



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:03 PM UTC

PDB ID : 2XCT / pdb_00002xct
Title : The twinned 3.35Å structure of S. aureus Gyrase complex with Ciprofloxacin and DNA
Authors : Bax, B.D.; Chan, P.; Eggleston, D.S.; Fosberry, A.; Gentry, D.R.; Gorrec, F.; Giordano, I.; Hann, M.M.; Hennessy, A.; Hibbs, M.; Huang, J.; Jones, E.; Jones, J.; Brown, K.K.; Lewis, C.J.; May, E.; Singh, O.; Spitzfaden, C.; Shen, C.; Shillings, A.; Theobald, A.; Wohlkonig, A.; Pearson, N.D.; Gwynn, M.N.
Deposited on : 2010-04-25
Resolution : 3.35 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)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

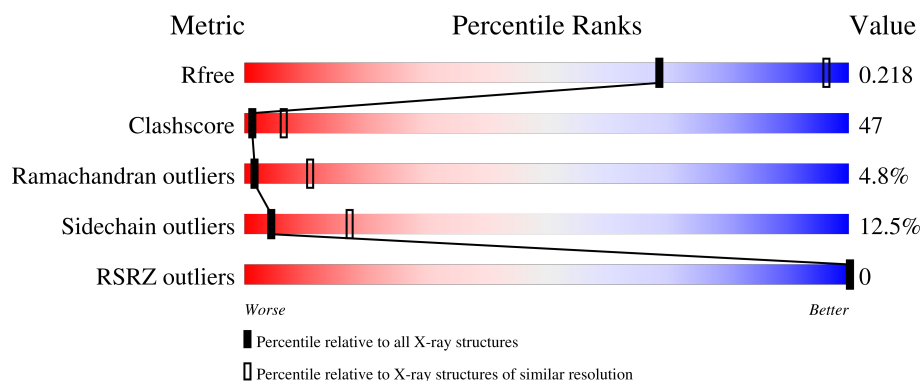
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

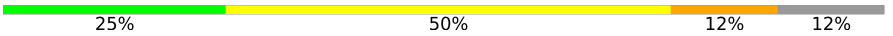
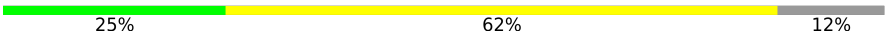
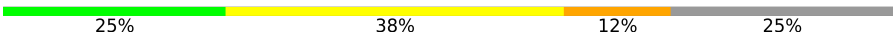
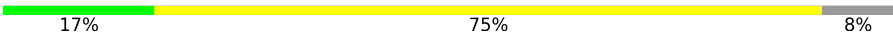
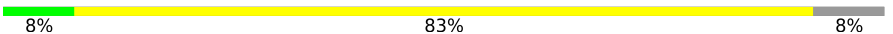
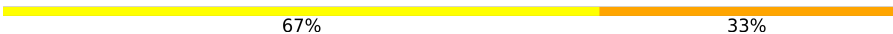
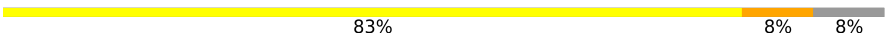
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Mol	Chain	Length	Quality of chain
1	B	692	
1	D	692	
1	S	692	

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
1	U	692	
2	E	8	
2	V	8	
3	F	8	
3	W	8	
4	G	12	
4	X	12	
5	H	12	
5	Y	12	

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
7	CPF	H	1020	-	-	X	-
7	CPF	X	1020	-	-	X	-
7	CPF	Y	1020	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 22370 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 DNA GYRASE SUBUNIT B, DNA GYRASE SUBUNIT A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	669	Total	C	N	O	S	0	2	0
			5262	3277	944	1015	26			
1	D	669	Total	C	N	O	S	0	1	0
			5151	3212	913	1001	25			
1	S	667	Total	C	N	O	S	0	0	1
			5199	3247	920	1007	25			
1	U	665	Total	C	N	O	S	0	0	0
			5193	3239	926	1003	25			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	409	MET	-	expression tag	UNP P66937
B	544	THR	-	insertion	UNP P66937
B	545	GLY	-	insertion	UNP P66937
B	1123	PHE	TYR	engineered mutation	UNP Q99XG5
D	409	MET	-	expression tag	UNP P66937
D	544	THR	-	insertion	UNP P66937
D	545	GLY	-	insertion	UNP P66937
D	1123	PHE	TYR	engineered mutation	UNP Q99XG5
S	409	MET	-	expression tag	UNP P66937
S	544	THR	-	insertion	UNP P66937
S	545	GLY	-	insertion	UNP P66937
S	1123	PHE	TYR	engineered mutation	UNP Q99XG5
U	409	MET	-	expression tag	UNP P66937
U	544	THR	-	insertion	UNP P66937
U	545	GLY	-	insertion	UNP P66937
U	1123	PHE	TYR	engineered mutation	UNP Q99XG5

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	7	Total	C	N	O	P	0	0	0
			147	69	27	44	7			
2	V	7	Total	C	N	O	P	0	0	0
			147	69	27	44	7			

- Molecule 3 is a DNA chain called 5'-D(AP*GP*CP*CP*GP*TP*AP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	7	Total	C	N	O	P	0	0	0
			145	68	28	42	7			
3	W	6	Total	C	N	O	P	0	0	0
			123	58	23	36	6			

- Molecule 4 is a DNA chain called 5'-D(GP*TP*AP*CP*CP*CP*AP*CP*GP*GP*CP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	11	Total	C	N	O	P	0	0	0
			220	105	42	63	10			
4	X	11	Total	C	N	O	P	0	0	0
			220	105	42	63	10			

- Molecule 5 is a DNA chain called 5'-D(GP*TP*AP*CP*AP*CP*CP*GP*CP*AP*CP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	12	Total	C	N	O	P	0	0	0
			240	115	47	67	11			
5	Y	11	Total	C	N	O	P	0	0	0
			219	105	42	62	10			

- Molecule 6 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

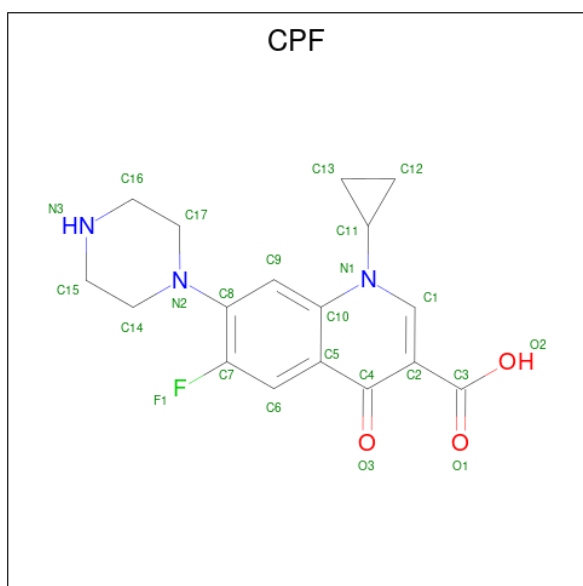
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Mn	0	0
			1	1		
6	D	1	Total	Mn	0	0
			1	1		
6	F	1	Total	Mn	0	0
			1	1		
6	G	1	Total	Mn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	S	1	Total	Mn	0	0
			1	1		
6	U	1	Total	Mn	0	0
			1	1		
6	W	2	Total	Mn	0	0
			2	2		

- Molecule 7 is 1-CYCLOPROPYL-6-FLUORO-4-OXO-7-PIPERAZIN-1-YL-1,4-DIHYDRO QUINOLINE-3-CARBOXYLIC ACID (CCD ID: CPF) (formula: $C_{17}H_{18}FN_3O_3$).

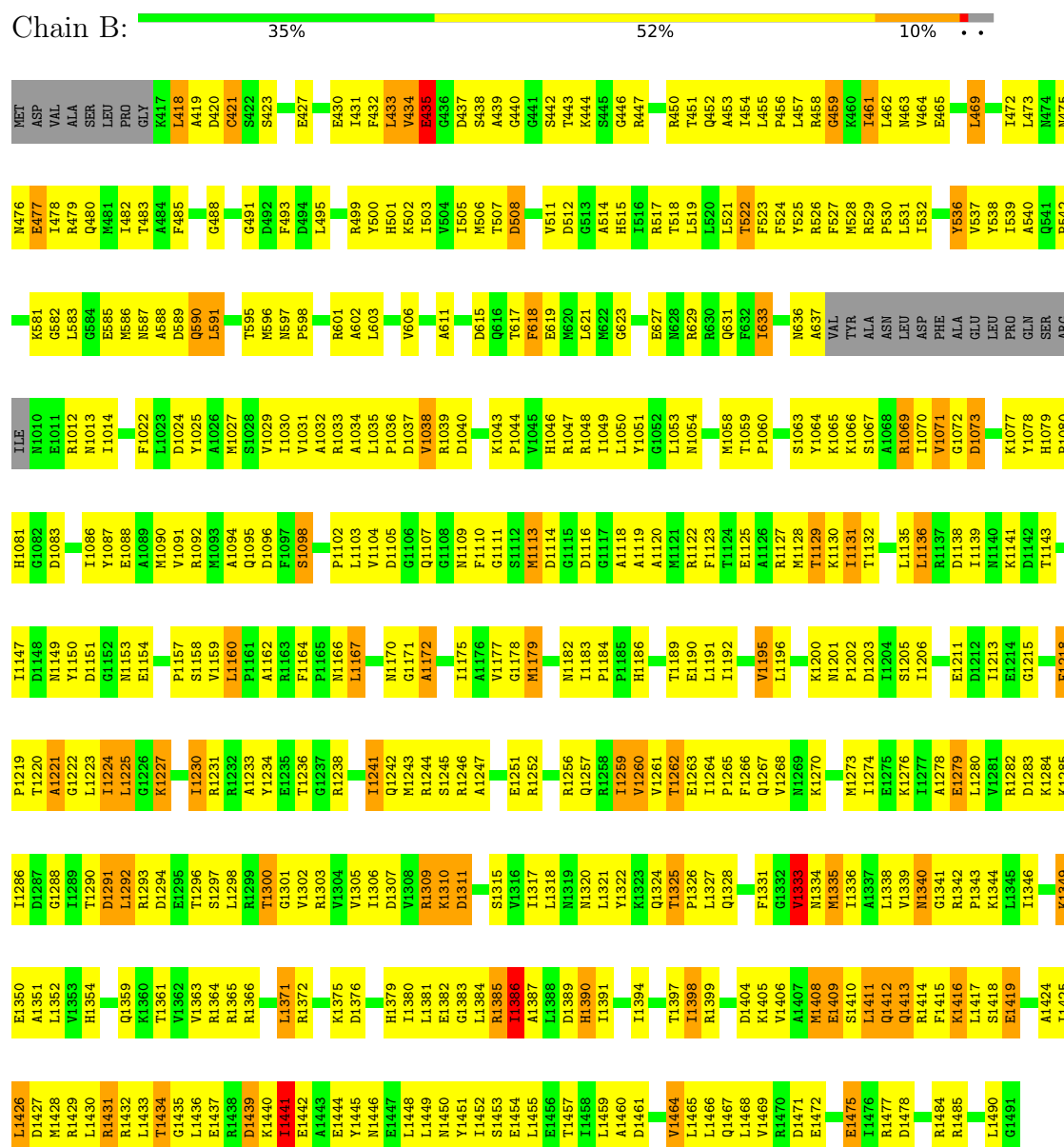


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	G	1	Total	C	F	N	O	0	0
			24	17	1	3	3		
7	H	1	Total	C	F	N	O	0	0
			24	17	1	3	3		
7	X	1	Total	C	F	N	O	0	0
			24	17	1	3	3		
7	Y	1	Total	C	F	N	O	0	0
			24	17	1	3	3		

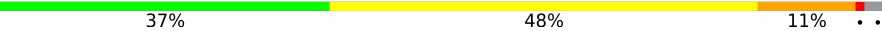
3 Residue-property plots

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

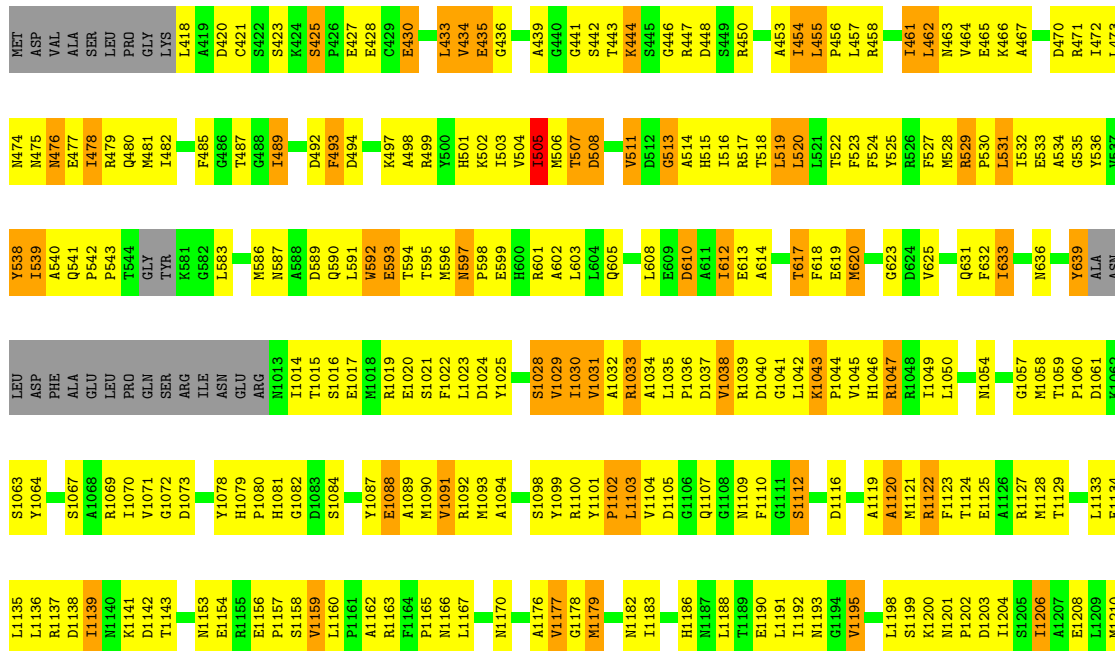
- Molecule 1: DNA GYRASE SUBUNIT B, DNA GYRASE SUBUNIT A

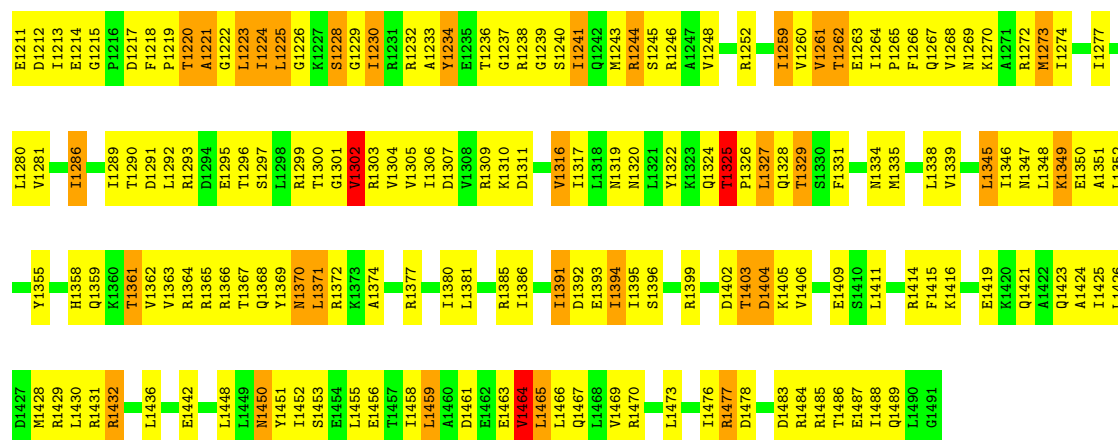


- Molecule 1: DNA GYRASE SUBUNIT B, DNA GYRASE SUBUNIT A

Chain D:  37% 48% 11% ..

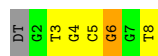
MET	ASP	VAL	ALA	SER	LEU	PRO	GLY	K417	L418	A419	D420	C421	S422	S423	S425	P426	E427	E428	C429	E430	L431	F432	L433	V434	E435	G436	D437	S438	A439	S442	T443	G446	R447	D448	S449	R450	T451	L452	A453	L454	L455	P456	L457	R458	G459	K460	L461	L462	N463	V464	L469	P470	R471	L472	L473																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
N474	N475	N476	N477	N478	N479	N480	N481	N482	N483	N484	N485	N486	N487	N488	N489	N490	N491	N492	N493	N494	N495	N496	N497	N498	N499	N500	N501	N502	N503	N504	N505	N506	N507	N508	N511	N512	N513	N514	N515	N516	N517	N518	N519	N520	N521	N522	N523	N524	N525	N526	N527	N528	N529	N530	N531	N532	N533	N534	N535	N536	N537																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
Y538	Y539	A540	Q541	P542	P543	T544	G545	T546	T547	T548	T549	T550	T551	T552	T553	T554	T555	T556	T557	T558	T559	T560	T561	T562	T563	T564	T565	T566	T567	T568	T569	T570	T571	T572	T573	T574	T575	T576	T577	T578	T579	T580	T581	T582	T583	T584	T585	T586	T587	T588	T589	T590	T591	T592	T593	T594	T595	T596	T597	T598	T599	T600	T601	T602	T603	T604	T605	T606	T607	T608	T609	T610	T611	T612	T613	T614	T615	T616	T617	T618	T619	T620	T621	T622	T623	T624	T625	T626	T627	T628	T629	T630	T631	T632	T633	T634	T635	T636	T637	T638	T639	T640	T641	T642	T643	T644	T645	T646	T647	T648	T649	T650	T651	T652	T653	T654	T655	T656	T657	T658	T659	T660	T661	T662	T663	T664	T665	T666	T667	T668	T669	T670	T671	T672	T673	T674	T675	T676	T677	T678	T679	T680	T681	T682	T683	T684	T685	T686	T687	T688	T689	T690	T691	T692	T693	T694	T695	T696	T697	T698	T699	T700	T701	T702	T703	T704	T705	T706	T707	T708	T709	T710	T711	T712	T713	T714	T715	T716	T717	T718	T719	T720	T721	T722	T723	T724	T725	T726	T727	T728	T729	T730	T731	T732	T733	T734	T735	T736	T737	T738	T739	T740	T741	T742	T743	T744	T745	T746	T747	T748	T749	T750	T751	T752	T753	T754	T755	T756	T757	T758	T759	T760	T761	T762	T763	T764	T765	T766	T767	T768	T769	T770	T771	T772	T773	T774	T775	T776	T777	T778	T779	T780	T781	T782	T783	T784	T785	T786	T787	T788	T789	T790	T791	T792	T793	T794	T795	T796	T797	T798	T799	T800	T801	T802	T803	T804	T805	T806	T807	T808	T809	T810	T811	T812	T813	T814	T815	T816	T817	T818	T819	T820	T821	T822	T823	T824	T825	T826	T827	T828	T829	T830	T831	T832	T833	T834	T835	T836	T837	T838	T839	T840	T841	T842	T843	T844	T845	T846	T847	T848	T849	T850	T851	T852	T853	T854	T855	T856	T857	T858	T859	T860	T861	T862	T863	T864	T865	T866	T867	T868	T869	T870	T871	T872	T873	T874	T875	T876	T877	T878	T879	T880	T881	T882	T883	T884	T885	T886	T887	T888	T889	T890	T891	T892	T893	T894	T895	T896	T897	T898	T899	T900	T901	T902	T903	T904	T905	T906	T907	T908	T909	T910	T911	T912	T913	T914	T915	T916	T917	T918	T919	T920	T921	T922	T923	T924	T925	T926	T927	T928	T929	T930	T931	T932	T933	T934	T935	T936	T937	T938	T939	T940	T941	T942	T943	T944	T945	T946	T947	T948	T949	T950	T951	T952	T953	T954	T955	T956	T957	T958	T959	T960	T961	T962	T963	T964	T965	T966	T967	T968	T969	T970	T971	T972	T973	T974	T975	T976	T977	T978	T979	T980	T981	T982	T983	T984	T985	T986	T987	T988	T989	T990	T991	T992	T993	T994	T995	T996	T997	T998	T999	T1000	T1001	T1002	T1003	T1004	T1005	T1006	T1007	T1008	T1009	T1010	T1011	T1012	T1013	T1014	T1015	T1016	T1017	T1018	T1019	T1020	T1021	T1022	T1023	T1024	T1025	T1026	T1027	T1028	T1029	T1030	T1031	T1032	T1033	T1034	T1035	T1036	T1037	T1038	T1039	T1040	T1041	T1042	T1043	T1044	T1045	T1046	T1047	T1048	T1049	T1050	T1051	T1052	T1053	T1054	T1055	T1056	T1057	T1058	T1059	T1060	T1061	T1062	T1063	T1064	T1065	T1066	T1067	T1068	T1069	T1070	T1071	T1072	T1073	T1074	T1075	T1076	T1077	T1078	T1079	T1080	T1081	T1082	T1083	T1084	T1085	T1086	T1087	T1088	T1089	T1090	T1091	T1092	T1093	T1094	T1095	T1096	T1097	T1098	T1099	T1100	T1101	T1102	T1103	T1104	T1105	T1106	T1107	T1108	T1109	T1110	T1111	T1112	T1113	T1114	T1115	T1116	T1117	T1118	T1119	T1120	T1121	T1122	T1123	T1124	T1125	T1126	T1127	T1128	T1129	T1130	T1131	T1132	T1133	T1134	T1135	T1136	T1137	T1138	T1139	T1140	T1141	T1142	T1143	T1144	T1145	T1146	T1147	T1148	T1149	T1150	T1151	T1152	T1153	T1154	T1155	T1156	T1157	T1158	T1159	T1160	T1161	T1162	T1163	T1164	T1165	T1166	T1167	T1168	T1169	T1170	T1171	T1172	T1173	T1174	T1175	T1176	T1177	T1178	T1179	T1180	T1181	T1182	T1183	T1184	T1185	T1186	T1187	T1188	T1189	T1190	T1191	T1192	T1193	T1194	T1195	T1196	T1197	T1198	T1199	T1200	T1201	T1202	T1203	T1204	T1205	T1206	T1207	T1208	T1209	T1210	T1211	T1212	T1213	T1214	T1215	T1216	T1217	T1218	T1219	T1220	T1221	T1222	T1223	T1224	T1225	T1226	T1227	T1228	T1229	T1230	T1231	T1232	T1233	T1234	T1235	T1236	T1237	T1238	T1239	T1240	T1241	T1242	T1243	T1244	T1245	T1246	T1247	T1248	T1249	T1250	T1251	T1252	T1253	T1254	T1255	T1256	T1257	T1258	T1259	T1260	T1261	T1262	T1263	T1264	T1265	T1266	T1267	T1268	T1269	T1270	T1271	T1272	T1273	T1274	T1275	T1276	T1277	T1278	T1279	T1280	T1281	T1282	T1283	T1284	T1285	T1286	T1287	T1288	T1289	T1290	T1291	T1292	T1293	T1294	T1295	T1296	T1297	T1298	T1299	T1300	T1301	T1302	T1303	T1304	T1305	T1306	T1307	T1308	T1309	T1310	T1311	T1312	T1313	T1314	T1315	T1316	T1317	T1318	T1319	T1320	T1321	T1322	T1323	T1324	T1325	T1326	T1327	T1328	T1329	T1330	T1331	T1332	T1333	T1334	T1335	T1336	T1337	T1338	T1339	T1340	T1341	T1342	T1343	T1344	T1345	T1346	T1347	T1348	T1349	T1350	T1351	T1352	T1353	T1354	T1355	T1356	T1357	T1358	T1359	T1360	T1361	T1362	T1363	T1364	T1365	T1366	T1367	T1368	T1369	T1370	T1371	T1372	T1373	T1374	T1375	T1376	T1377	T1378	T1379	T1380	T1381	T1382	T1383	T1384	T1385	T1386	T1387	T1388	T1389	T1390	T1391	T1392	T1393	T1394	T1395	T1396	T1397	T1398	T1399	T1400	T1401	T1402	T1403	T1404	T1405	T1406	T1407	T1408	T1409	T1410	T1411	T1412	T1413	T1414	T1415	T1416	T1417	T1418	T1419	T1420	T1421	T1422	T1423	T1424	T1425	T1426	T1427	T1428	T1429	T1430	T1431	T1432	T1433	T1434	T1435	T1436	T1437	T1438	T1439	T1440	T1441	T1442	T1443	T1444	T1445	T1446	T1447	T1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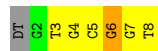
- Molecule 2: 5'-D(TP*GP*TP*GP*CP*GP*GP*T)-3'

Chain E: 25% 50% 12% 12%



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

Chain V: 12% 62% 12% 12%



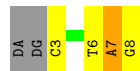
- Molecule 3: 5'-D(AP*GP*CP*CP*GP*TP*AP*G)-3'

Chain F: 25% 62% 12%



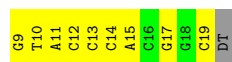
- Molecule 3: 5'-D(AP*GP*CP*CP*GP*TP*AP*G)-3'

Chain W: 25% 38% 12% 25%



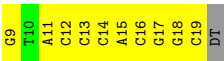
- Molecule 4: 5'-D(GP*TP*AP*CP*CP*CP*AP*CP*GP*GP*CP*T)-3'

Chain G: 17% 75% 8%



- Molecule 4: 5'-D(GP*TP*AP*CP*CP*CP*AP*CP*GP*GP*CP*T)-3'

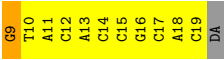
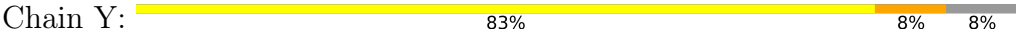
Chain X: 8% 83% 8%



● Molecule 5: 5'-D(GP*TP*AP*CP*AP*CP*CP*GP*CP*AP*CP*A)-3'



● Molecule 5: 5'-D(GP*TP*AP*CP*AP*CP*CP*GP*CP*AP*CP*A)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	88.98Å 123.17Å 170.42Å 90.00° 90.25° 90.00°	Depositor
Resolution (Å)	24.96 – 3.35 24.96 – 3.35	Depositor EDS
% Data completeness (in resolution range)	98.5 (24.96-3.35) 97.3 (24.96-3.35)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 3.38Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.166 , 0.236 0.167 , 0.218	Depositor DCC
R_{free} test set	2115 reflections (4.05%)	wwPDB-VP
Wilson B-factor (Å ²)	72.1	Xtriage
Anisotropy	0.604	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 33.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.277 for h,-k,-l	Xtriage
Reported twinning fraction	0.324 for h,-k,-l	Depositor
Outliers	0 of 52173 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22370	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	B	0.65	0/5332	1.07	20/7190 (0.3%)
1	D	0.63	0/5220	1.06	22/7063 (0.3%)
1	S	0.60	1/5269 (0.0%)	1.05	29/7112 (0.4%)
1	U	0.66	0/5263	1.11	37/7106 (0.5%)
2	E	0.48	0/164	1.36	1/252 (0.4%)
2	V	0.39	0/164	1.18	1/252 (0.4%)
3	F	0.40	0/162	1.14	0/248
3	W	0.37	0/137	1.17	1/209 (0.5%)
4	G	0.47	0/246	1.12	0/377
4	X	0.49	0/246	1.22	1/377 (0.3%)
5	H	0.67	0/269	1.71	8/412 (1.9%)
5	Y	0.46	0/245	1.47	5/375 (1.3%)
All	All	0.63	1/22717 (0.0%)	1.10	125/30973 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	639	TYR	C-N	-6.94	1.23	1.33

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	9	DG	C4'-C3'-O3'	10.62	125.94	110.00
1	B	1391	ILE	N-CA-C	10.30	120.22	110.53
1	U	1079	HIS	CA-C-N	-8.00	113.57	121.65
1	U	1079	HIS	C-N-CA	-8.00	113.57	121.65
1	B	1325	THR	CA-C-N	7.98	129.82	119.84
1	B	1325	THR	C-N-CA	7.98	129.82	119.84
5	Y	9	DG	O4'-C1'-N9	7.75	120.03	108.40
1	D	1160	LEU	CA-C-N	7.70	128.41	119.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1160	LEU	C-N-CA	7.70	128.41	119.47
1	U	1391	ILE	N-CA-C	7.70	118.44	110.36
5	H	9	DG	P-O3'-C3'	7.58	131.56	120.20
5	Y	9	DG	C1'-O4'-C4'	-7.56	98.36	109.70
1	S	1164	PHE	CA-C-N	7.55	129.28	119.84
1	S	1164	PHE	C-N-CA	7.55	129.28	119.84
1	D	1325	THR	CA-C-N	7.26	128.18	120.12
1	D	1325	THR	C-N-CA	7.26	128.18	120.12
1	U	1325	THR	N-CA-C	7.14	117.33	108.11
1	S	436	GLY	N-CA-C	7.00	121.74	112.65
1	B	469	LEU	N-CA-C	6.97	118.95	111.36
1	S	1035	LEU	CA-C-N	6.92	128.49	119.84
1	S	1035	LEU	C-N-CA	6.92	128.49	119.84
1	S	541	GLN	CA-C-N	6.81	124.63	119.66
1	S	541	GLN	C-N-CA	6.81	124.63	119.66
1	B	1419	GLU	N-CA-C	-6.75	103.01	111.11
1	S	1029	VAL	CB-CA-C	-6.70	100.31	111.29
1	U	1224	ILE	N-CA-C	6.68	117.51	107.75
5	H	17	DC	O4'-C1'-N1	-6.68	98.38	108.40
5	Y	9	DG	C4-N9-C1'	-6.67	116.99	127.00
1	D	1053	LEU	N-CA-C	-6.66	104.02	111.28
1	U	1112	SER	N-CA-C	6.65	117.02	108.24
1	D	425	SER	CA-C-N	6.64	128.14	119.84
1	D	425	SER	C-N-CA	6.64	128.14	119.84
1	D	442	SER	N-CA-C	-6.51	103.81	111.03
2	V	6	DG	O5'-C5'-C4'	-6.50	101.05	110.80
1	U	1464	VAL	CB-CA-C	-6.50	103.50	112.02
1	U	455	LEU	CA-C-N	6.46	127.44	120.13
1	U	455	LEU	C-N-CA	6.46	127.44	120.13
1	U	1178	GLY	N-CA-C	-6.45	107.02	114.69
1	U	1103	LEU	N-CA-C	-6.43	104.58	112.88
1	S	1156	GLU	CA-C-N	6.38	126.33	119.76
1	S	1156	GLU	C-N-CA	6.38	126.33	119.76
1	B	1071	VAL	CB-CA-C	-6.36	103.83	111.97
1	B	1178	GLY	N-CA-C	-6.36	107.34	115.42
1	S	1325	THR	CA-C-N	6.34	127.77	119.84
1	S	1325	THR	C-N-CA	6.34	127.77	119.84
1	D	1077	LYS	N-CA-C	6.23	119.04	111.82
1	D	1101	TYR	CA-C-N	6.22	127.20	119.98
1	D	1101	TYR	C-N-CA	6.22	127.20	119.98
1	D	1218	PHE	CA-C-N	6.17	126.06	119.28
1	D	1218	PHE	C-N-CA	6.17	126.06	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	425	SER	CA-C-N	6.16	125.56	118.85
1	U	425	SER	C-N-CA	6.16	125.56	118.85
1	U	539	ILE	CB-CA-C	-6.15	102.55	110.98
1	B	1241	ILE	N-CA-C	6.07	116.60	107.80
5	H	9	DG	O4'-C1'-N9	6.04	117.45	108.40
1	S	1239	GLY	N-CA-C	-6.01	103.10	111.09
1	U	505	ILE	CB-CA-C	-5.98	105.46	111.80
5	H	10	DT	O4'-C1'-N1	5.98	117.37	108.40
1	D	447	ARG	N-CA-C	5.87	118.74	110.23
1	S	539	ILE	CB-CA-C	-5.85	103.75	110.41
1	U	1442	GLU	N-CA-C	-5.84	104.99	111.36
1	U	597	ASN	CA-C-N	5.81	125.51	119.82
1	U	597	ASN	C-N-CA	5.81	125.51	119.82
1	S	1268	VAL	N-CA-C	5.77	116.78	108.48
5	H	16	DG	C1'-O4'-C4'	-5.74	101.09	109.70
1	U	1071	VAL	CB-CA-C	-5.73	104.37	111.94
1	U	1089	ALA	N-CA-C	-5.73	105.31	112.93
5	H	17	DC	C4'-C3'-O3'	-5.71	101.43	110.00
1	S	1261	VAL	N-CA-C	5.70	116.20	107.77
1	B	1441	ILE	CB-CA-C	-5.68	104.54	111.87
1	S	597	ASN	CA-C-N	5.67	126.93	119.84
1	S	597	ASN	C-N-CA	5.67	126.93	119.84
1	B	1218	PHE	CA-C-N	5.64	126.01	119.47
1	B	1218	PHE	C-N-CA	5.64	126.01	119.47
1	U	625	VAL	CB-CA-C	-5.58	106.32	112.68
1	U	1241	ILE	N-CA-C	5.56	115.87	107.75
1	B	1211	GLU	N-CA-C	-5.56	105.76	112.54
1	U	1327	LEU	N-CA-C	-5.51	105.82	112.54
1	D	1229	GLY	N-CA-C	-5.50	105.73	112.77
1	D	1079	HIS	CA-C-N	5.50	126.71	119.84
1	D	1079	HIS	C-N-CA	5.50	126.71	119.84
1	S	1322	TYR	N-CA-C	-5.45	106.33	112.87
1	S	1126	ALA	N-CA-C	5.42	117.42	109.24
1	B	1179	MET	N-CA-C	5.41	116.86	109.18
5	Y	9	DG	C8-N9-C1'	5.41	135.11	127.00
1	U	1234	TYR	N-CA-C	5.38	117.14	111.28
1	S	1022	PHE	N-CA-C	-5.37	105.09	111.69
1	U	1072	GLY	N-CA-C	-5.36	106.15	113.27
1	S	455	LEU	CA-C-N	5.35	125.35	120.21
1	S	455	LEU	C-N-CA	5.35	125.35	120.21
1	B	435	GLU	N-CA-C	5.32	116.76	111.07
1	U	1252	ARG	N-CA-C	5.30	117.74	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1225	LEU	N-CA-C	5.29	117.25	107.73
1	U	1391	ILE	CB-CA-C	-5.28	105.12	111.88
1	U	513	GLY	N-CA-C	-5.27	106.26	112.64
1	U	1043	LYS	CA-C-N	5.26	125.32	119.32
1	U	1043	LYS	C-N-CA	5.26	125.32	119.32
1	D	1335	MET	N-CA-C	5.26	117.51	109.62
5	H	9	DG	C8-N9-C1'	5.26	134.88	127.00
1	U	529	ARG	CA-C-N	-5.22	113.65	119.19
1	U	529	ARG	C-N-CA	-5.22	113.65	119.19
1	B	618	PHE	N-CA-C	-5.22	105.48	111.07
1	S	1107	GLN	N-CA-C	5.19	117.10	107.60
1	U	439	ALA	N-CA-C	-5.19	106.90	113.18
1	B	1160	LEU	CA-C-N	5.18	125.48	119.47
1	B	1160	LEU	C-N-CA	5.18	125.48	119.47
3	W	7	DA	O3'-P-O5'	-5.18	96.24	104.00
1	D	454	ILE	CB-CA-C	-5.17	103.12	110.83
1	D	1069	ARG	N-CA-C	-5.16	106.67	113.12
1	S	1440	LYS	N-CA-C	-5.16	105.34	111.69
1	S	472	ILE	CB-CA-C	-5.15	105.22	111.87
1	U	1047	ARG	N-CA-C	-5.15	105.09	111.33
1	B	1230	ILE	CB-CA-C	-5.14	105.30	111.88
1	U	1223	LEU	N-CA-C	5.12	117.59	109.50
1	D	1178	GLY	N-CA-C	-5.11	108.11	113.58
1	B	1333	VAL	N-CA-C	5.10	115.68	109.30
1	S	1438	ARG	N-CA-C	-5.06	106.35	112.88
1	U	1028	SER	N-CA-C	5.06	116.48	110.97
1	S	1249	ILE	N-CA-C	5.05	115.61	107.98
1	S	537	VAL	N-CA-C	5.05	115.31	107.28
4	X	16	DC	P-O3'-C3'	-5.04	112.63	120.20
5	Y	16	DG	C1'-O4'-C4'	-5.04	102.14	109.70
2	E	6	DG	O4'-C1'-N9	5.03	115.94	108.40
1	U	1273	MET	N-CA-C	-5.02	105.81	111.28
1	D	1051	TYR	N-CA-C	-5.01	106.34	112.90

There are no chirality outliers.

There are no planarity outliers.

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	B	5262	0	5259	473	0
1	D	5151	0	5043	472	0
1	S	5199	0	5178	534	0
1	U	5193	0	5163	490	0
2	E	147	0	80	8	0
2	V	147	0	80	8	0
3	F	145	0	79	14	0
3	W	123	0	68	8	0
4	G	220	0	124	27	0
4	X	220	0	124	35	0
5	H	240	0	135	38	0
5	Y	219	0	124	37	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	S	1	0	0	0	0
6	U	1	0	0	0	0
6	W	2	0	0	0	0
7	G	24	0	17	8	0
7	H	24	0	17	9	0
7	X	24	0	17	20	0
7	Y	24	0	17	10	0
All	All	22370	0	21525	2045	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 47.

All (2045) 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)
4:G:12:DC:N3	5:H:9:DG:N2	1.82	1.26
4:X:11:DA:N1	5:Y:10:DT:O4	1.78	1.15
5:H:11:DA:H2''	5:H:12:DC:C5'	1.86	1.06
1:U:1122:ARG:HH22	4:X:9:DG:H5''	1.18	1.06
1:D:1192:ILE:HD12	1:D:1477:ARG:HB2	1.39	1.05
1:U:1030:ILE:HG23	1:U:1035:LEU:HD12	1.39	1.04
4:X:9:DG:N2	5:Y:12:DC:O2	1.91	1.04
5:H:11:DA:C2'	5:H:12:DC:H5'	1.90	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:435:GLU:OE1	1:D:508:ASP:HB2	1.61	0.99
1:S:1277:ILE:HG12	1:S:1325:THR:HG21	1.45	0.99
1:S:1297:SER:HB2	1:S:1299:ARG:HH21	1.25	0.99
1:S:1309:ARG:HH11	1:S:1309:ARG:HG3	1.27	0.98
1:S:1256:ARG:HG2	1:S:1310:LYS:HB2	1.44	0.98
1:U:1059:THR:HA	1:U:1128:MET:HE3	1.45	0.98
1:D:495:LEU:HD21	1:D:534:ALA:HB2	1.45	0.98
5:H:11:DA:H2''	5:H:12:DC:H5'	0.99	0.98
1:S:458:ARG:NH2	1:S:480:GLN:HE22	1.63	0.96
4:X:13:DC:H1'	7:X:1020:CPF:H161	1.44	0.96
1:S:1342:ARG:HG2	1:S:1342:ARG:HH21	1.30	0.96
1:S:1299:ARG:H	1:S:1299:ARG:HD2	1.31	0.95
1:U:1042:LEU:HD11	1:U:1160:LEU:HD12	1.47	0.94
1:B:458:ARG:HB2	7:G:1020:CPF:H162	1.50	0.94
1:U:434:VAL:HG22	1:U:456:PRO:HA	1.47	0.93
1:B:1296:THR:HG23	1:B:1301:GLY:O	1.69	0.93
1:U:1122:ARG:HH12	4:X:9:DG:H3'	1.32	0.92
1:B:1431:ARG:HG3	1:D:1426:LEU:O	1.69	0.92
1:B:1408:MET:HB3	1:B:1412:GLN:HE21	1.36	0.91
1:S:1193:ASN:HA	1:S:1196:LEU:HD12	1.54	0.90
1:B:1256:ARG:HG2	1:B:1310:LYS:CB	2.02	0.90
1:S:1060:PRO:HG2	1:S:1133:LEU:HD11	1.55	0.89
1:U:1458:ILE:HA	1:U:1464:VAL:HG11	1.54	0.89
1:B:1371:LEU:HD11	1:B:1375:LYS:HE3	1.53	0.89
1:S:620:MET:HE1	1:U:1019:ARG:HH12	1.35	0.89
1:U:435:GLU:HG2	1:U:507:THR:HA	1.54	0.89
1:D:1027:MET:O	1:D:1031:VAL:HG22	1.71	0.89
1:B:585:GLU:O	1:D:1108:GLY:HA2	1.73	0.89
1:D:499:ARG:HH11	1:D:499:ARG:HG3	1.37	0.89
1:B:447:ARG:HA	1:B:596:MET:HE1	1.54	0.88
1:U:587:ASN:HB3	1:U:589:ASP:OD1	1.73	0.88
4:X:14:DC:H2''	4:X:15:DA:H5'	1.55	0.88
1:U:1122:ARG:NH2	4:X:9:DG:H5''	1.88	0.88
1:D:443:THR:HG22	1:D:454:ILE:HD11	1.56	0.88
3:F:8:DG:H5''	3:F:8:DG:H8	1.39	0.88
1:B:1095:GLN:HB2	1:B:1098:SER:HB2	1.54	0.87
1:D:636:ASN:HD22	1:D:636:ASN:N	1.72	0.87
1:S:1283:ASP:HB3	1:S:1285:LYS:HE3	1.56	0.87
1:D:454:ILE:HG22	1:D:456:PRO:HD3	1.57	0.87
1:D:437:ASP:CB	5:H:9:DG:H5''	2.05	0.87
1:S:1232:ARG:HG3	1:S:1232:ARG:HH11	1.38	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1049:ILE:O	1:D:1053:LEU:HG	1.72	0.87
1:U:1361:THR:O	1:U:1365:ARG:HG3	1.75	0.87
1:B:1461:ASP:HB3	1:B:1464:VAL:HG23	1.57	0.87
5:H:19:DC:H2'	5:H:19:DC:OP2	1.75	0.87
1:U:475:ASN:O	1:U:479:ARG:HG3	1.75	0.87
3:W:7:DA:H2''	3:W:8:DG:H5''	1.55	0.86
1:D:1030:ILE:CG2	1:D:1343:PRO:HG3	2.06	0.86
1:U:508:ASP:HB3	1:U:583:LEU:HD23	1.55	0.86
1:S:459:GLY:HA3	7:X:1020:CPF:H131	1.56	0.85
1:B:1153:ASN:O	1:B:1154:GLU:HG2	1.76	0.85
1:D:434:VAL:HG12	1:D:506:MET:HE3	1.58	0.85
1:S:443:THR:HG22	1:S:454:ILE:HD11	1.57	0.85
1:U:1368:GLN:HG2	1:U:1459:LEU:HD11	1.58	0.85
1:S:1325:THR:HB	1:S:1326:PRO:HD2	1.59	0.85
1:U:493:PHE:HZ	1:U:531:LEU:HB2	1.39	0.85
1:U:435:GLU:CG	1:U:507:THR:HA	2.04	0.85
1:B:1049:ILE:HG21	1:B:1090:MET:HG3	1.56	0.85
4:G:12:DC:N4	5:H:9:DG:H22	1.74	0.85
1:S:1013:ASN:HB3	1:S:1016:SER:HB2	1.57	0.85
1:B:430:GLU:HB3	1:B:502:LYS:HB2	1.58	0.84
1:S:459:GLY:CA	7:X:1020:CPF:H131	2.07	0.84
1:B:1363:VAL:HG13	1:B:1366:ARG:HH21	1.42	0.84
1:D:1049:ILE:HD13	1:D:1090:MET:HB2	1.58	0.83
1:B:1409:GLU:HA	1:B:1412:GLN:HG3	1.61	0.83
1:B:1222:GLY:O	1:B:1223:LEU:HD12	1.76	0.83
1:S:1232:ARG:HH11	1:S:1232:ARG:CG	1.92	0.83
1:B:435:GLU:HG3	1:B:508:ASP:OD1	1.77	0.83
1:S:1431:ARG:HG3	1:U:1426:LEU:HB3	1.60	0.83
4:X:13:DC:H1'	7:X:1020:CPF:C16	2.09	0.83
1:B:1230:ILE:HA	1:B:1241:ILE:HD11	1.58	0.82
4:X:9:DG:N1	5:Y:12:DC:N3	2.28	0.82
1:B:1066:LYS:HD3	1:B:1125:GLU:HG2	1.61	0.82
1:S:1309:ARG:HH11	1:S:1309:ARG:CG	1.92	0.82
1:U:1025:TYR:O	1:U:1029:VAL:HG23	1.78	0.82
1:S:1137:ARG:O	1:S:1138:ASP:HB2	1.76	0.82
1:S:1342:ARG:HH21	1:S:1342:ARG:CG	1.91	0.82
1:D:1064:TYR:HB3	1:D:1125:GLU:HB3	1.62	0.82
1:U:1192:ILE:HD12	1:U:1477:ARG:HB2	1.61	0.81
1:B:1071:VAL:HG13	1:B:1086:ILE:HG21	1.62	0.81
1:S:1295:GLU:HB2	1:S:1303:ARG:HG2	1.60	0.81
1:B:1425:ILE:O	1:D:1430:LEU:HD12	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:443:THR:HG23	1:D:596:MET:SD	2.20	0.81
1:U:461:ILE:HD11	1:U:477:GLU:HB3	1.61	0.81
1:U:522:THR:HA	1:U:618:PHE:CE2	2.15	0.81
1:B:1325:THR:HB	1:B:1326:PRO:HD2	1.60	0.81
1:D:493:PHE:CZ	1:D:495:LEU:HD13	2.16	0.81
1:D:458:ARG:HB2	7:H:1020:CPF:H172	1.59	0.81
1:D:1186:HIS:HB2	1:D:1191:LEU:HD11	1.60	0.81
3:F:8:DG:H5''	3:F:8:DG:C8	2.16	0.81
1:S:452:GLN:OE1	1:S:592:TRP:HZ3	1.63	0.81
1:S:1051:TYR:HH	1:S:1146:PHE:HE2	1.27	0.81
1:B:1138:ASP:HB3	1:B:1141:LYS:HD2	1.63	0.80
1:U:1054:ASN:HB2	1:U:1136:LEU:HD13	1.62	0.80
1:S:1342:ARG:HG2	1:S:1342:ARG:NH2	1.94	0.80
1:U:1450:ASN:HD22	1:U:1450:ASN:N	1.80	0.80
1:B:587:ASN:HB2	1:B:589:ASP:OD1	1.81	0.79
1:B:1245:SER:OG	1:B:1265:PRO:HD3	1.82	0.79
1:D:1030:ILE:HG21	1:D:1343:PRO:HG3	1.64	0.79
5:H:9:DG:H2'	5:H:10:DT:C5	2.17	0.79
1:U:458:ARG:HB3	7:Y:1020:CPF:H162	1.63	0.79
1:S:441:GLY:HA3	1:S:1109:ASN:HD21	1.48	0.79
4:X:12:DC:H42	5:Y:9:DG:H1	1.30	0.79
1:S:1071:VAL:HG12	1:S:1075:MET:HE2	1.65	0.79
1:U:1264:ILE:HG23	1:U:1302:VAL:HG11	1.64	0.79
1:B:606:VAL:HG11	1:B:1014:ILE:HD12	1.62	0.79
1:D:1319:ASN:HA	1:D:1322:TYR:HD2	1.47	0.79
1:S:1215:GLY:HA3	1:S:1488:ILE:HD11	1.63	0.79
1:S:1259:ILE:HD13	1:S:1318:LEU:HB2	1.64	0.79
4:X:9:DG:H5'	7:Y:1020:CPF:H1	1.65	0.79
1:D:1313:ASN:HD22	1:D:1316:VAL:HG23	1.46	0.79
4:G:10:DT:H2''	4:G:11:DA:C8	2.18	0.79
1:D:475:ASN:HD22	4:G:14:DC:H5'	1.46	0.79
1:U:1143:THR:HB	1:U:1362:VAL:HG13	1.64	0.79
1:D:1238:ARG:HG2	1:D:1334:ASN:HD22	1.48	0.78
1:B:1063:SER:O	1:B:1065:LYS:HE2	1.84	0.78
1:U:597:ASN:HD21	1:U:599:GLU:HG3	1.48	0.78
1:D:1231:ARG:HH11	1:D:1231:ARG:CG	1.95	0.78
1:S:1196:LEU:O	1:S:1200:LYS:HG3	1.83	0.78
4:G:9:DG:H5'	7:G:1020:CPF:H122	1.66	0.78
1:U:1105:ASP:HB3	1:U:1127:ARG:HG3	1.66	0.78
1:B:1244:ARG:HG2	1:B:1245:SER:H	1.49	0.78
1:D:1293:ARG:NH2	1:D:1305:VAL:HG11	1.99	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1466:LEU:O	1:S:1466:LEU:HD12	1.84	0.78
1:D:508:ASP:HA	1:D:583:LEU:HD23	1.66	0.77
1:D:1414:ARG:HD2	1:D:1415:PHE:CE1	2.19	0.77
1:B:1064:TYR:HB3	1:B:1125:GLU:HB3	1.65	0.77
1:D:495:LEU:HD21	1:D:534:ALA:CB	2.13	0.77
1:D:1273:MET:O	1:D:1277:ILE:HG13	1.85	0.77
1:S:502:LYS:HA	1:S:538:TYR:HE1	1.50	0.77
1:D:1064:TYR:CE2	1:D:1107:GLN:HB2	2.19	0.77
1:D:1363:VAL:HG13	1:D:1366:ARG:NH2	1.99	0.77
1:S:1100:ARG:HD2	1:S:1485:ARG:NH1	1.99	0.77
1:D:1448:LEU:O	1:D:1452:ILE:HG13	1.85	0.77
5:Y:12:DC:H2'	7:Y:1020:CPF:H141	1.65	0.77
1:U:1064:TYR:HB3	1:U:1125:GLU:HB3	1.65	0.77
1:S:471:ARG:HG2	1:S:471:ARG:HH11	1.49	0.77
1:B:1039:ARG:HH21	1:B:1159:VAL:HB	1.49	0.76
1:D:485:PHE:HE1	1:D:503:ILE:HG12	1.50	0.76
1:D:1383:GLY:H	1:D:1421:GLN:HE21	1.32	0.76
1:U:461:ILE:HG21	1:U:520:LEU:HD23	1.67	0.76
1:B:1051:TYR:CE2	1:B:1157:PRO:HD3	2.20	0.76
1:U:529:ARG:HA	1:U:532:ILE:HD12	1.65	0.76
1:U:540:ALA:HA	1:U:603:LEU:HD23	1.67	0.76
1:D:586:MET:HE2	1:D:590:GLN:HG3	1.67	0.76
1:B:434:VAL:HG21	1:B:440:GLY:CA	2.15	0.76
1:B:1038:VAL:HG13	1:B:1039:ARG:HG3	1.68	0.76
1:D:493:PHE:CE2	1:D:530:PRO:HB2	2.21	0.76
1:U:1191:LEU:O	1:U:1195:VAL:HG23	1.86	0.76
1:S:1241:ILE:HD12	1:S:1333:VAL:HG21	1.68	0.76
1:U:1165:PRO:HA	1:U:1355:TYR:CE2	2.20	0.76
1:B:1431:ARG:HH11	1:D:1423:GLN:CD	1.94	0.75
1:D:587:ASN:HB2	1:D:590:GLN:HB3	1.67	0.75
1:D:1296:THR:OG1	1:D:1302:VAL:HA	1.86	0.75
1:S:629:ARG:O	1:S:633:ILE:HG13	1.86	0.75
1:B:1058:MET:HG2	1:B:1065:LYS:HE3	1.67	0.75
1:B:1225:LEU:HD11	1:B:1244:ARG:CZ	2.15	0.75
1:S:494:ASP:HB3	1:S:497:LYS:HB2	1.68	0.75
1:S:1448:LEU:O	1:S:1452:ILE:HG13	1.86	0.75
1:S:1468:LEU:O	1:S:1471:ASP:HB2	1.86	0.75
1:S:443:THR:HG22	1:S:454:ILE:CD1	2.15	0.75
1:S:1111:GLY:HA2	1:S:1116:ASP:HB2	1.67	0.75
1:B:1123:PHE:O	1:D:585:GLU:HB3	1.86	0.75
1:S:1042:LEU:HD22	1:S:1046:HIS:HB3	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:620:MET:HE1	1:U:1019:ARG:NH1	2.02	0.75
1:S:1192:ILE:O	1:S:1196:LEU:HG	1.86	0.74
1:U:1358:HIS:O	1:U:1362:VAL:HG23	1.87	0.74
1:S:1254:GLY:HA3	1:S:1256:ARG:HH12	1.50	0.74
1:U:427:GLU:HA	1:U:501:HIS:CD2	2.22	0.74
1:B:1288:GLY:HA2	1:B:1309:ARG:NH1	2.02	0.74
1:S:1025:TYR:HA	1:U:511:VAL:HB	1.69	0.74
1:U:1034:ALA:O	1:U:1043:LYS:HE2	1.87	0.74
1:D:508:ASP:CG	1:D:583:LEU:HB2	2.13	0.74
1:S:1297:SER:HB2	1:S:1299:ARG:NH2	2.02	0.74
1:U:1218:PHE:HE2	1:U:1224:ILE:HD11	1.53	0.74
1:U:1377:ARG:HG2	1:U:1448:LEU:HD11	1.69	0.74
5:Y:18:DA:H2''	5:Y:19:DC:H5'	1.70	0.74
1:D:535:GLY:C	1:D:536:TYR:HD2	1.95	0.74
1:U:1182:ASN:O	1:U:1183:ILE:HG13	1.87	0.74
4:X:9:DG:N2	5:Y:12:DC:C2	2.51	0.74
1:B:1382:GLU:HG3	1:B:1445:TYR:HE2	1.52	0.74
1:B:469:LEU:HD12	1:B:472:ILE:HB	1.68	0.74
1:D:527:PHE:O	1:D:528:MET:HG2	1.88	0.74
1:B:433:LEU:HA	1:B:455:LEU:O	1.88	0.74
1:U:1265:PRO:HB2	1:U:1268:VAL:HG21	1.68	0.74
1:B:1031:VAL:HG23	1:B:1032:ALA:N	2.03	0.73
1:B:1219:PRO:HA	1:B:1485:ARG:HH11	1.52	0.73
1:B:1104:VAL:HG12	1:B:1105:ASP:H	1.53	0.73
5:H:10:DT:H2''	5:H:11:DA:N7	2.03	0.73
1:S:1306:ILE:O	1:S:1306:ILE:HG22	1.89	0.73
1:U:1448:LEU:O	1:U:1452:ILE:HG13	1.89	0.73
1:B:1029:VAL:O	1:B:1033:ARG:HB3	1.89	0.73
1:U:461:ILE:HD11	1:U:477:GLU:CB	2.18	0.73
1:U:1138:ASP:HA	1:U:1141:LYS:HE3	1.71	0.73
1:D:540:ALA:HA	1:D:603:LEU:HD22	1.70	0.73
1:D:531:LEU:HD11	1:D:536:TYR:HB2	1.70	0.73
1:B:1030:ILE:HG23	1:B:1035:LEU:HD12	1.69	0.73
1:D:1279:GLU:O	1:D:1283:ASP:HB2	1.89	0.73
1:U:1245:SER:OG	1:U:1264:ILE:HA	1.89	0.73
1:S:1350:GLU:O	1:S:1354:HIS:HD2	1.72	0.73
1:S:1408:MET:C	1:S:1412:GLN:HE21	1.96	0.73
1:S:1408:MET:O	1:S:1412:GLN:HG3	1.87	0.73
1:B:1192:ILE:HD13	1:B:1477:ARG:HB2	1.69	0.72
1:U:522:THR:HA	1:U:618:PHE:HE2	1.52	0.72
1:U:1299:ARG:H	1:U:1299:ARG:HD2	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:636:ASN:HD22	1:D:636:ASN:H	1.38	0.72
1:S:1204:ILE:HG13	1:S:1205:SER:H	1.53	0.72
1:S:1484:ARG:HG2	1:S:1486:THR:O	1.89	0.72
1:B:508:ASP:OD1	1:B:508:ASP:N	2.22	0.72
1:B:1046:HIS:HA	1:B:1049:ILE:HD12	1.71	0.72
1:B:1448:LEU:O	1:B:1452:ILE:HG13	1.90	0.72
1:D:430:GLU:HB2	1:D:502:LYS:O	1.90	0.72
1:S:1387:ALA:HA	1:S:1394:ILE:HG13	1.72	0.72
1:D:1259:ILE:HB	1:D:1306:ILE:HB	1.72	0.72
4:X:13:DC:N4	4:X:14:DC:C4	2.57	0.72
1:S:1079:HIS:NE2	1:S:1081:HIS:HD2	1.88	0.72
1:B:1113:MET:HE1	1:B:1302:VAL:HG22	1.71	0.71
4:G:12:DC:N4	5:H:9:DG:N2	2.38	0.71
1:S:1184:PRO:HB2	1:S:1216:PRO:HB3	1.72	0.71
1:D:1184:PRO:HB2	1:D:1216:PRO:HB3	1.71	0.71
1:S:1381:LEU:HD11	1:S:1444:GLU:OE2	1.90	0.71
1:U:1120:ALA:HB3	1:U:1123:PHE:CD1	2.24	0.71
1:U:1245:SER:OG	1:U:1265:PRO:HD3	1.90	0.71
1:U:1031:VAL:HA	1:U:1338:LEU:HD11	1.72	0.71
1:U:1206:ILE:O	1:U:1210:MET:HG3	1.89	0.71
1:D:543:PRO:HG3	1:D:594:THR:HB	1.72	0.71
1:D:1192:ILE:HD12	1:D:1477:ARG:CB	2.19	0.71
1:D:1468:LEU:O	1:D:1472:GLU:HG3	1.91	0.71
1:B:1381:LEU:HD13	1:B:1445:TYR:HA	1.71	0.71
1:S:1293:ARG:CZ	1:S:1293:ARG:HB2	2.21	0.71
1:U:1208:GLU:HA	1:U:1211:GLU:OE1	1.89	0.71
1:B:1071:VAL:HG13	1:B:1086:ILE:CG2	2.21	0.71
1:B:1408:MET:HB3	1:B:1412:GLN:NE2	2.04	0.71
1:B:1416:LYS:HA	1:B:1416:LYS:HE2	1.73	0.71
1:B:586:MET:HB3	1:B:590:GLN:HB3	1.71	0.71
1:S:1221:ALA:HB1	1:S:1485:ARG:O	1.90	0.71
1:B:459:GLY:HA2	2:E:8:DT:H2"	1.73	0.70
1:S:1233:ALA:HB1	1:S:1333:VAL:HG11	1.72	0.70
1:U:1059:THR:HG22	1:U:1128:MET:HE1	1.73	0.70
1:S:1286:ILE:HD12	1:S:1324:GLN:NE2	2.06	0.70
1:U:1135:LEU:HA	1:U:1162:ALA:HA	1.73	0.70
1:D:1242:GLN:NE2	1:D:1330:SER:HB3	2.05	0.70
1:S:1036:PRO:HA	1:S:1042:LEU:O	1.91	0.70
1:B:1408:MET:HE3	1:B:1412:GLN:HE22	1.57	0.70
1:S:1289:ILE:HG23	1:S:1306:ILE:HG23	1.74	0.70
1:B:1431:ARG:NH1	1:D:1423:GLN:HE22	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1136:LEU:HD23	1:U:1160:LEU:HD22	1.72	0.70
1:U:1292:LEU:HD12	1:U:1293:ARG:H	1.54	0.70
1:B:447:ARG:HD3	1:B:454:ILE:HD12	1.73	0.70
4:G:12:DC:H42	5:H:9:DG:N2	1.90	0.70
1:S:432:PHE:O	1:S:434:VAL:HG13	1.92	0.70
1:S:540:ALA:O	1:S:541:GLN:HG3	1.92	0.70
1:B:1104:VAL:HG12	1:B:1105:ASP:N	2.06	0.70
1:U:531:LEU:CD1	1:U:536:TYR:HB2	2.21	0.70
1:B:1238:ARG:HH11	1:B:1334:ASN:ND2	1.90	0.70
1:D:461:ILE:HG22	1:D:462:LEU:H	1.54	0.70
1:S:1026:ALA:O	1:S:1030:ILE:HG13	1.92	0.70
1:D:1204:ILE:H	1:D:1349:LYS:NZ	1.90	0.69
1:S:1090:MET:HA	1:S:1093:MET:HE2	1.74	0.69
4:G:11:DA:H2''	4:G:12:DC:H5'	1.73	0.69
1:S:1185:PRO:HD2	1:S:1218:PHE:CE1	2.27	0.69
1:S:1249:ILE:HD11	1:S:1318:LEU:HD23	1.72	0.69
4:G:12:DC:C4	5:H:9:DG:N2	2.41	0.69
1:S:423:SER:HB3	1:S:450:ARG:O	1.93	0.69
1:U:1080:PRO:HD2	1:U:1081:HIS:CD2	2.28	0.69
1:U:1153:ASN:C	1:U:1154:GLU:HG2	2.18	0.69
1:B:1431:ARG:NH1	1:D:1423:GLN:NE2	2.40	0.69
1:D:512:ASP:O	1:D:516:ILE:HG13	1.93	0.69
1:S:1026:ALA:HB1	1:U:633:ILE:HD11	1.75	0.69
1:S:1039:ARG:HH21	1:S:1159:VAL:HB	1.58	0.68
1:D:1029:VAL:HG11	1:D:1177:VAL:HG23	1.75	0.68
1:B:1408:MET:HE3	1:B:1412:GLN:NE2	2.08	0.68
1:S:1179:MET:O	5:Y:17:DC:H4'	1.93	0.68
1:U:494:ASP:OD1	1:U:497:LYS:HG3	1.93	0.68
1:B:469:LEU:HD13	1:B:472:ILE:HD12	1.75	0.68
1:D:587:ASN:HB2	1:D:590:GLN:CB	2.24	0.68
1:S:517:ARG:NH2	1:U:1021:SER:OG	2.26	0.68
1:S:1079:HIS:CE1	1:S:1081:HIS:HD2	2.11	0.68
1:U:464:VAL:O	1:U:472:ILE:HD11	1.93	0.68
1:U:487:THR:HG22	1:U:498:ALA:HB2	1.76	0.68
1:U:1093:MET:HG2	1:U:1099:TYR:CZ	2.29	0.68
1:S:1241:ILE:HD12	1:S:1333:VAL:CG2	2.24	0.68
1:B:1107:GLN:H	1:B:1110:PHE:HE1	1.41	0.68
1:S:1064:TYR:HE1	1:S:1127:ARG:CZ	2.07	0.68
1:S:1347:ASN:OD1	1:S:1347:ASN:N	2.24	0.67
1:B:1451:TYR:CE2	1:B:1455:LEU:HD11	2.28	0.67
1:U:1355:TYR:O	1:U:1359:GLN:HG2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1031:VAL:HA	1:D:1338:LEU:HD11	1.76	0.67
1:U:1222:GLY:N	1:U:1263:GLU:OE2	2.28	0.67
1:U:1458:ILE:HA	1:U:1464:VAL:CG1	2.24	0.67
1:B:1038:VAL:HG12	1:B:1338:LEU:O	1.95	0.67
1:D:1136:LEU:HD23	1:D:1160:LEU:HD22	1.77	0.67
1:D:1297:SER:C	1:D:1299:ARG:H	2.01	0.67
1:U:1346:ILE:HD12	1:U:1351:ALA:HA	1.76	0.67
1:B:464:VAL:HG22	1:B:522:THR:CG2	2.25	0.67
1:D:626:VAL:HG11	4:G:17:DG:H3'	1.76	0.67
1:S:1100:ARG:HH11	1:S:1100:ARG:HG3	1.60	0.67
1:S:587:ASN:HB2	1:S:590:GLN:HB2	1.75	0.67
1:B:636:ASN:O	1:B:637:ALA:O	2.13	0.67
2:E:3:DT:H3	5:H:18:DA:H61	1.42	0.67
1:S:1185:PRO:HD2	1:S:1218:PHE:CD1	2.30	0.67
1:S:1383:GLY:HA3	1:S:1421:GLN:HG2	1.77	0.67
1:B:1109:ASN:HB3	1:B:1119:ALA:HB2	1.77	0.67
1:B:1390:HIS:ND1	1:B:1390:HIS:N	2.43	0.67
5:Y:13:DA:N3	7:Y:1020:CPF:H161	2.09	0.67
1:D:434:VAL:CG1	1:D:506:MET:HE3	2.25	0.66
1:U:1243:MET:HE3	1:U:1329:THR:HG22	1.76	0.66
1:D:535:GLY:HA2	1:D:605:GLN:OE1	1.94	0.66
1:S:1299:ARG:H	1:S:1299:ARG:CD	2.02	0.66
1:U:421:CYS:H	1:U:453:ALA:HB2	1.60	0.66
1:S:1254:GLY:HA3	1:S:1256:ARG:NH1	2.11	0.66
1:S:1320:ASN:O	1:S:1324:GLN:HG3	1.95	0.66
1:D:1110:PHE:HE1	1:D:1124:THR:HB	1.61	0.66
1:D:1313:ASN:ND2	1:D:1316:VAL:HG23	2.10	0.66
1:S:1259:ILE:CD1	1:S:1318:LEU:HB2	2.24	0.66
1:S:1188:LEU:O	1:S:1192:ILE:HG13	1.95	0.66
1:U:425:SER:OG	1:U:428:GLU:HG2	1.95	0.66
1:U:434:VAL:HG23	1:U:436:GLY:H	1.59	0.66
1:S:540:ALA:HA	1:S:603:LEU:HD22	1.77	0.66
1:U:586:MET:HB2	1:U:591:LEU:CD1	2.25	0.66
1:B:1104:VAL:O	1:B:1129:THR:HG23	1.95	0.66
1:S:1101:TYR:HB3	1:S:1131:ILE:HD13	1.77	0.66
1:S:1232:ARG:HG3	1:S:1232:ARG:NH1	2.04	0.66
1:B:1286:ILE:HD12	1:B:1324:GLN:NE2	2.11	0.66
1:B:1430:LEU:O	1:B:1433:LEU:HG	1.96	0.66
1:D:419:ALA:HB1	1:D:447:ARG:HH12	1.61	0.66
1:D:1277:ILE:O	1:D:1281:VAL:HG23	1.96	0.66
1:D:1415:PHE:HB2	1:D:1417:LEU:HG	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1466:LEU:HD21	1:S:1470:ARG:HH21	1.61	0.66
1:B:461:ILE:HG22	1:B:462:LEU:H	1.59	0.65
1:D:1383:GLY:HA3	1:D:1421:GLN:HG2	1.78	0.65
1:S:1050:LEU:N	1:S:1050:LEU:HD23	2.10	0.65
1:D:586:MET:CE	1:D:590:GLN:HG3	2.26	0.65
1:D:1267:GLN:OE1	3:F:4:DC:H4'	1.96	0.65
1:S:1187:ASN:O	1:S:1191:LEU:HG	1.95	0.65
1:U:1100:ARG:HH12	1:U:1485:ARG:NE	1.95	0.65
1:D:508:ASP:OD1	1:D:583:LEU:HB2	1.97	0.65
1:S:461:ILE:HD11	1:S:477:GLU:HB2	1.78	0.65
1:S:543:PRO:HD2	1:S:586:MET:HE1	1.78	0.65
1:S:583:LEU:O	1:S:585:GLU:N	2.29	0.65
1:S:1067:SER:OG	1:S:1124:THR:O	2.13	0.65
1:U:1265:PRO:HB2	1:U:1268:VAL:CG2	2.26	0.65
4:X:18:DG:H2''	4:X:19:DC:C6	2.31	0.65
1:B:1325:THR:HB	1:B:1326:PRO:CD	2.25	0.65
1:U:1261:VAL:HG23	1:U:1304:VAL:O	1.95	0.65
1:D:620:MET:HE3	1:D:621:LEU:HG	1.78	0.65
1:S:1051:TYR:OH	1:S:1146:PHE:HE2	1.79	0.65
1:S:1256:ARG:CG	1:S:1310:LYS:HB2	2.23	0.65
1:S:1428:MET:HE3	1:U:1430:LEU:HD11	1.77	0.65
1:D:1280:LEU:HB3	1:D:1286:ILE:HG22	1.77	0.65
1:D:1395:ILE:O	1:D:1399:ARG:HG3	1.96	0.65
1:B:1346:ILE:HD12	1:B:1351:ALA:HA	1.78	0.65
1:D:433:LEU:HD23	1:D:455:LEU:HB3	1.78	0.65
1:D:1313:ASN:HD22	1:D:1316:VAL:H	1.44	0.65
1:S:589:ASP:CG	1:S:590:GLN:N	2.54	0.65
1:B:1273:MET:HG3	1:B:1326:PRO:HB2	1.78	0.65
1:D:430:GLU:CB	1:D:502:LYS:O	2.45	0.65
1:D:1132:THR:O	1:D:1135:LEU:HB2	1.97	0.65
1:U:461:ILE:HG21	1:U:520:LEU:CD2	2.26	0.65
1:U:1243:MET:SD	1:U:1266:PHE:HB3	2.37	0.65
1:U:1421:GLN:O	1:U:1425:ILE:HG13	1.97	0.65
5:Y:13:DA:C2	7:Y:1020:CPF:H161	2.31	0.65
1:B:1153:ASN:C	1:B:1154:GLU:HG2	2.21	0.65
1:B:1411:LEU:O	1:B:1415:PHE:HB2	1.97	0.65
1:S:1426:LEU:HB3	1:U:1431:ARG:HB3	1.79	0.65
1:B:1218:PHE:HB3	1:B:1266:PHE:HB2	1.79	0.65
1:B:1361:THR:O	1:B:1365:ARG:HG3	1.97	0.65
1:B:1381:LEU:HD12	1:B:1448:LEU:HD12	1.77	0.65
1:D:1031:VAL:HG12	1:D:1338:LEU:HD21	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:11:DA:H2"	5:Y:12:DC:OP2	1.96	0.65
1:B:597:ASN:HD22	1:B:598:PRO:HD2	1.61	0.64
1:S:531:LEU:O	1:S:536:TYR:HB2	1.96	0.64
1:S:1179:MET:O	1:S:1180:ALA:HB2	1.97	0.64
1:U:534:ALA:HB1	1:U:536:TYR:CE2	2.32	0.64
1:B:1183:ILE:HG12	1:B:1335:MET:HG2	1.79	0.64
1:B:1274:ILE:HD13	1:B:1294:ASP:HB2	1.79	0.64
1:B:1292:LEU:HG	1:B:1292:LEU:O	1.97	0.64
1:D:1050:LEU:N	1:D:1050:LEU:HD23	2.11	0.64
1:D:541:GLN:HE21	1:D:541:GLN:HA	1.61	0.64
2:E:4:DG:N2	5:H:18:DA:C2	2.65	0.64
1:S:525:TYR:HE2	1:S:526:ARG:NH1	1.96	0.64
1:S:529:ARG:O	1:S:533:GLU:HG3	1.98	0.64
1:U:427:GLU:HA	1:U:501:HIS:CG	2.32	0.64
1:D:1329:THR:HG22	1:D:1330:SER:H	1.62	0.64
1:D:1400:GLU:HG3	1:D:1400:GLU:O	1.95	0.64
1:S:1218:PHE:CG	1:S:1266:PHE:HB2	2.32	0.64
1:D:1049:ILE:C	1:D:1050:LEU:HD23	2.22	0.64
1:B:1346:ILE:HD12	1:B:1351:ALA:CA	2.28	0.64
1:D:493:PHE:HZ	1:D:495:LEU:HD13	1.62	0.64
1:D:1092:ARG:C	1:D:1094:ALA:H	2.04	0.64
1:S:1162:ALA:C	1:S:1164:PHE:H	2.03	0.64
1:B:447:ARG:CA	1:B:596:MET:HE1	2.26	0.64
1:B:1046:HIS:O	1:B:1047:ARG:C	2.40	0.64
1:B:1386:ILE:HG22	1:B:1387:ALA:N	2.11	0.64
1:U:632:PHE:HD1	1:U:636:ASN:ND2	1.96	0.64
1:U:1182:ASN:C	1:U:1183:ILE:HG13	2.23	0.64
1:B:540:ALA:HA	1:B:603:LEU:HD22	1.79	0.64
1:B:1029:VAL:HA	1:B:1033:ARG:CB	2.28	0.64
1:D:1196:LEU:O	1:D:1199:SER:OG	2.16	0.64
1:U:632:PHE:O	1:U:636:ASN:HB2	1.98	0.64
1:D:633:ILE:HG22	1:D:634:GLU:N	2.13	0.64
1:S:1245:SER:OG	1:S:1327:LEU:HD12	1.98	0.64
1:U:597:ASN:ND2	1:U:599:GLU:HG3	2.12	0.64
1:D:604:LEU:HD22	1:D:1012:ARG:HB2	1.80	0.64
1:S:1309:ARG:HG3	1:S:1309:ARG:NH1	2.05	0.64
1:B:1247:ALA:HA	1:B:1260:VAL:O	1.97	0.63
1:U:531:LEU:HD12	1:U:531:LEU:O	1.98	0.63
1:B:629:ARG:O	1:B:633:ILE:HG13	1.97	0.63
1:D:1030:ILE:HG22	1:D:1031:VAL:HG13	1.81	0.63
1:S:525:TYR:CE2	1:S:526:ARG:NH1	2.66	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1177:VAL:C	1:S:1179:MET:H	2.05	0.63
1:S:1452:ILE:O	1:S:1456:GLU:HG3	1.96	0.63
1:B:434:VAL:HG21	1:B:440:GLY:HA2	1.80	0.63
1:D:1231:ARG:HH11	1:D:1231:ARG:HG2	1.61	0.63
1:S:1025:TYR:CE2	1:U:515:HIS:CD2	2.86	0.63
1:S:1428:MET:HG3	1:S:1432:ARG:HG3	1.79	0.63
1:B:1215:GLY:HA2	1:B:1234:TYR:OH	1.99	0.63
1:D:1224:ILE:HD12	1:D:1486:THR:HG21	1.79	0.63
1:B:619:GLU:O	1:B:623:GLY:N	2.31	0.63
1:B:1247:ALA:HB2	1:B:1261:VAL:HG22	1.81	0.63
1:D:458:ARG:HD3	7:H:1020:CPF:H162	1.79	0.63
1:D:1440:LYS:O	1:D:1443:ALA:HB3	1.99	0.63
1:U:583:LEU:HD13	1:U:591:LEU:HD11	1.79	0.63
1:U:1335:MET:O	1:U:1345:LEU:HD12	1.98	0.63
1:B:430:GLU:CB	1:B:502:LYS:HB2	2.28	0.63
1:S:1130:LYS:HA	1:S:1133:LEU:HD12	1.81	0.63
1:S:1423:GLN:HA	1:S:1426:LEU:HD12	1.79	0.63
1:U:485:PHE:CE2	1:U:524:PHE:HE2	2.17	0.63
1:B:629:ARG:HB2	1:B:629:ARG:HH11	1.64	0.63
1:D:493:PHE:HE2	1:D:530:PRO:HB2	1.62	0.63
1:S:461:ILE:HD12	1:S:462:LEU:H	1.64	0.63
1:U:1042:LEU:CD1	1:U:1160:LEU:HD12	2.23	0.63
1:U:1157:PRO:C	1:U:1159:VAL:H	2.07	0.63
1:B:1380:ILE:HD12	1:B:1424:ALA:HB2	1.80	0.63
1:S:1258:ARG:HB3	1:S:1307:ASP:HA	1.80	0.63
1:U:1296:THR:HG23	1:U:1301:GLY:C	2.24	0.63
1:B:1029:VAL:C	1:B:1033:ARG:HB3	2.24	0.62
1:B:1413:GLN:HG2	1:B:1414:ARG:N	2.13	0.62
1:D:450:ARG:CZ	1:D:450:ARG:HB2	2.29	0.62
1:D:633:ILE:HD11	1:D:1026:ALA:HB1	1.80	0.62
1:U:530:PRO:HA	1:U:533:GLU:HG3	1.81	0.62
1:B:478:ILE:HG23	1:B:523:PHE:CZ	2.34	0.62
1:B:1027[B]:MET:HE2	1:B:1027[B]:MET:HA	1.80	0.62
1:B:1175:ILE:HD13	5:H:17:DC:N3	2.13	0.62
1:U:462:LEU:HG	1:U:463:ASN:N	2.12	0.62
1:U:485:PHE:HE2	1:U:524:PHE:HE2	1.46	0.62
1:B:1069:ARG:HG2	1:D:1072:GLY:O	2.00	0.62
1:D:541:GLN:HB2	1:D:602:ALA:HB3	1.79	0.62
1:D:1079:HIS:NE2	1:D:1081:HIS:HD2	1.96	0.62
1:U:586:MET:HB2	1:U:591:LEU:HD13	1.81	0.62
1:B:443:THR:HG22	1:B:454:ILE:HD11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1466:LEU:HD12	1:B:1466:LEU:O	1.98	0.62
3:F:8:DG:H8	3:F:8:DG:C5'	2.10	0.62
1:U:531:LEU:HD11	1:U:536:TYR:HB2	1.81	0.62
1:B:606:VAL:HG13	1:B:1014:ILE:HB	1.82	0.62
1:B:1292:LEU:HD13	1:B:1306:ILE:HG12	1.80	0.62
1:S:1045:VAL:O	1:S:1049:ILE:HG13	1.99	0.62
1:D:1231:ARG:HG2	1:D:1231:ARG:NH1	2.15	0.62
1:D:1391:ILE:HG23	1:D:1392:ASP:N	2.14	0.62
1:B:476:ASN:ND2	1:B:480:GLN:HG3	2.14	0.62
1:B:1066:LYS:HD3	1:B:1125:GLU:CG	2.30	0.62
1:S:621:LEU:O	1:S:629:ARG:HD3	2.00	0.62
1:U:435:GLU:HG3	1:U:507:THR:HA	1.80	0.62
1:S:1408:MET:SD	1:S:1426:LEU:HD11	2.39	0.62
1:U:508:ASP:CB	1:U:583:LEU:HD23	2.29	0.62
1:S:1314:ALA:HA	1:S:1317:ILE:HD12	1.80	0.62
1:S:1428:MET:HE3	1:U:1430:LEU:CD1	2.29	0.62
1:U:522:THR:CA	1:U:618:PHE:HE2	2.13	0.62
1:U:535:GLY:O	1:U:605:GLN:OE1	2.17	0.62
1:B:514:ALA:O	1:B:518:THR:HG23	2.00	0.62
1:B:1225:LEU:HD11	1:B:1244:ARG:NE	2.14	0.62
1:B:1029:VAL:HG13	1:B:1033:ARG:HD2	1.82	0.61
1:S:418:LEU:HG	1:S:418:LEU:O	2.00	0.61
1:U:1367:THR:HG21	1:U:1459:LEU:HD23	1.82	0.61
1:B:1409:GLU:CA	1:B:1412:GLN:HG3	2.30	0.61
1:B:1415:PHE:HB3	1:B:1417:LEU:HG	1.80	0.61
1:D:499:ARG:HG3	1:D:499:ARG:NH1	2.13	0.61
1:S:1191:LEU:O	1:S:1194:GLY:N	2.33	0.61
1:U:592:TRP:CD1	1:U:593:GLU:N	2.68	0.61
1:U:610:ASP:C	1:U:610:ASP:OD1	2.43	0.61
1:B:528:MET:O	1:B:531:LEU:HB3	2.00	0.61
1:B:1244:ARG:HG2	1:B:1245:SER:N	2.15	0.61
1:S:1177:VAL:O	1:S:1179:MET:N	2.32	0.61
1:S:1215:GLY:O	1:S:1217:ASP:N	2.34	0.61
1:U:493:PHE:CZ	1:U:531:LEU:HB2	2.29	0.61
1:B:431:ILE:HG22	1:B:503:ILE:HA	1.83	0.61
1:B:1290:THR:O	1:B:1291:ASP:HB2	2.00	0.61
1:S:1382:GLU:CG	1:S:1445:TYR:HE1	2.13	0.61
1:U:443:THR:HG23	1:U:596:MET:SD	2.40	0.61
1:B:1384:LEU:HD22	1:B:1428:MET:SD	2.40	0.61
1:D:1414:ARG:HD2	1:D:1415:PHE:CZ	2.35	0.61
1:S:1461:ASP:HB3	1:S:1464:VAL:HB	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1109:ASN:HB3	1:U:1119:ALA:HB2	1.81	0.61
1:S:1204:ILE:HG13	1:S:1205:SER:N	2.15	0.61
1:S:1329:THR:HG22	1:S:1330:SER:H	1.65	0.61
1:D:1381:LEU:O	1:D:1385:ARG:HG3	2.01	0.61
1:S:476:ASN:CG	1:S:480:GLN:HE21	2.09	0.61
1:S:519:LEU:HD23	1:S:622:MET:CE	2.30	0.61
1:B:1408:MET:O	1:B:1412:GLN:HG2	2.01	0.61
1:U:1067:SER:HB2	1:U:1121:MET:O	2.00	0.61
1:B:1431:ARG:HH12	1:D:1423:GLN:HE22	1.46	0.61
1:S:1344:LYS:NZ	1:S:1350:GLU:OE1	2.33	0.61
1:D:539:ILE:O	1:D:539:ILE:HG22	2.01	0.61
1:S:458:ARG:HH22	1:S:480:GLN:HE22	1.46	0.61
4:X:11:DA:C6	5:Y:10:DT:O4	2.53	0.61
1:B:1031:VAL:HG23	1:B:1032:ALA:H	1.64	0.60
1:B:1223:LEU:HD11	1:B:1246:ARG:CZ	2.31	0.60
1:D:1357:GLU:OE1	1:D:1357:GLU:HA	2.00	0.60
1:S:1398:ILE:HD11	1:S:1411:LEU:HD11	1.83	0.60
1:B:511:VAL:HB	1:B:1025:TYR:HA	1.83	0.60
1:B:1245:SER:OG	1:B:1264:ILE:HA	2.01	0.60
1:D:1292:LEU:CD1	1:D:1306:ILE:HG12	2.31	0.60
1:S:1071:VAL:HG13	1:S:1086:ILE:HD12	1.83	0.60
1:S:1255:GLY:HA3	1:S:1310:LYS:HE3	1.82	0.60
1:S:1399:ARG:CZ	1:U:1391:ILE:HG21	2.31	0.60
1:B:1387:ALA:HB2	1:B:1425:ILE:HD13	1.83	0.60
1:S:461:ILE:HD11	1:S:477:GLU:CB	2.32	0.60
1:S:1286:ILE:HD12	1:S:1324:GLN:HE22	1.66	0.60
1:U:420:ASP:HA	1:U:453:ALA:HB1	1.82	0.60
1:D:478:ILE:O	1:D:482:ILE:HG13	2.01	0.60
1:U:632:PHE:CD1	1:U:636:ASN:ND2	2.70	0.60
1:D:522:THR:HA	1:D:618:PHE:CE2	2.36	0.60
4:G:13:DC:O2	7:H:1020:CPF:H161	2.02	0.60
1:B:1149:ASN:C	1:B:1149:ASN:OD1	2.44	0.60
1:B:1259:ILE:HD13	1:B:1318:LEU:HB2	1.84	0.60
1:S:458:ARG:HD2	7:X:1020:CPF:H162	1.83	0.60
1:U:435:GLU:HG3	1:U:508:ASP:H	1.67	0.60
1:U:1186:HIS:NE2	1:U:1234:TYR:CE1	2.70	0.60
1:B:1219:PRO:HA	1:B:1485:ARG:NH1	2.16	0.60
1:B:1454:GLU:O	1:B:1457:THR:HB	2.02	0.60
1:U:1059:THR:HG22	1:U:1128:MET:CE	2.32	0.60
1:U:1064:TYR:CB	1:U:1125:GLU:HB3	2.31	0.60
1:B:443:THR:HG22	1:B:454:ILE:CD1	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1258:ARG:HD2	1:S:1305:VAL:CG1	2.32	0.60
1:U:1112:SER:OG	1:U:1116:ASP:OD1	2.19	0.60
1:B:1030:ILE:HG21	1:B:1343:PRO:HG3	1.84	0.59
1:B:1245:SER:HB3	1:B:1263:GLU:O	2.02	0.59
1:D:1049:ILE:HG22	1:D:1050:LEU:HD23	1.82	0.59
3:F:6:DT:C2	3:F:7:DA:C8	2.90	0.59
1:S:532:ILE:HD13	1:U:1014:ILE:HD12	1.83	0.59
1:S:1177:VAL:HG12	1:S:1178:GLY:N	2.17	0.59
1:B:514:ALA:HA	1:B:517:ARG:NH2	2.17	0.59
1:D:538:TYR:HA	1:D:604:LEU:O	2.03	0.59
1:U:511:VAL:O	1:U:514:ALA:HB3	2.02	0.59
1:D:435:GLU:HG3	1:D:516:ILE:HD12	1.83	0.59
1:D:1213:ILE:HG22	1:D:1213:ILE:O	2.02	0.59
1:S:1100:ARG:HA	1:S:1219:PRO:HB3	1.83	0.59
1:S:1029:VAL:O	1:S:1029:VAL:HG12	2.02	0.59
1:B:464:VAL:HG22	1:B:522:THR:HG23	1.84	0.59
1:S:1484:ARG:CG	1:S:1486:THR:O	2.49	0.59
1:U:1325:THR:C	1:U:1327:LEU:H	2.10	0.59
4:X:11:DA:N1	5:Y:10:DT:C4	2.66	0.59
1:B:469:LEU:CD1	1:B:472:ILE:HD12	2.32	0.59
1:D:475:ASN:ND2	4:G:14:DC:H5'	2.18	0.59
1:D:1051:TYR:O	1:D:1054:ASN:HB3	2.03	0.59
1:D:1133:LEU:O	1:D:1137:ARG:N	2.35	0.59
1:S:1403:THR:HG22	1:U:1436:LEU:HD12	1.84	0.59
1:U:1218:PHE:HD1	1:U:1266:PHE:CD2	2.20	0.59
1:D:1055:GLU:C	1:D:1057:GLY:H	2.10	0.59
4:G:10:DT:H2''	4:G:11:DA:N7	2.17	0.59
1:S:1368:GLN:O	1:S:1372:ARG:NH1	2.36	0.59
1:S:1403:THR:HG22	1:U:1436:LEU:CD1	2.32	0.59
1:U:1364:ARG:O	1:U:1367:THR:HB	2.02	0.59
3:W:8:DG:H5'	3:W:8:DG:C8	2.38	0.59
4:X:12:DC:C2	7:X:1020:CPF:H141	2.37	0.59
1:U:462:LEU:HA	5:Y:14:DC:O3'	2.03	0.59
1:B:1186:HIS:NE2	1:B:1234:TYR:OH	2.30	0.58
1:U:1087:TYR:O	1:U:1091:VAL:HB	2.03	0.58
1:B:1224:ILE:HA	1:B:1242:GLN:O	2.02	0.58
1:B:1024[A]:ASP:HA	1:B:1027[A]:MET:HE2	1.85	0.58
1:S:1067:SER:HB2	1:S:1121:MET:HB2	1.85	0.58
1:U:1183:ILE:HG12	1:U:1335:MET:HG2	1.83	0.58
3:W:8:DG:C4	7:X:1020:CPF:H132	2.38	0.58
1:D:1185:PRO:O	1:D:1217:ASP:N	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1406:VAL:O	1:S:1407:ALA:C	2.45	0.58
1:U:458:ARG:HH11	7:Y:1020:CPF:H152	1.68	0.58
1:U:1064:TYR:CD1	1:U:1127:ARG:HG2	2.38	0.58
1:B:597:ASN:O	1:B:601:ARG:HB3	2.02	0.58
1:S:587:ASN:HB2	1:S:590:GLN:CB	2.34	0.58
1:D:432:PHE:CD2	1:D:504:VAL:HB	2.39	0.58
1:D:1064:TYR:CD1	1:D:1127:ARG:HG2	2.37	0.58
1:D:1326:PRO:C	1:D:1328:GLN:N	2.60	0.58
1:B:447:ARG:CD	1:B:454:ILE:HD12	2.33	0.58
1:S:1042:LEU:HD22	1:S:1046:HIS:CB	2.33	0.58
1:S:1064:TYR:HE1	1:S:1127:ARG:NE	2.00	0.58
1:S:1185:PRO:HD3	1:S:1266:PHE:CE2	2.38	0.58
1:U:444:LYS:NZ	1:U:454:ILE:HD12	2.19	0.58
1:U:1190:GLU:O	1:U:1213:ILE:HG13	2.04	0.58
1:B:1051:TYR:CD2	1:B:1157:PRO:HD3	2.38	0.58
1:U:1049:ILE:HD13	1:U:1090:MET:HB2	1.86	0.58
1:B:463:ASN:OD1	1:B:465:GLU:HB3	2.04	0.58
1:B:525:TYR:O	1:B:529:ARG:HB2	2.04	0.58
1:B:1149:ASN:ND2	1:B:1154:GLU:HB2	2.19	0.58
1:D:443:THR:CG2	1:D:596:MET:SD	2.91	0.58
1:S:445:SER:O	1:S:588:ALA:HB1	2.04	0.58
1:S:602:ALA:C	1:S:603:LEU:HD23	2.28	0.58
1:B:1051:TYR:CZ	1:B:1157:PRO:HD3	2.39	0.58
1:B:1363:VAL:CG1	1:B:1468:LEU:HD23	2.34	0.58
1:D:1012:ARG:NH1	1:D:1016:SER:HB3	2.19	0.58
1:S:602:ALA:O	1:S:603:LEU:HD23	2.04	0.58
1:S:1060:PRO:O	1:S:1127:ARG:NH1	2.37	0.58
1:U:1380:ILE:HD12	1:U:1424:ALA:HB2	1.86	0.58
1:D:1132:THR:HG22	1:D:1136:LEU:HD11	1.86	0.57
1:S:1381:LEU:O	1:S:1385:ARG:HG3	2.04	0.57
1:U:1064:TYR:CE1	1:U:1127:ARG:HG2	2.39	0.57
1:U:1229:GLY:HA3	1:U:1240:SER:O	2.04	0.57
1:U:1347:ASN:ND2	1:U:1350:GLU:OE2	2.36	0.57
1:B:1096:ASP:HA	1:B:1102:PRO:HG3	1.86	0.57
1:S:620:MET:CE	1:U:1019:ARG:HH12	2.12	0.57
1:U:1060:PRO:CD	1:U:1133:LEU:HD21	2.34	0.57
1:U:1377:ARG:CG	1:U:1448:LEU:HD11	2.32	0.57
5:Y:12:DC:H2'	7:Y:1020:CPF:C14	2.32	0.57
1:B:1431:ARG:NH1	1:D:1423:GLN:CD	2.62	0.57
1:S:1093:MET:HE3	1:S:1104:VAL:HG21	1.85	0.57
1:U:1186:HIS:NE2	1:U:1234:TYR:HE1	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:597:ASN:HD22	1:B:598:PRO:CD	2.17	0.57
1:D:1362:VAL:HG12	1:D:1363:VAL:N	2.18	0.57
1:S:1451:TYR:HE2	1:S:1455:LEU:HD21	1.70	0.57
1:U:489:ILE:HG22	1:U:527:PHE:HB3	1.85	0.57
1:U:1014:ILE:O	1:U:1014:ILE:HG12	2.04	0.57
1:B:1022:PHE:O	1:B:1025:TYR:HB3	2.04	0.57
1:B:1064:TYR:CE2	1:B:1127:ARG:NH2	2.73	0.57
1:B:1149:ASN:HD22	1:B:1154:GLU:HB2	1.68	0.57
1:D:1176:ALA:HB3	1:D:1179:MET:O	2.04	0.57
1:S:1309:ARG:CG	1:S:1309:ARG:NH1	2.62	0.57
1:S:1321:LEU:C	1:S:1323:LYS:H	2.11	0.57
1:B:454:ILE:HG22	1:B:456:PRO:HD3	1.86	0.57
1:S:632:PHE:CE1	1:S:636:ASN:ND2	2.72	0.57
1:S:1319:ASN:O	1:S:1323:LYS:HG3	2.04	0.57
1:S:1451:TYR:CE2	1:S:1455:LEU:HD21	2.39	0.57
1:U:598:PRO:HA	1:U:601:ARG:NE	2.19	0.57
1:U:1059:THR:HA	1:U:1128:MET:CE	2.29	0.57
1:B:1270:LYS:O	1:B:1274:ILE:HG13	2.04	0.57
1:D:1329:THR:HG22	1:D:1330:SER:N	2.18	0.57
5:H:10:DT:H2"	5:H:11:DA:C8	2.39	0.57
1:S:1072:GLY:O	1:U:1069:ARG:HG3	2.05	0.57
1:D:443:THR:HG22	1:D:454:ILE:CD1	2.32	0.57
1:D:1338:LEU:HD23	1:D:1342:ARG:C	2.30	0.57
1:U:1038:VAL:HG13	1:U:1039:ARG:HG3	1.86	0.57
1:U:1244:ARG:HH21	1:U:1322:TYR:HB3	1.70	0.57
1:B:506:MET:SD	1:B:595:THR:HG21	2.45	0.57
1:S:456:PRO:O	1:S:457:LEU:HG	2.04	0.57
1:U:477:GLU:N	1:U:477:GLU:OE1	2.38	0.57
1:U:1268:VAL:HG12	1:U:1269:ASN:N	2.20	0.57
1:U:1280:LEU:HD13	1:U:1286:ILE:HD12	1.87	0.57
1:B:457:LEU:HD12	1:B:477:GLU:HG3	1.87	0.57
1:B:636:ASN:O	1:B:637:ALA:C	2.48	0.57
1:D:1087:TYR:HB2	1:D:1121:MET:HE2	1.86	0.57
1:D:1277:ILE:HB	1:D:1292:LEU:HD21	1.86	0.57
4:G:11:DA:N1	5:H:10:DT:O4	2.38	0.57
1:S:608:LEU:HD11	1:S:611:ALA:HA	1.87	0.57
1:B:501:HIS:HA	1:B:536:TYR:CD1	2.40	0.56
1:D:1449:LEU:HD23	1:D:1452:ILE:HD12	1.86	0.56
1:S:534:ALA:O	1:S:536:TYR:HD2	1.88	0.56
1:S:1217:ASP:HA	1:S:1486:THR:HB	1.87	0.56
1:S:1231:ARG:O	1:S:1235:GLU:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1215:GLY:HA3	1:U:1230:ILE:HD13	1.86	0.56
1:D:543:PRO:HG3	1:D:594:THR:CB	2.35	0.56
3:F:8:DG:C8	3:F:8:DG:C5'	2.86	0.56
1:B:1058:MET:SD	1:B:1065:LYS:HG3	2.46	0.56
1:B:1058:MET:HE2	1:B:1065:LYS:HG3	1.86	0.56
1:B:1200:LYS:O	1:B:1202:PRO:HD3	2.06	0.56
1:D:431:ILE:HG22	1:D:503:ILE:HG13	1.86	0.56
1:D:458:ARG:HB2	7:H:1020:CPF:C17	2.32	0.56
1:S:1042:LEU:HD13	1:S:1047:ARG:HA	1.87	0.56
1:S:1318:LEU:HD12	1:S:1318:LEU:O	2.05	0.56
1:U:473:LEU:C	1:U:474:ASN:HD22	2.14	0.56
1:U:1289:ILE:HG22	1:U:1290:THR:H	1.70	0.56
1:U:1289:ILE:HG22	1:U:1290:THR:N	2.18	0.56
1:U:1358:HIS:HD2	1:U:1359:GLN:HE21	1.52	0.56
1:U:1368:GLN:O	1:U:1372:ARG:HD3	2.04	0.56
5:Y:11:DA:H1'	5:Y:12:DC:H5''	1.87	0.56
1:U:1045:VAL:O	1:U:1049:ILE:HG13	2.06	0.56
1:U:1054:ASN:HB2	1:U:1136:LEU:CD1	2.34	0.56
1:U:1230:ILE:HA	1:U:1241:ILE:HD11	1.86	0.56
1:B:1270:LYS:NZ	1:B:1294:ASP:OD2	2.38	0.56
1:S:469:LEU:HG	1:S:473:LEU:HG	1.88	0.56
1:U:541:GLN:OE1	1:U:602:ALA:HB1	2.04	0.56
1:B:1029:VAL:HA	1:B:1033:ARG:HB2	1.88	0.56
1:B:1408:MET:O	1:B:1410:SER:N	2.39	0.56
1:D:526:ARG:C	1:D:527:PHE:CD1	2.84	0.56
1:U:1367:THR:CG2	1:U:1459:LEU:HD23	2.36	0.56
1:U:1464:VAL:HG12	1:U:1465:LEU:N	2.18	0.56
1:B:589:ASP:OD1	1:B:590:GLN:N	2.38	0.56
1:D:621:LEU:O	1:D:629:ARG:HD3	2.06	0.56
1:S:1068:ALA:HA	1:S:1121:MET:HE2	1.87	0.56
1:S:1071:VAL:CG2	1:S:1121:MET:HE1	2.36	0.56
1:S:1187:ASN:OD1	1:S:1190:GLU:N	2.38	0.56
1:S:1247:ALA:HA	1:S:1260:VAL:O	2.05	0.56
1:S:1283:ASP:CB	1:S:1285:LYS:HE3	2.34	0.56
1:S:1454:GLU:O	1:S:1457:THR:HB	2.06	0.56
1:B:1441:ILE:HG22	1:B:1442:GLU:N	2.20	0.56
1:D:1164:PHE:O	1:D:1166:ASN:N	2.39	0.56
1:S:543:PRO:HD3	1:S:594:THR:HB	1.88	0.56
1:U:508:ASP:HB3	1:U:583:LEU:CD2	2.30	0.56
1:U:1135:LEU:HD23	1:U:1162:ALA:HA	1.88	0.56
1:B:1079:HIS:CE1	1:B:1081:HIS:HD2	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1427:ASP:OD1	1:D:1431:ARG:NH2	2.39	0.56
1:D:472:ILE:O	1:D:478:ILE:HG21	2.05	0.56
1:S:461:ILE:O	1:S:519:LEU:HD13	2.04	0.56
1:U:1084:SER:O	1:U:1088:GLU:HB2	2.05	0.56
1:U:1273:MET:O	1:U:1277:ILE:HG13	2.06	0.56
1:D:501:HIS:O	1:D:536:TYR:HA	2.05	0.56
1:D:1110:PHE:CE1	1:D:1124:THR:HB	2.39	0.56
5:H:12:DC:H2'	5:H:13:DA:H5'	1.86	0.56
1:S:476:ASN:ND2	1:S:480:GLN:HE21	2.04	0.56
1:S:1288:GLY:O	1:S:1308:VAL:HG22	2.06	0.56
1:S:1382:GLU:HG2	1:S:1445:TYR:CE1	2.41	0.56
1:U:517:ARG:HD2	1:U:539:ILE:HG21	1.87	0.56
1:U:1153:ASN:O	1:U:1154:GLU:HG2	2.06	0.56
1:U:1192:ILE:HD12	1:U:1477:ARG:CB	2.33	0.56
1:B:1080:PRO:O	1:B:1081:HIS:CG	2.59	0.55
1:B:1196:LEU:O	1:B:1200:LYS:HG3	2.05	0.55
1:D:430:GLU:HA	1:D:500:TYR:HB3	1.89	0.55
1:D:1127:ARG:O	1:D:1128:MET:O	2.24	0.55
1:S:626:VAL:HG11	4:X:18:DG:OP2	2.06	0.55
1:S:1197:SER:OG	1:S:1212:ASP:OD2	2.23	0.55
1:S:1325:THR:HB	1:S:1326:PRO:CD	2.35	0.55
1:U:533:GLU:HA	1:U:608:LEU:HD22	1.87	0.55
1:U:598:PRO:HB3	1:U:601:ARG:NH2	2.21	0.55
1:U:1218:PHE:CD1	1:U:1266:PHE:CD2	2.94	0.55
1:B:1222:GLY:C	1:B:1223:LEU:HD12	2.30	0.55
1:D:474:ASN:O	1:D:479:ARG:HD2	2.07	0.55
1:D:1058:MET:HE2	1:D:1065:LYS:CB	2.36	0.55
1:S:1122:ARG:HH11	1:U:1082:GLY:HA2	1.71	0.55
1:S:1177:VAL:CG1	1:S:1178:GLY:N	2.70	0.55
1:S:1185:PRO:HG2	1:S:1219:PRO:HD2	1.87	0.55
1:U:1038:VAL:HG12	1:U:1338:LEU:O	2.07	0.55
1:D:514:ALA:O	1:D:518:THR:HG23	2.06	0.55
1:S:1215:GLY:HA2	1:S:1234:TYR:OH	2.06	0.55
1:D:539:ILE:HB	1:D:604:LEU:HB2	1.88	0.55
1:U:435:GLU:HG3	1:U:508:ASP:N	2.22	0.55
1:U:589:ASP:CG	1:U:590:GLN:H	2.14	0.55
1:B:437:ASP:OD2	4:G:10:DT:H5'	2.06	0.55
1:B:1079:HIS:CE1	1:B:1081:HIS:CD2	2.95	0.55
1:S:418:LEU:HD13	1:S:454:ILE:O	2.07	0.55
1:S:1039:ARG:NH2	1:S:1159:VAL:HB	2.20	0.55
1:S:1073:ASP:O	1:S:1077:LYS:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:460:LYS:O	4:G:14:DC:H1'	2.06	0.55
1:D:1296:THR:HG1	1:D:1302:VAL:HA	1.71	0.55
1:S:1344:LYS:NZ	1:S:1346:ILE:HG22	2.22	0.55
1:U:1233:ALA:O	1:U:1237:GLY:N	2.39	0.55
1:U:1362:VAL:O	1:U:1363:VAL:C	2.48	0.55
3:F:8:DG:H2'	7:H:1020:CPF:H132	1.88	0.55
1:S:456:PRO:C	1:S:457:LEU:HG	2.31	0.55
1:S:1467:GLN:OE1	1:S:1467:GLN:HA	2.07	0.55
1:U:1041:GLY:HA2	1:U:1167:LEU:HD13	1.89	0.55
1:D:454:ILE:CG2	1:D:456:PRO:HD3	2.35	0.55
5:H:9:DG:H2'	5:H:10:DT:C6	2.42	0.55
1:U:1220:THR:O	1:U:1221:ALA:HB3	2.05	0.55
4:X:13:DC:N4	4:X:14:DC:N3	2.55	0.55
1:B:1136:LEU:HD21	1:B:1160:LEU:HD13	1.89	0.55
1:D:508:ASP:CA	1:D:583:LEU:HD23	2.37	0.55
1:D:1041:GLY:HA2	1:D:1167:LEU:HD13	1.88	0.55
1:S:420:ASP:HA	1:S:453:ALA:HB1	1.89	0.55
5:Y:13:DA:P	5:Y:13:DA:H2'	2.47	0.55
1:B:1220:THR:O	1:B:1221:ALA:HB3	2.06	0.54
1:D:596:MET:O	1:D:598:PRO:HD3	2.07	0.54
1:D:1184:PRO:O	1:D:1186:HIS:CE1	2.60	0.54
1:D:1451:TYR:CE1	1:D:1455:LEU:HD21	2.42	0.54
1:S:459:GLY:N	7:X:1020:CPF:H131	2.22	0.54
1:S:1265:PRO:HB2	1:S:1268:VAL:HG21	1.87	0.54
1:B:629:ARG:HB2	1:B:629:ARG:NH1	2.23	0.54
1:U:1246:ARG:HG2	1:U:1262:THR:OG1	2.07	0.54
1:B:606:VAL:CG1	1:B:1014:ILE:HD12	2.37	0.54
1:D:495:LEU:CD2	1:D:534:ALA:HB2	2.30	0.54
1:U:601:ARG:HD2	1:U:603:LEU:HG	1.90	0.54
1:U:1234:TYR:O	1:U:1347:ASN:HB2	2.06	0.54
1:B:1071:VAL:C	1:B:1073:ASP:N	2.62	0.54
1:D:1111:GLY:O	1:D:1112:SER:HB3	2.07	0.54
3:F:8:DG:H2'	7:H:1020:CPF:C13	2.38	0.54
1:S:1100:ARG:HG3	1:S:1100:ARG:NH1	2.22	0.54
1:B:434:VAL:HG21	1:B:440:GLY:N	2.22	0.54
1:B:447:ARG:HA	1:B:596:MET:CE	2.33	0.54
1:B:1149:ASN:OD1	1:B:1149:ASN:O	2.26	0.54
1:B:1218:PHE:CB	1:B:1266:PHE:HB2	2.38	0.54
4:G:13:DC:H5''	4:G:13:DC:H6	1.73	0.54
1:S:1386:ILE:HG23	1:S:1390:HIS:HD2	1.73	0.54
1:S:1387:ALA:O	1:S:1391:ILE:HA	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1411:LEU:O	1:S:1415:PHE:HB2	2.08	0.54
1:U:430:GLU:HB2	1:U:502:LYS:HB2	1.89	0.54
1:U:1049:ILE:HB	1:U:1093:MET:HE1	1.89	0.54
4:X:9:DG:C2	5:Y:12:DC:N3	2.75	0.54
1:B:619:GLU:O	1:B:623:GLY:CA	2.55	0.54
1:B:1113:MET:CE	1:B:1302:VAL:HG22	2.37	0.54
1:B:1230:ILE:H	1:B:1230:ILE:HD12	1.71	0.54
1:B:1380:ILE:HD12	1:B:1424:ALA:CB	2.37	0.54
1:D:435:GLU:OE2	3:F:8:DG:O3'	2.26	0.54
1:D:1150:TYR:CE2	1:D:1151:ASP:HB3	2.42	0.54
1:D:1469:VAL:HG12	1:D:1473:LEU:CD1	2.37	0.54
1:U:463:ASN:ND2	1:U:466:LYS:HG3	2.22	0.54
4:X:13:DC:H1'	7:X:1020:CPF:N3	2.21	0.54
1:B:420:ASP:OD2	1:B:499:ARG:NH2	2.39	0.54
1:B:1037:ASP:HB3	1:B:1040:ASP:OD1	2.08	0.54
1:B:1129:THR:HB	1:B:1131:ILE:HG22	1.90	0.54
1:B:1243:MET:HE3	1:B:1265:PRO:HB3	1.89	0.54
1:D:1191:LEU:HD23	1:D:1213:ILE:HD13	1.90	0.54
1:S:437:ASP:HB3	5:Y:9:DG:H5'	1.90	0.54
1:S:458:ARG:CD	1:S:477:GLU:OE2	2.56	0.54
1:S:1192:ILE:HD12	1:S:1477:ARG:HB2	1.89	0.54
1:D:1369:TYR:CZ	1:D:1373:LYS:HD2	2.42	0.54
1:S:1264:ILE:HB	1:S:1265:PRO:CD	2.38	0.54
1:D:1067:SER:HB2	1:D:1121:MET:O	2.07	0.54
1:D:1191:LEU:O	1:D:1195:VAL:HG23	2.08	0.54
1:D:1227:LYS:O	1:D:1231:ARG:HB2	2.08	0.54
1:S:538:TYR:HB3	1:S:604:LEU:O	2.07	0.54
1:S:1059:THR:HB	1:S:1060:PRO:CD	2.38	0.54
1:U:430:GLU:HB3	1:U:502:LYS:HE2	1.89	0.54
1:U:1100:ARG:HH12	1:U:1485:ARG:CZ	2.20	0.54
1:U:1461:ASP:OD2	1:U:1463:GLU:N	2.40	0.54
1:B:1336:ILE:HG23	1:B:1344:LYS:O	2.08	0.54
1:D:1266:PHE:O	1:D:1267:GLN:HB2	2.08	0.54
5:H:9:DG:C2'	5:H:10:DT:C6	2.91	0.54
1:S:1276:LYS:O	1:S:1280:LEU:HG	2.07	0.54
1:S:1474:THR:HG23	1:S:1477:ARG:NH2	2.23	0.54
1:B:1283:ASP:O	1:B:1285:LYS:HG3	2.08	0.53
1:B:1349:LYS:O	1:B:1350:GLU:C	2.51	0.53
1:D:494:ASP:C	1:D:496:ALA:H	2.15	0.53
1:U:1232:ARG:HG2	1:U:1239:GLY:HA2	1.90	0.53
1:U:1234:TYR:CD1	1:U:1348:LEU:HD13	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1484:ARG:HD3	1:U:1486:THR:O	2.07	0.53
1:D:1384:LEU:O	1:D:1387:ALA:HB3	2.08	0.53
1:S:1177:VAL:CG1	1:S:1178:GLY:H	2.22	0.53
1:S:1190:GLU:HB3	1:S:1213:ILE:HA	1.91	0.53
1:U:470:ASP:O	1:U:474:ASN:ND2	2.41	0.53
1:U:1391:ILE:HG23	1:U:1392:ASP:N	2.23	0.53
1:B:522:THR:HG22	1:B:523:PHE:N	2.23	0.53
1:B:1382:GLU:HG3	1:B:1445:TYR:CE2	2.39	0.53
1:D:511:VAL:C	1:D:513:GLY:H	2.16	0.53
1:D:528:MET:O	1:D:531:LEU:HB3	2.08	0.53
1:D:1079:HIS:CE1	1:D:1081:HIS:HD2	2.26	0.53
4:X:13:DC:C1'	7:X:1020:CPF:H161	2.28	0.53
1:B:472:ILE:HD13	1:B:527:PHE:CZ	2.44	0.53
1:B:501:HIS:CD2	1:B:536:TYR:CE1	2.97	0.53
1:B:536:TYR:O	1:B:538:TYR:HD1	1.91	0.53
1:B:1361:THR:O	1:B:1361:THR:HG22	2.08	0.53
1:S:1087:TYR:O	1:S:1091:VAL:HG23	2.09	0.53
1:S:1100:ARG:NH2	1:S:1217:ASP:OD2	2.41	0.53
4:X:14:DC:H2'	4:X:15:DA:H8	1.73	0.53
1:D:482:ILE:HG23	1:D:489:ILE:HG23	1.91	0.53
1:D:1292:LEU:HD13	1:D:1306:ILE:HG12	1.90	0.53
1:D:1425:ILE:C	1:D:1427:ASP:H	2.17	0.53
1:U:1054:ASN:CB	1:U:1136:LEU:HD13	2.37	0.53
3:W:8:DG:H5'	3:W:8:DG:H8	1.71	0.53
1:B:493:PHE:CZ	1:B:531:LEU:HB2	2.43	0.53
1:D:1266:PHE:CE2	1:D:1267:GLN:HG3	2.44	0.53
1:D:1290:THR:OG1	1:D:1307:ASP:HB3	2.07	0.53
1:D:1369:TYR:CE2	1:D:1373:LYS:HD2	2.44	0.53
1:S:1202:PRO:HB2	1:S:1203:ASP:OD1	2.09	0.53
1:B:442:SER:HB2	1:B:591:LEU:HD23	1.91	0.53
1:B:1191:LEU:HD23	1:B:1213:ILE:HD13	1.91	0.53
1:D:1363:VAL:HG13	1:D:1366:ARG:HH21	1.70	0.53
1:S:468:ARG:O	1:S:472:ILE:HG13	2.09	0.53
1:S:1182:ASN:OD1	1:S:1331:PHE:CZ	2.62	0.53
1:S:1350:GLU:O	1:S:1354:HIS:CD2	2.56	0.53
1:U:444:LYS:HA	1:U:447:ARG:HG2	1.89	0.53
4:X:12:DC:O2	7:X:1020:CPF:H141	2.08	0.53
1:B:447:ARG:HD2	1:B:452:GLN:O	2.09	0.53
1:B:1262:THR:O	1:B:1263:GLU:HG3	2.08	0.53
1:U:591:LEU:O	1:U:592:TRP:C	2.51	0.53
1:U:1030:ILE:HG22	1:U:1031:VAL:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1100:ARG:NH1	1:U:1485:ARG:CZ	2.72	0.53
1:U:1091:VAL:O	1:U:1091:VAL:HG13	2.09	0.53
1:U:1190:GLU:HB3	1:U:1213:ILE:HA	1.91	0.53
1:U:1409:GLU:OE1	1:U:1409:GLU:HA	2.07	0.53
1:B:1325:THR:CB	1:B:1326:PRO:HD2	2.35	0.53
1:D:1071:VAL:HG11	1:D:1121:MET:HE1	1.91	0.53
1:D:1378:ALA:O	1:D:1382:GLU:HG3	2.08	0.53
4:G:11:DA:N1	5:H:10:DT:C4	2.77	0.53
5:H:18:DA:C5	5:H:19:DC:N4	2.76	0.53
1:S:1018:MET:HE2	1:U:618:PHE:CE2	2.44	0.53
1:S:1309:ARG:HD2	1:S:1309:ARG:O	2.09	0.53
1:U:493:PHE:HZ	1:U:531:LEU:CB	2.16	0.53
1:U:1037:ASP:O	1:U:1039:ARG:N	2.42	0.53
4:X:13:DC:C1'	7:X:1020:CPF:H142	2.39	0.53
1:D:1037:ASP:OD2	1:D:1038:VAL:N	2.42	0.52
1:D:1238:ARG:CG	1:D:1334:ASN:HD22	2.20	0.52
1:S:633:ILE:O	1:S:637:ALA:HB2	2.09	0.52
1:S:1026:ALA:CB	1:U:633:ILE:HD11	2.39	0.52
1:S:1289:ILE:HG12	1:S:1317:ILE:HG21	1.91	0.52
1:U:1046:HIS:O	1:U:1047:ARG:C	2.52	0.52
1:B:458:ARG:CB	7:G:1020:CPF:H162	2.30	0.52
1:B:1259:ILE:HG21	1:B:1318:LEU:HD13	1.91	0.52
1:B:1414:ARG:O	1:B:1415:PHE:CD1	2.63	0.52
1:D:636:ASN:N	1:D:636:ASN:ND2	2.42	0.52
1:D:1204:ILE:HG13	1:D:1205:SER:N	2.24	0.52
5:H:12:DC:H2''	5:H:13:DA:C5'	2.39	0.52
5:H:18:DA:H2''	5:H:19:DC:OP2	2.09	0.52
1:S:448:ASP:C	1:S:450:ARG:H	2.17	0.52
1:S:444:LYS:O	1:S:447:ARG:HG2	2.09	0.52
1:S:493:PHE:HE2	1:S:495:LEU:HB2	1.74	0.52
1:S:1077:LYS:O	1:S:1078:TYR:CG	2.62	0.52
1:S:1273:MET:HG3	1:S:1326:PRO:HB2	1.90	0.52
1:U:1136:LEU:O	1:U:1139:ILE:HB	2.08	0.52
1:B:1039:ARG:NH2	1:B:1159:VAL:HB	2.21	0.52
1:B:1190:GLU:CD	1:B:1484:ARG:HH21	2.16	0.52
1:D:454:ILE:HG22	1:D:456:PRO:CD	2.34	0.52
4:G:9:DG:H5'	7:G:1020:CPF:C12	2.37	0.52
1:S:506:MET:HG2	1:S:583:LEU:HD11	1.91	0.52
1:S:1151:ASP:C	1:S:1153:ASN:H	2.16	0.52
1:S:1224:ILE:O	1:S:1489:GLN:HB2	2.10	0.52
1:S:1321:LEU:C	1:S:1323:LYS:N	2.64	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:583:LEU:CD1	1:U:591:LEU:HD11	2.39	0.52
1:B:446:GLY:N	1:B:588:ALA:HB1	2.24	0.52
1:B:1149:ASN:O	1:B:1151:ASP:N	2.42	0.52
1:S:607:LYS:O	1:U:1014:ILE:HG22	2.09	0.52
1:B:1031:VAL:CG2	1:B:1032:ALA:N	2.70	0.52
1:B:1136:LEU:CD2	1:B:1160:LEU:HD13	2.40	0.52
1:D:1193:ASN:OD1	1:D:1193:ASN:N	2.41	0.52
1:D:1210:MET:SD	1:D:1234:TYR:HD2	2.31	0.52
1:S:1201:ASN:OD1	1:S:1202:PRO:HD2	2.09	0.52
1:S:1334:ASN:O	1:S:1336:ILE:N	2.42	0.52
1:U:1380:ILE:HD12	1:U:1424:ALA:CB	2.39	0.52
1:B:519:LEU:HD11	5:H:15:DC:H4'	1.91	0.52
1:S:418:LEU:C	1:S:418:LEU:HD12	2.35	0.52
1:S:1113:MET:C	1:S:1115:GLY:H	2.17	0.52
1:S:1139:ILE:HD12	1:S:1161:PRO:HD3	1.91	0.52
1:U:1101:TYR:N	1:U:1170:ASN:OD1	2.42	0.52
5:Y:13:DA:H2''	5:Y:14:DC:OP2	2.10	0.52
1:B:1363:VAL:HG21	1:B:1469:VAL:HG22	1.90	0.52
1:D:1079:HIS:NE2	1:D:1081:HIS:CD2	2.77	0.52
1:D:1367:THR:HG22	1:D:1459:LEU:HD21	1.91	0.52
1:D:1410:SER:O	1:D:1412:GLN:N	2.42	0.52
1:S:1092:ARG:HB3	1:S:1092:ARG:CZ	2.38	0.52
1:S:1162:ALA:C	1:S:1164:PHE:N	2.68	0.52
1:S:1243:MET:O	1:S:1328:GLN:HG3	2.10	0.52
1:S:1369:TYR:CD2	1:S:1370:ASN:N	2.78	0.52
1:U:442:SER:HB3	1:U:591:LEU:HD22	1.92	0.52
1:U:1163:ARG:NH2	1:U:1363:VAL:HG23	2.24	0.52
1:U:1186:HIS:NE2	1:U:1234:TYR:OH	2.42	0.52
1:U:1364:ARG:HB2	1:U:1465:LEU:HD11	1.90	0.52
1:U:1414:ARG:HB3	1:U:1415:PHE:CD1	2.44	0.52
1:B:602:ALA:O	1:B:603:LEU:HD23	2.09	0.52
1:B:1030:ILE:HG22	1:B:1031:VAL:N	2.23	0.52
1:D:422:SER:OG	1:D:450:ARG:HG2	2.10	0.52
1:D:1092:ARG:C	1:D:1094:ALA:N	2.64	0.52
1:S:521:LEU:HD21	1:S:606:VAL:HG11	1.91	0.52
1:S:1049:ILE:O	1:S:1053:LEU:HG	2.09	0.52
1:S:1258:ARG:HD2	1:S:1305:VAL:HG11	1.92	0.52
1:S:1344:LYS:HZ2	1:S:1346:ILE:HG22	1.75	0.52
1:S:1383:GLY:CA	1:S:1421:GLN:HG2	2.40	0.52
1:U:632:PHE:HD1	1:U:636:ASN:HD22	1.56	0.52
1:U:1040:ASP:CG	1:U:1042:LEU:HD12	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1091:VAL:O	1:U:1091:VAL:CG1	2.57	0.52
1:U:1476:ILE:C	1:U:1478:ASP:H	2.18	0.52
1:B:433:LEU:HD12	1:B:505:ILE:HG12	1.91	0.52
1:B:1218:PHE:O	1:B:1221:ALA:N	2.37	0.52
1:D:419:ALA:HB1	1:D:447:ARG:NH1	2.24	0.52
1:S:1289:ILE:CG1	1:S:1317:ILE:HG21	2.40	0.52
1:S:1490:LEU:HD12	1:S:1490:LEU:O	2.09	0.52
1:U:461:ILE:HG22	1:U:519:LEU:HD13	1.91	0.52
1:U:540:ALA:HA	1:U:603:LEU:CD2	2.38	0.52
1:B:1363:VAL:HG13	1:B:1366:ARG:NH2	2.20	0.51
1:D:1030:ILE:HG21	1:D:1343:PRO:CG	2.38	0.51
1:S:1382:GLU:CG	1:S:1445:TYR:CE1	2.93	0.51
1:U:478:ILE:O	1:U:482:ILE:HG13	2.09	0.51
1:U:501:HIS:O	1:U:536:TYR:HB3	2.10	0.51
1:B:621:LEU:O	1:B:629:ARG:CD	2.58	0.51
1:B:1201:ASN:C	1:B:1203:ASP:H	2.16	0.51
1:D:504:VAL:HG11	1:D:540:ALA:HB2	1.92	0.51
1:S:1387:ALA:HA	1:S:1394:ILE:CG1	2.40	0.51
1:U:1381:LEU:O	1:U:1385:ARG:HG3	2.10	0.51
1:B:1431:ARG:CG	1:D:1426:LEU:O	2.51	0.51
1:D:625:VAL:HG21	1:D:628:ASN:ND2	2.26	0.51
1:D:1469:VAL:HG12	1:D:1473:LEU:HD12	1.93	0.51
1:S:441:GLY:HA3	1:S:1109:ASN:ND2	2.20	0.51
1:S:494:ASP:CB	1:S:497:LYS:HD2	2.40	0.51
1:S:630:ARG:HA	1:S:633:ILE:HD12	1.92	0.51
1:S:1463:GLU:OE2	1:S:1466:LEU:HD23	2.10	0.51
1:U:485:PHE:O	1:U:499:ARG:HG3	2.10	0.51
1:U:592:TRP:CG	1:U:593:GLU:N	2.79	0.51
1:U:1041:GLY:HA2	1:U:1167:LEU:CD1	2.40	0.51
1:B:418:LEU:HD12	1:B:419:ALA:N	2.25	0.51
1:B:1151:ASP:OD1	1:B:1153:ASN:HB2	2.10	0.51
1:S:630:ARG:HG3	1:U:1179:MET:HE3	1.91	0.51
1:S:1051:TYR:CZ	1:S:1157:PRO:HD3	2.45	0.51
1:S:1071:VAL:HG12	1:S:1075:MET:CE	2.39	0.51
1:S:1391:ILE:O	1:S:1395:ILE:HG12	2.10	0.51
1:U:1037:ASP:C	1:U:1039:ARG:H	2.18	0.51
1:U:1267:GLN:OE1	1:U:1331:PHE:HE1	1.93	0.51
1:U:1301:GLY:O	1:U:1302:VAL:C	2.53	0.51
1:B:1309:ARG:O	1:B:1310:LYS:O	2.29	0.51
1:D:500:TYR:O	1:D:536:TYR:CD1	2.63	0.51
1:D:1055:GLU:C	1:D:1057:GLY:N	2.68	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1060:PRO:HD3	1:D:1128:MET:CB	2.41	0.51
2:E:8:DT:C2	7:G:1020:CPF:H132	2.45	0.51
1:S:1222:GLY:HA2	1:S:1263:GLU:HB3	1.92	0.51
1:S:1295:GLU:O	1:S:1300:THR:HG21	2.10	0.51
1:U:1201:ASN:O	1:U:1202:PRO:C	2.54	0.51
1:U:1452:ILE:O	1:U:1456:GLU:HG3	2.10	0.51
1:B:435:GLU:HG2	1:B:507:THR:HB	1.92	0.51
1:D:1105:ASP:O	1:D:1126:ALA:HA	2.11	0.51
1:S:1221:ALA:HA	1:S:1485:ARG:C	2.36	0.51
1:U:1030:ILE:HG12	1:U:1176:ALA:HB1	1.93	0.51
1:D:472:ILE:C	1:D:474:ASN:H	2.19	0.51
1:D:1179:MET:C	4:G:17:DG:H4'	2.36	0.51
1:S:1241:ILE:CD1	1:S:1333:VAL:HG21	2.38	0.51
1:S:1297:SER:HG	1:S:1300:THR:HG1	1.57	0.51
1:U:1290:THR:OG1	1:U:1291:ASP:N	2.43	0.51
1:U:1295:GLU:OE1	1:U:1305:VAL:HG21	2.10	0.51
1:B:1416:LYS:HE2	1:B:1416:LYS:CA	2.37	0.51
1:D:517:ARG:NH1	1:D:517:ARG:HB2	2.25	0.51
1:S:1321:LEU:HB3	1:S:1327:LEU:HD23	1.92	0.51
1:U:586:MET:HB2	1:U:591:LEU:HD12	1.93	0.51
1:U:1087:TYR:CZ	1:U:1121:MET:HA	2.45	0.51
1:B:1103:LEU:HD21	1:B:1170:ASN:HD21	1.76	0.51
1:B:1153:ASN:O	1:B:1154:GLU:CG	2.56	0.51
1:D:1390:HIS:HB3	1:D:1393:GLU:OE2	2.11	0.51
1:S:1122:ARG:NH1	1:U:1082:GLY:HA2	2.26	0.51
1:U:1320:ASN:HB3	1:U:1324:GLN:HE21	1.76	0.51
1:U:1335:MET:O	1:U:1345:LEU:CD1	2.59	0.51
1:B:1244:ARG:HA	1:B:1328:GLN:HG3	1.92	0.51
1:D:522:THR:HA	1:D:618:PHE:HE2	1.76	0.51
1:S:1151:ASP:O	1:S:1153:ASN:N	2.42	0.51
1:S:1355:TYR:O	1:S:1358:HIS:HB3	2.10	0.51
1:U:435:GLU:OE1	1:U:508:ASP:OD1	2.29	0.51
1:U:1093:MET:HB3	1:U:1104:VAL:HG23	1.92	0.51
1:U:1316:VAL:HA	1:U:1319:ASN:HB2	1.93	0.51
1:D:633:ILE:CD1	1:D:1026:ALA:HB1	2.41	0.50
1:D:1297:SER:C	1:D:1299:ARG:N	2.69	0.50
1:S:458:ARG:HD2	1:S:477:GLU:OE2	2.11	0.50
1:B:1104:VAL:CG1	1:B:1105:ASP:N	2.74	0.50
1:D:1390:HIS:O	1:D:1394:ILE:HG12	2.11	0.50
1:S:421:CYS:N	1:S:453:ALA:HB2	2.26	0.50
1:S:422:SER:O	1:S:424:LYS:HD2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1067:SER:CB	1:S:1121:MET:HB2	2.41	0.50
1:S:1071:VAL:CG1	1:S:1075:MET:HE2	2.37	0.50
1:S:1406:VAL:O	1:S:1408:MET:N	2.44	0.50
1:U:430:GLU:CB	1:U:502:LYS:HB2	2.41	0.50
1:D:1293:ARG:HH22	1:D:1305:VAL:HG11	1.77	0.50
1:S:459:GLY:HA3	7:X:1020:CPF:C13	2.37	0.50
1:S:597:ASN:HD22	1:S:598:PRO:HD2	1.76	0.50
1:S:1090:MET:HA	1:S:1093:MET:CE	2.40	0.50
1:S:1100:ARG:NH1	1:S:1101:TYR:CZ	2.79	0.50
1:S:1269:ASN:O	1:S:1270:LYS:C	2.54	0.50
1:S:1433:LEU:HD23	1:S:1433:LEU:N	2.26	0.50
1:U:481:MET:HG2	1:U:485:PHE:CZ	2.46	0.50
1:B:1080:PRO:C	1:B:1081:HIS:CG	2.89	0.50
1:D:514:ALA:O	1:D:517:ARG:HB3	2.12	0.50
1:D:1403:THR:OG1	1:D:1406:VAL:HG23	2.12	0.50
1:U:586:MET:HE2	1:U:591:LEU:HA	1.93	0.50
1:B:476:ASN:HD21	1:B:480:GLN:HG3	1.76	0.50
1:B:493:PHE:HZ	1:B:531:LEU:HB2	1.76	0.50
1:B:1040:ASP:OD2	1:B:1047:ARG:NH2	2.45	0.50
1:D:452:GLN:OE1	1:D:592:TRP:HZ3	1.95	0.50
1:D:540:ALA:HB1	1:D:595:THR:CG2	2.42	0.50
1:S:464:VAL:HG21	1:S:523:PHE:HA	1.94	0.50
1:S:471:ARG:HG2	1:S:471:ARG:NH1	2.20	0.50
1:S:1116:ASP:O	1:S:1118:ALA:N	2.44	0.50
1:S:1196:LEU:O	1:S:1200:LYS:HE3	2.11	0.50
1:S:1265:PRO:HB2	1:S:1268:VAL:CG2	2.42	0.50
1:B:1201:ASN:C	1:B:1201:ASN:OD1	2.55	0.50
1:B:1247:ALA:HA	1:B:1261:VAL:HA	1.93	0.50
1:B:1405:LYS:HE2	1:B:1409:GLU:OE1	2.12	0.50
1:D:1318:LEU:HG	1:D:1322:TYR:CE2	2.46	0.50
5:H:18:DA:C5	5:H:19:DC:C4	3.00	0.50
1:S:521:LEU:CD2	1:S:606:VAL:HG11	2.42	0.50
1:S:1246:ARG:NH2	1:S:1487:GLU:HB3	2.26	0.50
1:U:597:ASN:O	1:U:601:ARG:HB3	2.11	0.50
1:U:1270:LYS:O	1:U:1274:ILE:HG13	2.12	0.50
1:U:1349:LYS:O	1:U:1350:GLU:C	2.54	0.50
1:D:1150:TYR:CD2	1:D:1151:ASP:N	2.80	0.50
1:D:1204:ILE:H	1:D:1349:LYS:HZ1	1.58	0.50
1:S:1051:TYR:CZ	1:S:1146:PHE:HE2	2.29	0.50
1:S:1206:ILE:O	1:S:1210:MET:HG3	2.11	0.50
1:B:433:LEU:HB3	1:B:457:LEU:HD21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1059:THR:HA	1:B:1128:MET:HE3	1.94	0.50
1:B:1292:LEU:HA	1:B:1305:VAL:O	2.12	0.50
1:D:1408:MET:O	1:D:1412:GLN:HG3	2.12	0.50
1:D:1472:GLU:O	1:D:1476:ILE:HG12	2.12	0.50
1:S:1096:ASP:HA	1:S:1102:PRO:HG3	1.93	0.50
1:S:1381:LEU:HD13	1:S:1445:TYR:N	2.27	0.50
1:U:444:LYS:HZ2	1:U:454:ILE:HD12	1.77	0.50
1:U:592:TRP:HA	1:U:596:MET:HE2	1.94	0.50
1:U:1335:MET:HE3	1:U:1346:ILE:O	2.12	0.50
1:D:626:VAL:HA	1:D:629:ARG:NH2	2.27	0.50
1:D:1179:MET:O	4:G:17:DG:H4'	2.12	0.50
1:S:1037:ASP:O	1:S:1041:GLY:HA2	2.11	0.50
1:S:1072:GLY:C	1:U:1069:ARG:HG3	2.37	0.50
1:S:1193:ASN:CA	1:S:1196:LEU:HD12	2.36	0.50
1:S:1245:SER:CB	1:S:1261:VAL:HG11	2.41	0.50
1:U:433:LEU:HA	1:U:455:LEU:O	2.12	0.50
1:U:1157:PRO:O	1:U:1159:VAL:N	2.45	0.50
1:B:438:SER:O	1:B:439:ALA:C	2.55	0.49
1:B:493:PHE:CE2	1:B:530:PRO:HB2	2.46	0.49
1:D:1153:ASN:C	1:D:1154:GLU:HG2	2.36	0.49
1:D:1313:ASN:HB3	1:D:1316:VAL:CG2	2.42	0.49
1:D:1329:THR:CG2	1:D:1330:SER:H	2.24	0.49
1:U:1195:VAL:O	1:U:1198:LEU:HB3	2.11	0.49
1:U:1281:VAL:HG22	1:U:1289:ILE:HD12	1.94	0.49
1:U:1451:TYR:CE1	1:U:1455:LEU:HD21	2.47	0.49
1:D:475:ASN:C	1:D:475:ASN:OD1	2.54	0.49
1:D:604:LEU:HD13	1:D:1012:ARG:CB	2.42	0.49
1:D:1466:LEU:HD23	1:D:1470:ARG:HH22	1.77	0.49
1:S:463:ASN:C	1:S:463:ASN:OD1	2.55	0.49
1:S:1071:VAL:O	1:S:1074:VAL:N	2.46	0.49
1:U:1223:LEU:HD23	1:U:1487:GLU:OE2	2.12	0.49
1:B:1104:VAL:CG1	1:B:1105:ASP:H	2.22	0.49
1:D:587:ASN:O	1:D:591:LEU:HG	2.12	0.49
1:D:1060:PRO:HD3	1:D:1128:MET:HB2	1.94	0.49
1:S:455:LEU:HD12	1:S:456:PRO:HD2	1.93	0.49
1:S:1068:ALA:N	1:S:1121:MET:HE2	2.26	0.49
1:U:506:MET:SD	1:U:595:THR:HG21	2.51	0.49
1:U:1157:PRO:C	1:U:1159:VAL:N	2.68	0.49
1:B:525:TYR:HE2	1:B:526:ARG:NH1	2.10	0.49
1:B:611:ALA:O	1:B:615:ASP:OD2	2.30	0.49
1:D:461:ILE:HG22	1:D:462:LEU:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1030:ILE:HG23	1:S:1035:LEU:HD12	1.93	0.49
1:S:1401:SER:HB3	1:S:1406:VAL:HB	1.95	0.49
1:S:1432:ARG:O	1:S:1438:ARG:HG3	2.13	0.49
1:U:1198:LEU:C	1:U:1200:LYS:H	2.20	0.49
1:U:1292:LEU:HD12	1:U:1293:ARG:N	2.25	0.49
1:D:521:LEU:HD12	1:D:1018:MET:SD	2.53	0.49
1:D:602:ALA:C	1:D:603:LEU:HD23	2.38	0.49
1:S:418:LEU:O	1:S:420:ASP:N	2.43	0.49
1:U:476:ASN:O	1:U:480:GLN:N	2.40	0.49
1:U:1042:LEU:HD13	1:U:1047:ARG:HA	1.95	0.49
1:U:1090:MET:HG2	1:U:1090:MET:O	2.13	0.49
1:U:1193:ASN:HB3	1:U:1212:ASP:HB3	1.95	0.49
1:D:439:ALA:HB1	1:D:583:LEU:HD12	1.94	0.49
1:D:1068:ALA:HB2	1:D:1121:MET:HG3	1.94	0.49
1:D:1092:ARG:O	1:D:1094:ALA:N	2.46	0.49
1:S:525:TYR:HE2	1:S:526:ARG:HH12	1.60	0.49
1:S:1199:SER:HB2	1:S:1466:LEU:HD11	1.94	0.49
1:U:619:GLU:O	1:U:623:GLY:HA3	2.12	0.49
1:U:1104:VAL:HG12	1:U:1105:ASP:N	2.27	0.49
1:B:432:PHE:HB2	1:B:454:ILE:HG12	1.94	0.49
1:B:1094:ALA:HB2	1:B:1104:VAL:HB	1.94	0.49
1:B:1291:ASP:HB3	1:B:1307:ASP:OD2	2.13	0.49
1:S:1233:ALA:HB1	1:S:1333:VAL:CG1	2.40	0.49
1:S:1291:ASP:OD2	1:S:1292:LEU:N	2.46	0.49
1:S:1385:ARG:O	1:S:1388:LEU:HB2	2.12	0.49
1:U:1192:ILE:CD1	1:U:1477:ARG:HB2	2.38	0.49
1:U:1296:THR:HG23	1:U:1302:VAL:N	2.27	0.49
1:B:1382:GLU:CG	1:B:1445:TYR:HE2	2.22	0.49
1:D:539:ILE:O	1:D:540:ALA:O	2.31	0.49
2:E:6:DG:N2	5:H:16:DG:N2	2.61	0.49
1:S:481:MET:O	1:S:485:PHE:CG	2.66	0.49
1:U:420:ASP:HA	1:U:453:ALA:CB	2.43	0.49
1:U:464:VAL:HG21	1:U:523:PHE:HA	1.95	0.49
1:U:1138:ASP:OD2	1:U:1366:ARG:HD3	2.12	0.49
1:B:431:ILE:HA	1:B:453:ALA:O	2.13	0.49
1:B:1064:TYR:O	1:B:1065:LYS:HD3	2.12	0.49
1:B:1092:ARG:C	1:B:1094:ALA:H	2.21	0.49
1:D:523:PHE:HD2	1:D:524:PHE:CD2	2.31	0.49
1:D:540:ALA:HB1	1:D:595:THR:HG23	1.95	0.49
1:D:1185:PRO:O	1:D:1217:ASP:O	2.31	0.49
1:S:437:ASP:N	5:Y:9:DG:H5'	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:518:THR:HG21	1:U:1022:PHE:HB2	1.94	0.49
1:S:620:MET:CE	1:U:1019:ARG:NH1	2.74	0.49
1:B:1147:ILE:HG23	1:B:1158:SER:HB3	1.95	0.49
1:S:1103:LEU:HD22	1:S:1135:LEU:HD11	1.94	0.49
1:S:1224:ILE:HD12	1:S:1488:ILE:HG12	1.95	0.49
1:U:508:ASP:O	1:U:513:GLY:HA3	2.12	0.49
1:U:1067:SER:CB	1:U:1121:MET:O	2.60	0.49
1:B:1030:ILE:O	1:B:1035:LEU:HB2	2.13	0.48
1:B:1071:VAL:O	1:B:1072:GLY:C	2.55	0.48
1:B:1225:LEU:HB2	1:B:1242:GLN:HB2	1.95	0.48
1:D:1030:ILE:HG23	1:D:1343:PRO:HG3	1.93	0.48
5:H:20:DA:OP1	5:H:20:DA:H4'	2.12	0.48
1:S:1177:VAL:C	1:S:1179:MET:N	2.70	0.48
1:S:1203:ASP:OD1	1:S:1203:ASP:N	2.46	0.48
1:S:1381:LEU:CD2	1:S:1441:ILE:HG23	2.43	0.48
1:U:487:THR:HG22	1:U:498:ALA:CB	2.42	0.48
1:U:1032:ALA:O	1:U:1033:ARG:HB2	2.13	0.48
1:U:1461:ASP:HB3	1:U:1464:VAL:CG2	2.43	0.48
1:B:1230:ILE:HA	1:B:1241:ILE:CD1	2.38	0.48
1:B:1290:THR:O	1:B:1291:ASP:CB	2.60	0.48
1:D:1390:HIS:N	1:D:1390:HIS:ND1	2.60	0.48
1:S:437:ASP:H	5:Y:9:DG:H5'	1.78	0.48
1:S:447:ARG:HG3	1:S:447:ARG:O	2.12	0.48
1:S:1225:LEU:HD12	1:S:1242:GLN:HB3	1.95	0.48
1:U:1225:LEU:HD21	1:U:1244:ARG:HD2	1.95	0.48
1:B:1067:SER:O	1:B:1071:VAL:HG23	2.13	0.48
1:B:1382:GLU:O	1:B:1383:GLY:C	2.56	0.48
1:B:1389:ASP:HB2	1:B:1390:HIS:ND1	2.29	0.48
1:B:1434:THR:HG21	1:D:1404:ASP:OD1	2.13	0.48
1:B:1450:ASN:O	1:B:1453:SER:HB3	2.14	0.48
1:D:426:PRO:O	1:D:429:CYS:HB2	2.12	0.48
1:D:1238:ARG:HG2	1:D:1334:ASN:ND2	2.24	0.48
5:H:15:DC:H2''	5:H:16:DG:O4'	2.12	0.48
1:S:461:ILE:HD12	1:S:462:LEU:N	2.27	0.48
1:S:1159:VAL:HG22	1:S:1160:LEU:N	2.27	0.48
1:D:446:GLY:C	1:D:592:TRP:HB2	2.39	0.48
1:D:1467:GLN:O	1:D:1468:LEU:C	2.56	0.48
1:S:1046:HIS:HE1	2:V:6:DG:OP1	1.97	0.48
1:S:1064:TYR:CE1	1:S:1127:ARG:NE	2.82	0.48
1:S:1288:GLY:O	1:S:1308:VAL:HG13	2.13	0.48
1:U:1230:ILE:HG23	1:U:1234:TYR:CE2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:511:VAL:O	1:B:514:ALA:HB3	2.13	0.48
1:B:619:GLU:O	1:B:623:GLY:HA3	2.13	0.48
1:B:1405:LYS:O	1:B:1409:GLU:HG3	2.13	0.48
1:D:475:ASN:O	1:D:478:ILE:HB	2.14	0.48
1:D:494:ASP:HB3	1:D:497:LYS:HE3	1.95	0.48
1:U:1226:GLY:C	1:U:1228:SER:H	2.20	0.48
1:U:1416:LYS:HB3	1:U:1416:LYS:HE2	1.54	0.48
4:X:11:DA:H2	5:Y:10:DT:H3	1.61	0.48
1:B:1025:TYR:O	1:B:1029:VAL:HG23	2.14	0.48
1:S:1386:ILE:HG23	1:S:1390:HIS:CD2	2.48	0.48
1:S:1401:SER:HB3	1:S:1407:ALA:H	1.78	0.48
1:U:1110:PHE:HZ	1:U:1125:GLU:O	1.97	0.48
1:B:431:ILE:HG21	1:B:485:PHE:HE1	1.79	0.48
1:D:508:ASP:HA	1:D:583:LEU:CD2	2.41	0.48
1:S:1318:LEU:HD12	1:S:1318:LEU:C	2.39	0.48
1:S:1439:ASP:O	1:S:1443:ALA:CB	2.62	0.48
1:U:1040:ASP:O	1:U:1166:ASN:ND2	2.44	0.48
1:B:1071:VAL:C	1:B:1073:ASP:H	2.21	0.48
1:B:1384:LEU:O	1:B:1385:ARG:C	2.56	0.48
1:D:1195:VAL:HA	1:D:1198:LEU:HB3	1.95	0.48
1:D:1277:ILE:HB	1:D:1292:LEU:CD2	2.43	0.48
7:H:1020:CPF:H1	7:H:1020:CPF:H121	1.41	0.48
1:S:1084:SER:HB2	1:S:1088:GLU:OE1	2.14	0.48
2:V:4:DG:H2''	2:V:5:DC:H5'	1.96	0.48
1:B:1060:PRO:HG2	1:B:1130:LYS:HA	1.96	0.48
1:B:1265:PRO:O	1:B:1268:VAL:HB	2.14	0.48
1:B:1325:THR:CB	1:B:1326:PRO:CD	2.90	0.48
1:D:487:THR:HB	1:D:493:PHE:CE1	2.49	0.48
1:D:488:GLY:O	1:D:493:PHE:HD1	1.96	0.48
1:D:1410:SER:O	1:D:1411:LEU:C	2.57	0.48
3:F:6:DT:N3	3:F:7:DA:N7	2.62	0.48
1:S:493:PHE:CE2	1:S:530:PRO:HB2	2.49	0.48
1:U:470:ASP:OD1	1:U:471:ARG:N	2.47	0.48
1:U:1134:GLU:O	1:U:1163:ARG:HG2	2.13	0.48
1:B:1029:VAL:HA	1:B:1033:ARG:HB3	1.95	0.47
1:B:1431:ARG:NH1	1:D:1423:GLN:OE1	2.34	0.47
1:B:1475:GLU:HA	1:B:1478:ASP:HB2	1.96	0.47
1:D:532:ILE:HA	1:D:537:VAL:CG2	2.42	0.47
1:D:1185:PRO:HG2	1:D:1218:PHE:HA	1.96	0.47
1:D:1287:ASP:OD1	1:D:1287:ASP:N	2.47	0.47
1:D:1383:GLY:H	1:D:1421:GLN:NE2	2.06	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4:DG:H2''	2:E:5:DC:H5'	1.95	0.47
1:S:1404:ASP:OD2	1:U:1431:ARG:HB2	2.15	0.47
1:U:1093:MET:HG2	1:U:1099:TYR:CE2	2.49	0.47
1:U:1346:ILE:HA	1:U:1350:GLU:OE1	2.13	0.47
1:B:517:ARG:O	1:B:521:LEU:HG	2.14	0.47
1:B:525:TYR:CE2	1:B:526:ARG:NH1	2.82	0.47
1:B:1031:VAL:CG2	1:B:1032:ALA:H	2.25	0.47
1:B:1087:TYR:O	1:B:1090:MET:N	2.47	0.47
1:D:429:CYS:O	1:D:430:GLU:HB3	2.14	0.47
1:D:458:ARG:CB	7:H:1020:CPF:H172	2.39	0.47
1:D:1038:VAL:HG11	1:D:1339:VAL:HG22	1.96	0.47
1:S:1051:TYR:CE2	1:S:1157:PRO:HD3	2.48	0.47
1:S:1246:ARG:HH22	1:S:1487:GLU:HB3	1.79	0.47
1:U:1101:TYR:O	1:U:1102:PRO:C	2.57	0.47
1:B:485:PHE:HD2	1:B:528:MET:HE1	1.79	0.47
1:D:485:PHE:CZ	1:D:524:PHE:CZ	3.03	0.47
1:D:1127:ARG:O	1:D:1128:MET:C	2.57	0.47
1:S:1013:ASN:HB3	1:S:1016:SER:CB	2.36	0.47
1:S:1083:ASP:HA	1:S:1086:ILE:HG13	1.95	0.47
1:S:1377:ARG:O	1:S:1378:ALA:C	2.57	0.47
1:U:1030:ILE:C	1:U:1032:ALA:H	2.20	0.47
1:U:1225:LEU:N	1:U:1225:LEU:HD23	2.29	0.47
1:U:1406:VAL:O	1:U:1409:GLU:N	2.47	0.47
1:B:1120:ALA:HB3	1:B:1123:PHE:HD1	1.79	0.47
1:D:432:PHE:CD1	1:D:596:MET:HE3	2.48	0.47
1:D:485:PHE:CE2	1:D:524:PHE:CE2	3.02	0.47
1:D:1079:HIS:CD2	1:D:1081:HIS:HD2	2.32	0.47
1:D:1161:PRO:O	1:D:1162:ALA:C	2.56	0.47
1:D:1349:LYS:O	1:D:1350:GLU:C	2.57	0.47
5:H:12:DC:C2'	5:H:13:DA:O5'	2.63	0.47
1:S:418:LEU:O	1:S:418:LEU:CG	2.62	0.47
1:S:476:ASN:CG	1:S:480:GLN:NE2	2.71	0.47
1:S:1022:PHE:O	1:S:1025:TYR:HB3	2.14	0.47
1:S:1181:THR:OG1	1:S:1336:ILE:O	2.26	0.47
1:U:592:TRP:O	1:U:593:GLU:C	2.56	0.47
3:W:7:DA:H2''	3:W:8:DG:C5'	2.35	0.47
4:X:14:DC:H2'	4:X:15:DA:C8	2.49	0.47
1:B:512:ASP:OD2	2:E:8:DT:H5'	2.14	0.47
1:B:1080:PRO:HD2	1:B:1081:HIS:CD2	2.49	0.47
1:B:1406:VAL:O	1:B:1410:SER:N	2.47	0.47
1:D:536:TYR:CD2	1:D:536:TYR:N	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1241:ILE:HD12	1:D:1333:VAL:CG2	2.44	0.47
1:D:1483:ASP:OD1	1:D:1483:ASP:N	2.44	0.47
1:S:1091:VAL:HG12	1:S:1095:GLN:NE2	2.28	0.47
1:S:1093:MET:HB3	1:S:1104:VAL:HG23	1.95	0.47
1:S:1215:GLY:HA3	1:S:1488:ILE:CD1	2.40	0.47
1:U:1028:SER:O	1:U:1029:VAL:C	2.58	0.47
1:U:1230:ILE:HG23	1:U:1234:TYR:HE2	1.78	0.47
1:B:469:LEU:HG	1:B:473:LEU:HG	1.97	0.47
1:B:1467:GLN:NE2	1:B:1471:ASP:OD1	2.43	0.47
1:D:626:VAL:HG22	1:D:629:ARG:HH21	1.77	0.47
1:D:1402:ASP:CG	1:D:1403:THR:H	2.23	0.47
1:D:1445:TYR:CE1	1:D:1449:LEU:HD11	2.50	0.47
1:D:1461:ASP:OD1	1:D:1464:VAL:HG23	2.15	0.47
1:U:1022:PHE:CD2	1:U:1022:PHE:O	2.68	0.47
1:U:1031:VAL:HA	1:U:1338:LEU:CD1	2.42	0.47
1:U:1264:ILE:HB	1:U:1265:PRO:CD	2.43	0.47
1:U:1395:ILE:O	1:U:1399:ARG:HG3	2.15	0.47
1:B:452:GLN:HE22	1:B:596:MET:HB3	1.78	0.47
1:B:1245:SER:CB	1:B:1263:GLU:O	2.63	0.47
1:B:1349:LYS:O	1:B:1352:LEU:N	2.47	0.47
1:B:1431:ARG:HH12	1:D:1423:GLN:NE2	2.09	0.47
1:B:1468:LEU:O	1:B:1472:GLU:HG3	2.13	0.47
1:D:428:GLU:O	1:D:451:THR:HG22	2.15	0.47
1:D:1052:GLY:O	1:D:1056:GLN:HB2	2.15	0.47
1:D:1067:SER:C	1:D:1069:ARG:H	2.22	0.47
1:D:1163:ARG:NH2	1:D:1363:VAL:HG22	2.28	0.47
1:D:1231:ARG:HH11	1:D:1231:ARG:HG3	1.75	0.47
1:D:1391:ILE:CG2	1:D:1392:ASP:N	2.78	0.47
1:D:1461:ASP:O	1:D:1462:GLU:C	2.58	0.47
1:S:437:ASP:OD2	5:Y:10:DT:OP1	2.33	0.47
1:S:437:ASP:OD2	5:Y:10:DT:H5''	2.15	0.47
1:S:1261:VAL:HG12	1:S:1263:GLU:O	2.15	0.47
1:U:1122:ARG:NH1	4:X:9:DG:H3'	2.14	0.47
1:U:1137:ARG:O	1:U:1138:ASP:HB2	2.14	0.47
1:U:1291:ASP:OD2	1:U:1292:LEU:N	2.47	0.47
4:X:13:DC:C4	4:X:14:DC:C4	3.03	0.47
1:B:514:ALA:HA	1:B:517:ARG:CZ	2.45	0.47
1:D:446:GLY:O	1:D:592:TRP:HB2	2.14	0.47
1:S:424:LYS:O	1:S:426:PRO:HD3	2.14	0.47
1:S:495:LEU:HD11	1:S:534:ALA:CB	2.45	0.47
1:S:1466:LEU:HD11	1:S:1470:ARG:HE	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:493:PHE:HE2	1:U:530:PRO:HB2	1.79	0.47
1:U:1245:SER:HG	1:U:1265:PRO:HD3	1.78	0.47
5:Y:12:DC:C5'	5:Y:12:DC:H6	2.28	0.47
1:D:1104:VAL:CG1	1:D:1126:ALA:HB1	2.45	0.47
1:D:1224:ILE:HG21	1:D:1230:ILE:HD11	1.96	0.47
1:D:1226:GLY:C	1:D:1228:SER:H	2.22	0.47
1:S:418:LEU:CD1	1:S:454:ILE:O	2.63	0.47
1:S:423:SER:O	1:S:429:CYS:SG	2.73	0.47
1:S:1070:ILE:HD12	1:S:1126:ALA:HB3	1.97	0.47
1:B:1069:ARG:HE	1:B:1069:ARG:HB3	1.25	0.47
1:D:504:VAL:HG13	1:D:540:ALA:H	1.80	0.47
1:S:1111:GLY:CA	1:S:1116:ASP:HB2	2.43	0.47
1:B:444:LYS:HA	1:B:447:ARG:HH11	1.80	0.46
1:B:1432:ARG:HG2	1:B:1437:GLU:HB3	1.97	0.46
1:D:1165:PRO:O	1:D:1169:ALA:HB2	2.15	0.46
1:S:1204:ILE:CG1	1:S:1205:SER:N	2.77	0.46
1:S:1398:ILE:O	1:S:1399:ARG:C	2.58	0.46
1:B:432:PHE:HD2	1:B:506:MET:HE2	1.80	0.46
1:B:1135:LEU:HG	1:B:1164:PHE:HE2	1.81	0.46
1:D:1383:GLY:N	1:D:1421:GLN:HE21	2.08	0.46
1:S:1049:ILE:HG21	1:S:1093:MET:HE1	1.97	0.46
1:S:1406:VAL:O	1:S:1409:GLU:N	2.48	0.46
1:U:1020:GLU:O	1:U:1024:ASP:HB2	2.16	0.46
1:U:1092:ARG:NH1	1:U:1098:SER:HB3	2.30	0.46
1:B:1244:ARG:CG	1:B:1245:SER:H	2.23	0.46
1:D:1091:VAL:O	1:D:1094:ALA:HB3	2.15	0.46
1:D:1168:LEU:HD21	1:D:1351:ALA:HB1	1.97	0.46
1:S:1245:SER:HB2	1:S:1261:VAL:HG11	1.97	0.46
1:S:1309:ARG:HD2	1:S:1309:ARG:C	2.40	0.46
1:S:1425:ILE:O	1:S:1426:LEU:C	2.57	0.46
1:U:1467:GLN:OE1	1:U:1470:ARG:HD2	2.15	0.46
1:D:448:ASP:OD1	1:D:449:SER:N	2.48	0.46
1:D:494:ASP:C	1:D:496:ALA:N	2.73	0.46
1:D:1209:LEU:HD13	1:D:1352:LEU:CD1	2.46	0.46
1:U:504:VAL:HA	1:U:538:TYR:O	2.15	0.46
1:U:538:TYR:N	1:U:538:TYR:CD1	2.83	0.46
1:U:1268:VAL:CG1	1:U:1269:ASN:N	2.78	0.46
1:U:1402:ASP:OD2	1:U:1403:THR:HG23	2.15	0.46
1:B:1279:GLU:HA	1:B:1282:ARG:NH2	2.30	0.46
1:B:1408:MET:C	1:B:1410:SER:N	2.72	0.46
1:D:464:VAL:HG23	1:D:522:THR:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:471:ARG:O	1:D:472:ILE:C	2.59	0.46
1:D:1258:ARG:HD2	1:D:1305:VAL:HG13	1.96	0.46
1:B:1177:VAL:C	1:B:1179:MET:H	2.23	0.46
1:D:1182:ASN:ND2	1:D:1331:PHE:CZ	2.84	0.46
1:D:1242:GLN:HE21	1:D:1330:SER:HB3	1.79	0.46
1:D:1245:SER:HA	1:D:1263:GLU:O	2.16	0.46
5:H:9:DG:H2"	5:H:10:DT:C6	2.51	0.46
1:S:458:ARG:HB3	7:X:1020:CPF:H172	1.97	0.46
1:S:1079:HIS:NE2	1:S:1081:HIS:CD2	2.77	0.46
1:S:1293:ARG:NH2	1:S:1295:GLU:OE2	2.40	0.46
1:B:585:GLU:O	1:D:1108:GLY:CA	2.55	0.46
1:B:1047:ARG:HE	1:B:1047:ARG:HB2	1.54	0.46
1:D:522:THR:OG1	1:D:622:MET:HG3	2.16	0.46
1:D:526:ARG:NH1	1:D:615:ASP:OD1	2.41	0.46
1:D:604:LEU:CD2	1:D:1012:ARG:HB2	2.44	0.46
1:S:1291:ASP:HB3	1:S:1307:ASP:HB2	1.97	0.46
1:B:459:GLY:HA3	2:E:8:DT:O2	2.16	0.46
1:B:1131:ILE:HG13	1:B:1131:ILE:O	2.15	0.46
1:D:532:ILE:HA	1:D:537:VAL:HG21	1.97	0.46
1:D:539:ILE:HB	1:D:604:LEU:CB	2.46	0.46
1:D:1083:ASP:HB3	1:D:1121:MET:HE1	1.98	0.46
1:D:1261:VAL:O	1:D:1303:ARG:HA	2.15	0.46
1:D:1436:LEU:O	1:D:1440:LYS:N	2.33	0.46
1:S:1100:ARG:HD2	1:S:1485:ARG:HH11	1.80	0.46
1:S:1412:GLN:HB3	1:S:1417:LEU:O	2.15	0.46
1:U:1107:GLN:C	1:U:1110:PHE:HE1	2.24	0.46
1:B:1342:ARG:HB3	1:B:1343:PRO:HD2	1.96	0.46
1:D:1198:LEU:CD2	1:D:1352:LEU:HB2	2.46	0.46
1:D:1218:PHE:HE2	1:D:1224:ILE:HD11	1.81	0.46
1:S:1070:ILE:CD1	1:S:1126:ALA:HB3	2.46	0.46
1:S:1387:ALA:CA	1:S:1394:ILE:HG13	2.45	0.46
1:U:470:ASP:OD1	1:U:470:ASP:C	2.59	0.46
1:U:1037:ASP:C	1:U:1039:ARG:N	2.73	0.46
1:U:1165:PRO:CA	1:U:1355:TYR:CZ	2.99	0.46
1:U:1190:GLU:HB3	1:U:1212:ASP:O	2.16	0.46
4:X:13:DC:C6	7:X:1020:CPF:H142	2.51	0.46
1:B:526:ARG:HB3	1:B:527:PHE:CE1	2.51	0.46
1:B:1429:ARG:NH1	1:D:1427:ASP:O	2.48	0.46
1:D:543:PRO:HG3	1:D:594:THR:CG2	2.46	0.46
1:D:1101:TYR:HB3	1:D:1131:ILE:HD13	1.97	0.46
1:S:484:ALA:O	1:S:500:TYR:HE1	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:538:TYR:N	1:S:538:TYR:CD1	2.83	0.46
1:S:1101:TYR:HB3	1:S:1131:ILE:CD1	2.44	0.46
1:S:1245:SER:OG	1:S:1327:LEU:CD1	2.63	0.46
1:U:1262:THR:HA	1:U:1302:VAL:O	2.15	0.46
1:B:423:SER:HB2	1:B:450:ARG:O	2.16	0.45
1:B:427:GLU:CD	1:B:427:GLU:H	2.24	0.45
1:B:526:ARG:C	1:B:527:PHE:CD1	2.94	0.45
1:B:1039:ARG:HH21	1:B:1159:VAL:CB	2.24	0.45
1:D:526:ARG:HB2	1:D:527:PHE:CD1	2.51	0.45
1:D:1192:ILE:CD1	1:D:1477:ARG:HB2	2.28	0.45
1:D:1439:ASP:O	1:D:1440:LYS:C	2.59	0.45
1:D:1442:GLU:O	1:D:1442:GLU:HG3	2.15	0.45
1:S:1113:MET:C	1:S:1115:GLY:N	2.74	0.45
1:S:1371:LEU:HD11	1:S:1452:ILE:HG22	1.97	0.45
1:S:1404:ASP:HA	1:S:1407:ALA:HB3	1.97	0.45
1:U:1040:ASP:OD2	1:U:1159:VAL:HG23	2.17	0.45
2:V:5:DC:H2'	2:V:5:DC:O5'	2.17	0.45
1:B:1088:GLU:HA	1:B:1091:VAL:HB	1.97	0.45
1:B:1111:GLY:N	1:B:1118:ALA:HA	2.31	0.45
1:D:1080:PRO:HG3	1:D:1150:TYR:CD1	2.51	0.45
1:S:1027:MET:O	1:S:1028:SER:C	2.59	0.45
1:S:1033:ARG:CZ	2:V:7:DG:H4'	2.46	0.45
1:S:1079:HIS:CE1	1:S:1081:HIS:CD2	2.99	0.45
1:S:1213:ILE:HG22	1:S:1214:GLU:N	2.31	0.45
1:S:1346:ILE:HD12	1:S:1351:ALA:HB2	1.98	0.45
1:U:610:ASP:OD1	1:U:613:GLU:N	2.49	0.45
1:U:1038:VAL:HG22	1:U:1038:VAL:O	2.16	0.45
5:Y:14:DC:H2'	5:Y:15:DC:H6	1.82	0.45
1:B:526:ARG:CB	1:B:527:PHE:CD1	2.99	0.45
1:B:1225:LEU:HB2	1:B:1242:GLN:CB	2.47	0.45
1:B:1311:ASP:OD1	1:B:1311:ASP:N	2.49	0.45
1:B:1459:LEU:O	1:B:1461:ASP:N	2.44	0.45
1:D:528:MET:O	1:D:531:LEU:N	2.48	0.45
1:S:1149:ASN:ND2	1:S:1151:ASP:OD1	2.48	0.45
1:S:1201:ASN:HA	1:S:1202:PRO:HD3	1.80	0.45
1:S:1310:LYS:O	1:S:1311:ASP:HB2	2.16	0.45
1:U:1033:ARG:N	1:U:1044:PRO:HG2	2.31	0.45
2:V:8:DT:C2	7:Y:1020:CPF:H132	2.51	0.45
7:X:1020:CPF:H141	7:X:1020:CPF:F1	2.06	0.45
7:Y:1020:CPF:H9	7:Y:1020:CPF:H171	1.52	0.45
1:B:1293:ARG:NH2	1:B:1305:VAL:HG11	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1379:HIS:O	1:B:1382:GLU:HB2	2.16	0.45
1:D:527:PHE:O	1:D:528:MET:CG	2.60	0.45
1:S:1179:MET:O	1:S:1180:ALA:CB	2.62	0.45
1:S:1227:LYS:O	1:S:1230:ILE:HB	2.16	0.45
1:U:1028:SER:C	1:U:1030:ILE:N	2.71	0.45
1:B:1044:PRO:O	1:B:1048:ARG:HB2	2.16	0.45
1:B:1364:ARG:HB2	1:B:1465:LEU:HD21	1.99	0.45
1:B:1412:GLN:OE1	1:B:1419:GLU:HA	2.16	0.45
1:D:462:LEU:HA	4:G:14:DC:O3'	2.17	0.45
1:S:421:CYS:H	1:S:453:ALA:HB2	1.82	0.45
1:U:457:LEU:HD11	1:U:520:LEU:HD11	1.97	0.45
1:U:1218:PHE:CD1	1:U:1266:PHE:CG	3.05	0.45
1:U:1324:GLN:O	1:U:1325:THR:HG23	2.16	0.45
1:U:1368:GLN:O	1:U:1372:ARG:CD	2.64	0.45
1:B:1038:VAL:HG21	1:B:1354:HIS:CB	2.47	0.45
1:B:1066:LYS:HE3	1:B:1125:GLU:OE2	2.17	0.45
1:B:1445:TYR:CD1	1:B:1445:TYR:C	2.94	0.45
1:D:1019:ARG:O	1:D:1023:LEU:HB2	2.17	0.45
1:S:446:GLY:O	1:S:592:TRP:HB2	2.17	0.45
1:S:527:PHE:N	1:S:527:PHE:CD1	2.84	0.45
1:S:1029:VAL:HG13	1:S:1033:ARG:HB3	1.98	0.45
1:U:1217:ASP:OD2	1:U:1484:ARG:HA	2.17	0.45
1:U:1266:PHE:O	1:U:1268:VAL:HG23	2.16	0.45
1:U:1290:THR:CG2	1:U:1309:ARG:N	2.80	0.45
1:U:1368:GLN:CG	1:U:1459:LEU:HD11	2.39	0.45
1:U:1393:GLU:O	1:U:1396:SER:N	2.50	0.45
1:B:621:LEU:HD22	1:B:1022:PHE:CD2	2.52	0.45
1:B:1107:GLN:HG2	1:B:1125:GLU:OE1	2.17	0.45
1:B:1175:ILE:HD13	5:H:17:DC:C2	2.51	0.45
1:B:1363:VAL:HG11	1:B:1468:LEU:HD23	1.97	0.45
1:D:484:ALA:O	1:D:500:TYR:HE1	1.99	0.45
1:D:1273:MET:HE2	1:D:1273:MET:HB3	1.80	0.45
1:S:1322:TYR:O	1:S:1328:GLN:HB3	2.17	0.45
1:S:1369:TYR:CD2	1:S:1369:TYR:C	2.94	0.45
1:S:1448:LEU:O	1:S:1449:LEU:C	2.59	0.45
1:U:446:GLY:O	1:U:592:TRP:CE3	2.70	0.45
1:U:1204:ILE:HG23	1:U:1204:ILE:O	2.15	0.45
1:U:1310:LYS:HG2	1:U:1311:ASP:OD1	2.17	0.45
1:B:1012:ARG:HD2	1:B:1013:ASN:N	2.31	0.45
1:D:450:ARG:HB2	1:D:450:ARG:NH1	2.31	0.45
1:D:1310:LYS:O	1:D:1312:ALA:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1462:GLU:C	1:D:1464:VAL:H	2.25	0.45
1:S:457:LEU:O	1:S:459:GLY:N	2.50	0.45
1:S:1346:ILE:HG22	1:S:1350:GLU:OE1	2.16	0.45
1:U:536:TYR:O	1:U:538:TYR:CE1	2.70	0.45
1:U:541:GLN:HB2	1:U:602:ALA:HB3	1.99	0.45
1:U:1038:VAL:HG21	1:U:1339:VAL:HG22	1.98	0.45
1:U:1404:ASP:O	1:U:1405:LYS:C	2.60	0.45
1:B:527:PHE:CD1	1:B:527:PHE:N	2.85	0.45
1:B:587:ASN:CB	1:B:589:ASP:OD1	2.60	0.45
1:B:1446:ASN:HA	1:B:1449:LEU:HD12	1.99	0.45
1:D:1150:TYR:CD2	1:D:1151:ASP:HB3	2.51	0.45
1:S:1177:VAL:O	1:S:1179:MET:HG2	2.17	0.45
1:U:461:ILE:HG12	1:U:520:LEU:HD21	1.99	0.45
1:B:529:ARG:N	1:B:530:PRO:CD	2.80	0.45
1:B:621:LEU:O	1:B:629:ARG:HD2	2.17	0.45
1:D:446:GLY:O	1:D:592:TRP:CE3	2.70	0.45
1:D:1044:PRO:O	1:D:1046:HIS:N	2.50	0.45
1:D:1185:PRO:HG2	1:D:1217:ASP:O	2.17	0.45
1:D:1455:LEU:O	1:D:1459:LEU:HG	2.16	0.45
3:F:2:DG:N2	4:G:19:DC:O2	2.43	0.45
1:S:461:ILE:CD1	1:S:477:GLU:CB	2.94	0.45
1:S:1035:LEU:HA	1:S:1036:PRO:HD3	1.58	0.45
1:S:1068:ALA:CA	1:S:1121:MET:HE2	2.47	0.45
1:D:1031:VAL:HG12	1:D:1338:LEU:CD2	2.45	0.44
1:D:1064:TYR:CE2	1:D:1107:GLN:OE1	2.70	0.44
1:D:1433:LEU:C	1:D:1434:THR:O	2.60	0.44
7:H:1020:CPF:H142	7:H:1020:CPF:F1	2.07	0.44
1:S:459:GLY:HA3	3:W:8:DG:N3	2.32	0.44
1:S:597:ASN:HA	1:S:598:PRO:HD2	1.63	0.44
1:S:1093:MET:HE3	1:S:1093:MET:HB2	1.74	0.44
1:S:1388:LEU:CD2	1:S:1438:ARG:HG2	2.47	0.44
1:U:617:THR:HG22	1:U:618:PHE:N	2.32	0.44
1:U:1092:ARG:C	1:U:1094:ALA:H	2.25	0.44
1:U:1237:GLY:HA2	1:U:1335:MET:HE2	1.99	0.44
1:U:1243:MET:O	1:U:1244:ARG:HB2	2.17	0.44
2:V:3:DT:H2"	2:V:4:DG:OP2	2.17	0.44
4:X:9:DG:N1	5:Y:11:DA:N6	2.66	0.44
1:B:1278:ALA:C	1:B:1280:LEU:H	2.24	0.44
1:S:1083:ASP:OD2	1:S:1084:SER:N	2.50	0.44
1:S:1132:THR:O	1:S:1135:LEU:HB2	2.17	0.44
1:U:612:ILE:C	1:U:614:ALA:N	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1025:TYR:CZ	1:U:1029:VAL:HG21	2.52	0.44
1:D:626:VAL:HG22	4:G:17:DG:P	2.57	0.44
1:D:1184:PRO:HG3	1:D:1333:VAL:HG22	1.99	0.44
1:S:471:ARG:NH1	1:S:471:ARG:CG	2.80	0.44
1:S:1386:ILE:O	1:S:1387:ALA:C	2.60	0.44
1:U:1325:THR:C	1:U:1327:LEU:N	2.74	0.44
1:B:1071:VAL:O	1:B:1073:ASP:N	2.50	0.44
1:D:432:PHE:CE1	1:D:596:MET:HE3	2.52	0.44
1:D:494:ASP:CB	1:D:497:LYS:HE3	2.47	0.44
1:D:625:VAL:O	1:D:626:VAL:C	2.59	0.44
7:G:1020:CPF:H171	7:G:1020:CPF:H9	1.54	0.44
1:S:1221:ALA:HA	1:S:1486:THR:N	2.32	0.44
1:U:493:PHE:CE2	1:U:530:PRO:HB2	2.53	0.44
1:B:444:LYS:HA	1:B:447:ARG:HD3	2.00	0.44
1:B:1063:SER:O	1:B:1065:LYS:CE	2.60	0.44
1:B:1166:ASN:O	1:B:1167:LEU:C	2.60	0.44
1:D:597:ASN:HD22	1:D:598:PRO:HD2	1.83	0.44
1:S:522:THR:HA	1:S:618:PHE:CE2	2.53	0.44
1:S:597:ASN:HD22	1:S:598:PRO:CD	2.31	0.44
1:S:1221:ALA:CB	1:S:1485:ARG:O	2.62	0.44
1:U:529:ARG:O	1:U:533:GLU:HG3	2.17	0.44
1:U:1218:PHE:HD1	1:U:1266:PHE:CG	2.35	0.44
1:B:491:GLY:C	1:B:493:PHE:H	2.26	0.44
1:B:582:GLY:O	1:B:583:LEU:C	2.61	0.44
1:B:1162:ALA:C	1:B:1164:PHE:H	2.25	0.44
1:B:1191:LEU:CD2	1:B:1213:ILE:HD13	2.48	0.44
1:B:1331:PHE:HD2	1:B:1333:VAL:HG23	1.83	0.44
1:B:1394:ILE:O	1:B:1398:ILE:HG13	2.18	0.44
1:B:1405:LYS:NZ	1:B:1409:GLU:OE1	2.47	0.44
1:S:437:ASP:HB3	5:Y:9:DG:O3'	2.17	0.44
1:S:1129:THR:OG1	1:S:1131:ILE:HG23	2.17	0.44
1:U:462:LEU:HD11	1:U:467:ALA:HB2	1.99	0.44
1:U:520:LEU:HD22	1:U:520:LEU:HA	1.77	0.44
1:U:1025:TYR:CE2	1:U:1029:VAL:HG21	2.52	0.44
1:U:1104:VAL:CG1	1:U:1105:ASP:N	2.80	0.44
1:B:1054:ASN:HB2	1:B:1136:LEU:HD13	1.98	0.44
1:B:1058:MET:CE	1:B:1065:LYS:HG3	2.47	0.44
1:B:1430:LEU:O	1:B:1432:ARG:N	2.51	0.44
1:D:526:ARG:HB2	1:D:527:PHE:CE1	2.52	0.44
1:D:604:LEU:HD13	1:D:1012:ARG:HB2	2.00	0.44
1:D:1371:LEU:O	1:D:1372:ARG:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:458:ARG:NE	1:S:477:GLU:OE2	2.51	0.44
1:S:508:ASP:HB2	1:S:583:LEU:H	1.83	0.44
1:U:612:ILE:HD13	1:U:612:ILE:HA	1.83	0.44
1:B:1171:GLY:O	1:B:1172:ALA:HB2	2.18	0.44
1:B:1381:LEU:CD1	1:B:1448:LEU:HD12	2.46	0.44
1:D:474:ASN:O	1:D:475:ASN:C	2.59	0.44
1:D:536:TYR:HD2	1:D:536:TYR:N	2.16	0.44
1:D:1318:LEU:HG	1:D:1322:TYR:HE2	1.82	0.44
1:U:1093:MET:HA	1:U:1099:TYR:CD1	2.53	0.44
7:X:1020:CPF:H9	7:X:1020:CPF:H11	1.65	0.44
1:B:597:ASN:ND2	1:B:598:PRO:HD2	2.30	0.44
1:B:1218:PHE:HA	1:B:1219:PRO:HD2	1.79	0.44
1:B:1300:THR:CG2	1:B:1303:ARG:HD3	2.47	0.44
1:B:1435:GLY:O	1:B:1439:ASP:OD2	2.34	0.44
1:D:539:ILE:O	1:D:540:ALA:C	2.60	0.44
1:D:632:PHE:CE1	1:D:1019:ARG:NH2	2.86	0.44
1:S:475:ASN:O	1:S:478:ILE:HB	2.17	0.44
1:S:1417:LEU:HD22	1:S:1421:GLN:HB3	2.00	0.44
1:U:597:ASN:HA	1:U:598:PRO:HD2	1.84	0.44
1:U:1335:MET:C	1:U:1345:LEU:CD1	2.91	0.44
1:U:1381:LEU:HD12	1:U:1448:LEU:HD12	1.99	0.44
7:X:1020:CPF:F1	7:X:1020:CPF:C14	2.54	0.44
1:B:499:ARG:HB2	1:B:500:TYR:CD1	2.53	0.43
1:B:586:MET:H	1:B:586:MET:HG3	1.58	0.43
1:B:1317:ILE:O	1:B:1320:ASN:N	2.47	0.43
1:D:457:LEU:HD13	1:D:461:ILE:HD11	1.99	0.43
1:D:1454:GLU:O	1:D:1455:LEU:C	2.60	0.43
1:S:519:LEU:HD23	1:S:622:MET:HE3	2.00	0.43
1:S:1145:ASP:OD1	1:S:1145:ASP:N	2.49	0.43
1:S:1382:GLU:HG3	1:S:1445:TYR:HE1	1.80	0.43
1:B:444:LYS:O	1:B:447:ARG:NH1	2.51	0.43
1:B:1282:ARG:HG2	1:B:1283:ASP:OD1	2.17	0.43
1:B:1372:ARG:O	1:B:1376:ASP:HB2	2.18	0.43
1:D:449:SER:C	1:D:450:ARG:HG3	2.43	0.43
1:D:1314:ALA:O	1:D:1318:LEU:N	2.51	0.43
5:H:12:DC:H2''	5:H:13:DA:O5'	2.18	0.43
1:S:1215:GLY:H	1:S:1484:ARG:NH2	2.16	0.43
1:S:1358:HIS:HD2	1:S:1359:GLN:NE2	2.16	0.43
1:S:1381:LEU:HD11	1:S:1444:GLU:CD	2.42	0.43
1:U:1177:VAL:O	1:U:1177:VAL:HG12	2.17	0.43
1:U:1419:GLU:O	1:U:1423:GLN:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:6:DG:H1	5:Y:15:DC:N4	2.16	0.43
5:Y:13:DA:OP2	5:Y:13:DA:H8	2.01	0.43
1:B:444:LYS:CA	1:B:447:ARG:HH11	2.30	0.43
1:B:503:ILE:O	1:B:503:ILE:HG22	2.18	0.43
1:B:1107:GLN:HB3	1:B:1125:GLU:HB2	2.00	0.43
1:B:1230:ILE:O	1:B:1233:ALA:HB3	2.18	0.43
1:D:1051:TYR:CD2	1:D:1157:PRO:HD3	2.53	0.43
1:S:520:LEU:HD23	1:S:520:LEU:HA	1.76	0.43
1:S:1129:THR:OG1	1:S:1132:THR:OG1	2.29	0.43
1:S:1174:GLY:H	1:S:1181:THR:HG23	1.83	0.43
1:S:1220:THR:O	1:S:1221:ALA:HB3	2.18	0.43
1:S:1316:VAL:O	1:S:1317:ILE:C	2.61	0.43
1:S:1394:ILE:HD13	1:S:1415:PHE:CE1	2.52	0.43
1:U:433:LEU:HD12	1:U:505:ILE:HG12	2.00	0.43
1:U:592:TRP:HE3	1:U:596:MET:HE3	1.81	0.43
1:U:1188:LEU:HD12	1:U:1188:LEU:HA	1.71	0.43
1:U:1202:PRO:C	1:U:1204:ILE:H	2.26	0.43
1:B:420:ASP:OD1	1:B:421:CYS:N	2.51	0.43
1:B:447:ARG:CB	1:B:596:MET:HE1	2.48	0.43
1:B:1183:ILE:HA	1:B:1184:PRO:HD3	1.66	0.43
1:B:1415:PHE:CB	1:B:1417:LEU:HG	2.49	0.43
1:D:429:CYS:C	1:D:430:GLU:HG2	2.43	0.43
1:D:532:ILE:HD13	1:D:1014:ILE:HD12	2.01	0.43
1:D:1131:ILE:O	1:D:1131:ILE:CG1	2.66	0.43
1:D:1164:PHE:O	1:D:1164:PHE:CD1	2.71	0.43
1:S:1224:ILE:HD12	1:S:1488:ILE:CG1	2.48	0.43
1:S:1398:ILE:CD1	1:S:1411:LEU:HD11	2.48	0.43
1:S:1428:MET:HA	1:S:1432:ARG:NH1	2.32	0.43
1:U:435:GLU:HG3	1:U:507:THR:CA	2.48	0.43
1:U:443:THR:OG1	1:U:506:MET:HE1	2.18	0.43
1:U:531:LEU:HD12	1:U:531:LEU:C	2.44	0.43
4:X:13:DC:H1'	7:X:1020:CPF:H142	2.01	0.43
1:B:627:GLU:OE1	1:B:627:GLU:HA	2.18	0.43
1:B:1122:ARG:NH2	1:B:1123:PHE:CE1	2.86	0.43
1:B:1265:PRO:HB2	1:B:1268:VAL:CG2	2.48	0.43
1:B:1334:ASN:O	1:B:1336:ILE:HG13	2.18	0.43
1:D:525:TYR:HE2	1:D:526:ARG:NH1	2.16	0.43
1:D:1132:THR:O	1:D:1136:LEU:HD12	2.18	0.43
1:D:1462:GLU:O	1:D:1464:VAL:N	2.52	0.43
1:S:1075:MET:HE3	1:S:1075:MET:HB3	1.78	0.43
1:S:1185:PRO:O	1:S:1216:PRO:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1275:GLU:O	1:S:1279:GLU:HB2	2.19	0.43
1:S:1283:ASP:O	1:S:1284:LYS:HB2	2.17	0.43
1:U:418:LEU:HD13	1:U:455:LEU:HD13	2.00	0.43
1:U:1025:TYR:CZ	1:U:1029:VAL:CG2	3.01	0.43
1:U:1060:PRO:HD3	1:U:1133:LEU:HD21	2.00	0.43
1:B:1331:PHE:CD2	1:B:1333:VAL:HG23	2.53	0.43
1:D:496:ALA:C	1:D:498:ALA:H	2.26	0.43
1:D:1361:THR:O	1:D:1365:ARG:HG3	2.19	0.43
1:S:521:LEU:HD22	1:U:1014:ILE:HG13	2.00	0.43
1:S:1432:ARG:H	1:S:1432:ARG:HG2	1.58	0.43
1:S:1439:ASP:O	1:S:1443:ALA:HB3	2.18	0.43
1:S:1449:LEU:HA	1:S:1452:ILE:HD12	2.00	0.43
1:B:540:ALA:O	1:B:542:PRO:HD3	2.19	0.43
1:S:1185:PRO:HG2	1:S:1218:PHE:HD1	1.84	0.43
1:U:1058:MET:SD	1:U:1070:ILE:HG12	2.59	0.43
1:U:1176:ALA:O	1:U:1177:VAL:HG23	2.19	0.43
1:U:1361:THR:O	1:U:1365:ARG:CG	2.57	0.43
1:B:521:LEU:O	1:B:522:THR:C	2.61	0.43
1:B:1050:LEU:HD23	1:B:1053:LEU:HD12	2.01	0.43
1:B:1218:PHE:CG	1:B:1266:PHE:HB2	2.54	0.43
1:B:1411:LEU:HD23	1:B:1417:LEU:CD1	2.48	0.43
1:D:473:LEU:C	1:D:474:ASN:HD22	2.27	0.43
1:D:540:ALA:O	1:D:542:PRO:HD3	2.19	0.43
1:D:1425:ILE:HG23	1:D:1428:MET:CE	2.48	0.43
1:S:593:GLU:OE1	1:S:593:GLU:HA	2.18	0.43
1:S:1238:ARG:HA	1:S:1333:VAL:O	2.18	0.43
1:S:1245:SER:HB3	1:S:1261:VAL:HG11	2.01	0.43
1:U:464:VAL:HG23	1:U:465:GLU:N	2.32	0.43
1:U:1100:ARG:HA	1:U:1219:PRO:HG3	2.00	0.43
1:U:1110:PHE:CZ	1:U:1124:THR:HB	2.54	0.43
1:U:1467:GLN:OE1	1:U:1467:GLN:HA	2.19	0.43
7:X:1020:CPF:H122	5:Y:9:DG:O5'	2.18	0.43
1:B:488:GLY:O	1:B:493:PHE:HD1	2.01	0.43
1:B:1079:HIS:HA	1:B:1080:PRO:HD3	1.89	0.43
1:B:1426:LEU:HD23	1:B:1426:LEU:HA	1.75	0.43
1:D:435:GLU:OE1	1:D:508:ASP:CB	2.49	0.43
1:D:592:TRP:O	1:D:597:ASN:N	2.51	0.43
1:D:1186:HIS:HB2	1:D:1191:LEU:CD1	2.42	0.43
1:D:1186:HIS:CD2	1:D:1216:PRO:HA	2.54	0.43
1:D:1421:GLN:O	1:D:1425:ILE:HG13	2.19	0.43
3:F:6:DT:C4	3:F:7:DA:N7	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1146:PHE:C	1:S:1147:ILE:HG23	2.44	0.43
1:U:542:PRO:HA	1:U:543:PRO:HD3	1.86	0.43
1:U:639:TYR:N	1:U:639:TYR:CD1	2.87	0.43
1:U:1156:GLU:HB2	1:U:1157:PRO:HD2	2.01	0.43
1:B:463:ASN:C	1:B:465:GLU:H	2.27	0.43
1:B:1029:VAL:O	1:B:1029:VAL:HG12	2.18	0.43
1:B:1034:ALA:HA	1:B:1043:LYS:HD3	2.01	0.43
1:D:448:ASP:H	1:D:592:TRP:HZ3	1.66	0.43
1:D:500:TYR:HB2	1:D:503:ILE:HD11	2.01	0.43
1:D:1183:ILE:HA	1:D:1184:PRO:HD3	1.88	0.43
1:D:1366:ARG:O	1:D:1369:TYR:N	2.51	0.43
1:D:1425:ILE:C	1:D:1427:ASP:N	2.75	0.43
7:G:1020:CPF:H1	7:G:1020:CPF:H121	1.73	0.43
5:H:9:DG:C2'	5:H:10:DT:C5	2.94	0.43
1:S:1135:LEU:HD23	1:S:1162:ALA:HA	2.00	0.43
1:S:1224:ILE:HG23	1:S:1242:GLN:O	2.19	0.43
1:S:1348:LEU:O	1:S:1351:ALA:HB3	2.19	0.43
1:S:1456:GLU:O	1:S:1457:THR:C	2.62	0.43
1:U:441:GLY:O	1:U:442:SER:C	2.62	0.43
1:U:1035:LEU:HA	1:U:1036:PRO:HD3	1.75	0.43
1:U:1133:LEU:O	1:U:1137:ARG:N	2.52	0.43
1:B:495:LEU:HD12	1:B:495:LEU:O	2.19	0.42
1:B:1114:ASP:OD1	1:B:1270:LYS:NZ	2.48	0.42
1:B:1120:ALA:O	1:B:1122:ARG:N	2.52	0.42
1:B:1179:MET:HE2	1:B:1179:MET:HB3	1.85	0.42
1:B:1413:GLN:C	1:B:1415:PHE:H	2.26	0.42
1:D:458:ARG:HD2	1:D:477:GLU:HG3	2.01	0.42
1:D:1313:ASN:ND2	1:D:1316:VAL:H	2.12	0.42
1:S:515:HIS:O	1:S:516:ILE:C	2.62	0.42
1:S:1118:ALA:C	1:S:1119:ALA:O	2.62	0.42
1:S:1247:ALA:CB	1:S:1260:VAL:O	2.67	0.42
1:U:458:ARG:HB3	7:Y:1020:CPF:C16	2.43	0.42
1:U:592:TRP:O	1:U:596:MET:N	2.51	0.42
1:U:1165:PRO:CA	1:U:1355:TYR:CE2	2.97	0.42
1:U:1190:GLU:O	1:U:1213:ILE:CG1	2.66	0.42
1:U:1246:ARG:HB3	1:U:1263:GLU:HB2	2.01	0.42
1:U:1273:MET:SD	1:U:1327:LEU:HA	2.58	0.42
1:U:1450:ASN:HD22	1:U:1450:ASN:H	1.60	0.42
1:B:1027[B]:MET:HA	1:B:1027[B]:MET:CE	2.47	0.42
1:D:477:GLU:O	1:D:481:MET:HG3	2.18	0.42
1:D:1466:LEU:O	1:D:1470:ARG:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:493:PHE:CG	1:S:494:ASP:N	2.86	0.42
1:U:430:GLU:O	1:U:430:GLU:HG2	2.19	0.42
1:U:587:ASN:HB2	1:U:590:GLN:HB2	2.00	0.42
1:U:1119:ALA:O	1:U:1120:ALA:O	2.37	0.42
1:U:1165:PRO:HG3	1:U:1355:TYR:CE1	2.54	0.42
1:U:1238:ARG:CD	1:U:1345:LEU:HD21	2.48	0.42
1:U:1260:VAL:HG11	1:U:1303:ARG:NH1	2.34	0.42
1:B:418:LEU:HD12	1:B:418:LEU:C	2.44	0.42
1:B:473:LEU:O	1:B:479:ARG:HD2	2.19	0.42
1:B:1192:ILE:CD1	1:B:1477:ARG:HB2	2.42	0.42
1:D:1143:THR:HG21	1:D:1362:VAL:HG13	2.01	0.42
3:F:6:DT:O4	3:F:7:DA:N6	2.52	0.42
5:H:12:DC:H3'	5:H:12:DC:OP2	2.19	0.42
1:S:431:ILE:HG13	1:S:453:ALA:O	2.19	0.42
1:S:1038:VAL:HG21	1:S:1354:HIS:HB2	2.02	0.42
1:S:1265:PRO:O	1:S:1266:PHE:C	2.62	0.42
1:S:1293:ARG:HB2	1:S:1293:ARG:NH1	2.33	0.42
1:U:1070:ILE:O	1:U:1073:ASP:HB3	2.18	0.42
1:U:1121:MET:HE2	1:U:1121:MET:HB3	1.81	0.42
1:U:1281:VAL:CG2	1:U:1289:ILE:HD12	2.49	0.42
1:U:1293:ARG:HH12	1:U:1307:ASP:CG	2.27	0.42
1:U:1369:TYR:O	1:U:1370:ASN:C	2.61	0.42
1:U:1450:ASN:H	1:U:1450:ASN:ND2	2.16	0.42
1:B:493:PHE:CD2	1:B:530:PRO:HB2	2.55	0.42
1:B:1405:LYS:CE	1:B:1409:GLU:OE1	2.67	0.42
1:D:512:ASP:HA	1:D:515:HIS:HB3	2.00	0.42
1:D:1145:ASP:O	1:D:1158:SER:HB3	2.20	0.42
1:D:1179:MET:HE2	1:D:1179:MET:HB3	1.90	0.42
1:D:1199:SER:CB	1:D:1470:ARG:HE	2.33	0.42
1:D:1467:GLN:O	1:D:1470:ARG:N	2.52	0.42
1:S:1027:MET:O	1:S:1030:ILE:N	2.47	0.42
1:S:1437:GLU:O	1:S:1441:ILE:HG13	2.20	0.42
1:U:631:GLN:O	1:U:632:PHE:C	2.61	0.42
1:U:1186:HIS:CD2	1:U:1234:TYR:OH	2.72	0.42
1:U:1346:ILE:HD12	1:U:1351:ALA:CA	2.47	0.42
1:U:1411:LEU:HA	1:U:1411:LEU:HD23	1.74	0.42
1:B:478:ILE:CG2	1:B:523:PHE:CZ	3.02	0.42
1:B:1365:ARG:HE	1:B:1365:ARG:HB3	1.51	0.42
1:D:586:MET:HB2	1:D:591:LEU:HD21	2.01	0.42
1:D:591:LEU:HD23	1:D:591:LEU:HA	1.80	0.42
1:D:1187:ASN:OD1	1:D:1187:ASN:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:446:GLY:O	1:S:592:TRP:CE3	2.72	0.42
1:S:494:ASP:OD1	1:S:497:LYS:HE3	2.18	0.42
1:S:1317:ILE:H	1:S:1317:ILE:HG13	1.47	0.42
1:S:1457:THR:O	1:S:1464:VAL:HG11	2.20	0.42
1:U:1094:ALA:HB2	1:U:1104:VAL:HB	2.01	0.42
1:B:435:GLU:HB2	1:B:583:LEU:HD12	2.01	0.42
1:B:1036:PRO:HG3	1:B:1172:ALA:HB1	2.02	0.42
1:D:485:PHE:HZ	1:D:524:PHE:CZ	2.37	0.42
1:S:485:PHE:O	1:S:487:THR:HG23	2.19	0.42
1:S:1185:PRO:O	1:S:1186:HIS:ND1	2.53	0.42
1:S:1470:ARG:H	1:S:1470:ARG:HG3	1.62	0.42
1:U:441:GLY:C	1:U:443:THR:N	2.77	0.42
1:U:1453:SER:O	1:U:1456:GLU:HB2	2.19	0.42
1:B:1201:ASN:O	1:B:1203:ASP:N	2.52	0.42
1:D:1394:ILE:CD1	1:D:1415:PHE:CZ	3.03	0.42
4:G:14:DC:H2''	4:G:15:DA:H5'	2.02	0.42
7:G:1020:CPF:F1	7:G:1020:CPF:C14	2.58	0.42
1:S:475:ASN:O	1:S:476:ASN:C	2.63	0.42
1:U:421:CYS:N	1:U:453:ALA:HB2	2.32	0.42
1:U:514:ALA:O	1:U:518:THR:HG23	2.20	0.42
1:U:598:PRO:HB3	1:U:601:ARG:CZ	2.48	0.42
1:U:1035:LEU:HA	1:U:1035:LEU:HD23	1.88	0.42
1:U:1134:GLU:OE2	1:U:1137:ARG:HD3	2.19	0.42
1:U:1238:ARG:HD2	1:U:1345:LEU:HD21	2.01	0.42
1:U:1243:MET:HE2	1:U:1331:PHE:HB2	2.00	0.42
1:B:524:PHE:N	1:B:524:PHE:CD2	2.85	0.42
1:B:1195:VAL:HG12	1:B:1196:LEU:N	2.34	0.42
1:B:1286:ILE:O	1:B:1286:ILE:HG23	2.18	0.42
1:D:472:ILE:O	1:D:474:ASN:N	2.53	0.42
1:D:1467:GLN:OE1	1:D:1467:GLN:HA	2.20	0.42
1:S:1101:TYR:CB	1:S:1131:ILE:HD13	2.48	0.42
1:S:1138:ASP:OD1	1:S:1141:LYS:HD2	2.20	0.42
1:S:1217:ASP:HB2	1:S:1484:ARG:NH1	2.34	0.42
1:S:1219:PRO:HA	1:S:1485:ARG:HH11	1.84	0.42
1:U:492:ASP:O	1:U:494:ASP:N	2.53	0.42
1:U:1050:LEU:HD11	1:U:1103:LEU:HD13	2.01	0.42
1:U:1296:THR:HG22	1:U:1297:SER:N	2.35	0.42
1:U:1429:ARG:O	1:U:1432:ARG:HB2	2.19	0.42
4:X:17:DG:H2'	4:X:17:DG:O5'	2.20	0.42
1:B:519:LEU:O	1:B:522:THR:HB	2.19	0.42
1:B:1398:ILE:O	1:B:1399:ARG:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:535:GLY:C	1:D:536:TYR:CD2	2.86	0.42
1:D:611:ALA:O	1:D:615:ASP:HB2	2.19	0.42
1:D:1329:THR:CG2	1:D:1330:SER:N	2.81	0.42
1:D:1412:GLN:NE2	1:D:1419:GLU:HA	2.34	0.42
4:G:11:DA:H2"	4:G:12:DC:C5'	2.46	0.42
1:S:1259:ILE:HG22	1:S:1260:VAL:N	2.35	0.42
1:S:1296:THR:OG1	1:S:1303:ARG:N	2.47	0.42
1:S:1388:LEU:HD21	1:S:1438:ARG:HG2	2.02	0.42
1:U:527:PHE:C	1:U:528:MET:HG3	2.44	0.42
1:U:1264:ILE:CG2	1:U:1302:VAL:HG11	2.42	0.42
1:U:1295:GLU:HG3	1:U:1305:VAL:HG23	2.01	0.42
1:U:1425:ILE:O	1:U:1428:MET:HB3	2.20	0.42
1:U:1476:ILE:C	1:U:1478:ASP:N	2.78	0.42
1:B:500:TYR:O	1:B:501:HIS:HD2	2.03	0.42
1:B:1224:ILE:HD13	1:B:1241:ILE:CG2	2.49	0.42
1:B:1266:PHE:O	1:B:1267:GLN:HB2	2.19	0.42
1:B:1455:LEU:C	1:B:1457:THR:N	2.77	0.42
1:D:435:GLU:O	1:D:457:LEU:O	2.37	0.42
1:D:1013:ASN:HB3	1:D:1016:SER:HB2	2.01	0.42
1:S:1071:VAL:O	1:S:1075:MET:N	2.51	0.42
1:S:1134:GLU:CD	1:S:1479:ARG:HH22	2.27	0.42
1:S:1193:ASN:O	1:S:1197:SER:OG	2.37	0.42
1:S:1245:SER:HB3	1:S:1263:GLU:O	2.20	0.42
1:U:485:PHE:HB3	1:U:487:THR:HG23	2.02	0.42
1:U:1043:LYS:HB3	1:U:1044:PRO:HD2	2.01	0.42
1:U:1046:HIS:CE1	3:W:6:DT:OP1	2.73	0.42
1:U:1238:ARG:HH11	1:U:1334:ASN:ND2	2.18	0.42
1:B:1092:ARG:C	1:B:1094:ALA:N	2.77	0.41
1:D:1037:ASP:HB3	1:D:1040:ASP:OD1	2.20	0.41
1:D:1049:ILE:HG21	1:D:1090:MET:HB2	2.02	0.41
1:D:1293:ARG:CZ	1:D:1305:VAL:HG11	2.50	0.41
1:D:1454:GLU:O	1:D:1457:THR:N	2.53	0.41
1:D:1462:GLU:C	1:D:1464:VAL:N	2.77	0.41
1:S:485:PHE:C	1:S:487:THR:N	2.77	0.41
1:S:518:THR:O	1:S:519:LEU:C	2.62	0.41
1:S:636:ASN:O	1:U:1023:LEU:HD21	2.19	0.41
1:U:620:MET:HE2	1:U:620:MET:HB3	1.88	0.41
1:U:1192:ILE:O	1:U:1193:ASN:C	2.62	0.41
1:U:1320:ASN:CB	1:U:1324:GLN:HE21	2.33	0.41
1:B:465:GLU:CD	1:B:526:ARG:HH21	2.26	0.41
1:B:475:ASN:O	1:B:479:ARG:CD	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1381:LEU:HB3	1:B:1445:TYR:HD2	1.85	0.41
1:B:1381:LEU:HD21	1:B:1444:GLU:CD	2.46	0.41
1:D:493:PHE:CE2	1:D:495:LEU:HD13	2.55	0.41
1:S:620:MET:HE3	1:S:621:LEU:HD21	2.02	0.41
1:S:1064:TYR:CE2	1:S:1107:GLN:CB	3.03	0.41
1:U:462:LEU:HD11	1:U:467:ALA:CB	2.50	0.41
1:U:1057:GLY:C	1:U:1059:THR:H	2.29	0.41
1:U:1349:LYS:O	1:U:1352:LEU:N	2.53	0.41
1:U:1358:HIS:HD2	1:U:1359:GLN:NE2	2.17	0.41
1:B:515:HIS:HB2	1:B:1025:TYR:CG	2.54	0.41
1:B:532:ILE:HG12	1:B:537:VAL:HG21	2.02	0.41
1:B:536:TYR:N	1:B:536:TYR:CD2	2.88	0.41
1:B:618:PHE:O	1:B:619:GLU:C	2.61	0.41
1:B:1201:ASN:OD1	1:B:1201:ASN:O	2.38	0.41
1:B:1322:TYR:CD1	1:B:1327:LEU:HD23	2.55	0.41
1:D:540:ALA:C	1:D:542:PRO:HD3	2.45	0.41
1:D:625:VAL:CB	1:D:628:ASN:ND2	2.84	0.41
1:D:1198:LEU:HG	1:D:1198:LEU:O	2.20	0.41
1:D:1336:ILE:HA	1:D:1344:LYS:O	2.19	0.41
1:D:1357:GLU:OE1	1:D:1357:GLU:CA	2.65	0.41
1:S:1030:ILE:CG2	1:S:1343:PRO:HG3	2.50	0.41
1:S:1074:VAL:O	1:S:1074:VAL:HG12	2.21	0.41
1:S:1090:MET:HE1	1:S:1126:ALA:HB2	2.02	0.41
1:S:1193:ASN:HA	1:S:1196:LEU:HB2	2.02	0.41
1:S:1363:VAL:CG1	1:S:1468:LEU:HD23	2.50	0.41
1:U:493:PHE:CE2	1:U:531:LEU:N	2.88	0.41
1:U:1025:TYR:CD2	1:U:1025:TYR:C	2.96	0.41
1:U:1243:MET:O	1:U:1328:GLN:HG3	2.20	0.41
1:U:1391:ILE:O	1:U:1395:ILE:HG12	2.19	0.41
1:B:519:LEU:HA	1:B:519:LEU:HD23	1.73	0.41
1:B:1227:LYS:O	1:B:1231:ARG:HB2	2.20	0.41
1:B:1238:ARG:HG2	1:B:1334:ASN:HD22	1.85	0.41
1:B:1436:LEU:HD23	1:B:1440:LYS:HE3	2.01	0.41
1:S:437:ASP:H	5:Y:9:DG:C5'	2.32	0.41
1:S:627:GLU:O	1:S:629:ARG:N	2.53	0.41
1:S:1132:THR:C	1:S:1134:GLU:H	2.27	0.41
1:S:1445:TYR:CD2	1:S:1445:TYR:C	2.98	0.41
1:U:1036:PRO:HA	1:U:1042:LEU:O	2.20	0.41
1:U:1038:VAL:HG11	1:U:1339:VAL:HA	2.01	0.41
1:U:1214:GLU:HB3	1:U:1488:ILE:HD12	2.02	0.41
1:U:1371:LEU:HG	1:U:1372:ARG:N	2.30	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:457:LEU:CD1	1:B:477:GLU:HG3	2.50	0.41
1:B:1035:LEU:HA	1:B:1036:PRO:HD3	1.87	0.41
1:B:1049:ILE:O	1:B:1053:LEU:HG	2.21	0.41
1:B:1058:MET:HG2	1:B:1065:LYS:HG3	2.01	0.41
1:B:1066:LYS:O	1:B:1070:ILE:HG13	2.20	0.41
1:D:1164:PHE:HA	1:D:1165:PRO:HD3	1.89	0.41
1:S:1185:PRO:HD2	1:S:1218:PHE:HE1	1.83	0.41
1:U:482:ILE:HG12	1:U:523:PHE:HZ	1.85	0.41
1:U:503:ILE:HD13	1:U:531:LEU:HD11	2.03	0.41
1:U:1299:ARG:H	1:U:1299:ARG:CD	2.29	0.41
1:B:1404:ASP:O	1:B:1408:MET:HG2	2.20	0.41
1:D:421:CYS:SG	1:D:429:CYS:SG	3.07	0.41
1:D:442:SER:CB	1:D:591:LEU:HD12	2.50	0.41
1:D:506:MET:HB2	1:D:506:MET:HE2	1.78	0.41
1:D:1164:PHE:CD1	1:D:1164:PHE:C	2.98	0.41
1:S:540:ALA:C	1:S:541:GLN:HG3	2.46	0.41
1:S:1116:ASP:O	1:S:1117:GLY:C	2.64	0.41
1:U:1259:ILE:H	1:U:1259:ILE:HG13	1.70	0.41
1:U:1292:LEU:C	1:U:1293:ARG:HG3	2.46	0.41
1:B:1171:GLY:HA2	1:B:1184:PRO:O	2.21	0.41
1:B:1274:ILE:HG23	1:B:1292:LEU:HD11	2.02	0.41
1:D:497:LYS:H	1:D:497:LYS:HG3	1.64	0.41
1:D:1376:ASP:O	1:D:1380:ILE:HG12	2.21	0.41
1:D:1400:GLU:O	1:D:1400:GLU:CG	2.61	0.41
1:D:1484:ARG:HD3	1:D:1486:THR:O	2.20	0.41
1:S:1037:ASP:HA	1:S:1338:LEU:HB2	2.01	0.41
1:S:1218:PHE:C	1:S:1220:THR:H	2.29	0.41
1:S:1358:HIS:CD2	1:S:1359:GLN:HE21	2.39	0.41
1:U:1100:ARG:NH1	1:U:1485:ARG:NE	2.66	0.41
1:U:1450:ASN:N	1:U:1450:ASN:ND2	2.50	0.41
1:B:1077:LYS:HB3	1:B:1078:TYR:CE1	2.56	0.41
1:B:1221:ALA:HB2	1:B:1485:ARG:HB3	2.02	0.41
1:B:1339:VAL:O	1:B:1340:ASN:C	2.64	0.41
1:D:1402:ASP:OD2	1:D:1403:THR:HG23	2.20	0.41
1:D:1425:ILE:HG23	1:D:1428:MET:HE1	2.02	0.41
5:H:9:DG:H4'	5:H:10:DT:OP1	2.21	0.41
1:S:631:GLN:O	1:S:634:GLU:N	2.51	0.41
1:S:1038:VAL:HG12	1:S:1338:LEU:O	2.21	0.41
1:S:1074:VAL:O	1:S:1079:HIS:N	2.53	0.41
1:S:1075:MET:O	1:S:1075:MET:HG2	2.19	0.41
1:S:1121:MET:O	1:S:1122:ARG:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1132:THR:C	1:S:1134:GLU:N	2.75	0.41
1:S:1452:ILE:HG13	1:S:1452:ILE:H	1.43	0.41
1:U:1210:MET:HE2	1:U:1210:MET:HB3	1.81	0.41
1:U:1238:ARG:CG	1:U:1345:LEU:HD21	2.51	0.41
1:U:1320:ASN:HB3	1:U:1324:GLN:NE2	2.36	0.41
1:U:1369:TYR:CD2	1:U:1370:ASN:N	2.89	0.41
1:U:1393:GLU:O	1:U:1394:ILE:C	2.64	0.41
2:V:6:DG:H1	5:Y:15:DC:H42	1.68	0.41
1:B:1029:VAL:CA	1:B:1033:ARG:HB3	2.50	0.41
1:B:1064:TYR:CD1	1:B:1107:GLN:HB2	2.56	0.41
1:B:1252:ARG:HG2	1:B:1257:GLN:O	2.21	0.41
1:D:442:SER:HB2	1:D:591:LEU:HD12	2.02	0.41
1:D:469:LEU:HA	1:D:472:ILE:HD12	2.01	0.41
1:D:527:PHE:C	1:D:528:MET:CG	2.93	0.41
1:D:542:PRO:HA	1:D:543:PRO:HD3	1.79	0.41
1:D:587:ASN:HB2	1:D:590:GLN:HB2	2.02	0.41
1:D:589:ASP:C	1:D:591:LEU:N	2.78	0.41
1:D:620:MET:HE2	1:D:620:MET:HB3	1.90	0.41
1:D:630:ARG:O	1:D:633:ILE:HB	2.21	0.41
1:D:1013:ASN:HB3	1:D:1016:SER:CB	2.51	0.41
1:D:1150:TYR:CD2	1:D:1150:TYR:C	2.99	0.41
1:D:1266:PHE:CZ	1:D:1267:GLN:HG3	2.56	0.41
1:S:617:THR:O	1:S:621:LEU:HG	2.21	0.41
1:S:1150:TYR:CD2	1:S:1150:TYR:C	2.98	0.41
1:S:1161:PRO:O	1:S:1162:ALA:C	2.61	0.41
1:S:1288:GLY:O	1:S:1317:ILE:HD13	2.21	0.41
1:S:1309:ARG:HH11	1:S:1309:ARG:CB	2.32	0.41
1:S:1325:THR:CB	1:S:1326:PRO:CD	2.98	0.41
1:S:1331:PHE:HD2	1:S:1333:VAL:HG22	1.86	0.41
1:S:1335:MET:HE3	1:S:1346:ILE:O	2.21	0.41
1:U:1041:GLY:HA3	1:U:1167:LEU:HA	2.03	0.41
1:U:1295:GLU:N	1:U:1303:ARG:O	2.41	0.41
1:U:1355:TYR:CZ	1:U:1359:GLN:HG3	2.56	0.41
1:U:1381:LEU:CD1	1:U:1448:LEU:HD12	2.51	0.41
1:U:1399:ARG:HG3	1:U:1399:ARG:H	1.59	0.41
1:U:1476:ILE:O	1:U:1478:ASP:N	2.54	0.41
3:W:3:DC:H6	3:W:3:DC:H2'	1.68	0.41
4:X:17:DG:C2	4:X:18:DG:C2	3.08	0.41
1:B:472:ILE:HD13	1:B:527:PHE:HZ	1.85	0.41
1:B:525:TYR:HE2	1:B:526:ARG:HH12	1.68	0.41
1:B:1132:THR:O	1:B:1132:THR:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1245:SER:HG	1:B:1265:PRO:HD3	1.84	0.41
1:D:429:CYS:O	1:D:430:GLU:CB	2.68	0.41
1:D:517:ARG:HB2	1:D:517:ARG:CZ	2.51	0.41
1:D:1054:ASN:HA	1:D:1128:MET:HE2	2.02	0.41
1:D:1313:ASN:O	1:D:1317:ILE:HG13	2.21	0.41
1:D:1358:HIS:O	1:D:1358:HIS:CG	2.73	0.41
3:F:8:DG:C2	4:G:14:DC:O2	2.74	0.41
5:H:19:DC:H1'	5:H:20:DA:O4'	2.21	0.41
1:S:501:HIS:CD2	1:S:536:TYR:HH	2.38	0.41
1:U:464:VAL:HA	1:U:472:ILE:HG12	2.03	0.41
1:U:536:TYR:N	1:U:536:TYR:CD2	2.89	0.41
1:U:1269:ASN:CB	1:U:1272:ARG:NH1	2.84	0.41
5:Y:13:DA:OP2	5:Y:13:DA:C8	2.74	0.41
1:B:1162:ALA:O	1:B:1359:GLN:NE2	2.54	0.40
1:B:1385:ARG:O	1:B:1386:ILE:C	2.64	0.40
1:D:523:PHE:CD2	1:D:524:PHE:CE2	3.09	0.40
1:D:1160:LEU:HB3	1:D:1161:PRO:HD2	2.02	0.40
1:D:1437:GLU:O	1:D:1441:ILE:HG13	2.21	0.40
1:S:1100:ARG:NH1	1:S:1485:ARG:CZ	2.84	0.40
1:S:1185:PRO:HB2	1:S:1217:ASP:O	2.22	0.40
1:U:427:GLU:HA	1:U:501:HIS:CE1	2.56	0.40
1:U:1059:THR:CG2	1:U:1128:MET:CE	2.98	0.40
4:X:17:DG:C2	4:X:18:DG:N3	2.89	0.40
1:B:536:TYR:N	1:B:536:TYR:HD2	2.20	0.40
1:B:1418:SER:O	1:B:1419:GLU:C	2.62	0.40
1:D:501:HIS:HA	1:D:536:TYR:CD1	2.56	0.40
1:S:437:ASP:CB	5:Y:9:DG:H5'	2.51	0.40
1:S:608:LEU:O	1:S:608:LEU:HG	2.20	0.40
1:S:1273:MET:HA	1:S:1326:PRO:HG2	2.03	0.40
1:S:1364:ARG:O	1:S:1368:GLN:HG3	2.21	0.40
1:S:1390:HIS:HB3	1:S:1393:GLU:CB	2.51	0.40
1:U:525:TYR:OH	1:U:614:ALA:C	2.63	0.40
1:U:1195:VAL:O	1:U:1198:LEU:N	2.54	0.40
1:U:1374:ALA:HB1	1:U:1448:LEU:CD2	2.51	0.40
1:B:1225:LEU:HA	1:B:1225:LEU:HD23	1.79	0.40
1:B:1321:LEU:HD23	1:B:1321:LEU:HA	1.92	0.40
1:B:1408:MET:C	1:B:1412:GLN:CG	2.94	0.40
1:D:588:ALA:O	1:D:591:LEU:HB2	2.21	0.40
1:D:1012:ARG:NH2	1:D:1016:SER:O	2.54	0.40
1:S:517:ARG:NH2	1:U:1017:GLU:OE2	2.50	0.40
1:U:1165:PRO:HA	1:U:1355:TYR:CZ	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:12:DC:H6	5:Y:12:DC:H5'	1.87	0.40
1:B:1080:PRO:O	1:B:1081:HIS:ND1	2.55	0.40
1:B:1120:ALA:C	1:B:1122:ARG:N	2.79	0.40
1:B:1339:VAL:C	1:B:1341:GLY:N	2.79	0.40
1:D:461:ILE:H	1:D:461:ILE:HG13	1.67	0.40
1:D:1046:HIS:O	1:D:1047:ARG:C	2.64	0.40
1:D:1049:ILE:HD13	1:D:1090:MET:CB	2.42	0.40
1:D:1188:LEU:O	1:D:1192:ILE:HG13	2.21	0.40
1:D:1214:GLU:HB3	1:D:1488:ILE:HD12	2.04	0.40
1:D:1348:LEU:O	1:D:1349:LYS:C	2.63	0.40
1:D:1432:ARG:CG	1:D:1441:ILE:HD11	2.52	0.40
1:D:1438:ARG:O	1:D:1441:ILE:HB	2.22	0.40
1:S:465:GLU:OE1	1:S:465:GLU:O	2.38	0.40
1:U:448:ASP:OD1	1:U:448:ASP:C	2.65	0.40
1:B:443:THR:O	1:B:447:ARG:HB3	2.20	0.40
1:B:461:ILE:O	5:H:14:DC:H2''	2.21	0.40
1:B:598:PRO:HA	1:B:601:ARG:HD3	2.03	0.40
1:B:1103:LEU:HD21	1:B:1170:ASN:ND2	2.37	0.40
1:B:1182:ASN:ND2	1:B:1331:PHE:CE2	2.89	0.40
1:B:1283:ASP:O	1:B:1284:LYS:C	2.63	0.40
1:B:1411:LEU:HD23	1:B:1417:LEU:HD12	2.04	0.40
1:D:426:PRO:O	1:D:427:GLU:C	2.65	0.40
1:D:531:LEU:CD1	1:D:536:TYR:HB2	2.48	0.40
1:D:625:VAL:HB	1:D:628:ASN:ND2	2.37	0.40
1:D:630:ARG:O	1:D:631:GLN:C	2.64	0.40
1:D:1371:LEU:O	1:D:1374:ALA:N	2.50	0.40
1:S:1247:ALA:CA	1:S:1260:VAL:O	2.69	0.40
1:U:423:SER:HB3	1:U:450:ARG:O	2.21	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	B	667/692 (96%)	545 (82%)	100 (15%)	22 (3%)	3	17
1	D	664/692 (96%)	526 (79%)	108 (16%)	30 (4%)	2	12
1	S	661/692 (96%)	493 (75%)	123 (19%)	45 (7%)	1	6
1	U	659/692 (95%)	532 (81%)	97 (15%)	30 (5%)	2	11
All	All	2651/2768 (96%)	2096 (79%)	428 (16%)	127 (5%)	2	11

All (127) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1150	TYR
1	B	1291	ASP
1	B	1310	LYS
1	B	1409	GLU
1	B	1431	ARG
1	D	435	GLU
1	D	540	ALA
1	D	1128	MET
1	D	1434	THR
1	D	1483	ASP
1	S	583	LEU
1	S	627	GLU
1	S	1118	ALA
1	S	1138	ASP
1	S	1335	MET
1	S	1406	VAL
1	U	1038	VAL
1	U	1120	ALA
1	U	1142	ASP
1	U	1302	VAL
1	U	1477	ARG
1	B	1335	MET
1	B	1340	ASN
1	B	1408	MET
1	B	1460	ALA
1	D	427	GLU
1	D	493	PHE
1	D	585	GLU
1	D	633	ILE
1	D	1165	PRO
1	D	1167	LEU
1	D	1411	LEU
1	D	1426	LEU

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Mol	Chain	Res	Type
1	S	419	ALA
1	S	420	ASP
1	S	458	ARG
1	S	516	ILE
1	S	540	ALA
1	S	584	GLY
1	S	628	ASN
1	S	635	ASP
1	S	1027	MET
1	S	1054	ASN
1	S	1117	GLY
1	S	1119	ALA
1	S	1152	GLY
1	S	1178	GLY
1	S	1180	ALA
1	S	1284	LYS
1	S	1378	ALA
1	S	1379	HIS
1	S	1407	ALA
1	U	593	GLU
1	U	1030	ILE
1	U	1033	ARG
1	U	1158	SER
1	U	1159	VAL
1	U	1228	SER
1	B	1172	ALA
1	B	1221	ALA
1	B	1309	ARG
1	B	1434	THR
1	D	430	GLU
1	D	473	LEU
1	D	1045	VAL
1	D	1112	SER
1	D	1316	VAL
1	S	449	SER
1	S	468	ARG
1	S	1044	PRO
1	S	1165	PRO
1	S	1216	PRO
1	S	1227	LYS
1	U	519	LEU
1	U	592	TRP

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Mol	Chain	Res	Type
1	U	1199	SER
1	U	1244	ARG
1	B	1167	LEU
1	B	1276	LYS
1	B	1349	LYS
1	B	1386	ILE
1	D	423	SER
1	D	1149	ASN
1	S	448	ASP
1	S	475	ASN
1	S	1078	TYR
1	S	1171	GLY
1	S	1340	ASN
1	U	493	PHE
1	U	1063	SER
1	U	1489	GLN
1	B	581	LYS
1	B	1279	GLU
1	D	1068	ALA
1	D	1327	LEU
1	D	1367	THR
1	D	1371	LEU
1	S	1028	SER
1	S	1033	ARG
1	S	1137	ARG
1	S	1189	THR
1	S	1270	LYS
1	U	1326	PRO
1	U	1349	LYS
1	U	1370	ASN
1	B	633	ILE
1	D	1093	MET
1	D	1349	LYS
1	S	598	PRO
1	U	1203	ASP
1	U	1221	ALA
1	S	623	GLY
1	U	1102	PRO
1	D	1226	GLY
1	S	1202	PRO
1	S	1316	VAL
1	U	1195	VAL

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Mol	Chain	Res	Type
1	U	1206	ILE
1	B	461	ILE
1	D	1177	VAL
1	D	1441	ILE
1	U	1029	VAL
1	U	1177	VAL
1	U	1386	ILE
1	B	459	GLY
1	D	539	ILE
1	U	1394	ILE

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	B	563/591 (95%)	500 (89%)	63 (11%)	6	21
1	D	539/591 (91%)	471 (87%)	68 (13%)	4	17
1	S	555/591 (94%)	478 (86%)	77 (14%)	3	14
1	U	553/591 (94%)	486 (88%)	67 (12%)	5	18
All	All	2210/2364 (94%)	1935 (88%)	275 (12%)	4	18

All (275) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	418	LEU
1	B	421	CYS
1	B	433	LEU
1	B	434	VAL
1	B	435	GLU
1	B	451	THR
1	B	477	GLU
1	B	482	ILE
1	B	483	THR
1	B	508	ASP
1	B	522	THR

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Mol	Chain	Res	Type
1	B	536	TYR
1	B	539	ILE
1	B	590	GLN
1	B	591	LEU
1	B	617	THR
1	B	631	GLN
1	B	1038	VAL
1	B	1069	ARG
1	B	1073	ASP
1	B	1083	ASP
1	B	1098	SER
1	B	1113	MET
1	B	1116	ASP
1	B	1129	THR
1	B	1131	ILE
1	B	1136	LEU
1	B	1139	ILE
1	B	1143	THR
1	B	1189	THR
1	B	1195	VAL
1	B	1205	SER
1	B	1206	ILE
1	B	1224	ILE
1	B	1227	LYS
1	B	1236	THR
1	B	1251	GLU
1	B	1259	ILE
1	B	1260	VAL
1	B	1262	THR
1	B	1292	LEU
1	B	1297	SER
1	B	1298	LEU
1	B	1300	THR
1	B	1311	ASP
1	B	1315	SER
1	B	1333	VAL
1	B	1371	LEU
1	B	1385	ARG
1	B	1386	ILE
1	B	1390	HIS
1	B	1397	THR
1	B	1398	ILE

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Mol	Chain	Res	Type
1	B	1411	LEU
1	B	1412	GLN
1	B	1413	GLN
1	B	1416	LYS
1	B	1426	LEU
1	B	1439	ASP
1	B	1441	ILE
1	B	1464	VAL
1	B	1475	GLU
1	B	1490	LEU
1	D	422	SER
1	D	434	VAL
1	D	458	ARG
1	D	461	ILE
1	D	475	ASN
1	D	477	GLU
1	D	483	THR
1	D	499	ARG
1	D	507	THR
1	D	516	ILE
1	D	536	TYR
1	D	541	GLN
1	D	583	LEU
1	D	585	GLU
1	D	594	THR
1	D	603	LEU
1	D	620	MET
1	D	625	VAL
1	D	636	ASN
1	D	1028	SER
1	D	1045	VAL
1	D	1047	ARG
1	D	1058	MET
1	D	1063	SER
1	D	1070	ILE
1	D	1084	SER
1	D	1098	SER
1	D	1107	GLN
1	D	1122	ARG
1	D	1135	LEU
1	D	1136	LEU
1	D	1147	ILE

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Mol	Chain	Res	Type
1	D	1159	VAL
1	D	1168	LEU
1	D	1179	MET
1	D	1192	ILE
1	D	1193	ASN
1	D	1195	VAL
1	D	1204	ILE
1	D	1231	ARG
1	D	1245	SER
1	D	1258	ARG
1	D	1284	LYS
1	D	1296	THR
1	D	1299	ARG
1	D	1300	THR
1	D	1315	SER
1	D	1327	LEU
1	D	1344	LYS
1	D	1347	ASN
1	D	1352	LEU
1	D	1357	GLU
1	D	1360	LYS
1	D	1367	THR
1	D	1384	LEU
1	D	1385	ARG
1	D	1390	HIS
1	D	1393	GLU
1	D	1395	ILE
1	D	1396	SER
1	D	1400	GLU
1	D	1404	ASP
1	D	1408	MET
1	D	1426	LEU
1	D	1450	ASN
1	D	1465	LEU
1	D	1483	ASP
1	D	1490	LEU
1	S	418	LEU
1	S	428	GLU
1	S	445	SER
1	S	461	ILE
1	S	462	LEU
1	S	476	ASN

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Mol	Chain	Res	Type
1	S	477	GLU
1	S	483	THR
1	S	492	ASP
1	S	505	ILE
1	S	511	VAL
1	S	512	ASP
1	S	516	ILE
1	S	522	THR
1	S	538	TYR
1	S	544	THR
1	S	589	ASP
1	S	591	LEU
1	S	604	LEU
1	S	636	ASN
1	S	1038	VAL
1	S	1049	ILE
1	S	1058	MET
1	S	1067	SER
1	S	1085	SER
1	S	1086	ILE
1	S	1092	ARG
1	S	1096	ASP
1	S	1103	LEU
1	S	1124	THR
1	S	1131	ILE
1	S	1136	LEU
1	S	1143	THR
1	S	1145	ASP
1	S	1147	ILE
1	S	1168	LEU
1	S	1187	ASN
1	S	1189	THR
1	S	1195	VAL
1	S	1203	ASP
1	S	1204	ILE
1	S	1209	LEU
1	S	1220	THR
1	S	1228	SER
1	S	1232	ARG
1	S	1236	THR
1	S	1245	SER
1	S	1248	VAL

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Mol	Chain	Res	Type
1	S	1260	VAL
1	S	1261	VAL
1	S	1262	THR
1	S	1298	LEU
1	S	1299	ARG
1	S	1308	VAL
1	S	1309	ARG
1	S	1329	THR
1	S	1342	ARG
1	S	1345	LEU
1	S	1347	ASN
1	S	1348	LEU
1	S	1362	VAL
1	S	1367	THR
1	S	1369	TYR
1	S	1391	ILE
1	S	1392	ASP
1	S	1398	ILE
1	S	1418	SER
1	S	1433	LEU
1	S	1448	LEU
1	S	1450	ASN
1	S	1452	ILE
1	S	1453	SER
1	S	1458	ILE
1	S	1464	VAL
1	S	1466	LEU
1	S	1483	ASP
1	S	1486	THR
1	U	430	GLU
1	U	433	LEU
1	U	434	VAL
1	U	435	GLU
1	U	444	LYS
1	U	454	ILE
1	U	461	ILE
1	U	462	LEU
1	U	476	ASN
1	U	478	ILE
1	U	489	ILE
1	U	505	ILE
1	U	507	THR

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Mol	Chain	Res	Type
1	U	508	ASP
1	U	511	VAL
1	U	516	ILE
1	U	520	LEU
1	U	531	LEU
1	U	538	TYR
1	U	594	THR
1	U	610	ASP
1	U	612	ILE
1	U	617	THR
1	U	620	MET
1	U	633	ILE
1	U	639	TYR
1	U	1015	THR
1	U	1016	SER
1	U	1031	VAL
1	U	1061	ASP
1	U	1078	TYR
1	U	1088	GLU
1	U	1091	VAL
1	U	1122	ARG
1	U	1129	THR
1	U	1139	ILE
1	U	1179	MET
1	U	1220	THR
1	U	1225	LEU
1	U	1230	ILE
1	U	1236	THR
1	U	1248	VAL
1	U	1259	ILE
1	U	1261	VAL
1	U	1262	THR
1	U	1286	ILE
1	U	1300	THR
1	U	1302	VAL
1	U	1306	ILE
1	U	1316	VAL
1	U	1317	ILE
1	U	1325	THR
1	U	1329	THR
1	U	1345	LEU
1	U	1361	THR

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Mol	Chain	Res	Type
1	U	1371	LEU
1	U	1403	THR
1	U	1404	ASP
1	U	1432	ARG
1	U	1450	ASN
1	U	1459	LEU
1	U	1464	VAL
1	U	1465	LEU
1	U	1466	LEU
1	U	1469	VAL
1	U	1473	LEU
1	U	1483	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	476	ASN
1	B	501	HIS
1	B	587	ASN
1	B	590	GLN
1	B	597	ASN
1	B	600	HIS
1	B	605	GLN
1	B	628	ASN
1	B	1081	HIS
1	B	1170	ASN
1	B	1334	ASN
1	B	1347	ASN
1	B	1358	HIS
1	B	1359	GLN
1	B	1450	ASN
1	D	474	ASN
1	D	501	HIS
1	D	541	GLN
1	D	597	ASN
1	D	600	HIS
1	D	628	ASN
1	D	636	ASN
1	D	1013	ASN
1	D	1081	HIS
1	D	1313	ASN
1	D	1334	ASN

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Mol	Chain	Res	Type
1	D	1347	ASN
1	D	1358	HIS
1	D	1446	ASN
1	S	480	GLN
1	S	597	ASN
1	S	616	GLN
1	S	1046	HIS
1	S	1054	ASN
1	S	1081	HIS
1	S	1324	GLN
1	S	1358	HIS
1	S	1390	HIS
1	S	1412	GLN
1	U	474	ASN
1	U	515	HIS
1	U	597	ASN
1	U	605	GLN
1	U	636	ASN
1	U	1046	HIS
1	U	1107	GLN
1	U	1242	GLN
1	U	1313	ASN
1	U	1324	GLN
1	U	1358	HIS
1	U	1368	GLN
1	U	1450	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	CPF	H	1020	6	27,27,27	2.36	7 (25%)	40,40,40	2.80	18 (45%)
7	CPF	G	1020	6	27,27,27	2.29	5 (18%)	40,40,40	2.41	16 (40%)
7	CPF	X	1020	6	27,27,27	2.32	7 (25%)	40,40,40	2.30	14 (35%)
7	CPF	Y	1020	6	27,27,27	2.34	7 (25%)	40,40,40	2.68	19 (47%)

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
7	CPF	H	1020	6	-	6/12/22/22	0/4/4/4
7	CPF	G	1020	6	-	6/12/22/22	0/4/4/4
7	CPF	X	1020	6	-	4/12/22/22	0/4/4/4
7	CPF	Y	1020	6	-	2/12/22/22	0/4/4/4

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	1020	CPF	O3-C4	7.26	1.38	1.23
7	X	1020	CPF	O3-C4	6.57	1.36	1.23
7	H	1020	CPF	O3-C4	6.15	1.36	1.23
7	Y	1020	CPF	O2-C3	6.04	1.47	1.30
7	H	1020	CPF	O2-C3	5.96	1.46	1.30
7	X	1020	CPF	O2-C3	5.90	1.46	1.30
7	H	1020	CPF	C5-C4	-5.82	1.36	1.48
7	Y	1020	CPF	O3-C4	5.79	1.35	1.23
7	Y	1020	CPF	C5-C4	-5.61	1.37	1.48
7	G	1020	CPF	O2-C3	5.61	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	X	1020	CPF	C5-C4	-4.98	1.38	1.48
7	G	1020	CPF	C10-N1	-4.47	1.34	1.40
7	Y	1020	CPF	C10-N1	-4.32	1.34	1.40
7	G	1020	CPF	C5-C4	-4.29	1.39	1.48
7	H	1020	CPF	C10-N1	-3.80	1.35	1.40
7	X	1020	CPF	C10-N1	-3.63	1.35	1.40
7	H	1020	CPF	C2-C3	2.69	1.52	1.48
7	X	1020	CPF	C2-C4	-2.54	1.38	1.44
7	H	1020	CPF	C2-C4	-2.43	1.38	1.44
7	X	1020	CPF	C2-C3	2.33	1.52	1.48
7	Y	1020	CPF	C2-C4	-2.33	1.39	1.44
7	Y	1020	CPF	C2-C3	2.24	1.52	1.48
7	G	1020	CPF	C2-C4	-2.24	1.39	1.44
7	X	1020	CPF	C12-C11	2.16	1.53	1.48
7	H	1020	CPF	C12-C11	2.15	1.53	1.48
7	Y	1020	CPF	C13-C11	2.10	1.53	1.48

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	1020	CPF	C12-C11-N1	-7.26	107.38	118.87
7	H	1020	CPF	C13-C11-N1	-6.90	107.95	118.87
7	Y	1020	CPF	C12-C11-N1	-6.52	108.55	118.87
7	G	1020	CPF	C13-C11-N1	-6.47	108.63	118.87
7	H	1020	CPF	F1-C7-C8	5.93	124.02	118.37
7	X	1020	CPF	C13-C11-N1	-5.47	110.21	118.87
7	G	1020	CPF	C12-C11-N1	-5.45	110.24	118.87
7	Y	1020	CPF	C6-C7-C8	-5.10	118.85	123.35
7	Y	1020	CPF	C9-C8-N2	-4.82	115.56	122.59
7	Y	1020	CPF	C5-C4-C2	4.68	121.54	115.64
7	X	1020	CPF	C6-C7-C8	-4.58	119.31	123.35
7	H	1020	CPF	C14-N2-C17	4.48	121.64	111.57
7	X	1020	CPF	C14-N2-C17	4.45	121.59	111.57
7	Y	1020	CPF	F1-C7-C8	4.41	122.58	118.37
7	Y	1020	CPF	C13-C11-N1	-4.35	111.98	118.87
7	H	1020	CPF	O3-C4-C5	-4.31	114.67	121.57
7	X	1020	CPF	C12-C11-N1	-4.17	112.27	118.87
7	Y	1020	CPF	C14-N2-C17	4.13	120.87	111.57
7	H	1020	CPF	C5-C4-C2	4.07	120.78	115.64
7	H	1020	CPF	C1-C2-C4	-4.07	116.95	119.94
7	G	1020	CPF	C14-N2-C17	4.05	120.69	111.57
7	H	1020	CPF	C6-C7-C8	-3.88	119.92	123.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	1020	CPF	C9-C8-N2	-3.88	116.94	122.59
7	G	1020	CPF	C9-C8-C7	3.77	120.46	116.53
7	G	1020	CPF	C6-C7-C8	-3.75	120.04	123.35
7	X	1020	CPF	F1-C7-C8	3.73	121.93	118.37
7	Y	1020	CPF	C7-C8-N2	3.73	124.78	120.42
7	H	1020	CPF	C9-C8-C7	3.72	120.41	116.53
7	X	1020	CPF	C5-C4-C2	3.71	120.31	115.64
7	X	1020	CPF	C1-C2-C3	3.55	123.93	118.27
7	Y	1020	CPF	C2-C1-N1	-3.52	120.21	124.42
7	G	1020	CPF	C5-C10-N1	3.50	121.59	118.83
7	Y	1020	CPF	O3-C4-C5	-3.30	116.29	121.57
7	G	1020	CPF	C2-C1-N1	-3.29	120.47	124.42
7	H	1020	CPF	C6-C5-C10	3.26	122.61	118.76
7	X	1020	CPF	C9-C8-C7	3.24	119.91	116.53
7	Y	1020	CPF	C10-C5-C4	-3.11	118.42	121.38
7	Y	1020	CPF	C1-C2-C4	-3.07	117.69	119.94
7	G	1020	CPF	C16-C17-N2	-3.03	103.80	110.38
7	X	1020	CPF	C15-N3-C16	3.01	118.91	110.40
7	Y	1020	CPF	C9-C8-C7	3.00	119.66	116.53
7	X	1020	CPF	C2-C1-N1	-2.85	121.01	124.42
7	G	1020	CPF	C10-C5-C4	-2.83	118.69	121.38
7	H	1020	CPF	C17-N2-C8	2.81	122.86	116.19
7	Y	1020	CPF	C5-C10-N1	2.71	120.97	118.83
7	Y	1020	CPF	C1-C2-C3	2.71	122.58	118.27
7	H	1020	CPF	C9-C10-N1	2.70	122.82	120.49
7	G	1020	CPF	C5-C4-C2	2.66	119.00	115.64
7	X	1020	CPF	C1-C2-C4	-2.62	118.02	119.94
7	G	1020	CPF	C14-N2-C8	2.60	122.35	116.19
7	H	1020	CPF	C1-C2-C3	2.59	122.39	118.27
7	H	1020	CPF	C15-N3-C16	2.56	117.64	110.40
7	Y	1020	CPF	C14-N2-C8	2.53	122.20	116.19
7	H	1020	CPF	C10-N1-C1	2.43	121.47	119.64
7	G	1020	CPF	C15-N3-C16	2.40	117.19	110.40
7	X	1020	CPF	C3-C2-C4	-2.38	118.05	121.61
7	Y	1020	CPF	C15-N3-C16	2.32	116.96	110.40
7	H	1020	CPF	C2-C1-N1	-2.31	121.66	124.42
7	X	1020	CPF	O2-C3-O1	-2.28	118.47	123.90
7	G	1020	CPF	F1-C7-C8	2.26	120.53	118.37
7	G	1020	CPF	C9-C10-N1	-2.20	118.59	120.49
7	X	1020	CPF	C6-C5-C10	2.19	121.34	118.76
7	Y	1020	CPF	C6-C5-C10	2.17	121.33	118.76
7	G	1020	CPF	O3-C4-C2	-2.08	119.74	123.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	1020	CPF	C6-C5-C4	-2.06	116.48	119.94
7	Y	1020	CPF	C10-N1-C1	2.02	121.16	119.64
7	H	1020	CPF	O2-C3-O1	-2.01	119.12	123.90

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	H	1020	CPF	C12-C11-N1-C1
7	G	1020	CPF	C9-C8-N2-C14
7	Y	1020	CPF	C9-C8-N2-C14
7	X	1020	CPF	C9-C8-N2-C14
7	G	1020	CPF	C13-C11-N1-C1
7	G	1020	CPF	C7-C8-N2-C14
7	Y	1020	CPF	C7-C8-N2-C14
7	H	1020	CPF	C12-C11-N1-C10
7	X	1020	CPF	C7-C8-N2-C14
7	H	1020	CPF	C7-C8-N2-C17
7	X	1020	CPF	C12-C11-N1-C1
7	G	1020	CPF	C13-C11-N1-C10
7	X	1020	CPF	C12-C11-N1-C10
7	G	1020	CPF	C12-C11-N1-C1
7	H	1020	CPF	C13-C11-N1-C1
7	G	1020	CPF	C12-C11-N1-C10
7	H	1020	CPF	C9-C8-N2-C17
7	H	1020	CPF	C13-C11-N1-C10

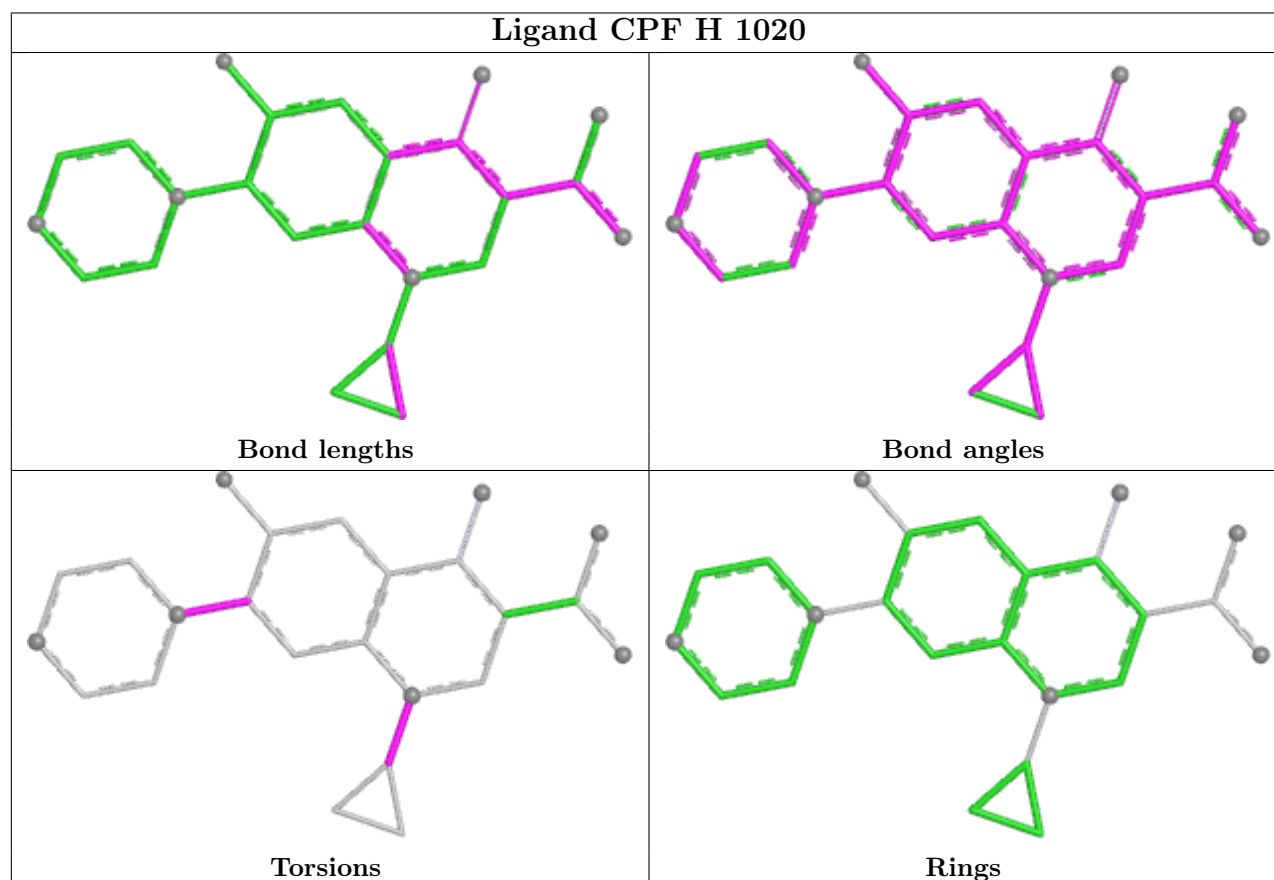
There are no ring outliers.

4 monomers are involved in 47 short contacts:

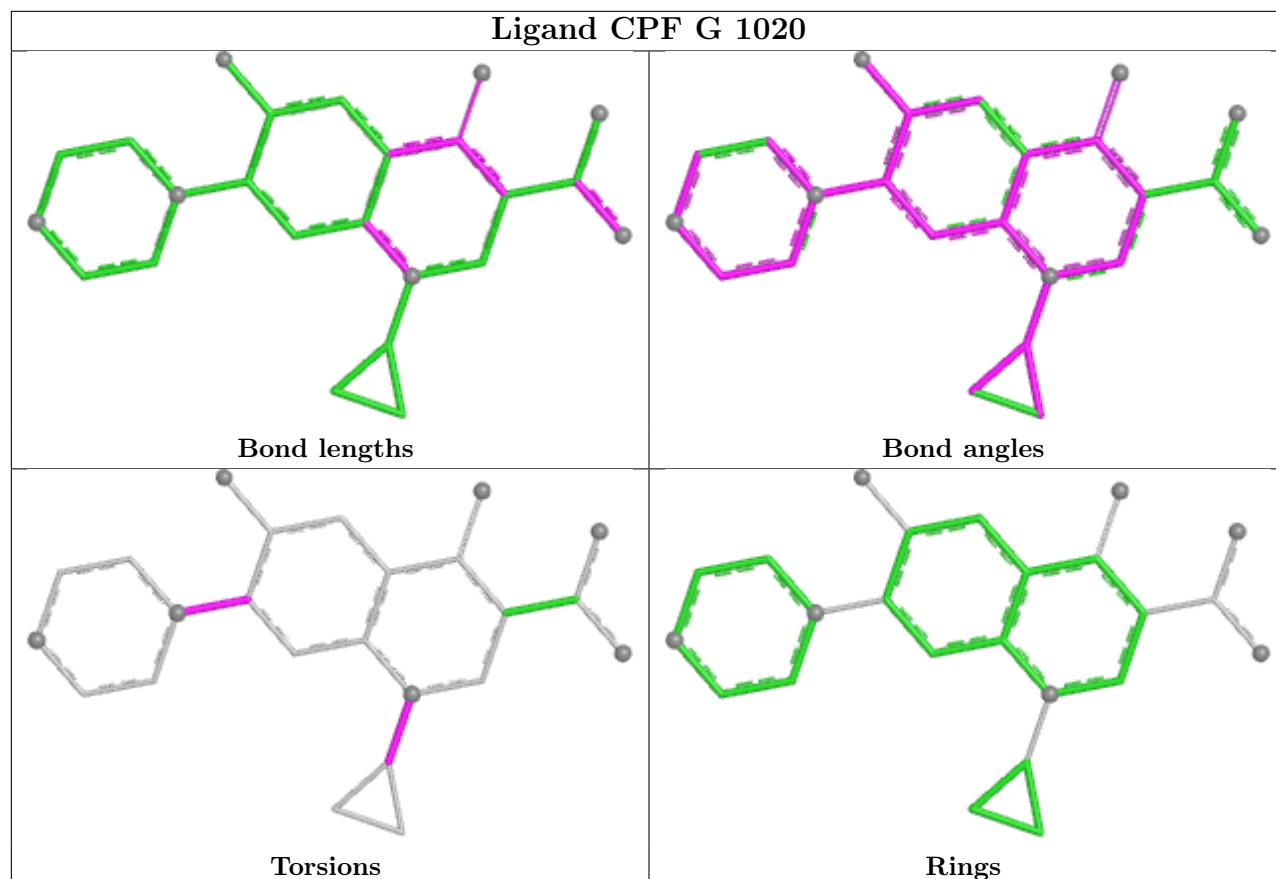
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	H	1020	CPF	9	0
7	G	1020	CPF	8	0
7	X	1020	CPF	20	0
7	Y	1020	CPF	10	0

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

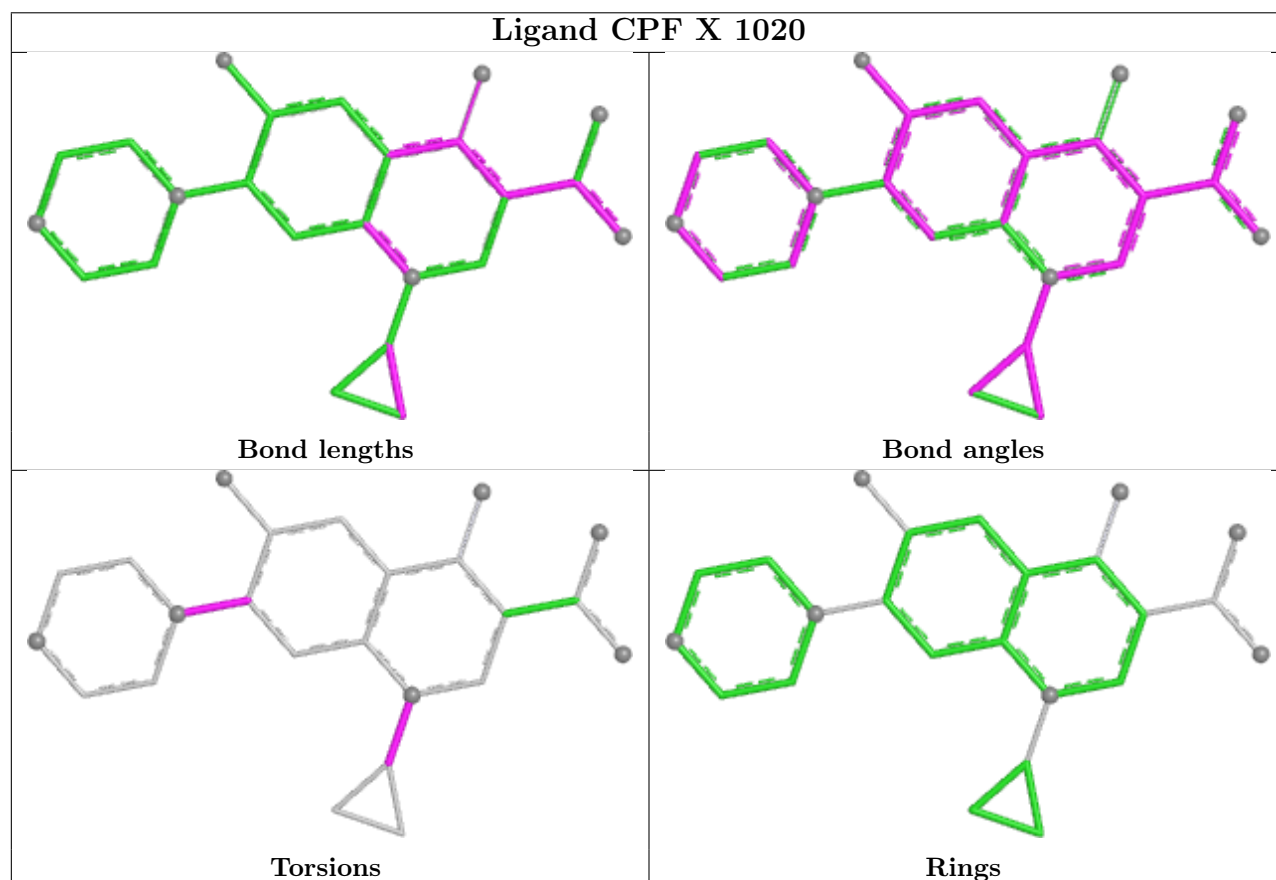
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

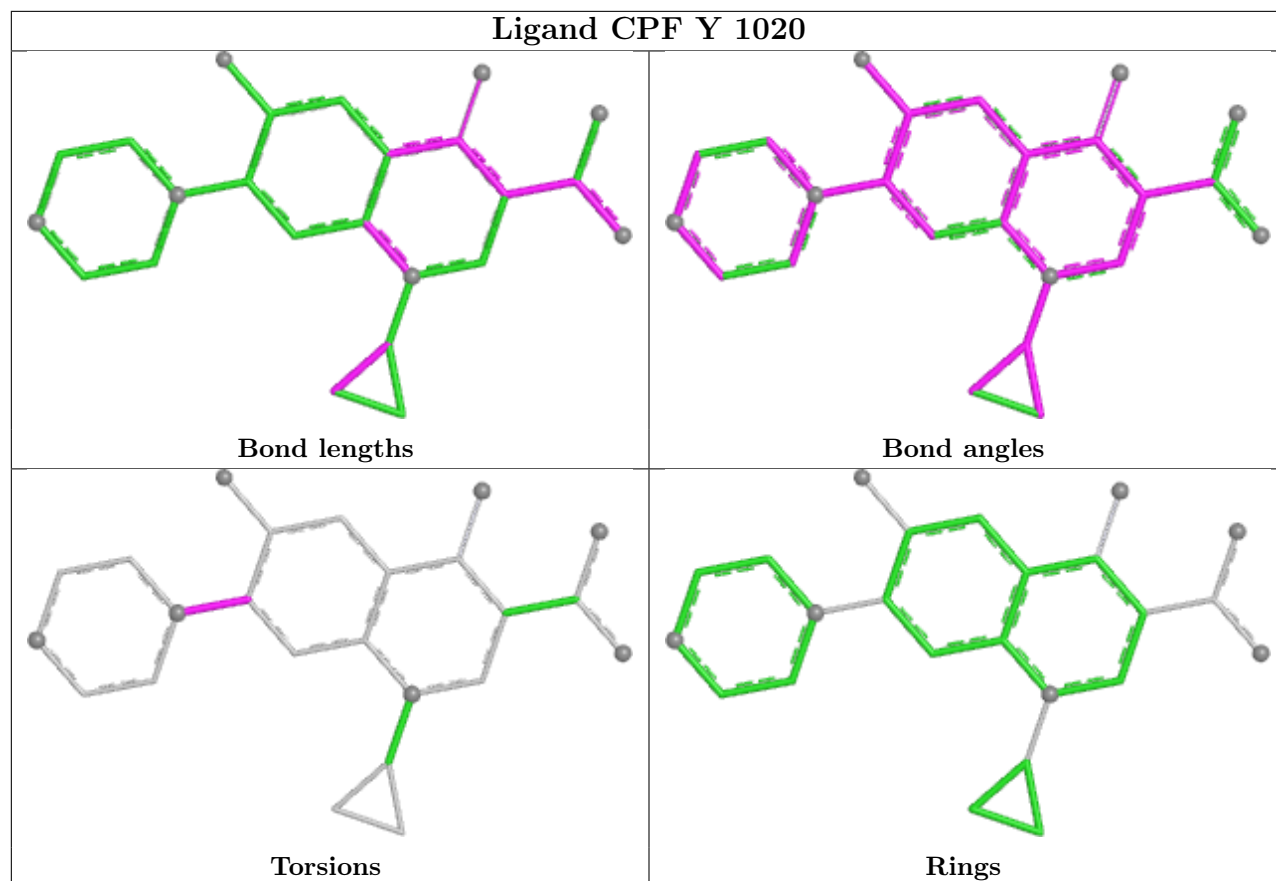


Ligand CPF G 1020



Ligand CPF X 1020





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](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	B	669/692 (96%)	-1.53	0 100 100	21, 64, 101, 143	2 (0%)
1	D	669/692 (96%)	-1.50	0 100 100	35, 68, 108, 143	1 (0%)
1	S	667/692 (96%)	-1.37	0 100 100	43, 78, 119, 218	0
1	U	665/692 (96%)	-1.43	0 100 100	39, 72, 110, 158	0
2	E	7/8 (87%)	-1.52	0 100 100	48, 52, 83, 89	0
2	V	7/8 (87%)	-1.53	0 100 100	51, 62, 76, 86	0
3	F	7/8 (87%)	-1.72	0 100 100	51, 57, 77, 80	0
3	W	6/8 (75%)	-1.56	0 100 100	62, 75, 86, 86	0
4	G	11/12 (91%)	-1.57	0 100 100	60, 67, 90, 120	0
4	X	11/12 (91%)	-1.37	0 100 100	68, 88, 102, 125	0
5	H	12/12 (100%)	-1.59	0 100 100	48, 77, 111, 123	0
5	Y	11/12 (91%)	-1.46	0 100 100	67, 75, 106, 117	0
All	All	2742/2848 (96%)	-1.46	0 100 100	21, 71, 112, 218	3 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

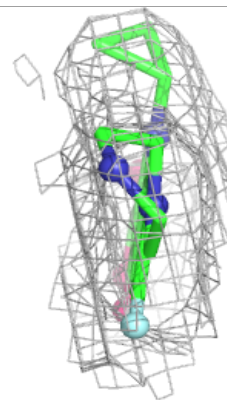
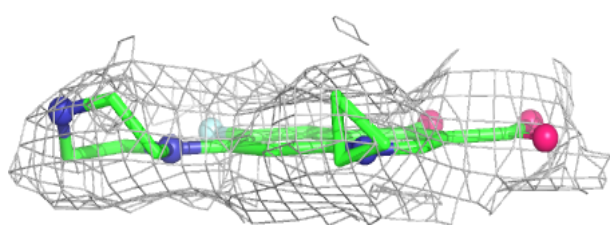
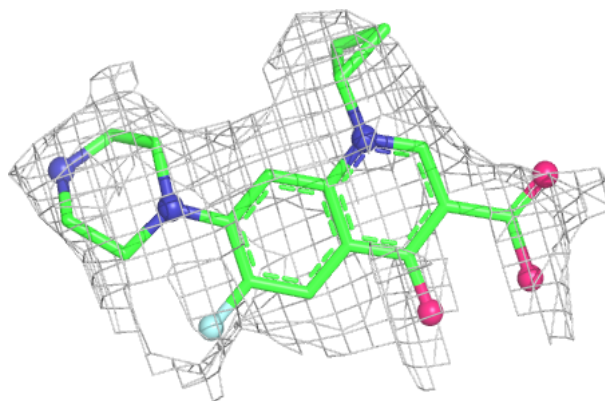
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MN	F	2000	1/1	0.98	0.03	86,86,86,86	0
7	CPF	G	1020	24/24	0.98	0.05	70,70,70,70	0
6	MN	W	2001	1/1	0.99	0.02	76,76,76,76	0
6	MN	W	2000	1/1	0.99	0.03	86,86,86,86	0
7	CPF	H	1020	24/24	0.99	0.04	86,86,86,86	0
7	CPF	X	1020	24/24	0.99	0.04	86,86,86,86	0
7	CPF	Y	1020	24/24	0.99	0.04	76,76,76,76	0
6	MN	B	2492	1/1	1.00	0.03	76,76,76,76	0
6	MN	G	2000	1/1	1.00	0.03	70,70,70,70	0
6	MN	S	2492	1/1	1.00	0.01	70,70,70,70	0
6	MN	U	2492	1/1	1.00	0.03	64,64,64,64	0
6	MN	D	2492	1/1	1.00	0.01	85,85,85,85	0

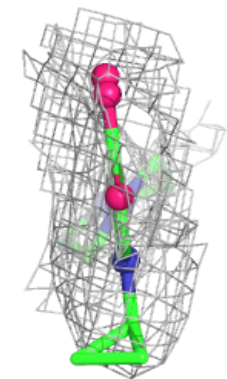
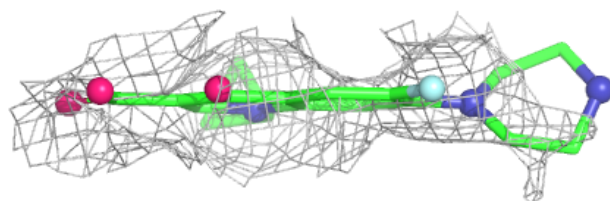
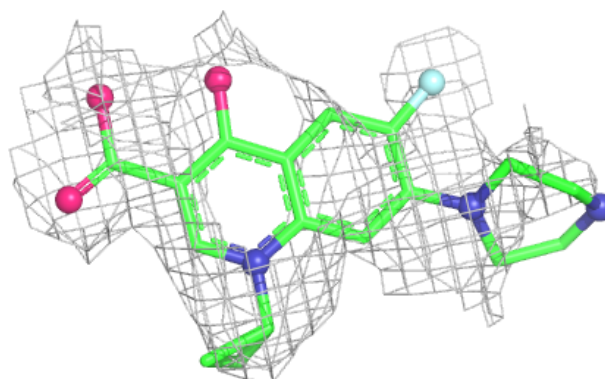
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around CPF G 1020:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

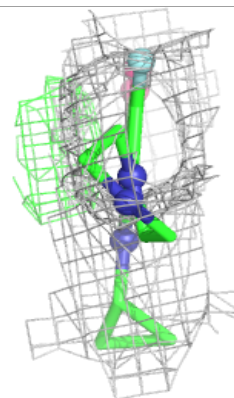
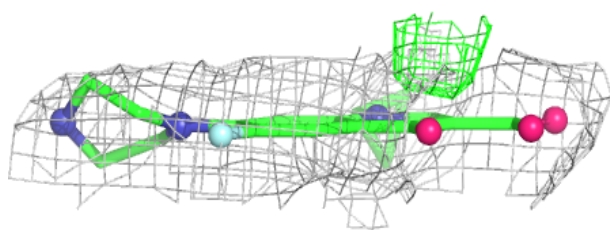
**Electron density around CPF H 1020:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

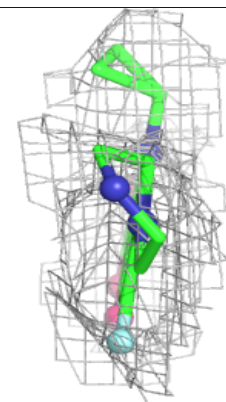
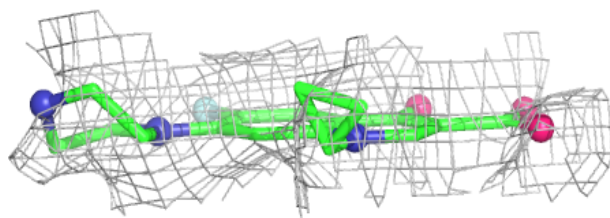
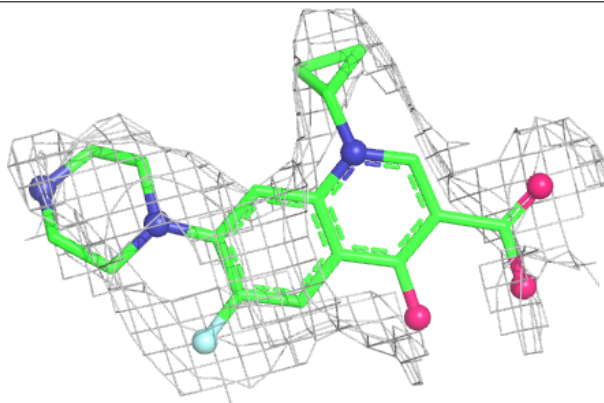


Electron density around CPF X 1020:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around CPF Y 1020:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.