Full wwPDB X-ray Structure Validation Report ⓘ

Dec 10, 2023 – 04:57 am GMT

PDB ID	:	2CKJ
Title	:	Human milk xanthine oxidoreductase
Authors	:	Pearson, A.R.; Godber, B.L.J.; Eisenthal, 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:

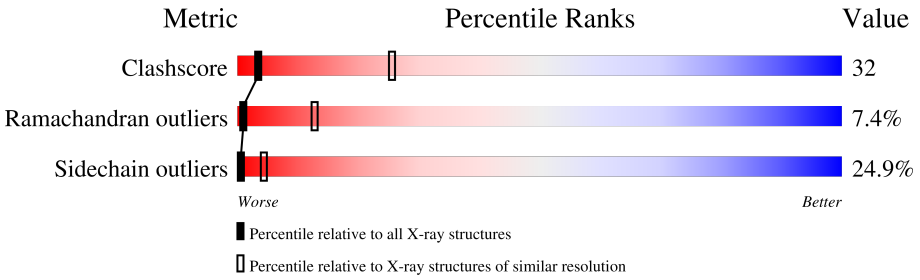
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.59 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	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1333	34% 34% 20% 6% 5%
1	B	1333	35% 35% 20% 7% .
1	C	1333	35% 36% 18% 8% .
1	D	1333	36% 34% 20% 7% .

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)

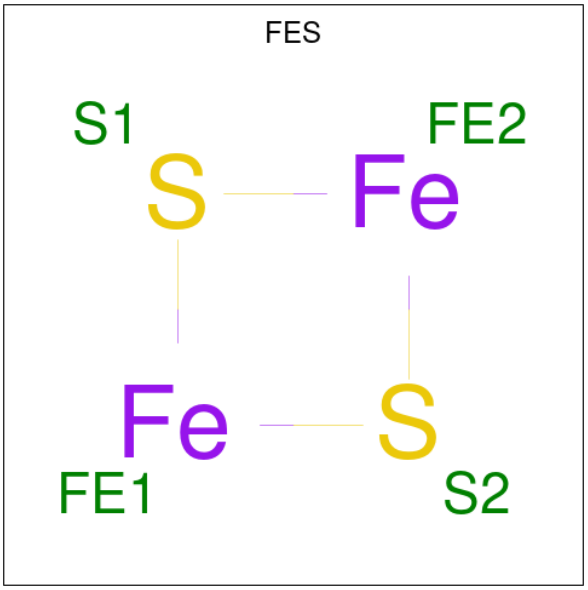
There are 6 unique types of molecules in this entry. The entry contains 39807 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: FES) (formula: Fe_2S_2).



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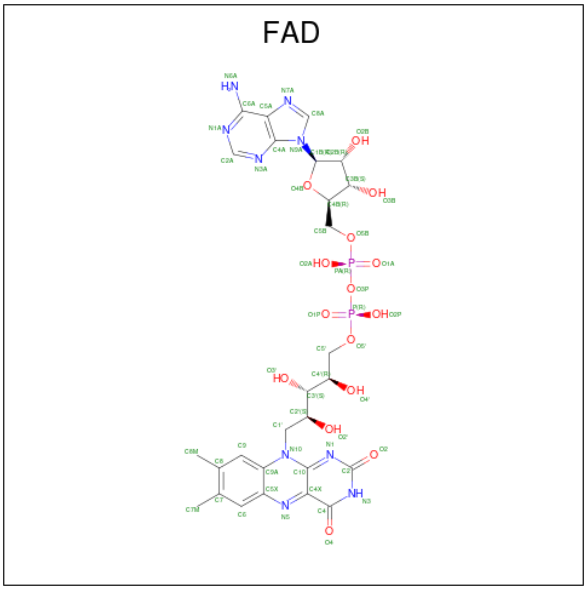
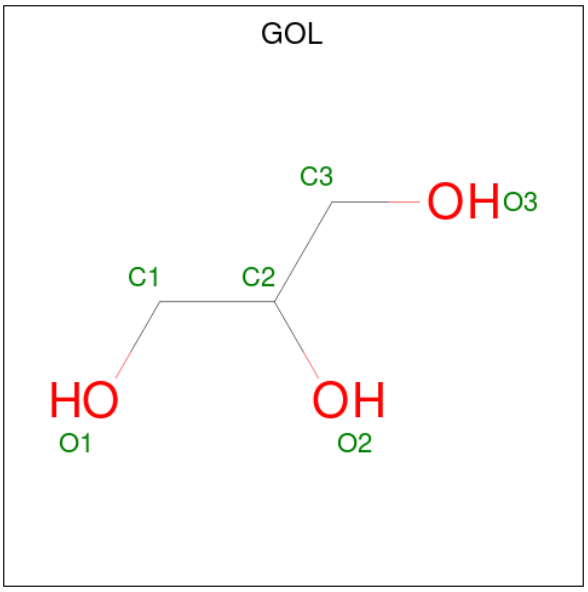
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Fe S 4 2 2	0	0
2	B	1	Total Fe S 4 2 2	0	0
2	C	1	Total Fe S 4 2 2	0	0
2	C	1	Total Fe S 4 2 2	0	0
2	D	1	Total Fe S 4 2 2	0	0
2	D	1	Total Fe S 4 2 2	0	0

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



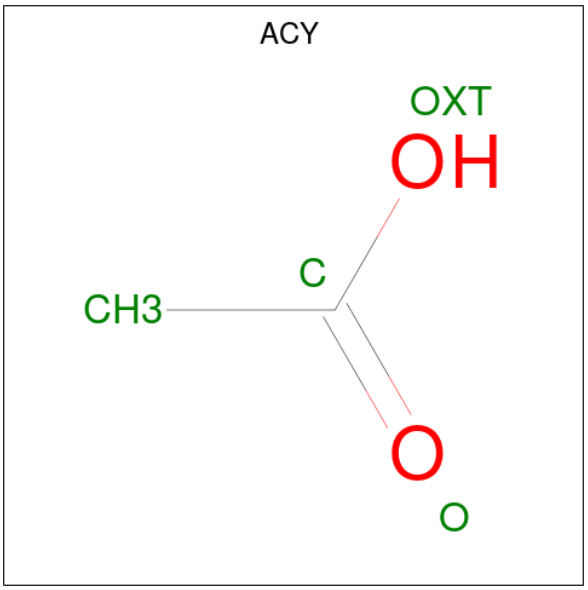
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 53 27 9 15 2	0	0
3	B	1	Total C N O P 53 27 9 15 2	0	0
3	C	1	Total C N O P 53 27 9 15 2	0	0
3	D	1	Total C N O P 53 27 9 15 2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



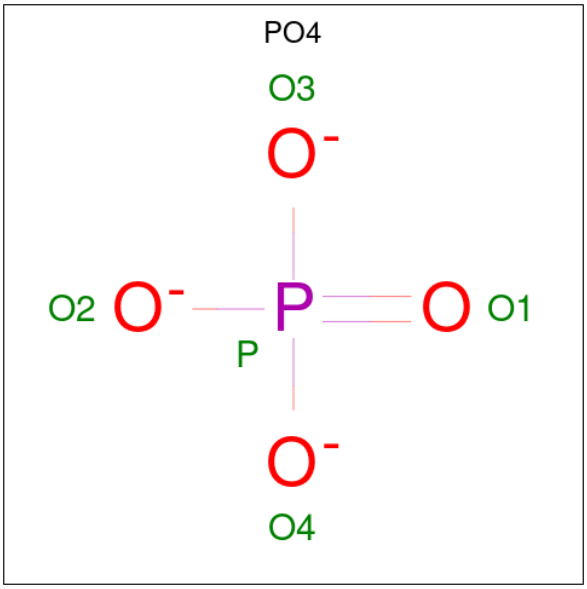
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0

- Molecule 5 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



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

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

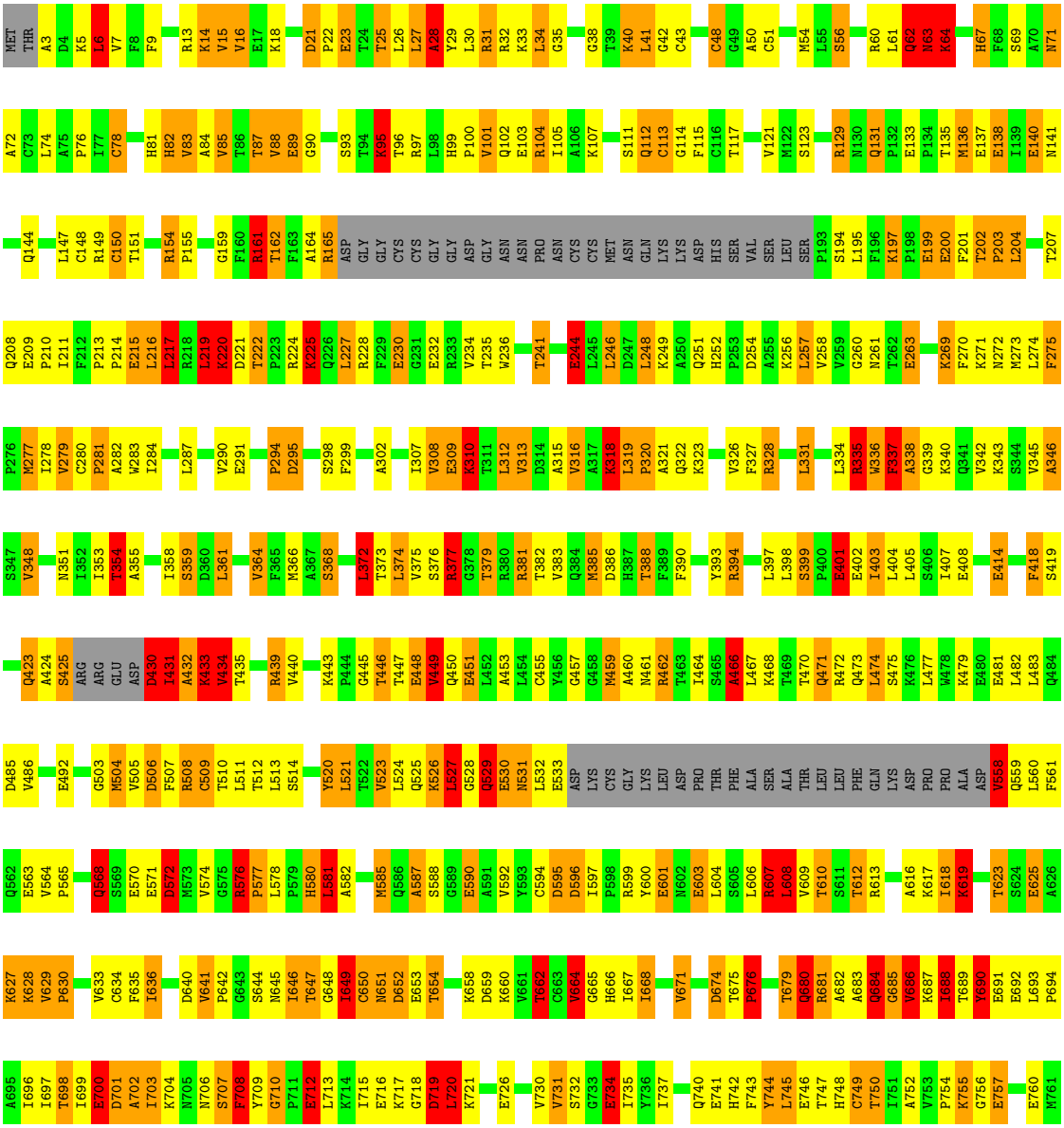
3 Residue-property plots (i)

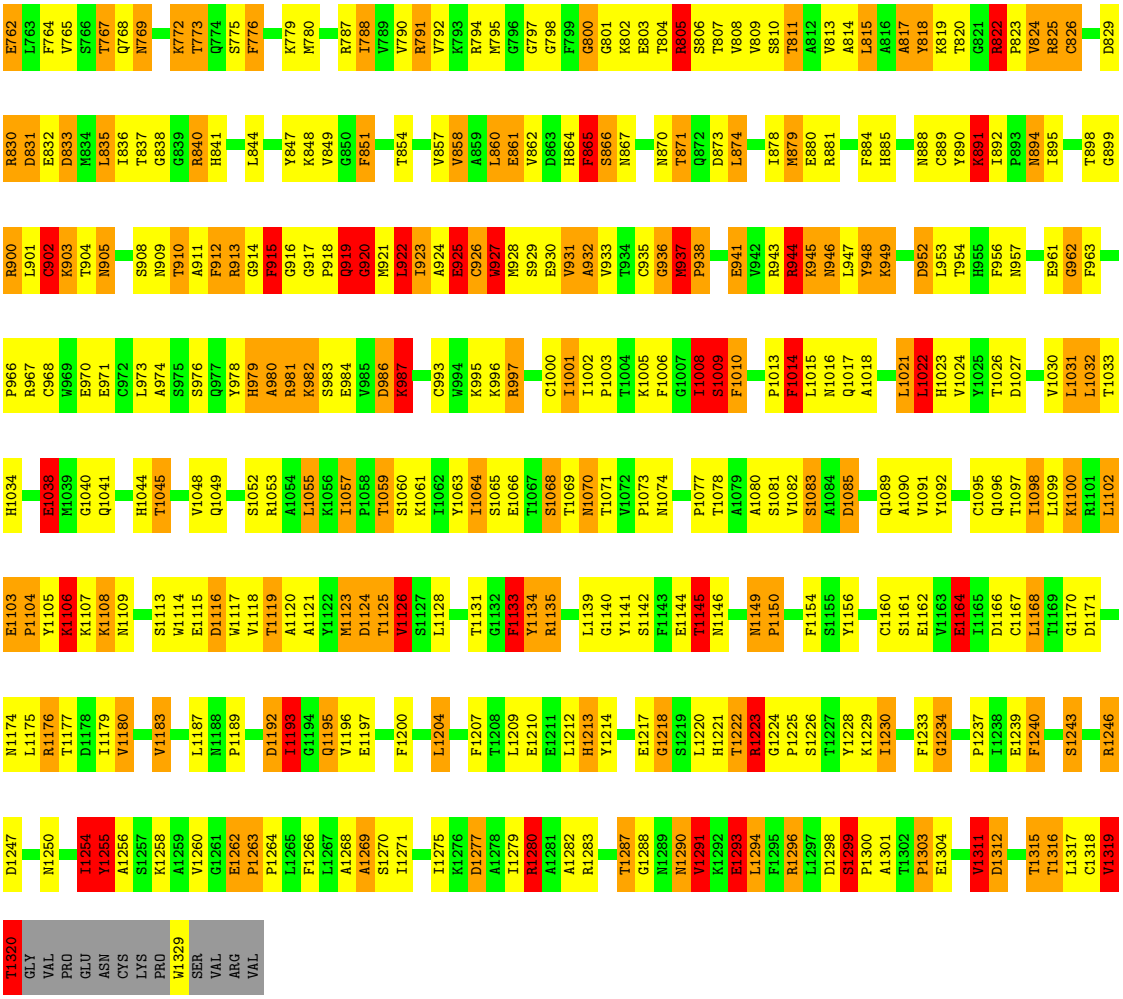
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

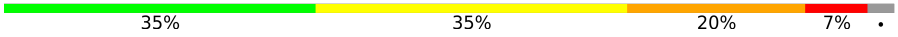
Chain A:

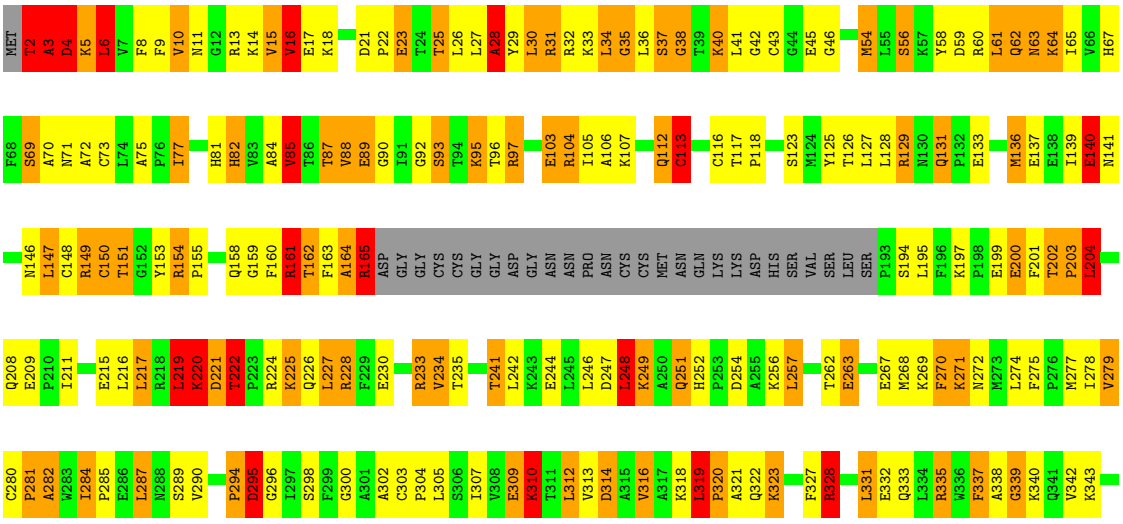


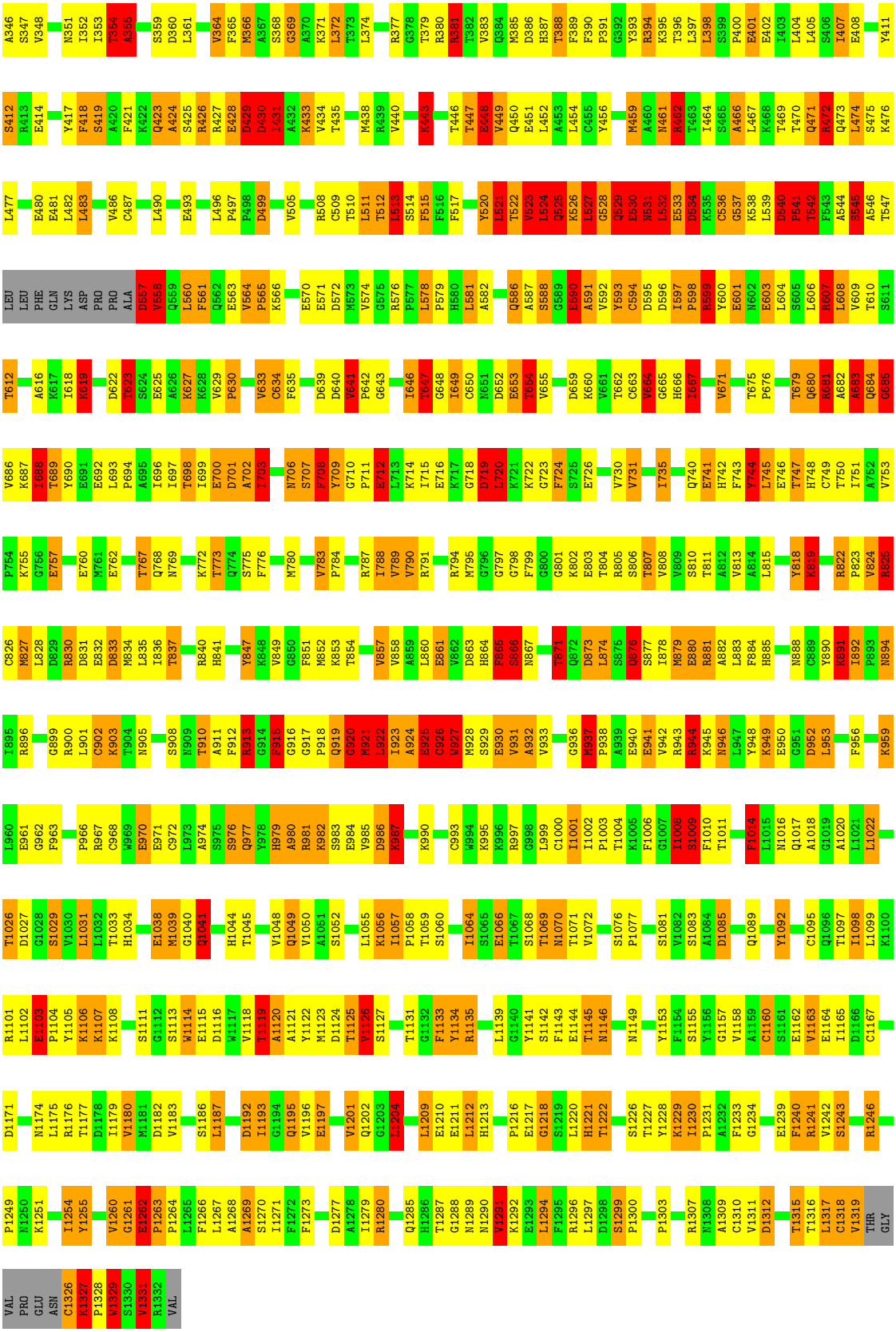


• Molecule 1: XANTHINE OXIDOREDUCTASE

Chain B:

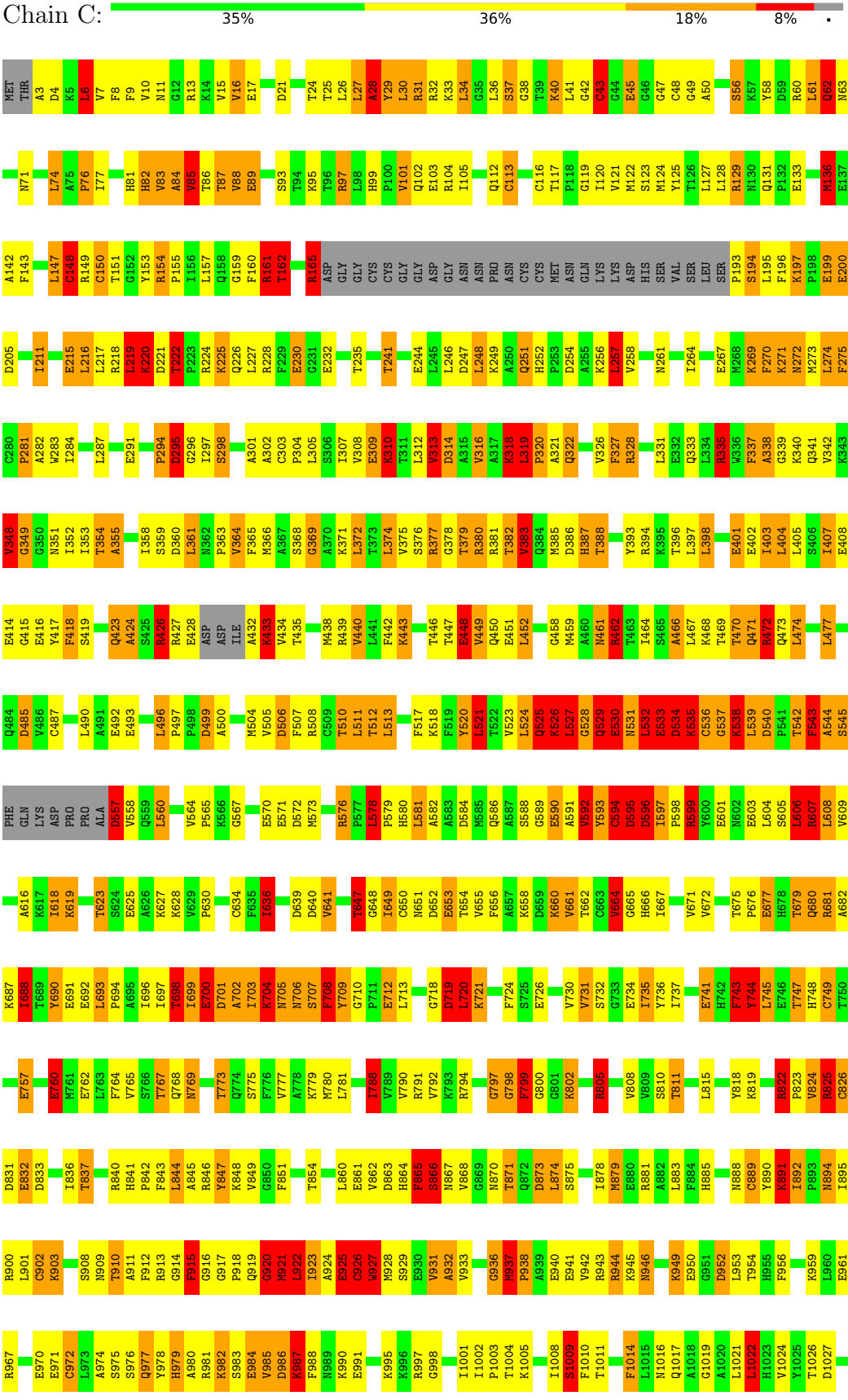


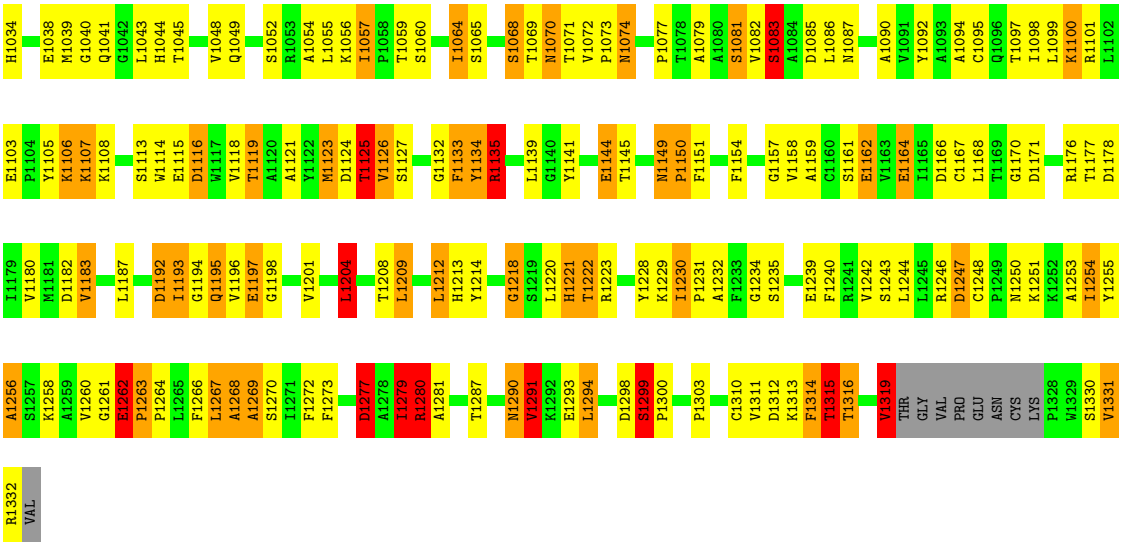




• Molecule 1: XANTHINE OXIDOREDUCTASE

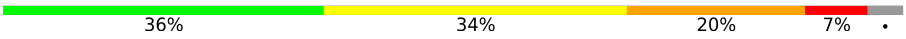
Chain C:

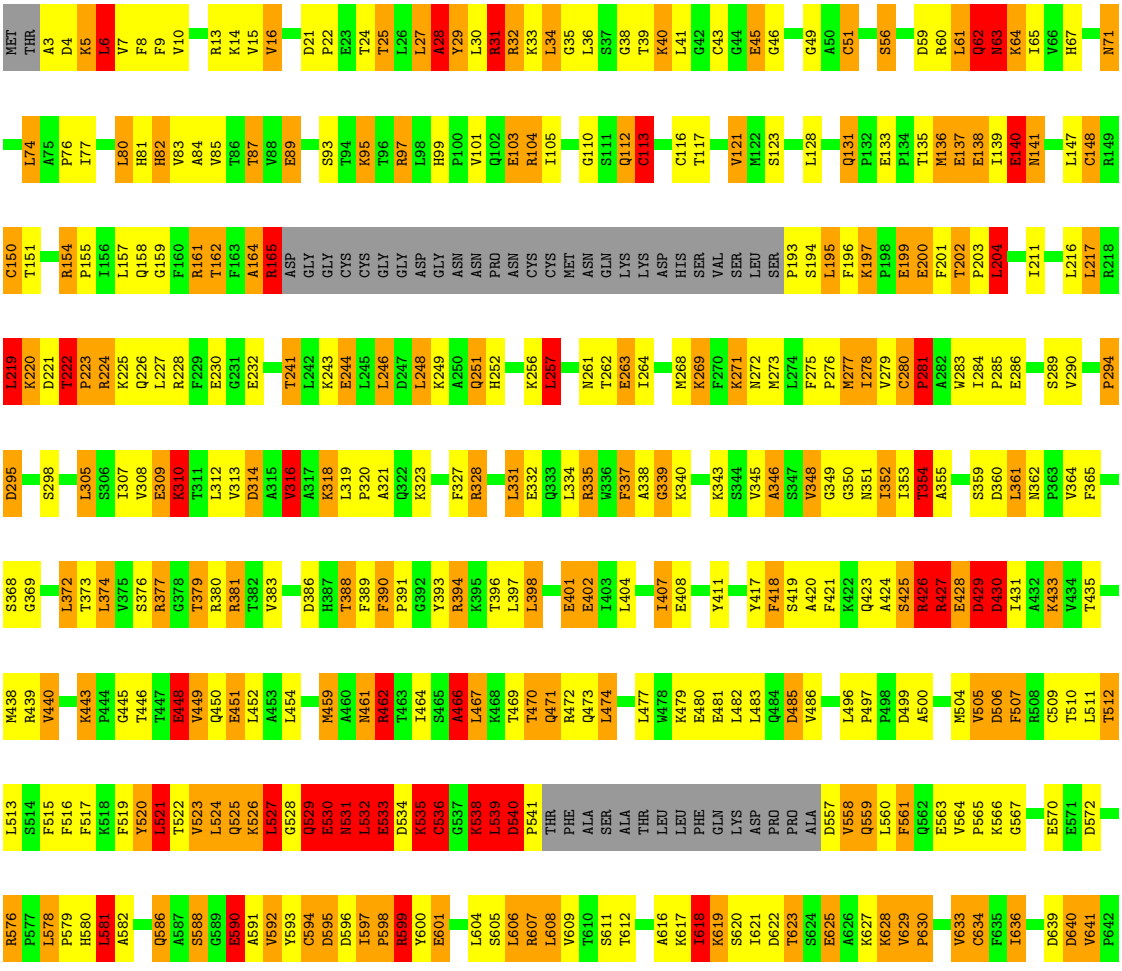


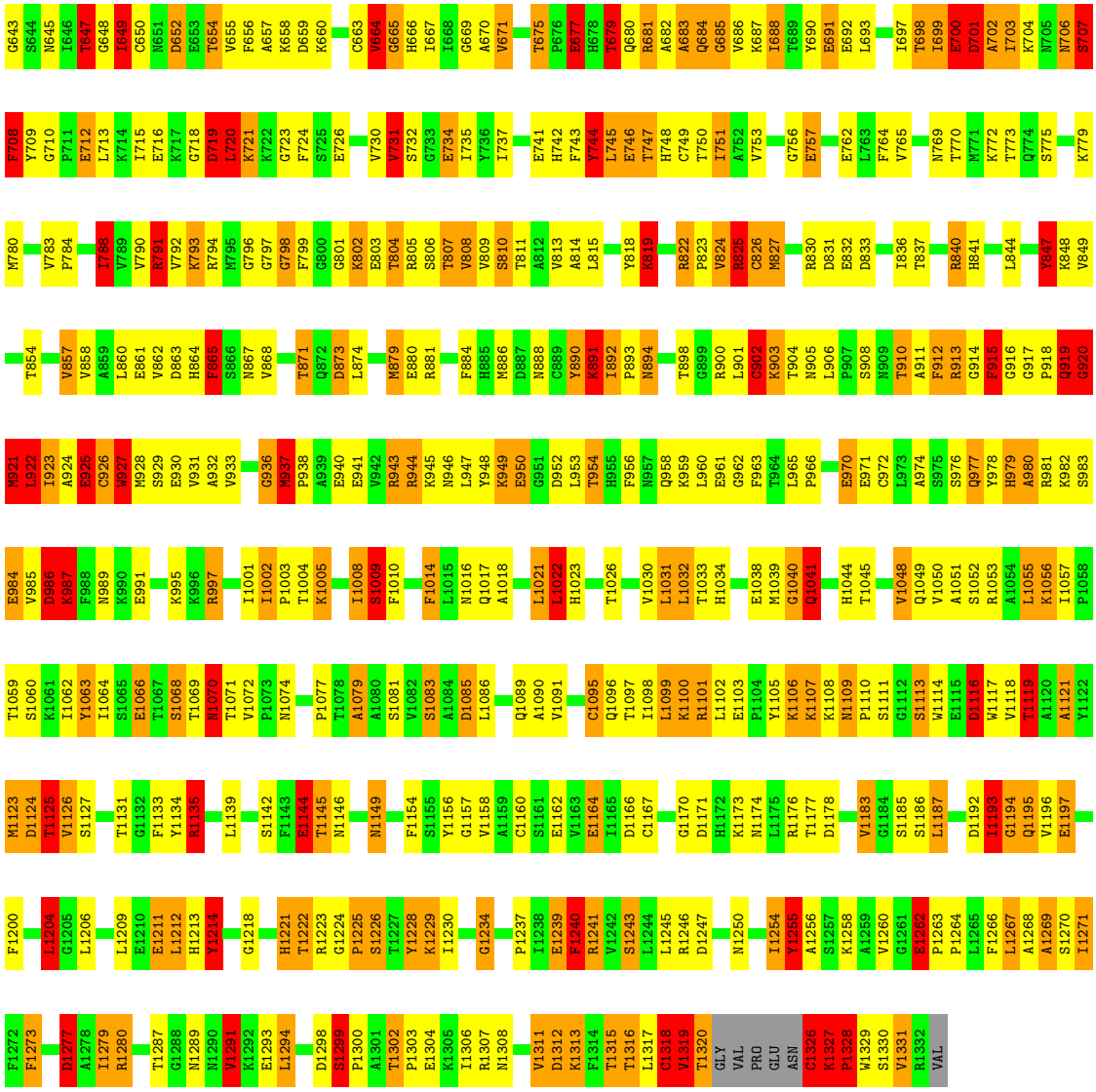


• Molecule 1: XANTHINE OXIDOREDUCTASE

Chain D:






G643 S644 N645 I646 T647 G648 I649 C650 N651 D652 E653 T654 V655 F656 A657 K658 D659 K660 C663 V664 G665 H666 I667 I668 G669 A670 V671 T675 P676 E677 H678 I679 Q680 R681 A682 A683 Q684 G685 V686 K687 I688 T689 Y690 E691 E692 L693 I697 T698 I699 E700 D701 A702 I703 K704 N705 N706 S707
F708 Y709 G710 P711 E712 L713 K714 I715 E716 K717 G718 D719 L720 K721 K722 G723 F724 S725 E726 V730 V731 S732 G733 E734 I735 Y736 I737 E741 H742 F743 Y744 L745 E746 T747 H748 C749 T750 I751 A752 V753 G756 E757 E762 L763 F764 V765 N769 T770 M771 K772 T773 Q774 S775 K779
M780 V783 P784 I788 V789 V790 R791 V792 K793 R794 M795 G796 G797 G798 F799 G800 G801 K802 E803 T804 R805 S806 T807 V808 V809 S810 T811 A812 V813 A814 L815 Y818 K819 R822 P823 V824 R825 C826 M827 R830 D831 E832 D833 I836 T837 R840 H841 L844 Y847 K848 V849
T854 V857 V858 A859 L860 E861 V862 D863 H864 F865 S866 N867 V868 T871 Q872 D873 L874 M879 E880 R881 F884 H885 M886 D887 N888 C889 Y890 K891 I892 P893 N894 T898 G899 R900 L901 C902 K903 T904 N905 L906 P907 S908 N909 T910 A911 F912 R913 G914 F915 G916 G917 P918 Q919 G920
M921 L922 I923 A924 E925 C926 W927 M928 S929 E930 V931 A932 V933 G936 M937 P938 A939 E940 E941 V942 R943 R944 K945 N946 L947 Y948 K949 E950 G951 D952 L953 T954 H955 F956 N957 Q958 K959 L960 E961 G962 F963 T964 L965 P966 E970 E971 C972 L973 A974 S975 S976 Q977 Y978 H979 A980 R981 K982 S983
E984 V985 D986 K987 F988 N989 K990 E991 K995 K996 R997 I1001 I1002 P1003 T1004 K1005 I1008 S1009 F1010 F1014 L1015 N1016 Q1017 A1018 L1021 L1022 H1023 T1026 V1030 L1031 L1032 T1033 H1034 E1038 M1039 G1040 Q1041 H1044 T1045 V1048 Q1049 V1050 A1051 S1052 R1053 A1054 L1055 K1056 I1057 P1058
T1059 S1060 K1061 I1062 Y1063 I1064 S1065 E1066 T1067 S1068 T1069 N1070 T1071 V1072 P1073 N1074 P1077 T1078 A1079 A1080 S1081 V1082 S1083 A1084 D1085 L1086 Q1089 A1090 V1091 C1095 Q1096 T1097 I1098 L1099 K1100 R1101 L1102 E1103 P1104 Y1105 K1106 K1107 K1108 N1109 P1110 S1111 G1112 S1113 W1114 E1115 D1116 W1117 V1118 T1119 A1120 A1121 Y1122
M1123 D1124 T1125 V1126 S1127 T1131 G1132 F1133 Y1134 R1135 L1139 S1142 F1143 E1144 T1145 N1146 N1149 F1154 S1155 Y1156 G1157 V1158 A1159 C1160 S1161 E1162 V1163 E1164 I1165 D1166 C1167 G1170 D1171 H1172 K1173 N1174 L1175 R1176 T1177 D1178 V1183 G1184 S1185 S1186 L1187 D1192 I1193 G1194 Q1195 V1196 E1197
F1200 L1204 G1205 L1206 L1209 E1210 E1211 L1212 H1213 Y1214 G1218 H1221 T1222 R1223 G1224 P1225 S1226 T1227 Y1228 K1229 I1230 G1234 P1237 I1238 E1239 F1240 R1241 V1242 S1243 L1244 L1245 R1246 D1247 N1250 I1254 Y1255 A1256 S1257 K1258 A1259 V1260 G1261 E1262 P1263 P1264 L1265 F1266 L1267 A1268 A1269 S1270 I1271
F1272 F1273 D1277 A1278 I1279 R1280 T1287 G1288 N1289 N1290 V1291 K1292 E1293 L1294 D1298 S1299 P1300 A1301 T1302 P1303 E1304 K1305 I1306 R1307 N1308 V1311 D1312 K1313 F1314 T1315 T1316 L1317 C1318 V1319 T1320 GLY VAL PRO GLU ASN C1326 K1327 P1328 W1329 S1330 V1331 R1332 VAL

4 Data and refinement statistics (i)

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 (i)

5.1 Standard geometry (i)

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

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	2.11	336/9969 (3.4%)	1.70	184/13492 (1.4%)
1	B	2.14	334/10160 (3.3%)	1.73	211/13751 (1.5%)
1	C	2.10	326/10113 (3.2%)	1.72	202/13685 (1.5%)
1	D	2.06	304/10118 (3.0%)	1.70	175/13693 (1.3%)
All	All	2.10	1300/40360 (3.2%)	1.71	772/54621 (1.4%)

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 (1300) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1318	CYS	CB-SG	17.07	2.11	1.82
1	A	762	GLU	CG-CD	16.49	1.76	1.51
1	A	78	CYS	CB-SG	16.00	2.09	1.82
1	B	3	ALA	N-CA	15.65	1.77	1.46
1	B	762	GLU	CD-OE1	15.23	1.42	1.25
1	D	1144	GLU	CG-CD	14.31	1.73	1.51
1	B	1162	GLU	CG-CD	13.95	1.72	1.51
1	D	1318	CYS	CB-SG	13.61	2.05	1.82
1	D	51	CYS	CB-SG	13.13	2.04	1.82
1	A	309	GLU	CG-CD	12.87	1.71	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	599	ARG	CG-CD	12.17	1.82	1.51
1	C	599	ARG	CG-CD	12.16	1.82	1.51
1	B	599	ARG	CG-CD	12.10	1.82	1.51
1	A	935	CYS	CB-SG	-12.07	1.61	1.82
1	B	393	TYR	CE1-CZ	11.97	1.54	1.38
1	B	40	LYS	CE-NZ	11.85	1.78	1.49
1	C	832	GLU	CG-CD	11.77	1.69	1.51
1	B	431	ILE	CA-CB	11.74	1.81	1.54
1	B	3	ALA	CA-CB	11.71	1.77	1.52
1	D	200	GLU	CD-OE2	11.53	1.38	1.25
1	B	1319	VAL	CA-CB	11.47	1.78	1.54
1	B	984	GLU	CG-CD	11.26	1.68	1.51
1	B	533	GLU	CG-CD	11.18	1.68	1.51
1	C	971	GLU	CD-OE1	11.10	1.37	1.25
1	D	861	GLU	CG-CD	11.00	1.68	1.51
1	A	1255	TYR	CD1-CE1	10.97	1.55	1.39
1	D	762	GLU	CD-OE2	10.91	1.37	1.25
1	A	150	CYS	CB-SG	-10.77	1.64	1.82
1	D	150	CYS	CB-SG	-10.75	1.64	1.82
1	A	971	GLU	CG-CD	10.72	1.68	1.51
1	C	1319	VAL	CA-CB	10.70	1.77	1.54
1	A	762	GLU	CD-OE1	10.52	1.37	1.25
1	B	23	GLU	CD-OE2	10.50	1.37	1.25
1	A	762	GLU	CD-OE2	10.48	1.37	1.25
1	D	927	TRP	CB-CG	-10.35	1.31	1.50
1	D	970	GLU	CG-CD	10.34	1.67	1.51
1	C	734	GLU	CG-CD	10.32	1.67	1.51
1	C	593	TYR	CB-CG	-10.28	1.36	1.51
1	A	402	GLU	CD-OE2	10.23	1.36	1.25
1	A	232	GLU	CG-CD	10.21	1.67	1.51
1	D	408	GLU	CG-CD	10.13	1.67	1.51
1	B	941	GLU	CG-CD	10.12	1.67	1.51
1	A	681	ARG	CZ-NH1	10.09	1.46	1.33
1	C	64	LYS	CD-CE	10.08	1.76	1.51
1	C	599	ARG	CB-CG	10.06	1.79	1.52
1	A	318	LYS	CD-CE	10.02	1.76	1.51
1	A	653	GLU	CG-CD	10.01	1.67	1.51
1	C	941	GLU	CG-CD	10.01	1.67	1.51
1	C	971	GLU	CG-CD	10.01	1.67	1.51
1	A	941	GLU	CG-CD	9.98	1.67	1.51
1	A	83	VAL	CB-CG1	-9.94	1.31	1.52
1	B	1310	CYS	CB-SG	-9.91	1.65	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	355	ALA	CA-CB	-9.91	1.31	1.52
1	C	1083	SER	CB-OG	9.82	1.55	1.42
1	D	200	GLU	CG-CD	9.82	1.66	1.51
1	A	971	GLU	CD-OE1	9.80	1.36	1.25
1	B	1291	VAL	CA-CB	9.80	1.75	1.54
1	C	200	GLU	CD-OE2	9.78	1.36	1.25
1	A	309	GLU	CD-OE2	9.78	1.36	1.25
1	C	29	TYR	CE1-CZ	-9.78	1.25	1.38
1	C	1291	VAL	CA-CB	9.76	1.75	1.54
1	A	1108	LYS	CD-CE	9.73	1.75	1.51
1	D	832	GLU	CD-OE2	9.71	1.36	1.25
1	B	692	GLU	CD-OE1	9.71	1.36	1.25
1	A	700	GLU	CD-OE1	9.68	1.36	1.25
1	D	1291	VAL	CA-CB	9.67	1.75	1.54
1	C	594	CYS	CB-SG	9.65	1.98	1.82
1	C	133	GLU	CD-OE2	9.64	1.36	1.25
1	C	269	LYS	CD-CE	9.64	1.75	1.51
1	D	903	LYS	CD-CE	9.49	1.75	1.51
1	C	318	LYS	CD-CE	9.48	1.75	1.51
1	C	762	GLU	CD-OE1	9.47	1.36	1.25
1	B	570	GLU	CG-CD	9.45	1.66	1.51
1	B	601	GLU	CG-CD	9.45	1.66	1.51
1	D	138	GLU	CG-CD	9.45	1.66	1.51
1	D	970	GLU	CD-OE2	9.43	1.36	1.25
1	D	762	GLU	CG-CD	9.39	1.66	1.51
1	B	1162	GLU	CD-OE2	9.36	1.35	1.25
1	A	818	TYR	CD2-CE2	9.33	1.53	1.39
1	D	762	GLU	CD-OE1	9.33	1.35	1.25
1	A	880	GLU	CG-CD	9.31	1.66	1.51
1	C	1144	GLU	CG-CD	9.30	1.66	1.51
1	D	1144	GLU	CB-CG	9.27	1.69	1.52
1	D	903	LYS	CE-NZ	9.26	1.72	1.49
1	B	533	GLU	CB-CG	9.25	1.69	1.52
1	A	984	GLU	CG-CD	9.24	1.65	1.51
1	B	401	GLU	CD-OE2	9.24	1.35	1.25
1	A	818	TYR	CD1-CE1	9.23	1.53	1.39
1	B	984	GLU	CD-OE2	9.21	1.35	1.25
1	C	1118	VAL	CB-CG1	-9.19	1.33	1.52
1	A	64	LYS	CD-CE	9.11	1.74	1.51
1	C	230	GLU	CG-CD	9.07	1.65	1.51
1	A	1108	LYS	CE-NZ	9.04	1.71	1.49
1	B	150	CYS	CB-SG	-9.03	1.66	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	903	LYS	CD-CE	9.01	1.73	1.51
1	A	451	GLU	CG-CD	9.01	1.65	1.51
1	C	28	ALA	CA-CB	8.98	1.71	1.52
1	A	1038	GLU	CD-OE1	8.96	1.35	1.25
1	B	625	GLU	CG-CD	8.95	1.65	1.51
1	D	570	GLU	CG-CD	8.95	1.65	1.51
1	A	625	GLU	CG-CD	8.94	1.65	1.51
1	B	1239	GLU	CD-OE2	8.93	1.35	1.25
1	C	625	GLU	CG-CD	8.90	1.65	1.51
1	D	332	GLU	CG-CD	8.88	1.65	1.51
1	C	402	GLU	CG-CD	8.85	1.65	1.51
1	B	593	TYR	CB-CG	-8.83	1.38	1.51
1	B	414	GLU	CG-CD	8.82	1.65	1.51
1	D	1331	VAL	CB-CG2	8.82	1.71	1.52
1	C	1239	GLU	CD-OE2	8.81	1.35	1.25
1	D	625	GLU	CG-CD	8.79	1.65	1.51
1	A	970	GLU	CG-CD	8.79	1.65	1.51
1	D	1291	VAL	CB-CG1	8.77	1.71	1.52
1	A	712	GLU	CG-CD	8.76	1.65	1.51
1	C	16	VAL	CB-CG2	-8.75	1.34	1.52
1	B	393	TYR	CD1-CE1	8.73	1.52	1.39
1	C	984	GLU	CD-OE2	8.70	1.35	1.25
1	A	903	LYS	CE-NZ	8.70	1.70	1.49
1	D	140	GLU	CG-CD	8.69	1.65	1.51
1	A	7	VAL	CB-CG2	-8.69	1.34	1.52
1	B	64	LYS	CD-CE	8.69	1.73	1.51
1	C	309	GLU	CD-OE2	8.65	1.35	1.25
1	C	601	GLU	CD-OE2	8.63	1.35	1.25
1	C	62	GLN	CG-CD	8.62	1.70	1.51
1	D	599	ARG	CB-CG	8.61	1.75	1.52
1	D	401	GLU	CB-CG	8.61	1.68	1.52
1	B	393	TYR	CD2-CE2	8.59	1.52	1.39
1	A	749	CYS	CB-SG	-8.58	1.67	1.82
1	D	832	GLU	CG-CD	8.54	1.64	1.51
1	B	789	VAL	CB-CG2	-8.53	1.34	1.52
1	B	1153	TYR	CD2-CE2	8.53	1.52	1.39
1	C	1162	GLU	CG-CD	8.52	1.64	1.51
1	C	1331	VAL	CA-CB	8.52	1.72	1.54
1	D	940	GLU	CG-CD	8.52	1.64	1.51
1	C	903	LYS	CE-NZ	8.50	1.70	1.49
1	A	617	LYS	CD-CE	8.50	1.72	1.51
1	D	971	GLU	CD-OE2	8.48	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	819	LYS	CD-CE	8.48	1.72	1.51
1	C	601	GLU	CD-OE1	8.45	1.34	1.25
1	A	1291	VAL	CA-CB	8.44	1.72	1.54
1	A	832	GLU	CG-CD	8.42	1.64	1.51
1	D	64	LYS	CD-CE	8.42	1.72	1.51
1	A	971	GLU	CD-OE2	8.38	1.34	1.25
1	A	336	TRP	CE3-CZ3	8.38	1.52	1.38
1	C	889	CYS	CB-SG	-8.38	1.68	1.82
1	D	448	GLU	CD-OE2	8.38	1.34	1.25
1	C	832	GLU	CD-OE2	8.37	1.34	1.25
1	B	481	GLU	CG-CD	8.36	1.64	1.51
1	C	140	GLU	CG-CD	8.35	1.64	1.51
1	A	7	VAL	CB-CG1	-8.35	1.35	1.52
1	C	133	GLU	CG-CD	8.34	1.64	1.51
1	B	712	GLU	CG-CD	8.33	1.64	1.51
1	D	280	CYS	CB-SG	-8.33	1.68	1.82
1	B	103	GLU	CD-OE1	8.32	1.34	1.25
1	C	33	LYS	CD-CE	8.30	1.72	1.51
1	A	283	TRP	CG-CD1	-8.28	1.25	1.36
1	C	971	GLU	CD-OE2	8.27	1.34	1.25
1	A	1162	GLU	CG-CD	8.26	1.64	1.51
1	A	133	GLU	CG-CD	8.25	1.64	1.51
1	D	941	GLU	CG-CD	8.24	1.64	1.51
1	C	1272	PHE	CD1-CE1	8.23	1.55	1.39
1	B	530	GLU	CG-CD	8.21	1.64	1.51
1	C	499	ASP	CB-CG	8.19	1.69	1.51
1	D	332	GLU	CB-CG	8.19	1.67	1.52
1	A	309	GLU	CD-OE1	8.16	1.34	1.25
1	C	408	GLU	CG-CD	8.15	1.64	1.51
1	B	741	GLU	CD-OE1	8.15	1.34	1.25
1	A	215	GLU	CD-OE1	8.14	1.34	1.25
1	A	269	LYS	CD-CE	8.14	1.71	1.51
1	A	915	PHE	CE1-CZ	8.13	1.52	1.37
1	D	712	GLU	CD-OE1	8.09	1.34	1.25
1	A	558	VAL	CB-CG1	8.06	1.69	1.52
1	A	803	GLU	CG-CD	8.05	1.64	1.51
1	A	1164	GLU	CG-CD	8.02	1.64	1.51
1	B	332	GLU	CG-CD	8.02	1.64	1.51
1	D	1063	TYR	CD1-CE1	8.01	1.51	1.39
1	C	140	GLU	CB-CG	8.00	1.67	1.52
1	D	310	LYS	CD-CE	8.00	1.71	1.51
1	B	113	CYS	CB-SG	-7.97	1.68	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	393	TYR	CG-CD2	7.97	1.49	1.39
1	B	1072	VAL	CB-CG1	7.96	1.69	1.52
1	D	133	GLU	CG-CD	7.94	1.63	1.51
1	D	1214	TYR	CD1-CE1	7.94	1.51	1.39
1	A	346	ALA	CA-CB	-7.93	1.35	1.52
1	D	1291	VAL	CB-CG2	7.92	1.69	1.52
1	A	318	LYS	CB-CG	7.92	1.74	1.52
1	D	961	GLU	CD-OE2	7.91	1.34	1.25
1	B	915	PHE	CE2-CZ	7.91	1.52	1.37
1	C	861	GLU	CD-OE1	7.90	1.34	1.25
1	A	653	GLU	CD-OE1	7.89	1.34	1.25
1	A	968	CYS	CB-SG	7.89	1.95	1.82
1	B	1262	GLU	CG-CD	7.87	1.63	1.51
1	D	408	GLU	CB-CG	7.87	1.67	1.52
1	A	40	LYS	CD-CE	7.86	1.71	1.51
1	B	940	GLU	CG-CD	7.86	1.63	1.51
1	A	432	ALA	CA-CB	7.86	1.69	1.52
1	C	805	ARG	CZ-NH2	7.86	1.43	1.33
1	D	1262	GLU	CD-OE2	7.85	1.34	1.25
1	C	1144	GLU	CB-CG	7.85	1.67	1.52
1	C	1239	GLU	CD-OE1	7.85	1.34	1.25
1	D	734	GLU	CG-CD	7.84	1.63	1.51
1	C	492	GLU	CG-CD	7.83	1.63	1.51
1	B	601	GLU	CD-OE2	7.83	1.34	1.25
1	A	408	GLU	CD-OE2	7.82	1.34	1.25
1	C	1154	PHE	CE1-CZ	7.82	1.52	1.37
1	D	1144	GLU	CD-OE2	7.81	1.34	1.25
1	A	16	VAL	CB-CG2	-7.80	1.36	1.52
1	A	1018	ALA	CA-CB	7.77	1.68	1.52
1	C	309	GLU	CD-OE1	7.76	1.34	1.25
1	A	619	LYS	CD-CE	7.76	1.70	1.51
1	B	762	GLU	CG-CD	7.76	1.63	1.51
1	D	1038	GLU	CD-OE1	7.76	1.34	1.25
1	D	269	LYS	CE-NZ	7.75	1.68	1.49
1	C	205	ASP	CB-CG	-7.75	1.35	1.51
1	B	448	GLU	CG-CD	7.74	1.63	1.51
1	B	481	GLU	CB-CG	7.74	1.66	1.52
1	C	485	ASP	CB-CG	7.74	1.68	1.51
1	A	1083	SER	CB-OG	7.74	1.52	1.42
1	B	968	CYS	CB-SG	-7.73	1.69	1.82
1	B	762	GLU	CD-OE2	7.73	1.34	1.25
1	D	915	PHE	CG-CD2	7.73	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	417	TYR	CD1-CE1	7.71	1.50	1.39
1	C	13	ARG	NE-CZ	7.71	1.43	1.33
1	C	749	CYS	CB-SG	-7.70	1.69	1.82
1	C	232	GLU	CG-CD	7.70	1.63	1.51
1	D	200	GLU	CD-OE1	7.69	1.34	1.25
1	A	752	ALA	CA-CB	-7.69	1.36	1.52
1	B	818	TYR	CD1-CE1	7.68	1.50	1.39
1	A	161	ARG	CG-CD	7.68	1.71	1.51
1	D	269	LYS	CD-CE	7.67	1.70	1.51
1	C	279	VAL	CB-CG1	-7.67	1.36	1.52
1	A	343	LYS	CD-CE	7.66	1.70	1.51
1	D	961	GLU	CD-OE1	7.65	1.34	1.25
1	A	200	GLU	CB-CG	7.63	1.66	1.52
1	A	1319	VAL	CA-CB	7.62	1.70	1.54
1	A	700	GLU	CG-CD	7.61	1.63	1.51
1	B	726	GLU	CG-CD	7.61	1.63	1.51
1	B	13	ARG	CG-CD	7.60	1.71	1.51
1	B	75	ALA	CA-CB	-7.59	1.36	1.52
1	B	599	ARG	CB-CG	7.59	1.73	1.52
1	B	23	GLU	CD-OE1	7.59	1.33	1.25
1	A	792	VAL	CB-CG1	-7.57	1.36	1.52
1	C	593	TYR	CG-CD1	-7.57	1.29	1.39
1	B	1197	GLU	CG-CD	7.57	1.63	1.51
1	B	408	GLU	CG-CD	7.56	1.63	1.51
1	B	825	ARG	CZ-NH2	7.56	1.42	1.33
1	A	903	LYS	CD-CE	7.56	1.70	1.51
1	B	970	GLU	CG-CD	7.56	1.63	1.51
1	B	571	GLU	CG-CD	7.55	1.63	1.51
1	D	1162	GLU	CG-CD	7.55	1.63	1.51
1	D	944	ARG	CB-CG	7.54	1.73	1.52
1	A	570	GLU	CG-CD	7.54	1.63	1.51
1	B	891	LYS	CD-CE	7.54	1.70	1.51
1	D	1135	ARG	NE-CZ	7.53	1.42	1.33
1	A	340	LYS	CD-CE	7.53	1.70	1.51
1	B	309	GLU	CD-OE2	7.51	1.33	1.25
1	C	13	ARG	CG-CD	7.50	1.70	1.51
1	A	961	GLU	CD-OE1	7.49	1.33	1.25
1	A	1134	TYR	CD1-CE1	7.47	1.50	1.39
1	D	505	VAL	CB-CG2	7.47	1.68	1.52
1	C	448	GLU	CB-CG	7.44	1.66	1.52
1	B	1229	LYS	CD-CE	7.44	1.69	1.51
1	C	769	ASN	C-O	7.43	1.37	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	597	ILE	CB-CG2	-7.42	1.29	1.52
1	A	54	MET	CG-SD	7.41	2.00	1.81
1	B	865	PHE	CD1-CE1	7.40	1.54	1.39
1	B	783	VAL	CB-CG2	-7.39	1.37	1.52
1	B	1211	GLU	CG-CD	7.39	1.63	1.51
1	A	818	TYR	CE1-CZ	7.38	1.48	1.38
1	B	267	GLU	CD-OE1	7.38	1.33	1.25
1	D	16	VAL	CB-CG2	-7.38	1.37	1.52
1	C	254	ASP	CB-CG	7.36	1.67	1.51
1	A	318	LYS	CG-CD	7.36	1.77	1.52
1	C	799	PHE	CD1-CE1	-7.36	1.24	1.39
1	A	746	GLU	CG-CD	7.35	1.62	1.51
1	A	660	LYS	CD-CE	7.35	1.69	1.51
1	D	133	GLU	CD-OE1	7.35	1.33	1.25
1	C	688	ILE	N-CA	7.35	1.61	1.46
1	A	492	GLU	CD-OE2	7.34	1.33	1.25
1	A	1319	VAL	CB-CG2	7.33	1.68	1.52
1	D	1173	LYS	CD-CE	7.33	1.69	1.51
1	D	861	GLU	CD-OE2	7.33	1.33	1.25
1	B	1103	GLU	CD-OE1	7.33	1.33	1.25
1	D	393	TYR	CE2-CZ	7.32	1.48	1.38
1	D	10	VAL	CB-CG2	-7.32	1.37	1.52
1	A	776	PHE	CB-CG	-7.31	1.39	1.51
1	A	927	TRP	CB-CG	-7.31	1.37	1.50
1	D	832	GLU	CB-CG	7.30	1.66	1.52
1	A	402	GLU	CG-CD	7.30	1.62	1.51
1	B	971	GLU	CD-OE1	7.29	1.33	1.25
1	A	1156	TYR	CE2-CZ	7.28	1.48	1.38
1	C	1164	GLU	CG-CD	7.28	1.62	1.51
1	B	103	GLU	CG-CD	7.27	1.62	1.51
1	C	1290	ASN	CB-CG	7.27	1.67	1.51
1	B	414	GLU	CB-CG	7.27	1.66	1.52
1	B	200	GLU	CD-OE1	7.27	1.33	1.25
1	A	62	GLN	CG-CD	7.26	1.67	1.51
1	A	1301	ALA	CA-CB	-7.25	1.37	1.52
1	B	267	GLU	CG-CD	7.25	1.62	1.51
1	B	671	VAL	CB-CG1	-7.25	1.37	1.52
1	A	95	LYS	CD-CE	7.24	1.69	1.51
1	C	609	VAL	CB-CG1	-7.24	1.37	1.52
1	A	138	GLU	CG-CD	7.23	1.62	1.51
1	B	140	GLU	CB-CG	7.23	1.65	1.52
1	D	1108	LYS	CD-CE	7.22	1.69	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	342	VAL	CB-CG2	-7.21	1.37	1.52
1	C	593	TYR	CG-CD2	-7.21	1.29	1.39
1	D	629	VAL	CB-CG1	-7.20	1.37	1.52
1	C	1239	GLU	CG-CD	7.20	1.62	1.51
1	B	279	VAL	CB-CG2	-7.19	1.37	1.52
1	A	310	LYS	CE-NZ	7.18	1.67	1.49
1	D	318	LYS	CD-CE	7.18	1.69	1.51
1	A	563	GLU	CG-CD	7.18	1.62	1.51
1	C	625	GLU	CD-OE1	7.18	1.33	1.25
1	A	200	GLU	CD-OE2	7.17	1.33	1.25
1	C	1319	VAL	CB-CG1	7.17	1.68	1.52
1	D	557	ASP	CB-CG	7.17	1.66	1.51
1	B	133	GLU	CD-OE1	7.16	1.33	1.25
1	D	617	LYS	CD-CE	7.15	1.69	1.51
1	D	408	GLU	CD-OE1	7.14	1.33	1.25
1	C	21	ASP	CB-CG	7.14	1.66	1.51
1	C	50	ALA	CA-CB	-7.14	1.37	1.52
1	C	762	GLU	CG-CD	7.14	1.62	1.51
1	D	1320	THR	CA-CB	7.14	1.72	1.53
1	B	1018	ALA	CA-CB	7.13	1.67	1.52
1	B	660	LYS	CD-CE	7.13	1.69	1.51
1	D	944	ARG	CG-CD	7.12	1.69	1.51
1	C	597	ILE	CB-CG2	-7.11	1.30	1.52
1	A	762	GLU	CB-CG	7.11	1.65	1.52
1	B	930	GLU	CD-OE2	7.11	1.33	1.25
1	B	1331	VAL	CA-CB	7.11	1.69	1.54
1	A	811	THR	CB-CG2	7.11	1.75	1.52
1	D	681	ARG	CZ-NH1	7.11	1.42	1.33
1	C	13	ARG	CD-NE	7.09	1.58	1.46
1	A	107	LYS	CD-CE	7.07	1.69	1.51
1	C	13	ARG	CZ-NH1	7.07	1.42	1.33
1	C	16	VAL	CB-CG1	-7.07	1.38	1.52
1	D	140	GLU	CB-CG	7.07	1.65	1.52
1	D	808	VAL	CB-CG2	-7.06	1.38	1.52
1	C	687	LYS	CD-CE	7.06	1.69	1.51
1	B	17	GLU	CG-CD	-7.06	1.41	1.51
1	B	309	GLU	CG-CD	7.05	1.62	1.51
1	A	716	GLU	CG-CD	7.04	1.62	1.51
1	A	603	GLU	CD-OE1	7.04	1.33	1.25
1	D	40	LYS	CB-CG	7.04	1.71	1.52
1	D	393	TYR	CD2-CE2	7.02	1.49	1.39
1	C	1082	VAL	CA-CB	-7.02	1.40	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	824	VAL	CB-CG2	-7.01	1.38	1.52
1	D	506	ASP	CB-CG	7.01	1.66	1.51
1	B	726	GLU	CB-CG	7.01	1.65	1.52
1	A	1255	TYR	CD2-CE2	7.00	1.49	1.39
1	D	1072	VAL	CA-CB	-6.99	1.40	1.54
1	D	393	TYR	CD1-CE1	6.99	1.49	1.39
1	B	2	THR	CA-C	6.99	1.71	1.52
1	B	832	GLU	CD-OE1	6.98	1.33	1.25
1	D	915	PHE	CE1-CZ	6.98	1.50	1.37
1	A	691	GLU	CB-CG	6.98	1.65	1.52
1	C	200	GLU	CG-CD	6.97	1.62	1.51
1	C	15	VAL	CB-CG2	-6.97	1.38	1.52
1	B	393	TYR	CB-CG	6.94	1.62	1.51
1	B	961	GLU	CB-CG	6.94	1.65	1.52
1	C	42	GLY	N-CA	6.92	1.56	1.46
1	C	570	GLU	CB-CG	6.92	1.65	1.52
1	D	103	GLU	CD-OE2	6.91	1.33	1.25
1	A	23	GLU	CD-OE2	6.91	1.33	1.25
1	C	433	LYS	CE-NZ	6.91	1.66	1.49
1	A	481	GLU	CD-OE2	6.90	1.33	1.25
1	D	140	GLU	CD-OE2	6.90	1.33	1.25
1	A	343	LYS	CE-NZ	6.90	1.66	1.49
1	D	675	THR	CA-CB	6.90	1.71	1.53
1	B	200	GLU	CD-OE2	6.89	1.33	1.25
1	B	1014	PHE	CD2-CE2	6.88	1.53	1.39
1	D	165	ARG	N-CA	6.88	1.60	1.46
1	A	335	ARG	CG-CD	6.88	1.69	1.51
1	A	137	GLU	CG-CD	6.87	1.62	1.51
1	C	1331	VAL	CA-C	6.87	1.70	1.52
1	A	803	GLU	CD-OE2	6.87	1.33	1.25
1	C	1310	CYS	CB-SG	-6.86	1.70	1.82
1	A	336	TRP	CE2-CZ2	6.86	1.51	1.39
1	C	88	VAL	CB-CG1	-6.86	1.38	1.52
1	A	600	TYR	CD1-CE1	-6.85	1.29	1.39
1	B	915	PHE	CE1-CZ	6.85	1.50	1.37
1	C	291	GLU	CG-CD	6.85	1.62	1.51
1	A	112	GLN	CG-CD	6.84	1.66	1.51
1	B	1163	VAL	CB-CG1	-6.83	1.38	1.52
1	D	1240	PHE	CB-CG	6.83	1.62	1.51
1	A	1312	ASP	CB-CG	6.82	1.66	1.51
1	C	972	CYS	CB-SG	6.82	1.93	1.82
1	D	978	TYR	CD2-CE2	6.82	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1090	ALA	CA-CB	-6.82	1.38	1.52
1	D	10	VAL	CA-CB	-6.82	1.40	1.54
1	B	593	TYR	CD1-CE1	6.80	1.49	1.39
1	A	408	GLU	CD-OE1	6.80	1.33	1.25
1	A	481	GLU	CG-CD	6.79	1.62	1.51
1	B	225	LYS	CD-CE	6.79	1.68	1.51
1	D	137	GLU	CD-OE1	6.79	1.33	1.25
1	C	40	LYS	CE-NZ	6.78	1.66	1.49
1	B	1126	VAL	CB-CG1	6.78	1.67	1.52
1	B	757	GLU	CB-CG	6.78	1.65	1.52
1	C	536	CYS	CB-SG	-6.77	1.70	1.82
1	B	451	GLU	CB-CG	6.75	1.65	1.52
1	A	1229	LYS	CE-NZ	6.75	1.66	1.49
1	B	1115	GLU	CD-OE1	6.74	1.33	1.25
1	A	200	GLU	CG-CD	6.74	1.62	1.51
1	D	726	GLU	CG-CD	6.74	1.62	1.51
1	B	2	THR	CA-CB	6.73	1.70	1.53
1	B	254	ASP	CB-CG	6.73	1.65	1.51
1	B	36	LEU	C-O	6.73	1.36	1.23
1	A	258	VAL	CA-CB	-6.72	1.40	1.54
1	D	570	GLU	CD-OE2	6.72	1.33	1.25
1	D	1109	ASN	CB-CG	6.72	1.66	1.51
1	B	570	GLU	CD-OE2	6.71	1.33	1.25
1	B	599	ARG	CD-NE	6.71	1.57	1.46
1	C	625	GLU	CB-CG	6.71	1.65	1.52
1	B	328	ARG	CG-CD	6.71	1.68	1.51
1	C	570	GLU	CD-OE2	6.71	1.33	1.25
1	A	558	VAL	CB-CG2	6.71	1.67	1.52
1	A	401	GLU	CG-CD	6.70	1.61	1.51
1	A	1134	TYR	CD2-CE2	6.69	1.49	1.39
1	C	364	VAL	CA-CB	-6.68	1.40	1.54
1	B	708	PHE	CB-CG	6.68	1.62	1.51
1	A	1171	ASP	CB-CG	6.68	1.65	1.51
1	C	348	VAL	CB-CG1	-6.68	1.38	1.52
1	B	971	GLU	CD-OE2	6.67	1.32	1.25
1	D	32	ARG	CG-CD	6.67	1.68	1.51
1	B	588	SER	CB-OG	6.67	1.50	1.42
1	C	726	GLU	CG-CD	6.67	1.61	1.51
1	D	1197	GLU	CD-OE1	6.67	1.32	1.25
1	B	681	ARG	CZ-NH1	6.66	1.41	1.33
1	C	97	ARG	CG-CD	6.66	1.68	1.51
1	D	411	TYR	CD2-CE2	6.65	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	653	GLU	CG-CD	6.65	1.61	1.51
1	B	1134	TYR	CG-CD1	-6.65	1.30	1.39
1	C	525	GLN	CB-CG	6.64	1.70	1.52
1	C	891	LYS	CD-CE	6.64	1.67	1.51
1	B	401	GLU	CG-CD	6.64	1.61	1.51
1	B	140	GLU	CD-OE1	6.64	1.32	1.25
1	D	1255	TYR	CE1-CZ	-6.64	1.29	1.38
1	C	165	ARG	CZ-NH2	6.64	1.41	1.33
1	B	1192	ASP	CB-CG	6.63	1.65	1.51
1	A	688	ILE	N-CA	6.63	1.59	1.46
1	C	427	ARG	CG-CD	6.62	1.68	1.51
1	D	629	VAL	CB-CG2	-6.62	1.39	1.52
1	A	451	GLU	CD-OE2	6.60	1.32	1.25
1	C	309	GLU	CG-CD	6.60	1.61	1.51
1	B	653	GLU	CG-CD	6.60	1.61	1.51
1	B	408	GLU	CD-OE1	6.59	1.32	1.25
1	C	961	GLU	CG-CD	6.59	1.61	1.51
1	D	1162	GLU	CB-CG	6.59	1.64	1.52
1	B	1239	GLU	CD-OE1	6.58	1.32	1.25
1	B	1038	GLU	CD-OE1	6.58	1.32	1.25
1	A	28	ALA	CA-CB	6.58	1.66	1.52
1	C	272	ASN	CB-CG	6.57	1.66	1.51
1	C	744	TYR	CE2-CZ	6.57	1.47	1.38
1	C	1038	GLU	CG-CD	6.56	1.61	1.51
1	C	1272	PHE	CB-CG	-6.56	1.40	1.51
1	C	779	LYS	CD-CE	6.56	1.67	1.51
1	D	433	LYS	CE-NZ	6.56	1.65	1.49
1	B	783	VAL	CB-CG1	-6.55	1.39	1.52
1	D	535	LYS	CB-CG	6.54	1.70	1.52
1	B	230	GLU	CD-OE1	6.54	1.32	1.25
1	A	291	GLU	CG-CD	6.53	1.61	1.51
1	C	1180	VAL	CA-CB	-6.53	1.41	1.54
1	B	263	GLU	CD-OE2	6.53	1.32	1.25
1	B	971	GLU	CG-CD	6.53	1.61	1.51
1	B	789	VAL	CA-CB	-6.52	1.41	1.54
1	A	817	ALA	CA-CB	-6.52	1.38	1.52
1	A	95	LYS	CE-NZ	6.52	1.65	1.49
1	D	430	ASP	CB-CG	6.51	1.65	1.51
1	C	1092	TYR	CD2-CE2	6.51	1.49	1.39
1	C	345	VAL	CB-CG1	-6.50	1.39	1.52
1	C	45	GLU	CB-CG	-6.50	1.39	1.52
1	D	793	LYS	CG-CD	6.50	1.74	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	655	VAL	CB-CG1	-6.50	1.39	1.52
1	D	712	GLU	CG-CD	6.49	1.61	1.51
1	B	342	VAL	CB-CG2	-6.49	1.39	1.52
1	B	1049	GLN	C-O	6.49	1.35	1.23
1	C	641	VAL	CB-CG1	-6.49	1.39	1.52
1	D	1063	TYR	CD2-CE2	6.49	1.49	1.39
1	D	33	LYS	CB-CG	6.48	1.70	1.52
1	A	279	VAL	CB-CG2	-6.48	1.39	1.52
1	C	103	GLU	CB-CG	6.48	1.64	1.52
1	B	480	GLU	CG-CD	6.47	1.61	1.51
1	B	819	LYS	CD-CE	6.46	1.67	1.51
1	D	1326	CYS	CB-SG	6.46	1.93	1.82
1	D	140	GLU	CD-OE1	6.46	1.32	1.25
1	D	138	GLU	CB-CG	6.46	1.64	1.52
1	B	417	TYR	CD1-CE1	6.45	1.49	1.39
1	D	984	GLU	CD-OE2	6.45	1.32	1.25
1	A	1120	ALA	CA-CB	-6.45	1.39	1.52
1	B	1171	ASP	CB-CG	6.45	1.65	1.51
1	D	309	GLU	CD-OE2	6.44	1.32	1.25
1	C	427	ARG	CB-CG	6.44	1.70	1.52
1	A	1193	ILE	CA-CB	6.43	1.69	1.54
1	C	818	TYR	CE1-CZ	6.43	1.47	1.38
1	A	16	VAL	CA-CB	-6.42	1.41	1.54
1	C	267	GLU	CD-OE1	6.42	1.32	1.25
1	C	712	GLU	CB-CG	6.42	1.64	1.52
1	C	408	GLU	CB-CG	6.42	1.64	1.52
1	B	1291	VAL	CB-CG1	6.42	1.66	1.52
1	A	140	GLU	CD-OE1	6.41	1.32	1.25
1	C	818	TYR	CD2-CE2	6.41	1.49	1.39
1	A	161	ARG	CB-CG	6.41	1.69	1.52
1	A	230	GLU	CD-OE2	6.41	1.32	1.25
1	A	533	GLU	N-CA	6.41	1.59	1.46
1	D	579	PRO	C-O	6.40	1.36	1.23
1	A	103	GLU	CG-CD	6.40	1.61	1.51
1	C	401	GLU	CG-CD	6.40	1.61	1.51
1	C	636	ILE	CA-CB	6.39	1.69	1.54
1	A	1162	GLU	CD-OE2	6.39	1.32	1.25
1	D	223	PRO	N-CA	6.39	1.58	1.47
1	A	1319	VAL	N-CA	6.39	1.59	1.46
1	C	58	TYR	CE1-CZ	-6.38	1.30	1.38
1	D	533	GLU	CB-CG	6.38	1.64	1.52
1	C	1251	LYS	CD-CE	6.38	1.67	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	880	GLU	CG-CD	6.38	1.61	1.51
1	C	83	VAL	CB-CG1	-6.37	1.39	1.52
1	D	340	LYS	CE-NZ	6.37	1.65	1.49
1	D	1083	SER	CA-C	6.37	1.69	1.52
1	C	811	THR	CB-CG2	6.37	1.73	1.52
1	B	10	VAL	CB-CG2	-6.37	1.39	1.52
1	B	21	ASP	CB-CG	6.37	1.65	1.51
1	A	530	GLU	CB-CG	6.37	1.64	1.52
1	D	230	GLU	CD-OE1	6.37	1.32	1.25
1	B	72	ALA	CA-CB	-6.36	1.39	1.52
1	C	557	ASP	CB-CG	6.35	1.65	1.51
1	D	310	LYS	CE-NZ	6.35	1.65	1.49
1	D	930	GLU	CG-CD	6.35	1.61	1.51
1	D	840	ARG	C-O	6.35	1.35	1.23
1	A	719	ASP	CB-CG	6.33	1.65	1.51
1	B	619	LYS	CB-CG	6.33	1.69	1.52
1	C	1208	THR	C-O	6.33	1.35	1.23
1	A	21	ASP	CB-CG	6.33	1.65	1.51
1	C	941	GLU	CD-OE1	6.33	1.32	1.25
1	D	971	GLU	CG-CD	6.33	1.61	1.51
1	A	199	GLU	CB-CG	6.32	1.64	1.52
1	C	17	GLU	CD-OE1	6.32	1.32	1.25
1	B	1048	VAL	CB-CG2	-6.32	1.39	1.52
1	A	446	THR	CB-CG2	6.32	1.73	1.52
1	A	971	GLU	CB-CG	6.32	1.64	1.52
1	A	140	GLU	CB-CG	6.31	1.64	1.52
1	B	1083	SER	CB-OG	6.31	1.50	1.42
1	D	905	ASN	CB-CG	6.31	1.65	1.51
1	C	407	ILE	CB-CG2	-6.31	1.33	1.52
1	A	687	LYS	CD-CE	6.30	1.67	1.51
1	B	586	GLN	CD-NE2	6.30	1.48	1.32
1	D	97	ARG	NE-CZ	6.29	1.41	1.33
1	C	275	PHE	CB-CG	-6.29	1.40	1.51
1	C	8	PHE	CD2-CE2	6.29	1.51	1.39
1	A	230	GLU	CD-OE1	6.29	1.32	1.25
1	B	448	GLU	CD-OE2	6.29	1.32	1.25
1	A	915	PHE	CG-CD2	6.29	1.48	1.38
1	B	570	GLU	CB-CG	6.28	1.64	1.52
1	A	1213	HIS	N-CA	6.28	1.58	1.46
1	B	428	GLU	CG-CD	6.28	1.61	1.51
1	B	200	GLU	CG-CD	6.28	1.61	1.51
1	D	1229	LYS	CD-CE	6.28	1.67	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	601	GLU	CD-OE1	6.27	1.32	1.25
1	D	515	PHE	CE2-CZ	6.27	1.49	1.37
1	B	719	ASP	CB-CG	6.26	1.65	1.51
1	D	1108	LYS	CE-NZ	6.26	1.64	1.49
1	B	1056	LYS	CD-CE	6.26	1.67	1.51
1	D	451	GLU	CG-CD	6.26	1.61	1.51
1	D	121	VAL	CB-CG1	6.26	1.66	1.52
1	D	625	GLU	CB-CG	6.26	1.64	1.52
1	A	1103	GLU	CG-CD	6.26	1.61	1.51
1	B	1290	ASN	CB-CG	6.26	1.65	1.51
1	D	348	VAL	CA-CB	-6.26	1.41	1.54
1	B	915	PHE	CG-CD2	6.25	1.48	1.38
1	D	704	LYS	CD-CE	6.25	1.66	1.51
1	A	1115	GLU	CG-CD	6.25	1.61	1.51
1	B	1234	GLY	CA-C	6.25	1.61	1.51
1	C	777	VAL	CB-CG2	-6.24	1.39	1.52
1	A	323	LYS	CD-CE	6.24	1.66	1.51
1	C	426	ARG	N-CA	6.24	1.58	1.46
1	D	808	VAL	CB-CG1	-6.24	1.39	1.52
1	B	1072	VAL	CB-CG2	-6.24	1.39	1.52
1	D	64	LYS	CG-CD	6.23	1.73	1.52
1	A	1229	LYS	CG-CD	6.23	1.73	1.52
1	B	1120	ALA	CA-CB	-6.22	1.39	1.52
1	C	371	LYS	CD-CE	6.22	1.66	1.51
1	A	27	LEU	C-O	6.22	1.35	1.23
1	A	805	ARG	CZ-NH2	6.22	1.41	1.33
1	C	599	ARG	NE-CZ	6.22	1.41	1.33
1	C	915	PHE	CG-CD2	6.20	1.48	1.38
1	B	603	GLU	CD-OE1	6.20	1.32	1.25
1	B	1153	TYR	CD1-CE1	6.20	1.48	1.39
1	B	1242	VAL	CB-CG2	-6.20	1.39	1.52
1	C	258	VAL	CB-CG1	-6.20	1.39	1.52
1	D	8	PHE	CE2-CZ	-6.20	1.25	1.37
1	A	64	LYS	CG-CD	6.19	1.73	1.52
1	A	861	GLU	CG-CD	6.19	1.61	1.51
1	C	230	GLU	CD-OE2	6.19	1.32	1.25
1	B	619	LYS	CD-CE	6.19	1.66	1.51
1	C	681	ARG	CG-CD	6.19	1.67	1.51
1	B	1319	VAL	CB-CG2	6.18	1.65	1.52
1	D	1100	LYS	CD-CE	6.18	1.66	1.51
1	B	1319	VAL	CB-CG1	6.18	1.65	1.52
1	C	691	GLU	CG-CD	6.18	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1291	VAL	CB-CG1	6.18	1.65	1.52
1	B	499	ASP	CB-CG	6.17	1.64	1.51
1	A	33	LYS	CD-CE	6.17	1.66	1.51
1	A	481	GLU	CD-OE1	6.17	1.32	1.25
1	C	32	ARG	CZ-NH2	6.17	1.41	1.33
1	D	803	GLU	CG-CD	6.17	1.61	1.51
1	A	690	TYR	CD2-CE2	-6.16	1.30	1.39
1	B	103	GLU	CD-OE2	6.16	1.32	1.25
1	B	1319	VAL	CA-C	6.16	1.69	1.52
1	A	1214	TYR	CD1-CE1	6.16	1.48	1.39
1	B	340	LYS	CD-CE	6.15	1.66	1.51
1	C	318	LYS	CG-CD	6.14	1.73	1.52
1	B	612	THR	CB-CG2	6.14	1.72	1.52
1	A	236	TRP	CE2-CZ2	-6.14	1.29	1.39
1	B	1291	VAL	N-CA	6.14	1.58	1.46
1	B	647	THR	CB-CG2	6.13	1.72	1.52
1	A	617	LYS	CE-NZ	6.13	1.64	1.49
1	B	395	LYS	CE-NZ	6.13	1.64	1.49
1	C	196	PHE	CB-CG	6.13	1.61	1.51
1	D	112	GLN	CG-CD	6.13	1.65	1.51
1	A	67	HIS	N-CA	6.12	1.58	1.46
1	D	1319	VAL	CA-CB	6.12	1.67	1.54
1	B	46	GLY	CA-C	6.12	1.61	1.51
1	C	138	GLU	CG-CD	6.12	1.61	1.51
1	B	402	GLU	CD-OE2	6.12	1.32	1.25
1	C	29	TYR	CG-CD2	-6.11	1.31	1.39
1	D	318	LYS	CG-CD	6.11	1.73	1.52
1	C	757	GLU	CD-OE2	6.10	1.32	1.25
1	A	199	GLU	CG-CD	6.10	1.61	1.51
1	A	425	SER	N-CA	6.09	1.58	1.46
1	B	332	GLU	CB-CG	6.09	1.63	1.52
1	D	1125	THR	CA-CB	6.09	1.69	1.53
1	A	800	GLY	N-CA	6.08	1.55	1.46
1	D	32	ARG	CZ-NH1	6.08	1.41	1.33
1	B	161	ARG	CZ-NH1	6.08	1.41	1.33
1	D	803	GLU	CD-OE2	6.08	1.32	1.25
1	B	1239	GLU	CG-CD	6.08	1.61	1.51
1	A	600	TYR	CB-CG	-6.08	1.42	1.51
1	D	133	GLU	CD-OE2	6.08	1.32	1.25
1	A	133	GLU	CD-OE1	6.07	1.32	1.25
1	D	232	GLU	CG-CD	6.07	1.61	1.51
1	C	218	ARG	CZ-NH1	6.07	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	22	PRO	CB-CG	-6.07	1.19	1.50
1	C	995	LYS	CE-NZ	6.06	1.64	1.49
1	D	731	VAL	CB-CG1	6.06	1.65	1.52
1	C	826	CYS	CB-SG	6.06	1.92	1.82
1	D	971	GLU	CD-OE1	6.06	1.32	1.25
1	B	401	GLU	CD-OE1	6.05	1.32	1.25
1	C	310	LYS	CD-CE	6.05	1.66	1.51
1	B	146	ASN	C-O	6.05	1.34	1.23
1	D	961	GLU	CG-CD	6.05	1.61	1.51
1	B	97	ARG	CG-CD	6.05	1.67	1.51
1	A	533	GLU	CG-CD	6.04	1.61	1.51
1	A	309	GLU	CB-CG	6.04	1.63	1.52
1	D	526	LYS	CD-CE	6.04	1.66	1.51
1	C	310	LYS	CE-NZ	6.04	1.64	1.49
1	A	13	ARG	CG-CD	6.04	1.67	1.51
1	C	64	LYS	CE-NZ	6.04	1.64	1.49
1	B	663	CYS	CB-SG	6.03	1.92	1.82
1	B	16	VAL	CB-CG2	-6.03	1.40	1.52
1	B	448	GLU	CB-CG	6.02	1.63	1.52
1	B	215	GLU	CD-OE2	6.02	1.32	1.25
1	D	1156	TYR	CD2-CE2	6.02	1.48	1.39
1	A	616	ALA	CA-C	-6.01	1.37	1.52
1	B	609	VAL	CB-CG2	-6.01	1.40	1.52
1	B	33	LYS	CD-CE	6.01	1.66	1.51
1	A	660	LYS	CE-NZ	6.00	1.64	1.49
1	B	941	GLU	CB-CG	6.00	1.63	1.52
1	D	393	TYR	CG-CD2	6.00	1.47	1.39
1	A	635	PHE	CE1-CZ	-6.00	1.25	1.37
1	A	746	GLU	CB-CG	6.00	1.63	1.52
1	A	902	CYS	CB-SG	-6.00	1.72	1.82
1	A	726	GLU	CD-OE2	6.00	1.32	1.25
1	A	636	ILE	CA-CB	5.99	1.68	1.54
1	B	741	GLU	CD-OE2	5.99	1.32	1.25
1	A	755	LYS	CD-CE	5.99	1.66	1.51
1	B	1092	TYR	CE2-CZ	5.99	1.46	1.38
1	C	85	VAL	CB-CG1	-5.99	1.40	1.52
1	A	13	ARG	CZ-NH1	5.99	1.40	1.33
1	C	1332	ARG	N-CA	5.99	1.58	1.46
1	A	479	LYS	CD-CE	5.97	1.66	1.51
1	B	861	GLU	CG-CD	5.97	1.60	1.51
1	C	1162	GLU	CD-OE2	5.97	1.32	1.25
1	A	402	GLU	CD-OE1	5.96	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	760	GLU	CD-OE1	5.96	1.32	1.25
1	C	757	GLU	CG-CD	5.96	1.60	1.51
1	D	445	GLY	N-CA	5.96	1.54	1.46
1	B	984	GLU	CD-OE1	5.96	1.32	1.25
1	D	45	GLU	CB-CG	-5.95	1.40	1.52
1	C	1256	ALA	CA-CB	-5.95	1.40	1.52
1	D	593	TYR	CD1-CE1	-5.95	1.30	1.39
1	B	1011	THR	N-CA	5.95	1.58	1.46
1	D	690	TYR	CE2-CZ	-5.95	1.30	1.38
1	B	927	TRP	CB-CG	-5.95	1.39	1.50
1	B	425	SER	N-CA	5.94	1.58	1.46
1	B	865	PHE	CD2-CE2	5.93	1.51	1.39
1	A	687	LYS	CG-CD	5.93	1.72	1.52
1	B	97	ARG	CB-CG	5.93	1.68	1.52
1	D	263	GLU	CD-OE2	5.93	1.32	1.25
1	B	903	LYS	CD-CE	5.93	1.66	1.51
1	A	984	GLU	CD-OE2	5.93	1.32	1.25
1	B	735	ILE	CB-CG2	5.93	1.71	1.52
1	C	340	LYS	CD-CE	5.92	1.66	1.51
1	C	603	GLU	CG-CD	5.92	1.60	1.51
1	B	712	GLU	CD-OE2	5.92	1.32	1.25
1	A	757	GLU	CB-CG	5.92	1.63	1.52
1	C	603	GLU	CD-OE1	5.92	1.32	1.25
1	C	375	VAL	CB-CG1	-5.91	1.40	1.52
1	D	332	GLU	CD-OE2	5.90	1.32	1.25
1	C	211	ILE	CB-CG2	5.89	1.71	1.52
1	C	45	GLU	CD-OE2	5.89	1.32	1.25
1	D	671	VAL	CB-CG1	-5.89	1.40	1.52
1	C	47	GLY	C-O	5.89	1.33	1.23
1	D	1262	GLU	CD-OE1	5.89	1.32	1.25
1	C	1038	GLU	CD-OE1	5.88	1.32	1.25
1	C	1094	ALA	CA-CB	-5.88	1.40	1.52
1	D	563	GLU	CB-CG	5.88	1.63	1.52
1	C	757	GLU	CD-OE1	5.88	1.32	1.25
1	A	685	GLY	C-O	-5.88	1.14	1.23
1	B	40	LYS	CD-CE	5.88	1.66	1.51
1	D	380	ARG	CZ-NH1	5.88	1.40	1.33
1	D	1331	VAL	CA-CB	5.87	1.67	1.54
1	B	16	VAL	CB-CG1	-5.87	1.40	1.52
1	C	1144	GLU	CD-OE1	5.87	1.32	1.25
1	C	927	TRP	CB-CG	-5.87	1.39	1.50
1	D	161	ARG	CG-CD	5.87	1.66	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1162	GLU	CD-OE1	5.87	1.32	1.25
1	A	101	VAL	C-O	-5.86	1.12	1.23
1	C	741	GLU	CD-OE1	5.86	1.32	1.25
1	D	799	PHE	CE2-CZ	-5.86	1.26	1.37
1	A	97	ARG	NE-CZ	5.86	1.40	1.33
1	C	481	GLU	CD-OE1	5.86	1.32	1.25
1	D	380	ARG	CZ-NH2	5.86	1.40	1.33
1	A	628	LYS	CB-CG	5.85	1.68	1.52
1	A	1320	THR	N-CA	5.85	1.58	1.46
1	B	566	LYS	CB-CG	5.85	1.68	1.52
1	C	202	THR	N-CA	5.85	1.58	1.46
1	A	649	ILE	CB-CG2	5.85	1.71	1.52
1	C	13	ARG	CZ-NH2	5.85	1.40	1.33
1	C	251	GLN	CG-CD	5.85	1.64	1.51
1	B	1056	LYS	CE-NZ	5.84	1.63	1.49
1	A	393	TYR	CD1-CE1	5.84	1.48	1.39
1	B	208	GLN	CG-CD	5.84	1.64	1.51
1	A	431	ILE	CG1-CD1	5.84	1.90	1.50
1	D	433	LYS	CD-CE	5.84	1.65	1.51
1	D	339	GLY	N-CA	5.84	1.54	1.46
1	A	443	LYS	CD-CE	5.83	1.65	1.51
1	D	5	LYS	CD-CE	5.83	1.65	1.51
1	C	165	ARG	CB-CG	5.83	1.68	1.52
1	A	32	ARG	CZ-NH2	5.83	1.40	1.33
1	A	485	ASP	CB-CG	5.83	1.64	1.51
1	C	199	GLU	CG-CD	5.82	1.60	1.51
1	C	698	THR	CA-CB	5.82	1.68	1.53
1	A	1183	VAL	CB-CG2	-5.82	1.40	1.52
1	A	1311	VAL	CA-CB	5.82	1.67	1.54
1	C	95	LYS	CD-CE	5.81	1.65	1.51
1	A	445	GLY	C-O	5.81	1.32	1.23
1	C	915	PHE	CE1-CZ	5.81	1.48	1.37
1	D	1095	CYS	CB-SG	-5.80	1.72	1.81
1	B	853	LYS	CD-CE	5.80	1.65	1.51
1	C	1312	ASP	CB-CG	5.80	1.64	1.51
1	D	199	GLU	CB-CG	5.80	1.63	1.52
1	B	880	GLU	CD-OE1	5.80	1.32	1.25
1	D	461	ASN	CB-CG	-5.80	1.37	1.51
1	A	236	TRP	CB-CG	5.79	1.60	1.50
1	C	647	THR	CB-CG2	5.79	1.71	1.52
1	A	1319	VAL	CA-C	5.78	1.68	1.52
1	A	1239	GLU	CG-CD	5.78	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	848	LYS	CD-CE	5.78	1.65	1.51
1	C	480	GLU	CB-CG	5.78	1.63	1.52
1	C	818	TYR	CD1-CE1	5.78	1.48	1.39
1	D	1229	LYS	CE-NZ	5.78	1.63	1.49
1	D	286	GLU	CD-OE2	5.77	1.31	1.25
1	C	48	CYS	C-O	5.77	1.34	1.23
1	D	818	TYR	CD1-CE1	5.76	1.48	1.39
1	A	137	GLU	CB-CG	5.76	1.63	1.52
1	B	402	GLU	CG-CD	5.74	1.60	1.51
1	C	1083	SER	CA-CB	5.74	1.61	1.52
1	D	110	GLY	C-O	5.74	1.32	1.23
1	B	811	THR	CB-CG2	5.73	1.71	1.52
1	B	443	LYS	CD-CE	5.73	1.65	1.51
1	D	13	ARG	CG-CD	5.73	1.66	1.51
1	D	137	GLU	CG-CD	5.73	1.60	1.51
1	D	507	PHE	CE1-CZ	-5.73	1.26	1.37
1	B	716	GLU	CD-OE1	5.73	1.31	1.25
1	C	753	VAL	CB-CG1	-5.73	1.40	1.52
1	D	599	ARG	CD-NE	5.72	1.56	1.46
1	A	1140	GLY	N-CA	5.72	1.54	1.46
1	C	365	PHE	CD1-CE1	5.72	1.50	1.39
1	D	1214	TYR	CD2-CE2	5.72	1.48	1.39
1	A	310	LYS	CD-CE	5.72	1.65	1.51
1	C	1291	VAL	CB-CG2	5.72	1.64	1.52
1	B	195	LEU	N-CA	5.72	1.57	1.46
1	A	1124	ASP	CB-CG	5.71	1.63	1.51
1	B	619	LYS	CE-NZ	5.71	1.63	1.49
1	C	480	GLU	CG-CD	5.71	1.60	1.51
1	A	970	GLU	CD-OE2	5.70	1.31	1.25
1	C	417	TYR	CE2-CZ	5.70	1.46	1.38
1	B	1144	GLU	CG-CD	5.70	1.60	1.51
1	B	1261	GLY	CA-C	5.70	1.60	1.51
1	C	342	VAL	CB-CG1	-5.70	1.40	1.52
1	D	691	GLU	CD-OE2	5.69	1.31	1.25
1	C	433	LYS	CD-CE	5.68	1.65	1.51
1	B	310	LYS	CE-NZ	5.68	1.63	1.49
1	C	279	VAL	CB-CG2	-5.68	1.41	1.52
1	C	1100	LYS	CD-CE	5.68	1.65	1.51
1	C	1166	ASP	CB-CG	5.68	1.63	1.51
1	C	687	LYS	CG-CD	5.67	1.71	1.52
1	D	1289	ASN	CB-CG	5.67	1.64	1.51
1	D	590	GLU	CD-OE1	5.67	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	744	TYR	CZ-OH	5.67	1.47	1.37
1	B	32	ARG	CZ-NH2	5.67	1.40	1.33
1	B	790	VAL	CB-CG2	-5.67	1.41	1.52
1	C	672	VAL	CB-CG1	-5.67	1.41	1.52
1	A	1304	GLU	CG-CD	5.67	1.60	1.51
1	C	269	LYS	CE-NZ	5.66	1.63	1.49
1	A	22	PRO	N-CA	-5.66	1.37	1.47
1	A	453	ALA	CA-CB	5.66	1.64	1.52
1	B	995	LYS	CE-NZ	5.65	1.63	1.49
1	A	18	LYS	CD-CE	5.65	1.65	1.51
1	A	225	LYS	CD-CE	5.64	1.65	1.51
1	C	318	LYS	CE-NZ	5.64	1.63	1.49
1	A	716	GLU	CD-OE2	5.64	1.31	1.25
1	C	101	VAL	CB-CG2	-5.64	1.41	1.52
1	D	1144	GLU	CD-OE1	5.64	1.31	1.25
1	B	808	VAL	CB-CG2	-5.64	1.41	1.52
1	D	417	TYR	CD1-CE1	5.64	1.47	1.39
1	C	1262	GLU	CD-OE1	5.64	1.31	1.25
1	B	270	PHE	CE2-CZ	5.63	1.48	1.37
1	C	199	GLU	CD-OE1	5.62	1.31	1.25
1	B	271	LYS	CD-CE	5.62	1.65	1.51
1	B	1229	LYS	CE-NZ	5.62	1.63	1.49
1	D	402	GLU	CG-CD	5.62	1.60	1.51
1	D	479	LYS	CB-CG	5.62	1.67	1.52
1	D	590	GLU	CD-OE2	5.62	1.31	1.25
1	A	434	VAL	CB-CG2	-5.62	1.41	1.52
1	B	13	ARG	CZ-NH1	5.62	1.40	1.33
1	B	97	ARG	NE-CZ	5.62	1.40	1.33
1	B	927	TRP	CZ3-CH2	5.61	1.49	1.40
1	C	613	ARG	CG-CD	5.61	1.66	1.51
1	D	601	GLU	CD-OE1	5.61	1.31	1.25
1	D	393	TYR	CE1-CZ	5.61	1.45	1.38
1	A	1290	ASN	CB-CG	5.61	1.64	1.51
1	A	1106	LYS	CD-CE	5.61	1.65	1.51
1	C	1164	GLU	CD-OE1	5.61	1.31	1.25
1	D	891	LYS	CG-CD	5.61	1.71	1.52
1	A	529	GLN	CB-CG	5.61	1.67	1.52
1	C	215	GLU	CB-CG	5.61	1.62	1.52
1	C	825	ARG	CZ-NH1	5.61	1.40	1.33
1	B	1031	LEU	C-O	5.60	1.33	1.23
1	D	788	ILE	CA-CB	-5.60	1.42	1.54
1	A	708	PHE	CB-CG	5.60	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	197	LYS	CD-CE	5.60	1.65	1.51
1	C	215	GLU	CD-OE1	5.60	1.31	1.25
1	A	820	THR	CB-CG2	-5.60	1.33	1.52
1	A	861	GLU	CD-OE1	5.60	1.31	1.25
1	C	408	GLU	CD-OE1	5.60	1.31	1.25
1	C	411	TYR	CB-CG	-5.60	1.43	1.51
1	A	625	GLU	CB-CG	5.60	1.62	1.52
1	C	326	VAL	CB-CG2	-5.60	1.41	1.52
1	B	73	CYS	CB-SG	5.59	1.91	1.82
1	C	1242	VAL	CB-CG2	-5.59	1.41	1.52
1	D	29	TYR	CD2-CE2	5.59	1.47	1.39
1	A	687	LYS	CE-NZ	5.59	1.63	1.49
1	C	1183	VAL	CB-CG1	-5.59	1.41	1.52
1	A	530	GLU	CG-CD	5.58	1.60	1.51
1	A	755	LYS	CE-NZ	5.58	1.63	1.49
1	A	962	GLY	C-O	5.58	1.32	1.23
1	C	318	LYS	CB-CG	5.58	1.67	1.52
1	A	107	LYS	CE-NZ	5.58	1.63	1.49
1	B	88	VAL	CB-CG2	-5.58	1.41	1.52
1	B	1331	VAL	N-CA	5.58	1.57	1.46
1	C	195	LEU	N-CA	5.58	1.57	1.46
1	B	64	LYS	CG-CD	5.58	1.71	1.52
1	D	712	GLU	CD-OE2	5.57	1.31	1.25
1	A	1154	PHE	CG-CD1	5.57	1.47	1.38
1	B	251	GLN	CG-CD	5.57	1.63	1.51
1	A	103	GLU	CB-CG	5.56	1.62	1.52
1	A	915	PHE	CE2-CZ	5.56	1.48	1.37
1	C	704	LYS	CD-CE	5.56	1.65	1.51
1	B	801	GLY	N-CA	-5.56	1.37	1.46
1	B	593	TYR	CA-CB	-5.55	1.41	1.53
1	C	1134	TYR	CE2-CZ	-5.55	1.31	1.38
1	A	414	GLU	CG-CD	5.55	1.60	1.51
1	A	848	LYS	CB-CG	5.55	1.67	1.52
1	B	1290	ASN	N-CA	5.55	1.57	1.46
1	D	62	GLN	CG-CD	5.55	1.63	1.51
1	D	1056	LYS	CD-CE	5.55	1.65	1.51
1	A	1229	LYS	CD-CE	5.55	1.65	1.51
1	D	251	GLN	CB-CG	5.55	1.67	1.52
1	A	475	SER	CA-CB	5.54	1.61	1.52
1	B	755	LYS	CD-CE	5.54	1.65	1.51
1	A	686	VAL	CB-CG1	-5.54	1.41	1.52
1	B	590	GLU	CG-CD	5.54	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	202	THR	CB-CG2	5.54	1.70	1.52
1	B	15	VAL	CB-CG2	-5.53	1.41	1.52
1	A	1164	GLU	CD-OE2	5.53	1.31	1.25
1	B	408	GLU	CD-OE2	5.53	1.31	1.25
1	D	448	GLU	CD-OE1	5.53	1.31	1.25
1	C	744	TYR	CZ-OH	5.53	1.47	1.37
1	C	735	ILE	CB-CG2	5.52	1.70	1.52
1	B	757	GLU	CG-CD	5.52	1.60	1.51
1	D	1211	GLU	CB-CG	5.52	1.62	1.52
1	B	515	PHE	CD1-CE1	-5.51	1.28	1.39
1	A	97	ARG	CG-CD	5.51	1.65	1.51
1	B	25	THR	CB-CG2	5.51	1.70	1.52
1	A	533	GLU	CB-CG	5.50	1.62	1.52
1	D	477	LEU	CG-CD2	5.50	1.72	1.51
1	B	803	GLU	CA-C	5.50	1.67	1.52
1	B	323	LYS	CD-CE	5.50	1.65	1.51
1	B	1108	LYS	CD-CE	5.50	1.65	1.51
1	A	50	ALA	CA-CB	-5.50	1.41	1.52
1	D	104	ARG	CZ-NH1	5.50	1.40	1.33
1	A	734	GLU	CG-CD	5.49	1.60	1.51
1	B	590	GLU	CD-OE1	5.49	1.31	1.25
1	D	891	LYS	CD-CE	5.49	1.65	1.51
1	B	23	GLU	CG-CD	5.49	1.60	1.51
1	B	136	MET	CG-SD	5.49	1.95	1.81
1	C	267	GLU	CG-CD	5.49	1.60	1.51
1	D	407	ILE	CB-CG2	-5.48	1.35	1.52
1	A	596	ASP	C-O	5.48	1.33	1.23
1	D	687	LYS	CD-CE	5.48	1.65	1.51
1	A	466	ALA	CA-CB	5.48	1.64	1.52
1	D	1160	CYS	CB-SG	-5.48	1.72	1.81
1	A	1233	PHE	CD1-CE1	5.48	1.50	1.39
1	A	97	ARG	CD-NE	5.47	1.55	1.46
1	B	1217	GLU	CD-OE2	5.47	1.31	1.25
1	C	978	TYR	CE1-CZ	5.47	1.45	1.38
1	D	847	TYR	CD1-CE1	5.47	1.47	1.39
1	C	200	GLU	CB-CG	5.47	1.62	1.52
1	A	915	PHE	CD2-CE2	5.47	1.50	1.39
1	A	1061	LYS	CE-NZ	5.47	1.62	1.49
1	D	97	ARG	CD-NE	5.47	1.55	1.46
1	A	1156	TYR	CE1-CZ	5.46	1.45	1.38
1	D	308	VAL	CB-CG2	-5.46	1.41	1.52
1	D	679	THR	CB-CG2	5.46	1.70	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	991	GLU	CD-OE2	5.45	1.31	1.25
1	A	803	GLU	CD-OE1	5.45	1.31	1.25
1	D	622	ASP	CB-CG	5.45	1.63	1.51
1	A	587	ALA	CA-CB	-5.44	1.41	1.52
1	C	940	GLU	CG-CD	5.44	1.60	1.51
1	D	1003	PRO	N-CA	-5.44	1.38	1.47
1	B	600	TYR	CB-CG	-5.44	1.43	1.51
1	C	64	LYS	CG-CD	5.44	1.71	1.52
1	A	215	GLU	CD-OE2	5.44	1.31	1.25
1	A	1293	GLU	CD-OE1	5.44	1.31	1.25
1	A	449	VAL	CA-CB	5.44	1.66	1.54
1	A	692	GLU	CD-OE1	5.44	1.31	1.25
1	C	656	PHE	CE1-CZ	5.44	1.47	1.37
1	B	865	PHE	CE1-CZ	5.43	1.47	1.37
1	B	1261	GLY	C-O	5.43	1.32	1.23
1	B	1328	PRO	N-CA	5.43	1.56	1.47
1	D	726	GLU	CD-OE1	5.43	1.31	1.25
1	A	687	LYS	CB-CG	5.43	1.67	1.52
1	D	1299	SER	CB-OG	5.43	1.49	1.42
1	C	393	TYR	CE1-CZ	5.43	1.45	1.38
1	D	1197	GLU	CD-OE2	5.43	1.31	1.25
1	A	716	GLU	CD-OE1	5.43	1.31	1.25
1	B	425	SER	CA-CB	5.43	1.61	1.52
1	D	21	ASP	CB-CG	5.43	1.63	1.51
1	D	1239	GLU	CG-CD	5.42	1.60	1.51
1	A	750	THR	CA-CB	5.42	1.67	1.53
1	B	687	LYS	CD-CE	5.42	1.64	1.51
1	D	9	PHE	CE2-CZ	5.42	1.47	1.37
1	B	1329	TRP	CB-CG	5.42	1.60	1.50
1	D	1066	GLU	CD-OE1	5.42	1.31	1.25
1	D	660	LYS	CD-CE	5.41	1.64	1.51
1	A	244	GLU	CB-CG	-5.41	1.41	1.52
1	D	915	PHE	CE2-CZ	5.41	1.47	1.37
1	D	323	LYS	CB-CG	5.41	1.67	1.52
1	A	676	PRO	N-CA	-5.41	1.38	1.47
1	D	563	GLU	CD-OE2	5.41	1.31	1.25
1	C	865	PHE	CE1-CZ	5.40	1.47	1.37
1	B	1260	VAL	CB-CG2	-5.40	1.41	1.52
1	C	658	LYS	CD-CE	5.40	1.64	1.51
1	D	1072	VAL	CB-CG2	-5.40	1.41	1.52
1	A	905	ASN	CB-CG	5.40	1.63	1.51
1	C	788	ILE	CA-CB	-5.39	1.42	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1135	ARG	CB-CG	5.39	1.67	1.52
1	D	601	GLU	CD-OE2	5.39	1.31	1.25
1	C	197	LYS	CB-CG	5.39	1.67	1.52
1	C	592	VAL	CB-CG2	5.39	1.64	1.52
1	D	443	LYS	CD-CE	5.39	1.64	1.51
1	A	15	VAL	CB-CG1	-5.38	1.41	1.52
1	A	446	THR	CA-CB	5.38	1.67	1.53
1	A	102	GLN	CA-C	-5.38	1.39	1.52
1	A	393	TYR	CD2-CE2	5.38	1.47	1.39
1	A	467	LEU	CG-CD1	5.38	1.71	1.51
1	C	819	LYS	CD-CE	5.38	1.64	1.51
1	D	566	LYS	CD-CE	5.38	1.64	1.51
1	B	803	GLU	CD-OE2	5.38	1.31	1.25
1	C	383	VAL	CB-CG1	-5.38	1.41	1.52
1	C	589	GLY	N-CA	-5.37	1.38	1.46
1	A	629	VAL	CB-CG2	-5.37	1.41	1.52
1	D	540	ASP	N-CA	5.37	1.57	1.46
1	C	84	ALA	CA-CB	-5.37	1.41	1.52
1	C	291	GLU	CD-OE1	5.37	1.31	1.25
1	D	586	GLN	CD-NE2	5.37	1.46	1.32
1	A	603	GLU	CG-CD	5.36	1.59	1.51
1	C	153	TYR	CZ-OH	-5.36	1.28	1.37
1	D	480	GLU	CG-CD	5.36	1.59	1.51
1	B	165	ARG	C-O	5.36	1.33	1.23
1	C	442	PHE	CE1-CZ	5.36	1.47	1.37
1	A	930	GLU	CD-OE2	5.36	1.31	1.25
1	C	660	LYS	CD-CE	5.36	1.64	1.51
1	A	570	GLU	CB-CG	5.36	1.62	1.52
1	D	677	GLU	CD-OE2	5.36	1.31	1.25
1	D	691	GLU	CD-OE1	5.36	1.31	1.25
1	D	1255	TYR	CG-CD1	-5.36	1.32	1.39
1	A	571	GLU	CD-OE2	5.36	1.31	1.25
1	B	234	VAL	CB-CG1	-5.36	1.41	1.52
1	B	161	ARG	CG-CD	5.35	1.65	1.51
1	C	33	LYS	CE-NZ	5.35	1.62	1.49
1	C	959	LYS	CB-CG	5.35	1.67	1.52
1	D	1289	ASN	N-CA	5.35	1.57	1.46
1	D	628	LYS	CG-CD	5.35	1.70	1.52
1	C	937	MET	CG-SD	5.35	1.95	1.81
1	A	944	ARG	CG-CD	5.34	1.65	1.51
1	D	36	LEU	C-O	5.34	1.33	1.23
1	A	616	ALA	CA-CB	-5.34	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	161	ARG	CZ-NH1	5.34	1.40	1.33
1	B	112	GLN	CG-CD	5.34	1.63	1.51
1	D	138	GLU	CD-OE2	5.34	1.31	1.25
1	B	1114	TRP	CB-CG	5.34	1.59	1.50
1	D	1171	ASP	CB-CG	5.34	1.62	1.51
1	A	668	ILE	C-O	5.33	1.33	1.23
1	A	1156	TYR	CD2-CE2	5.33	1.47	1.39
1	B	84	ALA	CA-CB	-5.33	1.41	1.52
1	D	332	GLU	CD-OE1	5.33	1.31	1.25
1	A	14	LYS	CD-CE	5.33	1.64	1.51
1	B	160	PHE	CD1-CE1	-5.33	1.28	1.39
1	B	1331	VAL	CB-CG2	5.33	1.64	1.52
1	A	269	LYS	CE-NZ	5.33	1.62	1.49
1	B	2	THR	CB-CG2	5.33	1.70	1.52
1	C	142	ALA	CA-CB	-5.32	1.41	1.52
1	A	601	GLU	CD-OE1	5.32	1.31	1.25
1	A	129	ARG	N-CA	-5.32	1.35	1.46
1	B	865	PHE	CE2-CZ	5.32	1.47	1.37
1	B	1103	GLU	CG-CD	5.32	1.59	1.51
1	D	133	GLU	CB-CG	5.32	1.62	1.52
1	B	1066	GLU	CD-OE1	5.32	1.31	1.25
1	C	133	GLU	CD-OE1	5.32	1.31	1.25
1	D	902	CYS	CB-SG	-5.31	1.73	1.81
1	A	364	VAL	CB-CG1	5.31	1.64	1.52
1	B	161	ARG	CB-CG	5.31	1.66	1.52
1	C	1107	LYS	CD-CE	5.31	1.64	1.51
1	C	1198	GLY	C-O	5.31	1.32	1.23
1	D	1200	PHE	CD1-CE1	-5.31	1.28	1.39
1	A	137	GLU	CD-OE2	5.30	1.31	1.25
1	A	359	SER	CB-OG	5.30	1.49	1.42
1	D	197	LYS	CD-CE	5.30	1.64	1.51
1	D	362	ASN	CB-CG	5.30	1.63	1.51
1	A	1010	PHE	CE2-CZ	-5.30	1.27	1.37
1	B	1115	GLU	CG-CD	5.30	1.59	1.51
1	B	825	ARG	CZ-NH1	5.30	1.40	1.33
1	B	876	GLN	CG-CD	5.30	1.63	1.51
1	D	1320	THR	CB-CG2	5.29	1.69	1.52
1	B	1155	SER	CB-OG	5.29	1.49	1.42
1	C	1290	ASN	N-CA	5.29	1.56	1.46
1	D	1331	VAL	CA-C	5.29	1.66	1.52
1	A	133	GLU	CD-OE2	5.28	1.31	1.25
1	B	592	VAL	CA-CB	-5.28	1.43	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	308	VAL	CB-CG2	-5.28	1.41	1.52
1	C	937	MET	CB-CG	5.28	1.68	1.51
1	A	691	GLU	CG-CD	5.28	1.59	1.51
1	B	853	LYS	CE-NZ	5.28	1.62	1.49
1	D	601	GLU	CG-CD	5.28	1.59	1.51
1	B	709	TYR	CD1-CE1	-5.28	1.31	1.39
1	B	772	LYS	N-CA	-5.28	1.35	1.46
1	C	1330	SER	CA-CB	5.28	1.60	1.52
1	A	769	ASN	C-O	5.27	1.33	1.23
1	A	1023	HIS	C-O	5.27	1.33	1.23
1	B	475	SER	CA-CB	5.27	1.60	1.52
1	B	546	ALA	CA-CB	5.27	1.63	1.52
1	C	7	VAL	CB-CG2	-5.27	1.41	1.52
1	D	1164	GLU	CG-CD	5.26	1.59	1.51
1	A	137	GLU	CD-OE1	5.26	1.31	1.25
1	C	1103	GLU	CD-OE2	5.26	1.31	1.25
1	D	200	GLU	CB-CG	5.26	1.62	1.52
1	C	672	VAL	CB-CG2	-5.26	1.41	1.52
1	D	639	ASP	CB-CG	5.26	1.62	1.51
1	C	481	GLU	CD-OE2	5.25	1.31	1.25
1	C	605	SER	CB-OG	5.25	1.49	1.42
1	B	712	GLU	CD-OE1	5.25	1.31	1.25
1	D	658	LYS	CE-NZ	5.25	1.62	1.49
1	B	414	GLU	CD-OE1	5.25	1.31	1.25
1	D	941	GLU	CB-CG	5.25	1.62	1.52
1	C	526	LYS	CG-CD	5.25	1.70	1.52
1	D	745	LEU	C-O	5.25	1.33	1.23
1	C	1106	LYS	CD-CE	5.24	1.64	1.51
1	D	690	TYR	CE1-CZ	5.24	1.45	1.38
1	A	492	GLU	CG-CD	5.24	1.59	1.51
1	B	364	VAL	CA-CB	-5.24	1.43	1.54
1	C	270	PHE	CE2-CZ	5.24	1.47	1.37
1	B	1309	ALA	CA-CB	-5.24	1.41	1.52
1	C	1331	VAL	CB-CG2	5.24	1.63	1.52
1	B	1122	TYR	CD1-CE1	5.23	1.47	1.39
1	D	647	THR	CA-CB	5.23	1.67	1.53
1	C	944	ARG	CB-CG	5.23	1.66	1.52
1	D	40	LYS	CE-NZ	5.23	1.62	1.49
1	C	402	GLU	CD-OE1	5.23	1.31	1.25
1	C	619	LYS	CD-CE	5.23	1.64	1.51
1	C	832	GLU	CB-CG	5.23	1.62	1.52
1	A	755	LYS	CG-CD	5.23	1.70	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	144	GLN	CB-CG	5.22	1.66	1.52
1	A	455	CYS	CB-SG	-5.22	1.73	1.81
1	A	1207	PHE	CE1-CZ	5.22	1.47	1.37
1	A	957	ASN	CB-CG	5.22	1.63	1.51
1	B	267	GLU	CD-OE2	5.22	1.31	1.25
1	C	413	ARG	CZ-NH1	5.22	1.39	1.33
1	A	815	LEU	C-O	5.22	1.33	1.23
1	C	1108	LYS	CD-CE	5.22	1.64	1.51
1	A	1223	ARG	CZ-NH1	5.22	1.39	1.33
1	A	25	THR	CA-CB	5.21	1.67	1.53
1	A	891	LYS	CD-CE	5.21	1.64	1.51
1	D	283	TRP	CG-CD1	-5.21	1.29	1.36
1	D	515	PHE	CE1-CZ	-5.21	1.27	1.37
1	D	1228	TYR	CG-CD2	-5.21	1.32	1.39
1	B	2	THR	N-CA	5.21	1.56	1.46
1	B	1251	LYS	CD-CE	5.21	1.64	1.51
1	C	1319	VAL	CB-CG2	5.21	1.63	1.52
1	B	8	PHE	CG-CD1	-5.21	1.30	1.38
1	B	1234	GLY	N-CA	5.20	1.53	1.46
1	D	832	GLU	CD-OE1	5.20	1.31	1.25
1	B	131	GLN	CG-CD	5.20	1.63	1.51
1	C	601	GLU	CG-CD	5.20	1.59	1.51
1	D	263	GLU	CD-OE1	5.20	1.31	1.25
1	A	1135	ARG	CB-CG	5.20	1.66	1.52
1	C	415	GLY	C-O	5.20	1.31	1.23
1	D	1005	LYS	CE-NZ	5.20	1.62	1.49
1	B	1249	PRO	N-CA	-5.19	1.38	1.47
1	C	49	GLY	N-CA	5.19	1.53	1.46
1	B	429	ASP	CB-CG	5.19	1.62	1.51
1	C	797	GLY	CA-C	-5.19	1.43	1.51
1	D	891	LYS	CE-NZ	5.19	1.62	1.49
1	A	308	VAL	CB-CG2	-5.19	1.42	1.52
1	A	1116	ASP	CB-CG	5.19	1.62	1.51
1	C	743	PHE	CG-CD2	-5.19	1.30	1.38
1	B	84	ALA	C-O	5.19	1.33	1.23
1	B	714	LYS	N-CA	5.19	1.56	1.46
1	A	819	LYS	CD-CE	5.18	1.64	1.51
1	D	890	TYR	CG-CD1	-5.18	1.32	1.39
1	B	857	VAL	CB-CG1	-5.18	1.42	1.52
1	B	952	ASP	CB-CG	5.18	1.62	1.51
1	B	1233	PHE	CE1-CZ	5.18	1.47	1.37
1	C	461	ASN	CB-CG	-5.18	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1207	PHE	CG-CD2	5.18	1.46	1.38
1	B	448	GLU	CD-OE1	5.17	1.31	1.25
1	C	322	GLN	CG-CD	5.17	1.62	1.51
1	D	959	LYS	CE-NZ	5.17	1.61	1.49
1	A	1266	PHE	CD2-CE2	-5.17	1.28	1.39
1	B	92	GLY	C-O	5.17	1.31	1.23
1	B	961	GLU	CD-OE1	5.17	1.31	1.25
1	B	600	TYR	CE2-CZ	5.16	1.45	1.38
1	C	896	ARG	CZ-NH2	5.16	1.39	1.33
1	C	1229	LYS	CE-NZ	5.16	1.61	1.49
1	B	85	VAL	CB-CG2	-5.16	1.42	1.52
1	B	1144	GLU	CD-OE1	5.16	1.31	1.25
1	B	61	LEU	CG-CD2	5.15	1.71	1.51
1	A	217	LEU	N-CA	5.15	1.56	1.46
1	B	106	ALA	CA-CB	5.15	1.63	1.52
1	B	808	VAL	C-O	5.15	1.33	1.23
1	C	493	GLU	CD-OE2	5.15	1.31	1.25
1	C	1118	VAL	CB-CG2	-5.15	1.42	1.52
1	A	609	VAL	C-O	5.15	1.33	1.23
1	A	646	ILE	CG1-CD1	5.15	1.85	1.50
1	B	431	ILE	CB-CG2	5.15	1.68	1.52
1	B	871	THR	C-O	5.15	1.33	1.23
1	D	223	PRO	CG-CD	5.15	1.67	1.50
1	B	8	PHE	CE2-CZ	-5.15	1.27	1.37
1	A	291	GLU	CB-CG	5.15	1.61	1.52
1	B	1211	GLU	CB-CG	5.14	1.61	1.52
1	A	824	VAL	CA-CB	-5.14	1.44	1.54
1	D	1223	ARG	CZ-NH1	5.14	1.39	1.33
1	A	890	TYR	C-O	5.14	1.33	1.23
1	D	402	GLU	CD-OE1	5.14	1.31	1.25
1	A	772	LYS	CE-NZ	5.13	1.61	1.49
1	C	414	GLU	CB-CG	5.13	1.61	1.52
1	B	818	TYR	CG-CD1	5.13	1.45	1.39
1	A	263	GLU	CD-OE1	5.13	1.31	1.25
1	B	940	GLU	CD-OE1	5.13	1.31	1.25
1	B	959	LYS	CG-CD	5.13	1.69	1.52
1	C	1192	ASP	CB-CG	5.13	1.62	1.51
1	D	485	ASP	CB-CG	5.13	1.62	1.51
1	A	1217	GLU	CB-CG	5.13	1.61	1.52
1	B	133	GLU	CG-CD	5.13	1.59	1.51
1	D	346	ALA	CA-CB	-5.13	1.41	1.52
1	C	140	GLU	CD-OE1	5.13	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	116	CYS	CB-SG	5.13	1.91	1.82
1	A	1061	LYS	CD-CE	5.12	1.64	1.51
1	C	58	TYR	CG-CD2	-5.12	1.32	1.39
1	C	341	GLN	CG-CD	5.12	1.62	1.51
1	C	792	VAL	CB-CG2	-5.12	1.42	1.52
1	D	1273	PHE	CD2-CE2	5.12	1.49	1.39
1	B	493	GLU	CD-OE2	5.12	1.31	1.25
1	B	646	ILE	CG1-CD1	5.12	1.85	1.50
1	C	43	CYS	CB-SG	-5.11	1.73	1.81
1	C	1054	ALA	CA-CB	-5.11	1.41	1.52
1	A	1320	THR	CA-CB	5.11	1.66	1.53
1	B	591	ALA	C-O	5.11	1.33	1.23
1	C	1221	HIS	C-O	5.11	1.33	1.23
1	C	101	VAL	CA-CB	-5.11	1.44	1.54
1	D	595	ASP	CB-CG	5.11	1.62	1.51
1	B	1006	PHE	CD1-CE1	5.10	1.49	1.39
1	D	770	THR	C-O	-5.10	1.13	1.23
1	A	472	ARG	CG-CD	5.10	1.64	1.51
1	A	848	LYS	CD-CE	5.10	1.64	1.51
1	B	635	PHE	CD1-CE1	5.10	1.49	1.39
1	A	764	PHE	CD1-CE1	5.10	1.49	1.39
1	A	236	TRP	CE3-CZ3	-5.09	1.29	1.38
1	C	1103	GLU	CD-OE1	5.09	1.31	1.25
1	A	97	ARG	CZ-NH1	5.09	1.39	1.33
1	B	107	LYS	CG-CD	5.09	1.69	1.52
1	D	138	GLU	CD-OE1	5.09	1.31	1.25
1	A	104	ARG	CG-CD	5.09	1.64	1.51
1	A	1123	MET	C-O	5.09	1.33	1.23
1	D	148	CYS	CB-SG	5.09	1.91	1.82
1	B	1014	PHE	C-O	-5.09	1.13	1.23
1	C	291	GLU	CD-OE2	5.09	1.31	1.25
1	C	1229	LYS	CD-CE	5.09	1.64	1.51
1	B	290	VAL	N-CA	5.08	1.56	1.46
1	B	1241	ARG	C-O	5.08	1.33	1.23
1	C	271	LYS	CD-CE	5.08	1.64	1.51
1	C	443	LYS	CD-CE	5.08	1.64	1.51
1	C	991	GLU	CD-OE1	5.08	1.31	1.25
1	D	481	GLU	CG-CD	5.08	1.59	1.51
1	A	646	ILE	CA-CB	-5.08	1.43	1.54
1	B	381	ARG	CG-CD	5.08	1.64	1.51
1	C	764	PHE	CD1-CE1	5.08	1.49	1.39
1	D	1090	ALA	CA-CB	-5.08	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	990	LYS	CD-CE	5.08	1.64	1.51
1	A	1006	PHE	CE1-CZ	5.08	1.47	1.37
1	C	125	TYR	C-O	5.08	1.32	1.23
1	C	1197	GLU	CG-CD	5.08	1.59	1.51
1	A	597	ILE	CB-CG2	-5.07	1.37	1.52
1	B	926	CYS	CB-SG	-5.07	1.73	1.81
1	D	621	ILE	CA-CB	-5.07	1.43	1.54
1	D	950	GLU	CG-CD	5.07	1.59	1.51
1	A	337	PHE	CG-CD1	-5.07	1.31	1.38
1	A	680	GLN	CB-CG	5.07	1.66	1.52
1	B	526	LYS	CD-CE	5.07	1.64	1.51
1	C	344	SER	CB-OG	5.07	1.48	1.42
1	C	571	GLU	CG-CD	5.07	1.59	1.51
1	C	1272	PHE	CD2-CE2	5.07	1.49	1.39
1	D	1255	TYR	CD2-CE2	5.07	1.47	1.39
1	C	1262	GLU	CG-CD	5.07	1.59	1.51
1	A	368	SER	C-O	5.07	1.32	1.23
1	A	23	GLU	CG-CD	5.06	1.59	1.51
1	C	743	PHE	CE1-CZ	-5.06	1.27	1.37
1	D	1056	LYS	CE-NZ	5.06	1.61	1.49
1	D	1255	TYR	CD1-CE1	5.06	1.47	1.39
1	B	930	GLU	CD-OE1	5.06	1.31	1.25
1	C	990	LYS	CD-CE	5.06	1.63	1.51
1	B	712	GLU	CB-CG	5.06	1.61	1.52
1	D	654	THR	C-O	5.06	1.32	1.23
1	D	411	TYR	CD1-CE1	5.05	1.47	1.39
1	A	700	GLU	CD-OE2	5.05	1.31	1.25
1	D	1101	ARG	CZ-NH1	5.05	1.39	1.33
1	D	1183	VAL	CA-CB	5.05	1.65	1.54
1	C	945	LYS	CD-CE	5.04	1.63	1.51
1	C	1277	ASP	CB-CG	5.04	1.62	1.51
1	A	945	LYS	CD-CE	5.04	1.63	1.51
1	C	836	ILE	CA-CB	-5.04	1.43	1.54
1	A	1100	LYS	CD-CE	5.04	1.63	1.51
1	B	1197	GLU	CD-OE1	5.04	1.31	1.25
1	B	158	GLN	CG-CD	5.04	1.62	1.51
1	D	790	VAL	CA-CB	-5.04	1.44	1.54
1	B	1160	CYS	CB-SG	5.04	1.90	1.82
1	A	144	GLN	CG-CD	5.03	1.62	1.51
1	B	627	LYS	CB-CG	5.03	1.66	1.52
1	B	746	GLU	CG-CD	5.03	1.59	1.51
1	D	978	TYR	CD1-CE1	5.03	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	160	PHE	CE1-CZ	-5.03	1.27	1.37
1	D	290	VAL	CB-CG2	5.03	1.63	1.52
1	C	283	TRP	N-CA	-5.03	1.36	1.46
1	A	318	LYS	CE-NZ	5.03	1.61	1.49
1	C	61	LEU	CG-CD1	5.03	1.70	1.51
1	C	492	GLU	CB-CG	5.03	1.61	1.52
1	D	593	TYR	CB-CG	-5.03	1.44	1.51
1	A	1059	THR	CB-CG2	5.02	1.69	1.52
1	B	472	ARG	CZ-NH1	5.02	1.39	1.33
1	D	726	GLU	CD-OE2	5.02	1.31	1.25
1	A	41	LEU	C-O	5.02	1.32	1.23
1	A	432	ALA	N-CA	5.02	1.56	1.46
1	C	1103	GLU	CG-CD	5.02	1.59	1.51
1	C	861	GLU	CG-CD	5.02	1.59	1.51
1	B	655	VAL	CB-CG1	-5.01	1.42	1.52
1	D	1119	THR	CB-CG2	5.01	1.68	1.52
1	A	468	LYS	CD-CE	5.01	1.63	1.51
1	D	1083	SER	CB-OG	5.01	1.48	1.42
1	C	451	GLU	CG-CD	5.01	1.59	1.51
1	A	283	TRP	CD2-CE2	-5.01	1.35	1.41
1	B	22	PRO	CB-CG	-5.01	1.25	1.50
1	D	113	CYS	CB-SG	-5.01	1.73	1.81
1	D	945	LYS	CD-CE	5.00	1.63	1.51
1	D	1121	ALA	N-CA	5.00	1.56	1.46
1	A	529	GLN	CG-CD	5.00	1.62	1.51
1	B	744	TYR	CZ-OH	5.00	1.46	1.37
1	C	278	ILE	CA-CB	-5.00	1.43	1.54
1	D	316	VAL	CB-CG1	5.00	1.63	1.52
1	C	472	ARG	CG-CD	5.00	1.64	1.51
1	D	1156	TYR	CG-CD2	5.00	1.45	1.39

All (772) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	794	ARG	NE-CZ-NH2	-14.57	113.02	120.30
1	A	830	ARG	NE-CZ-NH1	13.47	127.04	120.30
1	C	825	ARG	NE-CZ-NH2	-13.45	113.58	120.30
1	B	599	ARG	CG-CD-NE	13.40	139.94	111.80
1	C	599	ARG	NE-CZ-NH1	13.04	126.82	120.30
1	A	794	ARG	NE-CZ-NH1	12.28	126.44	120.30
1	D	1135	ARG	NE-CZ-NH1	12.09	126.34	120.30
1	C	584	ASP	CB-CG-OD1	11.75	128.87	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	980	ALA	N-CA-C	-11.62	79.64	111.00
1	B	532	LEU	CA-CB-CG	11.40	141.51	115.30
1	D	659	ASP	CB-CG-OD2	-11.30	108.13	118.30
1	D	6	LEU	CB-CG-CD2	-11.22	91.92	111.00
1	C	825	ARG	NE-CZ-NH1	11.11	125.85	120.30
1	C	794	ARG	NE-CZ-NH2	-11.09	114.76	120.30
1	A	681	ARG	NE-CZ-NH1	11.06	125.83	120.30
1	A	149	ARG	NE-CZ-NH2	10.96	125.78	120.30
1	B	136	MET	CG-SD-CE	10.93	117.69	100.20
1	A	681	ARG	NE-CZ-NH2	-10.85	114.88	120.30
1	D	532	LEU	CA-CB-CG	10.80	140.15	115.30
1	B	527	LEU	CA-CB-CG	10.74	140.00	115.30
1	D	794	ARG	NE-CZ-NH1	10.58	125.59	120.30
1	C	129	ARG	NE-CZ-NH1	10.49	125.55	120.30
1	C	829	ASP	CB-CG-OD2	-10.42	108.92	118.30
1	D	825	ARG	NE-CZ-NH1	-10.42	115.09	120.30
1	C	708	PHE	N-CA-CB	-10.41	91.86	110.60
1	C	314	ASP	CB-CG-OD1	-10.32	109.01	118.30
1	B	537	GLY	N-CA-C	-10.30	87.34	113.10
1	B	980	ALA	N-CA-C	-10.22	83.41	111.00
1	B	161	ARG	NE-CZ-NH1	10.21	125.40	120.30
1	D	791	ARG	NE-CZ-NH2	10.21	125.40	120.30
1	B	161	ARG	NE-CZ-NH2	-10.09	115.25	120.30
1	B	4	ASP	CB-CA-C	-10.03	90.35	110.40
1	C	866	SER	N-CA-C	9.95	137.85	111.00
1	A	1021	LEU	CB-CG-CD1	-9.94	94.11	111.00
1	A	831	ASP	CB-CG-OD1	-9.88	109.41	118.30
1	C	32	ARG	NE-CZ-NH1	-9.87	115.37	120.30
1	D	599	ARG	CG-CD-NE	9.83	132.44	111.80
1	C	1135	ARG	NE-CZ-NH1	9.82	125.21	120.30
1	B	720	LEU	CA-CB-CG	9.82	137.88	115.30
1	B	1280	ARG	NE-CZ-NH2	-9.82	115.39	120.30
1	B	1135	ARG	NE-CZ-NH1	9.81	125.21	120.30
1	D	97	ARG	NE-CZ-NH1	9.80	125.20	120.30
1	D	794	ARG	NE-CZ-NH2	-9.67	115.46	120.30
1	B	4	ASP	CB-CG-OD1	-9.66	109.61	118.30
1	D	618	ILE	CG1-CB-CG2	-9.60	90.28	111.40
1	C	1298	ASP	CB-CG-OD1	9.54	126.89	118.30
1	A	599	ARG	NE-CZ-NH2	-9.54	115.53	120.30
1	B	394	ARG	NE-CZ-NH2	-9.53	115.53	120.30
1	B	60	ARG	NE-CZ-NH1	9.52	125.06	120.30
1	A	161	ARG	NE-CZ-NH1	9.51	125.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1280	ARG	NE-CZ-NH1	9.41	125.01	120.30
1	A	161	ARG	NE-CZ-NH2	-9.41	115.60	120.30
1	D	927	TRP	CA-CB-CG	9.30	131.37	113.70
1	B	268	MET	CG-SD-CE	9.28	115.05	100.20
1	C	97	ARG	NE-CZ-NH1	9.27	124.93	120.30
1	A	840	ARG	NE-CZ-NH1	9.24	124.92	120.30
1	C	639	ASP	CB-CG-OD1	-9.19	110.03	118.30
1	B	3	ALA	N-CA-C	9.16	135.74	111.00
1	D	1307	ARG	NE-CZ-NH2	-9.13	115.74	120.30
1	D	952	ASP	CB-CG-OD1	9.10	126.49	118.30
1	C	980	ALA	N-CA-C	-9.09	86.46	111.00
1	A	903	LYS	CD-CE-NZ	9.06	132.54	111.70
1	A	720	LEU	CA-CB-CG	9.06	136.13	115.30
1	B	794	ARG	NE-CZ-NH2	-9.06	115.77	120.30
1	C	413	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	C	1331	VAL	CB-CA-C	9.02	128.53	111.40
1	D	599	ARG	CA-CB-CG	9.00	133.21	113.40
1	D	639	ASP	CB-CG-OD1	-8.96	110.24	118.30
1	A	97	ARG	NE-CZ-NH1	8.93	124.76	120.30
1	B	521	LEU	CB-CG-CD2	-8.92	95.84	111.00
1	B	228	ARG	NE-CZ-NH1	-8.90	115.85	120.30
1	C	927	TRP	CA-CB-CG	8.90	130.62	113.70
1	D	720	LEU	CA-CB-CG	8.90	135.78	115.30
1	C	685	GLY	N-CA-C	8.90	135.35	113.10
1	B	462	ARG	NE-CZ-NH1	-8.88	115.86	120.30
1	D	394	ARG	NE-CZ-NH1	8.85	124.72	120.30
1	A	607	ARG	NE-CZ-NH1	-8.82	115.89	120.30
1	B	927	TRP	CA-CB-CG	8.71	130.25	113.70
1	A	277	MET	CG-SD-CE	8.70	114.13	100.20
1	D	1101	ARG	NE-CZ-NH2	-8.69	115.96	120.30
1	D	136	MET	CG-SD-CE	8.68	114.08	100.20
1	D	1021	LEU	CB-CG-CD1	-8.67	96.26	111.00
1	A	708	PHE	N-CA-CB	-8.66	95.01	110.60
1	B	194	SER	N-CA-C	8.66	134.38	111.00
1	D	1031	LEU	CB-CG-CD1	-8.66	96.28	111.00
1	C	165	ARG	NE-CZ-NH2	8.66	124.63	120.30
1	C	532	LEU	CA-CB-CG	8.64	135.18	115.30
1	A	361	LEU	CB-CG-CD2	-8.64	96.31	111.00
1	B	708	PHE	N-CA-CB	-8.64	95.05	110.60
1	D	104	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	B	592	VAL	CB-CA-C	-8.62	95.03	111.40
1	A	1176	ARG	NE-CZ-NH1	-8.61	116.00	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	277	MET	CG-SD-CE	8.57	113.91	100.20
1	A	866	SER	N-CA-CB	-8.57	97.65	110.50
1	B	701	ASP	N-CA-C	-8.54	87.94	111.00
1	C	599	ARG	CA-CB-CG	8.51	132.12	113.40
1	A	685	GLY	N-CA-C	8.50	134.34	113.10
1	A	521	LEU	CB-CG-CD2	-8.45	96.63	111.00
1	B	1099	LEU	CB-CG-CD1	-8.41	96.71	111.00
1	D	685	GLY	N-CA-C	8.39	134.08	113.10
1	A	21	ASP	CB-CG-OD2	-8.34	110.79	118.30
1	C	720	LEU	CA-CB-CG	8.34	134.48	115.30
1	D	952	ASP	CB-CG-OD2	-8.34	110.80	118.30
1	A	394	ARG	NE-CZ-NH1	8.32	124.46	120.30
1	D	1298	ASP	CB-CG-OD2	-8.30	110.83	118.30
1	C	792	VAL	CB-CA-C	-8.24	95.75	111.40
1	D	1187	LEU	CB-CG-CD2	-8.23	97.01	111.00
1	A	840	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	A	701	ASP	N-CA-C	-8.22	88.81	111.00
1	D	31	ARG	NE-CZ-NH1	-8.21	116.19	120.30
1	B	4	ASP	N-CA-C	8.19	133.12	111.00
1	B	1116	ASP	CB-CG-OD1	-8.19	110.92	118.30
1	C	1229	LYS	CD-CE-NZ	8.19	130.53	111.70
1	C	1298	ASP	CB-CG-OD2	-8.18	110.94	118.30
1	D	1099	LEU	CB-CG-CD1	-8.18	97.10	111.00
1	C	1099	LEU	CA-CB-CG	8.16	134.08	115.30
1	C	607	ARG	NE-CZ-NH1	-8.14	116.23	120.30
1	A	640	ASP	CB-CG-OD1	-8.13	110.98	118.30
1	B	597	ILE	CB-CA-C	-8.13	95.34	111.60
1	B	1229	LYS	CD-CE-NZ	8.11	130.36	111.70
1	A	830	ARG	NE-CZ-NH2	-8.11	116.25	120.30
1	B	1307	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	D	1241	ARG	NE-CZ-NH2	-8.09	116.25	120.30
1	A	165	ARG	NE-CZ-NH2	8.06	124.33	120.30
1	A	599	ARG	NE-CZ-NH1	8.05	124.33	120.30
1	B	833	ASP	CB-CG-OD2	8.05	125.54	118.30
1	D	154	ARG	NE-CZ-NH2	8.03	124.32	120.30
1	B	1193	ILE	CB-CA-C	-8.03	95.54	111.60
1	C	404	LEU	CB-CG-CD1	-8.00	97.41	111.00
1	C	903	LYS	CD-CE-NZ	7.99	130.08	111.70
1	D	599	ARG	CB-CA-C	7.96	126.31	110.40
1	D	1229	LYS	CD-CE-NZ	7.95	129.99	111.70
1	C	606	LEU	CB-CG-CD2	-7.94	97.50	111.00
1	C	873	ASP	CB-CG-OD2	7.92	125.43	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	462	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	C	16	VAL	CG1-CB-CG2	-7.90	98.26	110.90
1	C	194	SER	N-CA-C	7.89	132.30	111.00
1	C	149	ARG	NE-CZ-NH2	7.88	124.24	120.30
1	C	157	LEU	CB-CG-CD1	-7.88	97.60	111.00
1	D	521	LEU	CB-CG-CD2	-7.84	97.67	111.00
1	C	584	ASP	CB-CG-OD2	-7.83	111.25	118.30
1	D	1298	ASP	CB-CG-OD1	7.83	125.35	118.30
1	C	88	VAL	CG1-CB-CG2	-7.82	98.38	110.90
1	C	122	MET	CG-SD-CE	-7.82	87.69	100.20
1	D	1085	ASP	CB-CG-OD2	-7.80	111.28	118.30
1	B	903	LYS	CD-CE-NZ	7.75	129.51	111.70
1	D	640	ASP	CB-CG-OD1	-7.74	111.33	118.30
1	B	863	ASP	CB-CG-OD2	7.74	125.26	118.30
1	A	216	LEU	N-CA-C	-7.72	90.15	111.00
1	D	533	GLU	N-CA-C	-7.72	90.16	111.00
1	A	1246	ARG	NE-CZ-NH1	-7.72	116.44	120.30
1	B	2	THR	C-N-CA	7.71	140.99	121.70
1	D	1271	ILE	CG1-CB-CG2	-7.71	94.45	111.40
1	C	205	ASP	CB-CG-OD1	-7.69	111.38	118.30
1	C	873	ASP	CB-CG-OD1	-7.65	111.42	118.30
1	B	529	GLN	N-CA-C	7.64	131.62	111.00
1	A	40	LYS	CD-CE-NZ	7.64	129.26	111.70
1	B	830	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	A	943	ARG	NE-CZ-NH2	7.63	124.12	120.30
1	B	431	ILE	CB-CA-C	7.63	126.86	111.60
1	D	426	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	C	361	LEU	CA-CB-CG	-7.60	97.82	115.30
1	D	28	ALA	N-CA-CB	7.58	120.72	110.10
1	C	247	ASP	CB-CG-OD2	-7.58	111.48	118.30
1	C	161	ARG	NE-CZ-NH2	-7.57	116.52	120.30
1	B	863	ASP	CB-CG-OD1	-7.56	111.50	118.30
1	A	194	SER	N-CA-C	7.52	131.31	111.00
1	B	953	LEU	CB-CG-CD2	-7.52	98.22	111.00
1	B	794	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	B	312	LEU	CB-CG-CD2	7.50	123.76	111.00
1	A	674	ASP	CB-CG-OD1	7.49	125.04	118.30
1	D	165	ARG	CA-CB-CG	-7.47	96.96	113.40
1	A	927	TRP	CA-CB-CG	7.47	127.89	113.70
1	B	1317	LEU	CB-CG-CD2	7.46	123.69	111.00
1	B	40	LYS	CD-CE-NZ	7.45	128.84	111.70
1	D	538	LYS	N-CA-C	7.45	131.13	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	866	SER	N-CA-C	7.45	131.12	111.00
1	C	1204	LEU	CB-CG-CD2	-7.44	98.34	111.00
1	C	753	VAL	C-N-CD	7.44	144.02	128.40
1	B	319	LEU	CB-CG-CD2	-7.44	98.36	111.00
1	D	903	LYS	CD-CE-NZ	7.43	128.80	111.70
1	B	995	LYS	CD-CE-NZ	7.43	128.78	111.70
1	C	599	ARG	CG-CD-NE	7.40	127.34	111.80
1	A	592	VAL	CB-CA-C	-7.39	97.35	111.40
1	C	1116	ASP	CB-CG-OD2	-7.39	111.65	118.30
1	D	194	SER	N-CA-C	7.38	130.93	111.00
1	A	6	LEU	CB-CG-CD2	-7.38	98.46	111.00
1	B	659	ASP	CB-CG-OD2	-7.37	111.67	118.30
1	A	944	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	C	1193	ILE	CB-CA-C	-7.34	96.92	111.60
1	C	701	ASP	N-CA-C	-7.34	91.19	111.00
1	C	380	ARG	NE-CZ-NH2	7.31	123.96	120.30
1	D	1277	ASP	CB-CG-OD1	-7.30	111.73	118.30
1	A	1018	ALA	N-CA-CB	7.28	120.29	110.10
1	D	314	ASP	CB-CG-OD1	-7.26	111.77	118.30
1	B	85	VAL	CB-CA-C	-7.24	97.64	111.40
1	C	597	ILE	CB-CA-C	-7.24	97.12	111.60
1	B	36	LEU	CB-CG-CD2	-7.24	98.69	111.00
1	B	1296	ARG	NE-CZ-NH2	7.22	123.91	120.30
1	C	149	ARG	NE-CZ-NH1	-7.19	116.70	120.30
1	D	1102	LEU	CB-CG-CD1	-7.19	98.77	111.00
1	D	844	LEU	CB-CG-CD2	7.19	123.22	111.00
1	C	204	LEU	CB-CG-CD2	7.17	123.19	111.00
1	C	138	GLU	OE1-CD-OE2	-7.17	114.70	123.30
1	B	840	ARG	NE-CZ-NH1	7.17	123.88	120.30
1	D	652	ASP	CB-CG-OD1	-7.16	111.85	118.30
1	C	1182	ASP	CB-CG-OD1	7.14	124.73	118.30
1	B	287	LEU	CB-CG-CD1	-7.13	98.87	111.00
1	B	927	TRP	N-CA-CB	-7.13	97.77	110.60
1	C	4	ASP	CB-CG-OD2	7.13	124.72	118.30
1	C	531	ASN	N-CA-C	-7.11	91.81	111.00
1	D	639	ASP	CB-CG-OD2	7.10	124.69	118.30
1	C	426	ARG	NE-CZ-NH1	7.09	123.85	120.30
1	A	866	SER	N-CA-C	7.07	130.08	111.00
1	C	413	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	B	1280	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	B	30	LEU	CB-CG-CD2	-7.04	99.03	111.00
1	C	595	ASP	CB-CG-OD2	7.01	124.61	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	195	LEU	N-CA-C	7.00	129.91	111.00
1	D	527	LEU	CA-CB-CG	6.99	131.38	115.30
1	A	1055	LEU	CB-CG-CD2	-6.98	99.14	111.00
1	A	215	GLU	OE1-CD-OE2	6.97	131.67	123.30
1	D	594	CYS	CA-CB-SG	-6.96	101.47	114.00
1	B	1064	ILE	CB-CA-C	-6.95	97.70	111.60
1	C	530	GLU	N-CA-C	6.93	129.72	111.00
1	B	59	ASP	CB-CG-OD1	6.93	124.54	118.30
1	D	708	PHE	N-CA-C	6.93	129.71	111.00
1	B	639	ASP	CB-CG-OD1	-6.91	112.08	118.30
1	B	17	GLU	OE1-CD-OE2	6.91	131.59	123.30
1	A	334	LEU	CB-CG-CD1	-6.90	99.26	111.00
1	C	596	ASP	CB-CG-OD2	6.89	124.50	118.30
1	A	1192	ASP	CB-CG-OD1	6.88	124.49	118.30
1	C	85	VAL	CB-CA-C	-6.88	98.33	111.40
1	C	521	LEU	CB-CG-CD2	-6.87	99.32	111.00
1	D	165	ARG	N-CA-CB	6.87	122.96	110.60
1	C	148	CYS	CA-CB-SG	6.86	126.35	114.00
1	C	1022	LEU	CA-CB-CG	6.86	131.08	115.30
1	A	394	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	D	195	LEU	N-CA-C	6.86	129.52	111.00
1	C	165	ARG	CB-CG-CD	6.85	129.40	111.60
1	C	829	ASP	CB-CG-OD1	6.85	124.46	118.30
1	D	104	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	D	165	ARG	CB-CG-CD	6.83	129.37	111.60
1	D	980	ALA	N-CA-C	-6.83	92.55	111.00
1	D	997	ARG	NE-CZ-NH1	-6.83	116.88	120.30
1	B	13	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	D	824	VAL	CB-CA-C	-6.81	98.46	111.40
1	C	477	LEU	CA-CB-CG	6.81	130.96	115.30
1	A	1247	ASP	CB-CG-OD1	6.80	124.42	118.30
1	A	1298	ASP	CB-CG-OD2	-6.80	112.18	118.30
1	B	924	ALA	N-CA-C	-6.80	92.64	111.00
1	C	364	VAL	CA-CB-CG2	-6.79	100.71	110.90
1	B	4	ASP	OD1-CG-OD2	6.79	136.20	123.30
1	D	32	ARG	NE-CZ-NH2	-6.77	116.91	120.30
1	C	1039	MET	CB-CA-C	-6.77	96.87	110.40
1	C	45	GLU	N-CA-CB	-6.76	98.42	110.60
1	C	927	TRP	N-CA-CB	-6.76	98.43	110.60
1	D	161	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	C	141	ASN	N-CA-CB	-6.76	98.43	110.60
1	D	361	LEU	CA-CB-CG	-6.75	99.76	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	313	VAL	CB-CA-C	-6.75	98.57	111.40
1	B	541	PRO	N-CA-C	6.72	129.58	112.10
1	B	165	ARG	NE-CZ-NH2	6.72	123.66	120.30
1	B	827	MET	CG-SD-CE	-6.72	89.45	100.20
1	D	606	LEU	CB-CG-CD2	-6.72	99.58	111.00
1	B	833	ASP	CB-CG-OD1	-6.71	112.26	118.30
1	B	46	GLY	N-CA-C	6.71	129.86	113.10
1	B	866	SER	N-CA-CB	-6.67	100.49	110.50
1	A	686	VAL	CG1-CB-CG2	-6.67	100.24	110.90
1	A	608	LEU	CB-CG-CD2	-6.66	99.67	111.00
1	D	535	LYS	N-CA-C	-6.63	93.09	111.00
1	B	6	LEU	CB-CG-CD2	-6.62	99.75	111.00
1	C	944	ARG	CA-CB-CG	6.60	127.93	113.40
1	B	60	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	A	1008	ILE	CG1-CB-CG2	-6.59	96.89	111.40
1	A	1319	VAL	N-CA-C	6.59	128.80	111.00
1	A	919	GLN	CA-C-N	-6.59	103.02	116.20
1	B	599	ARG	CA-CB-CG	6.56	127.83	113.40
1	C	1171	ASP	CB-CG-OD1	6.56	124.20	118.30
1	A	348	VAL	CB-CA-C	-6.55	98.96	111.40
1	B	1218	GLY	N-CA-C	6.54	129.44	113.10
1	D	927	TRP	N-CA-CB	-6.53	98.84	110.60
1	D	863	ASP	CB-CG-OD2	6.53	124.18	118.30
1	B	59	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	D	157	LEU	CB-CG-CD1	-6.51	99.94	111.00
1	B	787	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	B	558	VAL	CG1-CB-CG2	6.50	121.29	110.90
1	A	129	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	A	913	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	C	6	LEU	CB-CG-CD1	6.48	122.02	111.00
1	C	866	SER	N-CA-CB	-6.47	100.80	110.50
1	D	305	LEU	CB-CG-CD1	6.45	121.97	111.00
1	D	1204	LEU	CB-CG-CD2	-6.44	100.05	111.00
1	B	881	ARG	NE-CZ-NH1	-6.42	117.09	120.30
1	C	1031	LEU	CB-CG-CD1	-6.42	100.09	111.00
1	B	1319	VAL	CB-CA-C	6.42	123.59	111.40
1	D	361	LEU	CB-CG-CD2	-6.41	100.10	111.00
1	B	1022	LEU	CB-CA-C	6.41	122.38	110.20
1	B	1064	ILE	CG1-CB-CG2	-6.41	97.30	111.40
1	C	863	ASP	CB-CG-OD1	-6.41	112.53	118.30
1	C	136	MET	CG-SD-CE	6.41	110.45	100.20
1	D	36	LEU	CB-CG-CD2	-6.40	100.12	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	318	LYS	CD-CE-NZ	6.39	126.41	111.70
1	B	825	ARG	NE-CZ-NH1	-6.39	117.10	120.30
1	B	607	ARG	CB-CA-C	-6.39	97.61	110.40
1	B	295	ASP	CB-CG-OD1	-6.38	112.56	118.30
1	D	921	MET	N-CA-C	-6.36	93.83	111.00
1	C	921	MET	N-CA-C	-6.36	93.83	111.00
1	C	319	LEU	CB-CG-CD2	-6.36	100.19	111.00
1	A	312	LEU	CB-CG-CD2	6.34	121.78	111.00
1	C	572	ASP	CB-CG-OD1	6.34	124.00	118.30
1	D	581	LEU	CB-CG-CD2	-6.33	100.23	111.00
1	C	161	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	D	1160	CYS	CA-CB-SG	-6.32	102.62	114.00
1	A	165	ARG	N-CA-CB	6.32	121.97	110.60
1	A	195	LEU	N-CA-C	6.31	128.03	111.00
1	B	147	LEU	CA-CB-CG	6.30	129.80	115.30
1	A	219	LEU	CB-CG-CD2	6.29	121.70	111.00
1	A	943	ARG	NE-CZ-NH1	-6.27	117.16	120.30
1	D	848	LYS	CD-CE-NZ	6.26	126.09	111.70
1	A	717	LYS	CD-CE-NZ	6.26	126.09	111.70
1	C	40	LYS	CD-CE-NZ	6.25	126.08	111.70
1	A	381	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	A	345	VAL	N-CA-C	6.23	127.81	111.00
1	C	66	VAL	CB-CA-C	-6.22	99.58	111.40
1	A	927	TRP	N-CA-CB	-6.21	99.41	110.60
1	C	165	ARG	CA-CB-CG	-6.21	99.73	113.40
1	A	227	LEU	CB-CG-CD2	-6.21	100.44	111.00
1	B	461	ASN	CB-CA-C	-6.21	97.98	110.40
1	D	804	THR	CB-CA-C	-6.21	94.85	111.60
1	A	1085	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	D	943	ARG	NE-CZ-NH2	6.20	123.40	120.30
1	D	526	LYS	CD-CE-NZ	6.20	125.96	111.70
1	A	654	THR	CB-CA-C	-6.19	94.89	111.60
1	B	233	ARG	NE-CZ-NH2	6.19	123.39	120.30
1	A	377	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	B	149	ARG	NE-CZ-NH1	-6.19	117.21	120.30
1	B	913	ARG	NE-CZ-NH2	6.19	123.39	120.30
1	C	824	VAL	CB-CA-C	-6.18	99.66	111.40
1	D	995	LYS	CD-CE-NZ	6.17	125.90	111.70
1	B	277	MET	CG-SD-CE	6.16	110.06	100.20
1	A	467	LEU	N-CA-C	6.15	127.61	111.00
1	D	592	VAL	CB-CA-C	-6.15	99.71	111.40
1	A	995	LYS	CD-CE-NZ	6.15	125.84	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	372	LEU	CB-CG-CD2	6.15	121.45	111.00
1	C	216	LEU	N-CA-C	-6.15	94.41	111.00
1	C	607	ARG	CB-CA-C	-6.14	98.11	110.40
1	C	128	LEU	CA-CB-CG	-6.13	101.20	115.30
1	B	165	ARG	CA-CB-CG	-6.13	99.92	113.40
1	B	919	GLN	CA-C-N	-6.13	103.95	116.20
1	B	1031	LEU	CB-CG-CD1	-6.13	100.58	111.00
1	B	431	ILE	CA-CB-CG1	6.12	122.63	111.00
1	C	147	LEU	CB-CG-CD1	-6.12	100.59	111.00
1	C	461	ASN	CB-CA-C	-6.12	98.16	110.40
1	A	952	ASP	CB-CG-OD1	6.12	123.80	118.30
1	B	335	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	C	427	ARG	CD-NE-CZ	6.11	132.16	123.60
1	A	844	LEU	CB-CG-CD2	6.11	121.39	111.00
1	B	104	ARG	NE-CZ-NH1	-6.11	117.24	120.30
1	D	886	MET	CG-SD-CE	6.11	109.97	100.20
1	D	147	LEU	CA-CB-CG	6.10	129.34	115.30
1	B	242	LEU	CB-CG-CD1	6.10	121.37	111.00
1	D	792	VAL	CB-CA-C	-6.09	99.83	111.40
1	A	1204	LEU	CB-CG-CD2	-6.08	100.67	111.00
1	A	1193	ILE	CB-CA-C	-6.07	99.45	111.60
1	A	64	LYS	O-C-N	-6.07	112.99	122.70
1	B	328	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	C	794	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	D	461	ASN	CB-CA-C	-6.06	98.28	110.40
1	C	1261	GLY	N-CA-C	6.06	128.25	113.10
1	C	836	ILE	CB-CA-C	-6.06	99.49	111.60
1	D	701	ASP	N-CA-C	-6.06	94.65	111.00
1	D	1002	ILE	CG1-CB-CG2	-6.05	98.09	111.40
1	A	1223	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	D	194	SER	N-CA-CB	-6.04	101.43	110.50
1	B	825	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	D	1299	SER	CB-CA-C	-6.04	98.62	110.10
1	A	749	CYS	CA-CB-SG	-6.03	103.14	114.00
1	A	937	MET	N-CA-C	6.03	127.28	111.00
1	B	128	LEU	CB-CG-CD2	-6.03	100.75	111.00
1	B	824	VAL	CB-CA-C	-6.02	99.96	111.40
1	D	462	ARG	NE-CZ-NH1	-6.02	117.29	120.30
1	A	1319	VAL	CA-CB-CG2	6.01	119.91	110.90
1	C	49	GLY	N-CA-C	6.01	128.12	113.10
1	B	257	LEU	CB-CA-C	-6.01	98.78	110.20
1	A	925	GLU	N-CA-C	-6.00	94.79	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1031	LEU	N-CA-C	6.00	127.20	111.00
1	C	427	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	A	822	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	B	685	GLY	N-CA-C	5.98	128.06	113.10
1	D	128	LEU	CB-CG-CD2	-5.98	100.84	111.00
1	C	606	LEU	CA-CB-CG	5.98	129.04	115.30
1	D	827	MET	CG-SD-CE	-5.97	90.65	100.20
1	A	746	GLU	OE1-CD-OE2	-5.97	116.14	123.30
1	D	1022	LEU	CA-CB-CG	5.96	129.02	115.30
1	B	1187	LEU	CB-CG-CD2	-5.96	100.86	111.00
1	B	407	ILE	CG1-CB-CG2	-5.96	98.28	111.40
1	A	576	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	B	1031	LEU	CB-CG-CD2	5.95	121.12	111.00
1	A	935	CYS	CA-CB-SG	-5.95	103.30	114.00
1	B	545	SER	N-CA-C	5.94	127.04	111.00
1	A	310	LYS	CD-CE-NZ	5.94	125.36	111.70
1	A	342	VAL	CG1-CB-CG2	5.93	120.40	110.90
1	B	1317	LEU	CA-CB-CG	5.93	128.95	115.30
1	A	660	LYS	CD-CE-NZ	5.91	125.30	111.70
1	D	1166	ASP	CB-CG-OD1	5.91	123.62	118.30
1	C	1178	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	B	776	PHE	CB-CA-C	-5.89	98.61	110.40
1	D	681	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	B	1039	MET	CB-CG-SD	-5.89	94.73	112.40
1	C	165	ARG	N-CA-CB	5.88	121.19	110.60
1	D	335	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	403	ILE	CB-CA-C	-5.87	99.87	111.60
1	D	1135	ARG	NH1-CZ-NH2	-5.86	112.95	119.40
1	C	403	ILE	CB-CA-C	-5.86	99.88	111.60
1	A	898	THR	CB-CA-C	-5.86	95.79	111.60
1	A	136	MET	CG-SD-CE	5.85	109.56	100.20
1	A	570	GLU	OE1-CD-OE2	-5.85	116.28	123.30
1	B	1008	ILE	CG1-CB-CG2	-5.85	98.53	111.40
1	D	944	ARG	CA-CB-CG	5.84	126.25	113.40
1	B	641	VAL	C-N-CD	5.83	140.65	128.40
1	A	1175	LEU	N-CA-C	5.83	126.75	111.00
1	C	274	LEU	CB-CG-CD2	5.83	120.91	111.00
1	B	28	ALA	N-CA-CB	5.83	118.25	110.10
1	C	640	ASP	CB-CG-OD1	-5.82	113.06	118.30
1	B	65	ILE	CG1-CB-CG2	-5.81	98.61	111.40
1	A	104	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	D	576	ARG	NE-CZ-NH2	-5.81	117.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	527	LEU	CA-CB-CG	5.81	128.66	115.30
1	D	844	LEU	CB-CG-CD1	-5.81	101.12	111.00
1	C	335	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	C	347	SER	N-CA-CB	-5.80	101.80	110.50
1	B	598	PRO	N-CA-C	5.79	127.16	112.10
1	C	599	ARG	NH1-CZ-NH2	-5.79	113.03	119.40
1	B	23	GLU	OE1-CD-OE2	5.79	130.25	123.30
1	B	371	LYS	CD-CE-NZ	5.79	125.02	111.70
1	D	873	ASP	CB-CG-OD1	-5.79	113.09	118.30
1	C	1204	LEU	CB-CG-CD1	5.79	120.84	111.00
1	C	595	ASP	CB-CG-OD1	-5.79	113.09	118.30
1	B	165	ARG	N-CA-CB	5.78	121.01	110.60
1	B	131	GLN	CB-CA-C	5.78	121.96	110.40
1	C	529	GLN	N-CA-C	5.77	126.58	111.00
1	A	331	LEU	CA-CB-CG	5.76	128.55	115.30
1	C	822	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	1218	GLY	N-CA-C	5.76	127.50	113.10
1	D	600	TYR	CB-CA-C	-5.76	98.88	110.40
1	D	986	ASP	N-CA-C	-5.75	95.46	111.00
1	A	608	LEU	CA-CB-CG	5.75	128.53	115.30
1	B	279	VAL	CG1-CB-CG2	-5.75	101.70	110.90
1	C	830	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	D	1194	GLY	N-CA-C	-5.74	98.74	113.10
1	A	477	LEU	CA-CB-CG	5.74	128.50	115.30
1	B	744	TYR	C-N-CA	-5.74	107.36	121.70
1	D	863	ASP	CB-CG-OD1	-5.74	113.14	118.30
1	A	207	THR	CB-CA-C	-5.73	96.12	111.60
1	D	840	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	A	433	LYS	CD-CE-NZ	-5.73	98.52	111.70
1	A	27	LEU	CB-CG-CD1	-5.72	101.27	111.00
1	D	746	GLU	N-CA-C	-5.72	95.54	111.00
1	D	1312	ASP	CB-CG-OD1	5.72	123.45	118.30
1	B	355	ALA	N-CA-C	5.72	126.44	111.00
1	B	654	THR	CB-CA-C	-5.72	96.16	111.60
1	B	1071	THR	CA-CB-CG2	-5.72	104.39	112.40
1	C	335	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	D	24	THR	CA-CB-CG2	-5.71	104.41	112.40
1	A	690	TYR	CA-CB-CG	5.71	124.24	113.40
1	C	636	ILE	CA-CB-CG2	5.71	122.31	110.90
1	D	65	ILE	CG1-CB-CG2	-5.70	98.85	111.40
1	B	834	MET	CB-CG-SD	-5.70	95.30	112.40
1	B	1331	VAL	CB-CA-C	5.69	122.21	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	246	LEU	CB-CG-CD1	-5.68	101.34	111.00
1	A	610	THR	N-CA-C	5.68	126.35	111.00
1	B	1162	GLU	OE1-CD-OE2	-5.68	116.48	123.30
1	A	719	ASP	N-CA-CB	5.68	120.82	110.60
1	B	227	LEU	CB-CG-CD1	-5.67	101.36	111.00
1	D	1116	ASP	CB-CG-OD1	5.67	123.40	118.30
1	B	45	GLU	N-CA-CB	-5.66	100.40	110.60
1	B	609	VAL	CB-CA-C	-5.66	100.65	111.40
1	B	369	GLY	N-CA-C	-5.66	98.95	113.10
1	C	28	ALA	N-CA-CB	5.66	118.02	110.10
1	D	751	ILE	CG1-CB-CG2	-5.66	98.95	111.40
1	A	28	ALA	N-CA-CB	5.65	118.01	110.10
1	D	578	LEU	CB-CG-CD1	5.64	120.60	111.00
1	D	945	LYS	CD-CE-NZ	5.64	124.68	111.70
1	B	1048	VAL	CG1-CB-CG2	-5.64	101.88	110.90
1	D	1055	LEU	CA-CB-CG	5.64	128.27	115.30
1	A	829	ASP	CB-CA-C	-5.63	99.14	110.40
1	B	127	LEU	CB-CG-CD2	-5.63	101.43	111.00
1	D	39	THR	N-CA-C	-5.63	95.81	111.00
1	B	896	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	B	533	GLU	N-CA-CB	5.62	120.72	110.60
1	B	381	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	C	609	VAL	CB-CA-C	-5.62	100.72	111.40
1	C	345	VAL	N-CA-C	5.62	126.17	111.00
1	B	467	LEU	CB-CG-CD1	5.62	120.55	111.00
1	A	941	GLU	OE1-CD-OE2	-5.61	116.57	123.30
1	D	467	LEU	CB-CG-CD1	5.61	120.54	111.00
1	B	558	VAL	N-CA-CB	-5.61	99.16	111.50
1	B	825	ARG	NH1-CZ-NH2	5.61	125.57	119.40
1	C	608	LEU	CA-CB-CG	5.61	128.20	115.30
1	B	1182	ASP	CB-CG-OD1	5.61	123.35	118.30
1	C	37	SER	C-N-CA	-5.61	110.52	122.30
1	C	318	LYS	CD-CE-NZ	5.61	124.59	111.70
1	B	1192	ASP	CB-CG-OD1	5.60	123.34	118.30
1	B	1227	THR	CA-CB-CG2	-5.60	104.56	112.40
1	A	269	LYS	CD-CE-NZ	5.60	124.58	111.70
1	A	1320	THR	N-CA-CB	5.60	120.94	110.30
1	A	749	CYS	N-CA-C	5.59	126.10	111.00
1	B	1018	ALA	N-CA-CB	5.59	117.93	110.10
1	C	1178	ASP	CB-CG-OD1	5.59	123.33	118.30
1	C	1332	ARG	N-CA-C	5.59	126.09	111.00
1	C	36	LEU	CB-CG-CD1	-5.59	101.50	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	902	CYS	CA-CB-SG	-5.58	103.95	114.00
1	C	521	LEU	CA-CB-CG	-5.58	102.46	115.30
1	D	1086	LEU	CB-CG-CD2	-5.58	101.51	111.00
1	A	408	GLU	OE1-CD-OE2	5.58	129.99	123.30
1	C	128	LEU	CB-CG-CD2	-5.58	101.52	111.00
1	C	530	GLU	CA-C-N	-5.57	104.94	117.20
1	D	609	VAL	CB-CA-C	-5.57	100.82	111.40
1	B	233	ARG	NE-CZ-NH1	-5.57	117.52	120.30
1	B	1163	VAL	CB-CA-C	-5.57	100.82	111.40
1	D	1245	LEU	O-C-N	5.57	131.60	122.70
1	B	219	LEU	CB-CG-CD2	5.56	120.46	111.00
1	C	331	LEU	CB-CG-CD2	5.56	120.46	111.00
1	B	599	ARG	CB-CG-CD	-5.56	97.15	111.60
1	D	394	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	D	1171	ASP	CB-CG-OD1	5.56	123.30	118.30
1	A	1064	ILE	CB-CA-C	-5.55	100.49	111.60
1	D	141	ASN	N-CA-CB	-5.55	100.61	110.60
1	B	703	ILE	CB-CA-C	-5.55	100.50	111.60
1	A	508	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	A	671	VAL	CG1-CB-CG2	-5.55	102.03	110.90
1	C	599	ARG	CD-NE-CZ	5.54	131.36	123.60
1	C	119	GLY	N-CA-C	5.53	126.93	113.10
1	A	585	MET	CG-SD-CE	-5.53	91.36	100.20
1	C	1116	ASP	CB-CG-OD1	5.52	123.27	118.30
1	D	1328	PRO	N-CA-C	5.52	126.46	112.10
1	B	1098	ILE	CG1-CB-CG2	-5.52	99.26	111.40
1	B	1319	VAL	CA-C-O	5.52	131.69	120.10
1	C	719	ASP	N-CA-CB	5.52	120.53	110.60
1	D	335	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	572	ASP	CB-CG-OD1	5.52	123.27	118.30
1	D	49	GLY	N-CA-C	5.51	126.89	113.10
1	B	594	CYS	CA-CB-SG	-5.51	104.08	114.00
1	B	922	LEU	CB-CG-CD2	5.51	120.36	111.00
1	C	967	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	D	25	THR	OG1-CB-CG2	-5.51	97.33	110.00
1	C	257	LEU	CA-CB-CG	5.51	127.96	115.30
1	B	1234	GLY	N-CA-C	5.50	126.86	113.10
1	A	275	PHE	N-CA-C	-5.50	96.15	111.00
1	B	1180	VAL	CB-CA-C	-5.49	100.96	111.40
1	C	844	LEU	CB-CG-CD2	5.49	120.34	111.00
1	B	937	MET	N-CA-C	5.49	125.83	111.00
1	B	600	TYR	CB-CG-CD1	-5.49	117.71	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	720	LEU	N-CA-C	-5.49	96.18	111.00
1	D	898	THR	CB-CA-C	-5.49	96.78	111.60
1	D	1018	ALA	N-CA-CB	5.49	117.78	110.10
1	B	165	ARG	CB-CG-CD	5.49	125.86	111.60
1	C	472	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	C	247	ASP	CB-CG-OD1	5.48	123.24	118.30
1	A	21	ASP	CB-CG-OD1	5.48	123.23	118.30
1	A	131	GLN	N-CA-C	-5.48	96.20	111.00
1	B	37	SER	C-N-CA	-5.48	110.80	122.30
1	A	338	ALA	N-CA-C	5.47	125.78	111.00
1	D	1099	LEU	CA-CB-CG	5.47	127.89	115.30
1	D	97	ARG	CD-NE-CZ	5.47	131.25	123.60
1	B	787	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	B	593	TYR	CA-CB-CG	-5.46	103.03	113.40
1	D	756	GLY	N-CA-C	5.46	126.74	113.10
1	B	319	LEU	CA-CB-CG	-5.46	102.75	115.30
1	D	529	GLN	N-CA-C	5.46	125.73	111.00
1	D	719	ASP	N-CA-C	-5.43	96.33	111.00
1	D	1241	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	B	131	GLN	C-N-CD	5.43	139.81	128.40
1	B	1175	LEU	N-CA-C	5.43	125.65	111.00
1	D	868	VAL	CA-CB-CG2	-5.43	102.76	110.90
1	A	1299	SER	CB-CA-C	-5.42	99.79	110.10
1	C	405	LEU	CB-CG-CD1	-5.42	101.78	111.00
1	C	15	VAL	CG1-CB-CG2	-5.42	102.23	110.90
1	C	513	LEU	CA-CB-CG	5.41	127.75	115.30
1	D	5	LYS	CB-CA-C	5.41	121.23	110.40
1	C	30	LEU	CB-CG-CD2	-5.41	101.80	111.00
1	D	204	LEU	CB-CG-CD2	5.41	120.20	111.00
1	B	1241	ARG	N-CA-CB	-5.41	100.86	110.60
1	B	310	LYS	CD-CE-NZ	5.41	124.13	111.70
1	A	16	VAL	CA-CB-CG2	-5.40	102.80	110.90
1	A	662	THR	CA-CB-CG2	5.40	119.96	112.40
1	A	1229	LYS	CD-CE-NZ	5.40	124.11	111.70
1	A	1234	GLY	N-CA-C	5.39	126.57	113.10
1	A	97	ARG	CD-NE-CZ	5.39	131.14	123.60
1	A	1022	LEU	CA-CB-CG	5.39	127.69	115.30
1	B	248	LEU	CB-CG-CD1	5.38	120.16	111.00
1	D	1124	ASP	CB-CG-OD2	5.38	123.14	118.30
1	C	97	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	B	808	VAL	N-CA-CB	5.37	123.31	111.50
1	B	532	LEU	CB-CG-CD2	5.36	120.11	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	539	LEU	CA-CB-CG	-5.36	102.98	115.30
1	B	3	ALA	CB-CA-C	-5.35	102.07	110.10
1	C	1086	LEU	CA-CB-CG	-5.34	103.01	115.30
1	B	366	MET	CG-SD-CE	5.34	108.75	100.20
1	A	1168	LEU	CA-CB-CG	-5.34	103.01	115.30
1	C	533	GLU	N-CA-C	5.33	125.40	111.00
1	D	331	LEU	CA-CB-CG	5.33	127.56	115.30
1	C	127	LEU	CB-CG-CD1	-5.32	101.95	111.00
1	D	997	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	D	506	ASP	CB-CG-OD1	5.32	123.09	118.30
1	D	636	ILE	CA-CB-CG2	5.32	121.54	110.90
1	C	76	PRO	C-N-CA	-5.31	108.42	121.70
1	A	509	CYS	CA-CB-SG	-5.31	104.44	114.00
1	A	1166	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	B	967	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	A	880	GLU	OE1-CD-OE2	-5.31	116.93	123.30
1	C	705	ASN	CB-CA-C	-5.31	99.79	110.40
1	D	919	GLN	CA-C-N	-5.31	105.59	116.20
1	C	1031	LEU	N-CA-C	5.30	125.32	111.00
1	B	1026	THR	N-CA-C	5.29	125.30	111.00
1	D	345	VAL	N-CA-C	5.29	125.30	111.00
1	C	1011	THR	N-CA-CB	5.29	120.36	110.30
1	A	361	LEU	CB-CG-CD1	-5.29	102.01	111.00
1	A	1133	PHE	N-CA-CB	-5.29	101.09	110.60
1	D	268	MET	CG-SD-CE	5.28	108.65	100.20
1	C	536	CYS	CB-CA-C	-5.28	99.84	110.40
1	B	1111	SER	CB-CA-C	-5.28	100.07	110.10
1	D	7	VAL	CA-CB-CG1	-5.28	102.98	110.90
1	D	913	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	A	225	LYS	CD-CE-NZ	5.28	123.83	111.70
1	A	1126	VAL	CB-CA-C	-5.28	101.38	111.40
1	C	358	ILE	CG1-CB-CG2	-5.28	99.80	111.40
1	D	278	ILE	CB-CA-C	-5.28	101.05	111.60
1	A	111	SER	N-CA-C	-5.27	96.76	111.00
1	C	848	LYS	CD-CE-NZ	5.27	123.83	111.70
1	A	973	LEU	CA-CB-CG	5.27	127.42	115.30
1	B	467	LEU	N-CA-C	5.27	125.23	111.00
1	A	40	LYS	CB-CG-CD	5.27	125.30	111.60
1	B	1119	THR	N-CA-CB	5.27	120.31	110.30
1	D	1313	LYS	CD-CE-NZ	-5.27	99.58	111.70
1	D	936	GLY	N-CA-C	-5.27	99.94	113.10
1	B	789	VAL	CA-CB-CG2	-5.26	103.00	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	532	LEU	CB-CG-CD1	5.26	119.95	111.00
1	C	426	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	C	511	LEU	CB-CG-CD1	5.26	119.94	111.00
1	C	827	MET	CG-SD-CE	-5.26	91.79	100.20
1	A	27	LEU	C-N-CA	-5.25	108.56	121.70
1	B	339	GLY	N-CA-C	5.25	126.23	113.10
1	C	1064	ILE	CA-CB-CG1	5.25	120.98	111.00
1	B	521	LEU	CA-CB-CG	-5.25	103.23	115.30
1	D	539	LEU	CB-CG-CD2	5.24	119.91	111.00
1	A	568	GLN	N-CA-C	5.23	125.12	111.00
1	A	900	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	B	129	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	C	1194	GLY	N-CA-C	-5.23	100.03	113.10
1	C	1071	THR	CA-CB-CG2	-5.22	105.08	112.40
1	C	1223	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	C	1099	LEU	CB-CG-CD1	-5.22	102.13	111.00
1	A	197	LYS	C-N-CD	5.22	139.36	128.40
1	D	947	LEU	CA-CB-CG	-5.22	103.30	115.30
1	B	719	ASP	N-CA-CB	5.22	119.99	110.60
1	B	290	VAL	CB-CA-C	-5.21	101.49	111.40
1	C	922	LEU	CB-CG-CD2	5.21	119.86	111.00
1	A	641	VAL	C-N-CD	5.21	139.35	128.40
1	A	936	GLY	N-CA-C	-5.21	100.07	113.10
1	B	513	LEU	CA-CB-CG	5.21	127.28	115.30
1	C	592	VAL	CB-CA-C	-5.21	101.50	111.40
1	C	310	LYS	CD-CE-NZ	5.21	123.67	111.70
1	D	505	VAL	CG1-CB-CG2	5.21	119.23	110.90
1	A	833	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	1180	VAL	CB-CA-C	-5.20	101.52	111.40
1	A	1280	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	B	483	LEU	CB-CG-CD2	-5.20	102.16	111.00
1	D	80	LEU	CA-CB-CG	-5.20	103.33	115.30
1	B	1204	LEU	CA-CB-CG	5.20	127.25	115.30
1	A	776	PHE	CB-CA-C	-5.20	100.01	110.40
1	C	295	ASP	CB-CG-OD1	-5.20	113.62	118.30
1	A	165	ARG	CA-CB-CG	-5.19	101.98	113.40
1	A	467	LEU	CB-CG-CD1	5.19	119.82	111.00
1	C	719	ASP	N-CA-C	-5.19	96.99	111.00
1	D	1193	ILE	CG1-CB-CG2	-5.19	99.99	111.40
1	A	756	GLY	N-CA-C	5.18	126.06	113.10
1	B	97	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	B	405	LEU	CB-CG-CD2	5.18	119.81	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	543	PHE	N-CA-C	5.18	125.00	111.00
1	B	54	MET	N-CA-C	5.18	124.99	111.00
1	B	247	ASP	CB-CG-OD1	5.18	122.97	118.30
1	B	131	GLN	N-CA-C	-5.18	97.02	111.00
1	B	828	LEU	CB-CG-CD1	5.18	119.80	111.00
1	B	1297	LEU	CB-CG-CD1	-5.18	102.20	111.00
1	D	46	GLY	N-CA-C	5.18	126.04	113.10
1	A	318	LYS	CB-CG-CD	5.17	125.05	111.60
1	C	246	LEU	CB-CG-CD2	-5.17	102.21	111.00
1	B	246	LEU	CA-CB-CG	-5.17	103.41	115.30
1	B	1296	ARG	NE-CZ-NH1	-5.17	117.72	120.30
1	C	434	VAL	CB-CA-C	-5.17	101.58	111.40
1	B	913	ARG	NE-CZ-NH1	-5.17	117.72	120.30
1	A	315	ALA	CB-CA-C	5.16	117.84	110.10
1	C	1218	GLY	N-CA-C	5.16	126.00	113.10
1	B	195	LEU	N-CA-C	5.15	124.91	111.00
1	A	835	LEU	CB-CG-CD1	-5.15	102.25	111.00
1	C	936	GLY	N-CA-C	-5.15	100.23	113.10
1	D	1234	GLY	N-CA-C	5.15	125.97	113.10
1	D	1316	THR	CB-CA-C	-5.15	97.69	111.60
1	A	257	LEU	CB-CG-CD1	-5.15	102.25	111.00
1	B	667	ILE	CG1-CB-CG2	5.15	122.72	111.40
1	C	690	TYR	CA-CB-CG	5.15	123.18	113.40
1	C	427	ARG	N-CA-CB	5.14	119.86	110.60
1	A	1102	LEU	CB-CG-CD1	-5.14	102.26	111.00
1	D	246	LEU	CA-CB-CG	-5.14	103.48	115.30
1	A	628	LYS	CA-CB-CG	5.14	124.70	113.40
1	D	567	GLY	N-CA-C	5.14	125.94	113.10
1	B	619	LYS	CD-CE-NZ	5.13	123.51	111.70
1	C	254	ASP	CB-CG-OD1	5.13	122.92	118.30
1	D	360	ASP	CB-CG-OD2	5.12	122.91	118.30
1	C	539	LEU	CB-CG-CD1	-5.12	102.29	111.00
1	C	1220	LEU	CA-CB-CG	5.12	127.08	115.30
1	A	431	ILE	N-CA-CB	-5.12	99.02	110.80
1	A	617	LYS	CD-CE-NZ	5.12	123.48	111.70
1	A	1078	THR	CA-CB-CG2	-5.12	105.23	112.40
1	D	1101	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	C	599	ARG	CB-CA-C	5.11	120.63	110.40
1	C	339	GLY	N-CA-C	5.11	125.88	113.10
1	C	846	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	B	225	LYS	CD-CE-NZ	5.11	123.45	111.70
1	D	197	LYS	C-N-CD	5.11	139.13	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1038	GLU	CG-CD-OE2	-5.11	108.08	118.30
1	B	314	ASP	CB-CG-OD1	-5.11	113.70	118.30
1	B	1201	VAL	CG1-CB-CG2	-5.11	102.73	110.90
1	D	257	LEU	CB-CA-C	-5.10	100.51	110.20
1	A	681	ARG	CB-CG-CD	5.09	124.85	111.60
1	C	124	MET	CG-SD-CE	-5.09	92.05	100.20
1	D	40	LYS	CD-CE-NZ	5.09	123.41	111.70
1	B	808	VAL	CB-CA-C	-5.09	101.73	111.40
1	C	162	THR	OG1-CB-CG2	-5.09	98.30	110.00
1	A	603	GLU	C-N-CA	-5.08	108.99	121.70
1	B	919	GLN	N-CA-CB	5.08	119.75	110.60
1	B	688	ILE	CG1-CB-CG2	-5.08	100.22	111.40
1	B	557	ASP	CB-CG-OD1	5.08	122.87	118.30
1	C	27	LEU	C-N-CA	-5.08	109.00	121.70
1	B	1246	ARG	NE-CZ-NH2	5.08	122.84	120.30
1	A	1317	LEU	CA-CB-CG	5.07	126.96	115.30
1	D	572	ASP	CB-CG-OD1	5.07	122.86	118.30
1	A	619	LYS	CD-CE-NZ	5.07	123.35	111.70
1	C	222	THR	N-CA-CB	-5.06	100.68	110.30
1	D	334	LEU	CB-CG-CD2	-5.06	102.39	111.00
1	D	1039	MET	CB-CA-C	-5.06	100.27	110.40
1	A	652	ASP	CB-CA-C	-5.06	100.28	110.40
1	A	1098	ILE	CG1-CB-CG2	-5.06	100.27	111.40
1	A	430	ASP	C-N-CA	5.06	134.34	121.70
1	A	829	ASP	CB-CG-OD2	-5.05	113.75	118.30
1	C	572	ASP	CB-CG-OD2	-5.05	113.75	118.30
1	A	831	ASP	CB-CG-OD2	5.05	122.85	118.30
1	A	997	ARG	NE-CZ-NH1	-5.05	117.78	120.30
1	A	558	VAL	CG1-CB-CG2	5.05	118.98	110.90
1	C	219	LEU	CB-CG-CD1	-5.04	102.43	111.00
1	B	35	GLY	N-CA-C	5.04	125.70	113.10
1	B	147	LEU	CB-CA-C	-5.04	100.62	110.20
1	B	944	ARG	CA-CB-CG	5.04	124.48	113.40
1	C	537	GLY	N-CA-C	-5.04	100.51	113.10
1	C	313	VAL	CB-CA-C	-5.03	101.84	111.40
1	C	578	LEU	CB-CG-CD1	5.03	119.56	111.00
1	C	680	GLN	CB-CA-C	-5.03	100.33	110.40
1	D	954	THR	CA-CB-CG2	-5.03	105.35	112.40
1	C	165	ARG	NE-CZ-NH1	-5.03	117.79	120.30
1	A	131	GLN	CA-CB-CG	5.03	124.45	113.40
1	C	21	ASP	CB-CA-C	-5.03	100.35	110.40
1	C	246	LEU	CB-CG-CD1	-5.02	102.46	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1328	PRO	N-CA-C	5.02	125.14	112.10
1	A	232	GLU	OE1-CD-OE2	-5.02	117.28	123.30
1	D	515	PHE	CG-CD2-CE2	-5.02	115.28	120.80
1	A	299	PHE	CB-CA-C	-5.01	100.37	110.40
1	C	496	LEU	CB-CG-CD2	-5.01	102.48	111.00
1	D	681	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	A	920	GLY	N-CA-C	5.00	125.61	113.10
1	C	40	LYS	CB-CG-CD	5.00	124.60	111.60

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	Mainchain,Peptide
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	Mainchain,Peptide
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	Mainchain,Peptide
1	B	892	ILE	Peptide
1	B	920	GLY	Mainchain,Peptide
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	Mainchain,Peptide
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	Mainchain,Peptide
1	C	926	CYS	Peptide
1	C	936	GLY	Peptide
1	C	937	MET	Peptide
1	C	979	HIS	Mainchain,Peptide
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	Mainchain,Peptide
1	D	684	GLN	Mainchain,Peptide
1	D	699	ILE	Peptide
1	D	700	GLU	Peptide
1	D	707	SER	Mainchain,Peptide
1	D	718	GLY	Peptide
1	D	719	ASP	Peptide
1	D	731	VAL	Peptide
1	D	865	PHE	Mainchain,Peptide
1	D	891	LYS	Peptide
1	D	892	ILE	Peptide
1	D	919	GLN	Peptide
1	D	920	GLY	Mainchain,Peptide
1	D	926	CYS	Peptide
1	D	936	GLY	Peptide
1	D	937	MET	Peptide
1	D	979	HIS	Mainchain,Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9764	0	9788	628	0
1	B	9951	0	9967	711	0
1	C	9905	0	9922	648	0
1	D	9910	0	9929	634	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	12	0
3	B	53	0	29	6	0
3	C	53	0	29	10	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	10	0
5	D	4	0	3	0	0
6	D	5	0	0	1	0
All	All	39807	0	39758	2568	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 32.

All (2568) 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:C:688:ILE:CG1	1:C:688:ILE:CD1	1.81	1.56
1:A:811:THR:CB	1:A:811:THR:CG2	1.75	1.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:762:GLU:CG	1:A:762:GLU:CD	1.76	1.53
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: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:B:430:ASP:CG	1:B:1229:LYS:HE2	1.38	1.42
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:D:430:ASP:CG	1:D:1229:LYS:HE2	1.46	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: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:B:430:ASP:CG	1:B:1229:LYS:CE	2.17	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: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:A:159:GLY:O	1:A:162:THR:HG22	1.54	1.05
1:B:647:THR:HG23	1:B:648:GLY:N	1.63	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: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:B:534:ASP:CG	1:C:251:GLN:HB3	1.79	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:D:430:ASP:HB3	1:D:1229:LYS:HZ1	1.04	1.02
1:D:6:LEU:HD23	1:D:6:LEU:C	1.77	1.01
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:C:647:THR:CG2	1:C:648:GLY:N	2.17	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: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:910:THR:HG23	1:A:911:ALA:N	1.77	0.99
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:D:747:THR:HG23	1:D:827:MET:HE2	1.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:840:ARG:HA	4:D:3007:GOL:O1	1.64	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:430:ASP:CG	1:D:1229:LYS:CE	2.34	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: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:B:1213:HIS:H	1:B:1222:THR:CG2	1.81	0.93
1:D:459:MET:SD	1:D:512:THR:HG21	2.08	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:606:LEU:HD23	1:D:606:LEU:C	1.87	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:A:373:THR:C	1:A:374:LEU:HD23	1.90	0.92
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: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: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
1:D:1041:GLN:O	1:D:1041:GLN:HG2	1.72	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:698:THR:O	1:A:700:GLU:O	1.90	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: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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:920:GLY:HA2	1:A:921:MET:C	1.96	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
1:C:117:THR:O	1:C:121:VAL:HG23	1.78	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:D:27:LEU:O	1:D:28:ALA:CB	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:38:GLY:HA2	1:A:40:LYS:HE2	1.60	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:D:248:LEU:C	1:D:248:LEU:HD12	1.99	0.82
1:A:647:THR:CG2	1:A:648:GLY:N	2.22	0.82
1:D:530:GLU:C	1:D:532:LEU:H	1.83	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
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:A:248:LEU:C	1:A:248:LEU:HD12	2.01	0.81
1:C:533:GLU:HA	1:C:534:ASP:HB2	1.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1262:GLU:C	1:B:1264:PRO:HD2	2.02	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:B:910:THR:HG23	1:B:911:ALA:N	1.96	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:C:606:LEU:HD23	1:C:606:LEU:C	2.03	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
1:D:1081:SER:OG	1:D:1262:GLU:HG3	1.83	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: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:D:1293:GLU:O	1:D:1294:LEU:HD23	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1109:ASN:CG	1:C:1316:THR:HG21	2.04	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: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:A:1070:ASN:C	1:A:1070:ASN:HD22	1.85	0.78
1:C:1192:ASP:O	1:C:1193:ILE:HB	1.84	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:B:534:ASP:CG	1:C:251:GLN:CB	2.52	0.77
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:B:203:PRO:O	1:B:204:LEU:HB3	1.83	0.77
1:C:824:VAL:HG12	1:C:825:ARG:N	1.99	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:1195:GLN:HA	1:B:1195:GLN:NE2	1.99	0.75
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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:248:LEU:C	1:C:248:LEU:HD12	2.08	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:D:747:THR:HG23	1:D:827:MET:HE3	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:D:430:ASP:CB	1:D:1229:LYS:HZ1	1.93	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: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
1:C:113:CYS:HB3	1:C:150:CYS:SG	2.29	0.73
1:A:29:TYR:HE2	1:A:34:LEU:HD21	1.53	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:C:533:GLU:HG2	1:C:538:LYS:HZ1	1.54	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:B:864:HIS:HB2	1:B:879:MET:HE3	1.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:248:LEU:C	1:A:248:LEU:CD1	2.58	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
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:B:534:ASP:CB	1:C:251:GLN:HB2	2.21	0.71
1:B:701:ASP:O	1:B:702:ALA:C	2.30	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:523:VAL:HG12	1:B:524:LEU:H	0.61	0.70
1:B:917:GLY:H	1:B:918:PRO:HD2	1.56	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:B:3:ALA:CB	1:B:3:ALA:C	2.60	0.70
1:B:557:ASP:HB2	1:B:1240:PHE:H	1.57	0.70
1:C:533:GLU:HG2	1:C:538:LYS:HZ2	1.54	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:A:6:LEU:HD23	1:A:6:LEU:C	2.12	0.69
1:B:1311:VAL:HA	1:B:1315:THR:HG21	1.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1214:TYR:N	1:D:1214:TYR:CD1	2.58	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:588:SER:OG	1:C:590:GLU:HG2	1.93	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:1195:GLN:CA	1:C:1195:GLN:HE21	2.06	0.69
1:A:1021:LEU:HD12	1:A:1021:LEU:C	2.02	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
1:D:1021:LEU:HD12	1:D:1022:LEU:H	1.55	0.69
1:A:606:LEU:HD23	1:A:606:LEU:C	2.13	0.69
1:B:581:LEU:HG	1:B:1045:THR:HG23	1.72	0.69
1:B:1210:GLU:OE1	1:B:1228:TYR:OH	2.02	0.69
1:C:31:ARG:HG3	1:C:31:ARG:NH1	1.95	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: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:430:ASP:CG	1:B:1229:LYS:CD	2.58	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:920:GLY:CA	1:D:923:ILE:HG12	2.16	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:849:VAL:HG13	1:A:849:VAL:O	1.93	0.68
1:B:337:PHE:CD1	1:B:338:ALA:HB3	2.27	0.68
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:D:373:THR:C	1:D:374:LEU:HD23	2.13	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:D:840:ARG:HA	4:D:3007:GOL:HO1	1.59	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:ALA:CB	1:C:227:LEU:HD23	2.25	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:B:594:CYS:C	1:B:596:ASP:H	1.97	0.66
1:A:353:ILE:CG2	1:A:353:ILE:O	2.42	0.66
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: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:B:509:CYS:O	1:B:510:THR:C	2.34	0.65
1:C:104:ARG:HG2	1:C:201:PHE:CE1	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1192:ASP:O	1:B:1193:ILE:HB	1.96	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:D:248:LEU:C	1:D:248:LEU:CD1	2.64	0.65
1:B:6:LEU:C	1:B:6:LEU:HD23	2.17	0.65
1:B:88:VAL:HG13	1:B:89:GLU:N	2.10	0.65
1:B:606:LEU:HD23	1:B:606:LEU:C	2.14	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
1:A:840:ARG:HG3	4:A:3007:GOL:H31	1.78	0.65
1:A:1070:ASN:C	1:A:1070:ASN:ND2	2.49	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: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: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:B:251:GLN:HG3	1:B:252:HIS:CD2	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:749:CYS:HB2	1:B:827:MET:HG3	1.79	0.64
1:C:1279:ILE:O	1:C:1280:ARG:C	2.32	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:B:2:THR:C	1:B:4:ASP:OD1	2.36	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: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
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:C:1262:GLU:C	1:C:1264:PRO:HD2	2.18	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: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:216:LEU:O	1:A:217:LEU:HB2	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: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:864:HIS:HB2	1:A:879:MET:HE3	1.79	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:1106:LYS:HG2	1:D:1117:TRP:CZ2	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:THR:HG21	1:A:89:GLU:HG2	1.80	0.63
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:795:MET:CE	1:B:1039:MET:CG	2.77	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
1:D:840:ARG:CG	4:D:3007:GOL:O1	2.46	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: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: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:C:524:LEU:O	1:C:525:GLN:C	2.36	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:1289:ASN:CG	1:C:380:ARG:HH12	2.03	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:1002:ILE:HD13	1:B:1270:SER:HA	1.81	0.61
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: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:B:682:ALA:C	1:B:684:GLN:H	2.04	0.61
1:C:161:ARG:HG3	1:C:162:THR:N	2.16	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:C:892:ILE:HG23	1:C:892:ILE:O	2.00	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:C:693:LEU:HB3	1:C:694:PRO:CD	2.31	0.61
1:A:772:LYS:O	1:A:773:THR:C	2.35	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:C:459:MET:CE	1:C:459:MET:HA	2.31	0.61
1:C:701:ASP:O	1:C:702:ALA:C	2.37	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:D:780:MET:HE1	1:D:815:LEU:HB2	1.83	0.61
1:D:1260:VAL:O	1:D:1260:VAL:HG22	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:795:MET:CE	1:B:1039:MET:HG3	2.30	0.60
1:B:980:ALA:O	1:B:981:ARG:C	2.39	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: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
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: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:B:278:ILE:HG22	1:B:279:VAL:N	2.16	0.60
1:B:927:TRP:HE3	1:B:927:TRP:C	2.04	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: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: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:C:27:LEU:HD12	1:C:27:LEU:C	2.21	0.60
1:D:888:ASN:OD1	1:D:921:MET:HE3	2.01	0.60
1:A:366:MET:HA	1:A:385:MET:HG2	1.84	0.60
1:C:3:ALA:HB2	1:C:225:LYS:HZ2	1.66	0.60
1:C:1073:PRO:O	1:C:1074:ASN:HB2	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:824:VAL:HG12	1:A:825:ARG:N	2.16	0.59
1:B:257:LEU:O	3:B:3006:FAD:H2B	2.02	0.59
1:B:795:MET:HE1	1:B:1039:MET:CG	2.31	0.59
1:B:1292:LYS:CE	1:C:382:THR:HG21	2.26	0.59
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: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: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:A:215:GLU:C	1:A:216:LEU:O	2.32	0.59
1:A:1108:LYS:HZ2	1:C:1319:VAL:HG23	1.66	0.59
1:B:822:ARG:HB2	1:B:823:PRO:HD2	1.85	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: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: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:747:THR:CG2	1:D:827:MET:HE2	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1008:ILE:O	1:C:1009:SER:HB2	2.01	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
1:C:398:LEU:HD23	1:C:398:LEU:H	1.67	0.59
1:C:1293:GLU:O	1:C:1294:LEU:HD23	2.03	0.59
1:D:530:GLU:C	1:D:532:LEU:N	2.54	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:B:1014:PHE:CD1	1:B:1014:PHE:C	2.76	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:A:594:CYS:C	1:A:596:ASP:H	2.06	0.58
1:B:449:VAL:O	1:B:449:VAL:HG12	2.02	0.58
1:B:916:GLY:CA	4:B:3007:GOL:H32	2.32	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: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:921:MET:HE1	1:B:1004:THR:OG1	2.03	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:593:TYR:HB2	1:C:596:ASP:OD2	2.03	0.58
1:C:1192:ASP:O	1:C:1193:ILE:CB	2.47	0.58
1:D:701:ASP:O	1:D:702:ALA:C	2.40	0.58
1:A:353:ILE:O	1:A:353:ILE:HG22	2.04	0.58
1:A:649:ILE:O	1:A:649:ILE:CG1	2.51	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:C:682:ALA:C	1:C:684:GLN:H	2.07	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:512:THR:C	1:A:513:LEU:HD23	2.24	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: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:A:1014:PHE:C	1:A:1014:PHE:CD1	2.77	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:873:ASP:CG	1:A:874:LEU:H	2.07	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:459:MET:HA	1:C:459:MET:HE2	1.85	0.57
1:C:1195:GLN:CA	1:C:1195:GLN:NE2	2.65	0.57
1:D:594:CYS:C	1:D:596:ASP:H	2.07	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:262:THR:OG1	3:B:3006:FAD:O2P	2.21	0.57
1:C:3:ALA:HB2	1:C:225:LYS:HZ1	1.67	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: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: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: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:248:LEU:HD12	1:B:248:LEU:C	2.25	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:830:ARG:HG3	1:C:830:ARG:O	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:1014:PHE:C	1:A:1014:PHE:HD1	2.09	0.56
1:A:1102:LEU:O	1:A:1103:GLU:C	2.42	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: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:4:ASP:O	1:B:5:LYS:C	2.44	0.56
1:B:386:ASP:O	1:B:388:THR:N	2.38	0.56
1:B:878:ILE:HG12	1:B:915:PHE:CD1	2.40	0.56
1:B:937:MET:HB2	1:B:938:PRO:C	2.26	0.56
1:B:1263:PRO:N	1:B:1264:PRO:CD	2.68	0.56
1:C:248:LEU:C	1:C:248:LEU:CD1	2.73	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:C:269:LYS:HG2	1:C:270:PHE:CD1	2.40	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: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:888:ASN:OD1	1:B:921:MET:HE3	2.05	0.56
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:D:1070:ASN:C	1:D:1070:ASN:HD22	2.07	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:B:284:ILE:O	1:B:285:PRO:C	2.44	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: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: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: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:888:ASN:OD1	1:A:921:MET:HE3	2.06	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:750:THR:HG21	1:D:810:SER:HA	1.88	0.55
1:D:1206:LEU:HD12	1:D:1206:LEU:O	2.06	0.55
1:A:693:LEU:HB3	1:A:694:PRO:CD	2.36	0.55
1:A:1262:GLU:C	1:A:1264:PRO:HD2	2.26	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: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: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:888:ASN:OD1	1:C:921:MET:HE3	2.07	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:C:1034:HIS:CE1	1:C:1044:HIS:CD2	2.91	0.55
1:D:1142:SER:CB	1:D:1145:THR:CG2	2.84	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:A:682:ALA:C	1:A:684:GLN:H	2.10	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: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:C:449:VAL:O	1:C:449:VAL:CG1	2.46	0.55
1:C:520:TYR:C	1:C:520:TYR:CD2	2.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:D:81:HIS:O	1:D:82:HIS:HB2	2.08	0.54
1:A:788:ILE:N	1:A:788:ILE:CD1	2.70	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
1:A:165:ARG:HB2	1:A:165:ARG:NH1	2.22	0.54
1:A:423:GLN:CD	1:A:424:ALA:H	2.10	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:532:LEU:HA	1:B:534:ASP:H	1.71	0.54
1:B:1014:PHE:C	1:B:1014:PHE:HD1	2.10	0.54
1:C:29:TYR:HE2	1:C:34:LEU:HD21	1.73	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:A:71:ASN:ND2	1:A:71:ASN:N	2.55	0.54
1:B:377:ARG:HG3	1:B:377:ARG:O	2.08	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:4:ASP:O	1:D:5:LYS:C	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:891:LYS:HE2	1:D:949:LYS:CE	2.28	0.54
1:A:520:TYR:C	1:A:520:TYR:CD2	2.81	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:A:1108:LYS:HZ3	1:C:1319:VAL:HG23	1.73	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:D:312:LEU:N	1:D:312:LEU:CD1	2.71	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:D:927:TRP:HE3	1:D:927:TRP:C	2.11	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
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:826:CYS:SG	1:D:827:MET:N	2.81	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:A:864:HIS:C	1:A:865:PHE:CD1	2.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:482:LEU:O	1:D:486:VAL:HG23	2.08	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:780:MET:HE2	1:D:815:LEU:HB2	1.90	0.53
1:D:965:LEU:N	1:D:966:PRO:HD2	2.23	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: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: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: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:B:684:GLN:HA	1:B:684:GLN:NE2	2.22	0.53
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: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:160:PHE:O	1:C:161:ARG:C	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:507:PHE:CZ	1:D:511:LEU:CD1	2.90	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:1070:ASN:HD22	1:D:1071:THR:N	2.07	0.52
1:A:523:VAL:HG12	1:A:524:LEU:N	2.24	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:459:MET:HE3	1:C:508:ARG:HD2	1.91	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:A:509:CYS:O	1:A:510:THR:C	2.47	0.52
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:840:ARG:HG2	4:C:3007:GOL:HO1	1.74	0.52
1:C:871:THR:CG2	1:C:908:SER:HB2	2.36	0.52
1:C:1183:VAL:C	1:C:1258:LYS:HB2	2.29	0.52
1:D:1154:PHE:O	1:D:1258:LYS:HE2	2.10	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:1014:PHE:HD1	1:D:1014:PHE:C	2.13	0.52
1:A:572:ASP:C	1:A:572:ASP:OD1	2.48	0.52
1:A:1316:THR:O	1:A:1319:VAL:HG12	2.10	0.52
1:B:509:CYS:C	1:B:511:LEU:N	2.55	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:6:LEU:HD23	1:C:6:LEU:C	2.30	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: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: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:A:433:LYS:C	1:A:434:VAL:CG1	2.77	0.52
1:A:684:GLN:NE2	1:A:684:GLN:CA	2.65	0.52
1:B:520:TYR:C	1:B:520:TYR:CD2	2.83	0.52
1:B:708:PHE:HE1	1:B:900:ARG:NH2	2.08	0.52
1:B:927:TRP:CE3	1:B:927:TRP:C	2.82	0.52
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: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:1262:GLU:O	1:B:1263:PRO:C	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1263:PRO:N	1:C:1264:PRO:CD	2.72	0.51
1:D:520:TYR:C	1:D:520:TYR:CD2	2.84	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: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:698:THR:HG23	1:C:701:ASP:CG	2.30	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
1:D:440:VAL:HG23	1:D:452:LEU:HD12	1.93	0.51
1:A:312:LEU:N	1:A:312:LEU:HD12	2.25	0.51
1:B:372:LEU:HD21	1:B:385:MET:CE	2.40	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: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:795:MET:HE3	1:B:1039:MET:CG	2.41	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: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:B:528:GLY:CA	1:B:529:GLN:HB2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:795:MET:HE3	1:B:1039:MET:HG3	1.91	0.51
1:A:642:PRO:HG3	1:A:818:TYR:CE2	2.46	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:A:1022:LEU:C	1:A:1022:LEU:HD12	2.31	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:780:MET:C	1:D:780:MET:SD	2.89	0.51
1:D:1193:ILE:O	1:D:1194:GLY:C	2.49	0.51
1:B:599:ARG:CD	1:B:599:ARG:HB3	2.39	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
1:B:56:SER:HB3	1:B:67:HIS:CE1	2.45	0.51
1:B:248:LEU:C	1:B:248:LEU:CD1	2.80	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:D:71:ASN:H	1:D:71:ASN:HD22	1.58	0.51
1:A:372:LEU:HD21	1:A:385:MET:HE3	1.94	0.50
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:1133:PHE:CD1	1:D:1127:SER:HB2	2.46	0.50
1:B:723:GLY:O	1:B:724:PHE:HB2	2.11	0.50
1:B:824:VAL:HG12	1:B:825:ARG:N	2.25	0.50
1:C:154:ARG:HD3	1:C:1197:GLU:OE2	2.11	0.50
1:C:217:LEU:C	1:C:220:LYS:HG2	2.31	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:A:980:ALA:O	1:A:981:ARG:C	2.49	0.50
1:B:594:CYS:C	1:B:596:ASP:N	2.62	0.50
1:B:795:MET:HE1	1:B:1039:MET:HG3	1.93	0.50
1:B:873:ASP:CG	1:B:874:LEU:H	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:1070:ASN:C	1:D:1070:ASN:ND2	2.62	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
1:C:749:CYS:HB2	1:C:827:MET:HB2	1.94	0.50
1:D:888:ASN:OD1	1:D:921:MET:HE2	2.12	0.50
1:A:1224:GLY:O	1:A:1226:SER:N	2.44	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:B:867:ASN:C	1:B:867:ASN:OD1	2.49	0.50
1:C:316:VAL:HG21	1:C:328:ARG:HD3	1.94	0.50
1:C:946:ASN:ND2	1:C:946:ASN:N	2.60	0.50
1:D:467:LEU:HA	1:D:470:THR:HB	1.93	0.50
1:D:682:ALA:C	1:D:684:GLN:H	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:797:GLY:O	1:D:802:LYS:HE3	2.11	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:679:THR:HG22	1:B:680:GLN:N	2.27	0.49
1:B:878:ILE:CG2	4:B:3007:GOL:C1	2.81	0.49
1:B:1076:SER:O	1:B:1077:PRO:C	2.47	0.49
1:C:398:LEU:H	1:C:398:LEU:CD2	2.25	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:1089:GLN:HG2	1:A:1134:TYR:CD1	2.47	0.49
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:682:ALA:C	1:C:684:GLN:N	2.65	0.49
1:C:972:CYS:C	1:C:974:ALA:H	2.14	0.49
1:D:719:ASP:CA	1:D:720:LEU:HB3	2.42	0.49
1:A:595:ASP:HA	1:A:825:ARG:NH1	2.27	0.49
1:A:1065:SER:O	1:A:1065:SER:OG	2.28	0.49
1:A:1118:VAL:O	1:A:1119:THR:C	2.48	0.49
1:B:715:ILE:HG23	1:B:1146:ASN:HD21	1.77	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: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:HG3	1:A:830:ARG:O	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:734:GLU:HG2	1:A:1296:ARG:HH12	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:711:PRO:O	1:B:712:GLU:C	2.50	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: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: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: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:1125:THR:CG2	1:D:1135:ARG:HB2	2.40	0.49
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:B:795:MET:HE1	1:B:1039:MET:HG2	1.94	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:B:354:THR:HG23	1:B:354:THR:O	2.13	0.49
1:B:879:MET:HE3	1:B:899:GLY:HA3	1.94	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:A:87:THR:HG22	1:A:90:GLY:N	2.28	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:1133:PHE:CD2	1:C:1133:PHE:C	2.81	0.48
1:D:920:GLY:HA2	1:D:921:MET:C	2.34	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:D:1014:PHE:C	1:D:1014:PHE:CD1	2.85	0.48
1:A:910:THR:O	4:A:3007:GOL:H11	2.12	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:459:MET:HE3	1:B:508:ARG:HD2	1.95	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:D:430:ASP:CG	1:D:1229:LYS:CD	2.81	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:558:VAL:C	1:A:559:GLN:HG3	2.34	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:213:PRO:O	1:A:214:PRO:C	2.49	0.48
1:A:256:LYS:HE2	1:A:275:PHE:CD2	2.49	0.48
1:A:947:LEU:O	1:A:948:TYR:C	2.52	0.48
1:C:972:CYS:C	1:C:974:ALA:N	2.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:865:PHE:HD1	1:B:865:PHE:H	1.58	0.48
1:B:921:MET:CE	1:B:1004:THR:OG1	2.62	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:C:351:ASN:ND2	1:C:361:LEU:CB	2.70	0.48
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:C:864:HIS:HB2	1:C:879:MET:HE3	1.94	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: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: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:664:VAL:HG21	1:A:1218:GLY:C	2.32	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:1195:GLN:CA	1:B:1195:GLN:NE2	2.63	0.48
1:C:754:PRO:HD3	1:C:823:PRO:HA	1.96	0.48
1:C:760:GLU:OE1	1:D:1063:TYR:OH	2.28	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:1268:ALA:O	1:D:1269:ALA:C	2.51	0.47
1:A:513:LEU:N	1:A:513:LEU:CD2	2.51	0.47
1:A:1121:ALA:O	1:A:1126:VAL:HG23	2.15	0.47
1:B:154:ARG:HH11	1:B:1197:GLU:CD	2.14	0.47
1:B:702:ALA:HB1	1:B:902:CYS:HB3	1.97	0.47
1:B:767:THR:OG1	1:B:768:GLN:N	2.46	0.47
1:B:927:TRP:CE3	1:B:928:MET:HA	2.47	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: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: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:708:PHE:O	1:B:708:PHE:HD1	1.96	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:813:VAL:O	1:D:814:ALA:C	2.52	0.47
1:D:1077:PRO:HB2	1:D:1079:ALA:HB2	1.96	0.47
1:D:1279:ILE:O	1:D:1280:ARG:C	2.51	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: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
1:D:507:PHE:HB3	1:D:1304:GLU:HG3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:721:LYS:HD2	1:D:721:LYS:HA	1.58	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:888:ASN:OD1	1:B:921:MET:CE	2.62	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: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:372:LEU:HD22	1:B:407:ILE:CD1	2.37	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:C:101:VAL:HG12	1:C:101:VAL:O	2.14	0.47
1:C:433:LYS:O	1:C:458:GLY:HA3	2.14	0.47
1:C:842:PRO:HD2	1:C:867:ASN:HB3	1.96	0.47
1:C:1311:VAL:HA	1:C:1315:THR:HG21	1.96	0.47
1:D:62:GLN:O	1:D:63:ASN:C	2.53	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:772:LYS:O	1:D:773:THR:C	2.51	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:C:372:LEU:HD22	1:C:407:ILE:HD11	1.97	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:499:ASP:O	1:D:500:ALA:C	2.50	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:949:LYS:O	1:D:950:GLU:C	2.53	0.47
1:A:337:PHE:HZ	3:A:3006:FAD:HO2'	1.61	0.46
1:B:69:SER:O	1:B:70:ALA:HB2	2.15	0.46
1:B:578:LEU:HA	1:B:579:PRO:HD2	1.78	0.46
1:B:649:ILE:O	1:B:649:ILE:CG1	2.63	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:B:14:LYS:HG2	1:B:15:VAL:N	2.30	0.46
1:B:372:LEU:HD21	1:B:385:MET:HE3	1.97	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:C:1070:ASN:HD22	1:C:1070:ASN:C	2.17	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:1268:ALA:O	1:A:1269:ALA:C	2.54	0.46
1:B:606:LEU:HD23	1:B:607:ARG:CA	2.36	0.46
1:B:864:HIS:C	1:B:865:PHE:CD1	2.88	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
1:D:507:PHE:CG	1:D:1304:GLU:HA	2.50	0.46
3:D:3006:FAD:HM71	3:D:3006:FAD:HM83	1.74	0.46
1:A:62:GLN:O	1:A:63:ASN:C	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1250:ASN:O	1:A:1256:ALA:HA	2.16	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:C:83:VAL:HG12	1:C:84:ALA:N	2.29	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: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:B:1133:PHE:CD2	1:B:1133:PHE:C	2.89	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:1031:LEU:HD12	1:D:1031:LEU:HA	1.42	0.46
1:D:1183:VAL:C	1:D:1258:LYS:HB2	2.35	0.46
1:A:676:PRO:HA	1:A:679:THR:HB	1.97	0.46
1:A:701:ASP:O	1:A:702:ALA:C	2.53	0.46
1:B:219:LEU:HA	1:B:219:LEU:HD13	1.36	0.46
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:981:ARG:O	1:B:982:LYS:C	2.52	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:A:1224:GLY:C	1:A:1226:SER:H	2.18	0.46
1:B:88:VAL:C	1:B:90:GLY:H	2.18	0.46
1:B:509:CYS:C	1:B:511:LEU:H	2.18	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:A:234:VAL:HG12	1:A:235:THR:N	2.31	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: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:B:1118:VAL:C	1:B:1120:ALA:N	2.68	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:1090:ALA:HB1	1:C:1132:GLY:O	2.17	0.45
1:D:1113:SER:O	1:D:1116:ASP:HB2	2.15	0.45
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:D:641:VAL:HG11	1:D:645:ASN:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1196:VAL:HG12	1:C:1197:GLU:N	2.31	0.45
1:D:430:ASP:OD2	1:D:1229:LYS:CD	2.65	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: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:D:1055:LEU:O	1:D:1056:LYS:HB2	2.16	0.45
1:D:1185:SER:O	1:D:1186:SER:C	2.55	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:A:879:MET:HE3	1:A:899:GLY:HA3	1.98	0.45
1:B:851:PHE:CD2	1:B:851:PHE:N	2.84	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
1:C:612:THR:HG23	1:C:690:TYR:OH	2.17	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:428:GLU:CD	1:D:428:GLU:H	2.19	0.45
1:D:643:GLY:HA3	1:D:780:MET:O	2.16	0.45
1:A:737:ILE:HG23	1:A:1299:SER:HB3	1.99	0.45
1:B:1262:GLU:C	1:B:1264:PRO:CD	2.77	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:682:ALA:C	1:D:684:GLN:N	2.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:664:VAL:HG21	1:C:1218:GLY:C	2.36	0.45
1:C:703:ILE:C	1:C:705:ASN:N	2.70	0.45
1:A:698:THR:C	1:A:700:GLU:O	2.55	0.45
1:B:3:ALA:C	1:B:4:ASP:CG	2.73	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:B:1289:ASN:C	1:C:380:ARG:NH1	2.70	0.45
1:C:337:PHE:CD1	1:C:338:ALA:CB	3.00	0.45
1:C:499:ASP:O	1:C:500:ALA:C	2.55	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:1157:GLY:C	1:C:1158:VAL:HG23	2.37	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:386:ASP:C	1:C:388:THR:H	2.19	0.45
1:C:560:LEU:CD1	1:C:1243:SER:HB3	2.47	0.45
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:927:TRP:CE3	1:D:927:TRP:C	2.88	0.45
1:D:1176:ARG:HG3	1:D:1177:THR:H	1.82	0.45
1:A:698:THR:HG23	1:A:701:ASP:CG	2.37	0.45
1:A:1183:VAL:C	1:A:1258:LYS:HB2	2.37	0.45
1:B:1000:CYS:O	1:B:1160:CYS:HA	2.16	0.45
1:C:937:MET:CB	1:C:938:PRO:CA	2.92	0.45
1:A:588:SER:OG	1:A:590:GLU:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:768:GLN:HG2	1:B:795:MET:HE1	1.99	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: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:947:LEU:C	1:A:948:TYR:O	2.55	0.44
1:A:1055:LEU:HD23	1:A:1057:ILE:HD13	1.98	0.44
1:B:622:ASP:C	1:B:622:ASP:OD1	2.56	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: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:C:780:MET:HE2	1:C:815:LEU:HB2	1.98	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:373:THR:C	1:A:374:LEU:CD2	2.75	0.44
1:A:1034:HIS:HE1	1:A:1044:HIS:HD2	1.59	0.44
1:A:1262:GLU:O	1:A:1263:PRO:C	2.56	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:B:789:VAL:O	1:B:789:VAL:HG12	2.10	0.44
1:C:386:ASP:C	1:C:388:THR:N	2.71	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
1:D:922:LEU:O	1:D:926:CYS:HB2	2.18	0.44
1:A:851:PHE:CD2	1:A:851:PHE:N	2.84	0.44
1:B:1055:LEU:HD23	1:B:1057:ILE:CD1	2.46	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:246:LEU:HD21	1:A:375:VAL:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:920:GLY:HA2	1:C:922:LEU:CA	2.48	0.44
1:C:1027:ASP:OD2	1:C:1027:ASP:C	2.55	0.44
1:D:788:ILE:N	1:D:788:ILE:HD13	2.32	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:1144:GLU:C	1:A:1145:THR:HG22	2.38	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:883:LEU:C	1:B:885:HIS:H	2.21	0.44
1:B:999:LEU:HG	1:B:1000:CYS:N	2.32	0.44
1:C:281:PRO:O	1:C:282:ALA:HB3	2.17	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
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: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:1069:THR:O	1:B:1069:THR:OG1	2.21	0.44
1:C:215:GLU:C	1:C:216:LEU:O	2.50	0.44
1:D:864:HIS:HB2	1:D:879:MET:HE3	2.00	0.44
1:D:986:ASP:O	1:D:987:LYS:CB	2.65	0.44
1:A:700:GLU:O	1:A:701:ASP:CB	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:278:ILE:CG2	1:D:279:VAL:N	2.80	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:428:GLU:CD	1:B:428:GLU:H	2.21	0.44
1:B:461:ASN:CB	1:B:462:ARG:CG	2.89	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: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:248:LEU:HD12	1:B:248:LEU:O	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
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:C:1014:PHE:CD1	1:C:1014:PHE:C	2.92	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: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: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
3:A:3006:FAD:HM83	3:A:3006:FAD:HM71	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:923:ILE:O	1:B:924:ALA:C	2.53	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: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:D:594:CYS:C	1:D:596:ASP:N	2.71	0.43
1:A:209:GLU:HB3	1:A:210:PRO:HD2	1.99	0.43
1:A:372:LEU:HD21	1:A:385:MET:CE	2.48	0.43
1:A:927:TRP:HZ3	1:A:928:MET:CE	2.31	0.43
1:A:954:THR:C	1:A:956:PHE:H	2.20	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:720:LEU:H	1:B:722:LYS:H	1.66	0.43
1:C:505:VAL:O	1:C:505:VAL:HG12	2.18	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:841:HIS:N	4:D:3007:GOL:O1	2.46	0.43
1:D:847:TYR:CE1	1:D:927:TRP:HB2	2.54	0.43
1:D:972:CYS:C	1:D:974:ALA:H	2.19	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:A:373:THR:CA	1:A:374:LEU:HD23	2.49	0.43
1:B:629:VAL:HG13	1:B:630:PRO:HD2	2.01	0.43
1:B:682:ALA:C	1:B:684:GLN:N	2.67	0.43
1:B:1216:PRO:HD3	1:B:1329:TRP:O	2.17	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1285:GLN:HA	1:C:378:GLY:HA2	2.01	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
3:C:3006:FAD:HM71	3:C:3006:FAD:HM83	1.51	0.43
1:D:372:LEU:HB2	1:D:374:LEU:HD21	2.01	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: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:14:LYS:HG2	1:D:15:VAL:N	2.34	0.43
1:D:154:ARG:N	1:D:155:PRO:CD	2.80	0.43
1:D:404:LEU:CA	3:D:3006:FAD:H62A	2.30	0.43
1:D:1280:ARG:NH1	1:D:1280:ARG:CG	2.81	0.43
1:A:662:THR:O	1:A:905:ASN:HB3	2.18	0.43
1:A:1109:ASN:CG	1:A:1109:ASN:O	2.57	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:943:ARG:O	1:B:944:ARG:C	2.57	0.43
1:B:1102:LEU:O	1:B:1103:GLU:C	2.57	0.43
1:B:1192:ASP:O	1:B:1193:ILE:CB	2.59	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:429:ASP:O	1:D:430:ASP:CB	2.67	0.43
1:D:682:ALA:O	1:D:683:ALA:C	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:312:LEU:O	1:A:313:VAL:C	2.57	0.42
1:A:748:HIS:O	1:A:749:CYS:CB	2.53	0.42
1:A:1048:VAL:O	1:A:1049:GLN:C	2.57	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: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:1170:GLY:O	1:A:1303:PRO:HA	2.18	0.42
1:B:740:GLN:CG	1:B:741:GLU:N	2.82	0.42
1:B:795:MET:C	1:B:797:GLY:H	2.21	0.42
1:B:1174:ASN:OD1	1:B:1271:ILE:HD13	2.19	0.42
1:B:1268:ALA:O	1:B:1269:ALA:C	2.57	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: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:983:SER:O	1:D:984:GLU:C	2.57	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:353:ILE:C	1:B:355:ALA:N	2.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:703:ILE:O	1:C:704:LYS:C	2.57	0.42
1:C:744:TYR:CD1	1:C:744:TYR:N	2.81	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: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:767:THR:O	1:A:795:MET:HE2	2.18	0.42
1:A:931:VAL:O	1:A:932:ALA:C	2.57	0.42
1:A:966:PRO:HG2	1:A:967:ARG:H	1.84	0.42
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:616:ALA:CB	1:C:692:GLU:HA	2.49	0.42
1:C:1021:LEU:HD12	1:C:1021:LEU:C	2.32	0.42
1:C:1201:VAL:O	1:C:1204:LEU:HB3	2.19	0.42
1:D:6:LEU:C	1:D:6:LEU:CD2	2.59	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:715:ILE:HG22	1:D:716:GLU:N	2.34	0.42
1:D:1157:GLY:C	1:D:1158:VAL:HG23	2.40	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:459:MET:HA	1:A:459:MET:HE2	2.00	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:C:353:ILE:C	1:C:355:ALA:N	2.73	0.42
1:D:656:PHE:O	1:D:657:ALA:C	2.58	0.42
1:D:798:GLY:O	1:D:801:GLY:N	2.53	0.42
1:D:972:CYS:C	1:D:974:ALA:N	2.73	0.42
1:D:1053:ARG:HD2	1:D:1255:TYR:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1070:ASN:C	1:C:1070:ASN:ND2	2.72	0.42
1:C:1073:PRO:CD	1:D:1023:HIS:CD2	2.98	0.42
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:A:246:LEU:HD22	1:A:376:SER:C	2.40	0.42
1:A:742:HIS:HA	1:A:912:PHE:CE1	2.54	0.42
1:A:923:ILE:O	1:A:926:CYS:HB2	2.18	0.42
1:A:1103:GLU:O	1:A:1104:PRO:C	2.58	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:C	1:B:1120:ALA:H	2.23	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:THR:O	1:B:126:THR:HG22	2.20	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:161:ARG:CG	1:C:162:THR:N	2.82	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:D:248:LEU:O	1:D:248:LEU:CD1	2.67	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
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: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: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:B:1106:LYS:O	1:B:1107:LYS:C	2.59	0.42
1:C:99:HIS:O	1:C:102:GLN:N	2.51	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: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:650:CYS:O	1:A:651:ASN:C	2.58	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:A:1224:GLY:C	1:A:1226:SER:N	2.73	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: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:D:31:ARG:NH2	1:D:596:ASP:OD1	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:161:ARG:O	1:B:162:THR:C	2.58	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:972:CYS:C	1:B:974:ALA:H	2.23	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
1:D:396:THR:HB	1:D:397:LEU:H	1.68	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:386:ASP:C	1:A:388:THR:H	2.22	0.41
1:A:459:MET:HA	1:A:459:MET:HE3	2.02	0.41
1:A:681:ARG:O	1:A:684:GLN:HB3	2.20	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:B:346:ALA:HB1	3:B:3006:FAD:H4'	2.01	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:C:62:GLN:O	1:C:63:ASN:C	2.59	0.41
1:C:520:TYR:C	1:C:520:TYR:HD2	2.23	0.41
1:C:879:MET:HE3	1:C:899:GLY:HA3	2.01	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: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:1080:ALA:C	1:A:1082:VAL:H	2.24	0.41
1:A:1149:ASN:HD22	1:A:1149:ASN:HA	1.31	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:D:708:PHE:HB2	1:D:902:CYS:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:645:ASN:OD1	1:A:645:ASN:O	2.38	0.41
1:A:927:TRP:CE3	1:A:928:MET:CA	3.00	0.41
1:B:525:GLN:O	1:B:525:GLN:HG3	2.18	0.41
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: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:C:949:LYS:O	1:C:950:GLU:C	2.57	0.41
1:D:606:LEU:CD2	1:D:606:LEU:C	2.69	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:800:GLY:C	1:A:802:LYS:N	2.74	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:386:ASP:C	1:B:388:THR:H	2.24	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: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:A:1081:SER:HG	1:A:1262:GLU:HG3	1.83	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: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: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: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: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:719:ASP:CA	1:B:720:LEU:CB	2.99	0.41
1:B:917:GLY:O	1:B:921:MET:CB	2.68	0.41
1:C:348:VAL:O	1:C:349:GLY:C	2.59	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:100:PRO:O	1:A:101:VAL:C	2.56	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: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:3:ALA:HA	1:B:4:ASP:CG	2.41	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:806:SER:O	1:B:807:THR:C	2.59	0.41
1:B:841:HIS:CG	4:B:3007:GOL:HO1	2.39	0.41
1:B:1145:THR:O	1:B:1146:ASN:C	2.58	0.41
1:C:257:LEU:HD12	3:C:3006:FAD:C5A	2.50	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:533:GLU:CG	1:C:538:LYS:HZ1	2.26	0.41
1:C:578:LEU:HA	1:C:579:PRO:HD2	1.91	0.41
1:C:594:CYS:C	1:C:596:ASP:N	2.74	0.41
1:C:797:GLY:O	1:C:802:LYS:HE3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:881:ARG:O	1:C:881:ARG:CG	2.68	0.41
1:C:1014:PHE:C	1:C:1014:PHE:HD1	2.23	0.41
1:C:1073:PRO:O	1:C:1074:ASN:CB	2.65	0.41
1:C:1135:ARG:CB	1:D:1125:THR:CG2	2.99	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:636:ILE:HD12	1:D:636:ILE:HA	1.83	0.41
1:D:698:THR:C	1:D:700:GLU:O	2.59	0.41
1:D:1081:SER:HA	6:D:3009:PO4:O3	2.21	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:864:HIS:HB2	1:B:879:MET:CE	2.46	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:949:LYS:N	1:C:952:ASP:OD2	2.38	0.41
1:C:1253:ALA:O	1:C:1254:ILE:C	2.59	0.41
1:D:279:VAL:O	1:D:279:VAL:HG13	2.22	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: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:1124:ASP:O	1:B:1125:THR:CB	2.45	0.40
1:C:386:ASP:O	1:C:387:HIS:C	2.60	0.40
1:C:545:SER:O	1:C:546:ALA:CB	2.69	0.40
1:C:800:GLY:C	1:C:802:LYS:N	2.74	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:B:159:GLY:O	1:B:162:THR:CG2	2.52	0.40
1:B:564:VAL:O	1:B:565:PRO:C	2.58	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
1:C:543:PHE:O	1:C:544:ALA:CB	2.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:745:LEU:N	1:C:745:LEU:CD2	2.84	0.40
1:C:927:TRP:CE3	1:C:927:TRP:C	2.94	0.40
1:C:954:THR:C	1:C:956:PHE:N	2.75	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:D:1133:PHE:CD2	1:D:1133:PHE:C	2.95	0.40
1:A:28:ALA:H	1:A:31:ARG:H	1.68	0.40
1:A:524:LEU:O	1:A:527:LEU:HD12	2.21	0.40
1:A:585:MET:HE3	1:A:585:MET:HB2	1.92	0.40
1:A:824:VAL:CG1	1:A:825:ARG:N	2.83	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: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:504:MET:HG2	1:D:1304:GLU:CD	2.42	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:HE2	1:A:524:LEU:HD11	1.81	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: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:867:ASN:C	1:C:867:ASN:OD1	2.60	0.40
1:C:873:ASP:CG	1:C:874:LEU:H	2.24	0.40
1:C:883:LEU:C	1:C:885:HIS:H	2.25	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
1:D:195:LEU:O	1:D:196:PHE:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:ILE:O	1:D:285:PRO:C	2.59	0.40
1:D:496:LEU:HD23	1:D:496:LEU:HA	1.82	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: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: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	15
1	B	1281/1333 (96%)	1021 (80%)	158 (12%)	102 (8%)	1	11
1	C	1273/1333 (96%)	1011 (79%)	168 (13%)	94 (7%)	1	13
1	D	1275/1333 (96%)	1006 (79%)	174 (14%)	95 (8%)	1	12
All	All	5084/5332 (95%)	4040 (80%)	668 (13%)	376 (7%)	1	13

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

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Mol	Chain	Res	Type
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
1	B	433	LYS
1	B	449	VAL
1	B	471	GLN
1	B	472	ARG

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Mol	Chain	Res	Type
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
1	C	471	GLN
1	C	472	ARG
1	C	530	GLU
1	C	531	ASN

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Mol	Chain	Res	Type
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
1	D	666	HIS
1	D	683	ALA
1	D	685	GLY
1	D	702	ALA

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Mol	Chain	Res	Type
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
1	B	534	ASP
1	B	581	LEU
1	B	595	ASP
1	B	710	GLY

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Mol	Chain	Res	Type
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
1	D	524	LEU
1	D	525	GLN
1	D	536	CYS
1	D	707	SER

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Mol	Chain	Res	Type
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
1	C	204	LEU
1	C	320	PRO
1	C	433	LYS
1	C	529	GLN

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Mol	Chain	Res	Type
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
1	C	591	ALA
1	C	724	PHE
1	C	798	GLY
1	C	921	MET

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Mol	Chain	Res	Type
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
1	D	349	GLY
1	D	426	ARG
1	D	535	LYS
1	D	806	SER

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Mol	Chain	Res	Type
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 (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1067/1126 (95%)	807 (76%)	260 (24%)	0 4
1	B	1088/1126 (97%)	812 (75%)	276 (25%)	0 4
1	C	1082/1126 (96%)	814 (75%)	268 (25%)	0 4
1	D	1084/1126 (96%)	813 (75%)	271 (25%)	0 4
All	All	4321/4504 (96%)	3246 (75%)	1075 (25%)	0 4

All (1075) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	6	LEU
1	A	25	THR
1	A	31	ARG
1	A	34	LEU
1	A	41	LEU
1	A	48	CYS
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	82	HIS
1	A	85	VAL
1	A	87	THR
1	A	88	VAL
1	A	89	GLU
1	A	93	SER
1	A	95	LYS
1	A	105	ILE
1	A	113	CYS
1	A	123	SER
1	A	129	ARG
1	A	131	GLN
1	A	136	MET
1	A	154	ARG
1	A	161	ARG
1	A	197	LYS
1	A	199	GLU

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Mol	Chain	Res	Type
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	225	LYS
1	A	241	THR
1	A	244	GLU
1	A	248	LEU
1	A	249	LYS
1	A	277	MET
1	A	280	CYS
1	A	290	VAL
1	A	295	ASP
1	A	298	SER
1	A	307	ILE
1	A	310	LYS
1	A	316	VAL
1	A	318	LYS
1	A	319	LEU
1	A	328	ARG
1	A	335	ARG
1	A	348	VAL
1	A	354	THR
1	A	359	SER
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	418	PHE

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Mol	Chain	Res	Type
1	A	419	SER
1	A	425	SER
1	A	431	ILE
1	A	434	VAL
1	A	439	ARG
1	A	440	VAL
1	A	447	THR
1	A	450	GLN
1	A	459	MET
1	A	462	ARG
1	A	464	ILE
1	A	470	THR
1	A	474	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
1	A	558	VAL
1	A	564	VAL
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	623	THR
1	A	630	PRO
1	A	636	ILE
1	A	641	VAL

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Mol	Chain	Res	Type
1	A	644	SER
1	A	647	THR
1	A	649	ILE
1	A	650	CYS
1	A	654	THR
1	A	662	THR
1	A	664	VAL
1	A	671	VAL
1	A	674	ASP
1	A	675	THR
1	A	676	PRO
1	A	679	THR
1	A	680	GLN
1	A	684	GLN
1	A	686	VAL
1	A	688	ILE
1	A	690	TYR
1	A	698	THR
1	A	700	GLU
1	A	703	ILE
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	734	GLU
1	A	735	ILE
1	A	743	PHE
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

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Mol	Chain	Res	Type
1	A	788	ILE
1	A	791	ARG
1	A	805	ARG
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	851	PHE
1	A	854	THR
1	A	857	VAL
1	A	858	VAL
1	A	860	LEU
1	A	865	PHE
1	A	871	THR
1	A	879	MET
1	A	891	LYS
1	A	894	ASN
1	A	902	CYS
1	A	910	THR
1	A	912	PHE
1	A	915	PHE
1	A	922	LEU
1	A	925	GLU
1	A	927	TRP
1	A	929	SER
1	A	937	MET
1	A	944	ARG
1	A	946	ASN
1	A	949	LYS
1	A	953	LEU
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	1000	CYS
1	A	1001	ILE

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Mol	Chain	Res	Type
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	1032	LEU
1	A	1033	THR
1	A	1038	GLU
1	A	1045	THR
1	A	1052	SER
1	A	1057	ILE
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	1104	PRO
1	A	1106	LYS
1	A	1107	LYS
1	A	1114	TRP
1	A	1119	THR
1	A	1123	MET
1	A	1126	VAL
1	A	1131	THR
1	A	1133	PHE
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

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Mol	Chain	Res	Type
1	A	1222	THR
1	A	1223	ARG
1	A	1230	ILE
1	A	1240	PHE
1	A	1243	SER
1	A	1246	ARG
1	A	1254	ILE
1	A	1263	PRO
1	A	1277	ASP
1	A	1279	ILE
1	A	1280	ARG
1	A	1287	THR
1	A	1291	VAL
1	A	1294	LEU
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	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	69	SER
1	B	71	ASN
1	B	77	ILE
1	B	82	HIS
1	B	85	VAL
1	B	87	THR
1	B	89	GLU
1	B	93	SER
1	B	95	LYS

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Mol	Chain	Res	Type
1	B	97	ARG
1	B	103	GLU
1	B	105	ILE
1	B	113	CYS
1	B	118	PRO
1	B	123	SER
1	B	129	ARG
1	B	131	GLN
1	B	136	MET
1	B	149	ARG
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	225	LYS
1	B	226	GLN
1	B	241	THR
1	B	248	LEU
1	B	249	LYS
1	B	284	ILE
1	B	295	ASP
1	B	298	SER
1	B	307	ILE
1	B	310	LYS
1	B	314	ASP
1	B	316	VAL
1	B	318	LYS
1	B	319	LEU
1	B	328	ARG
1	B	331	LEU
1	B	335	ARG
1	B	348	VAL
1	B	354	THR

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Mol	Chain	Res	Type
1	B	359	SER
1	B	372	LEU
1	B	379	THR
1	B	381	ARG
1	B	383	VAL
1	B	388	THR
1	B	394	ARG
1	B	398	LEU
1	B	401	GLU
1	B	412	SER
1	B	418	PHE
1	B	419	SER
1	B	427	ARG
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	452	LEU
1	B	459	MET
1	B	462	ARG
1	B	464	ILE
1	B	470	THR
1	B	474	LEU
1	B	477	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	524	LEU
1	B	525	GLN
1	B	527	LEU
1	B	529	GLN
1	B	530	GLU
1	B	531	ASN
1	B	532	LEU

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Mol	Chain	Res	Type
1	B	533	GLU
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	560	LEU
1	B	561	PHE
1	B	564	VAL
1	B	572	ASP
1	B	576	ARG
1	B	578	LEU
1	B	590	GLU
1	B	598	PRO
1	B	599	ARG
1	B	601	GLU
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	634	CYS
1	B	641	VAL
1	B	647	THR
1	B	649	ILE
1	B	650	CYS
1	B	652	ASP
1	B	654	THR
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	681	ARG
1	B	686	VAL
1	B	688	ILE
1	B	689	THR

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Mol	Chain	Res	Type
1	B	698	THR
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	743	PHE
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	788	ILE
1	B	802	LYS
1	B	807	THR
1	B	819	LYS
1	B	822	ARG
1	B	825	ARG
1	B	826	CYS
1	B	830	ARG
1	B	831	ASP
1	B	837	THR
1	B	847	TYR
1	B	852	MET
1	B	854	THR
1	B	857	VAL
1	B	865	PHE
1	B	866	SER
1	B	871	THR
1	B	876	GLN
1	B	877	SER
1	B	879	MET
1	B	891	LYS

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Mol	Chain	Res	Type
1	B	894	ASN
1	B	902	CYS
1	B	910	THR
1	B	912	PHE
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	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	1052	SER
1	B	1057	ILE
1	B	1059	THR
1	B	1060	SER
1	B	1069	THR
1	B	1070	ASN
1	B	1085	ASP
1	B	1097	THR

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Mol	Chain	Res	Type
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	1126	VAL
1	B	1131	THR
1	B	1133	PHE
1	B	1135	ARG
1	B	1139	LEU
1	B	1143	PHE
1	B	1149	ASN
1	B	1167	CYS
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	1240	PHE
1	B	1243	SER
1	B	1246	ARG
1	B	1263	PRO
1	B	1277	ASP
1	B	1279	ILE
1	B	1280	ARG
1	B	1287	THR
1	B	1291	VAL
1	B	1294	LEU
1	B	1299	SER
1	B	1312	ASP
1	B	1315	THR
1	B	1316	THR
1	B	1317	LEU
1	B	1326	CYS
1	B	1327	LYS
1	B	1329	TRP

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Mol	Chain	Res	Type
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	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	82	HIS
1	C	85	VAL
1	C	87	THR
1	C	88	VAL
1	C	89	GLU
1	C	93	SER
1	C	97	ARG
1	C	105	ILE
1	C	113	CYS
1	C	123	SER
1	C	129	ARG
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
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	224	ARG
1	C	225	LYS
1	C	226	GLN

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Mol	Chain	Res	Type
1	C	228	ARG
1	C	241	THR
1	C	248	LEU
1	C	249	LYS
1	C	257	LEU
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	335	ARG
1	C	348	VAL
1	C	354	THR
1	C	359	SER
1	C	363	PRO
1	C	372	LEU
1	C	374	LEU
1	C	377	ARG
1	C	379	THR
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	418	PHE
1	C	423	GLN
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

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Mol	Chain	Res	Type
1	C	462	ARG
1	C	464	ILE
1	C	470	THR
1	C	474	LEU
1	C	477	LEU
1	C	483	LEU
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	540	ASP
1	C	542	THR
1	C	545	SER
1	C	547	THR
1	C	557	ASP
1	C	558	VAL
1	C	560	LEU
1	C	564	VAL
1	C	576	ARG
1	C	578	LEU
1	C	581	LEU
1	C	590	GLU
1	C	592	VAL
1	C	596	ASP
1	C	599	ARG
1	C	606	LEU
1	C	608	LEU
1	C	612	THR
1	C	618	ILE

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Mol	Chain	Res	Type
1	C	619	LYS
1	C	623	THR
1	C	628	LYS
1	C	630	PRO
1	C	634	CYS
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	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	693	LEU
1	C	698	THR
1	C	699	ILE
1	C	700	GLU
1	C	703	ILE
1	C	704	LYS
1	C	706	ASN
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	743	PHE
1	C	744	TYR
1	C	745	LEU
1	C	747	THR

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Mol	Chain	Res	Type
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	791	ARG
1	C	802	LYS
1	C	805	ARG
1	C	810	SER
1	C	822	ARG
1	C	825	ARG
1	C	826	CYS
1	C	830	ARG
1	C	831	ASP
1	C	837	THR
1	C	847	TYR
1	C	854	THR
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	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	937	MET
1	C	944	ARG
1	C	946	ASN
1	C	949	LYS
1	C	953	LEU
1	C	970	GLU
1	C	976	SER
1	C	977	GLN

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Mol	Chain	Res	Type
1	C	979	HIS
1	C	982	LYS
1	C	986	ASP
1	C	987	LYS
1	C	1001	ILE
1	C	1009	SER
1	C	1014	PHE
1	C	1017	GLN
1	C	1022	LEU
1	C	1026	THR
1	C	1043	LEU
1	C	1052	SER
1	C	1057	ILE
1	C	1059	THR
1	C	1060	SER
1	C	1065	SER
1	C	1068	SER
1	C	1070	ASN
1	C	1081	SER
1	C	1085	ASP
1	C	1097	THR
1	C	1098	ILE
1	C	1100	LYS
1	C	1106	LYS
1	C	1107	LYS
1	C	1114	TRP
1	C	1119	THR
1	C	1123	MET
1	C	1125	THR
1	C	1126	VAL
1	C	1133	PHE
1	C	1135	ARG
1	C	1139	LEU
1	C	1149	ASN
1	C	1161	SER
1	C	1167	CYS
1	C	1195	GLN
1	C	1204	LEU
1	C	1209	LEU
1	C	1212	LEU
1	C	1214	TYR
1	C	1221	HIS

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Mol	Chain	Res	Type
1	C	1222	THR
1	C	1230	ILE
1	C	1240	PHE
1	C	1246	ARG
1	C	1263	PRO
1	C	1277	ASP
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	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	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	93	SER
1	D	95	LYS
1	D	97	ARG
1	D	103	GLU
1	D	105	ILE
1	D	113	CYS
1	D	123	SER

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Mol	Chain	Res	Type
1	D	131	GLN
1	D	136	MET
1	D	161	ARG
1	D	162	THR
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	225	LYS
1	D	226	GLN
1	D	228	ARG
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	289	SER
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	335	ARG
1	D	348	VAL
1	D	352	ILE
1	D	354	THR
1	D	359	SER
1	D	372	LEU
1	D	374	LEU
1	D	377	ARG
1	D	379	THR
1	D	381	ARG

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Mol	Chain	Res	Type
1	D	383	VAL
1	D	388	THR
1	D	390	PHE
1	D	394	ARG
1	D	398	LEU
1	D	401	GLU
1	D	418	PHE
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	505	VAL
1	D	506	ASP
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	559	GLN
1	D	561	PHE
1	D	564	VAL
1	D	576	ARG

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Mol	Chain	Res	Type
1	D	578	LEU
1	D	588	SER
1	D	590	GLU
1	D	597	ILE
1	D	598	PRO
1	D	599	ARG
1	D	601	GLU
1	D	605	SER
1	D	608	LEU
1	D	612	THR
1	D	618	ILE
1	D	619	LYS
1	D	623	THR
1	D	630	PRO
1	D	633	VAL
1	D	634	CYS
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	663	CYS
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	698	THR
1	D	700	GLU
1	D	701	ASP
1	D	703	ILE
1	D	706	ASN
1	D	708	PHE
1	D	712	GLU
1	D	713	LEU
1	D	720	LEU
1	D	721	LYS

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Mol	Chain	Res	Type
1	D	730	VAL
1	D	731	VAL
1	D	732	SER
1	D	734	GLU
1	D	735	ILE
1	D	743	PHE
1	D	744	TYR
1	D	745	LEU
1	D	747	THR
1	D	753	VAL
1	D	757	GLU
1	D	775	SER
1	D	779	LYS
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	826	CYS
1	D	830	ARG
1	D	831	ASP
1	D	836	ILE
1	D	837	THR
1	D	847	TYR
1	D	854	THR
1	D	857	VAL
1	D	865	PHE
1	D	871	THR
1	D	879	MET
1	D	891	LYS
1	D	894	ASN
1	D	902	CYS
1	D	910	THR
1	D	912	PHE
1	D	915	PHE
1	D	921	MET
1	D	922	LEU
1	D	925	GLU
1	D	927	TRP

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Mol	Chain	Res	Type
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	1026	THR
1	D	1032	LEU
1	D	1033	THR
1	D	1041	GLN
1	D	1048	VAL
1	D	1052	SER
1	D	1057	ILE
1	D	1059	THR
1	D	1060	SER
1	D	1068	SER
1	D	1070	ASN
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	1116	ASP
1	D	1119	THR
1	D	1123	MET
1	D	1125	THR

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Mol	Chain	Res	Type
1	D	1126	VAL
1	D	1131	THR
1	D	1135	ARG
1	D	1139	LEU
1	D	1149	ASN
1	D	1167	CYS
1	D	1178	ASP
1	D	1195	GLN
1	D	1204	LEU
1	D	1211	GLU
1	D	1212	LEU
1	D	1214	TYR
1	D	1221	HIS
1	D	1222	THR
1	D	1226	SER
1	D	1230	ILE
1	D	1240	PHE
1	D	1243	SER
1	D	1246	ARG
1	D	1254	ILE
1	D	1277	ASP
1	D	1279	ILE
1	D	1280	ARG
1	D	1287	THR
1	D	1291	VAL
1	D	1294	LEU
1	D	1302	THR
1	D	1311	VAL
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	112	GLN

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Mol	Chain	Res	Type
1	A	252	HIS
1	A	261	ASN
1	A	351	ASN
1	A	531	ASN
1	A	684	GLN
1	A	742	HIS
1	A	748	HIS
1	A	768	GLN
1	A	894	ASN
1	A	946	ASN
1	A	958	GLN
1	A	977	GLN
1	A	1034	HIS
1	A	1044	HIS
1	A	1070	ASN
1	A	1146	ASN
1	A	1149	ASN
1	A	1195	GLN
1	B	63	ASN
1	B	71	ASN
1	B	112	GLN
1	B	252	HIS
1	B	272	ASN
1	B	351	ASN
1	B	423	GLN
1	B	525	GLN
1	B	531	ASN
1	B	684	GLN
1	B	748	HIS
1	B	768	GLN
1	B	864	HIS
1	B	894	ASN
1	B	946	ASN
1	B	958	GLN
1	B	977	GLN
1	B	1034	HIS
1	B	1044	HIS
1	B	1070	ASN
1	B	1149	ASN
1	B	1195	GLN
1	B	1213	HIS
1	C	71	ASN

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Mol	Chain	Res	Type
1	C	112	GLN
1	C	158	GLN
1	C	251	GLN
1	C	252	HIS
1	C	261	ASN
1	C	351	ASN
1	C	423	GLN
1	C	450	GLN
1	C	529	GLN
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	1023	HIS
1	C	1034	HIS
1	C	1044	HIS
1	C	1070	ASN
1	C	1149	ASN
1	C	1195	GLN
1	C	1213	HIS
1	D	71	ASN
1	D	81	HIS
1	D	158	GLN
1	D	252	HIS
1	D	351	ASN
1	D	615	HIS
1	D	651	ASN
1	D	684	GLN
1	D	706	ASN
1	D	748	HIS
1	D	768	GLN
1	D	864	HIS
1	D	894	ASN
1	D	958	GLN
1	D	977	GLN
1	D	992	ASN
1	D	1023	HIS

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Mol	Chain	Res	Type
1	D	1034	HIS
1	D	1044	HIS
1	D	1070	ASN
1	D	1149	ASN
1	D	1195	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides 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	$\#\|Z\| > 2$
2	FES	C	3002	1	0,4,4	-	-	-		
2	FES	A	3002	1	0,4,4	-	-	-		
2	FES	D	3002	1	0,4,4	-	-	-		
4	GOL	B	3007	-	5,5,5	0.61	0	5,5,5	0.75	0
4	GOL	D	3007	-	5,5,5	0.85	0	5,5,5	1.30	1 (20%)
3	FAD	B	3006	-	53,58,58	2.07	14 (26%)	68,89,89	2.32	25 (36%)
4	GOL	A	3007	-	5,5,5	0.59	0	5,5,5	0.95	0
3	FAD	D	3006	-	53,58,58	2.28	11 (20%)	68,89,89	2.46	28 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	GOL	C	3007	-	5,5,5	0.52	0	5,5,5	0.53	0
6	PO4	D	3009	-	4,4,4	1.07	0	6,6,6	1.86	1 (16%)
2	FES	D	3001	1	0,4,4	-	-	-		
2	FES	B	3001	1	0,4,4	-	-	-		
3	FAD	C	3006	-	53,58,58	2.02	14 (26%)	68,89,89	2.48	29 (42%)
3	FAD	A	3006	-	53,58,58	1.84	12 (22%)	68,89,89	1.99	25 (36%)
2	FES	A	3001	1	0,4,4	-	-	-		
2	FES	B	3002	1	0,4,4	-	-	-		
2	FES	C	3001	1	0,4,4	-	-	-		
5	ACY	D	3008	-	3,3,3	1.13	0	3,3,3	1.52	0

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
2	FES	C	3002	1	-	-	0/1/1/1
2	FES	A	3002	1	-	-	0/1/1/1
2	FES	D	3002	1	-	-	0/1/1/1
4	GOL	B	3007	-	-	2/4/4/4	-
4	GOL	D	3007	-	-	0/4/4/4	-
2	FES	C	3001	1	-	-	0/1/1/1
3	FAD	B	3006	-	-	8/30/50/50	0/6/6/6
4	GOL	A	3007	-	-	2/4/4/4	-
3	FAD	D	3006	-	-	9/30/50/50	0/6/6/6
4	GOL	C	3007	-	-	2/4/4/4	-
2	FES	D	3001	1	-	-	0/1/1/1
2	FES	B	3001	1	-	-	0/1/1/1
3	FAD	A	3006	-	-	6/30/50/50	0/6/6/6
2	FES	A	3001	1	-	-	0/1/1/1
2	FES	B	3002	1	-	-	0/1/1/1
3	FAD	C	3006	-	-	8/30/50/50	0/6/6/6

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3006	FAD	C2A-N3A	10.49	1.49	1.32
3	D	3006	FAD	C2A-N1A	7.07	1.47	1.33
3	B	3006	FAD	C2A-N3A	7.04	1.43	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3006	FAD	C2A-N3A	6.02	1.41	1.32
3	A	3006	FAD	C2A-N1A	5.43	1.44	1.33
3	A	3006	FAD	C2A-N3A	5.34	1.40	1.32
3	C	3006	FAD	C2A-N1A	5.23	1.43	1.33
3	B	3006	FAD	O4B-C1B	-4.64	1.34	1.41
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	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	D	3006	FAD	C5A-C4A	3.66	1.50	1.40
3	A	3006	FAD	C1'-N10	3.65	1.57	1.48
3	D	3006	FAD	C2B-C1B	3.47	1.59	1.53
3	C	3006	FAD	C10-N1	3.39	1.40	1.33
3	B	3006	FAD	O2'-C2'	-3.24	1.36	1.43
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	B	3006	FAD	C2B-C1B	-2.95	1.49	1.53
3	D	3006	FAD	C10-N10	2.91	1.43	1.37
3	A	3006	FAD	C5A-N7A	-2.72	1.29	1.39
3	C	3006	FAD	O4B-C4B	-2.70	1.39	1.45
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	A	3006	FAD	C4A-N3A	-2.64	1.32	1.35
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	D	3006	FAD	C6A-N1A	2.46	1.48	1.37
3	A	3006	FAD	C4X-C4	-2.43	1.35	1.44
3	A	3006	FAD	C8A-N7A	-2.43	1.30	1.34
3	B	3006	FAD	C8M-C8	2.40	1.55	1.51
3	B	3006	FAD	C5A-N7A	-2.40	1.31	1.39
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3006	FAD	O3'-C3'	-2.28	1.37	1.43
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	C	3006	FAD	C4A-N3A	-2.02	1.32	1.35

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	3006	FAD	C1B-N9A-C4A	6.77	138.54	126.64
3	C	3006	FAD	C1B-N9A-C4A	6.74	138.48	126.64
3	B	3006	FAD	C1B-N9A-C4A	6.65	138.32	126.64
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	P-O3P-PA	-4.73	116.61	132.83
3	D	3006	FAD	C8M-C8-C7	-4.72	111.07	120.74
3	C	3006	FAD	N6A-C6A-N1A	4.64	128.20	118.57
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	O5B-C5B-C4B	4.56	124.68	108.99
3	D	3006	FAD	O2-C2-N1	-4.52	114.34	121.83
3	A	3006	FAD	C5X-C9A-N10	4.50	122.60	117.95
3	B	3006	FAD	N3A-C2A-N1A	-4.46	121.71	128.68
3	A	3006	FAD	O5'-C5'-C4'	4.44	121.22	109.36
3	D	3006	FAD	N6A-C6A-N1A	4.36	127.63	118.57
3	A	3006	FAD	O3B-C3B-C4B	-4.33	98.53	111.05
3	C	3006	FAD	C5A-C6A-N6A	-4.29	113.84	120.35
3	D	3006	FAD	C5A-C6A-N6A	-4.28	113.85	120.35
3	B	3006	FAD	O3'-C3'-C2'	-4.27	98.50	108.81
3	C	3006	FAD	N3A-C2A-N1A	-4.24	122.05	128.68
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	O4'-C4'-C5'	-3.92	101.11	109.92
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	A	3006	FAD	N3A-C2A-N1A	-3.59	123.07	128.68
3	C	3006	FAD	O4B-C1B-C2B	3.54	112.10	106.93
3	A	3006	FAD	C1B-N9A-C4A	3.49	132.77	126.64
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	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	O4-C4-C4X	-3.12	118.33	126.60
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	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	D	3006	FAD	N3A-C2A-N1A	-2.99	124.00	128.68
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	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	C8M-C8-C9	-2.83	114.25	119.49
3	D	3006	FAD	C4A-C5A-N7A	2.80	112.32	109.40
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	D	3006	FAD	C5B-C4B-C3B	-2.64	105.28	115.18
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	B	3006	FAD	C4A-C5A-N7A	-2.61	106.68	109.40
3	C	3006	FAD	C4'-C3'-C2'	2.60	118.77	113.36
3	C	3006	FAD	C8M-C8-C9	2.56	124.23	119.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	3006	FAD	C9-C8-C7	-2.55	116.01	119.67
3	C	3006	FAD	C5'-C4'-C3'	-2.50	107.37	112.20
3	B	3006	FAD	C5A-C6A-N6A	-2.46	116.61	120.35
3	D	3006	FAD	O2B-C2B-C1B	2.43	119.84	110.85
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	C	3006	FAD	C3B-C2B-C1B	-2.31	97.51	100.98
3	A	3006	FAD	C5A-C6A-N6A	2.30	123.84	120.35
3	A	3006	FAD	O2B-C2B-C3B	-2.26	104.52	111.82
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	O3B-C3B-C2B	2.20	118.94	111.82
3	D	3006	FAD	C9A-C5X-N5	-2.19	120.05	122.43
3	D	3006	FAD	C5A-C6A-N1A	-2.15	115.47	120.35
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	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	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
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 (37) 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

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Mol	Chain	Res	Type	Atoms
3	B	3006	FAD	C5B-O5B-PA-O2A
3	B	3006	FAD	C5B-O5B-PA-O3P
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-C4B-C5B-O5B
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	B	3006	FAD	O4B-C4B-C5B-O5B
3	B	3006	FAD	C3B-C4B-C5B-O5B
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 81 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3002	FES	2	0
4	B	3007	GOL	14	0

Continued on next page...

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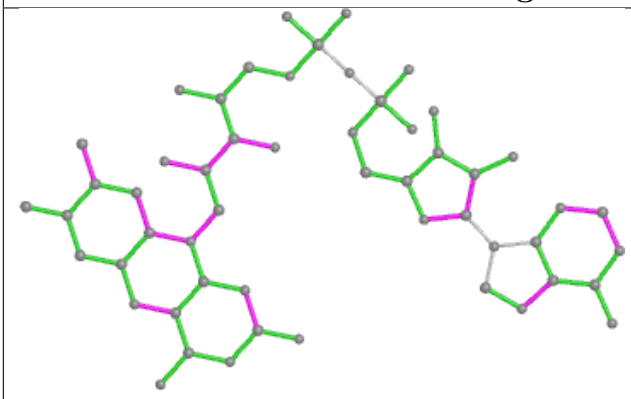
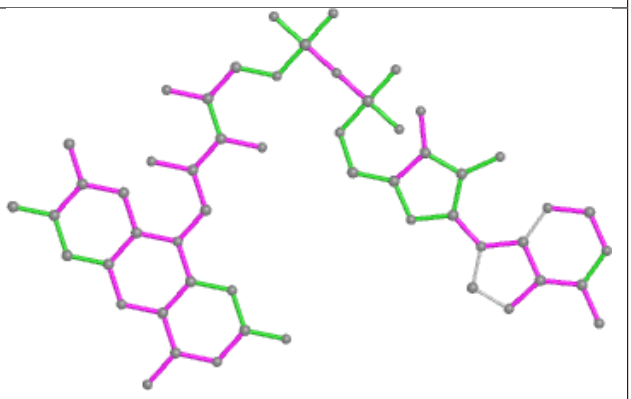
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	3007	GOL	10	0
3	B	3006	FAD	6	0
4	A	3007	GOL	6	0
3	D	3006	FAD	14	0
4	C	3007	GOL	4	0
6	D	3009	PO4	1	0
3	C	3006	FAD	10	0
3	A	3006	FAD	12	0
2	B	3002	FES	2	0

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

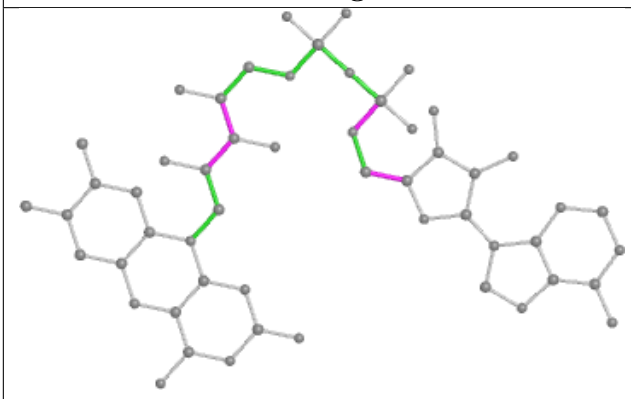
Ligand FAD B 3006



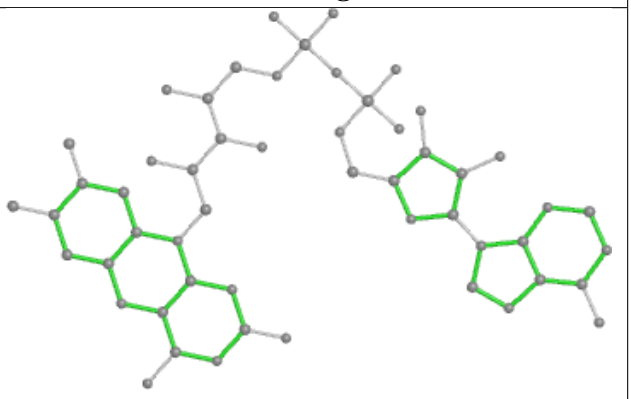
Bond lengths



Bond angles

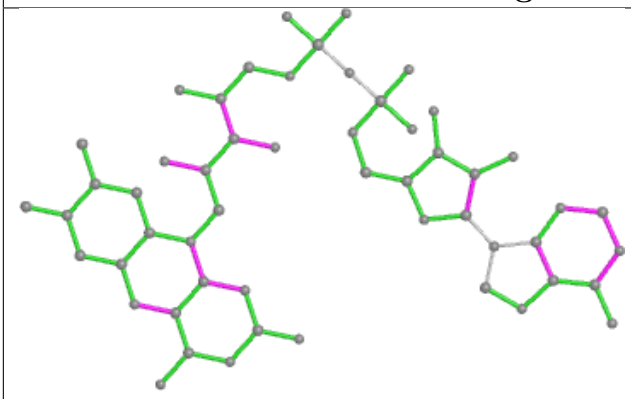


Torsions

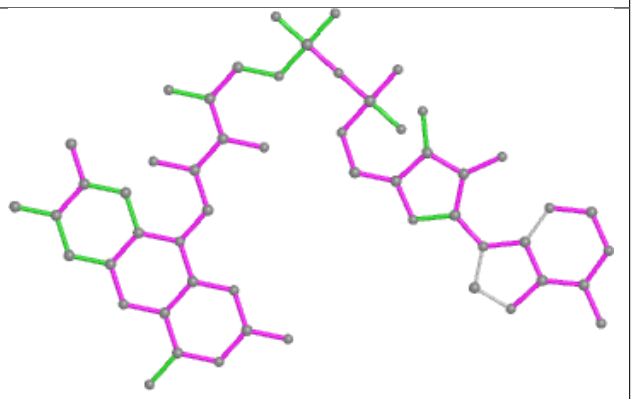


Rings

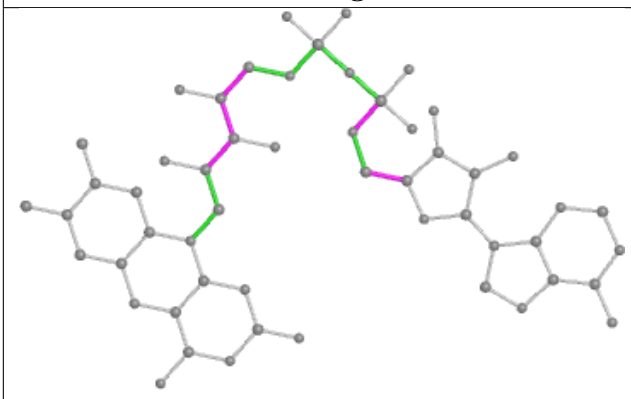
Ligand FAD D 3006



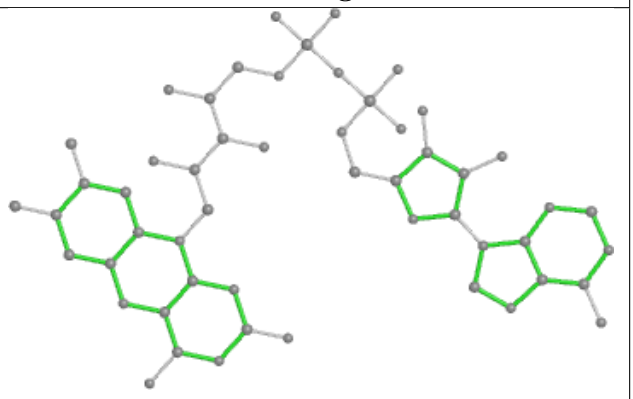
Bond lengths



Bond angles

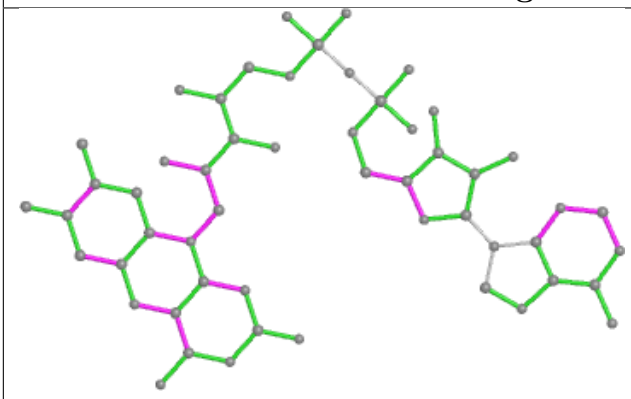


Torsions

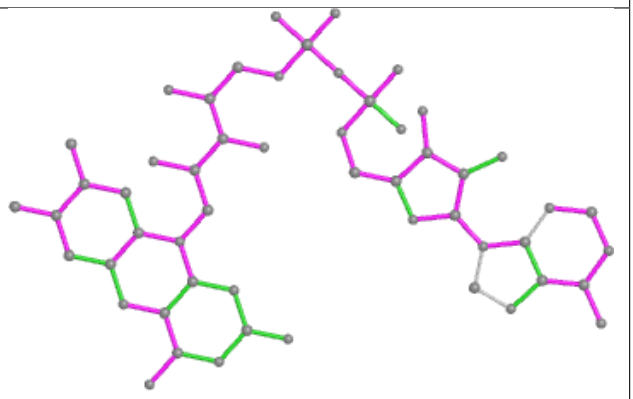


Rings

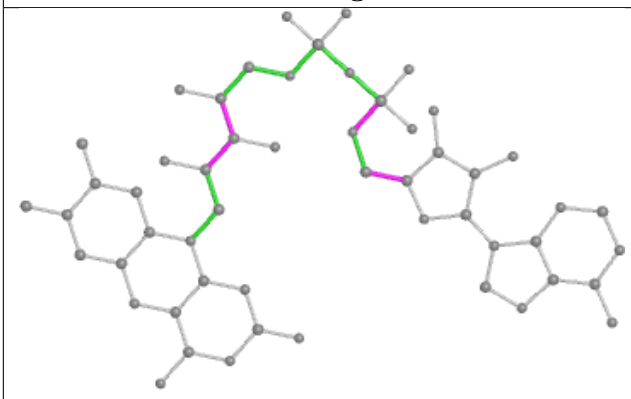
Ligand FAD C 3006



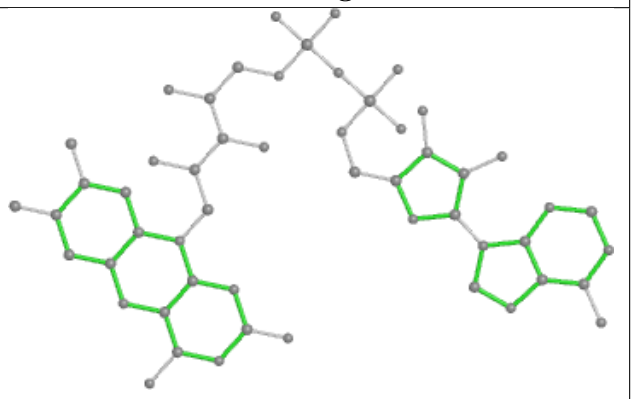
Bond lengths



Bond angles

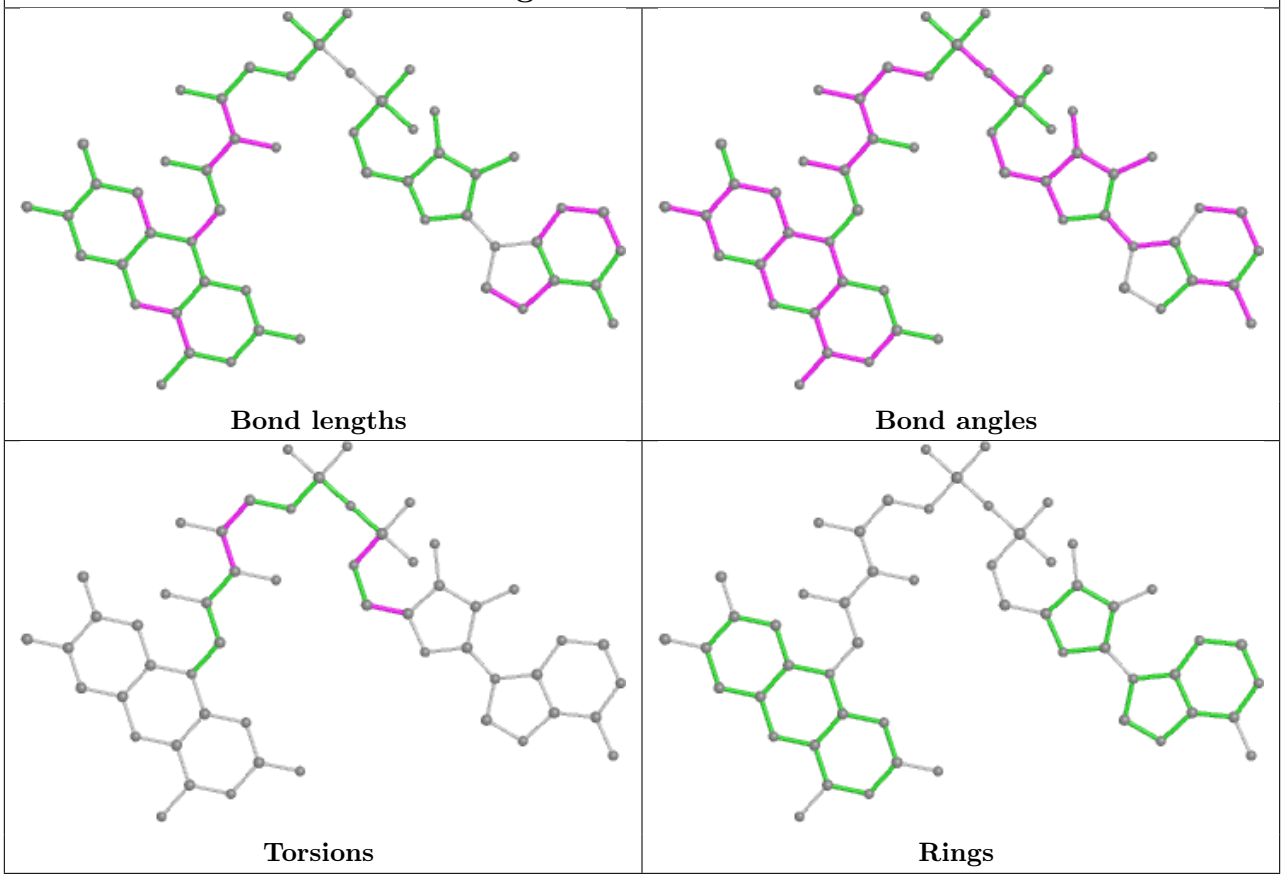


Torsions



Rings

Ligand FAD A 3006



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.