:ALA:O	1:A:1118:CYS:HB3	2.18	0.41
1:A:969:PRO:CD	1:A:970:PRO:CD	2.99	0.41
1:A:1044:PRO:HG2	1:A:1047:MET:HE3	2.03	0.41
1:A:1059:ASN:N	1:A:1059:ASN:HD22	2.19	0.41
1:A:1093:GLY:O	1:A:1094:THR:C	2.63	0.41
1:A:1458:VAL:HA	1:A:1459:PRO:HD3	1.66	0.41
1:A:1466:LEU:O	1:A:1468:VAL:N	2.54	0.41
1:B:240:ASN:HB3	1:B:327:TRP:CZ2	2.56	0.41
1:B:438:GLU:OE2	1:B:553:ALA:HB3	2.20	0.41
1:B:609:GLU:C	1:B:611:MET:N	2.77	0.41
1:B:782:ARG:C	1:B:784:SER:H	2.28	0.41
1:B:937:LYS:N	1:B:938:PRO:HD3	2.35	0.41
1:B:974:ILE:HD13	1:B:974:ILE:HG21	1.74	0.41
1:B:999:LYS:CG	1:B:1022:LEU:CD2	2.64	0.41
1:B:1009:ILE:C	1:B:1011:ALA:N	2.78	0.41
1:B:1250:VAL:HG13	1:B:1259:LEU:HD12	2.01	0.41
1:B:1335:LYS:HA	1:B:1354:THR:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1435:THR:CG2	1:B:1437:SER:CB	2.99	0.41
1:A:5:PHE:CD1	1:A:5:PHE:C	2.99	0.41
1:A:266:VAL:HG12	1:A:279:THR:HG22	1.94	0.41
1:A:461:MET:CE	1:A:461:MET:HA	2.51	0.41
1:A:513:SER:CA	1:A:520:MET:HE2	2.51	0.41
1:A:864:SER:HB3	1:A:1117:VAL:O	2.21	0.41
1:A:930:ILE:CD1	1:A:983:LEU:HD13	2.43	0.41
1:B:10:ASP:OD1	1:B:10:ASP:C	2.63	0.41
1:B:295:LYS:CG	1:B:390:MET:HE1	2.51	0.41
1:B:807:TYR:OH	1:B:1148:GLU:OE2	2.31	0.41
1:B:1099:ALA:C	1:B:1101:GLY:N	2.78	0.41
1:B:1153:LEU:HD23	1:B:1153:LEU:HA	1.42	0.41
1:B:1435:THR:O	1:B:1436:GLN:C	2.61	0.41
1:B:1446:ASP:O	1:B:1447:TRP:C	2.64	0.41
1:A:42:ASP:OD1	1:A:212:SER:OG	2.38	0.40
1:A:485:ILE:HD13	1:A:485:ILE:HG21	1.72	0.40
1:A:503:PHE:CE2	1:A:938:PRO:HB3	2.56	0.40
1:A:622:LEU:HA	1:A:739:PHE:HE1	1.86	0.40
1:A:677:GLU:O	1:A:678:ARG:C	2.64	0.40
1:A:1059:ASN:O	1:A:1060:ARG:C	2.63	0.40
1:A:1289:MET:CE	1:A:1289:MET:N	2.76	0.40
1:A:1458:VAL:CG1	1:A:1459:PRO:HD2	2.48	0.40
1:A:1468:VAL:HG12	1:A:1468:VAL:O	2.15	0.40
1:B:120:LYS:HE2	1:B:120:LYS:HA	2.00	0.40
1:B:240:ASN:HB3	1:B:327:TRP:CH2	2.56	0.40
1:B:387:PRO:HD3	1:B:1344:GLU:CD	2.42	0.40
1:B:410:LEU:HD12	1:B:410:LEU:N	2.36	0.40
1:B:561:TYR:CD1	1:B:561:TYR:O	2.74	0.40
1:B:636:LEU:O	1:B:637:ARG:C	2.65	0.40
1:B:853:PHE:CZ	1:B:1079:ILE:HD13	2.55	0.40
1:A:185:ALA:C	1:A:187:GLN:N	2.76	0.40
1:A:244:MET:HB2	1:A:244:MET:HE3	1.34	0.40
1:A:320:CYS:O	1:A:322:SER:N	2.54	0.40
1:A:464:ILE:CD1	1:A:779:TYR:CZ	2.94	0.40
1:A:492:TYR:CD2	1:A:761:GLN:HG2	2.57	0.40
1:A:528:ASN:O	1:A:529:LEU:HD23	2.21	0.40
1:A:628:HIS:O	1:A:629:THR:C	2.64	0.40
1:A:635:ASN:O	1:A:636:LEU:HD13	2.20	0.40
1:A:1131:THR:CG2	1:A:1133:GLU:HB2	2.52	0.40
1:A:1262:GLY:O	1:A:1263:HIS:C	2.63	0.40
1:B:80:ARG:O	1:B:80:ARG:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:GLU:H	1:B:186:GLU:HG3	1.05	0.40
1:B:280:VAL:O	1:B:281:PHE:C	2.62	0.40
1:B:330:PRO:HA	1:B:350:LEU:HB2	2.03	0.40
1:B:406:LEU:O	1:B:409:HIS:HB3	2.21	0.40
1:B:450:ARG:C	1:B:452:GLN:N	2.79	0.40
1:B:621:ILE:HG12	1:B:657:VAL:HG12	2.04	0.40
1:B:657:VAL:O	1:B:661:VAL:HG23	2.22	0.40
1:B:787:ARG:HH12	1:B:821:PRO:CB	2.34	0.40
1:B:1062:ARG:HH11	1:B:1062:ARG:HD3	1.40	0.40
1:B:1147:ARG:HH11	1:B:1147:ARG:HD3	1.75	0.40
1:B:1245:ARG:O	1:B:1246:LEU:C	2.63	0.40
1:A:183:PHE:HE1	1:A:188:LEU:HA	1.79	0.40
1:A:318:GLN:O	1:A:322:SER:OG	2.40	0.40
1:A:353:MET:HE2	1:A:366:GLY:N	2.36	0.40
1:A:390:MET:HG3	1:A:406:LEU:HD23	2.02	0.40
1:A:606:LEU:O	1:A:607:THR:HG22	2.21	0.40
1:A:836:ALA:HB1	1:A:837:PRO:CD	2.52	0.40
1:A:1401:LEU:HD11	1:A:1405:ILE:CD1	2.50	0.40
1:B:325:GLU:H	1:B:325:GLU:HG3	1.48	0.40
1:B:536:ASP:OD1	1:B:538:THR:N	2.54	0.40
1:B:547:SER:C	1:B:549:VAL:N	2.77	0.40
1:B:575:VAL:HG13	1:B:759:LEU:HD22	2.03	0.40
1:B:1222:LEU:HD12	1:B:1222:LEU:O	2.20	0.40
1:B:1357:VAL:CG1	1:B:1359:GLY:H	2.35	0.40
1:A:355:TYR:CZ	1:A:383:GLY:HA3	2.56	0.40
1:A:595:ASP:O	1:A:596:ALA:O	2.38	0.40
1:A:833:SER:HB2	1:A:1167:LEU:HD22	2.03	0.40
1:A:1374:VAL:HG12	1:A:1375:ILE:H	1.86	0.40
1:A:1395:TYR:HD2	1:A:1454:PHE:CE1	2.39	0.40
1:B:56:LYS:CG	1:B:71:LEU:HD22	2.48	0.40
1:B:246:ALA:O	1:B:247:HIS:C	2.61	0.40
1:B:298:LEU:HD23	1:B:324:MET:HG2	2.04	0.40
1:B:313:HIS:CD2	1:B:313:HIS:N	2.89	0.40
1:B:412:THR:O	1:B:412:THR:CG2	2.68	0.40
1:B:770:VAL:O	1:B:770:VAL:CG1	2.67	0.40
1:B:942:GLY:HA2	4:B:2475:AKG:O5	2.20	0.40
1:B:969:PRO:N	1:B:970:PRO:CD	2.84	0.40
1:B:1354:THR:HA	1:B:1372:THR:O	2.21	0.40
1:A:6:ILE:HB	1:A:205:ALA:HB3	2.03	0.40
1:A:148:LEU:O	1:A:151:ILE:HB	2.21	0.40
1:A:233:GLU:O	1:A:329:GLY:HA3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:894:PHE:CZ	1:A:924:GLN:HG3	2.56	0.40
1:A:1108:CYS:SG	5:A:2476:F3S:S2	3.20	0.40
1:A:1150:LEU:HD21	1:A:1158:LEU:HD12	2.04	0.40
1:A:1400:SER:C	1:A:1402:PRO:HD2	2.46	0.40
1:A:1406:ASN:OD1	1:A:1406:ASN:C	2.64	0.40
1:A:1427:LEU:O	1:A:1428:ILE:C	2.62	0.40
1:B:117:ILE:HD12	1:B:117:ILE:HG21	1.49	0.40
1:B:230:HIS:CE1	1:B:234:ILE:HG13	2.55	0.40
1:B:242:ASN:C	1:B:244:MET:H	2.28	0.40
1:B:297:MET:HE2	1:B:297:MET:HB3	1.67	0.40
1:B:495:LEU:O	1:B:497:HIS:N	2.55	0.40
1:B:948:LYS:C	1:B:950:THR:N	2.78	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1444/1479 (98%)	1152 (80%)	227 (16%)	65 (4%)	2	12
1	B	1444/1479 (98%)	1170 (81%)	211 (15%)	63 (4%)	2	12
All	All	2888/2958 (98%)	2322 (80%)	438 (15%)	128 (4%)	2	12

All (128) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	444	LYS
1	A	451	GLN
1	A	705	LEU
1	A	712	GLY
1	A	950	THR

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Mol	Chain	Res	Type
1	A	1062	ARG
1	A	1227	GLU
1	A	1339	ALA
1	A	1375	ILE
1	A	1376	LEU
1	A	1388	THR
1	A	1394	VAL
1	A	1408	GLU
1	A	1461	GLU
1	A	1467	GLU
1	B	249	THR
1	B	255	ALA
1	B	418	LYS
1	B	561	TYR
1	B	705	LEU
1	B	740	PRO
1	B	950	THR
1	B	1164	ARG
1	B	1467	GLU
1	A	53	LYS
1	A	54	PHE
1	A	249	THR
1	A	370	GLY
1	A	561	TYR
1	A	599	GLY
1	A	663	ALA
1	A	709	SER
1	A	745	ARG
1	A	939	GLY
1	A	1042	GLY
1	A	1160	GLU
1	A	1164	ARG
1	A	1317	THR
1	A	1439	PHE
1	A	1454	PHE
1	A	1460	LYS
1	B	25	LEU
1	B	421	GLN
1	B	444	LYS
1	B	451	GLN
1	B	562	MET
1	B	577	GLY

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Mol	Chain	Res	Type
1	B	610	ALA
1	B	747	SER
1	B	764	THR
1	B	868	HIS
1	B	884	SER
1	B	886	GLU
1	B	1160	GLU
1	B	1381	ASP
1	B	1408	GLU
1	B	1421	GLU
1	B	1432	VAL
1	B	1433	THR
1	B	1452	THR
1	B	1461	GLU
1	A	24	ALA
1	A	377	THR
1	A	432	THR
1	A	433	ALA
1	A	629	THR
1	A	740	PRO
1	A	974	ILE
1	A	1361	GLY
1	A	1381	ASP
1	A	1407	ASP
1	A	1438	ARG
1	B	663	ALA
1	B	721	GLY
1	B	745	ARG
1	B	869	GLY
1	B	1062	ARG
1	B	1071	GLY
1	B	1114	PRO
1	B	1142	LEU
1	B	1339	ALA
1	B	1438	ARG
1	B	1439	PHE
1	A	208	HIS
1	A	245	LYS
1	A	421	GLN
1	A	450	ARG
1	A	492	TYR
1	A	553	ALA

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Mol	Chain	Res	Type
1	A	844	GLU
1	A	915	PHE
1	B	326	PRO
1	B	475	ALA
1	B	496	HIS
1	B	856	PRO
1	B	974	ILE
1	B	1376	LEU
1	B	1407	ASP
1	B	1424	LEU
1	A	69	ASN
1	A	521	SER
1	A	654	TYR
1	A	962	GLY
1	A	1395	TYR
1	B	254	PRO
1	B	388	GLY
1	B	450	ARG
1	B	559	ARG
1	B	1078	ASP
1	A	217	PRO
1	B	290	THR
1	B	619	PRO
1	B	780	ARG
1	A	707	ILE
1	A	1185	PRO
1	B	61	VAL
1	A	619	PRO
1	A	1071	GLY
1	A	1261	PRO
1	A	1389	GLY
1	B	116	ILE
1	B	455	GLY
1	B	1394	VAL
1	A	372	VAL
1	B	774	PRO
1	B	953	ILE
1	B	657	VAL

5.3.2 Protein sidechains [i](#)

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	1184/1206 (98%)	933 (79%)	251 (21%)	1	6
1	B	1184/1206 (98%)	938 (79%)	246 (21%)	1	7
All	All	2368/2412 (98%)	1871 (79%)	497 (21%)	1	6

All (497) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	CYS
1	A	3	VAL
1	A	34	VAL
1	A	35	ASP
1	A	37	ASP
1	A	39	LYS
1	A	40	THR
1	A	47	HIS
1	A	52	GLN
1	A	59	VAL
1	A	62	ILE
1	A	68	ASP
1	A	69	ASN
1	A	76	VAL
1	A	78	LEU
1	A	80	ARG
1	A	81	ILE
1	A	109	GLN
1	A	112	ILE
1	A	113	ASN
1	A	117	ILE
1	A	120	LYS
1	A	131	ILE
1	A	142	GLU
1	A	143	GLN
1	A	146	LEU
1	A	156	GLU

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Mol	Chain	Res	Type
1	A	162	GLU
1	A	177	ILE
1	A	184	LEU
1	A	186	GLU
1	A	188	LEU
1	A	189	THR
1	A	196	LEU
1	A	198	GLU
1	A	207	TYR
1	A	209	GLN
1	A	210	ARG
1	A	215	THR
1	A	218	THR
1	A	227	MET
1	A	228	LEU
1	A	235	ASN
1	A	242	ASN
1	A	244	MET
1	A	249	THR
1	A	252	GLU
1	A	254	PRO
1	A	258	THR
1	A	261	GLN
1	A	263	LEU
1	A	267	ILE
1	A	269	VAL
1	A	279	THR
1	A	286	ARG
1	A	299	VAL
1	A	312	ASN
1	A	316	LEU
1	A	322	SER
1	A	335	MET
1	A	336	THR
1	A	342	VAL
1	A	347	ARG
1	A	351	ARG
1	A	353	MET
1	A	355	TYR
1	A	357	ILE
1	A	362	LEU
1	A	367	SER

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Mol	Chain	Res	Type
1	A	368	GLU
1	A	372	VAL
1	A	377	THR
1	A	380	ILE
1	A	390	MET
1	A	397	SER
1	A	405	GLU
1	A	413	LEU
1	A	417	ASP
1	A	420	VAL
1	A	429	LEU
1	A	430	VAL
1	A	439	PRO
1	A	440	SER
1	A	441	ASP
1	A	447	LEU
1	A	449	ARG
1	A	458	MET
1	A	461	MET
1	A	463	LEU
1	A	465	LEU
1	A	476	ILE
1	A	479	MET
1	A	483	SER
1	A	487	VAL
1	A	495	LEU
1	A	505	GLN
1	A	509	PRO
1	A	519	VAL
1	A	520	MET
1	A	525	ARG
1	A	526	LEU
1	A	529	LEU
1	A	534	ASP
1	A	537	GLU
1	A	544	GLN
1	A	559	ARG
1	A	564	ASP
1	A	569	ILE
1	A	572	THR
1	A	584	ASP
1	A	606	LEU

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Mol	Chain	Res	Type
1	A	607	THR
1	A	621	ILE
1	A	631	LEU
1	A	634	SER
1	A	636	LEU
1	A	637	ARG
1	A	638	THR
1	A	640	THR
1	A	642	LEU
1	A	644	VAL
1	A	650	LEU
1	A	658	LEU
1	A	665	THR
1	A	670	LEU
1	A	673	GLU
1	A	678	ARG
1	A	704	LEU
1	A	705	LEU
1	A	715	VAL
1	A	724	ASN
1	A	731	SER
1	A	734	LEU
1	A	746	ILE
1	A	764	THR
1	A	768	GLU
1	A	786	ASP
1	A	787	ARG
1	A	794	VAL
1	A	795	ILE
1	A	803	THR
1	A	806	SER
1	A	812	LYS
1	A	820	ARG
1	A	824	GLN
1	A	826	ARG
1	A	831	LEU
1	A	833	SER
1	A	842	GLU
1	A	850	ARG
1	A	851	LYS
1	A	855	THR
1	A	863	LEU

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Mol	Chain	Res	Type
1	A	875	MET
1	A	884	SER
1	A	889	GLU
1	A	912	SER
1	A	934	GLN
1	A	937	LYS
1	A	950	THR
1	A	952	MET
1	A	953	ILE
1	A	958	HIS
1	A	960	THR
1	A	966	ILE
1	A	970	PRO
1	A	978	GLU
1	A	982	GLN
1	A	983	LEU
1	A	1003	ARG
1	A	1008	THR
1	A	1015	LYS
1	A	1036	THR
1	A	1043	LEU
1	A	1057	THR
1	A	1058	LEU
1	A	1059	ASN
1	A	1062	ARG
1	A	1065	VAL
1	A	1066	ARG
1	A	1075	THR
1	A	1077	ARG
1	A	1085	LEU
1	A	1104	MET
1	A	1109	HIS
1	A	1119	VAL
1	A	1121	ASP
1	A	1122	ASP
1	A	1124	LEU
1	A	1131	THR
1	A	1142	LEU
1	A	1145	GLU
1	A	1157	SER
1	A	1161	VAL
1	A	1164	ARG

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Mol	Chain	Res	Type
1	A	1170	GLN
1	A	1171	VAL
1	A	1190	VAL
1	A	1206	GLU
1	A	1207	VAL
1	A	1211	LEU
1	A	1220	ARG
1	A	1222	LEU
1	A	1225	GLU
1	A	1229	MET
1	A	1246	LEU
1	A	1253	LYS
1	A	1261	PRO
1	A	1264	ILE
1	A	1267	ARG
1	A	1269	ARG
1	A	1271	THR
1	A	1274	GLN
1	A	1289	MET
1	A	1291	ASP
1	A	1301	SER
1	A	1304	THR
1	A	1308	ARG
1	A	1310	THR
1	A	1314	PRO
1	A	1317	THR
1	A	1318	ASN
1	A	1349	ARG
1	A	1355	VAL
1	A	1357	VAL
1	A	1360	CYS
1	A	1369	THR
1	A	1374	VAL
1	A	1379	VAL
1	A	1381	ASP
1	A	1382	ASN
1	A	1388	THR
1	A	1394	VAL
1	A	1398	ASP
1	A	1400	SER
1	A	1401	LEU
1	A	1402	PRO

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Mol	Chain	Res	Type
1	A	1408	GLU
1	A	1410	VAL
1	A	1419	HIS
1	A	1421	GLU
1	A	1422	SER
1	A	1424	LEU
1	A	1425	LYS
1	A	1428	ILE
1	A	1449	ARG
1	A	1452	THR
1	A	1461	GLU
1	A	1466	LEU
1	A	1470	VAL
1	A	1471	HIS
1	B	3	VAL
1	B	34	VAL
1	B	35	ASP
1	B	37	ASP
1	B	40	THR
1	B	47	HIS
1	B	59	VAL
1	B	62	ILE
1	B	68	ASP
1	B	76	VAL
1	B	80	ARG
1	B	81	ILE
1	B	92	ILE
1	B	109	GLN
1	B	113	ASN
1	B	117	ILE
1	B	120	LYS
1	B	143	GLN
1	B	146	LEU
1	B	156	GLU
1	B	173	SER
1	B	184	LEU
1	B	186	GLU
1	B	188	LEU
1	B	189	THR
1	B	198	GLU
1	B	209	GLN
1	B	210	ARG

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Mol	Chain	Res	Type
1	B	215	THR
1	B	218	THR
1	B	227	MET
1	B	235	ASN
1	B	241	VAL
1	B	242	ASN
1	B	247	HIS
1	B	249	THR
1	B	254	PRO
1	B	258	THR
1	B	260	MET
1	B	261	GLN
1	B	263	LEU
1	B	269	VAL
1	B	274	SER
1	B	279	THR
1	B	286	ARG
1	B	290	THR
1	B	297	MET
1	B	299	VAL
1	B	308	THR
1	B	312	ASN
1	B	316	LEU
1	B	317	ILE
1	B	322	SER
1	B	325	GLU
1	B	347	ARG
1	B	351	ARG
1	B	353	MET
1	B	362	LEU
1	B	367	SER
1	B	368	GLU
1	B	377	THR
1	B	380	ILE
1	B	385	LEU
1	B	389	GLU
1	B	390	MET
1	B	397	SER
1	B	402	ARG
1	B	405	GLU
1	B	412	THR
1	B	413	LEU

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Mol	Chain	Res	Type
1	B	417	ASP
1	B	420	VAL
1	B	422	ASN
1	B	423	THR
1	B	429	LEU
1	B	430	VAL
1	B	439	PRO
1	B	447	LEU
1	B	449	ARG
1	B	461	MET
1	B	462	GLU
1	B	468	MET
1	B	481	ASP
1	B	483	SER
1	B	487	VAL
1	B	491	LYS
1	B	495	LEU
1	B	500	ARG
1	B	501	GLN
1	B	519	VAL
1	B	520	MET
1	B	522	LEU
1	B	524	THR
1	B	526	LEU
1	B	534	ASP
1	B	537	GLU
1	B	538	THR
1	B	542	LEU
1	B	555	PHE
1	B	559	ARG
1	B	564	ASP
1	B	569	ILE
1	B	570	ASP
1	B	572	THR
1	B	584	ASP
1	B	592	GLU
1	B	593	THR
1	B	606	LEU
1	B	607	THR
1	B	608	ASP
1	B	621	ILE
1	B	622	LEU

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Mol	Chain	Res	Type
1	B	631	LEU
1	B	636	LEU
1	B	637	ARG
1	B	640	THR
1	B	642	LEU
1	B	658	LEU
1	B	659	ILE
1	B	665	THR
1	B	670	LEU
1	B	673	GLU
1	B	681	ARG
1	B	690	GLU
1	B	704	LEU
1	B	714	SER
1	B	717	SER
1	B	731	SER
1	B	746	ILE
1	B	751	LEU
1	B	764	THR
1	B	770	VAL
1	B	771	VAL
1	B	786	ASP
1	B	787	ARG
1	B	794	VAL
1	B	805	ASP
1	B	817	VAL
1	B	820	ARG
1	B	823	MET
1	B	824	GLN
1	B	826	ARG
1	B	833	SER
1	B	841	ASP
1	B	849	ILE
1	B	850	ARG
1	B	855	THR
1	B	859	SER
1	B	860	MET
1	B	884	SER
1	B	889	GLU
1	B	898	LYS
1	B	912	SER
1	B	918	THR

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Mol	Chain	Res	Type
1	B	934	GLN
1	B	937	LYS
1	B	950	THR
1	B	952	MET
1	B	958	HIS
1	B	960	THR
1	B	966	ILE
1	B	978	GLU
1	B	983	LEU
1	B	1001	VAL
1	B	1002	SER
1	B	1003	ARG
1	B	1008	THR
1	B	1015	LYS
1	B	1030	THR
1	B	1043	LEU
1	B	1050	SER
1	B	1057	THR
1	B	1058	LEU
1	B	1059	ASN
1	B	1062	ARG
1	B	1064	ARG
1	B	1065	VAL
1	B	1077	ARG
1	B	1079	ILE
1	B	1090	PHE
1	B	1098	ILE
1	B	1104	MET
1	B	1105	VAL
1	B	1109	HIS
1	B	1114	PRO
1	B	1119	VAL
1	B	1121	ASP
1	B	1122	ASP
1	B	1124	LEU
1	B	1129	VAL
1	B	1131	THR
1	B	1142	LEU
1	B	1145	GLU
1	B	1146	VAL
1	B	1147	ARG
1	B	1157	SER

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Mol	Chain	Res	Type
1	B	1161	VAL
1	B	1167	LEU
1	B	1169	HIS
1	B	1170	GLN
1	B	1171	VAL
1	B	1186	ARG
1	B	1190	VAL
1	B	1207	VAL
1	B	1229	MET
1	B	1237	ASN
1	B	1238	THR
1	B	1245	ARG
1	B	1246	LEU
1	B	1247	SER
1	B	1253	LYS
1	B	1261	PRO
1	B	1264	ILE
1	B	1265	THR
1	B	1269	ARG
1	B	1271	THR
1	B	1289	MET
1	B	1298	LYS
1	B	1308	ARG
1	B	1317	THR
1	B	1318	ASN
1	B	1344	GLU
1	B	1349	ARG
1	B	1355	VAL
1	B	1357	VAL
1	B	1360	CYS
1	B	1369	THR
1	B	1379	VAL
1	B	1381	ASP
1	B	1388	THR
1	B	1397	LEU
1	B	1398	ASP
1	B	1400	SER
1	B	1401	LEU
1	B	1408	GLU
1	B	1409	SER
1	B	1410	VAL
1	B	1421	GLU

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Mol	Chain	Res	Type
1	B	1422	SER
1	B	1435	THR
1	B	1449	ARG
1	B	1452	THR
1	B	1465	ARG
1	B	1466	LEU
1	B	1470	VAL
1	B	1471	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	A	47	HIS
1	A	52	GLN
1	A	113	ASN
1	A	143	GLN
1	A	163	GLN
1	A	209	GLN
1	A	214	ASN
1	A	230	HIS
1	A	235	ASN
1	A	240	ASN
1	A	242	ASN
1	A	261	GLN
1	A	313	HIS
1	A	318	GLN
1	A	321	ASN
1	A	452	GLN
1	A	505	GLN
1	A	643	ASN
1	A	653	HIS
1	A	724	ASN
1	A	738	HIS
1	A	755	GLN
1	A	788	HIS
1	A	796	HIS
1	A	800	GLN
1	A	824	GLN
1	A	924	GLN
1	A	943	GLN
1	A	982	GLN

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Mol	Chain	Res	Type
1	A	1026	ASN
1	A	1059	ASN
1	A	1205	ASN
1	A	1230	GLN
1	A	1274	GLN
1	A	1282	GLN
1	A	1293	ASN
1	A	1318	ASN
1	A	1320	ASN
1	A	1363	ASN
1	A	1382	ASN
1	A	1419	HIS
1	A	1471	HIS
1	B	30	HIS
1	B	47	HIS
1	B	52	GLN
1	B	113	ASN
1	B	143	GLN
1	B	165	ASN
1	B	208	HIS
1	B	214	ASN
1	B	235	ASN
1	B	240	ASN
1	B	242	ASN
1	B	247	HIS
1	B	321	ASN
1	B	422	ASN
1	B	452	GLN
1	B	497	HIS
1	B	505	GLN
1	B	544	GLN
1	B	643	ASN
1	B	653	HIS
1	B	738	HIS
1	B	755	GLN
1	B	762	HIS
1	B	788	HIS
1	B	800	GLN
1	B	824	GLN
1	B	943	GLN
1	B	982	GLN
1	B	1035	GLN

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Mol	Chain	Res	Type
1	B	1059	ASN
1	B	1137	ASN
1	B	1205	ASN
1	B	1274	GLN
1	B	1318	ASN
1	B	1363	ASN
1	B	1382	ASN
1	B	1419	HIS
1	B	1471	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	AKG	B	2475	-	9,9,9	3.58	4 (44%)	11,11,11	2.77	4 (36%)
2	OMT	B	2473	-	9,10,10	4.56	5 (55%)	9,14,14	6.31	5 (55%)
3	FMN	B	2474	-	33,33,33	1.38	4 (12%)	48,50,50	2.69	20 (41%)
3	FMN	A	2474	-	33,33,33	1.49	5 (15%)	48,50,50	2.80	18 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OMT	A	2473	-	9,10,10	4.70	5 (55%)	9,14,14	5.25	6 (66%)
4	AKG	A	2475	-	9,9,9	3.16	4 (44%)	11,11,11	2.99	4 (36%)
5	F3S	B	2476	1	0,9,9	-	-	-	-	-
5	F3S	A	2476	1	0,9,9	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AKG	B	2475	-	-	1/9/9/9	-
2	OMT	B	2473	-	-	5/10/10/10	-
3	FMN	B	2474	-	-	5/18/18/18	0/3/3/3
3	FMN	A	2474	-	-	7/18/18/18	0/3/3/3
2	OMT	A	2473	-	-	4/10/10/10	-
4	AKG	A	2475	-	-	2/9/9/9	-
5	F3S	B	2476	1	-	-	0/3/3/3
5	F3S	A	2476	1	-	-	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2473	OMT	CB-CG	-7.95	1.45	1.52
2	B	2473	OMT	CG-SD	-7.13	1.69	1.78
2	A	2473	OMT	CG-SD	-6.93	1.69	1.78
2	B	2473	OMT	CB-CG	-6.84	1.46	1.52
2	B	2473	OMT	OD1-SD	6.68	1.57	1.44
4	B	2475	AKG	O5-C2	6.47	1.36	1.23
4	B	2475	AKG	O1-C1	6.25	1.38	1.22
2	A	2473	OMT	OD2-SD	6.09	1.56	1.44
4	A	2475	AKG	O5-C2	5.97	1.35	1.23
2	B	2473	OMT	OD2-SD	5.49	1.55	1.44
2	A	2473	OMT	OD1-SD	5.19	1.54	1.44
4	A	2475	AKG	O1-C1	4.98	1.34	1.22
4	A	2475	AKG	O3-C5	4.32	1.36	1.22
2	A	2473	OMT	O-C	4.30	1.34	1.22
4	B	2475	AKG	O3-C5	4.21	1.35	1.22
2	B	2473	OMT	O-C	3.40	1.32	1.22
3	B	2474	FMN	C10-N1	3.28	1.39	1.33
4	B	2475	AKG	C3-C2	3.09	1.54	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2474	FMN	C9A-N10	-3.04	1.35	1.41
4	A	2475	AKG	C3-C2	2.91	1.54	1.51
3	A	2474	FMN	C9A-C5A	-2.87	1.36	1.41
3	A	2474	FMN	C4A-N5	2.77	1.36	1.30
3	A	2474	FMN	C10-N1	2.68	1.38	1.33
3	A	2474	FMN	O4'-C4'	-2.53	1.38	1.43
3	B	2474	FMN	C9A-C5A	-2.53	1.37	1.41
3	B	2474	FMN	C4A-N5	2.41	1.36	1.30
3	A	2474	FMN	C9A-N10	-2.32	1.37	1.41

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2473	OMT	OD2-SD-CG	-16.19	96.65	108.33
2	A	2473	OMT	OD2-SD-CE	-12.57	97.19	108.87
3	B	2474	FMN	C4'-C3'-C2'	-8.97	98.65	113.57
3	A	2474	FMN	O5'-P-O1P	-8.15	84.41	106.44
4	B	2475	AKG	C4-C3-C2	-7.61	98.63	112.91
4	A	2475	AKG	C4-C3-C2	-7.19	99.42	112.91
2	B	2473	OMT	OD1-SD-CE	-6.85	102.50	108.87
3	B	2474	FMN	O4'-C4'-C3'	-6.78	93.39	109.25
3	A	2474	FMN	O4'-C4'-C5'	-6.39	95.89	109.99
2	A	2473	OMT	CE-SD-CG	6.04	127.72	105.28
3	A	2474	FMN	O4'-C4'-C3'	-5.96	95.31	109.25
3	A	2474	FMN	O3P-P-O5'	5.60	121.28	106.67
3	A	2474	FMN	O2P-P-O5'	5.19	120.21	106.67
2	B	2473	OMT	OD1-SD-CG	4.96	111.91	108.33
3	B	2474	FMN	C5'-C4'-C3'	4.81	121.29	112.22
3	A	2474	FMN	C4'-C3'-C2'	-4.81	105.57	113.57
3	B	2474	FMN	C1'-N10-C9A	-4.31	112.26	120.63
4	A	2475	AKG	O1-C1-C2	4.24	127.09	121.81
3	A	2474	FMN	C9A-C5A-N5	-4.16	118.04	122.45
3	B	2474	FMN	C4-N3-C2	-4.14	118.28	125.64
2	A	2473	OMT	OD2-SD-CG	-4.04	105.42	108.33
3	A	2474	FMN	C4-N3-C2	-3.98	118.57	125.64
3	B	2474	FMN	C8M-C8-C9	3.88	126.41	119.57
3	B	2474	FMN	C4-C4A-C10	3.82	123.49	116.93
3	A	2474	FMN	O3P-P-O1P	-3.81	95.99	110.83
2	A	2473	OMT	OD2-SD-OD1	-3.76	110.16	117.22
3	B	2474	FMN	O3P-P-O2P	-3.67	94.03	107.80
4	A	2475	AKG	C3-C2-C1	3.66	122.07	115.86
3	A	2474	FMN	O2-C2-N3	-3.65	111.58	118.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2474	FMN	O2-C2-N3	-3.62	111.64	118.58
2	A	2473	OMT	OD1-SD-CE	-3.47	105.65	108.87
2	B	2473	OMT	CE-SD-CG	3.44	118.08	105.28
3	B	2474	FMN	C8M-C8-C7	-3.31	114.00	120.76
3	A	2474	FMN	C5A-C9A-N10	3.23	120.89	117.97
3	A	2474	FMN	C4-C4A-C10	3.23	122.46	116.93
2	B	2473	OMT	CB-CA-N	3.19	118.44	110.12
3	B	2474	FMN	O3P-P-O5'	3.04	114.60	106.67
3	B	2474	FMN	O2P-P-O5'	3.01	114.51	106.67
4	B	2475	AKG	C3-C2-C1	2.99	120.95	115.86
4	A	2475	AKG	O5-C2-C1	-2.87	115.56	119.67
2	A	2473	OMT	CB-CA-N	2.86	117.58	110.12
3	B	2474	FMN	C9A-C5A-N5	-2.74	119.55	122.45
3	A	2474	FMN	N3-C2-N1	2.71	125.25	119.50
3	A	2474	FMN	C1'-N10-C9A	-2.69	115.39	120.63
3	B	2474	FMN	C4A-C10-N1	-2.65	118.09	124.59
4	B	2475	AKG	C3-C4-C5	2.46	120.19	113.67
3	B	2474	FMN	N3-C2-N1	2.41	124.63	119.50
3	A	2474	FMN	C5A-N5-C4A	2.32	121.83	118.09
4	B	2475	AKG	O3-C5-C4	-2.30	115.80	123.09
3	A	2474	FMN	C10-C4A-N5	-2.26	120.20	124.81
3	A	2474	FMN	O3P-P-O2P	2.23	116.16	107.80
3	B	2474	FMN	C10-C4A-N5	-2.15	120.41	124.81
3	A	2474	FMN	C5'-C4'-C3'	2.13	116.24	112.22
3	B	2474	FMN	O2'-C2'-C3'	2.07	114.10	109.25
3	B	2474	FMN	C4A-C4-N3	2.05	118.48	113.25
3	B	2474	FMN	N10-C10-N1	2.01	124.42	118.51
3	B	2474	FMN	C7M-C7-C6	2.01	123.11	119.57

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2473	OMT	C-CA-CB-CG
2	A	2473	OMT	CB-CG-SD-OD1
2	A	2473	OMT	CB-CG-SD-OD2
2	B	2473	OMT	N-CA-CB-CG
2	B	2473	OMT	C-CA-CB-CG
2	B	2473	OMT	CB-CG-SD-OD1
2	B	2473	OMT	CB-CG-SD-OD2
3	A	2474	FMN	O4'-C4'-C5'-O5'
3	A	2474	FMN	C5'-O5'-P-O1P

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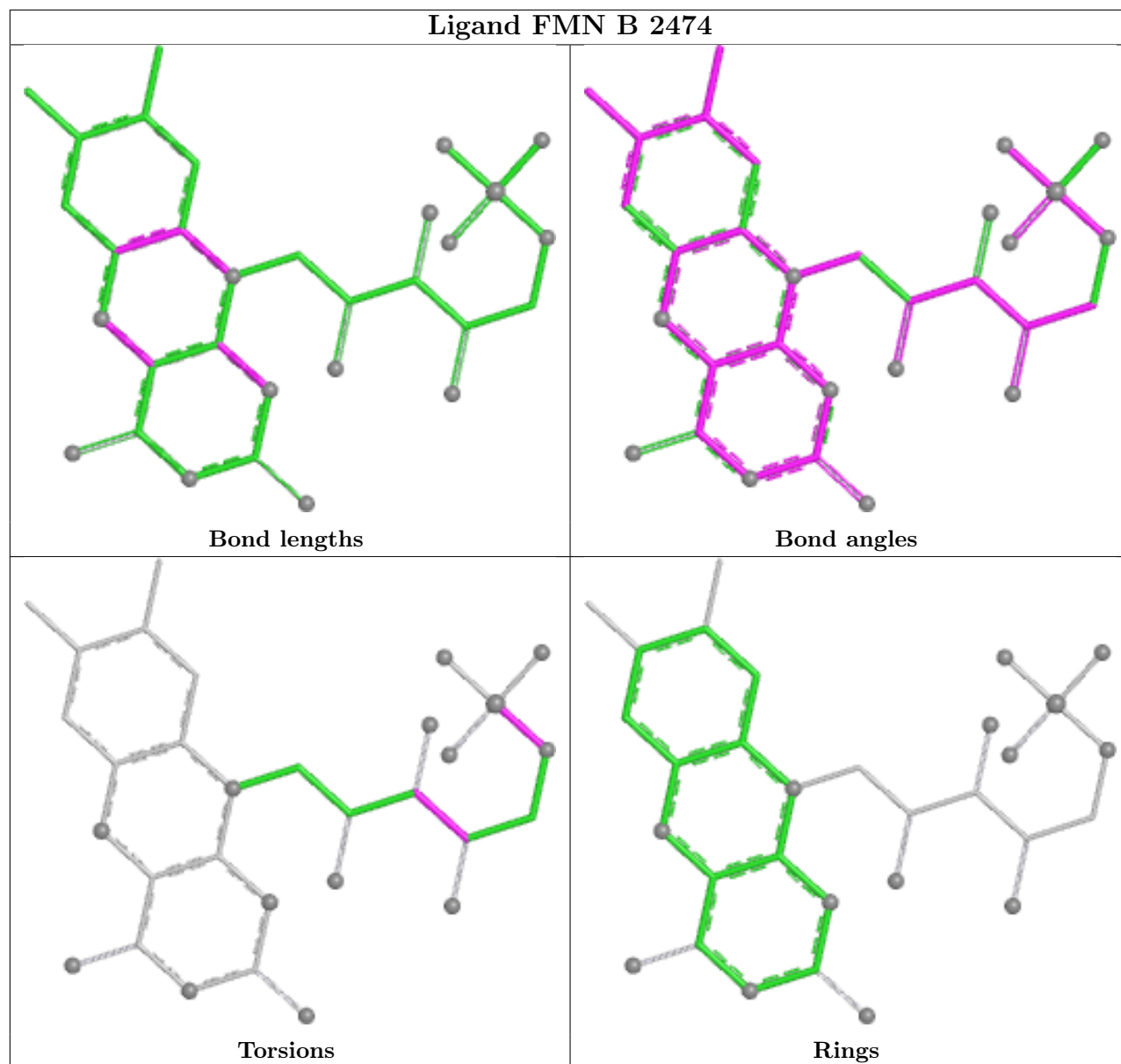
Mol	Chain	Res	Type	Atoms
3	A	2474	FMN	C5'-O5'-P-O3P
3	B	2474	FMN	C2'-C3'-C4'-O4'
3	B	2474	FMN	O3'-C3'-C4'-O4'
3	A	2474	FMN	C2'-C3'-C4'-O4'
3	A	2474	FMN	O3'-C3'-C4'-C5'
3	B	2474	FMN	O3'-C3'-C4'-C5'
3	A	2474	FMN	C2'-C3'-C4'-C5'
3	B	2474	FMN	C2'-C3'-C4'-C5'
3	A	2474	FMN	O3'-C3'-C4'-O4'
2	A	2473	OMT	CB-CG-SD-CE
2	B	2473	OMT	CB-CG-SD-CE
4	B	2475	AKG	C2-C3-C4-C5
3	B	2474	FMN	C5'-O5'-P-O2P
4	A	2475	AKG	C3-C4-C5-O4
4	A	2475	AKG	C3-C4-C5-O3

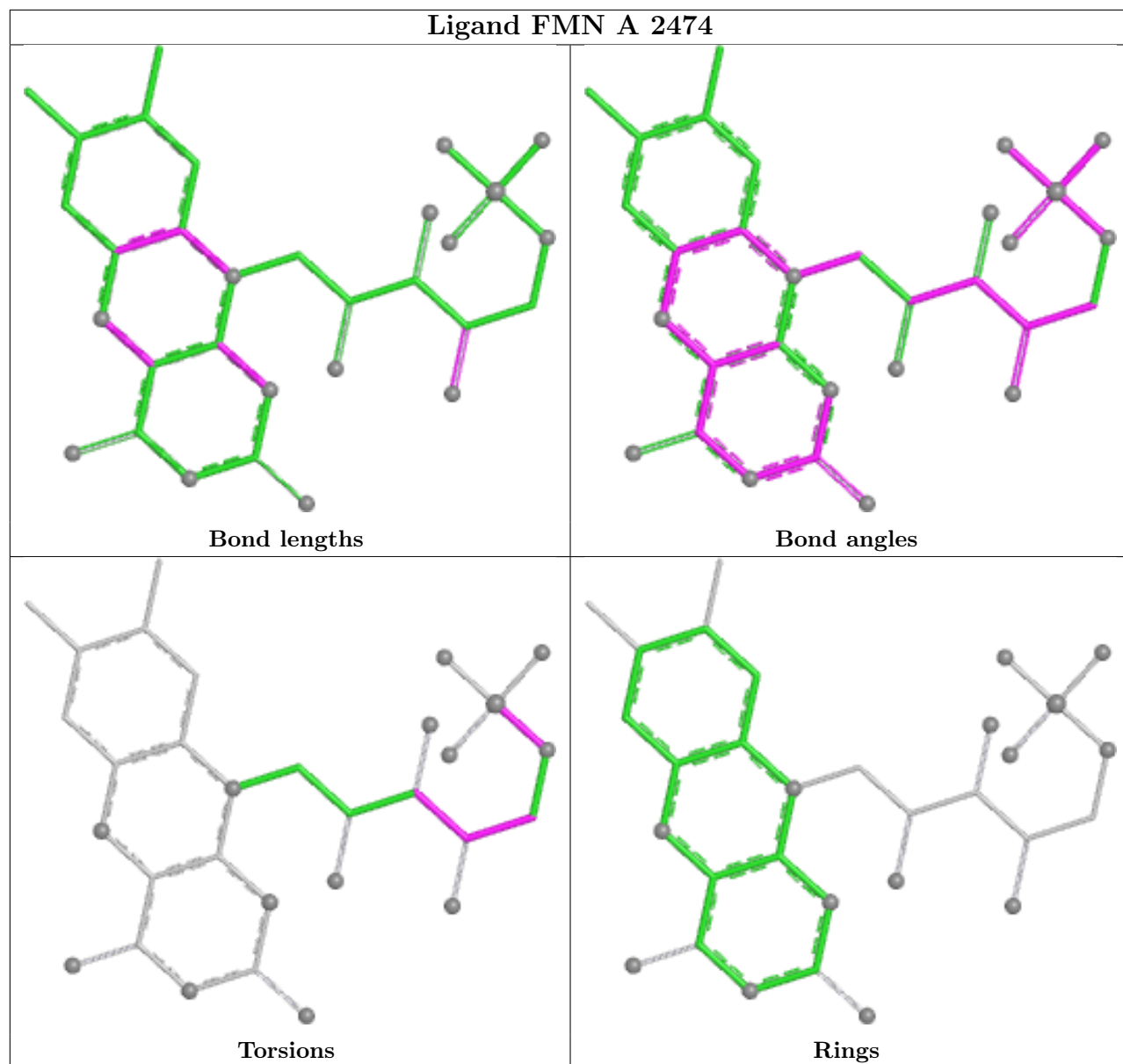
There are no ring outliers.

7 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2475	AKG	3	0
2	B	2473	OMT	2	0
3	B	2474	FMN	7	0
3	A	2474	FMN	5	0
2	A	2473	OMT	3	0
5	B	2476	F3S	3	0
5	A	2476	F3S	2	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.