



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2026 – 02:03 pm BST

PDB ID : 2CKJ / pdb_00002ckj
Title : Human milk xanthine oxidoreductase
Authors : Pearson, A.R.; Godber, B.L.J.; Eissenthal, R.; Taylor, G.L.; Harrison, R.
Deposited on : 2006-04-19
Resolution : 3.59 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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

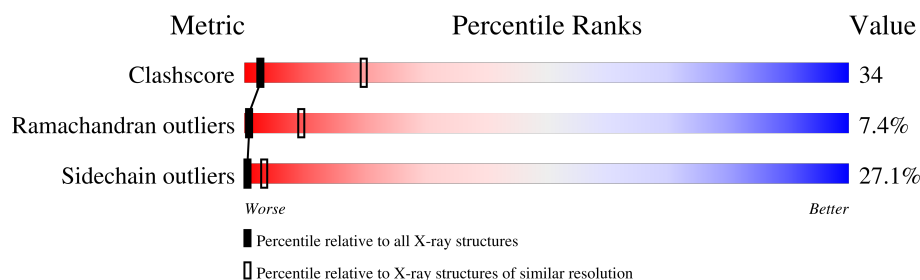
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.59 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1333	25% 35% 25% 10% 5%
1	B	1333	26% 36% 24% 11% .
1	C	1333	26% 36% 24% 11% .
1	D	1333	25% 38% 23% 10% .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FES	A	3002	-	-	X	-
2	FES	B	3002	-	-	X	-
4	GOL	A	3007	-	-	X	-
4	GOL	B	3007	-	-	X	-
4	GOL	C	3007	-	-	X	-
4	GOL	D	3007	-	-	X	-

2 Entry composition [i](#)

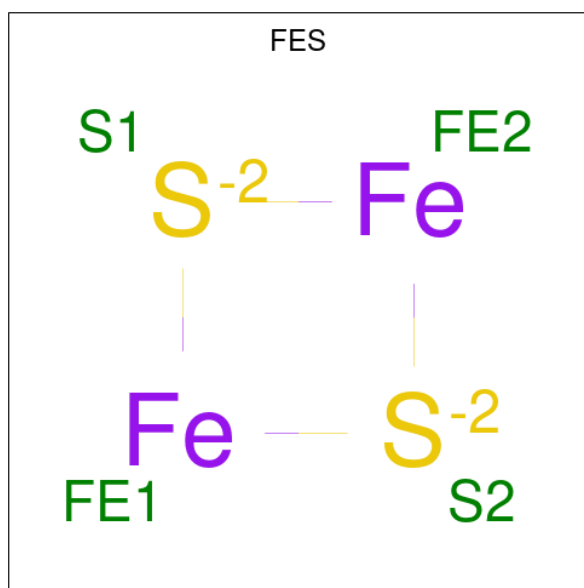
There are 6 unique types of molecules in this entry. The entry contains 39807 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 XANTHINE OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1264	Total	C	N	O	S	0	0	0
			9764	6195	1679	1826	64			
1	B	1289	Total	C	N	O	S	0	0	0
			9951	6307	1713	1865	66			
1	C	1283	Total	C	N	O	S	0	0	0
			9905	6280	1706	1854	65			
1	D	1283	Total	C	N	O	S	0	0	0
			9910	6281	1707	1856	66			

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



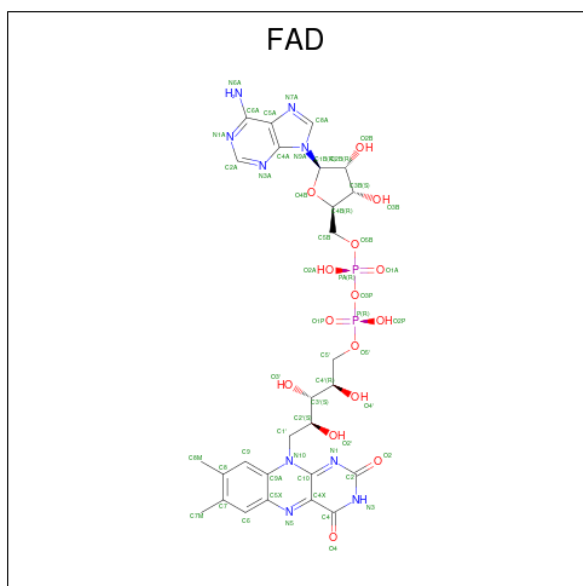
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	A	1	Total	Fe	S	0	0
			4	2	2		

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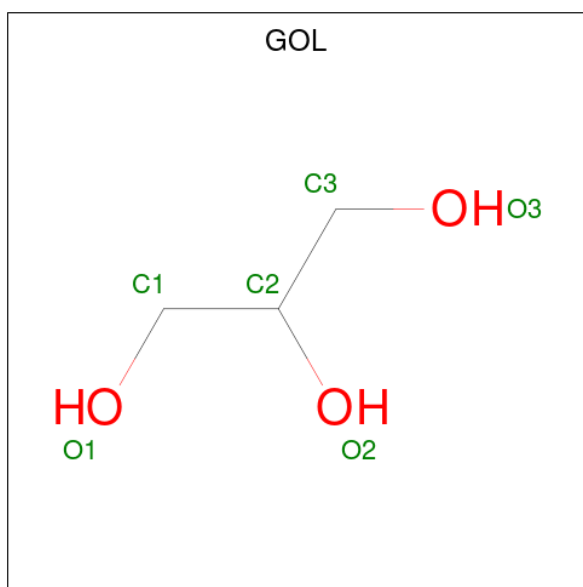
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		
2	C	1	Total	Fe	S	0	0
			4	2	2		
2	C	1	Total	Fe	S	0	0
			4	2	2		
2	D	1	Total	Fe	S	0	0
			4	2	2		
2	D	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



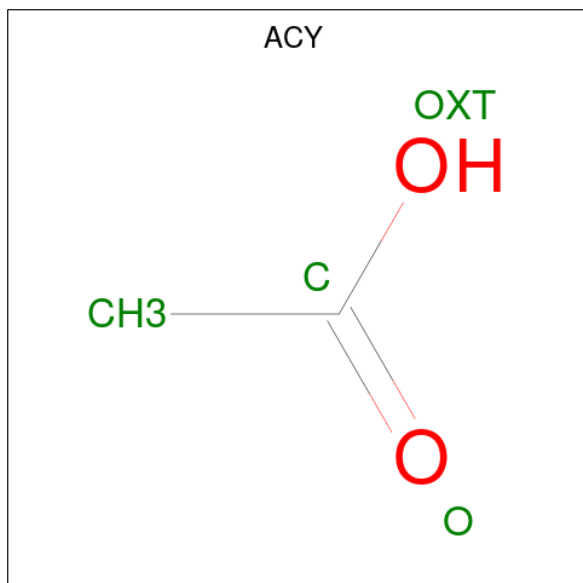
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	B	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	C	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	D	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



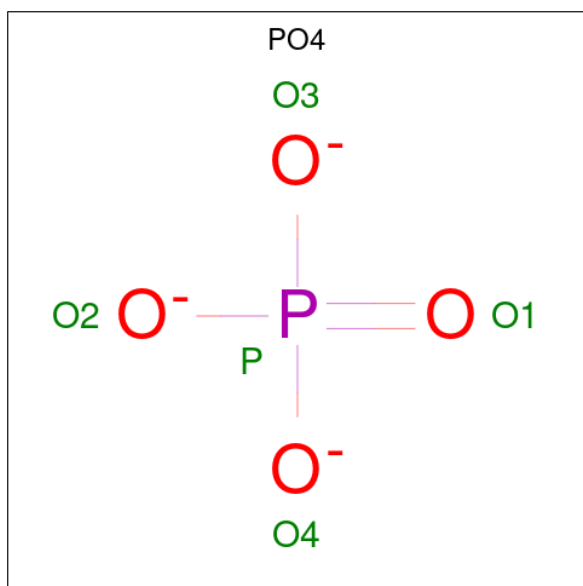
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is ACETIC ACID (CCD ID: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



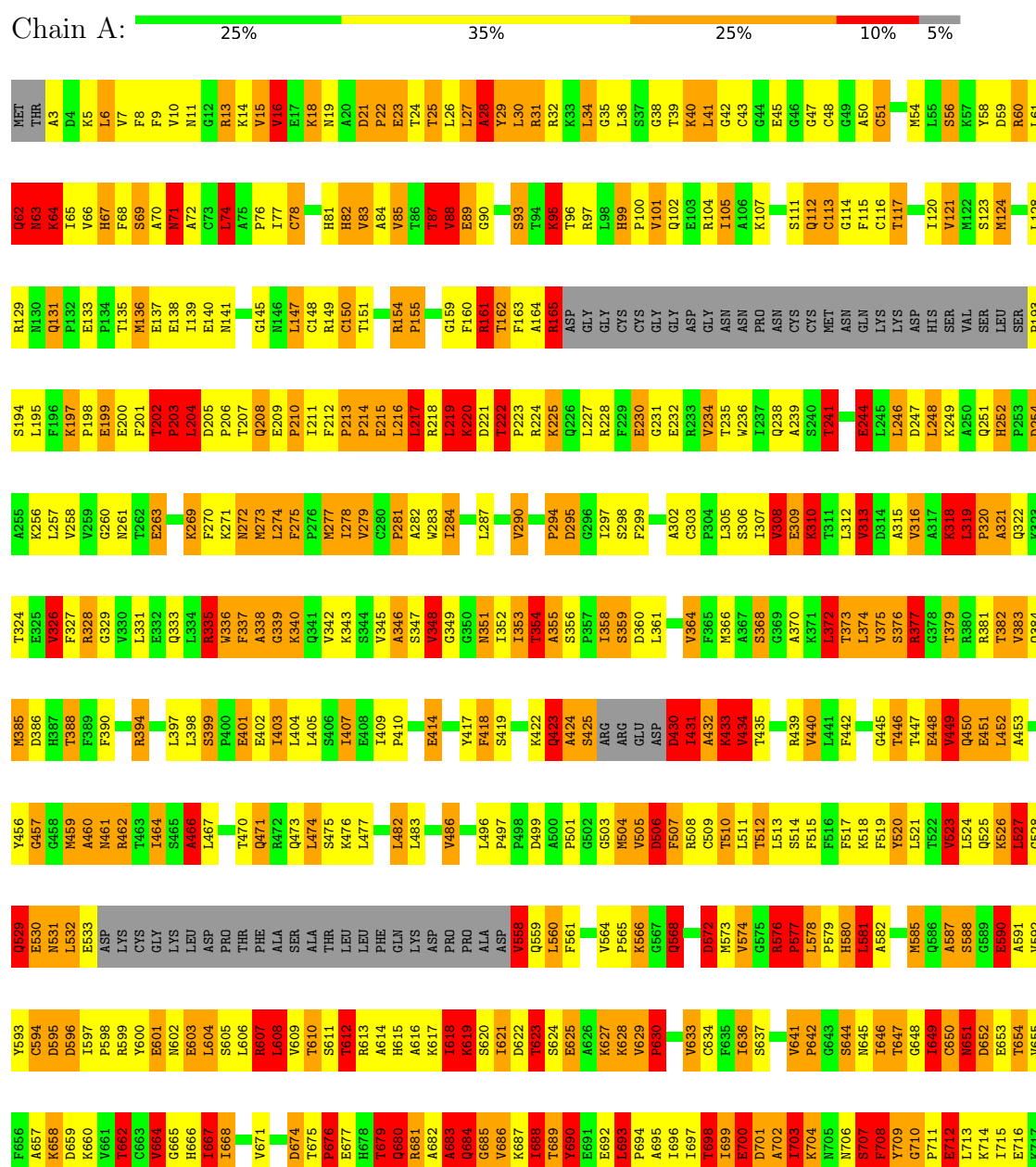
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	O	P	0	0
			5	4	1		

3 Residue-property plots

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

Note EDS was not executed.

• Molecule 1: XANTHINE OXIDOREDUCTASE



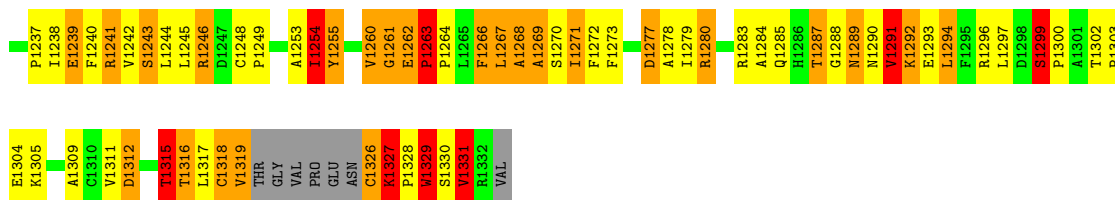
A1301	P1302	T1303	E1304	K1305	I1306	V1311	D1312	T1315	T1316	L1317	C1318	V1319	T1320	GLY	VAL	PRO	GLU	ASN	CYS	LYS	PRO	W1329	SER	VAL	ARG	VAL	A1268	A1269	S1270	I1271	A1274	L1275	K1276	D1277	A1278	I1279	R1280	A1281	L1282	R1283	A1284	Q1285	H1286	T1287	G1288	N1289	V1290	V1291	E1292	L1293	S1294	F1295	R1296	L1297	D1298	L1299	P1300															
I1236	P1237	I1238	E1239	D1240	R1241	V1242	S1243	L1244	R1245	D1246	D1247	C1248	P1249	N1250	I1254	V1255	A1256	S1257	K1258	A1259	V1260	G1261	E1262	P1263	P1264	A1268	A1269	S1270	I1271	A1274	L1275	K1276	D1277	A1278	I1279	R1280	A1281	L1282	R1283	A1284	Q1285	H1286	T1287	G1288	N1289	V1290	V1291	E1292	L1293	S1294	F1295	R1296	L1297	D1298	L1299	P1300																
C1167	L1168	T1169	G1170	D1171	K1172	K1173	M1174	L1175	R1176	T1177	D1178	C1248	P1249	N1250	V1183	L1187	M1188	P1189	A1190	L1191	D1192	G1193	G1194	P1195	V1196	E1197	F1200	L1204	G1205	L1206	L1209	E1210	E1211	L1212	H1213	G1218	S1219	L1220	H1221	T1222	R1223	G1224	P1225	S1226	T1227	V1228	L1229	F1229	A1230	P1231	L1232	L1233	L1234	L1235																		
L1102	E1103	P1104	Y1105	K1106	R1107	K1108	N1109	S1113	W1114	E1115	D1116	W1117	V1118	T1119	A1120	A1121	Y1122	M1123	D1124	T1125	Y1126	L1127	L1128	S1129	A1130	T1131	F1132	Y1133	R1134	T1135	P1137	N1138	L1139	G1140	Y1141	S1142	F1143	T1145	N1146	N1149	P1150	F1151	H1152	Y1153	A1154	G1157	V1158	A1159	C1160	S1161	E1164	D1166																				
Q1041	H1044	T1045	K1046	R1047	V1048	Q1049	V1050	A1051	S1052	R1053	A1054	L1055	K1056	T1057	P1058	T1059	S1060	K1061	Y1062	Y1063	I1064	S1065	T1066	S1068	N1070	T1071	V1072	P1073	N1074	T1075	S1076	P1077	T1078	A1079	A1080	S1081	S1082	S1083	A1084	D1085	L1086	N1087	G1088	Q1089	A1090	V1091	Y1092	A1093	A1094	C1095	Q1096	T1097	I1098	L1099	K1100	R1101																
Q977	Y978	H979	T1045	K1106	R981	K982	S983	V985	K987	E991	N992	C993	N994	K995	K996	R997	C1000	I1001	I1002	P1003	T1004	K1005	I1008	S1009	F1010	T1011	V1012	F1014	K944	N945	L947	Y948	K949	E950	G951	D952	L953	T954	H955	F956	K959	G962	F963	P966	R967	C902	K903	T904	N905	E970	E971	A974	M1039	S975	S976																	
A911	F912	G913	G914	G915	G916	G917	P918	Q919	G920	M921	L922	L923	A924	E925	C926	N927	M928	D863	H864	F865	E930	E931	A932	V933	T934	C935	E1004	G936	P937	P938	E941	V942	R943	K945	N946	L947	Y948	K949	E950	G951	D952	L953	T954	H955	F956	K959	G962	F963	P966	R967	C902	K903	T904	N905	E970	E971	A974	M1039	S975	S976												
L781	G782	V783	N786	K787	L788	V789	V790	V791	G920	V792	V793	G794	N795	G796	G797	V798	V799	G800	G801	E741	K802	E803	H742	T804	R805	Y744	L745	E746	T747	H748	C749	T750	T751	A812	H813	A814	L815	K755	P754	G756	E757	L758	T820	G759	E760	M761	P822	P823	E762	L763	R824	R825	C826	M827	L828	D829	R830	D831	T770	M771	K772	M834	K903	L835	S775	T837	V776	V777	A778	K909	R840	M790

● Molecule 1: XANTHINE OXIDOREDUCTASE

Chain B:  26% 36% 24% 11% .

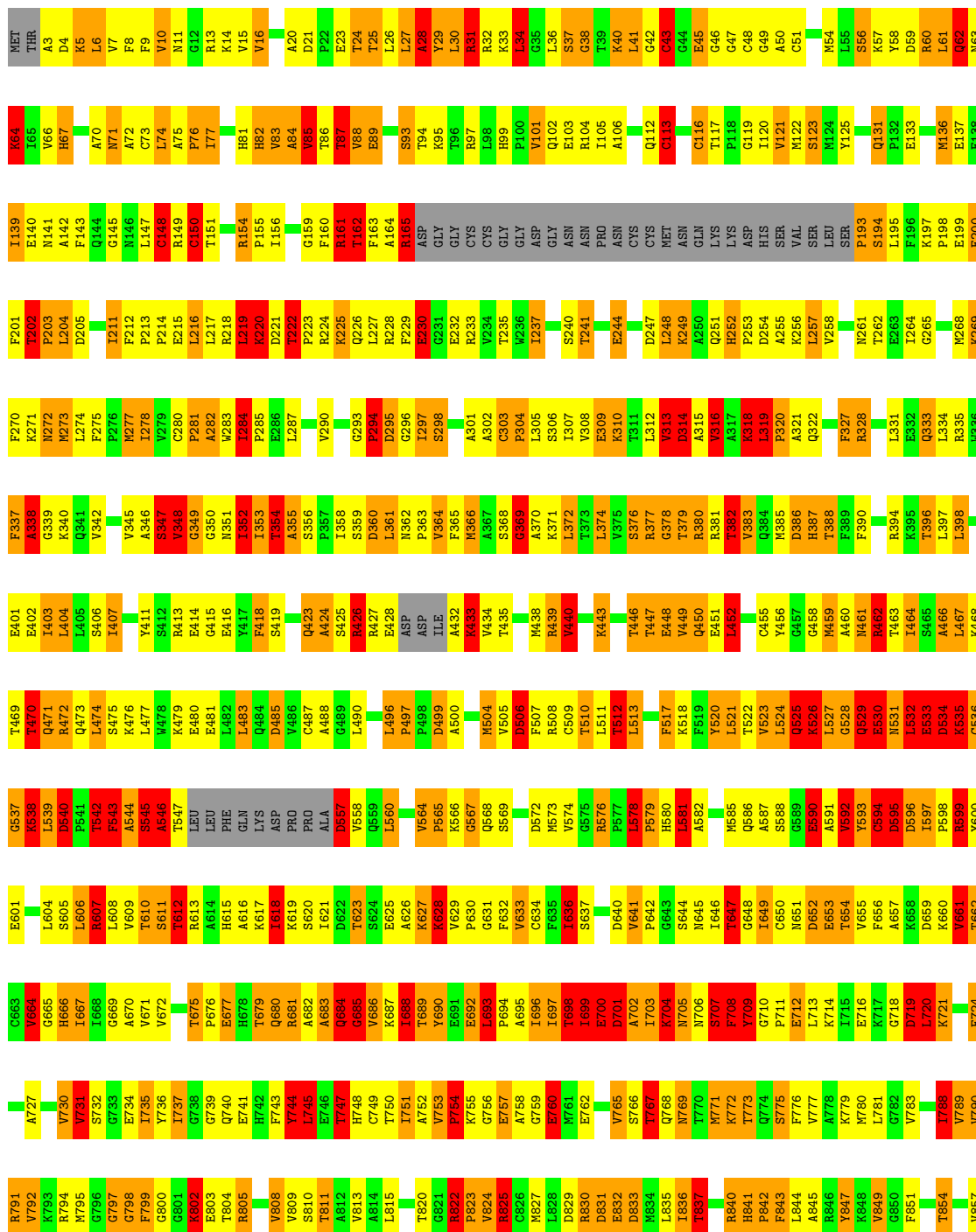
SER	P193	S194	L195	F196	K197	P198	E199	E200	F201	L202	L203	L204	D205		E209	P210	L211	L212	P213	C214	E215	L216	L217	R218	L219	K220	D221	L222	P223	R224	K225	Q226	L227	R228	F229	E230	G231	E232	R233	V234	L235	W236		A239	S240	T241		E244	L245	L246	D247	L248	K249	A250	Q251	H252	P253	D254	A255		
Q131	P132	E133	P134	L135	M136	K137	P138	E139	E140	A141	A142	F143	Q144	G145	N146	L147	C148	R149	A150	T151	G152	Y153	R154	P155		Q158	F159	F160	R161	T162	F163	A164	L165	ASP	GLY	GLY	CYS	CYS	GLY	GLY	ASP	GLY	ASN	ASN	PRD	CYS	MET	ASN	GLN	LYS	LYS	ASP	HIS	SER	VAL	SER	LEU				
M63	K64	I65	V66	H67	F68	S69	A70	M71	A72	C73	L74	A75	F76	I77		H81	H82	V83	A84	V85	T86	T87	V88	E89	G90	I91	G92	S93	T94	K95	T96	R97		V101	Q102	E103	R104	I105	A106	K107		S111	Q112	C113		G116	T117	P118		V121	M122	S123	M124	V125	T126	L127	M128	R129	V130		
MET	T2	A3	D4	K5	L6	V7	F8	N9	A10	V10	N11	G12	R13	K14	V15	E17	K18	N19	A20	D21	P22	E23	T24	T25	L26	L27	A28	E29	Y29	L30	R31	R32	K33	L34	G35	L36	S37	G38	T39		G40	L41	G42	C43	G44	E45			A50	C51	T52	V53	M54	L55	S56	K57	Y58	D59	R60	L61	Q62

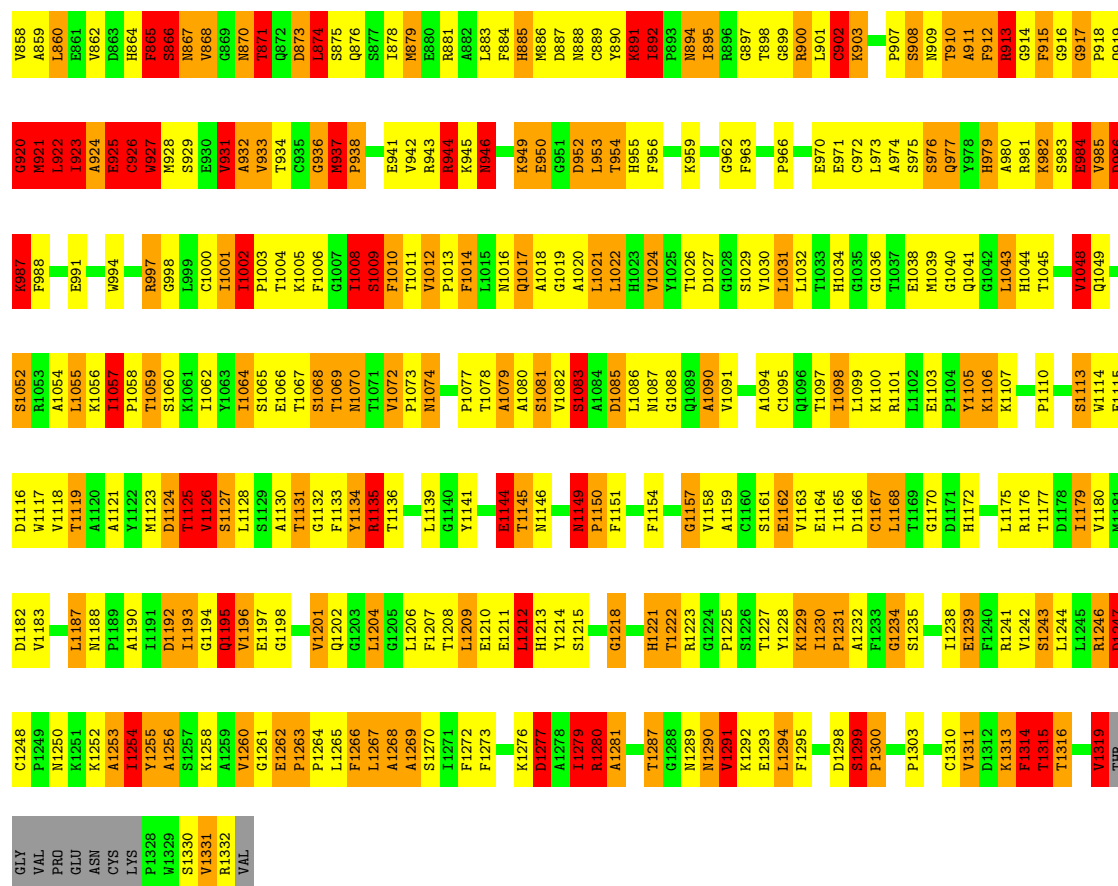
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K1173	S1111	G1042	T978	G914	F851	M786	L720	F656	V592	E530	Y456	F390	V326	L257
L1175	G1112	L1043	H979	F915	R852	M787	K721	A657	Y593	N531	M459	G391	L532	T262
L1176	S1113	H1044	A980	G916	R853	T788	K722	K658	C594	L532	A460	G392	R328	E263
T1177	K1114	T1045	R981	G917	T854	V789	F723	D659	D595	E533	N461	R394	D596	I264
D1178	E1115	K1046	K982	F918	G855	V790	F724	K660	D596	D534	R462	K395	L331	M288
I1179	D1116	M1047	S983	Q919	T856	R791	W730	V661	F597	K535	R463	K396	E332	K269
L1180	D1117	V1048	E984	G920	V857	V792	W731	T662	F598	C836	T463	L397	E333	M270
V1183	L1117	Q1049	V985	N921	R858	K793	W732	G663	R599	G537	L464	L398	L334	K271
T1118	L1118	V1050	D986	L922	A859	R794	G733	V664	E601	K538	A465	L399	L334	L274
V1189	T1119	A1051	R987	R923	L860	M795	G733	G665	N602	L539	A466	P400	F337	M272
G1184	A1120	S1052	F988	A924	E861	G796	E734	H666	N603	D540	L467	P400	F337	M273
S1185	E1121	R1053	N989	E925	V862	G797	L735	T667	E603	P541	K468	E401	A338	M273
S1186	T1122	A1054	C926	C926	D863	G798	W736	M671	L604	T842	T469		G339	L274
L1187	M1123	L1055	A927	A927	H864	F799	W737	V672	S605	F543	T470	L404	K340	F275
N1188	K1056	K1056	N928	N928	G800	G738	G738	V672	A544	A644	Q471	L405	K340	F276
P1189	T1125	P1057	S929	S929	R866	C801	G739	A673	R607	S545	Q472	S406	V342	M277
A1190	V1126	P1058	A994	E930	N867	K802	Q740	A673	L608	A546	Q473	I407	K343	L278
T1191	S1127	V1059	E811	V931	V868	E803	E741	T675	V609	T547	L474	E408	S344	V279
D1192		S1060	A932	A932	T871	T804	H742	P676	T610	LEU	S475	I409	V345	C280
I1193			V933	V933	Q872	R805	H743		S611	GLN	K476	P410	A346	P281
Q1194					D873	S806	L744		T612	LYS	L482	Y411	S347	A282
G1195					L874	T807	L745			ASP	L483	S412	V348	W283
V1196					S875	V809	T747		H615	PRO	A616	S412	V348	I284
E1197					Q876	S810	H748		K617	PRO	D485	F418	I352	P285
G1198					S877	T811	C749		K619	ALA	C487	F418	I353	E286
A1199					E940	T811	T750		K619	ALA	C487	F418	I353	L287
F1200					N879	A812	W751		D622	V583	L490	F420	A355	S289
Q1201					E890	A814	A752		D622	V583	L490	F420	A355	V290
V1202					R881	L815	W753		T693	D559	K422	K422	I358	
G1203					A822	A816	T754		S624	L560	Q423	Q423	S359	P284
L1204					L863	A817	K755		S624	L560	Q423	Q423	S359	P284
G1205					F884	V818	G756		E625	F561	L496	Q423	D360	D295
T1208					H885	K819	E757		K627	E563	P497	S425	D360	G296
E1210					N886	R819	E757		K627	E563	P497	S425	D360	G296
E1211					N887	R819	E757		K627	E563	P497	S425	D360	G296
L1212					N888	R819	E757		K627	E563	P497	S425	D360	G296
H1213					N889	R819	E757		K627	E563	P497	S425	D360	G296
P1216					N890	R819	E757		K627	E563	P497	S425	D360	G296
G1218					N891	R819	E757		K627	E563	P497	S425	D360	G296
S1219					N892	R819	E757		K627	E563	P497	S425	D360	G296
L1220					N893	R819	E757		K627	E563	P497	S425	D360	G296
H1221					N894	R819	E757		K627	E563	P497	S425	D360	G296
T1222					N895	R819	E757		K627	E563	P497	S425	D360	G296
R1223					N896	R819	E757		K627	E563	P497	S425	D360	G296
G1224					N897	R819	E757		K627	E563	P497	S425	D360	G296
P1225					N898	R819	E757		K627	E563	P497	S425	D360	G296
S1226					N899	R819	E757		K627	E563	P497	S425	D360	G296
T1227					N900	R819	E757		K627	E563	P497	S425	D360	G296
V1228					N901	R819	E757		K627	E563	P497	S425	D360	G296
K1229					N902	R819	E757		K627	E563	P497	S425	D360	G296
L1230					N903	R819	E757		K627	E563	P497	S425	D360	G296
P1231					N904	R819	E757		K627	E563	P497	S425	D360	G296
A1232					N905	R819	E757		K627	E563	P497	S425	D360	G296
F1233					N906	R819	E757		K627	E563	P497	S425	D360	G296
G1234					N907	R819	E757		K627	E563	P497	S425	D360	G296



• Molecule 1: XANTHINE OXIDOREDUCTASE

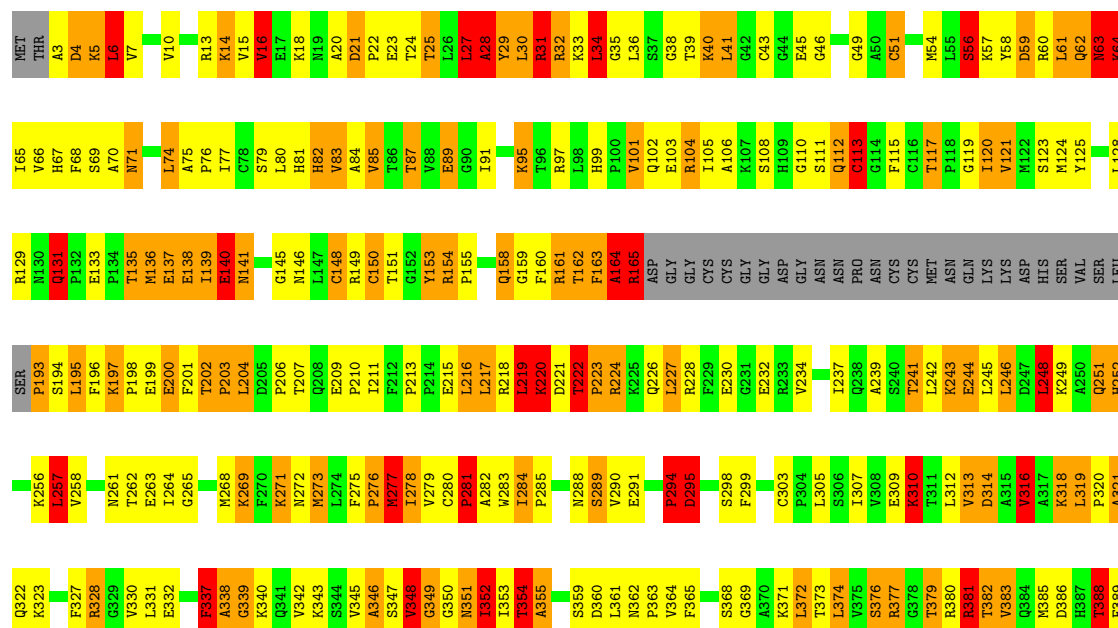
Chain C: 26% 36% 24% 11%





● Molecule 1: XANTHINE OXIDOREDUCTASE

Chain D: 25% 38% 23% 10% .



L1297	L1298	S1299	P1300	A1301	T1302	P1303	E1304	E1305	L1306	A1307	N1308	Y1311	D1312	K1313	F1314	T1315	T1316	L1317	C1318	T1319	T1320	GLY	VAL	PRO	GLU	ASN	C1326	K1327	P1328	W1329	S1330	R1332	VAL	F390	P391	R394	N461	T396	L397	L398	E401	E402	I403	I404	L405	S406	E408	Y411	S412	R413	E414	F418	S419	A420	F421	Q423	D426	S425	A432	K433	T435	M438	R439	V440	L441	F442	K443	P444	G445	T446	T447	E448	V449	Q450	E451	L452	A453	L454	C455	Y456	M459	A460	R462	T463	L464	S465	A466	L467	K468	T469	T470	Q471	R472	L474	S475	K476	W478	K479	E480	E481	L482	L483	Q484	D485	P486	S486	D557	V558	Q559	L560	F561	V564	P565	K566	Q567	Q568	S569	E570	E571	T510	L511	T512	L513	S514	P515	F516	F517	K518	F519	Y520	L521	T522	V523	L524	Q525	K526	L527	Q528	Q529	E530	N531	L532	E533	D534	K535	E536	G537	K538	L539	D540	P541	THR	PHE	ALA	SER	ALA	THR	LEU	LEU	PHE	GLN	LYS	ASP	PRO	PRO	ALA	D557	V558	Q559	L560	F561	V564	P565	K566	Q567	Q568	S569	E570	E571	T510	L511	T512	L513	S514	P515	F516	F517	K518	F519	Y520	L521	T522	V523	L524	Q525	E589	E590	V592	C594	D595	D596	L597	P598	R599	Y600	E601	L604	S605	L606	R607	R607	L608	V609	S611	T610	T612	R613	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	E659	E660	E661	E662	E663	E664	E665	E666	E667	E668	E669	E670	E671	E672	E673	E674	E675	E676	E677	E678	E679	E680	E681	E682	E683	E684	E685	E686	E687	E688	E689	E690	E691	E692	E693	E694	E695	E696	E697	E698	E699	E700	E701	E702	E703	E704	E705	E706	E707	E708	E709	E710	E711	E712	E713	E714	E715	E716	E717	E718	E719	E720	E721	E722	E723	E724	E725	E726	E727	E728	E729	E730	E731	E732	E733	E734	E735	E736	E737	E738	E739	E740	E741	E742	E743	E744	E745	E746	E747	E748	E749	E750	E751	E752	E753	E754	E755	E756	E757	E758	E759	E760	E761	E762	E763	E764	E765	E766	E767	E768	E769	E770	E771	E772	E773	E774	E775	E776	E777	E778	E779	E780	E781	E782	E783	E784	E785	E786	E787	E788	E789	E790	E791	E792	E793	E794	E795	E796	E797	E798	E799	E800	E801	E802	E803	E804	E805	E806	E807	E808	E809	E810	E811	E812	E813	E814	E815	E816	E817	E818	E819	E820	E821	E822	E823	E824	E825	E826	E827	E828	E829	E830	E831	E832	E833	E834	E835	E836	E837	E838	E839	E840	E841	E842	E843	E844	E845	E846	E847	E848	E849	E850	E851	E852	E853	E854	E855	E856	E857	E858	E859	E860	E861	E862	E863	E864	E865	E866	E867	E868	E869	E870	E871	E872	E873	E874	E875	E876	E877	E878	E879	E880	E881	E882	E883	E884	E885	E886	E887	E888	E889	E890	E891	E892	E893	E894	E895	E896	E897	E898	E899	E900	E901	E902	E903	E904	E905	E906	E907	E908	E909	E910	E911	E912	E913	E914	E915	E916	E917	E918	E919	E920	E921	E922	E923	E924	E925	E926	E927	E928	E929	E930	E931	E932	E933	E934	E935	E936	E937	E938	E939	E940	E941	E942	E943	E944	E945	E946	E947	E948	E949	E950	E951	E952	E953	E954	E955	E956	E957	E958	E959	E960	E961	E962	E963	E964	E965	E966	E967	E968	E969	E970	E971	E972	E973	E974	E975	E976	E977	E978	E979	E980	E981	E982	E983	E984	E985	E986	E987	E988	E989	E990	E991	E992	E993	E994	E995	E996	E997	E998	E999	E1000	E1001	E1002	E1003	E1004	E1005	E1006	E1007	E1008	E1009	E1010	E1011	E1012	E1013	E1014	E1015	E1016	E1017	E1018	E1019	E1020	E1021	E1022	E1023	E1024	E1025	E1026	E1027	E1028	E1029	E1030	E1031	E1032	E1033	E1034	E1035	E1036	E1037	E1038	E1039	E1040	E1041	E1042	E1043	E1044	E1045	E1046	E1047	E1048	E1049	E1050	E1051	E1052	E1053	E1054	E1055	E1056	E1057	E1058	E1059	E1060	E1061	E1062	E1063	E1064	E1065	E1066	E1067	E1068	E1069	E1070	E1071	E1072	E1073	E1074	E1075	E1076	E1077	E1078	E1079	E1080	E1081	E1082	E1083	E1084	E1085	E1086	E1087	E1088	E1089	E1090	E1091	E1092	E1093	E1094	E1095	E1096	E1097	E1098	E1099	E1100	E1101	E1102	E1103	E1104	E1105	E1106	E1107	E1108	E1109	E1110	E1111	E1112	E1113	E1114	E1115	E1116	E1117	E1118	E1119	E1120	E1121	E1122	E1123	E1124	E1125	E1126	E1127	E1128	E1129	E1130	E1131	E1132	E1133	E1134	E1135	E1136	E1137	E1138	E1139	E1140	E1141	E1142	E1143	E1144	E1145	E1146	E1147	E1148	E1149	E1150	E1151	E1152	E1153	E1154	E1155	E1156	E1157	E1158	E1159	E1160	E1161	E1162	E1163	E1164	E1165	E1166	E1167	E1168	E1169	E1170	E1171	E1172	E1173	E1174	E1175	E1176	E1177	E1178	E1179	E1180	E1181	E1182	E1183	E1184	E1185	E1186	E1187	E1188	E1189	E1190	E1191	E1192	E1193	E1194	E1195	E1196	E1197	E1198	E1199	E1200	E1201	E1202	E1203	E1204	E1205	E1206	E1207	E1208	E1209	E1210	E1211	E1212	E1213	E1214	E1215	E1216	E1217	E1218	E1219	E1220	E1221	E1222	E1223	E1224	E1225	E1226	E1227	E1228	E1229	E1230	E1231	E1232	E1233	E1234	E1235	E1236	E1237	E1238	E1239	E1240	E1241	E1242	E1243	E1244	E1245	E1246	E1247	E1248	E1249	E1250	E1251	E1252	E1253	E1254	E1255	E1256	E1257	E1258	E1259	E1260	E1261	E1262	E1263	E1264	E1265	E1266	E1267	E1268	E1269	E1270	E1271	E1272	E1273	E1274	E1275	E1276	E1277	E1278	E1279	E1280	E1281	E1282	E1283	E128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4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	197.73Å 197.73Å 285.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.76 – 3.59	Depositor
% Data completeness (in resolution range)	98.2 (30.76-3.59)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.178 , 0.258	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	39807	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FES, PO4, GOL, ACY, FAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	2.46	516/9969 (5.2%)	2.19	457/13492 (3.4%)
1	B	2.51	514/10160 (5.1%)	2.20	474/13751 (3.4%)
1	C	2.45	479/10113 (4.7%)	2.19	466/13685 (3.4%)
1	D	2.41	487/10118 (4.8%)	2.15	443/13693 (3.2%)
All	All	2.46	1996/40360 (4.9%)	2.18	1840/54621 (3.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	40
1	B	1	54
1	C	1	49
1	D	0	55
All	All	2	198

All (1996) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	3	ALA	N-CA	24.39	1.77	1.46
1	B	431	ILE	CA-CB	23.30	1.81	1.54
1	B	1289	ASN	CA-C	19.41	1.62	1.52
1	A	1289	ASN	CA-C	17.58	1.63	1.52
1	C	355	ALA	CA-CB	-17.42	1.31	1.52
1	C	1331	VAL	CA-CB	16.64	1.72	1.55
1	C	1331	VAL	CA-C	15.68	1.70	1.52
1	B	1291	VAL	CA-CB	15.34	1.75	1.54
1	C	1291	VAL	CA-CB	15.29	1.75	1.54
1	D	1291	VAL	CA-CB	15.15	1.75	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	675	THR	CA-CB	14.01	1.71	1.54
1	B	3	ALA	CA-CB	13.95	1.77	1.53
1	A	1291	VAL	CA-CB	13.24	1.72	1.54
1	B	783	VAL	CA-C	13.14	1.63	1.52
1	C	1082	VAL	CA-CB	-12.58	1.40	1.54
1	D	1083	SER	CA-C	12.50	1.69	1.52
1	A	616	ALA	CA-C	-12.48	1.37	1.52
1	C	636	ILE	CA-CB	12.34	1.69	1.54
1	C	688	ILE	N-CA	12.17	1.61	1.46
1	A	1319	VAL	CA-C	11.99	1.68	1.52
1	A	1319	VAL	CA-CB	11.97	1.70	1.54
1	D	348	VAL	CA-CB	-11.97	1.41	1.54
1	A	636	ILE	CA-CB	11.57	1.68	1.54
1	C	769	ASN	C-O	11.51	1.37	1.23
1	A	752	ALA	CA-CB	-11.46	1.36	1.53
1	A	1311	VAL	CA-CB	11.39	1.67	1.54
1	A	346	ALA	CA-CB	-11.36	1.35	1.53
1	B	1331	VAL	CA-CB	11.19	1.69	1.54
1	A	1193	ILE	CA-CB	11.17	1.69	1.54
1	A	1018	ALA	CA-CB	11.15	1.68	1.53
1	B	75	ALA	CA-CB	-11.13	1.36	1.53
1	A	258	VAL	CA-CB	-11.10	1.40	1.54
1	A	1301	ALA	CA-CB	-11.05	1.37	1.52
1	A	424	ALA	CA-C	10.98	1.59	1.53
1	B	697	ILE	CA-CB	-10.98	1.45	1.55
1	D	1331	VAL	CA-C	10.98	1.66	1.52
1	D	1072	VAL	CA-CB	-10.94	1.40	1.54
1	A	688	ILE	N-CA	10.79	1.59	1.46
1	A	102	GLN	CA-C	-10.79	1.39	1.52
1	C	364	VAL	CA-CB	-10.58	1.40	1.54
1	B	789	VAL	CA-CB	-10.58	1.41	1.54
1	C	28	ALA	CA-CB	10.56	1.71	1.53
1	B	36	LEU	C-O	10.56	1.36	1.23
1	A	1213	HIS	N-CA	10.52	1.58	1.46
1	D	10	VAL	CA-CB	-10.47	1.40	1.53
1	C	836	ILE	CA-CB	-10.42	1.43	1.54
1	D	788	ILE	CA-CB	-10.39	1.42	1.54
1	B	803	GLU	CA-C	10.35	1.67	1.52
1	D	579	PRO	C-O	10.34	1.36	1.23
1	A	67	HIS	N-CA	10.33	1.58	1.46
1	C	1180	VAL	CA-CB	-10.28	1.41	1.54
1	A	1319	VAL	N-CA	10.22	1.59	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	642	PRO	N-CA	-10.16	1.40	1.47
1	D	1291	VAL	CA-C	10.10	1.65	1.52
1	A	431	ILE	CG1-CD1	10.00	1.90	1.51
1	D	223	PRO	N-CA	10.00	1.58	1.46
1	C	788	ILE	CA-CB	-9.98	1.42	1.54
1	D	599	ARG	CG-CD	9.97	1.82	1.52
1	B	1011	THR	N-CA	9.97	1.58	1.46
1	C	599	ARG	CG-CD	9.97	1.82	1.52
1	C	50	ALA	CA-CB	-9.93	1.37	1.53
1	B	599	ARG	CG-CD	9.92	1.82	1.52
1	B	1049	GLN	C-O	9.88	1.35	1.24
1	A	762	GLU	CG-CD	9.85	1.76	1.52
1	B	431	ILE	CA-C	9.85	1.64	1.52
1	B	54	MET	CA-C	9.83	1.65	1.52
1	A	1090	ALA	CA-CB	-9.82	1.38	1.53
1	B	1291	VAL	N-CA	9.82	1.58	1.46
1	D	1327	LYS	CA-C	9.81	1.65	1.52
1	C	426	ARG	N-CA	9.80	1.58	1.46
1	B	40	LYS	CE-NZ	9.78	1.78	1.49
1	A	751	ILE	CA-CB	9.77	1.65	1.54
1	A	101	VAL	C-O	-9.73	1.12	1.24
1	D	1290	ASN	CA-C	9.73	1.65	1.52
1	D	538	LYS	CA-C	9.67	1.64	1.52
1	D	1319	VAL	CA-CB	9.66	1.67	1.54
1	A	681	ARG	CZ-NH1	9.58	1.46	1.32
1	D	840	ARG	C-O	9.52	1.35	1.23
1	B	70	ALA	CA-C	-9.50	1.40	1.52
1	A	890	TYR	CA-C	9.47	1.64	1.52
1	C	1208	THR	C-O	9.46	1.35	1.24
1	D	1183	VAL	CA-CB	9.45	1.65	1.54
1	A	817	ALA	CA-CB	-9.42	1.38	1.53
1	C	698	THR	CA-CB	9.40	1.68	1.53
1	A	16	VAL	CA-CB	-9.37	1.41	1.54
1	B	425	SER	N-CA	9.34	1.58	1.46
1	D	1125	THR	CA-CB	9.29	1.69	1.53
1	D	1331	VAL	CA-CB	9.28	1.67	1.54
1	A	1120	ALA	CA-CB	-9.25	1.39	1.53
1	D	1319	VAL	CA-C	9.23	1.64	1.52
1	D	621	ILE	CA-CB	-9.19	1.43	1.54
1	B	1018	ALA	CA-CB	9.18	1.67	1.54
1	A	111	SER	CA-C	-9.17	1.43	1.53
1	C	232	GLU	CA-C	-9.16	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	432	ALA	CA-CB	9.16	1.69	1.53
1	C	13	ARG	NE-CZ	9.11	1.43	1.33
1	A	28	ALA	CA-C	-9.10	1.40	1.52
1	B	1318	CYS	CB-SG	9.10	2.11	1.81
1	C	599	ARG	CB-CG	9.09	1.79	1.52
1	C	699	ILE	CA-CB	-9.09	1.44	1.54
1	C	150	CYS	CA-C	9.04	1.65	1.52
1	B	529	GLN	CA-C	9.04	1.64	1.52
1	B	146	ASN	C-O	9.03	1.34	1.24
1	B	1319	VAL	CA-CB	9.03	1.78	1.54
1	B	195	LEU	N-CA	9.02	1.57	1.46
1	A	71	ASN	CA-C	-9.01	1.41	1.52
1	C	925	GLU	CA-C	-8.99	1.40	1.52
1	B	762	GLU	CD-OE1	8.97	1.42	1.25
1	B	28	ALA	CA-C	-8.97	1.40	1.52
1	A	27	LEU	C-O	8.94	1.35	1.23
1	B	1331	VAL	N-CA	8.93	1.57	1.46
1	D	1289	ASN	CA-C	8.93	1.64	1.52
1	A	857	VAL	CA-C	8.93	1.63	1.52
1	B	1241	ARG	CA-C	8.92	1.63	1.52
1	D	111	SER	CA-C	-8.91	1.42	1.52
1	C	1256	ALA	CA-CB	-8.91	1.40	1.53
1	D	525	GLN	CA-C	8.90	1.64	1.52
1	D	1135	ARG	NE-CZ	8.90	1.42	1.33
1	D	339	GLY	N-CA	8.90	1.54	1.45
1	B	1031	LEU	C-O	8.88	1.33	1.23
1	B	1331	VAL	CA-C	8.85	1.64	1.52
1	D	688	ILE	N-CA	8.85	1.56	1.46
1	A	321	ALA	CA-C	8.83	1.64	1.52
1	D	337	PHE	CA-C	8.83	1.64	1.52
1	D	792	VAL	CA-C	-8.82	1.41	1.52
1	A	646	ILE	CG1-CD1	8.78	1.85	1.51
1	C	1018	ALA	C-O	-8.77	1.16	1.24
1	D	777	VAL	CA-CB	-8.76	1.44	1.54
1	C	13	ARG	CD-NE	8.76	1.58	1.46
1	C	195	LEU	N-CA	8.75	1.57	1.46
1	B	1290	ASN	N-CA	8.73	1.57	1.46
1	B	646	ILE	CG1-CD1	8.72	1.85	1.51
1	D	1318	CYS	CA-C	8.71	1.64	1.52
1	C	278	ILE	CA-CB	-8.68	1.43	1.54
1	C	1289	ASN	CA-C	8.66	1.64	1.52
1	B	2	THR	CA-C	8.65	1.71	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	422	LYS	CA-C	-8.62	1.41	1.52
1	B	1120	ALA	CA-CB	-8.61	1.39	1.53
1	C	122	MET	CA-C	-8.61	1.41	1.52
1	A	449	VAL	CA-CB	8.61	1.66	1.54
1	B	592	VAL	CA-CB	-8.59	1.43	1.54
1	D	1064	ILE	N-CA	8.58	1.55	1.46
1	A	78	CYS	CB-SG	8.55	2.09	1.81
1	D	1144	GLU	CG-CD	8.54	1.73	1.52
1	B	290	VAL	N-CA	8.54	1.56	1.46
1	B	1022	LEU	CA-C	8.53	1.62	1.52
1	B	72	ALA	CA-CB	-8.53	1.39	1.53
1	D	770	THR	C-O	-8.53	1.13	1.24
1	D	890	TYR	CA-C	8.49	1.62	1.52
1	D	59	ASP	C-O	-8.49	1.14	1.24
1	C	1187	LEU	CA-C	8.48	1.64	1.52
1	C	70	ALA	CA-C	-8.46	1.42	1.52
1	D	213	PRO	CA-C	-8.43	1.44	1.52
1	C	1319	VAL	CA-CB	8.43	1.77	1.54
1	A	1254	ILE	CA-C	8.42	1.63	1.52
1	D	1289	ASN	N-CA	8.42	1.57	1.46
1	C	1001	ILE	CA-C	8.40	1.63	1.52
1	C	202	THR	N-CA	8.39	1.58	1.45
1	B	714	LYS	N-CA	8.39	1.56	1.46
1	D	790	VAL	CA-CB	-8.38	1.44	1.54
1	C	1031	LEU	CA-C	8.37	1.63	1.53
1	A	646	ILE	CA-CB	-8.36	1.43	1.53
1	A	318	LYS	CG-CD	8.34	1.77	1.52
1	B	1162	GLU	CG-CD	8.33	1.72	1.52
1	A	1009	SER	CA-C	-8.33	1.41	1.52
1	C	1290	ASN	N-CA	8.32	1.56	1.46
1	B	599	ARG	CD-NE	8.29	1.57	1.46
1	D	36	LEU	C-O	8.29	1.33	1.23
1	A	460	ALA	CA-C	8.27	1.61	1.53
1	C	365	PHE	CA-C	8.27	1.63	1.52
1	D	790	VAL	C-O	-8.27	1.15	1.24
1	D	1121	ALA	N-CA	8.27	1.56	1.46
1	A	417	TYR	CA-C	8.26	1.62	1.52
1	C	597	ILE	CA-C	-8.24	1.44	1.52
1	B	382	THR	CA-CB	8.24	1.62	1.53
1	A	750	THR	CA-CB	8.20	1.67	1.52
1	D	1182	ASP	CA-C	8.20	1.63	1.52
1	A	878	ILE	CA-CB	-8.19	1.44	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	25	THR	CA-CB	8.18	1.67	1.53
1	D	679	THR	C-O	-8.18	1.14	1.24
1	D	600	TYR	CA-C	-8.18	1.42	1.53
1	A	450	GLN	CA-C	8.17	1.62	1.52
1	A	769	ASN	C-O	8.17	1.33	1.23
1	A	577	PRO	CA-C	8.16	1.61	1.53
1	B	84	ALA	CA-CB	-8.16	1.41	1.53
1	A	8	PHE	CA-C	-8.14	1.42	1.52
1	B	772	LYS	N-CA	-8.13	1.35	1.46
1	A	827	MET	N-CA	8.12	1.55	1.46
1	A	217	LEU	N-CA	8.11	1.56	1.46
1	D	1128	LEU	N-CA	-8.10	1.36	1.46
1	B	735	ILE	CA-CB	8.10	1.63	1.55
1	B	1232	ALA	CA-C	-8.08	1.41	1.53
1	A	609	VAL	C-O	8.08	1.33	1.24
1	C	499	ASP	CA-C	8.07	1.64	1.52
1	C	595	ASP	CA-C	8.07	1.63	1.52
1	B	874	LEU	CA-C	8.06	1.63	1.52
1	A	684	GLN	N-CA	-8.06	1.36	1.46
1	B	84	ALA	C-O	8.05	1.33	1.24
1	B	270	PHE	CA-C	-8.05	1.42	1.52
1	A	232	GLU	CA-C	-8.03	1.42	1.52
1	C	488	ALA	CA-C	8.03	1.63	1.52
1	C	84	ALA	CA-CB	-8.02	1.41	1.53
1	C	194	SER	N-CA	8.01	1.56	1.46
1	C	64	LYS	CD-CE	8.00	1.76	1.52
1	A	668	ILE	C-O	7.99	1.33	1.24
1	D	647	THR	CA-CB	7.98	1.67	1.53
1	D	673	ALA	CA-C	7.98	1.63	1.52
1	C	101	VAL	CA-CB	-7.98	1.44	1.54
1	C	1311	VAL	CA-CB	7.97	1.63	1.54
1	D	1287	THR	CA-CB	7.96	1.64	1.53
1	A	318	LYS	CD-CE	7.95	1.76	1.52
1	C	1094	ALA	CA-CB	-7.95	1.40	1.53
1	C	620	SER	C-O	7.95	1.32	1.23
1	B	655	VAL	CA-CB	-7.94	1.45	1.54
1	D	745	LEU	C-O	7.94	1.33	1.24
1	A	129	ARG	N-CA	-7.93	1.35	1.46
1	B	908	SER	C-O	-7.92	1.14	1.23
1	B	1327	LYS	CA-C	7.92	1.62	1.52
1	C	1265	LEU	N-CA	7.91	1.56	1.46
1	A	432	ALA	N-CA	7.91	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	775	SER	N-CA	7.89	1.55	1.46
1	D	1291	VAL	N-CA	7.88	1.56	1.46
1	B	653	GLU	N-CA	7.88	1.55	1.45
1	D	641	VAL	C-O	-7.87	1.14	1.24
1	D	763	LEU	CA-C	-7.87	1.42	1.52
1	A	54	MET	CG-SD	7.87	2.00	1.80
1	B	641	VAL	C-O	-7.86	1.14	1.24
1	D	28	ALA	N-CA	7.86	1.56	1.46
1	D	480	GLU	CA-C	7.86	1.63	1.52
1	C	48	CYS	C-O	7.84	1.34	1.24
1	D	440	VAL	CA-C	7.84	1.62	1.52
1	B	215	GLU	CA-C	7.84	1.63	1.52
1	D	822	ARG	CA-CB	-7.84	1.44	1.53
1	A	815	LEU	C-O	7.82	1.33	1.24
1	A	644	SER	CA-C	-7.82	1.42	1.52
1	B	1127	SER	CA-C	-7.81	1.42	1.52
1	D	149	ARG	CA-C	7.81	1.62	1.52
1	A	83	VAL	CA-CB	-7.81	1.44	1.54
1	D	121	VAL	N-CA	-7.80	1.37	1.46
1	A	615	HIS	N-CA	7.79	1.55	1.46
1	D	599	ARG	CB-CG	7.79	1.75	1.52
1	C	615	HIS	N-CA	7.78	1.55	1.46
1	B	635	PHE	CA-C	7.77	1.62	1.52
1	D	540	ASP	N-CA	7.76	1.57	1.46
1	B	689	THR	CA-CB	7.76	1.65	1.53
1	B	1137	PRO	N-CA	7.75	1.54	1.46
1	B	263	GLU	CA-C	-7.74	1.45	1.52
1	B	672	VAL	CA-CB	7.72	1.64	1.53
1	D	1290	ASN	N-CA	7.71	1.56	1.46
1	A	1108	LYS	CD-CE	7.71	1.75	1.52
1	C	1179	ILE	CA-C	7.71	1.62	1.52
1	A	309	GLU	CG-CD	7.68	1.71	1.52
1	A	803	GLU	CA-C	7.68	1.63	1.52
1	A	446	THR	CA-CB	7.68	1.67	1.53
1	B	364	VAL	CA-CB	-7.68	1.43	1.54
1	C	443	LYS	CA-C	7.67	1.62	1.52
1	A	616	ALA	C-O	-7.64	1.14	1.23
1	A	133	GLU	C-O	-7.64	1.16	1.24
1	A	1023	HIS	C-O	7.63	1.33	1.24
1	B	533	GLU	CA-C	7.63	1.62	1.53
1	C	269	LYS	CD-CE	7.63	1.75	1.52
1	C	42	GLY	N-CA	7.63	1.56	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	460	ALA	CA-CB	-7.63	1.43	1.54
1	A	689	THR	N-CA	7.62	1.55	1.46
1	B	1319	VAL	CA-C	7.62	1.69	1.52
1	D	903	LYS	CE-NZ	7.62	1.72	1.49
1	A	1291	VAL	N-CA	7.60	1.55	1.46
1	A	596	ASP	C-O	7.60	1.33	1.24
1	A	236	TRP	CA-C	-7.59	1.43	1.52
1	D	330	VAL	CA-CB	7.59	1.64	1.54
1	B	675	THR	C-O	-7.59	1.17	1.24
1	A	1311	VAL	CA-C	7.58	1.62	1.52
1	D	313	VAL	CA-CB	7.58	1.63	1.54
1	D	714	LYS	N-CA	7.58	1.55	1.46
1	D	1254	ILE	CA-C	7.58	1.62	1.52
1	A	22	PRO	N-CA	-7.57	1.37	1.47
1	A	28	ALA	CA-CB	7.57	1.66	1.53
1	D	463	THR	CA-CB	7.56	1.62	1.53
1	D	1331	VAL	N-CA	7.55	1.55	1.46
1	C	805	ARG	CZ-NH2	7.55	1.43	1.33
1	A	641	VAL	C-O	-7.54	1.15	1.25
1	A	223	PRO	N-CA	7.54	1.55	1.46
1	A	222	THR	C-N	7.53	1.42	1.33
1	C	907	PRO	C-O	7.53	1.32	1.23
1	C	688	ILE	CG1-CD1	7.53	1.81	1.51
1	B	205	ASP	N-CA	-7.53	1.39	1.46
1	C	62	GLN	CG-CD	7.53	1.70	1.52
1	D	1082	VAL	CA-CB	-7.53	1.44	1.54
1	C	803	GLU	CA-C	7.52	1.62	1.52
1	C	414	GLU	N-CA	7.51	1.56	1.46
1	A	263	GLU	CA-C	-7.51	1.46	1.52
1	C	574	VAL	CA-CB	-7.51	1.45	1.54
1	D	903	LYS	CD-CE	7.51	1.75	1.52
1	B	842	PRO	CA-C	7.51	1.60	1.52
1	B	526	LYS	CA-C	7.50	1.62	1.52
1	D	633	VAL	CA-C	-7.50	1.45	1.52
1	C	318	LYS	CD-CE	7.50	1.75	1.52
1	B	1330	SER	CA-C	7.49	1.62	1.52
1	B	1046	LYS	CA-C	7.48	1.62	1.52
1	D	346	ALA	CA-CB	-7.47	1.41	1.53
1	C	620	SER	N-CA	7.47	1.55	1.46
1	A	1101	ARG	CA-C	-7.47	1.42	1.52
1	A	212	PHE	CA-C	-7.47	1.43	1.52
1	A	50	ALA	CA-CB	-7.46	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	195	LEU	N-CA	7.45	1.56	1.46
1	C	283	TRP	N-CA	-7.45	1.36	1.46
1	C	686	VAL	CA-C	-7.45	1.43	1.52
1	D	97	ARG	NE-CZ	7.44	1.41	1.33
1	A	676	PRO	N-CA	-7.44	1.38	1.47
1	A	1108	LYS	CE-NZ	7.44	1.71	1.49
1	A	824	VAL	CA-CB	-7.43	1.44	1.54
1	A	890	TYR	C-O	7.43	1.33	1.24
1	D	1311	VAL	CA-CB	7.43	1.62	1.54
1	A	205	ASP	N-CA	-7.42	1.38	1.46
1	A	933	VAL	CA-C	-7.42	1.44	1.52
1	C	892	ILE	C-N	7.42	1.40	1.33
1	D	346	ALA	CA-C	-7.42	1.43	1.52
1	B	810	SER	C-O	7.41	1.32	1.24
1	B	961	GLU	CA-C	-7.41	1.42	1.53
1	B	597	ILE	CA-C	-7.41	1.45	1.52
1	A	637	SER	CA-C	-7.39	1.43	1.52
1	D	1090	ALA	CA-CB	-7.38	1.41	1.53
1	B	71	ASN	N-CA	7.38	1.55	1.46
1	B	101	VAL	CA-CB	-7.38	1.44	1.54
1	B	512	THR	C-O	-7.37	1.15	1.24
1	D	793	LYS	CG-CD	7.37	1.74	1.52
1	B	456	TYR	CA-C	7.37	1.61	1.52
1	B	1241	ARG	C-O	7.35	1.33	1.24
1	C	599	ARG	NE-CZ	7.35	1.41	1.33
1	C	609	VAL	CA-CB	-7.34	1.45	1.54
1	A	41	LEU	C-O	7.34	1.32	1.24
1	B	308	VAL	CA-CB	-7.34	1.46	1.54
1	A	925	GLU	CA-C	-7.33	1.43	1.52
1	C	689	THR	N-CA	7.33	1.54	1.46
1	B	1249	PRO	N-CA	-7.33	1.38	1.47
1	B	586	GLN	CD-NE2	7.32	1.48	1.33
1	B	792	VAL	C-O	-7.32	1.16	1.24
1	D	1318	CYS	CB-SG	7.32	2.05	1.81
1	A	802	LYS	N-CA	7.31	1.54	1.46
1	B	836	ILE	CA-C	7.31	1.62	1.52
1	C	1125	THR	CA-CB	7.31	1.65	1.53
1	B	472	ARG	CA-C	7.31	1.62	1.52
1	D	654	THR	C-O	7.31	1.32	1.24
1	D	734	GLU	N-CA	7.31	1.54	1.46
1	B	4	ASP	C-O	-7.30	1.14	1.24
1	D	599	ARG	CA-CB	7.30	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	364	VAL	CA-CB	-7.30	1.44	1.54
1	A	194	SER	N-CA	7.30	1.55	1.45
1	B	1175	LEU	N-CA	7.29	1.55	1.46
1	D	165	ARG	N-CA	7.29	1.60	1.46
1	D	117	THR	N-CA	-7.29	1.40	1.46
1	D	1003	PRO	N-CA	-7.28	1.38	1.47
1	B	775	SER	CA-C	-7.28	1.43	1.52
1	D	1319	VAL	N-CA	7.27	1.55	1.46
1	B	688	ILE	CG1-CD1	7.26	1.80	1.51
1	A	616	ALA	CA-CB	-7.26	1.41	1.53
1	C	824	VAL	CA-CB	-7.26	1.44	1.54
1	A	149	ARG	N-CA	7.25	1.55	1.46
1	C	427	ARG	N-CA	7.25	1.55	1.46
1	D	381	ARG	CA-C	7.25	1.62	1.52
1	B	825	ARG	CZ-NH2	7.25	1.42	1.33
1	D	194	SER	CA-C	7.23	1.62	1.53
1	A	1134	TYR	N-CA	7.23	1.54	1.46
1	B	582	ALA	CA-CB	-7.23	1.43	1.53
1	C	1062	ILE	N-CA	7.23	1.54	1.46
1	D	164	ALA	CA-CB	-7.23	1.42	1.53
1	A	1012	VAL	CA-CB	-7.22	1.44	1.54
1	A	1158	VAL	C-O	7.22	1.32	1.24
1	B	591	ALA	C-O	7.21	1.33	1.24
1	C	359	SER	CA-C	-7.20	1.43	1.52
1	C	470	THR	CA-C	7.20	1.62	1.52
1	A	64	LYS	CD-CE	7.19	1.74	1.52
1	A	59	ASP	CA-C	-7.19	1.43	1.52
1	C	1064	ILE	CA-CB	7.19	1.64	1.54
1	A	1191	ILE	CA-CB	-7.18	1.45	1.54
1	B	871	THR	C-O	7.18	1.33	1.23
1	C	1038	GLU	CA-CB	-7.18	1.44	1.53
1	A	497	PRO	C-N	7.17	1.43	1.34
1	A	685	GLY	C-O	-7.17	1.14	1.23
1	C	237	ILE	CA-CB	-7.17	1.45	1.54
1	C	268	MET	SD-CE	7.17	1.97	1.79
1	C	1231	PRO	C-O	7.17	1.31	1.23
1	A	905	ASN	CA-C	7.17	1.62	1.53
1	C	303	CYS	CA-C	-7.17	1.46	1.53
1	B	1328	PRO	N-CA	7.16	1.56	1.47
1	C	7	VAL	CA-CB	-7.16	1.45	1.54
1	A	318	LYS	CB-CG	7.16	1.74	1.52
1	D	239	ALA	CA-C	-7.16	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1124	ASP	CA-C	7.16	1.62	1.52
1	C	1198	GLY	C-O	7.16	1.32	1.23
1	C	125	TYR	C-O	7.15	1.32	1.24
1	A	903	LYS	CE-NZ	7.15	1.70	1.49
1	B	144	GLN	N-CA	7.14	1.54	1.46
1	C	874	LEU	CA-C	7.13	1.62	1.52
1	B	1183	VAL	CA-CB	7.13	1.62	1.54
1	B	688	ILE	CA-CB	7.13	1.64	1.54
1	C	802	LYS	CA-C	7.12	1.62	1.52
1	C	664	VAL	N-CA	7.12	1.55	1.46
1	C	735	ILE	N-CA	7.12	1.54	1.46
1	B	646	ILE	CA-CB	-7.12	1.45	1.53
1	B	1330	SER	N-CA	7.12	1.55	1.46
1	A	383	VAL	CA-CB	7.11	1.63	1.54
1	C	903	LYS	CD-CE	7.11	1.73	1.52
1	D	739	GLY	C-O	7.11	1.30	1.23
1	A	368	SER	C-O	7.11	1.32	1.24
1	C	568	GLN	N-CA	7.11	1.54	1.45
1	C	1207	PHE	CA-C	-7.10	1.43	1.52
1	D	599	ARG	CD-NE	7.09	1.56	1.46
1	A	587	ALA	CA-CB	-7.09	1.41	1.53
1	B	1018	ALA	N-CA	7.08	1.56	1.46
1	B	46	GLY	CA-C	7.08	1.61	1.51
1	B	818	TYR	CA-C	-7.08	1.43	1.52
1	C	370	ALA	CA-CB	-7.08	1.43	1.53
1	B	511	LEU	CA-C	7.07	1.61	1.52
1	C	873	ASP	CA-C	7.07	1.62	1.52
1	D	51	CYS	CB-SG	7.07	2.04	1.81
1	B	1234	GLY	CA-C	7.07	1.61	1.51
1	D	64	LYS	CG-CD	7.06	1.73	1.52
1	D	641	VAL	CA-C	-7.06	1.46	1.53
1	A	1229	LYS	CG-CD	7.06	1.73	1.52
1	D	689	THR	N-CA	7.06	1.54	1.46
1	C	60	ARG	N-CA	7.06	1.55	1.46
1	A	101	VAL	CA-CB	-7.05	1.44	1.54
1	A	1072	VAL	C-O	-7.05	1.15	1.24
1	C	382	THR	CA-C	7.05	1.61	1.53
1	A	811	THR	CB-CG2	7.05	1.75	1.52
1	B	333	GLN	CA-C	-7.05	1.43	1.52
1	D	243	LYS	CA-C	7.05	1.61	1.52
1	B	1164	GLU	N-CA	7.04	1.54	1.46
1	D	91	ILE	CA-CB	7.04	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	461	ASN	CA-C	-7.04	1.43	1.52
1	A	1057	ILE	CA-C	-7.03	1.45	1.52
1	B	1309	ALA	CA-CB	-7.02	1.41	1.53
1	C	832	GLU	CG-CD	7.02	1.69	1.52
1	A	64	LYS	CG-CD	7.02	1.73	1.52
1	A	102	GLN	C-O	-7.02	1.15	1.24
1	A	1123	MET	C-O	7.02	1.33	1.24
1	A	1008	ILE	CA-CB	-7.01	1.45	1.54
1	B	859	ALA	CA-C	7.01	1.61	1.52
1	C	593	TYR	CB-CG	-7.01	1.36	1.51
1	B	817	ALA	C-O	-7.01	1.16	1.24
1	C	1100	LYS	N-CA	-7.00	1.37	1.46
1	D	1193	ILE	CA-CB	6.99	1.64	1.54
1	B	1100	LYS	N-CA	-6.99	1.37	1.46
1	C	903	LYS	CE-NZ	6.99	1.70	1.49
1	B	1134	TYR	CA-C	6.96	1.61	1.52
1	D	836	ILE	C-O	6.96	1.31	1.24
1	B	542	THR	CA-CB	6.96	1.65	1.53
1	C	318	LYS	CG-CD	6.96	1.73	1.52
1	D	950	GLU	C-O	-6.95	1.15	1.23
1	B	808	VAL	C-O	6.95	1.33	1.24
1	C	452	LEU	CA-C	6.95	1.61	1.52
1	B	1050	VAL	CA-CB	-6.95	1.45	1.54
1	C	142	ALA	CA-CB	-6.95	1.41	1.53
1	B	593	TYR	CA-CB	-6.95	1.41	1.53
1	B	878	ILE	CA-CB	-6.93	1.46	1.54
1	A	97	ARG	NE-CZ	6.92	1.40	1.33
1	B	568	GLN	N-CA	6.92	1.54	1.45
1	C	1266	PHE	N-CA	-6.92	1.38	1.46
1	D	318	LYS	CG-CD	6.92	1.73	1.52
1	D	560	LEU	CA-C	6.92	1.60	1.52
1	A	497	PRO	CA-C	6.91	1.56	1.52
1	C	512	THR	CA-CB	6.91	1.65	1.53
1	C	758	ALA	CA-CB	-6.91	1.42	1.53
1	B	2	THR	C-N	6.91	1.43	1.33
1	D	1097	THR	CA-CB	6.91	1.64	1.53
1	C	162	THR	CA-CB	6.90	1.65	1.53
1	A	1243	SER	CA-C	-6.90	1.44	1.52
1	B	824	VAL	CA-CB	-6.90	1.45	1.54
1	B	982	LYS	CA-C	-6.89	1.44	1.52
1	B	1329	TRP	CA-C	6.89	1.61	1.52
1	C	156	ILE	CA-CB	-6.89	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	206	PRO	N-CA	-6.88	1.40	1.47
1	A	1021	LEU	C-O	6.88	1.32	1.23
1	B	607	ARG	CA-C	-6.88	1.43	1.52
1	D	40	LYS	N-CA	6.88	1.54	1.45
1	B	597	ILE	CB-CG2	-6.88	1.29	1.52
1	D	33	LYS	C-O	-6.87	1.15	1.24
1	A	614	ALA	CA-CB	-6.87	1.42	1.53
1	B	1073	PRO	CA-C	-6.87	1.45	1.52
1	B	599	ARG	CB-CG	6.86	1.73	1.52
1	A	653	GLU	N-CA	6.86	1.54	1.45
1	A	1290	ASN	CA-C	6.85	1.61	1.52
1	B	406	SER	N-CA	6.85	1.54	1.46
1	A	313	VAL	CA-CB	6.84	1.63	1.54
1	C	1238	ILE	CA-CB	-6.84	1.46	1.54
1	B	64	LYS	CD-CE	6.84	1.73	1.52
1	A	297	ILE	CA-CB	-6.84	1.45	1.54
1	C	28	ALA	CA-C	-6.83	1.43	1.52
1	D	200	GLU	CD-OE2	6.83	1.38	1.25
1	A	532	LEU	CA-C	6.83	1.61	1.52
1	D	923	ILE	C-O	6.82	1.32	1.24
1	D	385	MET	CA-C	6.82	1.61	1.52
1	D	944	ARG	CB-CG	6.82	1.73	1.52
1	A	105	ILE	CA-CB	-6.82	1.45	1.54
1	C	87	THR	C-O	-6.82	1.15	1.23
1	D	681	ARG	CZ-NH1	6.81	1.42	1.32
1	B	14	LYS	C-O	-6.80	1.15	1.23
1	B	447	THR	N-CA	6.80	1.54	1.46
1	B	510	THR	CA-C	-6.80	1.43	1.52
1	A	533	GLU	N-CA	6.79	1.59	1.46
1	C	1221	HIS	C-O	6.79	1.33	1.24
1	A	97	ARG	CD-NE	6.79	1.55	1.46
1	B	597	ILE	CA-CB	-6.79	1.45	1.54
1	A	607	ARG	C-O	6.78	1.32	1.24
1	D	97	ARG	CD-NE	6.78	1.55	1.46
1	D	338	ALA	CA-CB	-6.78	1.42	1.53
1	B	1222	THR	CA-CB	6.78	1.65	1.53
1	C	13	ARG	CZ-NH1	6.78	1.42	1.32
1	C	47	GLY	C-O	6.78	1.33	1.23
1	C	418	PHE	N-CA	6.78	1.54	1.46
1	A	749	CYS	CA-C	6.78	1.61	1.52
1	C	198	PRO	C-O	6.78	1.32	1.24
1	D	148	CYS	CA-C	-6.77	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	446	THR	N-CA	6.77	1.54	1.45
1	D	789	VAL	C-O	6.77	1.31	1.24
1	A	60	ARG	N-CA	6.77	1.54	1.46
1	B	1188	ASN	CA-C	6.77	1.61	1.52
1	A	370	ALA	CA-CB	-6.77	1.43	1.53
1	C	1020	ALA	CA-CB	-6.77	1.42	1.54
1	C	1287	THR	CA-CB	6.77	1.63	1.53
1	A	800	GLY	N-CA	6.76	1.55	1.45
1	B	1084	ALA	CA-CB	-6.76	1.42	1.53
1	D	441	LEU	CA-C	6.76	1.60	1.52
1	A	674	ASP	C-O	-6.76	1.15	1.24
1	C	499	ASP	CB-CG	6.76	1.69	1.52
1	B	900	ARG	CA-C	6.75	1.60	1.52
1	B	239	ALA	CA-C	-6.75	1.43	1.52
1	B	1068	SER	C-O	6.75	1.32	1.23
1	A	1228	TYR	C-O	6.74	1.32	1.23
1	B	809	VAL	CA-CB	-6.74	1.45	1.54
1	B	1290	ASN	CA-C	6.73	1.61	1.52
1	B	1072	VAL	CA-C	6.73	1.59	1.52
1	B	667	ILE	C-O	6.73	1.30	1.24
1	A	687	LYS	CG-CD	6.72	1.72	1.52
1	A	1299	SER	CA-C	-6.72	1.44	1.52
1	A	382	THR	CA-CB	6.72	1.63	1.52
1	C	600	TYR	CA-C	-6.72	1.44	1.53
1	D	58	TYR	N-CA	6.72	1.54	1.46
1	D	711	PRO	N-CA	6.72	1.55	1.47
1	B	984	GLU	CG-CD	6.71	1.68	1.52
1	C	595	ASP	C-O	6.71	1.32	1.24
1	C	1279	ILE	CA-C	6.71	1.61	1.52
1	C	14	LYS	C-O	-6.71	1.15	1.23
1	D	453	ALA	CA-C	6.71	1.60	1.52
1	D	675	THR	N-CA	6.71	1.51	1.45
1	A	475	SER	N-CA	6.70	1.55	1.46
1	D	630	PRO	C-O	-6.70	1.15	1.23
1	A	202	THR	N-CA	6.70	1.56	1.46
1	A	442	PHE	C-O	6.70	1.32	1.23
1	B	817	ALA	CA-CB	-6.70	1.43	1.53
1	C	594	CYS	N-CA	-6.70	1.37	1.46
1	C	535	LYS	CA-C	6.69	1.60	1.52
1	C	811	THR	CA-CB	-6.69	1.43	1.53
1	C	1054	ALA	CA-CB	-6.69	1.41	1.53
1	A	515	PHE	CA-C	-6.69	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1067	THR	C-O	6.69	1.32	1.24
1	A	617	LYS	CD-CE	6.68	1.72	1.52
1	A	823	PRO	C-O	6.68	1.31	1.23
1	C	777	VAL	CA-CB	-6.67	1.46	1.54
1	A	657	ALA	CA-CB	-6.67	1.42	1.53
1	A	963	PHE	C-O	6.67	1.31	1.24
1	B	414	GLU	CA-CB	6.67	1.61	1.53
1	D	819	LYS	CD-CE	6.67	1.72	1.52
1	D	952	ASP	N-CA	6.67	1.53	1.46
1	B	533	GLU	CG-CD	6.67	1.68	1.52
1	D	1021	LEU	CA-C	-6.66	1.44	1.52
1	C	684	GLN	C-O	-6.65	1.16	1.23
1	A	279	VAL	CA-CB	-6.65	1.46	1.54
1	A	1190	ALA	N-CA	6.65	1.54	1.46
1	A	783	VAL	C-N	6.64	1.42	1.33
1	C	353	ILE	CA-CB	-6.64	1.46	1.54
1	C	85	VAL	CA-CB	-6.64	1.46	1.54
1	B	97	ARG	NE-CZ	6.64	1.40	1.33
1	B	1134	TYR	N-CA	6.64	1.54	1.46
1	B	917	GLY	C-N	-6.63	1.25	1.34
1	D	445	GLY	N-CA	6.63	1.54	1.45
1	A	630	PRO	N-CA	-6.63	1.39	1.47
1	C	205	ASP	CB-CG	-6.63	1.35	1.52
1	B	414	GLU	N-CA	6.63	1.54	1.46
1	A	93	SER	CA-C	-6.62	1.44	1.52
1	D	477	LEU	CA-C	6.62	1.60	1.52
1	C	766	SER	CA-C	-6.62	1.46	1.53
1	C	316	VAL	N-CA	6.62	1.54	1.46
1	C	222	THR	C-N	6.61	1.41	1.33
1	D	64	LYS	CD-CE	6.61	1.72	1.52
1	B	393	TYR	CE1-CZ	6.61	1.54	1.38
1	D	1067	THR	CA-CB	6.61	1.63	1.53
1	B	122	MET	CA-C	-6.61	1.43	1.52
1	B	1316	THR	CA-CB	6.60	1.63	1.53
1	B	1242	VAL	N-CA	6.60	1.54	1.46
1	D	102	GLN	CA-C	-6.60	1.44	1.52
1	D	110	GLY	C-O	6.60	1.32	1.23
1	D	817	ALA	CA-C	6.60	1.61	1.52
1	C	843	PHE	CA-C	6.59	1.60	1.52
1	D	160	PHE	CA-C	-6.59	1.43	1.52
1	A	1254	ILE	N-CA	6.59	1.54	1.46
1	C	597	ILE	CB-CG2	-6.59	1.30	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	450	GLN	CA-C	6.59	1.61	1.52
1	A	1029	SER	C-O	6.58	1.31	1.23
1	B	769	ASN	C-O	6.58	1.32	1.23
1	D	1119	THR	N-CA	6.58	1.54	1.46
1	A	1238	ILE	N-CA	6.58	1.54	1.46
1	C	971	GLU	CD-OE1	6.58	1.37	1.25
1	C	1210	GLU	CA-C	6.58	1.61	1.52
1	D	1078	THR	CA-CB	-6.58	1.44	1.52
1	C	34	LEU	CA-C	-6.58	1.44	1.52
1	D	227	LEU	N-CA	6.58	1.53	1.46
1	C	835	LEU	C-O	6.57	1.32	1.24
1	C	1117	TRP	N-CA	-6.57	1.37	1.46
1	B	387	HIS	N-CA	6.57	1.54	1.46
1	D	630	PRO	CA-C	-6.57	1.44	1.52
1	A	568	GLN	N-CA	6.56	1.54	1.46
1	D	861	GLU	CG-CD	6.56	1.68	1.52
1	B	733	GLY	CA-C	6.55	1.59	1.51
1	D	16	VAL	CA-CB	-6.55	1.46	1.53
1	D	477	LEU	C-O	6.55	1.31	1.23
1	A	699	ILE	CA-CB	-6.54	1.47	1.54
1	A	1076	SER	C-O	-6.54	1.15	1.23
1	A	364	VAL	N-CA	-6.54	1.38	1.46
1	C	1292	LYS	CA-C	6.53	1.60	1.53
1	C	71	ASN	CA-C	-6.53	1.44	1.52
1	A	1046	LYS	C-O	6.53	1.31	1.24
1	B	688	ILE	CA-C	6.53	1.60	1.52
1	B	600	TYR	CA-C	-6.53	1.44	1.53
1	C	33	LYS	CD-CE	6.52	1.72	1.52
1	B	60	ARG	N-CA	6.52	1.54	1.46
1	A	922	LEU	CA-C	-6.51	1.44	1.52
1	A	1242	VAL	CA-CB	-6.51	1.46	1.54
1	C	1118	VAL	CA-CB	-6.51	1.46	1.54
1	A	1078	THR	CA-C	-6.51	1.44	1.52
1	A	1176	ARG	N-CA	6.51	1.54	1.45
1	B	583	ALA	N-CA	6.51	1.54	1.46
1	A	510	THR	N-CA	-6.50	1.37	1.46
1	A	194	SER	CA-C	6.50	1.61	1.53
1	D	1017	GLN	C-O	-6.50	1.16	1.23
1	B	149	ARG	CA-C	6.50	1.61	1.52
1	A	657	ALA	CA-C	-6.50	1.44	1.52
1	C	1289	ASN	N-CA	6.49	1.54	1.46
1	C	297	ILE	CA-CB	-6.49	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	804	THR	N-CA	6.49	1.53	1.46
1	D	1175	LEU	N-CA	6.49	1.53	1.46
1	B	1237	PRO	CA-C	6.48	1.60	1.52
1	D	232	GLU	C-O	-6.48	1.14	1.23
1	D	1078	THR	CA-C	-6.48	1.44	1.52
1	A	223	PRO	CA-C	6.48	1.60	1.52
1	C	1130	ALA	CA-CB	-6.47	1.42	1.53
1	D	762	GLU	CD-OE2	6.47	1.37	1.25
1	A	1222	THR	C-O	6.47	1.31	1.23
1	A	425	SER	N-CA	6.47	1.58	1.46
1	D	1320	THR	CA-CB	6.46	1.72	1.54
1	A	1166	ASP	CA-C	-6.46	1.45	1.52
1	C	545	SER	N-CA	6.45	1.54	1.46
1	D	1079	ALA	C-O	6.45	1.32	1.24
1	B	1261	GLY	CA-C	6.44	1.60	1.51
1	D	150	CYS	CA-C	6.44	1.61	1.52
1	C	366	MET	C-O	-6.44	1.16	1.24
1	B	841	HIS	N-CA	6.43	1.54	1.46
1	B	1267	LEU	C-O	-6.43	1.15	1.24
1	C	1083	SER	CB-OG	6.43	1.55	1.42
1	C	258	VAL	CA-CB	-6.43	1.46	1.54
1	C	687	LYS	CG-CD	6.43	1.71	1.52
1	D	139	ILE	C-O	-6.43	1.15	1.24
1	C	641	VAL	CA-C	-6.42	1.46	1.53
1	D	277	MET	C-O	-6.42	1.16	1.24
1	A	962	GLY	C-O	6.42	1.32	1.23
1	A	1212	LEU	CA-C	6.42	1.61	1.52
1	B	1246	ARG	N-CA	6.41	1.53	1.45
1	B	542	THR	CA-C	6.41	1.61	1.52
1	C	194	SER	CA-C	6.41	1.61	1.52
1	C	293	GLY	C-N	6.41	1.40	1.33
1	B	546	ALA	CA-CB	6.41	1.63	1.53
1	A	746	GLU	CA-C	-6.41	1.44	1.52
1	B	30	LEU	CA-C	-6.41	1.44	1.52
1	B	1305	LYS	C-O	-6.41	1.16	1.24
1	C	1182	ASP	CA-C	6.41	1.61	1.52
1	A	273	MET	N-CA	6.40	1.54	1.45
1	B	681	ARG	CZ-NH1	6.40	1.41	1.32
1	D	649	ILE	CA-CB	-6.40	1.46	1.54
1	A	199	GLU	C-O	-6.40	1.15	1.24
1	B	247	ASP	CA-C	-6.40	1.44	1.52
1	D	1141	TYR	C-O	-6.40	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	40	LYS	CA-C	6.39	1.62	1.53
1	B	1009	SER	C-O	-6.39	1.16	1.24
1	D	278	ILE	CA-CB	-6.39	1.46	1.54
1	A	971	GLU	CG-CD	6.39	1.68	1.52
1	A	1121	ALA	CA-CB	-6.39	1.43	1.53
1	D	289	SER	CA-C	6.39	1.61	1.52
1	A	1140	GLY	N-CA	6.39	1.54	1.45
1	A	269	LYS	CD-CE	6.38	1.71	1.52
1	C	485	ASP	CB-CG	6.38	1.68	1.52
1	A	445	GLY	C-O	6.38	1.32	1.23
1	A	1070	ASN	CA-C	-6.38	1.44	1.52
1	C	747	THR	N-CA	6.37	1.53	1.46
1	D	40	LYS	CB-CG	6.37	1.71	1.52
1	B	419	SER	N-CA	6.37	1.54	1.45
1	A	1305	LYS	C-O	-6.36	1.15	1.24
1	B	102	GLN	CA-C	-6.36	1.44	1.52
1	C	724	PHE	N-CA	6.36	1.54	1.46
1	A	601	GLU	C-O	-6.36	1.15	1.24
1	D	269	LYS	CE-NZ	6.36	1.68	1.49
1	B	24	THR	C-O	-6.36	1.16	1.24
1	B	409	ILE	CA-CB	-6.36	1.47	1.53
1	C	709	TYR	N-CA	6.36	1.54	1.46
1	D	891	LYS	CG-CD	6.36	1.71	1.52
1	A	808	VAL	N-CA	6.35	1.54	1.46
1	D	595	ASP	N-CA	6.35	1.54	1.46
1	A	418	PHE	N-CA	6.35	1.54	1.46
1	C	1332	ARG	N-CA	6.35	1.58	1.46
1	A	512	THR	CA-C	6.35	1.61	1.52
1	C	205	ASP	N-CA	-6.35	1.40	1.46
1	D	5	LYS	N-CA	-6.35	1.38	1.46
1	C	1167	CYS	CA-C	-6.34	1.43	1.52
1	D	614	ALA	CA-C	6.34	1.61	1.52
1	B	1071	THR	N-CA	-6.34	1.38	1.46
1	C	642	PRO	C-O	-6.34	1.15	1.24
1	C	106	ALA	C-O	-6.34	1.15	1.24
1	C	745	LEU	C-O	6.34	1.31	1.24
1	A	572	ASP	CA-C	6.33	1.61	1.52
1	A	618	ILE	CA-CB	6.33	1.63	1.54
1	C	165	ARG	CZ-NH2	6.33	1.41	1.33
1	C	771	MET	C-O	6.32	1.31	1.24
1	B	598	PRO	C-O	6.32	1.32	1.24
1	B	64	LYS	CG-CD	6.32	1.71	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	204	LEU	C-O	6.32	1.31	1.24
1	C	21	ASP	CA-C	-6.31	1.45	1.52
1	C	38	GLY	C-O	-6.31	1.15	1.24
1	C	811	THR	CB-CG2	6.31	1.73	1.52
1	C	1066	GLU	CA-C	-6.31	1.45	1.52
1	D	396	THR	C-O	-6.31	1.17	1.24
1	D	1064	ILE	C-O	6.31	1.30	1.24
1	C	783	VAL	C-O	6.31	1.32	1.24
1	D	878	ILE	CA-C	-6.31	1.45	1.52
1	D	1011	THR	N-CA	6.30	1.53	1.46
1	C	654	THR	C-O	6.30	1.31	1.24
1	B	21	ASP	C-O	-6.30	1.16	1.24
1	A	353	ILE	CA-CB	-6.30	1.47	1.54
1	A	1087	ASN	CA-C	-6.30	1.43	1.52
1	B	642	PRO	N-CA	-6.29	1.39	1.47
1	C	681	ARG	C-O	-6.29	1.16	1.24
1	D	59	ASP	CA-C	-6.29	1.45	1.52
1	C	1079	ALA	CA-CB	-6.29	1.42	1.53
1	C	1290	ASN	CB-CG	6.29	1.67	1.52
1	B	131	GLN	CA-C	6.29	1.60	1.52
1	D	121	VAL	CA-CB	-6.29	1.47	1.54
1	D	1314	PHE	N-CA	6.29	1.53	1.46
1	B	772	LYS	CA-C	-6.28	1.44	1.52
1	C	532	LEU	CA-C	6.28	1.61	1.52
1	A	62	GLN	CG-CD	6.28	1.67	1.52
1	B	342	VAL	CA-CB	-6.28	1.46	1.54
1	B	903	LYS	C-O	-6.28	1.16	1.23
1	B	759	GLY	C-O	-6.28	1.16	1.24
1	A	1076	SER	N-CA	6.27	1.54	1.45
1	B	615	HIS	N-CA	6.27	1.54	1.46
1	B	789	VAL	C-O	-6.27	1.17	1.24
1	D	672	VAL	N-CA	6.27	1.54	1.46
1	B	509	CYS	N-CA	-6.26	1.38	1.46
1	C	205	ASP	CA-CB	-6.26	1.45	1.53
1	D	239	ALA	CA-CB	-6.26	1.43	1.53
1	D	310	LYS	CD-CE	6.26	1.71	1.52
1	A	65	ILE	CA-CB	-6.26	1.46	1.54
1	A	903	LYS	C-O	-6.26	1.16	1.24
1	A	1192	ASP	C-O	-6.26	1.16	1.23
1	C	1212	LEU	CA-C	6.26	1.60	1.52
1	D	1236	ILE	C-O	6.26	1.32	1.24
1	C	842	PRO	CA-C	6.26	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1180	VAL	N-CA	-6.26	1.38	1.46
1	A	446	THR	CB-CG2	6.26	1.73	1.52
1	A	453	ALA	CA-CB	6.25	1.64	1.53
1	B	597	ILE	C-O	-6.25	1.16	1.24
1	B	141	ASN	N-CA	-6.25	1.38	1.46
1	C	751	ILE	N-CA	6.25	1.53	1.46
1	A	762	GLU	CD-OE1	6.25	1.37	1.25
1	B	703	ILE	CA-CB	-6.25	1.46	1.54
1	D	1330	SER	CA-C	6.25	1.60	1.52
1	B	758	ALA	N-CA	6.24	1.54	1.46
1	B	1261	GLY	C-O	6.24	1.32	1.23
1	B	23	GLU	CD-OE2	6.24	1.37	1.25
1	B	133	GLU	C-O	-6.24	1.16	1.24
1	A	83	VAL	CB-CG1	-6.23	1.31	1.52
1	A	161	ARG	CG-CD	6.23	1.71	1.52
1	D	598	PRO	CA-CB	-6.23	1.45	1.53
1	A	762	GLU	CD-OE2	6.23	1.37	1.25
1	B	127	LEU	C-O	-6.22	1.16	1.24
1	A	1228	TYR	CA-C	6.22	1.60	1.52
1	D	1001	ILE	CA-C	6.22	1.60	1.52
1	A	791	ARG	C-O	6.22	1.31	1.23
1	C	364	VAL	CA-C	-6.22	1.44	1.52
1	A	372	LEU	N-CA	6.21	1.53	1.45
1	A	1320	THR	N-CA	6.21	1.58	1.46
1	C	640	ASP	N-CA	6.21	1.53	1.45
1	B	708	PHE	C-O	-6.21	1.16	1.24
1	D	113	CYS	CA-C	6.21	1.61	1.52
1	A	466	ALA	CA-CB	6.20	1.64	1.53
1	D	586	GLN	CD-NE2	6.20	1.46	1.33
1	D	814	ALA	CA-C	6.19	1.61	1.52
1	B	475	SER	N-CA	6.19	1.55	1.46
1	A	69	SER	CA-C	-6.19	1.44	1.52
1	A	315	ALA	CA-C	6.19	1.61	1.52
1	B	427	ARG	N-CA	6.19	1.54	1.46
1	C	354	THR	C-O	6.19	1.31	1.24
1	D	591	ALA	C-O	6.19	1.31	1.24
1	C	757	GLU	CA-C	6.18	1.60	1.52
1	C	1126	VAL	CA-CB	-6.18	1.46	1.54
1	A	812	ALA	CA-C	6.18	1.60	1.52
1	A	66	VAL	C-O	6.18	1.31	1.24
1	B	434	VAL	C-O	-6.18	1.16	1.24
1	C	640	ASP	C-O	6.18	1.31	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	659	ASP	N-CA	6.17	1.54	1.46
1	C	923	ILE	CA-CB	-6.17	1.46	1.54
1	D	1263	PRO	CA-C	-6.17	1.46	1.52
1	B	786	ASN	N-CA	-6.17	1.38	1.46
1	D	257	LEU	CA-C	-6.17	1.45	1.52
1	D	630	PRO	CA-CB	-6.17	1.45	1.53
1	B	13	ARG	CG-CD	6.17	1.71	1.52
1	A	88	VAL	CA-CB	6.16	1.61	1.54
1	B	1199	ALA	CA-CB	-6.16	1.43	1.53
1	C	64	LYS	CG-CD	6.16	1.71	1.52
1	C	499	ASP	CA-CB	6.16	1.64	1.53
1	D	135	THR	N-CA	6.16	1.53	1.45
1	D	970	GLU	CG-CD	6.16	1.67	1.52
1	D	1059	THR	CA-C	6.16	1.61	1.52
1	D	1081	SER	C-O	6.16	1.31	1.24
1	D	382	THR	CA-CB	6.16	1.62	1.52
1	D	666	HIS	CA-CB	6.16	1.63	1.53
1	A	40	LYS	CD-CE	6.15	1.71	1.52
1	B	1121	ALA	CA-CB	-6.15	1.43	1.53
1	A	54	MET	C-O	6.15	1.30	1.24
1	C	734	GLU	CG-CD	6.15	1.67	1.52
1	B	1287	THR	CA-CB	6.15	1.61	1.53
1	C	711	PRO	C-O	-6.15	1.17	1.23
1	A	338	ALA	C-O	-6.15	1.16	1.24
1	C	1215	SER	C-N	6.14	1.41	1.33
1	A	1153	TYR	C-O	6.14	1.30	1.24
1	D	1117	TRP	N-CA	6.14	1.54	1.46
1	A	424	ALA	CA-CB	6.13	1.62	1.52
1	B	390	PHE	CA-C	-6.13	1.44	1.52
1	B	1245	LEU	CA-C	-6.13	1.44	1.52
1	B	784	PRO	N-CA	6.13	1.54	1.47
1	C	1058	PRO	N-CA	6.13	1.54	1.47
1	A	431	ILE	CB-CG1	6.13	1.65	1.53
1	D	268	MET	SD-CE	6.13	1.94	1.79
1	B	106	ALA	CA-CB	6.12	1.63	1.53
1	A	1233	PHE	CA-CB	-6.12	1.44	1.53
1	D	783	VAL	C-O	6.12	1.31	1.24
1	D	1243	SER	N-CA	6.12	1.53	1.46
1	A	623	THR	CA-CB	-6.12	1.42	1.53
1	A	680	GLN	C-O	-6.12	1.17	1.24
1	C	1106	LYS	C-O	-6.12	1.17	1.24
1	B	741	GLU	N-CA	6.12	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	232	GLU	N-CA	6.11	1.53	1.45
1	B	979	HIS	C-O	6.11	1.31	1.23
1	B	328	ARG	N-CA	6.11	1.54	1.46
1	D	1260	VAL	CA-CB	-6.11	1.46	1.55
1	D	70	ALA	CA-C	-6.11	1.45	1.52
1	C	1110	PRO	C-O	6.10	1.31	1.24
1	C	1059	THR	C-O	6.10	1.31	1.24
1	D	120	ILE	CA-CB	-6.10	1.46	1.54
1	B	1009	SER	CA-C	-6.10	1.44	1.52
1	D	649	ILE	C-O	-6.09	1.18	1.24
1	D	1054	ALA	N-CA	-6.09	1.38	1.46
1	D	566	LYS	N-CA	6.09	1.53	1.46
1	D	202	THR	N-CA	6.09	1.54	1.45
1	A	232	GLU	CG-CD	6.09	1.67	1.52
1	A	664	VAL	N-CA	6.09	1.53	1.46
1	D	1145	THR	CA-CB	6.08	1.63	1.53
1	A	210	PRO	CA-C	6.08	1.59	1.52
1	B	612	THR	CB-CG2	6.08	1.72	1.52
1	A	402	GLU	CD-OE2	6.08	1.36	1.25
1	A	1287	THR	CA-CB	6.08	1.61	1.53
1	C	13	ARG	CG-CD	6.08	1.70	1.52
1	C	670	ALA	C-O	-6.08	1.16	1.23
1	B	2	THR	CA-CB	6.08	1.70	1.54
1	C	543	PHE	CA-C	6.08	1.60	1.52
1	B	647	THR	CB-CG2	6.07	1.72	1.52
1	C	164	ALA	CA-C	6.07	1.59	1.52
1	C	913	ARG	CA-C	6.07	1.60	1.52
1	A	1034	HIS	CA-C	-6.07	1.45	1.52
1	A	303	CYS	CA-C	-6.07	1.47	1.53
1	A	858	VAL	C-O	-6.07	1.16	1.24
1	C	1006	PHE	C-O	6.07	1.30	1.24
1	A	241	THR	CA-CB	6.07	1.62	1.53
1	A	619	LYS	CD-CE	6.07	1.70	1.52
1	C	254	ASP	CB-CG	6.07	1.67	1.52
1	B	1293	GLU	N-CA	6.06	1.54	1.46
1	C	922	LEU	N-CA	6.06	1.54	1.46
1	D	628	LYS	CG-CD	6.06	1.70	1.52
1	C	8	PHE	CA-CB	-6.06	1.46	1.53
1	D	664	VAL	CA-CB	-6.06	1.46	1.54
1	D	466	ALA	CA-C	-6.06	1.44	1.52
1	D	153	TYR	CA-C	6.05	1.60	1.52
1	A	788	ILE	CA-CB	-6.05	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1180	VAL	CA-CB	-6.05	1.46	1.54
1	A	496	LEU	CA-C	6.05	1.59	1.52
1	C	362	ASN	N-CA	-6.04	1.42	1.46
1	A	425	SER	CA-C	6.04	1.65	1.52
1	C	121	VAL	CA-CB	-6.04	1.47	1.54
1	C	822	ARG	CA-CB	-6.04	1.45	1.53
1	D	1245	LEU	C-O	6.04	1.31	1.24
1	B	709	TYR	N-CA	6.04	1.53	1.46
1	C	644	SER	CA-C	-6.04	1.45	1.52
1	C	675	THR	C-O	-6.04	1.18	1.24
1	B	1226	SER	C-O	-6.04	1.16	1.24
1	D	408	GLU	CG-CD	6.04	1.67	1.52
1	A	760	GLU	CA-C	-6.04	1.45	1.52
1	D	833	ASP	CA-C	6.03	1.60	1.52
1	B	941	GLU	CG-CD	6.03	1.67	1.52
1	C	273	MET	SD-CE	6.03	1.94	1.79
1	B	15	VAL	CA-C	-6.03	1.45	1.52
1	D	640	ASP	CA-C	-6.03	1.44	1.52
1	D	1181	MET	C-O	-6.02	1.17	1.24
1	A	1274	ALA	CA-CB	-6.02	1.43	1.53
1	C	618	ILE	CA-CB	6.02	1.61	1.53
1	B	593	TYR	CB-CG	-6.02	1.38	1.51
1	B	1327	LYS	N-CA	6.02	1.54	1.46
1	C	463	THR	CA-CB	6.01	1.60	1.52
1	B	94	THR	C-O	-6.01	1.16	1.24
1	C	525	GLN	CB-CG	6.01	1.70	1.52
1	D	927	TRP	CB-CG	-6.01	1.31	1.50
1	A	621	ILE	C-O	-6.01	1.17	1.24
1	B	418	PHE	N-CA	6.00	1.53	1.46
1	D	22	PRO	CB-CG	-6.00	1.19	1.49
1	C	488	ALA	C-O	6.00	1.30	1.24
1	A	1138	ASN	N-CA	6.00	1.53	1.46
1	D	892	ILE	N-CA	6.00	1.53	1.46
1	C	434	VAL	CA-CB	-6.00	1.46	1.54
1	D	269	LYS	CD-CE	6.00	1.70	1.52
1	B	1066	GLU	C-O	-6.00	1.16	1.23
1	C	1193	ILE	N-CA	5.99	1.53	1.46
1	B	450	GLN	CA-C	5.99	1.60	1.52
1	A	112	GLN	CA-C	5.99	1.60	1.52
1	A	343	LYS	CD-CE	5.99	1.70	1.52
1	D	83	VAL	CA-CB	-5.99	1.45	1.55
1	A	923	ILE	N-CA	5.98	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1227	THR	N-CA	5.98	1.53	1.46
1	D	362	ASN	C-O	-5.98	1.18	1.24
1	D	586	GLN	C-O	5.98	1.31	1.24
1	A	1084	ALA	CA-CB	-5.98	1.43	1.53
1	D	754	PRO	C-O	-5.98	1.16	1.24
1	A	755	LYS	C-O	-5.98	1.16	1.24
1	B	682	ALA	CA-CB	-5.97	1.43	1.53
1	C	854	THR	CA-C	5.97	1.60	1.52
1	B	254	ASP	C-O	5.97	1.32	1.24
1	B	792	VAL	CA-C	-5.97	1.45	1.52
1	A	653	GLU	CG-CD	5.97	1.67	1.52
1	B	123	SER	N-CA	-5.97	1.39	1.46
1	C	941	GLU	CG-CD	5.97	1.67	1.52
1	A	414	GLU	N-CA	5.96	1.53	1.46
1	B	577	PRO	CA-C	5.96	1.58	1.53
1	C	971	GLU	CG-CD	5.96	1.67	1.52
1	D	154	ARG	C-N	5.96	1.42	1.33
1	D	476	LYS	N-CA	5.96	1.53	1.46
1	A	574	VAL	N-CA	5.96	1.53	1.46
1	B	1047	MET	N-CA	-5.96	1.38	1.46
1	B	1097	THR	CA-C	-5.96	1.45	1.52
1	C	54	MET	CA-C	5.96	1.60	1.52
1	D	477	LEU	CG-CD2	5.96	1.72	1.52
1	B	431	ILE	C-O	5.96	1.30	1.24
1	B	123	SER	CA-C	-5.96	1.45	1.52
1	C	1187	LEU	N-CA	5.96	1.53	1.46
1	C	757	GLU	C-O	5.95	1.31	1.24
1	A	829	ASP	C-O	5.95	1.31	1.23
1	A	593	TYR	CA-C	5.95	1.57	1.53
1	A	941	GLU	CG-CD	5.95	1.67	1.52
1	B	222	THR	CA-C	5.95	1.60	1.52
1	A	476	LYS	CA-C	5.95	1.60	1.52
1	A	1183	VAL	CA-CB	5.95	1.61	1.54
1	C	526	LYS	CG-CD	5.95	1.70	1.52
1	D	607	ARG	N-CA	5.94	1.53	1.46
1	B	158	GLN	C-O	-5.94	1.16	1.24
1	C	535	LYS	N-CA	5.94	1.53	1.45
1	B	592	VAL	N-CA	5.94	1.53	1.46
1	B	32	ARG	N-CA	-5.94	1.39	1.46
1	D	232	GLU	CA-C	-5.94	1.44	1.52
1	D	525	GLN	C-O	5.94	1.31	1.24
1	B	1220	LEU	N-CA	5.93	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1280	ARG	CA-C	-5.93	1.44	1.52
1	D	362	ASN	N-CA	-5.93	1.41	1.46
1	D	1093	ALA	CA-CB	-5.93	1.44	1.53
1	D	792	VAL	CA-CB	-5.93	1.46	1.54
1	B	282	ALA	N-CA	5.93	1.53	1.46
1	D	1225	PRO	C-O	5.92	1.31	1.24
1	A	755	LYS	CG-CD	5.92	1.70	1.52
1	B	92	GLY	C-O	5.92	1.31	1.23
1	B	610	THR	CA-C	-5.92	1.45	1.52
1	B	692	GLU	N-CA	-5.92	1.38	1.46
1	B	1271	ILE	CA-CB	-5.92	1.46	1.54
1	C	223	PRO	CA-C	5.92	1.58	1.52
1	A	99	HIS	C-O	-5.92	1.15	1.23
1	D	535	LYS	CB-CG	5.92	1.70	1.52
1	D	1051	ALA	CA-C	5.92	1.61	1.52
1	A	935	CYS	CB-SG	-5.92	1.61	1.81
1	B	370	ALA	CA-CB	-5.91	1.44	1.53
1	A	805	ARG	CZ-NH2	5.91	1.41	1.33
1	C	797	GLY	CA-C	-5.91	1.43	1.51
1	B	533	GLU	N-CA	5.91	1.53	1.46
1	C	841	HIS	N-CA	5.91	1.52	1.45
1	C	1145	THR	CA-CB	5.91	1.63	1.53
1	B	545	SER	N-CA	5.91	1.53	1.46
1	C	1227	THR	CA-CB	5.91	1.62	1.53
1	D	557	ASP	CB-CG	5.91	1.66	1.52
1	D	837	THR	N-CA	5.91	1.53	1.46
1	D	1032	LEU	C-O	5.91	1.30	1.23
1	C	455	CYS	CA-C	-5.90	1.45	1.52
1	A	903	LYS	CD-CE	5.90	1.70	1.52
1	B	57	LYS	C-O	-5.89	1.16	1.23
1	B	1186	SER	N-CA	5.89	1.53	1.46
1	A	112	GLN	CG-CD	5.89	1.66	1.52
1	B	1223	ARG	CA-C	5.89	1.60	1.52
1	C	360	ASP	C-O	-5.89	1.16	1.24
1	A	501	PRO	CA-C	5.89	1.59	1.52
1	A	937	MET	SD-CE	5.89	1.94	1.79
1	A	310	LYS	CE-NZ	5.88	1.67	1.49
1	B	793	LYS	CA-C	-5.88	1.46	1.52
1	A	601	GLU	N-CA	-5.88	1.38	1.46
1	D	303	CYS	CA-C	-5.88	1.47	1.53
1	B	891	LYS	CD-CE	5.88	1.70	1.52
1	C	21	ASP	CB-CG	5.88	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1245	LEU	C-O	5.88	1.31	1.24
1	B	799	PHE	C-O	-5.88	1.16	1.24
1	B	817	ALA	CA-C	-5.88	1.45	1.52
1	D	7	VAL	CA-CB	-5.88	1.46	1.54
1	B	88	VAL	CA-CB	-5.88	1.47	1.54
1	A	340	LYS	CD-CE	5.87	1.70	1.52
1	A	1100	LYS	CA-C	5.87	1.60	1.52
1	B	760	GLU	C-O	5.87	1.30	1.23
1	C	884	PHE	C-O	5.87	1.31	1.24
1	A	1090	ALA	N-CA	-5.87	1.39	1.46
1	D	33	LYS	CB-CG	5.87	1.70	1.52
1	D	215	GLU	CA-C	5.87	1.60	1.52
1	D	382	THR	CA-C	5.87	1.60	1.53
1	A	1082	VAL	CA-CB	-5.86	1.47	1.54
1	B	136	MET	CG-SD	5.86	1.95	1.80
1	C	32	ARG	CZ-NH2	5.86	1.41	1.33
1	C	809	VAL	C-O	-5.86	1.17	1.24
1	D	32	ARG	CZ-NH1	5.86	1.41	1.32
1	D	145	GLY	C-O	5.86	1.30	1.24
1	B	161	ARG	CZ-NH1	5.86	1.41	1.32
1	B	248	LEU	C-O	5.86	1.30	1.24
1	D	210	PRO	N-CA	-5.86	1.40	1.46
1	C	415	GLY	C-O	5.86	1.31	1.24
1	A	121	VAL	C-O	-5.86	1.17	1.24
1	A	1164	GLU	CA-C	5.86	1.59	1.52
1	C	10	VAL	C-O	-5.86	1.17	1.24
1	B	924	ALA	CA-C	-5.85	1.45	1.52
1	C	859	ALA	CA-CB	-5.85	1.43	1.53
1	B	1234	GLY	N-CA	5.85	1.53	1.45
1	B	1260	VAL	CA-CB	-5.85	1.46	1.54
1	D	200	GLU	CG-CD	5.85	1.66	1.52
1	A	683	ALA	C-N	-5.85	1.26	1.33
1	B	905	ASN	CA-C	5.85	1.60	1.53
1	C	218	ARG	CZ-NH1	5.85	1.41	1.32
1	A	599	ARG	CA-C	-5.85	1.45	1.53
1	D	708	PHE	C-O	-5.84	1.16	1.24
1	C	49	GLY	N-CA	5.84	1.53	1.45
1	B	1127	SER	C-O	-5.84	1.17	1.23
1	D	288	ASN	CA-C	-5.84	1.45	1.52
1	A	971	GLU	CD-OE1	5.83	1.36	1.25
1	C	407	ILE	CB-CG2	-5.83	1.33	1.52
1	C	620	SER	CA-C	5.83	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	427	ARG	CB-CG	5.83	1.70	1.52
1	A	749	CYS	N-CA	5.83	1.53	1.46
1	A	1222	THR	CA-CB	5.83	1.60	1.53
1	A	1098	ILE	CA-CB	5.83	1.61	1.54
1	A	1133	PHE	C-O	-5.83	1.16	1.23
1	A	69	SER	N-CA	5.83	1.52	1.45
1	A	351	ASN	CA-C	-5.83	1.45	1.52
1	A	309	GLU	CD-OE2	5.82	1.36	1.25
1	A	467	LEU	CG-CD1	5.82	1.71	1.52
1	C	200	GLU	CD-OE2	5.82	1.36	1.25
1	A	7	VAL	CA-CB	-5.82	1.46	1.54
1	B	462	ARG	CA-C	-5.82	1.45	1.53
1	D	1254	ILE	N-CA	5.82	1.53	1.46
1	B	264	ILE	CA-CB	-5.82	1.47	1.54
1	B	959	LYS	CG-CD	5.82	1.69	1.52
1	A	1260	VAL	CA-CB	-5.81	1.47	1.55
1	C	1280	ARG	C-O	-5.81	1.16	1.24
1	A	566	LYS	N-CA	5.81	1.53	1.46
1	A	326	VAL	C-O	-5.81	1.17	1.24
1	C	137	GLU	CA-C	5.81	1.60	1.52
1	D	959	LYS	CA-C	5.81	1.60	1.52
1	C	1057	ILE	N-CA	-5.81	1.39	1.46
1	D	644	SER	CA-C	-5.81	1.45	1.52
1	A	101	VAL	CA-C	-5.80	1.44	1.52
1	A	161	ARG	CB-CG	5.80	1.69	1.52
1	C	1179	ILE	CA-CB	-5.80	1.47	1.54
1	D	597	ILE	CA-CB	-5.80	1.43	1.53
1	B	279	VAL	CA-C	-5.80	1.45	1.52
1	B	1229	LYS	CD-CE	5.80	1.69	1.52
1	C	599	ARG	CA-CB	5.80	1.62	1.53
1	D	101	VAL	CA-CB	-5.79	1.46	1.54
1	A	195	LEU	N-CA	5.79	1.53	1.46
1	D	870	ASN	N-CA	5.79	1.52	1.46
1	C	67	HIS	N-CA	5.79	1.53	1.46
1	A	87	THR	CA-CB	-5.78	1.45	1.53
1	A	654	THR	N-CA	5.78	1.53	1.46
1	A	1223	ARG	N-CA	5.78	1.53	1.46
1	A	83	VAL	CA-C	5.78	1.60	1.52
1	C	585	MET	N-CA	-5.78	1.39	1.46
1	C	1011	THR	N-CA	5.78	1.53	1.46
1	D	832	GLU	CD-OE2	5.78	1.36	1.25
1	D	1109	ASN	CB-CG	5.78	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	21	ASP	C-O	-5.78	1.17	1.24
1	B	692	GLU	CD-OE1	5.78	1.36	1.25
1	D	748	HIS	N-CA	5.78	1.53	1.45
1	A	826	CYS	C-O	5.78	1.30	1.23
1	D	753	VAL	CA-CB	-5.78	1.46	1.54
1	A	676	PRO	C-O	5.77	1.31	1.24
1	A	13	ARG	CZ-NH1	5.77	1.40	1.32
1	B	107	LYS	CG-CD	5.77	1.69	1.52
1	B	538	LYS	N-CA	5.77	1.53	1.46
1	D	1144	GLU	CB-CG	5.77	1.69	1.52
1	A	1235	SER	N-CA	5.77	1.53	1.45
1	B	333	GLN	N-CA	-5.77	1.38	1.46
1	C	672	VAL	CA-CB	-5.77	1.46	1.54
1	D	944	ARG	CG-CD	5.77	1.69	1.52
1	B	937	MET	N-CA	5.77	1.54	1.46
1	D	321	ALA	CA-C	5.77	1.60	1.52
1	D	506	ASP	CB-CG	5.77	1.66	1.52
1	A	700	GLU	CD-OE1	5.76	1.36	1.25
1	B	544	ALA	CA-CB	5.76	1.62	1.53
1	D	699	ILE	N-CA	5.76	1.53	1.46
1	A	660	LYS	CA-C	5.76	1.59	1.52
1	D	75	ALA	CA-CB	-5.76	1.43	1.53
1	A	771	MET	CA-C	-5.76	1.45	1.52
1	B	511	LEU	C-O	5.76	1.30	1.24
1	B	533	GLU	CB-CG	5.76	1.69	1.52
1	D	322	GLN	CA-C	5.76	1.59	1.52
1	C	631	GLY	C-O	5.75	1.31	1.24
1	C	1118	VAL	CB-CG1	-5.75	1.33	1.52
1	D	79	SER	CA-C	5.75	1.60	1.52
1	D	242	LEU	CA-C	-5.75	1.45	1.52
1	B	239	ALA	C-O	-5.75	1.16	1.23
1	C	1315	THR	CA-C	5.75	1.60	1.52
1	A	45	GLU	N-CA	-5.75	1.38	1.46
1	C	934	THR	CA-C	5.75	1.60	1.52
1	C	1211	GLU	N-CA	5.74	1.53	1.46
1	C	133	GLU	CD-OE2	5.74	1.36	1.25
1	C	71	ASN	CG-ND2	5.74	1.45	1.33
1	A	36	LEU	CA-C	-5.73	1.45	1.53
1	B	314	ASP	CG-OD2	5.73	1.36	1.25
1	D	461	ASN	CB-CG	-5.73	1.37	1.52
1	D	525	GLN	N-CA	5.73	1.53	1.46
1	B	619	LYS	CB-CG	5.73	1.69	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1116	ASP	CA-C	-5.73	1.45	1.52
1	A	239	ALA	N-CA	5.73	1.52	1.45
1	C	647	THR	CB-CG2	5.73	1.71	1.52
1	D	70	ALA	CA-CB	-5.73	1.44	1.53
1	C	380	ARG	NE-CZ	5.73	1.39	1.33
1	A	660	LYS	CD-CE	5.72	1.69	1.52
1	B	1008	ILE	CA-CB	-5.72	1.47	1.54
1	C	596	ASP	C-N	5.72	1.39	1.33
1	B	892	ILE	CA-C	5.72	1.58	1.52
1	B	911	ALA	N-CA	5.72	1.53	1.46
1	C	83	VAL	CA-CB	-5.72	1.47	1.54
1	D	21	ASP	N-CA	5.72	1.55	1.46
1	B	1021	LEU	C-O	5.72	1.30	1.23
1	D	65	ILE	CA-CB	-5.72	1.47	1.54
1	C	937	MET	CG-SD	5.72	1.95	1.80
1	D	591	ALA	CA-CB	-5.72	1.43	1.53
1	A	355	ALA	CA-CB	-5.72	1.43	1.53
1	A	1255	TYR	CD1-CE1	5.72	1.55	1.38
1	A	1154	PHE	N-CA	5.71	1.53	1.46
1	C	1090	ALA	N-CA	-5.71	1.39	1.46
1	A	1070	ASN	C-O	-5.71	1.16	1.24
1	C	451	GLU	C-O	5.71	1.31	1.24
1	C	1154	PHE	C-O	5.71	1.31	1.23
1	D	1173	LYS	CD-CE	5.71	1.69	1.52
1	A	719	ASP	C-O	5.71	1.31	1.24
1	B	791	ARG	C-O	5.71	1.30	1.23
1	B	64	LYS	C-O	-5.71	1.16	1.23
1	C	543	PHE	N-CA	5.71	1.53	1.46
1	C	594	CYS	CA-C	-5.71	1.45	1.52
1	A	1073	PRO	N-CA	-5.71	1.41	1.46
1	A	745	LEU	C-O	5.70	1.31	1.24
1	D	1331	VAL	CB-CG2	5.70	1.71	1.52
1	B	1201	VAL	C-O	-5.70	1.17	1.24
1	C	1290	ASN	CA-CB	5.70	1.63	1.53
1	D	1127	SER	CA-C	5.70	1.60	1.52
1	B	16	VAL	CA-CB	-5.69	1.46	1.53
1	C	306	SER	C-O	-5.69	1.17	1.24
1	A	1190	ALA	C-O	-5.69	1.17	1.24
1	C	1272	PHE	CD1-CE1	5.69	1.55	1.38
1	A	318	LYS	CA-CB	5.69	1.61	1.53
1	D	700	GLU	N-CA	5.69	1.53	1.46
1	A	699	ILE	CA-C	-5.68	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	654	THR	CA-C	5.68	1.59	1.52
1	D	759	GLY	C-O	-5.68	1.16	1.24
1	D	900	ARG	N-CA	5.68	1.52	1.45
1	D	1075	THR	CA-C	-5.68	1.46	1.52
1	B	366	MET	C-O	-5.67	1.17	1.24
1	B	1297	LEU	N-CA	5.67	1.52	1.46
1	D	1103	GLU	N-CA	5.67	1.54	1.46
1	A	254	ASP	CA-C	5.67	1.60	1.52
1	B	811	THR	CB-CG2	5.67	1.71	1.52
1	D	380	ARG	CZ-NH1	5.67	1.40	1.32
1	C	253	PRO	CA-C	5.67	1.60	1.52
1	D	1291	VAL	CB-CG1	5.67	1.71	1.52
1	B	783	VAL	CA-CB	-5.67	1.50	1.55
1	C	783	VAL	CA-C	5.67	1.58	1.52
1	A	1297	LEU	CA-C	5.66	1.59	1.52
1	C	945	LYS	CG-CD	5.66	1.69	1.52
1	A	820	THR	CB-CG2	-5.66	1.33	1.52
1	B	735	ILE	CB-CG2	5.66	1.71	1.52
1	C	331	LEU	N-CA	5.66	1.53	1.46
1	C	433	LYS	CE-NZ	5.66	1.66	1.49
1	C	1066	GLU	C-O	-5.66	1.17	1.23
1	C	613	ARG	N-CA	5.65	1.52	1.45
1	A	1017	GLN	C-O	-5.65	1.16	1.23
1	B	347	SER	CA-C	5.65	1.60	1.52
1	A	278	ILE	CA-CB	-5.65	1.47	1.54
1	A	343	LYS	CE-NZ	5.65	1.66	1.49
1	C	272	ASN	CB-CG	5.65	1.66	1.52
1	D	831	ASP	CA-C	5.65	1.60	1.52
1	B	1156	TYR	C-O	5.65	1.30	1.23
1	D	34	LEU	CA-C	-5.65	1.45	1.52
1	A	206	PRO	CA-C	-5.64	1.47	1.52
1	B	1284	ALA	CA-CB	-5.64	1.43	1.53
1	C	1085	ASP	CG-OD2	5.64	1.36	1.25
1	D	497	PRO	C-O	-5.64	1.18	1.24
1	D	1332	ARG	CA-CB	5.64	1.64	1.53
1	A	216	LEU	CA-C	-5.64	1.45	1.53
1	B	1225	PRO	C-O	5.64	1.31	1.24
1	C	31	ARG	C-O	-5.64	1.17	1.24
1	C	762	GLU	CD-OE1	5.64	1.36	1.25
1	A	95	LYS	CD-CE	5.64	1.69	1.52
1	A	827	MET	SD-CE	5.63	1.93	1.79
1	B	570	GLU	CG-CD	5.63	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	601	GLU	CG-CD	5.63	1.66	1.52
1	C	211	ILE	CB-CG2	5.63	1.71	1.52
1	D	138	GLU	CG-CD	5.63	1.66	1.52
1	C	792	VAL	CA-CB	-5.62	1.47	1.54
1	B	546	ALA	N-CA	5.62	1.53	1.46
1	B	777	VAL	CA-C	5.62	1.59	1.52
1	D	529	GLN	N-CA	5.62	1.53	1.46
1	D	1108	LYS	CD-CE	5.62	1.69	1.52
1	A	442	PHE	CA-C	5.62	1.59	1.52
1	A	1018	ALA	C-O	-5.62	1.18	1.24
1	D	970	GLU	CD-OE2	5.62	1.36	1.25
1	A	560	LEU	CA-C	5.61	1.59	1.52
1	C	304	PRO	C-O	5.61	1.29	1.23
1	C	744	TYR	N-CA	5.61	1.53	1.45
1	A	1312	ASP	CB-CG	5.61	1.66	1.52
1	A	530	GLU	N-CA	5.61	1.53	1.46
1	C	452	LEU	C-O	5.61	1.30	1.23
1	D	535	LYS	CA-CB	5.61	1.62	1.53
1	B	70	ALA	CA-CB	-5.60	1.44	1.53
1	B	833	ASP	CA-CB	5.60	1.62	1.53
1	D	385	MET	N-CA	5.60	1.52	1.46
1	D	282	ALA	N-CA	5.60	1.53	1.46
1	A	120	ILE	CA-CB	-5.59	1.47	1.54
1	B	1225	PRO	N-CA	5.59	1.54	1.47
1	D	762	GLU	CG-CD	5.59	1.66	1.52
1	A	1209	LEU	CA-C	5.59	1.59	1.52
1	C	669	GLY	N-CA	5.59	1.52	1.45
1	A	604	LEU	N-CA	5.59	1.52	1.45
1	B	297	ILE	CA-C	5.59	1.59	1.52
1	A	649	ILE	CB-CG2	5.58	1.71	1.52
1	B	1263	PRO	C-N	5.58	1.40	1.34
1	A	453	ALA	N-CA	5.58	1.52	1.46
1	D	28	ALA	CA-C	-5.58	1.45	1.52
1	D	318	LYS	CD-CE	5.58	1.69	1.52
1	C	414	GLU	CA-CB	5.58	1.59	1.53
1	B	1020	ALA	N-CA	5.58	1.52	1.45
1	B	1162	GLU	CD-OE2	5.58	1.35	1.25
1	A	66	VAL	N-CA	5.58	1.52	1.46
1	C	1247	ASP	N-CA	5.58	1.53	1.46
1	D	1024	VAL	CA-C	5.58	1.59	1.52
1	B	871	THR	CA-C	5.57	1.59	1.52
1	A	1259	ALA	CA-C	5.57	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	13	ARG	NE-CZ	5.57	1.39	1.33
1	B	61	LEU	CG-CD2	5.57	1.71	1.52
1	D	679	THR	N-CA	-5.57	1.39	1.46
1	B	533	GLU	CA-CB	5.57	1.60	1.53
1	A	335	ARG	CG-CD	5.56	1.69	1.52
1	B	842	PRO	N-CA	-5.56	1.41	1.46
1	B	1135	ARG	NE-CZ	5.56	1.39	1.33
1	C	30	LEU	CA-C	-5.56	1.45	1.52
1	D	743	PHE	CA-C	5.56	1.60	1.53
1	C	1246	ARG	CD-NE	5.56	1.54	1.46
1	A	486	VAL	CA-CB	-5.56	1.48	1.54
1	D	762	GLU	CD-OE1	5.56	1.35	1.25
1	B	602	ASN	CA-C	5.56	1.60	1.53
1	B	637	SER	N-CA	5.56	1.53	1.46
1	D	652	ASP	CG-OD2	5.56	1.35	1.25
1	D	1137	PRO	CA-C	5.56	1.58	1.52
1	A	1011	THR	N-CA	5.55	1.53	1.46
1	B	1010	PHE	C-O	5.55	1.30	1.23
1	D	347	SER	CA-C	-5.55	1.46	1.52
1	D	617	LYS	CD-CE	5.55	1.69	1.52
1	C	40	LYS	CE-NZ	5.55	1.66	1.49
1	C	1135	ARG	NE-CZ	5.55	1.39	1.33
1	A	880	GLU	CG-CD	5.55	1.66	1.52
1	A	956	PHE	CA-C	5.55	1.59	1.52
1	A	1091	VAL	CA-CB	-5.55	1.48	1.54
1	D	1003	PRO	CA-C	5.55	1.60	1.52
1	D	380	ARG	CZ-NH2	5.55	1.40	1.33
1	C	1291	VAL	CA-C	5.55	1.59	1.52
1	A	1129	SER	CA-C	-5.54	1.45	1.52
1	B	194	SER	CA-C	5.54	1.61	1.53
1	C	378	GLY	C-O	-5.54	1.16	1.24
1	C	1144	GLU	CG-CD	5.54	1.66	1.52
1	B	459	MET	N-CA	5.54	1.53	1.46
1	D	1199	ALA	CA-CB	-5.54	1.44	1.53
1	C	13	ARG	CZ-NH2	5.54	1.40	1.33
1	C	254	ASP	CA-C	5.54	1.60	1.52
1	D	627	LYS	CA-C	5.54	1.60	1.52
1	B	660	LYS	CD-CE	5.54	1.69	1.52
1	B	254	ASP	CB-CG	5.54	1.65	1.52
1	A	628	LYS	CG-CD	5.53	1.69	1.52
1	B	2	THR	N-CA	5.53	1.56	1.46
1	B	509	CYS	CA-C	5.53	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	573	MET	CA-CB	-5.53	1.45	1.53
1	C	680	GLN	N-CA	5.53	1.52	1.46
1	D	532	LEU	N-CA	5.53	1.53	1.46
1	A	198	PRO	N-CA	-5.53	1.40	1.47
1	A	450	GLN	N-CA	5.53	1.52	1.46
1	B	254	ASP	CA-C	5.53	1.60	1.52
1	C	653	GLU	N-CA	5.53	1.52	1.45
1	C	752	ALA	CA-C	-5.53	1.46	1.52
1	C	913	ARG	C-O	5.53	1.30	1.24
1	D	54	MET	CA-C	5.53	1.59	1.52
1	A	711	PRO	CA-C	5.52	1.58	1.52
1	B	16	VAL	CA-C	-5.52	1.45	1.52
1	C	284	ILE	CA-CB	-5.52	1.47	1.54
1	A	1268	ALA	N-CA	5.52	1.53	1.46
1	A	1271	ILE	CA-CB	5.52	1.62	1.54
1	C	103	GLU	C-O	-5.52	1.17	1.24
1	C	994	TRP	CA-C	5.52	1.59	1.52
1	A	32	ARG	CZ-NH2	5.52	1.40	1.33
1	A	1229	LYS	CE-NZ	5.52	1.66	1.49
1	A	1301	ALA	CA-C	5.52	1.59	1.53
1	C	386	ASP	N-CA	5.52	1.52	1.46
1	C	868	VAL	C-O	5.52	1.30	1.24
1	C	628	LYS	CG-CD	5.52	1.69	1.52
1	B	375	VAL	N-CA	5.51	1.52	1.46
1	A	308	VAL	CA-CB	-5.51	1.48	1.54
1	B	765	VAL	C-O	-5.51	1.18	1.24
1	D	376	SER	N-CA	5.51	1.52	1.45
1	C	358	ILE	CA-CB	5.51	1.60	1.54
1	D	481	GLU	C-O	5.51	1.31	1.24
1	D	825	ARG	CA-C	-5.51	1.45	1.52
1	B	401	GLU	CD-OE2	5.50	1.35	1.25
1	A	336	TRP	CE2-CZ2	5.50	1.51	1.39
1	A	984	GLU	CG-CD	5.50	1.65	1.52
1	B	837	THR	CA-CB	5.50	1.62	1.53
1	B	1238	ILE	C-O	-5.50	1.18	1.24
1	C	462	ARG	CA-CB	-5.50	1.46	1.53
1	A	36	LEU	C-O	5.50	1.30	1.23
1	A	679	THR	N-CA	-5.50	1.39	1.46
1	C	116	CYS	CA-C	5.50	1.62	1.52
1	C	1090	ALA	CA-CB	-5.50	1.44	1.53
1	D	39	THR	CA-CB	-5.50	1.44	1.53
1	C	59	ASP	CA-C	-5.50	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	709	TYR	N-CA	5.49	1.53	1.46
1	B	789	VAL	CA-C	-5.49	1.45	1.52
1	A	1171	ASP	CB-CG	5.49	1.65	1.52
1	B	438	MET	N-CA	5.49	1.52	1.46
1	A	107	LYS	CD-CE	5.49	1.69	1.52
1	C	43	CYS	CA-C	-5.49	1.46	1.52
1	B	91	ILE	C-O	-5.49	1.18	1.24
1	B	984	GLU	CD-OE2	5.49	1.35	1.25
1	D	388	THR	CA-CB	5.49	1.62	1.53
1	A	1017	GLN	CA-C	-5.49	1.45	1.52
1	D	136	MET	CA-C	-5.49	1.45	1.52
1	B	985	VAL	CA-CB	-5.48	1.47	1.54
1	C	687	LYS	CD-CE	5.48	1.69	1.52
1	A	199	GLU	CA-C	-5.48	1.45	1.52
1	B	1136	THR	CA-C	5.48	1.59	1.52
1	C	1231	PRO	CA-C	5.48	1.59	1.52
1	A	736	TYR	N-CA	5.48	1.52	1.46
1	C	16	VAL	CB-CG2	-5.48	1.34	1.52
1	D	499	ASP	N-CA	5.48	1.53	1.46
1	D	873	ASP	CG-OD2	5.48	1.35	1.25
1	D	866	SER	N-CA	-5.48	1.39	1.47
1	D	414	GLU	N-CA	5.48	1.53	1.46
1	D	657	ALA	C-O	5.48	1.30	1.23
1	D	1232	ALA	CA-C	-5.48	1.45	1.53
1	D	202	THR	CB-CG2	5.47	1.70	1.52
1	B	129	ARG	CA-C	5.47	1.60	1.52
1	C	230	GLU	CA-C	-5.47	1.45	1.52
1	D	649	ILE	CG1-CD1	-5.47	1.30	1.51
1	A	608	LEU	CA-C	-5.47	1.46	1.52
1	A	619	LYS	C-O	5.47	1.30	1.24
1	B	1163	VAL	N-CA	5.47	1.52	1.46
1	D	915	PHE	CG-CD2	5.47	1.50	1.38
1	A	1125	THR	CA-CB	5.47	1.62	1.53
1	B	604	LEU	N-CA	5.47	1.52	1.45
1	C	427	ARG	NE-CZ	5.47	1.39	1.33
1	D	765	VAL	CA-CB	5.46	1.61	1.54
1	A	529	GLN	CA-C	5.46	1.60	1.52
1	C	93	SER	C-O	-5.46	1.17	1.23
1	C	823	PRO	N-CA	-5.46	1.40	1.47
1	D	937	MET	CA-C	-5.46	1.46	1.52
1	B	268	MET	SD-CE	5.46	1.93	1.79
1	C	481	GLU	N-CA	5.46	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	232	GLU	C-O	-5.46	1.17	1.23
1	A	1158	VAL	CA-C	5.46	1.59	1.52
1	C	1057	ILE	CA-CB	-5.46	1.47	1.54
1	A	959	LYS	N-CA	5.46	1.52	1.46
1	B	711	PRO	N-CA	5.46	1.54	1.47
1	B	764	PHE	C-O	5.46	1.30	1.24
1	C	791	ARG	CA-C	-5.46	1.45	1.52
1	B	813	VAL	CA-CB	-5.45	1.48	1.54
1	B	1192	ASP	CB-CG	5.45	1.65	1.52
1	D	1242	VAL	CA-CB	-5.45	1.47	1.54
1	D	1271	ILE	C-O	5.45	1.30	1.24
1	C	913	ARG	N-CA	5.45	1.53	1.46
1	C	1234	GLY	C-O	5.45	1.31	1.23
1	D	664	VAL	N-CA	5.45	1.53	1.46
1	A	1020	ALA	CA-C	5.45	1.59	1.52
1	B	25	THR	CB-CG2	5.45	1.70	1.52
1	C	917	GLY	C-O	5.45	1.31	1.24
1	A	464	ILE	N-CA	5.44	1.54	1.45
1	B	141	ASN	C-O	5.44	1.30	1.24
1	A	24	THR	C-O	-5.44	1.17	1.24
1	A	831	ASP	CG-OD2	5.44	1.35	1.25
1	D	873	ASP	CA-C	5.44	1.60	1.52
1	B	963	PHE	C-O	5.44	1.30	1.24
1	D	1244	LEU	CA-C	-5.44	1.45	1.52
1	A	7	VAL	CB-CG2	-5.44	1.34	1.52
1	C	925	GLU	C-O	-5.44	1.17	1.24
1	A	275	PHE	CA-C	-5.43	1.45	1.52
1	A	453	ALA	C-O	5.43	1.30	1.23
1	D	1274	ALA	N-CA	-5.43	1.39	1.46
1	A	600	TYR	CA-CB	-5.43	1.45	1.53
1	A	941	GLU	N-CA	5.43	1.52	1.46
1	C	15	VAL	C-O	5.43	1.30	1.24
1	C	119	GLY	C-O	5.43	1.31	1.23
1	A	1123	MET	SD-CE	5.43	1.93	1.79
1	B	13	ARG	CZ-NH1	5.43	1.40	1.32
1	B	512	THR	CA-C	-5.43	1.46	1.52
1	B	563	GLU	N-CA	5.43	1.52	1.45
1	B	650	CYS	N-CA	5.43	1.52	1.46
1	C	565	PRO	CA-C	5.43	1.60	1.52
1	C	1225	PRO	C-O	5.43	1.31	1.24
1	B	527	LEU	CA-C	5.43	1.60	1.52
1	B	687	LYS	CG-CD	5.43	1.68	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	674	ASP	N-CA	-5.43	1.38	1.46
1	D	807	THR	N-CA	-5.43	1.39	1.46
1	B	300	GLY	N-CA	5.43	1.51	1.45
1	B	762	GLU	C-O	-5.42	1.17	1.24
1	C	61	LEU	CG-CD1	5.42	1.70	1.52
1	A	373	THR	CA-C	-5.42	1.46	1.52
1	B	50	ALA	CA-CB	-5.42	1.44	1.53
1	B	328	ARG	CG-CD	5.42	1.68	1.52
1	C	530	GLU	C-O	5.42	1.30	1.24
1	A	215	GLU	CA-C	5.42	1.59	1.52
1	C	447	THR	CA-C	5.42	1.59	1.52
1	C	825	ARG	CZ-NH1	5.42	1.40	1.32
1	D	340	LYS	N-CA	5.42	1.53	1.46
1	B	317	ALA	CA-CB	5.42	1.62	1.53
1	C	440	VAL	C-O	5.41	1.29	1.24
1	C	739	GLY	N-CA	5.41	1.51	1.45
1	C	634	CYS	CA-C	5.41	1.60	1.52
1	A	1206	LEU	N-CA	5.41	1.53	1.46
1	B	28	ALA	N-CA	5.41	1.53	1.46
1	C	542	THR	CA-CB	5.41	1.62	1.53
1	A	499	ASP	CA-C	5.41	1.60	1.52
1	A	1183	VAL	N-CA	5.41	1.53	1.46
1	A	410	PRO	C-O	5.40	1.29	1.23
1	A	707	SER	CA-C	5.40	1.60	1.52
1	C	230	GLU	CG-CD	5.40	1.65	1.52
1	B	534	ASP	N-CA	5.40	1.53	1.46
1	C	1146	ASN	C-O	-5.40	1.17	1.24
1	D	905	ASN	CB-CG	5.40	1.65	1.52
1	D	1234	GLY	CA-C	5.40	1.59	1.51
1	A	832	GLU	C-O	5.40	1.30	1.24
1	A	1123	MET	CA-C	5.40	1.60	1.52
1	B	981	ARG	CA-C	5.40	1.60	1.52
1	D	216	LEU	N-CA	5.40	1.52	1.45
1	D	679	THR	CB-CG2	5.40	1.70	1.52
1	D	278	ILE	C-O	5.39	1.29	1.24
1	A	735	ILE	N-CA	5.39	1.52	1.46
1	D	32	ARG	CG-CD	5.39	1.68	1.52
1	B	767	THR	C-O	5.39	1.30	1.23
1	C	1330	SER	CA-C	5.39	1.59	1.52
1	D	41	LEU	CA-C	5.39	1.59	1.52
1	D	41	LEU	N-CA	5.39	1.52	1.46
1	B	857	VAL	CA-CB	5.39	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1008	ILE	CA-C	5.38	1.59	1.52
1	C	97	ARG	CD-NE	5.38	1.53	1.46
1	B	460	ALA	CA-CB	-5.38	1.44	1.53
1	A	11	ASN	C-O	-5.38	1.16	1.23
1	B	829	ASP	C-O	-5.38	1.16	1.23
1	B	920	GLY	C-O	-5.38	1.16	1.23
1	C	1276	LYS	CA-C	5.38	1.60	1.52
1	D	209	GLU	N-CA	5.38	1.53	1.45
1	D	678	HIS	CA-CB	-5.38	1.44	1.53
1	C	97	ARG	CG-CD	5.38	1.68	1.52
1	B	1155	SER	CA-C	5.38	1.59	1.52
1	D	809	VAL	CA-CB	-5.38	1.48	1.54
1	A	58	TYR	N-CA	5.37	1.52	1.46
1	A	891	LYS	CG-CD	5.37	1.68	1.52
1	B	97	ARG	CB-CG	5.37	1.68	1.52
1	B	443	LYS	CA-C	5.37	1.59	1.52
1	C	705	ASN	CA-C	-5.37	1.45	1.52
1	D	206	PRO	N-CA	5.37	1.54	1.47
1	D	509	CYS	N-CA	-5.37	1.39	1.46
1	A	21	ASP	CG-OD1	5.37	1.35	1.25
1	B	61	LEU	CA-C	5.37	1.59	1.52
1	A	991	GLU	CA-C	5.37	1.60	1.52
1	A	1054	ALA	CA-CB	-5.37	1.43	1.53
1	B	453	ALA	CA-CB	5.37	1.62	1.53
1	B	608	LEU	N-CA	5.37	1.52	1.45
1	A	814	ALA	CA-C	5.37	1.59	1.52
1	A	821	GLY	N-CA	5.37	1.52	1.45
1	B	273	MET	SD-CE	5.37	1.93	1.79
1	A	451	GLU	CG-CD	5.37	1.65	1.52
1	B	770	THR	N-CA	-5.37	1.40	1.46
1	C	10	VAL	CA-C	-5.37	1.45	1.52
1	D	433	LYS	CE-NZ	5.37	1.65	1.49
1	D	778	ALA	CA-C	5.37	1.59	1.52
1	D	1276	LYS	CA-C	5.37	1.59	1.52
1	D	265	GLY	C-O	5.36	1.31	1.23
1	D	766	SER	N-CA	-5.36	1.39	1.46
1	B	1329	TRP	N-CA	5.36	1.52	1.46
1	A	1241	ARG	CA-C	5.36	1.59	1.52
1	C	891	LYS	CG-CD	5.36	1.68	1.52
1	B	32	ARG	CZ-NH2	5.36	1.40	1.33
1	D	746	GLU	CA-C	-5.36	1.45	1.52
1	A	986	ASP	N-CA	5.36	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1116	ASP	CA-C	-5.36	1.46	1.52
1	B	1290	ASN	CB-CG	5.36	1.65	1.52
1	D	1024	VAL	N-CA	5.35	1.53	1.46
1	C	314	ASP	CA-C	5.35	1.59	1.52
1	D	1240	PHE	CB-CG	5.35	1.62	1.50
1	D	430	ASP	CB-CG	5.35	1.65	1.52
1	A	778	ALA	CA-C	5.35	1.59	1.52
1	B	646	ILE	N-CA	-5.35	1.39	1.46
1	C	427	ARG	CG-CD	5.35	1.68	1.52
1	D	239	ALA	C-O	-5.35	1.17	1.23
1	D	401	GLU	CB-CG	5.35	1.68	1.52
1	D	1084	ALA	CA-CB	-5.35	1.44	1.53
1	A	764	PHE	C-O	5.35	1.30	1.24
1	A	1038	GLU	CD-OE1	5.35	1.35	1.25
1	C	597	ILE	N-CA	5.35	1.53	1.46
1	B	358	ILE	CA-C	-5.34	1.46	1.52
1	D	68	PHE	C-O	5.34	1.30	1.23
1	A	1165	ILE	CA-CB	-5.34	1.45	1.55
1	C	376	SER	CA-C	-5.34	1.46	1.52
1	B	789	VAL	CB-CG2	-5.34	1.34	1.52
1	A	225	LYS	CG-CD	5.34	1.68	1.52
1	A	1276	LYS	N-CA	5.34	1.52	1.46
1	D	791	ARG	CA-C	5.34	1.59	1.52
1	C	149	ARG	CA-C	5.33	1.60	1.52
1	D	742	HIS	CA-C	-5.33	1.46	1.52
1	D	146	ASN	CA-C	5.33	1.58	1.52
1	A	95	LYS	CE-NZ	5.33	1.65	1.49
1	C	1157	GLY	N-CA	5.33	1.51	1.45
1	B	625	GLU	CG-CD	5.33	1.65	1.52
1	D	1122	TYR	N-CA	-5.33	1.40	1.46
1	C	566	LYS	CA-C	5.33	1.59	1.52
1	D	570	GLU	CG-CD	5.33	1.65	1.52
1	A	1182	ASP	CA-C	5.33	1.59	1.52
1	A	403	ILE	C-O	-5.33	1.18	1.24
1	A	625	GLU	CG-CD	5.33	1.65	1.52
1	B	1048	VAL	N-CA	5.33	1.52	1.46
1	B	1239	GLU	CD-OE2	5.33	1.35	1.25
1	D	33	LYS	CA-C	-5.33	1.45	1.52
1	A	64	LYS	CA-C	5.32	1.59	1.52
1	B	1161	SER	N-CA	5.32	1.52	1.46
1	D	104	ARG	CZ-NH1	5.32	1.40	1.32
1	D	948	TYR	CA-C	5.32	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	639	ASP	CG-OD2	5.32	1.35	1.25
1	B	1261	GLY	N-CA	5.32	1.53	1.45
1	C	1134	TYR	CA-C	5.32	1.59	1.52
1	C	1190	ALA	CA-C	-5.32	1.46	1.52
1	B	967	ARG	CA-C	5.32	1.59	1.52
1	D	1019	GLY	C-O	5.32	1.29	1.24
1	B	805	ARG	C-O	-5.31	1.17	1.24
1	A	588	SER	C-O	-5.31	1.16	1.23
1	C	662	THR	CA-CB	5.31	1.61	1.53
1	D	841	HIS	C-N	5.31	1.40	1.33
1	C	831	ASP	C-O	-5.31	1.18	1.24
1	D	1241	ARG	CA-C	5.31	1.59	1.53
1	A	748	HIS	CA-C	-5.31	1.45	1.53
1	A	1062	ILE	CA-CB	-5.31	1.48	1.54
1	B	901	LEU	N-CA	-5.30	1.38	1.46
1	C	139	ILE	CA-CB	5.30	1.61	1.54
1	C	506	ASP	N-CA	-5.30	1.39	1.46
1	D	1133	PHE	CA-C	5.30	1.59	1.52
1	D	412	SER	CA-C	5.30	1.59	1.52
1	A	628	LYS	CB-CG	5.30	1.68	1.52
1	B	1082	VAL	CA-CB	-5.30	1.48	1.54
1	C	625	GLU	CG-CD	5.30	1.65	1.52
1	C	689	THR	CA-CB	5.30	1.62	1.53
1	D	413	ARG	N-CA	5.30	1.52	1.45
1	D	875	SER	CA-C	5.30	1.60	1.52
1	D	1300	PRO	CA-C	5.30	1.59	1.52
1	C	60	ARG	CA-CB	5.30	1.62	1.53
1	A	339	GLY	N-CA	5.30	1.51	1.45
1	B	204	LEU	C-O	5.30	1.30	1.24
1	B	566	LYS	CB-CG	5.30	1.68	1.52
1	A	819	LYS	C-O	-5.29	1.18	1.24
1	B	1020	ALA	C-O	5.29	1.30	1.23
1	B	1171	ASP	CB-CG	5.29	1.65	1.52
1	C	439	ARG	N-CA	5.29	1.52	1.46
1	B	1024	VAL	N-CA	5.29	1.53	1.46
1	D	27	LEU	CA-C	-5.29	1.45	1.52
1	C	789	VAL	N-CA	5.29	1.52	1.46
1	D	571	GLU	CA-C	5.29	1.59	1.52
1	B	164	ALA	N-CA	-5.29	1.40	1.46
1	B	1193	ILE	N-CA	5.29	1.52	1.46
1	D	332	GLU	CG-CD	5.29	1.65	1.52
1	D	85	VAL	CA-CB	-5.29	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	161	ARG	C-O	5.29	1.30	1.24
1	A	1101	ARG	N-CA	-5.29	1.39	1.46
1	B	426	ARG	N-CA	5.29	1.53	1.46
1	B	1074	ASN	C-O	5.29	1.30	1.23
1	D	125	TYR	CA-CB	5.29	1.62	1.53
1	D	232	GLU	N-CA	5.29	1.52	1.46
1	D	258	VAL	CA-CB	-5.29	1.47	1.54
1	B	534	ASP	CA-C	5.28	1.59	1.52
1	C	599	ARG	CA-C	5.28	1.59	1.52
1	D	527	LEU	N-CA	5.28	1.53	1.46
1	C	165	ARG	CB-CG	5.28	1.68	1.52
1	C	1085	ASP	CG-OD1	5.28	1.35	1.25
1	B	4	ASP	N-CA	5.28	1.53	1.46
1	B	435	THR	CA-C	-5.28	1.46	1.52
1	C	735	ILE	CB-CG2	5.28	1.70	1.52
1	C	954	THR	CA-C	5.28	1.59	1.52
1	C	1082	VAL	N-CA	-5.28	1.40	1.46
1	B	801	GLY	N-CA	-5.28	1.37	1.45
1	B	937	MET	SD-CE	5.28	1.92	1.79
1	B	1069	THR	CA-C	-5.28	1.45	1.52
1	B	1268	ALA	N-CA	5.28	1.53	1.46
1	A	576	ARG	CA-C	-5.28	1.46	1.52
1	B	1144	GLU	CA-C	5.28	1.58	1.53
1	D	276	PRO	N-CA	-5.28	1.40	1.47
1	A	1083	SER	CA-C	5.28	1.59	1.52
1	C	594	CYS	CB-SG	5.28	1.98	1.81
1	D	139	ILE	CA-C	-5.27	1.45	1.52
1	B	453	ALA	C-O	5.27	1.29	1.23
1	B	760	GLU	N-CA	5.27	1.52	1.46
1	C	402	GLU	CG-CD	5.27	1.65	1.52
1	D	108	SER	C-O	5.27	1.30	1.24
1	D	526	LYS	CG-CD	5.27	1.68	1.52
1	D	794	ARG	N-CA	5.27	1.52	1.45
1	D	1254	ILE	CA-CB	5.27	1.61	1.54
1	A	918	PRO	N-CA	-5.27	1.40	1.47
1	D	931	VAL	CA-C	5.27	1.59	1.52
1	B	2	THR	CB-CG2	5.26	1.70	1.52
1	C	937	MET	CB-CG	5.26	1.68	1.52
1	D	376	SER	CA-C	5.26	1.59	1.52
1	D	636	ILE	CA-CB	5.26	1.61	1.54
1	D	854	THR	CA-C	5.26	1.59	1.52
1	D	351	ASN	C-O	5.26	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1187	LEU	CG-CD1	-5.26	1.35	1.52
1	D	657	ALA	N-CA	5.26	1.53	1.46
1	D	1021	LEU	CG-CD1	-5.26	1.35	1.52
1	C	1239	GLU	CD-OE2	5.26	1.35	1.25
1	D	149	ARG	N-CA	5.26	1.52	1.46
1	D	446	THR	C-O	5.26	1.30	1.23
1	A	360	ASP	CA-C	-5.26	1.45	1.52
1	A	1180	VAL	CA-CB	-5.26	1.47	1.54
1	B	225	LYS	CD-CE	5.26	1.68	1.52
1	B	236	TRP	CA-C	-5.26	1.46	1.52
1	C	1252	LYS	C-O	5.26	1.30	1.24
1	B	414	GLU	CG-CD	5.25	1.65	1.52
1	C	1210	GLU	C-O	5.25	1.30	1.24
1	C	1078	THR	CA-CB	-5.25	1.45	1.52
1	C	396	THR	CA-C	-5.25	1.47	1.53
1	C	396	THR	C-O	-5.25	1.18	1.24
1	C	1134	TYR	N-CA	5.25	1.52	1.46
1	D	829	ASP	N-CA	5.25	1.52	1.45
1	A	150	CYS	CB-SG	-5.24	1.64	1.81
1	B	340	LYS	CA-C	-5.24	1.45	1.52
1	B	708	PHE	CB-CG	5.24	1.62	1.50
1	B	946	ASN	N-CA	5.24	1.52	1.46
1	C	740	GLN	CA-C	5.24	1.59	1.52
1	C	885	HIS	CA-C	-5.24	1.45	1.52
1	B	439	ARG	C-O	5.24	1.29	1.23
1	B	220	LYS	C-O	5.24	1.30	1.24
1	B	783	VAL	C-O	5.24	1.30	1.24
1	D	269	LYS	CA-C	5.24	1.59	1.52
1	A	884	PHE	CA-C	5.24	1.59	1.52
1	D	207	THR	C-O	5.24	1.30	1.24
1	A	220	LYS	CA-C	5.24	1.59	1.52
1	D	150	CYS	CB-SG	-5.24	1.64	1.81
1	C	94	THR	CA-CB	5.24	1.63	1.53
1	D	112	GLN	CG-CD	5.24	1.65	1.52
1	D	461	ASN	C-O	-5.24	1.17	1.24
1	D	625	GLU	CG-CD	5.24	1.65	1.52
1	D	774	GLN	CA-C	5.24	1.59	1.52
1	D	847	TYR	CA-CB	-5.24	1.44	1.54
1	A	970	GLU	CG-CD	5.23	1.65	1.52
1	B	1067	THR	CA-C	5.23	1.58	1.52
1	D	1320	THR	CB-CG2	5.23	1.69	1.52
1	A	432	ALA	CA-C	5.23	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	506	ASP	CA-C	5.23	1.60	1.52
1	A	869	GLY	CA-C	5.23	1.58	1.52
1	B	21	ASP	CB-CG	5.23	1.65	1.52
1	D	539	LEU	CA-C	5.23	1.59	1.53
1	C	61	LEU	CG-CD2	5.23	1.69	1.52
1	A	865	PHE	N-CA	5.23	1.53	1.46
1	D	598	PRO	N-CA	-5.22	1.40	1.47
1	A	7	VAL	CB-CG1	-5.22	1.35	1.52
1	A	558	VAL	CB-CG1	5.22	1.69	1.52
1	A	1079	ALA	C-O	5.22	1.30	1.24
1	B	1312	ASP	CA-C	5.22	1.59	1.52
1	D	1251	LYS	N-CA	5.22	1.53	1.46
1	C	443	LYS	N-CA	5.22	1.53	1.46
1	A	712	GLU	CG-CD	5.22	1.65	1.52
1	C	557	ASP	CB-CG	5.22	1.65	1.52
1	D	1012	VAL	C-O	-5.22	1.17	1.24
1	D	646	ILE	CG1-CD1	5.21	1.72	1.51
1	C	1166	ASP	CA-C	-5.21	1.46	1.52
1	A	205	ASP	C-O	-5.21	1.20	1.25
1	A	456	TYR	C-O	5.21	1.29	1.24
1	B	459	MET	CA-C	5.21	1.59	1.52
1	A	347	SER	C-O	-5.21	1.17	1.23
1	B	7	VAL	CA-CB	-5.21	1.47	1.54
1	D	340	LYS	CE-NZ	5.21	1.65	1.49
1	A	452	LEU	C-O	5.21	1.29	1.23
1	C	595	ASP	N-CA	5.21	1.52	1.46
1	C	684	GLN	N-CA	-5.21	1.39	1.46
1	D	342	VAL	C-O	-5.21	1.18	1.24
1	A	1011	THR	C-O	5.21	1.30	1.24
1	A	1106	LYS	CG-CD	5.20	1.68	1.52
1	C	165	ARG	NE-CZ	5.20	1.38	1.33
1	C	404	LEU	N-CA	5.20	1.52	1.46
1	C	1018	ALA	CA-CB	5.20	1.61	1.54
1	D	863	ASP	N-CA	5.20	1.52	1.46
1	C	870	ASN	N-CA	5.20	1.51	1.46
1	A	956	PHE	CA-CB	5.20	1.61	1.53
1	C	356	SER	N-CA	5.20	1.53	1.45
1	A	719	ASP	CB-CG	5.20	1.65	1.52
1	B	68	PHE	N-CA	5.20	1.52	1.45
1	B	913	ARG	CA-C	5.20	1.59	1.52
1	C	225	LYS	N-CA	-5.20	1.39	1.45
1	D	1109	ASN	CA-CB	5.20	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	984	GLU	CD-OE2	5.20	1.35	1.25
1	B	1066	GLU	N-CA	5.20	1.52	1.45
1	B	1304	GLU	CA-C	-5.20	1.46	1.52
1	A	21	ASP	CB-CG	5.19	1.65	1.52
1	A	290	VAL	N-CA	5.19	1.52	1.46
1	D	119	GLY	C-O	5.19	1.30	1.23
1	B	57	LYS	CA-C	-5.19	1.46	1.52
1	C	1201	VAL	CA-CB	-5.19	1.47	1.54
1	D	66	VAL	CA-CB	-5.19	1.46	1.55
1	D	310	LYS	CE-NZ	5.19	1.65	1.49
1	B	563	GLU	C-O	5.19	1.30	1.23
1	A	1063	TYR	N-CA	5.19	1.52	1.46
1	B	1316	THR	C-O	5.19	1.30	1.24
1	C	1255	TYR	CA-CB	5.19	1.62	1.53
1	C	750	THR	C-O	5.18	1.29	1.23
1	B	300	GLY	C-O	-5.18	1.18	1.23
1	B	1150	PRO	CA-C	5.18	1.59	1.52
1	C	1242	VAL	CA-CB	-5.18	1.48	1.54
1	A	64	LYS	C-O	-5.18	1.17	1.23
1	C	675	THR	CA-C	-5.18	1.47	1.52
1	D	1049	GLN	N-CA	5.18	1.52	1.46
1	B	875	SER	C-O	5.18	1.30	1.24
1	B	1116	ASP	CG-OD2	5.18	1.35	1.25
1	C	822	ARG	C-O	-5.18	1.18	1.24
1	B	1111	SER	CA-CB	-5.17	1.46	1.53
1	D	140	GLU	CG-CD	5.17	1.65	1.52
1	D	584	ASP	C-O	5.17	1.30	1.24
1	A	161	ARG	CZ-NH1	5.17	1.40	1.32
1	A	655	VAL	C-O	-5.17	1.18	1.24
1	B	104	ARG	CA-C	-5.17	1.46	1.52
1	D	316	VAL	CA-C	5.17	1.59	1.52
1	D	443	LYS	CG-CD	5.17	1.68	1.52
1	C	29	TYR	CE1-CZ	-5.17	1.25	1.38
1	C	309	GLU	CD-OE2	5.17	1.35	1.25
1	C	605	SER	CA-C	-5.17	1.46	1.52
1	D	13	ARG	NE-CZ	5.17	1.38	1.33
1	C	265	GLY	N-CA	5.16	1.52	1.45
1	C	461	ASN	CB-CG	-5.16	1.39	1.52
1	D	710	GLY	N-CA	5.16	1.51	1.44
1	A	566	LYS	CA-C	5.16	1.59	1.52
1	A	884	PHE	C-O	5.16	1.30	1.24
1	B	1189	PRO	C-O	-5.16	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1298	ASP	CA-C	5.16	1.58	1.52
1	D	234	VAL	CA-C	5.16	1.59	1.52
1	A	74	LEU	N-CA	-5.16	1.40	1.46
1	A	818	TYR	N-CA	5.16	1.52	1.46
1	A	1064	ILE	C-O	5.16	1.29	1.24
1	D	1084	ALA	CA-C	-5.16	1.46	1.52
1	B	1072	VAL	CB-CG1	5.16	1.69	1.52
1	D	515	PHE	CA-C	5.16	1.60	1.52
1	B	1054	ALA	C-O	-5.16	1.18	1.24
1	C	348	VAL	N-CA	5.16	1.52	1.46
1	C	601	GLU	CD-OE2	5.16	1.35	1.25
1	C	1021	LEU	C-O	5.16	1.29	1.23
1	D	860	LEU	N-CA	5.15	1.52	1.46
1	C	139	ILE	CA-C	-5.15	1.45	1.52
1	A	604	LEU	CG-CD2	-5.15	1.35	1.52
1	B	885	HIS	CA-C	-5.15	1.45	1.52
1	B	1032	LEU	CA-C	-5.15	1.46	1.52
1	D	646	ILE	CA-C	-5.15	1.46	1.52
1	B	1011	THR	CA-C	5.15	1.59	1.52
1	B	1093	ALA	C-O	5.15	1.29	1.24
1	C	1154	PHE	CA-C	5.15	1.58	1.52
1	D	54	MET	CG-SD	5.15	1.93	1.80
1	D	944	ARG	NE-CZ	5.15	1.38	1.33
1	A	1230	ILE	CA-C	5.14	1.58	1.52
1	C	661	VAL	CA-CB	5.14	1.61	1.54
1	D	526	LYS	CA-C	5.14	1.59	1.52
1	B	22	PRO	CA-CB	-5.14	1.46	1.53
1	B	672	VAL	N-CA	5.14	1.53	1.46
1	B	719	ASP	CB-CG	5.14	1.65	1.52
1	D	1084	ALA	C-O	-5.14	1.17	1.24
1	C	425	SER	CA-C	5.14	1.59	1.52
1	D	277	MET	CA-C	-5.14	1.46	1.52
1	D	813	VAL	CA-CB	-5.14	1.48	1.54
1	C	891	LYS	CD-CE	5.14	1.67	1.52
1	D	1033	THR	CA-C	-5.14	1.46	1.52
1	B	807	THR	N-CA	-5.14	1.39	1.46
1	B	1211	GLU	CA-C	5.14	1.58	1.52
1	D	198	PRO	N-CA	-5.14	1.41	1.47
1	D	299	PHE	N-CA	5.14	1.52	1.46
1	B	452	LEU	N-CA	5.13	1.52	1.46
1	B	865	PHE	CD1-CE1	5.13	1.54	1.38
1	D	295	ASP	C-O	5.13	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	415	GLY	CA-C	5.13	1.58	1.51
1	B	546	ALA	CA-C	5.13	1.59	1.52
1	B	825	ARG	CZ-NH1	5.13	1.40	1.32
1	D	540	ASP	CA-C	5.13	1.59	1.52
1	D	1291	VAL	CB-CG2	5.13	1.69	1.52
1	C	1187	LEU	CG-CD2	-5.13	1.35	1.52
1	D	953	LEU	CA-C	5.13	1.58	1.52
1	B	776	PHE	CA-C	-5.13	1.45	1.52
1	C	1036	GLY	N-CA	5.13	1.50	1.44
1	A	1133	PHE	CA-C	5.13	1.59	1.52
1	C	198	PRO	N-CA	-5.13	1.41	1.47
1	D	432	ALA	CA-C	-5.13	1.46	1.53
1	A	1248	CYS	N-CA	5.12	1.53	1.46
1	C	212	PHE	CA-C	-5.12	1.46	1.52
1	D	577	PRO	CA-C	5.12	1.58	1.53
1	C	612	THR	CA-C	5.12	1.59	1.52
1	D	1108	LYS	CE-NZ	5.12	1.64	1.49
1	B	542	THR	N-CA	5.12	1.52	1.46
1	C	75	ALA	CA-CB	-5.12	1.44	1.53
1	C	229	PHE	CA-CB	-5.12	1.44	1.53
1	D	708	PHE	N-CA	-5.12	1.39	1.46
1	A	238	GLN	N-CA	-5.12	1.40	1.46
1	B	301	ALA	N-CA	5.12	1.52	1.46
1	C	808	VAL	N-CA	5.12	1.52	1.46
1	D	874	LEU	N-CA	5.12	1.52	1.46
1	C	581	LEU	CA-C	5.12	1.59	1.52
1	C	1260	VAL	N-CA	5.11	1.52	1.46
1	B	111	SER	CA-C	-5.11	1.46	1.52
1	B	580	HIS	CA-C	-5.11	1.46	1.52
1	B	1118	VAL	CA-CB	-5.11	1.47	1.54
1	A	277	MET	SD-CE	5.11	1.92	1.79
1	A	605	SER	N-CA	5.11	1.51	1.45
1	A	377	ARG	N-CA	5.11	1.52	1.46
1	B	574	VAL	CA-C	-5.11	1.47	1.52
1	D	381	ARG	N-CA	5.11	1.52	1.46
1	B	63	ASN	N-CA	5.11	1.52	1.46
1	A	679	THR	CA-CB	-5.10	1.45	1.53
1	A	1284	ALA	CA-C	5.10	1.59	1.52
1	B	313	VAL	N-CA	5.10	1.52	1.46
1	C	1289	ASN	CA-CB	5.10	1.62	1.53
1	A	776	PHE	CB-CG	-5.10	1.39	1.50
1	B	55	LEU	C-O	5.10	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	752	ALA	CA-CB	-5.10	1.45	1.53
1	B	289	SER	C-O	5.10	1.30	1.23
1	B	310	LYS	CG-CD	5.10	1.67	1.52
1	C	772	LYS	C-O	5.09	1.30	1.24
1	A	16	VAL	CA-C	-5.09	1.46	1.52
1	D	479	LYS	CB-CG	5.09	1.67	1.52
1	A	674	ASP	CA-CB	5.09	1.61	1.53
1	B	447	THR	CA-C	5.09	1.59	1.52
1	A	384	GLN	C-O	-5.09	1.17	1.24
1	A	924	ALA	C-O	5.09	1.30	1.23
1	A	1183	VAL	CA-C	5.09	1.59	1.52
1	C	1128	LEU	C-O	5.09	1.30	1.24
1	B	856	THR	CA-CB	-5.09	1.45	1.53
1	D	332	GLU	CB-CG	5.09	1.67	1.52
1	A	231	GLY	C-O	-5.09	1.17	1.23
1	C	1207	PHE	N-CA	-5.09	1.39	1.45
1	D	832	GLU	CG-CD	5.09	1.64	1.52
1	B	910	THR	CA-CB	-5.08	1.47	1.53
1	B	1315	THR	CA-CB	5.08	1.61	1.53
1	C	477	LEU	CA-C	5.08	1.58	1.52
1	B	1051	ALA	CA-CB	-5.08	1.44	1.53
1	B	150	CYS	CA-C	5.08	1.59	1.52
1	D	811	THR	N-CA	-5.08	1.40	1.46
1	B	657	ALA	C-O	5.08	1.29	1.23
1	D	273	MET	SD-CE	5.08	1.92	1.79
1	A	529	GLN	CB-CG	5.08	1.67	1.52
1	A	1083	SER	CB-OG	5.08	1.52	1.42
1	C	1201	VAL	CA-C	-5.08	1.45	1.52
1	C	849	VAL	C-N	5.08	1.38	1.33
1	A	1044	HIS	N-CA	-5.08	1.39	1.46
1	C	255	ALA	CA-CB	-5.08	1.45	1.53
1	C	976	SER	C-O	-5.08	1.17	1.24
1	C	1079	ALA	C-O	5.08	1.30	1.24
1	A	944	ARG	NE-CZ	5.07	1.38	1.33
1	C	1162	GLU	CG-CD	5.07	1.64	1.52
1	D	557	ASP	N-CA	5.07	1.55	1.46
1	D	1295	PHE	N-CA	5.07	1.52	1.46
1	D	572	ASP	C-O	5.07	1.29	1.24
1	D	940	GLU	CG-CD	5.07	1.64	1.52
1	C	426	ARG	CA-C	5.07	1.59	1.52
1	B	318	LYS	CA-CB	5.07	1.59	1.53
1	D	971	GLU	CD-OE2	5.07	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1254	ILE	C-O	5.07	1.30	1.24
1	B	499	ASP	CB-CG	5.07	1.64	1.52
1	C	1055	LEU	CA-CB	-5.07	1.45	1.53
1	D	456	TYR	N-CA	5.07	1.52	1.46
1	A	840	ARG	C-O	5.07	1.30	1.23
1	C	779	LYS	CD-CE	5.07	1.67	1.52
1	D	529	GLN	CA-C	5.07	1.59	1.52
1	C	413	ARG	CZ-NH1	5.06	1.39	1.32
1	D	106	ALA	CA-CB	5.06	1.61	1.53
1	B	284	ILE	CA-C	5.06	1.58	1.52
1	D	1083	SER	N-CA	5.06	1.52	1.46
1	D	407	ILE	CB-CG2	-5.06	1.35	1.52
1	A	1223	ARG	CZ-NH1	5.06	1.39	1.32
1	C	318	LYS	CB-CG	5.06	1.67	1.52
1	C	666	HIS	CA-CB	5.06	1.62	1.53
1	A	1181	MET	C-O	-5.06	1.18	1.24
1	B	593	TYR	CA-C	-5.06	1.46	1.52
1	C	825	ARG	C-O	5.06	1.30	1.23
1	B	16	VAL	C-N	-5.06	1.26	1.33
1	B	1124	ASP	CA-C	5.05	1.59	1.52
1	D	444	PRO	N-CA	5.05	1.53	1.47
1	D	937	MET	C-O	5.05	1.30	1.24
1	D	1131	THR	CA-CB	-5.05	1.45	1.53
1	A	934	THR	N-CA	5.05	1.52	1.46
1	C	601	GLU	CD-OE1	5.05	1.34	1.25
1	A	568	GLN	CA-C	5.05	1.59	1.52
1	A	788	ILE	CA-C	5.05	1.58	1.52
1	A	843	PHE	C-O	5.05	1.30	1.23
1	B	1244	LEU	N-CA	-5.05	1.39	1.46
1	A	433	LYS	N-CA	5.04	1.52	1.46
1	A	467	LEU	N-CA	5.04	1.52	1.46
1	A	477	LEU	C-O	5.04	1.29	1.23
1	B	1123	MET	SD-CE	5.04	1.92	1.79
1	C	1165	ILE	CG1-CD1	-5.04	1.32	1.51
1	D	1185	SER	N-CA	5.04	1.53	1.46
1	B	215	GLU	N-CA	-5.04	1.39	1.46
1	D	1084	ALA	N-CA	5.04	1.52	1.46
1	B	30	LEU	N-CA	-5.04	1.40	1.46
1	A	475	SER	CA-CB	5.04	1.61	1.53
1	B	318	LYS	CG-CD	5.04	1.67	1.52
1	B	863	ASP	CA-C	5.04	1.58	1.52
1	B	998	GLY	N-CA	5.04	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	27	LEU	N-CA	5.04	1.52	1.46
1	D	986	ASP	CA-C	-5.04	1.46	1.52
1	A	1154	PHE	CA-C	5.03	1.58	1.52
1	D	342	VAL	CA-C	-5.03	1.46	1.52
1	A	688	ILE	CA-C	5.03	1.58	1.52
1	A	848	LYS	CB-CG	5.03	1.67	1.52
1	B	346	ALA	CA-C	-5.03	1.46	1.52
1	B	1010	PHE	C-N	5.03	1.40	1.33
1	D	685	GLY	CA-C	-5.03	1.44	1.51
1	B	1130	ALA	CA-CB	-5.03	1.45	1.53
1	C	282	ALA	N-CA	5.03	1.52	1.46
1	D	34	LEU	CA-CB	-5.03	1.46	1.53
1	C	1144	GLU	N-CA	5.03	1.53	1.46
1	D	251	GLN	CB-CG	5.03	1.67	1.52
1	A	762	GLU	C-O	-5.02	1.17	1.23
1	A	667	ILE	CA-CB	-5.02	1.47	1.54
1	A	1210	GLU	C-O	-5.02	1.18	1.24
1	B	1213	HIS	N-CA	5.02	1.52	1.46
1	C	795	MET	CG-SD	5.02	1.93	1.80
1	D	223	PRO	CA-CB	5.02	1.60	1.53
1	B	863	ASP	N-CA	5.02	1.52	1.46
1	D	607	ARG	C-O	5.02	1.30	1.24
1	D	803	GLU	C-O	-5.02	1.17	1.24
1	A	102	GLN	N-CA	5.02	1.52	1.46
1	A	839	GLY	C-O	5.02	1.29	1.23
1	C	1313	LYS	CA-C	5.02	1.59	1.52
1	D	820	THR	C-O	5.02	1.30	1.24
1	A	236	TRP	CE2-CZ2	-5.02	1.29	1.39
1	A	1195	GLN	N-CA	-5.02	1.40	1.46
1	B	738	GLY	N-CA	5.02	1.52	1.45
1	B	1150	PRO	C-O	5.02	1.30	1.24
1	D	223	PRO	CA-C	5.02	1.58	1.52
1	D	619	LYS	CG-CD	5.02	1.67	1.52
1	C	1277	ASP	CA-C	-5.02	1.46	1.52
1	B	1283	ARG	C-O	-5.01	1.18	1.24
1	A	832	GLU	CG-CD	5.01	1.64	1.52
1	B	106	ALA	C-O	-5.01	1.17	1.24
1	B	536	CYS	CA-C	5.01	1.59	1.52
1	B	1245	LEU	C-O	5.01	1.30	1.24
1	C	462	ARG	CA-C	-5.01	1.46	1.53
1	D	671	VAL	C-O	5.01	1.30	1.24
1	A	617	LYS	CE-NZ	5.01	1.64	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	716	GLU	N-CA	5.01	1.52	1.46
1	A	839	GLY	N-CA	5.01	1.49	1.44
1	A	945	LYS	C-O	5.01	1.30	1.24
1	A	971	GLU	CD-OE2	5.01	1.34	1.25
1	B	46	GLY	C-O	5.01	1.31	1.24
1	B	783	VAL	C-N	5.01	1.40	1.33
1	C	427	ARG	CD-NE	5.01	1.53	1.46
1	B	395	LYS	CE-NZ	5.01	1.64	1.49
1	C	832	GLU	CD-OE2	5.01	1.34	1.25
1	D	448	GLU	CD-OE2	5.01	1.34	1.25
1	B	543	PHE	CA-C	5.00	1.58	1.52
1	D	1327	LYS	CA-CB	5.00	1.61	1.53

All (1840) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	194	SER	N-CA-C	18.64	134.38	110.33
1	A	216	LEU	N-CA-C	-16.47	90.15	110.41
1	C	194	SER	N-CA-C	16.14	132.30	110.35
1	A	194	SER	N-CA-C	15.94	131.31	110.43
1	B	753	VAL	N-CA-C	15.73	123.72	108.15
1	C	195	LEU	N-CA-C	15.59	129.91	111.82
1	D	194	SER	N-CA-C	15.45	130.93	110.53
1	A	980	ALA	N-CA-C	-14.63	79.64	110.80
1	B	1327	LYS	CA-C-N	14.05	137.41	119.84
1	B	1327	LYS	C-N-CA	14.05	137.41	119.84
1	D	538	LYS	N-CA-C	13.94	131.13	109.52
1	D	195	LEU	N-CA-C	13.92	129.52	112.54
1	A	467	LEU	N-CA-C	13.83	127.61	111.71
1	A	213	PRO	CA-C-N	-13.37	105.61	120.04
1	A	213	PRO	C-N-CA	-13.37	105.61	120.04
1	C	216	LEU	N-CA-C	-13.01	94.41	110.41
1	C	753	VAL	CA-C-N	-12.98	103.62	119.84
1	C	753	VAL	C-N-CA	-12.98	103.62	119.84
1	B	980	ALA	N-CA-C	-12.86	83.41	110.80
1	B	599	ARG	CG-CD-NE	12.70	139.94	112.00
1	C	866	SER	N-CA-C	12.70	137.85	110.80
1	D	213	PRO	CA-C-N	-12.57	106.47	120.04
1	D	213	PRO	C-N-CA	-12.57	106.47	120.04
1	A	505	VAL	N-CA-C	12.35	122.28	110.30
1	A	358	ILE	N-CA-C	12.16	122.73	111.91
1	B	1175	LEU	N-CA-C	12.12	125.65	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1331	VAL	CB-CA-C	12.04	128.53	111.80
1	D	202	THR	CA-C-N	11.98	134.81	119.84
1	D	202	THR	C-N-CA	11.98	134.81	119.84
1	C	213	PRO	CA-C-N	-11.92	107.22	120.45
1	C	213	PRO	C-N-CA	-11.92	107.22	120.45
1	C	708	PHE	N-CA-CB	-11.92	91.86	110.57
1	A	202	THR	CA-C-N	11.90	134.72	119.84
1	A	202	THR	C-N-CA	11.90	134.72	119.84
1	B	467	LEU	N-CA-C	11.76	125.23	111.71
1	B	3	ALA	N-CA-C	11.71	135.74	110.80
1	A	431	ILE	N-CA-CB	-11.68	99.02	112.34
1	A	195	LEU	N-CA-C	11.55	128.03	112.90
1	B	924	ALA	N-CA-C	-11.54	92.64	109.96
1	C	467	LEU	N-CA-C	11.53	123.85	111.28
1	C	533	GLU	N-CA-C	11.43	125.40	110.43
1	C	980	ALA	N-CA-C	-11.43	86.46	110.80
1	B	46	GLY	N-CA-C	11.37	129.86	115.42
1	C	701	ASP	N-CA-C	-11.36	91.19	108.00
1	B	592	VAL	CB-CA-C	-11.31	95.03	110.98
1	C	1175	LEU	N-CA-C	11.26	123.11	111.07
1	A	592	VAL	CB-CA-C	-11.25	97.35	110.96
1	B	797	GLY	N-CA-C	11.19	122.58	111.95
1	C	339	GLY	N-CA-C	11.07	125.88	112.48
1	D	467	LEU	N-CA-C	10.98	124.34	111.71
1	B	537	GLY	N-CA-C	-10.90	87.34	113.18
1	B	1312	ASP	N-CA-C	10.88	122.17	108.45
1	B	202	THR	CA-C-N	10.87	133.43	119.84
1	B	202	THR	C-N-CA	10.87	133.43	119.84
1	A	424	ALA	N-CA-C	10.86	119.17	108.75
1	B	431	ILE	CB-CA-C	10.76	126.86	110.83
1	B	701	ASP	N-CA-C	-10.73	87.94	110.80
1	C	792	VAL	CB-CA-C	-10.58	95.75	110.77
1	A	430	ASP	CA-C-N	10.50	134.34	122.48
1	A	430	ASP	C-N-CA	10.50	134.34	122.48
1	B	4	ASP	N-CA-C	10.48	133.12	110.80
1	B	131	GLN	CA-C-N	-10.47	108.22	120.89
1	B	131	GLN	C-N-CA	-10.47	108.22	120.89
1	D	1299	SER	N-CA-C	10.42	123.73	109.24
1	C	578	LEU	CA-C-N	10.33	130.40	119.76
1	C	578	LEU	C-N-CA	10.33	130.40	119.76
1	A	701	ASP	N-CA-C	-10.33	88.81	110.80
1	C	629	VAL	N-CA-C	10.29	117.48	108.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	129	ARG	N-CA-C	-10.22	100.22	112.89
1	B	2	THR	CA-C-N	10.18	140.99	121.54
1	B	2	THR	C-N-CA	10.18	140.99	121.54
1	C	85	VAL	CB-CA-C	-10.14	98.33	110.91
1	D	139	ILE	N-CA-C	-10.11	98.44	112.50
1	B	1011	THR	N-CA-C	10.10	121.88	111.07
1	A	348	VAL	CB-CA-C	-10.09	98.96	111.88
1	D	529	GLN	N-CA-C	10.09	125.73	113.12
1	B	4	ASP	CB-CA-C	-10.09	90.35	110.42
1	C	232	GLU	N-CA-C	-10.07	101.12	113.41
1	A	597	ILE	N-CA-C	-10.01	99.14	108.95
1	D	283	TRP	N-CA-C	-9.93	101.30	113.41
1	D	599	ARG	CB-CA-C	9.93	126.31	109.53
1	A	610	THR	N-CA-C	9.93	126.35	108.48
1	A	708	PHE	N-CA-CB	-9.91	95.01	110.57
1	D	430	ASP	N-CA-C	9.90	121.89	108.23
1	B	708	PHE	N-CA-CB	-9.88	95.05	110.57
1	D	1260	VAL	N-CA-C	9.83	123.05	113.71
1	D	355	ALA	N-CA-C	9.82	124.35	108.63
1	D	218	ARG	N-CA-C	-9.82	101.05	113.23
1	B	54	MET	N-CA-C	9.82	124.99	108.20
1	D	345	VAL	N-CA-C	9.82	125.30	113.22
1	A	345	VAL	N-CA-C	9.81	127.81	113.39
1	A	1031	LEU	N-CA-C	9.80	127.20	107.41
1	B	529	GLN	N-CA-C	9.78	131.62	110.80
1	B	590	GLU	N-CA-C	9.75	123.68	111.69
1	C	597	ILE	CA-C-N	9.75	132.03	119.84
1	C	597	ILE	C-N-CA	9.75	132.03	119.84
1	C	755	LYS	N-CA-C	9.74	123.12	111.82
1	B	85	VAL	CB-CA-C	-9.71	97.64	110.84
1	D	533	GLU	N-CA-C	-9.69	90.16	110.80
1	D	740	GLN	N-CA-C	9.68	124.22	108.55
1	B	783	VAL	N-CA-C	9.66	118.56	107.84
1	D	66	VAL	N-CA-C	9.65	124.03	109.17
1	A	340	LYS	N-CA-C	9.64	122.79	111.71
1	D	986	ASP	N-CA-C	-9.61	95.46	109.59
1	B	1193	ILE	CB-CA-C	-9.60	95.54	111.29
1	A	529	GLN	N-CA-C	9.60	122.60	110.61
1	D	599	ARG	CA-CB-CG	9.55	133.21	114.10
1	D	1299	SER	CA-C-N	9.55	131.78	119.84
1	D	1299	SER	C-N-CA	9.55	131.78	119.84
1	C	836	ILE	CB-CA-C	-9.54	99.49	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	866	SER	N-CA-C	9.54	131.12	110.80
1	B	535	LYS	N-CA-C	9.53	124.44	113.01
1	C	708	PHE	N-CA-C	9.51	124.38	109.07
1	D	464	ILE	N-CA-C	9.51	123.81	109.17
1	C	308	VAL	N-CA-C	-9.50	100.39	110.36
1	C	497	PRO	CA-C-N	-9.49	109.97	119.56
1	C	497	PRO	C-N-CA	-9.49	109.97	119.56
1	C	464	ILE	N-CA-C	9.47	122.53	109.46
1	A	1260	VAL	N-CA-C	9.45	122.69	113.71
1	A	1175	LEU	N-CA-C	9.38	126.75	111.37
1	A	1319	VAL	N-CA-C	9.36	128.80	109.34
1	C	685	GLY	N-CA-C	9.35	135.35	113.18
1	D	927	TRP	CA-CB-CG	9.35	131.37	113.60
1	D	599	ARG	CG-CD-NE	9.29	132.44	112.00
1	B	464	ILE	N-CA-C	9.26	123.55	109.20
1	C	641	VAL	N-CA-C	-9.26	99.88	108.95
1	A	596	ASP	N-CA-C	-9.25	102.12	113.50
1	C	811	THR	N-CA-C	9.25	120.97	111.07
1	D	1027	ASP	CA-C-N	-9.24	113.51	123.30
1	D	1027	ASP	C-N-CA	-9.24	113.51	123.30
1	A	783	VAL	CA-C-N	9.21	129.29	119.90
1	A	783	VAL	C-N-CA	9.21	129.29	119.90
1	B	195	LEU	N-CA-C	9.17	124.91	112.90
1	B	1329	TRP	N-CA-C	9.13	121.17	111.03
1	D	629	VAL	CA-C-N	9.13	129.69	119.83
1	D	629	VAL	C-N-CA	9.13	129.69	119.83
1	C	535	LYS	N-CA-C	9.08	122.87	109.07
1	A	866	SER	N-CA-C	9.05	130.08	110.80
1	B	345	VAL	N-CA-C	9.03	123.27	113.43
1	C	599	ARG	CA-CB-CG	9.01	132.12	114.10
1	B	1315	THR	CA-C-N	8.99	133.06	120.29
1	B	1315	THR	C-N-CA	8.99	133.06	120.29
1	B	868	VAL	N-CA-C	8.98	119.53	110.82
1	B	696	ILE	CA-C-N	-8.96	114.19	122.97
1	B	696	ILE	C-N-CA	-8.96	114.19	122.97
1	C	927	TRP	CA-CB-CG	8.96	130.62	113.60
1	D	746	GLU	N-CA-C	-8.96	95.54	109.25
1	A	1299	SER	CB-CA-C	-8.95	99.79	110.08
1	B	121	VAL	N-CA-C	-8.94	101.69	110.72
1	A	685	GLY	N-CA-C	8.93	134.34	113.18
1	C	531	ASN	N-CA-C	-8.91	91.81	110.80
1	A	461	ASN	N-CA-C	8.91	122.11	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	30	LEU	N-CA-C	-8.89	100.56	111.40
1	C	530	GLU	N-CA-C	8.88	129.72	110.80
1	D	708	PHE	N-CA-C	8.88	129.71	110.80
1	B	597	ILE	CA-C-N	8.86	130.91	119.84
1	B	597	ILE	C-N-CA	8.86	130.91	119.84
1	C	461	ASN	N-CA-C	8.83	123.06	111.75
1	A	836	ILE	N-CA-C	8.83	118.90	110.42
1	C	1038	GLU	N-CA-C	8.83	122.35	108.67
1	D	685	GLY	N-CA-C	8.82	134.08	113.18
1	D	840	ARG	CA-C-N	8.82	132.49	120.67
1	D	840	ARG	C-N-CA	8.82	132.49	120.67
1	A	991	GLU	N-CA-C	8.82	123.30	112.54
1	A	464	ILE	N-CA-C	8.81	122.74	109.17
1	C	31	ARG	N-CA-C	-8.81	100.86	111.69
1	B	597	ILE	CB-CA-C	-8.80	95.34	111.36
1	B	703	ILE	CB-CA-C	-8.79	100.50	112.02
1	C	567	GLY	N-CA-C	8.79	122.70	112.50
1	C	1039	MET	CB-CA-C	-8.79	96.87	111.02
1	B	1076	SER	CA-C-N	-8.79	110.93	119.89
1	B	1076	SER	C-N-CA	-8.79	110.93	119.89
1	A	232	GLU	N-CA-C	-8.77	102.74	113.97
1	C	611	SER	N-CA-C	8.77	123.23	110.42
1	B	456	TYR	N-CA-C	8.77	122.70	108.41
1	C	1031	LEU	N-CA-C	8.77	125.32	107.69
1	B	927	TRP	CA-CB-CG	8.76	130.25	113.60
1	C	1193	ILE	CB-CA-C	-8.76	96.92	111.29
1	B	1194	GLY	N-CA-C	-8.76	102.04	112.64
1	B	1064	ILE	CB-CA-C	-8.74	97.70	110.63
1	B	213	PRO	CA-C-N	-8.73	110.61	120.04
1	B	213	PRO	C-N-CA	-8.73	110.61	120.04
1	A	1318	CYS	N-CA-C	8.72	124.23	113.50
1	B	1223	ARG	N-CA-C	8.71	123.58	111.56
1	A	283	TRP	N-CA-C	-8.70	102.68	113.38
1	C	345	VAL	N-CA-C	8.69	126.17	113.39
1	C	164	ALA	N-CA-C	8.68	122.57	108.34
1	D	653	GLU	N-CA-C	8.65	122.86	110.14
1	A	275	PHE	N-CA-C	-8.64	96.15	109.64
1	C	777	VAL	N-CA-C	-8.63	102.31	110.42
1	C	1299	SER	CA-C-N	8.62	130.62	119.84
1	C	1299	SER	C-N-CA	8.62	130.62	119.84
1	D	316	VAL	N-CA-C	8.61	119.42	110.72
1	D	597	ILE	CA-C-N	8.60	130.59	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	597	ILE	C-N-CA	8.60	130.59	119.84
1	C	740	GLN	N-CA-C	8.59	123.44	108.75
1	B	21	ASP	CA-C-O	-8.59	112.97	119.32
1	D	568	GLN	N-CA-C	8.58	122.02	110.35
1	A	654	THR	CB-CA-C	-8.57	94.89	109.72
1	D	165	ARG	CA-CB-CG	-8.57	96.96	114.10
1	D	980	ALA	N-CA-C	-8.57	92.55	110.80
1	D	1223	ARG	N-CA-C	8.56	123.18	111.71
1	C	355	ALA	N-CA-C	8.55	122.31	108.63
1	D	456	TYR	N-CA-C	8.55	122.36	108.34
1	D	234	VAL	N-CA-C	8.52	121.84	108.89
1	B	497	PRO	CA-C-N	-8.49	110.98	119.56
1	B	497	PRO	C-N-CA	-8.49	110.98	119.56
1	D	610	THR	N-CA-C	8.49	123.49	109.06
1	B	622	ASP	N-CA-C	8.48	122.87	108.02
1	C	537	GLY	N-CA-C	-8.47	100.51	112.37
1	B	1048	VAL	N-CA-CB	8.46	119.84	110.62
1	C	867	ASN	N-CA-C	8.45	122.77	108.23
1	B	654	THR	CB-CA-C	-8.44	96.16	110.16
1	A	64	LYS	O-C-N	-8.42	112.99	123.17
1	B	1192	ASP	N-CA-C	-8.41	99.41	110.43
1	A	1094	ALA	N-CA-C	-8.41	102.20	111.36
1	D	865	PHE	CA-C-N	8.38	133.75	121.26
1	D	865	PHE	C-N-CA	8.38	133.75	121.26
1	A	329	GLY	N-CA-C	8.35	122.59	112.49
1	B	24	THR	CA-C-N	8.34	134.04	120.94
1	B	24	THR	C-N-CA	8.34	134.04	120.94
1	B	326	VAL	N-CA-C	-8.34	102.73	110.82
1	C	21	ASP	CB-CA-C	-8.33	100.35	109.85
1	D	535	LYS	N-CA-C	-8.31	93.09	110.80
1	B	541	PRO	N-CA-C	8.31	129.58	112.47
1	C	560	LEU	N-CA-C	8.30	122.09	109.23
1	C	470	THR	N-CA-C	8.28	121.12	111.02
1	D	756	GLY	N-CA-C	8.28	126.74	115.32
1	D	461	ASN	N-CA-C	8.28	122.34	111.75
1	A	527	LEU	CA-C-N	8.27	128.43	120.98
1	A	527	LEU	C-N-CA	8.27	128.43	120.98
1	C	653	GLU	N-CA-C	8.27	122.58	110.59
1	D	137	GLU	N-CA-C	8.25	121.39	111.82
1	D	340	LYS	N-CA-C	8.24	121.38	111.82
1	C	313	VAL	N-CA-CB	8.23	120.75	110.47
1	D	51	CYS	N-CA-C	-8.23	101.11	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	597	ILE	CB-CA-C	-8.23	102.00	110.89
1	C	808	VAL	N-CA-CB	8.22	121.72	110.54
1	B	900	ARG	N-CA-C	8.21	122.86	110.14
1	D	924	ALA	N-CA-C	-8.20	97.89	110.10
1	D	1191	ILE	N-CA-C	8.19	119.00	110.72
1	B	1218	GLY	N-CA-C	8.19	129.44	116.01
1	B	348	VAL	N-CA-C	-8.19	102.36	110.30
1	B	142	ALA	N-CA-C	-8.18	103.28	113.18
1	B	1289	ASN	N-CA-C	8.17	121.11	108.12
1	C	1010	PHE	CA-C-O	-8.17	112.66	121.56
1	A	728	ASP	N-CA-C	8.16	119.96	111.14
1	C	139	ILE	N-CA-C	-8.15	101.17	112.50
1	B	1000	CYS	N-CA-C	8.14	120.96	108.42
1	A	24	THR	CA-C-N	8.13	133.71	120.94
1	A	24	THR	C-N-CA	8.13	133.71	120.94
1	B	641	VAL	CA-C-N	-8.12	109.69	119.84
1	B	641	VAL	C-N-CA	-8.12	109.69	119.84
1	C	695	ALA	CA-C-N	-8.12	112.57	123.12
1	C	695	ALA	C-N-CA	-8.12	112.57	123.12
1	B	113	CYS	N-CA-C	8.10	120.83	111.11
1	C	596	ASP	N-CA-C	-8.08	104.56	114.75
1	B	731	VAL	N-CA-C	8.08	121.72	109.20
1	D	46	GLY	N-CA-C	8.07	126.04	115.47
1	A	359	SER	N-CA-C	-8.06	99.39	110.35
1	B	612	THR	N-CA-C	-8.05	102.50	112.88
1	D	858	VAL	N-CA-C	8.04	118.88	112.12
1	A	1081	SER	N-CA-C	-8.04	101.29	113.51
1	C	902	CYS	N-CA-C	8.03	122.79	109.46
1	C	629	VAL	CA-C-N	8.01	128.50	119.93
1	C	629	VAL	C-N-CA	8.01	128.50	119.93
1	B	319	LEU	CA-C-N	8.00	129.84	119.84
1	B	319	LEU	C-N-CA	8.00	129.84	119.84
1	C	59	ASP	N-CA-C	8.00	119.69	110.97
1	C	868	VAL	N-CA-C	8.00	118.80	110.72
1	D	440	VAL	N-CA-C	7.97	120.33	108.46
1	D	921	MET	N-CA-C	-7.97	93.83	110.80
1	C	921	MET	N-CA-C	-7.97	93.83	110.80
1	C	765	VAL	N-CA-C	7.96	118.86	108.35
1	A	1238	ILE	CA-C-N	-7.96	111.39	122.93
1	A	1238	ILE	C-N-CA	-7.96	111.39	122.93
1	C	1210	GLU	N-CA-C	7.95	121.42	109.25
1	D	701	ASP	N-CA-C	-7.95	94.65	108.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	765	VAL	N-CA-C	7.94	119.77	108.17
1	A	641	VAL	CA-C-N	-7.92	111.92	120.94
1	A	641	VAL	C-N-CA	-7.92	111.92	120.94
1	A	394	ARG	CA-C-O	-7.91	112.36	121.54
1	A	731	VAL	N-CA-C	7.91	120.53	109.29
1	C	652	ASP	CA-C-O	-7.91	112.04	120.42
1	A	937	MET	N-CA-C	7.90	127.28	109.81
1	C	163	PHE	CA-C-N	-7.89	111.64	122.77
1	C	163	PHE	C-N-CA	-7.89	111.64	122.77
1	C	1068	SER	N-CA-C	7.89	120.71	108.96
1	C	804	THR	CB-CA-C	-7.89	98.79	109.28
1	B	342	VAL	N-CA-C	-7.88	105.08	112.96
1	B	1029	SER	N-CA-C	7.88	121.61	110.50
1	A	928	MET	N-CA-C	7.87	119.49	111.07
1	C	165	ARG	CB-CG-CD	7.87	129.40	111.30
1	D	612	THR	N-CA-C	-7.87	102.73	112.88
1	C	837	THR	N-CA-C	7.87	119.86	111.28
1	D	803	GLU	N-CA-C	7.86	121.81	111.75
1	D	165	ARG	CB-CG-CD	7.86	129.37	111.30
1	D	792	VAL	CB-CA-C	-7.85	99.83	110.42
1	C	1048	VAL	N-CA-CB	7.85	119.52	110.65
1	B	1190	ALA	N-CA-C	-7.84	102.04	111.69
1	C	456	TYR	N-CA-C	7.84	121.20	108.34
1	B	969	TRP	N-CA-C	-7.84	102.42	110.97
1	C	390	PHE	CA-C-N	7.84	127.39	118.85
1	C	390	PHE	C-N-CA	7.84	127.39	118.85
1	B	747	THR	N-CA-C	-7.83	98.23	110.36
1	C	597	ILE	CB-CA-C	-7.83	97.12	111.36
1	D	804	THR	CB-CA-C	-7.83	94.85	110.42
1	D	675	THR	CA-C-N	-7.81	112.86	120.83
1	D	675	THR	C-N-CA	-7.81	112.86	120.83
1	D	731	VAL	N-CA-C	7.81	121.17	108.99
1	C	333	GLN	N-CA-C	-7.80	103.89	113.41
1	A	1218	GLY	N-CA-C	7.80	127.50	115.72
1	B	967	ARG	N-CA-C	7.80	119.78	111.28
1	D	592	VAL	CB-CA-C	-7.80	99.71	111.33
1	C	313	VAL	CB-CA-C	-7.79	101.84	112.04
1	A	756	GLY	N-CA-C	7.78	126.06	115.32
1	A	252	HIS	CB-CA-C	-7.77	101.52	111.15
1	B	902	CYS	N-CA-C	7.75	121.29	108.96
1	A	313	VAL	CB-CA-C	-7.75	98.57	111.29
1	D	4	ASP	CA-C-N	-7.74	109.56	121.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4	ASP	C-N-CA	-7.74	109.56	121.02
1	A	953	LEU	N-CA-C	7.74	122.16	109.24
1	B	744	TYR	CA-C-N	-7.73	107.36	120.58
1	B	744	TYR	C-N-CA	-7.73	107.36	120.58
1	C	870	ASN	N-CA-C	7.73	121.31	112.57
1	B	1299	SER	CB-CA-C	-7.73	101.19	110.08
1	C	767	THR	N-CA-C	7.73	120.91	109.24
1	A	560	LEU	N-CA-C	7.72	121.48	109.52
1	D	248	LEU	N-CA-C	-7.71	102.82	111.07
1	A	1000	CYS	N-CA-C	7.70	120.78	109.07
1	A	70	ALA	CA-C-N	-7.70	112.38	123.00
1	A	70	ALA	C-N-CA	-7.70	112.38	123.00
1	C	1192	ASP	N-CA-C	-7.69	100.37	110.53
1	A	898	THR	CB-CA-C	-7.69	95.79	110.24
1	C	46	GLY	N-CA-C	7.69	125.20	115.21
1	D	5	LYS	CB-CA-C	7.68	121.23	110.16
1	D	805	ARG	N-CA-C	7.68	119.73	111.36
1	C	833	ASP	N-CA-C	-7.68	102.84	111.14
1	D	614	ALA	N-CA-C	7.67	121.13	111.69
1	A	519	PHE	N-CA-C	-7.67	102.86	111.14
1	D	150	CYS	N-CA-C	7.66	120.71	111.82
1	A	197	LYS	CA-C-N	-7.66	111.95	120.45
1	A	197	LYS	C-N-CA	-7.66	111.95	120.45
1	A	1289	ASN	N-CA-C	7.65	121.10	108.48
1	B	232	GLU	N-CA-C	-7.65	104.47	113.88
1	B	752	ALA	CA-C-N	-7.64	114.84	123.25
1	B	752	ALA	C-N-CA	-7.64	114.84	123.25
1	B	1136	THR	CA-C-N	-7.64	112.33	120.66
1	B	1136	THR	C-N-CA	-7.64	112.33	120.66
1	A	738	GLY	N-CA-C	7.64	120.73	112.33
1	D	599	ARG	N-CA-C	-7.64	98.13	110.20
1	A	506	ASP	N-CA-C	7.64	122.04	112.87
1	C	194	SER	CA-C-N	7.63	131.92	120.31
1	C	194	SER	C-N-CA	7.63	131.92	120.31
1	A	18	LYS	N-CA-C	7.63	121.69	112.38
1	B	136	MET	CG-SD-CE	7.63	117.69	100.90
1	B	545	SER	N-CA-C	7.63	127.04	110.80
1	D	313	VAL	CB-CA-C	-7.63	102.05	112.04
1	C	1126	VAL	N-CA-C	7.61	120.77	108.97
1	B	611	SER	N-CA-C	7.61	121.00	110.35
1	A	1169	THR	N-CA-C	7.61	122.69	113.41
1	B	833	ASP	N-CA-C	-7.60	102.93	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	866	SER	N-CA-CB	-7.60	97.65	110.49
1	A	64	LYS	CA-C-N	-7.60	113.25	123.12
1	A	64	LYS	C-N-CA	-7.60	113.25	123.12
1	A	440	VAL	N-CA-C	7.60	119.69	108.45
1	A	746	GLU	N-CA-C	-7.59	98.57	109.96
1	D	1106	LYS	N-CA-C	-7.58	102.95	111.14
1	D	1311	VAL	N-CA-C	7.58	119.76	108.54
1	D	41	LEU	N-CA-C	7.56	121.24	109.07
1	B	20	ALA	CA-C-O	-7.56	112.30	120.92
1	B	736	TYR	N-CA-C	7.55	120.83	108.52
1	C	252	HIS	CA-C-N	7.55	128.20	120.04
1	C	252	HIS	C-N-CA	7.55	128.20	120.04
1	B	927	TRP	N-CA-CB	-7.53	97.77	110.49
1	A	771	MET	N-CA-C	7.52	120.20	111.02
1	C	1106	LYS	N-CA-C	-7.52	103.02	111.07
1	A	927	TRP	CA-CB-CG	7.52	127.89	113.60
1	A	925	GLU	N-CA-C	-7.52	94.79	110.80
1	B	609	VAL	CB-CA-C	-7.50	100.65	110.84
1	A	137	GLU	N-CA-C	7.49	120.10	111.11
1	D	1299	SER	CB-CA-C	-7.47	98.62	109.38
1	B	66	VAL	N-CA-C	7.46	120.65	109.17
1	C	406	SER	N-CA-C	7.46	120.54	108.76
1	D	1012	VAL	CA-C-N	-7.45	111.30	119.19
1	D	1012	VAL	C-N-CA	-7.45	111.30	119.19
1	A	578	LEU	CA-C-N	7.45	127.87	119.83
1	A	578	LEU	C-N-CA	7.45	127.87	119.83
1	D	406	SER	N-CA-C	7.44	120.68	108.99
1	B	600	TYR	N-CA-C	-7.44	100.93	110.53
1	A	351	ASN	N-CA-C	-7.44	102.54	111.69
1	D	937	MET	O-C-N	7.44	129.87	121.32
1	A	1293	GLU	CA-C-N	-7.43	111.78	123.23
1	A	1293	GLU	C-N-CA	-7.43	111.78	123.23
1	B	1152	HIS	N-CA-C	-7.43	104.06	113.43
1	A	614	ALA	N-CA-C	7.43	121.59	112.23
1	B	1241	ARG	N-CA-C	7.43	120.84	108.73
1	D	497	PRO	CA-C-N	-7.42	112.14	119.64
1	D	497	PRO	C-N-CA	-7.42	112.14	119.64
1	C	1179	ILE	N-CA-C	7.42	120.47	108.97
1	C	529	GLN	N-CA-C	7.41	126.58	110.80
1	A	868	VAL	N-CA-C	7.37	119.39	111.58
1	C	76	PRO	CA-C-N	-7.36	108.42	120.64
1	C	76	PRO	C-N-CA	-7.36	108.42	120.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	THR	CB-CA-C	-7.36	96.12	110.11
1	C	1299	SER	N-CA-C	7.35	119.46	109.24
1	D	342	VAL	N-CA-C	-7.35	106.33	113.53
1	A	1246	ARG	N-CA-C	7.34	122.00	110.32
1	B	355	ALA	N-CA-C	7.34	126.44	110.80
1	B	764	PHE	CA-C-N	-7.34	112.13	122.71
1	B	764	PHE	C-N-CA	-7.34	112.13	122.71
1	B	919	GLN	CA-C-O	7.34	129.01	120.49
1	A	633	VAL	N-CA-C	7.34	118.12	111.81
1	D	165	ARG	N-CA-CB	7.33	122.96	110.50
1	A	497	PRO	CA-C-O	-7.32	114.95	120.73
1	D	1245	LEU	O-C-N	7.32	131.60	123.04
1	B	783	VAL	CA-C-N	7.32	127.36	119.90
1	B	783	VAL	C-N-CA	7.32	127.36	119.90
1	C	620	SER	N-CA-C	7.31	119.26	108.14
1	A	149	ARG	NE-CZ-NH2	7.31	125.78	119.20
1	D	1302	THR	CA-C-N	7.31	128.98	119.84
1	D	1302	THR	C-N-CA	7.31	128.98	119.84
1	B	546	ALA	N-CA-C	7.30	119.14	111.03
1	D	1069	THR	CB-CA-C	-7.29	102.00	111.40
1	A	155	PRO	CB-CA-C	-7.27	100.12	112.26
1	D	771	MET	N-CA-C	7.26	118.98	111.14
1	B	653	GLU	N-CA-C	7.26	121.34	109.94
1	D	154	ARG	O-C-N	7.26	126.94	120.48
1	C	319	LEU	CA-C-N	7.25	128.91	119.84
1	C	319	LEU	C-N-CA	7.25	128.91	119.84
1	C	924	ALA	N-CA-C	-7.25	99.29	110.10
1	B	937	MET	N-CA-C	7.25	125.83	109.81
1	C	836	ILE	N-CA-C	7.25	117.77	110.23
1	C	41	LEU	N-CA-C	7.24	120.31	108.52
1	D	496	LEU	N-CA-C	7.24	120.93	109.64
1	D	348	VAL	CB-CA-C	-7.22	102.45	111.70
1	B	1022	LEU	CB-CA-C	7.22	122.38	109.38
1	A	1193	ILE	CB-CA-C	-7.22	99.45	111.29
1	B	558	VAL	N-CA-CB	-7.21	99.16	112.43
1	B	532	LEU	CA-CB-CG	7.20	141.51	116.30
1	A	1134	TYR	N-CA-C	7.20	119.33	108.46
1	D	138	GLU	N-CA-C	-7.20	103.97	112.89
1	B	431	ILE	CA-CB-CG1	7.20	122.63	110.40
1	C	64	LYS	CA-C-N	-7.20	113.77	123.12
1	C	64	LYS	C-N-CA	-7.20	113.77	123.12
1	B	216	LEU	N-CA-C	-7.19	101.06	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	165	ARG	CA-CB-CG	-7.19	99.73	114.10
1	A	749	CYS	N-CA-C	7.18	126.10	110.80
1	A	21	ASP	CB-CA-C	-7.17	101.67	109.85
1	A	1223	ARG	N-CA-C	7.17	121.45	111.56
1	D	633	VAL	CB-CA-C	-7.17	103.89	110.91
1	B	1018	ALA	N-CA-C	7.16	117.95	108.07
1	A	591	ALA	CA-C-N	7.16	131.32	122.37
1	A	591	ALA	C-N-CA	7.16	131.32	122.37
1	A	857	VAL	N-CA-C	7.16	119.43	109.55
1	B	1210	GLU	N-CA-C	7.15	120.33	108.96
1	C	927	TRP	N-CA-CB	-7.14	98.43	110.49
1	C	45	GLU	N-CA-CB	-7.13	98.42	110.41
1	C	141	ASN	N-CA-CB	-7.13	98.43	110.49
1	D	1174	ASN	CA-C-N	7.13	130.70	120.79
1	D	1174	ASN	C-N-CA	7.13	130.70	120.79
1	B	598	PRO	N-CA-C	7.13	127.16	112.47
1	D	961	GLU	N-CA-C	7.13	121.03	110.48
1	B	749	CYS	N-CA-C	7.13	119.22	108.46
1	D	587	ALA	N-CA-C	-7.12	104.59	113.28
1	A	15	VAL	CA-C-N	-7.12	113.29	123.11
1	A	15	VAL	C-N-CA	-7.12	113.29	123.11
1	A	423	GLN	N-CA-C	7.12	121.16	109.06
1	A	403	ILE	CB-CA-C	-7.11	99.87	110.82
1	C	1080	ALA	N-CA-C	7.10	120.55	110.68
1	A	496	LEU	N-CA-C	7.09	119.82	109.04
1	B	1111	SER	CB-CA-C	-7.09	100.07	111.28
1	B	165	ARG	CA-CB-CG	-7.09	99.92	114.10
1	D	1175	LEU	N-CA-C	7.09	119.67	111.02
1	D	1293	GLU	CA-C-N	-7.08	112.33	123.24
1	D	1293	GLU	C-N-CA	-7.08	112.33	123.24
1	D	824	VAL	CB-CA-C	-7.08	98.46	110.71
1	D	319	LEU	CA-C-N	7.08	128.69	119.84
1	D	319	LEU	C-N-CA	7.08	128.69	119.84
1	C	617	LYS	CA-C-N	-7.08	114.11	123.17
1	C	617	LYS	C-N-CA	-7.08	114.11	123.17
1	A	612	THR	N-CA-C	-7.07	104.26	113.17
1	C	699	ILE	N-CA-C	7.07	117.58	110.23
1	D	1319	VAL	N-CA-C	7.07	124.05	109.34
1	B	440	VAL	N-CA-C	7.07	118.99	108.46
1	B	1043	LEU	N-CA-C	-7.07	103.57	111.28
1	B	953	LEU	N-CA-C	7.07	120.70	108.76
1	C	66	VAL	CB-CA-C	-7.07	99.58	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	759	GLY	N-CA-C	-7.06	104.83	115.00
1	A	604	LEU	N-CA-C	7.06	120.83	110.59
1	D	465	SER	N-CA-C	7.06	121.33	109.76
1	A	772	LYS	CA-C-N	-7.05	110.09	120.38
1	A	772	LYS	C-N-CA	-7.05	110.09	120.38
1	C	824	VAL	CB-CA-C	-7.04	99.66	110.50
1	A	338	ALA	N-CA-C	7.03	125.78	110.80
1	C	340	LYS	N-CA-C	7.03	121.12	112.54
1	C	150	CYS	N-CA-C	7.03	119.97	111.82
1	C	403	ILE	CB-CA-C	-7.02	99.88	110.55
1	C	997	ARG	N-CA-C	7.02	120.94	109.85
1	D	29	TYR	N-CA-C	-7.02	103.63	111.28
1	A	1188	ASN	CA-C-N	7.02	126.65	119.56
1	A	1188	ASN	C-N-CA	7.02	126.65	119.56
1	D	622	ASP	N-CA-C	7.01	120.29	108.02
1	D	1118	VAL	N-CA-C	-7.01	104.36	110.74
1	D	609	VAL	CB-CA-C	-7.01	100.82	110.77
1	A	902	CYS	N-CA-C	7.01	121.09	109.46
1	B	200	GLU	N-CA-C	-7.00	104.62	113.72
1	B	333	GLN	N-CA-C	-7.00	104.38	113.12
1	A	333	GLN	N-CA-C	-6.99	104.89	113.41
1	C	868	VAL	O-C-N	6.98	129.02	121.83
1	A	51	CYS	N-CA-C	-6.98	103.34	112.41
1	C	40	LYS	CA-C-N	-6.97	113.29	123.05
1	C	40	LYS	C-N-CA	-6.97	113.29	123.05
1	C	599	ARG	CG-CD-NE	6.97	127.34	112.00
1	D	1024	VAL	N-CA-C	6.97	117.69	107.37
1	B	323	LYS	N-CA-C	-6.96	103.46	112.23
1	B	45	GLU	N-CA-CB	-6.96	100.40	110.56
1	C	540	ASP	CA-C-N	6.95	127.36	119.92
1	C	540	ASP	C-N-CA	6.95	127.36	119.92
1	C	636	ILE	CA-CB-CG2	6.95	122.31	110.50
1	B	808	VAL	N-CA-CB	6.93	123.31	110.77
1	A	339	GLY	N-CA-C	6.92	120.79	111.72
1	C	1000	CYS	N-CA-C	6.92	119.70	108.76
1	B	755	LYS	CA-C-N	-6.92	113.74	123.08
1	B	755	LYS	C-N-CA	-6.92	113.74	123.08
1	C	1188	ASN	CA-C-N	6.92	126.55	119.56
1	C	1188	ASN	C-N-CA	6.92	126.55	119.56
1	C	944	ARG	CA-CB-CG	6.91	127.93	114.10
1	D	906	LEU	N-CA-C	-6.91	98.33	109.58
1	A	602	ASN	CA-C-N	-6.90	113.20	122.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	602	ASN	C-N-CA	-6.90	113.20	122.72
1	C	382	THR	N-CA-C	6.90	118.70	107.32
1	C	1168	LEU	N-CA-C	6.89	120.17	111.69
1	D	791	ARG	NE-CZ-NH2	6.89	125.40	119.20
1	D	927	TRP	N-CA-CB	-6.89	98.84	110.49
1	C	1011	THR	N-CA-CB	6.89	120.36	110.16
1	D	1233	PHE	N-CA-C	-6.89	103.70	111.07
1	A	935	CYS	N-CA-C	6.89	119.37	111.11
1	C	610	THR	N-CA-C	6.88	120.87	108.69
1	C	1195	GLN	N-CA-C	6.88	119.36	111.11
1	A	794	ARG	NE-CZ-NH2	-6.87	113.02	119.20
1	A	1126	VAL	CB-CA-C	-6.86	101.38	111.19
1	B	599	ARG	CA-CB-CG	6.86	127.83	114.10
1	B	720	LEU	N-CA-C	-6.86	96.18	110.80
1	B	944	ARG	N-CA-C	-6.86	103.82	111.71
1	B	461	ASN	CB-CA-C	-6.84	97.98	110.63
1	B	511	LEU	N-CA-C	6.84	118.81	111.36
1	B	1299	SER	N-CA-C	6.84	120.71	108.47
1	C	10	VAL	CB-CA-C	-6.83	102.61	110.73
1	B	1272	PHE	N-CA-C	6.83	118.72	111.28
1	C	840	ARG	N-CA-C	-6.82	100.18	110.28
1	D	898	THR	CB-CA-C	-6.82	96.78	111.11
1	D	868	VAL	N-CA-C	6.82	118.44	111.00
1	C	811	THR	CA-CB-OG1	-6.82	99.37	109.60
1	D	532	LEU	CA-CB-CG	6.81	140.15	116.30
1	A	736	TYR	N-CA-C	6.81	119.62	108.52
1	C	131	GLN	CA-C-N	-6.81	112.65	120.89
1	C	131	GLN	C-N-CA	-6.81	112.65	120.89
1	D	618	ILE	CG1-CB-CG2	-6.81	90.28	110.70
1	B	1026	THR	N-CA-C	6.81	125.30	110.80
1	D	1241	ARG	N-CA-C	6.80	121.02	107.62
1	D	917	GLY	CA-C-N	6.80	126.43	119.56
1	D	917	GLY	C-N-CA	6.80	126.43	119.56
1	B	710	GLY	CA-C-N	6.80	127.04	119.90
1	B	710	GLY	C-N-CA	6.80	127.04	119.90
1	A	1064	ILE	CB-CA-C	-6.80	100.49	110.62
1	A	27	LEU	CA-C-N	-6.79	108.56	121.54
1	A	27	LEU	C-N-CA	-6.79	108.56	121.54
1	D	719	ASP	N-CA-C	-6.79	96.33	110.80
1	D	1328	PRO	N-CA-C	6.79	126.46	112.47
1	C	695	ALA	N-CA-C	6.79	120.52	109.59
1	B	257	LEU	CB-CA-C	-6.78	98.78	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	609	VAL	CB-CA-C	-6.78	100.72	110.83
1	D	991	GLU	N-CA-C	6.78	121.25	113.19
1	B	1266	PHE	N-CA-C	6.77	119.50	111.71
1	A	808	VAL	N-CA-CB	6.77	118.93	110.47
1	B	527	LEU	CA-CB-CG	6.77	140.00	116.30
1	A	1260	VAL	CB-CA-C	-6.77	104.27	110.63
1	D	1127	SER	N-CA-C	6.77	120.18	110.10
1	B	700	GLU	N-CA-C	-6.76	101.61	110.33
1	B	1031	LEU	N-CA-C	6.76	122.10	107.49
1	C	54	MET	N-CA-C	6.76	119.54	108.52
1	D	915	PHE	CB-CA-C	-6.76	101.05	111.66
1	A	165	ARG	N-CA-CB	6.75	121.97	110.50
1	B	1224	GLY	CA-C-N	6.75	128.28	119.84
1	B	1224	GLY	C-N-CA	6.75	128.28	119.84
1	D	20	ALA	CA-C-O	-6.75	113.60	121.16
1	D	1285	GLN	N-CA-C	6.74	118.41	111.14
1	B	1180	VAL	CB-CA-C	-6.73	100.96	110.12
1	B	1135	ARG	N-CA-C	-6.73	98.00	109.24
1	C	596	ASP	O-C-N	6.73	129.92	121.64
1	B	64	LYS	O-C-N	-6.73	115.36	123.10
1	A	460	ALA	CA-C-N	6.73	129.59	120.38
1	A	460	ALA	C-N-CA	6.73	129.59	120.38
1	B	911	ALA	N-CA-C	6.73	119.98	110.23
1	A	568	GLN	N-CA-C	6.72	125.12	110.80
1	D	1172	HIS	N-CA-C	6.72	119.63	109.41
1	A	456	TYR	N-CA-C	6.72	119.36	108.41
1	D	1331	VAL	N-CA-C	6.72	123.31	109.34
1	A	1050	VAL	N-CA-C	6.71	116.81	110.30
1	A	431	ILE	CB-CG1-CD1	6.70	127.87	113.80
1	C	371	LYS	N-CA-C	6.70	121.70	107.70
1	A	737	ILE	CB-CA-C	-6.70	101.80	110.98
1	D	158	GLN	N-CA-C	-6.70	104.92	113.23
1	A	862	VAL	N-CA-C	6.69	117.94	108.17
1	A	770	THR	CB-CA-C	6.67	122.00	110.79
1	C	20	ALA	N-CA-C	6.67	120.05	110.24
1	C	517	PHE	N-CA-C	-6.67	103.94	111.07
1	C	352	ILE	CB-CA-C	-6.67	103.29	112.02
1	C	543	PHE	N-CA-C	6.67	125.00	110.80
1	B	382	THR	N-CA-C	6.66	119.79	107.60
1	B	1331	VAL	CB-CA-C	6.66	122.21	111.29
1	C	1069	THR	N-CA-C	-6.66	103.20	112.25
1	A	1120	ALA	N-CA-C	6.66	118.22	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	635	PHE	O-C-N	-6.65	115.63	123.22
1	A	755	LYS	N-CA-C	6.65	119.36	111.71
1	B	5	LYS	N-CA-C	-6.65	102.71	111.02
1	D	1313	LYS	CA-C-N	6.64	131.64	120.88
1	D	1313	LYS	C-N-CA	6.64	131.64	120.88
1	B	1315	THR	O-C-N	6.64	129.16	122.12
1	B	41	LEU	N-CA-C	6.63	119.33	108.52
1	D	953	LEU	N-CA-C	6.63	119.96	108.76
1	D	835	LEU	CA-C-N	6.62	128.90	120.56
1	D	835	LEU	C-N-CA	6.62	128.90	120.56
1	C	1001	ILE	N-CA-CB	-6.62	103.73	112.34
1	D	323	LYS	N-CA-C	-6.62	104.14	111.82
1	D	910	THR	N-CA-C	6.61	117.00	108.34
1	B	22	PRO	CB-CA-C	-6.61	102.47	111.85
1	B	716	GLU	N-CA-C	6.61	119.93	108.76
1	D	113	CYS	N-CA-C	6.61	119.32	111.33
1	C	1134	TYR	N-CA-C	6.61	119.25	108.55
1	C	745	LEU	N-CA-C	6.60	118.27	111.14
1	C	425	SER	CA-C-N	6.60	134.15	121.54
1	C	425	SER	C-N-CA	6.60	134.15	121.54
1	A	1180	VAL	CB-CA-C	-6.60	101.52	110.42
1	B	194	SER	CA-C-N	6.60	133.66	121.52
1	B	194	SER	C-N-CA	6.60	133.66	121.52
1	C	592	VAL	CB-CA-C	-6.60	101.50	111.33
1	D	1165	ILE	CB-CA-C	-6.60	102.15	111.38
1	D	617	LYS	N-CA-C	-6.58	101.04	110.59
1	A	695	ALA	N-CA-C	6.58	119.14	108.41
1	C	1187	LEU	N-CA-C	6.58	119.27	111.71
1	A	1259	ALA	N-CA-C	6.58	119.29	110.35
1	C	986	ASP	N-CA-C	-6.57	100.17	109.96
1	A	641	VAL	N-CA-C	-6.57	101.80	108.96
1	D	347	SER	CA-C-O	-6.57	113.75	120.71
1	C	27	LEU	CA-C-N	-6.56	109.00	121.54
1	C	27	LEU	C-N-CA	-6.56	109.00	121.54
1	A	1123	MET	N-CA-C	6.56	120.38	112.38
1	B	569	SER	N-CA-C	6.56	119.27	110.35
1	C	808	VAL	CB-CA-C	-6.56	103.29	112.14
1	A	919	GLN	CA-C-O	6.55	128.35	120.81
1	A	927	TRP	N-CA-CB	-6.55	99.41	110.49
1	A	313	VAL	N-CA-CB	6.55	122.04	111.23
1	A	653	GLU	N-CA-C	6.55	119.77	110.14
1	C	1223	ARG	N-CA-C	6.55	121.21	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	744	TYR	N-CA-C	-6.54	101.90	110.53
1	D	1105	TYR	N-CA-C	-6.54	104.33	112.90
1	A	83	VAL	CB-CA-C	-6.54	101.94	111.68
1	A	692	GLU	N-CA-C	6.54	120.62	107.41
1	B	824	VAL	CB-CA-C	-6.53	99.96	110.28
1	A	1193	ILE	N-CA-CB	6.53	122.01	111.23
1	D	1126	VAL	N-CA-C	6.53	117.88	108.48
1	A	1086	LEU	N-CA-C	6.52	118.39	111.28
1	B	283	TRP	N-CA-C	-6.52	105.14	113.23
1	A	29	TYR	N-CA-C	-6.52	104.17	111.28
1	A	10	VAL	N-CA-C	6.51	117.26	107.75
1	A	308	VAL	CB-CA-C	-6.51	103.54	111.88
1	A	1045	THR	N-CA-C	-6.51	104.03	112.23
1	D	727	ALA	N-CA-C	6.51	120.14	109.72
1	A	1133	PHE	N-CA-CB	-6.50	101.09	111.43
1	D	1035	GLY	N-CA-C	6.50	122.32	113.99
1	B	840	ARG	CA-C-N	6.50	129.49	120.65
1	B	840	ARG	C-N-CA	6.50	129.49	120.65
1	A	97	ARG	N-CA-C	-6.50	98.01	109.06
1	B	808	VAL	CB-CA-C	-6.50	101.73	112.26
1	B	776	PHE	CB-CA-C	-6.50	98.61	110.63
1	B	51	CYS	N-CA-C	-6.49	103.97	112.41
1	D	636	ILE	CA-CB-CG2	6.49	121.54	110.50
1	D	830	ARG	N-CA-CB	6.49	119.39	109.91
1	A	252	HIS	CA-C-N	6.49	126.12	119.56
1	A	252	HIS	C-N-CA	6.49	126.12	119.56
1	A	603	GLU	CA-C-N	-6.49	108.99	122.03
1	A	603	GLU	C-N-CA	-6.49	108.99	122.03
1	B	340	LYS	N-CA-C	6.49	120.46	112.54
1	D	69	SER	CA-CB-OG	-6.49	98.12	111.10
1	B	533	GLU	N-CA-CB	6.49	120.72	111.25
1	C	506	ASP	N-CA-C	-6.49	105.38	113.55
1	C	719	ASP	N-CA-C	-6.49	96.99	110.80
1	C	137	GLU	N-CA-C	6.48	118.34	111.28
1	B	1246	ARG	N-CA-C	6.47	120.09	110.52
1	D	1039	MET	CB-CA-C	-6.46	100.27	110.94
1	C	523	VAL	N-CA-C	-6.46	104.35	110.42
1	A	629	VAL	CA-C-N	6.46	126.84	119.93
1	A	629	VAL	C-N-CA	6.46	126.84	119.93
1	A	1065	SER	N-CA-C	6.46	121.82	113.88
1	A	903	LYS	CD-CE-NZ	6.45	132.54	111.90
1	C	464	ILE	O-C-N	6.45	128.12	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	731	VAL	O-C-N	6.45	128.69	122.69
1	B	1205	GLY	N-CA-C	-6.45	104.69	112.49
1	B	618	ILE	CB-CA-C	6.44	118.40	110.73
1	B	607	ARG	CB-CA-C	-6.43	97.61	110.42
1	B	268	MET	CG-SD-CE	6.43	115.05	100.90
1	B	375	VAL	N-CA-C	6.43	119.56	108.95
1	C	1260	VAL	N-CA-C	6.43	122.71	109.34
1	D	752	ALA	CA-C-N	-6.43	110.24	122.13
1	D	752	ALA	C-N-CA	-6.43	110.24	122.13
1	C	640	ASP	O-C-N	6.42	130.25	122.48
1	D	278	ILE	CB-CA-C	-6.42	101.05	110.62
1	D	1068	SER	N-CA-C	6.42	118.94	109.24
1	C	599	ARG	CB-CA-C	6.42	120.63	109.65
1	B	135	THR	N-CA-C	-6.42	99.75	109.95
1	B	1319	VAL	CB-CA-C	6.42	123.59	111.40
1	B	1027	ASP	CA-C-N	-6.41	115.81	123.44
1	B	1027	ASP	C-N-CA	-6.41	115.81	123.44
1	D	917	GLY	O-C-N	6.41	123.38	121.07
1	A	1286	HIS	N-CA-C	6.41	119.77	112.97
1	C	641	VAL	CB-CA-C	6.41	117.81	110.89
1	D	825	ARG	NE-CZ-NH1	-6.41	115.09	121.50
1	A	145	GLY	N-CA-C	6.41	121.72	114.67
1	B	1319	VAL	CA-C-O	6.41	131.69	120.80
1	D	313	VAL	N-CA-CB	6.40	118.47	110.47
1	C	350	GLY	N-CA-C	6.40	120.64	112.83
1	D	630	PRO	CB-CA-C	-6.40	103.58	111.64
1	B	711	PRO	N-CA-C	6.40	120.46	110.80
1	D	1316	THR	CB-CA-C	-6.40	97.69	110.42
1	B	862	VAL	N-CA-C	6.39	117.50	108.17
1	C	569	SER	N-CA-C	6.39	118.81	110.43
1	C	696	ILE	CA-C-N	-6.39	110.47	121.97
1	C	696	ILE	C-N-CA	-6.39	110.47	121.97
1	A	1176	ARG	N-CA-C	6.39	118.78	109.07
1	C	579	PRO	CB-CA-C	-6.39	103.22	111.46
1	B	252	HIS	O-C-N	6.37	126.09	121.12
1	C	917	GLY	CA-C-N	6.37	126.29	119.28
1	C	917	GLY	C-N-CA	6.37	126.29	119.28
1	C	1289	ASN	N-CA-C	6.37	124.37	110.80
1	A	838	GLY	CA-C-N	6.36	128.85	122.30
1	A	838	GLY	C-N-CA	6.36	128.85	122.30
1	D	842	PRO	CA-C-O	-6.36	114.18	122.19
1	C	1043	LEU	CA-C-N	-6.36	110.65	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1043	LEU	C-N-CA	-6.36	110.65	120.31
1	C	1261	GLY	N-CA-C	6.36	128.25	113.18
1	D	802	LYS	N-CA-C	6.36	120.67	112.41
1	C	911	ALA	N-CA-C	6.35	119.57	110.10
1	A	703	ILE	CB-CA-C	-6.34	103.73	112.04
1	B	865	PHE	CA-C-N	6.34	133.66	121.54
1	B	865	PHE	C-N-CA	6.34	133.66	121.54
1	A	797	GLY	N-CA-C	6.34	120.03	111.72
1	B	741	GLU	N-CA-C	6.34	119.87	110.48
1	C	461	ASN	CB-CA-C	-6.34	98.16	110.46
1	C	23	GLU	CA-C-N	-6.34	113.25	122.19
1	C	23	GLU	C-N-CA	-6.34	113.25	122.19
1	A	652	ASP	CB-CA-C	-6.33	100.28	110.79
1	B	165	ARG	CB-CG-CD	6.33	125.86	111.30
1	B	533	GLU	CA-C-N	6.33	133.64	121.54
1	B	533	GLU	C-N-CA	6.33	133.64	121.54
1	D	1182	ASP	N-CA-C	6.33	119.12	108.23
1	A	608	LEU	CA-C-O	-6.33	113.70	121.11
1	C	680	GLN	CB-CA-C	-6.33	100.33	110.84
1	D	1011	THR	N-CA-C	6.32	117.97	111.14
1	C	886	MET	N-CA-C	6.32	118.97	111.71
1	B	230	GLU	N-CA-C	6.32	119.19	108.90
1	C	123	SER	O-C-N	6.32	128.66	122.09
1	C	1100	LYS	N-CA-C	-6.31	104.40	111.28
1	A	355	ALA	N-CA-C	6.31	124.24	110.80
1	A	832	GLU	N-CA-C	-6.31	104.49	111.36
1	C	49	GLY	N-CA-C	6.31	128.12	113.18
1	C	794	ARG	N-CA-C	6.31	118.36	108.96
1	D	1127	SER	CA-C-N	-6.30	112.65	122.67
1	D	1127	SER	C-N-CA	-6.30	112.65	122.67
1	A	497	PRO	O-C-N	6.30	124.11	121.15
1	D	817	ALA	N-CA-C	6.30	118.70	111.02
1	C	731	VAL	N-CA-CB	6.29	119.51	112.34
1	C	1043	LEU	N-CA-C	-6.29	104.34	111.07
1	C	165	ARG	N-CA-CB	6.29	121.19	110.50
1	D	1149	ASN	N-CA-C	6.29	122.51	109.11
1	D	836	ILE	CB-CA-C	-6.29	103.92	111.97
1	C	1024	VAL	N-CA-C	6.29	116.67	107.37
1	D	475	SER	N-CA-C	6.28	119.91	111.24
1	D	461	ASN	CB-CA-C	-6.28	98.28	110.46
1	B	1134	TYR	N-CA-C	6.28	118.06	108.52
1	B	557	ASP	CA-C-N	6.28	131.49	122.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	557	ASP	C-N-CA	6.28	131.49	122.45
1	B	685	GLY	N-CA-C	6.28	128.06	113.18
1	A	744	TYR	CA-C-N	-6.27	109.86	120.58
1	A	744	TYR	C-N-CA	-6.27	109.86	120.58
1	A	1127	SER	CA-C-N	-6.27	112.70	122.67
1	A	1127	SER	C-N-CA	-6.27	112.70	122.67
1	A	111	SER	N-CA-C	-6.27	96.76	107.23
1	A	59	ASP	N-CA-C	6.26	117.91	111.14
1	C	600	TYR	CA-C-N	-6.26	109.41	121.94
1	C	600	TYR	C-N-CA	-6.26	109.41	121.94
1	C	1243	SER	CA-C-N	6.26	129.72	120.95
1	C	1243	SER	C-N-CA	6.26	129.72	120.95
1	B	1172	HIS	N-CA-C	6.26	118.47	109.14
1	C	898	THR	CB-CA-C	-6.26	99.48	112.44
1	D	6	LEU	CB-CG-CD2	-6.26	91.92	110.70
1	B	27	LEU	CA-C-N	-6.25	109.59	121.54
1	B	27	LEU	C-N-CA	-6.25	109.59	121.54
1	B	898	THR	CB-CA-C	-6.25	99.54	111.48
1	D	558	VAL	N-CA-C	6.25	117.36	108.42
1	B	1028	GLY	N-CA-C	6.25	121.10	113.79
1	B	64	LYS	CA-C-N	-6.25	114.79	123.10
1	B	64	LYS	C-N-CA	-6.25	114.79	123.10
1	C	825	ARG	NE-CZ-NH2	-6.25	113.58	119.20
1	D	593	TYR	CA-C-N	-6.25	112.55	122.17
1	D	593	TYR	C-N-CA	-6.25	112.55	122.17
1	C	24	THR	CA-C-N	6.24	131.33	122.09
1	C	24	THR	C-N-CA	6.24	131.33	122.09
1	D	194	SER	N-CA-CB	-6.24	101.43	110.36
1	A	1117	TRP	N-CA-C	6.24	119.99	112.38
1	D	1158	VAL	N-CA-C	6.24	116.04	108.06
1	D	1314	PHE	N-CA-C	6.23	119.28	111.24
1	A	530	GLU	N-CA-C	6.23	124.06	110.80
1	C	1064	ILE	CA-CB-CG1	6.22	120.98	110.40
1	D	1193	ILE	N-CA-CB	6.22	121.49	111.23
1	D	339	GLY	N-CA-C	6.22	120.52	112.68
1	C	202	THR	CA-C-N	6.22	127.61	119.84
1	C	202	THR	C-N-CA	6.22	127.61	119.84
1	D	1115	GLU	N-CA-C	-6.21	104.61	111.82
1	A	1101	ARG	N-CA-C	-6.21	104.41	112.23
1	D	654	THR	N-CA-C	6.20	118.84	108.73
1	C	892	ILE	N-CA-CB	-6.20	102.53	111.21
1	D	751	ILE	CB-CA-C	-6.20	102.25	110.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	75	ALA	CA-C-N	6.19	126.11	119.85
1	B	75	ALA	C-N-CA	6.19	126.11	119.85
1	C	75	ALA	CA-C-N	6.19	126.11	119.85
1	C	75	ALA	C-N-CA	6.19	126.11	119.85
1	A	746	GLU	O-C-N	6.19	130.54	122.93
1	B	808	VAL	O-C-N	6.19	128.79	121.80
1	D	163	PHE	CA-C-N	-6.19	113.47	122.44
1	D	163	PHE	C-N-CA	-6.19	113.47	122.44
1	C	607	ARG	CB-CA-C	-6.18	98.11	110.42
1	B	165	ARG	N-CA-CB	6.18	121.01	110.50
1	A	954	THR	N-CA-C	6.18	118.53	110.43
1	D	841	HIS	CA-C-O	-6.18	113.62	119.80
1	A	594	CYS	N-CA-C	6.18	123.95	110.80
1	C	1067	THR	CA-C-N	-6.18	111.74	121.87
1	C	1067	THR	C-N-CA	-6.18	111.74	121.87
1	D	822	ARG	CA-C-N	6.17	126.12	119.76
1	D	822	ARG	C-N-CA	6.17	126.12	119.76
1	A	840	ARG	CA-C-N	6.17	128.94	120.67
1	A	840	ARG	C-N-CA	6.17	128.94	120.67
1	C	32	ARG	N-CA-C	6.17	121.64	112.94
1	D	314	ASP	CB-CA-C	6.17	119.74	109.56
1	C	51	CYS	N-CA-C	-6.17	103.91	112.30
1	B	720	LEU	CA-CB-CG	6.17	137.88	116.30
1	C	1172	HIS	N-CA-C	6.16	118.78	109.23
1	D	1208	THR	CB-CA-C	-6.16	99.99	109.29
1	A	131	GLN	N-CA-C	-6.16	96.20	109.81
1	D	59	ASP	N-CA-C	6.16	117.86	111.03
1	D	352	ILE	CB-CA-C	-6.16	104.09	111.97
1	D	1085	ASP	CA-C-N	-6.16	110.95	120.31
1	D	1085	ASP	C-N-CA	-6.16	110.95	120.31
1	C	1192	ASP	CA-C-O	-6.16	114.73	121.87
1	D	1011	THR	N-CA-CB	6.16	119.00	110.07
1	B	599	ARG	CB-CG-CD	-6.15	97.15	111.30
1	A	716	GLU	N-CA-C	6.15	119.52	109.06
1	B	1328	PRO	N-CA-C	6.15	125.14	112.47
1	C	1149	ASN	N-CA-C	6.15	122.58	108.93
1	C	820	THR	CA-C-O	6.14	126.92	119.31
1	B	218	ARG	N-CA-C	-6.14	105.62	113.23
1	D	635	PHE	N-CA-C	6.14	118.69	108.20
1	C	32	ARG	NE-CZ-NH1	-6.13	115.37	121.50
1	B	568	GLN	N-CA-C	6.13	119.15	110.50
1	B	672	VAL	N-CA-C	6.13	117.03	107.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	290	VAL	CB-CA-C	-6.13	101.49	110.81
1	D	709	TYR	N-CA-C	6.13	123.85	110.80
1	D	1254	ILE	N-CA-C	6.13	122.08	109.34
1	B	390	PHE	CA-C-N	6.12	127.49	119.84
1	B	390	PHE	C-N-CA	6.12	127.49	119.84
1	D	34	LEU	N-CA-C	-6.12	105.12	112.59
1	C	557	ASP	CA-C-N	6.12	131.86	122.25
1	C	557	ASP	C-N-CA	6.12	131.86	122.25
1	A	747	THR	N-CA-C	-6.12	100.34	109.94
1	B	348	VAL	N-CA-CB	6.12	117.28	110.62
1	B	1173	LYS	N-CA-C	-6.12	100.66	110.14
1	A	719	ASP	N-CA-CB	6.11	120.82	110.49
1	A	117	THR	N-CA-C	6.11	120.80	112.55
1	A	597	ILE	CB-CA-C	-6.11	104.29	110.89
1	A	829	ASP	CB-CA-C	-6.11	99.14	109.83
1	A	199	GLU	N-CA-C	-6.11	105.59	113.16
1	C	860	LEU	N-CA-C	6.11	118.00	107.93
1	D	1190	ALA	N-CA-C	-6.11	104.55	111.14
1	C	1010	PHE	N-CA-C	-6.10	101.89	110.50
1	C	338	ALA	N-CA-C	6.10	123.80	110.80
1	A	737	ILE	N-CA-C	6.10	116.89	107.99
1	D	1281	ALA	N-CA-C	6.09	119.55	111.75
1	D	1194	GLY	N-CA-C	-6.09	98.74	113.18
1	C	1218	GLY	N-CA-C	6.09	126.00	116.01
1	A	1306	ILE	CB-CA-C	-6.09	104.06	112.04
1	A	40	LYS	CB-CG-CD	6.09	125.30	111.30
1	C	759	GLY	N-CA-C	-6.08	106.85	115.43
1	D	431	ILE	N-CA-C	6.08	118.63	109.20
1	B	495	HIS	N-CA-C	-6.08	101.48	110.48
1	C	233	ARG	CB-CA-C	-6.08	101.31	109.16
1	C	1196	VAL	N-CA-C	6.08	116.56	110.23
1	A	740	GLN	N-CA-C	6.08	118.36	108.76
1	D	641	VAL	CA-C-O	-6.08	114.06	119.71
1	D	944	ARG	CA-CB-CG	6.08	126.25	114.10
1	C	590	GLU	N-CA-C	6.07	119.95	112.54
1	D	1097	THR	N-CA-C	-6.07	104.73	111.71
1	B	578	LEU	CA-C-N	6.07	126.01	119.76
1	B	578	LEU	C-N-CA	6.07	126.01	119.76
1	C	1094	ALA	N-CA-C	-6.07	104.78	111.82
1	B	59	ASP	N-CA-C	6.07	117.97	111.36
1	C	434	VAL	CB-CA-C	-6.07	101.58	110.62
1	B	1278	ALA	N-CA-C	-6.07	104.78	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	799	PHE	CA-C-O	-6.06	111.84	120.51
1	A	1241	ARG	N-CA-C	6.06	118.56	108.20
1	B	919	GLN	N-CA-CB	6.06	119.75	109.87
1	A	165	ARG	CA-CB-CG	-6.06	101.98	114.10
1	C	944	ARG	CA-C-N	6.06	128.40	120.28
1	C	944	ARG	C-N-CA	6.06	128.40	120.28
1	D	937	MET	N-CA-C	6.06	123.20	109.81
1	A	214	PRO	N-CA-C	-6.06	106.09	114.27
1	A	244	GLU	N-CA-C	6.06	119.77	112.38
1	B	792	VAL	CA-C-N	-6.05	111.22	122.60
1	B	792	VAL	C-N-CA	-6.05	111.22	122.60
1	D	1131	THR	CB-CA-C	-6.05	98.22	111.71
1	D	28	ALA	N-CA-CB	6.05	120.72	110.49
1	D	439	ARG	N-CA-C	6.05	119.34	109.24
1	D	590	GLU	N-CA-C	6.05	119.85	112.23
1	B	880	GLU	N-CA-C	-6.05	104.61	111.14
1	B	813	VAL	CB-CA-C	-6.04	104.23	111.97
1	B	593	TYR	CA-CB-CG	-6.04	103.03	113.90
1	A	786	ASN	N-CA-C	-6.04	105.49	112.92
1	B	1192	ASP	CA-C-O	-6.04	115.23	121.87
1	D	836	ILE	N-CA-C	6.04	116.22	110.42
1	D	1057	ILE	N-CA-C	-6.04	101.21	108.45
1	C	427	ARG	N-CA-C	-6.03	105.18	112.54
1	C	165	ARG	NE-CZ-NH2	6.03	124.63	119.20
1	B	578	LEU	CB-CA-C	6.03	118.07	109.08
1	C	534	ASP	N-CA-C	-6.03	97.96	110.80
1	D	1031	LEU	N-CA-C	6.03	120.30	107.70
1	A	1011	THR	N-CA-CB	6.03	119.05	110.13
1	A	1232	ALA	CA-C-O	-6.02	114.24	121.89
1	C	633	VAL	N-CA-C	6.02	117.39	111.67
1	B	452	LEU	N-CA-C	6.01	119.34	108.69
1	A	277	MET	CG-SD-CE	6.01	114.13	100.90
1	A	937	MET	CA-C-N	6.01	127.35	119.84
1	A	937	MET	C-N-CA	6.01	127.35	119.84
1	B	560	LEU	N-CA-C	6.01	118.31	109.24
1	B	771	MET	N-CA-C	6.00	117.82	111.28
1	C	122	MET	CG-SD-CE	-6.00	87.69	100.90
1	B	369	GLY	N-CA-C	-6.00	98.95	113.18
1	B	1035	GLY	N-CA-C	6.00	120.15	112.83
1	C	686	VAL	N-CA-C	-6.00	99.94	108.58
1	C	5	LYS	CA-C-O	-6.00	114.32	120.80
1	C	753	VAL	N-CA-C	6.00	121.84	108.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1254	ILE	N-CA-C	6.00	121.81	109.34
1	D	39	THR	N-CA-C	-6.00	95.81	107.62
1	D	680	GLN	CB-CA-C	-6.00	100.78	110.74
1	C	532	LEU	N-CA-C	-6.00	104.87	111.82
1	A	1064	ILE	CA-C-N	-5.99	112.05	122.36
1	A	1064	ILE	C-N-CA	-5.99	112.05	122.36
1	D	136	MET	CG-SD-CE	5.99	114.08	100.90
1	D	1019	GLY	O-C-N	5.99	127.83	123.27
1	D	632	PHE	CA-C-N	-5.99	116.48	122.77
1	D	632	PHE	C-N-CA	-5.99	116.48	122.77
1	B	1039	MET	CB-CG-SD	-5.99	94.73	112.70
1	D	57	LYS	CA-C-O	-5.99	114.86	121.33
1	A	356	SER	CA-C-O	-5.99	114.18	120.70
1	A	621	ILE	CA-C-N	-5.99	114.33	123.07
1	A	621	ILE	C-N-CA	-5.99	114.33	123.07
1	B	131	GLN	CB-CA-C	5.99	121.96	110.17
1	D	25	THR	OG1-CB-CG2	-5.98	97.33	109.30
1	C	16	VAL	CA-C-N	-5.98	114.81	122.77
1	C	16	VAL	C-N-CA	-5.98	114.81	122.77
1	A	318	LYS	CB-CG-CD	5.98	125.05	111.30
1	C	1052	SER	CB-CA-C	-5.98	100.69	110.85
1	D	870	ASN	N-CA-C	5.98	119.33	112.57
1	A	1018	ALA	N-CA-CB	5.97	120.29	110.97
1	B	59	ASP	CA-C-O	-5.96	114.10	120.42
1	B	73	CYS	N-CA-C	-5.96	105.58	112.92
1	C	946	ASN	N-CA-C	5.96	117.60	110.44
1	D	382	THR	N-CA-C	5.96	119.72	107.37
1	A	1081	SER	CB-CA-C	5.96	115.73	109.83
1	B	1011	THR	N-CA-CB	5.96	118.65	110.01
1	C	193	PRO	CA-C-N	5.96	129.74	120.75
1	C	193	PRO	C-N-CA	5.96	129.74	120.75
1	D	1188	ASN	CA-C-N	5.96	125.57	119.56
1	D	1188	ASN	C-N-CA	5.96	125.57	119.56
1	D	197	LYS	CA-C-N	-5.95	113.85	120.45
1	D	197	LYS	C-N-CA	-5.95	113.85	120.45
1	B	655	VAL	CB-CA-C	-5.95	104.27	111.88
1	C	719	ASP	N-CA-CB	5.94	120.53	110.49
1	B	1292	LYS	CA-C-N	5.94	129.55	121.05
1	B	1292	LYS	C-N-CA	5.94	129.55	121.05
1	B	240	SER	N-CA-C	5.94	120.92	113.43
1	B	735	ILE	N-CA-C	5.94	116.08	107.88
1	D	24	THR	CA-C-N	5.93	130.26	120.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	24	THR	C-N-CA	5.93	130.26	120.94
1	D	744	TYR	N-CA-C	-5.93	101.70	110.48
1	B	652	ASP	N-CA-CB	5.93	118.61	110.01
1	C	841	HIS	N-CA-C	5.93	116.87	109.57
1	B	1229	LYS	N-CA-C	5.93	119.08	107.57
1	C	1012	VAL	CA-C-N	-5.93	112.47	119.05
1	C	1012	VAL	C-N-CA	-5.93	112.47	119.05
1	D	672	VAL	N-CA-C	5.93	116.40	107.75
1	A	23	GLU	N-CA-C	5.92	120.35	113.18
1	A	714	LYS	N-CA-C	5.92	118.29	108.99
1	C	646	ILE	CB-CA-C	5.92	119.23	111.53
1	B	770	THR	CB-CA-C	5.92	120.25	110.90
1	C	669	GLY	N-CA-C	5.92	119.15	110.80
1	B	866	SER	N-CA-CB	-5.92	100.49	110.49
1	C	277	MET	CG-SD-CE	5.92	113.91	100.90
1	D	815	LEU	N-CA-C	5.92	117.73	111.28
1	D	820	THR	CA-C-O	5.92	126.22	119.18
1	B	774	GLN	N-CA-C	5.91	117.40	111.07
1	B	1158	VAL	N-CA-C	5.91	116.04	107.88
1	B	587	ALA	CA-C-N	-5.91	113.38	122.60
1	B	587	ALA	C-N-CA	-5.91	113.38	122.60
1	B	697	ILE	O-C-N	5.91	126.34	121.85
1	D	1064	ILE	CB-CA-C	-5.91	101.82	110.62
1	C	1193	ILE	N-CA-CB	5.91	120.98	111.23
1	B	695	ALA	CA-C-N	-5.91	115.34	122.90
1	B	695	ALA	C-N-CA	-5.91	115.34	122.90
1	D	672	VAL	O-C-N	-5.91	116.94	123.20
1	A	802	LYS	N-CA-C	5.90	120.08	112.41
1	D	1311	VAL	CB-CA-C	5.90	117.99	111.08
1	A	1077	PRO	CB-CA-C	-5.90	103.84	111.39
1	B	1245	LEU	O-C-N	5.90	129.94	123.04
1	B	1100	LYS	N-CA-C	-5.89	104.98	111.82
1	B	1293	GLU	CA-C-N	-5.89	113.71	123.37
1	B	1293	GLU	C-N-CA	-5.89	113.71	123.37
1	A	681	ARG	CB-CG-CD	5.89	124.85	111.30
1	A	808	VAL	N-CA-C	5.89	117.33	110.62
1	D	807	THR	N-CA-C	5.89	118.46	111.33
1	D	1037	THR	N-CA-C	5.89	119.14	109.72
1	A	809	VAL	N-CA-C	5.88	115.95	110.42
1	B	530	GLU	N-CA-C	5.88	123.33	110.80
1	C	808	VAL	O-C-N	5.88	127.58	121.87
1	D	85	VAL	CB-CA-C	-5.88	102.85	110.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1294	LEU	CA-C-N	-5.87	114.41	122.93
1	A	1294	LEU	C-N-CA	-5.87	114.41	122.93
1	D	1051	ALA	N-CA-C	5.87	119.97	112.34
1	B	1241	ARG	N-CA-CB	-5.86	100.86	110.42
1	C	705	ASN	CB-CA-C	-5.86	99.79	109.99
1	D	66	VAL	CB-CA-C	-5.86	103.17	111.38
1	D	600	TYR	CB-CA-C	-5.86	98.88	111.78
1	B	638	ALA	N-CA-C	5.86	119.25	111.75
1	B	991	GLU	N-CA-C	5.86	120.04	113.01
1	C	1048	VAL	CB-CA-C	-5.86	104.31	111.87
1	D	783	VAL	N-CA-C	5.86	115.48	108.45
1	C	675	THR	CA-C-O	-5.86	115.11	120.50
1	A	215	GLU	N-CA-C	5.85	117.74	111.36
1	C	1289	ASN	CA-C-N	5.85	132.71	121.54
1	C	1289	ASN	C-N-CA	5.85	132.71	121.54
1	A	1224	GLY	CA-C-N	5.85	127.15	119.84
1	A	1224	GLY	C-N-CA	5.85	127.15	119.84
1	C	730	VAL	N-CA-C	5.85	117.06	107.24
1	D	141	ASN	N-CA-CB	-5.85	100.61	110.49
1	D	340	LYS	CA-C-N	5.85	129.95	120.60
1	D	340	LYS	C-N-CA	5.85	129.95	120.60
1	A	775	SER	CA-C-O	-5.84	114.68	120.70
1	D	232	GLU	N-CA-C	-5.84	106.69	113.88
1	D	500	ALA	CA-C-N	-5.84	114.29	120.66
1	D	500	ALA	C-N-CA	-5.84	114.29	120.66
1	A	433	LYS	CA-C-N	-5.84	116.13	121.97
1	A	433	LYS	C-N-CA	-5.84	116.13	121.97
1	A	431	ILE	N-CA-C	5.84	117.58	109.29
1	A	1301	ALA	N-CA-C	5.84	118.67	108.52
1	D	164	ALA	N-CA-C	5.84	117.90	107.80
1	C	1136	THR	N-CA-C	-5.83	101.16	109.62
1	A	611	SER	N-CA-C	5.83	118.93	110.42
1	D	149	ARG	N-CA-C	5.83	118.51	111.40
1	C	1008	ILE	N-CA-C	5.83	116.25	107.80
1	C	1229	LYS	CD-CE-NZ	5.82	130.53	111.90
1	A	745	LEU	N-CA-C	5.82	118.85	111.69
1	A	1319	VAL	CA-C-N	5.82	132.18	121.70
1	A	1319	VAL	C-N-CA	5.82	132.18	121.70
1	A	622	ASP	N-CA-C	5.82	118.20	108.02
1	A	688	ILE	N-CA-C	5.82	117.98	108.97
1	D	257	LEU	CB-CA-C	-5.81	100.51	110.22
1	C	887	ASP	N-CA-C	5.81	118.39	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1119	THR	N-CA-CB	5.81	120.31	110.49
1	C	1211	GLU	CA-C-N	-5.81	113.49	122.09
1	C	1211	GLU	C-N-CA	-5.81	113.49	122.09
1	A	222	THR	CA-C-N	5.81	126.00	120.31
1	A	222	THR	C-N-CA	5.81	126.00	120.31
1	B	111	SER	N-CA-C	-5.81	98.81	108.34
1	D	133	GLU	N-CA-C	-5.81	98.15	108.55
1	B	834	MET	CB-CG-SD	-5.80	95.30	112.70
1	C	119	GLY	N-CA-C	5.80	126.93	113.18
1	D	460	ALA	CA-C-N	5.80	128.85	120.38
1	D	460	ALA	C-N-CA	5.80	128.85	120.38
1	B	635	PHE	CA-C-O	5.80	126.56	120.36
1	D	517	PHE	N-CA-C	-5.80	104.59	111.03
1	C	1215	SER	CA-C-N	5.80	125.66	119.28
1	C	1215	SER	C-N-CA	5.80	125.66	119.28
1	A	258	VAL	N-CA-C	5.79	116.93	108.53
1	C	688	ILE	CB-CA-C	-5.79	101.62	110.95
1	A	434	VAL	CA-C-O	5.79	124.54	120.66
1	B	1065	SER	N-CA-C	5.79	120.38	112.68
1	D	703	ILE	N-CA-C	5.79	115.86	110.42
1	A	599	ARG	CA-C-N	-5.79	112.66	122.67
1	A	599	ARG	C-N-CA	-5.79	112.66	122.67
1	A	1274	ALA	N-CA-C	-5.79	105.11	111.82
1	B	131	GLN	N-CA-C	-5.79	97.02	109.81
1	B	874	LEU	N-CA-C	5.79	123.12	110.80
1	C	40	LYS	CB-CG-CD	5.78	124.60	111.30
1	D	49	GLY	N-CA-C	5.78	126.89	113.18
1	B	1302	THR	N-CA-C	5.78	117.88	109.84
1	C	40	LYS	N-CA-C	5.78	119.07	110.52
1	A	1236	ILE	CA-C-N	5.78	125.78	119.89
1	A	1236	ILE	C-N-CA	5.78	125.78	119.89
1	C	1098	ILE	N-CA-CB	5.78	117.96	110.57
1	A	59	ASP	CA-C-O	-5.77	114.75	120.70
1	A	578	LEU	N-CA-C	-5.77	102.50	109.72
1	B	1234	GLY	N-CA-C	5.77	126.86	113.18
1	B	1229	LYS	CD-CE-NZ	5.77	130.36	111.90
1	A	892	ILE	N-CA-CB	-5.77	103.13	111.21
1	C	937	MET	N-CA-C	5.77	122.56	109.81
1	B	775	SER	CA-C-O	-5.76	113.84	120.24
1	A	1097	THR	N-CA-C	-5.75	105.15	111.82
1	C	122	MET	O-C-N	5.75	128.71	122.15
1	C	611	SER	CA-C-O	5.75	126.70	120.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1064	ILE	CB-CA-C	-5.75	102.05	110.62
1	B	193	PRO	CA-C-N	5.75	131.18	120.95
1	B	193	PRO	C-N-CA	5.75	131.18	120.95
1	B	680	GLN	N-CA-C	5.75	123.05	110.80
1	A	690	TYR	CA-CB-CG	5.75	124.24	113.90
1	B	1330	SER	N-CA-C	5.75	123.04	110.80
1	C	632	PHE	CA-C-N	-5.75	115.79	122.63
1	C	632	PHE	C-N-CA	-5.75	115.79	122.63
1	A	655	VAL	N-CA-C	5.74	117.17	110.62
1	A	1191	ILE	N-CA-C	5.74	116.47	110.62
1	C	866	SER	N-CA-CB	-5.74	100.80	110.49
1	B	1238	ILE	CA-C-N	-5.73	114.62	122.93
1	B	1238	ILE	C-N-CA	-5.73	114.62	122.93
1	B	1184	GLY	N-CA-C	-5.73	102.25	112.22
1	A	461	ASN	CB-CA-C	-5.73	100.94	110.68
1	C	73	CYS	N-CA-C	-5.72	105.63	113.30
1	C	1091	VAL	CB-CA-C	-5.72	104.56	111.88
1	D	753	VAL	N-CA-C	5.72	121.24	108.88
1	B	863	ASP	N-CA-C	5.72	117.85	108.52
1	B	1163	VAL	CA-C-O	-5.72	115.22	121.28
1	C	776	PHE	N-CA-C	-5.72	105.80	112.89
1	B	673	ALA	N-CA-C	5.72	119.23	108.65
1	D	892	ILE	CA-C-N	5.72	126.21	120.04
1	D	892	ILE	C-N-CA	5.72	126.21	120.04
1	C	476	LYS	CA-C-N	-5.71	113.70	122.62
1	C	476	LYS	C-N-CA	-5.71	113.70	122.62
1	D	695	ALA	N-CA-C	5.71	118.79	109.59
1	A	759	GLY	N-CA-C	-5.71	107.49	114.92
1	C	530	GLU	CA-C-N	5.71	132.45	121.54
1	C	530	GLU	C-N-CA	5.71	132.45	121.54
1	C	1310	CYS	CB-CA-C	-5.71	103.56	112.12
1	D	1085	ASP	N-CA-CB	5.71	118.34	110.07
1	A	165	ARG	NE-CZ-NH2	5.70	124.33	119.20
1	B	831	ASP	N-CA-C	5.70	120.78	111.37
1	C	427	ARG	N-CA-CB	5.70	119.86	110.39
1	C	1206	LEU	CA-C-N	-5.70	113.19	122.26
1	C	1206	LEU	C-N-CA	-5.70	113.19	122.26
1	B	1188	ASN	CA-C-N	5.70	125.80	119.87
1	B	1188	ASN	C-N-CA	5.70	125.80	119.87
1	A	1106	LYS	N-CA-C	-5.70	104.98	111.14
1	C	16	VAL	CG1-CB-CG2	-5.70	98.26	110.80
1	C	364	VAL	CA-CB-CG2	-5.70	100.71	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1101	ARG	N-CA-C	5.70	117.49	111.28
1	D	25	THR	N-CA-CB	-5.70	101.97	110.17
1	C	34	LEU	N-CA-C	-5.69	105.01	112.41
1	C	859	ALA	N-CA-C	5.69	117.72	109.07
1	D	652	ASP	N-CA-CB	5.69	118.49	110.12
1	B	1067	THR	CA-C-N	-5.69	113.26	122.36
1	B	1067	THR	C-N-CA	-5.69	113.26	122.36
1	C	1295	PHE	N-CA-C	5.69	118.75	109.59
1	C	727	ALA	N-CA-C	5.69	118.49	109.50
1	C	757	GLU	N-CA-C	5.69	118.51	109.24
1	C	513	LEU	N-CA-C	5.68	118.25	111.71
1	D	154	ARG	NE-CZ-NH2	5.68	124.32	119.20
1	A	585	MET	N-CA-C	5.68	118.24	111.71
1	A	1238	ILE	N-CA-CB	5.68	117.07	110.65
1	A	193	PRO	CA-C-N	5.68	130.47	120.87
1	A	193	PRO	C-N-CA	5.68	130.47	120.87
1	A	847	TYR	N-CA-C	5.68	117.60	109.14
1	C	903	LYS	CD-CE-NZ	5.68	130.08	111.90
1	D	237	ILE	N-CA-C	5.68	116.03	107.80
1	D	294	PRO	N-CA-C	-5.68	108.78	114.68
1	D	636	ILE	CB-CA-C	5.68	119.40	111.34
1	A	620	SER	CA-CB-OG	-5.67	99.75	111.10
1	B	795	MET	N-CA-C	5.67	118.82	109.85
1	C	937	MET	CA-C-N	5.67	126.93	119.84
1	C	937	MET	C-N-CA	5.67	126.93	119.84
1	D	1295	PHE	N-CA-C	5.67	119.07	109.76
1	A	30	LEU	N-CA-C	-5.67	105.01	111.14
1	A	1311	VAL	N-CA-C	5.67	117.34	109.80
1	B	16	VAL	CA-C-N	-5.67	115.00	123.00
1	B	16	VAL	C-N-CA	-5.67	115.00	123.00
1	B	772	LYS	N-CA-C	-5.67	104.57	112.45
1	A	720	LEU	CA-CB-CG	5.67	136.13	116.30
1	A	615	HIS	CA-C-O	-5.66	112.35	120.11
1	A	1254	ILE	N-CA-C	5.66	121.12	109.34
1	C	564	VAL	N-CA-CB	5.66	115.82	109.99
1	D	194	SER	CA-C-N	5.66	130.17	120.72
1	D	194	SER	C-N-CA	5.66	130.17	120.72
1	B	44	GLY	CA-C-N	5.66	131.70	122.65
1	B	44	GLY	C-N-CA	5.66	131.70	122.65
1	A	272	ASN	N-CA-C	5.66	122.84	110.80
1	D	1229	LYS	CD-CE-NZ	5.65	129.99	111.90
1	B	228	ARG	NE-CZ-NH1	-5.65	115.85	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	637	SER	N-CA-C	5.65	116.83	108.86
1	D	299	PHE	N-CA-C	5.65	117.62	108.41
1	D	657	ALA	O-C-N	5.65	129.90	123.12
1	A	1234	GLY	N-CA-C	5.65	126.57	113.18
1	B	577	PRO	N-CA-C	5.65	120.11	112.48
1	B	937	MET	O-C-N	5.65	127.82	121.32
1	B	462	ARG	NE-CZ-NH1	-5.64	115.86	121.50
1	C	88	VAL	CG1-CB-CG2	-5.64	98.38	110.80
1	C	316	VAL	N-CA-CB	5.64	118.21	110.54
1	B	508	ARG	CA-C-O	5.64	126.92	121.00
1	A	788	ILE	N-CA-C	5.64	116.42	108.36
1	C	334	LEU	CA-C-N	-5.64	112.28	120.29
1	C	334	LEU	C-N-CA	-5.64	112.28	120.29
1	C	641	VAL	CA-C-N	-5.64	114.51	120.94
1	C	641	VAL	C-N-CA	-5.64	114.51	120.94
1	D	1065	SER	N-CA-C	5.64	120.43	112.93
1	A	457	GLY	CA-C-O	-5.63	116.46	121.64
1	C	1029	SER	N-CA-C	5.63	118.82	110.48
1	B	708	PHE	N-CA-C	5.63	118.13	109.07
1	B	1004	THR	CB-CA-C	-5.63	100.92	109.99
1	B	709	TYR	N-CA-C	5.63	122.79	110.80
1	C	57	LYS	N-CA-C	5.63	117.65	108.76
1	D	75	ALA	CA-C-N	5.63	125.81	119.90
1	D	75	ALA	C-N-CA	5.63	125.81	119.90
1	A	590	GLU	N-CA-C	5.63	119.32	112.23
1	D	922	LEU	N-CA-C	-5.62	98.82	110.80
1	A	1318	CYS	CA-C-N	5.62	132.09	121.97
1	A	1318	CYS	C-N-CA	5.62	132.09	121.97
1	B	719	ASP	N-CA-CB	5.62	119.99	110.49
1	D	594	CYS	CA-CB-SG	-5.62	101.47	114.40
1	A	324	THR	CB-CA-C	-5.62	104.25	111.22
1	B	804	THR	CB-CA-C	-5.62	99.24	110.42
1	D	68	PHE	N-CA-C	5.62	117.81	108.99
1	D	831	ASP	N-CA-C	5.62	118.12	111.33
1	A	607	ARG	NE-CZ-NH1	-5.61	115.89	121.50
1	A	139	ILE	N-CA-C	-5.61	103.92	111.44
1	C	1287	THR	N-CA-C	-5.61	105.03	112.94
1	A	579	PRO	N-CA-C	5.61	119.67	111.03
1	B	1315	THR	N-CA-C	-5.61	105.17	111.28
1	C	699	ILE	CB-CA-C	-5.61	104.52	111.70
1	C	149	ARG	NE-CZ-NH2	5.60	124.24	119.20
1	D	1161	SER	N-CA-C	5.60	118.53	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	470	THR	N-CA-C	5.60	117.85	111.02
1	D	501	PRO	N-CA-C	-5.60	102.42	111.77
1	A	1319	VAL	CA-CB-CG2	5.60	119.91	110.40
1	C	101	VAL	N-CA-C	-5.60	104.72	112.50
1	C	72	ALA	N-CA-C	5.59	119.73	113.02
1	D	569	SER	N-CA-C	5.59	117.96	110.35
1	D	31	ARG	N-CA-C	-5.59	104.68	112.45
1	D	936	GLY	N-CA-C	-5.59	99.94	113.18
1	B	406	SER	N-CA-C	5.59	118.30	108.75
1	C	37	SER	CA-C-N	-5.59	110.52	121.53
1	C	37	SER	C-N-CA	-5.59	110.52	121.53
1	D	453	ALA	N-CA-C	5.58	118.56	109.06
1	C	744	TYR	CA-C-N	-5.58	112.85	120.44
1	C	744	TYR	C-N-CA	-5.58	112.85	120.44
1	A	1189	PRO	CB-CA-C	-5.58	103.53	111.68
1	B	739	GLY	CA-C-O	-5.58	114.66	122.36
1	D	216	LEU	N-CA-C	-5.58	103.12	110.43
1	B	211	ILE	CA-C-O	-5.57	114.41	120.71
1	B	430	ASP	N-CA-C	5.57	122.67	110.80
1	A	1192	ASP	N-CA-C	-5.57	102.23	110.48
1	C	145	GLY	N-CA-C	5.57	124.65	115.34
1	A	662	THR	CA-CB-CG2	5.57	119.96	110.50
1	D	720	LEU	CA-CB-CG	5.57	135.78	116.30
1	D	902	CYS	N-CA-C	5.57	117.77	109.25
1	D	1118	VAL	CB-CA-C	5.57	119.29	111.94
1	B	251	GLN	CA-C-N	-5.56	117.38	122.28
1	B	251	GLN	C-N-CA	-5.56	117.38	122.28
1	C	692	GLU	N-CA-C	5.56	118.10	107.75
1	A	767	THR	N-CA-C	5.56	118.64	109.85
1	D	874	LEU	N-CA-C	5.56	122.64	110.80
1	A	247	ASP	N-CA-C	-5.56	104.85	111.69
1	D	769	ASN	N-CA-C	5.56	118.09	107.75
1	D	115	PHE	N-CA-C	5.56	118.53	111.69
1	C	214	PRO	N-CA-C	-5.56	107.40	114.35
1	B	1133	PHE	N-CA-C	5.55	117.41	109.14
1	D	944	ARG	CB-CA-C	5.55	120.12	110.68
1	A	1320	THR	N-CA-CB	5.55	120.94	111.50
1	A	624	SER	N-CA-C	5.55	117.41	111.36
1	D	808	VAL	N-CA-CB	5.55	120.14	110.65
1	C	1194	GLY	N-CA-C	-5.55	100.03	113.18
1	B	37	SER	CA-C-N	-5.54	110.80	121.78
1	B	37	SER	C-N-CA	-5.54	110.80	121.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	611	SER	N-CA-C	5.54	118.06	110.24
1	A	422	LYS	CA-C-N	-5.54	112.84	122.37
1	A	422	LYS	C-N-CA	-5.54	112.84	122.37
1	C	88	VAL	N-CA-CB	5.54	116.66	110.51
1	C	564	VAL	CA-C-N	5.54	126.77	119.84
1	C	564	VAL	C-N-CA	5.54	126.77	119.84
1	A	685	GLY	CA-C-N	-5.54	115.22	122.37
1	A	685	GLY	C-N-CA	-5.54	115.22	122.37
1	B	4	ASP	OD1-CG-OD2	5.54	136.20	122.90
1	C	427	ARG	CD-NE-CZ	5.54	132.16	124.40
1	D	193	PRO	CA-C-N	5.54	131.05	120.97
1	D	193	PRO	C-N-CA	5.54	131.05	120.97
1	D	1133	PHE	N-CA-CB	-5.54	102.65	111.62
1	A	830	ARG	NE-CZ-NH1	5.54	127.04	121.50
1	A	1151	PHE	N-CA-C	5.54	118.70	109.96
1	B	989	ASN	N-CA-C	5.54	117.75	111.11
1	C	712	GLU	N-CA-C	5.54	118.50	110.42
1	D	608	LEU	CA-C-N	5.54	130.46	123.10
1	D	608	LEU	C-N-CA	5.54	130.46	123.10
1	D	718	GLY	CA-C-N	5.54	132.11	121.54
1	D	718	GLY	C-N-CA	5.54	132.11	121.54
1	C	280	CYS	CA-C-N	5.53	126.76	119.84
1	C	280	CYS	C-N-CA	5.53	126.76	119.84
1	D	1052	SER	CB-CA-C	-5.53	101.44	110.85
1	A	936	GLY	N-CA-C	-5.53	100.07	113.18
1	A	1021	LEU	CB-CG-CD1	-5.53	94.11	110.70
1	C	1241	ARG	N-CA-C	5.53	117.78	107.99
1	D	371	LYS	N-CA-C	5.53	119.26	107.70
1	B	16	VAL	CA-C-O	5.53	126.56	120.48
1	D	289	SER	N-CA-C	5.53	118.66	110.48
1	B	1163	VAL	CB-CA-C	-5.52	100.82	110.71
1	A	783	VAL	O-C-N	5.52	125.59	121.72
1	B	27	LEU	O-C-N	-5.52	115.50	123.07
1	A	1129	SER	N-CA-C	-5.52	98.92	108.69
1	A	1129	SER	CA-CB-OG	5.52	122.14	111.10
1	B	737	ILE	CB-CA-C	-5.52	103.42	110.98
1	D	777	VAL	CB-CA-C	-5.52	104.91	111.81
1	B	1010	PHE	CA-C-O	-5.51	115.12	121.19
1	C	212	PHE	CA-C-N	5.51	126.06	120.38
1	C	212	PHE	C-N-CA	5.51	126.06	120.38
1	C	463	THR	CA-C-N	-5.51	116.37	122.27
1	C	463	THR	C-N-CA	-5.51	116.37	122.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	756	GLY	N-CA-C	5.51	121.25	114.69
1	A	523	VAL	O-C-N	5.51	127.83	121.94
1	B	339	GLY	N-CA-C	5.51	126.23	113.18
1	A	1176	ARG	NE-CZ-NH1	-5.50	116.00	121.50
1	B	903	LYS	CD-CE-NZ	5.50	129.51	111.90
1	C	994	TRP	N-CA-C	5.50	121.77	114.12
1	D	944	ARG	CA-C-N	5.50	127.65	120.28
1	D	944	ARG	C-N-CA	5.50	127.65	120.28
1	C	162	THR	OG1-CB-CG2	-5.50	98.30	109.30
1	B	1065	SER	CA-C-N	5.50	130.88	121.87
1	B	1065	SER	C-N-CA	5.50	130.88	121.87
1	C	672	VAL	O-C-N	-5.50	117.47	123.18
1	B	87	THR	CA-C-O	-5.49	115.21	121.58
1	A	246	LEU	N-CA-C	5.49	118.02	111.71
1	C	581	LEU	N-CA-C	5.49	122.49	110.80
1	A	1299	SER	N-CA-C	5.49	118.29	108.47
1	A	693	LEU	N-CA-C	5.48	118.75	109.87
1	A	523	VAL	N-CA-C	-5.48	105.27	110.42
1	D	849	VAL	N-CA-C	5.48	115.94	107.78
1	C	714	LYS	N-CA-C	5.48	117.41	108.76
1	C	1314	PHE	N-CA-C	5.48	119.96	112.68
1	D	703	ILE	CB-CA-C	-5.48	104.81	111.87
1	C	70	ALA	CA-C-O	-5.47	114.98	121.06
1	B	1193	ILE	N-CA-CB	5.47	120.26	111.23
1	B	841	HIS	N-CA-C	5.47	117.35	109.48
1	C	936	GLY	N-CA-C	-5.47	100.23	113.18
1	A	943	ARG	NE-CZ-NH2	5.46	124.12	119.20
1	B	1260	VAL	N-CA-C	5.46	120.71	109.34
1	C	1163	VAL	CA-C-O	-5.46	116.22	121.63
1	D	1297	LEU	N-CA-C	5.46	117.30	108.34
1	D	36	LEU	CB-CA-C	-5.46	101.82	111.22
1	D	863	ASP	N-CA-C	5.46	117.66	107.99
1	A	863	ASP	N-CA-C	5.46	117.63	108.73
1	B	1127	SER	CA-C-N	-5.46	114.42	122.83
1	B	1127	SER	C-N-CA	-5.46	114.42	122.83
1	C	688	ILE	N-CA-C	5.46	117.19	108.89
1	A	124	MET	N-CA-C	5.46	117.68	111.02
1	A	698	THR	N-CA-C	5.46	118.19	110.50
1	C	64	LYS	O-C-N	-5.45	117.03	123.25
1	A	830	ARG	N-CA-CB	5.45	117.92	110.01
1	A	986	ASP	N-CA-CB	5.45	118.54	109.60
1	B	997	ARG	N-CA-C	5.45	118.46	109.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	22	PRO	CA-C-N	-5.45	112.52	122.38
1	D	22	PRO	C-N-CA	-5.45	112.52	122.38
1	A	532	LEU	CA-C-N	5.45	131.50	121.70
1	A	532	LEU	C-N-CA	5.45	131.50	121.70
1	A	581	LEU	N-CA-C	5.45	122.40	110.80
1	A	1037	THR	CA-C-N	-5.45	115.53	122.77
1	A	1037	THR	C-N-CA	-5.45	115.53	122.77
1	C	87	THR	CA-C-N	-5.45	113.58	120.60
1	C	87	THR	C-N-CA	-5.45	113.58	120.60
1	C	222	THR	N-CA-CB	-5.45	100.68	110.37
1	C	309	GLU	CA-C-N	5.45	128.12	120.28
1	C	309	GLU	C-N-CA	5.45	128.12	120.28
1	C	1202	GLN	N-CA-C	5.45	117.92	111.33
1	B	301	ALA	N-CA-C	5.44	119.02	112.38
1	C	1253	ALA	N-CA-C	5.44	117.67	109.23
1	C	564	VAL	CB-CA-C	-5.44	105.67	111.00
1	C	1281	ALA	N-CA-C	5.44	122.39	110.80
1	D	525	GLN	N-CA-C	5.44	122.39	110.80
1	D	765	VAL	N-CA-C	5.44	115.96	108.12
1	D	577	PRO	N-CA-C	5.44	119.82	112.48
1	D	1291	VAL	CA-C-N	5.44	132.29	123.37
1	D	1291	VAL	C-N-CA	5.44	132.29	123.37
1	A	278	ILE	CB-CA-C	-5.44	102.52	110.62
1	A	819	LYS	CG-CD-CE	5.44	123.81	111.30
1	D	743	PHE	N-CA-C	5.44	118.84	111.17
1	B	703	ILE	N-CA-C	5.44	115.64	110.53
1	D	604	LEU	N-CA-C	5.43	118.56	110.52
1	D	252	HIS	CA-C-N	5.43	125.04	119.56
1	D	252	HIS	C-N-CA	5.43	125.04	119.56
1	D	900	ARG	N-CA-C	5.43	118.56	110.14
1	A	40	LYS	CD-CE-NZ	5.43	129.26	111.90
1	B	71	ASN	N-CA-CB	5.43	119.27	110.43
1	B	899	GLY	N-CA-C	5.43	119.23	110.87
1	D	707	SER	CA-C-N	5.42	131.90	121.54
1	D	707	SER	C-N-CA	5.42	131.90	121.54
1	C	347	SER	N-CA-CB	-5.42	101.80	110.63
1	A	208	GLN	N-CA-CB	-5.42	102.33	110.73
1	B	276	PRO	CA-C-N	-5.42	115.13	122.77
1	B	276	PRO	C-N-CA	-5.42	115.13	122.77
1	B	772	LYS	CA-C-N	-5.42	112.96	120.38
1	B	772	LYS	C-N-CA	-5.42	112.96	120.38
1	D	1271	ILE	CG1-CB-CG2	-5.42	94.45	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	424	ALA	CA-C-N	5.42	131.45	121.70
1	A	424	ALA	C-N-CA	5.42	131.45	121.70
1	C	249	LYS	N-CA-C	5.42	117.94	111.71
1	B	735	ILE	CB-CA-C	-5.41	104.28	111.80
1	C	348	VAL	CB-CA-C	-5.41	102.41	111.29
1	A	629	VAL	N-CA-C	5.41	114.05	109.02
1	B	655	VAL	N-CA-C	5.41	116.04	110.36
1	D	775	SER	N-CA-CB	5.41	117.91	110.07
1	A	198	PRO	N-CA-C	-5.41	107.59	114.35
1	D	16	VAL	N-CA-C	5.41	114.53	106.85
1	A	1022	LEU	CB-CA-C	5.40	119.13	110.16
1	C	316	VAL	N-CA-C	5.40	116.13	110.62
1	A	67	HIS	N-CA-C	5.40	117.76	109.07
1	A	1315	THR	N-CA-C	-5.40	105.47	111.36
1	D	1234	GLY	N-CA-C	5.40	125.97	113.18
1	B	770	THR	N-CA-C	5.40	116.97	111.14
1	A	431	ILE	CB-CA-C	-5.39	104.36	111.70
1	C	532	LEU	CA-CB-CG	5.39	135.18	116.30
1	C	71	ASN	N-CA-CB	5.39	119.22	110.43
1	C	1310	CYS	N-CA-C	5.39	117.70	109.62
1	C	1332	ARG	N-CA-C	5.39	126.09	111.00
1	A	1137	PRO	CA-C-O	-5.39	115.40	122.19
1	C	955	HIS	N-CA-C	-5.39	106.41	112.87
1	A	203	PRO	CA-C-N	-5.38	111.25	121.54
1	A	203	PRO	C-N-CA	-5.38	111.25	121.54
1	C	991	GLU	N-CA-C	5.38	119.72	113.20
1	D	567	GLY	N-CA-C	5.38	125.94	113.18
1	D	465	SER	CA-C-N	5.38	131.82	121.54
1	D	465	SER	C-N-CA	5.38	131.82	121.54
1	A	36	LEU	O-C-N	5.38	130.00	123.01
1	A	7	VAL	CA-C-N	-5.38	113.75	122.36
1	A	7	VAL	C-N-CA	-5.38	113.75	122.36
1	A	1210	GLU	O-C-N	-5.38	117.20	123.27
1	B	1126	VAL	N-CA-C	5.38	117.13	108.85
1	C	652	ASP	N-CA-CB	5.38	118.12	110.16
1	D	59	ASP	N-CA-CB	5.38	117.77	109.98
1	D	860	LEU	N-CA-C	5.38	117.94	108.75
1	D	885	HIS	N-CA-C	5.38	120.52	112.94
1	A	1245	LEU	O-C-N	5.37	129.34	123.22
1	A	801	GLY	N-CA-C	-5.37	107.12	113.99
1	C	87	THR	CA-C-O	-5.37	115.35	121.58
1	D	564	VAL	CA-C-N	5.37	126.55	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	564	VAL	C-N-CA	5.37	126.55	119.84
1	B	1248	CYS	N-CA-C	5.36	121.66	109.81
1	C	20	ALA	CA-C-O	-5.36	115.12	120.96
1	D	600	TYR	N-CA-C	-5.36	102.05	110.36
1	D	58	TYR	N-CA-C	5.36	118.36	109.46
1	D	474	LEU	CA-C-N	5.36	130.56	122.68
1	D	474	LEU	C-N-CA	5.36	130.56	122.68
1	D	666	HIS	CA-CB-CG	5.36	119.16	113.80
1	D	752	ALA	N-CA-C	5.36	118.19	109.24
1	D	919	GLN	N-CA-CB	5.35	118.25	109.95
1	A	922	LEU	N-CA-C	-5.35	99.40	110.80
1	C	1017	GLN	N-CA-C	5.35	118.15	109.06
1	C	1131	THR	N-CA-C	5.35	116.82	110.19
1	C	596	ASP	CA-C-N	5.35	132.02	122.13
1	C	596	ASP	C-N-CA	5.35	132.02	122.13
1	D	83	VAL	CB-CA-C	-5.35	103.89	111.38
1	A	598	PRO	N-CA-C	5.34	119.62	111.34
1	D	222	THR	N-CA-CB	-5.34	100.86	110.37
1	B	1289	ASN	CA-C-N	5.34	131.75	121.54
1	B	1289	ASN	C-N-CA	5.34	131.75	121.54
1	C	58	TYR	N-CA-C	5.34	117.42	109.25
1	C	247	ASP	CB-CA-C	-5.34	102.46	110.90
1	A	1010	PHE	CA-C-O	-5.34	115.18	121.16
1	B	865	PHE	CB-CA-C	-5.34	103.37	110.79
1	C	716	GLU	N-CA-C	5.34	118.16	109.24
1	D	246	LEU	N-CA-C	5.34	117.85	111.71
1	D	54	MET	N-CA-C	5.34	117.11	108.41
1	C	240	SER	N-CA-C	5.34	120.16	113.43
1	B	510	THR	N-CA-C	-5.33	104.92	111.75
1	D	220	LYS	N-CA-C	5.33	122.16	110.80
1	A	944	ARG	CB-CA-C	5.33	119.74	110.68
1	A	1069	THR	CB-CA-C	-5.33	103.73	111.14
1	B	540	ASP	CA-C-N	5.33	126.50	119.84
1	B	540	ASP	C-N-CA	5.33	126.50	119.84
1	B	891	LYS	CB-CA-C	5.33	118.54	109.53
1	D	778	ALA	N-CA-C	5.33	117.78	111.33
1	A	731	VAL	N-CA-CB	5.33	118.42	112.34
1	B	1197	GLU	CA-C-N	5.33	126.01	119.99
1	B	1197	GLU	C-N-CA	5.33	126.01	119.99
1	D	594	CYS	N-CA-C	5.33	119.26	112.12
1	A	776	PHE	N-CA-CB	5.33	119.23	110.39
1	B	1277	ASP	N-CA-C	-5.33	105.39	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	200	GLU	CB-CA-C	5.33	118.98	110.09
1	A	212	PHE	O-C-N	5.32	126.13	121.18
1	B	154	ARG	O-C-N	5.32	124.58	120.38
1	B	818	TYR	CB-CA-C	-5.32	102.53	110.88
1	C	59	ASP	CA-C-O	-5.32	115.41	121.00
1	C	599	ARG	NE-CZ-NH1	5.32	126.82	121.50
1	A	19	ASN	N-CA-C	5.32	119.00	112.03
1	C	536	CYS	CB-CA-C	-5.32	99.84	110.42
1	C	1105	TYR	CA-C-N	5.32	127.35	120.44
1	C	1105	TYR	C-N-CA	5.32	127.35	120.44
1	A	318	LYS	CG-CD-CE	5.31	123.52	111.30
1	B	512	THR	CA-C-O	-5.31	115.23	121.07
1	D	514	SER	N-CA-C	-5.31	105.39	111.07
1	C	667	ILE	N-CA-CB	-5.31	104.92	110.82
1	B	1039	MET	CB-CA-C	-5.31	102.18	110.94
1	C	1065	SER	CA-C-O	-5.31	113.56	119.67
1	D	31	ARG	NE-CZ-NH1	-5.31	116.19	121.50
1	A	1105	TYR	N-CA-C	-5.30	106.65	113.23
1	B	297	ILE	CB-CA-C	5.30	118.46	110.98
1	C	865	PHE	CA-C-N	5.30	131.67	121.54
1	C	865	PHE	C-N-CA	5.30	131.67	121.54
1	A	628	LYS	CA-CB-CG	5.30	124.70	114.10
1	B	883	LEU	N-CA-C	-5.30	105.15	111.03
1	B	1022	LEU	N-CA-C	5.30	118.12	109.59
1	C	522	THR	CB-CA-C	-5.30	99.36	110.17
1	A	1030	VAL	O-C-N	5.29	128.54	122.93
1	B	40	LYS	CD-CE-NZ	5.29	128.84	111.90
1	B	836	ILE	N-CA-C	5.29	120.35	109.34
1	C	496	LEU	N-CA-C	5.29	118.14	110.14
1	D	621	ILE	N-CA-CB	-5.29	104.11	111.41
1	D	906	LEU	CA-C-N	5.29	125.21	119.76
1	D	906	LEU	C-N-CA	5.29	125.21	119.76
1	A	1108	LYS	CG-CD-CE	5.29	123.46	111.30
1	B	383	VAL	N-CA-C	5.29	116.91	108.87
1	C	380	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	D	203	PRO	N-CA-C	5.29	123.36	112.47
1	B	35	GLY	N-CA-C	5.28	125.70	113.18
1	D	245	LEU	N-CA-C	-5.28	104.96	111.40
1	D	903	LYS	CD-CE-NZ	5.28	128.80	111.90
1	A	417	TYR	N-CA-C	5.28	118.01	109.40
1	D	154	ARG	CA-C-N	5.28	124.73	119.24
1	D	154	ARG	C-N-CA	5.28	124.73	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	770	THR	CB-CA-C	5.28	120.36	110.70
1	C	361	LEU	CA-CB-CG	-5.28	97.82	116.30
1	B	793	LYS	N-CA-C	-5.28	105.66	112.68
1	A	1078	THR	N-CA-C	-5.28	98.06	107.98
1	B	995	LYS	CD-CE-NZ	5.28	128.78	111.90
1	C	113	CYS	O-C-N	5.28	128.18	122.11
1	A	651	ASN	CA-C-O	-5.27	112.97	120.51
1	B	906	LEU	N-CA-C	-5.27	99.91	108.82
1	B	19	ASN	N-CA-C	5.27	118.94	112.03
1	B	533	GLU	CB-CA-C	5.27	120.19	111.23
1	B	769	ASN	N-CA-C	5.27	117.80	107.57
1	A	1055	LEU	N-CA-C	-5.27	107.02	113.50
1	C	876	GLN	CA-CB-CG	-5.27	103.56	114.10
1	B	1169	THR	N-CA-C	5.27	119.84	113.41
1	B	1189	PRO	CB-CA-C	-5.27	103.48	111.44
1	C	607	ARG	NE-CZ-NH1	-5.27	116.23	121.50
1	B	578	LEU	N-CA-C	-5.27	103.13	109.72
1	A	377	ARG	N-CA-C	5.27	116.83	108.67
1	A	147	LEU	CA-C-O	-5.26	115.01	120.70
1	B	1085	ASP	CA-C-N	-5.26	112.31	120.31
1	B	1085	ASP	C-N-CA	-5.26	112.31	120.31
1	C	690	TYR	N-CA-C	5.26	118.06	109.59
1	A	689	THR	N-CA-C	5.26	116.97	108.34
1	D	767	THR	N-CA-C	5.26	117.67	109.52
1	D	1295	PHE	O-C-N	5.26	129.34	123.19
1	B	53	VAL	N-CA-C	5.26	116.28	108.65
1	B	1299	SER	N-CA-CB	5.26	116.85	110.17
1	A	194	SER	CA-C-N	5.26	131.20	121.52
1	A	194	SER	C-N-CA	5.26	131.20	121.52
1	A	1192	ASP	CA-C-O	-5.26	115.42	121.47
1	C	369	GLY	N-CA-C	-5.26	100.72	113.18
1	D	59	ASP	CA-C-O	-5.26	115.48	120.90
1	A	898	THR	N-CA-C	5.25	117.85	109.81
1	B	25	THR	N-CA-CB	-5.25	102.60	110.17
1	D	1208	THR	N-CA-C	5.25	122.62	114.64
1	C	707	SER	CA-C-N	5.25	130.25	123.00
1	C	707	SER	C-N-CA	5.25	130.25	123.00
1	A	591	ALA	N-CA-C	-5.25	102.28	110.10
1	D	431	ILE	O-C-N	5.25	128.22	122.76
1	A	600	TYR	CA-C-N	-5.25	111.44	121.94
1	A	600	TYR	C-N-CA	-5.25	111.44	121.94
1	A	610	THR	CB-CA-C	-5.25	100.88	109.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	646	ILE	CB-CA-C	5.25	118.48	111.19
1	D	880	GLU	N-CA-C	-5.25	105.46	111.07
1	A	920	GLY	N-CA-C	5.25	125.61	113.18
1	D	27	LEU	CA-C-N	-5.24	111.53	121.54
1	D	27	LEU	C-N-CA	-5.24	111.53	121.54
1	C	871	THR	N-CA-C	-5.24	100.55	108.52
1	D	1153	TYR	CA-C-O	-5.24	115.54	121.25
1	A	507	PHE	N-CA-C	-5.24	105.21	111.03
1	D	1182	ASP	CA-C-O	5.24	126.64	120.98
1	B	1263	PRO	O-C-N	5.24	127.64	121.46
1	B	1296	ARG	NE-CZ-NH2	5.24	123.91	119.20
1	C	645	ASN	CA-C-N	-5.24	115.77	123.10
1	C	645	ASN	C-N-CA	-5.24	115.77	123.10
1	B	1330	SER	CA-C-N	5.23	131.39	121.97
1	B	1330	SER	C-N-CA	5.23	131.39	121.97
1	B	307	ILE	CA-C-N	-5.23	113.85	120.60
1	B	307	ILE	C-N-CA	-5.23	113.85	120.60
1	D	131	GLN	CA-C-N	-5.23	114.56	120.89
1	D	131	GLN	C-N-CA	-5.23	114.56	120.89
1	A	869	GLY	N-CA-C	5.23	121.73	112.53
1	B	1133	PHE	N-CA-CB	-5.23	103.15	111.62
1	D	1265	LEU	CA-C-N	-5.23	112.87	120.29
1	D	1265	LEU	C-N-CA	-5.23	112.87	120.29
1	A	163	PHE	CB-CA-C	-5.22	101.07	110.37
1	B	659	ASP	N-CA-C	5.22	121.93	110.80
1	C	440	VAL	N-CA-C	5.22	116.24	108.46
1	A	1035	GLY	N-CA-C	5.22	120.08	113.24
1	B	161	ARG	CB-CG-CD	5.22	123.30	111.30
1	B	431	ILE	N-CA-C	5.22	115.48	108.17
1	C	1125	THR	CB-CA-C	5.22	120.81	110.42
1	D	383	VAL	N-CA-C	5.22	116.80	108.87
1	C	509	CYS	N-CA-C	5.22	117.37	111.11
1	D	610	THR	CB-CA-C	-5.22	98.79	109.38
1	A	1133	PHE	N-CA-C	5.21	117.33	109.41
1	C	294	PRO	N-CA-C	-5.21	107.83	114.35
1	D	847	TYR	N-CA-C	5.21	117.11	109.24
1	A	773	THR	N-CA-CB	5.21	118.38	110.14
1	A	814	ALA	CA-C-N	5.21	127.27	120.28
1	A	814	ALA	C-N-CA	5.21	127.27	120.28
1	D	1192	ASP	N-CA-C	-5.21	103.65	110.53
1	B	334	LEU	CA-C-N	-5.21	111.82	120.68
1	B	334	LEU	C-N-CA	-5.21	111.82	120.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1066	GLU	N-CA-C	5.21	116.72	108.96
1	B	23	GLU	N-CA-C	5.21	119.26	113.01
1	B	827	MET	CG-SD-CE	-5.21	89.45	100.90
1	C	813	VAL	N-CA-C	5.21	115.83	110.36
1	D	360	ASP	N-CA-C	-5.21	106.98	113.38
1	A	65	ILE	CB-CA-C	-5.20	103.36	110.96
1	A	375	VAL	N-CA-C	5.20	117.54	108.90
1	A	890	TYR	N-CA-C	5.20	117.97	109.59
1	B	65	ILE	CA-C-O	-5.20	114.98	120.39
1	D	591	ALA	CA-C-N	5.20	128.06	120.98
1	D	591	ALA	C-N-CA	5.20	128.06	120.98
1	B	886	MET	N-CA-C	5.20	118.72	112.38
1	C	396	THR	CB-CA-C	-5.20	102.45	114.41
1	A	709	TYR	N-CA-C	5.20	121.87	110.80
1	C	148	CYS	CA-CB-SG	5.20	126.35	114.40
1	A	88	VAL	N-CA-CB	5.20	116.63	110.55
1	A	865	PHE	CB-CA-C	-5.20	104.61	111.42
1	C	1300	PRO	N-CA-C	-5.20	101.77	112.47
1	C	720	LEU	CA-CB-CG	5.19	134.48	116.30
1	B	944	ARG	CA-CB-CG	5.19	124.48	114.10
1	C	680	GLN	N-CA-C	5.19	119.88	111.37
1	A	47	GLY	N-CA-C	5.19	125.48	113.18
1	B	294	PRO	N-CA-C	-5.19	107.87	114.35
1	C	262	THR	CA-C-O	5.19	125.92	119.12
1	B	460	ALA	CA-C-N	5.19	127.75	120.28
1	B	460	ALA	C-N-CA	5.19	127.75	120.28
1	C	612	THR	N-CA-C	-5.18	106.64	113.17
1	D	97	ARG	N-CA-C	-5.18	100.25	109.06
1	A	424	ALA	CA-C-O	5.18	121.59	118.33
1	C	83	VAL	CB-CA-C	-5.18	103.96	111.68
1	D	278	ILE	N-CA-C	5.18	115.94	108.48
1	A	131	GLN	CA-CB-CG	5.18	124.45	114.10
1	C	693	LEU	N-CA-C	5.18	118.26	109.87
1	D	919	GLN	CA-C-O	5.18	126.59	120.69
1	B	652	ASP	CA-C-O	-5.18	115.38	120.82
1	C	475	SER	N-CA-C	5.18	118.38	111.24
1	D	923	ILE	N-CA-CB	5.17	119.77	111.23
1	A	608	LEU	O-C-N	5.17	129.60	123.24
1	D	485	ASP	N-CA-C	-5.17	105.77	111.71
1	A	636	ILE	CA-CB-CG2	5.17	119.28	110.50
1	B	500	ALA	CA-C-N	-5.17	115.41	120.52
1	B	500	ALA	C-N-CA	-5.17	115.41	120.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	669	GLY	CA-C-O	-5.17	115.96	121.38
1	C	696	ILE	N-CA-C	5.16	115.29	107.80
1	D	1038	GLU	N-CA-C	5.16	116.67	108.67
1	A	218	ARG	N-CA-C	-5.16	105.84	111.82
1	B	610	THR	CA-C-N	5.16	129.00	121.31
1	B	610	THR	C-N-CA	5.16	129.00	121.31
1	A	593	TYR	CA-C-N	-5.16	111.69	121.54
1	A	593	TYR	C-N-CA	-5.16	111.69	121.54
1	B	278	ILE	N-CA-C	5.16	115.91	108.48
1	C	237	ILE	CB-CA-C	-5.16	103.46	110.42
1	C	690	TYR	CA-CB-CG	5.15	123.18	113.90
1	A	299	PHE	CB-CA-C	-5.15	100.37	109.70
1	B	246	LEU	N-CA-C	5.15	118.34	111.75
1	C	587	ALA	CA-C-N	-5.15	114.51	122.49
1	C	587	ALA	C-N-CA	-5.15	114.51	122.49
1	B	475	SER	N-CA-C	5.15	118.34	111.24
1	B	847	TYR	N-CA-C	5.15	117.63	109.50
1	C	25	THR	N-CA-CB	-5.14	101.90	110.23
1	C	900	ARG	CA-C-N	-5.14	115.37	123.13
1	C	900	ARG	C-N-CA	-5.14	115.37	123.13
1	A	39	THR	CA-C-O	-5.14	115.63	121.39
1	B	164	ALA	N-CA-C	5.14	117.17	108.02
1	D	667	ILE	N-CA-CB	-5.14	105.12	110.82
1	B	513	LEU	CA-C-N	5.14	127.16	120.28
1	B	513	LEU	C-N-CA	5.14	127.16	120.28
1	B	602	ASN	CA-C-N	-5.14	115.63	122.72
1	B	602	ASN	C-N-CA	-5.14	115.63	122.72
1	B	263	GLU	N-CA-C	-5.13	105.24	112.12
1	B	1261	GLY	N-CA-C	5.13	125.35	113.18
1	D	819	LYS	CG-CD-CE	5.13	123.11	111.30
1	B	1316	THR	N-CA-C	5.13	116.95	111.36
1	C	803	GLU	N-CA-CB	-5.13	102.32	110.22
1	B	334	LEU	N-CA-C	5.13	119.01	112.34
1	C	908	SER	N-CA-C	5.13	117.66	109.96
1	A	919	GLN	N-CA-CB	5.13	117.49	109.85
1	A	1206	LEU	N-CA-C	5.13	118.32	111.75
1	B	470	THR	N-CA-C	5.13	117.28	111.02
1	A	865	PHE	CA-C-N	5.13	131.33	121.54
1	A	865	PHE	C-N-CA	5.13	131.33	121.54
1	C	60	ARG	N-CA-CB	5.13	119.16	110.49
1	A	746	GLU	N-CA-CB	5.13	117.49	109.85
1	B	681	ARG	N-CA-C	5.13	117.53	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1064	ILE	CA-C-O	-5.13	114.67	120.67
1	D	587	ALA	CA-C-N	-5.12	114.61	122.60
1	D	587	ALA	C-N-CA	-5.12	114.61	122.60
1	A	943	ARG	N-CA-C	-5.12	105.15	111.40
1	B	987	LYS	N-CA-C	-5.12	99.89	110.80
1	D	937	MET	CA-C-N	5.12	126.24	119.84
1	D	937	MET	C-N-CA	5.12	126.24	119.84
1	D	818	TYR	CA-C-N	5.12	127.41	120.65
1	D	818	TYR	C-N-CA	5.12	127.41	120.65
1	D	1160	CYS	CA-CB-SG	-5.12	102.62	114.40
1	A	1052	SER	CB-CA-C	-5.11	102.82	110.90
1	B	756	GLY	N-CA-C	5.11	120.81	114.37
1	B	892	ILE	N-CA-CB	-5.11	104.05	111.21
1	A	1229	LYS	CA-C-O	-5.11	115.86	121.58
1	B	225	LYS	CA-C-N	-5.11	113.03	120.75
1	B	225	LYS	C-N-CA	-5.11	113.03	120.75
1	C	618	ILE	CB-CA-C	5.11	116.76	111.09
1	D	941	GLU	N-CA-C	-5.11	105.71	111.28
1	B	939	ALA	N-CA-C	5.11	117.51	111.33
1	D	659	ASP	N-CA-C	5.11	121.68	110.80
1	A	1027	ASP	CA-C-N	-5.11	115.29	123.31
1	A	1027	ASP	C-N-CA	-5.11	115.29	123.31
1	B	290	VAL	N-CA-CB	5.11	120.66	111.21
1	B	1211	GLU	CA-C-N	-5.11	115.04	122.65
1	B	1211	GLU	C-N-CA	-5.11	115.04	122.65
1	A	779	LYS	N-CA-CB	5.11	117.41	110.01
1	C	1002	ILE	CA-C-N	5.11	126.22	119.84
1	C	1002	ILE	C-N-CA	5.11	126.22	119.84
1	C	1208	THR	CB-CA-C	-5.11	99.73	110.45
1	D	56	SER	N-CA-C	-5.11	101.83	109.95
1	C	1086	LEU	N-CA-CB	5.10	117.41	110.01
1	A	1011	THR	CB-CA-C	-5.10	102.23	110.79
1	A	1172	HIS	N-CA-C	5.10	117.42	109.52
1	A	1196	VAL	N-CA-CB	5.10	115.97	110.62
1	D	1129	SER	CA-CB-OG	5.10	121.30	111.10
1	A	851	PHE	N-CA-C	5.09	116.99	108.99
1	B	435	THR	N-CA-C	-5.09	101.45	109.50
1	B	657	ALA	O-C-N	5.09	129.19	122.97
1	A	319	LEU	CA-C-N	5.09	126.21	119.84
1	A	319	LEU	C-N-CA	5.09	126.21	119.84
1	D	641	VAL	N-CA-C	-5.09	103.96	108.95
1	A	683	ALA	CA-C-O	5.09	127.79	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	840	ARG	O-C-N	5.09	129.34	122.82
1	B	160	PHE	N-CA-C	5.09	119.11	113.01
1	D	246	LEU	O-C-N	5.08	128.17	122.22
1	D	10	VAL	CB-CA-C	-5.08	104.38	110.99
1	D	411	TYR	N-CA-C	-5.08	103.82	110.53
1	A	1076	SER	CB-CA-C	5.08	117.45	109.27
1	B	68	PHE	N-CA-C	5.08	116.79	109.07
1	C	1099	LEU	CA-CB-CG	5.08	134.08	116.30
1	D	1004	THR	N-CA-C	5.08	116.24	108.52
1	C	1083	SER	CA-CB-OG	5.08	121.25	111.10
1	B	370	ALA	CA-C-O	-5.08	115.68	121.82
1	A	376	SER	N-CA-C	-5.07	101.70	108.34
1	A	1219	SER	N-CA-C	-5.07	100.98	109.24
1	D	1318	CYS	CA-C-N	5.07	131.09	121.97
1	D	1318	CYS	C-N-CA	5.07	131.09	121.97
1	B	155	PRO	CB-CA-C	-5.06	103.83	112.64
1	D	291	GLU	N-CA-C	5.06	116.67	108.26
1	A	116	CYS	N-CA-C	-5.06	107.08	113.20
1	A	932	ALA	CA-C-N	-5.06	116.38	122.35
1	A	932	ALA	C-N-CA	-5.06	116.38	122.35
1	C	686	VAL	O-C-N	5.06	128.72	122.95
1	C	1127	SER	CA-C-N	-5.06	114.62	122.67
1	C	1127	SER	C-N-CA	-5.06	114.62	122.67
1	B	215	GLU	CA-CB-CG	-5.06	103.98	114.10
1	B	512	THR	N-CA-C	-5.06	104.84	111.02
1	A	1246	ARG	NE-CZ-NH1	-5.06	116.44	121.50
1	B	1030	VAL	CA-C-O	-5.06	114.75	120.67
1	C	476	LYS	CA-C-O	5.06	124.77	119.91
1	D	997	ARG	N-CA-C	5.06	117.85	109.85
1	D	1085	ASP	CB-CA-C	-5.06	102.91	110.90
1	A	8	PHE	CA-C-N	-5.06	115.35	122.94
1	A	8	PHE	C-N-CA	-5.06	115.35	122.94
1	B	163	PHE	CA-C-N	-5.06	115.68	122.86
1	B	163	PHE	C-N-CA	-5.06	115.68	122.86
1	C	414	GLU	N-CA-C	5.06	116.43	109.15
1	C	627	LYS	N-CA-CB	5.06	119.04	110.49
1	C	953	LEU	N-CA-C	5.06	117.66	109.06
1	A	667	ILE	N-CA-C	5.05	115.56	108.89
1	B	272	ASN	N-CA-C	5.05	121.57	110.80
1	B	564	VAL	CB-CA-C	-5.05	106.24	110.94
1	C	636	ILE	CB-CA-C	5.05	117.18	110.91
1	B	161	ARG	N-CA-C	-5.05	105.05	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1106	LYS	N-CA-C	-5.05	105.46	110.97
1	A	825	ARG	CB-CG-CD	5.05	122.92	111.30
1	A	862	VAL	CB-CA-C	-5.05	102.30	110.28
1	A	1183	VAL	CA-C-O	5.05	124.65	119.35
1	B	278	ILE	CB-CA-C	-5.05	103.09	110.62
1	A	68	PHE	N-CA-C	5.05	116.48	108.96
1	A	7	VAL	CB-CA-C	-5.05	103.26	110.12
1	A	133	GLU	N-CA-CB	-5.04	104.79	111.40
1	B	453	ALA	N-CA-C	5.04	117.56	108.48
1	C	758	ALA	N-CA-C	5.04	118.56	111.90
1	A	1153	TYR	N-CA-C	-5.04	100.77	107.88
1	B	1208	THR	CB-CA-C	-5.04	101.68	109.29
1	A	1081	SER	CA-C-O	5.04	123.31	119.18
1	B	485	ASP	N-CA-C	-5.04	105.98	111.82
1	D	30	LEU	CA-C-O	5.04	125.89	120.70
1	A	220	LYS	N-CA-C	5.04	121.53	110.80
1	C	161	ARG	CB-CG-CD	5.04	122.89	111.30
1	D	468	LYS	N-CA-C	-5.04	105.68	111.07
1	D	1080	ALA	N-CA-C	5.04	120.05	113.20
1	A	356	SER	CA-C-N	5.03	125.06	119.32
1	A	356	SER	C-N-CA	5.03	125.06	119.32
1	A	751	ILE	N-CA-C	-5.03	100.53	108.23
1	D	1105	TYR	CB-CA-C	5.03	119.78	109.67
1	C	720	LEU	N-CA-C	-5.03	100.09	110.80
1	D	829	ASP	N-CA-C	-5.03	103.08	110.52
1	A	1002	ILE	CA-C-N	5.03	126.12	119.84
1	A	1002	ILE	C-N-CA	5.03	126.12	119.84
1	B	345	VAL	CA-C-N	-5.03	114.23	121.42
1	B	345	VAL	C-N-CA	-5.03	114.23	121.42
1	A	1090	ALA	N-CA-C	5.02	116.44	111.07
1	C	1055	LEU	CA-C-O	5.02	124.67	119.14
1	B	496	LEU	N-CA-C	5.02	117.47	109.64
1	C	423	GLN	N-CA-C	5.02	116.59	108.26
1	A	667	ILE	N-CA-CB	-5.02	105.06	110.53
1	C	692	GLU	N-CA-CB	-5.02	102.11	110.39
1	A	69	SER	CA-CB-OG	-5.02	101.06	111.10
1	A	921	MET	N-CA-C	-5.01	100.12	110.80
1	B	58	TYR	N-CA-C	5.01	117.78	109.46
1	B	147	LEU	CB-CA-C	-5.01	100.62	109.70
1	D	735	ILE	CA-C-O	-5.01	116.03	121.19
1	C	258	VAL	N-CA-C	5.01	115.19	108.17
1	C	760	GLU	N-CA-C	5.01	117.50	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1001	ILE	N-CA-CB	-5.01	104.57	111.99
1	D	1035	GLY	CA-C-O	-5.01	113.74	119.65
1	A	234	VAL	N-CA-C	5.01	116.56	108.85
1	A	102	GLN	CB-CA-C	-5.01	102.38	110.79
1	C	485	ASP	N-CA-C	-5.01	105.90	111.36
1	B	1052	SER	CB-CA-C	-5.00	102.35	110.85
1	B	55	LEU	N-CA-C	5.00	117.71	109.76
1	D	751	ILE	CA-C-O	-5.00	115.04	120.84

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	165	ARG	CA
1	C	165	ARG	CA

All (198) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1299	SER	Peptide
1	A	1318	CYS	Peptide
1	A	1319	VAL	Peptide
1	A	140	GLU	Peptide
1	A	164	ALA	Peptide
1	A	202	THR	Peptide
1	A	222	THR	Peptide
1	A	294	PRO	Peptide
1	A	337	PHE	Peptide
1	A	339	GLY	Peptide
1	A	354	THR	Peptide
1	A	423	GLN	Peptide
1	A	430	ASP	Peptide
1	A	446	THR	Peptide
1	A	460	ALA	Peptide
1	A	466	ALA	Peptide
1	A	504	MET	Peptide
1	A	527	LEU	Peptide
1	A	528	GLY	Peptide
1	A	529	GLN	Peptide
1	A	531	ASN	Peptide
1	A	664	VAL	Peptide
1	A	665	GLY	Peptide
1	A	684	GLN	Peptide

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Mol	Chain	Res	Type	Group
1	A	700	GLU	Peptide
1	A	707	SER	Peptide
1	A	718	GLY	Peptide
1	A	719	ASP	Peptide
1	A	731	VAL	Peptide
1	A	838	GLY	Peptide
1	A	865	PHE	Peptide,Mainchain
1	A	891	LYS	Peptide
1	A	892	ILE	Peptide
1	A	919	GLN	Peptide
1	A	920	GLY	Peptide
1	A	926	CYS	Peptide
1	A	936	GLY	Peptide
1	A	937	MET	Peptide
1	A	979	HIS	Peptide
1	B	1299	SER	Peptide
1	B	1327	LYS	Peptide
1	B	1331	VAL	Peptide
1	B	140	GLU	Peptide
1	B	164	ALA	Peptide
1	B	202	THR	Peptide
1	B	221	ASP	Peptide
1	B	222	THR	Peptide
1	B	271	LYS	Peptide
1	B	294	PRO	Peptide
1	B	3	ALA	Peptide
1	B	337	PHE	Peptide
1	B	339	GLY	Peptide
1	B	354	THR	Peptide
1	B	38	GLY	Peptide
1	B	423	GLN	Peptide
1	B	424	ALA	Peptide
1	B	430	ASP	Peptide
1	B	431	ILE	Peptide
1	B	443	LYS	Peptide
1	B	446	THR	Peptide
1	B	466	ALA	Peptide
1	B	523	VAL	Peptide
1	B	528	GLY	Peptide,Mainchain
1	B	530	GLU	Peptide
1	B	531	ASN	Peptide
1	B	532	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	B	534	ASP	Peptide
1	B	536	CYS	Peptide
1	B	540	ASP	Peptide
1	B	541	PRO	Peptide
1	B	542	THR	Peptide
1	B	544	ALA	Peptide
1	B	590	GLU	Peptide
1	B	623	THR	Peptide
1	B	664	VAL	Peptide
1	B	665	GLY	Peptide
1	B	683	ALA	Peptide
1	B	684	GLN	Peptide
1	B	707	SER	Peptide
1	B	708	PHE	Peptide
1	B	718	GLY	Peptide
1	B	719	ASP	Peptide
1	B	731	VAL	Peptide
1	B	865	PHE	Peptide,Mainchain
1	B	892	ILE	Peptide
1	B	920	GLY	Peptide,Mainchain
1	B	926	CYS	Peptide
1	B	936	GLY	Peptide
1	B	937	MET	Peptide
1	B	979	HIS	Peptide
1	C	1079	ALA	Peptide
1	C	1144	GLU	Peptide
1	C	1268	ALA	Peptide
1	C	1299	SER	Peptide
1	C	140	GLU	Peptide
1	C	150	CYS	Peptide
1	C	193	PRO	Peptide
1	C	202	THR	Peptide
1	C	222	THR	Peptide
1	C	294	PRO	Peptide
1	C	337	PHE	Peptide
1	C	354	THR	Peptide
1	C	424	ALA	Peptide
1	C	443	LYS	Peptide
1	C	446	THR	Peptide
1	C	466	ALA	Peptide
1	C	504	MET	Peptide
1	C	528	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	C	530	GLU	Peptide
1	C	532	LEU	Peptide
1	C	533	GLU	Peptide
1	C	534	ASP	Peptide
1	C	535	LYS	Peptide
1	C	536	CYS	Peptide
1	C	538	LYS	Peptide
1	C	540	ASP	Peptide
1	C	546	ALA	Peptide
1	C	567	GLY	Peptide
1	C	664	VAL	Peptide
1	C	665	GLY	Peptide
1	C	683	ALA	Peptide
1	C	684	GLN	Peptide
1	C	700	GLU	Peptide
1	C	707	SER	Peptide,Mainchain
1	C	708	PHE	Peptide
1	C	718	GLY	Peptide
1	C	719	ASP	Peptide
1	C	731	VAL	Peptide
1	C	865	PHE	Peptide
1	C	891	LYS	Peptide
1	C	892	ILE	Peptide
1	C	920	GLY	Peptide,Mainchain
1	C	926	CYS	Peptide
1	C	936	GLY	Peptide
1	C	937	MET	Peptide
1	C	979	HIS	Peptide,Mainchain
1	D	1079	ALA	Peptide
1	D	1144	GLU	Peptide
1	D	1299	SER	Peptide
1	D	131	GLN	Peptide
1	D	1327	LYS	Peptide
1	D	140	GLU	Peptide
1	D	164	ALA	Peptide
1	D	193	PRO	Peptide
1	D	202	THR	Peptide
1	D	222	THR	Peptide
1	D	271	LYS	Peptide
1	D	281	PRO	Peptide
1	D	294	PRO	Peptide
1	D	337	PHE	Peptide

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Mol	Chain	Res	Type	Group
1	D	339	GLY	Peptide
1	D	354	THR	Peptide
1	D	429	ASP	Peptide
1	D	431	ILE	Peptide
1	D	443	LYS	Peptide
1	D	446	THR	Peptide
1	D	466	ALA	Peptide
1	D	527	LEU	Peptide
1	D	528	GLY	Peptide
1	D	530	GLU	Peptide
1	D	532	LEU	Peptide
1	D	533	GLU	Peptide
1	D	535	LYS	Peptide
1	D	536	CYS	Peptide
1	D	538	LYS	Peptide
1	D	540	ASP	Peptide
1	D	649	ILE	Peptide
1	D	664	VAL	Peptide
1	D	665	GLY	Peptide,Mainchain
1	D	684	GLN	Peptide,Mainchain
1	D	699	ILE	Peptide
1	D	700	GLU	Peptide
1	D	707	SER	Peptide,Mainchain
1	D	718	GLY	Peptide
1	D	719	ASP	Peptide
1	D	731	VAL	Peptide
1	D	865	PHE	Peptide,Mainchain
1	D	891	LYS	Peptide
1	D	892	ILE	Peptide
1	D	919	GLN	Peptide
1	D	920	GLY	Peptide,Mainchain
1	D	926	CYS	Peptide
1	D	936	GLY	Peptide
1	D	937	MET	Peptide
1	D	979	HIS	Peptide,Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9764	0	9788	663	0
1	B	9951	0	9967	736	0
1	C	9905	0	9922	680	0
1	D	9910	0	9929	674	0
2	A	8	0	0	2	0
2	B	8	0	0	2	0
2	C	8	0	0	0	0
2	D	8	0	0	0	0
3	A	53	0	30	10	0
3	B	53	0	29	6	0
3	C	53	0	29	9	0
3	D	53	0	29	14	0
4	A	6	0	8	6	0
4	B	6	0	8	14	0
4	C	6	0	8	4	0
4	D	6	0	8	11	0
5	D	4	0	3	0	0
6	D	5	0	0	1	0
All	All	39807	0	39758	2697	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 34.

All (2697) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:793:LYS:CG	1:D:793:LYS:CD	1.74	1.62
1:C:1319:VAL:CA	1:C:1319:VAL:CB	1.77	1.61
1:D:903:LYS:CD	1:D:903:LYS:CE	1.75	1.61
1:B:1319:VAL:CA	1:B:1319:VAL:CB	1.78	1.61
1:A:318:LYS:CE	1:A:318:LYS:CD	1.76	1.61
1:C:599:ARG:CB	1:C:599:ARG:CG	1.79	1.59
1:D:599:ARG:CG	1:D:599:ARG:CB	1.75	1.59
1:C:269:LYS:CE	1:C:269:LYS:CD	1.75	1.59
1:C:318:LYS:CD	1:C:318:LYS:CE	1.74	1.59
1:C:1291:VAL:CA	1:C:1291:VAL:CB	1.75	1.59
1:D:1291:VAL:CA	1:D:1291:VAL:CB	1.75	1.59
1:B:3:ALA:CA	1:B:3:ALA:CB	1.77	1.59
1:B:431:ILE:CB	1:B:431:ILE:CA	1.81	1.58
1:A:1108:LYS:CE	1:A:1108:LYS:CD	1.75	1.58
1:A:762:GLU:CG	1:A:762:GLU:CD	1.76	1.57
1:C:688:ILE:CG1	1:C:688:ILE:CD1	1.81	1.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:811:THR:CB	1:A:811:THR:CG2	1.75	1.56
1:A:318:LYS:CD	1:A:318:LYS:CG	1.77	1.56
1:C:64:LYS:CE	1:C:64:LYS:CD	1.76	1.56
1:B:688:ILE:CD1	1:B:688:ILE:CG1	1.80	1.56
1:B:1291:VAL:CA	1:B:1291:VAL:CB	1.75	1.55
1:B:599:ARG:CG	1:B:599:ARG:CD	1.82	1.54
1:C:903:LYS:NZ	1:C:903:LYS:CE	1.70	1.54
1:C:599:ARG:CG	1:C:599:ARG:CD	1.82	1.53
1:D:599:ARG:CG	1:D:599:ARG:CD	1.82	1.53
1:A:646:ILE:CG1	1:A:646:ILE:CD1	1.86	1.51
1:A:903:LYS:NZ	1:A:903:LYS:CE	1.70	1.51
1:A:1108:LYS:CE	1:A:1108:LYS:NZ	1.71	1.51
1:D:269:LYS:NZ	1:D:269:LYS:CE	1.68	1.51
1:D:903:LYS:CE	1:D:903:LYS:NZ	1.72	1.51
1:A:431:ILE:CG1	1:A:431:ILE:CD1	1.90	1.49
1:B:646:ILE:CG1	1:B:646:ILE:CD1	1.85	1.49
1:D:606:LEU:HD23	1:D:607:ARG:N	1.18	1.48
1:B:3:ALA:CA	1:B:3:ALA:N	1.77	1.47
1:B:430:ASP:CG	1:B:1229:LYS:HE2	1.38	1.46
1:B:40:LYS:NZ	1:B:40:LYS:CE	1.78	1.44
1:D:51:CYS:CB	1:D:51:CYS:SG	2.04	1.44
1:D:1318:CYS:CB	1:D:1318:CYS:SG	2.05	1.44
1:A:1109:ASN:HB2	1:C:1316:THR:CG2	1.50	1.42
1:D:430:ASP:CG	1:D:1229:LYS:HE2	1.46	1.40
1:B:1318:CYS:SG	1:B:1318:CYS:CB	2.11	1.39
1:A:78:CYS:SG	1:A:78:CYS:CB	2.09	1.38
1:B:1289:ASN:HB2	1:C:380:ARG:NH1	1.02	1.35
1:B:1289:ASN:CB	1:C:380:ARG:NH1	1.90	1.34
1:D:159:GLY:O	1:D:162:THR:HG22	1.27	1.33
1:A:606:LEU:HD23	1:A:607:ARG:N	1.40	1.32
1:D:31:ARG:HH11	1:D:31:ARG:CG	1.41	1.31
1:B:647:THR:CG2	1:B:648:GLY:H	1.43	1.31
1:C:647:THR:CG2	1:C:648:GLY:H	1.42	1.31
1:D:699:ILE:O	1:D:702:ALA:HB3	1.26	1.27
1:B:606:LEU:HD23	1:B:607:ARG:N	1.45	1.26
1:B:916:GLY:N	4:B:3007:GOL:H32	1.50	1.26
1:B:534:ASP:OD1	1:C:251:GLN:HB3	1.36	1.25
1:D:430:ASP:HB3	1:D:1229:LYS:NZ	1.51	1.24
1:B:430:ASP:HB3	1:B:1229:LYS:NZ	1.51	1.23
1:A:1109:ASN:CB	1:C:1316:THR:HG21	1.69	1.23
1:A:647:THR:CG2	1:A:648:GLY:H	1.51	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:ASP:OD2	1:B:1229:LYS:CD	1.88	1.21
1:B:699:ILE:O	1:B:702:ALA:HB3	1.41	1.19
1:C:606:LEU:HD23	1:C:607:ARG:N	1.55	1.19
1:B:523:VAL:HG12	1:B:524:LEU:N	1.36	1.18
1:D:606:LEU:CD2	1:D:607:ARG:H	1.56	1.18
1:A:31:ARG:HH11	1:A:31:ARG:CG	1.55	1.18
1:D:430:ASP:CB	1:D:1229:LYS:HE2	1.72	1.18
1:B:430:ASP:CG	1:B:1229:LYS:CE	2.17	1.17
1:C:607:ARG:HE	1:C:679:THR:CG2	1.56	1.17
1:C:159:GLY:O	1:C:162:THR:HG22	1.42	1.16
1:A:607:ARG:HE	1:A:679:THR:HG23	1.09	1.16
1:B:607:ARG:HE	1:B:679:THR:CG2	1.57	1.16
1:A:699:ILE:O	1:A:702:ALA:HB3	1.44	1.15
1:A:31:ARG:HH11	1:A:31:ARG:HG3	1.05	1.14
1:D:607:ARG:HE	1:D:679:THR:HG23	0.97	1.14
1:A:910:THR:HG23	1:A:911:ALA:H	1.11	1.14
1:D:606:LEU:CD2	1:D:607:ARG:N	2.10	1.14
1:A:27:LEU:O	1:A:28:ALA:CB	1.96	1.13
1:C:376:SER:HB3	1:C:379:THR:OG1	1.48	1.13
1:D:920:GLY:HA3	1:D:923:ILE:HG12	1.28	1.13
1:A:374:LEU:N	1:A:374:LEU:HD23	1.51	1.13
1:B:937:MET:HB2	1:B:938:PRO:CA	1.74	1.12
1:B:937:MET:HB2	1:B:938:PRO:HA	1.16	1.12
1:C:31:ARG:HH11	1:C:31:ARG:HG3	1.11	1.11
1:A:607:ARG:HE	1:A:679:THR:CG2	1.62	1.11
1:D:937:MET:HB2	1:D:938:PRO:HA	1.28	1.11
1:C:27:LEU:O	1:C:28:ALA:CB	1.98	1.11
1:B:607:ARG:HE	1:B:679:THR:HG23	1.13	1.11
1:B:27:LEU:O	1:B:28:ALA:CB	1.95	1.10
1:B:878:ILE:HG21	4:B:3007:GOL:H11	1.21	1.10
1:D:747:THR:HG23	1:D:827:MET:CE	1.82	1.10
1:D:31:ARG:HH11	1:D:31:ARG:HG3	1.12	1.10
1:B:540:ASP:CB	1:B:541:PRO:HD3	1.80	1.09
1:D:374:LEU:N	1:D:374:LEU:HD23	1.57	1.09
1:B:523:VAL:CG1	1:B:524:LEU:H	1.50	1.09
1:C:920:GLY:HA3	1:C:923:ILE:HG12	1.35	1.08
1:B:540:ASP:HB3	1:B:541:PRO:HD3	1.30	1.08
1:D:430:ASP:CB	1:D:1229:LYS:CE	2.31	1.08
1:D:607:ARG:NE	1:D:679:THR:HG23	1.69	1.08
1:C:927:TRP:HE3	1:C:928:MET:N	1.51	1.07
1:B:31:ARG:HH11	1:B:31:ARG:CG	1.67	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1312:ASP:H	1:B:1315:THR:CG2	1.66	1.07
1:B:534:ASP:CG	1:C:251:GLN:HB3	1.79	1.07
1:C:607:ARG:HE	1:C:679:THR:HG23	1.15	1.07
1:D:647:THR:HG23	1:D:648:GLY:H	1.04	1.06
1:D:159:GLY:O	1:D:162:THR:CG2	2.03	1.06
1:A:647:THR:HG23	1:A:648:GLY:N	1.66	1.06
1:C:647:THR:HG23	1:C:648:GLY:N	1.66	1.06
1:D:6:LEU:HD23	1:D:6:LEU:C	1.77	1.06
1:A:159:GLY:O	1:A:162:THR:HG22	1.54	1.05
1:B:540:ASP:HB3	1:B:541:PRO:CD	1.84	1.05
1:D:607:ARG:HE	1:D:679:THR:CG2	1.71	1.04
1:A:1109:ASN:HB2	1:C:1316:THR:HG21	1.06	1.03
1:B:647:THR:HG23	1:B:648:GLY:N	1.63	1.03
1:D:430:ASP:HB3	1:D:1229:LYS:CE	1.86	1.03
1:D:920:GLY:CA	1:D:923:ILE:H	1.72	1.03
1:B:920:GLY:HA3	1:B:923:ILE:HG12	1.40	1.03
1:B:1291:VAL:HA	1:C:380:ARG:HE	1.23	1.03
1:A:997:ARG:HG2	1:A:1164:GLU:HB2	1.37	1.02
1:A:920:GLY:HA3	1:A:923:ILE:H	1.17	1.02
1:D:916:GLY:HA2	1:D:919:GLN:OE1	1.58	1.02
1:A:865:PHE:N	1:A:865:PHE:CD1	2.26	1.02
1:D:523:VAL:HG12	1:D:524:LEU:N	1.75	1.02
1:B:1289:ASN:CB	1:C:380:ARG:HH12	1.59	1.02
1:A:606:LEU:CD2	1:A:607:ARG:H	1.74	1.01
1:B:31:ARG:HH11	1:B:31:ARG:HG3	1.22	1.01
1:C:594:CYS:H	1:C:596:ASP:HB2	1.23	1.01
1:A:1109:ASN:HB2	1:C:1316:THR:HG23	1.40	1.01
1:B:430:ASP:HB3	1:B:1229:LYS:HZ3	0.84	1.01
1:B:871:THR:HG23	1:B:908:SER:HB2	1.43	1.00
1:D:430:ASP:CG	1:D:1229:LYS:CE	2.34	1.00
1:D:891:LYS:HE2	1:D:949:LYS:HE3	1.43	1.00
1:B:2:THR:O	1:B:4:ASP:OD1	1.78	1.00
1:D:604:LEU:HD21	1:D:822:ARG:NH1	1.77	1.00
1:A:664:VAL:HG21	1:A:1218:GLY:O	1.61	1.00
1:A:1195:GLN:NE2	1:A:1195:GLN:HA	1.77	0.99
1:C:699:ILE:O	1:C:702:ALA:HB3	1.61	0.99
1:C:607:ARG:NE	1:C:679:THR:HG23	1.78	0.99
1:D:31:ARG:HH11	1:D:31:ARG:HG2	1.27	0.99
1:B:927:TRP:HE3	1:B:928:MET:N	1.58	0.99
1:B:3:ALA:N	1:B:3:ALA:HA	1.76	0.98
1:B:1133:PHE:HD2	1:B:1134:TYR:N	1.61	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:ARG:NE	1:A:679:THR:HG23	1.78	0.98
1:B:431:ILE:CB	1:B:431:ILE:HA	1.92	0.98
1:C:647:THR:HG23	1:C:648:GLY:H	0.82	0.98
1:C:890:TYR:OH	1:C:943:ARG:HD3	1.63	0.98
1:D:606:LEU:HD23	1:D:606:LEU:C	1.87	0.98
1:B:219:LEU:O	1:B:221:ASP:N	1.97	0.98
1:B:1292:LYS:HE3	1:C:382:THR:HG21	1.44	0.97
1:A:1213:HIS:H	1:A:1222:THR:CG2	1.77	0.97
1:B:430:ASP:OD2	1:B:1229:LYS:HD2	1.61	0.97
1:D:747:THR:HG23	1:D:827:MET:HE2	1.45	0.97
1:D:840:ARG:HA	4:D:3007:GOL:O1	1.64	0.97
1:A:373:THR:C	1:A:374:LEU:HD23	1.90	0.97
1:A:647:THR:HG23	1:A:648:GLY:H	0.80	0.96
1:C:1133:PHE:HD2	1:C:1134:TYR:N	1.62	0.96
1:B:606:LEU:CD2	1:B:607:ARG:N	2.29	0.96
1:D:1312:ASP:H	1:D:1315:THR:CG2	1.78	0.96
1:A:1213:HIS:H	1:A:1222:THR:HG21	1.29	0.96
1:A:1124:ASP:O	1:A:1125:THR:HB	1.63	0.96
1:B:216:LEU:O	1:B:217:LEU:HB2	1.66	0.96
1:B:372:LEU:HD21	1:B:385:MET:HE3	1.45	0.96
1:D:31:ARG:CG	1:D:31:ARG:NH1	2.16	0.96
1:B:159:GLY:O	1:B:162:THR:HG22	1.65	0.95
1:B:878:ILE:HG21	4:B:3007:GOL:C1	1.94	0.95
1:D:647:THR:CG2	1:D:648:GLY:H	1.76	0.95
1:B:917:GLY:N	1:B:918:PRO:HD2	1.82	0.95
1:C:1133:PHE:CD2	1:C:1134:TYR:N	2.34	0.95
1:D:430:ASP:CB	1:D:1229:LYS:NZ	2.29	0.95
1:A:684:GLN:HE21	1:A:684:GLN:HA	1.31	0.95
1:A:374:LEU:N	1:A:374:LEU:CD2	2.30	0.95
1:B:701:ASP:O	1:B:703:ILE:N	2.00	0.95
1:C:1213:HIS:H	1:C:1222:THR:HG21	1.30	0.95
1:A:1195:GLN:HA	1:A:1195:GLN:HE21	1.29	0.95
1:D:31:ARG:HG2	1:D:31:ARG:NH1	1.81	0.95
1:C:524:LEU:HA	1:C:527:LEU:HD12	1.48	0.95
1:D:699:ILE:O	1:D:702:ALA:CB	2.16	0.94
1:D:216:LEU:O	1:D:217:LEU:HB2	1.66	0.94
1:D:461:ASN:HB3	1:D:462:ARG:HG3	1.48	0.94
1:B:1124:ASP:O	1:B:1125:THR:HB	1.65	0.94
1:D:372:LEU:N	1:D:372:LEU:HD23	1.81	0.94
1:D:430:ASP:HB3	1:D:1229:LYS:HZ1	1.27	0.94
1:B:1213:HIS:H	1:B:1222:THR:CG2	1.81	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:459:MET:SD	1:D:512:THR:HG21	2.08	0.93
1:B:534:ASP:HB2	1:C:251:GLN:HB2	1.47	0.93
1:C:594:CYS:O	1:C:597:ILE:HG12	1.68	0.93
1:D:699:ILE:HD13	1:D:867:ASN:HB2	1.50	0.93
1:A:699:ILE:HD13	1:A:867:ASN:HB2	1.48	0.93
1:B:1133:PHE:CD2	1:B:1134:TYR:N	2.36	0.93
1:C:701:ASP:O	1:C:703:ILE:N	2.02	0.93
1:B:693:LEU:N	1:B:693:LEU:HD12	1.84	0.93
1:D:523:VAL:HG12	1:D:524:LEU:H	1.33	0.93
1:B:294:PRO:HD2	1:B:295:ASP:HB2	1.50	0.92
1:D:372:LEU:HD23	1:D:372:LEU:H	1.32	0.92
1:A:513:LEU:N	1:A:513:LEU:HD23	1.83	0.92
1:A:927:TRP:HE3	1:A:928:MET:N	1.67	0.92
1:A:910:THR:HG23	1:A:911:ALA:N	1.77	0.92
1:B:606:LEU:HD23	1:B:607:ARG:H	1.29	0.92
1:A:910:THR:CG2	1:A:911:ALA:N	2.33	0.92
1:B:647:THR:HG23	1:B:648:GLY:H	0.78	0.92
1:B:916:GLY:H	4:B:3007:GOL:H32	1.07	0.92
1:C:693:LEU:N	1:C:693:LEU:CD1	2.32	0.92
1:D:937:MET:HB2	1:D:938:PRO:CA	1.92	0.92
1:B:607:ARG:NE	1:B:679:THR:HG23	1.84	0.91
1:B:606:LEU:CD2	1:B:607:ARG:H	1.82	0.91
1:B:937:MET:CB	1:B:938:PRO:HA	1.98	0.91
1:D:483:LEU:HB2	1:D:520:TYR:CE1	2.05	0.91
1:B:430:ASP:CB	1:B:1229:LYS:HZ3	1.80	0.91
1:D:374:LEU:N	1:D:374:LEU:CD2	2.30	0.91
1:D:920:GLY:HA3	1:D:923:ILE:H	1.34	0.91
1:A:433:LYS:O	1:A:434:VAL:HG12	1.70	0.91
1:C:217:LEU:O	1:C:220:LYS:HG2	1.70	0.91
1:A:31:ARG:CG	1:A:31:ARG:NH1	2.27	0.91
1:A:606:LEU:CD2	1:A:607:ARG:N	2.29	0.91
1:B:921:MET:HE1	1:B:1004:THR:OG1	1.70	0.90
1:B:428:GLU:O	1:B:429:ASP:O	1.88	0.90
1:A:924:ALA:O	1:A:925:GLU:HB2	1.71	0.90
1:B:27:LEU:O	1:B:28:ALA:HB2	1.70	0.90
1:C:924:ALA:O	1:C:925:GLU:HB2	1.67	0.90
1:C:31:ARG:HH11	1:C:31:ARG:CG	1.84	0.90
1:D:219:LEU:O	1:D:221:ASP:N	2.04	0.90
1:D:701:ASP:O	1:D:703:ILE:N	2.05	0.90
1:D:871:THR:HG23	1:D:908:SER:CB	2.01	0.90
1:B:430:ASP:CB	1:B:1229:LYS:HE2	2.02	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:795:MET:HE3	1:B:1039:MET:CG	2.01	0.90
1:D:1041:GLN:O	1:D:1041:GLN:HG2	1.72	0.89
1:A:698:THR:O	1:A:700:GLU:O	1.90	0.89
1:A:920:GLY:HA2	1:A:921:MET:C	1.96	0.89
1:C:16:VAL:O	1:C:16:VAL:HG12	1.72	0.89
1:C:920:GLY:CA	1:C:923:ILE:H	1.86	0.89
1:A:372:LEU:HD22	1:A:407:ILE:HD11	1.54	0.89
1:B:927:TRP:CE3	1:B:928:MET:N	2.40	0.89
1:C:351:ASN:ND2	1:C:361:LEU:HB2	1.88	0.89
1:D:404:LEU:N	3:D:3006:FAD:N6A	2.20	0.89
1:C:927:TRP:CE3	1:C:928:MET:N	2.40	0.89
1:B:647:THR:CG2	1:B:648:GLY:N	2.15	0.89
1:C:241:THR:HG23	1:C:244:GLU:HG2	1.52	0.89
1:A:937:MET:HB2	1:A:938:PRO:HA	1.55	0.89
1:D:165:ARG:HB2	1:D:165:ARG:NH1	1.88	0.89
1:C:533:GLU:HG2	1:C:538:LYS:NZ	1.87	0.89
1:D:647:THR:HG23	1:D:648:GLY:N	1.86	0.89
1:B:924:ALA:O	1:B:925:GLU:HB2	1.68	0.89
1:A:1195:GLN:HE21	1:A:1195:GLN:CA	1.79	0.88
1:D:927:TRP:HE3	1:D:928:MET:N	1.70	0.88
1:A:203:PRO:O	1:A:204:LEU:HB3	1.70	0.88
1:B:698:THR:O	1:B:700:GLU:O	1.90	0.88
1:C:1313:LYS:HB2	1:C:1314:PHE:CE2	2.08	0.88
1:D:649:ILE:HG13	1:D:649:ILE:O	1.70	0.88
1:B:429:ASP:O	1:B:430:ASP:HB2	1.73	0.88
1:B:865:PHE:N	1:B:865:PHE:CD1	2.39	0.88
1:B:540:ASP:CB	1:B:541:PRO:CD	2.45	0.88
1:C:449:VAL:O	1:C:449:VAL:HG12	1.74	0.88
1:D:888:ASN:OD1	1:D:921:MET:HE2	1.74	0.87
1:D:1192:ASP:O	1:D:1193:ILE:HB	1.72	0.87
1:A:27:LEU:O	1:A:28:ALA:HB3	1.74	0.87
1:A:43:CYS:N	2:A:3002:FES:S2	2.47	0.87
1:A:946:ASN:HD22	1:A:946:ASN:H	1.20	0.87
1:D:248:LEU:C	1:D:248:LEU:HD12	1.99	0.87
1:D:693:LEU:N	1:D:693:LEU:HD12	1.89	0.87
1:A:860:LEU:HD22	1:A:927:TRP:HZ2	1.38	0.87
1:D:530:GLU:C	1:D:532:LEU:H	1.83	0.87
1:B:430:ASP:CB	1:B:1229:LYS:CE	2.52	0.87
1:C:1045:THR:O	1:C:1049:GLN:HG3	1.74	0.87
1:D:924:ALA:O	1:D:925:GLU:HB2	1.74	0.87
1:B:43:CYS:N	2:B:3002:FES:S2	2.47	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:483:LEU:HB2	1:D:520:TYR:CD1	2.09	0.86
1:D:507:PHE:CZ	1:D:511:LEU:HD11	2.09	0.86
1:A:1021:LEU:HD12	1:A:1022:LEU:N	1.89	0.86
1:A:1133:PHE:HD2	1:A:1134:TYR:N	1.74	0.86
1:D:1213:HIS:H	1:D:1222:THR:CG2	1.87	0.86
1:B:430:ASP:HB3	1:B:1229:LYS:CE	2.05	0.86
1:D:540:ASP:HB2	1:D:541:PRO:HD3	1.57	0.86
1:A:606:LEU:HD23	1:A:607:ARG:H	1.08	0.86
1:D:917:GLY:N	1:D:918:PRO:HD2	1.90	0.86
1:A:946:ASN:HD22	1:A:946:ASN:N	1.72	0.86
1:C:251:GLN:HG3	1:C:252:HIS:CD2	2.10	0.86
1:A:248:LEU:C	1:A:248:LEU:HD12	2.01	0.85
1:A:927:TRP:HZ3	1:A:928:MET:HE2	1.41	0.85
1:C:664:VAL:HG21	1:C:1218:GLY:O	1.75	0.85
1:A:3:ALA:CB	1:A:227:LEU:HD23	2.06	0.85
1:B:997:ARG:HG2	1:B:1164:GLU:HB2	1.58	0.85
1:D:165:ARG:HB2	1:D:165:ARG:HH11	1.39	0.85
1:C:1313:LYS:HB2	1:C:1314:PHE:CD2	2.11	0.85
1:A:31:ARG:HG3	1:A:31:ARG:NH1	1.86	0.85
1:C:251:GLN:HG3	1:C:252:HIS:HD2	1.40	0.85
1:B:430:ASP:OD2	1:B:1229:LYS:HD3	1.73	0.85
1:B:1262:GLU:C	1:B:1264:PRO:HD2	2.02	0.85
1:C:920:GLY:HA2	1:C:923:ILE:H	1.39	0.85
1:A:113:CYS:HA	1:A:1040:GLY:HA3	1.57	0.85
1:D:404:LEU:H	3:D:3006:FAD:H61A	1.21	0.85
1:D:1312:ASP:H	1:D:1315:THR:HG21	1.41	0.85
1:C:219:LEU:O	1:C:221:ASP:N	2.10	0.85
1:A:701:ASP:O	1:A:703:ILE:N	2.10	0.84
1:C:607:ARG:NE	1:C:679:THR:CG2	2.37	0.84
1:D:604:LEU:HD21	1:D:822:ARG:HH11	1.40	0.84
1:A:83:VAL:HG12	1:A:84:ALA:N	1.93	0.84
1:D:165:ARG:HH11	1:D:165:ARG:CB	1.90	0.84
1:B:337:PHE:HD1	1:B:338:ALA:HB3	1.40	0.84
1:C:1044:HIS:HD2	1:C:1064:ILE:HD13	1.43	0.84
1:A:3:ALA:HB1	1:A:227:LEU:CD2	2.08	0.84
1:A:920:GLY:CA	1:A:923:ILE:H	1.90	0.84
1:C:1135:ARG:HB2	1:D:1125:THR:HG21	1.59	0.84
1:D:840:ARG:HG3	4:D:3007:GOL:O1	1.77	0.84
1:A:920:GLY:HA2	1:A:922:LEU:N	1.93	0.84
1:B:511:LEU:CD2	1:B:515:PHE:CE1	2.60	0.84
1:B:523:VAL:CG1	1:B:524:LEU:N	2.13	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:THR:O	1:C:121:VAL:HG23	1.78	0.84
1:C:606:LEU:HD23	1:C:606:LEU:C	2.03	0.84
1:D:203:PRO:O	1:D:204:LEU:HB3	1.77	0.84
1:A:604:LEU:HD21	1:A:822:ARG:NH1	1.93	0.83
1:A:748:HIS:O	1:A:749:CYS:HB3	1.75	0.83
1:C:459:MET:HE2	1:C:459:MET:HA	1.59	0.83
1:B:795:MET:HE3	1:B:1039:MET:HG3	1.59	0.83
1:A:27:LEU:O	1:A:28:ALA:HB2	1.78	0.83
1:C:871:THR:HG23	1:C:908:SER:HB2	1.60	0.83
1:B:693:LEU:N	1:B:693:LEU:CD1	2.42	0.83
1:C:606:LEU:CD2	1:C:607:ARG:N	2.41	0.83
1:D:910:THR:HG23	1:D:911:ALA:N	1.91	0.83
1:A:1002:ILE:HG23	1:A:1003:PRO:HD2	1.61	0.83
1:D:404:LEU:H	3:D:3006:FAD:H62A	1.25	0.83
1:A:1109:ASN:CG	1:C:1316:THR:HG21	2.04	0.83
1:A:38:GLY:HA2	1:A:40:LYS:HE2	1.60	0.83
1:A:1070:ASN:C	1:A:1070:ASN:HD22	1.85	0.83
1:B:1213:HIS:H	1:B:1222:THR:HG21	1.42	0.83
1:D:372:LEU:N	1:D:372:LEU:CD2	2.40	0.83
1:A:404:LEU:H	3:A:3006:FAD:H61A	1.27	0.83
1:C:507:PHE:CZ	1:C:511:LEU:HD11	2.14	0.83
1:B:1068:SER:OG	1:B:1069:THR:N	2.11	0.82
1:D:256:LYS:O	1:D:278:ILE:HG23	1.79	0.82
1:A:647:THR:CG2	1:A:648:GLY:N	2.22	0.82
1:C:647:THR:CG2	1:C:648:GLY:N	2.17	0.82
1:B:534:ASP:CG	1:C:251:GLN:CB	2.52	0.82
1:C:27:LEU:O	1:C:28:ALA:HB2	1.80	0.82
1:D:241:THR:HG23	1:D:244:GLU:HG2	1.60	0.82
1:D:865:PHE:CD1	1:D:865:PHE:N	2.44	0.82
1:C:1073:PRO:HD3	1:D:1023:HIS:CD2	2.15	0.82
1:D:693:LEU:N	1:D:693:LEU:CD1	2.41	0.82
1:D:425:SER:O	1:D:426:ARG:HB2	1.79	0.82
1:B:557:ASP:O	1:B:557:ASP:OD1	1.98	0.82
1:B:1195:GLN:HA	1:B:1195:GLN:HE21	1.43	0.82
1:C:257:LEU:O	3:C:3006:FAD:H2B	1.79	0.82
1:A:483:LEU:HB2	1:A:520:TYR:CE1	2.14	0.81
1:B:461:ASN:HB3	1:B:462:ARG:HG2	1.61	0.81
1:D:871:THR:HG23	1:D:908:SER:HB2	1.61	0.81
1:A:507:PHE:CE1	1:A:511:LEU:HD11	2.14	0.81
1:A:649:ILE:HG13	1:A:649:ILE:O	1.80	0.81
1:B:31:ARG:CG	1:B:31:ARG:NH1	2.39	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:878:ILE:CG2	4:B:3007:GOL:H11	2.08	0.81
1:C:461:ASN:HB3	1:C:462:ARG:CG	2.11	0.81
1:C:592:VAL:HG23	1:D:757:GLU:OE2	1.80	0.81
1:C:533:GLU:HA	1:C:534:ASP:HB2	1.62	0.81
1:D:27:LEU:O	1:D:28:ALA:CB	2.24	0.81
1:C:709:TYR:CE1	1:C:903:LYS:HG3	2.14	0.81
1:D:920:GLY:HA2	1:D:923:ILE:H	1.44	0.81
1:D:1124:ASP:O	1:D:1125:THR:HB	1.80	0.81
1:A:3:ALA:HB1	1:A:227:LEU:HD23	1.62	0.81
1:B:1289:ASN:HB2	1:C:380:ARG:HH11	1.01	0.81
1:C:27:LEU:O	1:C:28:ALA:HB3	1.81	0.81
1:C:461:ASN:HB3	1:C:462:ARG:HG2	1.62	0.81
1:C:693:LEU:H	1:C:693:LEU:HD13	1.45	0.81
1:C:891:LYS:HE2	1:C:949:LYS:HE3	1.62	0.81
1:B:27:LEU:O	1:B:28:ALA:HB3	1.81	0.81
1:C:116:CYS:SG	1:C:148:CYS:HB2	2.20	0.80
1:C:606:LEU:HD23	1:C:607:ARG:H	1.45	0.80
1:C:865:PHE:N	1:C:865:PHE:CD1	2.49	0.80
1:C:1021:LEU:HD12	1:C:1022:LEU:N	1.96	0.80
1:A:219:LEU:O	1:A:221:ASP:N	2.13	0.80
1:A:1133:PHE:CD2	1:A:1134:TYR:N	2.49	0.80
1:D:439:ARG:NH2	1:D:451:GLU:OE1	2.15	0.80
1:A:16:VAL:O	1:A:16:VAL:HG12	1.82	0.80
1:C:1068:SER:OG	1:C:1069:THR:N	2.15	0.80
1:C:1101:ARG:NH1	1:C:1127:SER:HB3	1.96	0.80
1:D:38:GLY:HA2	1:D:40:LYS:CE	2.11	0.80
1:A:860:LEU:HD22	1:A:927:TRP:CZ2	2.17	0.80
1:B:38:GLY:HA2	1:B:40:LYS:CE	2.12	0.79
1:D:1213:HIS:H	1:D:1222:THR:HG21	1.46	0.79
1:A:148:CYS:SG	1:A:151:THR:HG23	2.21	0.79
1:D:449:VAL:O	1:D:449:VAL:HG12	1.81	0.79
1:C:910:THR:HG23	1:C:911:ALA:H	1.46	0.79
1:A:346:ALA:HB1	3:A:3006:FAD:H4'	1.63	0.79
1:B:372:LEU:HD22	1:B:407:ILE:HD11	1.64	0.79
1:C:1213:HIS:H	1:C:1222:THR:CG2	1.95	0.79
1:A:159:GLY:O	1:A:162:THR:CG2	2.31	0.79
1:B:430:ASP:OD1	1:B:1229:LYS:HE2	1.81	0.79
1:B:461:ASN:HB3	1:B:462:ARG:CG	2.12	0.79
1:B:540:ASP:HB2	1:B:541:PRO:HD3	1.63	0.79
1:B:980:ALA:O	1:B:982:LYS:N	2.16	0.79
1:C:910:THR:HG23	1:C:911:ALA:N	1.98	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1081:SER:OG	1:D:1262:GLU:HG3	1.83	0.79
1:A:372:LEU:HD21	1:A:385:MET:HE3	1.65	0.79
1:A:439:ARG:NH2	1:A:451:GLU:OE1	2.15	0.79
1:C:920:GLY:HA3	1:C:923:ILE:CG1	2.13	0.79
1:A:1210:GLU:OE1	1:A:1228:TYR:OH	1.98	0.79
1:B:708:PHE:HB2	1:B:901:LEU:O	1.82	0.79
1:B:937:MET:CB	1:B:938:PRO:CA	2.60	0.78
1:C:248:LEU:C	1:C:248:LEU:HD12	2.08	0.78
1:C:593:TYR:O	1:C:594:CYS:HB2	1.81	0.78
1:A:865:PHE:N	1:A:865:PHE:HD1	1.75	0.78
1:A:921:MET:HE1	1:A:1004:THR:OG1	1.82	0.78
1:D:1293:GLU:O	1:D:1294:LEU:HD23	1.82	0.78
1:D:540:ASP:HB2	1:D:541:PRO:CD	2.13	0.78
1:D:963:PHE:CE2	1:D:966:PRO:HD3	2.18	0.78
1:B:910:THR:HG23	1:B:911:ALA:N	1.96	0.78
1:C:923:ILE:O	1:C:926:CYS:HB3	1.83	0.78
1:C:937:MET:HB2	1:C:938:PRO:HA	1.66	0.78
1:C:1021:LEU:HD12	1:C:1022:LEU:H	1.48	0.78
1:D:430:ASP:OD1	1:D:1229:LYS:HE2	1.83	0.78
1:B:87:THR:CG2	1:B:89:GLU:HG2	2.14	0.78
1:B:1312:ASP:H	1:B:1315:THR:HG22	1.47	0.78
1:A:432:ALA:O	1:A:433:LYS:HG2	1.84	0.78
1:B:871:THR:CG2	1:B:908:SER:HB2	2.13	0.78
1:B:1326:CYS:O	1:B:1327:LYS:HD3	1.83	0.78
1:C:376:SER:OG	1:C:377:ARG:N	2.14	0.78
1:D:6:LEU:HD23	1:D:6:LEU:O	1.85	0.77
1:D:523:VAL:CG1	1:D:524:LEU:N	2.46	0.77
1:A:684:GLN:HA	1:A:684:GLN:NE2	1.98	0.77
1:C:1262:GLU:H	1:C:1263:PRO:CD	1.98	0.77
1:D:1312:ASP:O	1:D:1315:THR:HG23	1.84	0.77
1:A:506:ASP:OD1	1:A:506:ASP:N	2.17	0.77
1:A:809:VAL:O	1:A:813:VAL:HG23	1.84	0.77
1:C:1319:VAL:CB	1:C:1319:VAL:HA	2.12	0.77
1:A:923:ILE:O	1:A:926:CYS:HB3	1.84	0.77
1:A:38:GLY:HA2	1:A:40:LYS:CE	2.14	0.77
1:A:1316:THR:O	1:A:1319:VAL:HG11	1.85	0.77
1:B:148:CYS:SG	1:B:151:THR:HG23	2.24	0.77
1:B:203:PRO:O	1:B:204:LEU:HB3	1.83	0.77
1:D:251:GLN:HG3	1:D:252:HIS:CD2	2.19	0.77
1:D:1142:SER:HB3	1:D:1145:THR:HG21	1.67	0.77
1:C:1044:HIS:CD2	1:C:1064:ILE:HD13	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1192:ASP:O	1:C:1193:ILE:HB	1.84	0.76
1:D:1101:ARG:NH1	1:D:1127:SER:HB3	2.00	0.76
1:A:699:ILE:CD1	1:A:867:ASN:HB2	2.14	0.76
1:C:3:ALA:HB2	1:C:225:LYS:NZ	2.01	0.76
1:C:698:THR:HG23	1:C:701:ASP:OD2	1.85	0.76
1:C:741:GLU:HB3	1:C:1228:TYR:CZ	2.20	0.76
1:A:920:GLY:HA3	1:A:923:ILE:HG12	1.67	0.76
1:A:1081:SER:OG	1:A:1262:GLU:HG3	1.85	0.76
1:C:607:ARG:HE	1:C:679:THR:HG22	1.48	0.76
1:B:1291:VAL:HA	1:C:380:ARG:NE	2.00	0.76
1:C:594:CYS:N	1:C:596:ASP:HB2	1.99	0.76
1:C:1034:HIS:HE1	1:C:1044:HIS:CD2	2.04	0.76
1:A:248:LEU:C	1:A:248:LEU:CD1	2.58	0.76
1:A:879:MET:HE3	1:A:899:GLY:HA3	1.68	0.76
1:A:1192:ASP:O	1:A:1193:ILE:HB	1.86	0.76
1:D:117:THR:O	1:D:121:VAL:HG23	1.86	0.76
1:D:433:LYS:HZ3	1:D:504:MET:HE1	1.51	0.76
1:C:37:SER:HB2	1:C:596:ASP:OD1	1.86	0.76
1:C:440:VAL:HG23	1:C:452:LEU:HD12	1.68	0.76
1:D:606:LEU:HD23	1:D:607:ARG:H	0.93	0.76
1:A:461:ASN:HB3	1:A:462:ARG:HG3	1.66	0.76
1:B:871:THR:HG23	1:B:908:SER:CB	2.15	0.76
1:B:1195:GLN:HE21	1:B:1195:GLN:CA	1.99	0.76
1:B:1319:VAL:CB	1:B:1319:VAL:HA	2.08	0.75
1:C:1124:ASP:O	1:C:1125:THR:HB	1.85	0.75
1:B:701:ASP:O	1:B:702:ALA:C	2.30	0.75
1:D:560:LEU:HD12	1:D:1243:SER:HB3	1.68	0.75
1:D:1121:ALA:O	1:D:1126:VAL:HG23	1.86	0.75
1:A:294:PRO:HD2	1:A:295:ASP:HB2	1.68	0.75
1:A:607:ARG:NE	1:A:679:THR:CG2	2.44	0.75
1:A:1311:VAL:HA	1:A:1315:THR:HG21	1.68	0.75
1:C:113:CYS:HA	1:C:1040:GLY:HA3	1.67	0.75
1:D:747:THR:HG23	1:D:827:MET:HE3	1.69	0.75
1:D:709:TYR:CE1	1:D:903:LYS:HG3	2.22	0.75
1:D:927:TRP:CE3	1:D:928:MET:N	2.54	0.75
1:A:871:THR:HG23	1:A:908:SER:HB2	1.69	0.75
1:A:946:ASN:N	1:A:946:ASN:ND2	2.32	0.75
1:B:431:ILE:CA	1:B:431:ILE:HB	2.09	0.75
1:B:1003:PRO:HA	1:B:1158:VAL:HG22	1.69	0.75
1:B:1055:LEU:O	1:B:1056:LYS:HB2	1.86	0.75
1:C:937:MET:HB2	1:C:938:PRO:CA	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:404:LEU:N	3:D:3006:FAD:H62A	1.81	0.75
1:A:1044:HIS:HD2	1:A:1064:ILE:HD13	1.52	0.75
1:D:963:PHE:HE2	1:D:966:PRO:HD3	1.51	0.75
1:C:274:LEU:HG	1:C:274:LEU:O	1.85	0.75
1:D:56:SER:HB3	1:D:67:HIS:ND1	2.01	0.75
1:A:1070:ASN:HD22	1:A:1071:THR:N	1.85	0.75
1:C:927:TRP:HE3	1:C:928:MET:CA	2.00	0.75
1:D:1133:PHE:CD2	1:D:1134:TYR:N	2.54	0.75
1:A:699:ILE:O	1:A:702:ALA:CB	2.30	0.74
1:A:891:LYS:HE2	1:A:949:LYS:HE3	1.68	0.74
1:B:1142:SER:HB3	1:B:1145:THR:HG21	1.69	0.74
1:B:1289:ASN:CB	1:C:380:ARG:HH11	1.75	0.74
1:A:811:THR:CG2	1:A:811:THR:HB	2.12	0.74
1:B:3:ALA:CB	1:B:3:ALA:C	2.60	0.74
1:C:1157:GLY:O	1:C:1158:VAL:HG23	1.87	0.74
1:B:511:LEU:HD21	1:B:515:PHE:CZ	2.22	0.74
1:B:499:ASP:HB3	1:B:1327:LYS:HG2	1.68	0.74
1:C:56:SER:HB3	1:C:67:HIS:CE1	2.21	0.74
1:A:927:TRP:CE3	1:A:928:MET:N	2.55	0.74
1:B:769:ASN:ND2	1:B:1077:PRO:HG3	2.02	0.74
1:B:1195:GLN:HA	1:B:1195:GLN:NE2	1.99	0.74
1:D:1021:LEU:HD12	1:D:1022:LEU:N	2.02	0.74
1:B:520:TYR:CE2	1:B:524:LEU:HD12	2.22	0.74
1:C:351:ASN:HD22	1:C:361:LEU:HB2	1.51	0.74
1:D:840:ARG:CA	4:D:3007:GOL:O1	2.35	0.74
1:A:203:PRO:O	1:A:204:LEU:CB	2.35	0.74
1:B:916:GLY:H	4:B:3007:GOL:C3	1.94	0.74
1:D:38:GLY:HA2	1:D:40:LYS:HE2	1.70	0.74
1:A:664:VAL:CG2	1:A:1218:GLY:O	2.36	0.73
1:A:1316:THR:O	1:A:1319:VAL:CG1	2.36	0.73
1:A:606:LEU:HD23	1:A:606:LEU:C	2.13	0.73
1:B:599:ARG:CD	1:B:599:ARG:CB	2.66	0.73
1:C:56:SER:HB3	1:C:67:HIS:ND1	2.02	0.73
1:C:920:GLY:HA2	1:C:923:ILE:N	2.03	0.73
1:B:879:MET:HE3	1:B:899:GLY:HA3	1.69	0.73
1:C:248:LEU:HD12	1:C:248:LEU:O	1.88	0.73
1:A:1293:GLU:O	1:A:1294:LEU:HD23	1.88	0.73
1:B:433:LYS:HB3	1:B:434:VAL:HG23	1.71	0.73
1:B:1044:HIS:CD2	1:B:1064:ILE:HD13	2.23	0.73
1:D:910:THR:HG23	1:D:911:ALA:H	1.50	0.73
1:B:372:LEU:HD23	1:B:372:LEU:N	2.02	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:ASP:CG	1:B:1229:LYS:CD	2.58	0.73
1:C:113:CYS:HB3	1:C:150:CYS:SG	2.29	0.73
1:B:594:CYS:C	1:B:596:ASP:H	1.97	0.73
1:C:533:GLU:HG2	1:C:538:LYS:HZ2	1.51	0.73
1:A:29:TYR:HE2	1:A:34:LEU:HD21	1.53	0.73
1:A:6:LEU:HD23	1:A:6:LEU:C	2.12	0.73
1:B:1034:HIS:HE1	1:B:1044:HIS:CD2	2.06	0.73
1:A:29:TYR:CE2	1:A:34:LEU:HD21	2.23	0.73
1:D:858:VAL:O	1:D:894:ASN:ND2	2.21	0.73
1:B:87:THR:HG21	1:B:89:GLU:HG2	1.71	0.72
1:A:937:MET:HB2	1:A:938:PRO:CA	2.16	0.72
1:C:693:LEU:HB3	1:C:694:PRO:HD2	1.71	0.72
1:A:1044:HIS:CD2	1:A:1064:ILE:HD13	2.23	0.72
1:D:925:GLU:O	1:D:1273:PHE:CZ	2.43	0.72
1:D:926:CYS:H	1:D:928:MET:H	1.34	0.72
1:D:1034:HIS:HE1	1:D:1044:HIS:CD2	2.06	0.72
1:B:588:SER:OG	1:B:590:GLU:HG2	1.90	0.72
1:B:1121:ALA:O	1:B:1126:VAL:HG23	1.90	0.72
1:C:910:THR:CG2	1:C:911:ALA:N	2.53	0.72
1:C:241:THR:HG23	1:C:244:GLU:CG	2.18	0.72
1:C:337:PHE:HD1	1:C:338:ALA:HB3	1.55	0.72
1:A:693:LEU:HB3	1:A:694:PRO:HD2	1.72	0.72
1:C:824:VAL:HG12	1:C:825:ARG:N	1.99	0.72
1:D:373:THR:C	1:D:374:LEU:HD23	2.13	0.72
1:A:1213:HIS:N	1:A:1222:THR:HG21	2.05	0.72
1:A:1108:LYS:NZ	1:C:1319:VAL:HG23	2.04	0.71
1:B:309:GLU:O	1:B:313:VAL:HG23	1.90	0.71
1:B:865:PHE:N	1:B:865:PHE:HD1	1.87	0.71
1:D:251:GLN:HG3	1:D:252:HIS:HD2	1.55	0.71
1:A:881:ARG:HD2	1:A:915:PHE:HB3	1.73	0.71
1:A:31:ARG:HH11	1:A:31:ARG:HG2	1.52	0.71
1:A:87:THR:HG23	1:A:89:GLU:N	2.05	0.71
1:B:849:VAL:O	1:B:849:VAL:HG13	1.91	0.71
1:C:693:LEU:N	1:C:693:LEU:HD12	2.04	0.71
1:B:891:LYS:HE2	1:B:949:LYS:HE3	1.71	0.71
1:D:31:ARG:HG3	1:D:31:ARG:NH1	1.95	0.71
1:D:1010:PHE:HB2	1:D:1016:ASN:ND2	2.06	0.71
1:A:135:THR:HG23	1:A:138:GLU:OE1	1.90	0.71
1:B:287:LEU:O	1:B:302:ALA:HB3	1.90	0.71
1:B:594:CYS:O	1:B:597:ILE:HG12	1.90	0.71
1:D:461:ASN:HB3	1:D:462:ARG:CG	2.19	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:472:ARG:HD2	1:D:485:ASP:OD2	1.91	0.71
1:D:538:LYS:HB3	1:D:539:LEU:O	1.90	0.71
1:A:76:PRO:HD3	1:A:261:ASN:ND2	2.06	0.71
1:B:431:ILE:HA	1:B:431:ILE:HB	1.70	0.71
1:C:693:LEU:N	1:C:693:LEU:HD13	2.04	0.71
1:D:87:THR:HG23	1:D:89:GLU:H	1.54	0.71
1:A:604:LEU:HD21	1:A:822:ARG:HH11	1.53	0.71
1:B:606:LEU:CG	1:B:607:ARG:H	2.04	0.71
1:D:1002:ILE:HD13	1:D:1270:SER:HA	1.71	0.71
1:D:1142:SER:HB3	1:D:1145:THR:CG2	2.20	0.71
1:A:840:ARG:HG2	4:A:3007:GOL:O1	1.90	0.71
1:C:917:GLY:N	1:C:918:PRO:HD2	2.06	0.71
1:D:148:CYS:SG	1:D:151:THR:HG23	2.30	0.71
1:D:647:THR:CG2	1:D:648:GLY:N	2.45	0.71
1:A:1192:ASP:O	1:A:1193:ILE:CB	2.39	0.71
1:A:927:TRP:CZ3	1:A:928:MET:HE2	2.25	0.71
1:B:534:ASP:CB	1:C:251:GLN:HB2	2.21	0.71
1:A:87:THR:HG23	1:A:89:GLU:H	1.54	0.70
1:A:376:SER:HB3	1:A:379:THR:OG1	1.91	0.70
1:B:1289:ASN:HB2	1:C:380:ARG:HH12	0.89	0.70
1:C:604:LEU:HD21	1:C:822:ARG:NH1	2.05	0.70
1:D:461:ASN:CB	1:D:462:ARG:HG3	2.19	0.70
1:A:471:GLN:O	1:A:474:LEU:HB2	1.91	0.70
1:A:574:VAL:HG13	1:A:1187:LEU:HD22	1.72	0.70
1:A:580:HIS:O	1:A:582:ALA:N	2.23	0.70
1:A:865:PHE:HD1	1:A:865:PHE:H	1.39	0.70
1:A:56:SER:HB3	1:A:67:HIS:ND1	2.06	0.70
1:B:520:TYR:HE2	1:B:524:LEU:HD12	1.54	0.70
1:B:684:GLN:HA	1:B:684:GLN:HE21	1.56	0.70
1:B:917:GLY:N	1:B:918:PRO:CD	2.53	0.70
1:C:165:ARG:NH1	1:C:165:ARG:HB2	2.06	0.70
1:C:296:GLY:N	1:C:411:TYR:CE1	2.59	0.70
1:C:871:THR:HG23	1:C:908:SER:CB	2.20	0.70
1:B:795:MET:HE3	1:B:1039:MET:HG2	1.71	0.70
1:B:932:ALA:HB2	1:B:942:VAL:HG21	1.73	0.70
1:C:404:LEU:H	3:C:3006:FAD:H62A	1.39	0.70
1:B:88:VAL:CG1	1:B:89:GLU:N	2.55	0.70
1:B:509:CYS:O	1:B:510:THR:C	2.34	0.70
1:B:523:VAL:HG12	1:B:524:LEU:H	0.61	0.70
1:B:606:LEU:HD23	1:B:606:LEU:C	2.14	0.70
1:B:917:GLY:H	1:B:918:PRO:HD2	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:LEU:C	1:B:6:LEU:HD23	2.17	0.70
1:B:682:ALA:O	1:B:684:GLN:N	2.25	0.70
1:C:557:ASP:OD1	1:C:557:ASP:N	2.24	0.70
1:B:699:ILE:O	1:B:702:ALA:CB	2.31	0.70
1:B:1291:VAL:N	1:C:380:ARG:NH2	2.40	0.70
1:C:483:LEU:HB2	1:C:520:TYR:CE1	2.26	0.70
1:D:113:CYS:HB3	1:D:150:CYS:SG	2.31	0.70
1:A:917:GLY:N	1:A:918:PRO:HD2	2.05	0.70
1:A:1021:LEU:HD12	1:A:1021:LEU:C	2.02	0.70
1:B:557:ASP:HB2	1:B:1240:PHE:H	1.57	0.70
1:D:433:LYS:NZ	1:D:504:MET:HE1	2.07	0.70
1:A:461:ASN:HB3	1:A:462:ARG:CG	2.22	0.69
1:D:871:THR:CG2	1:D:908:SER:HB2	2.22	0.69
1:D:1192:ASP:O	1:D:1193:ILE:CB	2.34	0.69
1:B:1311:VAL:HA	1:B:1315:THR:HG21	1.74	0.69
1:C:927:TRP:HZ3	1:C:928:MET:HE2	1.58	0.69
1:D:860:LEU:HD22	1:D:927:TRP:HZ2	1.57	0.69
1:D:881:ARG:HD2	1:D:915:PHE:HB3	1.74	0.69
1:D:1311:VAL:HA	1:D:1315:THR:HG21	1.73	0.69
1:C:376:SER:HB3	1:C:379:THR:HG1	1.58	0.69
1:C:386:ASP:OD1	1:C:388:THR:HG22	1.93	0.69
1:D:1214:TYR:N	1:D:1214:TYR:CD1	2.58	0.69
1:B:1210:GLU:OE1	1:B:1228:TYR:OH	2.02	0.69
1:D:113:CYS:HA	1:D:1040:GLY:HA3	1.74	0.69
1:D:891:LYS:CE	1:D:949:LYS:HE3	2.20	0.69
1:A:708:PHE:HB2	1:A:901:LEU:O	1.93	0.69
1:C:3:ALA:HB2	1:C:225:LYS:HZ2	1.57	0.69
1:C:588:SER:OG	1:C:590:GLU:HG2	1.93	0.69
1:D:124:MET:HE3	1:D:128:LEU:HD11	1.74	0.69
1:D:780:MET:HE1	1:D:815:LEU:HB2	1.75	0.69
1:A:217:LEU:O	1:A:220:LYS:HG2	1.92	0.69
1:A:281:PRO:O	1:A:282:ALA:HB3	1.92	0.69
1:B:29:TYR:CE2	1:B:34:LEU:HD21	2.27	0.69
1:B:372:LEU:N	1:B:372:LEU:CD2	2.54	0.69
1:B:708:PHE:HB3	1:B:902:CYS:HA	1.75	0.69
1:C:459:MET:HE3	1:C:508:ARG:HD2	1.74	0.69
1:C:1195:GLN:CA	1:C:1195:GLN:HE21	2.06	0.69
1:C:294:PRO:HD2	1:C:295:ASP:HB2	1.75	0.69
1:C:808:VAL:O	1:C:811:THR:HG22	1.91	0.69
1:D:101:VAL:O	1:D:101:VAL:HG12	1.91	0.69
1:D:937:MET:CB	1:D:938:PRO:HA	2.16	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1021:LEU:HD12	1:D:1022:LEU:H	1.55	0.69
1:B:581:LEU:HG	1:B:1045:THR:HG23	1.72	0.69
1:C:31:ARG:HG3	1:C:31:ARG:NH1	1.95	0.69
1:C:1279:ILE:O	1:C:1280:ARG:C	2.32	0.69
1:D:248:LEU:HD12	1:D:248:LEU:O	1.93	0.69
1:D:927:TRP:HE3	1:D:928:MET:CA	2.05	0.69
1:B:751:ILE:HD13	1:B:825:ARG:NH2	2.07	0.69
1:C:533:GLU:HG2	1:C:538:LYS:HZ1	1.57	0.69
1:B:2:THR:C	1:B:4:ASP:OD1	2.36	0.68
1:C:364:VAL:O	1:C:368:SER:HB2	1.92	0.68
1:D:529:GLN:O	1:D:530:GLU:HB2	1.93	0.68
1:B:249:LYS:NZ	1:B:400:PRO:O	2.24	0.68
1:B:1291:VAL:CA	1:B:1291:VAL:HB	2.15	0.68
1:D:616:ALA:HB1	1:D:691:GLU:O	1.93	0.68
1:B:719:ASP:HA	1:B:720:LEU:HB3	1.75	0.68
1:C:43:CYS:HB2	1:C:45:GLU:HB3	1.75	0.68
1:C:148:CYS:SG	1:C:151:THR:HG23	2.32	0.68
1:C:348:VAL:HG23	1:C:349:GLY:H	1.59	0.68
1:D:1005:LYS:HG3	1:D:1005:LYS:O	1.92	0.68
1:B:693:LEU:CD1	1:B:693:LEU:H	2.06	0.68
1:B:841:HIS:HB2	4:B:3007:GOL:O1	1.93	0.68
1:D:1004:THR:HG22	1:D:1267:LEU:HD21	1.74	0.68
1:B:429:ASP:O	1:B:430:ASP:CB	2.40	0.68
1:C:1125:THR:HG21	1:D:1135:ARG:HB2	1.75	0.68
1:D:248:LEU:C	1:D:248:LEU:CD1	2.64	0.68
1:D:920:GLY:CA	1:D:923:ILE:HG12	2.16	0.68
1:D:1004:THR:CG2	1:D:1267:LEU:HD21	2.24	0.68
1:A:87:THR:HG23	1:A:88:VAL:N	2.09	0.68
1:C:606:LEU:CD2	1:C:607:ARG:H	2.02	0.68
1:C:765:VAL:HG12	1:C:767:THR:HG22	1.75	0.68
1:C:860:LEU:HD22	1:C:927:TRP:HZ2	1.59	0.68
1:C:1262:GLU:C	1:C:1264:PRO:HD2	2.18	0.68
1:A:923:ILE:O	1:A:926:CYS:CB	2.42	0.68
1:B:860:LEU:HD22	1:B:927:TRP:CZ2	2.28	0.68
1:C:87:THR:HG23	1:C:89:GLU:H	1.58	0.68
1:C:471:GLN:O	1:C:474:LEU:HB2	1.93	0.68
1:D:920:GLY:CA	1:D:923:ILE:N	2.52	0.68
1:A:161:ARG:HG3	1:A:162:THR:N	2.07	0.68
1:D:294:PRO:HD2	1:D:295:ASP:HB2	1.74	0.68
1:D:780:MET:CE	1:D:815:LEU:HB2	2.24	0.68
1:B:337:PHE:CD1	1:B:338:ALA:HB3	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:890:TYR:OH	1:B:943:ARG:HD3	1.94	0.68
1:C:404:LEU:H	3:C:3006:FAD:H61A	1.40	0.68
1:D:920:GLY:HA3	1:D:923:ILE:CG1	2.17	0.68
1:A:433:LYS:O	1:A:434:VAL:CG1	2.42	0.67
1:C:1266:PHE:O	1:C:1268:ALA:N	2.27	0.67
1:D:425:SER:O	1:D:426:ARG:CB	2.42	0.67
1:D:459:MET:SD	1:D:512:THR:CG2	2.83	0.67
1:A:931:VAL:O	1:A:933:VAL:N	2.27	0.67
1:C:403:ILE:HG13	1:C:403:ILE:O	1.95	0.67
1:B:607:ARG:NE	1:B:679:THR:CG2	2.43	0.67
1:D:910:THR:CG2	1:D:911:ALA:N	2.57	0.67
1:C:404:LEU:N	3:C:3006:FAD:N6A	2.40	0.67
1:D:83:VAL:HG12	1:D:84:ALA:N	2.08	0.67
1:A:1277:ASP:O	1:A:1280:ARG:HB2	1.95	0.67
1:B:534:ASP:OD1	1:C:251:GLN:CB	2.29	0.67
1:B:372:LEU:HD23	1:B:372:LEU:H	1.58	0.67
1:B:649:ILE:O	1:B:649:ILE:HG13	1.95	0.67
1:A:607:ARG:HE	1:A:679:THR:HG22	1.56	0.67
1:A:693:LEU:HD12	1:A:693:LEU:N	2.10	0.67
1:A:849:VAL:HG13	1:A:849:VAL:O	1.93	0.67
1:B:448:GLU:O	1:B:449:VAL:HB	1.93	0.67
1:B:708:PHE:CB	1:B:902:CYS:HA	2.25	0.67
1:D:822:ARG:HB2	1:D:823:PRO:HD2	1.77	0.67
1:A:840:ARG:CG	4:A:3007:GOL:O1	2.43	0.67
1:B:610:THR:HG22	1:B:667:ILE:HA	1.76	0.67
1:C:3:ALA:CB	1:C:227:LEU:HD23	2.25	0.67
1:A:888:ASN:OD1	1:A:921:MET:HE2	1.95	0.67
1:B:709:TYR:CE1	1:B:903:LYS:HG3	2.30	0.67
1:B:804:THR:O	1:B:807:THR:HG23	1.95	0.67
1:B:931:VAL:HG12	1:B:932:ALA:N	2.10	0.67
1:B:1008:ILE:O	1:B:1009:SER:HB2	1.93	0.67
1:D:847:TYR:CD2	1:D:847:TYR:N	2.62	0.67
1:A:956:PHE:HB2	1:A:1141:TYR:CE1	2.30	0.67
1:C:708:PHE:HB2	1:C:901:LEU:O	1.95	0.67
1:C:1279:ILE:O	1:C:1280:ARG:O	2.12	0.67
1:D:203:PRO:O	1:D:204:LEU:CB	2.42	0.67
1:D:920:GLY:HA2	1:D:922:LEU:N	2.10	0.67
1:C:524:LEU:O	1:C:525:GLN:C	2.36	0.66
1:A:353:ILE:CG2	1:A:353:ILE:O	2.42	0.66
1:B:1289:ASN:CG	1:C:380:ARG:HH12	2.03	0.66
1:D:530:GLU:C	1:D:532:LEU:N	2.54	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:699:ILE:HD13	1:B:867:ASN:HB2	1.77	0.66
1:C:87:THR:HG23	1:C:89:GLU:N	2.11	0.66
1:D:1315:THR:O	1:D:1319:VAL:CG2	2.44	0.66
1:C:31:ARG:CG	1:C:31:ARG:NH1	2.52	0.66
1:C:676:PRO:O	1:C:679:THR:HG22	1.94	0.66
1:D:699:ILE:CD1	1:D:867:ASN:HB2	2.22	0.66
1:D:448:GLU:O	1:D:449:VAL:HB	1.95	0.66
1:A:946:ASN:H	1:A:946:ASN:ND2	1.92	0.66
1:D:404:LEU:HB3	3:D:3006:FAD:N6A	2.11	0.66
1:A:682:ALA:O	1:A:684:GLN:N	2.29	0.66
1:B:682:ALA:C	1:B:684:GLN:H	2.04	0.66
1:B:927:TRP:HE3	1:B:928:MET:CA	2.07	0.66
1:C:165:ARG:CB	1:C:165:ARG:HH11	2.08	0.66
1:C:216:LEU:O	1:C:217:LEU:HB2	1.95	0.66
1:D:257:LEU:HD12	3:D:3006:FAD:C5A	2.26	0.66
1:D:257:LEU:O	3:D:3006:FAD:H2B	1.96	0.66
1:D:376:SER:HB3	1:D:379:THR:OG1	1.95	0.66
1:B:860:LEU:HD22	1:B:927:TRP:HZ2	1.61	0.66
1:D:920:GLY:HA2	1:D:923:ILE:N	2.10	0.66
1:A:1262:GLU:H	1:A:1263:PRO:CD	2.08	0.66
1:D:337:PHE:HD1	1:D:338:ALA:HB3	1.61	0.66
1:D:698:THR:HG23	1:D:701:ASP:OD2	1.96	0.66
1:A:482:LEU:O	1:A:486:VAL:HG23	1.96	0.66
1:C:1041:GLN:O	1:C:1041:GLN:HG2	1.96	0.66
1:D:263:GLU:HG2	1:D:354:THR:OG1	1.96	0.66
1:D:374:LEU:HD23	1:D:374:LEU:H	1.56	0.66
1:B:456:TYR:CE2	1:B:512:THR:HG22	2.31	0.65
1:C:104:ARG:HG2	1:C:201:PHE:CE1	2.30	0.65
1:D:154:ARG:N	1:D:155:PRO:HD2	2.11	0.65
1:A:805:ARG:O	1:A:808:VAL:HG22	1.96	0.65
1:A:1010:PHE:HB2	1:A:1016:ASN:ND2	2.11	0.65
1:B:932:ALA:CB	1:B:942:VAL:HG21	2.25	0.65
1:C:701:ASP:O	1:C:702:ALA:C	2.37	0.65
1:B:1291:VAL:N	1:C:380:ARG:HH21	1.94	0.65
1:C:1195:GLN:NE2	1:C:1195:GLN:HA	2.09	0.65
1:B:88:VAL:HG13	1:B:89:GLU:N	2.10	0.65
1:B:980:ALA:O	1:B:981:ARG:C	2.39	0.65
1:D:890:TYR:OH	1:D:943:ARG:HD3	1.96	0.65
1:A:1034:HIS:HE1	1:A:1044:HIS:CD2	2.15	0.65
1:D:27:LEU:O	1:D:28:ALA:HB3	1.95	0.65
1:D:87:THR:HG23	1:D:89:GLU:N	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:840:ARG:HG3	4:A:3007:GOL:H31	1.78	0.65
1:B:509:CYS:O	1:B:511:LEU:N	2.30	0.65
1:B:747:THR:HG23	1:B:827:MET:CE	2.27	0.65
1:B:927:TRP:HE3	1:B:927:TRP:C	2.04	0.65
1:B:1101:ARG:NH1	1:B:1127:SER:HB3	2.12	0.65
1:C:203:PRO:O	1:C:204:LEU:HB3	1.97	0.65
1:D:698:THR:O	1:D:700:GLU:O	2.15	0.65
1:C:275:PHE:N	1:C:275:PHE:CD1	2.64	0.65
1:C:1048:VAL:HG12	1:C:1049:GLN:N	2.10	0.65
1:C:376:SER:CB	1:C:379:THR:OG1	2.36	0.65
1:C:894:ASN:N	1:C:894:ASN:ND2	2.44	0.65
1:A:646:ILE:CD1	1:A:646:ILE:CB	2.73	0.65
1:B:1034:HIS:HE1	1:B:1044:HIS:HD2	1.43	0.65
1:A:662:THR:HG1	1:A:870:ASN:HD22	1.42	0.65
1:B:113:CYS:HA	1:B:1040:GLY:HA3	1.78	0.65
1:B:139:ILE:HD11	1:B:164:ALA:HB2	1.77	0.65
1:B:154:ARG:HD3	1:B:1197:GLU:OE2	1.97	0.65
1:B:530:GLU:N	1:B:530:GLU:OE2	2.29	0.65
1:C:333:GLN:NE2	1:C:360:ASP:HB3	2.12	0.65
1:D:1174:ASN:O	1:D:1237:PRO:HA	1.97	0.65
1:B:920:GLY:CA	1:B:923:ILE:H	2.11	0.64
1:C:1081:SER:OG	1:C:1262:GLU:HG3	1.97	0.64
1:A:871:THR:HG23	1:A:908:SER:CB	2.27	0.64
1:C:27:LEU:C	1:C:27:LEU:HD12	2.21	0.64
1:C:372:LEU:HD21	1:C:385:MET:HE3	1.79	0.64
1:C:737:ILE:HG23	1:C:1299:SER:HB3	1.79	0.64
1:D:997:ARG:HG2	1:D:1164:GLU:HB2	1.78	0.64
1:A:772:LYS:O	1:A:773:THR:C	2.35	0.64
1:B:251:GLN:HG3	1:B:252:HIS:CD2	2.33	0.64
1:B:749:CYS:HB2	1:B:827:MET:HG3	1.79	0.64
1:C:920:GLY:HA3	1:C:923:ILE:H	1.62	0.64
1:D:824:VAL:HG12	1:D:825:ARG:N	2.10	0.64
1:A:1002:ILE:HG23	1:A:1003:PRO:CD	2.27	0.64
1:A:215:GLU:C	1:A:216:LEU:O	2.32	0.64
1:B:216:LEU:O	1:B:217:LEU:CB	2.38	0.64
1:C:496:LEU:HD23	1:C:497:PRO:HD2	1.78	0.64
1:D:1266:PHE:CE2	1:D:1269:ALA:HB2	2.33	0.64
1:B:1192:ASP:O	1:B:1193:ILE:HB	1.96	0.64
1:C:1291:VAL:CA	1:C:1291:VAL:HB	2.14	0.64
1:D:1326:CYS:O	1:D:1327:LYS:HG2	1.98	0.64
1:C:769:ASN:ND2	1:C:1077:PRO:HG3	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:917:GLY:N	1:D:918:PRO:CD	2.59	0.64
1:D:920:GLY:HA3	1:D:923:ILE:N	2.10	0.64
1:A:612:THR:HG23	1:A:690:TYR:OH	1.97	0.63
1:A:744:TYR:N	1:A:744:TYR:CD1	2.64	0.63
1:B:483:LEU:HB2	1:B:520:TYR:CE1	2.32	0.63
1:D:372:LEU:HD22	1:D:407:ILE:CD1	2.27	0.63
1:D:871:THR:HG23	1:D:908:SER:OG	1.96	0.63
1:B:946:ASN:H	1:B:946:ASN:HD22	1.45	0.63
1:D:51:CYS:SG	1:D:71:ASN:HB2	2.38	0.63
1:D:1068:SER:OG	1:D:1069:THR:N	2.30	0.63
1:A:594:CYS:C	1:A:596:ASP:H	2.06	0.63
1:B:521:LEU:HD21	1:B:537:GLY:HA2	1.80	0.63
1:B:946:ASN:HD22	1:B:946:ASN:N	1.94	0.63
1:C:542:THR:HG23	1:C:542:THR:O	1.98	0.63
1:A:399:SER:OG	1:A:401:GLU:OE1	2.15	0.63
1:B:327:PHE:N	1:B:327:PHE:HD1	1.97	0.63
1:B:741:GLU:HB3	1:B:1228:TYR:CZ	2.33	0.63
1:B:1014:PHE:CD1	1:B:1014:PHE:C	2.76	0.63
1:B:431:ILE:H	1:B:1229:LYS:NZ	1.97	0.63
1:C:372:LEU:N	1:C:372:LEU:CD2	2.61	0.63
1:C:607:ARG:CD	1:C:679:THR:HG23	2.28	0.63
1:D:1174:ASN:OD1	1:D:1271:ILE:HD13	1.97	0.63
1:A:927:TRP:HE3	1:A:928:MET:CA	2.11	0.63
1:B:664:VAL:HG21	1:B:1218:GLY:O	1.99	0.63
1:A:920:GLY:HA3	1:A:923:ILE:N	2.02	0.63
1:C:1262:GLU:H	1:C:1263:PRO:HD3	1.63	0.63
1:D:888:ASN:OD1	1:D:921:MET:CE	2.47	0.63
1:D:701:ASP:O	1:D:702:ALA:C	2.40	0.63
1:D:1106:LYS:HG2	1:D:1117:TRP:CZ2	2.34	0.63
1:A:87:THR:HG21	1:A:89:GLU:HG2	1.80	0.63
1:C:682:ALA:C	1:C:684:GLN:H	2.07	0.63
1:A:56:SER:HB3	1:A:67:HIS:HD1	1.64	0.62
1:A:512:THR:C	1:A:513:LEU:HD23	2.24	0.62
1:A:698:THR:HG23	1:A:701:ASP:OD2	1.99	0.62
1:B:1289:ASN:CA	1:C:380:ARG:NH1	2.61	0.62
1:C:6:LEU:HD23	1:C:6:LEU:O	1.99	0.62
1:D:1008:ILE:O	1:D:1009:SER:HB2	1.98	0.62
1:A:62:GLN:O	1:A:64:LYS:HB2	1.99	0.62
1:B:482:LEU:O	1:B:486:VAL:HG23	1.99	0.62
1:B:916:GLY:N	4:B:3007:GOL:C3	2.45	0.62
1:D:56:SER:HB3	1:D:67:HIS:CE1	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:840:ARG:CG	4:D:3007:GOL:O1	2.46	0.62
1:A:1014:PHE:C	1:A:1014:PHE:CD1	2.77	0.62
1:C:3:ALA:HB1	1:C:227:LEU:CD2	2.29	0.62
1:C:404:LEU:N	3:C:3006:FAD:H62A	1.97	0.62
1:D:62:GLN:O	1:D:64:LYS:HB2	1.99	0.62
1:C:27:LEU:HD12	1:C:28:ALA:N	2.15	0.62
1:C:604:LEU:HD21	1:C:822:ARG:HH11	1.64	0.62
1:D:1069:THR:O	1:D:1069:THR:OG1	2.10	0.62
1:A:873:ASP:CG	1:A:874:LEU:H	2.07	0.62
1:C:649:ILE:HG13	1:C:649:ILE:O	1.99	0.62
1:C:751:ILE:HG12	1:C:825:ARG:HB2	1.82	0.62
1:C:865:PHE:N	1:C:865:PHE:HD1	1.94	0.62
1:D:594:CYS:C	1:D:596:ASP:H	2.07	0.62
1:B:374:LEU:HD12	1:B:374:LEU:N	2.15	0.62
1:C:372:LEU:N	1:C:372:LEU:HD23	2.13	0.62
1:C:377:ARG:O	1:C:377:ARG:HG3	1.97	0.62
1:C:920:GLY:CA	1:C:923:ILE:HG12	2.22	0.62
1:C:946:ASN:H	1:C:946:ASN:HD22	1.46	0.62
1:D:372:LEU:HD22	1:D:407:ILE:HD11	1.82	0.62
1:D:750:THR:OG1	1:D:765:VAL:HG13	1.99	0.62
1:B:607:ARG:HE	1:B:679:THR:HG22	1.57	0.62
1:C:699:ILE:HD13	1:C:867:ASN:HB2	1.82	0.62
1:A:404:LEU:HB3	3:A:3006:FAD:N6A	2.15	0.62
1:A:1213:HIS:H	1:A:1222:THR:HG22	1.64	0.62
1:B:137:GLU:HG2	1:B:137:GLU:O	1.99	0.62
1:B:910:THR:CG2	1:B:911:ALA:N	2.63	0.62
1:B:1055:LEU:CD1	1:B:1095:CYS:SG	2.88	0.62
1:B:1291:VAL:CA	1:C:380:ARG:HE	2.06	0.62
1:D:625:GLU:OE2	1:D:628:LYS:HE2	1.99	0.62
1:D:1096:GLN:HA	1:D:1099:LEU:HD12	1.80	0.62
1:B:248:LEU:HD12	1:B:248:LEU:C	2.25	0.61
1:B:560:LEU:HD12	1:B:1243:SER:HB3	1.81	0.61
1:B:1089:GLN:HG2	1:B:1134:TYR:CD1	2.35	0.61
1:C:849:VAL:HG13	1:C:849:VAL:O	2.00	0.61
1:A:104:ARG:HG2	1:A:201:PHE:CE1	2.35	0.61
1:A:124:MET:HE3	1:A:128:LEU:HD11	1.81	0.61
1:A:216:LEU:O	1:A:217:LEU:HB2	1.98	0.61
1:B:234:VAL:HG12	1:B:235:THR:N	2.15	0.61
1:B:1002:ILE:HG23	1:B:1003:PRO:HD2	1.83	0.61
1:D:430:ASP:CB	1:D:1229:LYS:HZ3	2.14	0.61
1:B:1002:ILE:HD13	1:B:1270:SER:HA	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1142:SER:HB3	1:B:1145:THR:CG2	2.30	0.61
1:D:1044:HIS:HD2	1:D:1064:ILE:HD13	1.64	0.61
1:C:921:MET:HE1	1:C:1004:THR:OG1	1.99	0.61
1:C:997:ARG:HG2	1:C:1164:GLU:HB2	1.82	0.61
1:D:241:THR:HG23	1:D:244:GLU:CG	2.29	0.61
1:A:1014:PHE:C	1:A:1014:PHE:HD1	2.09	0.61
1:C:698:THR:O	1:C:700:GLU:O	2.19	0.61
1:C:748:HIS:HD2	1:C:833:ASP:OD1	1.83	0.61
1:B:87:THR:HG23	1:B:89:GLU:N	2.15	0.61
1:B:136:MET:HE3	1:B:161:ARG:HA	1.80	0.61
1:B:4:ASP:O	1:B:5:LYS:C	2.44	0.61
1:B:304:PRO:HA	1:B:346:ALA:O	2.00	0.61
1:B:693:LEU:HB3	1:B:694:PRO:HD2	1.82	0.61
1:B:937:MET:HB2	1:B:938:PRO:C	2.26	0.61
1:C:693:LEU:HB3	1:C:694:PRO:CD	2.31	0.61
1:B:1312:ASP:H	1:B:1315:THR:HG21	1.63	0.61
1:B:1312:ASP:N	1:B:1315:THR:CG2	2.51	0.61
1:D:507:PHE:CE1	1:D:511:LEU:HD11	2.35	0.61
1:A:520:TYR:CE2	1:A:524:LEU:HD11	2.36	0.61
1:A:693:LEU:CD1	1:A:693:LEU:H	2.14	0.61
1:B:327:PHE:HD1	1:B:327:PHE:H	1.48	0.61
1:B:696:ILE:HG23	1:B:701:ASP:HB3	1.83	0.61
1:C:1115:GLU:N	1:C:1115:GLU:OE1	2.29	0.61
1:A:676:PRO:O	1:A:679:THR:HG22	2.01	0.61
1:B:284:ILE:O	1:B:285:PRO:C	2.44	0.61
1:C:790:VAL:O	1:C:1069:THR:HG23	2.01	0.61
1:C:1055:LEU:HD13	1:C:1095:CYS:SG	2.41	0.61
1:A:56:SER:HB3	1:A:67:HIS:CE1	2.35	0.60
1:B:312:LEU:HB3	1:B:331:LEU:HD11	1.82	0.60
1:B:574:VAL:HG13	1:B:1187:LEU:HD22	1.82	0.60
1:B:1081:SER:OG	1:B:1262:GLU:HG3	2.01	0.60
1:B:1092:TYR:O	1:B:1095:CYS:HB2	2.01	0.60
1:C:256:LYS:O	1:C:278:ILE:HG23	2.00	0.60
1:C:386:ASP:O	1:C:388:THR:N	2.34	0.60
1:C:684:GLN:HA	1:C:684:GLN:HE21	1.66	0.60
1:A:527:LEU:HD12	1:A:527:LEU:N	2.16	0.60
1:C:104:ARG:HG2	1:C:201:PHE:CD1	2.36	0.60
1:C:942:VAL:O	1:C:946:ASN:ND2	2.34	0.60
1:D:1070:ASN:C	1:D:1070:ASN:HD22	2.07	0.60
1:A:251:GLN:HG3	1:A:252:HIS:CD2	2.36	0.60
1:A:603:GLU:HG3	1:A:823:PRO:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1108:LYS:HZ3	1:C:1319:VAL:HG23	1.67	0.60
1:B:795:MET:CE	1:B:1039:MET:CG	2.77	0.60
1:C:461:ASN:HB3	1:C:462:ARG:HG3	1.81	0.60
1:C:719:ASP:HA	1:C:720:LEU:HB3	1.82	0.60
1:D:560:LEU:CD1	1:D:1243:SER:HB3	2.29	0.60
1:D:581:LEU:HG	1:D:1045:THR:HG23	1.83	0.60
1:D:1260:VAL:O	1:D:1260:VAL:HG22	1.99	0.60
1:A:423:GLN:NE2	1:A:424:ALA:H	1.98	0.60
1:A:693:LEU:N	1:A:693:LEU:CD1	2.64	0.60
1:A:1102:LEU:O	1:A:1103:GLU:C	2.42	0.60
1:B:278:ILE:HG22	1:B:279:VAL:N	2.16	0.60
1:B:459:MET:HE3	1:B:508:ARG:HD2	1.83	0.60
1:C:3:ALA:HB1	1:C:227:LEU:HD23	1.83	0.60
1:C:1008:ILE:O	1:C:1009:SER:CB	2.49	0.60
1:C:1195:GLN:HE21	1:C:1195:GLN:HA	1.66	0.60
1:C:1262:GLU:N	1:C:1263:PRO:CD	2.58	0.60
1:D:471:GLN:O	1:D:474:LEU:HB2	2.02	0.60
1:C:374:LEU:HD22	1:C:398:LEU:HD22	1.84	0.60
1:C:840:ARG:CG	4:C:3007:GOL:O1	2.48	0.60
1:B:528:GLY:HA2	1:B:529:GLN:HB2	1.83	0.60
1:C:840:ARG:HG3	4:C:3007:GOL:O1	2.01	0.60
1:D:1044:HIS:CD2	1:D:1064:ILE:HD13	2.37	0.60
1:A:1262:GLU:C	1:A:1264:PRO:HD2	2.26	0.60
1:B:241:THR:HG23	1:B:244:GLU:HG2	1.83	0.60
1:C:822:ARG:HB2	1:C:823:PRO:HD2	1.83	0.60
1:C:892:ILE:HG23	1:C:892:ILE:O	2.00	0.60
1:D:1142:SER:CB	1:D:1145:THR:HG21	2.31	0.60
1:A:1055:LEU:HD13	1:A:1095:CYS:SG	2.41	0.60
1:B:520:TYR:HE2	1:B:524:LEU:CD1	2.15	0.60
1:A:366:MET:HA	1:A:385:MET:HG2	1.84	0.60
1:A:403:ILE:HG13	1:A:403:ILE:O	2.00	0.60
1:C:366:MET:HA	1:C:385:MET:HG2	1.84	0.60
1:C:664:VAL:CG2	1:C:1218:GLY:O	2.48	0.60
1:C:1319:VAL:CA	1:C:1319:VAL:HB	2.17	0.60
1:D:860:LEU:HD22	1:D:927:TRP:CZ2	2.37	0.60
1:D:865:PHE:N	1:D:865:PHE:HD1	1.95	0.60
1:D:1302:THR:O	1:D:1306:ILE:HG13	2.02	0.60
1:A:209:GLU:HA	1:A:209:GLU:OE2	2.02	0.59
1:A:682:ALA:C	1:A:684:GLN:H	2.10	0.59
1:B:257:LEU:O	3:B:3006:FAD:H2B	2.02	0.59
1:B:1292:LYS:CE	1:C:382:THR:HG21	2.26	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:697:ILE:HG22	1:C:698:THR:N	2.16	0.59
1:C:709:TYR:HE1	1:C:903:LYS:HG3	1.66	0.59
1:A:335:ARG:HG3	1:A:336:TRP:CD1	2.36	0.59
1:A:459:MET:HE2	1:A:459:MET:HA	1.83	0.59
1:A:697:ILE:HG22	1:A:698:THR:N	2.17	0.59
1:B:6:LEU:HD23	1:B:6:LEU:O	2.02	0.59
1:C:248:LEU:C	1:C:248:LEU:CD1	2.73	0.59
1:C:1213:HIS:N	1:C:1222:THR:HG21	2.12	0.59
1:D:697:ILE:O	1:D:904:THR:HG21	2.01	0.59
1:B:822:ARG:HB2	1:B:823:PRO:HD2	1.85	0.59
1:B:888:ASN:OD1	1:B:921:MET:HE2	2.02	0.59
1:C:520:TYR:C	1:C:520:TYR:CD2	2.79	0.59
1:C:542:THR:O	1:C:542:THR:CG2	2.50	0.59
1:A:274:LEU:HG	1:A:274:LEU:O	2.03	0.59
1:A:423:GLN:CD	1:A:424:ALA:H	2.10	0.59
1:A:503:GLY:O	1:A:504:MET:HB2	2.02	0.59
1:A:610:THR:HG22	1:A:667:ILE:HA	1.84	0.59
1:B:923:ILE:O	1:B:926:CYS:HB3	2.02	0.59
1:D:840:ARG:HA	4:D:3007:GOL:HO1	1.65	0.59
1:A:509:CYS:O	1:A:511:LEU:N	2.36	0.59
1:C:927:TRP:CE3	1:C:928:MET:CA	2.85	0.59
1:D:1176:ARG:HG3	1:D:1177:THR:N	2.16	0.59
1:A:461:ASN:CB	1:A:462:ARG:HG3	2.31	0.59
1:A:931:VAL:HG12	1:A:932:ALA:N	2.17	0.59
1:B:1041:GLN:HG2	1:B:1041:GLN:O	2.00	0.59
1:C:372:LEU:HD23	1:C:372:LEU:H	1.67	0.59
1:C:611:SER:OG	1:C:661:VAL:HG21	2.02	0.59
1:C:1010:PHE:HB2	1:C:1016:ASN:ND2	2.17	0.59
1:D:606:LEU:CG	1:D:607:ARG:H	2.14	0.59
1:D:923:ILE:O	1:D:926:CYS:HB3	2.03	0.59
1:B:1289:ASN:CA	1:C:380:ARG:HH11	2.16	0.59
1:C:881:ARG:HD2	1:C:915:PHE:HB3	1.83	0.59
1:C:1250:ASN:O	1:C:1256:ALA:HA	2.03	0.59
1:D:916:GLY:CA	1:D:919:GLN:OE1	2.43	0.59
1:A:1160:CYS:O	1:A:1177:THR:HA	2.03	0.59
1:B:799:PHE:N	1:B:799:PHE:CD1	2.70	0.59
1:B:1195:GLN:HG2	1:B:1260:VAL:HG13	1.85	0.59
1:C:1008:ILE:O	1:C:1009:SER:HB2	2.01	0.59
1:C:1073:PRO:O	1:C:1074:ASN:HB2	2.02	0.59
1:D:312:LEU:N	1:D:312:LEU:HD12	2.17	0.59
1:C:374:LEU:CD2	1:C:398:LEU:HD22	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:398:LEU:HD23	1:C:398:LEU:H	1.67	0.59
1:C:879:MET:HE3	1:C:899:GLY:HA3	1.85	0.59
1:C:1293:GLU:O	1:C:1294:LEU:HD23	2.03	0.59
1:A:337:PHE:HD1	1:A:338:ALA:HB3	1.67	0.59
1:B:860:LEU:HD12	1:B:861:GLU:N	2.18	0.59
1:D:276:PRO:HD2	1:D:277:MET:H	1.67	0.59
1:D:521:LEU:O	1:D:524:LEU:HB2	2.03	0.59
1:D:769:ASN:ND2	1:D:1077:PRO:HG3	2.18	0.59
1:B:916:GLY:CA	4:B:3007:GOL:H32	2.32	0.58
1:B:1014:PHE:C	1:B:1014:PHE:HD1	2.10	0.58
1:C:824:VAL:CG1	1:C:825:ARG:N	2.64	0.58
1:C:1055:LEU:CD1	1:C:1095:CYS:SG	2.91	0.58
1:D:4:ASP:O	1:D:5:LYS:C	2.42	0.58
1:A:520:TYR:C	1:A:520:TYR:CD2	2.81	0.58
1:A:1002:ILE:CG2	1:A:1003:PRO:HD2	2.32	0.58
1:A:1260:VAL:O	1:A:1260:VAL:HG22	2.02	0.58
1:B:423:GLN:NE2	1:B:424:ALA:H	2.01	0.58
1:B:449:VAL:O	1:B:449:VAL:HG12	2.02	0.58
1:B:1262:GLU:H	1:B:1263:PRO:CD	2.17	0.58
1:C:773:THR:HG22	1:C:790:VAL:HG21	1.84	0.58
1:D:664:VAL:HG21	1:D:1218:GLY:O	2.03	0.58
1:D:841:HIS:HB2	4:D:3007:GOL:H12	1.86	0.58
1:D:1051:ALA:HB2	1:D:1091:VAL:CG1	2.33	0.58
1:D:1312:ASP:N	1:D:1315:THR:HG21	2.16	0.58
1:A:824:VAL:HG12	1:A:825:ARG:N	2.16	0.58
1:A:1124:ASP:O	1:A:1125:THR:CB	2.35	0.58
1:C:301:ALA:O	1:C:349:GLY:HA3	2.03	0.58
1:C:524:LEU:O	1:C:526:LYS:N	2.36	0.58
1:D:427:ARG:HD3	1:D:428:GLU:OE1	2.04	0.58
1:A:3:ALA:HB3	1:A:227:LEU:HD23	1.82	0.58
1:B:117:THR:CG2	1:B:587:ALA:HA	2.34	0.58
1:B:1311:VAL:HG13	1:B:1315:THR:HG21	1.85	0.58
1:C:949:LYS:HG3	1:C:952:ASP:OD2	2.03	0.58
1:D:87:THR:CG2	1:D:89:GLU:HG2	2.33	0.58
1:D:535:LYS:HB2	1:D:536:CYS:HB2	1.84	0.58
1:D:927:TRP:HE3	1:D:927:TRP:C	2.11	0.58
1:A:31:ARG:NH1	1:A:31:ARG:HG2	2.10	0.58
1:A:623:THR:CG2	1:A:627:LYS:HE3	2.34	0.58
1:B:38:GLY:HA2	1:B:40:LYS:HE2	1.84	0.58
1:B:662:THR:O	1:B:905:ASN:HB3	2.04	0.58
1:C:593:TYR:HB2	1:C:596:ASP:OD2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1192:ASP:O	1:C:1193:ILE:CB	2.47	0.58
1:A:353:ILE:O	1:A:353:ILE:HG22	2.04	0.58
1:A:1070:ASN:C	1:A:1070:ASN:ND2	2.49	0.58
1:B:881:ARG:HD2	1:B:915:PHE:HB3	1.86	0.58
1:B:956:PHE:HB2	1:B:1141:TYR:CE1	2.38	0.58
1:D:747:THR:CG2	1:D:827:MET:HE2	2.26	0.58
1:D:927:TRP:HE3	1:D:928:MET:HA	1.67	0.58
1:D:1213:HIS:H	1:D:1222:THR:HG22	1.67	0.58
1:A:214:PRO:O	1:A:216:LEU:O	2.21	0.58
1:A:459:MET:HA	1:A:459:MET:CE	2.33	0.58
1:A:864:HIS:C	1:A:865:PHE:CD1	2.81	0.58
1:B:509:CYS:C	1:B:511:LEU:N	2.55	0.58
1:C:682:ALA:O	1:C:684:GLN:N	2.37	0.58
1:C:1034:HIS:HE1	1:C:1044:HIS:HD2	1.51	0.58
1:A:241:THR:HG23	1:A:244:GLU:HG2	1.85	0.58
1:B:262:THR:OG1	3:B:3006:FAD:O2P	2.21	0.58
1:B:366:MET:HA	1:B:385:MET:HG2	1.85	0.58
1:B:461:ASN:HB3	1:B:462:ARG:HG3	1.86	0.58
1:B:623:THR:CG2	1:B:627:LYS:HE3	2.34	0.58
1:C:159:GLY:O	1:C:162:THR:CG2	2.35	0.58
1:D:535:LYS:CB	1:D:536:CYS:HB2	2.34	0.58
1:D:633:VAL:HG12	1:D:634:CYS:N	2.19	0.58
1:B:946:ASN:N	1:B:946:ASN:ND2	2.51	0.58
1:C:320:PRO:O	1:C:322:GLN:N	2.36	0.58
1:C:1004:THR:HG22	1:C:1267:LEU:HD21	1.86	0.58
1:D:104:ARG:HG2	1:D:201:PHE:CE1	2.38	0.58
1:B:113:CYS:HB3	1:B:150:CYS:SG	2.43	0.57
1:D:87:THR:HG21	1:D:89:GLU:HG2	1.85	0.57
1:A:351:ASN:ND2	1:A:361:LEU:HB2	2.19	0.57
1:A:404:LEU:N	3:A:3006:FAD:H61A	1.98	0.57
1:A:1002:ILE:HD13	1:A:1270:SER:HA	1.87	0.57
1:B:681:ARG:O	1:B:684:GLN:HB3	2.04	0.57
1:B:748:HIS:O	1:B:749:CYS:HB2	2.05	0.57
1:B:878:ILE:HG12	1:B:915:PHE:CE1	2.39	0.57
1:B:1004:THR:HG22	1:B:1267:LEU:HD21	1.85	0.57
1:C:202:THR:HB	1:C:203:PRO:HD3	1.86	0.57
1:C:1195:GLN:CA	1:C:1195:GLN:NE2	2.65	0.57
1:D:604:LEU:HD21	1:D:822:ARG:HH12	1.66	0.57
1:A:684:GLN:HE21	1:A:684:GLN:CA	2.03	0.57
1:B:469:THR:O	1:B:473:GLN:HG2	2.05	0.57
1:C:305:LEU:HD12	1:C:346:ALA:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:430:ASP:HB3	1:D:1229:LYS:HE2	1.50	0.57
1:B:104:ARG:HD3	1:B:162:THR:HG21	1.86	0.57
1:A:709:TYR:CE1	1:A:903:LYS:HG3	2.40	0.57
1:B:700:GLU:HA	1:B:703:ILE:HG13	1.86	0.57
1:C:160:PHE:O	1:C:161:ARG:C	2.45	0.57
1:C:440:VAL:CG2	1:C:452:LEU:HD12	2.32	0.57
1:C:788:ILE:N	1:C:788:ILE:CD1	2.67	0.57
1:D:715:ILE:HG23	1:D:1146:ASN:HD21	1.70	0.57
1:D:892:ILE:HG23	1:D:892:ILE:O	2.03	0.57
1:B:795:MET:CE	1:B:1039:MET:HG3	2.30	0.57
1:B:1262:GLU:C	1:B:1264:PRO:CD	2.77	0.57
1:A:3:ALA:HB2	1:A:225:LYS:NZ	2.19	0.57
1:A:257:LEU:O	3:A:3006:FAD:H2B	2.03	0.57
1:A:688:ILE:H	1:A:688:ILE:HD13	1.69	0.57
1:A:926:CYS:H	1:A:928:MET:H	1.50	0.57
1:B:29:TYR:HE2	1:B:34:LEU:HD21	1.69	0.57
1:B:920:GLY:HA2	1:B:922:LEU:N	2.20	0.57
1:C:87:THR:HG21	1:C:89:GLU:HG2	1.87	0.57
1:D:433:LYS:HD3	1:D:504:MET:SD	2.43	0.57
1:D:684:GLN:HE21	1:D:684:GLN:HA	1.70	0.57
1:A:248:LEU:HD12	1:A:248:LEU:O	2.04	0.57
1:A:310:LYS:HA	1:A:313:VAL:HG23	1.85	0.57
1:A:509:CYS:O	1:A:510:THR:C	2.47	0.57
1:A:849:VAL:O	1:A:849:VAL:CG1	2.52	0.57
1:A:963:PHE:CE2	1:A:966:PRO:HD3	2.40	0.57
1:B:327:PHE:N	1:B:327:PHE:CD1	2.69	0.57
1:B:745:LEU:N	1:B:745:LEU:HD23	2.18	0.57
1:B:931:VAL:O	1:B:933:VAL:N	2.38	0.57
1:B:1034:HIS:CE1	1:B:1044:HIS:CD2	2.90	0.57
1:D:278:ILE:HG22	1:D:279:VAL:N	2.19	0.57
1:D:719:ASP:HA	1:D:720:LEU:HB3	1.86	0.57
1:D:783:VAL:HB	1:D:784:PRO:HD2	1.87	0.57
1:A:1021:LEU:HD12	1:A:1022:LEU:H	1.65	0.57
1:B:795:MET:CE	1:B:1039:MET:HG2	2.35	0.57
1:C:269:LYS:HG2	1:C:270:PHE:CE1	2.39	0.57
1:C:1183:VAL:C	1:C:1258:LYS:HB2	2.29	0.57
1:D:507:PHE:CB	1:D:1304:GLU:HG3	2.34	0.57
1:D:710:GLY:O	1:D:900:ARG:NH1	2.38	0.57
1:D:746:GLU:HB2	1:D:796:GLY:HA3	1.86	0.57
1:D:1034:HIS:HE1	1:D:1044:HIS:HD2	1.52	0.57
1:A:71:ASN:ND2	1:A:71:ASN:H	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:LYS:C	1:A:434:VAL:CG1	2.77	0.57
1:B:534:ASP:CB	1:C:251:GLN:CB	2.82	0.57
1:C:487:CYS:O	1:C:513:LEU:HD21	2.04	0.57
1:C:606:LEU:CG	1:C:607:ARG:H	2.18	0.57
1:D:582:ALA:O	1:D:586:GLN:HG3	2.05	0.57
1:D:682:ALA:O	1:D:684:GLN:N	2.37	0.57
1:D:983:SER:O	1:D:985:VAL:N	2.38	0.57
1:A:115:PHE:HD2	1:A:745:LEU:HB3	1.70	0.56
1:A:404:LEU:N	3:A:3006:FAD:N6A	2.53	0.56
1:A:520:TYR:CE2	1:A:524:LEU:CD1	2.88	0.56
1:A:1002:ILE:CG2	1:A:1003:PRO:CD	2.83	0.56
1:B:883:LEU:O	1:B:885:HIS:N	2.38	0.56
1:D:216:LEU:O	1:D:217:LEU:CB	2.40	0.56
1:D:737:ILE:HG23	1:D:1299:SER:HB3	1.87	0.56
1:D:1014:PHE:HD1	1:D:1014:PHE:C	2.13	0.56
1:B:256:LYS:HE2	1:B:275:PHE:CE2	2.40	0.56
1:B:461:ASN:CB	1:B:462:ARG:HG3	2.35	0.56
1:C:6:LEU:HD23	1:C:6:LEU:C	2.30	0.56
1:C:165:ARG:HB2	1:C:165:ARG:HH11	1.66	0.56
1:C:530:GLU:N	1:C:530:GLU:OE2	2.37	0.56
1:D:604:LEU:CD2	1:D:822:ARG:HH11	2.15	0.56
1:A:113:CYS:HB3	1:A:150:CYS:SG	2.45	0.56
1:A:841:HIS:N	4:A:3007:GOL:O1	2.31	0.56
1:A:1109:ASN:ND2	1:C:1316:THR:HG21	2.20	0.56
1:B:386:ASP:O	1:B:388:THR:N	2.38	0.56
1:B:520:TYR:C	1:B:520:TYR:CD2	2.83	0.56
1:B:878:ILE:HG12	1:B:915:PHE:CD1	2.40	0.56
1:B:927:TRP:CE3	1:B:927:TRP:C	2.82	0.56
1:B:1263:PRO:N	1:B:1264:PRO:CD	2.68	0.56
1:C:459:MET:CE	1:C:508:ARG:HD2	2.35	0.56
1:B:926:CYS:H	1:B:928:MET:H	1.51	0.56
1:B:1262:GLU:O	1:B:1263:PRO:C	2.45	0.56
1:C:269:LYS:HG2	1:C:270:PHE:CD1	2.40	0.56
1:C:780:MET:HE1	1:C:815:LEU:HB2	1.87	0.56
1:C:1183:VAL:O	1:C:1258:LYS:HB2	2.06	0.56
1:D:448:GLU:O	1:D:449:VAL:CB	2.53	0.56
1:D:454:LEU:HB2	1:D:466:ALA:HB2	1.87	0.56
1:A:354:THR:O	1:A:354:THR:HG23	2.04	0.56
1:A:649:ILE:O	1:A:649:ILE:CG1	2.51	0.56
1:A:768:GLN:NE2	1:A:802:LYS:H	2.04	0.56
1:B:16:VAL:O	1:B:16:VAL:HG12	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1291:VAL:CA	1:C:380:ARG:HH21	2.18	0.56
1:D:3:ALA:CB	1:D:227:LEU:HD23	2.35	0.56
1:A:1262:GLU:N	1:A:1263:PRO:CD	2.68	0.56
1:B:511:LEU:HD21	1:B:515:PHE:CE1	2.37	0.56
1:B:910:THR:HG23	1:B:911:ALA:H	1.69	0.56
1:C:382:THR:HG22	1:C:382:THR:O	2.06	0.56
1:C:459:MET:HA	1:C:459:MET:CE	2.31	0.56
1:C:698:THR:HG23	1:C:701:ASP:CG	2.30	0.56
1:D:1268:ALA:O	1:D:1271:ILE:N	2.32	0.56
1:A:154:ARG:HD3	1:A:1197:GLU:OE2	2.05	0.56
1:A:860:LEU:HD11	1:A:862:VAL:CG2	2.36	0.56
1:A:1055:LEU:HD23	1:A:1057:ILE:CD1	2.35	0.56
1:C:87:THR:CG2	1:C:89:GLU:HG2	2.36	0.56
1:C:699:ILE:CD1	1:C:867:ASN:HB2	2.34	0.56
1:C:1314:PHE:CD2	1:C:1314:PHE:N	2.70	0.56
1:D:677:GLU:O	1:D:681:ARG:HG3	2.05	0.56
1:A:719:ASP:HA	1:A:720:LEU:HB3	1.87	0.56
1:B:864:HIS:CB	1:B:879:MET:HE1	2.36	0.56
1:B:916:GLY:HA2	1:B:919:GLN:OE1	2.05	0.56
1:B:1213:HIS:N	1:B:1222:THR:HG21	2.16	0.56
1:C:1133:PHE:CD2	1:C:1133:PHE:C	2.81	0.56
1:C:1135:ARG:CB	1:D:1125:THR:HG21	2.35	0.56
1:D:923:ILE:O	1:D:926:CYS:CB	2.54	0.56
1:D:1326:CYS:O	1:D:1327:LYS:CG	2.54	0.56
1:A:3:ALA:HB3	1:A:227:LEU:HA	1.87	0.56
1:B:137:GLU:O	1:B:137:GLU:CG	2.54	0.56
1:B:202:THR:CB	1:B:203:PRO:HD3	2.35	0.56
1:B:430:ASP:CB	1:B:1229:LYS:NZ	2.44	0.56
1:B:1008:ILE:O	1:B:1009:SER:CB	2.53	0.56
1:D:921:MET:HE1	1:D:1004:THR:OG1	2.06	0.56
1:D:1224:GLY:O	1:D:1226:SER:N	2.39	0.56
1:D:1315:THR:O	1:D:1319:VAL:HG23	2.05	0.56
1:A:165:ARG:HB2	1:A:165:ARG:HH11	1.71	0.56
1:A:956:PHE:HB2	1:A:1141:TYR:HE1	1.70	0.56
1:B:112:GLN:HE21	1:B:150:CYS:HB3	1.71	0.56
1:C:1105:TYR:N	1:C:1105:TYR:CD1	2.74	0.56
1:A:351:ASN:HD22	1:A:361:LEU:HB2	1.71	0.55
1:A:1022:LEU:C	1:A:1022:LEU:HD12	2.31	0.55
1:C:653:GLU:OE2	1:C:805:ARG:NH1	2.39	0.55
1:C:914:GLY:N	1:C:1262:GLU:OE2	2.35	0.55
1:C:931:VAL:O	1:C:933:VAL:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1266:PHE:CE2	1:C:1269:ALA:HB2	2.41	0.55
1:D:3:ALA:HB1	1:D:227:LEU:HD23	1.88	0.55
1:D:750:THR:HG21	1:D:810:SER:HA	1.88	0.55
1:D:780:MET:C	1:D:780:MET:SD	2.89	0.55
1:D:1193:ILE:O	1:D:1194:GLY:C	2.49	0.55
1:D:1206:LEU:HD12	1:D:1206:LEU:O	2.06	0.55
1:A:572:ASP:C	1:A:572:ASP:OD1	2.48	0.55
1:A:693:LEU:HB3	1:A:694:PRO:CD	2.36	0.55
1:B:31:ARG:NH1	1:B:31:ARG:HG2	2.22	0.55
1:B:337:PHE:O	1:B:343:LYS:HE2	2.06	0.55
1:B:788:ILE:N	1:B:788:ILE:CD1	2.68	0.55
1:C:1055:LEU:O	1:C:1056:LYS:HB2	2.06	0.55
1:A:316:VAL:HG21	1:A:328:ARG:HD3	1.88	0.55
1:B:248:LEU:C	1:B:248:LEU:CD1	2.80	0.55
1:B:693:LEU:H	1:B:693:LEU:HD13	1.70	0.55
1:A:279:VAL:O	1:A:279:VAL:HG13	2.05	0.55
1:B:3:ALA:C	1:B:4:ASP:CG	2.73	0.55
1:B:927:TRP:CE3	1:B:928:MET:CA	2.88	0.55
1:C:560:LEU:HD12	1:C:1243:SER:HB3	1.87	0.55
1:C:988:PHE:CD2	1:C:997:ARG:HG3	2.41	0.55
1:D:708:PHE:O	1:D:708:PHE:HD1	1.89	0.55
1:A:769:ASN:HD22	1:A:1077:PRO:HG3	1.71	0.55
1:B:303:CYS:O	1:B:347:SER:HA	2.06	0.55
1:B:788:ILE:N	1:B:788:ILE:HD13	2.20	0.55
1:B:873:ASP:CG	1:B:874:LEU:H	2.13	0.55
1:C:217:LEU:C	1:C:220:LYS:HG2	2.31	0.55
1:C:1034:HIS:CE1	1:C:1044:HIS:CD2	2.91	0.55
1:D:520:TYR:C	1:D:520:TYR:CD2	2.84	0.55
1:D:1142:SER:CB	1:D:1145:THR:CG2	2.84	0.55
1:A:980:ALA:O	1:A:981:ARG:C	2.49	0.55
1:B:87:THR:HG23	1:B:89:GLU:H	1.71	0.55
1:B:558:VAL:HG12	1:B:1241:ARG:HG3	1.88	0.55
1:A:42:GLY:N	2:A:3002:FES:S2	2.72	0.55
1:A:99:HIS:CE1	1:A:101:VAL:HG23	2.41	0.55
1:B:38:GLY:HA2	1:B:40:LYS:CD	2.36	0.55
1:B:769:ASN:HD22	1:B:1077:PRO:HG3	1.71	0.55
1:B:878:ILE:HD13	4:B:3007:GOL:H11	1.87	0.55
1:C:161:ARG:HG3	1:C:162:THR:N	2.16	0.55
1:A:1255:TYR:O	1:A:1256:ALA:HB3	2.07	0.55
1:B:3:ALA:HB1	1:B:3:ALA:O	2.04	0.55
1:B:594:CYS:C	1:B:596:ASP:N	2.62	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:956:PHE:HB2	1:B:1141:TYR:HE1	1.70	0.55
1:B:1292:LYS:HE3	1:C:382:THR:CG2	2.29	0.55
1:D:539:LEU:HD22	1:D:540:ASP:H	1.71	0.55
1:B:1291:VAL:CB	1:B:1291:VAL:C	2.75	0.55
1:C:449:VAL:O	1:C:449:VAL:CG1	2.46	0.55
1:C:998:GLY:O	1:C:1162:GLU:HA	2.07	0.55
1:D:424:ALA:O	1:D:425:SER:CB	2.54	0.55
1:D:469:THR:O	1:D:473:GLN:HG2	2.06	0.55
1:A:1312:ASP:O	1:A:1315:THR:HG23	2.06	0.55
1:B:202:THR:HB	1:B:203:PRO:HD3	1.88	0.55
1:B:679:THR:HG22	1:B:680:GLN:H	1.72	0.55
1:C:423:GLN:HE21	1:C:424:ALA:N	2.05	0.55
1:C:679:THR:CG2	1:C:680:GLN:N	2.70	0.55
1:C:703:ILE:O	1:C:705:ASN:N	2.39	0.55
1:A:26:LEU:HD23	1:A:72:ALA:HB1	1.88	0.54
1:A:1005:LYS:HG3	1:A:1005:LYS:O	2.06	0.54
1:B:404:LEU:HB3	3:B:3006:FAD:N6A	2.23	0.54
1:B:867:ASN:C	1:B:867:ASN:OD1	2.49	0.54
1:C:303:CYS:O	1:C:347:SER:HA	2.06	0.54
1:C:623:THR:CG2	1:C:627:LYS:HE3	2.37	0.54
1:C:771:MET:HE3	1:C:772:LYS:HE2	1.89	0.54
1:D:682:ALA:C	1:D:684:GLN:H	2.15	0.54
1:A:1002:ILE:HG22	1:A:1003:PRO:N	2.21	0.54
1:D:76:PRO:HG2	1:D:76:PRO:O	2.07	0.54
1:A:372:LEU:CD2	1:A:407:ILE:HD11	2.33	0.54
1:A:581:LEU:HG	1:A:1045:THR:HG23	1.88	0.54
1:A:895:ILE:HG23	1:A:895:ILE:O	2.07	0.54
1:D:310:LYS:HA	1:D:313:VAL:HG23	1.89	0.54
1:C:682:ALA:C	1:C:684:GLN:N	2.65	0.54
1:D:81:HIS:O	1:D:82:HIS:HB2	2.08	0.54
1:D:1070:ASN:C	1:D:1070:ASN:ND2	2.62	0.54
1:A:788:ILE:N	1:A:788:ILE:CD1	2.70	0.54
1:A:1118:VAL:O	1:A:1119:THR:C	2.48	0.54
1:C:309:GLU:O	1:C:313:VAL:HG23	2.07	0.54
1:D:16:VAL:O	1:D:16:VAL:HG12	2.07	0.54
1:D:27:LEU:HD12	1:D:28:ALA:N	2.22	0.54
1:D:112:GLN:HE21	1:D:150:CYS:HB3	1.72	0.54
1:D:741:GLU:HB3	1:D:1228:TYR:CZ	2.43	0.54
1:D:1105:TYR:N	1:D:1105:TYR:CD1	2.75	0.54
1:D:1133:PHE:O	1:D:1134:TYR:HB2	2.06	0.54
1:A:71:ASN:H	1:A:71:ASN:HD22	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ARG:HB2	1:A:165:ARG:NH1	2.22	0.54
1:A:664:VAL:HG21	1:A:1218:GLY:C	2.32	0.54
1:A:791:ARG:NH1	1:A:1066:GLU:OE1	2.40	0.54
1:B:81:HIS:O	1:B:82:HIS:HB2	2.08	0.54
1:B:428:GLU:O	1:B:429:ASP:C	2.50	0.54
1:B:532:LEU:HA	1:B:534:ASP:H	1.71	0.54
1:C:29:TYR:HE2	1:C:34:LEU:HD21	1.73	0.54
1:C:972:CYS:C	1:C:974:ALA:H	2.14	0.54
1:D:312:LEU:H	1:D:312:LEU:CD1	2.20	0.54
1:D:509:CYS:O	1:D:512:THR:OG1	2.23	0.54
1:D:511:LEU:O	1:D:513:LEU:N	2.41	0.54
1:C:147:LEU:HD13	1:C:1230:ILE:HD11	1.87	0.54
1:C:353:ILE:O	1:C:353:ILE:CG2	2.56	0.54
1:C:920:GLY:HA2	1:C:922:LEU:N	2.23	0.54
1:D:891:LYS:HE2	1:D:949:LYS:CE	2.28	0.54
1:B:154:ARG:N	1:B:155:PRO:HD2	2.23	0.54
1:B:320:PRO:O	1:B:322:GLN:N	2.39	0.54
1:C:736:TYR:HD1	1:C:843:PHE:O	1.90	0.54
1:C:748:HIS:CD2	1:C:837:THR:HG21	2.42	0.54
1:D:1133:PHE:HD2	1:D:1134:TYR:N	2.01	0.54
1:A:256:LYS:HE2	1:A:275:PHE:CE2	2.43	0.54
1:B:676:PRO:O	1:B:679:THR:HG22	2.08	0.54
1:B:744:TYR:N	1:B:744:TYR:CD1	2.75	0.54
1:C:927:TRP:CZ3	1:C:928:MET:HE2	2.41	0.54
1:D:312:LEU:N	1:D:312:LEU:CD1	2.71	0.54
1:A:1108:LYS:HZ2	1:C:1319:VAL:HG23	1.73	0.54
1:B:23:GLU:OE2	1:B:233:ARG:HB2	2.08	0.54
1:C:448:GLU:O	1:C:449:VAL:HB	2.07	0.54
1:C:851:PHE:N	1:C:851:PHE:CD2	2.75	0.54
1:A:81:HIS:O	1:A:82:HIS:HB2	2.08	0.53
1:D:351:ASN:HD22	1:D:361:LEU:HB2	1.74	0.53
1:D:361:LEU:HB3	1:D:365:PHE:CE1	2.43	0.53
1:D:423:GLN:OE1	1:D:423:GLN:HA	2.09	0.53
1:A:885:HIS:HB3	1:A:921:MET:HG3	1.90	0.53
1:A:1109:ASN:CB	1:C:1316:THR:CG2	2.40	0.53
1:B:1055:LEU:HD13	1:B:1095:CYS:SG	2.48	0.53
1:B:1260:VAL:HG22	1:B:1260:VAL:O	2.08	0.53
1:C:595:ASP:OD1	1:C:825:ARG:HD3	2.08	0.53
1:C:1230:ILE:HB	1:C:1231:PRO:CD	2.38	0.53
1:D:27:LEU:HD12	1:D:31:ARG:HB2	1.90	0.53
1:D:271:LYS:O	1:D:273:MET:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:747:THR:CG2	1:D:827:MET:CE	2.73	0.53
1:A:858:VAL:O	1:A:894:ASN:ND2	2.42	0.53
1:A:1041:GLN:O	1:A:1041:GLN:HG2	2.05	0.53
1:B:323:LYS:HA	1:B:412:SER:O	2.07	0.53
1:B:633:VAL:O	1:B:634:CYS:HB3	2.07	0.53
1:B:925:GLU:O	1:B:1273:PHE:CZ	2.61	0.53
1:C:337:PHE:CD1	1:C:338:ALA:HB3	2.39	0.53
1:D:1250:ASN:O	1:D:1256:ALA:HA	2.08	0.53
1:A:335:ARG:HG3	1:A:336:TRP:NE1	2.22	0.53
1:B:377:ARG:HG3	1:B:377:ARG:O	2.08	0.53
1:B:927:TRP:CZ3	1:B:928:MET:HE2	2.43	0.53
1:C:830:ARG:HG3	1:C:830:ARG:O	2.04	0.53
1:C:926:CYS:H	1:C:928:MET:H	1.56	0.53
1:D:101:VAL:O	1:D:101:VAL:CG1	2.55	0.53
1:D:482:LEU:O	1:D:486:VAL:HG23	2.08	0.53
1:D:920:GLY:HA2	1:D:921:MET:C	2.34	0.53
1:D:1031:LEU:HD12	1:D:1063:TYR:O	2.09	0.53
1:A:625:GLU:OE2	1:A:628:LYS:HE2	2.09	0.53
1:C:353:ILE:O	1:C:353:ILE:HG22	2.08	0.53
1:C:1010:PHE:HB2	1:C:1016:ASN:HD21	1.74	0.53
1:D:965:LEU:N	1:D:966:PRO:HD2	2.23	0.53
1:A:71:ASN:ND2	1:A:71:ASN:N	2.55	0.53
1:B:217:LEU:O	1:B:220:LYS:HG2	2.09	0.53
1:B:448:GLU:O	1:B:449:VAL:CB	2.55	0.53
1:B:711:PRO:O	1:B:712:GLU:C	2.50	0.53
1:C:9:PHE:O	1:C:85:VAL:HG23	2.08	0.53
1:C:847:TYR:CE1	1:C:927:TRP:HB2	2.44	0.53
1:C:1083:SER:O	1:C:1087:ASN:ND2	2.39	0.53
1:D:313:VAL:HA	1:D:331:LEU:HD21	1.91	0.53
1:D:633:VAL:O	1:D:634:CYS:HB3	2.09	0.53
1:D:1014:PHE:C	1:D:1014:PHE:CD1	2.85	0.53
1:D:1197:GLU:HG2	1:D:1240:PHE:CZ	2.44	0.53
1:D:1280:ARG:HH11	1:D:1280:ARG:HG3	1.73	0.53
1:A:241:THR:HG23	1:A:244:GLU:CG	2.38	0.53
1:A:558:VAL:C	1:A:559:GLN:HG3	2.34	0.53
1:A:588:SER:OG	1:A:590:GLU:CG	2.57	0.53
1:D:386:ASP:OD1	1:D:388:THR:HG22	2.08	0.53
1:D:1008:ILE:O	1:D:1009:SER:CB	2.56	0.53
1:A:741:GLU:HB3	1:A:1228:TYR:CZ	2.43	0.53
1:A:947:LEU:O	1:A:948:TYR:C	2.52	0.53
1:B:684:GLN:HA	1:B:684:GLN:NE2	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:506:ASP:O	1:C:510:THR:OG1	2.26	0.53
1:C:708:PHE:HD1	1:C:708:PHE:O	1.91	0.53
1:A:3:ALA:HB2	1:A:225:LYS:HZ2	1.74	0.53
1:A:9:PHE:O	1:A:85:VAL:HG23	2.09	0.53
1:B:523:VAL:O	1:B:526:LYS:N	2.29	0.53
1:D:693:LEU:CD1	1:D:693:LEU:H	2.20	0.53
1:D:702:ALA:HB1	1:D:902:CYS:HB3	1.91	0.53
1:B:404:LEU:H	3:B:3006:FAD:H61A	1.57	0.53
1:B:1044:HIS:HD2	1:B:1064:ILE:HD13	1.72	0.53
1:D:430:ASP:CG	1:D:1229:LYS:CD	2.81	0.53
1:A:529:GLN:O	1:A:529:GLN:HG2	2.08	0.52
1:A:606:LEU:CG	1:A:607:ARG:H	2.21	0.52
1:A:920:GLY:CA	1:A:922:LEU:N	2.70	0.52
1:B:3:ALA:CB	1:B:3:ALA:O	2.57	0.52
1:B:353:ILE:O	1:B:355:ALA:N	2.42	0.52
1:B:927:TRP:HE3	1:B:928:MET:HA	1.73	0.52
1:B:1045:THR:O	1:B:1049:GLN:HG3	2.09	0.52
1:C:466:ALA:CB	1:C:470:THR:HB	2.39	0.52
1:C:472:ARG:HD2	1:C:485:ASP:OD2	2.08	0.52
1:D:507:PHE:CZ	1:D:511:LEU:CD1	2.90	0.52
1:A:864:HIS:CB	1:A:879:MET:HE1	2.40	0.52
1:A:864:HIS:HB2	1:A:879:MET:HE1	1.92	0.52
1:A:920:GLY:HA2	1:A:922:LEU:CB	2.40	0.52
1:B:364:VAL:O	1:B:368:SER:HB2	2.09	0.52
1:B:604:LEU:HD21	1:B:822:ARG:NH1	2.25	0.52
1:C:698:THR:OG1	1:C:700:GLU:HG2	2.10	0.52
1:D:826:CYS:SG	1:D:827:MET:N	2.81	0.52
1:D:1070:ASN:HD22	1:D:1071:THR:N	2.07	0.52
1:A:765:VAL:HG12	1:A:767:THR:HG22	1.91	0.52
1:B:676:PRO:HA	1:B:679:THR:HB	1.92	0.52
1:B:748:HIS:HD2	1:B:833:ASP:OD1	1.93	0.52
1:B:920:GLY:HA2	1:B:923:ILE:H	1.74	0.52
1:C:610:THR:HG22	1:C:667:ILE:HA	1.91	0.52
1:C:719:ASP:CA	1:C:720:LEU:HB3	2.39	0.52
1:D:251:GLN:CG	1:D:252:HIS:HD2	2.22	0.52
1:D:561:PHE:CD2	1:D:561:PHE:N	2.76	0.52
1:D:608:LEU:HD23	1:D:608:LEU:H	1.74	0.52
1:A:76:PRO:HD3	1:A:261:ASN:HD22	1.71	0.52
1:A:313:VAL:N	1:A:331:LEU:HD21	2.24	0.52
1:A:372:LEU:CD2	1:A:372:LEU:N	2.73	0.52
1:B:154:ARG:HH11	1:B:1197:GLU:CD	2.14	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:472:ARG:HG2	1:B:473:GLN:NE2	2.24	0.52
1:B:1262:GLU:N	1:B:1263:PRO:CD	2.72	0.52
1:C:507:PHE:CE2	1:C:511:LEU:HD11	2.44	0.52
1:C:871:THR:CG2	1:C:908:SER:HB2	2.36	0.52
1:D:1154:PHE:O	1:D:1258:LYS:HE2	2.10	0.52
1:D:1268:ALA:O	1:D:1269:ALA:C	2.51	0.52
1:A:523:VAL:HG12	1:A:524:LEU:N	2.24	0.52
1:A:1113:SER:O	1:A:1116:ASP:HB2	2.10	0.52
1:B:447:THR:O	1:B:448:GLU:HB2	2.09	0.52
1:B:930:GLU:HG2	1:B:1294:LEU:HD22	1.91	0.52
1:C:741:GLU:HG3	1:C:743:PHE:H	1.75	0.52
1:C:860:LEU:HD22	1:C:927:TRP:CZ2	2.43	0.52
1:A:257:LEU:HD12	3:A:3006:FAD:C5A	2.40	0.52
1:C:582:ALA:O	1:C:586:GLN:HG3	2.10	0.52
1:D:386:ASP:OD2	1:D:388:THR:HB	2.09	0.52
1:D:1041:GLN:O	1:D:1041:GLN:CG	2.49	0.52
1:D:1213:HIS:N	1:D:1222:THR:HG21	2.20	0.52
1:D:1279:ILE:O	1:D:1280:ARG:C	2.51	0.52
1:A:1055:LEU:CD1	1:A:1095:CYS:SG	2.98	0.52
1:A:1189:PRO:O	1:A:1193:ILE:HG13	2.09	0.52
1:C:895:ILE:HG23	1:C:895:ILE:O	2.09	0.52
1:C:1263:PRO:N	1:C:1264:PRO:HD2	2.25	0.52
1:D:629:VAL:HG13	1:D:630:PRO:HD2	1.92	0.52
1:A:1316:THR:O	1:A:1319:VAL:HG12	2.10	0.52
1:B:920:GLY:HA3	1:B:923:ILE:H	1.74	0.52
1:B:1176:ARG:HG3	1:B:1177:THR:N	2.25	0.52
1:B:1285:GLN:HA	1:C:378:GLY:N	2.25	0.52
1:C:346:ALA:HB1	3:C:3006:FAD:H4'	1.92	0.52
1:C:432:ALA:O	1:C:433:LYS:HB2	2.10	0.52
1:C:972:CYS:C	1:C:974:ALA:N	2.66	0.52
1:D:418:PHE:CD2	1:D:438:MET:O	2.63	0.52
1:B:534:ASP:HB2	1:C:251:GLN:CB	2.30	0.52
1:C:312:LEU:N	1:C:312:LEU:CD1	2.72	0.52
1:C:708:PHE:HB3	1:C:902:CYS:HA	1.92	0.52
1:C:923:ILE:O	1:C:926:CYS:CB	2.57	0.52
1:D:62:GLN:O	1:D:63:ASN:C	2.53	0.52
1:D:927:TRP:CE3	1:D:928:MET:HA	2.45	0.52
1:A:372:LEU:HD22	1:A:407:ILE:CD1	2.33	0.52
1:A:377:ARG:HG3	1:A:377:ARG:O	2.10	0.52
1:A:386:ASP:OD1	1:A:388:THR:HG22	2.10	0.52
1:B:708:PHE:HE1	1:B:900:ARG:NH2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1193:ILE:HA	1:B:1196:VAL:HB	1.91	0.52
1:C:618:ILE:O	1:C:618:ILE:HG12	2.10	0.52
1:D:95:LYS:HD3	1:D:590:GLU:OE1	2.10	0.52
1:D:352:ILE:HG22	1:D:353:ILE:HG13	1.92	0.52
1:D:599:ARG:CB	1:D:599:ARG:CD	2.85	0.52
1:D:772:LYS:O	1:D:773:THR:C	2.51	0.52
1:D:847:TYR:N	1:D:847:TYR:HD2	2.07	0.52
1:D:1010:PHE:HB2	1:D:1016:ASN:HD21	1.71	0.52
1:A:607:ARG:CD	1:A:679:THR:HG23	2.40	0.51
1:A:1014:PHE:HD1	1:A:1014:PHE:O	1.92	0.51
1:A:1092:TYR:O	1:A:1095:CYS:HB2	2.10	0.51
1:B:42:GLY:N	2:B:3002:FES:S2	2.75	0.51
1:B:1263:PRO:N	1:B:1264:PRO:HD2	2.23	0.51
1:C:679:THR:HG22	1:C:680:GLN:H	1.75	0.51
1:C:708:PHE:CD1	1:C:708:PHE:N	2.71	0.51
1:C:1263:PRO:N	1:C:1264:PRO:CD	2.72	0.51
1:D:459:MET:HE2	1:D:459:MET:HA	1.92	0.51
1:D:499:ASP:O	1:D:500:ALA:C	2.50	0.51
1:D:748:HIS:HD2	1:D:833:ASP:OD1	1.92	0.51
1:A:797:GLY:O	1:A:802:LYS:HE3	2.11	0.51
1:B:117:THR:HG22	1:B:587:ALA:HA	1.93	0.51
1:B:522:THR:HA	1:B:525:GLN:HB3	1.91	0.51
1:B:607:ARG:CD	1:B:679:THR:HG23	2.40	0.51
1:B:879:MET:O	1:B:882:ALA:HB3	2.10	0.51
1:B:1285:GLN:HA	1:C:378:GLY:H	1.75	0.51
1:C:1004:THR:CG2	1:C:1267:LEU:HD21	2.41	0.51
1:C:1121:ALA:O	1:C:1126:VAL:HG23	2.11	0.51
1:D:420:ALA:O	1:D:421:PHE:CD2	2.63	0.51
1:A:87:THR:CG2	1:A:89:GLU:HG2	2.39	0.51
1:A:87:THR:CG2	1:A:89:GLU:N	2.73	0.51
1:A:682:ALA:C	1:A:684:GLN:N	2.68	0.51
1:A:697:ILE:O	1:A:904:THR:HG21	2.10	0.51
1:B:1002:ILE:HD13	1:B:1270:SER:CA	2.40	0.51
1:B:1118:VAL:O	1:B:1120:ALA:N	2.43	0.51
1:B:1291:VAL:CA	1:B:1291:VAL:CG2	2.83	0.51
1:C:251:GLN:CG	1:C:252:HIS:HD2	2.20	0.51
1:C:309:GLU:O	1:C:313:VAL:CG2	2.58	0.51
1:C:748:HIS:O	1:C:749:CYS:HB2	2.10	0.51
1:C:937:MET:CB	1:C:938:PRO:HA	2.40	0.51
1:D:71:ASN:ND2	1:D:71:ASN:H	2.08	0.51
1:D:426:ARG:NH2	1:D:429:ASP:O	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:440:VAL:HG23	1:D:452:LEU:HD12	1.93	0.51
1:D:949:LYS:O	1:D:950:GLU:C	2.53	0.51
1:A:312:LEU:N	1:A:312:LEU:HD12	2.25	0.51
1:A:373:THR:C	1:A:374:LEU:CD2	2.75	0.51
1:B:389:PHE:O	1:B:391:PRO:HD3	2.10	0.51
1:D:1048:VAL:HG12	1:D:1049:GLN:N	2.26	0.51
1:A:213:PRO:O	1:A:214:PRO:C	2.49	0.51
1:A:847:TYR:CD2	1:A:847:TYR:N	2.78	0.51
1:A:1031:LEU:HD12	1:A:1063:TYR:O	2.11	0.51
1:B:941:GLU:O	1:B:945:LYS:HB2	2.09	0.51
1:C:946:ASN:HD22	1:C:946:ASN:N	2.09	0.51
1:D:139:ILE:O	1:D:141:ASN:N	2.43	0.51
1:D:165:ARG:NH1	1:D:165:ARG:CB	2.60	0.51
1:D:588:SER:OG	1:D:590:GLU:HG2	2.11	0.51
1:D:606:LEU:CD2	1:D:606:LEU:C	2.69	0.51
1:A:326:VAL:HG13	1:A:418:PHE:CE1	2.45	0.51
1:A:754:PRO:O	1:A:754:PRO:HG2	2.10	0.51
1:A:1268:ALA:O	1:A:1269:ALA:C	2.54	0.51
1:B:528:GLY:CA	1:B:529:GLN:HB2	2.41	0.51
1:B:864:HIS:C	1:B:865:PHE:CD1	2.88	0.51
1:D:504:MET:HE2	1:D:1304:GLU:HB2	1.93	0.51
1:A:62:GLN:O	1:A:63:ASN:C	2.53	0.51
1:A:642:PRO:HG3	1:A:818:TYR:CE2	2.46	0.51
1:C:1070:ASN:HD22	1:C:1070:ASN:C	2.17	0.51
1:D:99:HIS:CE1	1:D:101:VAL:HG23	2.46	0.51
1:D:351:ASN:HB2	3:D:3006:FAD:O4'	2.10	0.51
1:B:87:THR:HG23	1:B:89:GLU:HG2	1.91	0.51
1:B:209:GLU:HA	1:B:209:GLU:OE2	2.11	0.51
1:B:361:LEU:HB3	1:B:365:PHE:CE1	2.45	0.51
1:B:741:GLU:HG3	1:B:742:HIS:N	2.23	0.51
1:D:346:ALA:HB1	3:D:3006:FAD:H4'	1.93	0.51
1:D:748:HIS:O	1:D:749:CYS:HB2	2.11	0.51
1:D:1183:VAL:C	1:D:1258:LYS:HB2	2.35	0.51
1:A:767:THR:O	1:A:795:MET:HE2	2.10	0.51
1:A:1224:GLY:C	1:A:1226:SER:H	2.18	0.51
1:B:599:ARG:CD	1:B:599:ARG:HB3	2.39	0.51
1:B:1133:PHE:CD2	1:B:1133:PHE:C	2.89	0.51
1:B:1213:HIS:H	1:B:1222:THR:HG22	1.68	0.51
1:C:440:VAL:HG23	1:C:452:LEU:CD1	2.38	0.51
1:C:677:GLU:O	1:C:681:ARG:HG3	2.11	0.51
1:D:1197:GLU:HG2	1:D:1240:PHE:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:701:ASP:O	1:A:702:ALA:C	2.53	0.51
1:B:56:SER:HB3	1:B:67:HIS:CE1	2.45	0.51
1:B:421:PHE:HB3	1:B:515:PHE:CE2	2.45	0.51
1:B:560:LEU:CD1	1:B:1243:SER:HB3	2.41	0.51
1:B:791:ARG:NH1	1:B:1066:GLU:OE1	2.44	0.51
1:B:981:ARG:O	1:B:982:LYS:C	2.52	0.51
1:D:71:ASN:H	1:D:71:ASN:HD22	1.58	0.51
1:A:1055:LEU:HD23	1:A:1057:ILE:HD11	1.93	0.50
1:B:165:ARG:HH11	1:B:165:ARG:HB2	1.76	0.50
1:B:511:LEU:HD23	1:B:515:PHE:CD1	2.46	0.50
1:C:1021:LEU:HD12	1:C:1021:LEU:C	2.32	0.50
1:C:1133:PHE:CD1	1:D:1127:SER:HB2	2.46	0.50
1:D:813:VAL:O	1:D:814:ALA:C	2.52	0.50
1:B:723:GLY:O	1:B:724:PHE:HB2	2.11	0.50
1:B:768:GLN:HG2	1:B:795:MET:HE1	1.93	0.50
1:C:154:ARG:HD3	1:C:1197:GLU:OE2	2.11	0.50
1:D:309:GLU:O	1:D:313:VAL:HG23	2.11	0.50
1:A:686:VAL:HG22	1:A:686:VAL:O	2.11	0.50
1:B:509:CYS:C	1:B:511:LEU:H	2.18	0.50
1:C:154:ARG:N	1:C:155:PRO:HD2	2.26	0.50
1:A:269:LYS:HG2	1:A:270:PHE:CD1	2.46	0.50
1:A:322:GLN:HG2	1:A:414:GLU:OE1	2.11	0.50
1:A:432:ALA:HA	1:A:508:ARG:HD3	1.93	0.50
1:B:202:THR:HB	1:B:203:PRO:CD	2.41	0.50
1:C:38:GLY:HA2	1:C:40:LYS:CE	2.41	0.50
1:C:312:LEU:CD1	1:C:312:LEU:H	2.24	0.50
1:D:599:ARG:CG	1:D:599:ARG:HB2	2.20	0.50
1:A:560:LEU:HD12	1:A:1243:SER:HB3	1.94	0.50
1:A:769:ASN:ND2	1:A:1077:PRO:HG3	2.26	0.50
1:A:878:ILE:HG12	1:A:915:PHE:CE1	2.47	0.50
1:B:986:ASP:O	1:B:987:LYS:CB	2.59	0.50
1:B:1044:HIS:CD2	1:B:1064:ILE:CD1	2.94	0.50
1:B:1055:LEU:HD23	1:B:1057:ILE:HD11	1.92	0.50
1:B:1089:GLN:HB3	1:B:1134:TYR:CG	2.47	0.50
1:B:1118:VAL:C	1:B:1120:ALA:N	2.68	0.50
1:C:497:PRO:HG2	1:C:500:ALA:HB2	1.93	0.50
1:C:1170:GLY:O	1:C:1303:PRO:HA	2.11	0.50
1:A:83:VAL:CG1	1:A:84:ALA:N	2.68	0.50
1:A:878:ILE:HG12	1:A:915:PHE:CD1	2.46	0.50
1:A:1263:PRO:N	1:A:1264:PRO:HD2	2.26	0.50
1:C:679:THR:HG22	1:C:680:GLN:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:749:CYS:HB2	1:C:827:MET:HB2	1.94	0.50
1:A:1224:GLY:O	1:A:1226:SER:N	2.44	0.50
1:B:88:VAL:C	1:B:90:GLY:H	2.18	0.50
1:B:949:LYS:HG3	1:B:952:ASP:OD2	2.11	0.50
1:B:1038:GLU:HG3	1:B:1040:GLY:H	1.75	0.50
1:C:769:ASN:HD22	1:C:1077:PRO:HG3	1.77	0.50
1:D:496:LEU:HD23	1:D:497:PRO:HD2	1.93	0.50
1:B:389:PHE:O	1:B:391:PRO:CD	2.60	0.50
1:B:594:CYS:O	1:B:597:ILE:CG1	2.59	0.50
1:B:708:PHE:CE1	1:B:900:ARG:CZ	2.94	0.50
1:B:750:THR:HG21	1:B:810:SER:HA	1.93	0.50
1:C:316:VAL:HG21	1:C:328:ARG:HD3	1.94	0.50
1:D:428:GLU:CD	1:D:428:GLU:H	2.19	0.50
1:D:467:LEU:HA	1:D:470:THR:HB	1.93	0.50
1:A:95:LYS:O	1:A:96:THR:HG23	2.11	0.50
1:A:708:PHE:CB	1:A:902:CYS:HA	2.42	0.50
1:A:1174:ASN:O	1:A:1237:PRO:HA	2.12	0.50
1:B:337:PHE:CD1	1:B:338:ALA:CB	2.94	0.50
1:B:511:LEU:HD23	1:B:515:PHE:CE1	2.45	0.50
1:B:708:PHE:CD1	1:B:708:PHE:N	2.66	0.50
1:B:841:HIS:CG	4:B:3007:GOL:O1	2.64	0.50
1:B:849:VAL:O	1:B:849:VAL:CG1	2.60	0.50
1:D:682:ALA:C	1:D:684:GLN:N	2.69	0.50
1:D:797:GLY:O	1:D:802:LYS:HE3	2.11	0.50
1:D:864:HIS:HB2	1:D:879:MET:HE1	1.94	0.50
1:D:1125:THR:O	1:D:1125:THR:HG22	2.12	0.50
1:A:633:VAL:O	1:A:634:CYS:HB3	2.11	0.49
1:A:835:LEU:HD22	1:A:1223:ARG:HH12	1.77	0.49
1:B:366:MET:HE2	1:B:387:HIS:HA	1.94	0.49
1:B:679:THR:HG22	1:B:680:GLN:N	2.27	0.49
1:B:864:HIS:HB3	1:B:879:MET:HE1	1.94	0.49
1:B:878:ILE:CG2	4:B:3007:GOL:C1	2.81	0.49
1:B:1289:ASN:C	1:C:380:ARG:NH1	2.70	0.49
1:C:398:LEU:H	1:C:398:LEU:CD2	2.25	0.49
1:C:664:VAL:HG21	1:C:1218:GLY:C	2.36	0.49
1:C:829:ASP:HB2	1:C:832:GLU:HG3	1.94	0.49
1:C:916:GLY:HA2	1:C:919:GLN:OE1	2.11	0.49
1:D:857:VAL:CG2	1:D:858:VAL:N	2.75	0.49
1:A:327:PHE:O	1:A:331:LEU:HD12	2.12	0.49
1:A:698:THR:C	1:A:700:GLU:O	2.55	0.49
1:A:1089:GLN:HG2	1:A:1134:TYR:CD1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:483:LEU:HD12	1:B:483:LEU:O	2.12	0.49
1:C:256:LYS:HD2	3:C:3006:FAD:O2B	2.12	0.49
1:C:528:GLY:O	1:C:530:GLU:OE2	2.30	0.49
1:C:1157:GLY:C	1:C:1158:VAL:HG23	2.37	0.49
1:D:719:ASP:CA	1:D:720:LEU:HB3	2.42	0.49
1:D:1185:SER:O	1:D:1186:SER:C	2.55	0.49
1:A:595:ASP:HA	1:A:825:ARG:NH1	2.27	0.49
1:B:715:ILE:HG23	1:B:1146:ASN:HD21	1.77	0.49
1:B:1076:SER:O	1:B:1077:PRO:C	2.47	0.49
1:B:1230:ILE:HB	1:B:1231:PRO:CD	2.42	0.49
1:C:537:GLY:O	1:C:538:LYS:HD3	2.12	0.49
1:D:353:ILE:O	1:D:355:ALA:N	2.46	0.49
1:D:616:ALA:HB2	1:D:692:GLU:HA	1.94	0.49
1:D:684:GLN:HA	1:D:684:GLN:NE2	2.27	0.49
1:D:927:TRP:CE3	1:D:927:TRP:C	2.88	0.49
1:A:6:LEU:HD23	1:A:6:LEU:O	2.13	0.49
1:A:165:ARG:HH11	1:A:165:ARG:CB	2.24	0.49
1:A:830:ARG:O	1:A:830:ARG:HG3	2.13	0.49
1:B:203:PRO:O	1:B:204:LEU:CB	2.53	0.49
1:C:327:PHE:N	1:C:327:PHE:CD1	2.80	0.49
1:C:374:LEU:HD11	1:C:383:VAL:CG1	2.42	0.49
1:C:849:VAL:O	1:C:849:VAL:CG1	2.60	0.49
1:A:698:THR:HG23	1:A:701:ASP:CG	2.37	0.49
1:A:734:GLU:HG2	1:A:1296:ARG:HH12	1.76	0.49
1:A:1183:VAL:C	1:A:1258:LYS:HB2	2.37	0.49
1:B:593:TYR:CD2	1:B:593:TYR:N	2.78	0.49
1:B:682:ALA:O	1:B:685:GLY:HA3	2.12	0.49
1:B:1020:ALA:HB1	1:B:1033:THR:O	2.12	0.49
1:C:418:PHE:HD2	1:C:419:SER:N	2.10	0.49
1:C:499:ASP:O	1:C:500:ALA:C	2.55	0.49
1:C:1069:THR:O	1:C:1069:THR:OG1	2.23	0.49
1:C:1232:ALA:O	1:C:1235:SER:HB2	2.12	0.49
1:D:864:HIS:CB	1:D:879:MET:HE1	2.43	0.49
1:A:520:TYR:HE2	1:A:524:LEU:CD1	2.25	0.49
1:B:165:ARG:HB2	1:B:165:ARG:NH1	2.26	0.49
1:B:622:ASP:C	1:B:622:ASP:OD1	2.56	0.49
1:B:891:LYS:HD2	1:B:952:ASP:OD2	2.13	0.49
1:C:287:LEU:O	1:C:302:ALA:HB3	2.13	0.49
1:C:703:ILE:C	1:C:705:ASN:N	2.70	0.49
1:C:946:ASN:ND2	1:C:946:ASN:N	2.60	0.49
1:C:1125:THR:CG2	1:D:1135:ARG:HB2	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:809:VAL:O	1:D:813:VAL:HG23	2.13	0.49
1:D:1107:LYS:O	1:D:1110:PRO:HD3	2.13	0.49
1:A:337:PHE:CD1	1:A:338:ALA:HB3	2.48	0.49
1:A:623:THR:HG23	1:A:623:THR:O	2.12	0.49
1:A:1262:GLU:O	1:A:1263:PRO:C	2.56	0.49
1:C:386:ASP:C	1:C:388:THR:N	2.71	0.49
1:C:840:ARG:HG2	4:C:3007:GOL:HO1	1.78	0.49
1:D:708:PHE:HB2	1:D:901:LEU:O	2.13	0.49
1:D:804:THR:O	1:D:807:THR:HG23	2.13	0.49
1:A:658:LYS:O	1:A:659:ASP:HB2	2.13	0.49
1:A:742:HIS:CE1	1:A:801:GLY:CA	2.95	0.49
1:A:1008:ILE:O	1:A:1009:SER:HB2	2.12	0.49
1:A:1142:SER:CB	1:A:1145:THR:HG21	2.43	0.49
1:B:1157:GLY:O	1:B:1158:VAL:HG23	2.12	0.49
1:C:975:SER:O	1:C:977:GLN:HG2	2.12	0.49
1:C:1002:ILE:HG23	1:C:1003:PRO:HD2	1.95	0.49
1:C:1003:PRO:HA	1:C:1158:VAL:HG22	1.95	0.49
1:D:364:VAL:O	1:D:368:SER:HB2	2.13	0.49
1:A:256:LYS:O	1:A:278:ILE:HG23	2.12	0.49
1:A:1144:GLU:C	1:A:1145:THR:HG22	2.38	0.49
1:B:354:THR:HG23	1:B:354:THR:O	2.13	0.49
1:C:374:LEU:CD2	1:C:398:LEU:CD2	2.90	0.49
1:C:543:PHE:HB3	1:C:544:ALA:H	1.35	0.49
1:C:1027:ASP:OD2	1:C:1027:ASP:C	2.55	0.49
1:A:87:THR:HG22	1:A:90:GLY:N	2.28	0.49
1:B:883:LEU:C	1:B:885:HIS:H	2.21	0.49
1:B:1201:VAL:O	1:B:1204:LEU:HB3	2.13	0.49
1:C:230:GLU:HG3	1:C:235:THR:HG23	1.95	0.49
1:D:350:GLY:O	1:D:354:THR:HB	2.13	0.49
1:D:972:CYS:C	1:D:974:ALA:H	2.19	0.49
1:A:604:LEU:HD11	1:A:822:ARG:HH11	1.77	0.48
1:A:1002:ILE:CG2	1:A:1003:PRO:N	2.76	0.48
1:B:374:LEU:HD23	1:B:398:LEU:HD22	1.95	0.48
1:B:1262:GLU:H	1:B:1263:PRO:HD3	1.78	0.48
1:C:757:GLU:OE2	1:D:592:VAL:HG23	2.13	0.48
1:C:1135:ARG:HB2	1:D:1125:THR:CG2	2.39	0.48
1:C:1195:GLN:HG2	1:C:1260:VAL:HG13	1.95	0.48
1:D:45:GLU:CG	1:D:45:GLU:O	2.61	0.48
1:D:618:ILE:O	1:D:618:ILE:HG12	2.12	0.48
1:A:740:GLN:HG2	1:A:741:GLU:N	2.27	0.48
1:A:773:THR:HG22	1:A:790:VAL:HG21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:ILE:O	1:B:353:ILE:HG22	2.13	0.48
1:C:798:GLY:O	1:C:800:GLY:N	2.46	0.48
1:D:594:CYS:C	1:D:596:ASP:N	2.71	0.48
1:B:161:ARG:O	1:B:163:PHE:N	2.46	0.48
1:B:841:HIS:CB	4:B:3007:GOL:O1	2.59	0.48
1:C:1248:CYS:SG	1:C:1248:CYS:O	2.72	0.48
1:D:316:VAL:HG21	1:D:328:ARG:HD3	1.96	0.48
1:D:429:ASP:O	1:D:430:ASP:HB2	2.12	0.48
1:A:910:THR:O	4:A:3007:GOL:H11	2.12	0.48
1:A:947:LEU:C	1:A:948:TYR:O	2.55	0.48
1:B:95:LYS:O	1:B:96:THR:HG23	2.14	0.48
1:B:234:VAL:CG1	1:B:235:THR:N	2.76	0.48
1:B:1319:VAL:CA	1:B:1319:VAL:HB	2.17	0.48
1:C:780:MET:CE	1:C:815:LEU:HB2	2.44	0.48
1:C:845:ALA:CB	1:C:923:ILE:HD12	2.43	0.48
1:C:1014:PHE:CD1	1:C:1014:PHE:C	2.92	0.48
1:D:607:ARG:NE	1:D:679:THR:CG2	2.51	0.48
1:D:841:HIS:HB2	4:D:3007:GOL:C1	2.43	0.48
1:D:980:ALA:O	1:D:983:SER:N	2.47	0.48
1:A:281:PRO:O	1:A:282:ALA:CB	2.59	0.48
1:A:618:ILE:HG12	1:A:618:ILE:O	2.12	0.48
1:B:921:MET:O	1:B:1266:PHE:CE2	2.66	0.48
1:C:487:CYS:HB3	1:C:513:LEU:HD22	1.96	0.48
1:C:708:PHE:CB	1:C:902:CYS:HA	2.44	0.48
1:C:708:PHE:CE1	1:C:900:ARG:CZ	2.97	0.48
1:C:1127:SER:HA	1:D:1133:PHE:CE1	2.49	0.48
1:D:76:PRO:HD3	1:D:261:ASN:ND2	2.28	0.48
1:A:256:LYS:HE2	1:A:275:PHE:CD2	2.49	0.48
1:B:923:ILE:O	1:B:924:ALA:C	2.53	0.48
1:B:927:TRP:HZ3	1:B:928:MET:HE2	1.79	0.48
1:C:386:ASP:C	1:C:388:THR:H	2.19	0.48
1:D:1068:SER:OG	1:D:1070:ASN:ND2	2.46	0.48
1:B:679:THR:CG2	1:B:680:GLN:N	2.76	0.48
1:B:865:PHE:HD1	1:B:865:PHE:H	1.58	0.48
1:C:874:LEU:O	1:C:878:ILE:HG13	2.14	0.48
1:D:377:ARG:HG3	1:D:377:ARG:O	2.12	0.48
1:D:623:THR:CG2	1:D:627:LYS:HE3	2.44	0.48
1:A:202:THR:HB	1:A:203:PRO:HD3	1.95	0.48
1:B:104:ARG:HG2	1:B:201:PHE:CE1	2.49	0.48
1:B:428:GLU:CD	1:B:428:GLU:H	2.21	0.48
1:C:351:ASN:ND2	1:C:361:LEU:CB	2.70	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:647:THR:HG22	1:C:648:GLY:N	2.19	0.48
1:C:845:ALA:HB3	1:C:923:ILE:HD12	1.95	0.48
1:A:112:GLN:NE2	1:A:150:CYS:O	2.46	0.48
1:A:228:ARG:NH2	1:A:230:GLU:OE2	2.47	0.48
1:A:954:THR:C	1:A:956:PHE:H	2.20	0.48
1:A:1142:SER:HB3	1:A:1145:THR:HG21	1.96	0.48
1:B:93:SER:HB2	1:B:590:GLU:OE2	2.14	0.48
1:B:147:LEU:HD13	1:B:1230:ILE:HD11	1.94	0.48
1:B:438:MET:HB3	1:B:454:LEU:CD2	2.44	0.48
1:B:799:PHE:CE2	1:B:1202:GLN:NE2	2.82	0.48
1:B:888:ASN:OD1	1:B:921:MET:CE	2.62	0.48
1:B:1001:ILE:HG23	1:B:1001:ILE:O	2.14	0.48
1:B:1105:TYR:N	1:B:1105:TYR:CD1	2.82	0.48
1:B:1142:SER:CB	1:B:1145:THR:HG21	2.40	0.48
1:C:319:LEU:HA	1:C:320:PRO:HD2	1.69	0.48
1:D:284:ILE:H	1:D:284:ILE:HG12	1.36	0.48
1:D:788:ILE:N	1:D:788:ILE:CD1	2.76	0.48
1:A:287:LEU:O	1:A:302:ALA:HB3	2.14	0.48
1:A:312:LEU:CD1	1:A:312:LEU:H	2.27	0.48
1:A:588:SER:OG	1:A:590:GLU:HG3	2.14	0.48
1:A:804:THR:O	1:A:807:THR:HG23	2.14	0.48
1:A:1193:ILE:HA	1:A:1196:VAL:HB	1.95	0.48
1:B:795:MET:C	1:B:797:GLY:H	2.21	0.48
1:B:1195:GLN:CA	1:B:1195:GLN:NE2	2.63	0.48
1:C:215:GLU:C	1:C:216:LEU:O	2.50	0.48
1:C:754:PRO:HD3	1:C:823:PRO:HA	1.96	0.48
1:C:946:ASN:H	1:C:946:ASN:ND2	2.12	0.48
1:C:1113:SER:O	1:C:1116:ASP:HB2	2.14	0.48
1:D:608:LEU:N	1:D:608:LEU:CD2	2.77	0.48
1:D:693:LEU:H	1:D:693:LEU:HD13	1.79	0.48
1:D:697:ILE:O	1:D:904:THR:CG2	2.61	0.48
1:B:642:PRO:HG3	1:B:818:TYR:CE2	2.49	0.47
1:B:1102:LEU:O	1:B:1103:GLU:C	2.57	0.47
1:C:3:ALA:HB2	1:C:225:LYS:HZ1	1.76	0.47
1:D:337:PHE:CD1	1:D:338:ALA:HB3	2.45	0.47
1:D:707:SER:HB3	1:D:708:PHE:HB3	1.96	0.47
1:D:1055:LEU:HD13	1:D:1095:CYS:SG	2.54	0.47
1:D:1187:LEU:HA	1:D:1187:LEU:HD23	1.61	0.47
1:A:483:LEU:HB2	1:A:520:TYR:CD1	2.48	0.47
1:A:841:HIS:HA	1:A:909:ASN:HD22	1.80	0.47
1:A:894:ASN:ND2	1:A:894:ASN:N	2.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:LEU:O	1:B:274:LEU:HG	2.13	0.47
1:B:858:VAL:O	1:B:894:ASN:ND2	2.46	0.47
1:B:943:ARG:O	1:B:944:ARG:C	2.57	0.47
1:B:1209:LEU:HD12	1:B:1209:LEU:HA	1.61	0.47
1:C:139:ILE:HG21	1:C:139:ILE:HD13	1.53	0.47
1:C:1159:ALA:HB2	1:C:1267:LEU:HD13	1.96	0.47
1:D:682:ALA:O	1:D:683:ALA:C	2.57	0.47
1:D:840:ARG:HG3	4:D:3007:GOL:HO1	1.74	0.47
1:A:513:LEU:N	1:A:513:LEU:CD2	2.51	0.47
1:A:1048:VAL:O	1:A:1049:GLN:C	2.57	0.47
1:A:1121:ALA:O	1:A:1126:VAL:HG23	2.15	0.47
1:B:702:ALA:HB1	1:B:902:CYS:HB3	1.97	0.47
1:B:927:TRP:CE3	1:B:928:MET:HA	2.47	0.47
1:B:1186:SER:OG	1:B:1192:ASP:OD2	2.24	0.47
1:C:312:LEU:N	1:C:312:LEU:HD12	2.29	0.47
1:C:860:LEU:HD11	1:C:927:TRP:HE1	1.79	0.47
1:C:1266:PHE:O	1:C:1267:LEU:C	2.58	0.47
1:D:746:GLU:CB	1:D:796:GLY:HA3	2.44	0.47
1:D:958:GLN:HG3	1:D:1149:ASN:HD21	1.80	0.47
1:A:310:LYS:CA	1:A:313:VAL:HG23	2.44	0.47
1:A:312:LEU:O	1:A:313:VAL:C	2.57	0.47
1:A:1096:GLN:HA	1:A:1099:LEU:HD12	1.95	0.47
1:B:316:VAL:HG21	1:B:328:ARG:HD3	1.97	0.47
1:B:682:ALA:C	1:B:684:GLN:N	2.67	0.47
1:B:708:PHE:O	1:B:708:PHE:HD1	1.96	0.47
1:B:767:THR:OG1	1:B:768:GLN:N	2.46	0.47
1:C:10:VAL:O	1:C:10:VAL:HG12	2.09	0.47
1:C:271:LYS:O	1:C:273:MET:HG3	2.14	0.47
1:C:352:ILE:HG22	1:C:353:ILE:N	2.27	0.47
1:D:742:HIS:HA	1:D:912:PHE:CE1	2.50	0.47
1:D:1077:PRO:HB2	1:D:1079:ALA:HB2	1.96	0.47
1:D:1291:VAL:CB	1:D:1291:VAL:N	2.72	0.47
1:A:248:LEU:CD1	1:A:248:LEU:O	2.62	0.47
1:A:715:ILE:HG23	1:A:1146:ASN:HD21	1.80	0.47
1:A:888:ASN:OD1	1:A:921:MET:CE	2.62	0.47
1:B:263:GLU:HG2	1:B:354:THR:OG1	2.13	0.47
1:B:1057:ILE:HB	1:B:1058:PRO:CD	2.44	0.47
1:B:1268:ALA:O	1:B:1269:ALA:C	2.57	0.47
1:C:879:MET:HE3	1:C:899:GLY:CA	2.44	0.47
1:C:1044:HIS:CD2	1:C:1064:ILE:CD1	2.93	0.47
1:C:1195:GLN:HE21	1:C:1195:GLN:N	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:507:PHE:HB3	1:D:1304:GLU:HG3	1.95	0.47
1:D:721:LYS:HD2	1:D:721:LYS:HA	1.58	0.47
1:D:983:SER:O	1:D:984:GLU:C	2.57	0.47
1:A:740:GLN:CG	1:A:741:GLU:N	2.78	0.47
1:A:749:CYS:HB2	1:A:826:CYS:O	2.15	0.47
1:A:1038:GLU:HG3	1:A:1040:GLY:H	1.79	0.47
1:B:140:GLU:HB3	1:B:141:ASN:HB2	1.96	0.47
1:B:741:GLU:CG	1:B:742:HIS:N	2.77	0.47
1:B:1010:PHE:HB2	1:B:1016:ASN:ND2	2.29	0.47
1:C:269:LYS:HB3	1:C:270:PHE:HD1	1.80	0.47
1:C:452:LEU:HD23	1:C:470:THR:OG1	2.14	0.47
1:C:573:MET:HA	1:C:576:ARG:HG3	1.96	0.47
1:C:676:PRO:HA	1:C:679:THR:HB	1.97	0.47
1:C:931:VAL:HG12	1:C:932:ALA:N	2.30	0.47
1:D:264:ILE:HD11	3:D:3006:FAD:H3B	1.97	0.47
1:D:656:PHE:CD2	1:D:669:GLY:HA2	2.49	0.47
1:A:104:ARG:HG2	1:A:201:PHE:CD1	2.50	0.47
1:A:742:HIS:CE1	1:A:801:GLY:HA2	2.49	0.47
1:A:916:GLY:HA2	1:A:919:GLN:OE1	2.15	0.47
1:A:931:VAL:O	1:A:932:ALA:C	2.57	0.47
1:A:1200:PHE:CE1	1:A:1268:ALA:HA	2.50	0.47
1:B:289:SER:O	1:B:300:GLY:N	2.39	0.47
1:B:353:ILE:C	1:B:355:ALA:N	2.72	0.47
1:B:372:LEU:HD22	1:B:407:ILE:CD1	2.37	0.47
1:B:698:THR:C	1:B:700:GLU:O	2.58	0.47
1:B:719:ASP:CA	1:B:720:LEU:HB3	2.43	0.47
1:B:847:TYR:N	1:B:847:TYR:CD2	2.82	0.47
1:B:1118:VAL:C	1:B:1120:ALA:H	2.23	0.47
1:C:101:VAL:HG12	1:C:101:VAL:O	2.14	0.47
1:C:353:ILE:C	1:C:355:ALA:N	2.73	0.47
1:C:433:LYS:O	1:C:458:GLY:HA3	2.14	0.47
1:C:606:LEU:C	1:C:606:LEU:CD2	2.82	0.47
1:C:842:PRO:HD2	1:C:867:ASN:HB3	1.96	0.47
1:C:1291:VAL:CB	1:C:1291:VAL:C	2.80	0.47
1:C:1311:VAL:HA	1:C:1315:THR:HG21	1.96	0.47
1:D:276:PRO:HD2	1:D:277:MET:N	2.29	0.47
1:D:483:LEU:CB	1:D:520:TYR:CE1	2.90	0.47
1:D:656:PHE:O	1:D:657:ALA:C	2.58	0.47
1:D:1053:ARG:O	1:D:1053:ARG:HG2	2.13	0.47
1:A:353:ILE:HD11	1:A:404:LEU:HB2	1.97	0.47
1:A:386:ASP:C	1:A:388:THR:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:372:LEU:HD22	1:C:407:ILE:HD11	1.97	0.47
1:C:703:ILE:O	1:C:704:LYS:C	2.57	0.47
1:C:745:LEU:N	1:C:745:LEU:HD23	2.30	0.47
1:D:137:GLU:HA	1:D:140:GLU:HB2	1.95	0.47
1:D:849:VAL:HG13	1:D:849:VAL:O	2.15	0.47
1:A:14:LYS:HG2	1:A:15:VAL:N	2.29	0.47
1:A:1103:GLU:O	1:A:1104:PRO:C	2.58	0.47
1:A:1168:LEU:HD23	1:A:1168:LEU:HA	1.65	0.47
1:B:117:THR:HG21	1:B:587:ALA:HA	1.97	0.47
1:B:310:LYS:HA	1:B:313:VAL:HG23	1.96	0.47
1:C:496:LEU:CD2	1:C:497:PRO:HD2	2.44	0.47
1:C:747:THR:HG23	1:C:827:MET:CE	2.45	0.47
1:C:986:ASP:O	1:C:987:LYS:CB	2.62	0.47
1:D:517:PHE:CZ	1:D:521:LEU:HD11	2.49	0.47
1:D:1176:ARG:HD2	1:D:1239:GLU:HG3	1.96	0.47
1:A:284:ILE:HB	1:A:287:LEU:HD12	1.96	0.47
1:A:308:VAL:HG12	1:A:309:GLU:N	2.26	0.47
1:A:431:ILE:CD1	1:A:431:ILE:H	2.26	0.47
1:C:310:LYS:HA	1:C:313:VAL:HG23	1.97	0.47
1:C:925:GLU:O	1:C:1273:PHE:CZ	2.68	0.47
1:D:276:PRO:CD	1:D:277:MET:H	2.28	0.47
1:D:791:ARG:NH1	1:D:1066:GLU:OE2	2.48	0.47
1:B:578:LEU:HA	1:B:579:PRO:HD2	1.78	0.46
1:B:1266:PHE:CE2	1:B:1269:ALA:HB2	2.50	0.46
1:C:696:ILE:CG2	1:C:702:ALA:H	2.28	0.46
1:C:840:ARG:HG2	4:C:3007:GOL:O1	2.14	0.46
1:C:1193:ILE:HA	1:C:1196:VAL:HB	1.96	0.46
1:D:135:THR:HG23	1:D:138:GLU:OE1	2.15	0.46
1:D:608:LEU:H	1:D:608:LEU:CD2	2.28	0.46
1:D:1157:GLY:C	1:D:1158:VAL:HG23	2.40	0.46
1:A:246:LEU:HD22	1:A:376:SER:C	2.40	0.46
1:B:14:LYS:HG2	1:B:15:VAL:N	2.30	0.46
1:B:606:LEU:HG	1:B:607:ARG:H	1.80	0.46
1:B:833:ASP:O	1:B:837:THR:HG23	2.15	0.46
1:B:1106:LYS:O	1:B:1107:LYS:C	2.59	0.46
1:A:701:ASP:O	1:A:704:LYS:N	2.48	0.46
1:A:748:HIS:HD2	1:A:833:ASP:OD1	1.97	0.46
1:A:1224:GLY:C	1:A:1226:SER:N	2.73	0.46
1:B:606:LEU:HD23	1:B:607:ARG:CA	2.36	0.46
1:B:972:CYS:O	1:B:976:SER:HB3	2.16	0.46
1:C:618:ILE:HG22	1:C:660:LYS:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:507:PHE:CG	1:D:1304:GLU:HA	2.50	0.46
1:A:99:HIS:HE1	1:A:101:VAL:HG23	1.79	0.46
1:A:256:LYS:CE	1:A:275:PHE:CE2	2.99	0.46
1:A:435:THR:O	1:A:457:GLY:N	2.40	0.46
1:A:860:LEU:HD12	1:A:861:GLU:N	2.31	0.46
1:A:941:GLU:O	1:A:945:LYS:HB2	2.16	0.46
1:A:1109:ASN:CG	1:A:1109:ASN:O	2.57	0.46
1:A:1250:ASN:O	1:A:1256:ALA:HA	2.16	0.46
1:B:161:ARG:O	1:B:162:THR:C	2.58	0.46
1:B:278:ILE:CG2	1:B:279:VAL:N	2.79	0.46
1:B:374:LEU:N	1:B:374:LEU:CD1	2.78	0.46
1:B:972:CYS:C	1:B:974:ALA:H	2.23	0.46
1:C:112:GLN:HE21	1:C:150:CYS:HB3	1.79	0.46
1:D:262:THR:OG1	3:D:3006:FAD:O2P	2.22	0.46
1:D:558:VAL:HG12	1:D:1241:ARG:HG3	1.97	0.46
1:D:688:ILE:H	1:D:688:ILE:HD13	1.80	0.46
1:D:723:GLY:O	1:D:724:PHE:HB2	2.15	0.46
1:A:279:VAL:O	1:A:279:VAL:CG1	2.63	0.46
1:A:358:ILE:HG13	1:A:430:ASP:O	2.16	0.46
1:A:1161:SER:HA	1:A:1176:ARG:O	2.15	0.46
1:B:69:SER:O	1:B:70:ALA:HB2	2.15	0.46
1:C:62:GLN:O	1:C:63:ASN:C	2.59	0.46
1:C:520:TYR:C	1:C:520:TYR:HD2	2.23	0.46
1:D:80:LEU:O	1:D:83:VAL:HG23	2.15	0.46
1:D:104:ARG:HG2	1:D:201:PHE:CD1	2.50	0.46
1:D:841:HIS:H	4:D:3007:GOL:C1	2.28	0.46
1:D:931:VAL:HG12	1:D:932:ALA:N	2.31	0.46
1:A:251:GLN:HG3	1:A:252:HIS:HD2	1.77	0.46
1:A:278:ILE:HG22	1:A:279:VAL:N	2.30	0.46
1:A:1014:PHE:CD1	1:A:1014:PHE:O	2.68	0.46
1:A:1195:GLN:NE2	1:A:1195:GLN:CA	2.45	0.46
1:B:699:ILE:CD1	1:B:867:ASN:HB2	2.45	0.46
1:B:901:LEU:HA	1:B:901:LEU:HD23	1.60	0.46
1:C:527:LEU:HB2	1:C:528:GLY:H	1.40	0.46
1:C:805:ARG:HD2	1:C:805:ARG:HA	1.71	0.46
1:D:616:ALA:CB	1:D:692:GLU:HA	2.46	0.46
1:D:972:CYS:C	1:D:974:ALA:N	2.73	0.46
1:D:1031:LEU:HD12	1:D:1031:LEU:HA	1.42	0.46
1:A:676:PRO:HA	1:A:679:THR:HB	1.97	0.46
1:A:1080:ALA:C	1:A:1082:VAL:H	2.24	0.46
1:B:219:LEU:HA	1:B:219:LEU:HD13	1.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:963:PHE:CE2	1:B:966:PRO:HD3	2.51	0.46
1:B:1057:ILE:HB	1:B:1058:PRO:HD2	1.98	0.46
1:B:1212:LEU:HD12	1:B:1212:LEU:HA	1.71	0.46
1:C:353:ILE:O	1:C:355:ALA:N	2.49	0.46
1:C:708:PHE:O	1:C:708:PHE:CD1	2.68	0.46
1:C:949:LYS:O	1:C:950:GLU:C	2.57	0.46
1:C:956:PHE:HB2	1:C:1141:TYR:CE1	2.51	0.46
1:D:38:GLY:HA2	1:D:40:LYS:CD	2.46	0.46
1:D:914:GLY:N	1:D:1262:GLU:OE2	2.46	0.46
1:D:927:TRP:CE3	1:D:928:MET:CA	2.91	0.46
1:D:1144:GLU:O	1:D:1145:THR:HB	2.16	0.46
1:A:397:LEU:HD23	1:A:397:LEU:HA	1.73	0.46
1:A:576:ARG:HB3	1:A:577:PRO:HD2	1.98	0.46
1:B:607:ARG:HB2	1:B:679:THR:HG23	1.97	0.46
1:B:864:HIS:HB2	1:B:879:MET:CE	2.46	0.46
1:B:1176:ARG:CG	1:B:1177:THR:N	2.77	0.46
1:D:1214:TYR:N	1:D:1214:TYR:HD1	2.08	0.46
1:A:74:LEU:HA	1:A:74:LEU:HD23	1.58	0.46
1:C:351:ASN:HD21	1:C:361:LEU:HB2	1.75	0.46
1:D:389:PHE:O	1:D:391:PRO:HD3	2.14	0.46
1:D:965:LEU:O	1:D:965:LEU:HG	2.16	0.46
1:D:1055:LEU:CD1	1:D:1095:CYS:SG	3.04	0.46
1:A:117:THR:O	1:A:121:VAL:HG23	2.16	0.46
1:B:372:LEU:HD11	1:B:385:MET:CE	2.46	0.46
1:B:380:ARG:HG3	1:B:380:ARG:O	2.16	0.46
1:B:396:THR:HB	1:B:397:LEU:H	1.54	0.46
1:B:1163:VAL:O	1:B:1163:VAL:HG23	2.15	0.46
1:C:348:VAL:O	1:C:349:GLY:C	2.59	0.46
1:C:1070:ASN:C	1:C:1070:ASN:ND2	2.72	0.46
1:D:472:ARG:HG2	1:D:473:GLN:NE2	2.31	0.46
1:D:847:TYR:HB3	1:D:862:VAL:HG22	1.98	0.46
1:D:1119:THR:O	1:D:1123:MET:HG3	2.14	0.46
1:A:702:ALA:HB1	1:A:902:CYS:HB3	1.98	0.45
1:A:750:THR:HB	1:A:813:VAL:HG21	1.96	0.45
1:C:83:VAL:HG12	1:C:84:ALA:N	2.29	0.45
1:C:327:PHE:H	1:C:327:PHE:HD1	1.64	0.45
1:C:593:TYR:O	1:C:594:CYS:CB	2.46	0.45
1:C:594:CYS:C	1:C:596:ASP:N	2.74	0.45
1:C:1090:ALA:HB1	1:C:1132:GLY:O	2.17	0.45
1:D:459:MET:HE3	1:D:508:ARG:HD2	1.97	0.45
1:D:1113:SER:O	1:D:1116:ASP:HB2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ASP:O	1:A:23:GLU:N	2.49	0.45
1:A:312:LEU:N	1:A:312:LEU:CD1	2.79	0.45
1:A:423:GLN:NE2	1:A:424:ALA:N	2.62	0.45
1:A:608:LEU:HD23	1:A:608:LEU:H	1.81	0.45
1:B:431:ILE:H	1:B:1229:LYS:HZ1	1.62	0.45
1:B:700:GLU:O	1:B:701:ASP:HB2	2.15	0.45
1:B:913:ARG:HD3	1:B:1202:GLN:OE1	2.15	0.45
1:B:1145:THR:O	1:B:1146:ASN:C	2.58	0.45
1:D:641:VAL:HG11	1:D:645:ASN:HB2	1.99	0.45
1:D:698:THR:C	1:D:700:GLU:O	2.59	0.45
1:A:619:LYS:HB2	1:A:689:THR:O	2.16	0.45
1:A:697:ILE:CG2	1:A:698:THR:N	2.79	0.45
1:A:1068:SER:OG	1:A:1069:THR:N	2.46	0.45
1:A:1073:PRO:O	1:A:1074:ASN:HB2	2.16	0.45
1:A:1213:HIS:N	1:A:1222:THR:CG2	2.62	0.45
1:A:1262:GLU:H	1:A:1263:PRO:HD2	1.80	0.45
1:B:351:ASN:ND2	1:B:361:LEU:HB2	2.31	0.45
1:B:745:LEU:HD22	1:B:745:LEU:HA	1.58	0.45
1:C:386:ASP:O	1:C:387:HIS:C	2.60	0.45
1:C:1196:VAL:HG12	1:C:1197:GLU:N	2.31	0.45
1:C:1253:ALA:O	1:C:1254:ILE:C	2.59	0.45
1:D:430:ASP:OD2	1:D:1229:LYS:CD	2.65	0.45
1:A:100:PRO:O	1:A:101:VAL:C	2.56	0.45
1:A:241:THR:O	1:A:284:ILE:HD12	2.15	0.45
1:A:776:PHE:N	1:A:776:PHE:CD1	2.83	0.45
1:A:835:LEU:HA	1:A:835:LEU:HD12	1.69	0.45
1:B:3:ALA:HA	1:B:4:ASP:CG	2.41	0.45
1:B:386:ASP:C	1:B:388:THR:H	2.24	0.45
1:B:688:ILE:CD1	1:B:688:ILE:H	2.30	0.45
1:B:847:TYR:CE1	1:B:927:TRP:HB2	2.51	0.45
1:B:1187:LEU:HA	1:B:1187:LEU:HD23	1.68	0.45
1:C:1014:PHE:C	1:C:1014:PHE:HD1	2.23	0.45
1:D:1055:LEU:O	1:D:1056:LYS:HB2	2.16	0.45
1:A:113:CYS:SG	1:A:114:GLY:N	2.89	0.45
1:A:271:LYS:O	1:A:273:MET:N	2.49	0.45
1:A:448:GLU:O	1:A:449:VAL:HB	2.16	0.45
1:B:564:VAL:O	1:B:565:PRO:C	2.58	0.45
1:B:851:PHE:CD2	1:B:851:PHE:N	2.84	0.45
1:B:879:MET:HE3	1:B:899:GLY:CA	2.43	0.45
1:C:275:PHE:H	1:C:275:PHE:HD1	1.63	0.45
1:C:327:PHE:N	1:C:327:PHE:HD1	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:612:THR:HG23	1:C:690:TYR:OH	2.17	0.45
1:C:927:TRP:CE3	1:C:927:TRP:C	2.94	0.45
1:C:1149:ASN:HD22	1:C:1149:ASN:HA	1.37	0.45
1:D:27:LEU:HD11	1:D:31:ARG:HG3	1.99	0.45
1:D:643:GLY:HA3	1:D:780:MET:O	2.16	0.45
1:D:1133:PHE:CD2	1:D:1133:PHE:C	2.95	0.45
1:A:737:ILE:HG23	1:A:1299:SER:HB3	1.99	0.45
1:B:1311:VAL:CA	1:B:1315:THR:HG21	2.45	0.45
1:C:304:PRO:HA	1:C:346:ALA:O	2.16	0.45
1:C:467:LEU:HD12	1:C:468:LYS:N	2.32	0.45
1:D:264:ILE:H	1:D:264:ILE:HG12	1.47	0.45
1:D:327:PHE:N	1:D:327:PHE:CD1	2.85	0.45
1:D:504:MET:HG2	1:D:1304:GLU:CD	2.42	0.45
1:A:154:ARG:N	1:A:155:PRO:HD2	2.32	0.45
1:A:914:GLY:N	1:A:1262:GLU:OE2	2.35	0.45
1:B:27:LEU:HD12	1:B:31:ARG:HB2	1.99	0.45
1:B:534:ASP:CB	1:C:251:GLN:HE21	2.29	0.45
1:C:483:LEU:HB2	1:C:520:TYR:CD1	2.51	0.45
1:C:873:ASP:CG	1:C:874:LEU:H	2.24	0.45
1:C:883:LEU:C	1:C:885:HIS:H	2.25	0.45
1:B:31:ARG:HG3	1:B:31:ARG:NH1	2.07	0.45
1:B:165:ARG:HH11	1:B:165:ARG:CB	2.29	0.45
1:B:496:LEU:HD23	1:B:497:PRO:HD2	1.98	0.45
1:B:643:GLY:HA3	1:B:780:MET:O	2.17	0.45
1:B:920:GLY:HA2	1:B:923:ILE:N	2.31	0.45
1:B:937:MET:CG	1:B:938:PRO:HA	2.47	0.45
1:C:337:PHE:CD1	1:C:338:ALA:CB	3.00	0.45
1:C:844:LEU:HD12	1:C:844:LEU:HA	1.64	0.45
1:C:1055:LEU:HD23	1:C:1057:ILE:HD13	1.98	0.45
1:C:1176:ARG:HG3	1:C:1177:THR:N	2.32	0.45
1:D:3:ALA:HB1	1:D:227:LEU:CD2	2.46	0.45
1:D:352:ILE:O	1:D:355:ALA:HB2	2.16	0.45
1:D:857:VAL:HG23	1:D:858:VAL:N	2.32	0.45
1:D:865:PHE:HD1	1:D:865:PHE:H	1.63	0.45
1:D:1304:GLU:HG2	1:D:1308:ASN:ND2	2.32	0.45
1:A:980:ALA:O	1:A:982:LYS:N	2.50	0.45
1:A:1197:GLU:HG2	1:A:1240:PHE:CZ	2.52	0.45
1:B:161:ARG:HG3	1:B:162:THR:N	2.32	0.45
1:B:352:ILE:O	1:B:355:ALA:HB2	2.17	0.45
1:B:426:ARG:NH2	1:B:430:ASP:OD2	2.49	0.45
1:C:560:LEU:CD1	1:C:1243:SER:HB3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:THR:OG1	1:D:243:LYS:N	2.50	0.45
1:D:424:ALA:O	1:D:425:SER:OG	2.34	0.45
1:D:539:LEU:HD22	1:D:540:ASP:N	2.32	0.45
1:D:1176:ARG:HG3	1:D:1177:THR:H	1.82	0.45
1:A:509:CYS:C	1:A:511:LEU:N	2.71	0.45
1:B:864:HIS:HB2	1:B:879:MET:HE1	1.99	0.45
1:B:1000:CYS:O	1:B:1160:CYS:HA	2.16	0.45
1:C:864:HIS:CB	1:C:879:MET:HE1	2.47	0.45
1:C:937:MET:CB	1:C:938:PRO:CA	2.92	0.45
1:C:1022:LEU:C	1:C:1022:LEU:HD12	2.42	0.45
1:A:588:SER:OG	1:A:590:GLU:HG2	2.17	0.44
1:B:256:LYS:O	1:B:278:ILE:HG23	2.17	0.44
1:B:281:PRO:O	1:B:282:ALA:HB3	2.16	0.44
1:B:772:LYS:O	1:B:773:THR:C	2.60	0.44
1:B:926:CYS:H	1:B:928:MET:N	2.15	0.44
1:B:1179:ILE:HG21	1:B:1179:ILE:HD13	1.38	0.44
1:C:636:ILE:HD12	1:C:636:ILE:HA	1.61	0.44
1:C:768:GLN:HE22	1:C:800:GLY:H	1.64	0.44
1:C:867:ASN:C	1:C:867:ASN:OD1	2.60	0.44
1:D:43:CYS:HB2	1:D:45:GLU:HB3	1.99	0.44
1:D:59:ASP:OD1	1:D:61:LEU:N	2.46	0.44
1:A:147:LEU:HD13	1:A:1230:ILE:HD11	1.99	0.44
1:A:840:ARG:HG3	4:A:3007:GOL:O1	2.17	0.44
1:A:1055:LEU:HD23	1:A:1057:ILE:HD13	1.98	0.44
1:B:773:THR:HG22	1:B:790:VAL:HG21	1.99	0.44
1:B:1031:LEU:HA	1:B:1031:LEU:HD12	1.79	0.44
1:B:1070:ASN:HD22	1:B:1070:ASN:N	2.15	0.44
1:C:4:ASP:O	1:C:5:LYS:C	2.61	0.44
1:C:10:VAL:O	1:C:11:ASN:HB2	2.15	0.44
1:C:29:TYR:CE2	1:C:34:LEU:HD21	2.51	0.44
1:C:269:LYS:CE	1:C:269:LYS:CG	2.84	0.44
1:D:158:GLN:HE22	1:D:559:GLN:HE22	1.64	0.44
1:D:986:ASP:HA	1:D:989:ASN:HB2	2.00	0.44
1:A:1034:HIS:HE1	1:A:1044:HIS:HD2	1.59	0.44
1:B:257:LEU:HD12	3:B:3006:FAD:C5A	2.47	0.44
1:B:361:LEU:HA	1:B:361:LEU:HD23	1.39	0.44
1:C:471:GLN:HB3	1:C:472:ARG:H	1.69	0.44
1:C:1291:VAL:CA	1:C:1291:VAL:CG2	2.86	0.44
1:D:29:TYR:CE2	1:D:34:LEU:HD21	2.52	0.44
1:D:496:LEU:CD2	1:D:497:PRO:HD2	2.48	0.44
1:D:805:ARG:O	1:D:808:VAL:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:922:LEU:O	1:D:926:CYS:HB2	2.18	0.44
1:A:772:LYS:C	1:A:774:GLN:N	2.75	0.44
1:A:851:PHE:CD2	1:A:851:PHE:N	2.84	0.44
1:A:1053:ARG:O	1:A:1054:ALA:C	2.57	0.44
1:B:873:ASP:CG	1:B:874:LEU:N	2.75	0.44
1:B:1055:LEU:HD23	1:B:1057:ILE:CD1	2.46	0.44
1:C:594:CYS:C	1:C:596:ASP:H	2.25	0.44
1:C:1119:THR:O	1:C:1123:MET:HG3	2.18	0.44
1:A:42:GLY:HA3	1:A:48:CYS:SG	2.57	0.44
1:A:234:VAL:HG12	1:A:235:THR:N	2.31	0.44
1:A:246:LEU:HD21	1:A:375:VAL:HG23	1.99	0.44
1:A:260:GLY:N	3:A:3006:FAD:O1P	2.48	0.44
1:A:364:VAL:O	1:A:368:SER:HB2	2.18	0.44
1:A:629:VAL:HA	1:A:630:PRO:HD3	1.88	0.44
1:A:1141:TYR:CB	1:A:1150:PRO:HB3	2.48	0.44
1:A:1142:SER:OG	1:A:1145:THR:HG21	2.18	0.44
1:A:1176:ARG:CG	1:A:1177:THR:N	2.81	0.44
1:A:1312:ASP:H	1:A:1315:THR:HG23	1.82	0.44
1:B:588:SER:OG	1:B:590:GLU:CG	2.62	0.44
1:C:372:LEU:HD22	1:C:407:ILE:CD1	2.47	0.44
1:C:719:ASP:O	1:C:894:ASN:OD1	2.35	0.44
1:C:864:HIS:HB2	1:C:879:MET:HE1	1.99	0.44
1:C:920:GLY:HA2	1:C:922:LEU:CA	2.48	0.44
1:C:954:THR:C	1:C:956:PHE:N	2.75	0.44
1:D:153:TYR:O	1:D:154:ARG:C	2.59	0.44
1:D:520:TYR:C	1:D:520:TYR:HD2	2.25	0.44
1:D:585:MET:HB2	1:D:585:MET:HE3	1.55	0.44
1:D:788:ILE:N	1:D:788:ILE:HD13	2.32	0.44
1:D:889:CYS:C	1:D:948:TYR:HD2	2.26	0.44
1:A:227:LEU:HD23	1:A:227:LEU:HA	1.75	0.44
1:A:629:VAL:HG13	1:A:630:PRO:HD2	1.99	0.44
1:A:1176:ARG:HG3	1:A:1177:THR:N	2.32	0.44
1:B:593:TYR:HB2	1:B:596:ASP:OD2	2.17	0.44
1:B:664:VAL:CG2	1:B:1218:GLY:O	2.65	0.44
1:B:999:LEU:HG	1:B:1000:CYS:N	2.32	0.44
1:C:847:TYR:CD2	1:C:847:TYR:N	2.84	0.44
1:C:1168:LEU:HA	1:C:1168:LEU:HD23	1.56	0.44
1:D:27:LEU:O	1:D:28:ALA:HB2	2.14	0.44
1:D:138:GLU:O	1:D:141:ASN:HB3	2.18	0.44
1:D:611:SER:HB3	1:D:665:GLY:HA2	2.00	0.44
1:D:1213:HIS:O	1:D:1221:HIS:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:CYS:C	1:A:596:ASP:N	2.75	0.44
1:A:688:ILE:H	1:A:688:ILE:CD1	2.30	0.44
1:A:708:PHE:O	1:A:708:PHE:HD1	2.00	0.44
1:A:1106:LYS:HG2	1:A:1117:TRP:CZ2	2.53	0.44
1:A:1118:VAL:C	1:A:1120:ALA:N	2.73	0.44
1:A:1263:PRO:N	1:A:1264:PRO:CD	2.81	0.44
1:A:1319:VAL:HG13	1:A:1320:THR:N	2.32	0.44
1:B:58:TYR:CE2	1:B:220:LYS:HD2	2.52	0.44
1:B:791:ARG:HB3	1:B:1068:SER:HB2	1.99	0.44
1:B:805:ARG:HA	1:B:805:ARG:HD2	1.59	0.44
1:B:1042:GLY:O	1:B:1043:LEU:C	2.60	0.44
1:B:1069:THR:O	1:B:1069:THR:OG1	2.21	0.44
1:D:353:ILE:C	1:D:355:ALA:N	2.74	0.44
1:D:780:MET:HE2	1:D:815:LEU:HB2	1.99	0.44
1:D:986:ASP:O	1:D:987:LYS:CB	2.65	0.44
1:A:21:ASP:O	1:A:22:PRO:C	2.61	0.44
1:A:652:ASP:CG	1:A:872:GLN:H	2.25	0.44
1:A:700:GLU:O	1:A:701:ASP:CB	2.66	0.44
1:A:788:ILE:N	1:A:788:ILE:HD13	2.33	0.44
1:A:1319:VAL:HG13	1:A:1320:THR:O	2.17	0.44
1:B:880:GLU:O	1:B:883:LEU:N	2.48	0.44
1:B:963:PHE:HE2	1:B:966:PRO:HD3	1.82	0.44
1:B:1002:ILE:CG2	1:B:1003:PRO:HD2	2.48	0.44
1:D:517:PHE:CZ	1:D:521:LEU:CD1	3.00	0.44
1:D:608:LEU:HA	1:D:670:ALA:HA	2.00	0.44
1:A:202:THR:CB	1:A:203:PRO:HD3	2.45	0.44
1:A:337:PHE:CE2	3:A:3006:FAD:C2	3.00	0.44
1:A:473:GLN:HA	1:A:473:GLN:OE1	2.17	0.44
1:A:708:PHE:HB3	1:A:902:CYS:HA	2.00	0.44
1:A:1280:ARG:CG	1:A:1280:ARG:HH11	2.31	0.44
1:B:461:ASN:CB	1:B:462:ARG:CG	2.89	0.44
1:C:281:PRO:O	1:C:282:ALA:HB3	2.17	0.44
1:D:561:PHE:N	1:D:561:PHE:HD2	2.15	0.44
1:D:607:ARG:CD	1:D:679:THR:HG23	2.43	0.44
1:D:808:VAL:O	1:D:811:THR:HG22	2.17	0.44
1:A:722:LYS:C	1:A:723:GLY:O	2.56	0.43
1:A:800:GLY:C	1:A:802:LYS:N	2.74	0.43
1:A:1034:HIS:CE1	1:A:1044:HIS:CD2	3.01	0.43
1:B:62:GLN:O	1:B:64:LYS:HB2	2.18	0.43
1:B:851:PHE:CD1	1:B:931:VAL:HG22	2.53	0.43
1:B:1254:ILE:HG13	1:B:1255:TYR:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:PRO:HD3	1:C:261:ASN:ND2	2.33	0.43
1:C:956:PHE:HB2	1:C:1141:TYR:HE1	1.83	0.43
1:D:594:CYS:O	1:D:597:ILE:HG13	2.18	0.43
1:D:629:VAL:HA	1:D:630:PRO:HD3	1.90	0.43
1:D:1170:GLY:O	1:D:1303:PRO:HA	2.18	0.43
1:A:1128:LEU:HA	1:A:1128:LEU:HD23	1.79	0.43
1:A:1195:GLN:HG2	1:A:1260:VAL:HG13	1.99	0.43
1:B:3:ALA:HA	1:B:4:ASP:OD2	2.18	0.43
1:B:471:GLN:O	1:B:474:LEU:HB2	2.17	0.43
1:B:762:GLU:C	1:B:763:LEU:HD12	2.43	0.43
1:C:296:GLY:N	1:C:411:TYR:CD1	2.86	0.43
1:C:466:ALA:HB1	1:C:470:THR:HB	2.00	0.43
1:C:841:HIS:HA	1:C:909:ASN:HD22	1.83	0.43
1:A:461:ASN:HB3	1:A:462:ARG:HG2	2.00	0.43
1:A:684:GLN:NE2	1:A:684:GLN:CA	2.65	0.43
1:A:937:MET:CB	1:A:938:PRO:HA	2.36	0.43
1:A:944:ARG:O	1:A:947:LEU:HD12	2.17	0.43
1:A:1013:PRO:O	1:A:1015:LEU:N	2.51	0.43
1:B:333:GLN:NE2	1:B:360:ASP:HB3	2.34	0.43
1:B:483:LEU:HD22	1:B:520:TYR:CD1	2.52	0.43
1:B:520:TYR:C	1:B:520:TYR:HD2	2.24	0.43
1:C:76:PRO:O	1:C:77:ILE:C	2.56	0.43
1:C:699:ILE:H	1:C:699:ILE:HG12	1.58	0.43
1:C:917:GLY:N	1:C:918:PRO:CD	2.79	0.43
1:D:124:MET:HE2	1:D:163:PHE:CD1	2.53	0.43
1:D:310:LYS:CA	1:D:313:VAL:HG23	2.48	0.43
1:D:524:LEU:HD23	1:D:524:LEU:HA	1.73	0.43
1:A:209:GLU:HB3	1:A:210:PRO:HD2	1.99	0.43
1:A:698:THR:O	1:A:699:ILE:C	2.60	0.43
1:A:1008:ILE:O	1:A:1009:SER:CB	2.65	0.43
1:A:1283:ARG:O	1:A:1287:THR:HB	2.18	0.43
1:B:228:ARG:HG3	1:B:228:ARG:NH1	2.33	0.43
1:B:248:LEU:HD12	1:B:248:LEU:O	2.18	0.43
1:B:312:LEU:O	1:B:313:VAL:C	2.61	0.43
1:B:720:LEU:H	1:B:722:LYS:H	1.66	0.43
1:C:937:MET:HB2	1:C:938:PRO:C	2.43	0.43
1:D:278:ILE:CG2	1:D:279:VAL:N	2.80	0.43
1:D:507:PHE:CD2	1:D:1304:GLU:HA	2.53	0.43
1:D:511:LEU:HD23	1:D:511:LEU:HA	1.93	0.43
1:D:806:SER:O	1:D:807:THR:C	2.60	0.43
1:D:841:HIS:N	4:D:3007:GOL:O1	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:847:TYR:CE1	1:D:927:TRP:HB2	2.54	0.43
1:D:1263:PRO:N	1:D:1264:PRO:HD2	2.33	0.43
1:A:327:PHE:N	1:A:327:PHE:CD1	2.87	0.43
1:B:629:VAL:HG13	1:B:630:PRO:HD2	2.01	0.43
1:B:961:GLU:O	1:B:962:GLY:C	2.61	0.43
1:B:1216:PRO:HD3	1:B:1329:TRP:O	2.17	0.43
1:C:241:THR:HG23	1:C:244:GLU:CD	2.44	0.43
1:C:312:LEU:H	1:C:312:LEU:HD13	1.83	0.43
1:C:461:ASN:CB	1:C:462:ARG:HG3	2.47	0.43
1:C:720:LEU:HD13	1:C:721:LYS:N	2.34	0.43
1:C:798:GLY:O	1:C:799:PHE:C	2.62	0.43
1:C:943:ARG:O	1:C:944:ARG:C	2.60	0.43
1:C:1034:HIS:ND1	1:C:1034:HIS:N	2.67	0.43
1:D:703:ILE:H	1:D:703:ILE:HG13	1.63	0.43
1:D:886:MET:HE1	1:D:897:GLY:HA3	2.01	0.43
1:D:1114:TRP:O	1:D:1118:VAL:HG23	2.18	0.43
1:A:254:ASP:OD1	1:A:254:ASP:N	2.42	0.43
1:A:867:ASN:OD1	1:A:867:ASN:C	2.61	0.43
1:A:1024:VAL:HG22	1:A:1030:VAL:HG22	2.00	0.43
1:B:10:VAL:O	1:B:11:ASN:HB2	2.19	0.43
1:C:113:CYS:CA	1:C:1040:GLY:HA3	2.42	0.43
1:C:284:ILE:H	1:C:284:ILE:HG12	1.57	0.43
1:C:1209:LEU:HA	1:C:1209:LEU:HD12	1.55	0.43
1:C:1247:ASP:O	1:C:1248:CYS:HB3	2.19	0.43
1:C:1262:GLU:O	1:C:1263:PRO:C	2.60	0.43
1:D:27:LEU:HD12	1:D:27:LEU:C	2.43	0.43
1:D:744:TYR:N	1:D:744:TYR:CD1	2.84	0.43
1:D:892:ILE:HA	1:D:893:PRO:HD3	1.89	0.43
1:A:1002:ILE:HD13	1:A:1270:SER:CA	2.48	0.43
1:B:251:GLN:HG3	1:B:252:HIS:HD2	1.82	0.43
1:B:448:GLU:O	1:B:476:LYS:O	2.37	0.43
1:B:806:SER:O	1:B:807:THR:C	2.59	0.43
1:B:1285:GLN:HA	1:C:378:GLY:HA2	2.01	0.43
1:C:524:LEU:C	1:C:526:LYS:N	2.77	0.43
1:C:545:SER:O	1:C:546:ALA:HB2	2.18	0.43
1:C:580:HIS:O	1:C:582:ALA:N	2.52	0.43
1:C:721:LYS:HD2	1:C:721:LYS:HA	1.70	0.43
1:C:799:PHE:CD1	1:C:799:PHE:N	2.86	0.43
1:C:1187:LEU:HA	1:C:1187:LEU:HD23	1.79	0.43
1:D:350:GLY:C	3:D:3006:FAD:H5'1	2.44	0.43
1:D:372:LEU:HB2	1:D:374:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:511:LEU:C	1:D:513:LEU:N	2.75	0.43
1:D:707:SER:CB	1:D:708:PHE:HB3	2.49	0.43
1:A:815:LEU:HA	1:A:815:LEU:HD12	1.88	0.43
1:A:1271:ILE:O	1:A:1275:ILE:HG13	2.19	0.43
1:B:835:LEU:HD12	1:B:835:LEU:HA	1.66	0.43
1:B:920:GLY:HA2	1:B:921:MET:C	2.43	0.43
1:C:26:LEU:HA	1:C:77:ILE:HG22	2.00	0.43
1:C:136:MET:SD	1:C:161:ARG:HB2	2.59	0.43
1:C:466:ALA:HB3	1:C:470:THR:HB	2.00	0.43
1:C:917:GLY:H	1:C:918:PRO:HD2	1.80	0.43
1:C:1002:ILE:HD13	1:C:1270:SER:HA	2.00	0.43
1:C:1019:GLY:O	1:C:1072:VAL:HG21	2.19	0.43
1:D:154:ARG:N	1:D:155:PRO:CD	2.80	0.43
1:D:219:LEU:C	1:D:221:ASP:H	2.14	0.43
1:D:404:LEU:CA	3:D:3006:FAD:H62A	2.30	0.43
1:D:937:MET:HE3	1:D:937:MET:HB3	1.96	0.43
1:D:1193:ILE:C	1:D:1195:GLN:N	2.73	0.43
1:D:1280:ARG:NH1	1:D:1280:ARG:CG	2.81	0.43
1:A:650:CYS:O	1:A:651:ASN:C	2.58	0.43
1:A:662:THR:O	1:A:905:ASN:HB3	2.18	0.43
1:B:209:GLU:OE2	1:B:209:GLU:CA	2.66	0.43
1:B:708:PHE:HB2	1:B:902:CYS:HA	1.96	0.43
1:B:972:CYS:C	1:B:974:ALA:N	2.76	0.43
1:B:1192:ASP:O	1:B:1193:ILE:CB	2.59	0.43
1:C:626:ALA:C	1:C:628:LYS:H	2.27	0.43
1:C:1230:ILE:HB	1:C:1231:PRO:HD2	2.01	0.43
1:D:83:VAL:CG1	1:D:84:ALA:N	2.79	0.43
1:D:284:ILE:O	1:D:285:PRO:C	2.59	0.43
1:D:429:ASP:O	1:D:430:ASP:CB	2.67	0.43
1:A:696:ILE:HG23	1:A:701:ASP:HB3	2.01	0.43
1:A:811:THR:CG2	1:A:811:THR:CA	2.83	0.43
1:A:1179:ILE:HG22	1:A:1180:VAL:N	2.33	0.43
1:B:9:PHE:O	1:B:85:VAL:HG23	2.18	0.43
1:B:161:ARG:CG	1:B:162:THR:N	2.82	0.43
1:B:373:THR:C	1:B:374:LEU:HD12	2.44	0.43
1:C:30:LEU:HA	1:C:30:LEU:HD23	1.77	0.43
1:C:662:THR:HG1	1:C:870:ASN:HD22	1.65	0.43
1:C:708:PHE:HE1	1:C:900:ARG:CZ	2.32	0.43
1:C:1032:LEU:HD23	1:C:1032:LEU:HA	1.59	0.43
1:D:937:MET:CB	1:D:938:PRO:CA	2.77	0.43
1:A:88:VAL:CG1	1:A:89:GLU:N	2.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:748:HIS:O	1:A:749:CYS:CB	2.53	0.42
1:B:309:GLU:O	1:B:313:VAL:CG2	2.64	0.42
1:B:418:PHE:CD2	1:B:438:MET:O	2.73	0.42
1:B:622:ASP:OD1	1:B:623:THR:N	2.52	0.42
1:B:715:ILE:HG21	1:B:715:ILE:HD13	1.78	0.42
1:B:883:LEU:C	1:B:885:HIS:N	2.77	0.42
1:C:396:THR:HB	1:C:397:LEU:H	1.56	0.42
1:C:1031:LEU:HA	1:C:1031:LEU:HD12	1.65	0.42
1:D:361:LEU:HA	1:D:361:LEU:HD23	1.11	0.42
1:D:804:THR:HG21	1:D:873:ASP:OD2	2.19	0.42
1:A:517:PHE:O	1:A:518:LYS:C	2.63	0.42
1:A:1170:GLY:O	1:A:1303:PRO:HA	2.18	0.42
1:B:1174:ASN:OD1	1:B:1271:ILE:HD13	2.19	0.42
1:C:43:CYS:HB2	1:C:45:GLU:CB	2.44	0.42
1:C:120:ILE:HG23	1:C:143:PHE:CE1	2.53	0.42
1:C:335:ARG:H	1:C:335:ARG:HG2	1.71	0.42
1:C:1133:PHE:HD2	1:C:1133:PHE:C	2.17	0.42
1:C:1212:LEU:HD12	1:C:1212:LEU:HA	1.44	0.42
1:C:1244:LEU:HA	1:C:1244:LEU:HD23	1.64	0.42
1:D:561:PHE:HD2	1:D:561:PHE:H	1.66	0.42
1:D:894:ASN:ND2	1:D:894:ASN:N	2.66	0.42
1:D:958:GLN:NE2	1:D:1154:PHE:CZ	2.87	0.42
1:D:963:PHE:CE2	1:D:966:PRO:CD	2.98	0.42
1:D:1195:GLN:HA	1:D:1195:GLN:NE2	2.34	0.42
1:A:560:LEU:CD1	1:A:1243:SER:HB3	2.48	0.42
1:A:919:GLN:OE1	1:A:919:GLN:N	2.49	0.42
1:B:241:THR:HG23	1:B:244:GLU:CG	2.49	0.42
1:B:824:VAL:HG12	1:B:825:ARG:N	2.25	0.42
1:B:1319:VAL:CA	1:B:1319:VAL:CG1	2.89	0.42
1:C:361:LEU:HA	1:C:361:LEU:HD23	1.14	0.42
1:C:744:TYR:CD1	1:C:744:TYR:N	2.81	0.42
1:C:800:GLY:C	1:C:802:LYS:N	2.74	0.42
1:C:868:VAL:HG22	1:C:875:SER:HB3	2.01	0.42
1:C:888:ASN:HB3	1:C:889:CYS:H	1.55	0.42
1:D:276:PRO:CD	1:D:277:MET:N	2.79	0.42
1:D:511:LEU:C	1:D:513:LEU:H	2.26	0.42
1:D:1030:VAL:HG11	1:D:1062:ILE:HG12	2.01	0.42
1:D:1125:THR:O	1:D:1125:THR:CG2	2.67	0.42
1:D:1280:ARG:HH11	1:D:1280:ARG:CG	2.32	0.42
1:A:78:CYS:SG	1:A:78:CYS:CA	3.00	0.42
1:A:966:PRO:HG2	1:A:967:ARG:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1105:TYR:CD1	1:A:1105:TYR:N	2.87	0.42
1:B:688:ILE:HG12	1:B:690:TYR:CZ	2.54	0.42
1:B:1038:GLU:OE2	1:B:1041:GLN:N	2.43	0.42
1:C:505:VAL:O	1:C:505:VAL:HG12	2.18	0.42
1:C:616:ALA:CB	1:C:692:GLU:HA	2.49	0.42
1:C:983:SER:O	1:C:984:GLU:C	2.61	0.42
1:C:1012:VAL:O	1:C:1013:PRO:C	2.62	0.42
1:C:1201:VAL:O	1:C:1204:LEU:HB3	2.19	0.42
1:D:337:PHE:O	1:D:343:LYS:HE2	2.19	0.42
1:D:531:ASN:O	1:D:533:GLU:HA	2.19	0.42
1:D:619:LYS:O	1:D:620:SER:HB3	2.19	0.42
1:D:1157:GLY:O	1:D:1158:VAL:HG23	2.19	0.42
1:D:1212:LEU:HA	1:D:1212:LEU:HD12	1.78	0.42
1:A:607:ARG:CB	1:A:679:THR:HG23	2.50	0.42
1:A:734:GLU:HG2	1:A:1296:ARG:NH1	2.34	0.42
1:B:116:CYS:SG	1:B:148:CYS:HB2	2.59	0.42
1:B:296:GLY:N	1:B:411:TYR:CE1	2.88	0.42
1:B:783:VAL:HB	1:B:784:PRO:HD2	2.01	0.42
1:B:986:ASP:O	1:B:987:LYS:HB3	2.19	0.42
1:B:1119:THR:O	1:B:1123:MET:HG3	2.19	0.42
1:C:81:HIS:O	1:C:82:HIS:HB2	2.19	0.42
1:C:203:PRO:O	1:C:204:LEU:CB	2.63	0.42
1:D:798:GLY:O	1:D:801:GLY:N	2.53	0.42
1:D:1053:ARG:HD2	1:D:1255:TYR:CE2	2.54	0.42
1:D:1109:ASN:O	1:D:1111:SER:N	2.52	0.42
1:D:1176:ARG:CG	1:D:1177:THR:N	2.82	0.42
1:D:1263:PRO:N	1:D:1264:PRO:CD	2.83	0.42
1:A:574:VAL:HB	1:A:1053:ARG:HH21	1.84	0.42
1:A:607:ARG:CZ	1:A:680:GLN:HG2	2.49	0.42
1:A:613:ARG:HH11	1:A:613:ARG:HG3	1.84	0.42
1:A:650:CYS:O	1:A:652:ASP:N	2.52	0.42
1:A:983:SER:O	1:A:984:GLU:C	2.61	0.42
1:B:95:LYS:HD3	1:B:590:GLU:OE1	2.19	0.42
1:B:154:ARG:NH1	1:B:1197:GLU:OE1	2.53	0.42
1:B:354:THR:O	1:B:354:THR:CG2	2.68	0.42
1:B:608:LEU:HD23	1:B:608:LEU:H	1.84	0.42
1:B:835:LEU:HB3	1:B:836:ILE:H	1.55	0.42
1:B:860:LEU:HD12	1:B:861:GLU:H	1.84	0.42
1:C:599:ARG:CB	1:C:599:ARG:CD	2.94	0.42
1:C:703:ILE:C	1:C:705:ASN:H	2.27	0.42
1:C:1073:PRO:CD	1:D:1023:HIS:CD2	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1316:THR:O	1:C:1319:VAL:HG12	2.19	0.42
1:D:139:ILE:HD11	1:D:164:ALA:HB2	2.02	0.42
1:D:372:LEU:HD22	1:D:407:ILE:HD12	2.00	0.42
1:D:1022:LEU:C	1:D:1022:LEU:HD12	2.44	0.42
1:A:742:HIS:HA	1:A:912:PHE:CE1	2.54	0.42
1:A:806:SER:O	1:A:807:THR:C	2.61	0.42
1:A:923:ILE:O	1:A:926:CYS:HB2	2.18	0.42
1:A:1237:PRO:HG2	1:A:1240:PHE:CD1	2.54	0.42
1:B:607:ARG:CB	1:B:679:THR:HG23	2.50	0.42
1:B:640:ASP:OD1	1:B:819:LYS:HE2	2.19	0.42
1:B:688:ILE:CD1	1:B:688:ILE:CB	2.84	0.42
1:B:697:ILE:HG22	1:B:698:THR:N	2.34	0.42
1:B:815:LEU:O	1:B:818:TYR:HB3	2.20	0.42
1:B:985:VAL:HG12	1:B:986:ASP:N	2.33	0.42
1:B:1118:VAL:O	1:B:1119:THR:C	2.62	0.42
1:B:1165:ILE:HG21	1:B:1165:ILE:HD13	1.79	0.42
1:B:1180:VAL:HA	1:B:1243:SER:O	2.19	0.42
1:C:74:LEU:HA	1:C:74:LEU:HD23	1.77	0.42
1:C:860:LEU:CD1	1:C:927:TRP:HE1	2.32	0.42
1:C:1313:LYS:HB2	1:C:1314:PHE:HE2	1.74	0.42
1:D:982:LYS:O	1:D:983:SER:C	2.63	0.42
1:D:1262:GLU:C	1:D:1264:PRO:HD2	2.45	0.42
1:A:160:PHE:O	1:A:161:ARG:C	2.62	0.42
1:A:271:LYS:O	1:A:273:MET:HG3	2.20	0.42
1:A:668:ILE:HG21	1:A:668:ILE:HD13	1.72	0.42
1:A:1001:ILE:HG23	1:A:1001:ILE:O	2.20	0.42
1:A:1010:PHE:HB2	1:A:1016:ASN:HD21	1.84	0.42
1:A:1312:ASP:H	1:A:1315:THR:CG2	2.32	0.42
1:B:305:LEU:HD23	1:B:305:LEU:HA	1.67	0.42
1:B:1002:ILE:CD1	1:B:1270:SER:HA	2.49	0.42
1:C:1314:PHE:N	1:C:1314:PHE:HD2	2.16	0.42
1:D:224:ARG:H	1:D:224:ARG:HG2	1.63	0.42
1:A:963:PHE:HE2	1:A:966:PRO:HD3	1.83	0.42
1:A:1081:SER:OG	1:A:1262:GLU:CG	2.62	0.42
1:B:269:LYS:O	1:B:269:LYS:CG	2.68	0.42
1:B:459:MET:HA	1:B:459:MET:CE	2.49	0.42
1:B:619:LYS:HB2	1:B:689:THR:O	2.20	0.42
1:B:680:GLN:O	1:B:683:ALA:HB3	2.20	0.42
1:B:748:HIS:O	1:B:749:CYS:CB	2.62	0.42
1:B:924:ALA:O	1:B:925:GLU:CB	2.52	0.42
1:D:404:LEU:CB	3:D:3006:FAD:N6A	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1045:THR:O	1:D:1049:GLN:HG3	2.20	0.42
1:D:1271:ILE:HD13	1:D:1271:ILE:HG21	1.55	0.42
1:D:1291:VAL:CA	1:D:1291:VAL:CG2	2.87	0.42
1:A:30:LEU:HA	1:A:30:LEU:HD23	1.78	0.42
1:A:787:ARG:C	1:A:788:ILE:CD1	2.93	0.42
1:A:860:LEU:HD11	1:A:862:VAL:HG23	2.02	0.42
1:A:888:ASN:HB3	1:A:889:CYS:H	1.46	0.42
1:A:994:TRP:C	1:A:1167:CYS:HG	2.28	0.42
1:B:813:VAL:H	1:B:813:VAL:HG23	1.63	0.42
1:B:860:LEU:CD2	1:B:927:TRP:HZ2	2.29	0.42
1:C:99:HIS:O	1:C:102:GLN:N	2.51	0.42
1:C:314:ASP:O	1:C:315:ALA:C	2.63	0.42
1:C:322:GLN:NE2	1:C:416:GLU:H	2.18	0.42
1:D:71:ASN:ND2	1:D:71:ASN:N	2.67	0.42
1:D:640:ASP:OD1	1:D:819:LYS:HE2	2.20	0.42
1:D:678:HIS:O	1:D:679:THR:C	2.60	0.42
1:D:1315:THR:H	1:D:1315:THR:HG22	1.56	0.42
1:A:51:CYS:SG	1:A:71:ASN:HB2	2.60	0.41
1:A:526:LYS:HD2	1:A:526:LYS:O	2.20	0.41
1:A:787:ARG:O	1:A:788:ILE:HD12	2.19	0.41
1:A:949:LYS:HG3	1:A:952:ASP:OD2	2.20	0.41
1:B:30:LEU:HA	1:B:30:LEU:HD23	1.66	0.41
1:B:517:PHE:CZ	1:B:521:LEU:HD11	2.54	0.41
1:B:798:GLY:C	1:B:799:PHE:HD1	2.28	0.41
1:C:269:LYS:O	1:C:269:LYS:HG3	2.20	0.41
1:C:682:ALA:O	1:C:685:GLY:HA3	2.20	0.41
1:C:1087:ASN:O	1:C:1088:GLY:C	2.63	0.41
1:D:31:ARG:NH2	1:D:596:ASP:OD1	2.52	0.41
1:D:43:CYS:HB3	1:D:1225:PRO:HG3	2.02	0.41
1:D:137:GLU:O	1:D:137:GLU:HG2	2.19	0.41
1:D:879:MET:HE3	1:D:899:GLY:HA3	2.01	0.41
1:D:1032:LEU:HA	1:D:1032:LEU:HD23	1.72	0.41
1:A:313:VAL:HA	1:A:331:LEU:HD21	2.03	0.41
1:A:787:ARG:C	1:A:788:ILE:HD12	2.45	0.41
1:A:864:HIS:O	1:A:899:GLY:HA2	2.19	0.41
1:A:1195:GLN:HG2	1:A:1260:VAL:CG1	2.50	0.41
1:B:418:PHE:HD2	1:B:419:SER:N	2.18	0.41
1:B:511:LEU:HD23	1:B:511:LEU:O	2.20	0.41
1:B:708:PHE:CD1	1:B:708:PHE:O	2.72	0.41
1:B:1004:THR:O	1:B:1004:THR:HG23	2.19	0.41
1:B:1213:HIS:O	1:B:1221:HIS:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284:ILE:O	1:C:285:PRO:C	2.64	0.41
1:D:14:LYS:HG2	1:D:15:VAL:N	2.34	0.41
1:D:139:ILE:C	1:D:141:ASN:N	2.75	0.41
1:D:396:THR:HB	1:D:397:LEU:H	1.68	0.41
1:D:430:ASP:HB2	1:D:1229:LYS:HZ3	1.82	0.41
1:D:516:PHE:O	1:D:519:PHE:HB3	2.21	0.41
1:D:607:ARG:HB2	1:D:679:THR:CG2	2.51	0.41
1:D:708:PHE:O	1:D:708:PHE:CD1	2.72	0.41
1:D:956:PHE:HA	1:D:1146:ASN:OD1	2.20	0.41
1:A:585:MET:HE3	1:A:585:MET:HB2	1.52	0.41
1:A:681:ARG:O	1:A:684:GLN:HB3	2.20	0.41
1:A:954:THR:C	1:A:956:PHE:N	2.78	0.41
1:A:996:LYS:HG3	1:A:1282:ALA:HB2	2.01	0.41
1:A:1254:ILE:HG13	1:A:1255:TYR:N	2.36	0.41
1:A:1279:ILE:O	1:A:1280:ARG:C	2.63	0.41
1:B:346:ALA:HB1	3:B:3006:FAD:H4'	2.01	0.41
1:B:461:ASN:C	1:B:462:ARG:CG	2.88	0.41
1:B:1085:ASP:N	1:B:1085:ASP:OD1	2.52	0.41
1:B:1291:VAL:N	1:C:380:ARG:CZ	2.82	0.41
1:D:348:VAL:O	1:D:349:GLY:C	2.62	0.41
1:D:751:ILE:HB	1:D:764:PHE:HB2	2.02	0.41
1:D:824:VAL:CG1	1:D:825:ARG:N	2.76	0.41
1:D:906:LEU:HD23	1:D:906:LEU:HA	1.77	0.41
1:D:983:SER:C	1:D:985:VAL:N	2.75	0.41
1:A:326:VAL:O	1:A:327:PHE:C	2.63	0.41
1:A:646:ILE:O	1:A:646:ILE:HG23	2.21	0.41
1:A:780:MET:O	1:A:780:MET:SD	2.78	0.41
1:A:937:MET:H	1:A:937:MET:HG2	1.65	0.41
1:A:1149:ASN:HD22	1:A:1149:ASN:HA	1.31	0.41
1:B:800:GLY:C	1:B:802:LYS:N	2.76	0.41
1:C:927:TRP:CE3	1:C:928:MET:HA	2.54	0.41
1:C:983:SER:O	1:C:985:VAL:N	2.53	0.41
1:C:1024:VAL:HG22	1:C:1030:VAL:HG22	2.01	0.41
1:C:1048:VAL:O	1:C:1049:GLN:C	2.64	0.41
1:D:708:PHE:HB2	1:D:902:CYS:HA	2.02	0.41
1:D:771:MET:HE3	1:D:772:LYS:HE2	2.03	0.41
1:A:645:ASN:OD1	1:A:645:ASN:O	2.38	0.41
1:A:795:MET:C	1:A:797:GLY:H	2.27	0.41
1:A:927:TRP:CE3	1:A:928:MET:CA	3.00	0.41
1:B:117:THR:O	1:B:118:PRO:C	2.61	0.41
1:B:525:GLN:O	1:B:525:GLN:HG3	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:531:ASN:HD22	1:B:531:ASN:HA	1.66	0.41
1:B:574:VAL:HG13	1:B:1187:LEU:CD2	2.49	0.41
1:B:607:ARG:HB2	1:B:679:THR:CG2	2.50	0.41
1:B:653:GLU:HB2	1:B:654:THR:H	1.68	0.41
1:B:836:ILE:HG23	1:B:836:ILE:HD13	1.88	0.41
1:B:1080:ALA:C	1:B:1082:VAL:H	2.28	0.41
1:C:316:VAL:CG2	1:C:328:ARG:HD3	2.50	0.41
1:C:590:GLU:HG2	1:C:590:GLU:H	1.66	0.41
1:D:960:LEU:HD13	1:D:963:PHE:CE1	2.56	0.41
1:A:40:LYS:HB3	1:A:115:PHE:CZ	2.56	0.41
1:A:561:PHE:CD2	1:A:561:PHE:N	2.88	0.41
1:A:931:VAL:C	1:A:933:VAL:N	2.77	0.41
1:A:1032:LEU:HD11	1:A:1091:VAL:HG13	2.03	0.41
1:B:280:CYS:HA	1:B:281:PRO:HD3	1.83	0.41
1:B:582:ALA:O	1:B:586:GLN:HG3	2.20	0.41
1:B:892:ILE:HG23	1:B:892:ILE:O	2.21	0.41
1:B:1183:VAL:HG21	1:B:1186:SER:HB2	2.03	0.41
1:C:912:PHE:O	1:C:913:ARG:C	2.63	0.41
1:C:963:PHE:CE2	1:C:966:PRO:HD3	2.56	0.41
1:D:280:CYS:HA	1:D:281:PRO:HD3	1.95	0.41
1:D:656:PHE:CE2	1:D:669:GLY:HA2	2.55	0.41
1:D:1195:GLN:HE21	1:D:1195:GLN:CA	2.34	0.41
1:A:386:ASP:O	1:A:388:THR:N	2.53	0.41
1:A:449:VAL:O	1:A:449:VAL:HG12	2.21	0.41
1:A:1031:LEU:HD12	1:A:1031:LEU:HA	1.74	0.41
1:B:269:LYS:HB3	1:B:270:PHE:HD1	1.86	0.41
1:B:487:CYS:HB3	1:B:513:LEU:HD13	2.02	0.41
1:B:649:ILE:O	1:B:649:ILE:CG1	2.63	0.41
1:B:1027:ASP:OD2	1:B:1029:SER:OG	2.38	0.41
1:C:418:PHE:CD2	1:C:438:MET:O	2.73	0.41
1:C:517:PHE:CZ	1:C:521:LEU:HD11	2.54	0.41
1:C:626:ALA:C	1:C:628:LYS:N	2.78	0.41
1:C:862:VAL:O	1:C:897:GLY:HA2	2.20	0.41
1:D:256:LYS:HE2	1:D:275:PHE:CE2	2.55	0.41
1:D:305:LEU:HA	1:D:305:LEU:HD23	1.77	0.41
1:D:390:PHE:CD1	1:D:390:PHE:N	2.89	0.41
1:D:398:LEU:HD13	1:D:402:GLU:HB3	2.02	0.41
1:D:715:ILE:HG22	1:D:716:GLU:N	2.34	0.41
1:D:923:ILE:O	1:D:924:ALA:C	2.61	0.41
1:A:213:PRO:C	1:A:215:GLU:N	2.77	0.41
1:A:263:GLU:HG2	1:A:354:THR:OG1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:ILE:HA	1:A:407:ILE:HD12	1.44	0.41
1:A:606:LEU:HD23	1:A:607:ARG:CA	2.37	0.41
1:A:986:ASP:O	1:A:987:LYS:CB	2.69	0.41
1:A:1145:THR:O	1:A:1146:ASN:C	2.63	0.41
1:B:26:LEU:HA	1:B:77:ILE:HG22	2.03	0.41
1:B:54:MET:SD	1:B:126:THR:HG23	2.60	0.41
1:B:319:LEU:HA	1:B:320:PRO:HD2	1.58	0.41
1:B:524:LEU:HD22	1:B:530:GLU:HB2	2.03	0.41
1:B:603:GLU:OE2	1:B:825:ARG:NH2	2.53	0.41
1:B:641:VAL:CG2	1:B:643:GLY:H	2.33	0.41
1:B:917:GLY:O	1:B:921:MET:CB	2.68	0.41
1:C:760:GLU:OE1	1:D:1063:TYR:OH	2.28	0.41
1:C:788:ILE:N	1:C:788:ILE:HD13	2.35	0.41
1:C:888:ASN:O	1:C:1005:LYS:HG2	2.21	0.41
1:D:1277:ASP:O	1:D:1280:ARG:HB2	2.21	0.41
1:D:1302:THR:HG22	1:D:1303:PRO:HD2	2.03	0.41
1:D:1328:PRO:HB2	1:D:1329:TRP:H	1.67	0.41
1:A:51:CYS:SG	1:A:71:ASN:CB	3.09	0.41
1:A:348:VAL:O	1:A:349:GLY:C	2.64	0.41
1:A:613:ARG:HG3	1:A:613:ARG:NH1	2.36	0.41
1:A:814:ALA:O	1:A:817:ALA:HB3	2.21	0.41
1:A:873:ASP:CG	1:A:874:LEU:N	2.77	0.41
1:A:1195:GLN:HE21	1:A:1195:GLN:N	2.14	0.41
1:A:1210:GLU:HB3	1:A:1228:TYR:CZ	2.56	0.41
1:A:1280:ARG:HH11	1:A:1280:ARG:HG3	1.86	0.41
1:B:202:THR:HA	1:B:203:PRO:HD3	1.85	0.41
1:B:313:VAL:O	1:B:316:VAL:HG12	2.21	0.41
1:B:490:LEU:HD23	1:B:490:LEU:HA	1.92	0.41
1:B:604:LEU:HD21	1:B:822:ARG:HH11	1.85	0.41
1:B:682:ALA:O	1:B:683:ALA:C	2.64	0.41
1:B:841:HIS:CG	4:B:3007:GOL:HO1	2.39	0.41
1:C:257:LEU:HD12	3:C:3006:FAD:C5A	2.50	0.41
1:C:314:ASP:C	1:C:316:VAL:N	2.78	0.41
1:C:337:PHE:HZ	3:C:3006:FAD:O2'	2.04	0.41
1:C:368:SER:O	1:C:369:GLY:O	2.39	0.41
1:C:490:LEU:HD23	1:C:490:LEU:HA	1.89	0.41
1:C:518:LYS:HG2	1:C:539:LEU:HD21	2.03	0.41
1:C:578:LEU:HA	1:C:579:PRO:HD2	1.91	0.41
1:C:618:ILE:HG23	1:C:659:ASP:C	2.45	0.41
1:C:797:GLY:O	1:C:802:LYS:HE3	2.21	0.41
1:C:1073:PRO:O	1:C:1074:ASN:CB	2.65	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1135:ARG:CB	1:D:1125:THR:CG2	2.99	0.41
1:D:21:ASP:C	1:D:23:GLU:N	2.78	0.41
1:D:32:ARG:NH1	1:D:677:GLU:OE2	2.48	0.41
1:D:219:LEU:HD13	1:D:219:LEU:HA	1.68	0.41
1:D:327:PHE:N	1:D:327:PHE:HD1	2.18	0.41
1:D:351:ASN:ND2	1:D:361:LEU:HB2	2.34	0.41
1:D:424:ALA:C	1:D:425:SER:HG	2.28	0.41
1:D:636:ILE:HD12	1:D:636:ILE:HA	1.83	0.41
1:D:1081:SER:HA	6:D:3009:PO4:O3	2.21	0.41
1:D:1087:ASN:O	1:D:1088:GLY:C	2.64	0.41
1:A:340:LYS:C	1:A:342:VAL:H	2.28	0.41
1:A:708:PHE:HB2	1:A:902:CYS:HA	2.02	0.41
1:A:745:LEU:HD22	1:A:745:LEU:HA	1.79	0.41
1:B:126:THR:O	1:B:126:THR:HG22	2.20	0.41
1:B:326:VAL:O	1:B:327:PHE:C	2.62	0.41
1:B:1285:GLN:HA	1:C:378:GLY:CA	2.51	0.41
1:C:219:LEU:HA	1:C:219:LEU:HD13	1.51	0.41
1:C:597:ILE:HA	1:C:598:PRO:HD2	1.74	0.41
1:C:881:ARG:O	1:C:881:ARG:CG	2.68	0.41
1:C:949:LYS:N	1:C:952:ASP:OD2	2.38	0.41
1:D:279:VAL:O	1:D:279:VAL:HG13	2.22	0.41
1:D:883:LEU:C	1:D:885:HIS:H	2.29	0.41
1:D:1193:ILE:HA	1:D:1196:VAL:HB	2.03	0.41
1:A:281:PRO:HB2	1:A:282:ALA:H	1.80	0.40
1:A:346:ALA:CB	3:A:3006:FAD:H4'	2.43	0.40
1:A:788:ILE:HD12	1:A:788:ILE:HA	1.72	0.40
1:B:305:LEU:O	1:B:306:SER:C	2.63	0.40
1:B:390:PHE:HA	1:B:391:PRO:HD2	1.78	0.40
1:B:876:GLN:NE2	1:B:880:GLU:OE2	2.53	0.40
1:B:1253:ALA:O	1:B:1254:ILE:C	2.64	0.40
1:D:747:THR:OG1	1:D:748:HIS:N	2.54	0.40
1:D:1034:HIS:CE1	1:D:1044:HIS:CD2	2.97	0.40
1:D:1106:LYS:HA	1:D:1117:TRP:NE1	2.36	0.40
1:A:117:THR:HG21	1:A:587:ALA:HA	2.02	0.40
1:A:506:ASP:HA	1:A:509:CYS:HB3	2.03	0.40
1:A:682:ALA:O	1:A:683:ALA:C	2.63	0.40
1:A:1157:GLY:C	1:A:1158:VAL:HG23	2.46	0.40
1:B:159:GLY:O	1:B:162:THR:CG2	2.52	0.40
1:B:641:VAL:HG22	1:B:643:GLY:H	1.86	0.40
1:B:1311:VAL:HG13	1:B:1315:THR:CG2	2.51	0.40
1:C:398:LEU:CD2	1:C:398:LEU:N	2.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:543:PHE:O	1:C:544:ALA:CB	2.68	0.40
1:C:745:LEU:N	1:C:745:LEU:CD2	2.84	0.40
1:C:982:LYS:O	1:C:985:VAL:HB	2.21	0.40
1:C:1277:ASP:O	1:C:1280:ARG:HB2	2.21	0.40
1:D:99:HIS:HE1	1:D:101:VAL:HG23	1.83	0.40
1:D:222:THR:HA	1:D:223:PRO:HD3	1.99	0.40
1:D:841:HIS:ND1	4:D:3007:GOL:H11	2.37	0.40
1:A:28:ALA:H	1:A:31:ARG:H	1.68	0.40
1:A:136:MET:HE3	1:A:161:ARG:HA	2.03	0.40
1:A:524:LEU:O	1:A:527:LEU:HD12	2.21	0.40
1:A:824:VAL:CG1	1:A:825:ARG:N	2.83	0.40
1:B:141:ASN:C	1:B:143:PHE:H	2.28	0.40
1:B:216:LEU:H	1:B:216:LEU:HG	1.58	0.40
1:B:351:ASN:HD22	1:B:361:LEU:HB2	1.85	0.40
1:B:561:PHE:CD2	1:B:561:PHE:N	2.89	0.40
1:C:86:THR:HG22	1:C:87:THR:N	2.36	0.40
1:C:201:PHE:N	1:C:201:PHE:CD2	2.88	0.40
1:C:297:ILE:CG2	1:C:298:SER:N	2.83	0.40
1:C:469:THR:O	1:C:473:GLN:HG2	2.21	0.40
1:C:700:GLU:C	1:C:701:ASP:O	2.59	0.40
1:C:1193:ILE:H	1:C:1196:VAL:HG23	1.86	0.40
1:D:45:GLU:O	1:D:45:GLU:HG2	2.21	0.40
1:D:165:ARG:HH11	1:D:165:ARG:CG	2.34	0.40
1:D:1209:LEU:HA	1:D:1209:LEU:HD12	1.75	0.40
1:A:319:LEU:HA	1:A:320:PRO:HD2	1.76	0.40
1:A:372:LEU:HD23	1:A:372:LEU:H	1.87	0.40
1:A:520:TYR:C	1:A:520:TYR:HD2	2.27	0.40
1:A:520:TYR:HE2	1:A:524:LEU:HD11	1.81	0.40
1:A:883:LEU:C	1:A:885:HIS:H	2.30	0.40
1:A:937:MET:HE3	1:A:937:MET:HB3	2.02	0.40
1:A:949:LYS:O	1:A:950:GLU:C	2.63	0.40
1:A:1280:ARG:CG	1:A:1280:ARG:NH1	2.83	0.40
1:B:227:LEU:HA	1:B:227:LEU:HD23	1.91	0.40
1:B:407:ILE:HD12	1:B:407:ILE:HA	1.71	0.40
1:B:616:ALA:HA	1:B:693:LEU:HD13	2.04	0.40
1:C:43:CYS:HB2	1:C:45:GLU:H	1.85	0.40
1:C:479:LYS:O	1:C:480:GLU:C	2.64	0.40
1:C:737:ILE:HG23	1:C:1299:SER:CB	2.47	0.40
1:C:781:LEU:HD23	1:C:781:LEU:HA	1.74	0.40
1:C:1150:PRO:HD2	1:C:1151:PHE:H	1.86	0.40
1:D:74:LEU:HD23	1:D:74:LEU:HA	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:ILE:O	1:D:121:VAL:C	2.62	0.40
1:D:195:LEU:O	1:D:196:PHE:HB3	2.22	0.40
1:D:496:LEU:HD23	1:D:496:LEU:HA	1.82	0.40
1:D:931:VAL:O	1:D:932:ALA:C	2.61	0.40
1:D:958:GLN:NE2	1:D:1154:PHE:HZ	2.20	0.40
1:D:1186:SER:OG	1:D:1192:ASP:OD2	2.26	0.40
1:A:74:LEU:O	1:A:261:ASN:ND2	2.54	0.40
1:A:305:LEU:O	1:A:306:SER:C	2.65	0.40
1:A:710:GLY:O	1:A:900:ARG:NH1	2.55	0.40
1:B:563:GLU:HG3	1:B:564:VAL:N	2.35	0.40
1:B:851:PHE:CG	1:B:931:VAL:HG22	2.56	0.40
1:C:533:GLU:CB	1:C:535:LYS:H	2.35	0.40
1:C:656:PHE:O	1:C:657:ALA:C	2.65	0.40
1:D:139:ILE:C	1:D:141:ASN:H	2.30	0.40
1:D:985:VAL:O	1:D:986:ASP:C	2.64	0.40
1:D:1089:GLN:HG2	1:D:1134:TYR:CD1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1255/1333 (94%)	1002 (80%)	168 (13%)	85 (7%)	1	11
1	B	1281/1333 (96%)	1021 (80%)	158 (12%)	102 (8%)	1	8
1	C	1273/1333 (96%)	1011 (79%)	168 (13%)	94 (7%)	1	9
1	D	1275/1333 (96%)	1006 (79%)	174 (14%)	95 (8%)	1	9
All	All	5084/5332 (95%)	4040 (80%)	668 (13%)	376 (7%)	1	9

All (376) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	ALA
1	A	219	LEU
1	A	220	LYS
1	A	272	ASN
1	A	449	VAL
1	A	466	ALA
1	A	530	GLU
1	A	581	LEU
1	A	607	ARG
1	A	651	ASN
1	A	666	HIS
1	A	683	ALA
1	A	685	GLY
1	A	702	ALA
1	A	719	ASP
1	A	920	GLY
1	A	922	LEU
1	A	925	GLU
1	A	927	TRP
1	A	931	VAL
1	A	932	ALA
1	A	937	MET
1	A	987	LYS
1	A	1083	SER
1	A	1125	THR
1	A	1145	THR
1	A	1193	ILE
1	A	1254	ILE
1	A	1255	TYR
1	A	1269	ALA
1	A	1291	VAL
1	A	1319	VAL
1	B	3	ALA
1	B	4	ASP
1	B	28	ALA
1	B	162	THR
1	B	220	LYS
1	B	272	ASN
1	B	281	PRO
1	B	321	ALA
1	B	381	ARG
1	B	387	HIS
1	B	429	ASP

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Mol	Chain	Res	Type
1	B	433	LYS
1	B	449	VAL
1	B	471	GLN
1	B	472	ARG
1	B	523	VAL
1	B	524	LEU
1	B	525	GLN
1	B	529	GLN
1	B	536	CYS
1	B	540	ASP
1	B	541	PRO
1	B	542	THR
1	B	545	SER
1	B	565	PRO
1	B	607	ARG
1	B	666	HIS
1	B	683	ALA
1	B	685	GLY
1	B	702	ALA
1	B	719	ASP
1	B	866	SER
1	B	920	GLY
1	B	922	LEU
1	B	923	ILE
1	B	925	GLU
1	B	927	TRP
1	B	937	MET
1	B	981	ARG
1	B	987	LYS
1	B	1009	SER
1	B	1125	THR
1	B	1145	THR
1	B	1255	TYR
1	B	1291	VAL
1	B	1331	VAL
1	C	28	ALA
1	C	60	ARG
1	C	220	LYS
1	C	272	ASN
1	C	321	ALA
1	C	426	ARG
1	C	449	VAL

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Mol	Chain	Res	Type
1	C	471	GLN
1	C	472	ARG
1	C	530	GLU
1	C	531	ASN
1	C	543	PHE
1	C	544	ALA
1	C	546	ALA
1	C	565	PRO
1	C	581	LEU
1	C	666	HIS
1	C	683	ALA
1	C	685	GLY
1	C	702	ALA
1	C	704	LYS
1	C	719	ASP
1	C	866	SER
1	C	920	GLY
1	C	925	GLU
1	C	927	TRP
1	C	937	MET
1	C	987	LYS
1	C	1009	SER
1	C	1083	SER
1	C	1125	THR
1	C	1145	THR
1	C	1267	LEU
1	C	1269	ALA
1	C	1280	ARG
1	C	1291	VAL
1	D	28	ALA
1	D	220	LYS
1	D	272	ASN
1	D	321	ALA
1	D	425	SER
1	D	449	VAL
1	D	530	GLU
1	D	531	ASN
1	D	534	ASP
1	D	565	PRO
1	D	581	LEU
1	D	595	ASP
1	D	607	ARG

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Mol	Chain	Res	Type
1	D	666	HIS
1	D	683	ALA
1	D	685	GLY
1	D	702	ALA
1	D	719	ASP
1	D	920	GLY
1	D	923	ILE
1	D	925	GLU
1	D	927	TRP
1	D	937	MET
1	D	948	TYR
1	D	987	LYS
1	D	1041	GLN
1	D	1125	THR
1	D	1255	TYR
1	D	1269	ALA
1	D	1291	VAL
1	D	1327	LYS
1	D	1328	PRO
1	A	35	GLY
1	A	162	THR
1	A	217	LEU
1	A	281	PRO
1	A	471	GLN
1	A	565	PRO
1	A	568	GLN
1	A	595	ASP
1	A	720	LEU
1	A	806	SER
1	A	866	SER
1	A	913	ARG
1	A	923	ILE
1	A	962	GLY
1	A	1009	SER
1	A	1234	GLY
1	A	1300	PRO
1	B	63	ASN
1	B	219	LEU
1	B	282	ALA
1	B	355	ALA
1	B	448	GLU
1	B	466	ALA

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Mol	Chain	Res	Type
1	B	534	ASP
1	B	581	LEU
1	B	595	ASP
1	B	710	GLY
1	B	720	LEU
1	B	874	LEU
1	B	884	PHE
1	B	913	ARG
1	B	932	ALA
1	B	948	TYR
1	B	962	GLY
1	B	1119	THR
1	B	1146	ASN
1	B	1254	ILE
1	B	1288	GLY
1	B	1300	PRO
1	B	1327	LYS
1	C	162	THR
1	C	281	PRO
1	C	349	GLY
1	C	369	GLY
1	C	525	GLN
1	C	534	ASP
1	C	594	CYS
1	C	595	ASP
1	C	607	ARG
1	C	710	GLY
1	C	720	LEU
1	C	913	ARG
1	C	922	LEU
1	C	923	ILE
1	C	931	VAL
1	C	932	ALA
1	C	962	GLY
1	C	1234	GLY
1	C	1281	ALA
1	C	1300	PRO
1	D	63	ASN
1	D	204	LEU
1	D	281	PRO
1	D	427	ARG
1	D	512	THR

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Mol	Chain	Res	Type
1	D	524	LEU
1	D	525	GLN
1	D	536	CYS
1	D	707	SER
1	D	708	PHE
1	D	720	LEU
1	D	884	PHE
1	D	913	ARG
1	D	922	LEU
1	D	954	THR
1	D	981	ARG
1	D	1009	SER
1	D	1083	SER
1	D	1145	THR
1	D	1204	LEU
1	D	1254	ILE
1	D	1331	VAL
1	A	60	ARG
1	A	141	ASN
1	A	204	LEU
1	A	580	HIS
1	A	664	VAL
1	A	706	ASN
1	A	874	LEU
1	A	884	PHE
1	A	948	TYR
1	A	978	TYR
1	A	1288	GLY
1	A	1293	GLU
1	B	35	GLY
1	B	153	TYR
1	B	204	LEU
1	B	217	LEU
1	B	532	LEU
1	B	538	LYS
1	B	591	ALA
1	B	798	GLY
1	B	926	CYS
1	B	931	VAL
1	B	1041	GLN
1	B	1261	GLY
1	B	1269	ALA

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Mol	Chain	Res	Type
1	C	204	LEU
1	C	320	PRO
1	C	433	LYS
1	C	529	GLN
1	C	651	ASN
1	C	664	VAL
1	C	706	ASN
1	C	799	PHE
1	C	926	CYS
1	C	938	PRO
1	C	1074	ASN
1	C	1255	TYR
1	C	1315	THR
1	D	60	ARG
1	D	219	LEU
1	D	381	ARG
1	D	429	ASP
1	D	466	ALA
1	D	540	ASP
1	D	598	PRO
1	D	874	LEU
1	D	921	MET
1	D	1074	ASN
1	D	1193	ILE
1	D	1267	LEU
1	D	1300	PRO
1	D	1313	LYS
1	A	63	ASN
1	A	321	ALA
1	A	355	ALA
1	A	433	LYS
1	A	627	LYS
1	A	712	GLU
1	A	974	ALA
1	B	222	THR
1	B	426	ARG
1	B	527	LEU
1	B	873	ASP
1	B	977	GLN
1	B	1303	PRO
1	C	387	HIS
1	C	512	THR

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Mol	Chain	Res	Type
1	C	591	ALA
1	C	724	PHE
1	C	798	GLY
1	C	921	MET
1	C	952	ASP
1	C	981	ARG
1	C	1247	ASP
1	C	1290	ASN
1	D	222	THR
1	D	369	GLY
1	D	448	GLU
1	D	527	LEU
1	D	580	HIS
1	D	591	ALA
1	D	706	ASN
1	D	1070	ASN
1	D	1247	ASP
1	A	222	THR
1	A	320	PRO
1	A	448	GLU
1	A	532	LEU
1	A	981	ARG
1	A	1014	PHE
1	A	1280	ARG
1	A	1290	ASN
1	A	1296	ARG
1	A	1303	PRO
1	B	37	SER
1	B	125	TYR
1	B	320	PRO
1	B	369	GLY
1	B	921	MET
1	B	1026	THR
1	B	1103	GLU
1	C	222	THR
1	C	709	TYR
1	C	754	PRO
1	C	984	GLU
1	C	985	VAL
1	C	1254	ILE
1	D	217	LEU
1	D	320	PRO

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Mol	Chain	Res	Type
1	D	349	GLY
1	D	426	ARG
1	D	535	LYS
1	D	806	SER
1	D	977	GLN
1	D	1103	GLU
1	A	1225	PRO
1	A	1262	GLU
1	B	530	GLU
1	B	706	ASN
1	B	724	PHE
1	C	219	LEU
1	C	338	ALA
1	C	448	GLU
1	C	874	LEU
1	C	1150	PRO
1	D	471	GLN
1	D	1225	PRO
1	A	710	GLY
1	A	938	PRO
1	B	203	PRO
1	B	664	VAL
1	B	1262	GLU
1	C	1279	ILE
1	D	1234	GLY
1	A	1150	PRO
1	C	264	ILE
1	D	1040	GLY
1	D	1262	GLU
1	A	798	GLY
1	C	203	PRO
1	C	1262	GLU
1	D	35	GLY
1	D	798	GLY
1	B	1050	VAL
1	D	962	GLY
1	D	1050	VAL
1	A	203	PRO
1	D	664	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1067/1126 (95%)	781 (73%)	286 (27%)	0	3
1	B	1088/1126 (97%)	794 (73%)	294 (27%)	0	3
1	C	1082/1126 (96%)	787 (73%)	295 (27%)	0	3
1	D	1084/1126 (96%)	786 (72%)	298 (28%)	0	3
All	All	4321/4504 (96%)	3148 (73%)	1173 (27%)	0	3

All (1173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	6	LEU
1	A	13	ARG
1	A	16	VAL
1	A	18	LYS
1	A	25	THR
1	A	31	ARG
1	A	34	LEU
1	A	41	LEU
1	A	56	SER
1	A	61	LEU
1	A	62	GLN
1	A	63	ASN
1	A	64	LYS
1	A	69	SER
1	A	71	ASN
1	A	74	LEU
1	A	77	ILE
1	A	82	HIS
1	A	85	VAL
1	A	87	THR
1	A	88	VAL
1	A	89	GLU
1	A	93	SER

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Mol	Chain	Res	Type
1	A	95	LYS
1	A	105	ILE
1	A	113	CYS
1	A	123	SER
1	A	131	GLN
1	A	136	MET
1	A	154	ARG
1	A	161	ARG
1	A	165	ARG
1	A	197	LYS
1	A	199	GLU
1	A	200	GLU
1	A	208	GLN
1	A	211	ILE
1	A	219	LEU
1	A	220	LYS
1	A	224	ARG
1	A	230	GLU
1	A	241	THR
1	A	244	GLU
1	A	248	LEU
1	A	249	LYS
1	A	274	LEU
1	A	277	MET
1	A	284	ILE
1	A	290	VAL
1	A	295	ASP
1	A	298	SER
1	A	307	ILE
1	A	308	VAL
1	A	310	LYS
1	A	313	VAL
1	A	316	VAL
1	A	318	LYS
1	A	319	LEU
1	A	326	VAL
1	A	328	ARG
1	A	335	ARG
1	A	348	VAL
1	A	352	ILE
1	A	354	THR
1	A	359	SER

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Mol	Chain	Res	Type
1	A	372	LEU
1	A	374	LEU
1	A	377	ARG
1	A	379	THR
1	A	381	ARG
1	A	382	THR
1	A	383	VAL
1	A	385	MET
1	A	388	THR
1	A	390	PHE
1	A	394	ARG
1	A	398	LEU
1	A	399	SER
1	A	401	GLU
1	A	405	LEU
1	A	407	ILE
1	A	409	ILE
1	A	419	SER
1	A	425	SER
1	A	431	ILE
1	A	434	VAL
1	A	440	VAL
1	A	447	THR
1	A	450	GLN
1	A	452	LEU
1	A	459	MET
1	A	462	ARG
1	A	464	ILE
1	A	470	THR
1	A	474	LEU
1	A	482	LEU
1	A	505	VAL
1	A	506	ASP
1	A	514	SER
1	A	520	TYR
1	A	521	LEU
1	A	523	VAL
1	A	525	GLN
1	A	526	LYS
1	A	527	LEU
1	A	529	GLN
1	A	531	ASN

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Mol	Chain	Res	Type
1	A	558	VAL
1	A	564	VAL
1	A	566	LYS
1	A	568	GLN
1	A	572	ASP
1	A	576	ARG
1	A	577	PRO
1	A	578	LEU
1	A	581	LEU
1	A	590	GLU
1	A	601	GLU
1	A	608	LEU
1	A	612	THR
1	A	618	ILE
1	A	619	LYS
1	A	621	ILE
1	A	623	THR
1	A	630	PRO
1	A	636	ILE
1	A	641	VAL
1	A	644	SER
1	A	647	THR
1	A	649	ILE
1	A	650	CYS
1	A	654	THR
1	A	658	LYS
1	A	662	THR
1	A	664	VAL
1	A	667	ILE
1	A	671	VAL
1	A	674	ASP
1	A	675	THR
1	A	676	PRO
1	A	677	GLU
1	A	679	THR
1	A	680	GLN
1	A	686	VAL
1	A	688	ILE
1	A	690	TYR
1	A	693	LEU
1	A	698	THR
1	A	700	GLU

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Mol	Chain	Res	Type
1	A	703	ILE
1	A	704	LYS
1	A	707	SER
1	A	708	PHE
1	A	712	GLU
1	A	713	LEU
1	A	720	LEU
1	A	721	LYS
1	A	730	VAL
1	A	731	VAL
1	A	732	SER
1	A	735	ILE
1	A	737	ILE
1	A	744	TYR
1	A	745	LEU
1	A	747	THR
1	A	755	LYS
1	A	757	GLU
1	A	760	GLU
1	A	767	THR
1	A	773	THR
1	A	775	SER
1	A	779	LYS
1	A	781	LEU
1	A	788	ILE
1	A	789	VAL
1	A	790	VAL
1	A	791	ARG
1	A	792	VAL
1	A	810	SER
1	A	822	ARG
1	A	825	ARG
1	A	826	CYS
1	A	831	ASP
1	A	836	ILE
1	A	837	THR
1	A	854	THR
1	A	857	VAL
1	A	858	VAL
1	A	860	LEU
1	A	865	PHE
1	A	871	THR

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Mol	Chain	Res	Type
1	A	879	MET
1	A	891	LYS
1	A	894	ASN
1	A	895	ILE
1	A	902	CYS
1	A	910	THR
1	A	915	PHE
1	A	922	LEU
1	A	925	GLU
1	A	927	TRP
1	A	929	SER
1	A	933	VAL
1	A	937	MET
1	A	944	ARG
1	A	946	ASN
1	A	949	LYS
1	A	950	GLU
1	A	953	LEU
1	A	970	GLU
1	A	976	SER
1	A	979	HIS
1	A	982	LYS
1	A	983	SER
1	A	986	ASP
1	A	987	LYS
1	A	993	CYS
1	A	1001	ILE
1	A	1008	ILE
1	A	1009	SER
1	A	1014	PHE
1	A	1017	GLN
1	A	1022	LEU
1	A	1026	THR
1	A	1027	ASP
1	A	1029	SER
1	A	1032	LEU
1	A	1033	THR
1	A	1038	GLU
1	A	1045	THR
1	A	1052	SER
1	A	1056	LYS
1	A	1057	ILE

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Mol	Chain	Res	Type
1	A	1059	THR
1	A	1060	SER
1	A	1068	SER
1	A	1070	ASN
1	A	1085	ASP
1	A	1097	THR
1	A	1098	ILE
1	A	1100	LYS
1	A	1103	GLU
1	A	1104	PRO
1	A	1106	LYS
1	A	1107	LYS
1	A	1114	TRP
1	A	1119	THR
1	A	1125	THR
1	A	1126	VAL
1	A	1131	THR
1	A	1135	ARG
1	A	1139	LEU
1	A	1145	THR
1	A	1149	ASN
1	A	1164	GLU
1	A	1167	CYS
1	A	1195	GLN
1	A	1204	LEU
1	A	1209	LEU
1	A	1212	LEU
1	A	1220	LEU
1	A	1221	HIS
1	A	1222	THR
1	A	1223	ARG
1	A	1230	ILE
1	A	1236	ILE
1	A	1239	GLU
1	A	1243	SER
1	A	1246	ARG
1	A	1254	ILE
1	A	1262	GLU
1	A	1263	PRO
1	A	1271	ILE
1	A	1277	ASP
1	A	1279	ILE

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Mol	Chain	Res	Type
1	A	1280	ARG
1	A	1287	THR
1	A	1291	VAL
1	A	1294	LEU
1	A	1302	THR
1	A	1311	VAL
1	A	1315	THR
1	A	1316	THR
1	A	1320	THR
1	A	1329	TRP
1	B	2	THR
1	B	4	ASP
1	B	5	LYS
1	B	6	LEU
1	B	15	VAL
1	B	16	VAL
1	B	18	LYS
1	B	25	THR
1	B	31	ARG
1	B	34	LEU
1	B	41	LEU
1	B	56	SER
1	B	61	LEU
1	B	62	GLN
1	B	63	ASN
1	B	64	LYS
1	B	65	ILE
1	B	69	SER
1	B	71	ASN
1	B	77	ILE
1	B	82	HIS
1	B	85	VAL
1	B	87	THR
1	B	88	VAL
1	B	89	GLU
1	B	93	SER
1	B	95	LYS
1	B	97	ARG
1	B	103	GLU
1	B	105	ILE
1	B	113	CYS
1	B	118	PRO

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Mol	Chain	Res	Type
1	B	123	SER
1	B	129	ARG
1	B	131	GLN
1	B	136	MET
1	B	151	THR
1	B	154	ARG
1	B	161	ARG
1	B	165	ARG
1	B	197	LYS
1	B	199	GLU
1	B	200	GLU
1	B	204	LEU
1	B	211	ILE
1	B	219	LEU
1	B	220	LYS
1	B	222	THR
1	B	224	ARG
1	B	226	GLN
1	B	241	THR
1	B	244	GLU
1	B	248	LEU
1	B	249	LYS
1	B	257	LEU
1	B	284	ILE
1	B	295	ASP
1	B	298	SER
1	B	307	ILE
1	B	310	LYS
1	B	313	VAL
1	B	314	ASP
1	B	316	VAL
1	B	318	LYS
1	B	319	LEU
1	B	328	ARG
1	B	348	VAL
1	B	352	ILE
1	B	354	THR
1	B	359	SER
1	B	372	LEU
1	B	379	THR
1	B	381	ARG
1	B	382	THR

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Mol	Chain	Res	Type
1	B	383	VAL
1	B	388	THR
1	B	394	ARG
1	B	398	LEU
1	B	401	GLU
1	B	407	ILE
1	B	419	SER
1	B	426	ARG
1	B	427	ARG
1	B	428	GLU
1	B	430	ASP
1	B	431	ILE
1	B	435	THR
1	B	440	VAL
1	B	443	LYS
1	B	447	THR
1	B	450	GLN
1	B	451	GLU
1	B	452	LEU
1	B	459	MET
1	B	462	ARG
1	B	464	ILE
1	B	470	THR
1	B	474	LEU
1	B	505	VAL
1	B	511	LEU
1	B	512	THR
1	B	513	LEU
1	B	514	SER
1	B	520	TYR
1	B	521	LEU
1	B	522	THR
1	B	523	VAL
1	B	524	LEU
1	B	525	GLN
1	B	526	LYS
1	B	527	LEU
1	B	529	GLN
1	B	530	GLU
1	B	531	ASN
1	B	532	LEU
1	B	533	GLU

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Mol	Chain	Res	Type
1	B	539	LEU
1	B	541	PRO
1	B	542	THR
1	B	545	SER
1	B	547	THR
1	B	557	ASP
1	B	558	VAL
1	B	561	PHE
1	B	564	VAL
1	B	566	LYS
1	B	572	ASP
1	B	578	LEU
1	B	590	GLU
1	B	597	ILE
1	B	598	PRO
1	B	599	ARG
1	B	601	GLU
1	B	606	LEU
1	B	608	LEU
1	B	612	THR
1	B	618	ILE
1	B	619	LYS
1	B	623	THR
1	B	630	PRO
1	B	633	VAL
1	B	636	ILE
1	B	641	VAL
1	B	646	ILE
1	B	647	THR
1	B	649	ILE
1	B	650	CYS
1	B	652	ASP
1	B	654	THR
1	B	655	VAL
1	B	664	VAL
1	B	667	ILE
1	B	671	VAL
1	B	675	THR
1	B	679	THR
1	B	680	GLN
1	B	686	VAL
1	B	688	ILE

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Mol	Chain	Res	Type
1	B	689	THR
1	B	697	ILE
1	B	698	THR
1	B	699	ILE
1	B	700	GLU
1	B	703	ILE
1	B	706	ASN
1	B	707	SER
1	B	708	PHE
1	B	712	GLU
1	B	720	LEU
1	B	730	VAL
1	B	731	VAL
1	B	735	ILE
1	B	744	TYR
1	B	745	LEU
1	B	747	THR
1	B	753	VAL
1	B	757	GLU
1	B	760	GLU
1	B	767	THR
1	B	773	THR
1	B	775	SER
1	B	776	PHE
1	B	783	VAL
1	B	788	ILE
1	B	789	VAL
1	B	802	LYS
1	B	807	THR
1	B	822	ARG
1	B	825	ARG
1	B	826	CYS
1	B	830	ARG
1	B	831	ASP
1	B	836	ILE
1	B	837	THR
1	B	852	MET
1	B	854	THR
1	B	857	VAL
1	B	858	VAL
1	B	865	PHE
1	B	866	SER

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Mol	Chain	Res	Type
1	B	871	THR
1	B	876	GLN
1	B	877	SER
1	B	879	MET
1	B	891	LYS
1	B	894	ASN
1	B	902	CYS
1	B	910	THR
1	B	915	PHE
1	B	921	MET
1	B	922	LEU
1	B	925	GLU
1	B	927	TRP
1	B	929	SER
1	B	931	VAL
1	B	933	VAL
1	B	937	MET
1	B	944	ARG
1	B	946	ASN
1	B	949	LYS
1	B	950	GLU
1	B	953	LEU
1	B	959	LYS
1	B	970	GLU
1	B	976	SER
1	B	977	GLN
1	B	979	HIS
1	B	982	LYS
1	B	983	SER
1	B	986	ASP
1	B	987	LYS
1	B	993	CYS
1	B	1001	ILE
1	B	1008	ILE
1	B	1009	SER
1	B	1014	PHE
1	B	1017	GLN
1	B	1022	LEU
1	B	1029	SER
1	B	1041	GLN
1	B	1043	LEU
1	B	1052	SER

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Mol	Chain	Res	Type
1	B	1057	ILE
1	B	1059	THR
1	B	1060	SER
1	B	1069	THR
1	B	1070	ASN
1	B	1077	PRO
1	B	1085	ASP
1	B	1097	THR
1	B	1098	ILE
1	B	1104	PRO
1	B	1106	LYS
1	B	1107	LYS
1	B	1113	SER
1	B	1114	TRP
1	B	1119	THR
1	B	1125	THR
1	B	1126	VAL
1	B	1131	THR
1	B	1135	ARG
1	B	1139	LEU
1	B	1149	ASN
1	B	1164	GLU
1	B	1167	CYS
1	B	1173	LYS
1	B	1195	GLN
1	B	1204	LEU
1	B	1209	LEU
1	B	1212	LEU
1	B	1220	LEU
1	B	1221	HIS
1	B	1222	THR
1	B	1226	SER
1	B	1230	ILE
1	B	1239	GLU
1	B	1243	SER
1	B	1246	ARG
1	B	1254	ILE
1	B	1263	PRO
1	B	1277	ASP
1	B	1279	ILE
1	B	1280	ARG
1	B	1287	THR

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Mol	Chain	Res	Type
1	B	1291	VAL
1	B	1294	LEU
1	B	1299	SER
1	B	1315	THR
1	B	1316	THR
1	B	1317	LEU
1	B	1326	CYS
1	B	1327	LYS
1	B	1329	TRP
1	B	1331	VAL
1	C	6	LEU
1	C	24	THR
1	C	25	THR
1	C	31	ARG
1	C	34	LEU
1	C	36	LEU
1	C	41	LEU
1	C	43	CYS
1	C	56	SER
1	C	61	LEU
1	C	62	GLN
1	C	64	LYS
1	C	71	ASN
1	C	74	LEU
1	C	77	ILE
1	C	82	HIS
1	C	85	VAL
1	C	87	THR
1	C	88	VAL
1	C	89	GLU
1	C	93	SER
1	C	95	LYS
1	C	105	ILE
1	C	113	CYS
1	C	123	SER
1	C	131	GLN
1	C	136	MET
1	C	148	CYS
1	C	154	ARG
1	C	161	ARG
1	C	162	THR
1	C	165	ARG

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Mol	Chain	Res	Type
1	C	194	SER
1	C	197	LYS
1	C	199	GLU
1	C	200	GLU
1	C	211	ILE
1	C	219	LEU
1	C	220	LYS
1	C	222	THR
1	C	224	ARG
1	C	226	GLN
1	C	228	ARG
1	C	230	GLU
1	C	237	ILE
1	C	241	THR
1	C	244	GLU
1	C	248	LEU
1	C	249	LYS
1	C	257	LEU
1	C	277	MET
1	C	284	ILE
1	C	290	VAL
1	C	295	ASP
1	C	298	SER
1	C	307	ILE
1	C	310	LYS
1	C	313	VAL
1	C	314	ASP
1	C	316	VAL
1	C	318	LYS
1	C	319	LEU
1	C	327	PHE
1	C	328	ARG
1	C	342	VAL
1	C	347	SER
1	C	348	VAL
1	C	352	ILE
1	C	354	THR
1	C	363	PRO
1	C	372	LEU
1	C	374	LEU
1	C	377	ARG
1	C	379	THR

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Mol	Chain	Res	Type
1	C	381	ARG
1	C	382	THR
1	C	383	VAL
1	C	388	THR
1	C	394	ARG
1	C	398	LEU
1	C	401	GLU
1	C	426	ARG
1	C	428	GLU
1	C	435	THR
1	C	439	ARG
1	C	440	VAL
1	C	447	THR
1	C	450	GLN
1	C	452	LEU
1	C	459	MET
1	C	462	ARG
1	C	464	ILE
1	C	470	THR
1	C	474	LEU
1	C	483	LEU
1	C	504	MET
1	C	506	ASP
1	C	510	THR
1	C	512	THR
1	C	520	TYR
1	C	521	LEU
1	C	523	VAL
1	C	524	LEU
1	C	525	GLN
1	C	526	LYS
1	C	527	LEU
1	C	529	GLN
1	C	530	GLU
1	C	532	LEU
1	C	533	GLU
1	C	534	ASP
1	C	535	LYS
1	C	538	LYS
1	C	539	LEU
1	C	540	ASP
1	C	542	THR

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Mol	Chain	Res	Type
1	C	545	SER
1	C	547	THR
1	C	557	ASP
1	C	558	VAL
1	C	564	VAL
1	C	572	ASP
1	C	576	ARG
1	C	578	LEU
1	C	581	LEU
1	C	590	GLU
1	C	592	VAL
1	C	599	ARG
1	C	606	LEU
1	C	608	LEU
1	C	612	THR
1	C	618	ILE
1	C	619	LYS
1	C	621	ILE
1	C	623	THR
1	C	628	LYS
1	C	630	PRO
1	C	633	VAL
1	C	636	ILE
1	C	641	VAL
1	C	647	THR
1	C	649	ILE
1	C	650	CYS
1	C	652	ASP
1	C	654	THR
1	C	655	VAL
1	C	661	VAL
1	C	664	VAL
1	C	671	VAL
1	C	675	THR
1	C	677	GLU
1	C	679	THR
1	C	684	GLN
1	C	686	VAL
1	C	688	ILE
1	C	689	THR
1	C	693	LEU
1	C	697	ILE

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Mol	Chain	Res	Type
1	C	698	THR
1	C	699	ILE
1	C	700	GLU
1	C	701	ASP
1	C	703	ILE
1	C	704	LYS
1	C	707	SER
1	C	708	PHE
1	C	712	GLU
1	C	713	LEU
1	C	720	LEU
1	C	721	LYS
1	C	730	VAL
1	C	731	VAL
1	C	732	SER
1	C	735	ILE
1	C	737	ILE
1	C	744	TYR
1	C	745	LEU
1	C	747	THR
1	C	753	VAL
1	C	754	PRO
1	C	760	GLU
1	C	767	THR
1	C	773	THR
1	C	775	SER
1	C	788	ILE
1	C	789	VAL
1	C	790	VAL
1	C	791	ARG
1	C	792	VAL
1	C	802	LYS
1	C	810	SER
1	C	822	ARG
1	C	825	ARG
1	C	830	ARG
1	C	831	ASP
1	C	836	ILE
1	C	837	THR
1	C	847	TYR
1	C	854	THR
1	C	857	VAL

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Mol	Chain	Res	Type
1	C	858	VAL
1	C	865	PHE
1	C	866	SER
1	C	871	THR
1	C	879	MET
1	C	891	LYS
1	C	894	ASN
1	C	895	ILE
1	C	902	CYS
1	C	910	THR
1	C	912	PHE
1	C	915	PHE
1	C	921	MET
1	C	922	LEU
1	C	925	GLU
1	C	927	TRP
1	C	929	SER
1	C	931	VAL
1	C	933	VAL
1	C	937	MET
1	C	944	ARG
1	C	946	ASN
1	C	949	LYS
1	C	950	GLU
1	C	953	LEU
1	C	959	LYS
1	C	970	GLU
1	C	973	LEU
1	C	976	SER
1	C	977	GLN
1	C	979	HIS
1	C	982	LYS
1	C	986	ASP
1	C	987	LYS
1	C	1001	ILE
1	C	1002	ILE
1	C	1008	ILE
1	C	1009	SER
1	C	1014	PHE
1	C	1017	GLN
1	C	1022	LEU
1	C	1026	THR

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Mol	Chain	Res	Type
1	C	1043	LEU
1	C	1048	VAL
1	C	1052	SER
1	C	1057	ILE
1	C	1059	THR
1	C	1060	SER
1	C	1070	ASN
1	C	1072	VAL
1	C	1081	SER
1	C	1085	ASP
1	C	1097	THR
1	C	1098	ILE
1	C	1103	GLU
1	C	1106	LYS
1	C	1107	LYS
1	C	1113	SER
1	C	1114	TRP
1	C	1119	THR
1	C	1125	THR
1	C	1126	VAL
1	C	1131	THR
1	C	1135	ARG
1	C	1139	LEU
1	C	1144	GLU
1	C	1149	ASN
1	C	1161	SER
1	C	1167	CYS
1	C	1179	ILE
1	C	1195	GLN
1	C	1204	LEU
1	C	1209	LEU
1	C	1212	LEU
1	C	1214	TYR
1	C	1221	HIS
1	C	1222	THR
1	C	1229	LYS
1	C	1230	ILE
1	C	1239	GLU
1	C	1246	ARG
1	C	1254	ILE
1	C	1263	PRO
1	C	1277	ASP

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Mol	Chain	Res	Type
1	C	1279	ILE
1	C	1280	ARG
1	C	1287	THR
1	C	1291	VAL
1	C	1294	LEU
1	C	1299	SER
1	C	1314	PHE
1	C	1315	THR
1	C	1316	THR
1	C	1319	VAL
1	C	1331	VAL
1	D	6	LEU
1	D	14	LYS
1	D	16	VAL
1	D	18	LYS
1	D	25	THR
1	D	27	LEU
1	D	30	LEU
1	D	31	ARG
1	D	34	LEU
1	D	41	LEU
1	D	56	SER
1	D	61	LEU
1	D	62	GLN
1	D	63	ASN
1	D	64	LYS
1	D	71	ASN
1	D	74	LEU
1	D	77	ILE
1	D	82	HIS
1	D	85	VAL
1	D	87	THR
1	D	89	GLU
1	D	95	LYS
1	D	103	GLU
1	D	105	ILE
1	D	113	CYS
1	D	123	SER
1	D	131	GLN
1	D	136	MET
1	D	161	ARG
1	D	162	THR

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Mol	Chain	Res	Type
1	D	165	ARG
1	D	197	LYS
1	D	199	GLU
1	D	200	GLU
1	D	211	ILE
1	D	219	LEU
1	D	220	LYS
1	D	224	ARG
1	D	226	GLN
1	D	228	ARG
1	D	230	GLU
1	D	241	THR
1	D	244	GLU
1	D	246	LEU
1	D	248	LEU
1	D	249	LYS
1	D	257	LEU
1	D	277	MET
1	D	284	ILE
1	D	289	SER
1	D	290	VAL
1	D	295	ASP
1	D	298	SER
1	D	307	ILE
1	D	310	LYS
1	D	314	ASP
1	D	316	VAL
1	D	318	LYS
1	D	319	LEU
1	D	328	ARG
1	D	348	VAL
1	D	352	ILE
1	D	354	THR
1	D	359	SER
1	D	363	PRO
1	D	372	LEU
1	D	374	LEU
1	D	377	ARG
1	D	379	THR
1	D	381	ARG
1	D	382	THR
1	D	383	VAL

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Mol	Chain	Res	Type
1	D	388	THR
1	D	390	PHE
1	D	394	ARG
1	D	398	LEU
1	D	401	GLU
1	D	403	ILE
1	D	405	LEU
1	D	419	SER
1	D	426	ARG
1	D	427	ARG
1	D	428	GLU
1	D	430	ASP
1	D	435	THR
1	D	440	VAL
1	D	450	GLN
1	D	459	MET
1	D	462	ARG
1	D	464	ILE
1	D	470	THR
1	D	474	LEU
1	D	479	LYS
1	D	505	VAL
1	D	510	THR
1	D	520	TYR
1	D	521	LEU
1	D	522	THR
1	D	523	VAL
1	D	525	GLN
1	D	526	LYS
1	D	529	GLN
1	D	530	GLU
1	D	531	ASN
1	D	532	LEU
1	D	535	LYS
1	D	536	CYS
1	D	539	LEU
1	D	540	ASP
1	D	558	VAL
1	D	561	PHE
1	D	564	VAL
1	D	576	ARG
1	D	578	LEU

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Mol	Chain	Res	Type
1	D	581	LEU
1	D	590	GLU
1	D	592	VAL
1	D	597	ILE
1	D	598	PRO
1	D	601	GLU
1	D	605	SER
1	D	608	LEU
1	D	609	VAL
1	D	612	THR
1	D	618	ILE
1	D	619	LYS
1	D	621	ILE
1	D	623	THR
1	D	628	LYS
1	D	630	PRO
1	D	633	VAL
1	D	634	CYS
1	D	636	ILE
1	D	641	VAL
1	D	647	THR
1	D	649	ILE
1	D	650	CYS
1	D	652	ASP
1	D	654	THR
1	D	655	VAL
1	D	661	VAL
1	D	664	VAL
1	D	667	ILE
1	D	671	VAL
1	D	675	THR
1	D	677	GLU
1	D	679	THR
1	D	680	GLN
1	D	686	VAL
1	D	688	ILE
1	D	697	ILE
1	D	698	THR
1	D	699	ILE
1	D	700	GLU
1	D	701	ASP
1	D	703	ILE

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Mol	Chain	Res	Type
1	D	704	LYS
1	D	706	ASN
1	D	708	PHE
1	D	712	GLU
1	D	713	LEU
1	D	720	LEU
1	D	721	LYS
1	D	730	VAL
1	D	731	VAL
1	D	732	SER
1	D	734	GLU
1	D	735	ILE
1	D	744	TYR
1	D	745	LEU
1	D	747	THR
1	D	753	VAL
1	D	757	GLU
1	D	765	VAL
1	D	773	THR
1	D	775	SER
1	D	776	PHE
1	D	779	LYS
1	D	783	VAL
1	D	788	ILE
1	D	791	ARG
1	D	802	LYS
1	D	807	THR
1	D	810	SER
1	D	819	LYS
1	D	822	ARG
1	D	825	ARG
1	D	830	ARG
1	D	831	ASP
1	D	836	ILE
1	D	837	THR
1	D	846	ARG
1	D	847	TYR
1	D	854	THR
1	D	857	VAL
1	D	858	VAL
1	D	865	PHE
1	D	871	THR

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Mol	Chain	Res	Type
1	D	878	ILE
1	D	879	MET
1	D	891	LYS
1	D	894	ASN
1	D	902	CYS
1	D	910	THR
1	D	915	PHE
1	D	921	MET
1	D	922	LEU
1	D	925	GLU
1	D	927	TRP
1	D	929	SER
1	D	933	VAL
1	D	937	MET
1	D	944	ARG
1	D	946	ASN
1	D	949	LYS
1	D	953	LEU
1	D	970	GLU
1	D	976	SER
1	D	977	GLN
1	D	979	HIS
1	D	982	LYS
1	D	986	ASP
1	D	987	LYS
1	D	1001	ILE
1	D	1008	ILE
1	D	1009	SER
1	D	1014	PHE
1	D	1017	GLN
1	D	1022	LEU
1	D	1024	VAL
1	D	1026	THR
1	D	1030	VAL
1	D	1032	LEU
1	D	1033	THR
1	D	1041	GLN
1	D	1043	LEU
1	D	1045	THR
1	D	1048	VAL
1	D	1052	SER
1	D	1057	ILE

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Mol	Chain	Res	Type
1	D	1059	THR
1	D	1060	SER
1	D	1068	SER
1	D	1070	ASN
1	D	1072	VAL
1	D	1085	ASP
1	D	1097	THR
1	D	1098	ILE
1	D	1100	LYS
1	D	1106	LYS
1	D	1107	LYS
1	D	1113	SER
1	D	1119	THR
1	D	1125	THR
1	D	1126	VAL
1	D	1131	THR
1	D	1135	ARG
1	D	1139	LEU
1	D	1144	GLU
1	D	1149	ASN
1	D	1167	CYS
1	D	1178	ASP
1	D	1187	LEU
1	D	1195	GLN
1	D	1204	LEU
1	D	1212	LEU
1	D	1214	TYR
1	D	1220	LEU
1	D	1221	HIS
1	D	1222	THR
1	D	1226	SER
1	D	1230	ILE
1	D	1236	ILE
1	D	1243	SER
1	D	1246	ARG
1	D	1251	LYS
1	D	1254	ILE
1	D	1271	ILE
1	D	1277	ASP
1	D	1279	ILE
1	D	1280	ARG
1	D	1287	THR

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Mol	Chain	Res	Type
1	D	1291	VAL
1	D	1294	LEU
1	D	1302	THR
1	D	1303	PRO
1	D	1311	VAL
1	D	1313	LYS
1	D	1315	THR
1	D	1316	THR
1	D	1317	LEU
1	D	1318	CYS
1	D	1319	VAL
1	D	1320	THR
1	D	1326	CYS
1	D	1330	SER
1	D	1331	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (126) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	63	ASN
1	A	71	ASN
1	A	112	GLN
1	A	208	GLN
1	A	226	GLN
1	A	252	HIS
1	A	261	ASN
1	A	351	ASN
1	A	684	GLN
1	A	706	ASN
1	A	742	HIS
1	A	748	HIS
1	A	768	GLN
1	A	894	ASN
1	A	946	ASN
1	A	977	GLN
1	A	1017	GLN
1	A	1034	HIS
1	A	1044	HIS
1	A	1070	ASN
1	A	1089	GLN
1	A	1146	ASN

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Mol	Chain	Res	Type
1	A	1149	ASN
1	A	1195	GLN
1	A	1213	HIS
1	B	11	ASN
1	B	71	ASN
1	B	112	GLN
1	B	130	ASN
1	B	144	GLN
1	B	238	GLN
1	B	252	HIS
1	B	261	ASN
1	B	272	ASN
1	B	322	GLN
1	B	333	GLN
1	B	351	ASN
1	B	423	GLN
1	B	495	HIS
1	B	525	GLN
1	B	531	ASN
1	B	651	ASN
1	B	684	GLN
1	B	748	HIS
1	B	905	ASN
1	B	946	ASN
1	B	958	GLN
1	B	977	GLN
1	B	1023	HIS
1	B	1034	HIS
1	B	1044	HIS
1	B	1070	ASN
1	B	1087	ASN
1	B	1149	ASN
1	B	1195	GLN
1	B	1213	HIS
1	C	71	ASN
1	C	112	GLN
1	C	144	GLN
1	C	158	GLN
1	C	208	GLN
1	C	226	GLN
1	C	238	GLN
1	C	251	GLN

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Mol	Chain	Res	Type
1	C	252	HIS
1	C	261	ASN
1	C	322	GLN
1	C	351	ASN
1	C	423	GLN
1	C	473	GLN
1	C	529	GLN
1	C	531	ASN
1	C	615	HIS
1	C	684	GLN
1	C	706	ASN
1	C	748	HIS
1	C	768	GLN
1	C	894	ASN
1	C	909	ASN
1	C	946	ASN
1	C	958	GLN
1	C	1017	GLN
1	C	1023	HIS
1	C	1034	HIS
1	C	1044	HIS
1	C	1070	ASN
1	C	1089	GLN
1	C	1149	ASN
1	C	1195	GLN
1	C	1213	HIS
1	C	1286	HIS
1	C	1289	ASN
1	D	11	ASN
1	D	63	ASN
1	D	71	ASN
1	D	81	HIS
1	D	112	GLN
1	D	144	GLN
1	D	158	GLN
1	D	252	HIS
1	D	322	GLN
1	D	351	ASN
1	D	531	ASN
1	D	615	HIS
1	D	651	ASN
1	D	680	GLN

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Mol	Chain	Res	Type
1	D	684	GLN
1	D	706	ASN
1	D	748	HIS
1	D	864	HIS
1	D	894	ASN
1	D	946	ASN
1	D	958	GLN
1	D	977	GLN
1	D	992	ASN
1	D	1023	HIS
1	D	1034	HIS
1	D	1044	HIS
1	D	1070	ASN
1	D	1149	ASN
1	D	1195	GLN
1	D	1213	HIS
1	D	1286	HIS
1	D	1289	ASN
1	D	1308	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 ⓘ

18 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GOL	A	3007	-	5,5,5	0.59	0	5,5,5	0.95	0
2	FES	B	3002	1	0,4,4	-	-	-		
2	FES	D	3002	1	0,4,4	-	-	-		
4	GOL	D	3007	-	5,5,5	0.85	0	5,5,5	1.30	1 (20%)
2	FES	D	3001	1	0,4,4	-	-	-		
2	FES	A	3002	1	0,4,4	-	-	-		
2	FES	C	3002	1	0,4,4	-	-	-		
3	FAD	C	3006	-	56,58,58	2.01	17 (30%)	81,89,89	2.78	39 (48%)
3	FAD	D	3006	-	56,58,58	2.27	14 (25%)	81,89,89	2.86	39 (48%)
5	ACY	D	3008	-	3,3,3	1.13	0	3,3,3	1.52	0
6	PO4	D	3009	-	4,4,4	1.07	0	6,6,6	1.86	1 (16%)
2	FES	A	3001	1	0,4,4	-	-	-		
3	FAD	A	3006	-	56,58,58	1.79	11 (19%)	81,89,89	2.13	33 (40%)
4	GOL	B	3007	-	5,5,5	0.61	0	5,5,5	0.75	0
4	GOL	C	3007	-	5,5,5	0.52	0	5,5,5	0.53	0
2	FES	B	3001	1	0,4,4	-	-	-		
3	FAD	B	3006	-	56,58,58	1.93	14 (25%)	81,89,89	2.78	36 (44%)
2	FES	C	3001	1	0,4,4	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	3007	-	-	2/4/4/4	-
2	FES	B	3002	1	-	-	0/1/1/1
2	FES	D	3002	1	-	-	0/1/1/1
4	GOL	D	3007	-	-	0/4/4/4	-
2	FES	D	3001	1	-	-	0/1/1/1
2	FES	A	3002	1	-	-	0/1/1/1
3	FAD	C	3006	-	-	9/34/50/50	0/6/6/6
3	FAD	D	3006	-	-	11/34/50/50	0/6/6/6
2	FES	C	3002	1	-	-	0/1/1/1
4	GOL	B	3007	-	-	2/4/4/4	-
3	FAD	A	3006	-	-	8/34/50/50	0/6/6/6
4	GOL	C	3007	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FES	A	3001	1	-	-	0/1/1/1
2	FES	B	3001	1	-	-	0/1/1/1
3	FAD	B	3006	-	-	10/34/50/50	0/6/6/6
2	FES	C	3001	1	-	-	0/1/1/1

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3006	FAD	C2A-N3A	8.12	1.49	1.33
3	D	3006	FAD	C2A-N1A	7.07	1.47	1.33
3	D	3006	FAD	C5A-C4A	6.22	1.50	1.39
3	A	3006	FAD	C2A-N1A	5.43	1.44	1.33
3	C	3006	FAD	C2A-N1A	5.23	1.43	1.33
3	B	3006	FAD	C2A-N3A	5.13	1.43	1.33
3	A	3006	FAD	C5A-N7A	-4.85	1.29	1.39
3	B	3006	FAD	C2A-N1A	4.61	1.42	1.33
3	C	3006	FAD	C4X-N5	4.45	1.39	1.30
3	A	3006	FAD	C4X-N5	4.26	1.39	1.30
3	C	3006	FAD	C2A-N3A	4.25	1.41	1.33
3	B	3006	FAD	C5A-N7A	-4.23	1.31	1.39
3	D	3006	FAD	C6A-N1A	4.14	1.48	1.35
3	B	3006	FAD	C9A-N10	3.91	1.48	1.41
3	D	3006	FAD	C4X-N5	3.90	1.38	1.30
3	B	3006	FAD	C4X-N5	3.90	1.38	1.30
3	C	3006	FAD	O2'-C2'	-3.88	1.35	1.43
3	A	3006	FAD	C1'-N10	3.65	1.57	1.48
3	A	3006	FAD	C2A-N3A	3.65	1.40	1.33
3	C	3006	FAD	C8A-N7A	3.43	1.38	1.31
3	C	3006	FAD	C5A-N7A	-3.40	1.32	1.39
3	C	3006	FAD	C10-N1	3.39	1.40	1.33
3	D	3006	FAD	C5A-N7A	-3.36	1.32	1.39
3	B	3006	FAD	O2'-C2'	-3.24	1.36	1.43
3	D	3006	FAD	C8A-N9A	3.19	1.43	1.37
3	B	3006	FAD	O4B-C1B	-3.12	1.34	1.42
3	C	3006	FAD	C9A-N10	3.10	1.46	1.41
3	C	3006	FAD	C1'-C2'	-3.08	1.48	1.52
3	B	3006	FAD	C1'-N10	3.06	1.55	1.48
3	C	3006	FAD	C8-C7	-3.03	1.33	1.40
3	D	3006	FAD	C8A-N7A	2.99	1.37	1.31
3	D	3006	FAD	C10-N10	2.91	1.43	1.37
3	A	3006	FAD	C4A-N9A	-2.88	1.31	1.37
3	C	3006	FAD	O4B-C4B	-2.70	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3006	FAD	O3'-C3'	-2.69	1.36	1.43
3	B	3006	FAD	C2'-C3'	-2.68	1.48	1.53
3	B	3006	FAD	O3'-C3'	-2.65	1.36	1.43
3	C	3006	FAD	C5A-C4A	2.60	1.43	1.39
3	C	3006	FAD	C8A-N9A	2.53	1.42	1.37
3	B	3006	FAD	C9-C9A	2.51	1.43	1.39
3	D	3006	FAD	O2'-C2'	-2.49	1.38	1.43
3	A	3006	FAD	C4X-C4	-2.43	1.35	1.44
3	B	3006	FAD	C8M-C8	2.40	1.55	1.51
3	C	3006	FAD	C6-C5X	-2.39	1.36	1.40
3	C	3006	FAD	C4X-C4	-2.34	1.35	1.44
3	C	3006	FAD	C5B-C4B	2.33	1.58	1.51
3	A	3006	FAD	C9-C9A	2.32	1.43	1.39
3	A	3006	FAD	C2'-C3'	-2.32	1.49	1.53
3	C	3006	FAD	C1'-N10	2.30	1.54	1.48
3	A	3006	FAD	O3'-C3'	-2.28	1.37	1.43
3	B	3006	FAD	C8A-N7A	2.19	1.35	1.31
3	B	3006	FAD	C2-N1	2.09	1.41	1.36
3	A	3006	FAD	C4'-C3'	-2.08	1.49	1.53
3	D	3006	FAD	C10-N1	2.05	1.37	1.33
3	D	3006	FAD	C4'-C3'	-2.03	1.49	1.53
3	D	3006	FAD	C1B-N9A	2.00	1.52	1.46

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3006	FAD	C2B-C1B-N9A	8.80	135.59	113.30
3	B	3006	FAD	C5A-C4A-N3A	-8.10	116.18	126.75
3	C	3006	FAD	C2B-C1B-N9A	7.43	132.11	113.30
3	C	3006	FAD	C5A-C4A-N3A	-7.15	117.42	126.75
3	B	3006	FAD	C6A-C5A-C4A	7.01	126.60	117.18
3	B	3006	FAD	C2B-C1B-N9A	6.61	130.05	113.30
3	A	3006	FAD	C2B-C1B-N9A	6.47	129.70	113.30
3	D	3006	FAD	C4A-N9A-C8A	-6.35	98.85	105.73
3	C	3006	FAD	C6A-C5A-C4A	6.26	125.60	117.18
3	D	3006	FAD	C6A-C5A-C4A	6.01	125.26	117.18
3	C	3006	FAD	O2'-C2'-C1'	-5.79	95.79	109.80
3	D	3006	FAD	C4-C4X-C10	5.74	126.43	116.79
3	B	3006	FAD	C1B-N9A-C8A	-5.47	114.78	127.14
3	D	3006	FAD	C5A-C4A-N3A	-5.26	119.88	126.75
3	D	3006	FAD	N9A-C8A-N7A	5.26	121.11	113.91
3	B	3006	FAD	N3A-C4A-N9A	5.21	135.66	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3006	FAD	C6A-C5A-N7A	-5.18	122.36	132.02
3	D	3006	FAD	C4A-N9A-C1B	5.01	138.54	126.59
3	C	3006	FAD	C4A-N9A-C1B	4.99	138.48	126.59
3	B	3006	FAD	C4A-N9A-C1B	4.92	138.32	126.59
3	B	3006	FAD	P-O3P-PA	-4.73	116.61	132.83
3	D	3006	FAD	C8M-C8-C7	-4.72	111.07	120.74
3	B	3006	FAD	O2'-C2'-C3'	-4.63	97.85	109.10
3	B	3006	FAD	C9A-C5X-N5	-4.61	117.42	122.43
3	C	3006	FAD	C6A-C5A-N7A	-4.56	123.51	132.02
3	C	3006	FAD	O5B-C5B-C4B	4.56	124.68	108.99
3	D	3006	FAD	O2-C2-N1	-4.52	114.34	121.83
3	C	3006	FAD	N6A-C6A-N1A	4.50	128.20	118.35
3	A	3006	FAD	C5X-C9A-N10	4.50	122.60	117.95
3	C	3006	FAD	C1B-N9A-C8A	-4.45	117.09	127.14
3	A	3006	FAD	O5'-C5'-C4'	4.44	121.22	109.36
3	C	3006	FAD	C5A-C6A-N6A	-4.41	113.84	123.43
3	B	3006	FAD	N3A-C2A-N1A	-4.41	121.71	128.60
3	D	3006	FAD	C5A-C6A-N6A	-4.40	113.85	123.43
3	C	3006	FAD	N3A-C4A-N9A	4.37	134.29	127.08
3	A	3006	FAD	O3B-C3B-C4B	-4.33	98.53	111.05
3	B	3006	FAD	O3'-C3'-C2'	-4.27	98.50	108.81
3	A	3006	FAD	C6A-C5A-C4A	4.26	122.91	117.18
3	D	3006	FAD	N6A-C6A-N1A	4.24	127.63	118.35
3	C	3006	FAD	N3A-C2A-N1A	-4.19	122.05	128.60
3	B	3006	FAD	C5X-C9A-N10	4.19	122.28	117.95
3	D	3006	FAD	C10-C4X-N5	-4.18	115.98	124.86
3	C	3006	FAD	O4-C4-C4X	-3.99	116.02	126.60
3	C	3006	FAD	C8M-C8-C7	-3.94	112.66	120.74
3	B	3006	FAD	C5A-N7A-C8A	3.94	109.11	103.51
3	B	3006	FAD	O4'-C4'-C5'	-3.92	101.11	109.92
3	B	3006	FAD	C2A-N3A-C4A	3.82	120.78	111.75
3	A	3006	FAD	O4B-C1B-N9A	3.81	115.58	108.06
3	A	3006	FAD	C5B-C4B-C3B	-3.81	100.90	115.18
3	D	3006	FAD	P-O3P-PA	-3.81	119.75	132.83
3	D	3006	FAD	O2B-C2B-C3B	-3.78	99.59	111.82
3	C	3006	FAD	C1'-N10-C9A	3.73	126.73	120.51
3	C	3006	FAD	C2B-C3B-C4B	3.73	109.89	102.64
3	D	3006	FAD	O4B-C4B-C3B	3.72	112.48	105.11
3	D	3006	FAD	C4X-C10-N10	3.72	121.92	116.48
3	D	3006	FAD	C4X-C10-N1	-3.66	116.23	124.73
3	A	3006	FAD	O4'-C4'-C3'	-3.61	100.33	109.10
3	C	3006	FAD	C2A-N3A-C4A	3.55	120.13	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3006	FAD	N3A-C2A-N1A	-3.54	123.07	128.60
3	D	3006	FAD	C1'-N10-C9A	-3.49	114.69	120.51
3	C	3006	FAD	C5X-C9A-N10	3.49	121.55	117.95
3	C	3006	FAD	C7M-C7-C8	-3.38	113.82	120.74
3	C	3006	FAD	O5B-PA-O1A	-3.38	95.88	109.07
3	B	3006	FAD	C8M-C8-C7	3.34	127.59	120.74
6	D	3009	PO4	O3-P-O2	-3.29	97.40	107.97
3	B	3006	FAD	C4-N3-C2	-3.28	119.58	125.64
3	D	3006	FAD	O2'-C2'-C1'	-3.26	101.91	109.80
3	D	3006	FAD	O2'-C2'-C3'	-3.24	101.23	109.10
3	B	3006	FAD	C4A-C5A-N7A	-3.24	106.68	110.62
3	D	3006	FAD	C5A-N7A-C8A	-3.18	98.98	103.51
3	C	3006	FAD	O4'-C4'-C3'	3.18	116.83	109.10
3	D	3006	FAD	C5X-N5-C4X	3.17	123.34	118.07
3	A	3006	FAD	O5B-C5B-C4B	3.16	119.87	108.99
3	B	3006	FAD	C5A-C6A-N6A	-3.13	116.61	123.43
3	B	3006	FAD	O4-C4-C4X	-3.12	118.33	126.60
3	C	3006	FAD	C4A-N9A-C8A	-3.10	102.37	105.73
3	A	3006	FAD	C9A-C5X-N5	-3.09	119.07	122.43
3	C	3006	FAD	C9A-N10-C10	-3.08	115.96	120.77
3	B	3006	FAD	C4B-O4B-C1B	-3.07	102.70	109.47
3	B	3006	FAD	C4-C4X-C10	3.06	121.93	116.79
3	A	3006	FAD	P-O3P-PA	-3.04	122.41	132.83
3	B	3006	FAD	O2'-C2'-C1'	-3.00	102.54	109.80
3	B	3006	FAD	C9A-N10-C10	-2.98	116.13	120.77
3	A	3006	FAD	O2'-C2'-C3'	-2.96	101.91	109.10
3	B	3006	FAD	C4X-C10-N10	2.95	120.80	116.48
3	D	3006	FAD	N3A-C2A-N1A	-2.94	124.00	128.60
3	D	3006	FAD	O2B-C2B-C1B	2.94	119.84	110.02
3	A	3006	FAD	C9A-N10-C10	-2.93	116.20	120.77
3	D	3006	FAD	O5B-C5B-C4B	2.92	119.03	108.99
3	C	3006	FAD	O3'-C3'-C4'	-2.90	101.82	108.81
3	B	3006	FAD	C6A-C5A-N7A	-2.86	126.69	132.02
3	B	3006	FAD	C8M-C8-C9	-2.83	114.25	119.49
3	A	3006	FAD	O4-C4-C4X	-2.80	119.18	126.60
3	A	3006	FAD	C7M-C7-C6	2.78	124.62	119.49
3	B	3006	FAD	N9A-C8A-N7A	-2.73	110.18	113.91
3	D	3006	FAD	N3A-C4A-N9A	2.69	131.51	127.08
3	D	3006	FAD	C1B-N9A-C8A	-2.69	121.07	127.14
3	C	3006	FAD	O4B-C1B-N9A	2.69	113.35	108.06
3	D	3006	FAD	C5B-C4B-C3B	-2.64	105.28	115.18
3	A	3006	FAD	C1B-N9A-C8A	-2.64	121.18	127.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3006	FAD	C9-C9A-C5X	-2.63	115.14	120.11
3	B	3006	FAD	C9A-C9-C8	2.62	124.58	119.30
3	C	3006	FAD	O3'-C3'-C2'	-2.61	102.50	108.81
3	C	3006	FAD	C4'-C3'-C2'	2.60	118.77	113.36
3	A	3006	FAD	C4A-N9A-C1B	2.59	132.77	126.59
3	A	3006	FAD	C6A-C5A-N7A	-2.58	127.20	132.02
3	C	3006	FAD	C8M-C8-C9	2.56	124.23	119.49
3	B	3006	FAD	C9-C8-C7	-2.55	116.01	119.67
3	C	3006	FAD	O4B-C1B-C2B	2.51	112.10	106.64
3	C	3006	FAD	C5'-C4'-C3'	-2.50	107.37	112.20
3	D	3006	FAD	O4B-C1B-N9A	2.48	112.94	108.06
3	D	3006	FAD	C5A-C4A-N9A	2.42	108.60	105.78
3	C	3006	FAD	C6-C7-C8	2.38	123.08	119.67
3	C	3006	FAD	O3B-C3B-C2B	2.38	119.52	111.82
3	D	3006	FAD	O2-C2-N3	2.38	123.27	118.65
3	B	3006	FAD	C5X-N5-C4X	2.35	121.98	118.07
3	A	3006	FAD	C4-N3-C2	-2.34	121.32	125.64
3	D	3006	FAD	C4-N3-C2	-2.31	121.38	125.64
3	A	3006	FAD	O2B-C2B-C3B	-2.26	104.52	111.82
3	A	3006	FAD	C5A-C4A-N3A	-2.24	123.83	126.75
3	A	3006	FAD	C9A-C9-C8	2.23	123.80	119.30
3	C	3006	FAD	O2P-P-O5'	-2.22	97.43	107.75
3	A	3006	FAD	C4B-O4B-C1B	-2.22	104.58	109.47
3	D	3006	FAD	C2A-N3A-C4A	2.20	116.95	111.75
3	A	3006	FAD	O3B-C3B-C2B	2.20	118.94	111.82
3	D	3006	FAD	C9A-C5X-N5	-2.19	120.05	122.43
3	A	3006	FAD	C5A-N7A-C8A	2.18	106.61	103.51
3	C	3006	FAD	C5A-C4A-N9A	2.16	108.29	105.78
3	D	3006	FAD	O3'-C3'-C2'	-2.15	103.62	108.81
3	A	3006	FAD	C7M-C7-C8	-2.14	116.34	120.74
3	C	3006	FAD	P-O5'-C5'	-2.14	109.11	121.68
3	C	3006	FAD	C4-C4X-N5	-2.12	115.21	118.23
3	A	3006	FAD	N9A-C8A-N7A	-2.10	111.05	113.91
3	B	3006	FAD	C1'-N10-C9A	2.09	124.00	120.51
3	A	3006	FAD	C4X-C4-N3	2.08	118.47	113.19
3	C	3006	FAD	C3B-C2B-C1B	-2.06	97.51	101.43
3	C	3006	FAD	O2P-P-O1P	2.06	122.44	112.24
3	A	3006	FAD	C4X-C10-N10	2.06	119.50	116.48
3	A	3006	FAD	C9-C9A-C5X	-2.06	116.22	120.11
3	A	3006	FAD	O4B-C4B-C3B	2.05	109.17	105.11
3	D	3006	FAD	C4B-O4B-C1B	-2.05	104.96	109.47
3	B	3006	FAD	C5A-C4A-N9A	2.04	108.16	105.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	3007	GOL	O2-C2-C3	2.04	118.09	109.12
3	D	3006	FAD	O5B-PA-O1A	-2.03	101.13	109.07
3	D	3006	FAD	C5'-C4'-C3'	-2.03	108.29	112.20
3	B	3006	FAD	C4X-C4-N3	2.02	118.33	113.19
3	A	3006	FAD	O4'-C4'-C5'	2.02	114.45	109.92
3	C	3006	FAD	P-O3P-PA	-2.01	125.92	132.83
3	B	3006	FAD	O3B-C3B-C4B	-2.01	105.24	111.05

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	3006	FAD	C5B-O5B-PA-O3P
3	B	3006	FAD	C5B-O5B-PA-O1A
3	B	3006	FAD	C5B-O5B-PA-O2A
3	B	3006	FAD	C5B-O5B-PA-O3P
3	B	3006	FAD	O4B-C1B-N9A-C4A
3	B	3006	FAD	C2'-C3'-C4'-O4'
3	C	3006	FAD	C5B-O5B-PA-O1A
3	C	3006	FAD	C5B-O5B-PA-O2A
3	C	3006	FAD	C5B-O5B-PA-O3P
3	C	3006	FAD	C1'-C2'-C3'-O3'
3	D	3006	FAD	C5B-O5B-PA-O3P
3	D	3006	FAD	C1'-C2'-C3'-O3'
3	D	3006	FAD	O4'-C4'-C5'-O5'
4	A	3007	GOL	O1-C1-C2-C3
4	C	3007	GOL	C1-C2-C3-O3
3	C	3006	FAD	C2'-C3'-C4'-O4'
3	D	3006	FAD	C2'-C3'-C4'-O4'
4	A	3007	GOL	O1-C1-C2-O2
3	C	3006	FAD	C3B-C4B-C5B-O5B
4	B	3007	GOL	O1-C1-C2-C3
3	C	3006	FAD	C2'-C3'-C4'-C5'
4	C	3007	GOL	O2-C2-C3-O3
3	C	3006	FAD	O4B-C4B-C5B-O5B
3	D	3006	FAD	C3'-C4'-C5'-O5'
4	B	3007	GOL	O1-C1-C2-O2
3	A	3006	FAD	O4'-C4'-C5'-O5'
3	D	3006	FAD	O4B-C1B-N9A-C4A
3	B	3006	FAD	O4B-C1B-N9A-C8A
3	D	3006	FAD	O4B-C4B-C5B-O5B
3	A	3006	FAD	O4B-C1B-N9A-C4A

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Mol	Chain	Res	Type	Atoms
3	C	3006	FAD	O4B-C1B-N9A-C4A
3	B	3006	FAD	C2'-C3'-C4'-C5'
3	A	3006	FAD	C5B-O5B-PA-O1A
3	A	3006	FAD	C5B-O5B-PA-O2A
3	D	3006	FAD	C5B-O5B-PA-O1A
3	D	3006	FAD	C5B-O5B-PA-O2A
3	B	3006	FAD	C1'-C2'-C3'-O3'
3	D	3006	FAD	C2'-C3'-C4'-C5'
3	D	3006	FAD	O4B-C1B-N9A-C8A
3	B	3006	FAD	O4B-C4B-C5B-O5B
3	B	3006	FAD	C3B-C4B-C5B-O5B
3	A	3006	FAD	O4B-C1B-N9A-C8A
3	A	3006	FAD	C3B-C4B-C5B-O5B
3	A	3006	FAD	C2'-C3'-C4'-O4'

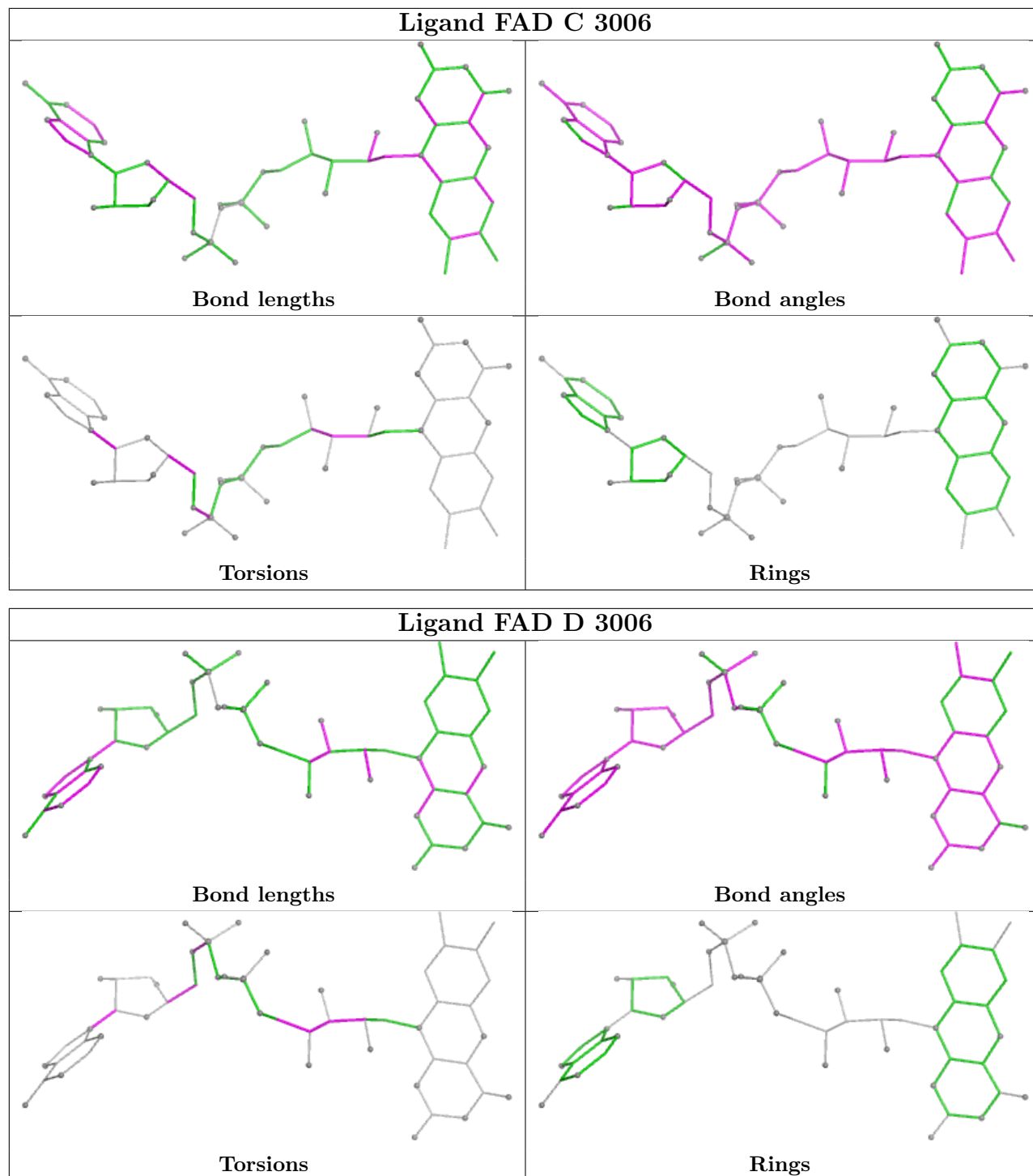
There are no ring outliers.

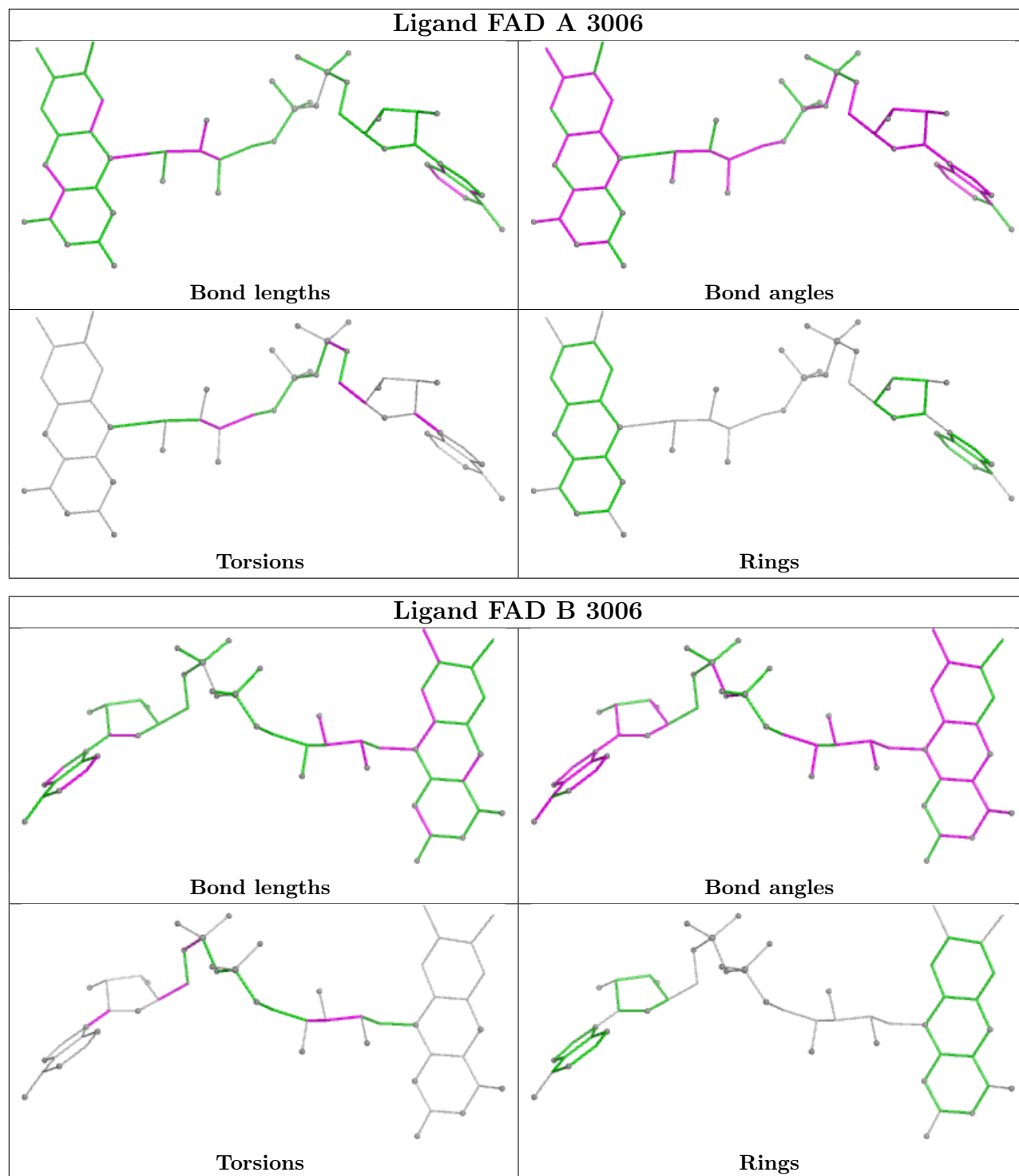
11 monomers are involved in 79 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3007	GOL	6	0
2	B	3002	FES	2	0
4	D	3007	GOL	11	0
2	A	3002	FES	2	0
3	C	3006	FAD	9	0
3	D	3006	FAD	14	0
6	D	3009	PO4	1	0
3	A	3006	FAD	10	0
4	B	3007	GOL	14	0
4	C	3007	GOL	4	0
3	B	3006	FAD	6	0

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

equivalents in the CSD to analyse the geometry.





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.