Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 03:42 am GMT

PDB ID	:	6H03
EMDB ID	:	EMD-0106
Title	:	OPEN CONFORMATION OF THE MEMBRANE ATTACK COMPLEX
Authors	:	Menny, A.; Serna, M.; Boyd, C.M.; Gardner, S.; Joseph, A.P.; Topf, M.; Bubeck, D.
Deposited on	:	2018-07-06
Resolution	:	5.60 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
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:

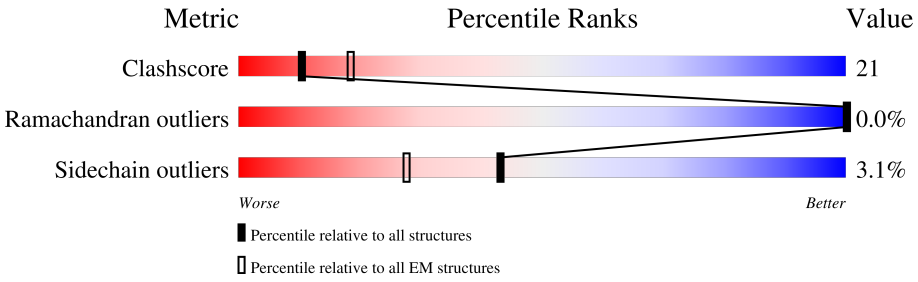
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 5.60 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1580	43% 59% 17% • 23%
2	C	537	10% 74% 21% •
3	D	821	25% 63% 16% • 20%
4	E	182	27% 74% 17% 9%
5	F	554	12% 66% 25% • 8%
6	B	913	35% 59% 16% • 24%
7	G	538	14% 58% 33% • 7%
7	H	538	6% 56% 36% • 7%

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Mol	Chain	Length	Quality of chain
7	I	538	6% 56% 36% • 7%
7	J	538	6% 55% 36% • 7%
7	K	538	6% 56% 36% • 7%
7	L	538	5% 53% 39% • 7%
7	M	538	5% 54% 37% • 7%
7	N	538	8% 55% 36% • 7%
7	O	538	6% 54% 38% • 7%
7	P	538	8% 53% 39% • 7%
7	Q	538	7% 54% 37% • 7%
7	R	538	9% 53% 39% • 7%
7	S	538	12% 53% 39% • 7%
7	T	538	17% 53% 38% • 7%
7	U	538	21% 53% 38% • 7%
7	V	538	32% 51% 40% • 7%
7	W	538	51% 51% 41% • 7%
7	X	538	82% 56% 36% • 7%
8	Y	3	100% 100%
9	Z	2	100% 50% 50%
9	a	2	100% 50% 50%
9	b	2	50% 50% 50%
9	c	2	50% 50% 50%
9	d	2	50% 50% 50%
9	e	2	50% 50% 50%
9	f	2	50% 50% 50%
9	g	2	50% 50% 50%

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Mol	Chain	Length	Quality of chain
9	h	2	50% 50% 50%
9	i	2	50% 50% 50%
9	j	2	50% 50% 50%
9	k	2	50% 50% 50%
9	l	2	50% 50% 50%
9	m	2	50% 50% 50%
9	n	2	50% 50% 50%
9	o	2	100% 50% 50%
9	p	2	100% 50% 50%
9	q	2	100% 50% 50%
9	r	2	100% 50% 50%
9	s	2	100% 50% 50%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 102310 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Complement C5,Complement C5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1223	9686	6226	1594	1839	27	0	0

- Molecule 2 is a protein called Complement component C8 beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	513	4119	2576	729	780	34	0	0

- Molecule 3 is a protein called Complement component C7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	657	5129	3190	896	1001	42	0	0

- Molecule 4 is a protein called Complement component C8 gamma chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	165	1295	828	224	239	4	0	0

- Molecule 5 is a protein called Complement component C8 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	511	4017	2492	701	787	37	0	0

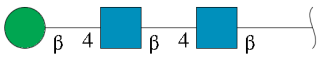
- Molecule 6 is a protein called Complement component C6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	B	690	5427	3367	952	1058	50	0	0

- Molecule 7 is a protein called Complement component C9.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	501	Total	C	N	O	S	0	0
			3977	2488	691	767	31		
7	P	501	Total	C	N	O	S	0	0
			3977	2488	691	767	31		
7	H	501	Total	C	N	O	S	0	0
			3977	2488	691	767	31		
7	I	501	Total	C	N	O	S	0	0
			3977	2488	691	767	31		
7	J	501	Total	C	N	O	S	0	0
			3977	2488	691	767	31		
7	K	501	Total	C	N	O	S	0	0
			3977	2488	691	767	31		
7	L	501	Total	C	N	O	S	0	0
			3977	2488	691	767	31		
7	M	501	Total	C	N	O	S	0	0
			3977	2488	691	767	31		
7	N	501	Total	C	N	O	S	0	0
			3973	2486	690	766	31		
7	O	501	Total	C	N	O	S	0	0
			3977	2488	691	767	31		
7	Q	501	Total	C	N	O	S	0	0
			3977	2488	691	767	31		
7	R	501	Total	C	N	O	S	0	0
			3977	2488	691	767	31		
7	S	501	Total	C	N	O	S	0	0
			3977	2488	691	767	31		
7	T	501	Total	C	N	O	S	0	0
			3977	2488	691	767	31		
7	U	501	Total	C	N	O	S	0	0
			3977	2488	691	767	31		
7	V	501	Total	C	N	O	S	0	0
			3951	2474	686	760	31		
7	W	501	Total	C	N	O	S	0	0
			3941	2466	682	762	31		
7	X	501	Total	C	N	O	S	0	0
			3977	2488	691	767	31		

- Molecule 8 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
8	Y	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 9 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	Z	2	Total	C	N	O	0	0
			28	16	2	10		
9	a	2	Total	C	N	O	0	0
			28	16	2	10		
9	b	2	Total	C	N	O	0	0
			28	16	2	10		
9	c	2	Total	C	N	O	0	0
			28	16	2	10		
9	d	2	Total	C	N	O	0	0
			28	16	2	10		
9	e	2	Total	C	N	O	0	0
			28	16	2	10		
9	f	2	Total	C	N	O	0	0
			28	16	2	10		
9	g	2	Total	C	N	O	0	0
			28	16	2	10		
9	h	2	Total	C	N	O	0	0
			28	16	2	10		
9	i	2	Total	C	N	O	0	0
			28	16	2	10		
9	j	2	Total	C	N	O	0	0
			28	16	2	10		
9	k	2	Total	C	N	O	0	0
			28	16	2	10		
9	l	2	Total	C	N	O	0	0
			28	16	2	10		
9	m	2	Total	C	N	O	0	0
			28	16	2	10		

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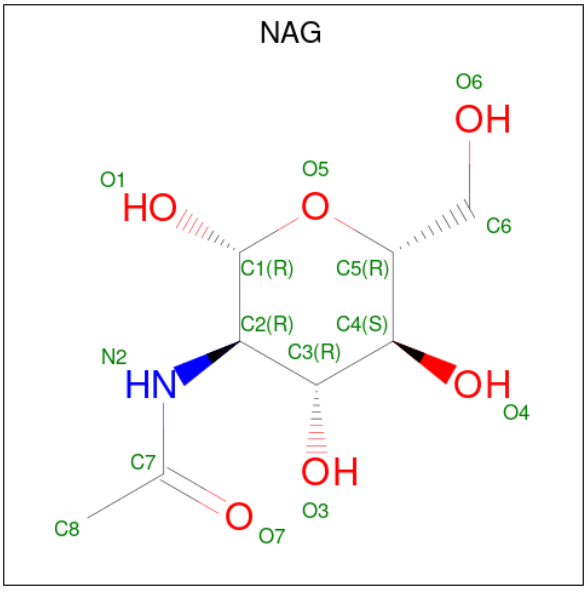
Mol	Chain	Residues	Atoms	AltConf	Trace
9	n	2	Total C N O 28 16 2 10	0	0
9	o	2	Total C N O 28 16 2 10	0	0
9	p	2	Total C N O 28 16 2 10	0	0
9	q	2	Total C N O 28 16 2 10	0	0
9	r	2	Total C N O 28 16 2 10	0	0
9	s	2	Total C N O 28 16 2 10	0	0

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	AltConf
10	F	1	Total C N O 14 8 1 5	0
10	G	1	Total C N O 28 16 2 10	0
10	G	1	Total C N O 28 16 2 10	0
10	P	1	Total C N O 28 16 2 10	0
10	P	1	Total C N O 28 16 2 10	0

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Mol	Chain	Residues	Atoms				AltConf
10	H	1	Total	C	N	O	0
			28	16	2	10	
10	H	1	Total	C	N	O	0
			28	16	2	10	
10	I	1	Total	C	N	O	0
			28	16	2	10	
10	I	1	Total	C	N	O	0
			28	16	2	10	
10	J	1	Total	C	N	O	0
			28	16	2	10	
10	J	1	Total	C	N	O	0
			28	16	2	10	
10	K	1	Total	C	N	O	0
			28	16	2	10	
10	K	1	Total	C	N	O	0
			28	16	2	10	
10	L	1	Total	C	N	O	0
			28	16	2	10	
10	L	1	Total	C	N	O	0
			28	16	2	10	
10	M	1	Total	C	N	O	0
			28	16	2	10	
10	M	1	Total	C	N	O	0
			28	16	2	10	
10	N	1	Total	C	N	O	0
			28	16	2	10	
10	N	1	Total	C	N	O	0
			28	16	2	10	
10	O	1	Total	C	N	O	0
			28	16	2	10	
10	O	1	Total	C	N	O	0
			28	16	2	10	
10	Q	1	Total	C	N	O	0
			28	16	2	10	
10	Q	1	Total	C	N	O	0
			28	16	2	10	
10	R	1	Total	C	N	O	0
			28	16	2	10	
10	R	1	Total	C	N	O	0
			28	16	2	10	
10	S	1	Total	C	N	O	0
			28	16	2	10	

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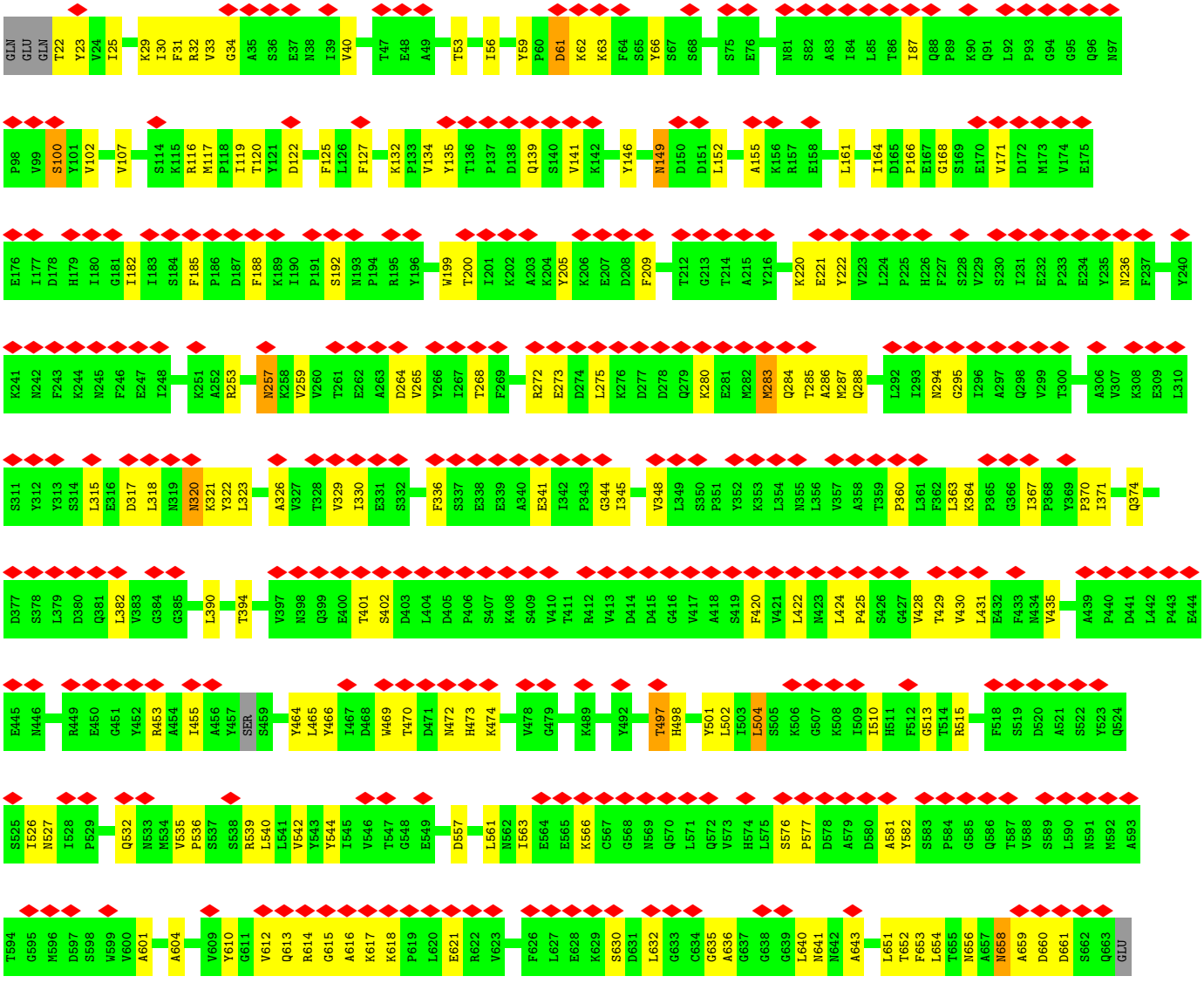
Mol	Chain	Residues	Atoms				AltConf
10	S	1	Total	C	N	O	0
			28	16	2	10	
10	T	1	Total	C	N	O	0
			28	16	2	10	
10	T	1	Total	C	N	O	0
			28	16	2	10	
10	U	1	Total	C	N	O	0
			28	16	2	10	
10	U	1	Total	C	N	O	0
			28	16	2	10	
10	V	1	Total	C	N	O	0
			28	16	2	10	
10	V	1	Total	C	N	O	0
			28	16	2	10	
10	W	1	Total	C	N	O	0
			28	16	2	10	
10	W	1	Total	C	N	O	0
			28	16	2	10	
10	X	1	Total	C	N	O	0
			28	16	2	10	
10	X	1	Total	C	N	O	0
			28	16	2	10	

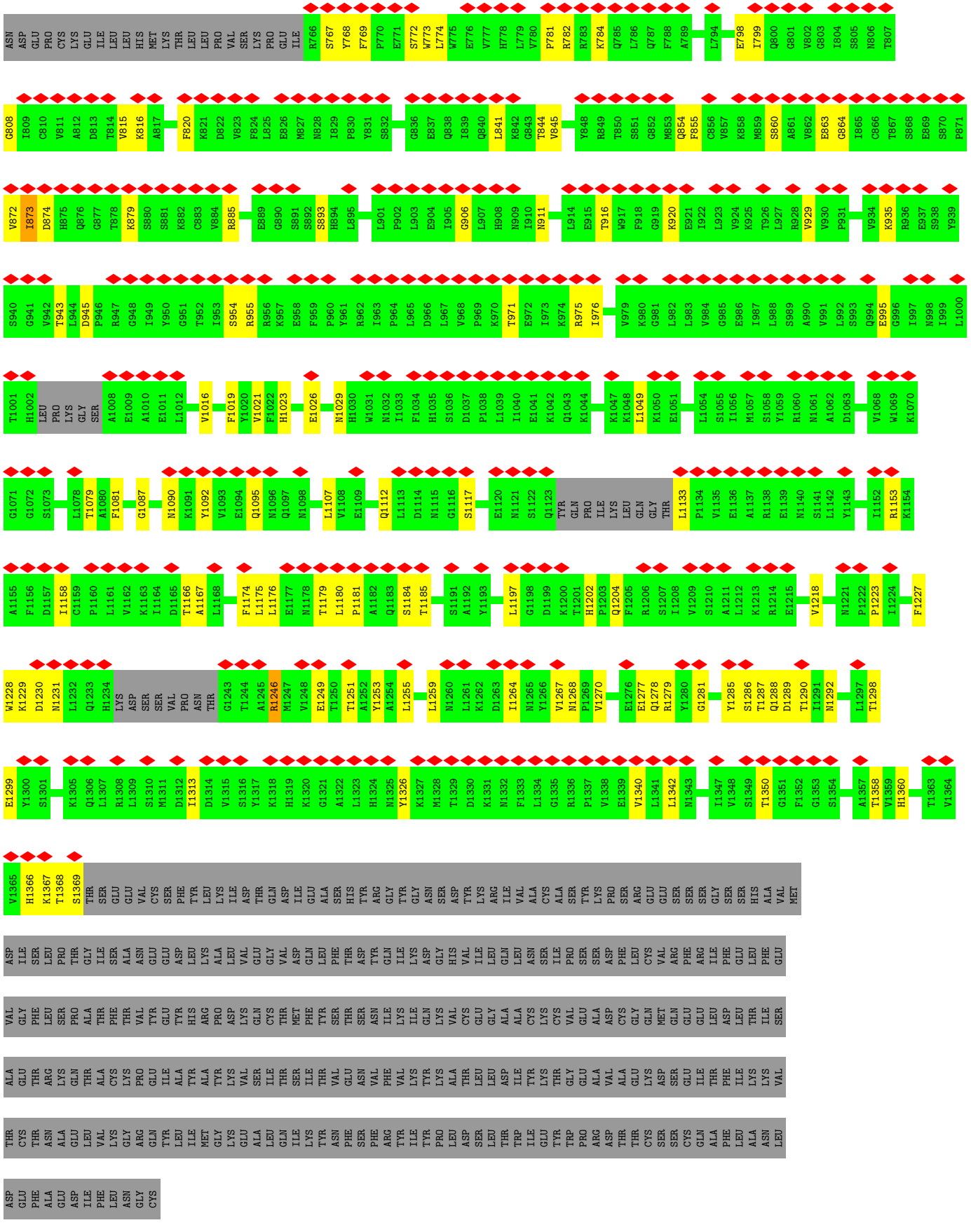
3 Residue-property plots (i)

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 and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Complement C5,Complement C5

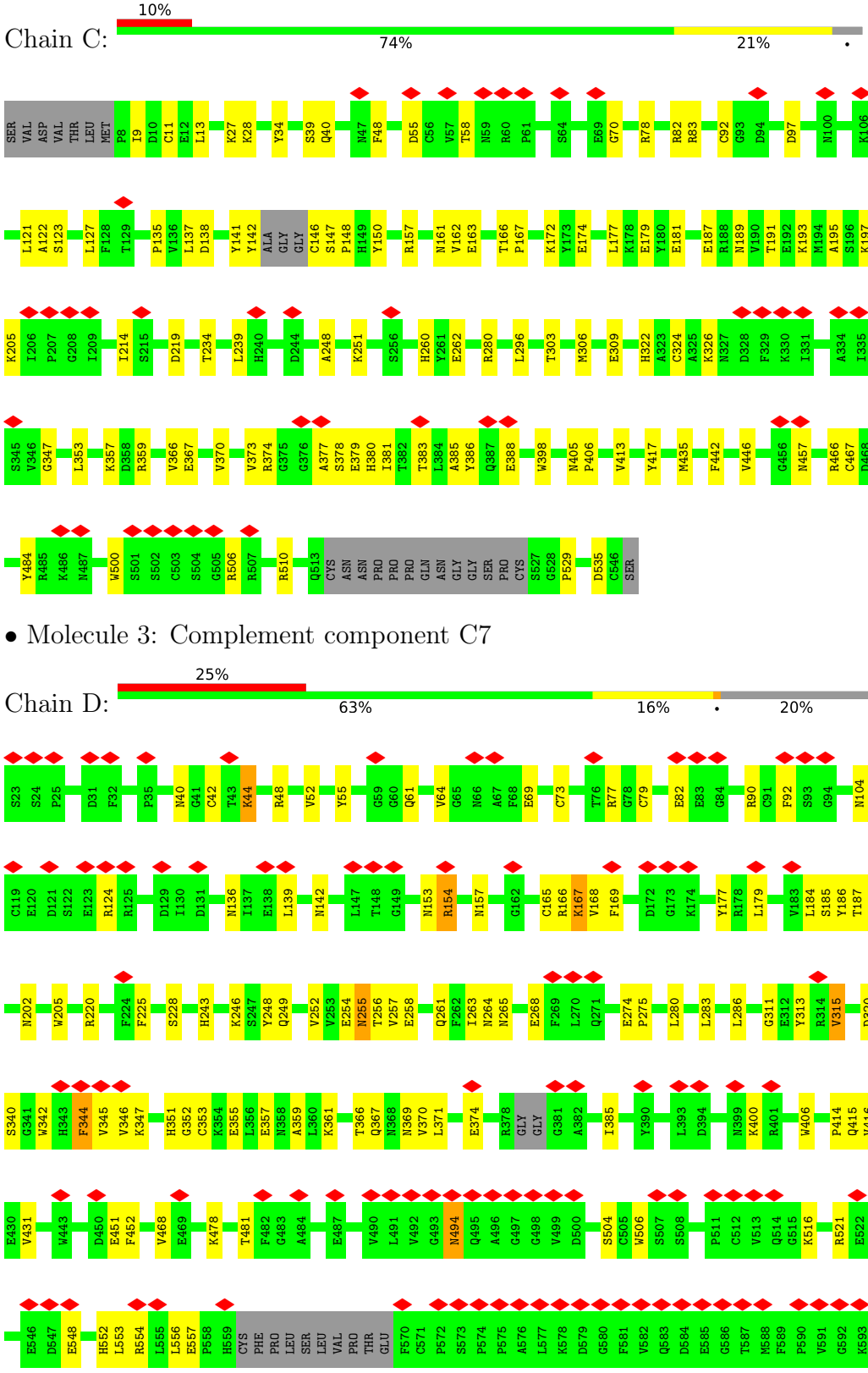
Chain A:




ASN ASP GLU PRO CYS LYS GLU ILE LEU LEU HIS MET LYS THR LEU LEU PRO VAL SER LYS PRO GLU ILE
R766 S767 Y768 F769 P770 E771 S772 W773 L774 W775 E776 V777 H778 L779 V780 P781 R782 R783 K784 Q785 L786 Q787 F788 A789 L794 E798 I799 Q800 G801 V802 G803 I804 S805 N806 T807
G808 I809 C810 V811 A812 D813 T814 V815 K816 A817 F820 K821 D822 V823 F824 L825 E826 M827 N828 I829 P830 Y831 S832 G836 E837 Q838 I839 Q840 L841 K842 G843 T844 V845 Y848 R849 T850 S851 G852 M853 Q854 F855 C856 V857 K858 M859 S860 A861 V862 E863 G864 I865 C866 T867 S868 E869 S870 P871
V872 I873 D874 H875 Q876 G877 T878 K879 S880 S881 K882 C883 V884 R885 E889 G890 S891 S892 S893 H894 L895 L901 P902 L903 E904 T905 G906 L907 H908 N909 I910 N911 L914 E915 T916 W917 F918 G919 K920 E921 I922 L923 V924 K925 T926 L927 R928 V929 V930 P931 V934 K935 R936 E937 S938 Y939
S940 G941 V942 T943 L944 D945 P946 R947 G948 I949 Y950 G951 T952 I953 S954 R955 R956 K957 E958 F959 P960 Y961 R962 I963 P964 L965 D966 L967 V968 P969 K970 T971 E972 I973 K974 R975 T976 V979 K980 G981 L982 L983 V984 G985 E986 I987 L988 S989 A990 V991 L992 S993 Q994 E995 G996 I997 N998 I999 L1000
T1001 H1002 LEU PRO LYS GLY SER A1008 E1009 A1010 E1011 L1012 V1016 F1019 Y1020 V1021 F1022 H1023 E1026 N1029 H1030 W1031 N1032 I1033 F1034 H1035 S1036 D1037 P1038 L1039 I1040 E1041 K1042 Q1043 K1044 K1047 K1048 L1049 K1050 E1051 L1054 S1055 I1056 M1057 S1058 Y1059 R1060 N1061 A1062 D1063 V1068 W1069 K1070
G1071 G1072 S1073 L1078 T1079 A1080 F1081 G1087 N1090 K1091 Y1092 V1093 E1094 Q1095 N1096 Q1097 N1098 L1107 V1108 E1109 Q1112 L1113 D1114 N1115 G1116 S1117 E1120 N1121 S1122 Q1123 TYR GLN PRO ILE LYS LEU GLN GLY THR L1133 P1134 V1135 E1136 A1137 R1138 E1139 N1140 S1141 L1142 Y1143 I1152 R1153 K1154
A1155 F1156 D1157 I1158 C1159 P1160 L1161 V1162 K1163 I1164 D1165 T1166 A1167 L1168 F1174 L1175 L1176 E1177 N1178 T1179 L1180 P1181 A1182 Q1183 S1184 T1185 S1191 A1192 Y1193 L1197 G1198 D1199 K1200 T1201 H1202 P1203 Q1204 F1205 R1206 S1207 I1208 V1209 S1210 A1211 L1212 K1213 R1214 E1215 V1218 N1221 P1222 P1223 I1224 F1227
W1228 K1229 D1230 N1231 L1232 Q1233 H1234 LYS ASP SER SER VAL PRO ASN THR G1243 T1244 A1245 R1246 M1247 V1248 E1249 T1250 T1251 A1252 Y1253 A1254 L1255 L1259 N1260 L1261 K1262 D1263 I1264 N1265 Y1266 V1267 N1268 P1269 V1270 E1276 E1277 Q1278 R1279 Y1280 G1281 Y1285 S1286 T1287 Q1288 D1289 T1290 I1291 N1292 L1297 T1298
E1299 Y1300 S1301 K1305 Q1306 L1307 R1308 L1309 S1310 M1311 D1312 I1313 D1314 V1315 S1316 Y1317 K1318 H1319 K1320 G1321 A1322 L1323 H1324 N1325 Y1326 K1327 M1328 T1329 D1330 K1331 N1332 F1333 L1334 G1335 R1336 P1337 V1338 E1339 V1340 L1341 L1342 N1343 I1347 V1348 S1349 T1350 G1351 F1352 G1353 S1354 A1357 T1358 Y1359 H1360 T1363 V1364
V1365 H1366 K1367 T1368 S1369 THR SER GLU GLU VAL CYS SER PHE TYR LEU LYS ALA LEU VAL GLU GLY GLY VAL ASP GLN LEU ASP ILE GLU ALA SER HIS TYR ARG GLY TYR GLY ASN SER ASP TYR LYS ARG ILE VAL ALA CYS ALA SER TYR LYS PRO SER ARG GLU GLU SER SER SER GLY SER SER SER HIS ALA VAL MET
ASP ILE SER LEU PRO THR GLY ILE SER LEU PHE THR ASP GLN ILE LYS ASP GLY HIS VAL ILE LEU GLN LEU LEU ASN SER ILE PRO SER SER ASP PHE LEU CYS VAL ARG PHE ARG ILE PHE GLU LEU PHE GLU
VAL GLY PHE LEU SER PRO ALA THR PHE THR VAL TYR GLU TYR HIS ARG PRO ASP LYS GLN CYS THR MET PHE TYR SER THR SER ASN ILE LYS ILE GLN LYS VAL CYS GLU GLY ALA ALA CYS LYS CYS VAL GLU ALA ASP CYS GLY GLN MET GLN GLU GLU LEU ASP LEU THR ILE SER
ALA GLU THR ARG LYS GLN THR ALA CYS LYS PRO GLU ILE ALA TYR ALA TYR LYS VAL SER ILE THR SER ILE THR VAL GLU ASN VAL PHE VAL LYS TYR LYS VAL ALA THR LEU LEU ASP ILE TYR LYS THR GLY GLU ALA ASP CYS GLU ILE ASP LEU THR PHE ILE LYS VAL
THR CYS THR ASN ALA GLU LEU VAL LYS GLY ARG GLN TYR LEU ILE MET GLY LYS GLU ALA LEU GLN ILE LYS TYR ASN PHE SER PHE ARG TYR ILE ASP SER LEU THR TRP ILE GLU TYR TRP PRO ARG ASP THR THR CYS SER GLN ALA PHE LEU ALA ASN LEU
ASP GLU PHE ALA GLU ASP ILE PHE LEU ASN GLY CYS

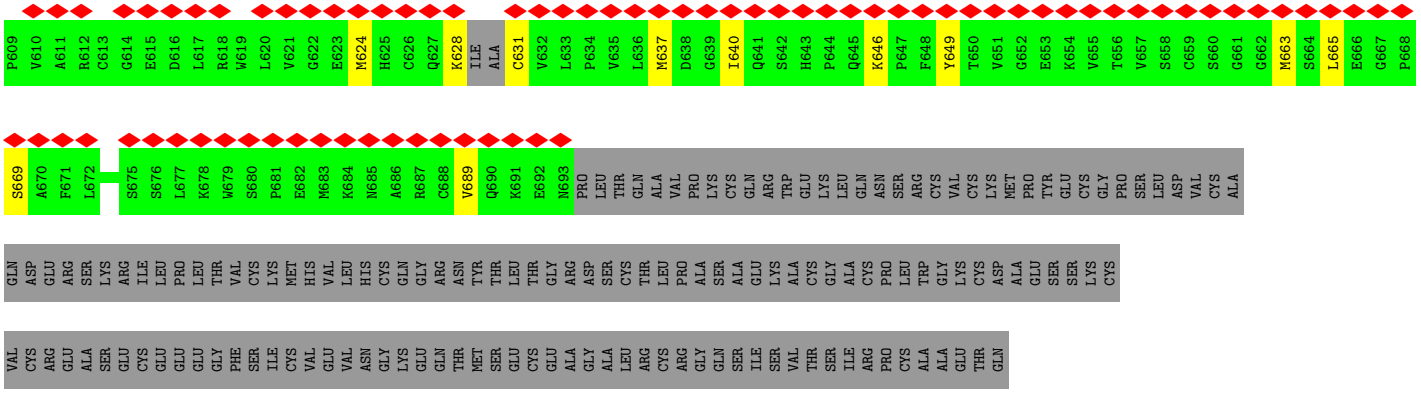
• Molecule 2: Complement component C8 beta chain

Chain C:



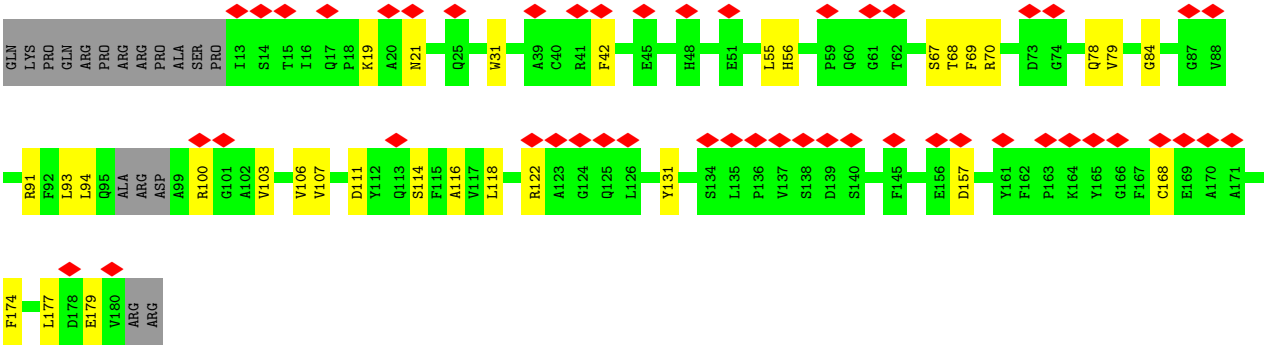
• Molecule 3: Complement component C7

Chain D:



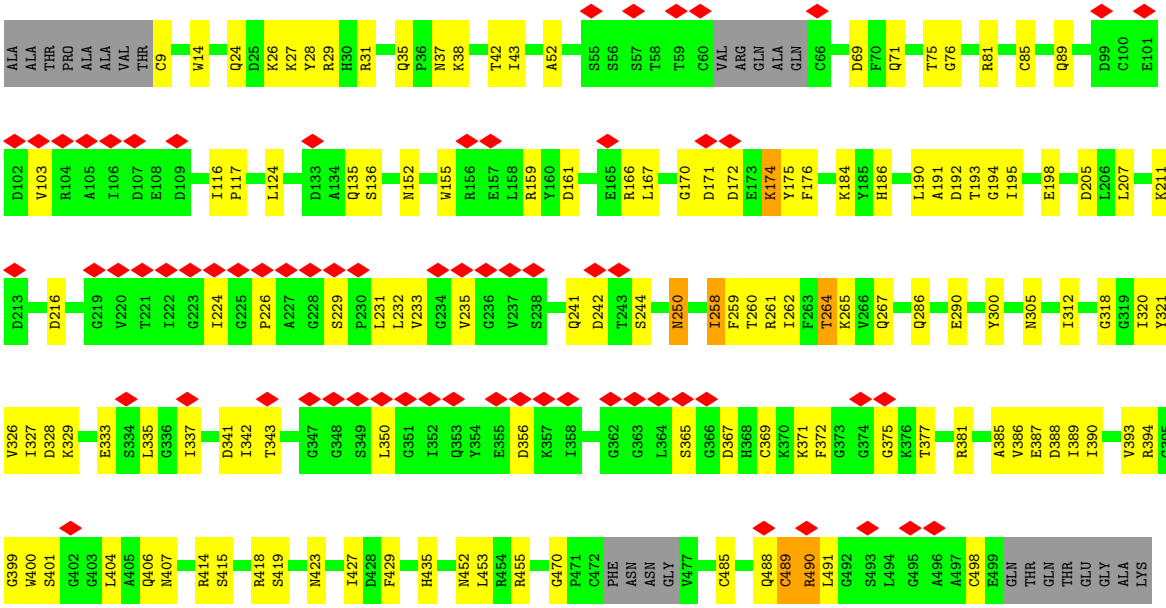
• Molecule 4: Complement component C8 gamma chain

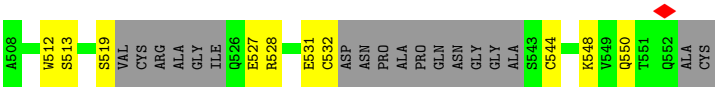
Chain E:



• Molecule 5: Complement component C8 alpha chain

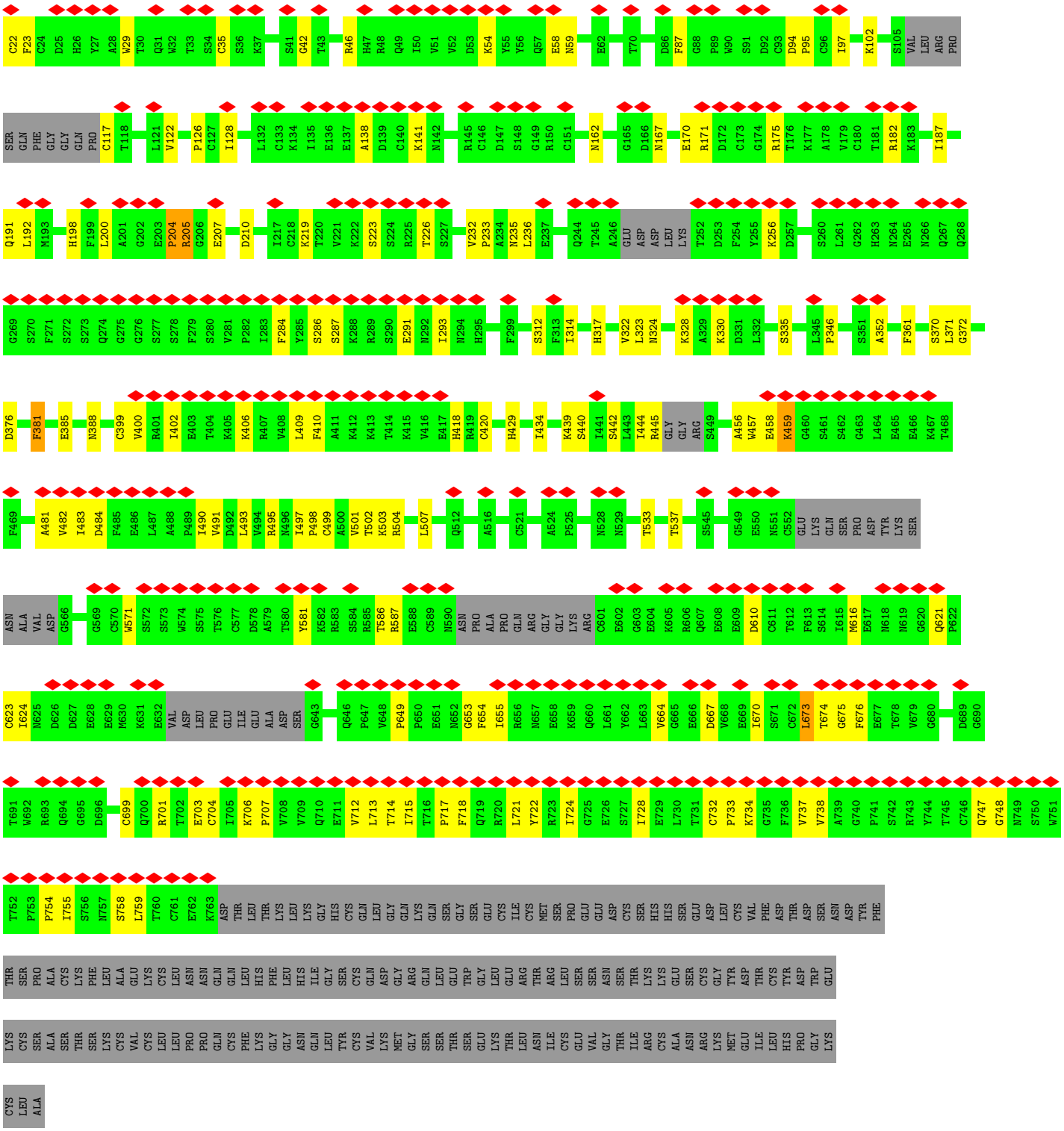
Chain F:





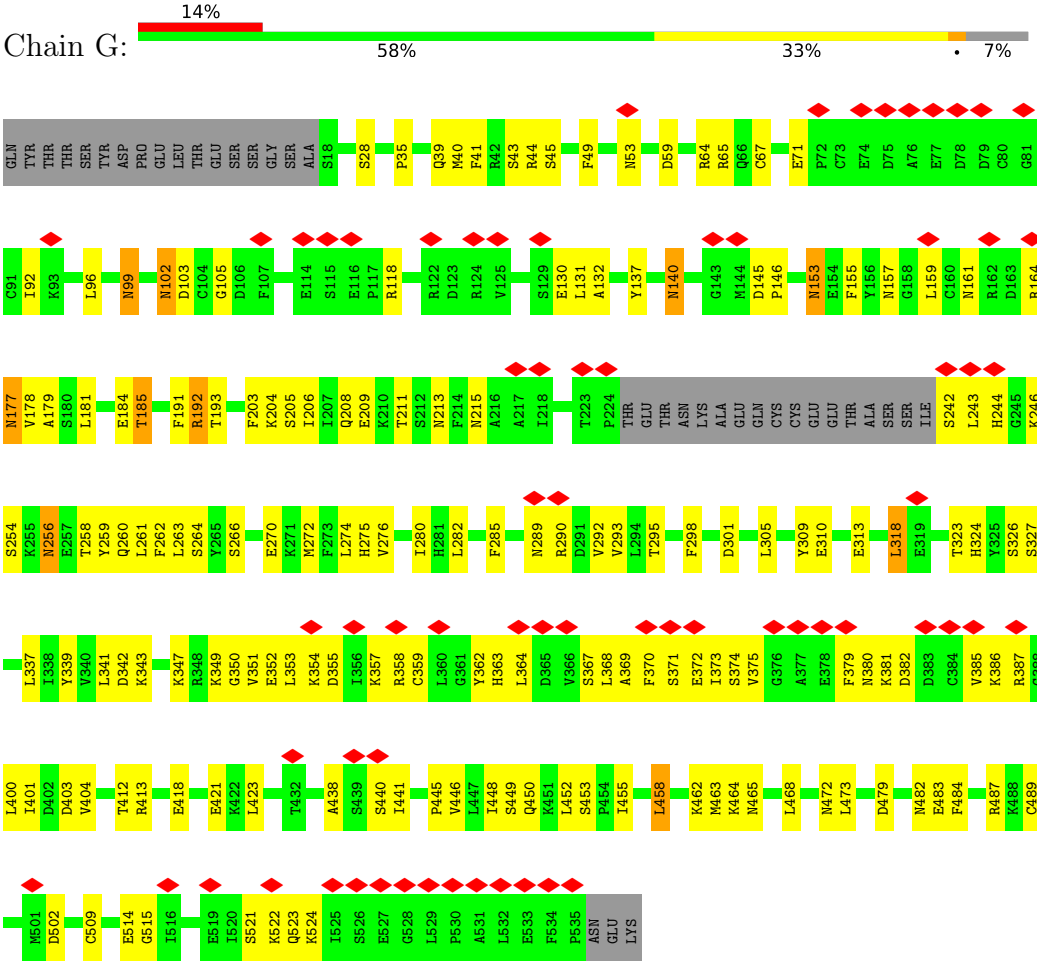
• Molecule 6: Complement component C6

Chain B:



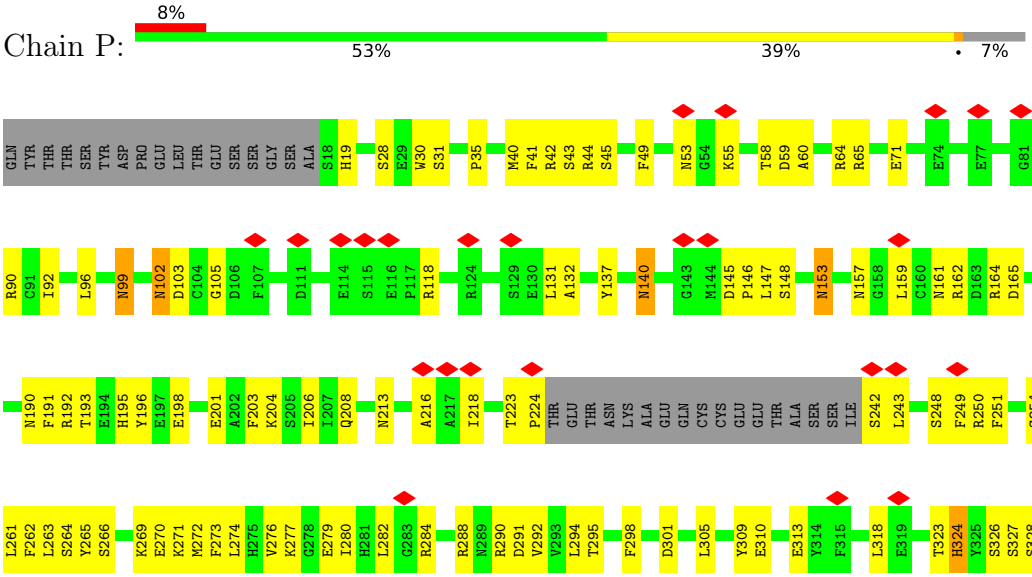
• Molecule 7: Complement component C9

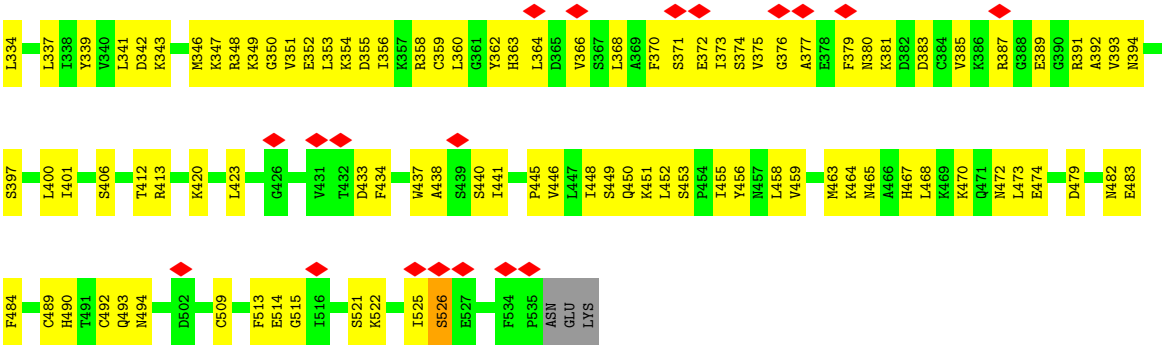
Chain G:



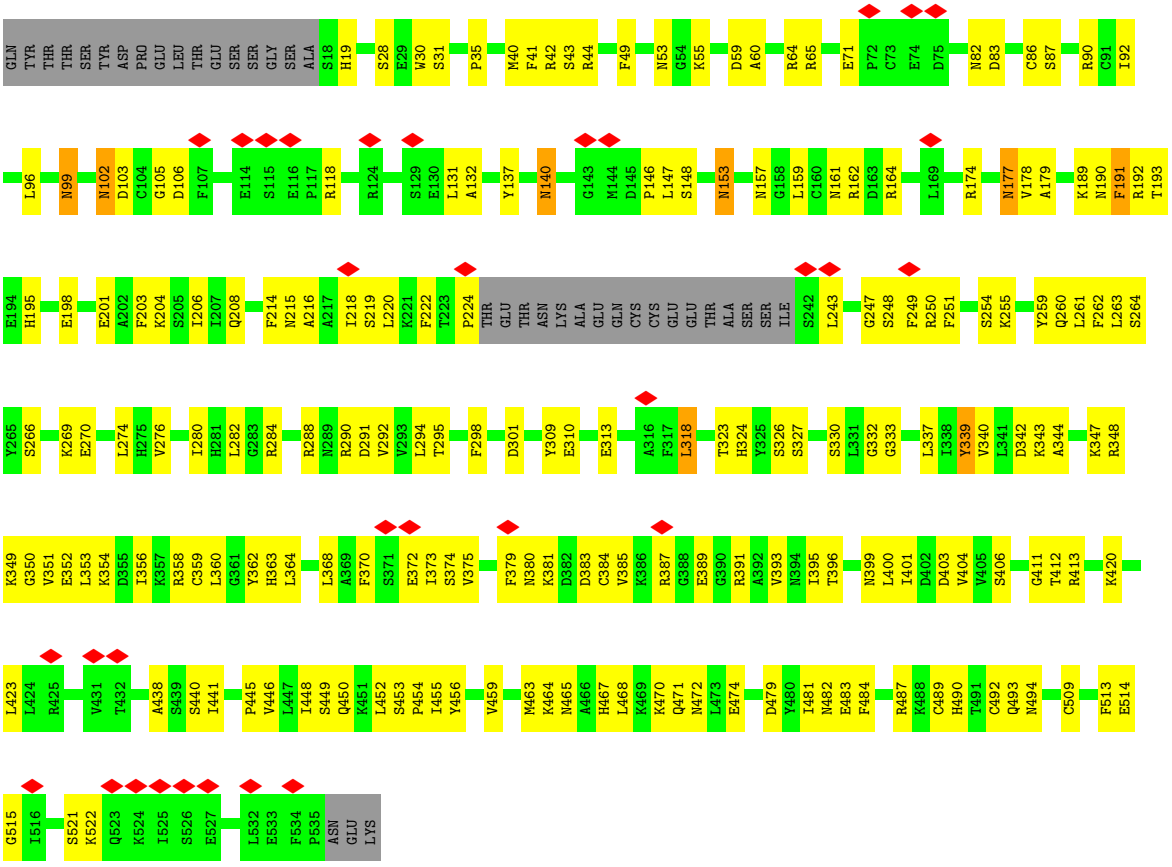
• Molecule 7: Complement component C9

Chain P:

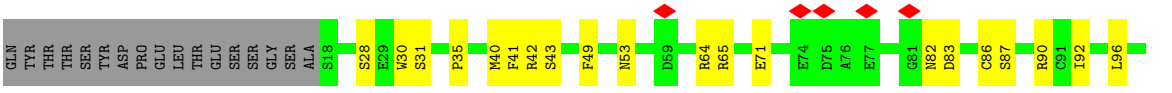


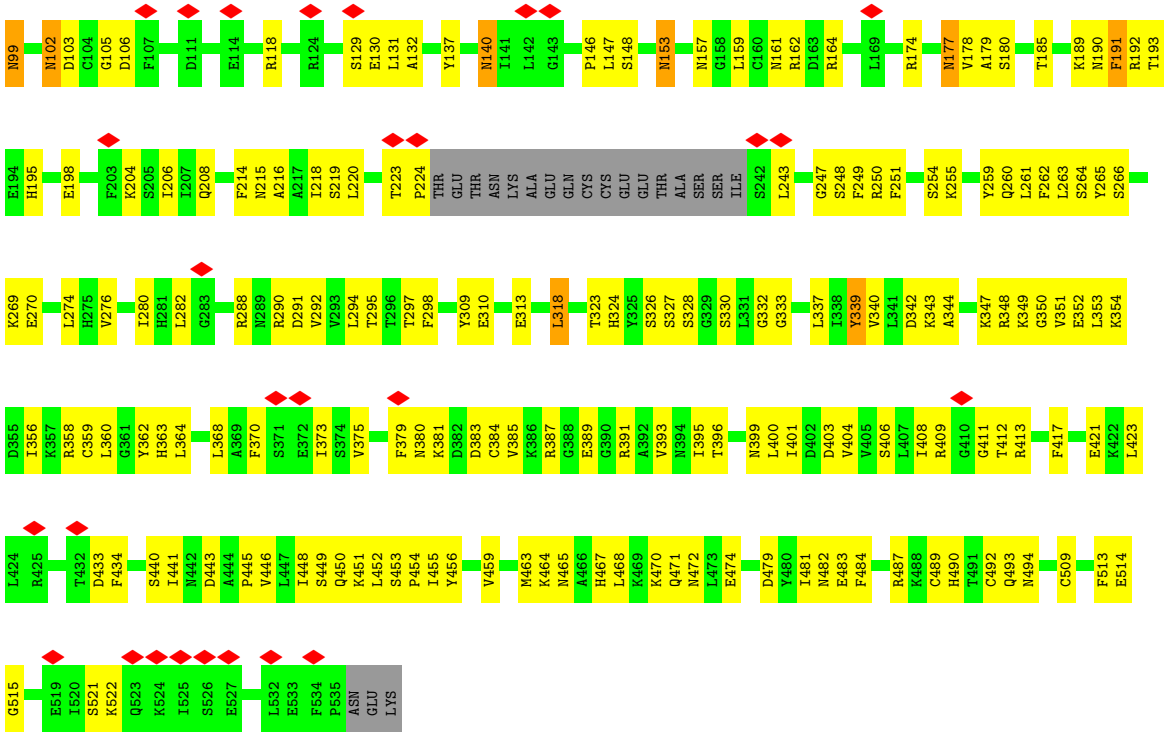


• Molecule 7: Complement component C9



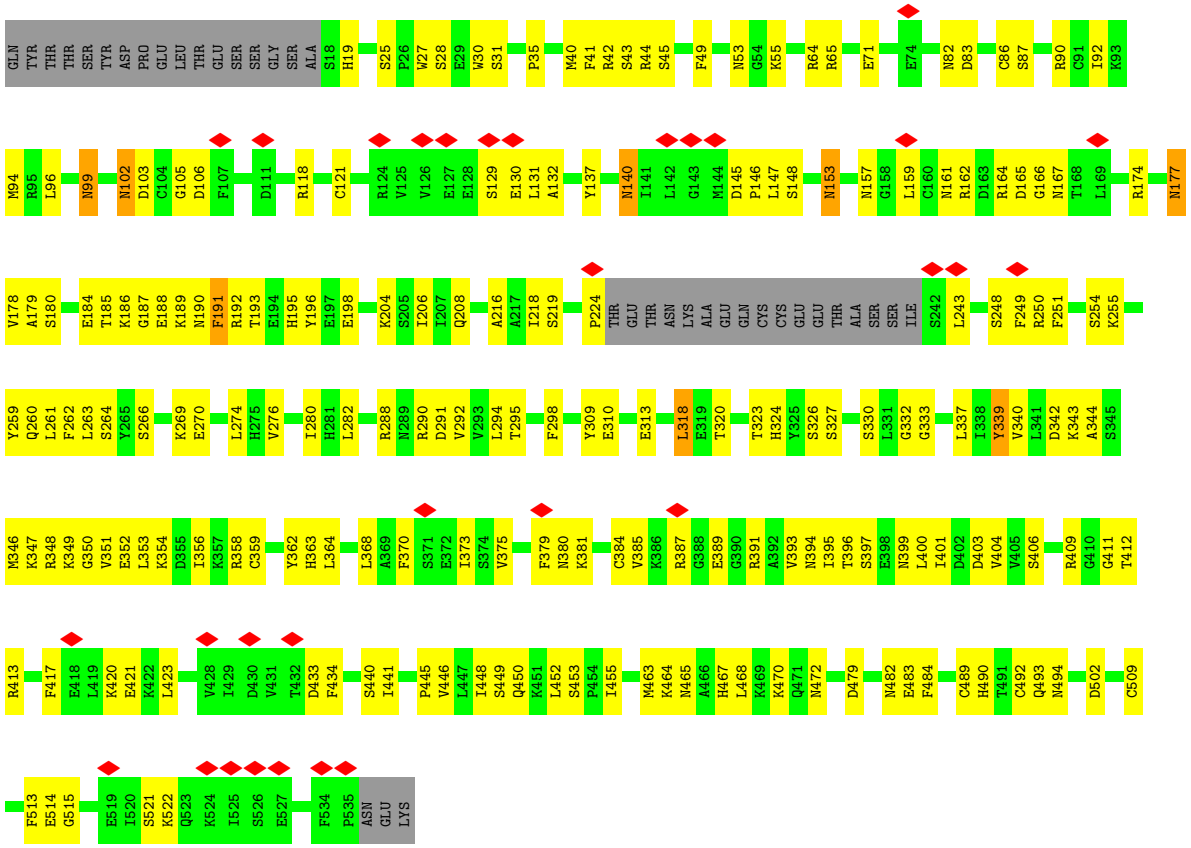
• Molecule 7: Complement component C9





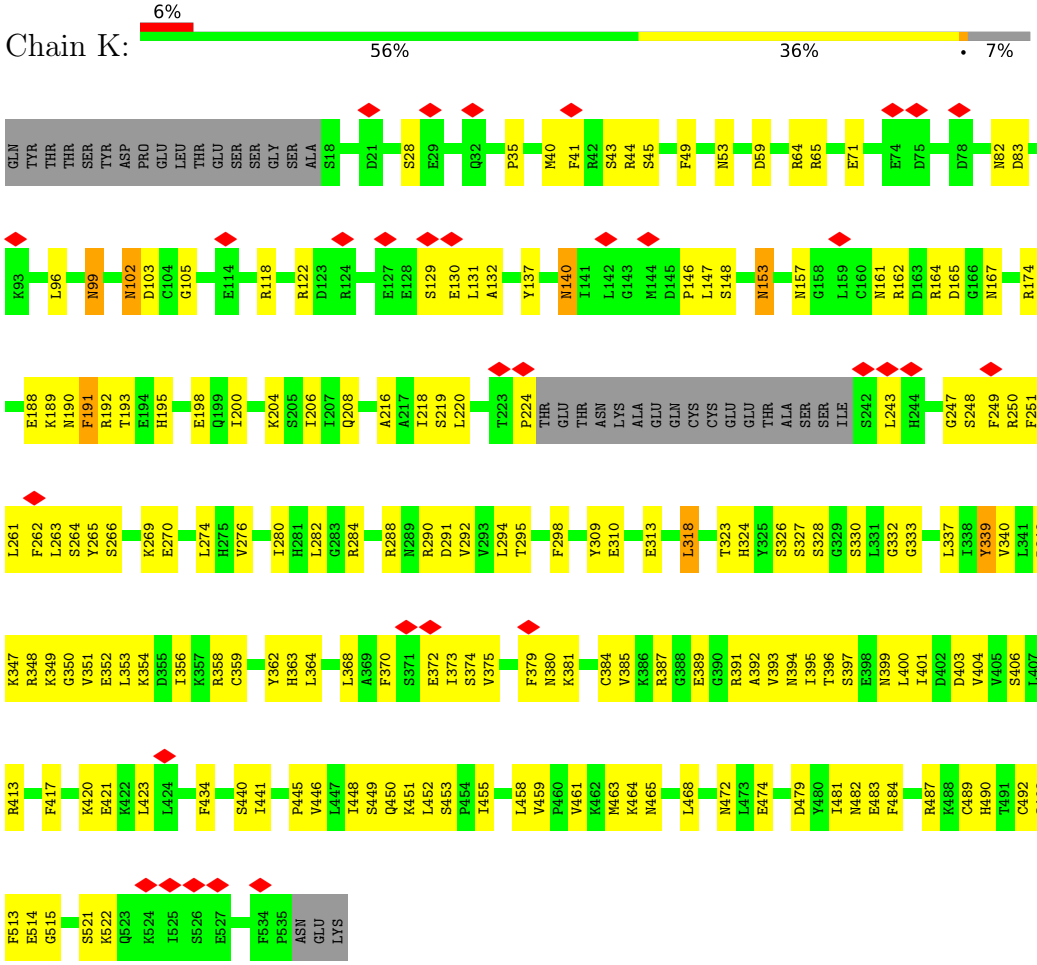
• Molecule 7: Complement component C9

Chain J:



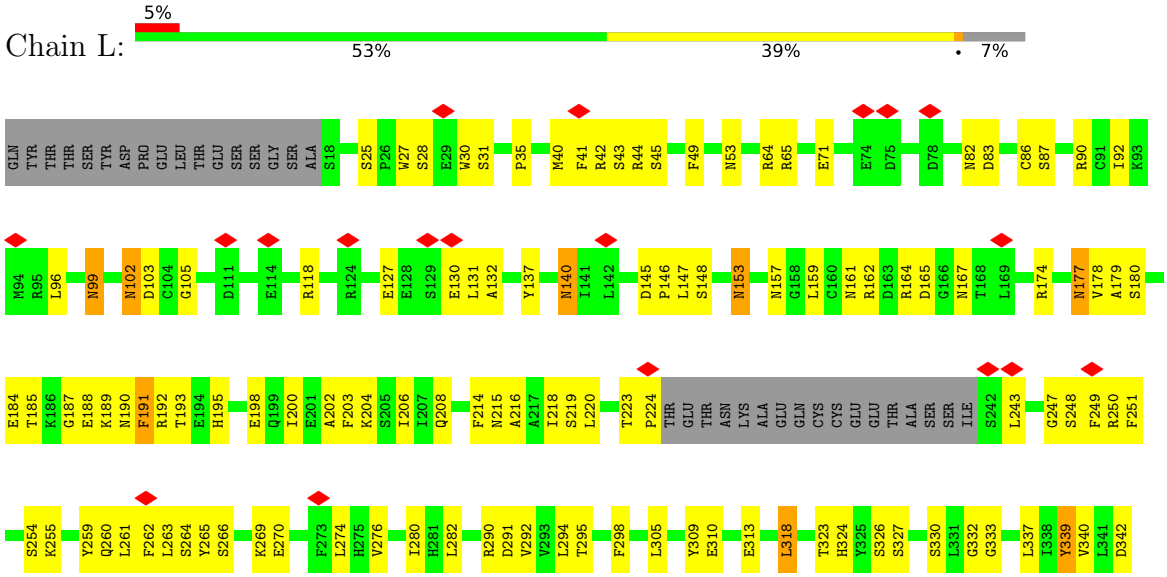
• Molecule 7: Complement component C9

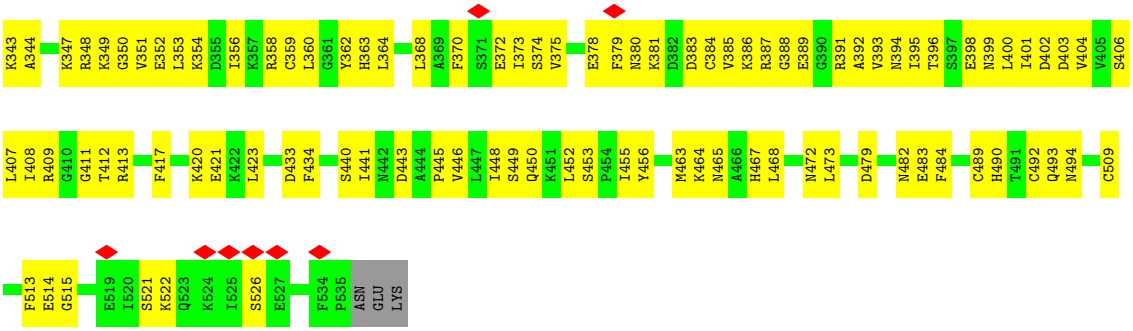
Chain K:



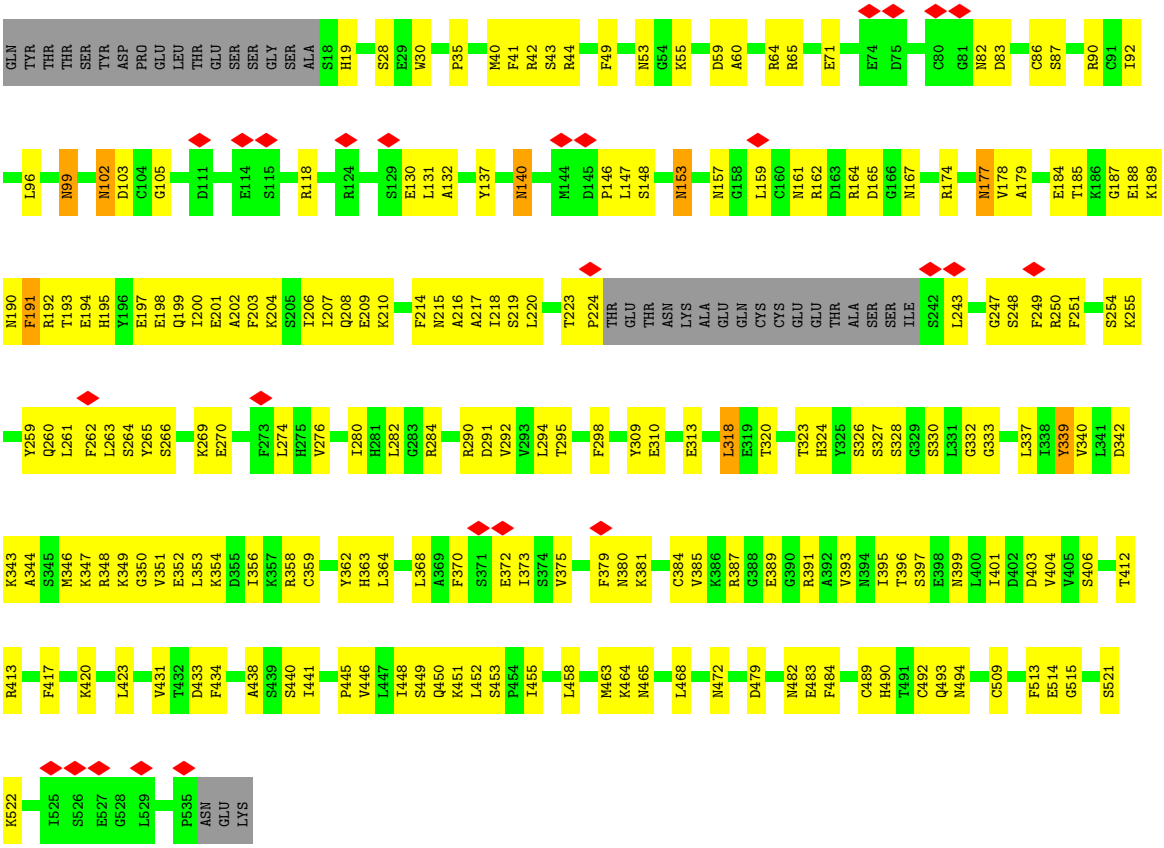
• Molecule 7: Complement component C9

Chain L:

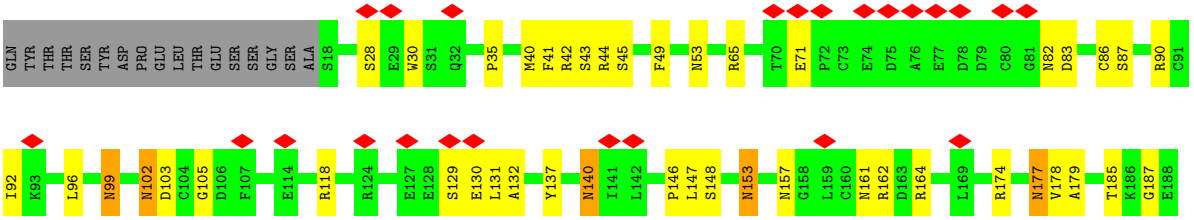


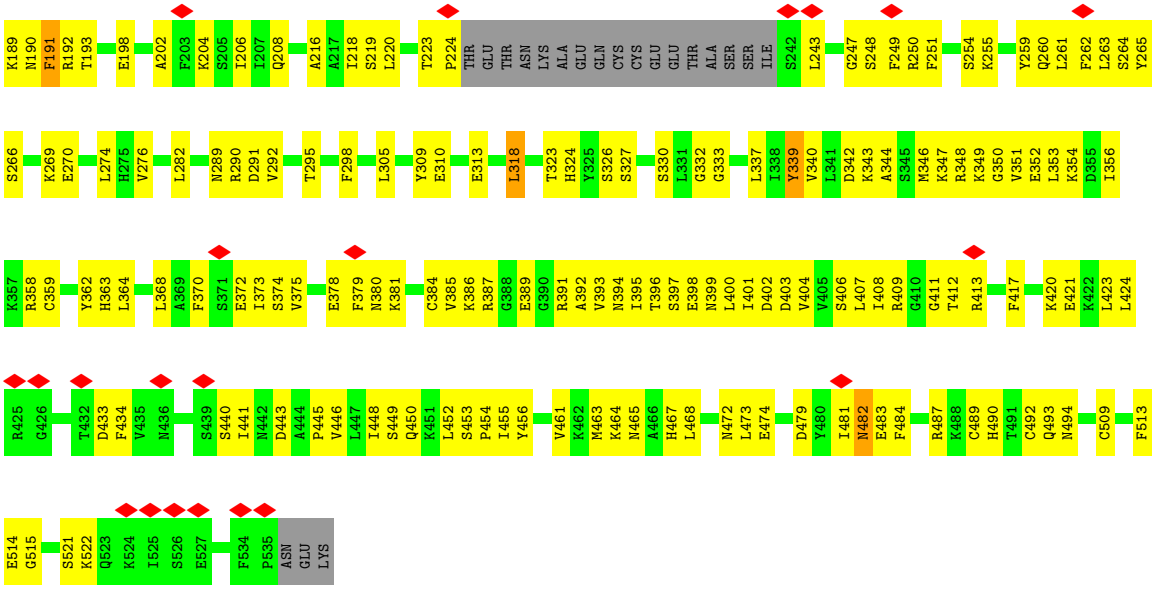


• Molecule 7: Complement component C9



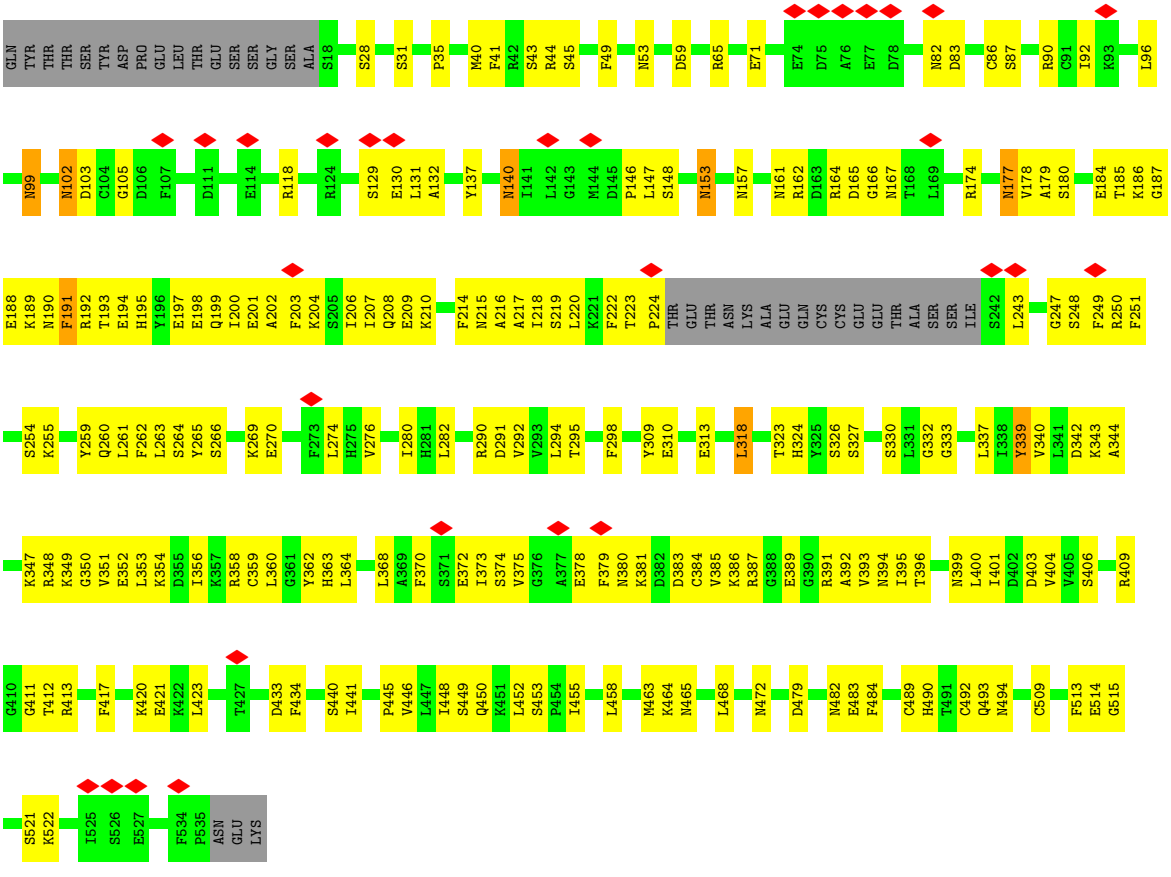
• Molecule 7: Complement component C9





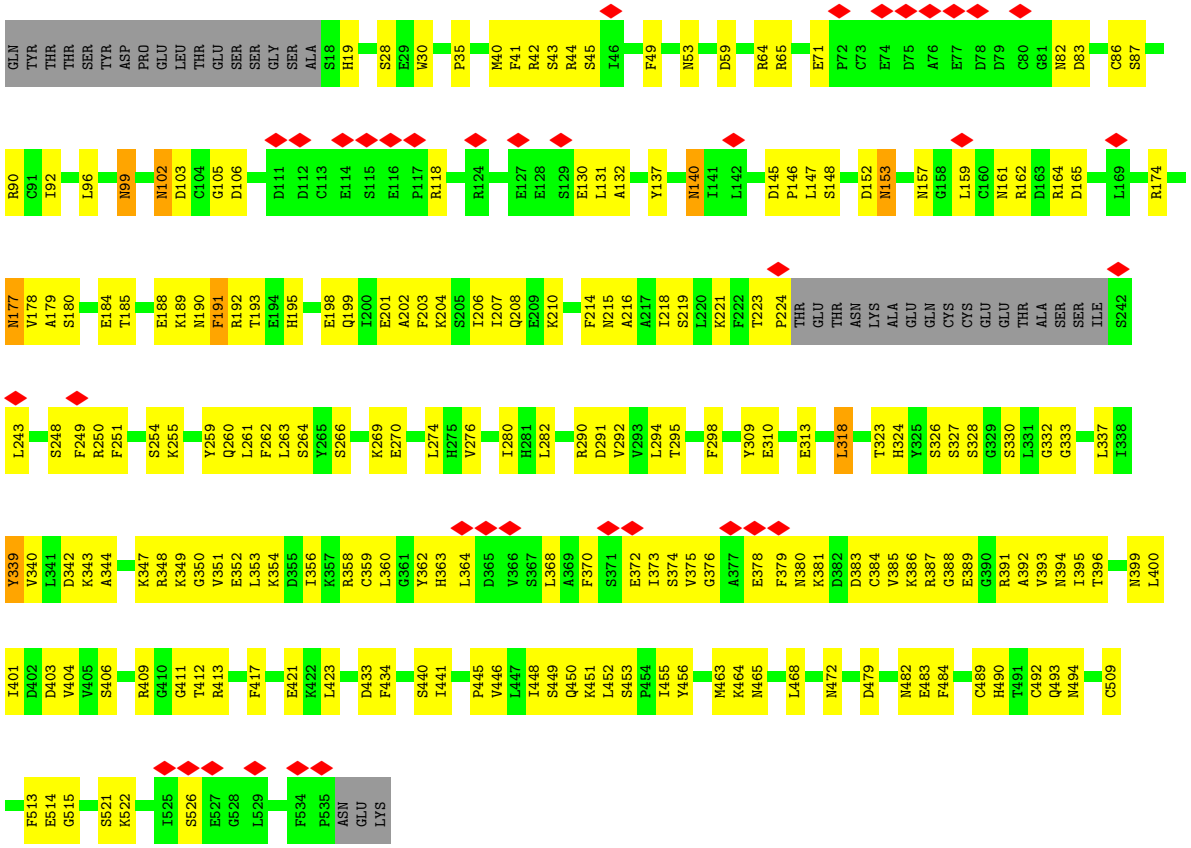
• Molecule 7: Complement component C9

Chain O:



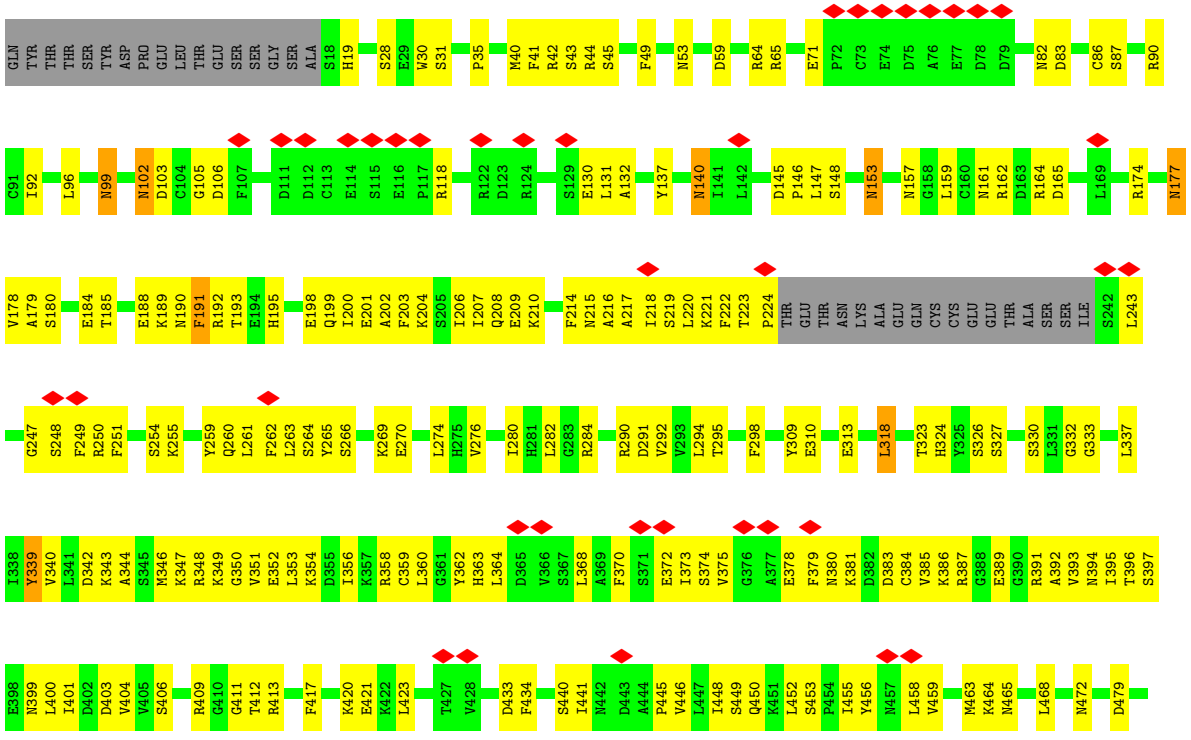
• Molecule 7: Complement component C9

Chain Q:



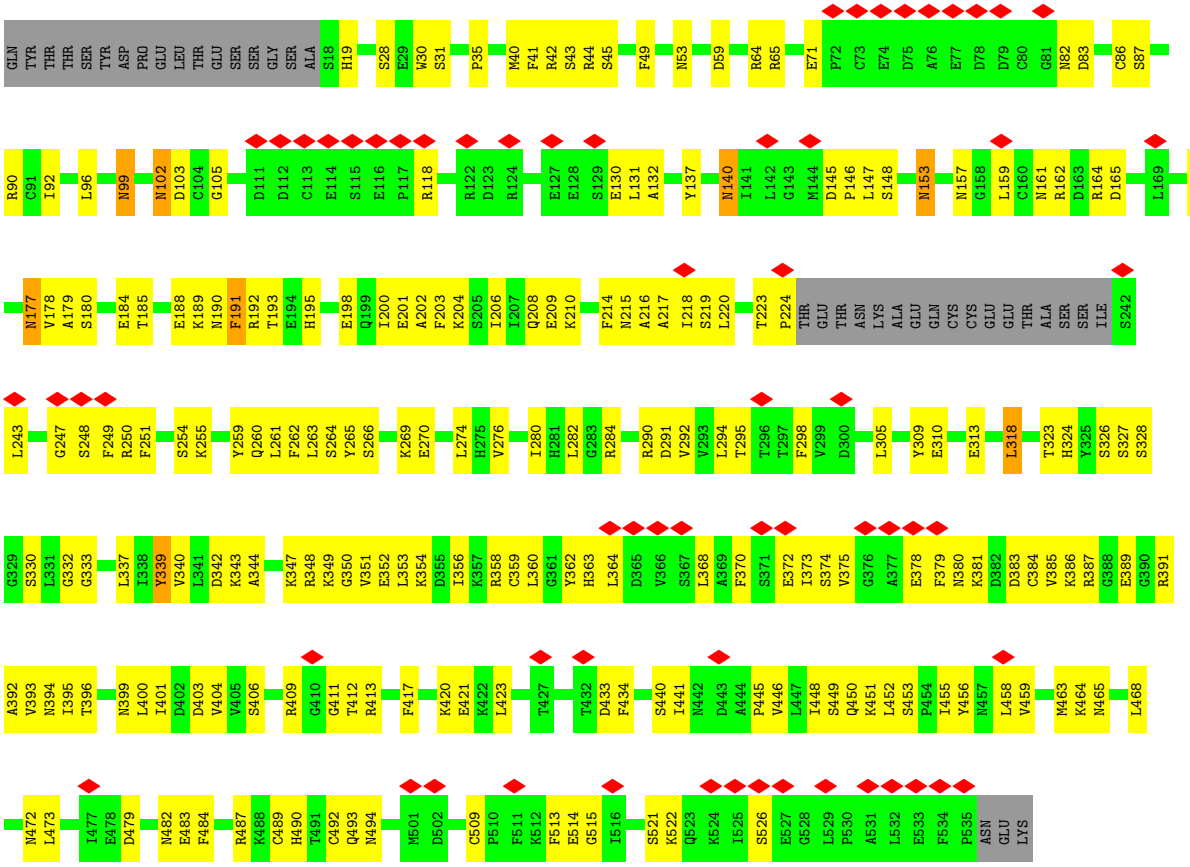
• Molecule 7: Complement component C9

Chain R:



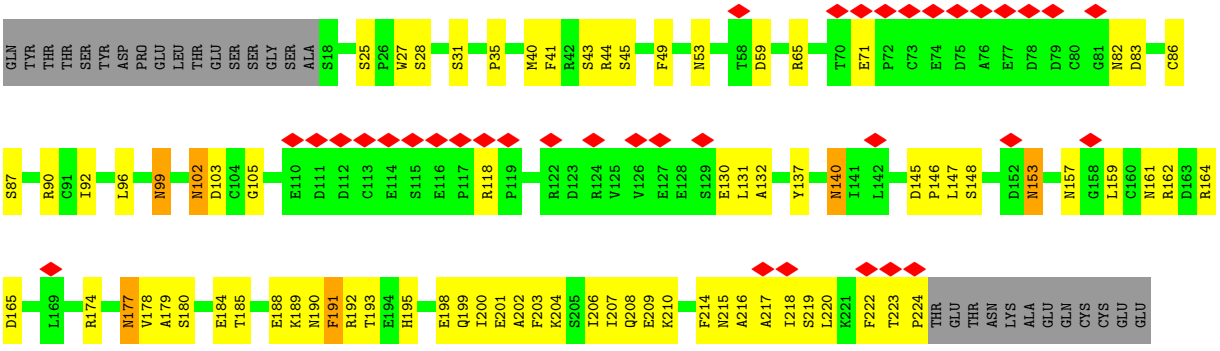
• Molecule 7: Complement component C9

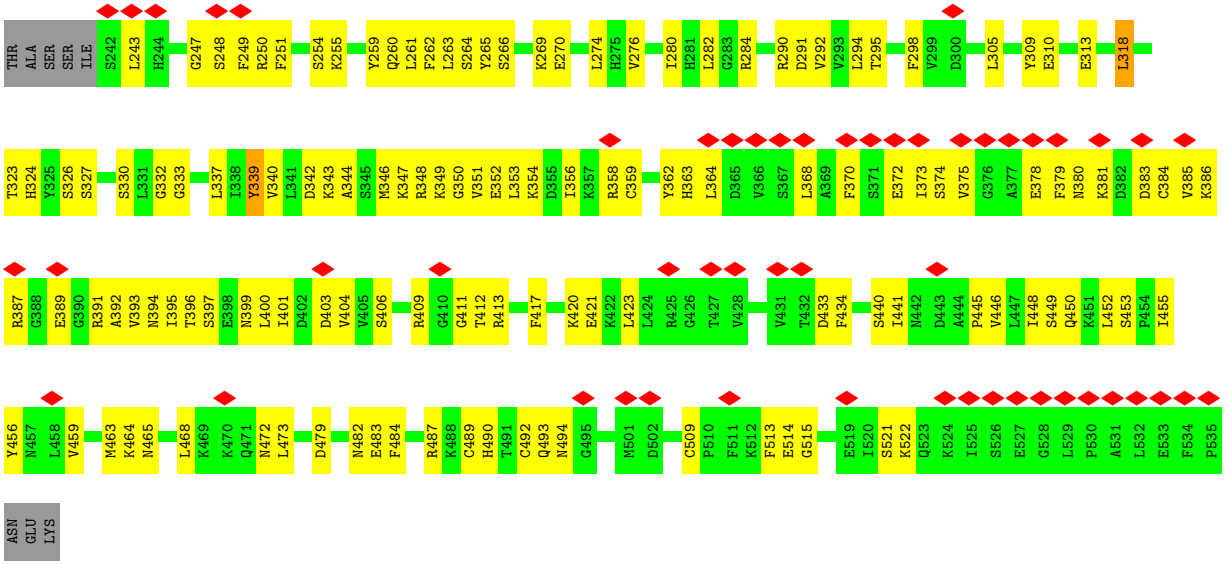
Chain S:



• Molecule 7: Complement component C9

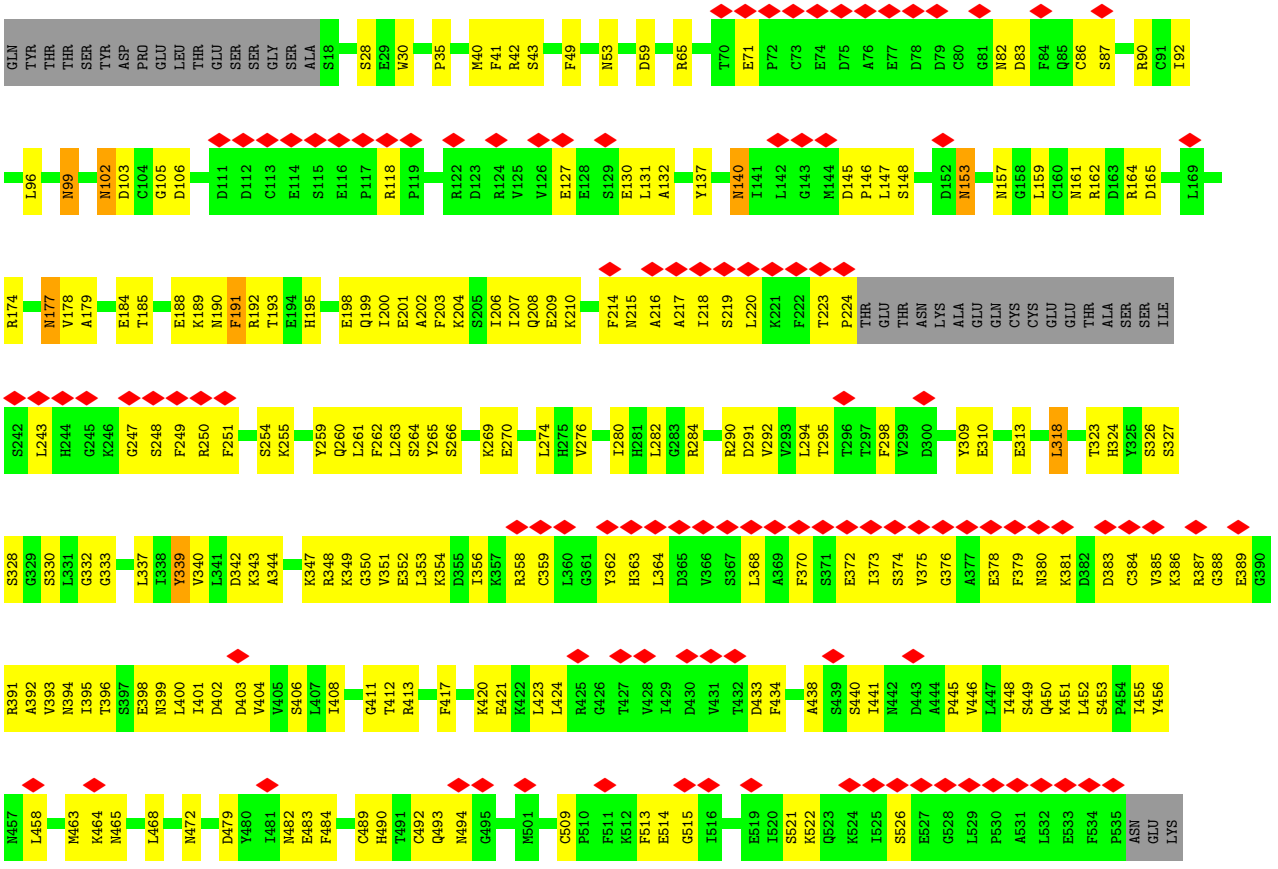
Chain T:





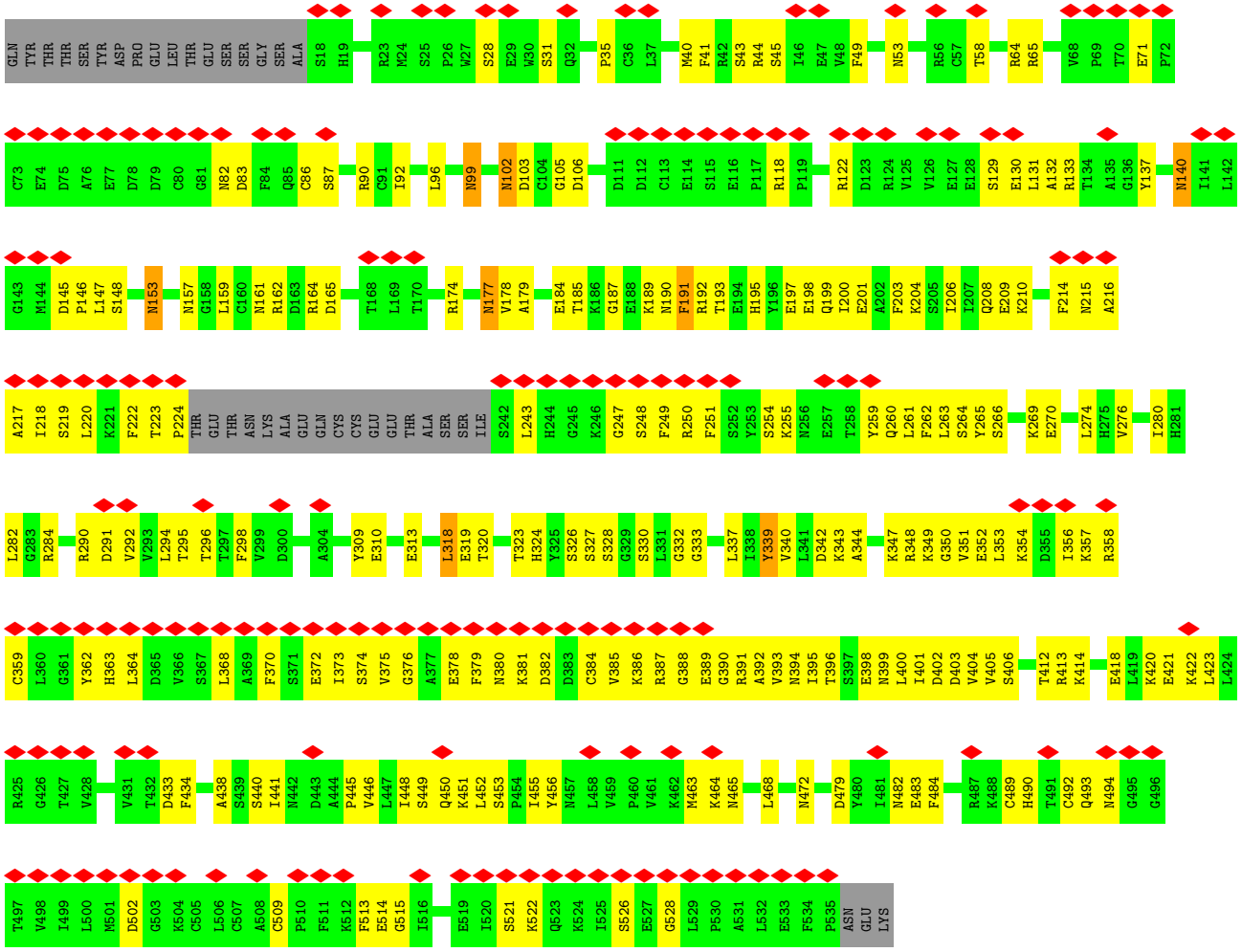
• Molecule 7: Complement component C9

Chain U:



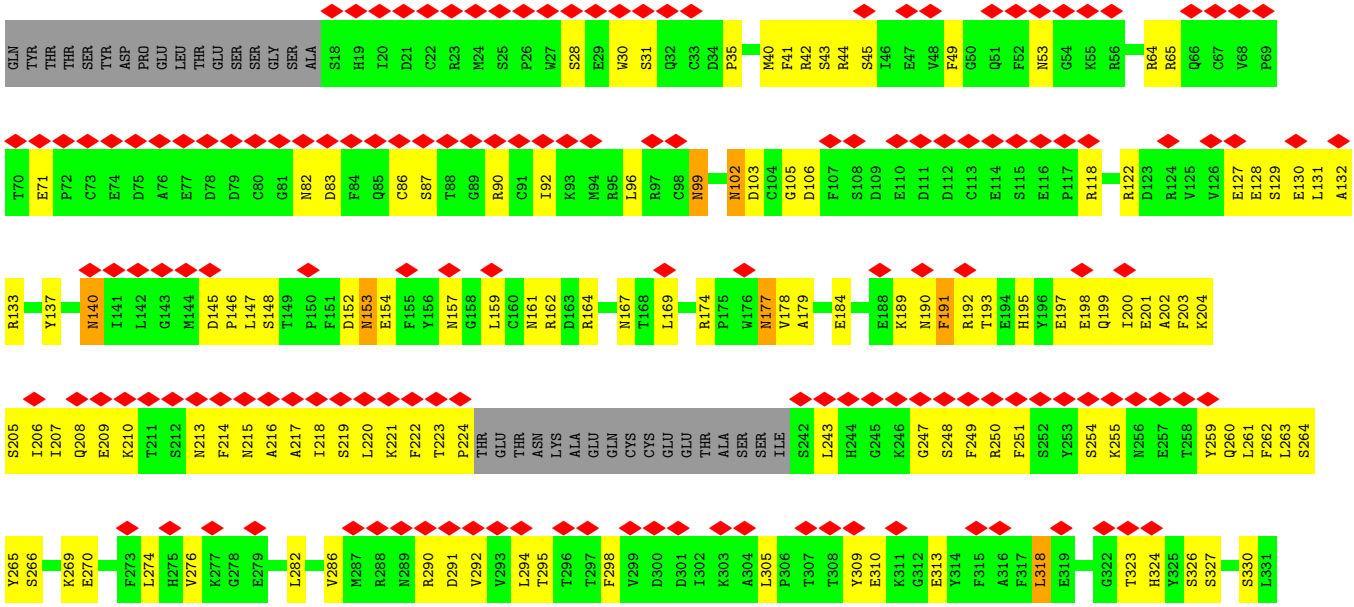
• Molecule 7: Complement component C9

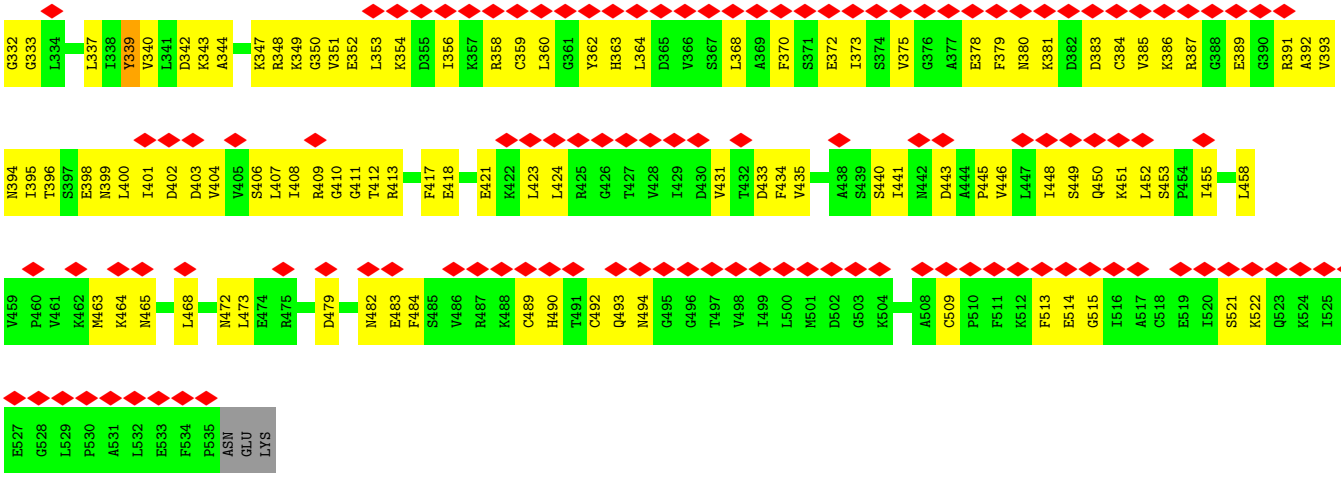
Chain V:



• Molecule 7: Complement component C9

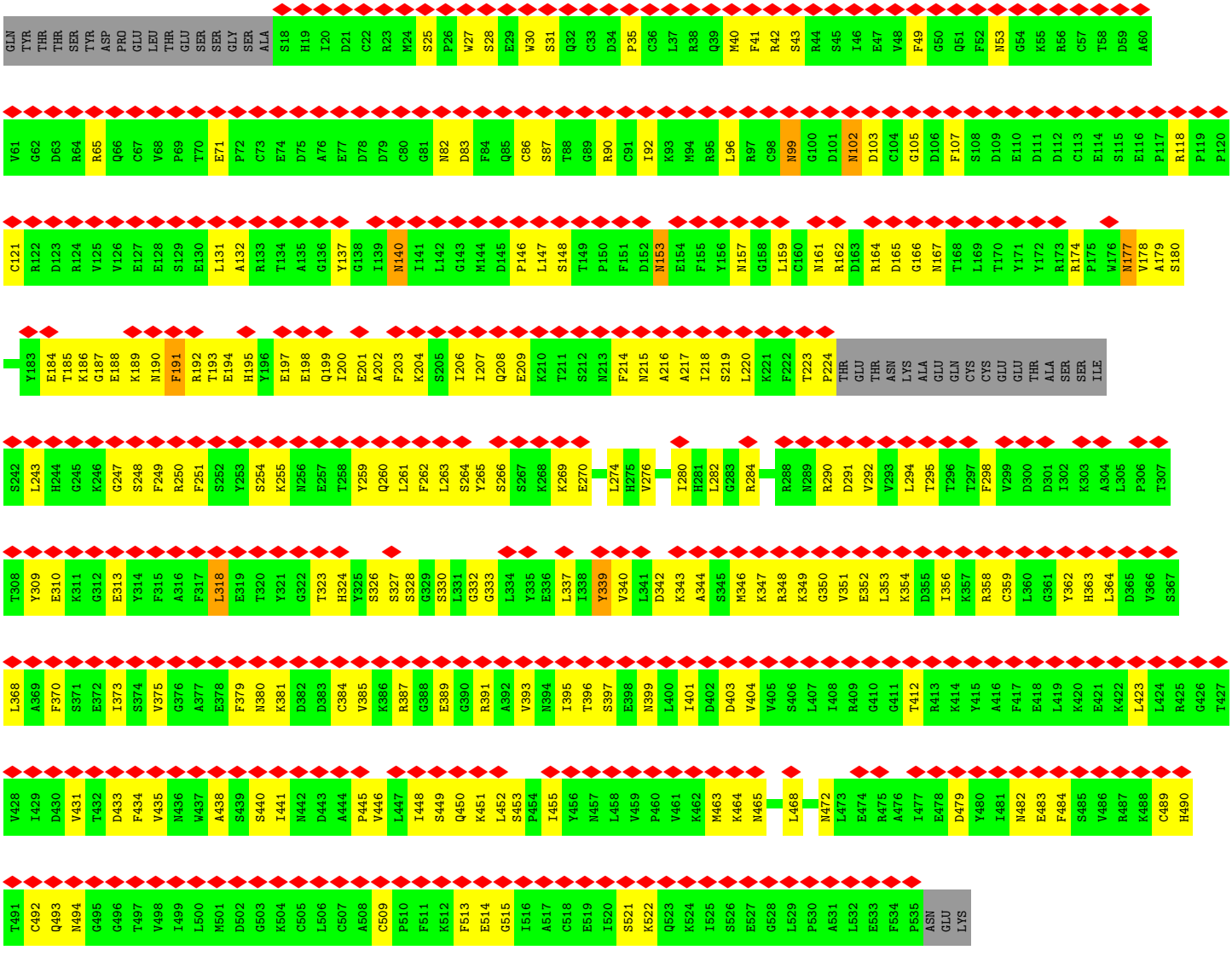
Chain W:





• Molecule 7: Complement component C9

Chain X:

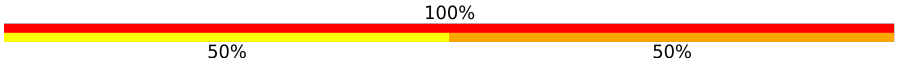


• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:

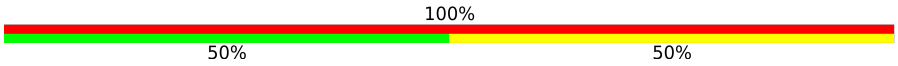
• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:



• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:



• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l:

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

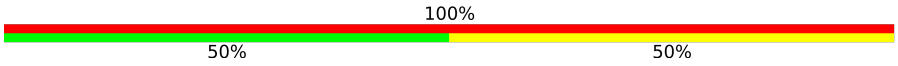
Chain m:

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain n:

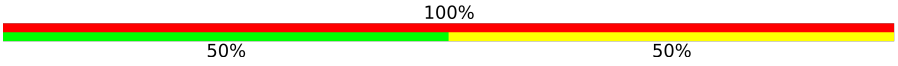
• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o:



• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:

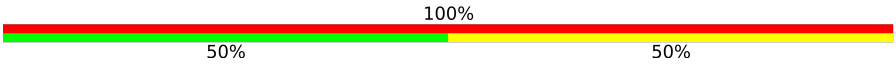


• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain q:

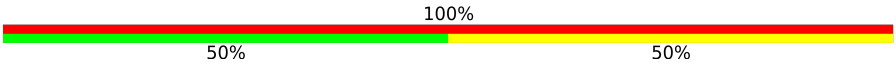
• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r:



• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain s:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	81968	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.308	Depositor
Minimum map value	-0.146	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	498.24, 498.24, 498.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.384, 1.384, 1.384	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.24	0/9902	0.44	1/13446 (0.0%)
2	C	0.24	0/4211	0.42	0/5677
3	D	0.25	0/5254	0.44	0/7104
4	E	0.24	0/1323	0.41	0/1794
5	F	0.25	0/4096	0.42	0/5509
6	B	0.25	0/5540	0.42	0/7476
7	G	0.25	0/4054	0.43	0/5458
7	H	0.25	0/4054	0.43	0/5458
7	I	0.25	0/4054	0.43	0/5458
7	J	0.25	0/4054	0.43	0/5458
7	K	0.25	0/4054	0.43	0/5458
7	L	0.25	0/4054	0.43	0/5458
7	M	0.25	0/4054	0.43	0/5458
7	N	0.26	0/4050	0.43	0/5453
7	O	0.25	0/4054	0.43	0/5458
7	P	0.25	0/4054	0.43	0/5458
7	Q	0.25	0/4054	0.43	0/5458
7	R	0.25	0/4054	0.43	0/5458
7	S	0.25	0/4054	0.43	0/5458
7	T	0.26	0/4054	0.43	0/5458
7	U	0.26	0/4054	0.43	0/5458
7	V	0.25	0/4028	0.43	0/5427
7	W	0.26	0/4017	0.43	0/5412
7	X	0.25	0/4054	0.43	0/5458
All	All	0.25	0/103231	0.43	1/139168 (0.0%)

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	1
3	D	0	1
5	F	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	61	ASP	C-N-CA	5.28	134.89	121.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	SER	Peptide
3	D	557	GLU	Peptide
5	F	488	GLN	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	9686	0	9674	179	0
2	C	4119	0	3949	77	0
3	D	5129	0	4822	119	0
4	E	1295	0	1259	20	0
5	F	4017	0	3796	120	0
6	B	5427	0	5152	116	0
7	G	3977	0	3841	181	0
7	H	3977	0	3839	214	0
7	I	3977	0	3839	254	0
7	J	3977	0	3839	256	0
7	K	3977	0	3838	222	0
7	L	3977	0	3839	272	0
7	M	3977	0	3836	293	0
7	N	3973	0	3833	316	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	O	3977	0	3839	296	0
7	P	3977	0	3841	212	0
7	Q	3977	0	3839	244	0
7	R	3977	0	3839	249	0
7	S	3977	0	3839	239	0
7	T	3977	0	3839	242	0
7	U	3977	0	3839	276	0
7	V	3951	0	3799	414	0
7	W	3941	0	3782	495	0
7	X	3977	0	3839	306	0
8	Y	39	0	31	0	0
9	Z	28	0	25	2	0
9	a	28	0	25	0	0
9	b	28	0	25	0	0
9	c	28	0	25	0	0
9	d	28	0	25	0	0
9	e	28	0	25	0	0
9	f	28	0	25	0	0
9	g	28	0	25	0	0
9	h	28	0	25	0	0
9	i	28	0	25	0	0
9	j	28	0	25	0	0
9	k	28	0	25	0	0
9	l	28	0	25	0	0
9	m	28	0	25	0	0
9	n	28	0	25	0	0
9	o	28	0	25	0	0
9	p	28	0	25	0	0
9	q	28	0	25	0	0
9	r	28	0	25	0	0
9	s	28	0	25	0	0
10	F	14	0	13	1	0
10	G	28	0	26	0	0
10	H	28	0	26	0	0
10	I	28	0	26	0	0
10	J	28	0	26	0	0
10	K	28	0	26	0	0
10	L	28	0	26	0	0
10	M	28	0	26	0	0
10	N	28	0	26	0	0
10	O	28	0	26	0	0
10	P	28	0	26	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	Q	28	0	26	0	0
10	R	28	0	26	0	0
10	S	28	0	26	0	0
10	T	28	0	26	0	0
10	U	28	0	26	0	0
10	V	28	0	26	0	0
10	W	28	0	26	0	0
10	X	28	0	26	0	0
All	All	102310	0	98663	4218	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 21.

All (4218) 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)
3:D:225:PHE:CD1	3:D:342:TRP:HB2	1.32	1.62
3:D:225:PHE:CE1	3:D:342:TRP:HB2	1.32	1.61
7:V:58:THR:HG21	7:W:452:LEU:CB	1.21	1.60
7:W:421:GLU:CB	7:X:434:PHE:HD2	1.17	1.58
7:V:58:THR:CG2	7:W:452:LEU:HB3	1.17	1.56
6:B:586:THR:CG2	7:X:107:PHE:CD2	1.82	1.53
7:V:414:LYS:HA	7:W:435:VAL:CG1	1.31	1.53
7:V:133:ARG:HH12	7:W:164:ARG:CB	1.29	1.46
7:G:524:LYS:HG3	7:P:196:TYR:CD2	1.51	1.45
7:P:372:GLU:CG	7:H:222:PHE:HE1	1.30	1.45
6:B:586:THR:HG21	7:X:107:PHE:CD2	0.94	1.45
7:V:64:ARG:HH12	7:W:291:ASP:N	1.11	1.43
7:Q:372:GLU:CG	7:R:223:THR:O	1.66	1.43
7:W:417:PHE:CZ	7:X:280:ILE:HG13	1.54	1.42
7:I:413:ARG:NH1	7:J:282:LEU:HA	1.33	1.40
7:V:64:ARG:NH1	7:W:290:ARG:CB	1.83	1.39
7:W:421:GLU:CB	7:X:434:PHE:CD2	2.06	1.36
7:P:372:GLU:CG	7:H:222:PHE:CE1	2.06	1.36
7:M:65:ARG:HB2	7:N:467:HIS:CG	1.61	1.35
7:M:44:ARG:NH2	7:N:474:GLU:OE2	1.61	1.34
7:W:413:ARG:NH1	7:X:282:LEU:HG	1.38	1.32
7:P:242:SER:CB	7:P:371:SER:OG	1.76	1.32
7:M:19:HIS:NE2	7:N:487:ARG:HD2	1.38	1.32
7:W:421:GLU:HB3	7:X:434:PHE:CD2	1.62	1.32
7:Q:372:GLU:CB	7:R:223:THR:O	1.78	1.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:225:PHE:CD1	3:D:342:TRP:CB	2.14	1.31
6:B:586:THR:CG2	7:X:107:PHE:HD2	1.23	1.31
7:V:380:ASN:HD22	7:W:215:ASN:CB	1.44	1.31
7:G:524:LYS:HE3	7:P:196:TYR:CD2	1.64	1.30
7:W:421:GLU:OE1	7:X:434:PHE:CB	1.80	1.29
7:W:412:THR:HA	7:X:167:ASN:OD1	1.26	1.29
6:B:586:THR:CG2	7:X:107:PHE:CE2	2.14	1.28
7:P:242:SER:HB3	7:P:371:SER:OG	1.14	1.27
7:N:372:GLU:CG	7:O:223:THR:O	1.83	1.26
7:S:372:GLU:CG	7:T:223:THR:O	1.84	1.26
7:V:133:ARG:NH1	7:W:164:ARG:HB3	1.48	1.25
7:I:370:PHE:CB	7:I:373:ILE:HB	1.26	1.25
7:J:370:PHE:CB	7:J:373:ILE:HB	1.26	1.25
7:Q:370:PHE:CB	7:Q:373:ILE:HB	1.26	1.25
7:V:64:ARG:NH1	7:W:291:ASP:H	1.35	1.25
7:V:386:LYS:CB	7:W:209:GLU:HB3	1.66	1.24
7:G:524:LYS:CG	7:P:196:TYR:CD2	2.20	1.24
7:R:370:PHE:CB	7:R:373:ILE:HB	1.26	1.24
7:L:372:GLU:CG	7:M:223:THR:O	1.86	1.23
7:V:392:ALA:CB	7:W:203:PHE:HB2	1.66	1.23
7:H:370:PHE:CB	7:H:373:ILE:HB	1.26	1.23
7:N:370:PHE:CB	7:N:373:ILE:HB	1.26	1.23
7:O:370:PHE:CB	7:O:373:ILE:HB	1.26	1.23
7:N:421:GLU:OE1	7:O:434:PHE:HB2	1.39	1.22
7:P:372:GLU:HG3	7:H:222:PHE:CE1	1.69	1.22
7:W:421:GLU:OE1	7:X:434:PHE:HB2	1.07	1.22
3:D:225:PHE:CE1	3:D:342:TRP:CB	2.21	1.22
7:U:374:SER:O	7:V:220:LEU:HD12	1.34	1.22
7:R:372:GLU:CG	7:S:223:THR:O	1.88	1.21
7:M:30:TRP:HH2	7:N:467:HIS:NE2	1.36	1.21
7:O:372:GLU:CG	7:Q:223:THR:O	1.89	1.21
7:U:391:ARG:NH2	7:V:204:LYS:HE3	1.52	1.21
7:P:372:GLU:HG2	7:H:222:PHE:CE1	1.67	1.20
7:I:413:ARG:NH1	7:J:282:LEU:CA	2.03	1.20
7:T:370:PHE:CB	7:T:373:ILE:CB	2.12	1.20
7:K:370:PHE:CB	7:K:373:ILE:HB	1.26	1.20
7:L:370:PHE:CB	7:L:373:ILE:CB	2.12	1.19
7:U:380:ASN:O	7:V:214:PHE:CD1	1.95	1.19
7:W:370:PHE:CB	7:W:373:ILE:HB	1.26	1.19
5:F:231:LEU:HD23	5:F:232:LEU:N	1.55	1.19
7:X:370:PHE:CB	7:X:373:ILE:CB	2.12	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:370:PHE:CB	7:S:373:ILE:HB	1.26	1.19
7:M:370:PHE:CB	7:M:373:ILE:CB	2.12	1.18
7:V:133:ARG:NH2	7:W:164:ARG:HD3	1.57	1.18
7:G:524:LYS:CG	7:P:196:TYR:CE2	2.26	1.18
7:U:370:PHE:CB	7:U:373:ILE:HB	1.26	1.18
7:O:372:GLU:CB	7:Q:223:THR:O	1.91	1.18
7:U:339:TYR:HB2	7:U:404:VAL:HG22	1.25	1.18
7:M:339:TYR:HB2	7:M:404:VAL:HG22	1.25	1.17
7:V:414:LYS:CA	7:W:435:VAL:CG1	2.22	1.17
7:I:370:PHE:CB	7:I:373:ILE:CB	2.12	1.17
7:L:370:PHE:CB	7:L:373:ILE:HB	1.26	1.17
7:J:370:PHE:CB	7:J:373:ILE:CB	2.12	1.17
7:V:339:TYR:HB2	7:V:404:VAL:HG22	1.25	1.17
7:O:372:GLU:HG3	7:Q:223:THR:O	1.42	1.16
7:H:370:PHE:CB	7:H:373:ILE:CB	2.12	1.16
7:N:339:TYR:HB2	7:N:404:VAL:HG22	1.25	1.16
7:T:370:PHE:HB2	7:T:373:ILE:CA	1.76	1.16
7:V:64:ARG:NH1	7:W:290:ARG:CA	2.08	1.16
7:J:370:PHE:HB2	7:J:373:ILE:CA	1.76	1.16
7:M:370:PHE:CB	7:M:373:ILE:HB	1.26	1.16
7:S:370:PHE:HB2	7:S:373:ILE:CA	1.76	1.16
7:U:370:PHE:CB	7:U:373:ILE:CB	2.12	1.16
7:V:396:THR:HB	7:W:199:GLN:OE1	1.43	1.16
7:O:370:PHE:CB	7:O:373:ILE:CB	2.12	1.16
7:Q:370:PHE:HB2	7:Q:373:ILE:CA	1.76	1.16
7:R:370:PHE:HB2	7:R:373:ILE:CA	1.76	1.16
7:U:378:GLU:OE1	7:V:217:ALA:HB3	1.46	1.16
7:V:370:PHE:HB2	7:V:373:ILE:CA	1.76	1.15
7:X:339:TYR:HB2	7:X:404:VAL:HG22	1.25	1.15
7:I:130:GLU:CD	7:J:165:ASP:HA	1.66	1.15
7:W:443:ASP:OD2	7:X:167:ASN:O	1.63	1.15
7:G:524:LYS:CE	7:P:196:TYR:CD2	2.29	1.15
7:O:370:PHE:HB2	7:O:373:ILE:CA	1.76	1.15
7:V:414:LYS:CA	7:W:435:VAL:HG11	1.77	1.15
7:W:370:PHE:HB2	7:W:373:ILE:CA	1.76	1.15
7:R:339:TYR:HB2	7:R:404:VAL:HG22	1.25	1.15
7:S:372:GLU:HG3	7:T:223:THR:O	1.44	1.15
7:N:370:PHE:HB2	7:N:373:ILE:CA	1.76	1.15
7:V:106:ASP:OD2	7:W:122:ARG:CB	1.95	1.15
7:W:130:GLU:HG3	7:X:165:ASP:HA	1.17	1.15
7:H:370:PHE:HB2	7:H:373:ILE:CA	1.76	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:370:PHE:HB2	7:I:373:ILE:CA	1.76	1.14
7:N:400:LEU:HD12	7:O:195:HIS:HB2	1.20	1.14
7:O:339:TYR:HB2	7:O:404:VAL:HG22	1.25	1.14
7:V:392:ALA:HB3	7:W:203:PHE:CB	1.76	1.14
7:I:339:TYR:HB2	7:I:404:VAL:HG22	1.25	1.14
7:K:370:PHE:HB2	7:K:373:ILE:CA	1.76	1.14
7:M:370:PHE:HB2	7:M:373:ILE:CA	1.76	1.14
7:U:370:PHE:HB2	7:U:373:ILE:CA	1.76	1.14
7:W:339:TYR:HB2	7:W:404:VAL:HG22	1.25	1.14
6:B:586:THR:HG21	7:X:107:PHE:CE2	1.80	1.14
7:G:524:LYS:CE	7:P:196:TYR:CE2	2.30	1.13
7:U:372:GLU:HG3	7:V:224:PRO:HA	1.28	1.13
7:W:400:LEU:HD12	7:X:195:HIS:HB2	1.30	1.13
7:L:370:PHE:HB2	7:L:373:ILE:CA	1.76	1.13
7:Q:370:PHE:HB2	7:Q:373:ILE:CB	1.77	1.13
7:V:145:ASP:OD2	7:W:184:GLU:CB	1.97	1.13
7:S:339:TYR:HB2	7:S:404:VAL:HG22	1.25	1.13
7:X:370:PHE:CB	7:X:373:ILE:HB	1.26	1.13
7:J:339:TYR:HB2	7:J:404:VAL:HG22	1.25	1.12
7:K:339:TYR:HB2	7:K:404:VAL:HG22	1.25	1.12
7:V:380:ASN:HD22	7:W:215:ASN:HB2	1.05	1.12
7:X:370:PHE:HB2	7:X:373:ILE:CA	1.76	1.12
7:T:370:PHE:CB	7:T:373:ILE:HB	1.26	1.12
7:Q:370:PHE:CB	7:Q:373:ILE:CB	2.12	1.12
7:R:370:PHE:HB2	7:R:373:ILE:CB	1.77	1.12
7:T:339:TYR:HB2	7:T:404:VAL:HG22	1.25	1.12
7:K:370:PHE:CB	7:K:373:ILE:CB	2.12	1.11
7:Q:372:GLU:HG3	7:R:223:THR:O	1.30	1.11
7:V:370:PHE:HB2	7:V:373:ILE:HB	1.31	1.11
7:S:372:GLU:CB	7:T:223:THR:O	1.97	1.11
7:V:370:PHE:CB	7:V:373:ILE:HB	1.26	1.11
7:W:421:GLU:HB2	7:X:434:PHE:CD2	1.73	1.11
7:K:370:PHE:HB2	7:K:373:ILE:CB	1.77	1.11
7:L:370:PHE:HB2	7:L:373:ILE:CB	1.77	1.11
7:L:370:PHE:HB2	7:L:373:ILE:HB	1.31	1.11
7:Q:370:PHE:HB2	7:Q:373:ILE:HB	1.31	1.11
7:S:370:PHE:CB	7:S:373:ILE:CB	2.12	1.11
7:N:370:PHE:HB2	7:N:373:ILE:CB	1.77	1.11
7:L:372:GLU:HG3	7:M:223:THR:O	1.48	1.10
7:J:370:PHE:HB2	7:J:373:ILE:CB	1.77	1.10
7:N:370:PHE:CB	7:N:373:ILE:CB	2.12	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:V:528:GLY:HA3	7:W:200:ILE:CD1	1.80	1.10
7:W:370:PHE:CB	7:W:373:ILE:CB	2.12	1.10
7:R:370:PHE:CB	7:R:373:ILE:CB	2.12	1.09
7:U:374:SER:O	7:V:220:LEU:CD1	1.98	1.09
7:W:370:PHE:HB2	7:W:373:ILE:CB	1.77	1.09
7:M:370:PHE:HB2	7:M:373:ILE:HB	1.31	1.09
7:N:372:GLU:HG3	7:O:223:THR:O	1.49	1.09
7:L:339:TYR:HB2	7:L:404:VAL:HG22	1.25	1.09
7:L:372:GLU:CB	7:M:223:THR:O	2.00	1.09
7:O:370:PHE:HB2	7:O:373:ILE:HB	1.30	1.09
7:R:372:GLU:CB	7:S:223:THR:O	1.99	1.09
7:V:414:LYS:HA	7:W:435:VAL:HG13	1.22	1.09
7:O:189:LYS:HE2	7:O:191:PHE:CE1	1.88	1.09
7:T:189:LYS:HE2	7:T:191:PHE:CE1	1.88	1.09
5:F:229:SER:HB3	5:F:356:ASP:OD2	1.52	1.08
7:M:189:LYS:HE2	7:M:191:PHE:CE1	1.88	1.08
7:R:372:GLU:HG3	7:S:223:THR:O	1.53	1.08
7:W:189:LYS:HE2	7:W:191:PHE:CE1	1.88	1.08
7:N:189:LYS:HE2	7:N:191:PHE:CE1	1.88	1.08
7:Q:339:TYR:HB2	7:Q:404:VAL:HG22	1.25	1.08
7:S:189:LYS:HE2	7:S:191:PHE:CE1	1.88	1.08
7:V:380:ASN:ND2	7:W:215:ASN:HB2	1.66	1.08
7:X:370:PHE:HB2	7:X:373:ILE:CB	1.77	1.08
7:P:525:ILE:O	7:P:526:SER:O	1.71	1.08
7:I:189:LYS:HE2	7:I:191:PHE:CE1	1.88	1.08
7:J:189:LYS:HE2	7:J:191:PHE:CE1	1.88	1.08
7:L:189:LYS:HE2	7:L:191:PHE:CE1	1.88	1.08
7:M:65:ARG:HD2	7:N:467:HIS:CD2	1.87	1.08
7:R:189:LYS:HE2	7:R:191:PHE:CE1	1.88	1.08
7:V:189:LYS:HE2	7:V:191:PHE:CE1	1.88	1.08
7:V:386:LYS:HB3	7:W:209:GLU:HB3	1.35	1.08
7:W:130:GLU:CG	7:X:165:ASP:HA	1.82	1.08
7:U:189:LYS:HE2	7:U:191:PHE:CE1	1.88	1.08
7:V:370:PHE:HB2	7:V:373:ILE:CB	1.77	1.08
7:H:339:TYR:HB2	7:H:404:VAL:HG22	1.25	1.07
7:M:64:ARG:O	7:N:467:HIS:ND1	1.86	1.07
7:O:370:PHE:HB2	7:O:373:ILE:CB	1.77	1.07
7:V:386:LYS:HD2	7:W:209:GLU:OE1	1.52	1.07
7:H:189:LYS:HE2	7:H:191:PHE:CE1	1.88	1.07
7:L:421:GLU:OE1	7:M:434:PHE:HB2	1.54	1.07
7:X:189:LYS:HE2	7:X:191:PHE:CE1	1.88	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:V:380:ASN:O	7:W:214:PHE:CD1	2.07	1.07
7:K:189:LYS:HE2	7:K:191:PHE:CE1	1.88	1.07
7:Q:189:LYS:HE2	7:Q:191:PHE:CE1	1.88	1.07
7:Q:372:GLU:HB3	7:R:223:THR:O	1.46	1.07
7:W:417:PHE:CZ	7:X:280:ILE:CG1	2.38	1.07
7:V:380:ASN:HB2	7:W:215:ASN:HB2	1.35	1.06
7:G:372:GLU:HG3	7:P:224:PRO:CA	1.83	1.06
7:H:370:PHE:HB2	7:H:373:ILE:CB	1.77	1.06
7:M:370:PHE:HB2	7:M:373:ILE:CB	1.77	1.06
7:K:190:ASN:C	7:K:191:PHE:HD1	1.59	1.06
7:T:370:PHE:HB2	7:T:373:ILE:HB	1.31	1.06
7:I:190:ASN:C	7:I:191:PHE:HD1	1.59	1.06
7:N:413:ARG:HH11	7:O:282:LEU:HA	1.14	1.06
7:X:190:ASN:C	7:X:191:PHE:HD1	1.59	1.06
7:G:372:GLU:CG	7:P:224:PRO:HA	1.86	1.05
7:M:190:ASN:C	7:M:191:PHE:HD1	1.59	1.05
7:U:380:ASN:HD22	7:V:215:ASN:HB2	1.14	1.05
7:N:190:ASN:C	7:N:191:PHE:HD1	1.59	1.05
7:J:190:ASN:C	7:J:191:PHE:HD1	1.59	1.05
7:L:421:GLU:HB3	7:M:434:PHE:HD2	1.15	1.05
7:R:372:GLU:HB3	7:S:223:THR:O	1.55	1.05
7:U:370:PHE:HB2	7:U:373:ILE:CB	1.77	1.05
7:V:133:ARG:HH12	7:W:164:ARG:HB3	0.89	1.05
7:P:374:SER:O	7:H:220:LEU:CD1	2.05	1.05
7:V:422:LYS:HG3	7:W:431:VAL:HG11	1.34	1.05
7:W:413:ARG:NH1	7:X:282:LEU:CG	2.19	1.05
7:W:421:GLU:HB3	7:X:434:PHE:HD2	0.91	1.05
7:H:190:ASN:C	7:H:191:PHE:HD1	1.59	1.05
7:K:370:PHE:HB2	7:K:373:ILE:HB	1.31	1.05
7:T:190:ASN:C	7:T:191:PHE:HD1	1.59	1.05
7:U:190:ASN:C	7:U:191:PHE:HD1	1.59	1.05
7:Q:190:ASN:C	7:Q:191:PHE:HD1	1.59	1.04
7:W:130:GLU:HA	7:X:164:ARG:O	1.56	1.04
7:W:190:ASN:C	7:W:191:PHE:HD1	1.59	1.04
6:B:586:THR:HG22	7:X:107:PHE:CE2	1.86	1.04
7:I:370:PHE:HB2	7:I:373:ILE:CB	1.77	1.04
7:L:190:ASN:C	7:L:191:PHE:HD1	1.59	1.04
7:V:391:ARG:HH21	7:W:204:LYS:HG3	1.16	1.04
7:K:370:PHE:HB2	7:K:373:ILE:N	1.73	1.04
7:V:370:PHE:HB2	7:V:373:ILE:N	1.73	1.04
7:M:65:ARG:CB	7:N:467:HIS:CG	2.40	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:190:ASN:C	7:S:191:PHE:HD1	1.59	1.04
7:T:370:PHE:HB2	7:T:373:ILE:CB	1.77	1.04
7:U:370:PHE:HB2	7:U:373:ILE:N	1.73	1.04
7:P:374:SER:O	7:H:220:LEU:HD13	1.56	1.03
7:M:65:ARG:CA	7:N:467:HIS:HB2	1.87	1.03
7:L:370:PHE:HB2	7:L:373:ILE:N	1.73	1.03
7:R:190:ASN:C	7:R:191:PHE:HD1	1.59	1.03
7:S:370:PHE:HB2	7:S:373:ILE:CB	1.77	1.03
7:X:370:PHE:HB2	7:X:373:ILE:HB	1.31	1.03
7:G:524:LYS:HG3	7:P:196:TYR:CG	1.93	1.03
7:G:524:LYS:HE2	7:P:196:TYR:HE2	1.20	1.03
7:L:372:GLU:HB3	7:M:223:THR:O	1.58	1.03
7:N:372:GLU:CB	7:O:223:THR:O	2.06	1.03
7:V:190:ASN:C	7:V:191:PHE:HD1	1.59	1.03
7:V:370:PHE:CB	7:V:373:ILE:CB	2.12	1.03
7:W:370:PHE:HB2	7:W:373:ILE:N	1.73	1.03
7:W:421:GLU:CD	7:X:434:PHE:HB2	1.79	1.03
7:G:243:LEU:CD1	7:G:370:PHE:CD1	2.42	1.03
7:G:372:GLU:HG3	7:P:224:PRO:HA	1.04	1.03
7:N:413:ARG:NH1	7:O:282:LEU:HG	1.72	1.03
7:I:370:PHE:HB2	7:I:373:ILE:N	1.73	1.03
7:R:370:PHE:HB2	7:R:373:ILE:N	1.73	1.03
7:N:370:PHE:HB2	7:N:373:ILE:HB	1.31	1.02
7:G:524:LYS:HG2	7:P:196:TYR:CE2	1.93	1.02
7:H:370:PHE:HB2	7:H:373:ILE:N	1.73	1.02
7:M:65:ARG:HA	7:N:467:HIS:HB2	1.04	1.02
7:O:190:ASN:C	7:O:191:PHE:HD1	1.59	1.02
7:O:372:GLU:HB3	7:Q:223:THR:O	1.57	1.02
7:S:370:PHE:HB2	7:S:373:ILE:N	1.73	1.02
7:J:370:PHE:HB2	7:J:373:ILE:N	1.73	1.02
7:M:370:PHE:HB2	7:M:373:ILE:N	1.73	1.02
7:S:370:PHE:HB2	7:S:373:ILE:HB	1.31	1.02
7:W:421:GLU:OE1	7:X:434:PHE:CG	2.12	1.02
7:X:370:PHE:HB2	7:X:373:ILE:N	1.73	1.02
7:N:370:PHE:HB2	7:N:373:ILE:N	1.73	1.02
7:U:370:PHE:HB2	7:U:373:ILE:HB	1.31	1.02
7:W:400:LEU:HD12	7:X:195:HIS:CB	1.90	1.02
7:T:370:PHE:HB2	7:T:373:ILE:N	1.73	1.02
7:W:403:ASP:HA	7:X:192:ARG:HG2	1.40	1.02
7:O:370:PHE:HB2	7:O:373:ILE:N	1.73	1.01
7:S:372:GLU:HB3	7:T:223:THR:O	1.57	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:105:GLY:HA2	7:V:159:LEU:HD22	1.42	1.01
7:U:400:LEU:HD12	7:V:195:HIS:HB2	1.39	1.01
7:J:370:PHE:HB2	7:J:373:ILE:HB	1.31	1.01
7:L:421:GLU:CB	7:M:434:PHE:HD2	1.71	1.01
7:Q:370:PHE:HB2	7:Q:373:ILE:N	1.73	1.01
7:W:413:ARG:HH11	7:X:282:LEU:HA	1.22	1.01
7:M:30:TRP:CH2	7:N:467:HIS:NE2	2.29	1.01
7:V:133:ARG:HH22	7:W:164:ARG:CD	1.72	1.01
3:D:225:PHE:HD1	3:D:342:TRP:CB	1.62	1.01
7:W:408:ILE:N	7:X:187:GLY:O	1.93	1.01
7:N:391:ARG:NH2	7:O:204:LYS:HE3	1.76	1.00
7:N:421:GLU:OE1	7:O:434:PHE:CB	2.08	1.00
7:U:380:ASN:O	7:V:214:PHE:CE1	2.14	1.00
7:H:370:PHE:HB2	7:H:373:ILE:HB	1.31	1.00
7:N:413:ARG:NH1	7:O:282:LEU:HA	1.75	1.00
7:V:414:LYS:HA	7:W:435:VAL:HG11	1.02	1.00
7:I:370:PHE:HB2	7:I:373:ILE:HB	1.31	0.99
7:U:391:ARG:NE	7:V:204:LYS:HE2	1.78	0.99
7:V:386:LYS:CD	7:W:209:GLU:HB3	1.91	0.99
7:I:413:ARG:HH11	7:J:282:LEU:CA	1.71	0.99
7:R:370:PHE:HB2	7:R:373:ILE:HB	1.31	0.99
7:V:58:THR:HG23	7:W:452:LEU:HB3	1.44	0.99
7:T:372:GLU:CG	7:U:223:THR:O	2.09	0.99
7:N:417:PHE:CZ	7:O:280:ILE:HG13	1.97	0.98
7:O:190:ASN:O	7:O:191:PHE:CD1	2.17	0.98
7:K:190:ASN:O	7:K:191:PHE:CD1	2.17	0.98
7:N:190:ASN:O	7:N:191:PHE:CD1	2.17	0.98
7:L:190:ASN:O	7:L:191:PHE:CD1	2.17	0.98
7:Q:190:ASN:O	7:Q:191:PHE:CD1	2.17	0.98
7:T:190:ASN:O	7:T:191:PHE:CD1	2.17	0.98
7:U:190:ASN:O	7:U:191:PHE:CD1	2.17	0.98
7:M:190:ASN:O	7:M:191:PHE:CD1	2.17	0.98
7:V:133:ARG:HH12	7:W:164:ARG:HB2	1.25	0.98
7:V:190:ASN:O	7:V:191:PHE:CD1	2.17	0.98
7:H:190:ASN:O	7:H:191:PHE:CD1	2.17	0.98
7:S:190:ASN:O	7:S:191:PHE:CD1	2.17	0.98
7:V:133:ARG:HH22	7:W:164:ARG:HD3	0.84	0.98
7:G:243:LEU:CD1	7:G:370:PHE:CE1	2.47	0.97
7:R:190:ASN:O	7:R:191:PHE:CD1	2.17	0.97
7:X:190:ASN:O	7:X:191:PHE:CD1	2.17	0.97
5:F:229:SER:CB	5:F:356:ASP:OD2	2.10	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:190:ASN:O	7:I:191:PHE:CD1	2.17	0.97
7:Q:339:TYR:HB3	7:Q:404:VAL:HG13	1.46	0.97
7:V:414:LYS:O	7:W:435:VAL:HG21	1.63	0.97
7:W:190:ASN:O	7:W:191:PHE:CD1	2.17	0.97
7:G:243:LEU:HD11	7:G:370:PHE:CE1	1.99	0.97
7:G:524:LYS:HE3	7:P:196:TYR:HD2	1.04	0.97
7:T:339:TYR:HB3	7:T:404:VAL:HG13	1.46	0.97
7:X:339:TYR:HB3	7:X:404:VAL:HG13	1.46	0.97
7:O:339:TYR:HB3	7:O:404:VAL:HG13	1.47	0.97
7:V:133:ARG:NH2	7:W:164:ARG:CD	2.27	0.97
7:H:339:TYR:HB3	7:H:404:VAL:HG13	1.47	0.97
7:U:339:TYR:HB3	7:U:404:VAL:HG13	1.46	0.97
7:W:408:ILE:O	7:X:187:GLY:N	1.98	0.97
7:J:339:TYR:HB3	7:J:404:VAL:HG13	1.46	0.97
7:T:370:PHE:CD1	7:T:373:ILE:HD12	2.00	0.97
7:I:130:GLU:OE2	7:J:165:ASP:HA	1.63	0.97
7:M:370:PHE:CD1	7:M:373:ILE:HD12	2.00	0.97
7:J:190:ASN:O	7:J:191:PHE:CD1	2.17	0.96
7:H:64:ARG:NH2	7:I:459:VAL:O	1.97	0.96
7:W:339:TYR:HB3	7:W:404:VAL:HG13	1.46	0.96
7:N:339:TYR:HB3	7:N:404:VAL:HG13	1.47	0.96
7:V:370:PHE:CD1	7:V:373:ILE:HD12	2.00	0.96
7:W:400:LEU:HD12	7:X:195:HIS:CG	2.00	0.96
7:I:339:TYR:HB3	7:I:404:VAL:HG13	1.46	0.96
7:N:130:GLU:HG3	7:O:164:ARG:O	1.66	0.96
7:K:370:PHE:CD1	7:K:373:ILE:HD12	2.00	0.96
7:N:370:PHE:CD1	7:N:373:ILE:HD12	2.00	0.96
7:N:380:ASN:HD22	7:O:215:ASN:HB2	1.26	0.96
7:W:421:GLU:HB2	7:X:434:PHE:HD2	1.10	0.96
7:H:59:ASP:OD1	7:I:456:TYR:OH	1.83	0.96
7:I:64:ARG:O	7:J:467:HIS:ND1	1.98	0.96
7:I:130:GLU:OE2	7:J:165:ASP:OD1	1.80	0.96
7:K:339:TYR:HB3	7:K:404:VAL:HG13	1.46	0.96
7:R:370:PHE:CD1	7:R:373:ILE:HD12	2.00	0.96
7:V:380:ASN:CB	7:W:215:ASN:HB2	1.94	0.96
7:W:370:PHE:CD1	7:W:373:ILE:HD12	2.00	0.96
7:W:412:THR:CA	7:X:167:ASN:OD1	2.13	0.95
7:X:370:PHE:CD1	7:X:373:ILE:HD12	2.00	0.95
7:J:370:PHE:CD1	7:J:373:ILE:HD12	2.00	0.95
7:L:370:PHE:CD1	7:L:373:ILE:HD12	2.00	0.95
7:W:130:GLU:HG3	7:X:165:ASP:CA	1.95	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:339:TYR:HB3	7:L:404:VAL:HG13	1.46	0.95
7:U:370:PHE:CD1	7:U:373:ILE:HD12	2.00	0.95
7:O:370:PHE:CD1	7:O:373:ILE:HD12	2.00	0.95
7:S:339:TYR:HB3	7:S:404:VAL:HG13	1.47	0.95
7:V:402:ASP:HB2	7:W:193:THR:CG2	1.96	0.95
7:I:411:GLY:O	7:J:185:THR:CG2	2.14	0.95
3:D:225:PHE:HE1	3:D:342:TRP:HB2	1.21	0.95
7:S:370:PHE:CD1	7:S:373:ILE:HD12	2.00	0.95
7:V:395:ILE:HG13	7:W:199:GLN:O	1.67	0.95
7:I:370:PHE:CD1	7:I:373:ILE:HD12	2.00	0.95
7:T:400:LEU:HD12	7:U:195:HIS:HB2	1.48	0.95
7:P:242:SER:CB	7:P:371:SER:HG	1.66	0.95
7:P:372:GLU:HG2	7:H:222:PHE:HE1	0.79	0.95
7:R:339:TYR:HB3	7:R:404:VAL:HG13	1.47	0.95
7:V:58:THR:HG21	7:W:452:LEU:HB2	1.47	0.95
7:V:339:TYR:HB3	7:V:404:VAL:HG13	1.46	0.95
7:K:400:LEU:HD12	7:L:195:HIS:HB2	1.49	0.94
7:M:339:TYR:HB3	7:M:404:VAL:HG13	1.46	0.94
7:V:64:ARG:HH11	7:W:290:ARG:CB	1.60	0.94
7:V:133:ARG:NH1	7:W:164:ARG:CB	2.13	0.94
7:G:524:LYS:HE2	7:P:196:TYR:CE2	1.98	0.94
7:H:370:PHE:CD1	7:H:373:ILE:HD12	2.00	0.94
7:H:391:ARG:NH2	7:I:204:LYS:HE3	1.82	0.94
7:I:421:GLU:OE1	7:J:434:PHE:HD2	1.48	0.94
7:L:421:GLU:HB3	7:M:434:PHE:CD2	2.02	0.94
7:M:55:LYS:HE3	7:N:481:ILE:HG23	1.48	0.94
7:M:372:GLU:CB	7:N:223:THR:O	2.14	0.94
7:Q:370:PHE:CD1	7:Q:373:ILE:HD12	2.00	0.94
7:V:357:LYS:HE2	7:W:209:GLU:OE1	1.67	0.94
7:W:412:THR:OG1	7:X:167:ASN:HB3	1.66	0.94
7:U:391:ARG:NH2	7:V:204:LYS:CE	2.30	0.94
7:X:189:LYS:HE2	7:X:191:PHE:CZ	2.03	0.94
7:I:189:LYS:HE2	7:I:191:PHE:CZ	2.03	0.94
7:V:392:ALA:HB3	7:W:203:PHE:HB2	0.94	0.94
7:V:64:ARG:CZ	7:W:290:ARG:HA	1.97	0.94
7:M:313:GLU:CD	7:N:290:ARG:NH2	2.20	0.94
7:V:64:ARG:NH1	7:W:291:ASP:N	1.96	0.94
7:M:189:LYS:HE2	7:M:191:PHE:CZ	2.03	0.94
7:S:189:LYS:HE2	7:S:191:PHE:CZ	2.03	0.94
7:V:64:ARG:HH12	7:W:290:ARG:C	1.71	0.94
7:Q:370:PHE:HB2	7:Q:373:ILE:H	1.33	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:370:PHE:N	7:J:373:ILE:O	2.01	0.93
7:O:370:PHE:N	7:O:373:ILE:O	2.01	0.93
7:T:370:PHE:N	7:T:373:ILE:O	2.01	0.93
7:M:65:ARG:HB2	7:N:467:HIS:ND1	1.83	0.93
7:T:380:ASN:HD22	7:U:215:ASN:HB2	1.32	0.93
7:R:370:PHE:N	7:R:373:ILE:O	2.01	0.93
7:K:189:LYS:HE2	7:K:191:PHE:CZ	2.03	0.93
7:N:189:LYS:HE2	7:N:191:PHE:CZ	2.03	0.93
7:U:370:PHE:HB2	7:U:373:ILE:H	1.33	0.93
7:U:370:PHE:N	7:U:373:ILE:O	2.01	0.93
7:V:386:LYS:HB3	7:W:209:GLU:CB	1.98	0.93
7:H:370:PHE:N	7:H:373:ILE:O	2.01	0.93
7:I:412:THR:OG1	7:J:167:ASN:OD1	1.85	0.93
7:N:372:GLU:HB3	7:O:223:THR:O	1.64	0.93
7:N:370:PHE:N	7:N:373:ILE:O	2.01	0.93
7:N:400:LEU:HD12	7:O:195:HIS:CB	1.99	0.93
7:Q:189:LYS:HE2	7:Q:191:PHE:CZ	2.03	0.93
7:U:189:LYS:HE2	7:U:191:PHE:CZ	2.03	0.93
7:V:370:PHE:N	7:V:373:ILE:O	2.01	0.93
7:W:413:ARG:HH12	7:X:282:LEU:HG	1.11	0.93
7:O:370:PHE:HB2	7:O:373:ILE:H	1.33	0.93
7:W:370:PHE:N	7:W:373:ILE:O	2.01	0.93
7:H:189:LYS:HE2	7:H:191:PHE:CZ	2.03	0.93
7:Q:370:PHE:N	7:Q:373:ILE:O	2.01	0.93
7:V:64:ARG:CZ	7:W:290:ARG:CB	2.46	0.93
7:M:313:GLU:CD	7:N:290:ARG:HH22	1.71	0.92
7:R:189:LYS:HE2	7:R:191:PHE:CZ	2.03	0.92
7:T:189:LYS:HE2	7:T:191:PHE:CZ	2.03	0.92
7:L:370:PHE:N	7:L:373:ILE:O	2.01	0.92
7:X:370:PHE:N	7:X:373:ILE:O	2.01	0.92
7:K:370:PHE:N	7:K:373:ILE:O	2.01	0.92
7:L:189:LYS:HE2	7:L:191:PHE:CZ	2.03	0.92
7:O:189:LYS:HE2	7:O:191:PHE:CZ	2.03	0.92
7:M:370:PHE:N	7:M:373:ILE:O	2.01	0.92
7:N:421:GLU:OE1	7:O:434:PHE:CD2	2.22	0.92
7:H:370:PHE:HB2	7:H:373:ILE:H	1.33	0.92
7:I:413:ARG:CZ	7:J:282:LEU:HA	2.00	0.92
7:V:320:THR:HG23	7:W:179:ALA:HB1	1.49	0.92
7:I:370:PHE:N	7:I:373:ILE:O	2.02	0.92
7:J:189:LYS:HE2	7:J:191:PHE:CZ	2.03	0.92
7:M:19:HIS:NE2	7:N:487:ARG:CD	2.30	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:V:189:LYS:HE2	7:V:191:PHE:CZ	2.03	0.92
7:V:414:LYS:CA	7:W:435:VAL:HG13	1.92	0.92
7:L:417:PHE:CZ	7:M:280:ILE:HG13	2.04	0.92
7:T:391:ARG:NH2	7:U:204:LYS:HE3	1.83	0.92
7:V:380:ASN:HD22	7:W:215:ASN:HB3	1.34	0.92
7:J:400:LEU:HD12	7:K:195:HIS:HB2	1.52	0.91
7:V:380:ASN:ND2	7:W:215:ASN:CB	2.27	0.91
7:I:130:GLU:HG3	7:J:164:ARG:O	1.69	0.91
7:S:370:PHE:N	7:S:373:ILE:O	2.01	0.91
7:W:189:LYS:HE2	7:W:191:PHE:CZ	2.03	0.91
7:W:400:LEU:CD1	7:X:195:HIS:HB2	2.01	0.91
7:W:417:PHE:CE2	7:X:280:ILE:HG13	2.04	0.91
7:K:370:PHE:HB2	7:K:373:ILE:H	1.33	0.91
7:W:370:PHE:HB2	7:W:373:ILE:H	1.33	0.91
7:M:65:ARG:HA	7:N:467:HIS:CB	1.98	0.91
7:V:370:PHE:HB2	7:V:373:ILE:H	1.33	0.90
7:N:406:SER:O	7:O:188:GLU:HB2	1.70	0.90
7:V:391:ARG:NH2	7:W:204:LYS:HG3	1.85	0.90
7:M:370:PHE:HB2	7:M:373:ILE:H	1.33	0.90
7:I:370:PHE:HB2	7:I:373:ILE:H	1.33	0.90
7:L:370:PHE:HB2	7:L:373:ILE:H	1.33	0.90
7:X:370:PHE:HB2	7:X:373:ILE:H	1.33	0.89
7:J:370:PHE:HB2	7:J:373:ILE:H	1.33	0.89
7:L:394:ASN:HB2	7:M:201:GLU:HB2	1.53	0.89
7:W:370:PHE:HB2	7:W:373:ILE:HB	1.31	0.89
7:G:524:LYS:CD	7:P:196:TYR:CD2	2.55	0.89
7:K:339:TYR:CB	7:K:404:VAL:HG22	2.03	0.88
7:G:243:LEU:HD11	7:G:370:PHE:HE1	1.38	0.88
7:K:413:ARG:HH11	7:L:282:LEU:HA	1.39	0.88
7:M:417:PHE:HE1	7:N:187:GLY:HA3	1.38	0.88
7:T:370:PHE:HB2	7:T:373:ILE:H	1.33	0.88
7:M:339:TYR:CB	7:M:404:VAL:HG22	2.04	0.88
7:R:370:PHE:HB2	7:R:373:ILE:H	1.33	0.88
7:T:339:TYR:CB	7:T:404:VAL:HG22	2.03	0.88
7:V:386:LYS:N	7:W:209:GLU:O	2.06	0.88
7:W:339:TYR:CB	7:W:404:VAL:HG22	2.04	0.88
7:S:339:TYR:CB	7:S:404:VAL:HG22	2.04	0.88
7:H:44:ARG:NH2	7:I:474:GLU:OE2	2.07	0.88
7:Q:339:TYR:CB	7:Q:404:VAL:HG22	2.03	0.88
7:L:130:GLU:HG3	7:M:165:ASP:HA	1.56	0.88
7:I:421:GLU:OE1	7:J:434:PHE:CD2	2.26	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:339:TYR:CB	7:J:404:VAL:HG22	2.03	0.88
7:U:391:ARG:HH21	7:V:204:LYS:HE3	1.33	0.88
7:W:406:SER:O	7:X:188:GLU:HB2	1.74	0.88
7:W:421:GLU:OE1	7:X:434:PHE:CD2	2.27	0.88
7:L:339:TYR:CB	7:L:404:VAL:HG22	2.03	0.88
7:U:384:CYS:O	7:V:210:LYS:HG3	1.73	0.88
6:B:586:THR:HG22	7:X:107:PHE:HE2	1.33	0.87
7:U:391:ARG:HE	7:V:204:LYS:HE2	1.35	0.87
7:L:413:ARG:NH1	7:M:282:LEU:HG	1.90	0.87
7:W:400:LEU:HD12	7:X:195:HIS:CD2	2.09	0.87
7:N:413:ARG:NH1	7:O:282:LEU:CA	2.36	0.87
7:I:148:SER:HB3	7:J:180:SER:HB2	1.57	0.87
7:N:339:TYR:CB	7:N:404:VAL:HG22	2.04	0.87
7:V:384:CYS:O	7:W:210:LYS:HG3	1.75	0.87
7:G:524:LYS:HE3	7:P:196:TYR:CE2	2.05	0.87
7:U:339:TYR:CB	7:U:404:VAL:HG22	2.04	0.87
7:H:19:HIS:NE2	7:I:487:ARG:HD2	1.89	0.87
7:N:190:ASN:O	7:N:191:PHE:HD1	1.55	0.87
7:O:339:TYR:CB	7:O:404:VAL:HG22	2.04	0.87
7:G:243:LEU:HD12	7:G:370:PHE:CD1	2.09	0.87
7:N:413:ARG:HH11	7:O:282:LEU:CA	1.87	0.87
7:Q:190:ASN:O	7:Q:191:PHE:HD1	1.55	0.87
7:X:339:TYR:CB	7:X:404:VAL:HG22	2.04	0.87
7:G:524:LYS:HG3	7:P:196:TYR:CE2	2.00	0.86
7:K:190:ASN:C	7:K:191:PHE:CD1	2.49	0.86
7:N:130:GLU:CD	7:O:165:ASP:HA	1.94	0.86
7:N:370:PHE:HB2	7:N:373:ILE:H	1.33	0.86
7:I:190:ASN:O	7:I:191:PHE:HD1	1.55	0.86
7:M:190:ASN:C	7:M:191:PHE:CD1	2.49	0.86
7:X:190:ASN:O	7:X:191:PHE:HD1	1.55	0.86
7:N:400:LEU:CD1	7:O:195:HIS:HB2	2.04	0.86
7:R:339:TYR:CB	7:R:404:VAL:HG22	2.03	0.86
7:S:370:PHE:CD1	7:S:373:ILE:CD1	2.59	0.86
7:V:528:GLY:HA3	7:W:200:ILE:HD12	1.55	0.86
7:L:370:PHE:CD1	7:L:373:ILE:CD1	2.59	0.86
7:W:370:PHE:CD1	7:W:373:ILE:CD1	2.59	0.86
7:N:413:ARG:CZ	7:O:282:LEU:HG	2.04	0.86
7:T:370:PHE:CD1	7:T:373:ILE:CD1	2.59	0.86
7:M:370:PHE:CD1	7:M:373:ILE:CD1	2.59	0.86
7:O:190:ASN:C	7:O:191:PHE:CD1	2.49	0.86
7:T:190:ASN:C	7:T:191:PHE:CD1	2.49	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:V:370:PHE:CD1	7:V:373:ILE:CD1	2.59	0.86
7:V:528:GLY:CA	7:W:200:ILE:HD13	2.06	0.86
7:W:417:PHE:CE2	7:X:280:ILE:CD1	2.57	0.86
7:P:372:GLU:HG3	7:H:222:PHE:CZ	2.10	0.86
7:H:370:PHE:CD1	7:H:373:ILE:CD1	2.59	0.86
7:N:130:GLU:OE2	7:O:165:ASP:HA	1.76	0.86
7:N:391:ARG:HH21	7:O:204:LYS:HE3	1.41	0.86
3:D:225:PHE:HD1	3:D:342:TRP:CG	1.93	0.86
7:P:374:SER:HB3	7:H:220:LEU:HD12	1.58	0.86
7:Q:370:PHE:CD1	7:Q:373:ILE:CD1	2.59	0.86
7:Q:400:LEU:HD12	7:R:195:HIS:HB2	1.57	0.86
7:T:190:ASN:O	7:T:191:PHE:HD1	1.55	0.86
7:V:390:GLY:N	7:W:205:SER:O	2.09	0.86
7:I:339:TYR:CB	7:I:404:VAL:HG22	2.03	0.86
7:M:190:ASN:O	7:M:191:PHE:HD1	1.55	0.86
7:U:190:ASN:C	7:U:191:PHE:CD1	2.49	0.86
7:T:372:GLU:OE1	7:U:223:THR:O	1.94	0.85
7:I:370:PHE:CD1	7:I:373:ILE:CD1	2.59	0.85
7:K:413:ARG:NH1	7:L:282:LEU:HA	1.91	0.85
7:T:380:ASN:O	7:U:214:PHE:CD1	2.27	0.85
7:U:190:ASN:O	7:U:191:PHE:HD1	1.55	0.85
7:V:339:TYR:CB	7:V:404:VAL:HG22	2.03	0.85
7:X:370:PHE:CD1	7:X:373:ILE:CD1	2.59	0.85
7:N:190:ASN:C	7:N:191:PHE:CD1	2.49	0.85
7:V:190:ASN:O	7:V:191:PHE:HD1	1.55	0.85
7:P:250:ARG:HB2	7:P:363:HIS:HB3	1.56	0.85
7:J:370:PHE:CD1	7:J:373:ILE:CD1	2.59	0.85
7:L:190:ASN:C	7:L:191:PHE:CD1	2.49	0.85
7:R:370:PHE:CD1	7:R:373:ILE:CD1	2.59	0.85
7:S:190:ASN:C	7:S:191:PHE:CD1	2.49	0.85
7:U:370:PHE:CD1	7:U:373:ILE:CD1	2.59	0.85
7:V:422:LYS:HG3	7:W:431:VAL:CG1	2.06	0.85
7:K:370:PHE:CD1	7:K:373:ILE:CD1	2.59	0.85
7:V:386:LYS:HB3	7:W:209:GLU:N	1.91	0.85
7:W:190:ASN:O	7:W:191:PHE:HD1	1.55	0.85
7:O:370:PHE:CD1	7:O:373:ILE:CD1	2.59	0.85
7:R:190:ASN:C	7:R:191:PHE:CD1	2.49	0.85
7:H:339:TYR:CB	7:H:404:VAL:HG22	2.04	0.85
7:I:413:ARG:HH11	7:J:282:LEU:HA	0.95	0.85
7:N:370:PHE:CD1	7:N:373:ILE:CD1	2.59	0.85
7:V:106:ASP:CG	7:W:122:ARG:CB	2.44	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:370:PHE:HB2	7:S:373:ILE:H	1.33	0.85
7:U:392:ALA:HB3	7:V:203:PHE:H	1.41	0.85
7:N:421:GLU:CB	7:O:434:PHE:HD2	1.89	0.84
7:V:528:GLY:HA3	7:W:200:ILE:HD13	1.54	0.84
7:L:421:GLU:CB	7:M:434:PHE:CD2	2.60	0.84
7:V:386:LYS:HB3	7:W:209:GLU:CA	2.07	0.84
7:P:64:ARG:NH2	7:H:459:VAL:O	2.09	0.84
7:N:403:ASP:HA	7:O:192:ARG:HG2	1.58	0.84
7:S:190:ASN:O	7:S:191:PHE:HD1	1.55	0.84
7:V:386:LYS:HD3	7:W:209:GLU:CB	2.07	0.84
7:V:391:ARG:HE	7:W:204:LYS:HG2	1.42	0.84
7:G:524:LYS:CE	7:P:196:TYR:HD2	1.80	0.84
7:V:129:SER:OG	7:W:169:LEU:CD1	2.25	0.84
7:V:386:LYS:CD	7:W:209:GLU:CB	2.54	0.84
7:R:190:ASN:O	7:R:191:PHE:HD1	1.55	0.84
7:U:372:GLU:HG3	7:V:224:PRO:CA	2.07	0.84
7:V:106:ASP:HB3	7:W:122:ARG:CB	2.07	0.84
7:I:411:GLY:O	7:J:185:THR:HG22	1.77	0.84
7:H:190:ASN:C	7:H:191:PHE:CD1	2.49	0.84
7:L:380:ASN:HD22	7:M:215:ASN:HB2	1.42	0.84
7:W:391:ARG:NH2	7:X:204:LYS:HE3	1.91	0.84
7:K:190:ASN:O	7:K:191:PHE:HD1	1.55	0.84
7:Q:189:LYS:HE2	7:Q:191:PHE:HE1	1.43	0.84
7:Q:190:ASN:C	7:Q:191:PHE:CD1	2.49	0.84
7:T:189:LYS:HE2	7:T:191:PHE:HE1	1.43	0.84
7:P:372:GLU:CG	7:H:222:PHE:CZ	2.61	0.83
7:G:524:LYS:NZ	7:P:271:LYS:HD3	1.93	0.83
7:I:129:SER:HB2	7:J:164:ARG:NH1	1.92	0.83
7:M:189:LYS:HE2	7:M:191:PHE:HE1	1.43	0.83
7:V:320:THR:CG2	7:W:179:ALA:HB1	2.08	0.83
7:U:391:ARG:HH21	7:V:204:LYS:CE	1.90	0.83
7:I:408:ILE:HG22	7:J:187:GLY:O	1.79	0.83
7:K:391:ARG:NH2	7:L:204:LYS:HE3	1.94	0.83
7:S:400:LEU:HD12	7:T:195:HIS:HB2	1.60	0.83
7:U:189:LYS:HE2	7:U:191:PHE:HE1	1.43	0.83
7:W:190:ASN:C	7:W:191:PHE:CD1	2.49	0.83
7:X:326:SER:HB3	7:X:450:GLN:HE21	1.44	0.83
7:H:326:SER:HB3	7:H:450:GLN:HE21	1.44	0.83
7:U:326:SER:HB3	7:U:450:GLN:HE21	1.44	0.83
7:J:64:ARG:NH2	7:K:459:VAL:O	2.12	0.83
7:G:326:SER:HB3	7:G:450:GLN:HE21	1.44	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:242:SER:HB2	7:P:371:SER:OG	1.78	0.82
7:L:189:LYS:HE2	7:L:191:PHE:HE1	1.43	0.82
7:M:326:SER:HB3	7:M:450:GLN:HE21	1.44	0.82
7:V:386:LYS:CB	7:W:209:GLU:CB	2.54	0.82
7:W:407:LEU:HA	7:X:188:GLU:HA	1.61	0.82
7:J:326:SER:HB3	7:J:450:GLN:HE21	1.44	0.82
7:O:190:ASN:O	7:O:191:PHE:HD1	1.55	0.82
7:H:190:ASN:O	7:H:191:PHE:HD1	1.55	0.82
7:H:391:ARG:HH21	7:I:204:LYS:HE3	1.43	0.82
7:I:130:GLU:CG	7:J:165:ASP:HA	2.09	0.82
7:I:411:GLY:O	7:J:185:THR:HG21	1.76	0.82
7:K:372:GLU:CG	7:L:223:THR:O	2.26	0.82
7:I:189:LYS:HE2	7:I:191:PHE:HE1	1.43	0.82
7:J:190:ASN:C	7:J:191:PHE:CD1	2.49	0.82
7:V:502:ASP:OD2	7:W:451:LYS:HA	1.78	0.82
7:V:190:ASN:C	7:V:191:PHE:CD1	2.49	0.82
7:N:326:SER:HB3	7:N:450:GLN:HE21	1.44	0.82
7:O:326:SER:HB3	7:O:450:GLN:HE21	1.44	0.82
7:V:64:ARG:CZ	7:W:290:ARG:CA	2.54	0.82
7:W:421:GLU:OE2	7:X:431:VAL:O	1.97	0.82
7:X:190:ASN:C	7:X:191:PHE:CD1	2.49	0.82
7:W:413:ARG:CZ	7:X:282:LEU:HG	2.09	0.82
7:K:189:LYS:HE2	7:K:191:PHE:HE1	1.43	0.82
7:V:326:SER:HB3	7:V:450:GLN:HE21	1.44	0.82
7:J:406:SER:O	7:K:188:GLU:HB2	1.79	0.82
7:M:417:PHE:HE2	7:N:185:THR:HG1	1.26	0.82
7:L:326:SER:HB3	7:L:450:GLN:HE21	1.44	0.82
7:W:326:SER:HB3	7:W:450:GLN:HE21	1.44	0.81
7:I:412:THR:HG1	7:J:167:ASN:CG	1.82	0.81
7:Q:326:SER:HB3	7:Q:450:GLN:HE21	1.44	0.81
7:P:372:GLU:O	7:H:222:PHE:CD1	2.33	0.81
7:I:190:ASN:C	7:I:191:PHE:CD1	2.49	0.81
7:K:130:GLU:HG3	7:L:164:ARG:O	1.80	0.81
7:L:391:ARG:HH22	7:M:202:ALA:HB1	1.42	0.81
7:Q:380:ASN:HD22	7:R:215:ASN:HB2	1.43	0.81
7:S:189:LYS:HE2	7:S:191:PHE:HE1	1.43	0.81
7:V:386:LYS:HB2	7:W:209:GLU:HB3	1.63	0.81
7:W:413:ARG:HH11	7:X:282:LEU:CA	1.93	0.81
7:W:418:GLU:HB2	7:X:435:VAL:HG22	1.63	0.81
7:P:326:SER:HB3	7:P:450:GLN:HE21	1.44	0.81
7:I:413:ARG:NH1	7:J:282:LEU:O	2.14	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:380:ASN:HD22	7:V:215:ASN:CB	1.92	0.81
7:V:133:ARG:NH2	7:W:164:ARG:CZ	2.43	0.81
7:I:64:ARG:O	7:J:467:HIS:CE1	2.33	0.81
7:I:417:PHE:CE1	7:J:187:GLY:HA3	2.16	0.81
7:K:479:ASP:O	7:K:483:GLU:HB2	1.81	0.81
7:W:394:ASN:HB2	7:X:201:GLU:HB2	1.62	0.81
7:J:391:ARG:HH21	7:K:204:LYS:HE3	1.45	0.81
7:N:380:ASN:O	7:O:214:PHE:CD1	2.34	0.81
7:T:372:GLU:HG3	7:U:223:THR:O	1.81	0.81
7:U:400:LEU:HD12	7:V:195:HIS:CB	2.11	0.81
7:V:479:ASP:O	7:V:483:GLU:HB2	1.81	0.81
7:N:392:ALA:HB3	7:O:203:PHE:H	1.46	0.81
7:S:479:ASP:O	7:S:483:GLU:HB2	1.81	0.81
7:R:400:LEU:HD12	7:S:195:HIS:HB2	1.62	0.81
7:T:374:SER:O	7:U:220:LEU:HD12	1.81	0.81
7:H:189:LYS:HE2	7:H:191:PHE:HE1	1.43	0.81
7:H:479:ASP:O	7:H:483:GLU:HB2	1.81	0.81
7:R:326:SER:HB3	7:R:450:GLN:HE21	1.44	0.81
7:Q:479:ASP:O	7:Q:483:GLU:HB2	1.81	0.80
3:D:225:PHE:CZ	3:D:340:SER:OG	2.34	0.80
7:P:479:ASP:O	7:P:483:GLU:HB2	1.82	0.80
7:K:326:SER:HB3	7:K:450:GLN:HE21	1.44	0.80
7:T:479:ASP:O	7:T:483:GLU:HB2	1.81	0.80
7:U:479:ASP:O	7:U:483:GLU:HB2	1.81	0.80
7:H:105:GLY:HA2	7:I:159:LEU:HD22	1.63	0.80
7:M:372:GLU:HG3	7:N:223:THR:O	1.82	0.80
7:O:479:ASP:O	7:O:483:GLU:HB2	1.81	0.80
7:J:479:ASP:O	7:J:483:GLU:HB2	1.81	0.80
7:L:400:LEU:HD12	7:M:195:HIS:HB2	1.63	0.80
7:M:372:GLU:HB3	7:N:223:THR:O	1.80	0.80
7:I:326:SER:HB3	7:I:450:GLN:HE21	1.44	0.80
7:I:479:ASP:O	7:I:483:GLU:HB2	1.81	0.80
7:M:479:ASP:O	7:M:483:GLU:HB2	1.81	0.80
7:U:413:ARG:HG2	7:V:438:ALA:HB1	1.63	0.80
7:W:412:THR:OG1	7:X:167:ASN:CB	2.28	0.80
7:N:412:THR:HA	7:O:167:ASN:OD1	1.80	0.80
7:O:391:ARG:HH22	7:Q:202:ALA:HB1	1.43	0.80
7:V:106:ASP:CB	7:W:122:ARG:CB	2.60	0.80
7:W:404:VAL:N	7:X:191:PHE:O	2.14	0.80
7:S:326:SER:HB3	7:S:450:GLN:HE21	1.44	0.80
5:F:371:LYS:HB3	7:G:209:GLU:HB3	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:65:ARG:HB2	7:N:467:HIS:CD2	2.16	0.80
7:T:326:SER:HB3	7:T:450:GLN:HE21	1.44	0.80
7:W:130:GLU:OE2	7:X:166:GLY:N	2.14	0.80
7:M:417:PHE:CE1	7:N:187:GLY:HA3	2.17	0.80
7:S:380:ASN:HD22	7:T:215:ASN:HB2	1.47	0.80
7:W:479:ASP:O	7:W:483:GLU:HB2	1.81	0.80
7:N:130:GLU:CG	7:O:165:ASP:HA	2.11	0.80
7:R:189:LYS:HE2	7:R:191:PHE:HE1	1.43	0.80
7:V:414:LYS:O	7:W:435:VAL:CG2	2.30	0.80
7:T:372:GLU:CD	7:U:223:THR:O	2.20	0.79
7:I:148:SER:HB3	7:J:180:SER:CB	2.12	0.79
7:L:412:THR:HA	7:M:167:ASN:OD1	1.81	0.79
7:L:479:ASP:O	7:L:483:GLU:HB2	1.81	0.79
7:P:272:MET:HB3	7:P:341:LEU:HB3	1.64	0.79
7:R:479:ASP:O	7:R:483:GLU:HB2	1.81	0.79
7:N:130:GLU:HG3	7:O:165:ASP:HA	1.64	0.79
7:R:391:ARG:NH2	7:S:204:LYS:HE3	1.98	0.79
7:L:190:ASN:O	7:L:191:PHE:HD1	1.55	0.79
7:V:400:LEU:HB2	7:W:195:HIS:CD2	2.18	0.79
7:J:190:ASN:O	7:J:191:PHE:HD1	1.55	0.79
7:L:400:LEU:HD12	7:M:195:HIS:CD2	2.18	0.79
7:V:402:ASP:HB2	7:W:193:THR:HG21	1.62	0.79
7:T:59:ASP:OD1	7:U:456:TYR:OH	2.00	0.79
7:V:189:LYS:HE2	7:V:191:PHE:HE1	1.43	0.79
1:A:61:ASP:HB2	1:A:62:LYS:HB3	1.64	0.79
7:P:264:SER:HB3	7:P:349:LYS:HB3	1.63	0.79
7:V:388:GLY:HA3	7:W:207:ILE:HG22	1.64	0.79
7:X:189:LYS:HE2	7:X:191:PHE:HE1	1.43	0.79
7:X:479:ASP:O	7:X:483:GLU:HB2	1.81	0.79
7:G:208:GLN:HB2	7:G:259:TYR:HB2	1.63	0.79
7:I:413:ARG:NH1	7:J:282:LEU:C	2.36	0.79
7:W:392:ALA:HB3	7:X:203:PHE:H	1.48	0.79
5:F:155:TRP:HE1	5:F:171:ASP:HA	1.49	0.78
7:N:479:ASP:O	7:N:483:GLU:HB2	1.81	0.78
7:V:386:LYS:CG	7:W:209:GLU:HB3	2.13	0.78
7:Q:264:SER:HB3	7:Q:349:LYS:HB3	1.66	0.78
7:Q:391:ARG:NH2	7:R:204:LYS:HE3	1.98	0.78
7:T:391:ARG:HH21	7:U:204:LYS:HE3	1.46	0.78
7:U:386:LYS:CD	7:V:209:GLU:HB3	2.12	0.78
7:K:264:SER:HB3	7:K:349:LYS:HB3	1.66	0.78
7:G:372:GLU:CG	7:P:223:THR:O	2.31	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:264:SER:HB3	7:O:349:LYS:HB3	1.66	0.78
7:R:264:SER:HB3	7:R:349:LYS:HB3	1.66	0.78
7:O:189:LYS:HE2	7:O:191:PHE:HE1	1.43	0.78
7:X:264:SER:HB3	7:X:349:LYS:HB3	1.66	0.78
6:B:586:THR:CB	7:X:107:PHE:CD2	2.67	0.78
7:J:264:SER:HB3	7:J:349:LYS:HB3	1.66	0.78
7:W:409:ARG:HD3	7:X:184:GLU:OE2	1.84	0.78
7:W:424:LEU:HD11	7:X:191:PHE:CZ	2.19	0.78
7:U:380:ASN:ND2	7:V:215:ASN:HB2	1.96	0.77
7:N:189:LYS:HE2	7:N:191:PHE:HE1	1.43	0.77
7:U:264:SER:HB3	7:U:349:LYS:HB3	1.66	0.77
7:U:386:LYS:HD2	7:V:209:GLU:HB3	1.67	0.77
1:A:283:MET:HA	1:A:284:GLN:HB3	1.67	0.77
7:P:514:GLU:HB2	7:P:522:LYS:HB2	1.65	0.77
7:R:380:ASN:HD22	7:S:215:ASN:HB2	1.49	0.77
7:V:386:LYS:HD3	7:W:209:GLU:HB2	1.67	0.77
7:V:402:ASP:O	7:W:193:THR:HG22	1.83	0.77
7:W:189:LYS:HE2	7:W:191:PHE:HE1	1.43	0.77
7:V:414:LYS:CB	7:W:435:VAL:HG11	2.15	0.77
7:W:413:ARG:NH1	7:X:282:LEU:HA	2.00	0.77
7:W:421:GLU:HB2	7:X:434:PHE:CE2	2.19	0.77
7:G:250:ARG:HB2	7:G:363:HIS:HB2	1.67	0.77
7:K:372:GLU:HB3	7:L:223:THR:O	1.83	0.77
5:F:265:LYS:HB2	5:F:427:ILE:HD11	1.66	0.77
7:U:391:ARG:CZ	7:V:204:LYS:HE3	2.14	0.77
7:V:394:ASN:CB	7:W:201:GLU:OE1	2.33	0.77
3:D:416:VAL:HG12	3:D:419:GLN:HE21	1.49	0.76
7:L:264:SER:HB3	7:L:349:LYS:HB3	1.66	0.76
7:L:400:LEU:HD12	7:M:195:HIS:CG	2.20	0.76
7:M:59:ASP:OD1	7:N:456:TYR:OH	2.01	0.76
7:T:264:SER:HB3	7:T:349:LYS:HB3	1.66	0.76
2:C:336:GLU:N	2:C:336:GLU:OE1	2.18	0.76
7:I:264:SER:HB3	7:I:349:LYS:HB3	1.66	0.76
7:S:264:SER:HB3	7:S:349:LYS:HB3	1.66	0.76
7:V:380:ASN:HB2	7:W:215:ASN:CB	2.14	0.76
3:D:225:PHE:HE1	3:D:342:TRP:CB	1.79	0.76
7:G:177:ASN:HD21	7:G:292:VAL:HG23	1.50	0.76
7:P:372:GLU:OE1	7:H:222:PHE:HZ	1.68	0.76
7:K:372:GLU:HG3	7:L:223:THR:O	1.86	0.76
7:N:264:SER:HB3	7:N:349:LYS:HB3	1.66	0.76
3:D:192:ILE:HG23	6:B:444:ILE:HG23	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:69:ASP:HB3	5:F:81:ARG:HG3	1.67	0.76
7:V:404:VAL:O	7:W:191:PHE:HB2	1.85	0.76
7:W:264:SER:HB3	7:W:349:LYS:HB3	1.66	0.76
7:N:409:ARG:HD3	7:O:184:GLU:OE2	1.85	0.76
7:U:391:ARG:HH21	7:V:204:LYS:HG3	1.50	0.76
7:P:380:ASN:HD22	7:H:215:ASN:HB2	1.51	0.76
7:V:264:SER:HB3	7:V:349:LYS:HB3	1.66	0.76
7:P:372:GLU:O	7:H:222:PHE:CE1	2.39	0.76
7:I:130:GLU:CG	7:J:164:ARG:O	2.33	0.76
7:O:400:LEU:HD12	7:Q:195:HIS:HB2	1.67	0.76
7:M:208:GLN:HB2	7:M:259:TYR:HB2	1.68	0.76
7:V:133:ARG:NH2	7:W:164:ARG:NH2	2.33	0.76
3:D:225:PHE:HZ	3:D:340:SER:OG	1.67	0.75
7:I:208:GLN:HB2	7:I:259:TYR:HB2	1.68	0.75
7:G:243:LEU:CD1	7:G:370:PHE:HD1	2.00	0.75
7:L:413:ARG:HH11	7:M:282:LEU:HA	1.51	0.75
7:U:391:ARG:CZ	7:V:204:LYS:CE	2.64	0.75
7:P:59:ASP:OD1	7:H:456:TYR:OH	2.04	0.75
7:N:380:ASN:HD22	7:O:215:ASN:CB	1.99	0.75
7:S:391:ARG:NH2	7:T:204:LYS:HE3	2.00	0.75
7:O:208:GLN:HB2	7:O:259:TYR:HB2	1.68	0.75
7:H:208:GLN:HB2	7:H:259:TYR:HB2	1.68	0.75
7:U:208:GLN:HB2	7:U:259:TYR:HB2	1.68	0.75
7:X:208:GLN:HB2	7:X:259:TYR:HB2	1.68	0.75
6:B:586:THR:CG2	7:X:107:PHE:HE2	1.91	0.75
7:I:106:ASP:OD2	7:J:121:CYS:HA	1.87	0.75
7:I:191:PHE:HA	7:I:276:VAL:HG12	1.69	0.75
7:J:189:LYS:HE2	7:J:191:PHE:HE1	1.43	0.75
7:M:191:PHE:HA	7:M:276:VAL:HG12	1.69	0.75
7:M:264:SER:HB3	7:M:349:LYS:HB3	1.66	0.75
7:N:191:PHE:HA	7:N:276:VAL:HG12	1.69	0.75
7:O:191:PHE:HA	7:O:276:VAL:HG12	1.69	0.75
7:Q:208:GLN:HB2	7:Q:259:TYR:HB2	1.68	0.75
7:S:208:GLN:HB2	7:S:259:TYR:HB2	1.68	0.75
7:U:411:GLY:O	7:V:185:THR:HG21	1.87	0.75
7:M:372:GLU:CG	7:N:223:THR:O	2.34	0.75
7:N:421:GLU:OE1	7:O:434:PHE:CG	2.40	0.75
7:U:145:ASP:OD2	7:V:284:ARG:NH1	2.19	0.75
7:U:191:PHE:HA	7:U:276:VAL:HG12	1.69	0.75
7:J:409:ARG:HD3	7:K:184:GLU:OE2	1.86	0.75
7:O:130:GLU:HG3	7:Q:164:ARG:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:391:ARG:HH22	7:T:202:ALA:HB1	1.52	0.74
7:T:208:GLN:HB2	7:T:259:TYR:HB2	1.68	0.74
7:V:64:ARG:NH1	7:W:290:ARG:C	2.35	0.74
7:H:264:SER:HB3	7:H:349:LYS:HB3	1.66	0.74
7:J:391:ARG:NH2	7:K:204:LYS:HE3	2.02	0.74
7:T:191:PHE:HA	7:T:276:VAL:HG12	1.69	0.74
7:K:191:PHE:HA	7:K:276:VAL:HG12	1.69	0.74
7:K:208:GLN:HB2	7:K:259:TYR:HB2	1.68	0.74
7:N:129:SER:HB2	7:O:164:ARG:NH1	2.01	0.74
7:N:208:GLN:HB2	7:N:259:TYR:HB2	1.68	0.74
7:S:59:ASP:OD1	7:T:456:TYR:OH	2.05	0.74
7:U:386:LYS:HB3	7:V:209:GLU:H	1.53	0.74
7:W:208:GLN:HB2	7:W:259:TYR:HB2	1.68	0.74
7:L:208:GLN:HB2	7:L:259:TYR:HB2	1.68	0.74
7:Q:413:ARG:HH11	7:R:282:LEU:HA	1.53	0.74
7:V:208:GLN:HB2	7:V:259:TYR:HB2	1.68	0.74
7:L:403:ASP:HA	7:M:192:ARG:HG2	1.69	0.74
7:V:352:GLU:HB3	7:V:391:ARG:HB3	1.70	0.74
5:F:258:ILE:HG23	5:F:327:ILE:HB	1.67	0.74
7:H:391:ARG:HH21	7:I:204:LYS:CE	2.00	0.74
7:T:352:GLU:HB3	7:T:391:ARG:HB3	1.70	0.74
7:U:352:GLU:HB3	7:U:391:ARG:HB3	1.70	0.74
7:V:380:ASN:CG	7:W:215:ASN:HB2	2.07	0.74
7:W:127:GLU:HG2	7:X:164:ARG:HH22	1.53	0.74
7:W:413:ARG:CZ	7:X:282:LEU:HD12	2.17	0.74
7:H:352:GLU:HB3	7:H:391:ARG:HB3	1.70	0.74
7:H:372:GLU:OE1	7:I:223:THR:O	2.04	0.74
7:L:391:ARG:HH21	7:M:204:LYS:HG3	1.52	0.74
7:N:417:PHE:CE2	7:O:280:ILE:HG13	2.22	0.74
7:U:372:GLU:CB	7:V:223:THR:O	2.31	0.74
7:J:413:ARG:NH1	7:K:282:LEU:HG	2.02	0.74
7:N:391:ARG:HE	7:O:204:LYS:HE2	1.53	0.74
7:Q:191:PHE:HA	7:Q:276:VAL:HG12	1.69	0.74
7:X:191:PHE:HA	7:X:276:VAL:HG12	1.69	0.74
7:G:264:SER:HB3	7:G:349:LYS:HB3	1.70	0.74
7:I:521:SER:O	7:I:522:LYS:HB3	1.88	0.74
7:M:55:LYS:HZ1	7:N:482:ASN:HB2	1.53	0.74
7:P:380:ASN:O	7:H:214:PHE:CD1	2.40	0.74
7:L:191:PHE:HA	7:L:276:VAL:HG12	1.69	0.74
7:M:352:GLU:HB3	7:M:391:ARG:HB3	1.70	0.74
7:Q:352:GLU:HB3	7:Q:391:ARG:HB3	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:R:208:GLN:HB2	7:R:259:TYR:HB2	1.68	0.73
7:V:191:PHE:HA	7:V:276:VAL:HG12	1.69	0.73
7:V:394:ASN:O	7:W:201:GLU:HB2	1.88	0.73
7:V:394:ASN:HB2	7:W:201:GLU:OE1	1.88	0.73
7:W:145:ASP:OD2	7:X:284:ARG:NH1	2.21	0.73
7:M:521:SER:O	7:M:522:LYS:HB3	1.88	0.73
7:N:421:GLU:OE1	7:O:434:PHE:HD2	1.70	0.73
7:U:521:SER:O	7:U:522:LYS:HB3	1.88	0.73
7:W:191:PHE:HA	7:W:276:VAL:HG12	1.69	0.73
7:W:446:VAL:HG21	7:X:184:GLU:HG3	1.69	0.73
7:G:254:SER:HB3	7:G:359:CYS:HB3	1.69	0.73
7:H:191:PHE:HA	7:H:276:VAL:HG12	1.69	0.73
7:J:130:GLU:HG3	7:K:164:ARG:O	1.89	0.73
7:L:521:SER:O	7:L:522:LYS:HB3	1.88	0.73
7:O:352:GLU:HB3	7:O:391:ARG:HB3	1.70	0.73
7:V:372:GLU:O	7:W:222:PHE:HA	1.88	0.73
7:V:390:GLY:O	7:W:204:LYS:HA	1.88	0.73
7:Q:391:ARG:HH22	7:R:202:ALA:HB1	1.51	0.73
7:R:352:GLU:HB3	7:R:391:ARG:HB3	1.70	0.73
7:X:521:SER:O	7:X:522:LYS:HB3	1.88	0.73
7:J:191:PHE:HA	7:J:276:VAL:HG12	1.69	0.73
7:J:352:GLU:HB3	7:J:391:ARG:HB3	1.70	0.73
7:Q:521:SER:O	7:Q:522:LYS:HB3	1.88	0.73
7:G:244:HIS:HB2	7:G:369:ALA:HB3	1.71	0.73
7:Q:372:GLU:HB3	7:R:223:THR:C	2.08	0.73
7:W:404:VAL:HB	7:X:191:PHE:HB2	1.70	0.73
7:L:392:ALA:HB3	7:M:203:PHE:H	1.53	0.73
7:M:417:PHE:HE2	7:N:185:THR:OG1	1.71	0.73
7:N:374:SER:O	7:O:220:LEU:HD12	1.86	0.73
7:V:421:GLU:CB	7:W:431:VAL:HG12	2.19	0.73
7:W:417:PHE:HZ	7:X:280:ILE:HG13	1.44	0.73
7:J:208:GLN:HB2	7:J:259:TYR:HB2	1.68	0.73
7:K:352:GLU:HB3	7:K:391:ARG:HB3	1.70	0.73
7:N:521:SER:O	7:N:522:LYS:HB3	1.88	0.73
7:R:191:PHE:HA	7:R:276:VAL:HG12	1.69	0.73
7:M:339:TYR:HB2	7:M:404:VAL:CG2	2.15	0.73
7:V:250:ARG:HB2	7:V:363:HIS:HB3	1.71	0.73
3:D:225:PHE:HD1	3:D:342:TRP:CD1	2.06	0.72
7:W:521:SER:O	7:W:522:LYS:HB3	1.88	0.72
3:D:254:GLU:HB2	3:D:313:TYR:HB3	1.71	0.72
3:D:225:PHE:CD1	3:D:342:TRP:CG	2.74	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:216:ALA:H	7:P:251:PHE:HB3	1.55	0.72
7:H:521:SER:O	7:H:522:LYS:HB3	1.88	0.72
7:T:250:ARG:HB2	7:T:363:HIS:HB3	1.71	0.72
7:I:250:ARG:HB2	7:I:363:HIS:HB3	1.71	0.72
7:J:521:SER:O	7:J:522:LYS:HB3	1.88	0.72
7:S:250:ARG:HB2	7:S:363:HIS:HB3	1.71	0.72
7:W:250:ARG:HB2	7:W:363:HIS:HB3	1.71	0.72
7:I:352:GLU:HB3	7:I:391:ARG:HB3	1.70	0.72
7:L:352:GLU:HB3	7:L:391:ARG:HB3	1.70	0.72
7:O:521:SER:O	7:O:522:LYS:HB3	1.88	0.72
7:S:352:GLU:HB3	7:S:391:ARG:HB3	1.70	0.72
2:C:201:SER:O	3:D:346:VAL:CB	2.37	0.72
5:F:231:LEU:HD23	5:F:232:LEU:H	1.49	0.72
7:L:404:VAL:HB	7:M:191:PHE:HB2	1.72	0.72
7:N:352:GLU:HB3	7:N:391:ARG:HB3	1.70	0.72
7:S:191:PHE:HA	7:S:276:VAL:HG12	1.69	0.72
7:W:413:ARG:CZ	7:X:282:LEU:CG	2.66	0.72
7:K:406:SER:O	7:L:188:GLU:HB2	1.90	0.72
7:N:412:THR:OG1	7:O:167:ASN:CG	2.28	0.72
7:R:521:SER:O	7:R:522:LYS:HB3	1.88	0.72
7:S:339:TYR:HB2	7:S:404:VAL:CG2	2.15	0.72
7:H:250:ARG:HB2	7:H:363:HIS:HB3	1.71	0.72
7:I:130:GLU:CB	7:J:164:ARG:O	2.37	0.72
7:Q:374:SER:O	7:R:220:LEU:HD12	1.90	0.72
7:V:133:ARG:NH2	7:W:164:ARG:NE	2.37	0.72
7:X:352:GLU:HB3	7:X:391:ARG:HB3	1.70	0.72
7:K:521:SER:O	7:K:522:LYS:HB3	1.88	0.72
7:W:128:GLU:O	7:X:164:ARG:NH2	2.22	0.72
7:P:105:GLY:HA2	7:H:159:LEU:HD22	1.72	0.72
7:M:250:ARG:HB2	7:M:363:HIS:HB3	1.71	0.72
7:V:133:ARG:CZ	7:W:164:ARG:NE	2.53	0.72
7:V:339:TYR:HB2	7:V:404:VAL:CG2	2.15	0.72
7:X:250:ARG:HB2	7:X:363:HIS:HB3	1.71	0.72
7:J:250:ARG:HB2	7:J:363:HIS:HB3	1.71	0.71
7:Q:250:ARG:HB2	7:Q:363:HIS:HB3	1.71	0.71
7:Q:380:ASN:HD22	7:R:215:ASN:CB	2.02	0.71
7:S:413:ARG:HH11	7:T:282:LEU:HA	1.55	0.71
7:V:421:GLU:CB	7:W:431:VAL:HA	2.20	0.71
5:F:389:ILE:HB	7:G:191:PHE:HB3	1.72	0.71
7:M:64:ARG:HD2	7:N:461:VAL:HG23	1.72	0.71
7:N:412:THR:OG1	7:O:167:ASN:OD1	2.07	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:R:250:ARG:HB2	7:R:363:HIS:HB3	1.71	0.71
7:M:64:ARG:C	7:N:467:HIS:HD1	1.92	0.71
7:N:378:GLU:OE1	7:O:217:ALA:HB3	1.89	0.71
7:Q:413:ARG:NH1	7:R:282:LEU:HA	2.05	0.71
7:W:424:LEU:HD11	7:X:191:PHE:CE2	2.25	0.71
7:M:19:HIS:CD2	7:N:487:ARG:HD2	2.23	0.71
7:U:391:ARG:HH21	7:V:204:LYS:CG	2.02	0.71
7:W:400:LEU:O	7:X:194:GLU:HB2	1.91	0.71
7:G:342:ASP:HB3	7:G:401:ILE:HB	1.71	0.71
7:V:372:GLU:O	7:W:222:PHE:CD1	2.44	0.71
7:W:352:GLU:HB3	7:W:391:ARG:HB3	1.70	0.71
7:M:30:TRP:HH2	7:N:467:HIS:CE1	2.07	0.71
7:O:250:ARG:HB2	7:O:363:HIS:HB3	1.71	0.71
7:U:250:ARG:HB2	7:U:363:HIS:HB3	1.71	0.71
7:G:372:GLU:OE1	7:P:223:THR:O	2.08	0.71
7:K:250:ARG:HB2	7:K:363:HIS:HB3	1.71	0.71
7:K:372:GLU:CB	7:L:223:THR:O	2.39	0.71
7:U:339:TYR:HB2	7:U:404:VAL:CG2	2.15	0.71
7:N:391:ARG:NE	7:O:204:LYS:HE2	2.06	0.71
7:N:412:THR:OG1	7:O:167:ASN:CB	2.38	0.71
7:Q:380:ASN:O	7:R:214:PHE:CD1	2.44	0.71
7:Q:380:ASN:HB2	7:R:215:ASN:HB2	1.71	0.71
7:P:204:LYS:HD2	7:P:263:LEU:HD23	1.73	0.71
7:H:391:ARG:NH2	7:I:204:LYS:CE	2.53	0.71
7:Q:391:ARG:HH21	7:R:204:LYS:HG3	1.55	0.71
7:U:372:GLU:HB3	7:V:223:THR:O	1.90	0.71
7:H:400:LEU:HD12	7:I:195:HIS:HB2	1.73	0.71
7:I:413:ARG:NH1	7:J:282:LEU:HG	2.06	0.71
7:L:380:ASN:HD22	7:M:215:ASN:CB	2.02	0.71
7:N:372:GLU:CD	7:O:223:THR:O	2.30	0.71
7:O:413:ARG:HH11	7:Q:282:LEU:HA	1.54	0.71
7:G:352:GLU:HB3	7:G:391:ARG:HB3	1.73	0.70
7:W:412:THR:OG1	7:X:167:ASN:CG	2.29	0.70
7:L:250:ARG:HB2	7:L:363:HIS:HB3	1.71	0.70
7:L:400:LEU:HD12	7:M:195:HIS:CB	2.21	0.70
7:N:250:ARG:HB2	7:N:363:HIS:HB3	1.71	0.70
7:W:216:ALA:HB3	7:W:251:PHE:HB3	1.73	0.70
7:I:106:ASP:N	7:J:159:LEU:HD13	2.05	0.70
7:L:216:ALA:HB3	7:L:251:PHE:HB3	1.73	0.70
7:T:521:SER:O	7:T:522:LYS:HB3	1.88	0.70
6:B:754:PRO:HB2	6:B:758:SER:HA	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:242:SER:HB3	7:G:371:SER:HA	1.72	0.70
7:N:421:GLU:CB	7:O:434:PHE:CD2	2.73	0.70
7:W:380:ASN:HD22	7:X:215:ASN:HB2	1.56	0.70
7:P:271:LYS:HG2	7:P:342:ASP:OD1	1.91	0.70
7:N:413:ARG:HH12	7:O:282:LEU:HG	1.55	0.70
7:O:363:HIS:ND1	7:O:380:ASN:OD1	2.25	0.70
7:Q:216:ALA:HB3	7:Q:251:PHE:HB3	1.73	0.70
7:R:339:TYR:HB2	7:R:404:VAL:CG2	2.15	0.70
7:H:363:HIS:ND1	7:H:380:ASN:OD1	2.25	0.70
7:J:417:PHE:CZ	7:K:280:ILE:HG13	2.26	0.70
7:R:216:ALA:HB3	7:R:251:PHE:HB3	1.74	0.70
7:S:521:SER:O	7:S:522:LYS:HB3	1.88	0.70
7:V:133:ARG:CZ	7:W:164:ARG:CZ	2.70	0.70
7:W:129:SER:HA	7:X:164:ARG:CZ	2.20	0.70
3:D:184:LEU:H	3:D:264:ASN:HA	1.55	0.70
5:F:267:GLN:HA	5:F:318:GLY:HA3	1.74	0.70
7:I:339:TYR:HB2	7:I:404:VAL:CG2	2.15	0.70
7:V:64:ARG:HD3	7:W:290:ARG:CB	2.22	0.70
7:G:479:ASP:O	7:G:483:GLU:HB2	1.92	0.70
7:P:30:TRP:HH2	7:H:467:HIS:CE1	2.10	0.70
7:O:339:TYR:HB2	7:O:404:VAL:CG2	2.15	0.70
7:S:216:ALA:HB3	7:S:251:PHE:HB3	1.73	0.70
7:V:396:THR:CB	7:W:199:GLN:OE1	2.32	0.70
7:K:391:ARG:HH21	7:L:204:LYS:HE3	1.56	0.70
7:R:363:HIS:ND1	7:R:380:ASN:OD1	2.25	0.70
2:C:197:LYS:HB2	3:D:351:HIS:HB2	1.74	0.70
7:K:216:ALA:HB3	7:K:251:PHE:HB3	1.73	0.70
7:W:391:ARG:HH21	7:X:204:LYS:HE3	1.54	0.70
7:X:339:TYR:HB2	7:X:404:VAL:CG2	2.15	0.70
7:J:216:ALA:HB3	7:J:251:PHE:HB3	1.73	0.69
7:M:65:ARG:CD	7:N:467:HIS:CD2	2.71	0.69
7:N:411:GLY:O	7:O:185:THR:HG21	1.91	0.69
7:W:417:PHE:CE2	7:X:280:ILE:CG1	2.69	0.69
2:C:123:SER:HA	2:C:135:PRO:HA	1.74	0.69
7:H:42:ARG:HH22	7:I:471:GLN:CD	1.95	0.69
7:L:421:GLU:OE1	7:M:434:PHE:CB	2.37	0.69
7:N:216:ALA:HB3	7:N:251:PHE:HB3	1.73	0.69
7:N:394:ASN:O	7:O:200:ILE:HA	1.91	0.69
7:T:216:ALA:HB3	7:T:251:PHE:HB3	1.73	0.69
7:V:319:GLU:OE2	7:W:451:LYS:HD3	1.91	0.69
7:P:65:ARG:HD2	7:H:467:HIS:CD2	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:352:GLU:HB3	7:P:391:ARG:HB3	1.74	0.69
7:O:216:ALA:HB3	7:O:251:PHE:HB3	1.73	0.69
7:O:413:ARG:NH1	7:Q:282:LEU:HA	2.08	0.69
7:U:386:LYS:O	7:V:208:GLN:OE1	2.10	0.69
7:K:363:HIS:ND1	7:K:380:ASN:OD1	2.25	0.69
7:N:363:HIS:ND1	7:N:380:ASN:OD1	2.25	0.69
7:N:421:GLU:HB2	7:O:434:PHE:HD2	1.55	0.69
7:Q:384:CYS:O	7:R:210:LYS:HG3	1.92	0.69
7:R:59:ASP:OD1	7:S:456:TYR:OH	2.09	0.69
7:W:413:ARG:CZ	7:X:282:LEU:CD1	2.70	0.69
7:K:413:ARG:NH1	7:L:282:LEU:HG	2.07	0.69
7:V:216:ALA:HB3	7:V:251:PHE:HB3	1.73	0.69
5:F:89:GLN:HB2	7:G:159:LEU:HD22	1.74	0.69
7:G:272:MET:HB3	7:G:341:LEU:HB3	1.73	0.69
7:P:254:SER:HB3	7:P:359:CYS:HB3	1.74	0.69
7:M:363:HIS:ND1	7:M:380:ASN:OD1	2.25	0.69
7:Q:339:TYR:HB2	7:Q:404:VAL:CG2	2.15	0.69
7:S:363:HIS:ND1	7:S:380:ASN:OD1	2.25	0.69
6:B:701:ARG:HD2	6:B:748:GLY:HA2	1.73	0.69
7:I:413:ARG:CZ	7:J:282:LEU:HG	2.23	0.69
7:K:59:ASP:OD1	7:L:456:TYR:OH	2.09	0.69
7:R:413:ARG:HH11	7:S:282:LEU:HA	1.57	0.69
7:T:391:ARG:HE	7:U:204:LYS:HE2	1.58	0.69
7:U:413:ARG:HD3	7:V:280:ILE:HD11	1.75	0.69
7:V:64:ARG:NH2	7:W:290:ARG:HA	2.07	0.69
7:W:394:ASN:O	7:X:200:ILE:HA	1.93	0.69
7:J:44:ARG:NH2	7:K:474:GLU:OE2	2.25	0.69
7:J:363:HIS:ND1	7:J:380:ASN:OD1	2.25	0.69
7:L:363:HIS:ND1	7:L:380:ASN:OD1	2.25	0.69
7:M:65:ARG:HG3	7:N:467:HIS:HB3	1.75	0.69
7:M:216:ALA:HB3	7:M:251:PHE:HB3	1.73	0.69
7:V:372:GLU:CB	7:W:223:THR:O	2.40	0.69
7:G:394:ASN:HB3	7:P:201:GLU:HB2	1.73	0.69
7:G:524:LYS:CD	7:P:196:TYR:CE2	2.73	0.69
7:I:216:ALA:HB3	7:I:251:PHE:HB3	1.73	0.69
7:J:64:ARG:HD2	7:K:461:VAL:CG2	2.23	0.69
7:P:380:ASN:HB2	7:H:215:ASN:HB2	1.75	0.69
7:I:417:PHE:HE1	7:J:187:GLY:HA3	1.58	0.69
7:M:65:ARG:CB	7:N:467:HIS:CB	2.71	0.69
7:R:102:ASN:ND2	7:R:105:GLY:O	2.26	0.69
7:T:413:ARG:HH11	7:U:282:LEU:HA	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:421:GLU:HB3	7:V:434:PHE:HD2	1.57	0.69
7:W:354:LYS:HB3	7:W:389:GLU:HB3	1.75	0.69
7:X:363:HIS:ND1	7:X:380:ASN:OD1	2.25	0.69
7:G:524:LYS:HZ1	7:P:271:LYS:HD3	1.59	0.68
7:J:339:TYR:HB2	7:J:404:VAL:CG2	2.15	0.68
7:O:354:LYS:HB3	7:O:389:GLU:HB3	1.75	0.68
7:Q:354:LYS:HB3	7:Q:389:GLU:HB3	1.75	0.68
7:U:216:ALA:HB3	7:U:251:PHE:HB3	1.73	0.68
7:U:413:ARG:HH11	7:V:282:LEU:HA	1.57	0.68
7:V:129:SER:OG	7:W:169:LEU:HD11	1.93	0.68
7:X:354:LYS:HB3	7:X:389:GLU:HB3	1.75	0.68
7:H:216:ALA:HB3	7:H:251:PHE:HB3	1.73	0.68
7:O:102:ASN:ND2	7:O:105:GLY:O	2.27	0.68
7:V:526:SER:HB3	7:W:198:GLU:HG2	1.74	0.68
7:I:102:ASN:ND2	7:I:105:GLY:O	2.27	0.68
7:L:391:ARG:NH2	7:M:204:LYS:HE3	2.08	0.68
2:C:201:SER:HB3	3:D:347:LYS:HB3	1.75	0.68
5:F:399:GLY:HA2	7:G:280:ILE:HD11	1.74	0.68
7:P:204:LYS:HB2	7:P:263:LEU:HB3	1.74	0.68
7:H:102:ASN:ND2	7:H:105:GLY:O	2.27	0.68
7:M:55:LYS:CE	7:N:481:ILE:HG23	2.23	0.68
7:S:102:ASN:ND2	7:S:105:GLY:O	2.27	0.68
7:S:354:LYS:HB3	7:S:389:GLU:HB3	1.75	0.68
7:W:413:ARG:NH1	7:X:282:LEU:CA	2.55	0.68
7:H:370:PHE:HD2	7:H:373:ILE:C	1.97	0.68
7:L:339:TYR:HB2	7:L:404:VAL:CG2	2.15	0.68
7:N:424:LEU:HD11	7:O:191:PHE:CZ	2.27	0.68
7:Q:370:PHE:HD2	7:Q:373:ILE:C	1.97	0.68
7:R:354:LYS:HB3	7:R:389:GLU:HB3	1.75	0.68
7:U:102:ASN:ND2	7:U:105:GLY:O	2.26	0.68
7:V:296:THR:HG21	7:W:159:LEU:HD23	1.75	0.68
7:W:102:ASN:ND2	7:W:105:GLY:O	2.26	0.68
7:X:216:ALA:HB3	7:X:251:PHE:HB3	1.73	0.68
7:K:102:ASN:ND2	7:K:105:GLY:O	2.27	0.68
7:L:102:ASN:ND2	7:L:105:GLY:O	2.26	0.68
7:Q:59:ASP:OD1	7:R:456:TYR:OH	2.11	0.68
7:R:370:PHE:HD2	7:R:373:ILE:C	1.97	0.68
7:V:354:LYS:HB3	7:V:389:GLU:HB3	1.75	0.68
7:W:339:TYR:HB2	7:W:404:VAL:CG2	2.15	0.68
7:W:417:PHE:CE2	7:X:280:ILE:HD11	2.28	0.68
5:F:229:SER:HB2	5:F:356:ASP:OD2	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:297:THR:CG2	7:J:288:ARG:NH2	2.57	0.68
7:I:354:LYS:HB3	7:I:389:GLU:HB3	1.75	0.68
7:J:130:GLU:HG3	7:K:165:ASP:HA	1.75	0.68
7:S:413:ARG:NH1	7:T:282:LEU:HA	2.09	0.68
1:A:860:SER:HB3	1:A:911:ASN:HB2	1.76	0.68
7:M:354:LYS:HB3	7:M:389:GLU:HB3	1.75	0.68
7:Q:102:ASN:ND2	7:Q:105:GLY:O	2.27	0.68
7:R:391:ARG:HH22	7:S:202:ALA:HB1	1.59	0.68
7:S:370:PHE:HD2	7:S:373:ILE:C	1.97	0.68
2:C:146:CYS:N	3:D:113:SER:HG	1.92	0.68
7:J:413:ARG:HH11	7:K:282:LEU:HA	1.58	0.68
7:L:354:LYS:HB3	7:L:389:GLU:HB3	1.75	0.68
7:N:421:GLU:HB2	7:O:434:PHE:CD2	2.29	0.68
7:O:370:PHE:HD2	7:O:373:ILE:C	1.97	0.68
7:T:363:HIS:ND1	7:T:380:ASN:OD1	2.25	0.68
7:X:102:ASN:ND2	7:X:105:GLY:O	2.26	0.68
5:F:337:ILE:HG12	5:F:377:THR:HG23	1.76	0.68
7:K:339:TYR:HB2	7:K:404:VAL:CG2	2.15	0.68
7:M:102:ASN:ND2	7:M:105:GLY:O	2.26	0.68
7:N:384:CYS:O	7:O:210:LYS:HG3	1.94	0.68
7:Q:363:HIS:ND1	7:Q:380:ASN:OD1	2.25	0.68
3:D:311:GLY:HA2	3:D:415:GLN:HG3	1.76	0.67
4:E:94:LEU:HB3	4:E:103:VAL:HB	1.76	0.67
7:J:102:ASN:ND2	7:J:105:GLY:O	2.27	0.67
7:J:354:LYS:HB3	7:J:389:GLU:HB3	1.75	0.67
7:V:363:HIS:ND1	7:V:380:ASN:OD1	2.25	0.67
7:X:370:PHE:HD2	7:X:373:ILE:C	1.97	0.67
7:K:354:LYS:HB3	7:K:389:GLU:HB3	1.75	0.67
7:W:410:GLY:C	7:X:185:THR:CG2	2.63	0.67
7:G:330:SER:HB2	7:G:449:SER:H	1.59	0.67
7:L:145:ASP:OD2	7:M:284:ARG:NH1	2.27	0.67
7:T:102:ASN:ND2	7:T:105:GLY:O	2.26	0.67
7:T:372:GLU:CB	7:U:223:THR:O	2.42	0.67
7:U:354:LYS:HB3	7:U:389:GLU:HB3	1.75	0.67
7:V:106:ASP:OD2	7:W:122:ARG:C	2.33	0.67
7:G:243:LEU:HD13	7:G:370:PHE:HD1	1.60	0.67
7:V:378:GLU:CB	7:W:217:ALA:O	2.42	0.67
2:C:179:GLU:HB2	3:D:369:ASN:HB2	1.77	0.67
7:P:206:ILE:HB	7:P:261:LEU:HB2	1.75	0.67
7:P:368:LEU:HB2	7:P:375:VAL:HB	1.77	0.67
7:K:370:PHE:HD2	7:K:373:ILE:C	1.97	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:R:189:LYS:CE	7:R:191:PHE:CE1	2.75	0.67
7:T:354:LYS:HB3	7:T:389:GLU:HB3	1.75	0.67
3:D:124:ARG:O	6:B:167:ASN:ND2	2.28	0.67
7:G:102:ASN:ND2	7:G:105:GLY:O	2.27	0.67
7:I:297:THR:HG23	7:J:288:ARG:HH22	1.60	0.67
7:N:102:ASN:ND2	7:N:105:GLY:O	2.26	0.67
7:R:374:SER:O	7:S:220:LEU:HD12	1.94	0.67
7:R:413:ARG:NH1	7:S:282:LEU:HA	2.09	0.67
7:T:370:PHE:HD2	7:T:373:ILE:C	1.97	0.67
7:P:262:PHE:HB3	7:P:351:VAL:HB	1.75	0.67
7:L:105:GLY:HA2	7:M:159:LEU:HD22	1.77	0.67
7:V:370:PHE:HD2	7:V:373:ILE:C	1.97	0.67
7:V:422:LYS:CG	7:W:431:VAL:HG11	2.20	0.67
7:W:370:PHE:HD2	7:W:373:ILE:C	1.97	0.67
7:H:354:LYS:HB3	7:H:389:GLU:HB3	1.75	0.67
7:L:413:ARG:HG2	7:M:438:ALA:HB1	1.77	0.67
7:R:105:GLY:HA2	7:S:159:LEU:HD22	1.76	0.67
2:C:181:GLU:HB2	3:D:367:GLN:HB2	1.76	0.67
3:D:225:PHE:CD1	3:D:342:TRP:CA	2.78	0.67
7:G:412:THR:N	7:G:440:SER:OG	2.28	0.67
7:H:30:TRP:HH2	7:I:467:HIS:CE1	2.13	0.67
7:M:370:PHE:CB	7:M:373:ILE:H	2.08	0.67
7:N:413:ARG:NH1	7:O:282:LEU:CG	2.54	0.67
7:W:189:LYS:CE	7:W:191:PHE:CE1	2.75	0.67
7:I:130:GLU:OE2	7:J:165:ASP:CA	2.39	0.66
7:N:394:ASN:HB2	7:O:201:GLU:HB2	1.77	0.66
7:X:368:LEU:HB2	7:X:375:VAL:HB	1.78	0.66
7:J:370:PHE:HD2	7:J:373:ILE:C	1.97	0.66
7:K:368:LEU:HB2	7:K:375:VAL:HB	1.78	0.66
7:N:370:PHE:HD2	7:N:373:ILE:C	1.97	0.66
7:T:372:GLU:HB3	7:U:223:THR:O	1.95	0.66
7:P:102:ASN:ND2	7:P:105:GLY:O	2.28	0.66
7:K:130:GLU:OE2	7:L:165:ASP:HA	1.95	0.66
7:N:380:ASN:ND2	7:O:215:ASN:HB2	2.05	0.66
7:N:412:THR:OG1	7:O:167:ASN:HB3	1.96	0.66
7:R:391:ARG:HH21	7:S:204:LYS:HG3	1.60	0.66
7:P:162:ARG:HD3	7:P:164:ARG:HD2	1.77	0.66
7:P:372:GLU:OE1	7:H:222:PHE:CZ	2.48	0.66
7:I:86:CYS:SG	7:I:87:SER:N	2.69	0.66
7:I:363:HIS:ND1	7:I:380:ASN:OD1	2.25	0.66
7:J:502:ASP:OD2	7:K:452:LEU:N	2.23	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:86:CYS:SG	7:K:87:SER:N	2.69	0.66
7:L:368:LEU:HB2	7:L:375:VAL:HB	1.77	0.66
7:M:86:CYS:SG	7:M:87:SER:N	2.69	0.66
7:M:391:ARG:HH22	7:N:202:ALA:HB1	1.58	0.66
7:O:86:CYS:SG	7:O:87:SER:N	2.69	0.66
7:S:86:CYS:SG	7:S:87:SER:N	2.69	0.66
7:S:368:LEU:HB2	7:S:375:VAL:HB	1.78	0.66
7:S:380:ASN:O	7:T:214:PHE:CD1	2.49	0.66
7:V:396:THR:O	7:W:199:GLN:HB3	1.94	0.66
7:L:64:ARG:HH11	7:M:290:ARG:NE	1.93	0.66
7:L:370:PHE:HD2	7:L:373:ILE:C	1.97	0.66
7:N:354:LYS:HB3	7:N:389:GLU:HB3	1.75	0.66
7:R:86:CYS:SG	7:R:87:SER:N	2.69	0.66
7:T:368:LEU:HB2	7:T:375:VAL:HB	1.78	0.66
7:X:86:CYS:SG	7:X:87:SER:N	2.69	0.66
7:J:86:CYS:SG	7:J:87:SER:N	2.69	0.66
7:Q:391:ARG:NE	7:R:204:LYS:HE2	2.11	0.66
7:U:363:HIS:ND1	7:U:380:ASN:OD1	2.25	0.66
7:P:86:CYS:SG	7:P:87:SER:N	2.69	0.66
7:P:372:GLU:O	7:H:222:PHE:HD1	1.79	0.66
7:R:380:ASN:O	7:S:214:PHE:CD1	2.49	0.66
7:S:356:ILE:HB	7:S:387:ARG:HB2	1.78	0.66
7:U:403:ASP:HA	7:V:192:ARG:HG2	1.76	0.66
7:V:58:THR:CG2	7:W:452:LEU:CB	2.10	0.66
7:W:86:CYS:SG	7:W:87:SER:N	2.69	0.66
7:W:363:HIS:ND1	7:W:380:ASN:OD1	2.25	0.66
7:P:64:ARG:H	7:H:470:LYS:HZ3	1.43	0.66
7:K:356:ILE:HB	7:K:387:ARG:HB2	1.78	0.66
7:N:368:LEU:HB2	7:N:375:VAL:HB	1.77	0.66
7:O:189:LYS:CE	7:O:191:PHE:CE1	2.75	0.66
7:V:370:PHE:CB	7:V:373:ILE:H	2.08	0.66
5:F:528:ARG:HB3	5:F:550:GLN:HB3	1.78	0.66
7:J:368:LEU:HB2	7:J:375:VAL:HB	1.78	0.66
7:U:370:PHE:CB	7:U:373:ILE:H	2.08	0.66
7:U:394:ASN:HB2	7:V:201:GLU:HB2	1.77	0.66
7:V:86:CYS:SG	7:V:87:SER:N	2.69	0.66
7:J:64:ARG:CZ	7:K:461:VAL:HB	2.26	0.66
7:M:370:PHE:HD2	7:M:373:ILE:C	1.97	0.66
7:Q:86:CYS:SG	7:Q:87:SER:N	2.69	0.66
7:U:86:CYS:SG	7:U:87:SER:N	2.69	0.66
7:U:368:LEU:HB2	7:U:375:VAL:HB	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:71:GLN:HE21	5:F:76:GLY:HA2	1.60	0.65
7:I:130:GLU:HG3	7:J:165:ASP:HA	1.78	0.65
7:I:370:PHE:HD2	7:I:373:ILE:C	1.97	0.65
7:N:356:ILE:HB	7:N:387:ARG:HB2	1.78	0.65
7:R:368:LEU:HB2	7:R:375:VAL:HB	1.77	0.65
7:U:391:ARG:NE	7:V:204:LYS:CE	2.57	0.65
3:D:252:VAL:H	3:D:315:VAL:HG12	1.62	0.65
7:P:44:ARG:NH2	7:H:474:GLU:OE2	2.29	0.65
7:H:86:CYS:SG	7:H:87:SER:N	2.69	0.65
7:I:359:CYS:HA	7:I:384:CYS:HA	1.79	0.65
7:V:162:ARG:HD3	7:V:164:ARG:HD2	1.79	0.65
7:V:359:CYS:HA	7:V:384:CYS:HA	1.79	0.65
7:W:368:LEU:HB2	7:W:375:VAL:HB	1.77	0.65
4:E:68:THR:HB	4:E:79:VAL:HB	1.79	0.65
7:P:360:LEU:HB3	7:P:383:ASP:HB3	1.77	0.65
7:M:189:LYS:CE	7:M:191:PHE:CE1	2.75	0.65
7:N:391:ARG:HH21	7:O:204:LYS:CE	2.09	0.65
7:T:86:CYS:SG	7:T:87:SER:N	2.69	0.65
2:C:191:THR:HB	3:D:357:GLU:HB3	1.79	0.65
7:V:102:ASN:ND2	7:V:105:GLY:O	2.26	0.65
7:W:106:ASP:OD2	7:X:121:CYS:HA	1.96	0.65
7:P:354:LYS:HB3	7:P:389:GLU:HB3	1.77	0.65
7:H:368:LEU:HB2	7:H:375:VAL:HB	1.78	0.65
7:J:359:CYS:HA	7:J:384:CYS:HA	1.79	0.65
7:L:380:ASN:HB2	7:M:215:ASN:HB2	1.77	0.65
7:N:86:CYS:SG	7:N:87:SER:N	2.69	0.65
7:Q:130:GLU:HG3	7:R:164:ARG:O	1.97	0.65
7:T:378:GLU:OE1	7:U:217:ALA:HB3	1.95	0.65
7:U:413:ARG:NH1	7:V:282:LEU:HA	2.10	0.65
7:V:320:THR:HG23	7:W:179:ALA:CB	2.24	0.65
7:W:400:LEU:CG	7:X:195:HIS:HB2	2.27	0.65
7:W:417:PHE:CD2	7:X:280:ILE:CD1	2.80	0.65
9:Z:1:NAG:H5	9:Z:2:NAG:HN2	1.62	0.65
7:K:370:PHE:CB	7:K:373:ILE:H	2.08	0.65
7:M:359:CYS:HA	7:M:384:CYS:HA	1.79	0.65
7:T:339:TYR:HB2	7:T:404:VAL:CG2	2.15	0.65
1:A:336:PHE:HE2	1:A:844:THR:HG22	1.60	0.65
7:H:359:CYS:HA	7:H:384:CYS:HA	1.79	0.65
7:O:359:CYS:HA	7:O:384:CYS:HA	1.79	0.65
7:V:368:LEU:HB2	7:V:375:VAL:HB	1.78	0.65
1:A:286:ALA:HB1	1:A:288:GLN:HG3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:339:TYR:HB2	7:H:404:VAL:CG2	2.15	0.65
7:I:106:ASP:HB2	7:J:159:LEU:CD1	2.27	0.65
7:Q:359:CYS:HA	7:Q:384:CYS:HA	1.79	0.65
7:U:162:ARG:HD3	7:U:164:ARG:HD2	1.79	0.65
7:G:64:ARG:NH2	7:P:459:VAL:O	2.30	0.65
7:L:86:CYS:SG	7:L:87:SER:N	2.69	0.65
7:N:130:GLU:HA	7:O:164:ARG:O	1.96	0.65
7:R:356:ILE:HB	7:R:387:ARG:HB2	1.78	0.65
7:S:359:CYS:HA	7:S:384:CYS:HA	1.79	0.65
7:S:370:PHE:CB	7:S:373:ILE:H	2.08	0.65
7:T:392:ALA:HB3	7:U:203:PHE:H	1.62	0.65
3:D:190:VAL:HA	3:D:257:VAL:HG21	1.79	0.65
7:G:524:LYS:HZ2	7:P:271:LYS:HD3	1.62	0.65
7:H:189:LYS:CE	7:H:191:PHE:CE1	2.75	0.65
7:K:162:ARG:HD3	7:K:164:ARG:HD2	1.79	0.65
7:K:189:LYS:CE	7:K:191:PHE:CE1	2.75	0.65
7:S:374:SER:O	7:T:220:LEU:HD12	1.97	0.65
7:U:398:GLU:OE1	7:V:197:GLU:OE1	2.15	0.65
7:W:370:PHE:CB	7:W:373:ILE:H	2.08	0.65
7:G:260:GLN:HB3	7:G:353:LEU:HB3	1.80	0.64
7:P:342:ASP:HB3	7:P:401:ILE:HB	1.78	0.64
7:I:370:PHE:CB	7:I:373:ILE:H	2.08	0.64
7:K:359:CYS:HA	7:K:384:CYS:HA	1.79	0.64
7:L:64:ARG:NH1	7:M:290:ARG:NE	2.45	0.64
7:N:413:ARG:CZ	7:O:282:LEU:CG	2.74	0.64
7:U:370:PHE:HD2	7:U:373:ILE:C	1.97	0.64
7:V:189:LYS:CE	7:V:191:PHE:CE1	2.75	0.64
7:W:356:ILE:HB	7:W:387:ARG:HB2	1.78	0.64
5:F:369:CYS:HB3	7:G:211:THR:HB	1.78	0.64
5:F:388:ASP:HA	7:G:192:ARG:HA	1.78	0.64
7:P:412:THR:N	7:P:440:SER:OG	2.29	0.64
7:I:189:LYS:CE	7:I:191:PHE:CE1	2.75	0.64
7:J:421:GLU:OE1	7:K:434:PHE:HB2	1.97	0.64
7:L:356:ILE:HB	7:L:387:ARG:HB2	1.78	0.64
7:M:55:LYS:NZ	7:N:482:ASN:HB2	2.12	0.64
7:O:368:LEU:HB2	7:O:375:VAL:HB	1.78	0.64
7:Q:368:LEU:HB2	7:Q:375:VAL:HB	1.77	0.64
7:Q:370:PHE:CB	7:Q:373:ILE:H	2.08	0.64
7:R:204:LYS:HD2	7:R:263:LEU:HD23	1.80	0.64
7:U:356:ILE:HB	7:U:387:ARG:HB2	1.78	0.64
7:V:133:ARG:HH21	7:W:164:ARG:NH2	1.94	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:V:414:LYS:N	7:W:435:VAL:HG13	2.12	0.64
7:W:130:GLU:HG3	7:X:164:ARG:O	1.96	0.64
7:I:368:LEU:HB2	7:I:375:VAL:HB	1.78	0.64
7:K:421:GLU:OE1	7:L:434:PHE:HB2	1.97	0.64
7:L:162:ARG:HD3	7:L:164:ARG:HD2	1.79	0.64
7:M:356:ILE:HB	7:M:387:ARG:HB2	1.78	0.64
7:N:162:ARG:HD3	7:N:164:ARG:HD2	1.79	0.64
7:N:337:LEU:HD22	7:N:423:LEU:HD21	1.80	0.64
7:N:421:GLU:HB3	7:O:434:PHE:HD2	1.61	0.64
7:O:356:ILE:HB	7:O:387:ARG:HB2	1.78	0.64
7:O:370:PHE:CB	7:O:373:ILE:H	2.08	0.64
7:Q:204:LYS:HD2	7:Q:263:LEU:HD23	1.80	0.64
7:T:356:ILE:HB	7:T:387:ARG:HB2	1.78	0.64
7:T:413:ARG:NH1	7:U:282:LEU:HA	2.12	0.64
7:U:337:LEU:HD22	7:U:423:LEU:HD21	1.80	0.64
7:W:407:LEU:CB	7:X:188:GLU:HB3	2.27	0.64
7:X:337:LEU:HD22	7:X:423:LEU:HD21	1.80	0.64
7:G:354:LYS:HB3	7:G:389:GLU:HB3	1.79	0.64
7:O:204:LYS:HD2	7:O:263:LEU:HD23	1.80	0.64
7:O:380:ASN:HB2	7:Q:215:ASN:HB2	1.80	0.64
7:X:356:ILE:HB	7:X:387:ARG:HB2	1.78	0.64
1:A:1176:LEU:HD22	1:A:1204:GLN:HB3	1.78	0.64
1:A:1313:ILE:HB	1:A:1326:TYR:HB2	1.80	0.64
3:D:167:LYS:H	3:D:167:LYS:HD2	1.62	0.64
5:F:9:CYS:N	5:F:42:THR:O	2.31	0.64
7:J:356:ILE:HB	7:J:387:ARG:HB2	1.78	0.64
7:O:421:GLU:OE1	7:Q:434:PHE:HB2	1.98	0.64
7:S:130:GLU:HG3	7:T:164:ARG:O	1.97	0.64
7:U:189:LYS:CE	7:U:191:PHE:CE1	2.75	0.64
7:V:356:ILE:HB	7:V:387:ARG:HB2	1.78	0.64
1:A:1087:GLY:HA2	1:A:1090:ASN:HD22	1.62	0.64
1:A:1153:ARG:HG2	1:A:1197:LEU:HB3	1.80	0.64
7:H:162:ARG:HD3	7:H:164:ARG:HD2	1.79	0.64
7:H:356:ILE:HB	7:H:387:ARG:HB2	1.78	0.64
7:I:356:ILE:HB	7:I:387:ARG:HB2	1.78	0.64
7:O:162:ARG:HD3	7:O:164:ARG:HD2	1.79	0.64
7:O:337:LEU:HD22	7:O:423:LEU:HD21	1.80	0.64
7:Q:356:ILE:HB	7:Q:387:ARG:HB2	1.78	0.64
7:T:337:LEU:HD22	7:T:423:LEU:HD21	1.80	0.64
7:T:391:ARG:NE	7:U:204:LYS:HE2	2.11	0.64
7:U:400:LEU:CD1	7:V:195:HIS:HB2	2.22	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:V:204:LYS:HD2	7:V:263:LEU:HD23	1.80	0.64
7:V:391:ARG:HA	7:W:203:PHE:O	1.96	0.64
7:W:162:ARG:HD3	7:W:164:ARG:HD2	1.79	0.64
5:F:489:CYS:HB3	5:F:491:LEU:H	1.61	0.64
7:J:403:ASP:HA	7:K:192:ARG:HG2	1.79	0.64
7:J:412:THR:N	7:J:440:SER:OG	2.30	0.64
7:K:204:LYS:HD2	7:K:263:LEU:HD23	1.80	0.64
7:K:337:LEU:HD22	7:K:423:LEU:HD21	1.80	0.64
7:L:337:LEU:HD22	7:L:423:LEU:HD21	1.80	0.64
7:N:421:GLU:HB3	7:O:434:PHE:CD2	2.33	0.64
7:V:403:ASP:OD1	7:W:191:PHE:O	2.15	0.64
7:X:370:PHE:CB	7:X:373:ILE:H	2.08	0.64
5:F:235:VAL:HA	5:F:350:LEU:HG	1.80	0.64
7:G:174:ARG:NH2	7:G:179:ALA:O	2.31	0.64
7:M:368:LEU:HB2	7:M:375:VAL:HB	1.78	0.64
7:S:337:LEU:HD22	7:S:423:LEU:HD21	1.80	0.64
7:W:407:LEU:HB3	7:X:188:GLU:HB3	1.80	0.64
5:F:327:ILE:HG12	5:F:387:GLU:HG3	1.80	0.64
7:G:86:CYS:SG	7:G:87:SER:N	2.71	0.64
7:J:337:LEU:HD22	7:J:423:LEU:HD21	1.80	0.64
7:N:359:CYS:HA	7:N:384:CYS:HA	1.79	0.64
7:S:204:LYS:HD2	7:S:263:LEU:HD23	1.80	0.64
7:T:370:PHE:CB	7:T:373:ILE:H	2.08	0.64
7:V:337:LEU:HD22	7:V:423:LEU:HD21	1.80	0.64
7:X:204:LYS:HD2	7:X:263:LEU:HD23	1.80	0.64
7:X:359:CYS:HA	7:X:384:CYS:HA	1.79	0.64
1:A:1228:TRP:H	1:A:1251:THR:HG22	1.62	0.64
7:G:266:SER:HB3	7:G:347:LYS:HB2	1.81	0.64
7:H:380:ASN:O	7:I:214:PHE:CD1	2.51	0.64
7:L:421:GLU:OE2	7:M:431:VAL:O	2.16	0.64
7:Q:162:ARG:HD3	7:Q:164:ARG:HD2	1.79	0.64
7:S:412:THR:N	7:S:440:SER:OG	2.30	0.64
7:U:359:CYS:HA	7:U:384:CYS:HA	1.79	0.64
7:V:388:GLY:N	7:W:207:ILE:O	2.31	0.64
7:W:204:LYS:HD2	7:W:263:LEU:HD23	1.80	0.64
7:P:337:LEU:HD22	7:P:423:LEU:HD21	1.79	0.63
7:I:413:ARG:NH2	7:J:282:LEU:HG	2.13	0.63
7:L:359:CYS:HA	7:L:384:CYS:HA	1.79	0.63
7:N:130:GLU:CG	7:O:164:ARG:O	2.45	0.63
7:S:162:ARG:HD3	7:S:164:ARG:HD2	1.79	0.63
7:T:403:ASP:HA	7:U:192:ARG:HG2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:V:386:LYS:HB3	7:W:209:GLU:H	1.62	0.63
7:W:400:LEU:CD1	7:X:195:HIS:CD2	2.81	0.63
7:X:162:ARG:HD3	7:X:164:ARG:HD2	1.79	0.63
5:F:26:LYS:HE3	7:G:462:LYS:HB3	1.80	0.63
7:G:204:LYS:HB2	7:G:263:LEU:HB3	1.81	0.63
7:J:162:ARG:HD3	7:J:164:ARG:HD2	1.79	0.63
7:M:162:ARG:HD3	7:M:164:ARG:HD2	1.79	0.63
7:M:337:LEU:HD22	7:M:423:LEU:HD21	1.80	0.63
7:R:162:ARG:HD3	7:R:164:ARG:HD2	1.79	0.63
7:R:359:CYS:HA	7:R:384:CYS:HA	1.79	0.63
7:S:189:LYS:CE	7:S:191:PHE:CE1	2.75	0.63
7:T:105:GLY:HA2	7:U:159:LEU:HD22	1.80	0.63
7:T:359:CYS:HA	7:T:384:CYS:HA	1.79	0.63
7:P:265:TYR:HB2	7:P:348:ARG:HH11	1.62	0.63
7:K:412:THR:N	7:K:440:SER:OG	2.30	0.63
7:N:339:TYR:HB2	7:N:404:VAL:CG2	2.15	0.63
7:N:411:GLY:O	7:O:185:THR:CG2	2.45	0.63
7:R:412:THR:N	7:R:440:SER:OG	2.30	0.63
7:V:388:GLY:HA3	7:W:207:ILE:CG2	2.27	0.63
7:G:243:LEU:HD13	7:G:370:PHE:CD1	2.29	0.63
7:G:324:HIS:HA	7:G:455:ILE:HG13	1.79	0.63
7:G:404:VAL:HB	7:P:191:PHE:HB3	1.79	0.63
7:H:413:ARG:HD3	7:I:280:ILE:HD11	1.80	0.63
7:I:162:ARG:HD3	7:I:164:ARG:HD2	1.79	0.63
7:V:392:ALA:HB3	7:W:203:PHE:CG	2.33	0.63
7:V:394:ASN:HB3	7:W:201:GLU:OE1	1.98	0.63
3:D:77:ARG:HD2	3:D:286:LEU:HD21	1.81	0.63
7:G:262:PHE:HB3	7:G:351:VAL:HB	1.80	0.63
7:P:208:GLN:HB2	7:P:259:TYR:HB2	1.79	0.63
7:J:204:LYS:HD2	7:J:263:LEU:HD23	1.80	0.63
7:L:204:LYS:HD2	7:L:263:LEU:HD23	1.80	0.63
7:O:189:LYS:CE	7:O:191:PHE:CZ	2.82	0.63
7:Q:380:ASN:ND2	7:R:215:ASN:HB2	2.12	0.63
7:V:129:SER:OG	7:W:169:LEU:HD12	1.97	0.63
7:W:129:SER:HB2	7:X:164:ARG:NH1	2.14	0.63
7:Q:337:LEU:HD22	7:Q:423:LEU:HD21	1.80	0.63
7:U:130:GLU:HG3	7:V:165:ASP:HA	1.79	0.63
7:V:412:THR:N	7:V:440:SER:OG	2.30	0.63
7:W:359:CYS:HA	7:W:384:CYS:HA	1.79	0.63
5:F:231:LEU:HD23	5:F:231:LEU:C	2.17	0.63
7:Q:392:ALA:HB3	7:R:203:PHE:H	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:367:ASP:HB3	7:G:213:ASN:HB2	1.81	0.63
7:H:42:ARG:NH2	7:I:471:GLN:OE1	2.29	0.63
7:I:297:THR:HG23	7:J:288:ARG:NH2	2.14	0.63
7:K:380:ASN:HD22	7:L:215:ASN:HB2	1.63	0.63
7:M:204:LYS:HD2	7:M:263:LEU:HD23	1.80	0.63
6:B:95:PRO:HB3	6:B:346:PRO:HB3	1.81	0.63
7:P:324:HIS:HA	7:P:455:ILE:HG13	1.81	0.63
7:I:106:ASP:HB2	7:J:159:LEU:HD13	1.80	0.63
7:J:206:ILE:HB	7:J:261:LEU:HB2	1.81	0.63
7:K:189:LYS:CE	7:K:191:PHE:CZ	2.82	0.63
7:L:412:THR:OG1	7:M:167:ASN:HB3	1.99	0.63
7:N:370:PHE:CB	7:N:373:ILE:H	2.08	0.63
7:N:391:ARG:NH2	7:O:204:LYS:CE	2.57	0.63
7:O:412:THR:N	7:O:440:SER:OG	2.30	0.63
7:R:337:LEU:HD22	7:R:423:LEU:HD21	1.80	0.63
7:U:204:LYS:HD2	7:U:263:LEU:HD23	1.80	0.63
7:P:330:SER:HB2	7:P:449:SER:H	1.63	0.62
7:I:204:LYS:HD2	7:I:263:LEU:HD23	1.80	0.62
7:J:370:PHE:CB	7:J:373:ILE:H	2.08	0.62
7:L:206:ILE:HB	7:L:261:LEU:HB2	1.81	0.62
7:M:412:THR:N	7:M:440:SER:OG	2.30	0.62
7:O:391:ARG:HH21	7:Q:204:LYS:HG3	1.63	0.62
7:L:189:LYS:CE	7:L:191:PHE:CE1	2.75	0.62
7:L:421:GLU:HB2	7:M:434:PHE:CD2	2.33	0.62
7:N:189:LYS:CE	7:N:191:PHE:CE1	2.75	0.62
7:V:380:ASN:O	7:W:214:PHE:CE1	2.51	0.62
7:W:395:ILE:HA	7:X:199:GLN:O	1.99	0.62
7:X:206:ILE:HB	7:X:261:LEU:HB2	1.81	0.62
2:C:83:ARG:NH2	3:D:115:ASP:O	2.31	0.62
7:H:337:LEU:HD22	7:H:423:LEU:HD21	1.80	0.62
7:N:386:LYS:HB3	7:O:209:GLU:H	1.64	0.62
3:D:255:ASN:ND2	3:D:311:GLY:O	2.32	0.62
7:H:65:ARG:HD2	7:I:467:HIS:CD2	2.34	0.62
7:K:255:LYS:HG3	7:K:358:ARG:HG2	1.82	0.62
7:L:370:PHE:CB	7:L:373:ILE:H	2.08	0.62
7:T:162:ARG:HD3	7:T:164:ARG:HD2	1.79	0.62
7:U:372:GLU:HB3	7:V:223:THR:C	2.19	0.62
7:V:378:GLU:O	7:W:216:ALA:HA	1.99	0.62
7:V:400:LEU:H	7:W:195:HIS:HB2	1.63	0.62
7:W:189:LYS:CE	7:W:191:PHE:CZ	2.82	0.62
7:W:337:LEU:HD22	7:W:423:LEU:HD21	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:W:417:PHE:CD2	7:X:280:ILE:HD12	2.34	0.62
1:A:152:LEU:HB3	1:A:808:GLY:HA2	1.81	0.62
3:D:552:HIS:HB2	3:D:556:LEU:HA	1.82	0.62
3:D:553:LEU:HG	6:B:126:PRO:HG2	1.81	0.62
7:H:204:LYS:HD2	7:H:263:LEU:HD23	1.80	0.62
7:N:412:THR:CA	7:O:167:ASN:OD1	2.47	0.62
7:R:255:LYS:HG3	7:R:358:ARG:HG2	1.82	0.62
7:S:262:PHE:HB3	7:S:351:VAL:HB	1.82	0.62
7:T:255:LYS:HG3	7:T:358:ARG:HG2	1.82	0.62
7:U:421:GLU:OE1	7:V:434:PHE:CD2	2.52	0.62
7:X:255:LYS:HG3	7:X:358:ARG:HG2	1.82	0.62
2:C:148:PRO:HA	2:C:157:ARG:HH22	1.64	0.62
7:G:465:ASN:HD21	7:G:468:LEU:HD23	1.64	0.62
7:I:255:LYS:HG3	7:I:358:ARG:HG2	1.82	0.62
7:J:262:PHE:HB3	7:J:351:VAL:HB	1.82	0.62
7:J:342:ASP:HB3	7:J:401:ILE:HB	1.82	0.62
7:K:262:PHE:HB3	7:K:351:VAL:HB	1.82	0.62
7:L:324:HIS:HA	7:L:455:ILE:HG13	1.82	0.62
7:Q:206:ILE:HB	7:Q:261:LEU:HB2	1.81	0.62
7:Q:255:LYS:HG3	7:Q:358:ARG:HG2	1.82	0.62
7:Q:324:HIS:HA	7:Q:455:ILE:HG13	1.82	0.62
7:S:206:ILE:HB	7:S:261:LEU:HB2	1.81	0.62
7:V:357:LYS:CE	7:W:209:GLU:OE1	2.46	0.62
7:X:262:PHE:HB3	7:X:351:VAL:HB	1.82	0.62
7:K:206:ILE:HB	7:K:261:LEU:HB2	1.81	0.62
7:L:262:PHE:HB3	7:L:351:VAL:HB	1.82	0.62
7:L:408:ILE:N	7:M:187:GLY:O	2.29	0.62
7:T:189:LYS:CE	7:T:191:PHE:CZ	2.81	0.62
7:T:374:SER:O	7:U:220:LEU:CD1	2.47	0.62
7:W:413:ARG:NH1	7:X:282:LEU:CB	2.62	0.62
7:P:358:ARG:HB2	7:P:385:VAL:HB	1.82	0.62
7:P:525:ILE:O	7:P:526:SER:C	2.38	0.62
7:I:337:LEU:HD22	7:I:423:LEU:HD21	1.80	0.62
7:N:342:ASP:HB3	7:N:401:ILE:HB	1.82	0.62
7:N:412:THR:N	7:N:440:SER:OG	2.31	0.62
7:O:255:LYS:HG3	7:O:358:ARG:HG2	1.82	0.62
7:T:324:HIS:HA	7:T:455:ILE:HG13	1.82	0.62
7:T:412:THR:N	7:T:440:SER:OG	2.30	0.62
7:W:410:GLY:O	7:X:185:THR:CG2	2.48	0.62
7:I:99:ASN:ND2	7:I:118:ARG:O	2.33	0.62
7:M:99:ASN:ND2	7:M:118:ARG:O	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:204:LYS:HD2	7:N:263:LEU:HD23	1.80	0.62
7:R:99:ASN:ND2	7:R:118:ARG:O	2.33	0.62
7:T:421:GLU:OE1	7:U:434:PHE:HB2	1.99	0.62
5:F:159:ARG:NH2	5:F:172:ASP:OD2	2.32	0.62
7:G:99:ASN:ND2	7:G:118:ARG:O	2.33	0.62
7:H:189:LYS:CE	7:H:191:PHE:CZ	2.82	0.62
7:H:255:LYS:HG3	7:H:358:ARG:HG2	1.82	0.62
7:H:412:THR:N	7:H:440:SER:OG	2.30	0.62
7:K:413:ARG:NH1	7:L:282:LEU:CA	2.62	0.62
7:N:400:LEU:HD12	7:O:195:HIS:CG	2.33	0.62
7:Q:394:ASN:HB2	7:R:201:GLU:HB2	1.82	0.62
7:U:99:ASN:ND2	7:U:118:ARG:O	2.33	0.62
7:W:412:THR:N	7:W:440:SER:OG	2.30	0.62
1:A:612:VAL:O	1:A:615:GLY:N	2.33	0.61
1:A:781:PRO:HD2	1:A:784:LYS:HB2	1.82	0.61
4:E:69:PHE:HB3	4:E:168:CYS:HB2	1.80	0.61
7:O:99:ASN:ND2	7:O:118:ARG:O	2.33	0.61
7:O:342:ASP:HB3	7:O:401:ILE:HB	1.82	0.61
7:O:406:SER:O	7:Q:188:GLU:HB2	2.00	0.61
7:S:391:ARG:HH21	7:T:204:LYS:HG3	1.63	0.61
7:W:413:ARG:NH2	7:X:282:LEU:CD1	2.62	0.61
3:D:166:ARG:NH2	6:B:207:GLU:OE1	2.32	0.61
3:D:504:SER:HB3	3:D:524:ASN:HB2	1.82	0.61
6:B:287:SER:HA	6:B:406:LYS:HG2	1.81	0.61
7:H:262:PHE:HB3	7:H:351:VAL:HB	1.82	0.61
7:K:358:ARG:O	7:K:385:VAL:N	2.32	0.61
7:O:59:ASP:OD1	7:Q:456:TYR:OH	2.17	0.61
7:S:324:HIS:HA	7:S:455:ILE:HG13	1.82	0.61
7:T:204:LYS:HD2	7:T:263:LEU:HD23	1.80	0.61
7:V:342:ASP:HB3	7:V:401:ILE:HB	1.82	0.61
7:V:395:ILE:CG1	7:W:199:GLN:O	2.46	0.61
7:W:64:ARG:NH1	7:X:290:ARG:NE	2.48	0.61
7:W:324:HIS:HA	7:W:455:ILE:HG13	1.82	0.61
7:P:99:ASN:ND2	7:P:118:ARG:O	2.34	0.61
7:H:99:ASN:ND2	7:H:118:ARG:O	2.33	0.61
7:M:320:THR:OG1	7:N:289:ASN:HB3	2.01	0.61
7:Q:262:PHE:HB3	7:Q:351:VAL:HB	1.82	0.61
7:S:99:ASN:ND2	7:S:118:ARG:O	2.33	0.61
7:U:412:THR:N	7:U:440:SER:OG	2.30	0.61
7:W:99:ASN:ND2	7:W:118:ARG:O	2.33	0.61
7:P:145:ASP:OD2	7:H:284:ARG:NH1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:206:ILE:HB	7:H:261:LEU:HB2	1.81	0.61
7:K:409:ARG:HD3	7:L:184:GLU:OE2	2.00	0.61
7:L:99:ASN:ND2	7:L:118:ARG:O	2.33	0.61
7:L:412:THR:N	7:L:440:SER:OG	2.30	0.61
7:O:380:ASN:HD22	7:Q:215:ASN:HB2	1.65	0.61
7:Q:99:ASN:ND2	7:Q:118:ARG:O	2.33	0.61
7:T:262:PHE:HB3	7:T:351:VAL:HB	1.82	0.61
7:V:99:ASN:ND2	7:V:118:ARG:O	2.33	0.61
1:A:1175:LEU:O	1:A:1179:THR:OG1	2.15	0.61
7:M:313:GLU:OE2	7:N:290:ARG:NH2	2.33	0.61
7:N:443:ASP:OD2	7:O:167:ASN:O	2.17	0.61
7:T:206:ILE:HB	7:T:261:LEU:HB2	1.81	0.61
7:U:386:LYS:HD3	7:V:209:GLU:HB3	1.83	0.61
2:C:378:SER:OG	2:C:380:HIS:NE2	2.34	0.61
7:K:521:SER:O	7:K:522:LYS:CB	2.49	0.61
7:N:206:ILE:HB	7:N:261:LEU:HB2	1.81	0.61
7:R:370:PHE:CB	7:R:373:ILE:H	2.08	0.61
7:S:255:LYS:HG3	7:S:358:ARG:HG2	1.82	0.61
7:U:206:ILE:HB	7:U:261:LEU:HB2	1.81	0.61
7:U:255:LYS:HG3	7:U:358:ARG:HG2	1.82	0.61
7:V:255:LYS:HG3	7:V:358:ARG:HG2	1.81	0.61
7:X:324:HIS:HA	7:X:455:ILE:HG13	1.82	0.61
2:C:202:PHE:H	2:C:214:ILE:HB	1.64	0.61
7:G:204:LYS:HD2	7:G:263:LEU:HD23	1.82	0.61
7:P:19:HIS:NE2	7:H:487:ARG:HD2	2.15	0.61
7:H:370:PHE:CB	7:H:373:ILE:H	2.08	0.61
7:K:324:HIS:HA	7:K:455:ILE:HG13	1.82	0.61
7:N:189:LYS:CE	7:N:191:PHE:CZ	2.82	0.61
7:N:255:LYS:HG3	7:N:358:ARG:HG2	1.82	0.61
7:R:324:HIS:HA	7:R:455:ILE:HG13	1.82	0.61
7:S:204:LYS:HB2	7:S:263:LEU:HB3	1.83	0.61
7:S:521:SER:O	7:S:522:LYS:CB	2.49	0.61
7:W:130:GLU:CD	7:X:165:ASP:HA	2.21	0.61
7:X:99:ASN:ND2	7:X:118:ARG:O	2.33	0.61
2:C:78:ARG:NH1	2:C:142:TYR:OH	2.34	0.61
7:G:333:GLY:H	7:G:448:ILE:HD11	1.64	0.61
7:P:174:ARG:NH2	7:P:179:ALA:O	2.33	0.61
7:P:256:ASN:OD1	7:P:256:ASN:N	2.33	0.61
7:H:204:LYS:HB2	7:H:263:LEU:HB3	1.83	0.61
7:L:204:LYS:HB2	7:L:263:LEU:HB3	1.83	0.61
7:N:408:ILE:N	7:O:187:GLY:O	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:206:ILE:HB	7:O:261:LEU:HB2	1.81	0.61
7:O:324:HIS:HA	7:O:455:ILE:HG13	1.82	0.61
7:U:262:PHE:HB3	7:U:351:VAL:HB	1.82	0.61
7:V:262:PHE:HB3	7:V:351:VAL:HB	1.82	0.61
7:V:386:LYS:HD2	7:W:209:GLU:HB3	1.82	0.61
7:V:391:ARG:HE	7:W:204:LYS:CG	2.14	0.61
7:W:358:ARG:O	7:W:385:VAL:N	2.31	0.61
7:X:204:LYS:HB2	7:X:263:LEU:HB3	1.83	0.61
2:C:341:SER:H	5:F:224:ILE:HG12	1.65	0.61
6:B:223:SER:HB3	6:B:226:THR:HB	1.82	0.61
7:H:55:LYS:HE3	7:I:481:ILE:HG23	1.81	0.61
7:H:413:ARG:NH1	7:I:282:LEU:HA	2.16	0.61
7:I:206:ILE:HB	7:I:261:LEU:HB2	1.81	0.61
7:I:324:HIS:HA	7:I:455:ILE:HG13	1.82	0.61
7:J:99:ASN:ND2	7:J:118:ARG:O	2.33	0.61
7:M:206:ILE:HB	7:M:261:LEU:HB2	1.81	0.61
7:M:342:ASP:HB3	7:M:401:ILE:HB	1.82	0.61
7:N:262:PHE:HB3	7:N:351:VAL:HB	1.82	0.61
7:O:413:ARG:NH1	7:Q:282:LEU:HG	2.15	0.61
7:Q:189:LYS:CE	7:Q:191:PHE:CE1	2.75	0.61
7:Q:342:ASP:HB3	7:Q:401:ILE:HB	1.82	0.61
7:T:99:ASN:ND2	7:T:118:ARG:O	2.33	0.61
7:T:384:CYS:O	7:U:210:LYS:HG3	2.01	0.61
7:V:374:SER:O	7:W:220:LEU:HG	2.00	0.61
7:W:204:LYS:HB2	7:W:263:LEU:HB3	1.83	0.61
7:W:402:ASP:OD2	7:X:193:THR:HG23	2.00	0.61
7:X:412:THR:N	7:X:440:SER:OG	2.31	0.61
5:F:195:ILE:HB	5:F:262:ILE:HD12	1.82	0.61
7:G:372:GLU:HG3	7:P:223:THR:O	2.00	0.61
7:G:372:GLU:HB3	7:P:223:THR:O	2.00	0.61
7:H:324:HIS:HA	7:H:455:ILE:HG13	1.82	0.61
7:H:358:ARG:O	7:H:385:VAL:N	2.32	0.61
7:H:521:SER:O	7:H:522:LYS:CB	2.49	0.61
7:I:412:THR:N	7:I:440:SER:OG	2.30	0.61
7:J:255:LYS:HG3	7:J:358:ARG:HG2	1.82	0.61
7:K:417:PHE:CZ	7:L:280:ILE:HG13	2.35	0.61
7:M:262:PHE:HB3	7:M:351:VAL:HB	1.82	0.61
7:M:324:HIS:HA	7:M:455:ILE:HG13	1.82	0.61
7:M:521:SER:O	7:M:522:LYS:CB	2.49	0.61
7:R:391:ARG:NE	7:S:204:LYS:HE2	2.16	0.61
7:S:342:ASP:HB3	7:S:401:ILE:HB	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:391:ARG:HH21	7:U:204:LYS:CE	2.14	0.61
7:V:189:LYS:CE	7:V:191:PHE:CZ	2.82	0.61
7:X:521:SER:O	7:X:522:LYS:CB	2.49	0.61
2:C:359:ARG:HB3	5:F:205:ASP:HB3	1.83	0.60
7:K:99:ASN:ND2	7:K:118:ARG:O	2.33	0.60
7:L:413:ARG:HH12	7:M:282:LEU:HG	1.62	0.60
7:O:391:ARG:NH2	7:Q:204:LYS:HE3	2.15	0.60
7:Q:403:ASP:HA	7:R:192:ARG:HG2	1.82	0.60
7:R:206:ILE:HB	7:R:261:LEU:HB2	1.81	0.60
7:U:324:HIS:HA	7:U:455:ILE:HG13	1.82	0.60
7:H:342:ASP:HB3	7:H:401:ILE:HB	1.82	0.60
7:J:324:HIS:HA	7:J:455:ILE:HG13	1.82	0.60
7:L:342:ASP:HB3	7:L:401:ILE:HB	1.82	0.60
7:Q:412:THR:N	7:Q:440:SER:OG	2.30	0.60
7:T:521:SER:O	7:T:522:LYS:CB	2.49	0.60
7:V:64:ARG:HH12	7:W:291:ASP:H	0.63	0.60
7:W:391:ARG:HH22	7:X:202:ALA:HB1	1.65	0.60
3:D:44:LYS:HB2	3:D:73:CYS:HB3	1.83	0.60
7:I:130:GLU:HA	7:J:164:ARG:O	2.01	0.60
7:I:262:PHE:HB3	7:I:351:VAL:HB	1.82	0.60
7:L:255:LYS:HG3	7:L:358:ARG:HG2	1.82	0.60
7:L:282:LEU:HD13	7:L:445:PRO:HB3	1.84	0.60
7:L:380:ASN:O	7:M:214:PHE:CD1	2.55	0.60
7:L:384:CYS:O	7:M:210:LYS:HG3	2.01	0.60
7:M:255:LYS:HG3	7:M:358:ARG:HG2	1.82	0.60
7:N:282:LEU:HD13	7:N:445:PRO:HB3	1.83	0.60
7:Q:189:LYS:CE	7:Q:191:PHE:CZ	2.82	0.60
7:R:342:ASP:HB3	7:R:401:ILE:HB	1.82	0.60
7:W:521:SER:O	7:W:522:LYS:CB	2.49	0.60
7:X:189:LYS:CE	7:X:191:PHE:CZ	2.82	0.60
1:A:1288:GLN:O	1:A:1292:ASN:ND2	2.33	0.60
2:C:385:ALA:HB1	5:F:193:THR:HG21	1.82	0.60
3:D:187:THR:OG1	3:D:261:GLN:NE2	2.35	0.60
5:F:27:LYS:HB2	5:F:52:ALA:HB3	1.83	0.60
7:G:524:LYS:NZ	7:P:271:LYS:CD	2.65	0.60
7:J:19:HIS:NE2	7:K:487:ARG:HD2	2.16	0.60
7:K:342:ASP:HB3	7:K:401:ILE:HB	1.82	0.60
7:K:421:GLU:OE1	7:L:434:PHE:HD2	1.84	0.60
7:M:313:GLU:HG3	7:N:290:ARG:HH21	1.65	0.60
7:N:424:LEU:HD11	7:O:191:PHE:CE2	2.37	0.60
7:Q:204:LYS:HB2	7:Q:263:LEU:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:R:262:PHE:HB3	7:R:351:VAL:HB	1.82	0.60
7:T:204:LYS:HB2	7:T:263:LEU:HB3	1.83	0.60
7:V:206:ILE:HB	7:V:261:LEU:HB2	1.81	0.60
7:V:324:HIS:HA	7:V:455:ILE:HG13	1.82	0.60
7:W:206:ILE:HB	7:W:261:LEU:HB2	1.81	0.60
7:W:255:LYS:HG3	7:W:358:ARG:HG2	1.82	0.60
3:D:139:LEU:HD23	3:D:142:ASN:HD22	1.66	0.60
7:J:189:LYS:CE	7:J:191:PHE:CE1	2.75	0.60
7:L:130:GLU:CG	7:M:165:ASP:HA	2.30	0.60
7:L:378:GLU:OE1	7:M:217:ALA:HB3	2.00	0.60
7:O:282:LEU:HD13	7:O:445:PRO:HB3	1.83	0.60
7:T:342:ASP:HB3	7:T:401:ILE:HB	1.82	0.60
7:U:282:LEU:HD13	7:U:445:PRO:HB3	1.84	0.60
7:U:342:ASP:HB3	7:U:401:ILE:HB	1.82	0.60
7:W:409:ARG:CB	7:X:186:LYS:HA	2.31	0.60
2:C:357:LYS:HB3	5:F:207:LEU:HB3	1.82	0.60
5:F:231:LEU:CD2	5:F:232:LEU:N	2.49	0.60
7:J:521:SER:O	7:J:522:LYS:CB	2.49	0.60
7:L:443:ASP:OD2	7:M:167:ASN:O	2.19	0.60
7:N:330:SER:HB2	7:N:449:SER:H	1.67	0.60
7:Q:330:SER:HB2	7:Q:449:SER:H	1.67	0.60
7:R:204:LYS:HB2	7:R:263:LEU:HB3	1.83	0.60
7:S:403:ASP:HA	7:T:192:ARG:HG2	1.82	0.60
7:U:521:SER:O	7:U:522:LYS:CB	2.49	0.60
7:W:262:PHE:HB3	7:W:351:VAL:HB	1.82	0.60
7:W:407:LEU:HA	7:X:188:GLU:CA	2.28	0.60
7:X:330:SER:HB2	7:X:449:SER:H	1.67	0.60
7:X:342:ASP:HB3	7:X:401:ILE:HB	1.82	0.60
7:I:282:LEU:HD13	7:I:445:PRO:HB3	1.83	0.60
7:J:330:SER:HB2	7:J:449:SER:H	1.67	0.60
7:N:99:ASN:ND2	7:N:118:ARG:O	2.33	0.60
7:N:408:ILE:O	7:O:187:GLY:N	2.32	0.60
7:Q:282:LEU:HD13	7:Q:445:PRO:HB3	1.83	0.60
7:Q:521:SER:O	7:Q:522:LYS:CB	2.49	0.60
7:S:384:CYS:O	7:T:210:LYS:HG3	2.01	0.60
7:I:342:ASP:HB3	7:I:401:ILE:HB	1.82	0.60
7:L:330:SER:HB2	7:L:449:SER:H	1.67	0.60
7:O:204:LYS:HB2	7:O:263:LEU:HB3	1.83	0.60
7:V:204:LYS:HB2	7:V:263:LEU:HB3	1.83	0.60
7:W:342:ASP:HB3	7:W:401:ILE:HB	1.82	0.60
7:W:411:GLY:O	7:X:185:THR:HG21	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:X:189:LYS:CE	7:X:191:PHE:CE1	2.75	0.60
7:H:282:LEU:HD13	7:H:445:PRO:HB3	1.83	0.60
7:J:189:LYS:CE	7:J:191:PHE:CZ	2.82	0.60
7:J:204:LYS:HB2	7:J:263:LEU:HB3	1.83	0.60
7:K:421:GLU:OE1	7:L:434:PHE:CD2	2.55	0.60
7:L:218:ILE:HG23	7:L:249:PHE:HB2	1.84	0.60
7:M:218:ILE:HG23	7:M:249:PHE:HB2	1.84	0.60
7:O:218:ILE:HG23	7:O:249:PHE:HB2	1.84	0.60
7:G:256:ASN:HB3	7:G:357:LYS:HB2	1.84	0.60
7:G:524:LYS:HZ2	7:P:271:LYS:CD	2.15	0.60
7:H:330:SER:HB2	7:H:449:SER:H	1.67	0.60
7:K:330:SER:HB2	7:K:449:SER:H	1.67	0.60
7:K:403:ASP:HA	7:L:192:ARG:HG2	1.84	0.60
7:T:330:SER:HB2	7:T:449:SER:H	1.67	0.60
7:V:521:SER:O	7:V:522:LYS:CB	2.49	0.60
2:C:138:ASP:O	2:C:161:ASN:ND2	2.35	0.59
5:F:452:ASN:OD1	5:F:455:ARG:NH2	2.35	0.59
7:K:282:LEU:HD13	7:K:445:PRO:HB3	1.84	0.59
7:N:204:LYS:HB2	7:N:263:LEU:HB3	1.83	0.59
7:N:218:ILE:HG23	7:N:249:PHE:HB2	1.84	0.59
7:N:324:HIS:HA	7:N:455:ILE:HG13	1.82	0.59
7:N:386:LYS:HE2	7:O:207:ILE:HG23	1.84	0.59
7:O:262:PHE:HB3	7:O:351:VAL:HB	1.82	0.59
7:R:282:LEU:HD13	7:R:445:PRO:HB3	1.84	0.59
7:S:218:ILE:HG23	7:S:249:PHE:HB2	1.84	0.59
7:T:218:ILE:HG23	7:T:249:PHE:HB2	1.84	0.59
7:T:358:ARG:O	7:T:385:VAL:N	2.32	0.59
7:V:414:LYS:HG2	7:W:435:VAL:CG1	2.32	0.59
6:B:586:THR:CB	7:X:107:PHE:CE2	2.86	0.59
7:G:105:GLY:HA2	7:P:159:LEU:HD22	1.83	0.59
7:I:358:ARG:O	7:I:385:VAL:N	2.32	0.59
7:J:358:ARG:O	7:J:385:VAL:N	2.32	0.59
7:N:408:ILE:HG22	7:O:187:GLY:O	2.02	0.59
7:R:330:SER:HB2	7:R:449:SER:H	1.67	0.59
7:W:218:ILE:HG23	7:W:249:PHE:HB2	1.84	0.59
7:L:380:ASN:ND2	7:M:215:ASN:HB2	2.13	0.59
7:L:521:SER:O	7:L:522:LYS:CB	2.49	0.59
7:S:380:ASN:HD22	7:T:215:ASN:CB	2.13	0.59
7:T:189:LYS:CE	7:T:191:PHE:CE1	2.75	0.59
7:T:386:LYS:O	7:U:208:GLN:OE1	2.20	0.59
7:G:392:ALA:HB3	7:P:203:PHE:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:130:GLU:CD	7:L:165:ASP:HA	2.22	0.59
7:M:174:ARG:NH2	7:M:179:ALA:O	2.36	0.59
7:U:204:LYS:HB2	7:U:263:LEU:HB3	1.83	0.59
1:A:40:VAL:HG11	1:A:502:LEU:HD21	1.83	0.59
5:F:42:THR:OG1	7:G:487:ARG:NH2	2.36	0.59
7:P:282:LEU:HD13	7:P:445:PRO:HB3	1.85	0.59
7:I:174:ARG:NH2	7:I:179:ALA:O	2.36	0.59
7:K:204:LYS:HB2	7:K:263:LEU:HB3	1.83	0.59
7:L:189:LYS:CE	7:L:191:PHE:CZ	2.82	0.59
7:N:521:SER:O	7:N:522:LYS:CB	2.49	0.59
7:Q:378:GLU:OE1	7:R:217:ALA:HB3	2.02	0.59
7:U:59:ASP:OD1	7:V:456:TYR:OH	2.20	0.59
7:U:330:SER:HB2	7:U:449:SER:H	1.67	0.59
7:X:174:ARG:NH2	7:X:179:ALA:O	2.36	0.59
2:C:193:LYS:HB3	3:D:355:GLU:HB3	1.84	0.59
7:G:258:THR:HB	7:G:355:ASP:HB3	1.84	0.59
7:H:174:ARG:NH2	7:H:179:ALA:O	2.36	0.59
7:I:521:SER:O	7:I:522:LYS:CB	2.49	0.59
7:Q:218:ILE:HG23	7:Q:249:PHE:HB2	1.84	0.59
7:R:358:ARG:O	7:R:385:VAL:N	2.31	0.59
7:T:417:PHE:CZ	7:U:280:ILE:HG13	2.38	0.59
7:U:398:GLU:HB3	7:V:197:GLU:HB3	1.84	0.59
7:V:174:ARG:NH2	7:V:179:ALA:O	2.36	0.59
7:V:218:ILE:HG23	7:V:249:PHE:HB2	1.84	0.59
7:V:282:LEU:HD13	7:V:445:PRO:HB3	1.83	0.59
7:W:282:LEU:HD13	7:W:445:PRO:HB3	1.84	0.59
7:W:372:GLU:CG	7:X:223:THR:O	2.50	0.59
7:W:404:VAL:O	7:X:190:ASN:HB2	2.03	0.59
7:P:372:GLU:HG2	7:P:372:GLU:O	2.02	0.59
7:H:218:ILE:HG23	7:H:249:PHE:HB2	1.84	0.59
7:I:330:SER:HB2	7:I:449:SER:H	1.67	0.59
7:J:174:ARG:NH2	7:J:179:ALA:O	2.36	0.59
7:J:282:LEU:HD13	7:J:445:PRO:HB3	1.83	0.59
7:M:189:LYS:CE	7:M:191:PHE:HE1	2.15	0.59
7:N:386:LYS:O	7:O:208:GLN:OE1	2.21	0.59
7:Q:105:GLY:HA2	7:R:159:LEU:HD22	1.85	0.59
7:T:174:ARG:NH2	7:T:179:ALA:O	2.36	0.59
7:T:282:LEU:HD13	7:T:445:PRO:HB3	1.84	0.59
7:U:218:ILE:HG23	7:U:249:PHE:HB2	1.84	0.59
7:W:330:SER:HB2	7:W:449:SER:H	1.67	0.59
2:C:234:THR:HG22	2:C:309:GLU:HA	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:218:ILE:HG23	7:I:249:PHE:HB2	1.84	0.59
7:M:177:ASN:HD21	7:M:292:VAL:HG23	1.68	0.59
7:M:189:LYS:CE	7:M:191:PHE:CZ	2.82	0.59
7:M:282:LEU:HD13	7:M:445:PRO:HB3	1.83	0.59
7:O:330:SER:HB2	7:O:449:SER:H	1.67	0.59
7:Q:174:ARG:NH2	7:Q:179:ALA:O	2.36	0.59
7:R:218:ILE:HG23	7:R:249:PHE:HB2	1.84	0.59
7:R:521:SER:O	7:R:522:LYS:CB	2.49	0.59
7:S:174:ARG:NH2	7:S:179:ALA:O	2.36	0.59
7:T:406:SER:O	7:U:188:GLU:HB2	2.03	0.59
7:W:174:ARG:NH2	7:W:179:ALA:O	2.36	0.59
7:G:145:ASP:OD2	7:P:284:ARG:NH1	2.36	0.59
7:G:270:GLU:HB3	7:G:343:LYS:HB2	1.83	0.59
7:P:514:GLU:CB	7:P:522:LYS:HD2	2.32	0.59
7:I:87:SER:OG	7:J:94:MET:CE	2.51	0.59
7:K:218:ILE:HG23	7:K:249:PHE:HB2	1.84	0.59
7:L:64:ARG:NH1	7:M:290:ARG:HE	2.01	0.59
7:L:174:ARG:NH2	7:L:179:ALA:O	2.36	0.59
7:M:65:ARG:CA	7:N:467:HIS:CB	2.70	0.59
7:O:358:ARG:O	7:O:385:VAL:N	2.32	0.59
7:S:177:ASN:HD21	7:S:292:VAL:HG23	1.68	0.59
7:S:391:ARG:NE	7:T:204:LYS:HE2	2.17	0.59
7:S:392:ALA:HB3	7:T:203:PHE:H	1.68	0.59
7:T:177:ASN:HD21	7:T:292:VAL:HG23	1.68	0.59
7:G:364:LEU:HB3	7:G:379:PHE:HB2	1.83	0.59
7:P:153:ASN:HD21	7:P:178:VAL:HG23	1.68	0.59
7:P:301:ASP:OD1	7:H:288:ARG:NH2	2.35	0.59
7:J:64:ARG:NH1	7:K:461:VAL:HB	2.18	0.59
7:K:174:ARG:NH2	7:K:179:ALA:O	2.36	0.59
7:M:204:LYS:HB2	7:M:263:LEU:HB3	1.83	0.59
7:O:174:ARG:NH2	7:O:179:ALA:O	2.36	0.59
7:R:174:ARG:NH2	7:R:179:ALA:O	2.36	0.59
7:R:177:ASN:HD21	7:R:292:VAL:HG23	1.68	0.59
7:T:400:LEU:HD12	7:U:195:HIS:CB	2.27	0.59
7:V:330:SER:HB2	7:V:449:SER:H	1.67	0.59
7:W:402:ASP:OD2	7:X:193:THR:CG2	2.50	0.59
7:X:218:ILE:HG23	7:X:249:PHE:HB2	1.84	0.59
7:G:246:LYS:HB2	7:G:367:SER:HB3	1.84	0.58
7:G:372:GLU:CD	7:P:223:THR:O	2.42	0.58
7:I:191:PHE:HD1	7:I:191:PHE:N	2.01	0.58
7:J:218:ILE:HG23	7:J:249:PHE:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:65:ARG:HG3	7:N:467:HIS:CB	2.33	0.58
7:S:189:LYS:CE	7:S:191:PHE:CZ	2.82	0.58
7:U:174:ARG:NH2	7:U:179:ALA:O	2.36	0.58
7:U:388:GLY:O	7:V:206:ILE:HG23	2.03	0.58
7:X:189:LYS:CE	7:X:191:PHE:HE1	2.15	0.58
7:I:204:LYS:HB2	7:I:263:LEU:HB3	1.83	0.58
7:L:413:ARG:NH1	7:M:282:LEU:HA	2.18	0.58
7:M:330:SER:HB2	7:M:449:SER:H	1.67	0.58
7:N:174:ARG:NH2	7:N:179:ALA:O	2.36	0.58
7:S:282:LEU:HD13	7:S:445:PRO:HB3	1.83	0.58
7:W:398:GLU:OE1	7:X:197:GLU:OE1	2.21	0.58
4:E:56:HIS:HB3	4:E:67:SER:HB2	1.86	0.58
7:H:380:ASN:O	7:I:214:PHE:CE1	2.56	0.58
7:K:177:ASN:HD21	7:K:292:VAL:HG23	1.68	0.58
7:U:372:GLU:O	7:V:222:PHE:HA	2.04	0.58
7:Q:406:SER:O	7:R:188:GLU:HB2	2.03	0.58
7:R:191:PHE:HD1	7:R:191:PHE:N	2.01	0.58
7:S:406:SER:O	7:T:188:GLU:HB2	2.02	0.58
7:T:413:ARG:NH1	7:U:282:LEU:HG	2.18	0.58
2:C:195:ALA:HB3	3:D:353:CYS:HB2	1.86	0.58
2:C:353:LEU:HD23	5:F:211:LYS:HB3	1.86	0.58
5:F:171:ASP:O	5:F:174:LYS:NZ	2.34	0.58
7:J:177:ASN:HD21	7:J:292:VAL:HG23	1.68	0.58
7:L:191:PHE:HD1	7:L:191:PHE:N	2.01	0.58
7:N:413:ARG:NH1	7:O:282:LEU:O	2.36	0.58
1:A:253:ARG:HH22	1:A:257:ASN:HD22	1.49	0.58
7:P:177:ASN:HD21	7:P:292:VAL:HG23	1.68	0.58
7:I:412:THR:OG1	7:J:167:ASN:CG	2.37	0.58
7:K:411:GLY:O	7:L:185:THR:HG21	2.04	0.58
7:N:130:GLU:HG3	7:O:165:ASP:CA	2.33	0.58
7:O:177:ASN:HD21	7:O:292:VAL:HG23	1.68	0.58
7:R:380:ASN:HB2	7:S:215:ASN:HB2	1.86	0.58
7:S:330:SER:HB2	7:S:449:SER:H	1.67	0.58
7:V:189:LYS:CE	7:V:191:PHE:HE1	2.15	0.58
7:X:282:LEU:HD13	7:X:445:PRO:HB3	1.83	0.58
1:A:323:LEU:H	1:A:345:ILE:H	1.51	0.58
1:A:364:LYS:NZ	1:A:557:ASP:OD2	2.35	0.58
7:L:358:ARG:O	7:L:385:VAL:N	2.32	0.58
7:N:177:ASN:HD21	7:N:292:VAL:HG23	1.68	0.58
7:N:191:PHE:HD1	7:N:191:PHE:N	2.01	0.58
7:Q:378:GLU:O	7:R:216:ALA:HA	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:358:ARG:O	7:S:385:VAL:N	2.31	0.58
7:U:358:ARG:O	7:U:385:VAL:N	2.32	0.58
7:G:350:GLY:O	7:G:393:VAL:N	2.36	0.58
7:P:65:ARG:HB2	7:H:467:HIS:ND1	2.18	0.58
7:V:177:ASN:HD21	7:V:292:VAL:HG23	1.68	0.58
7:X:191:PHE:HD1	7:X:191:PHE:N	2.01	0.58
6:B:256:LYS:HA	6:B:314:ILE:HG22	1.86	0.58
6:B:409:LEU:HD22	6:B:410:PHE:HB2	1.85	0.58
7:I:189:LYS:CE	7:I:191:PHE:CZ	2.82	0.58
7:L:404:VAL:N	7:M:191:PHE:O	2.34	0.58
7:O:521:SER:O	7:O:522:LYS:CB	2.49	0.58
7:R:384:CYS:O	7:S:210:LYS:HG3	2.03	0.58
7:S:380:ASN:HB2	7:T:215:ASN:HB2	1.86	0.58
5:F:377:THR:HB	7:G:203:PHE:HB2	1.86	0.58
7:G:164:ARG:NH2	7:G:171:TYR:OH	2.36	0.58
7:G:524:LYS:HG2	7:P:196:TYR:CZ	2.38	0.58
7:H:191:PHE:HD1	7:H:191:PHE:N	2.01	0.58
7:L:374:SER:O	7:M:220:LEU:HD12	2.03	0.58
7:S:372:GLU:HB3	7:T:223:THR:C	2.24	0.58
7:V:376:GLY:O	7:W:218:ILE:HG13	2.04	0.58
1:A:63:LYS:HE3	3:D:554:ARG:HH21	1.69	0.57
7:N:358:ARG:O	7:N:385:VAL:N	2.31	0.57
7:Q:191:PHE:HD1	7:Q:191:PHE:N	2.01	0.57
7:Q:391:ARG:HE	7:R:204:LYS:HE2	1.68	0.57
7:V:58:THR:HG22	7:W:452:LEU:HD23	1.86	0.57
7:W:130:GLU:CA	7:X:164:ARG:O	2.44	0.57
6:B:501:VAL:HB	6:B:624:ILE:HG21	1.86	0.57
7:G:413:ARG:HD3	7:P:280:ILE:HD11	1.86	0.57
7:H:177:ASN:HD21	7:H:292:VAL:HG23	1.68	0.57
7:H:189:LYS:CE	7:H:191:PHE:HE1	2.15	0.57
7:Q:372:GLU:CD	7:R:223:THR:O	2.41	0.57
7:U:177:ASN:HD21	7:U:292:VAL:HG23	1.68	0.57
7:V:392:ALA:HB2	7:W:203:PHE:HB2	1.79	0.57
1:A:854:GLN:HB3	1:A:885:ARG:HB3	1.86	0.57
1:A:1277:GLU:HG3	1:A:1278:GLN:H	1.69	0.57
3:D:136:ASN:HB3	3:D:414:PRO:HG3	1.87	0.57
6:B:490:ILE:HG13	6:B:493:LEU:HD12	1.86	0.57
7:P:42:ARG:HH22	7:H:471:GLN:CD	2.07	0.57
7:I:417:PHE:CE2	7:J:280:ILE:HG13	2.39	0.57
7:S:189:LYS:CE	7:S:191:PHE:HE1	2.15	0.57
7:S:413:ARG:NH1	7:T:282:LEU:HG	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ILE:HB	1:A:200:THR:HB	1.85	0.57
1:A:535:VAL:HG23	1:A:536:PRO:HD3	1.86	0.57
7:P:191:PHE:HA	7:P:276:VAL:HG12	1.86	0.57
7:I:189:LYS:CE	7:I:191:PHE:HE1	2.15	0.57
7:L:177:ASN:HD21	7:L:292:VAL:HG23	1.68	0.57
7:M:313:GLU:CG	7:N:290:ARG:NH2	2.68	0.57
7:N:372:GLU:HB3	7:O:223:THR:C	2.25	0.57
7:R:189:LYS:CE	7:R:191:PHE:CZ	2.82	0.57
7:W:177:ASN:HD21	7:W:292:VAL:HG23	1.68	0.57
7:W:421:GLU:CB	7:X:434:PHE:CE2	2.80	0.57
7:W:446:VAL:HG21	7:X:184:GLU:CG	2.34	0.57
7:X:177:ASN:HD21	7:X:292:VAL:HG23	1.68	0.57
7:M:191:PHE:HD1	7:M:191:PHE:N	2.01	0.57
7:O:403:ASP:HA	7:Q:192:ARG:HG2	1.86	0.57
7:Q:177:ASN:HD21	7:Q:292:VAL:HG23	1.68	0.57
7:W:413:ARG:HD3	7:X:441:ILE:HG23	1.86	0.57
1:A:53:THR:HB	1:A:107:VAL:HB	1.87	0.57
1:A:656:ASN:HD21	3:D:82:GLU:HB2	1.69	0.57
2:C:466:ARG:NH1	2:C:467:CYS:O	2.37	0.57
5:F:259:PHE:HB2	5:F:326:VAL:HG22	1.85	0.57
7:N:189:LYS:CE	7:N:191:PHE:HE1	2.15	0.57
7:Q:358:ARG:O	7:Q:385:VAL:N	2.31	0.57
7:U:189:LYS:CE	7:U:191:PHE:HE1	2.15	0.57
7:X:358:ARG:O	7:X:385:VAL:N	2.31	0.57
1:A:995:GLU:HG2	1:A:1021:VAL:HG21	1.85	0.57
3:D:165:CYS:SG	6:B:162:ASN:ND2	2.78	0.57
7:L:395:ILE:HA	7:M:199:GLN:O	2.04	0.57
7:T:394:ASN:O	7:U:200:ILE:HA	2.05	0.57
7:V:58:THR:HG21	7:W:452:LEU:CG	2.23	0.57
7:W:413:ARG:NH2	7:X:282:LEU:HD12	2.20	0.57
1:A:259:VAL:HB	1:A:295:GLY:HA3	1.85	0.57
3:D:256:THR:HG22	3:D:257:VAL:H	1.68	0.57
7:K:189:LYS:CE	7:K:191:PHE:HE1	2.15	0.57
7:R:189:LYS:CE	7:R:191:PHE:HE1	2.15	0.57
7:T:391:ARG:NH2	7:U:204:LYS:CE	2.64	0.57
1:A:540:LEU:HD23	1:A:561:LEU:HD11	1.87	0.57
3:D:320:ASP:HB3	3:D:370:VAL:HG23	1.87	0.57
7:I:177:ASN:HD21	7:I:292:VAL:HG23	1.68	0.57
7:R:380:ASN:HD22	7:S:215:ASN:CB	2.16	0.57
7:S:105:GLY:HA2	7:T:159:LEU:HD22	1.86	0.57
7:W:410:GLY:N	7:X:185:THR:HG23	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:703:GLU:HG2	6:B:721:LEU:HD13	1.87	0.57
7:J:413:ARG:NH1	7:K:282:LEU:HA	2.20	0.57
7:L:130:GLU:HA	7:M:164:ARG:O	2.04	0.57
7:M:358:ARG:O	7:M:385:VAL:N	2.32	0.57
7:U:189:LYS:CE	7:U:191:PHE:CZ	2.82	0.57
1:A:268:THR:HB	1:A:326:ALA:HB3	1.87	0.56
7:J:391:ARG:HH21	7:K:204:LYS:CE	2.16	0.56
7:S:324:HIS:CE1	7:S:452:LEU:HD21	2.40	0.56
7:W:324:HIS:CE1	7:W:452:LEU:HD21	2.40	0.56
7:W:372:GLU:HB3	7:X:223:THR:O	2.04	0.56
7:W:400:LEU:HB2	7:X:195:HIS:N	2.20	0.56
7:W:417:PHE:CZ	7:X:280:ILE:CD1	2.87	0.56
2:C:34:TYR:HA	2:C:280:ARG:HH12	1.70	0.56
6:B:732:CYS:HB3	6:B:737:VAL:HA	1.88	0.56
7:J:189:LYS:CE	7:J:191:PHE:HE1	2.15	0.56
7:R:324:HIS:CE1	7:R:452:LEU:HD21	2.40	0.56
1:A:1279:ARG:HG2	1:A:1281:GLY:HA3	1.85	0.56
3:D:111:GLU:HG2	3:D:274:GLU:HB2	1.87	0.56
6:B:581:TYR:HD2	6:B:610:ASP:HB2	1.68	0.56
10:P:603:NAG:H83	10:P:603:NAG:H3	1.87	0.56
7:K:324:HIS:CE1	7:K:452:LEU:HD21	2.40	0.56
7:M:65:ARG:CG	7:N:467:HIS:CG	2.88	0.56
7:N:324:HIS:CE1	7:N:452:LEU:HD21	2.41	0.56
7:O:417:PHE:CZ	7:Q:280:ILE:HG13	2.41	0.56
7:Q:413:ARG:NH1	7:R:282:LEU:HG	2.21	0.56
7:S:191:PHE:CD1	7:S:191:PHE:N	2.73	0.56
7:U:394:ASN:O	7:V:201:GLU:N	2.36	0.56
6:B:87:PHE:HB3	6:B:102:LYS:HE2	1.86	0.56
6:B:713:LEU:HA	6:B:714:THR:OG1	2.05	0.56
7:G:59:ASP:OD1	7:P:456:TYR:OH	2.21	0.56
7:G:372:GLU:HB3	7:P:223:THR:C	2.25	0.56
7:L:400:LEU:CD1	7:M:195:HIS:HB2	2.33	0.56
7:O:394:ASN:HB2	7:Q:201:GLU:HB2	1.86	0.56
7:T:324:HIS:CE1	7:T:452:LEU:HD21	2.41	0.56
1:A:283:MET:HA	1:A:284:GLN:CB	2.33	0.56
1:A:315:LEU:HD23	1:A:318:LEU:HG	1.87	0.56
1:A:1249:GLU:HG2	1:A:1289:ASP:HB2	1.87	0.56
7:K:191:PHE:HD1	7:K:191:PHE:N	2.01	0.56
7:L:324:HIS:CE1	7:L:452:LEU:HD21	2.40	0.56
7:L:408:ILE:O	7:M:187:GLY:N	2.38	0.56
7:Q:324:HIS:CE1	7:Q:452:LEU:HD21	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Q:376:GLY:O	7:R:218:ILE:HG13	2.06	0.56
7:V:324:HIS:CE1	7:V:452:LEU:HD21	2.40	0.56
7:W:148:SER:HB3	7:X:180:SER:HB2	1.88	0.56
5:F:399:GLY:HA3	7:G:438:ALA:HB1	1.86	0.56
7:P:198:GLU:HB3	7:P:269:LYS:HB2	1.87	0.56
7:I:130:GLU:HG3	7:J:165:ASP:CA	2.34	0.56
7:L:386:LYS:HB3	7:M:209:GLU:H	1.70	0.56
7:M:55:LYS:HE3	7:N:481:ILE:CG2	2.31	0.56
7:R:372:GLU:HB3	7:S:223:THR:C	2.23	0.56
7:V:386:LYS:HD2	7:W:209:GLU:CB	2.35	0.56
1:A:32:ARG:NH2	1:A:630:SER:O	2.39	0.56
1:A:273:GLU:HA	1:A:321:LYS:HB2	1.87	0.56
6:B:328:LYS:NZ	6:B:330:LYS:O	2.31	0.56
7:M:19:HIS:CD2	7:N:487:ARG:CD	2.85	0.56
7:M:60:ALA:H	7:N:454:PRO:HG2	1.69	0.56
7:O:191:PHE:HD1	7:O:191:PHE:N	2.01	0.56
7:T:130:GLU:HG3	7:U:165:ASP:HA	1.87	0.56
7:U:191:PHE:HD1	7:U:191:PHE:N	2.01	0.56
1:A:1287:THR:HB	1:A:1290:THR:HB	1.87	0.56
7:G:90:ARG:NH1	7:G:103:ASP:OD1	2.37	0.56
7:I:130:GLU:CA	7:J:164:ARG:O	2.53	0.56
7:I:324:HIS:CE1	7:I:452:LEU:HD21	2.40	0.56
7:J:324:HIS:CE1	7:J:452:LEU:HD21	2.41	0.56
7:K:412:THR:HG1	7:L:167:ASN:CG	2.09	0.56
7:L:417:PHE:CZ	7:M:280:ILE:CG1	2.84	0.56
7:L:421:GLU:OE1	7:M:434:PHE:CD2	2.58	0.56
7:O:189:LYS:CE	7:O:191:PHE:HE1	2.15	0.56
7:R:403:ASP:HA	7:S:192:ARG:HG2	1.87	0.56
7:X:370:PHE:CG	7:X:373:ILE:CD1	2.89	0.56
3:D:124:ARG:HG2	6:B:171:ARG:HA	1.88	0.56
7:K:130:GLU:HG3	7:L:165:ASP:HA	1.88	0.56
7:L:198:GLU:HB3	7:L:269:LYS:HB2	1.88	0.56
4:E:107:VAL:HG22	4:E:118:LEU:HG	1.87	0.56
7:H:153:ASN:HD21	7:H:178:VAL:HG23	1.71	0.56
7:J:153:ASN:HD21	7:J:178:VAL:HG23	1.71	0.56
7:J:270:GLU:HB3	7:J:343:LYS:HB2	1.88	0.56
7:M:413:ARG:NH1	7:N:282:LEU:O	2.38	0.56
7:P:394:ASN:HB2	7:H:201:GLU:HB2	1.87	0.55
7:H:324:HIS:CE1	7:H:452:LEU:HD21	2.40	0.55
7:I:409:ARG:HD3	7:J:184:GLU:OE2	2.05	0.55
7:K:198:GLU:HB3	7:K:269:LYS:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:30:TRP:CH2	7:N:467:HIS:CE1	2.90	0.55
7:O:130:GLU:OE2	7:Q:165:ASP:HA	2.06	0.55
7:R:270:GLU:HB3	7:R:343:LYS:HB2	1.89	0.55
7:R:370:PHE:CG	7:R:373:ILE:CD1	2.89	0.55
7:T:153:ASN:HD21	7:T:178:VAL:HG23	1.71	0.55
7:T:391:ARG:HH22	7:U:202:ALA:HB1	1.70	0.55
7:V:153:ASN:HD21	7:V:178:VAL:HG23	1.71	0.55
7:W:409:ARG:HB3	7:X:186:LYS:HA	1.89	0.55
7:I:153:ASN:HD21	7:I:178:VAL:HG23	1.71	0.55
7:O:324:HIS:CE1	7:O:452:LEU:HD21	2.40	0.55
7:Q:153:ASN:HD21	7:Q:178:VAL:HG23	1.71	0.55
7:R:378:GLU:OE1	7:S:217:ALA:HB3	2.07	0.55
7:U:106:ASP:H	7:V:159:LEU:HD13	1.71	0.55
7:V:270:GLU:HB3	7:V:343:LYS:HB2	1.88	0.55
1:A:604:ALA:O	1:A:772:SER:OG	2.22	0.55
7:P:58:THR:HG21	7:H:452:LEU:HD23	1.88	0.55
7:H:391:ARG:HE	7:I:204:LYS:HE2	1.71	0.55
7:J:129:SER:HA	7:K:164:ARG:CZ	2.36	0.55
7:R:198:GLU:HB3	7:R:269:LYS:HB2	1.88	0.55
7:S:270:GLU:HB3	7:S:343:LYS:HB2	1.88	0.55
7:T:380:ASN:O	7:U:214:PHE:CE1	2.59	0.55
7:U:324:HIS:CE1	7:U:452:LEU:HD21	2.41	0.55
1:A:371:ILE:HD12	1:A:422:LEU:HD13	1.89	0.55
2:C:366:VAL:HG12	5:F:198:GLU:HA	1.88	0.55
7:M:324:HIS:CE1	7:M:452:LEU:HD21	2.41	0.55
7:N:270:GLU:HB3	7:N:343:LYS:HB2	1.89	0.55
7:N:370:PHE:CG	7:N:373:ILE:CD1	2.89	0.55
7:S:198:GLU:HB3	7:S:269:LYS:HB2	1.88	0.55
7:U:198:GLU:HB3	7:U:269:LYS:HB2	1.88	0.55
7:V:370:PHE:CG	7:V:373:ILE:CD1	2.89	0.55
7:W:413:ARG:HD3	7:X:441:ILE:CG2	2.37	0.55
1:A:149:ASN:HB2	1:A:155:ALA:HB2	1.88	0.55
1:A:286:ALA:HA	1:A:287:MET:HB2	1.87	0.55
7:G:44:ARG:NH2	7:P:474:GLU:OE2	2.38	0.55
7:L:153:ASN:HD21	7:L:178:VAL:HG23	1.71	0.55
7:L:407:LEU:HA	7:M:188:GLU:HA	1.87	0.55
7:M:413:ARG:HG3	7:N:185:THR:OG1	2.07	0.55
7:R:392:ALA:HB3	7:S:203:PHE:H	1.71	0.55
7:S:153:ASN:HD21	7:S:178:VAL:HG23	1.71	0.55
7:U:270:GLU:HB3	7:U:343:LYS:HB2	1.88	0.55
7:V:394:ASN:HB2	7:W:201:GLU:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:W:370:PHE:CG	7:W:373:ILE:CD1	2.89	0.55
1:A:539:ARG:NH2	1:A:635:GLY:O	2.35	0.55
3:D:525:ASN:O	3:D:527:PRO:HD3	2.06	0.55
7:G:372:GLU:CB	7:P:223:THR:O	2.55	0.55
7:P:363:HIS:ND1	7:P:380:ASN:OD1	2.31	0.55
7:I:130:GLU:OE2	7:J:166:GLY:N	2.40	0.55
7:J:370:PHE:CG	7:J:373:ILE:CD1	2.89	0.55
7:L:270:GLU:HB3	7:L:343:LYS:HB2	1.89	0.55
7:Q:270:GLU:HB3	7:Q:343:LYS:HB2	1.88	0.55
7:V:528:GLY:CA	7:W:200:ILE:CD1	2.62	0.55
7:X:324:HIS:CE1	7:X:452:LEU:HD21	2.40	0.55
6:B:200:LEU:O	6:B:533:THR:OG1	2.24	0.55
6:B:291:GLU:HA	6:B:402:ILE:HG22	1.89	0.55
7:H:191:PHE:CD1	7:H:191:PHE:N	2.73	0.55
7:I:198:GLU:HB3	7:I:269:LYS:HB2	1.88	0.55
7:M:65:ARG:CB	7:N:467:HIS:HB2	2.36	0.55
7:M:153:ASN:HD21	7:M:178:VAL:HG23	1.71	0.55
7:M:191:PHE:CD1	7:M:191:PHE:N	2.73	0.55
7:N:153:ASN:HD21	7:N:178:VAL:HG23	1.71	0.55
7:N:198:GLU:HB3	7:N:269:LYS:HB2	1.88	0.55
7:Q:191:PHE:CD1	7:Q:191:PHE:N	2.73	0.55
7:Q:198:GLU:HB3	7:Q:269:LYS:HB2	1.88	0.55
7:T:189:LYS:CE	7:T:191:PHE:HE1	2.15	0.55
7:J:370:PHE:HB2	7:J:373:ILE:C	2.28	0.55
7:N:372:GLU:OE1	7:O:223:THR:O	2.25	0.55
7:O:370:PHE:CG	7:O:373:ILE:CD1	2.89	0.55
7:S:394:ASN:HB2	7:T:201:GLU:HB2	1.88	0.55
1:A:171:VAL:HG21	1:A:199:TRP:HZ3	1.71	0.55
3:D:185:SER:HB2	6:B:207:GLU:H	1.72	0.55
7:J:198:GLU:HB3	7:J:269:LYS:HB2	1.88	0.55
7:L:370:PHE:CG	7:L:373:ILE:CD1	2.89	0.55
7:U:370:PHE:CG	7:U:373:ILE:CD1	2.89	0.55
7:V:392:ALA:O	7:W:202:ALA:HA	2.07	0.55
7:W:189:LYS:CE	7:W:191:PHE:HE1	2.15	0.55
9:Z:1:NAG:H3	9:Z:1:NAG:H83	1.88	0.55
2:C:147:SER:O	2:C:157:ARG:NH1	2.40	0.55
3:D:142:ASN:HA	3:D:154:ARG:HA	1.89	0.55
5:F:264:THR:HG23	5:F:321:TYR:HB3	1.90	0.55
7:G:39:GLN:NE2	7:G:310:GLU:OE2	2.40	0.55
7:H:370:PHE:HB2	7:H:373:ILE:C	2.27	0.55
7:M:64:ARG:NH1	7:N:461:VAL:HB	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:153:ASN:HD21	7:O:178:VAL:HG23	1.71	0.55
7:V:398:GLU:O	7:W:197:GLU:CB	2.54	0.55
7:W:370:PHE:CD2	7:W:373:ILE:C	2.81	0.55
3:D:552:HIS:HB2	3:D:556:LEU:HD23	1.89	0.54
7:G:206:ILE:HB	7:G:261:LEU:HB2	1.89	0.54
7:G:413:ARG:HG2	7:P:438:ALA:HB1	1.88	0.54
7:P:356:ILE:HB	7:P:387:ARG:HB2	1.89	0.54
7:I:270:GLU:HB3	7:I:343:LYS:HB2	1.89	0.54
7:J:191:PHE:HD1	7:J:191:PHE:N	2.01	0.54
7:L:372:GLU:HB3	7:M:223:THR:C	2.26	0.54
7:S:391:ARG:HE	7:T:204:LYS:HE2	1.71	0.54
5:F:250:ASN:HB3	5:F:335:LEU:HB2	1.88	0.54
5:F:365:SER:HB3	7:G:215:ASN:H	1.72	0.54
6:B:198:HIS:N	6:B:204:PRO:O	2.31	0.54
7:H:270:GLU:HB3	7:H:343:LYS:HB2	1.88	0.54
7:K:270:GLU:HB3	7:K:343:LYS:HB2	1.88	0.54
7:L:189:LYS:CE	7:L:191:PHE:HE1	2.15	0.54
7:Q:189:LYS:CE	7:Q:191:PHE:HE1	2.15	0.54
7:T:198:GLU:HB3	7:T:269:LYS:HB2	1.88	0.54
7:U:153:ASN:HD21	7:U:178:VAL:HG23	1.71	0.54
7:U:421:GLU:HB3	7:V:434:PHE:CD2	2.40	0.54
7:V:198:GLU:HB3	7:V:269:LYS:HB2	1.88	0.54
7:W:391:ARG:HE	7:X:204:LYS:HE2	1.73	0.54
6:B:324:ASN:OD1	6:B:370:SER:OG	2.25	0.54
7:L:402:ASP:HB2	7:M:193:THR:HG22	1.88	0.54
7:M:65:ARG:HB2	7:N:467:HIS:CE1	2.42	0.54
7:O:198:GLU:HB3	7:O:269:LYS:HB2	1.88	0.54
7:T:270:GLU:HB3	7:T:343:LYS:HB2	1.88	0.54
7:V:357:LYS:HE2	7:W:209:GLU:CD	2.28	0.54
5:F:244:SER:HB3	5:F:341:ASP:HB2	1.90	0.54
7:Q:386:LYS:HB3	7:R:209:GLU:H	1.72	0.54
7:R:153:ASN:HD21	7:R:178:VAL:HG23	1.71	0.54
7:S:421:GLU:OE1	7:T:434:PHE:HB2	2.07	0.54
7:V:391:ARG:HH22	7:W:202:ALA:HB1	1.72	0.54
1:A:1360:HIS:NE2	6:B:667:ASP:OD2	2.41	0.54
7:K:380:ASN:O	7:L:214:PHE:CD1	2.60	0.54
7:K:391:ARG:HE	7:L:204:LYS:HE2	1.73	0.54
7:M:65:ARG:HD2	7:N:467:HIS:HD2	1.60	0.54
7:O:370:PHE:HB2	7:O:373:ILE:C	2.27	0.54
7:U:378:GLU:HB3	7:V:217:ALA:H	1.72	0.54
7:W:198:GLU:HB2	7:W:269:LYS:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:W:386:LYS:HE2	7:X:207:ILE:HG23	1.89	0.54
2:C:163:GLU:HG3	3:D:275:PRO:HG2	1.88	0.54
7:G:282:LEU:HD13	7:G:445:PRO:HB3	1.89	0.54
7:P:270:GLU:O	7:P:343:LYS:N	2.35	0.54
7:P:514:GLU:CG	7:P:522:LYS:HD2	2.38	0.54
7:I:191:PHE:CD1	7:I:191:PHE:N	2.73	0.54
7:I:417:PHE:CZ	7:J:280:ILE:HG13	2.43	0.54
7:M:370:PHE:HB2	7:M:373:ILE:C	2.27	0.54
7:N:395:ILE:HA	7:O:199:GLN:O	2.07	0.54
7:R:370:PHE:HB2	7:R:373:ILE:C	2.28	0.54
7:S:391:ARG:HH21	7:T:204:LYS:HE3	1.73	0.54
7:S:417:PHE:CZ	7:T:280:ILE:HG13	2.43	0.54
7:U:370:PHE:HB2	7:U:373:ILE:C	2.27	0.54
1:A:1286:SER:HB2	1:A:1287:THR:HA	1.89	0.54
5:F:117:PRO:HG3	7:G:164:ARG:HE	1.72	0.54
7:G:522:LYS:O	7:G:522:LYS:HG2	2.07	0.54
7:P:324:HIS:CE1	7:P:452:LEU:HD21	2.41	0.54
7:M:198:GLU:HB3	7:M:269:LYS:HB2	1.88	0.54
7:Q:370:PHE:CG	7:Q:373:ILE:CD1	2.89	0.54
7:V:358:ARG:O	7:V:385:VAL:N	2.32	0.54
7:W:153:ASN:HD21	7:W:178:VAL:HG23	1.71	0.54
5:F:231:LEU:HD23	5:F:232:LEU:CA	2.34	0.54
7:H:198:GLU:HB3	7:H:269:LYS:HB2	1.88	0.54
7:K:137:TYR:HB3	7:K:146:PRO:HB3	1.90	0.54
7:M:270:GLU:HB3	7:M:343:LYS:HB2	1.88	0.54
7:T:370:PHE:CG	7:T:373:ILE:CD1	2.89	0.54
7:V:370:PHE:HB2	7:V:373:ILE:C	2.27	0.54
7:X:153:ASN:HD21	7:X:178:VAL:HG23	1.71	0.54
1:A:127:PHE:HB2	1:A:146:TYR:HB2	1.90	0.54
1:A:430:VAL:HG21	1:A:453:ARG:HH21	1.72	0.54
5:F:389:ILE:N	7:G:191:PHE:O	2.28	0.54
7:N:130:GLU:OE2	7:O:165:ASP:CA	2.53	0.54
7:N:409:ARG:HA	7:O:186:LYS:HA	1.90	0.54
7:O:270:GLU:HB3	7:O:343:LYS:HB2	1.88	0.54
7:X:198:GLU:HB3	7:X:269:LYS:HB2	1.88	0.54
3:D:478:LYS:O	3:D:481:THR:OG1	2.24	0.54
5:F:470:GLY:N	5:F:485:CYS:SG	2.75	0.54
7:G:463:MET:HG2	7:G:464:LYS:H	1.73	0.54
7:K:153:ASN:HD21	7:K:178:VAL:HG23	1.71	0.54
7:R:391:ARG:HE	7:S:204:LYS:HE2	1.72	0.54
7:W:407:LEU:HB3	7:X:188:GLU:CB	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:798:GLU:HG2	1:A:816:LYS:HG3	1.90	0.53
7:M:137:TYR:HB3	7:M:146:PRO:HB3	1.90	0.53
7:V:376:GLY:O	7:W:218:ILE:HD12	2.08	0.53
7:W:270:GLU:HB3	7:W:343:LYS:HB2	1.88	0.53
1:A:182:ILE:HD13	1:A:601:ALA:HB2	1.91	0.53
5:F:242:ASP:HB2	5:F:343:THR:HB	1.89	0.53
7:H:137:TYR:HB3	7:H:146:PRO:HB3	1.90	0.53
7:L:386:LYS:HE2	7:M:207:ILE:HG23	1.91	0.53
7:N:148:SER:HB3	7:O:180:SER:HB2	1.90	0.53
7:T:35:PRO:HG3	7:T:71:GLU:HB2	1.90	0.53
7:U:191:PHE:CD1	7:U:191:PHE:N	2.73	0.53
7:X:137:TYR:HB3	7:X:146:PRO:HB3	1.90	0.53
7:X:270:GLU:HB3	7:X:343:LYS:HB2	1.89	0.53
6:B:713:LEU:HB2	6:B:715:ILE:HB	1.91	0.53
7:P:83:ASP:HB3	7:P:92:ILE:HG23	1.90	0.53
7:P:521:SER:O	7:P:522:LYS:HB3	2.08	0.53
7:I:137:TYR:HB3	7:I:146:PRO:HB3	1.90	0.53
7:I:333:GLY:H	7:I:448:ILE:HD11	1.74	0.53
7:J:130:GLU:CG	7:K:165:ASP:HA	2.39	0.53
7:J:412:THR:HA	7:K:167:ASN:OD1	2.08	0.53
7:Q:137:TYR:HB3	7:Q:146:PRO:HB3	1.90	0.53
7:Q:411:GLY:O	7:R:185:THR:HG21	2.08	0.53
7:R:411:GLY:O	7:S:185:THR:HG21	2.08	0.53
7:T:411:GLY:O	7:U:185:THR:HG21	2.08	0.53
7:U:137:TYR:HB3	7:U:146:PRO:HB3	1.90	0.53
7:W:398:GLU:HB3	7:X:197:GLU:HB3	1.90	0.53
7:X:370:PHE:HB2	7:X:373:ILE:C	2.27	0.53
1:A:975:ARG:HB2	1:A:1340:VAL:HB	1.90	0.53
2:C:9:ILE:HD11	2:C:40:GLN:HB3	1.91	0.53
2:C:189:ASN:HB2	3:D:359:ALA:HB3	1.90	0.53
6:B:372:GLY:N	6:B:481:ALA:O	2.42	0.53
7:H:35:PRO:HG3	7:H:71:GLU:HB2	1.91	0.53
7:I:35:PRO:HG3	7:I:71:GLU:HB2	1.91	0.53
7:I:65:ARG:HB2	7:J:467:HIS:CE1	2.43	0.53
7:I:400:LEU:HD12	7:J:195:HIS:HB2	1.90	0.53
7:L:391:ARG:NE	7:M:204:LYS:HE2	2.23	0.53
7:O:35:PRO:HG3	7:O:71:GLU:HB2	1.91	0.53
7:S:370:PHE:HB2	7:S:373:ILE:C	2.28	0.53
1:A:469:TRP:HE1	1:A:473:HIS:HA	1.73	0.53
7:H:391:ARG:NE	7:I:204:LYS:HE2	2.23	0.53
7:S:137:TYR:HB3	7:S:146:PRO:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:137:TYR:HB3	7:T:146:PRO:HB3	1.90	0.53
7:U:35:PRO:HG3	7:U:71:GLU:HB2	1.91	0.53
7:G:140:ASN:HA	7:G:323:THR:HG22	1.91	0.53
7:H:370:PHE:CG	7:H:373:ILE:CD1	2.89	0.53
7:K:370:PHE:HB2	7:K:373:ILE:C	2.28	0.53
7:L:400:LEU:O	7:M:194:GLU:HB2	2.09	0.53
7:M:333:GLY:H	7:M:448:ILE:HD11	1.74	0.53
7:N:137:TYR:HB3	7:N:146:PRO:HB3	1.90	0.53
7:O:380:ASN:HD22	7:Q:215:ASN:CB	2.21	0.53
7:Q:35:PRO:HG3	7:Q:71:GLU:HB2	1.91	0.53
7:Q:421:GLU:OE1	7:R:434:PHE:HB2	2.09	0.53
7:R:137:TYR:HB3	7:R:146:PRO:HB3	1.91	0.53
7:S:35:PRO:HG3	7:S:71:GLU:HB2	1.91	0.53
7:V:35:PRO:HG3	7:V:71:GLU:HB2	1.91	0.53
7:X:333:GLY:H	7:X:448:ILE:HD11	1.74	0.53
1:A:132:LYS:NZ	1:A:134:VAL:O	2.42	0.53
7:I:406:SER:O	7:J:188:GLU:HB2	2.09	0.53
7:R:130:GLU:HG3	7:S:164:ARG:O	2.08	0.53
7:T:370:PHE:HB2	7:T:373:ILE:C	2.27	0.53
5:F:229:SER:HB2	5:F:356:ASP:CG	2.28	0.53
5:F:328:ASP:N	5:F:386:VAL:O	2.41	0.53
7:G:83:ASP:HB3	7:G:92:ILE:HG23	1.90	0.53
7:G:191:PHE:HA	7:G:276:VAL:HG12	1.90	0.53
7:K:35:PRO:HG3	7:K:71:GLU:HB2	1.91	0.53
7:K:391:ARG:HH21	7:L:204:LYS:CE	2.21	0.53
7:M:463:MET:HG2	7:M:464:LYS:H	1.74	0.53
7:N:35:PRO:HG3	7:N:71:GLU:HB2	1.91	0.53
7:N:333:GLY:H	7:N:448:ILE:HD11	1.74	0.53
7:O:333:GLY:H	7:O:448:ILE:HD11	1.74	0.53
7:Q:463:MET:HG2	7:Q:464:LYS:H	1.74	0.53
1:A:971:THR:HG21	1:A:1366:HIS:HB2	1.91	0.53
3:D:225:PHE:CD1	3:D:342:TRP:CD1	2.91	0.53
7:G:337:LEU:HD22	7:G:423:LEU:HD21	1.90	0.53
7:P:514:GLU:HG3	7:P:522:LYS:HD2	1.90	0.53
7:H:333:GLY:H	7:H:448:ILE:HD11	1.74	0.53
7:J:333:GLY:H	7:J:448:ILE:HD11	1.74	0.53
7:J:463:MET:HG2	7:J:464:LYS:H	1.74	0.53
7:J:514:GLU:HG2	7:J:515:GLY:H	1.74	0.53
7:L:35:PRO:HG3	7:L:71:GLU:HB2	1.91	0.53
7:Q:417:PHE:CZ	7:R:280:ILE:HG13	2.44	0.53
7:S:333:GLY:H	7:S:448:ILE:HD11	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:370:PHE:CG	7:S:373:ILE:CD1	2.89	0.53
7:S:372:GLU:CD	7:T:223:THR:O	2.47	0.53
7:V:191:PHE:CD1	7:V:191:PHE:N	2.73	0.53
1:A:275:LEU:HB3	1:A:322:TYR:HE2	1.73	0.53
3:D:48:ARG:HH11	3:D:69:GLU:HB3	1.73	0.53
7:N:340:VAL:N	7:N:403:ASP:O	2.39	0.53
7:T:380:ASN:HD22	7:U:215:ASN:CB	2.15	0.53
7:U:333:GLY:H	7:U:448:ILE:HD11	1.74	0.53
7:V:413:ARG:C	7:W:435:VAL:HG13	2.28	0.53
7:X:35:PRO:HG3	7:X:71:GLU:HB2	1.91	0.53
1:A:192:SER:HB3	1:A:976:ILE:HD11	1.91	0.52
3:D:280:LEU:HD12	3:D:283:LEU:HD12	1.91	0.52
7:N:129:SER:HA	7:O:164:ARG:CZ	2.38	0.52
7:N:391:ARG:HH22	7:O:202:ALA:HB1	1.72	0.52
7:O:514:GLU:HG2	7:O:515:GLY:H	1.74	0.52
7:Q:19:HIS:NE2	7:R:487:ARG:HD2	2.23	0.52
7:Q:514:GLU:HG2	7:Q:515:GLY:H	1.74	0.52
7:R:35:PRO:HG3	7:R:71:GLU:HB2	1.91	0.52
7:S:514:GLU:HG2	7:S:515:GLY:H	1.74	0.52
7:V:463:MET:HG2	7:V:464:LYS:H	1.74	0.52
7:W:137:TYR:HB3	7:W:146:PRO:HB3	1.90	0.52
7:H:374:SER:O	7:I:220:LEU:HD12	2.08	0.52
7:L:463:MET:HG2	7:L:464:LYS:H	1.74	0.52
7:M:340:VAL:N	7:M:403:ASP:O	2.39	0.52
7:M:362:TYR:HB3	7:M:381:LYS:HB3	1.92	0.52
7:N:362:TYR:HB3	7:N:381:LYS:HB3	1.92	0.52
7:Q:370:PHE:HB2	7:Q:373:ILE:C	2.28	0.52
7:R:362:TYR:HB3	7:R:381:LYS:HB3	1.92	0.52
7:T:333:GLY:H	7:T:448:ILE:HD11	1.74	0.52
7:T:421:GLU:OE1	7:U:434:PHE:CD2	2.62	0.52
7:T:514:GLU:HG2	7:T:515:GLY:H	1.74	0.52
7:U:463:MET:HG2	7:U:464:LYS:H	1.74	0.52
7:U:514:GLU:HG2	7:U:515:GLY:H	1.74	0.52
7:V:333:GLY:H	7:V:448:ILE:HD11	1.74	0.52
7:W:35:PRO:HG3	7:W:71:GLU:HB2	1.91	0.52
7:W:463:MET:HG2	7:W:464:LYS:H	1.74	0.52
7:X:463:MET:HG2	7:X:464:LYS:H	1.74	0.52
1:A:59:TYR:HB2	1:A:100:SER:HB3	1.90	0.52
6:B:233:PRO:HD2	6:B:236:LEU:HD12	1.91	0.52
7:L:411:GLY:O	7:M:185:THR:HG21	2.10	0.52
7:M:514:GLU:HG2	7:M:515:GLY:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:409:ARG:HD3	7:Q:184:GLU:OE2	2.10	0.52
7:R:391:ARG:HH21	7:S:204:LYS:HE3	1.72	0.52
7:V:64:ARG:CD	7:W:290:ARG:CB	2.88	0.52
7:W:406:SER:O	7:X:188:GLU:CB	2.51	0.52
4:E:42:PHE:HB2	5:F:166:ARG:HD2	1.91	0.52
7:G:514:GLU:HG2	7:G:515:GLY:H	1.75	0.52
7:H:270:GLU:O	7:H:343:LYS:N	2.40	0.52
7:I:463:MET:HG2	7:I:464:LYS:H	1.74	0.52
7:K:411:GLY:O	7:L:185:THR:CG2	2.57	0.52
7:K:514:GLU:HG2	7:K:515:GLY:H	1.74	0.52
7:L:406:SER:O	7:M:188:GLU:HB2	2.08	0.52
7:O:362:TYR:HB3	7:O:381:LYS:HB3	1.92	0.52
7:Q:270:GLU:O	7:Q:343:LYS:N	2.39	0.52
7:W:370:PHE:HB2	7:W:373:ILE:C	2.28	0.52
1:A:430:VAL:HG12	1:A:455:ILE:HA	1.90	0.52
6:B:649:PRO:HB2	6:B:653:GLY:HA2	1.90	0.52
7:G:309:TYR:H	7:G:472:ASN:HD21	1.58	0.52
7:G:358:ARG:O	7:G:385:VAL:N	2.40	0.52
7:J:137:TYR:HB3	7:J:146:PRO:HB3	1.90	0.52
7:N:514:GLU:HG2	7:N:515:GLY:H	1.74	0.52
7:Q:362:TYR:HB3	7:Q:381:LYS:HB3	1.92	0.52
7:R:64:ARG:NH2	7:S:459:VAL:O	2.43	0.52
7:R:372:GLU:CD	7:S:223:THR:O	2.45	0.52
7:S:340:VAL:N	7:S:403:ASP:O	2.39	0.52
7:S:362:TYR:HB3	7:S:381:LYS:HB3	1.92	0.52
7:T:370:PHE:CD2	7:T:373:ILE:C	2.81	0.52
7:T:372:GLU:HG3	7:U:224:PRO:HA	1.90	0.52
1:A:363:LEU:HD13	1:A:431:LEU:HD23	1.91	0.52
1:A:473:HIS:N	1:A:474:LYS:HA	2.25	0.52
7:G:523:GLN:O	7:G:523:GLN:HG2	2.10	0.52
7:M:64:ARG:O	7:N:467:HIS:CG	2.61	0.52
7:R:270:GLU:O	7:R:343:LYS:N	2.39	0.52
7:R:340:VAL:N	7:R:403:ASP:O	2.39	0.52
7:S:19:HIS:NE2	7:T:487:ARG:HD2	2.25	0.52
7:S:191:PHE:HD1	7:S:191:PHE:N	2.01	0.52
7:S:378:GLU:OE1	7:T:217:ALA:HB3	2.09	0.52
7:S:463:MET:HG2	7:S:464:LYS:H	1.74	0.52
7:V:528:GLY:HA2	7:W:200:ILE:HD13	1.90	0.52
7:W:129:SER:HB2	7:X:164:ARG:HH11	1.73	0.52
7:W:404:VAL:CB	7:X:191:PHE:HB2	2.37	0.52
6:B:322:VAL:HG12	6:B:323:LEU:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:442:SER:HB2	6:B:459:LYS:NZ	2.24	0.52
7:G:324:HIS:CE1	7:G:452:LEU:HD11	2.45	0.52
7:P:35:PRO:HG3	7:P:71:GLU:HB2	1.92	0.52
7:P:374:SER:CB	7:H:220:LEU:HD12	2.35	0.52
7:P:514:GLU:HG2	7:P:515:GLY:H	1.75	0.52
7:H:370:PHE:CD2	7:H:373:ILE:C	2.80	0.52
7:K:391:ARG:NE	7:L:204:LYS:HE2	2.25	0.52
7:L:137:TYR:HB3	7:L:146:PRO:HB3	1.90	0.52
7:N:191:PHE:CD1	7:N:191:PHE:N	2.73	0.52
7:O:463:MET:HG2	7:O:464:LYS:H	1.74	0.52
7:R:463:MET:HG2	7:R:464:LYS:H	1.74	0.52
3:D:220:ARG:HG2	3:D:228:SER:HA	1.92	0.52
7:P:255:LYS:HG3	7:P:358:ARG:HG2	1.90	0.52
7:P:463:MET:HG2	7:P:464:LYS:H	1.74	0.52
7:L:370:PHE:HB2	7:L:373:ILE:C	2.27	0.52
7:L:446:VAL:HG21	7:M:184:GLU:HG3	1.91	0.52
7:T:362:TYR:HB3	7:T:381:LYS:HB3	1.92	0.52
7:V:362:TYR:HB3	7:V:381:LYS:HB3	1.92	0.52
7:V:388:GLY:O	7:W:206:ILE:HG23	2.09	0.52
7:W:191:PHE:CD1	7:W:191:PHE:N	2.73	0.52
7:W:372:GLU:HG3	7:X:223:THR:O	2.10	0.52
7:W:391:ARG:HH21	7:X:204:LYS:CE	2.21	0.52
7:W:417:PHE:CG	7:X:280:ILE:HD12	2.45	0.52
7:P:193:THR:HA	7:P:274:LEU:HB3	1.90	0.52
7:H:514:GLU:HG2	7:H:515:GLY:H	1.74	0.52
7:I:131:LEU:HG	7:I:132:ALA:H	1.75	0.52
7:I:370:PHE:HB2	7:I:373:ILE:C	2.27	0.52
7:J:35:PRO:HG3	7:J:71:GLU:HB2	1.91	0.52
7:J:83:ASP:HB3	7:J:92:ILE:HG23	1.92	0.52
7:N:400:LEU:HD12	7:O:195:HIS:CD2	2.45	0.52
7:R:191:PHE:CD1	7:R:191:PHE:N	2.73	0.52
5:F:320:ILE:O	5:F:394:ARG:N	2.41	0.52
7:G:92:ILE:HB	7:G:96:LEU:HB3	1.92	0.52
7:H:362:TYR:HB3	7:H:381:LYS:HB3	1.92	0.52
7:I:83:ASP:HB3	7:I:92:ILE:HG23	1.92	0.52
7:I:362:TYR:HB3	7:I:381:LYS:HB3	1.92	0.52
7:K:463:MET:HG2	7:K:464:LYS:H	1.74	0.52
7:N:463:MET:HG2	7:N:464:LYS:H	1.74	0.52
7:R:333:GLY:H	7:R:448:ILE:HD11	1.74	0.52
7:S:411:GLY:O	7:T:185:THR:HG21	2.10	0.52
7:V:137:TYR:HB3	7:V:146:PRO:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:W:391:ARG:NE	7:X:204:LYS:HE2	2.25	0.52
7:W:514:GLU:HG2	7:W:515:GLY:H	1.74	0.52
2:C:322:HIS:NE2	2:C:324:CYS:SG	2.83	0.51
3:D:42:CYS:N	3:D:79:CYS:SG	2.83	0.51
6:B:654:PHE:HB2	6:B:673:LEU:HD23	1.92	0.51
6:B:738:VAL:HG11	6:B:759:LEU:HB2	1.92	0.51
7:P:270:GLU:HB3	7:P:343:LYS:HB2	1.91	0.51
7:P:413:ARG:HD3	7:H:280:ILE:HD11	1.92	0.51
7:J:92:ILE:HB	7:J:96:LEU:HB3	1.92	0.51
7:J:270:GLU:O	7:J:343:LYS:N	2.40	0.51
7:J:320:THR:HG23	7:K:288:ARG:HG3	1.92	0.51
7:O:380:ASN:HD22	7:Q:215:ASN:HD22	1.58	0.51
7:Q:333:GLY:H	7:Q:448:ILE:HD11	1.74	0.51
7:Q:391:ARG:HH21	7:R:204:LYS:HE3	1.73	0.51
7:T:83:ASP:HB3	7:T:92:ILE:HG23	1.92	0.51
7:T:191:PHE:HD1	7:T:191:PHE:N	2.01	0.51
7:U:83:ASP:HB3	7:U:92:ILE:HG23	1.92	0.51
7:W:92:ILE:HB	7:W:96:LEU:HB3	1.92	0.51
2:C:386:TYR:CE2	2:C:388:GLU:HB3	2.45	0.51
6:B:287:SER:OG	6:B:406:LYS:HE2	2.10	0.51
7:G:35:PRO:HG3	7:G:71:GLU:HB2	1.92	0.51
7:G:301:ASP:OD1	7:P:288:ARG:NH2	2.43	0.51
7:H:463:MET:HG2	7:H:464:LYS:H	1.74	0.51
7:I:409:ARG:HA	7:J:186:LYS:HA	1.91	0.51
7:K:270:GLU:O	7:K:343:LYS:N	2.39	0.51
7:K:362:TYR:HB3	7:K:381:LYS:HB3	1.92	0.51
7:L:362:TYR:HB3	7:L:381:LYS:HB3	1.92	0.51
7:M:35:PRO:HG3	7:M:71:GLU:HB2	1.91	0.51
7:Q:92:ILE:HB	7:Q:96:LEU:HB3	1.92	0.51
7:Q:400:LEU:HD12	7:R:195:HIS:CB	2.35	0.51
7:V:131:LEU:HG	7:V:132:ALA:H	1.75	0.51
1:A:283:MET:HB2	1:A:285:THR:N	2.25	0.51
2:C:374:ARG:HG2	5:F:190:LEU:HG	1.91	0.51
3:D:194:ASN:ND2	6:B:456:ALA:O	2.41	0.51
7:M:83:ASP:HB3	7:M:92:ILE:HG23	1.92	0.51
7:O:137:TYR:HB3	7:O:146:PRO:HB3	1.91	0.51
7:U:374:SER:O	7:V:220:LEU:HD13	2.01	0.51
7:V:92:ILE:HB	7:V:96:LEU:HB3	1.93	0.51
7:V:514:GLU:HG2	7:V:515:GLY:H	1.74	0.51
7:X:83:ASP:HB3	7:X:92:ILE:HG23	1.92	0.51
1:A:322:TYR:HB3	1:A:344:GLY:HA3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:249:GLN:NE2	3:D:494:ASN:OD1	2.43	0.51
5:F:406:GLN:HG3	5:F:407:ASN:N	2.25	0.51
7:I:297:THR:CG2	7:J:288:ARG:CZ	2.88	0.51
7:I:421:GLU:OE1	7:J:434:PHE:HB2	2.10	0.51
7:J:320:THR:CG2	7:K:288:ARG:HG3	2.40	0.51
7:J:370:PHE:CD2	7:J:373:ILE:C	2.80	0.51
7:K:92:ILE:HB	7:K:96:LEU:HB3	1.93	0.51
7:K:333:GLY:H	7:K:448:ILE:HD11	1.74	0.51
7:K:391:ARG:HH22	7:L:202:ALA:HB1	1.75	0.51
7:L:266:SER:HB3	7:L:347:LYS:HB2	1.92	0.51
7:L:514:GLU:HG2	7:L:515:GLY:H	1.74	0.51
7:O:392:ALA:HB3	7:Q:203:PHE:H	1.75	0.51
7:T:463:MET:HG2	7:T:464:LYS:H	1.74	0.51
7:W:404:VAL:HB	7:X:191:PHE:CB	2.39	0.51
7:X:514:GLU:HG2	7:X:515:GLY:H	1.74	0.51
3:D:191:LYS:HA	6:B:445:ARG:HA	1.91	0.51
7:P:137:TYR:HB3	7:P:146:PRO:HB3	1.93	0.51
7:J:55:LYS:HE3	7:K:481:ILE:HG23	1.92	0.51
7:J:64:ARG:HD2	7:K:461:VAL:HG23	1.91	0.51
7:J:130:GLU:HA	7:K:164:ARG:O	2.10	0.51
7:K:83:ASP:HB3	7:K:92:ILE:HG23	1.92	0.51
7:L:92:ILE:HB	7:L:96:LEU:HB3	1.92	0.51
7:O:191:PHE:CD1	7:O:191:PHE:N	2.73	0.51
7:S:64:ARG:NH2	7:T:459:VAL:O	2.43	0.51
7:S:130:GLU:HG3	7:T:165:ASP:HA	1.92	0.51
7:U:400:LEU:HD12	7:V:195:HIS:CG	2.45	0.51
7:V:83:ASP:HB3	7:V:92:ILE:HG23	1.92	0.51
7:W:270:GLU:O	7:W:343:LYS:N	2.39	0.51
7:X:260:GLN:HB3	7:X:353:LEU:HB3	1.93	0.51
1:A:844:THR:OG1	1:A:893:SER:OG	2.21	0.51
6:B:59:ASN:O	6:B:388:ASN:ND2	2.44	0.51
6:B:712:VAL:HG21	6:B:759:LEU:HD11	1.93	0.51
7:P:257:GLU:HA	7:P:356:ILE:HA	1.92	0.51
7:H:30:TRP:HH2	7:I:467:HIS:NE2	2.08	0.51
7:L:131:LEU:HG	7:L:132:ALA:H	1.75	0.51
7:Q:266:SER:HB3	7:Q:347:LYS:HB2	1.93	0.51
7:S:409:ARG:HD3	7:T:184:GLU:OE2	2.11	0.51
7:U:92:ILE:HB	7:U:96:LEU:HB3	1.92	0.51
7:U:417:PHE:CZ	7:V:280:ILE:HG13	2.45	0.51
1:A:120:THR:HG22	1:A:122:ASP:H	1.75	0.51
7:J:131:LEU:HG	7:J:132:ALA:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:131:LEU:HG	7:K:132:ALA:H	1.76	0.51
7:L:83:ASP:HB3	7:L:92:ILE:HG23	1.92	0.51
7:L:372:GLU:CD	7:M:223:THR:O	2.46	0.51
7:N:131:LEU:HG	7:N:132:ALA:H	1.75	0.51
7:O:131:LEU:HG	7:O:132:ALA:H	1.75	0.51
7:O:260:GLN:HB3	7:O:353:LEU:HB3	1.93	0.51
7:Q:260:GLN:HB3	7:Q:353:LEU:HB3	1.93	0.51
7:S:131:LEU:HG	7:S:132:ALA:H	1.75	0.51
7:X:191:PHE:CD1	7:X:191:PHE:N	2.73	0.51
7:X:266:SER:HB3	7:X:347:LYS:HB2	1.92	0.51
3:D:344:PHE:HD2	3:D:345:VAL:HG23	1.76	0.51
5:F:342:ILE:HG23	5:F:372:PHE:HB2	1.92	0.51
7:I:260:GLN:HB3	7:I:353:LEU:HB3	1.93	0.51
7:J:260:GLN:HB3	7:J:353:LEU:HB3	1.93	0.51
7:M:260:GLN:HB3	7:M:353:LEU:HB3	1.93	0.51
7:N:400:LEU:O	7:O:194:GLU:HB2	2.10	0.51
7:O:92:ILE:HB	7:O:96:LEU:HB3	1.92	0.51
7:Q:374:SER:HB3	7:R:221:LYS:HG2	1.93	0.51
7:U:131:LEU:HG	7:U:132:ALA:H	1.75	0.51
7:U:387:ARG:HA	7:V:208:GLN:HE22	1.75	0.51
7:W:266:SER:HB3	7:W:347:LYS:HB2	1.93	0.51
7:W:362:TYR:HB3	7:W:381:LYS:HB3	1.92	0.51
7:W:409:ARG:HA	7:X:185:THR:O	2.10	0.51
2:C:380:HIS:CE1	2:C:398:TRP:HD1	2.28	0.51
3:D:55:TYR:OH	3:D:451:GLU:O	2.29	0.51
7:P:341:LEU:HD11	7:P:343:LYS:HE3	1.93	0.51
7:H:131:LEU:HG	7:H:132:ALA:H	1.75	0.51
7:I:92:ILE:HB	7:I:96:LEU:HB3	1.92	0.51
7:J:340:VAL:N	7:J:403:ASP:O	2.39	0.51
7:K:191:PHE:CD1	7:K:191:PHE:N	2.73	0.51
7:K:309:TYR:H	7:K:472:ASN:HD21	1.59	0.51
7:M:131:LEU:HG	7:M:132:ALA:H	1.75	0.51
7:N:413:ARG:NH1	7:O:282:LEU:C	2.63	0.51
7:Q:83:ASP:HB3	7:Q:92:ILE:HG23	1.92	0.51
7:Q:372:GLU:O	7:R:222:PHE:HA	2.10	0.51
7:R:514:GLU:HG2	7:R:515:GLY:H	1.74	0.51
7:V:376:GLY:O	7:W:218:ILE:CG1	2.59	0.51
7:W:131:LEU:HG	7:W:132:ALA:H	1.76	0.51
7:W:404:VAL:HB	7:X:191:PHE:N	2.26	0.51
7:X:340:VAL:N	7:X:403:ASP:O	2.39	0.51
1:A:640:LEU:HG	1:A:641:ASN:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:187:ILE:HD11	6:B:232:VAL:HG22	1.93	0.51
7:J:64:ARG:HD2	7:K:461:VAL:HG21	1.93	0.51
7:K:148:SER:HB3	7:L:180:SER:HB2	1.92	0.51
7:O:266:SER:HB3	7:O:347:LYS:HB2	1.93	0.51
7:R:266:SER:HB3	7:R:347:LYS:HB2	1.93	0.51
7:R:394:ASN:HB2	7:S:201:GLU:HB2	1.92	0.51
7:R:406:SER:O	7:S:188:GLU:HB2	2.11	0.51
7:V:260:GLN:HB3	7:V:353:LEU:HB3	1.93	0.51
7:W:83:ASP:HB3	7:W:92:ILE:HG23	1.92	0.51
7:W:333:GLY:H	7:W:448:ILE:HD11	1.74	0.51
7:X:362:TYR:HB3	7:X:381:LYS:HB3	1.92	0.51
3:D:92:PHE:HB2	3:D:114:ALA:HB2	1.93	0.50
3:D:225:PHE:CE1	3:D:342:TRP:CA	2.92	0.50
7:G:363:HIS:ND1	7:G:380:ASN:OD1	2.36	0.50
7:I:413:ARG:HH11	7:J:282:LEU:C	2.09	0.50
7:I:514:GLU:HG2	7:I:515:GLY:H	1.74	0.50
7:J:266:SER:HB3	7:J:347:LYS:HB2	1.93	0.50
7:J:362:TYR:HB3	7:J:381:LYS:HB3	1.92	0.50
7:K:129:SER:HB2	7:L:164:ARG:NH1	2.25	0.50
7:N:260:GLN:HB3	7:N:353:LEU:HB3	1.93	0.50
7:S:380:ASN:ND2	7:T:215:ASN:HB2	2.21	0.50
7:T:260:GLN:HB3	7:T:353:LEU:HB3	1.93	0.50
7:T:386:LYS:HB3	7:U:209:GLU:H	1.77	0.50
7:U:362:TYR:HB3	7:U:381:LYS:HB3	1.92	0.50
7:W:130:GLU:HG3	7:X:164:ARG:C	2.32	0.50
7:W:407:LEU:HA	7:X:187:GLY:O	2.10	0.50
1:A:1185:THR:HB	1:A:1230:ASP:HA	1.93	0.50
6:B:586:THR:CB	7:X:107:PHE:HD2	2.10	0.50
7:I:413:ARG:CZ	7:J:282:LEU:CG	2.88	0.50
7:L:127:GLU:HG2	7:M:164:ARG:HH22	1.76	0.50
7:L:333:GLY:H	7:L:448:ILE:HD11	1.74	0.50
7:L:526:SER:HB2	7:M:198:GLU:OE2	2.10	0.50
7:M:130:GLU:HG3	7:N:164:ARG:O	2.11	0.50
7:Q:131:LEU:HG	7:Q:132:ALA:H	1.75	0.50
7:S:92:ILE:HB	7:S:96:LEU:HB3	1.92	0.50
7:X:92:ILE:HB	7:X:96:LEU:HB3	1.93	0.50
1:A:1079:THR:HG21	1:A:1107:LEU:HD11	1.93	0.50
2:C:70:GLY:HA2	2:C:82:ARG:HH11	1.77	0.50
4:E:79:VAL:HA	4:E:177:LEU:HB3	1.93	0.50
6:B:138:ALA:O	6:B:141:LYS:NZ	2.42	0.50
7:P:260:GLN:HB3	7:P:353:LEU:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:266:SER:HB3	7:K:347:LYS:HB2	1.93	0.50
7:M:370:PHE:CG	7:M:373:ILE:CD1	2.89	0.50
7:N:130:GLU:OE2	7:O:166:GLY:N	2.43	0.50
7:N:370:PHE:HB2	7:N:373:ILE:C	2.27	0.50
7:R:92:ILE:HB	7:R:96:LEU:HB3	1.93	0.50
7:S:266:SER:HB3	7:S:347:LYS:HB2	1.92	0.50
1:A:581:ALA:HB1	1:A:820:PHE:HB3	1.93	0.50
1:A:1112:GLN:HE22	1:A:1167:ALA:HA	1.76	0.50
1:A:1231:ASN:HB2	1:A:1246:ARG:HH21	1.77	0.50
7:H:83:ASP:HB3	7:H:92:ILE:HG23	1.92	0.50
7:K:347:LYS:HG2	7:K:396:THR:HG23	1.94	0.50
7:O:270:GLU:O	7:O:343:LYS:N	2.39	0.50
7:R:83:ASP:HB3	7:R:92:ILE:HG23	1.92	0.50
7:R:347:LYS:HG2	7:R:396:THR:HG23	1.94	0.50
7:U:309:TYR:H	7:U:472:ASN:HD21	1.60	0.50
7:V:266:SER:HB3	7:V:347:LYS:HB2	1.93	0.50
7:V:309:TYR:H	7:V:472:ASN:HD21	1.60	0.50
7:X:131:LEU:HG	7:X:132:ALA:H	1.75	0.50
2:C:377:ALA:HA	2:C:381:ILE:HG21	1.94	0.50
3:D:188:PHE:H	6:B:192:LEU:HD11	1.77	0.50
7:I:64:ARG:HG2	7:J:470:LYS:HZ2	1.77	0.50
7:I:266:SER:HB3	7:I:347:LYS:HB2	1.93	0.50
7:K:130:GLU:CG	7:L:165:ASP:HA	2.42	0.50
7:N:266:SER:HB3	7:N:347:LYS:HB2	1.93	0.50
7:T:92:ILE:HB	7:T:96:LEU:HB3	1.93	0.50
7:T:131:LEU:HG	7:T:132:ALA:H	1.76	0.50
7:T:266:SER:HB3	7:T:347:LYS:HB2	1.93	0.50
7:T:394:ASN:HB2	7:U:201:GLU:HB2	1.93	0.50
7:W:64:ARG:NH1	7:X:290:ARG:HE	2.10	0.50
7:W:64:ARG:HH11	7:X:290:ARG:CZ	2.25	0.50
1:A:955:ARG:NH2	1:A:1350:THR:O	2.45	0.50
2:C:92:CYS:H	2:C:97:ASP:HB2	1.76	0.50
6:B:95:PRO:HG2	6:B:97:ILE:O	2.11	0.50
7:L:347:LYS:HG2	7:L:396:THR:HG23	1.94	0.50
7:M:92:ILE:HB	7:M:96:LEU:HB3	1.93	0.50
7:R:260:GLN:HB3	7:R:353:LEU:HB3	1.93	0.50
7:V:64:ARG:HH22	7:W:292:VAL:HG12	1.75	0.50
7:V:347:LYS:HG2	7:V:396:THR:HG23	1.94	0.50
7:W:64:ARG:HH11	7:X:290:ARG:NE	2.08	0.50
2:C:239:LEU:O	2:C:303:THR:HA	2.11	0.50
2:C:510:ARG:NH1	2:C:529:PRO:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:35:GLN:HE22	5:F:38:LYS:HE3	1.76	0.50
5:F:85:CYS:HB3	5:F:103:VAL:HG11	1.93	0.50
5:F:259:PHE:HA	5:F:326:VAL:HA	1.94	0.50
6:B:219:LYS:HG3	6:B:232:VAL:HB	1.94	0.50
7:P:333:GLY:H	7:P:448:ILE:HD11	1.75	0.50
7:J:309:TYR:H	7:J:472:ASN:HD21	1.60	0.50
7:J:347:LYS:HG2	7:J:396:THR:HG23	1.94	0.50
7:M:266:SER:HB3	7:M:347:LYS:HB2	1.92	0.50
7:N:83:ASP:HB3	7:N:92:ILE:HG23	1.92	0.50
7:N:413:ARG:NH2	7:O:282:LEU:HG	2.26	0.50
7:R:19:HIS:NE2	7:S:487:ARG:HD2	2.27	0.50
7:S:270:GLU:O	7:S:343:LYS:N	2.39	0.50
7:U:270:GLU:O	7:U:343:LYS:N	2.40	0.50
7:U:347:LYS:HG2	7:U:396:THR:HG23	1.94	0.50
7:U:394:ASN:O	7:V:200:ILE:HA	2.11	0.50
7:W:260:GLN:HB3	7:W:353:LEU:HB3	1.93	0.50
1:A:1279:ARG:O	1:A:1281:GLY:HA2	2.12	0.50
5:F:216:ASP:O	5:F:241:GLN:N	2.45	0.50
5:F:400:TRP:CZ2	5:F:415:SER:HB2	2.46	0.50
5:F:489:CYS:HA	5:F:498:CYS:HB2	1.93	0.50
5:F:513:SER:OG	5:F:531:GLU:N	2.43	0.50
7:I:270:GLU:O	7:I:343:LYS:N	2.39	0.50
7:J:394:ASN:O	7:K:200:ILE:HA	2.11	0.50
7:N:380:ASN:HB2	7:O:215:ASN:HB2	1.94	0.50
7:Q:340:VAL:N	7:Q:403:ASP:O	2.39	0.50
7:V:372:GLU:O	7:W:222:PHE:HD1	1.95	0.50
1:A:394:THR:O	1:A:401:THR:OG1	2.30	0.50
1:A:1227:PHE:HE2	1:A:1229:LYS:HE3	1.77	0.50
7:G:137:TYR:HB3	7:G:146:PRO:HB3	1.94	0.50
7:P:310:GLU:HG2	7:P:313:GLU:H	1.77	0.50
7:H:65:ARG:HB2	7:I:467:HIS:ND1	2.27	0.50
7:H:347:LYS:HG2	7:H:396:THR:HG23	1.94	0.50
7:J:290:ARG:HG2	7:J:291:ASP:H	1.77	0.50
7:M:313:GLU:CG	7:N:290:ARG:HH21	2.24	0.50
7:M:347:LYS:HG2	7:M:396:THR:HG23	1.94	0.50
7:N:92:ILE:HB	7:N:96:LEU:HB3	1.92	0.50
7:Q:391:ARG:HH21	7:R:204:LYS:CG	2.24	0.50
7:R:309:TYR:H	7:R:472:ASN:HD21	1.59	0.50
7:S:83:ASP:HB3	7:S:92:ILE:HG23	1.92	0.50
7:S:260:GLN:HB3	7:S:353:LEU:HB3	1.93	0.50
7:S:310:GLU:HG2	7:S:313:GLU:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:V:376:GLY:O	7:W:218:ILE:CD1	2.60	0.50
7:W:404:VAL:HB	7:X:191:PHE:H	1.76	0.50
1:A:25:ILE:HB	1:A:654:LEU:HB2	1.94	0.49
1:A:62:LYS:HD3	6:B:128:ILE:HD12	1.94	0.49
1:A:658:ASN:HD22	1:A:659:ALA:H	1.59	0.49
3:D:61:GLN:HE21	3:D:64:VAL:HG23	1.77	0.49
6:B:676:PHE:HB3	6:B:699:CYS:HB3	1.94	0.49
7:P:92:ILE:HB	7:P:96:LEU:HB3	1.93	0.49
7:H:413:ARG:HH11	7:I:282:LEU:HA	1.77	0.49
7:I:309:TYR:H	7:I:472:ASN:HD21	1.60	0.49
7:R:131:LEU:HG	7:R:132:ALA:H	1.75	0.49
7:S:90:ARG:NH1	7:S:103:ASP:OD1	2.44	0.49
7:S:309:TYR:H	7:S:472:ASN:HD21	1.60	0.49
7:T:270:GLU:O	7:T:343:LYS:N	2.39	0.49
7:T:347:LYS:HG2	7:T:396:THR:HG23	1.94	0.49
7:U:340:VAL:N	7:U:403:ASP:O	2.39	0.49
7:X:290:ARG:HG2	7:X:291:ASP:H	1.77	0.49
1:A:220:LYS:HG2	1:A:221:GLU:H	1.77	0.49
1:A:767:SER:HB2	1:A:768:TYR:HB3	1.93	0.49
7:P:243:LEU:HD12	7:P:370:PHE:CE1	2.47	0.49
7:H:92:ILE:HB	7:H:96:LEU:HB3	1.92	0.49
7:H:309:TYR:H	7:H:472:ASN:HD21	1.59	0.49
7:I:347:LYS:HG2	7:I:396:THR:HG23	1.94	0.49
7:K:260:GLN:HB3	7:K:353:LEU:HB3	1.93	0.49
7:K:413:ARG:CZ	7:L:282:LEU:HG	2.42	0.49
7:L:260:GLN:HB3	7:L:353:LEU:HB3	1.93	0.49
7:Q:309:TYR:H	7:Q:472:ASN:HD21	1.60	0.49
7:T:309:TYR:H	7:T:472:ASN:HD21	1.59	0.49
2:C:373:VAL:HB	5:F:191:ALA:HB3	1.94	0.49
4:E:70:ARG:HH21	5:F:167:LEU:HB2	1.77	0.49
7:P:327:SER:HB2	7:P:453:SER:HB2	1.94	0.49
7:K:90:ARG:NH1	7:K:103:ASP:OD1	2.44	0.49
7:L:290:ARG:HG2	7:L:291:ASP:H	1.77	0.49
7:N:309:TYR:H	7:N:472:ASN:HD21	1.59	0.49
7:N:391:ARG:CZ	7:O:204:LYS:HE3	2.40	0.49
7:O:309:TYR:H	7:O:472:ASN:HD21	1.60	0.49
7:S:290:ARG:HG2	7:S:291:ASP:H	1.77	0.49
7:T:130:GLU:HG3	7:U:164:ARG:O	2.11	0.49
7:T:290:ARG:HG2	7:T:291:ASP:H	1.78	0.49
7:V:310:GLU:HG2	7:V:313:GLU:H	1.77	0.49
7:W:309:TYR:H	7:W:472:ASN:HD21	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:X:310:GLU:HG2	7:X:313:GLU:H	1.77	0.49
5:F:394:ARG:NH1	7:G:184:GLU:OE2	2.46	0.49
7:H:90:ARG:NH1	7:H:103:ASP:OD1	2.44	0.49
7:H:266:SER:HB3	7:H:347:LYS:HB2	1.93	0.49
7:J:310:GLU:HG2	7:J:313:GLU:H	1.77	0.49
7:J:421:GLU:OE1	7:K:434:PHE:CD2	2.65	0.49
7:K:290:ARG:HG2	7:K:291:ASP:H	1.78	0.49
7:L:270:GLU:O	7:L:343:LYS:N	2.40	0.49
7:O:310:GLU:HG2	7:O:313:GLU:H	1.77	0.49
7:Q:409:ARG:HD3	7:R:184:GLU:OE2	2.12	0.49
7:R:310:GLU:HG2	7:R:313:GLU:H	1.77	0.49
7:T:310:GLU:HG2	7:T:313:GLU:H	1.77	0.49
7:U:421:GLU:OE1	7:V:434:PHE:HD2	1.96	0.49
7:W:347:LYS:HG2	7:W:396:THR:HG23	1.94	0.49
1:A:1342:LEU:HD23	1:A:1342:LEU:H	1.78	0.49
2:C:11:CYS:HB2	2:C:39:SER:HB3	1.94	0.49
4:E:157:ASP:OD2	6:B:182:ARG:NH2	2.36	0.49
7:P:140:ASN:HA	7:P:323:THR:HG22	1.93	0.49
7:M:290:ARG:HG2	7:M:291:ASP:H	1.77	0.49
7:M:313:GLU:HG3	7:N:290:ARG:NH2	2.28	0.49
7:O:372:GLU:HB3	7:Q:223:THR:C	2.29	0.49
7:Q:290:ARG:HG2	7:Q:291:ASP:H	1.77	0.49
7:Q:347:LYS:HG2	7:Q:396:THR:HG23	1.94	0.49
7:R:332:GLY:O	7:R:446:VAL:N	2.46	0.49
7:U:260:GLN:HB3	7:U:353:LEU:HB3	1.93	0.49
7:U:266:SER:HB3	7:U:347:LYS:HB2	1.93	0.49
7:X:295:THR:HG23	7:X:298:PHE:H	1.78	0.49
2:C:177:LEU:HD23	3:D:371:LEU:HD11	1.94	0.49
7:G:130:GLU:HG3	7:P:165:ASP:HA	1.94	0.49
7:I:290:ARG:HG2	7:I:291:ASP:H	1.77	0.49
7:I:413:ARG:NH1	7:J:282:LEU:CB	2.72	0.49
7:K:140:ASN:HA	7:K:323:THR:HG22	1.95	0.49
7:K:413:ARG:HH11	7:L:282:LEU:CA	2.19	0.49
7:L:309:TYR:H	7:L:472:ASN:HD21	1.60	0.49
7:M:309:TYR:H	7:M:472:ASN:HD21	1.60	0.49
7:N:290:ARG:HG2	7:N:291:ASP:H	1.77	0.49
7:O:83:ASP:HB3	7:O:92:ILE:HG23	1.92	0.49
7:O:290:ARG:HG2	7:O:291:ASP:H	1.77	0.49
7:R:413:ARG:NH1	7:S:282:LEU:HG	2.27	0.49
7:U:370:PHE:CB	7:U:373:ILE:N	2.62	0.49
7:V:90:ARG:NH1	7:V:103:ASP:OD1	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:V:133:ARG:NH1	7:W:164:ARG:HB2	2.04	0.49
7:V:270:GLU:O	7:V:343:LYS:N	2.39	0.49
7:W:310:GLU:HG2	7:W:313:GLU:H	1.77	0.49
7:X:309:TYR:H	7:X:472:ASN:HD21	1.60	0.49
1:A:265:VAL:HG13	1:A:329:VAL:HG22	1.95	0.49
1:A:424:LEU:HD23	1:A:428:VAL:HG21	1.94	0.49
5:F:387:GLU:O	7:G:193:THR:N	2.40	0.49
6:B:385:GLU:HA	6:B:434:ILE:HG22	1.95	0.49
7:G:347:LYS:HG2	7:G:396:THR:HG23	1.95	0.49
7:P:218:ILE:HG23	7:P:249:PHE:HB2	1.94	0.49
7:P:370:PHE:HB2	7:P:373:ILE:HB	1.94	0.49
7:H:260:GLN:HB3	7:H:353:LEU:HB3	1.93	0.49
7:I:332:GLY:O	7:I:446:VAL:N	2.46	0.49
7:K:400:LEU:HD12	7:L:195:HIS:CB	2.34	0.49
7:N:391:ARG:HH21	7:O:204:LYS:HG3	1.77	0.49
7:Q:310:GLU:HG2	7:Q:313:GLU:H	1.77	0.49
7:Q:332:GLY:O	7:Q:446:VAL:N	2.46	0.49
7:R:370:PHE:CD2	7:R:373:ILE:C	2.80	0.49
7:T:295:THR:HG23	7:T:298:PHE:H	1.78	0.49
7:U:290:ARG:HG2	7:U:291:ASP:H	1.77	0.49
7:U:376:GLY:O	7:V:218:ILE:HD12	2.12	0.49
6:B:192:LEU:HD23	6:B:482:VAL:HG23	1.95	0.49
7:G:332:GLY:N	7:G:446:VAL:O	2.45	0.49
7:H:140:ASN:HA	7:H:323:THR:HG22	1.95	0.49
7:H:332:GLY:O	7:H:446:VAL:N	2.46	0.49
7:J:90:ARG:NH1	7:J:103:ASP:OD1	2.44	0.49
7:K:295:THR:HG23	7:K:298:PHE:H	1.78	0.49
7:Q:140:ASN:HA	7:Q:323:THR:HG22	1.95	0.49
7:R:290:ARG:HG2	7:R:291:ASP:H	1.78	0.49
7:T:340:VAL:N	7:T:403:ASP:O	2.39	0.49
7:U:310:GLU:HG2	7:U:313:GLU:H	1.77	0.49
7:U:332:GLY:O	7:U:446:VAL:N	2.46	0.49
7:V:398:GLU:H	7:W:197:GLU:CB	2.26	0.49
7:W:140:ASN:HA	7:W:323:THR:HG22	1.95	0.49
7:W:295:THR:HG23	7:W:298:PHE:H	1.78	0.49
1:A:141:VAL:HB	1:A:188:PHE:HB3	1.94	0.49
2:C:127:LEU:HD22	2:C:413:VAL:HG11	1.94	0.49
5:F:190:LEU:N	5:F:267:GLN:HE21	2.10	0.49
5:F:389:ILE:O	7:G:191:PHE:N	2.40	0.49
7:J:145:ASP:OD2	7:K:284:ARG:NH1	2.46	0.49
7:K:310:GLU:HG2	7:K:313:GLU:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:348:ARG:HB2	7:K:395:ILE:HG23	1.95	0.49
7:M:295:THR:HG23	7:M:298:PHE:H	1.78	0.49
7:M:310:GLU:HG2	7:M:313:GLU:H	1.77	0.49
7:O:347:LYS:HG2	7:O:396:THR:HG23	1.94	0.49
7:S:348:ARG:HB2	7:S:395:ILE:HG23	1.95	0.49
7:X:347:LYS:HG2	7:X:396:THR:HG23	1.94	0.49
6:B:29:TRP:HB3	6:B:46:ARG:HD2	1.95	0.49
7:G:382:ASP:HB3	7:P:213:ASN:H	1.77	0.49
7:P:380:ASN:HD22	7:H:215:ASN:CB	2.24	0.49
7:I:140:ASN:HA	7:I:323:THR:HG22	1.95	0.49
7:J:191:PHE:CD1	7:J:191:PHE:N	2.73	0.49
7:U:295:THR:HG23	7:U:298:PHE:H	1.78	0.49
7:V:133:ARG:CZ	7:W:164:ARG:CD	2.89	0.49
1:A:429:THR:HG22	1:A:430:VAL:HG13	1.93	0.48
1:A:1176:LEU:HD13	1:A:1202:HIS:CE1	2.48	0.48
3:D:452:PHE:HB2	3:D:468:VAL:HG11	1.95	0.48
6:B:293:ILE:HA	6:B:400:VAL:HG12	1.94	0.48
6:B:717:PRO:HD2	6:B:728:ILE:HG13	1.95	0.48
7:J:140:ASN:HA	7:J:323:THR:HG22	1.95	0.48
7:L:310:GLU:HG2	7:L:313:GLU:H	1.77	0.48
7:R:130:GLU:HG3	7:S:165:ASP:HA	1.94	0.48
7:U:526:SER:HB2	7:V:198:GLU:OE2	2.13	0.48
7:V:382:ASP:HB3	7:W:213:ASN:O	2.12	0.48
7:W:410:GLY:H	7:X:185:THR:HG23	1.77	0.48
7:X:140:ASN:HA	7:X:323:THR:HG22	1.95	0.48
2:C:248:ALA:HB3	2:C:296:LEU:HB2	1.94	0.48
3:D:225:PHE:CE2	3:D:340:SER:OG	2.65	0.48
3:D:385:ILE:HD13	3:D:406:TRP:HE1	1.78	0.48
7:P:131:LEU:HG	7:P:132:ALA:H	1.78	0.48
7:I:310:GLU:HG2	7:I:313:GLU:H	1.77	0.48
7:L:295:THR:HG23	7:L:298:PHE:H	1.78	0.48
7:L:332:GLY:N	7:L:446:VAL:O	2.47	0.48
7:M:332:GLY:N	7:M:446:VAL:O	2.47	0.48
7:N:407:LEU:HA	7:O:188:GLU:CB	2.42	0.48
7:O:105:GLY:HA2	7:Q:159:LEU:HD22	1.94	0.48
7:R:140:ASN:HA	7:R:323:THR:HG22	1.95	0.48
7:R:295:THR:HG23	7:R:298:PHE:H	1.78	0.48
7:T:348:ARG:HB2	7:T:395:ILE:HG23	1.95	0.48
7:U:332:GLY:N	7:U:446:VAL:O	2.47	0.48
7:V:140:ASN:HA	7:V:323:THR:HG22	1.95	0.48
7:W:391:ARG:NH2	7:X:204:LYS:CE	2.71	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:X:348:ARG:HB2	7:X:395:ILE:HG23	1.95	0.48
5:F:155:TRP:CD1	5:F:174:LYS:HB3	2.48	0.48
7:G:362:TYR:O	7:G:381:LYS:N	2.47	0.48
7:G:387:ARG:NH1	7:P:208:GLN:OE1	2.47	0.48
7:H:290:ARG:HG2	7:H:291:ASP:H	1.77	0.48
7:I:446:VAL:HG21	7:J:184:GLU:CD	2.33	0.48
7:J:348:ARG:HB2	7:J:395:ILE:HG23	1.95	0.48
7:N:295:THR:HG23	7:N:298:PHE:H	1.78	0.48
7:O:384:CYS:O	7:Q:210:LYS:HG3	2.12	0.48
7:V:391:ARG:NH2	7:W:203:PHE:O	2.46	0.48
7:X:332:GLY:O	7:X:446:VAL:N	2.46	0.48
1:A:1255:LEU:HB2	1:A:1270:VAL:HG11	1.94	0.48
3:D:663:MET:HB3	3:D:689:VAL:HG21	1.95	0.48
4:E:177:LEU:HD23	4:E:179:GLU:H	1.78	0.48
7:I:370:PHE:CD2	7:I:373:ILE:C	2.81	0.48
7:M:266:SER:O	7:M:347:LYS:N	2.40	0.48
7:M:370:PHE:CD2	7:M:373:ILE:C	2.81	0.48
7:O:332:GLY:N	7:O:446:VAL:O	2.47	0.48
7:V:414:LYS:HA	7:W:435:VAL:CB	2.29	0.48
3:D:416:VAL:HG12	3:D:419:GLN:NE2	2.23	0.48
4:E:122:ARG:NH1	5:F:161:ASP:OD1	2.46	0.48
5:F:195:ILE:HG13	5:F:262:ILE:HB	1.94	0.48
7:P:295:THR:HG23	7:P:298:PHE:H	1.78	0.48
7:H:310:GLU:HG2	7:H:313:GLU:H	1.77	0.48
7:I:413:ARG:HH12	7:J:282:LEU:HG	1.77	0.48
7:L:386:LYS:HB3	7:M:209:GLU:N	2.28	0.48
7:N:332:GLY:N	7:N:446:VAL:O	2.47	0.48
7:N:332:GLY:O	7:N:446:VAL:N	2.46	0.48
7:Q:295:THR:HG23	7:Q:298:PHE:H	1.78	0.48
7:S:295:THR:HG23	7:S:298:PHE:H	1.78	0.48
7:S:332:GLY:O	7:S:446:VAL:N	2.46	0.48
7:T:90:ARG:NH1	7:T:103:ASP:OD1	2.44	0.48
7:W:191:PHE:HD1	7:W:191:PHE:N	2.01	0.48
1:A:773:TRP:CE3	1:A:774:LEU:HB2	2.49	0.48
3:D:631:CYS:HB2	3:D:649:TYR:HB2	1.95	0.48
7:G:357:LYS:HE2	7:G:386:LYS:HE3	1.96	0.48
7:P:309:TYR:H	7:P:472:ASN:HD21	1.61	0.48
7:H:348:ARG:HB2	7:H:395:ILE:HG23	1.95	0.48
7:I:295:THR:HG23	7:I:298:PHE:H	1.78	0.48
7:L:348:ARG:HB2	7:L:395:ILE:HG23	1.95	0.48
7:S:140:ASN:HA	7:S:323:THR:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:327:SER:HB2	7:U:453:SER:HB2	1.96	0.48
7:U:404:VAL:HB	7:V:191:PHE:HB2	1.95	0.48
7:W:410:GLY:O	7:X:185:THR:HG21	2.12	0.48
2:C:121:LEU:HD11	2:C:296:LEU:HD21	1.96	0.48
3:D:338:LYS:O	3:D:352:GLY:N	2.42	0.48
5:F:329:LYS:HA	5:F:385:ALA:HA	1.96	0.48
6:B:674:THR:HA	6:B:675:GLY:HA2	1.61	0.48
7:P:266:SER:O	7:P:347:LYS:N	2.41	0.48
7:H:340:VAL:N	7:H:403:ASP:O	2.39	0.48
7:J:327:SER:HB2	7:J:453:SER:HB2	1.96	0.48
7:M:90:ARG:NH1	7:M:103:ASP:OD1	2.44	0.48
7:N:310:GLU:HG2	7:N:313:GLU:H	1.77	0.48
7:Q:372:GLU:HB3	7:R:223:THR:H	1.79	0.48
7:T:332:GLY:N	7:T:446:VAL:O	2.47	0.48
7:V:295:THR:HG23	7:V:298:PHE:H	1.78	0.48
7:V:348:ARG:HB2	7:V:395:ILE:HG23	1.95	0.48
1:A:501:TYR:CZ	1:A:513:GLY:HA3	2.49	0.48
1:A:943:THR:HA	1:A:1358:THR:HA	1.95	0.48
7:H:295:THR:HG23	7:H:298:PHE:H	1.78	0.48
7:H:327:SER:HB2	7:H:453:SER:HB2	1.96	0.48
7:I:90:ARG:NH1	7:I:103:ASP:OD1	2.44	0.48
7:L:266:SER:O	7:L:347:LYS:N	2.40	0.48
7:L:394:ASN:O	7:M:200:ILE:HA	2.12	0.48
7:S:332:GLY:N	7:S:446:VAL:O	2.47	0.48
7:V:290:ARG:HG2	7:V:291:ASP:H	1.77	0.48
7:V:340:VAL:N	7:V:403:ASP:O	2.39	0.48
7:X:219:SER:HA	7:X:248:SER:HA	1.96	0.48
7:G:96:LEU:HD11	7:G:103:ASP:HB2	1.95	0.48
7:P:90:ARG:NH1	7:P:103:ASP:OD1	2.42	0.48
7:H:313:GLU:CD	7:I:290:ARG:NH2	2.67	0.48
7:K:327:SER:HB2	7:K:453:SER:HB2	1.96	0.48
7:N:347:LYS:HG2	7:N:396:THR:HG23	1.94	0.48
7:N:348:ARG:HB2	7:N:395:ILE:HG23	1.95	0.48
7:O:391:ARG:NE	7:Q:204:LYS:HE2	2.29	0.48
7:R:254:SER:HB3	7:R:359:CYS:HB3	1.96	0.48
7:W:348:ARG:HB2	7:W:395:ILE:HG23	1.95	0.48
7:X:332:GLY:N	7:X:446:VAL:O	2.47	0.48
7:G:264:SER:N	7:G:349:LYS:O	2.36	0.48
7:G:343:LYS:HG2	7:G:400:LEU:HD22	1.95	0.48
7:J:295:THR:HG23	7:J:298:PHE:H	1.78	0.48
7:N:402:ASP:HB2	7:O:193:THR:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:295:THR:HG23	7:O:298:PHE:H	1.78	0.48
7:Q:64:ARG:NH2	7:R:459:VAL:O	2.47	0.48
7:S:347:LYS:HG2	7:S:396:THR:HG23	1.94	0.48
7:U:140:ASN:HA	7:U:323:THR:HG22	1.95	0.48
7:V:332:GLY:O	7:V:446:VAL:N	2.46	0.48
7:X:254:SER:HB3	7:X:359:CYS:HB3	1.96	0.48
1:A:1016:VAL:HG21	1:A:1081:PHE:HE2	1.79	0.47
5:F:89:GLN:HG3	7:G:159:LEU:HD13	1.95	0.47
5:F:388:ASP:N	5:F:388:ASP:OD1	2.47	0.47
7:M:219:SER:HA	7:M:248:SER:HA	1.96	0.47
7:N:219:SER:HA	7:N:248:SER:HA	1.96	0.47
7:N:398:GLU:HB3	7:O:197:GLU:HB3	1.96	0.47
7:Q:219:SER:HA	7:Q:248:SER:HA	1.96	0.47
7:R:90:ARG:NH1	7:R:103:ASP:OD1	2.44	0.47
7:R:145:ASP:OD2	7:S:284:ARG:NH1	2.47	0.47
7:R:332:GLY:N	7:R:446:VAL:O	2.47	0.47
7:R:348:ARG:HB2	7:R:395:ILE:HG23	1.95	0.47
7:T:140:ASN:HA	7:T:323:THR:HG22	1.95	0.47
7:T:332:GLY:O	7:T:446:VAL:N	2.46	0.47
7:U:90:ARG:NH1	7:U:103:ASP:OD1	2.44	0.47
7:U:348:ARG:HB2	7:U:395:ILE:HG23	1.95	0.47
7:V:418:GLU:HA	7:W:431:VAL:HB	1.96	0.47
7:W:332:GLY:N	7:W:446:VAL:O	2.47	0.47
2:C:475:SER:HB3	2:C:480:CYS:HB3	1.96	0.47
3:D:257:VAL:HG13	3:D:258:GLU:H	1.79	0.47
6:B:22:CYS:SG	6:B:23:PHE:N	2.87	0.47
6:B:399:CYS:HB2	6:B:420:CYS:HB3	1.67	0.47
6:B:724:ILE:HG23	6:B:747:GLN:HA	1.95	0.47
7:I:332:GLY:N	7:I:446:VAL:O	2.47	0.47
7:J:332:GLY:O	7:J:446:VAL:N	2.46	0.47
7:K:254:SER:HB3	7:K:359:CYS:HB3	1.96	0.47
7:L:332:GLY:O	7:L:446:VAL:N	2.46	0.47
7:L:417:PHE:CE2	7:M:280:ILE:CD1	2.97	0.47
7:M:332:GLY:O	7:M:446:VAL:N	2.46	0.47
7:Q:148:SER:HB3	7:R:180:SER:HB2	1.96	0.47
7:Q:370:PHE:CD2	7:Q:373:ILE:C	2.80	0.47
7:U:402:ASP:HB2	7:V:193:THR:O	2.14	0.47
7:W:254:SER:HB3	7:W:359:CYS:HB3	1.96	0.47
1:A:61:ASP:HB2	1:A:62:LYS:CB	2.42	0.47
1:A:1218:VAL:HB	1:A:1223:PRO:HB3	1.96	0.47
7:I:348:ARG:HB2	7:I:395:ILE:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:140:ASN:HA	7:L:323:THR:HG22	1.95	0.47
7:M:65:ARG:CG	7:N:467:HIS:CB	2.92	0.47
7:M:140:ASN:HA	7:M:323:THR:HG22	1.95	0.47
7:N:140:ASN:HA	7:N:323:THR:HG22	1.95	0.47
7:N:266:SER:O	7:N:347:LYS:N	2.39	0.47
7:Q:332:GLY:N	7:Q:446:VAL:O	2.47	0.47
7:S:254:SER:HB3	7:S:359:CYS:HB3	1.96	0.47
7:T:421:GLU:HB3	7:U:434:PHE:HD2	1.79	0.47
7:V:254:SER:HB3	7:V:359:CYS:HB3	1.96	0.47
7:V:319:GLU:HG2	7:W:286:VAL:HG11	1.96	0.47
7:V:378:GLU:CB	7:W:217:ALA:H	2.26	0.47
7:V:413:ARG:O	7:W:435:VAL:HG22	2.14	0.47
7:W:327:SER:HB2	7:W:453:SER:HB2	1.96	0.47
1:A:272:ARG:HA	1:A:280:LYS:HG3	1.95	0.47
3:D:280:LEU:HD23	3:D:431:VAL:HG11	1.96	0.47
7:P:248:SER:OG	7:P:250:ARG:NH2	2.48	0.47
7:P:290:ARG:HG2	7:P:291:ASP:H	1.78	0.47
7:J:332:GLY:N	7:J:446:VAL:O	2.47	0.47
7:K:340:VAL:N	7:K:403:ASP:O	2.39	0.47
7:L:90:ARG:NH1	7:L:103:ASP:OD1	2.44	0.47
7:O:140:ASN:HA	7:O:323:THR:HG22	1.95	0.47
7:O:254:SER:HB3	7:O:359:CYS:HB3	1.96	0.47
7:Q:394:ASN:O	7:R:200:ILE:HA	2.15	0.47
7:T:145:ASP:OD2	7:U:284:ARG:NH1	2.47	0.47
7:T:219:SER:HA	7:T:248:SER:HA	1.96	0.47
7:V:332:GLY:N	7:V:446:VAL:O	2.47	0.47
7:V:414:LYS:CG	7:W:435:VAL:HG11	2.44	0.47
7:V:502:ASP:OD2	7:W:451:LYS:CA	2.56	0.47
7:W:332:GLY:O	7:W:446:VAL:N	2.46	0.47
1:A:464:TYR:O	1:A:544:TYR:OH	2.33	0.47
4:E:91:ARG:HG2	4:E:106:VAL:HG22	1.95	0.47
4:E:116:ALA:HB3	4:E:131:TYR:HB2	1.97	0.47
7:G:295:THR:HG23	7:G:298:PHE:H	1.79	0.47
7:G:332:GLY:O	7:G:446:VAL:N	2.46	0.47
7:L:327:SER:HB2	7:L:453:SER:HB2	1.96	0.47
7:M:372:GLU:HB2	7:N:223:THR:O	2.11	0.47
7:N:327:SER:HB2	7:N:453:SER:HB2	1.96	0.47
7:O:219:SER:HA	7:O:248:SER:HA	1.96	0.47
7:R:417:PHE:CZ	7:S:280:ILE:HG13	2.49	0.47
7:T:386:LYS:HE2	7:U:207:ILE:HG23	1.96	0.47
7:V:421:GLU:CB	7:W:431:VAL:CG1	2.91	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:350:GLY:O	7:P:393:VAL:N	2.47	0.47
7:H:332:GLY:N	7:H:446:VAL:O	2.47	0.47
7:H:411:GLY:O	7:I:185:THR:HG21	2.14	0.47
7:I:254:SER:HB3	7:I:359:CYS:HB3	1.96	0.47
7:I:413:ARG:NH1	7:J:282:LEU:CG	2.77	0.47
7:K:332:GLY:O	7:K:446:VAL:N	2.46	0.47
7:K:332:GLY:N	7:K:446:VAL:O	2.47	0.47
7:Q:130:GLU:HG3	7:R:165:ASP:HA	1.95	0.47
7:T:327:SER:HB2	7:T:453:SER:HB2	1.96	0.47
7:U:391:ARG:HH21	7:V:204:LYS:CD	2.26	0.47
1:A:320:ASN:HD21	1:A:348:VAL:HG22	1.80	0.47
3:D:189:GLN:HB3	6:B:192:LEU:HD21	1.97	0.47
3:D:199:GLU:O	3:D:248:TYR:HB2	2.14	0.47
7:I:219:SER:HA	7:I:248:SER:HA	1.96	0.47
7:J:254:SER:HB3	7:J:359:CYS:HB3	1.96	0.47
7:K:391:ARG:NH2	7:L:204:LYS:CE	2.71	0.47
7:K:408:ILE:HG22	7:L:187:GLY:O	2.15	0.47
7:L:219:SER:HA	7:L:248:SER:HA	1.96	0.47
7:L:413:ARG:NH1	7:M:282:LEU:CG	2.73	0.47
7:M:348:ARG:HB2	7:M:395:ILE:HG23	1.95	0.47
7:N:339:TYR:HB3	7:N:404:VAL:CG1	2.33	0.47
7:O:130:GLU:HG3	7:Q:165:ASP:HA	1.95	0.47
7:O:465:ASN:HD21	7:O:468:LEU:HD23	1.80	0.47
7:Q:348:ARG:HB2	7:Q:395:ILE:HG23	1.95	0.47
7:Q:350:GLY:O	7:Q:393:VAL:N	2.48	0.47
7:T:254:SER:HB3	7:T:359:CYS:HB3	1.96	0.47
7:T:350:GLY:O	7:T:393:VAL:N	2.48	0.47
7:T:370:PHE:CB	7:T:373:ILE:N	2.62	0.47
7:T:400:LEU:CD1	7:U:195:HIS:HB2	2.33	0.47
7:U:106:ASP:OD2	7:V:122:ARG:N	2.41	0.47
7:U:219:SER:HA	7:U:248:SER:HA	1.96	0.47
7:V:133:ARG:NH2	7:W:164:ARG:HH21	2.13	0.47
7:V:372:GLU:CB	7:W:223:THR:C	2.83	0.47
7:W:154:GLU:OE2	7:X:162:ARG:NH1	2.47	0.47
7:W:219:SER:HA	7:W:248:SER:HA	1.96	0.47
7:X:327:SER:HB2	7:X:453:SER:HB2	1.96	0.47
3:D:516:LYS:HD2	3:D:542:SER:HB3	1.96	0.47
6:B:704:CYS:SG	6:B:722:TYR:HB2	2.55	0.47
7:G:153:ASN:HD21	7:G:178:VAL:HG23	1.79	0.47
7:I:148:SER:CB	7:J:180:SER:HB3	2.45	0.47
7:J:129:SER:HB2	7:K:164:ARG:NH1	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:189:LYS:HE2	7:J:191:PHE:HZ	1.73	0.47
7:M:254:SER:HB3	7:M:359:CYS:HB3	1.96	0.47
7:M:320:THR:OG1	7:N:289:ASN:CB	2.62	0.47
7:N:130:GLU:OE2	7:O:165:ASP:OD1	2.32	0.47
7:S:219:SER:HA	7:S:248:SER:HA	1.96	0.47
7:S:327:SER:HB2	7:S:453:SER:HB2	1.96	0.47
7:T:421:GLU:OE1	7:U:434:PHE:HD2	1.98	0.47
7:V:394:ASN:O	7:W:201:GLU:CB	2.61	0.47
7:W:391:ARG:HH21	7:X:204:LYS:HG3	1.80	0.47
1:A:535:VAL:HA	1:A:563:ILE:HD11	1.96	0.47
1:A:1259:LEU:HD13	1:A:1299:GLU:HB2	1.96	0.47
6:B:35:CYS:SG	6:B:42:GLY:HA3	2.55	0.47
6:B:483:ILE:HG13	6:B:484:ASP:H	1.80	0.47
7:K:370:PHE:CD2	7:K:373:ILE:C	2.80	0.47
7:M:65:ARG:CG	7:N:467:HIS:CD2	2.98	0.47
7:N:413:ARG:NH1	7:O:282:LEU:CB	2.77	0.47
7:Q:41:PHE:CD1	7:Q:310:GLU:HG3	2.50	0.47
7:T:465:ASN:HD21	7:T:468:LEU:HD23	1.80	0.47
7:U:389:GLU:HA	7:V:206:ILE:HG12	1.97	0.47
7:W:129:SER:HA	7:X:164:ARG:NH1	2.30	0.47
7:W:129:SER:CB	7:X:164:ARG:NH1	2.78	0.47
1:A:465:LEU:HD11	1:A:542:VAL:HB	1.97	0.47
1:A:497:THR:HG23	1:A:498:HIS:H	1.79	0.47
7:I:327:SER:HB2	7:I:453:SER:HB2	1.96	0.47
7:I:350:GLY:O	7:I:393:VAL:N	2.48	0.47
7:I:465:ASN:HD21	7:I:468:LEU:HD23	1.80	0.47
7:K:350:GLY:O	7:K:393:VAL:N	2.48	0.47
7:L:254:SER:HB3	7:L:359:CYS:HB3	1.96	0.47
7:N:129:SER:CB	7:O:164:ARG:NH1	2.74	0.47
7:R:41:PHE:CD1	7:R:310:GLU:HG3	2.50	0.47
7:S:394:ASN:O	7:T:200:ILE:HA	2.15	0.47
7:T:409:ARG:HD3	7:U:184:GLU:OE2	2.15	0.47
7:U:370:PHE:CD2	7:U:373:ILE:C	2.80	0.47
7:V:106:ASP:OD2	7:W:122:ARG:CA	2.60	0.47
7:V:219:SER:HA	7:V:248:SER:HA	1.96	0.47
7:W:41:PHE:CD1	7:W:310:GLU:HG3	2.50	0.47
7:W:465:ASN:HD21	7:W:468:LEU:HD23	1.80	0.47
1:A:371:ILE:HB	1:A:420:PHE:HB2	1.96	0.46
5:F:14:TRP:HB3	5:F:29:ARG:HD2	1.97	0.46
5:F:397:SER:HB3	5:F:401:SER:H	1.80	0.46
7:P:41:PHE:CD1	7:P:310:GLU:HG3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:41:PHE:CD1	7:H:310:GLU:HG3	2.50	0.46
7:L:340:VAL:N	7:L:403:ASP:O	2.39	0.46
7:L:465:ASN:HD21	7:L:468:LEU:HD23	1.80	0.46
7:M:64:ARG:HD2	7:N:461:VAL:CG2	2.42	0.46
7:N:465:ASN:HD21	7:N:468:LEU:HD23	1.80	0.46
7:O:348:ARG:HB2	7:O:395:ILE:HG23	1.95	0.46
7:R:350:GLY:O	7:R:393:VAL:N	2.48	0.46
7:V:327:SER:HB2	7:V:453:SER:HB2	1.96	0.46
7:X:266:SER:O	7:X:347:LYS:N	2.40	0.46
1:A:31:PHE:HB2	1:A:119:ILE:HG22	1.97	0.46
1:A:166:PRO:HD3	1:A:199:TRP:CD2	2.50	0.46
2:C:373:VAL:O	5:F:191:ALA:N	2.47	0.46
7:H:65:ARG:HA	7:I:467:HIS:HB2	1.97	0.46
7:H:350:GLY:O	7:H:393:VAL:N	2.48	0.46
7:I:148:SER:HB3	7:J:180:SER:HB3	1.91	0.46
7:J:219:SER:HA	7:J:248:SER:HA	1.96	0.46
7:K:41:PHE:CD1	7:K:310:GLU:HG3	2.50	0.46
7:K:219:SER:HA	7:K:248:SER:HA	1.96	0.46
7:N:370:PHE:CD2	7:N:373:ILE:C	2.81	0.46
7:Q:327:SER:HB2	7:Q:453:SER:HB2	1.96	0.46
7:R:189:LYS:HE2	7:R:191:PHE:HZ	1.73	0.46
7:R:219:SER:HA	7:R:248:SER:HA	1.96	0.46
7:R:327:SER:HB2	7:R:453:SER:HB2	1.96	0.46
7:U:378:GLU:HB3	7:V:217:ALA:O	2.15	0.46
7:V:320:THR:HG21	7:W:179:ALA:HB1	1.95	0.46
7:X:465:ASN:HD21	7:X:468:LEU:HD23	1.80	0.46
3:D:40:ASN:CB	3:D:286:LEU:HD12	2.44	0.46
7:P:332:GLY:O	7:P:446:VAL:N	2.47	0.46
7:H:374:SER:O	7:I:220:LEU:CD1	2.63	0.46
7:I:370:PHE:CG	7:I:373:ILE:CD1	2.89	0.46
7:M:41:PHE:CD1	7:M:310:GLU:HG3	2.50	0.46
7:O:189:LYS:HE2	7:O:191:PHE:HZ	1.73	0.46
7:O:327:SER:HB2	7:O:453:SER:HB2	1.96	0.46
7:S:41:PHE:CD1	7:S:310:GLU:HG3	2.50	0.46
2:C:187:GLU:HB3	3:D:361:LYS:HB3	1.97	0.46
6:B:442:SER:HB2	6:B:459:LYS:HZ2	1.79	0.46
7:G:327:SER:HB2	7:G:453:SER:HB2	1.96	0.46
7:H:219:SER:HA	7:H:248:SER:HA	1.96	0.46
7:H:254:SER:HB3	7:H:359:CYS:HB3	1.96	0.46
7:I:189:LYS:HE2	7:I:191:PHE:HZ	1.73	0.46
7:J:41:PHE:CD1	7:J:310:GLU:HG3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:465:ASN:HD21	7:J:468:LEU:HD23	1.80	0.46
7:L:41:PHE:CD1	7:L:310:GLU:HG3	2.50	0.46
7:M:270:GLU:O	7:M:343:LYS:N	2.39	0.46
7:M:465:ASN:HD21	7:M:468:LEU:HD23	1.80	0.46
7:O:41:PHE:CD1	7:O:310:GLU:HG3	2.50	0.46
7:Q:254:SER:HB3	7:Q:359:CYS:HB3	1.96	0.46
7:Q:386:LYS:O	7:R:208:GLN:OE1	2.34	0.46
7:S:350:GLY:O	7:S:393:VAL:N	2.48	0.46
7:V:405:VAL:HG12	7:W:190:ASN:HA	1.97	0.46
1:A:364:LYS:HG2	1:A:466:TYR:CD1	2.51	0.46
1:A:799:ILE:HD11	1:A:815:VAL:HB	1.98	0.46
2:C:484:TYR:HB2	5:F:198:GLU:HG3	1.97	0.46
5:F:324:ILE:HB	5:F:390:ILE:HB	1.97	0.46
6:B:655:ILE:HG12	6:B:670:ILE:HG22	1.98	0.46
7:G:368:LEU:HB2	7:G:375:VAL:HB	1.97	0.46
7:J:350:GLY:O	7:J:393:VAL:N	2.48	0.46
7:M:327:SER:HB2	7:M:453:SER:HB2	1.96	0.46
7:N:398:GLU:OE1	7:O:197:GLU:OE1	2.32	0.46
7:O:340:VAL:N	7:O:403:ASP:O	2.39	0.46
7:O:350:GLY:O	7:O:393:VAL:N	2.48	0.46
7:O:411:GLY:O	7:Q:185:THR:HG21	2.15	0.46
7:Q:130:GLU:OE2	7:R:165:ASP:HA	2.15	0.46
7:R:206:ILE:O	7:R:261:LEU:N	2.46	0.46
7:U:421:GLU:CB	7:V:434:PHE:HD2	2.26	0.46
7:U:465:ASN:HD21	7:U:468:LEU:HD23	1.80	0.46
7:W:370:PHE:CB	7:W:373:ILE:N	2.62	0.46
7:W:407:LEU:HA	7:X:188:GLU:CB	2.45	0.46
1:A:253:ARG:HE	1:A:259:VAL:HG12	1.81	0.46
1:A:863:GLU:HA	1:A:864:GLY:HA2	1.52	0.46
2:C:306:MET:HG3	2:C:367:GLU:HB3	1.98	0.46
2:C:417:TYR:HB3	2:C:435:MET:HB3	1.96	0.46
7:H:370:PHE:CB	7:H:373:ILE:N	2.62	0.46
7:L:350:GLY:O	7:L:393:VAL:N	2.48	0.46
7:L:400:LEU:CG	7:M:195:HIS:HB2	2.45	0.46
7:Q:373:ILE:HG12	7:R:222:PHE:HD1	1.81	0.46
7:Q:388:GLY:O	7:R:206:ILE:HG23	2.16	0.46
7:T:41:PHE:CD1	7:T:310:GLU:HG3	2.50	0.46
7:U:254:SER:HB3	7:U:359:CYS:HB3	1.96	0.46
7:V:339:TYR:HB3	7:V:404:VAL:CG1	2.33	0.46
7:W:410:GLY:O	7:X:185:THR:HG23	2.16	0.46
2:C:506:ARG:NH2	2:C:535:ASP:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:174:PHE:HB2	5:F:414:ARG:NE	2.30	0.46
5:F:393:VAL:HG21	5:F:404:LEU:HD23	1.98	0.46
7:G:131:LEU:HG	7:G:132:ALA:H	1.79	0.46
7:G:270:GLU:O	7:G:343:LYS:N	2.35	0.46
7:K:328:SER:O	7:K:451:LYS:N	2.42	0.46
7:N:350:GLY:O	7:N:393:VAL:N	2.48	0.46
7:N:413:ARG:CZ	7:O:282:LEU:HA	2.42	0.46
7:O:380:ASN:ND2	7:Q:215:ASN:HD22	2.13	0.46
7:Q:191:PHE:O	7:Q:192:ARG:HG3	2.16	0.46
7:Q:370:PHE:CD1	7:Q:373:ILE:HD13	2.49	0.46
7:Q:526:SER:HB2	7:R:198:GLU:OE2	2.15	0.46
7:R:465:ASN:HD21	7:R:468:LEU:HD23	1.80	0.46
7:U:350:GLY:O	7:U:393:VAL:N	2.48	0.46
7:V:191:PHE:O	7:V:192:ARG:HG3	2.16	0.46
7:V:465:ASN:HD21	7:V:468:LEU:HD23	1.80	0.46
7:W:394:ASN:CB	7:X:201:GLU:HB2	2.41	0.46
7:X:90:ARG:NH1	7:X:103:ASP:OD1	2.44	0.46
1:A:472:ASN:HA	1:A:474:LYS:HD2	1.97	0.46
1:A:767:SER:HA	1:A:768:TYR:HA	1.69	0.46
2:C:122:ALA:HA	2:C:137:LEU:HD12	1.98	0.46
4:E:111:ASP:OD2	4:E:114:SER:OG	2.24	0.46
6:B:409:LEU:HA	6:B:410:PHE:HA	1.70	0.46
7:P:60:ALA:H	7:H:454:PRO:HG2	1.81	0.46
7:H:106:ASP:H	7:I:159:LEU:HD13	1.80	0.46
7:K:394:ASN:O	7:L:200:ILE:HA	2.16	0.46
7:N:254:SER:HB3	7:N:359:CYS:HB3	1.96	0.46
7:N:404:VAL:O	7:O:190:ASN:HB2	2.16	0.46
7:O:332:GLY:O	7:O:446:VAL:N	2.46	0.46
7:O:378:GLU:O	7:Q:216:ALA:HA	2.16	0.46
7:Q:386:LYS:HE2	7:R:207:ILE:HG23	1.98	0.46
7:Q:465:ASN:HD21	7:Q:468:LEU:HD23	1.80	0.46
7:R:106:ASP:H	7:S:159:LEU:HD13	1.81	0.46
7:U:41:PHE:CD1	7:U:310:GLU:HG3	2.50	0.46
7:V:41:PHE:CD1	7:V:310:GLU:HG3	2.50	0.46
7:V:380:ASN:HB2	7:W:215:ASN:N	2.31	0.46
7:V:414:LYS:HA	7:W:435:VAL:CG2	2.46	0.46
7:W:129:SER:CA	7:X:164:ARG:NH1	2.79	0.46
4:E:31:TRP:HB2	4:E:55:LEU:HB3	1.97	0.46
7:P:413:ARG:HG2	7:H:438:ALA:HB1	1.97	0.46
7:J:191:PHE:O	7:J:192:ARG:HG3	2.16	0.46
7:J:370:PHE:CB	7:J:373:ILE:N	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:41:PHE:CD1	7:N:310:GLU:HG3	2.50	0.46
7:R:191:PHE:O	7:R:192:ARG:HG3	2.16	0.46
7:S:148:SER:HB3	7:T:180:SER:HB2	1.98	0.46
7:S:191:PHE:O	7:S:192:ARG:HG3	2.16	0.46
7:T:383:ASP:OD1	7:U:210:LYS:HE3	2.16	0.46
6:B:322:VAL:HB	6:B:371:LEU:O	2.16	0.46
7:G:373:ILE:HG22	7:G:374:SER:N	2.31	0.46
7:I:106:ASP:CA	7:J:159:LEU:HD13	2.45	0.46
7:N:372:GLU:O	7:O:222:PHE:HA	2.16	0.46
7:O:380:ASN:O	7:Q:214:PHE:CD1	2.69	0.46
7:Q:391:ARG:CZ	7:R:204:LYS:HE3	2.43	0.46
7:S:386:LYS:HB3	7:T:209:GLU:H	1.79	0.46
7:T:391:ARG:HH21	7:U:204:LYS:HG3	1.81	0.46
7:V:58:THR:CG2	7:W:452:LEU:CG	2.89	0.46
7:W:380:ASN:O	7:X:214:PHE:CD1	2.69	0.46
1:A:995:GLU:HB2	6:B:616:MET:HG2	1.97	0.45
7:H:370:PHE:CD1	7:H:373:ILE:HD13	2.49	0.45
7:I:106:ASP:H	7:J:159:LEU:HD13	1.77	0.45
7:I:191:PHE:O	7:I:192:ARG:HG3	2.16	0.45
7:I:340:VAL:N	7:I:403:ASP:O	2.39	0.45
7:T:191:PHE:O	7:T:192:ARG:HG3	2.16	0.45
7:U:391:ARG:CZ	7:V:204:LYS:HE2	2.26	0.45
7:V:526:SER:HB3	7:W:198:GLU:CG	2.44	0.45
7:X:41:PHE:CD1	7:X:310:GLU:HG3	2.50	0.45
1:A:315:LEU:HG	1:A:317:ASP:H	1.81	0.45
1:A:1090:ASN:OD1	1:A:1095:GLN:HB2	2.16	0.45
7:J:206:ILE:O	7:J:261:LEU:N	2.46	0.45
7:K:413:ARG:NH1	7:L:282:LEU:O	2.50	0.45
7:L:421:GLU:OE1	7:M:434:PHE:CG	2.68	0.45
7:O:220:LEU:O	7:O:247:GLY:N	2.49	0.45
7:O:266:SER:O	7:O:347:LYS:N	2.40	0.45
7:V:414:LYS:CG	7:W:435:VAL:CG1	2.94	0.45
7:X:370:PHE:CB	7:X:373:ILE:N	2.62	0.45
1:A:283:MET:HB2	1:A:285:THR:H	1.81	0.45
1:A:873:ILE:HA	1:A:874:ASP:HA	1.60	0.45
7:J:421:GLU:OE1	7:K:434:PHE:HD2	1.98	0.45
7:K:392:ALA:HB3	7:L:203:PHE:H	1.80	0.45
7:O:380:ASN:HD22	7:Q:215:ASN:ND2	2.14	0.45
7:R:391:ARG:HH21	7:S:204:LYS:CG	2.25	0.45
7:S:514:GLU:HB2	7:S:522:LYS:HB2	1.99	0.45
7:U:191:PHE:O	7:U:192:ARG:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:V:58:THR:CG2	7:W:452:LEU:HD23	2.45	0.45
7:V:191:PHE:HD1	7:V:191:PHE:N	2.01	0.45
1:A:510:ILE:H	1:A:510:ILE:HG13	1.63	0.45
1:A:540:LEU:HD23	1:A:561:LEU:HD21	1.99	0.45
1:A:617:LYS:O	1:A:618:LYS:HG2	2.17	0.45
3:D:179:LEU:HD21	3:D:186:TYR:HB2	1.98	0.45
3:D:637:MET:HB2	3:D:640:ILE:HG12	1.99	0.45
5:F:231:LEU:HD21	5:F:233:VAL:HG23	1.99	0.45
7:G:193:THR:HG22	7:G:274:LEU:HD22	1.99	0.45
7:J:130:GLU:OE2	7:K:165:ASP:HA	2.16	0.45
7:J:177:ASN:ND2	7:J:292:VAL:HG23	2.32	0.45
7:K:191:PHE:O	7:K:192:ARG:HG3	2.16	0.45
7:K:374:SER:O	7:L:220:LEU:HD12	2.16	0.45
7:L:191:PHE:CD1	7:L:191:PHE:N	2.73	0.45
7:L:514:GLU:HB2	7:L:522:LYS:HB2	1.99	0.45
7:N:270:GLU:O	7:N:343:LYS:N	2.39	0.45
7:R:514:GLU:HB2	7:R:522:LYS:HB2	1.99	0.45
7:W:402:ASP:HB2	7:X:193:THR:HG22	1.98	0.45
7:X:514:GLU:HB2	7:X:522:LYS:HB2	1.99	0.45
2:C:260:HIS:HD2	2:C:262:GLU:HB2	1.80	0.45
3:D:52:VAL:HB	3:D:55:TYR:HE1	1.81	0.45
7:G:358:ARG:HB3	7:G:385:VAL:HB	1.98	0.45
7:P:433:ASP:OD1	7:P:434:PHE:N	2.50	0.45
7:H:220:LEU:O	7:H:247:GLY:N	2.49	0.45
7:I:41:PHE:CD1	7:I:310:GLU:HG3	2.50	0.45
7:K:266:SER:O	7:K:347:LYS:N	2.40	0.45
7:K:465:ASN:HD21	7:K:468:LEU:HD23	1.80	0.45
7:L:386:LYS:CD	7:M:209:GLU:HB3	2.47	0.45
7:L:391:ARG:HH21	7:M:204:LYS:CG	2.25	0.45
7:M:191:PHE:O	7:M:192:ARG:HG3	2.16	0.45
7:O:479:ASP:O	7:O:483:GLU:CB	2.61	0.45
7:Q:90:ARG:NH1	7:Q:103:ASP:OD1	2.44	0.45
7:V:380:ASN:ND2	7:W:215:ASN:HB3	2.15	0.45
7:W:106:ASP:N	7:X:159:LEU:HD13	2.32	0.45
7:X:189:LYS:CE	7:X:191:PHE:HZ	2.29	0.45
3:D:607:GLY:HA3	3:D:624:MET:HG2	1.98	0.45
5:F:116:ILE:HG22	5:F:176:PHE:HB3	1.99	0.45
7:G:305:LEU:HD21	7:G:473:LEU:HD11	1.98	0.45
7:I:370:PHE:HE2	7:I:375:VAL:HG23	1.82	0.45
7:I:514:GLU:HB2	7:I:522:LYS:HB2	1.99	0.45
7:N:191:PHE:O	7:N:192:ARG:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:413:ARG:HH11	7:O:282:LEU:C	2.20	0.45
7:S:177:ASN:ND2	7:S:292:VAL:HG23	2.32	0.45
7:S:220:LEU:O	7:S:247:GLY:N	2.49	0.45
7:S:465:ASN:HD21	7:S:468:LEU:HD23	1.80	0.45
7:T:370:PHE:HE2	7:T:375:VAL:HG23	1.82	0.45
1:A:363:LEU:HD21	1:A:428:VAL:HG13	1.97	0.45
2:C:383:THR:OG1	5:F:414:ARG:HG2	2.16	0.45
5:F:28:TYR:OH	7:G:290:ARG:NH1	2.34	0.45
5:F:152:ASN:HD21	5:F:174:LYS:HA	1.81	0.45
5:F:192:ASP:OD1	5:F:192:ASP:N	2.50	0.45
5:F:312:ILE:HG23	5:F:429:PHE:HB2	1.99	0.45
7:H:191:PHE:O	7:H:192:ARG:HG3	2.16	0.45
7:H:465:ASN:HD21	7:H:468:LEU:HD23	1.80	0.45
7:J:370:PHE:CB	7:J:373:ILE:CG1	2.93	0.45
7:K:105:GLY:HA2	7:L:159:LEU:HD22	1.98	0.45
7:L:391:ARG:HE	7:M:204:LYS:HE2	1.81	0.45
7:O:370:PHE:HE2	7:O:375:VAL:HG23	1.82	0.45
7:O:514:GLU:HB2	7:O:522:LYS:HB2	1.99	0.45
7:S:378:GLU:O	7:T:216:ALA:HA	2.17	0.45
7:S:400:LEU:HD12	7:T:195:HIS:CB	2.38	0.45
7:U:424:LEU:HD11	7:V:191:PHE:CE2	2.51	0.45
7:W:350:GLY:O	7:W:393:VAL:N	2.48	0.45
7:W:370:PHE:HE2	7:W:375:VAL:HG23	1.82	0.45
6:B:491:VAL:HG23	6:B:507:LEU:HD23	1.98	0.45
7:G:403:ASP:HA	7:P:192:ARG:HG2	1.98	0.45
7:I:87:SER:OG	7:J:94:MET:HE1	2.16	0.45
7:K:64:ARG:O	7:L:467:HIS:ND1	2.47	0.45
7:O:90:ARG:NH1	7:O:103:ASP:OD1	2.44	0.45
7:V:189:LYS:CE	7:V:191:PHE:HZ	2.29	0.45
7:V:414:LYS:HG2	7:W:435:VAL:HG11	1.96	0.45
7:W:220:LEU:O	7:W:247:GLY:N	2.49	0.45
2:C:113:ASP:OD1	2:C:114:GLN:N	2.47	0.45
6:B:122:VAL:HG21	6:B:352:ALA:HB1	1.98	0.45
6:B:733:PRO:HA	6:B:734:LYS:HA	1.67	0.45
7:H:65:ARG:HB2	7:I:467:HIS:CG	2.51	0.45
7:H:266:SER:O	7:H:347:LYS:N	2.40	0.45
7:M:206:ILE:O	7:M:261:LEU:N	2.46	0.45
7:N:370:PHE:HE2	7:N:375:VAL:HG23	1.82	0.45
7:Q:266:SER:O	7:Q:347:LYS:N	2.40	0.45
7:R:346:MET:N	7:R:397:SER:O	2.45	0.45
7:S:145:ASP:OD2	7:T:284:ARG:NH1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:386:LYS:HE2	7:T:207:ILE:HG23	1.99	0.45
7:U:370:PHE:CD1	7:U:373:ILE:HD13	2.49	0.45
7:V:177:ASN:ND2	7:V:292:VAL:HG23	2.32	0.45
7:V:350:GLY:O	7:V:393:VAL:N	2.48	0.45
7:V:389:GLU:HA	7:W:205:SER:O	2.17	0.45
7:V:391:ARG:NE	7:W:204:LYS:HG2	2.21	0.45
7:V:400:LEU:HB2	7:W:195:HIS:CG	2.52	0.45
7:W:514:GLU:HB2	7:W:522:LYS:HB2	1.99	0.45
2:C:251:LYS:HE3	3:D:153:ASN:HD21	1.81	0.45
3:D:261:GLN:HG3	3:D:263:ILE:HG12	1.99	0.45
4:E:78:GLN:O	4:E:177:LEU:N	2.48	0.45
6:B:502:THR:HG23	6:B:621:GLN:HE21	1.82	0.45
7:I:177:ASN:ND2	7:I:292:VAL:HG23	2.32	0.45
7:L:191:PHE:O	7:L:192:ARG:HG3	2.16	0.45
7:O:130:GLU:CD	7:Q:165:ASP:HA	2.37	0.45
7:Q:395:ILE:HA	7:R:199:GLN:O	2.17	0.45
7:R:370:PHE:CB	7:R:373:ILE:N	2.62	0.45
7:R:370:PHE:HE2	7:R:375:VAL:HG23	1.82	0.45
7:R:391:ARG:NH2	7:S:204:LYS:CE	2.75	0.45
7:S:130:GLU:OE2	7:T:165:ASP:HA	2.17	0.45
7:W:191:PHE:O	7:W:192:ARG:HG3	2.16	0.45
7:W:404:VAL:HB	7:X:191:PHE:CA	2.47	0.45
7:X:177:ASN:ND2	7:X:292:VAL:HG23	2.32	0.45
3:D:506:TRP:HE1	3:D:521:ARG:HE	1.64	0.44
3:D:646:LYS:HB2	3:D:649:TYR:HE1	1.82	0.44
5:F:320:ILE:HB	5:F:394:ARG:HB2	1.98	0.44
5:F:435:HIS:HB3	5:F:453:LEU:HD22	2.00	0.44
7:G:92:ILE:HG13	7:G:96:LEU:H	1.82	0.44
7:J:266:SER:O	7:J:347:LYS:N	2.40	0.44
7:J:411:GLY:O	7:K:185:THR:HG21	2.18	0.44
7:M:339:TYR:HB3	7:M:404:VAL:CG1	2.33	0.44
7:N:346:MET:N	7:N:397:SER:O	2.45	0.44
7:O:191:PHE:O	7:O:192:ARG:HG3	2.16	0.44
7:Q:328:SER:O	7:Q:451:LYS:N	2.42	0.44
7:R:489:CYS:SG	7:R:490:HIS:N	2.90	0.44
7:S:266:SER:O	7:S:347:LYS:N	2.40	0.44
7:S:339:TYR:HB3	7:S:404:VAL:CG1	2.33	0.44
7:W:340:VAL:N	7:W:403:ASP:O	2.39	0.44
7:W:372:GLU:CB	7:X:223:THR:O	2.64	0.44
1:A:370:PRO:HG2	1:A:470:THR:HG21	1.98	0.44
1:A:515:ARG:HG3	1:A:526:ILE:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:92:CYS:HB2	2:C:97:ASP:HB2	1.99	0.44
2:C:197:LYS:HG2	2:C:219:ASP:HA	1.98	0.44
7:P:328:SER:O	7:P:451:LYS:N	2.43	0.44
7:H:64:ARG:H	7:I:470:LYS:HZ3	1.65	0.44
7:J:106:ASP:OD2	7:K:122:ARG:N	2.50	0.44
7:J:489:CYS:SG	7:J:490:HIS:N	2.90	0.44
7:N:90:ARG:NH1	7:N:103:ASP:OD1	2.44	0.44
7:T:266:SER:O	7:T:347:LYS:N	2.40	0.44
7:U:489:CYS:SG	7:U:490:HIS:N	2.90	0.44
7:W:130:GLU:OE2	7:X:165:ASP:C	2.54	0.44
7:X:191:PHE:O	7:X:192:ARG:HG3	2.16	0.44
7:X:270:GLU:O	7:X:343:LYS:N	2.39	0.44
7:X:370:PHE:HE2	7:X:375:VAL:HG23	1.82	0.44
1:A:30:ILE:H	1:A:632:LEU:HD13	1.82	0.44
3:D:665:LEU:HD23	3:D:669:SER:HA	1.99	0.44
7:I:328:SER:O	7:I:451:LYS:N	2.42	0.44
7:K:489:CYS:SG	7:K:490:HIS:N	2.90	0.44
7:M:514:GLU:HB2	7:M:522:LYS:HB2	1.99	0.44
7:O:374:SER:HB3	7:Q:221:LYS:HG2	1.98	0.44
7:R:148:SER:HB3	7:S:180:SER:HB2	1.99	0.44
7:R:421:GLU:OE1	7:S:434:PHE:HB2	2.17	0.44
1:A:577:PRO:O	1:A:582:TYR:OH	2.29	0.44
7:G:280:ILE:HG23	7:G:441:ILE:HD13	2.00	0.44
7:G:333:GLY:N	7:G:448:ILE:HD11	2.32	0.44
7:P:279:GLU:HA	7:P:334:LEU:HA	1.99	0.44
7:H:514:GLU:HB2	7:H:522:LYS:HB2	1.99	0.44
7:I:106:ASP:CB	7:J:159:LEU:HD13	2.47	0.44
7:J:391:ARG:HE	7:K:204:LYS:HE2	1.81	0.44
7:J:514:GLU:HB2	7:J:522:LYS:HB2	1.99	0.44
7:M:346:MET:N	7:M:397:SER:O	2.45	0.44
7:N:189:LYS:HE2	7:N:191:PHE:HZ	1.73	0.44
7:N:391:ARG:CZ	7:O:204:LYS:CE	2.94	0.44
7:N:404:VAL:HB	7:O:191:PHE:H	1.82	0.44
7:Q:28:SER:HB2	7:Q:43:SER:HB3	2.00	0.44
7:R:360:LEU:N	7:R:383:ASP:O	2.44	0.44
7:T:489:CYS:SG	7:T:490:HIS:N	2.90	0.44
7:V:328:SER:O	7:V:451:LYS:N	2.42	0.44
7:V:370:PHE:HE2	7:V:375:VAL:HG23	1.82	0.44
7:W:130:GLU:OE2	7:X:165:ASP:HA	2.17	0.44
7:W:400:LEU:HB2	7:X:195:HIS:H	1.81	0.44
7:X:28:SER:HB2	7:X:43:SER:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:MET:SD	1:A:283:MET:N	2.81	0.44
2:C:110:HIS:HB2	2:C:112:MET:SD	2.57	0.44
2:C:442:PHE:O	2:C:446:VAL:HG22	2.18	0.44
3:D:323:LYS:HE3	3:D:367:GLN:HE21	1.83	0.44
3:D:554:ARG:HG2	6:B:128:ILE:HG21	1.99	0.44
7:J:479:ASP:O	7:J:483:GLU:CB	2.61	0.44
7:K:514:GLU:HB2	7:K:522:LYS:HB2	1.99	0.44
7:L:220:LEU:O	7:L:247:GLY:N	2.49	0.44
7:L:492:CYS:SG	7:L:493:GLN:N	2.91	0.44
7:M:350:GLY:O	7:M:393:VAL:N	2.48	0.44
7:M:492:CYS:SG	7:M:493:GLN:N	2.91	0.44
7:N:206:ILE:O	7:N:261:LEU:N	2.46	0.44
7:Q:145:ASP:OD2	7:R:284:ARG:NH1	2.51	0.44
7:U:40:MET:HB2	7:U:65:ARG:HB3	2.00	0.44
7:U:328:SER:O	7:U:451:LYS:N	2.42	0.44
7:W:417:PHE:CD2	7:X:280:ILE:HD11	2.49	0.44
7:W:492:CYS:SG	7:W:493:GLN:N	2.91	0.44
6:B:497:ILE:HB	6:B:498:PRO:HD2	2.00	0.44
7:P:196:TYR:HB2	7:P:271:LYS:HB2	2.00	0.44
7:I:220:LEU:O	7:I:247:GLY:N	2.49	0.44
7:J:28:SER:HB2	7:J:43:SER:HB3	2.00	0.44
7:J:370:PHE:HE2	7:J:375:VAL:HG23	1.82	0.44
7:M:189:LYS:CE	7:M:191:PHE:HZ	2.29	0.44
7:O:28:SER:HB2	7:O:43:SER:HB3	2.00	0.44
7:R:28:SER:HB2	7:R:43:SER:HB3	2.00	0.44
7:S:370:PHE:CD1	7:S:373:ILE:HD13	2.50	0.44
7:T:220:LEU:O	7:T:247:GLY:N	2.49	0.44
7:U:370:PHE:HE2	7:U:375:VAL:HG23	1.82	0.44
7:V:266:SER:O	7:V:347:LYS:N	2.40	0.44
7:W:105:GLY:HA2	7:X:159:LEU:HD22	1.99	0.44
7:W:189:LYS:HE2	7:W:191:PHE:HZ	1.73	0.44
7:X:346:MET:N	7:X:397:SER:O	2.45	0.44
1:A:768:TYR:HA	1:A:769:PHE:HA	1.76	0.44
2:C:338:VAL:HG12	2:C:339:TYR:N	2.33	0.44
3:D:139:LEU:HD23	3:D:142:ASN:ND2	2.31	0.44
3:D:139:LEU:HA	3:D:142:ASN:HD22	1.83	0.44
7:H:40:MET:HB2	7:H:65:ARG:HB3	2.00	0.44
7:J:189:LYS:CE	7:J:191:PHE:HZ	2.29	0.44
7:M:28:SER:HB2	7:M:43:SER:HB3	2.00	0.44
7:N:370:PHE:CB	7:N:373:ILE:CG1	2.93	0.44
7:N:514:GLU:HB2	7:N:522:LYS:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:400:LEU:HD12	7:Q:195:HIS:CB	2.43	0.44
7:T:387:ARG:HA	7:U:208:GLN:HE22	1.82	0.44
7:W:479:ASP:O	7:W:483:GLU:CB	2.61	0.44
7:X:489:CYS:SG	7:X:490:HIS:N	2.90	0.44
2:C:473:VAL:HG21	5:F:194:GLY:HA3	1.98	0.44
5:F:519:SER:HB3	5:F:527:GLU:H	1.83	0.44
7:G:193:THR:HA	7:G:274:LEU:HD22	2.00	0.44
7:I:28:SER:HB2	7:I:43:SER:HB3	2.00	0.44
7:K:40:MET:HB2	7:K:65:ARG:HB3	2.00	0.44
7:L:40:MET:HB2	7:L:65:ARG:HB3	2.00	0.44
7:L:392:ALA:HB3	7:M:203:PHE:N	2.29	0.44
7:M:370:PHE:CD1	7:M:373:ILE:HD13	2.49	0.44
7:N:189:LYS:CE	7:N:191:PHE:HZ	2.29	0.44
7:N:386:LYS:CD	7:O:209:GLU:HB3	2.47	0.44
7:Q:177:ASN:ND2	7:Q:292:VAL:HG23	2.32	0.44
7:T:395:ILE:HA	7:U:199:GLN:O	2.18	0.44
7:V:220:LEU:O	7:V:247:GLY:N	2.49	0.44
7:W:409:ARG:HA	7:X:186:LYS:HA	2.00	0.44
7:W:418:GLU:HB2	7:X:435:VAL:CG2	2.41	0.44
7:X:40:MET:HB2	7:X:65:ARG:HB3	2.00	0.44
7:X:370:PHE:CD2	7:X:373:ILE:C	2.80	0.44
1:A:102:VAL:HG12	1:A:117:MET:O	2.18	0.44
1:A:360:PRO:HG3	1:A:636:ALA:HB3	2.00	0.44
1:A:1023:HIS:ND1	1:A:1298:THR:HG21	2.33	0.44
1:A:1285:TYR:N	1:A:1286:SER:HA	2.32	0.44
3:D:274:GLU:HB3	3:D:275:PRO:HD3	2.00	0.44
5:F:333:GLU:HG2	5:F:381:ARG:HG3	1.99	0.44
5:F:407:ASN:OD1	10:F:601:NAG:N2	2.51	0.44
6:B:581:TYR:CD2	6:B:610:ASP:HB2	2.51	0.44
7:I:40:MET:HB2	7:I:65:ARG:HB3	2.00	0.44
7:N:489:CYS:SG	7:N:490:HIS:N	2.90	0.44
7:O:177:ASN:ND2	7:O:292:VAL:HG23	2.32	0.44
7:O:370:PHE:CD1	7:O:373:ILE:HD13	2.49	0.44
7:Q:372:GLU:OE1	7:R:223:THR:HB	2.18	0.44
7:Q:514:GLU:HB2	7:Q:522:LYS:HB2	1.99	0.44
7:R:40:MET:HB2	7:R:65:ARG:HB3	2.00	0.44
7:W:266:SER:O	7:W:347:LYS:N	2.40	0.44
2:C:379:GLU:OE1	5:F:418:ARG:NE	2.47	0.43
7:G:49:PHE:CE2	7:G:484:PHE:HB2	2.53	0.43
7:P:366:VAL:HB	7:P:377:ALA:HB3	2.00	0.43
7:H:177:ASN:ND2	7:H:292:VAL:HG23	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:492:CYS:SG	7:H:493:GLN:N	2.91	0.43
7:I:193:THR:HA	7:I:274:LEU:HB3	2.00	0.43
7:M:370:PHE:HE2	7:M:375:VAL:HG23	1.82	0.43
7:O:380:ASN:ND2	7:Q:215:ASN:HB2	2.32	0.43
7:Q:370:PHE:HE2	7:Q:375:VAL:HG23	1.82	0.43
7:T:193:THR:HA	7:T:274:LEU:HB3	2.01	0.43
7:U:189:LYS:CE	7:U:191:PHE:HZ	2.29	0.43
7:V:391:ARG:NH2	7:W:203:PHE:C	2.71	0.43
7:W:28:SER:HB2	7:W:43:SER:HB3	2.00	0.43
7:W:130:GLU:HG3	7:X:165:ASP:N	2.30	0.43
7:X:479:ASP:O	7:X:483:GLU:CB	2.61	0.43
1:A:1184:SER:OG	1:A:1230:ASP:OD1	2.37	0.43
2:C:141:TYR:HE1	2:C:157:ARG:HG3	1.83	0.43
5:F:327:ILE:HG23	5:F:387:GLU:HB2	1.99	0.43
6:B:317:HIS:CD2	6:B:376:ASP:HB3	2.52	0.43
7:P:177:ASN:ND2	7:P:292:VAL:HG23	2.31	0.43
7:H:339:TYR:HB3	7:H:404:VAL:CG1	2.33	0.43
7:J:313:GLU:HG3	7:K:290:ARG:HH21	1.84	0.43
7:K:370:PHE:CB	7:K:373:ILE:N	2.62	0.43
7:K:370:PHE:HE2	7:K:375:VAL:HG23	1.82	0.43
7:M:370:PHE:CB	7:M:373:ILE:CG1	2.92	0.43
7:N:400:LEU:HB2	7:O:195:HIS:H	1.83	0.43
7:R:380:ASN:ND2	7:S:215:ASN:HB2	2.24	0.43
7:U:193:THR:HA	7:U:274:LEU:HB3	2.00	0.43
7:V:28:SER:HB2	7:V:43:SER:HB3	2.00	0.43
7:V:206:ILE:O	7:V:261:LEU:N	2.46	0.43
7:V:404:VAL:O	7:W:191:PHE:CB	2.63	0.43
1:A:205:TYR:HB2	1:A:209:PHE:HB2	2.00	0.43
6:B:499:CYS:HA	6:B:624:ILE:O	2.18	0.43
7:G:274:LEU:HD11	7:G:339:TYR:CE2	2.53	0.43
7:G:502:ASP:OD2	7:P:452:LEU:N	2.44	0.43
7:I:370:PHE:CB	7:I:373:ILE:CG1	2.92	0.43
7:K:220:LEU:O	7:K:247:GLY:N	2.49	0.43
7:L:360:LEU:N	7:L:383:ASP:O	2.44	0.43
7:M:344:ALA:HB3	7:M:399:ASN:HB2	2.01	0.43
7:N:28:SER:HB2	7:N:43:SER:HB3	2.00	0.43
7:O:189:LYS:CE	7:O:191:PHE:HZ	2.29	0.43
7:R:193:THR:HA	7:R:274:LEU:HB3	2.00	0.43
7:S:189:LYS:CE	7:S:191:PHE:HZ	2.29	0.43
7:T:380:ASN:ND2	7:U:215:ASN:HB2	2.16	0.43
7:T:514:GLU:HB2	7:T:522:LYS:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:177:ASN:ND2	7:U:292:VAL:HG23	2.32	0.43
7:W:370:PHE:CD1	7:W:373:ILE:HD13	2.50	0.43
1:A:253:ARG:HH22	1:A:257:ASN:ND2	2.15	0.43
3:D:202:ASN:HA	3:D:246:LYS:HB3	2.01	0.43
3:D:268:GLU:H	3:D:429:LYS:NZ	2.16	0.43
5:F:37:ASN:HD22	5:F:43:ILE:HG22	1.81	0.43
5:F:184:LYS:HG3	5:F:186:HIS:H	1.83	0.43
6:B:418:HIS:NE2	6:B:420:CYS:SG	2.92	0.43
7:G:310:GLU:HG2	7:G:313:GLU:H	1.83	0.43
7:J:40:MET:HB2	7:J:65:ARG:HB3	2.00	0.43
7:J:413:ARG:HH12	7:K:282:LEU:HG	1.82	0.43
7:L:206:ILE:O	7:L:261:LEU:N	2.46	0.43
7:M:479:ASP:O	7:M:483:GLU:CB	2.61	0.43
7:Q:413:ARG:NH1	7:R:282:LEU:CA	2.79	0.43
7:S:370:PHE:HE2	7:S:375:VAL:HG23	1.82	0.43
7:T:346:MET:N	7:T:397:SER:O	2.45	0.43
7:U:514:GLU:HB2	7:U:522:LYS:HB2	1.99	0.43
7:V:130:GLU:OE2	7:W:167:ASN:O	2.36	0.43
7:W:378:GLU:OE1	7:X:217:ALA:HB3	2.19	0.43
7:W:489:CYS:SG	7:W:490:HIS:N	2.90	0.43
3:D:205:TRP:N	3:D:243:HIS:O	2.51	0.43
6:B:59:ASN:HD21	6:B:429:HIS:CE1	2.37	0.43
6:B:284:PHE:CD2	6:B:284:PHE:O	2.70	0.43
7:P:255:LYS:HE3	7:P:358:ARG:HE	1.83	0.43
7:P:392:ALA:HB3	7:H:203:PHE:H	1.84	0.43
7:J:406:SER:OG	7:J:420:LYS:NZ	2.48	0.43
7:J:412:THR:OG1	7:K:167:ASN:HB3	2.18	0.43
7:K:193:THR:HA	7:K:274:LEU:HB3	2.00	0.43
7:L:370:PHE:CD1	7:L:373:ILE:HD13	2.50	0.43
7:N:406:SER:OG	7:N:420:LYS:NZ	2.49	0.43
7:O:370:PHE:CD2	7:O:373:ILE:C	2.81	0.43
7:R:386:LYS:HB3	7:S:209:GLU:H	1.82	0.43
7:S:492:CYS:SG	7:S:493:GLN:N	2.91	0.43
7:T:28:SER:HB2	7:T:43:SER:HB3	2.00	0.43
7:T:370:PHE:CB	7:T:373:ILE:CG1	2.92	0.43
7:U:224:PRO:HG3	7:U:243:LEU:HD23	2.01	0.43
7:U:344:ALA:HB3	7:U:399:ASN:HB2	2.01	0.43
7:V:489:CYS:SG	7:V:490:HIS:N	2.90	0.43
7:W:413:ARG:O	7:X:438:ALA:HB1	2.19	0.43
1:A:1026:GLU:HG2	1:A:1092:TYR:HE1	1.83	0.43
3:D:603:TYR:HA	3:D:628:LYS:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:706:LYS:HG2	6:B:707:PRO:HD2	2.00	0.43
7:P:406:SER:OG	7:P:420:LYS:NZ	2.47	0.43
7:H:193:THR:HA	7:H:274:LEU:HB3	2.00	0.43
7:K:28:SER:HB2	7:K:43:SER:HB3	2.00	0.43
7:K:339:TYR:HB3	7:K:404:VAL:CG1	2.33	0.43
7:K:370:PHE:CD1	7:K:373:ILE:HD13	2.49	0.43
7:K:492:CYS:SG	7:K:493:GLN:N	2.91	0.43
7:L:400:LEU:CD1	7:M:195:HIS:CD2	2.96	0.43
7:T:370:PHE:CD1	7:T:373:ILE:HD13	2.50	0.43
7:V:40:MET:HB2	7:V:65:ARG:HB3	2.00	0.43
7:V:344:ALA:HB3	7:V:399:ASN:HB2	2.01	0.43
7:W:90:ARG:NH1	7:W:103:ASP:OD1	2.44	0.43
7:X:344:ALA:HB3	7:X:399:ASN:HB2	2.01	0.43
1:A:265:VAL:HG22	1:A:329:VAL:HG13	2.01	0.43
1:A:855:PHE:HA	1:A:916:THR:HG23	2.00	0.43
1:A:1019:PHE:CD1	1:A:1049:LEU:HG	2.54	0.43
5:F:159:ARG:HE	5:F:170:GLY:HA2	1.84	0.43
6:B:286:SER:O	6:B:287:SER:HB2	2.19	0.43
7:P:256:ASN:HB3	10:P:604:NAG:HN2	1.83	0.43
7:P:465:ASN:HD21	7:P:468:LEU:HD23	1.82	0.43
7:K:224:PRO:HG3	7:K:243:LEU:HD23	2.01	0.43
7:L:147:LEU:HG	7:L:148:SER:H	1.84	0.43
7:N:40:MET:HB2	7:N:65:ARG:HB3	2.00	0.43
7:O:40:MET:HB2	7:O:65:ARG:HB3	2.00	0.43
7:O:489:CYS:SG	7:O:490:HIS:N	2.90	0.43
7:Q:492:CYS:SG	7:Q:493:GLN:N	2.91	0.43
7:T:224:PRO:HG3	7:T:243:LEU:HD23	2.01	0.43
7:U:147:LEU:HG	7:U:148:SER:H	1.84	0.43
7:W:344:ALA:HB3	7:W:399:ASN:HB2	2.01	0.43
1:A:374:GLN:HE21	1:A:382:LEU:HB3	1.83	0.43
1:A:652:THR:OG1	1:A:660:ASP:OD2	2.25	0.43
3:D:184:LEU:HD13	3:D:265:ASN:HB2	2.00	0.43
4:E:174:PHE:HB2	5:F:414:ARG:HE	1.84	0.43
5:F:375:GLY:N	7:G:205:SER:O	2.52	0.43
7:G:28:SER:HB2	7:G:43:SER:HB3	2.00	0.43
7:P:280:ILE:HG21	7:P:437:TRP:HE1	1.83	0.43
7:I:206:ILE:O	7:I:261:LEU:N	2.46	0.43
7:I:492:CYS:SG	7:I:493:GLN:N	2.91	0.43
7:L:28:SER:HB2	7:L:43:SER:HB3	2.00	0.43
7:L:224:PRO:HG3	7:L:243:LEU:HD23	2.01	0.43
7:L:370:PHE:HE2	7:L:375:VAL:HG23	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:193:THR:HA	7:M:274:LEU:HB3	2.01	0.43
7:M:224:PRO:HG3	7:M:243:LEU:HD23	2.01	0.43
7:N:177:ASN:ND2	7:N:292:VAL:HG23	2.32	0.43
7:N:387:ARG:HA	7:O:208:GLN:HE22	1.84	0.43
7:O:344:ALA:HB3	7:O:399:ASN:HB2	2.01	0.43
7:R:177:ASN:ND2	7:R:292:VAL:HG23	2.32	0.43
7:R:220:LEU:O	7:R:247:GLY:N	2.49	0.43
7:S:364:LEU:N	7:S:379:PHE:O	2.49	0.43
7:U:396:THR:HB	7:V:199:GLN:HB3	2.01	0.43
1:A:390:LEU:HB3	1:A:435:VAL:HG22	2.00	0.43
4:E:84:GLY:O	4:E:93:LEU:N	2.40	0.43
6:B:205:ARG:HG3	6:B:361:PHE:C	2.39	0.43
7:P:489:CYS:SG	7:P:490:HIS:N	2.91	0.43
7:H:42:ARG:NH2	7:I:471:GLN:CD	2.70	0.43
7:H:224:PRO:HG3	7:H:243:LEU:HD23	2.01	0.43
7:N:407:LEU:HA	7:O:188:GLU:HB3	1.99	0.43
7:Q:193:THR:HA	7:Q:274:LEU:HB3	2.00	0.43
7:T:49:PHE:CE2	7:T:484:PHE:HB2	2.54	0.43
7:U:28:SER:HB2	7:U:43:SER:HB3	2.00	0.43
7:U:380:ASN:O	7:V:214:PHE:HD1	1.82	0.43
7:W:49:PHE:CE2	7:W:484:PHE:HB2	2.54	0.43
7:W:189:LYS:CE	7:W:191:PHE:HZ	2.29	0.43
7:X:193:THR:HA	7:X:274:LEU:HB3	2.00	0.43
7:X:220:LEU:O	7:X:247:GLY:N	2.49	0.43
1:A:1279:ARG:C	1:A:1281:GLY:HA2	2.39	0.43
2:C:28:LYS:NZ	2:C:55:ASP:OD1	2.51	0.43
7:H:364:LEU:N	7:H:379:PHE:O	2.49	0.43
7:I:147:LEU:HG	7:I:148:SER:H	1.84	0.43
7:I:344:ALA:HB3	7:I:399:ASN:HB2	2.01	0.43
7:I:360:LEU:N	7:I:383:ASP:O	2.44	0.43
7:I:522:LYS:HE2	7:J:196:TYR:OH	2.19	0.43
7:J:346:MET:N	7:J:397:SER:O	2.45	0.43
7:K:479:ASP:O	7:K:483:GLU:CB	2.61	0.43
7:Q:40:MET:HB2	7:Q:65:ARG:HB3	2.00	0.43
7:R:370:PHE:CB	7:R:373:ILE:CG1	2.92	0.43
7:S:193:THR:HA	7:S:274:LEU:HB3	2.00	0.43
7:S:370:PHE:CB	7:S:373:ILE:N	2.62	0.43
7:U:413:ARG:CD	7:V:280:ILE:HD11	2.48	0.43
7:V:492:CYS:SG	7:V:493:GLN:N	2.91	0.43
7:W:406:SER:N	7:X:189:LYS:O	2.52	0.43
7:X:147:LEU:HG	7:X:148:SER:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:THR:OG1	1:A:23:TYR:N	2.49	0.42
6:B:210:ASP:O	6:B:235:ASN:ND2	2.52	0.42
7:P:49:PHE:CE2	7:P:484:PHE:HB2	2.54	0.42
7:J:193:THR:HA	7:J:274:LEU:HB3	2.00	0.42
7:L:380:ASN:ND2	7:M:215:ASN:HD22	2.17	0.42
7:M:413:ARG:NH1	7:N:282:LEU:HA	2.34	0.42
7:N:49:PHE:CE2	7:N:484:PHE:HB2	2.54	0.42
7:N:479:ASP:O	7:N:483:GLU:CB	2.61	0.42
7:Q:224:PRO:HG3	7:Q:243:LEU:HD23	2.01	0.42
7:Q:421:GLU:OE1	7:R:434:PHE:CD2	2.72	0.42
7:S:28:SER:HB2	7:S:43:SER:HB3	2.00	0.42
7:S:489:CYS:SG	7:S:490:HIS:N	2.90	0.42
7:T:189:LYS:CE	7:T:191:PHE:HZ	2.29	0.42
7:U:479:ASP:O	7:U:483:GLU:CB	2.61	0.42
7:V:224:PRO:HG3	7:V:243:LEU:HD23	2.01	0.42
7:V:402:ASP:HB2	7:W:193:THR:HG22	1.92	0.42
7:W:206:ILE:O	7:W:261:LEU:N	2.46	0.42
1:A:134:VAL:HG22	1:A:613:GLN:HE22	1.84	0.42
1:A:501:TYR:CE2	1:A:513:GLY:HA3	2.54	0.42
1:A:872:VAL:HG12	1:A:879:LYS:HG3	2.00	0.42
6:B:586:THR:HB	7:X:107:PHE:CE2	2.54	0.42
7:G:489:CYS:SG	7:G:490:HIS:N	2.91	0.42
7:K:346:MET:N	7:K:397:SER:O	2.45	0.42
7:L:193:THR:HA	7:L:274:LEU:HB3	2.01	0.42
7:L:344:ALA:HB3	7:L:399:ASN:HB2	2.01	0.42
7:L:378:GLU:O	7:M:216:ALA:HA	2.19	0.42
7:M:40:MET:HB2	7:M:65:ARG:HB3	2.00	0.42
7:M:147:LEU:HG	7:M:148:SER:H	1.84	0.42
7:N:147:LEU:HG	7:N:148:SER:H	1.84	0.42
7:N:193:THR:HA	7:N:274:LEU:HB3	2.00	0.42
7:T:177:ASN:ND2	7:T:292:VAL:HG23	2.32	0.42
7:U:318:LEU:HD11	7:U:323:THR:HB	2.02	0.42
7:W:360:LEU:N	7:W:383:ASP:O	2.44	0.42
7:W:386:LYS:HB3	7:X:209:GLU:H	1.84	0.42
1:A:1158:ILE:H	1:A:1158:ILE:HG13	1.71	0.42
2:C:166:THR:HB	3:D:139:LEU:HG	2.01	0.42
7:P:147:LEU:HG	7:P:148:SER:H	1.84	0.42
7:P:206:ILE:O	7:P:261:LEU:N	2.49	0.42
7:P:274:LEU:HD11	7:P:339:TYR:CE1	2.54	0.42
7:H:28:SER:HB2	7:H:43:SER:HB3	2.00	0.42
7:H:147:LEU:HG	7:H:148:SER:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:489:CYS:SG	7:H:490:HIS:N	2.90	0.42
7:I:224:PRO:HG3	7:I:243:LEU:HD23	2.01	0.42
7:M:64:ARG:C	7:N:467:HIS:ND1	2.63	0.42
7:M:177:ASN:ND2	7:M:292:VAL:HG23	2.32	0.42
7:N:318:LEU:HD11	7:N:323:THR:HB	2.02	0.42
7:O:129:SER:HB2	7:Q:164:ARG:NH1	2.33	0.42
7:O:364:LEU:N	7:O:379:PHE:O	2.49	0.42
7:R:224:PRO:HG3	7:R:243:LEU:HD23	2.01	0.42
7:R:364:LEU:HD23	7:R:379:PHE:HB2	2.01	0.42
7:R:409:ARG:HD3	7:S:184:GLU:OE2	2.19	0.42
7:S:40:MET:HB2	7:S:65:ARG:HB3	2.00	0.42
7:S:386:LYS:O	7:T:208:GLN:OE1	2.36	0.42
7:T:344:ALA:HB3	7:T:399:ASN:HB2	2.01	0.42
7:U:421:GLU:OE1	7:V:434:PHE:HB2	2.19	0.42
1:A:29:LYS:HA	1:A:652:THR:HG22	2.01	0.42
1:A:1253:TYR:OH	1:A:1288:GLN:NE2	2.52	0.42
2:C:296:LEU:HB3	2:C:406:PRO:HB2	2.01	0.42
3:D:258:GLU:HB2	3:D:415:GLN:NE2	2.34	0.42
3:D:400:LYS:HZ3	6:B:458:GLU:HB2	1.85	0.42
5:F:231:LEU:C	5:F:231:LEU:CD2	2.86	0.42
7:P:55:LYS:HE3	7:H:481:ILE:HG23	2.00	0.42
7:P:332:GLY:N	7:P:446:VAL:O	2.51	0.42
7:P:380:ASN:ND2	7:H:215:ASN:HB2	2.27	0.42
7:H:49:PHE:CE2	7:H:484:PHE:HB2	2.54	0.42
7:H:370:PHE:HE2	7:H:375:VAL:HG23	1.82	0.42
7:H:380:ASN:HD22	7:I:215:ASN:HB2	1.84	0.42
7:J:49:PHE:CE2	7:J:484:PHE:HB2	2.54	0.42
7:L:130:GLU:HG3	7:M:164:ARG:O	2.18	0.42
7:M:489:CYS:SG	7:M:490:HIS:N	2.90	0.42
7:N:344:ALA:HB3	7:N:399:ASN:HB2	2.00	0.42
7:O:224:PRO:HG3	7:O:243:LEU:HD23	2.01	0.42
7:O:413:ARG:NH1	7:Q:282:LEU:CA	2.79	0.42
7:Q:49:PHE:CE2	7:Q:484:PHE:HB2	2.54	0.42
7:Q:386:LYS:HB3	7:R:209:GLU:N	2.33	0.42
7:R:49:PHE:CE2	7:R:484:PHE:HB2	2.54	0.42
7:S:391:ARG:CZ	7:T:204:LYS:HE3	2.50	0.42
7:S:479:ASP:O	7:S:483:GLU:CB	2.61	0.42
7:W:40:MET:HB2	7:W:65:ARG:HB3	2.00	0.42
6:B:94:ASP:N	6:B:95:PRO:HD3	2.34	0.42
6:B:317:HIS:HD2	6:B:376:ASP:HB3	1.84	0.42
6:B:571:TRP:CE2	6:B:587:ARG:HD3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:204:LYS:N	7:G:263:LEU:O	2.48	0.42
7:P:400:LEU:HD12	7:H:195:HIS:HB2	2.01	0.42
7:H:60:ALA:H	7:I:454:PRO:HG2	1.85	0.42
7:H:189:LYS:CE	7:H:191:PHE:HZ	2.29	0.42
7:I:189:LYS:CE	7:I:191:PHE:HZ	2.29	0.42
7:I:364:LEU:HD23	7:I:379:PHE:HB2	2.01	0.42
7:K:49:PHE:CE2	7:K:484:PHE:HB2	2.54	0.42
7:K:147:LEU:HG	7:K:148:SER:H	1.84	0.42
7:L:189:LYS:CE	7:L:191:PHE:HZ	2.29	0.42
7:L:370:PHE:CB	7:L:373:ILE:CG1	2.93	0.42
7:N:364:LEU:HD23	7:N:379:PHE:HB2	2.01	0.42
7:O:386:LYS:HE2	7:Q:207:ILE:HG23	2.02	0.42
7:R:406:SER:OG	7:R:420:LYS:NZ	2.49	0.42
7:R:492:CYS:SG	7:R:493:GLN:N	2.91	0.42
7:S:49:PHE:CE2	7:S:484:PHE:HB2	2.54	0.42
7:U:364:LEU:N	7:U:379:PHE:O	2.49	0.42
7:U:406:SER:OG	7:U:420:LYS:NZ	2.49	0.42
7:V:49:PHE:CE2	7:V:484:PHE:HB2	2.54	0.42
7:V:193:THR:HA	7:V:274:LEU:HB3	2.00	0.42
7:V:370:PHE:CD2	7:V:373:ILE:C	2.81	0.42
7:W:402:ASP:HB2	7:X:193:THR:O	2.18	0.42
1:A:264:ASP:N	1:A:330:ILE:O	2.51	0.42
2:C:174:GLU:HA	3:D:374:GLU:HA	2.01	0.42
3:D:139:LEU:HA	3:D:142:ASN:ND2	2.35	0.42
6:B:117:CYS:N	6:B:537:THR:HG1	2.18	0.42
7:H:344:ALA:HB3	7:H:399:ASN:HB2	2.01	0.42
7:I:489:CYS:SG	7:I:490:HIS:N	2.90	0.42
7:K:406:SER:OG	7:K:420:LYS:NZ	2.48	0.42
7:M:65:ARG:CB	7:N:467:HIS:CD2	2.92	0.42
7:O:193:THR:HA	7:O:274:LEU:HB3	2.00	0.42
7:Q:344:ALA:HB3	7:Q:399:ASN:HB2	2.01	0.42
7:Q:411:GLY:O	7:R:185:THR:CG2	2.67	0.42
7:S:344:ALA:HB3	7:S:399:ASN:HB2	2.01	0.42
7:X:339:TYR:HB3	7:X:404:VAL:CG1	2.33	0.42
1:A:401:THR:OG1	1:A:402:SER:N	2.53	0.42
1:A:643:ALA:HA	1:A:653:PHE:HE1	1.84	0.42
1:A:1246:ARG:H	1:A:1246:ARG:HD3	1.85	0.42
2:C:13:LEU:HD12	2:C:48:PHE:CZ	2.54	0.42
2:C:40:GLN:NE2	2:C:469:CYS:SG	2.93	0.42
7:I:297:THR:HG21	7:J:288:ARG:CZ	2.49	0.42
7:L:394:ASN:O	7:M:201:GLU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:409:ARG:HD3	7:M:184:GLU:OE2	2.19	0.42
7:O:49:PHE:CE2	7:O:484:PHE:HB2	2.54	0.42
7:O:364:LEU:HD23	7:O:379:PHE:HB2	2.01	0.42
7:Q:106:ASP:H	7:R:159:LEU:HD13	1.84	0.42
7:T:421:GLU:CB	7:U:434:PHE:HD2	2.33	0.42
7:U:333:GLY:HA3	7:U:441:ILE:HD11	2.02	0.42
7:V:318:LEU:HD11	7:V:323:THR:HB	2.01	0.42
7:W:127:GLU:HG2	7:X:164:ARG:NH2	2.28	0.42
7:W:364:LEU:HD23	7:W:379:PHE:HB2	2.01	0.42
7:X:333:GLY:HA3	7:X:441:ILE:HD11	2.02	0.42
7:X:350:GLY:O	7:X:393:VAL:N	2.48	0.42
1:A:576:SER:HB3	1:A:577:PRO:HD3	2.01	0.42
1:A:845:VAL:O	1:A:893:SER:OG	2.38	0.42
3:D:548:GLU:O	3:D:552:HIS:N	2.45	0.42
5:F:531:GLU:HG2	5:F:532:CYS:H	1.85	0.42
6:B:210:ASP:HB2	6:B:335:SER:HA	2.02	0.42
6:B:409:LEU:HD13	6:B:410:PHE:N	2.35	0.42
7:G:40:MET:HG3	7:G:67:CYS:HB2	2.01	0.42
7:H:206:ILE:O	7:H:261:LEU:N	2.46	0.42
7:I:64:ARG:HG2	7:J:470:LYS:NZ	2.35	0.42
7:I:129:SER:HB2	7:J:164:ARG:CZ	2.48	0.42
7:J:19:HIS:CE1	7:K:487:ARG:HD2	2.55	0.42
7:K:206:ILE:O	7:K:261:LEU:N	2.46	0.42
7:M:189:LYS:HE2	7:M:191:PHE:HZ	1.73	0.42
7:R:266:SER:O	7:R:347:LYS:N	2.40	0.42
7:U:266:SER:O	7:U:347:LYS:N	2.40	0.42
7:U:294:LEU:HD23	7:U:298:PHE:HD2	1.85	0.42
7:U:364:LEU:HD23	7:U:379:PHE:HB2	2.01	0.42
7:V:333:GLY:HA3	7:V:441:ILE:HD11	2.02	0.42
7:V:380:ASN:HB2	7:W:215:ASN:CA	2.49	0.42
7:W:224:PRO:HG3	7:W:243:LEU:HD23	2.01	0.42
7:W:370:PHE:CB	7:W:373:ILE:CG1	2.93	0.42
7:X:224:PRO:HG3	7:X:243:LEU:HD23	2.01	0.42
7:X:328:SER:O	7:X:451:LYS:N	2.42	0.42
2:C:118:ILE:HD11	2:C:162:VAL:HG21	2.01	0.42
3:D:115:ASP:C	3:D:117:ASP:H	2.23	0.42
7:G:65:ARG:HD2	7:P:467:HIS:CD2	2.55	0.42
7:J:147:LEU:HG	7:J:148:SER:H	1.84	0.42
7:J:224:PRO:HG3	7:J:243:LEU:HD23	2.01	0.42
7:J:318:LEU:HD11	7:J:323:THR:HB	2.01	0.42
7:K:318:LEU:HD11	7:K:323:THR:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:333:GLY:HA3	7:M:441:ILE:HD11	2.02	0.42
7:N:224:PRO:HG3	7:N:243:LEU:HD23	2.01	0.42
7:Q:294:LEU:HD23	7:Q:298:PHE:HD2	1.85	0.42
7:S:224:PRO:HG3	7:S:243:LEU:HD23	2.01	0.42
7:S:395:ILE:HA	7:T:199:GLN:O	2.18	0.42
7:S:406:SER:OG	7:S:420:LYS:NZ	2.48	0.42
7:T:206:ILE:O	7:T:261:LEU:N	2.46	0.42
7:T:318:LEU:HD11	7:T:323:THR:HB	2.01	0.42
7:T:339:TYR:CD1	7:T:339:TYR:C	2.94	0.42
7:T:364:LEU:HD23	7:T:379:PHE:HB2	2.02	0.42
7:U:411:GLY:O	7:V:185:THR:CG2	2.65	0.42
7:V:147:LEU:HG	7:V:148:SER:H	1.84	0.42
7:V:339:TYR:CD1	7:V:339:TYR:C	2.94	0.42
7:W:147:LEU:HG	7:W:148:SER:H	1.84	0.42
7:W:193:THR:HA	7:W:274:LEU:HB3	2.00	0.42
7:W:294:LEU:HD23	7:W:298:PHE:HD2	1.85	0.42
7:W:333:GLY:HA3	7:W:441:ILE:HD11	2.02	0.42
7:W:404:VAL:O	7:X:190:ASN:CB	2.66	0.42
7:X:492:CYS:SG	7:X:493:GLN:N	2.91	0.42
1:A:1180:LEU:HB2	1:A:1181:PRO:HD3	2.02	0.42
5:F:512:TRP:CE2	5:F:544:CYS:HB3	2.55	0.42
7:P:40:MET:HB2	7:P:65:ARG:HB3	2.02	0.42
7:P:190:ASN:OD1	7:P:277:LYS:N	2.49	0.42
7:P:492:CYS:SG	7:P:493:GLN:N	2.91	0.42
7:H:360:LEU:N	7:H:383:ASP:O	2.44	0.42
7:H:372:GLU:HG3	7:I:224:PRO:HA	2.02	0.42
7:K:177:ASN:ND2	7:K:292:VAL:HG23	2.32	0.42
7:L:489:CYS:SG	7:L:490:HIS:N	2.90	0.42
7:M:318:LEU:HD11	7:M:323:THR:HB	2.01	0.42
7:M:339:TYR:C	7:M:339:TYR:CD1	2.94	0.42
7:N:130:GLU:CB	7:O:164:ARG:O	2.68	0.42
7:N:374:SER:O	7:O:220:LEU:CD1	2.64	0.42
7:Q:318:LEU:HD11	7:Q:323:THR:HB	2.01	0.42
7:Q:339:TYR:CD1	7:Q:339:TYR:C	2.94	0.42
7:R:344:ALA:HB3	7:R:399:ASN:HB2	2.01	0.42
7:T:191:PHE:CD1	7:T:191:PHE:N	2.73	0.42
7:U:220:LEU:O	7:U:247:GLY:N	2.49	0.42
7:W:394:ASN:O	7:X:201:GLU:N	2.53	0.42
7:X:339:TYR:CD1	7:X:339:TYR:C	2.94	0.42
7:X:364:LEU:HD23	7:X:379:PHE:HB2	2.01	0.42
2:C:326:LYS:HG2	2:C:347:GLY:HA3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:336:GLU:HA	2:C:337:GLU:HA	1.59	0.41
5:F:397:SER:HB2	5:F:419:SER:HB3	2.02	0.41
6:B:715:ILE:HG12	6:B:728:ILE:HG12	2.01	0.41
7:G:64:ARG:H	7:P:470:LYS:HZ3	1.67	0.41
7:P:372:GLU:CD	7:H:222:PHE:CZ	2.93	0.41
7:I:49:PHE:CE2	7:I:484:PHE:HB2	2.54	0.41
7:I:87:SER:OG	7:J:94:MET:HE2	2.20	0.41
7:I:333:GLY:HA3	7:I:441:ILE:HD11	2.02	0.41
7:K:189:LYS:CE	7:K:191:PHE:HZ	2.29	0.41
7:L:364:LEU:HD23	7:L:379:PHE:HB2	2.01	0.41
7:L:391:ARG:HH21	7:M:204:LYS:HE3	1.84	0.41
7:N:333:GLY:HA3	7:N:441:ILE:HD11	2.02	0.41
7:N:386:LYS:HD2	7:O:209:GLU:HB3	2.02	0.41
7:O:162:ARG:HB3	7:O:164:ARG:HG3	2.02	0.41
7:O:294:LEU:HD23	7:O:298:PHE:HD2	1.85	0.41
7:O:318:LEU:HD11	7:O:323:THR:HB	2.02	0.41
7:O:492:CYS:SG	7:O:493:GLN:N	2.91	0.41
7:Q:421:GLU:OE1	7:R:434:PHE:HD2	2.03	0.41
7:R:147:LEU:HG	7:R:148:SER:H	1.84	0.41
7:S:318:LEU:HD11	7:S:323:THR:HB	2.02	0.41
7:T:40:MET:HB2	7:T:65:ARG:HB3	2.00	0.41
7:T:333:GLY:HA3	7:T:441:ILE:HD11	2.02	0.41
7:U:127:GLU:HG2	7:V:164:ARG:HH22	1.85	0.41
7:U:370:PHE:CB	7:U:373:ILE:CG1	2.93	0.41
7:V:406:SER:OG	7:V:420:LYS:NZ	2.49	0.41
1:A:935:LYS:HD2	1:A:1367:LYS:HB2	2.02	0.41
5:F:490:ARG:H	5:F:498:CYS:HB3	1.86	0.41
7:G:192:ARG:HD2	7:G:275:HIS:H	1.84	0.41
7:G:387:ARG:HD3	7:P:208:GLN:HE22	1.85	0.41
7:H:406:SER:OG	7:H:420:LYS:NZ	2.49	0.41
7:I:479:ASP:O	7:I:483:GLU:CB	2.61	0.41
7:K:344:ALA:HB3	7:K:399:ASN:HB2	2.01	0.41
7:K:364:LEU:N	7:K:379:PHE:O	2.49	0.41
7:L:294:LEU:HD23	7:L:298:PHE:HD2	1.85	0.41
7:L:398:GLU:OE1	7:M:197:GLU:OE1	2.38	0.41
7:M:294:LEU:HD23	7:M:298:PHE:HD2	1.85	0.41
7:N:339:TYR:CD1	7:N:339:TYR:C	2.94	0.41
7:O:395:ILE:HA	7:Q:199:GLN:O	2.19	0.41
7:R:294:LEU:HD23	7:R:298:PHE:HD2	1.85	0.41
7:U:49:PHE:CE2	7:U:484:PHE:HB2	2.54	0.41
7:U:162:ARG:HB3	7:U:164:ARG:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:V:162:ARG:HB3	7:V:164:ARG:HG3	2.03	0.41
7:V:364:LEU:HD23	7:V:379:PHE:HB2	2.02	0.41
7:W:339:TYR:CD1	7:W:339:TYR:C	2.94	0.41
7:X:49:PHE:CE2	7:X:484:PHE:HB2	2.54	0.41
1:A:945:ASP:N	1:A:954:SER:O	2.45	0.41
5:F:324:ILE:N	5:F:390:ILE:O	2.37	0.41
5:F:512:TRP:CZ2	5:F:544:CYS:HB3	2.55	0.41
6:B:495:ARG:HA	6:B:504:ARG:HH21	1.85	0.41
7:P:242:SER:HB3	7:P:371:SER:CB	2.32	0.41
7:P:294:LEU:HD23	7:P:298:PHE:HD2	1.85	0.41
7:P:362:TYR:HB3	7:P:381:LYS:HB3	2.00	0.41
7:I:443:ASP:OD2	7:J:167:ASN:O	2.39	0.41
7:J:333:GLY:HA3	7:J:441:ILE:HD11	2.02	0.41
7:J:344:ALA:HB3	7:J:399:ASN:HB2	2.01	0.41
7:Q:364:LEU:HD23	7:Q:379:PHE:HB2	2.02	0.41
7:Q:364:LEU:N	7:Q:379:PHE:O	2.49	0.41
7:S:294:LEU:HD23	7:S:298:PHE:HD2	1.85	0.41
7:S:339:TYR:C	7:S:339:TYR:CD1	2.94	0.41
7:S:421:GLU:OE1	7:T:434:PHE:CD2	2.73	0.41
7:T:147:LEU:HG	7:T:148:SER:H	1.84	0.41
7:V:364:LEU:N	7:V:379:PHE:O	2.49	0.41
7:W:318:LEU:HD11	7:W:323:THR:HB	2.01	0.41
7:X:162:ARG:HB3	7:X:164:ARG:HG3	2.02	0.41
7:X:318:LEU:HD11	7:X:323:THR:HB	2.01	0.41
1:A:1166:THR:HG23	6:B:718:PHE:CE2	2.55	0.41
7:G:400:LEU:HD12	7:P:195:HIS:CD2	2.55	0.41
7:P:243:LEU:HD12	7:P:370:PHE:CD1	2.54	0.41
7:H:364:LEU:HD23	7:H:379:PHE:HB2	2.01	0.41
7:K:364:LEU:HD23	7:K:379:PHE:HB2	2.01	0.41
7:L:49:PHE:CE2	7:L:484:PHE:HB2	2.54	0.41
7:L:318:LEU:HD11	7:L:323:THR:HB	2.02	0.41
7:L:333:GLY:HA3	7:L:441:ILE:HD11	2.02	0.41
7:L:388:GLY:O	7:M:206:ILE:HG23	2.20	0.41
7:L:479:ASP:O	7:L:483:GLU:CB	2.61	0.41
7:M:49:PHE:CE2	7:M:484:PHE:HB2	2.54	0.41
7:M:328:SER:O	7:M:451:LYS:N	2.42	0.41
7:N:220:LEU:O	7:N:247:GLY:N	2.49	0.41
7:N:391:ARG:NE	7:O:204:LYS:CE	2.80	0.41
7:Q:333:GLY:HA3	7:Q:441:ILE:HD11	2.02	0.41
7:Q:374:SER:O	7:R:220:LEU:HA	2.21	0.41
7:S:370:PHE:CD2	7:S:373:ILE:C	2.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:162:ARG:HB3	7:T:164:ARG:HG3	2.02	0.41
7:U:339:TYR:CD1	7:U:339:TYR:C	2.94	0.41
7:U:383:ASP:OD1	7:V:210:LYS:HE3	2.21	0.41
1:A:56:ILE:O	1:A:66:TYR:N	2.50	0.41
1:A:139:GLN:NE2	1:A:222:TYR:OH	2.53	0.41
1:A:394:THR:HG21	1:A:425:PRO:HD2	2.03	0.41
1:A:504:LEU:HD13	1:A:651:LEU:HD11	2.02	0.41
5:F:135:GLN:NE2	7:G:289:ASN:H	2.18	0.41
7:P:44:ARG:HG2	7:P:45:SER:H	1.86	0.41
7:P:346:MET:N	7:P:397:SER:O	2.51	0.41
7:H:148:SER:HB3	7:I:180:SER:HB2	2.02	0.41
7:H:301:ASP:OD1	7:I:288:ARG:NH2	2.53	0.41
7:J:492:CYS:SG	7:J:493:GLN:N	2.91	0.41
7:K:294:LEU:HD23	7:K:298:PHE:HD2	1.85	0.41
7:L:406:SER:OG	7:L:420:LYS:NZ	2.48	0.41
7:N:492:CYS:SG	7:N:493:GLN:N	2.91	0.41
7:O:206:ILE:O	7:O:261:LEU:N	2.46	0.41
7:S:433:ASP:OD1	7:S:434:PHE:N	2.54	0.41
7:T:406:SER:OG	7:T:420:LYS:NZ	2.48	0.41
7:U:380:ASN:HB2	7:V:215:ASN:HB2	2.02	0.41
7:U:446:VAL:HG21	7:V:184:GLU:HG3	2.02	0.41
7:V:386:LYS:CD	7:W:209:GLU:HB2	2.35	0.41
7:X:370:PHE:CB	7:X:373:ILE:CG1	2.93	0.41
1:A:515:ARG:HH22	1:A:527:ASN:H	1.68	0.41
3:D:184:LEU:HD11	6:B:361:PHE:CE1	2.55	0.41
6:B:167:ASN:OD1	6:B:170:GLU:HB2	2.19	0.41
7:G:418:GLU:HA	7:G:421:GLU:HG2	2.02	0.41
7:P:258:THR:N	7:P:355:ASP:O	2.53	0.41
7:I:266:SER:O	7:I:347:LYS:N	2.40	0.41
7:J:162:ARG:HB3	7:J:164:ARG:HG3	2.03	0.41
7:K:333:GLY:HA3	7:K:441:ILE:HD11	2.02	0.41
7:K:339:TYR:C	7:K:339:TYR:CD1	2.94	0.41
7:L:339:TYR:HB3	7:L:404:VAL:CG1	2.33	0.41
7:R:339:TYR:CD1	7:R:339:TYR:C	2.94	0.41
7:S:333:GLY:HA3	7:S:441:ILE:HD11	2.02	0.41
7:T:44:ARG:HG2	7:T:45:SER:H	1.86	0.41
7:U:492:CYS:SG	7:U:493:GLN:N	2.91	0.41
7:V:370:PHE:CB	7:V:373:ILE:N	2.62	0.41
7:V:380:ASN:HB2	7:W:215:ASN:H	1.85	0.41
7:W:162:ARG:HB3	7:W:164:ARG:HG3	2.02	0.41
1:A:1368:THR:HA	1:A:1369:SER:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:167:PRO:HA	2:C:248:ALA:HA	2.02	0.41
3:D:313:TYR:HB2	3:D:406:TRP:CH2	2.56	0.41
6:B:54:LYS:NZ	6:B:58:GLU:OE2	2.41	0.41
7:G:251:PHE:HD1	7:G:362:TYR:HD1	1.69	0.41
7:G:458:LEU:O	7:G:458:LEU:HD13	2.20	0.41
7:G:522:LYS:NZ	7:P:273:PHE:CD2	2.88	0.41
7:H:162:ARG:HB3	7:H:164:ARG:HG3	2.02	0.41
7:I:318:LEU:HD11	7:I:323:THR:HB	2.01	0.41
7:J:294:LEU:HD23	7:J:298:PHE:HD2	1.85	0.41
7:K:44:ARG:HG2	7:K:45:SER:H	1.86	0.41
7:K:421:GLU:OE1	7:L:434:PHE:CB	2.68	0.41
7:M:364:LEU:HD23	7:M:379:PHE:HB2	2.02	0.41
7:M:391:ARG:HH21	7:N:204:LYS:HG3	1.86	0.41
7:O:147:LEU:HG	7:O:148:SER:H	1.84	0.41
7:O:339:TYR:CD1	7:O:339:TYR:C	2.94	0.41
7:Q:370:PHE:CB	7:Q:373:ILE:CG1	2.93	0.41
7:Q:391:ARG:NH2	7:R:204:LYS:CE	2.76	0.41
7:Q:433:ASP:OD1	7:Q:434:PHE:N	2.54	0.41
7:Q:489:CYS:SG	7:Q:490:HIS:N	2.90	0.41
7:R:318:LEU:HD11	7:R:323:THR:HB	2.01	0.41
7:S:364:LEU:HD23	7:S:379:PHE:HB2	2.01	0.41
7:S:391:ARG:NH2	7:T:204:LYS:CE	2.79	0.41
7:S:391:ARG:HH21	7:T:204:LYS:CG	2.30	0.41
7:S:526:SER:HB2	7:T:198:GLU:OE2	2.21	0.41
7:T:413:ARG:HG2	7:U:438:ALA:HB1	2.02	0.41
7:U:376:GLY:O	7:V:218:ILE:CD1	2.69	0.41
7:W:364:LEU:N	7:W:379:PHE:O	2.49	0.41
7:X:433:ASP:OD1	7:X:434:PHE:N	2.54	0.41
1:A:364:LYS:HZ2	1:A:466:TYR:HD1	1.69	0.41
1:A:661:ASP:OD1	1:A:661:ASP:N	2.53	0.41
1:A:1117:SER:HB2	1:A:1174:PHE:CZ	2.56	0.41
1:A:1264:ILE:HG22	1:A:1268:ASN:HD21	1.85	0.41
5:F:400:TRP:CE2	5:F:415:SER:HB2	2.55	0.41
7:P:31:SER:OG	7:P:41:PHE:HB3	2.21	0.41
7:P:305:LEU:HD21	7:P:473:LEU:HD11	2.03	0.41
7:P:356:ILE:O	7:P:387:ARG:N	2.50	0.41
7:H:333:GLY:HA3	7:H:441:ILE:HD11	2.02	0.41
7:I:294:LEU:HD23	7:I:298:PHE:HD2	1.85	0.41
7:I:421:GLU:OE1	7:J:434:PHE:CB	2.68	0.41
7:I:433:ASP:OD1	7:I:434:PHE:N	2.54	0.41
7:L:177:ASN:ND2	7:L:292:VAL:HG23	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:370:PHE:CD2	7:L:373:ILE:C	2.81	0.41
7:N:162:ARG:HB3	7:N:164:ARG:HG3	2.02	0.41
7:O:433:ASP:OD1	7:O:434:PHE:N	2.54	0.41
7:R:433:ASP:OD1	7:R:434:PHE:N	2.54	0.41
7:T:294:LEU:HD23	7:T:298:PHE:HD2	1.85	0.41
7:T:433:ASP:OD1	7:T:434:PHE:N	2.54	0.41
7:U:387:ARG:HA	7:V:208:GLN:NE2	2.34	0.41
7:V:31:SER:OG	7:V:41:PHE:HB3	2.21	0.41
7:V:374:SER:HB3	7:W:221:LYS:H	1.85	0.41
7:V:392:ALA:N	7:W:203:PHE:O	2.54	0.41
7:W:339:TYR:HB3	7:W:404:VAL:CG1	2.33	0.41
7:W:433:ASP:OD1	7:W:434:PHE:N	2.54	0.41
7:X:370:PHE:CD1	7:X:373:ILE:HD13	2.50	0.41
1:A:125:PHE:HZ	1:A:630:SER:HB2	1.85	0.41
1:A:341:GLU:O	1:A:614:ARG:NH2	2.54	0.41
1:A:532:GLN:NE2	1:A:566:LYS:O	2.54	0.41
1:A:658:ASN:ND2	1:A:659:ALA:H	2.19	0.41
1:A:906:GLY:H	1:A:929:VAL:HG22	1.86	0.41
1:A:1255:LEU:HD11	1:A:1267:VAL:HG13	2.03	0.41
3:D:166:ARG:HB2	3:D:179:LEU:HB2	2.02	0.41
3:D:168:VAL:HG13	3:D:177:TYR:HB2	2.03	0.41
6:B:497:ILE:HD12	6:B:503:LYS:HE3	2.03	0.41
7:G:155:PHE:HD2	7:G:293:VAL:HG21	1.86	0.41
7:G:181:LEU:HA	7:G:285:PHE:HA	2.03	0.41
7:G:339:TYR:HA	7:G:404:VAL:HA	2.02	0.41
7:G:521:SER:O	7:G:522:LYS:HB3	2.21	0.41
7:P:162:ARG:HB3	7:P:164:ARG:HG3	2.03	0.41
7:H:31:SER:OG	7:H:41:PHE:HB3	2.21	0.41
7:H:294:LEU:HD23	7:H:298:PHE:HD2	1.85	0.41
7:H:318:LEU:HD11	7:H:323:THR:HB	2.01	0.41
7:I:339:TYR:CD1	7:I:339:TYR:C	2.94	0.41
7:I:370:PHE:CD1	7:I:373:ILE:HD13	2.50	0.41
7:I:413:ARG:CZ	7:J:282:LEU:CA	2.78	0.41
7:I:413:ARG:HH22	7:J:282:LEU:HG	1.84	0.41
7:J:364:LEU:HD23	7:J:379:PHE:HB2	2.02	0.41
7:L:31:SER:OG	7:L:41:PHE:HB3	2.21	0.41
7:L:339:TYR:CD1	7:L:339:TYR:C	2.94	0.41
7:L:370:PHE:CB	7:L:373:ILE:N	2.62	0.41
7:M:265:TYR:HD1	7:M:348:ARG:HG2	1.86	0.41
7:O:370:PHE:CB	7:O:373:ILE:CG1	2.93	0.41
7:O:391:ARG:HE	7:Q:204:LYS:HE2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:406:SER:OG	7:O:420:LYS:NZ	2.48	0.41
7:Q:147:LEU:HG	7:Q:148:SER:H	1.84	0.41
7:R:31:SER:OG	7:R:41:PHE:HB3	2.21	0.41
7:R:391:ARG:HH21	7:S:204:LYS:CE	2.34	0.41
7:R:421:GLU:OE1	7:S:434:PHE:CD2	2.74	0.41
7:S:328:SER:O	7:S:451:LYS:N	2.42	0.41
7:T:265:TYR:HD1	7:T:348:ARG:HG2	1.86	0.41
7:T:391:ARG:CZ	7:U:204:LYS:HE3	2.47	0.41
7:T:492:CYS:SG	7:T:493:GLN:N	2.91	0.41
7:U:206:ILE:O	7:U:261:LEU:N	2.46	0.41
7:U:433:ASP:OD1	7:U:434:PHE:N	2.54	0.41
7:V:294:LEU:HD23	7:V:298:PHE:HD2	1.85	0.41
7:W:44:ARG:HG2	7:W:45:SER:H	1.86	0.41
1:A:618:LYS:HG3	1:A:621:GLU:HG3	2.02	0.41
2:C:303:THR:HG22	2:C:370:VAL:O	2.21	0.41
3:D:400:LYS:HA	6:B:457:TRP:CD1	2.56	0.41
5:F:124:LEU:HD23	5:F:136:SER:HA	2.03	0.41
7:G:41:PHE:CD1	7:G:310:GLU:HG3	2.56	0.41
7:G:292:VAL:HG11	7:G:458:LEU:HD22	2.03	0.41
7:P:376:GLY:O	7:H:218:ILE:HD12	2.21	0.41
7:I:413:ARG:NE	7:J:282:LEU:HA	2.35	0.41
7:K:265:TYR:HD1	7:K:348:ARG:HG2	1.86	0.41
7:M:162:ARG:HB3	7:M:164:ARG:HG3	2.03	0.41
7:M:370:PHE:CB	7:M:373:ILE:N	2.62	0.41
7:M:433:ASP:OD1	7:M:434:PHE:N	2.54	0.41
7:N:30:TRP:CZ2	7:N:42:ARG:HD2	2.56	0.41
7:N:44:ARG:HG2	7:N:45:SER:H	1.86	0.41
7:N:305:LEU:HD21	7:N:473:LEU:HD11	2.03	0.41
7:N:370:PHE:CD1	7:N:373:ILE:HD13	2.49	0.41
7:O:31:SER:OG	7:O:41:PHE:HB3	2.21	0.41
7:O:360:LEU:N	7:O:383:ASP:O	2.44	0.41
7:S:31:SER:OG	7:S:41:PHE:HB3	2.21	0.41
7:S:44:ARG:HG2	7:S:45:SER:H	1.86	0.41
7:S:265:TYR:HD1	7:S:348:ARG:HG2	1.86	0.41
7:U:105:GLY:HA2	7:V:159:LEU:CD2	2.32	0.41
7:W:133:ARG:NE	7:X:164:ARG:HD3	2.36	0.41
7:X:30:TRP:CZ2	7:X:42:ARG:HD2	2.57	0.41
7:X:31:SER:OG	7:X:41:PHE:HB3	2.21	0.41
1:A:34:GLY:N	1:A:87:ILE:O	2.44	0.40
1:A:610:TYR:HB3	1:A:616:ALA:HB3	2.03	0.40
2:C:500:TRP:CE3	2:C:506:ARG:HB3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:196:PHE:HB2	6:B:440:SER:OG	2.20	0.40
5:F:397:SER:O	7:G:185:THR:OG1	2.32	0.40
7:G:44:ARG:HG2	7:G:45:SER:H	1.85	0.40
7:G:318:LEU:HD22	7:G:318:LEU:HA	1.95	0.40
7:H:30:TRP:CZ2	7:H:42:ARG:HD2	2.56	0.40
7:H:339:TYR:CD1	7:H:339:TYR:C	2.94	0.40
7:I:162:ARG:HB3	7:I:164:ARG:HG3	2.02	0.40
7:J:44:ARG:HG2	7:J:45:SER:H	1.86	0.40
7:J:339:TYR:CD1	7:J:339:TYR:C	2.94	0.40
7:K:458:LEU:O	7:K:458:LEU:HD13	2.22	0.40
7:L:305:LEU:HD21	7:L:473:LEU:HD11	2.03	0.40
7:L:400:LEU:HB2	7:M:195:HIS:HB2	2.03	0.40
7:M:30:TRP:CZ2	7:M:42:ARG:HD2	2.57	0.40
7:M:406:SER:OG	7:M:420:LYS:NZ	2.49	0.40
7:N:433:ASP:OD1	7:N:434:PHE:N	2.54	0.40
7:O:148:SER:HB3	7:Q:180:SER:HB2	2.02	0.40
7:O:333:GLY:HA3	7:O:441:ILE:HD11	2.02	0.40
7:Q:162:ARG:HB3	7:Q:164:ARG:HG3	2.03	0.40
7:Q:206:ILE:O	7:Q:261:LEU:N	2.46	0.40
7:Q:386:LYS:CD	7:R:209:GLU:HB3	2.51	0.40
7:R:44:ARG:HG2	7:R:45:SER:H	1.86	0.40
7:R:333:GLY:HA3	7:R:441:ILE:HD11	2.02	0.40
7:S:30:TRP:CZ2	7:S:42:ARG:HD2	2.57	0.40
7:S:147:LEU:HG	7:S:148:SER:H	1.84	0.40
7:S:162:ARG:HB3	7:S:164:ARG:HG3	2.02	0.40
7:U:265:TYR:HD1	7:U:348:ARG:HG2	1.86	0.40
7:V:433:ASP:OD1	7:V:434:PHE:N	2.54	0.40
7:W:31:SER:OG	7:W:41:PHE:HB3	2.21	0.40
7:X:206:ILE:O	7:X:261:LEU:N	2.46	0.40
7:X:294:LEU:HD23	7:X:298:PHE:HD2	1.85	0.40
1:A:33:VAL:HA	1:A:87:ILE:HB	2.03	0.40
1:A:168:GLY:HA3	6:B:664:VAL:HG12	2.03	0.40
3:D:324:LEU:HD12	3:D:366:THR:HB	2.03	0.40
5:F:24:GLN:NE2	5:F:290:GLU:HB3	2.36	0.40
5:F:324:ILE:HG22	5:F:326:VAL:HG23	2.02	0.40
5:F:396:GLY:O	5:F:423:ASN:HB3	2.21	0.40
7:G:40:MET:HB2	7:G:65:ARG:HB3	2.02	0.40
7:G:244:HIS:N	7:G:369:ALA:O	2.53	0.40
7:G:292:VAL:HG21	7:G:458:LEU:HD21	2.03	0.40
7:P:333:GLY:HA3	7:P:441:ILE:HD11	2.04	0.40
7:I:31:SER:OG	7:I:41:PHE:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:370:PHE:CD1	7:J:373:ILE:HD13	2.49	0.40
7:K:412:THR:HA	7:L:167:ASN:OD1	2.21	0.40
7:L:433:ASP:OD1	7:L:434:PHE:N	2.54	0.40
7:M:391:ARG:NH2	7:N:204:LYS:HE3	2.36	0.40
7:M:458:LEU:O	7:M:458:LEU:HD13	2.22	0.40
7:O:421:GLU:OE1	7:Q:434:PHE:CD2	2.75	0.40
7:Q:130:GLU:CD	7:R:165:ASP:HA	2.42	0.40
7:T:31:SER:OG	7:T:41:PHE:HB3	2.21	0.40
7:U:394:ASN:CB	7:V:201:GLU:HB2	2.47	0.40
7:V:265:TYR:HD1	7:V:348:ARG:HG2	1.86	0.40
7:W:30:TRP:CZ2	7:W:42:ARG:HD2	2.56	0.40
1:A:367:ILE:HD13	1:A:466:TYR:CD2	2.56	0.40
3:D:169:PHE:HE1	6:B:191:GLN:HB2	1.86	0.40
5:F:75:THR:HG22	5:F:286:GLN:NE2	2.36	0.40
5:F:300:TYR:CE2	5:F:452:ASN:HB3	2.56	0.40
6:B:717:PRO:O	6:B:722:TYR:OH	2.25	0.40
7:P:30:TRP:CH2	7:H:467:HIS:CE1	3.00	0.40
7:H:372:GLU:CD	7:I:223:THR:O	2.60	0.40
7:I:130:GLU:HG3	7:J:165:ASP:CB	2.52	0.40
7:I:413:ARG:CZ	7:J:282:LEU:CB	3.00	0.40
7:J:433:ASP:OD1	7:J:434:PHE:N	2.54	0.40
7:L:25:SER:OG	7:L:27:TRP:NE1	2.55	0.40
7:L:30:TRP:CZ3	7:L:42:ARG:HB2	2.57	0.40
7:L:265:TYR:HD1	7:L:348:ARG:HG2	1.86	0.40
7:N:265:TYR:HD1	7:N:348:ARG:HG2	1.87	0.40
7:O:44:ARG:HG2	7:O:45:SER:H	1.86	0.40
7:O:265:TYR:HD1	7:O:348:ARG:HG2	1.86	0.40
7:O:400:LEU:HD12	7:Q:195:HIS:CD2	2.57	0.40
7:O:458:LEU:O	7:O:458:LEU:HD13	2.22	0.40
7:Q:152:ASP:HB2	7:Q:295:THR:HA	2.04	0.40
7:Q:360:LEU:N	7:Q:383:ASP:O	2.45	0.40
7:R:30:TRP:CZ3	7:R:42:ARG:HB2	2.57	0.40
7:R:189:LYS:CE	7:R:191:PHE:HZ	2.29	0.40
7:S:30:TRP:CZ3	7:S:42:ARG:HB2	2.57	0.40
7:S:318:LEU:HD22	7:S:318:LEU:HA	1.94	0.40
7:T:305:LEU:HD21	7:T:473:LEU:HD11	2.03	0.40
7:U:30:TRP:CZ2	7:U:42:ARG:HD2	2.57	0.40
7:U:30:TRP:CZ3	7:U:42:ARG:HB2	2.57	0.40
7:U:458:LEU:HD13	7:U:458:LEU:O	2.22	0.40
7:V:44:ARG:HG2	7:V:45:SER:H	1.86	0.40
7:V:318:LEU:HD22	7:V:318:LEU:HA	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:W:152:ASP:HB2	7:W:295:THR:HA	2.04	0.40
7:W:458:LEU:HD13	7:W:458:LEU:O	2.22	0.40
7:X:265:TYR:HD1	7:X:348:ARG:HG2	1.86	0.40
1:A:161:LEU:HD22	1:A:185:PHE:CD2	2.56	0.40
1:A:1285:TYR:H	1:A:1288:GLN:H	1.70	0.40
4:E:19:LYS:N	4:E:107:VAL:O	2.47	0.40
6:B:755:ILE:H	6:B:755:ILE:HG13	1.77	0.40
7:P:28:SER:HB2	7:P:43:SER:HB3	2.03	0.40
7:P:364:LEU:HB3	7:P:379:PHE:HB2	2.04	0.40
7:I:30:TRP:CZ3	7:I:42:ARG:HB2	2.57	0.40
7:J:30:TRP:CZ2	7:J:42:ARG:HD2	2.57	0.40
7:N:400:LEU:HB2	7:O:195:HIS:N	2.37	0.40
7:Q:30:TRP:CZ2	7:Q:42:ARG:HD2	2.57	0.40
7:Q:44:ARG:HG2	7:Q:45:SER:H	1.86	0.40
7:Q:380:ASN:CB	7:R:215:ASN:HB2	2.48	0.40
7:S:305:LEU:HD21	7:S:473:LEU:HD11	2.04	0.40
7:S:458:LEU:O	7:S:458:LEU:HD13	2.22	0.40
7:U:400:LEU:HB2	7:V:195:HIS:HB2	2.02	0.40
7:V:370:PHE:CB	7:V:373:ILE:CG1	2.93	0.40
7:V:396:THR:O	7:W:199:GLN:CB	2.67	0.40
7:W:265:TYR:HD1	7:W:348:ARG:HG2	1.86	0.40
7:X:25:SER:OG	7:X:27:TRP:NE1	2.55	0.40
1:A:132:LYS:HB2	1:A:135:TYR:CE1	2.56	0.40
6:B:312:SER:O	6:B:381:PHE:N	2.37	0.40
6:B:673:LEU:HD13	6:B:674:THR:N	2.36	0.40
7:G:492:CYS:SG	7:G:493:GLN:N	2.93	0.40
7:P:334:LEU:HD23	7:P:448:ILE:HG23	2.03	0.40
7:H:42:ARG:HH12	7:I:471:GLN:NE2	2.19	0.40
7:I:30:TRP:CZ2	7:I:42:ARG:HD2	2.57	0.40
7:I:265:TYR:HD1	7:I:348:ARG:HG2	1.86	0.40
7:J:25:SER:OG	7:J:27:TRP:NE1	2.55	0.40
7:J:31:SER:OG	7:J:41:PHE:HB3	2.21	0.40
7:K:162:ARG:HB3	7:K:164:ARG:HG3	2.02	0.40
7:L:44:ARG:HG2	7:L:45:SER:H	1.86	0.40
7:L:64:ARG:HH11	7:M:290:ARG:CZ	2.35	0.40
7:L:417:PHE:CE2	7:M:280:ILE:HG13	2.53	0.40
7:M:30:TRP:CZ3	7:M:42:ARG:HB2	2.57	0.40
7:M:220:LEU:O	7:M:247:GLY:N	2.49	0.40
7:N:130:GLU:CA	7:O:164:ARG:O	2.65	0.40
7:R:265:TYR:HD1	7:R:348:ARG:HG2	1.86	0.40
7:R:394:ASN:O	7:S:200:ILE:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:R:421:GLU:OE1	7:S:434:PHE:HD2	2.05	0.40
7:R:458:LEU:HD13	7:R:458:LEU:O	2.22	0.40
7:S:360:LEU:N	7:S:383:ASP:O	2.44	0.40
7:S:372:GLU:O	7:T:222:PHE:HA	2.22	0.40
7:T:25:SER:OG	7:T:27:TRP:NE1	2.55	0.40
7:U:408:ILE:N	7:V:187:GLY:O	2.49	0.40
7:V:396:THR:H	7:W:199:GLN:HB3	1.87	0.40
7:W:30:TRP:CZ3	7:W:42:ARG:HB2	2.57	0.40
7:W:177:ASN:ND2	7:W:292:VAL:HG23	2.32	0.40
7:W:305:LEU:HD21	7:W:473:LEU:HD11	2.03	0.40
7:W:404:VAL:O	7:X:191:PHE:N	2.53	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 PDB entries followed by that with respect to all EM entries.

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	1211/1580 (77%)	1144 (94%)	67 (6%)	0	100 100
2	C	505/537 (94%)	482 (95%)	23 (5%)	0	100 100
3	D	649/821 (79%)	590 (91%)	58 (9%)	1 (0%)	47 81
4	E	161/182 (88%)	160 (99%)	1 (1%)	0	100 100
5	F	499/554 (90%)	474 (95%)	23 (5%)	2 (0%)	34 72
6	B	676/913 (74%)	645 (95%)	30 (4%)	1 (0%)	51 85
7	G	497/538 (92%)	460 (93%)	37 (7%)	0	100 100
7	H	497/538 (92%)	460 (93%)	37 (7%)	0	100 100
7	I	497/538 (92%)	458 (92%)	39 (8%)	0	100 100
7	J	497/538 (92%)	458 (92%)	39 (8%)	0	100 100
7	K	497/538 (92%)	458 (92%)	39 (8%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	L	497/538 (92%)	459 (92%)	38 (8%)	0	100	100
7	M	497/538 (92%)	459 (92%)	38 (8%)	0	100	100
7	N	497/538 (92%)	458 (92%)	39 (8%)	0	100	100
7	O	497/538 (92%)	459 (92%)	38 (8%)	0	100	100
7	P	497/538 (92%)	454 (91%)	42 (8%)	1 (0%)	47	81
7	Q	497/538 (92%)	458 (92%)	39 (8%)	0	100	100
7	R	497/538 (92%)	459 (92%)	38 (8%)	0	100	100
7	S	497/538 (92%)	458 (92%)	39 (8%)	0	100	100
7	T	497/538 (92%)	458 (92%)	39 (8%)	0	100	100
7	U	497/538 (92%)	460 (93%)	37 (7%)	0	100	100
7	V	497/538 (92%)	459 (92%)	38 (8%)	0	100	100
7	W	497/538 (92%)	459 (92%)	38 (8%)	0	100	100
7	X	497/538 (92%)	458 (92%)	39 (8%)	0	100	100
All	All	12647/14271 (89%)	11747 (93%)	895 (7%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	P	526	SER
3	D	344	PHE
5	F	226	PRO
5	F	489	CYS
6	B	204	PRO

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 PDB entries followed by that with respect to all EM entries.

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	1083/1403 (77%)	1066 (98%)	17 (2%)	62	79
2	C	453/473 (96%)	446 (98%)	7 (2%)	65	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	571/714 (80%)	558 (98%)	13 (2%)	50	70
4	E	134/149 (90%)	132 (98%)	2 (2%)	65	80
5	F	437/466 (94%)	426 (98%)	11 (2%)	47	68
6	B	610/810 (75%)	603 (99%)	7 (1%)	73	84
7	G	440/477 (92%)	423 (96%)	17 (4%)	32	57
7	H	440/477 (92%)	424 (96%)	16 (4%)	35	59
7	I	440/477 (92%)	424 (96%)	16 (4%)	35	59
7	J	440/477 (92%)	424 (96%)	16 (4%)	35	59
7	K	440/477 (92%)	424 (96%)	16 (4%)	35	59
7	L	440/477 (92%)	424 (96%)	16 (4%)	35	59
7	M	440/477 (92%)	424 (96%)	16 (4%)	35	59
7	N	439/477 (92%)	423 (96%)	16 (4%)	35	59
7	O	440/477 (92%)	424 (96%)	16 (4%)	35	59
7	P	440/477 (92%)	423 (96%)	17 (4%)	32	57
7	Q	440/477 (92%)	424 (96%)	16 (4%)	35	59
7	R	440/477 (92%)	424 (96%)	16 (4%)	35	59
7	S	440/477 (92%)	424 (96%)	16 (4%)	35	59
7	T	440/477 (92%)	424 (96%)	16 (4%)	35	59
7	U	440/477 (92%)	424 (96%)	16 (4%)	35	59
7	V	434/477 (91%)	418 (96%)	16 (4%)	34	58
7	W	433/477 (91%)	417 (96%)	16 (4%)	34	58
7	X	440/477 (92%)	424 (96%)	16 (4%)	35	59
All	All	11194/12601 (89%)	10847 (97%)	347 (3%)	43	62

All (347) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	ARG
1	A	149	ASN
1	A	236	ASN
1	A	257	ASN
1	A	283	MET
1	A	294	ASN
1	A	320	ASN

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Mol	Chain	Res	Type
1	A	497	THR
1	A	504	LEU
1	A	658	ASN
1	A	782	ARG
1	A	841	LEU
1	A	873	ILE
1	A	920	LYS
1	A	1029	ASN
1	A	1133	LEU
1	A	1246	ARG
2	C	27	LYS
2	C	58	THR
2	C	150	TYR
2	C	172	LYS
2	C	205	LYS
2	C	405	ASN
2	C	457	ASN
3	D	44	LYS
3	D	90	ARG
3	D	104	ASN
3	D	154	ARG
3	D	157	ASN
3	D	167	LYS
3	D	191	LYS
3	D	255	ASN
3	D	315	VAL
3	D	422	THR
3	D	494	ASN
3	D	525	ASN
3	D	533	ARG
4	E	21	ASN
4	E	100	ARG
5	F	31	ARG
5	F	174	LYS
5	F	175	TYR
5	F	250	ASN
5	F	258	ILE
5	F	260	THR
5	F	261	ARG
5	F	264	THR
5	F	305	ASN
5	F	490	ARG

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Mol	Chain	Res	Type
5	F	548	LYS
6	B	175	ARG
6	B	205	ARG
6	B	381	PHE
6	B	439	LYS
6	B	459	LYS
6	B	623	CYS
6	B	673	LEU
7	G	53	ASN
7	G	82	ASN
7	G	99	ASN
7	G	102	ASN
7	G	140	ASN
7	G	153	ASN
7	G	157	ASN
7	G	161	ASN
7	G	177	ASN
7	G	185	THR
7	G	192	ARG
7	G	256	ASN
7	G	318	LEU
7	G	458	LEU
7	G	482	ASN
7	G	494	ASN
7	G	509	CYS
7	P	53	ASN
7	P	82	ASN
7	P	99	ASN
7	P	102	ASN
7	P	140	ASN
7	P	153	ASN
7	P	157	ASN
7	P	161	ASN
7	P	177	ASN
7	P	256	ASN
7	P	318	LEU
7	P	324	HIS
7	P	458	LEU
7	P	482	ASN
7	P	494	ASN
7	P	509	CYS
7	P	513	PHE

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Mol	Chain	Res	Type
7	H	53	ASN
7	H	82	ASN
7	H	99	ASN
7	H	102	ASN
7	H	140	ASN
7	H	153	ASN
7	H	157	ASN
7	H	161	ASN
7	H	177	ASN
7	H	191	PHE
7	H	318	LEU
7	H	339	TYR
7	H	482	ASN
7	H	494	ASN
7	H	509	CYS
7	H	513	PHE
7	I	53	ASN
7	I	82	ASN
7	I	99	ASN
7	I	102	ASN
7	I	140	ASN
7	I	153	ASN
7	I	157	ASN
7	I	161	ASN
7	I	177	ASN
7	I	191	PHE
7	I	318	LEU
7	I	339	TYR
7	I	482	ASN
7	I	494	ASN
7	I	509	CYS
7	I	513	PHE
7	J	53	ASN
7	J	82	ASN
7	J	99	ASN
7	J	102	ASN
7	J	140	ASN
7	J	153	ASN
7	J	157	ASN
7	J	161	ASN
7	J	177	ASN
7	J	191	PHE

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Mol	Chain	Res	Type
7	J	318	LEU
7	J	339	TYR
7	J	482	ASN
7	J	494	ASN
7	J	509	CYS
7	J	513	PHE
7	K	53	ASN
7	K	82	ASN
7	K	99	ASN
7	K	102	ASN
7	K	140	ASN
7	K	153	ASN
7	K	157	ASN
7	K	161	ASN
7	K	177	ASN
7	K	191	PHE
7	K	318	LEU
7	K	339	TYR
7	K	482	ASN
7	K	494	ASN
7	K	509	CYS
7	K	513	PHE
7	L	53	ASN
7	L	82	ASN
7	L	99	ASN
7	L	102	ASN
7	L	140	ASN
7	L	153	ASN
7	L	157	ASN
7	L	161	ASN
7	L	177	ASN
7	L	191	PHE
7	L	318	LEU
7	L	339	TYR
7	L	482	ASN
7	L	494	ASN
7	L	509	CYS
7	L	513	PHE
7	M	53	ASN
7	M	82	ASN
7	M	99	ASN
7	M	102	ASN

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Mol	Chain	Res	Type
7	M	140	ASN
7	M	153	ASN
7	M	157	ASN
7	M	161	ASN
7	M	177	ASN
7	M	191	PHE
7	M	318	LEU
7	M	339	TYR
7	M	482	ASN
7	M	494	ASN
7	M	509	CYS
7	M	513	PHE
7	N	53	ASN
7	N	82	ASN
7	N	99	ASN
7	N	102	ASN
7	N	140	ASN
7	N	153	ASN
7	N	157	ASN
7	N	161	ASN
7	N	177	ASN
7	N	191	PHE
7	N	318	LEU
7	N	339	TYR
7	N	482	ASN
7	N	494	ASN
7	N	509	CYS
7	N	513	PHE
7	O	53	ASN
7	O	82	ASN
7	O	99	ASN
7	O	102	ASN
7	O	140	ASN
7	O	153	ASN
7	O	157	ASN
7	O	161	ASN
7	O	177	ASN
7	O	191	PHE
7	O	318	LEU
7	O	339	TYR
7	O	482	ASN
7	O	494	ASN

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Mol	Chain	Res	Type
7	O	509	CYS
7	O	513	PHE
7	Q	53	ASN
7	Q	82	ASN
7	Q	99	ASN
7	Q	102	ASN
7	Q	140	ASN
7	Q	153	ASN
7	Q	157	ASN
7	Q	161	ASN
7	Q	177	ASN
7	Q	191	PHE
7	Q	318	LEU
7	Q	339	TYR
7	Q	482	ASN
7	Q	494	ASN
7	Q	509	CYS
7	Q	513	PHE
7	R	53	ASN
7	R	82	ASN
7	R	99	ASN
7	R	102	ASN
7	R	140	ASN
7	R	153	ASN
7	R	157	ASN
7	R	161	ASN
7	R	177	ASN
7	R	191	PHE
7	R	318	LEU
7	R	339	TYR
7	R	482	ASN
7	R	494	ASN
7	R	509	CYS
7	R	513	PHE
7	S	53	ASN
7	S	82	ASN
7	S	99	ASN
7	S	102	ASN
7	S	140	ASN
7	S	153	ASN
7	S	157	ASN
7	S	161	ASN

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Mol	Chain	Res	Type
7	S	177	ASN
7	S	191	PHE
7	S	318	LEU
7	S	339	TYR
7	S	482	ASN
7	S	494	ASN
7	S	509	CYS
7	S	513	PHE
7	T	53	ASN
7	T	82	ASN
7	T	99	ASN
7	T	102	ASN
7	T	140	ASN
7	T	153	ASN
7	T	157	ASN
7	T	161	ASN
7	T	177	ASN
7	T	191	PHE
7	T	318	LEU
7	T	339	TYR
7	T	482	ASN
7	T	494	ASN
7	T	509	CYS
7	T	513	PHE
7	U	53	ASN
7	U	82	ASN
7	U	99	ASN
7	U	102	ASN
7	U	140	ASN
7	U	153	ASN
7	U	157	ASN
7	U	161	ASN
7	U	177	ASN
7	U	191	PHE
7	U	318	LEU
7	U	339	TYR
7	U	482	ASN
7	U	494	ASN
7	U	509	CYS
7	U	513	PHE
7	V	53	ASN
7	V	82	ASN

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Mol	Chain	Res	Type
7	V	99	ASN
7	V	102	ASN
7	V	140	ASN
7	V	153	ASN
7	V	157	ASN
7	V	161	ASN
7	V	177	ASN
7	V	191	PHE
7	V	318	LEU
7	V	339	TYR
7	V	482	ASN
7	V	494	ASN
7	V	509	CYS
7	V	513	PHE
7	W	53	ASN
7	W	82	ASN
7	W	99	ASN
7	W	102	ASN
7	W	140	ASN
7	W	153	ASN
7	W	157	ASN
7	W	161	ASN
7	W	177	ASN
7	W	191	PHE
7	W	318	LEU
7	W	339	TYR
7	W	482	ASN
7	W	494	ASN
7	W	509	CYS
7	W	513	PHE
7	X	53	ASN
7	X	82	ASN
7	X	99	ASN
7	X	102	ASN
7	X	140	ASN
7	X	153	ASN
7	X	157	ASN
7	X	161	ASN
7	X	177	ASN
7	X	191	PHE
7	X	318	LEU
7	X	339	TYR

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Mol	Chain	Res	Type
7	X	482	ASN
7	X	494	ASN
7	X	509	CYS
7	X	513	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (323) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	ASN
1	A	236	ASN
1	A	294	ASN
1	A	320	ASN
1	A	613	GLN
1	A	658	ASN
1	A	998	ASN
1	A	1029	ASN
1	A	1090	ASN
1	A	1204	GLN
1	A	1260	ASN
1	A	1288	GLN
1	A	1292	ASN
2	C	168	GLN
2	C	233	HIS
2	C	249	HIS
2	C	260	HIS
2	C	405	ASN
2	C	457	ASN
3	D	61	GLN
3	D	104	ASN
3	D	157	ASN
3	D	189	GLN
3	D	210	HIS
3	D	238	HIS
3	D	249	GLN
3	D	255	ASN
3	D	261	GLN
3	D	282	HIS
3	D	525	ASN
4	E	21	ASN
4	E	46	GLN
4	E	104	HIS
5	F	24	GLN

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Mol	Chain	Res	Type
5	F	35	GLN
5	F	71	GLN
5	F	120	GLN
5	F	135	GLN
5	F	186	HIS
5	F	250	ASN
5	F	267	GLN
5	F	270	HIS
5	F	305	ASN
6	B	57	GLN
6	B	59	ASN
6	B	317	HIS
6	B	333	HIS
6	B	429	HIS
6	B	621	GLN
7	G	53	ASN
7	G	82	ASN
7	G	99	ASN
7	G	140	ASN
7	G	153	ASN
7	G	157	ASN
7	G	161	ASN
7	G	167	ASN
7	G	177	ASN
7	G	275	HIS
7	G	465	ASN
7	G	482	ASN
7	G	494	ASN
7	P	53	ASN
7	P	82	ASN
7	P	99	ASN
7	P	102	ASN
7	P	140	ASN
7	P	153	ASN
7	P	157	ASN
7	P	161	ASN
7	P	177	ASN
7	P	195	HIS
7	P	275	HIS
7	P	442	ASN
7	P	450	GLN
7	P	465	ASN

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Mol	Chain	Res	Type
7	P	482	ASN
7	P	494	ASN
7	H	53	ASN
7	H	82	ASN
7	H	99	ASN
7	H	140	ASN
7	H	153	ASN
7	H	157	ASN
7	H	161	ASN
7	H	167	ASN
7	H	177	ASN
7	H	195	HIS
7	H	275	HIS
7	H	281	HIS
7	H	465	ASN
7	H	482	ASN
7	H	494	ASN
7	I	39	GLN
7	I	53	ASN
7	I	82	ASN
7	I	99	ASN
7	I	102	ASN
7	I	140	ASN
7	I	153	ASN
7	I	157	ASN
7	I	161	ASN
7	I	177	ASN
7	I	208	GLN
7	I	275	HIS
7	I	281	HIS
7	I	465	ASN
7	I	482	ASN
7	I	494	ASN
7	J	53	ASN
7	J	82	ASN
7	J	99	ASN
7	J	140	ASN
7	J	153	ASN
7	J	157	ASN
7	J	161	ASN
7	J	177	ASN
7	J	275	HIS

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Mol	Chain	Res	Type
7	J	281	HIS
7	J	450	GLN
7	J	465	ASN
7	J	482	ASN
7	J	494	ASN
7	K	53	ASN
7	K	82	ASN
7	K	99	ASN
7	K	140	ASN
7	K	153	ASN
7	K	157	ASN
7	K	161	ASN
7	K	177	ASN
7	K	208	GLN
7	K	275	HIS
7	K	281	HIS
7	K	465	ASN
7	K	482	ASN
7	K	494	ASN
7	L	53	ASN
7	L	82	ASN
7	L	99	ASN
7	L	102	ASN
7	L	140	ASN
7	L	153	ASN
7	L	157	ASN
7	L	161	ASN
7	L	177	ASN
7	L	275	HIS
7	L	281	HIS
7	L	380	ASN
7	L	450	GLN
7	L	465	ASN
7	L	482	ASN
7	L	494	ASN
7	M	53	ASN
7	M	82	ASN
7	M	99	ASN
7	M	102	ASN
7	M	140	ASN
7	M	153	ASN
7	M	157	ASN

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Mol	Chain	Res	Type
7	M	161	ASN
7	M	177	ASN
7	M	195	HIS
7	M	275	HIS
7	M	281	HIS
7	M	450	GLN
7	M	465	ASN
7	M	482	ASN
7	M	494	ASN
7	N	39	GLN
7	N	53	ASN
7	N	82	ASN
7	N	99	ASN
7	N	102	ASN
7	N	140	ASN
7	N	153	ASN
7	N	157	ASN
7	N	161	ASN
7	N	177	ASN
7	N	275	HIS
7	N	281	HIS
7	N	450	GLN
7	N	465	ASN
7	N	482	ASN
7	N	494	ASN
7	O	53	ASN
7	O	82	ASN
7	O	99	ASN
7	O	140	ASN
7	O	153	ASN
7	O	157	ASN
7	O	161	ASN
7	O	177	ASN
7	O	195	HIS
7	O	275	HIS
7	O	281	HIS
7	O	465	ASN
7	O	482	ASN
7	O	494	ASN
7	Q	53	ASN
7	Q	82	ASN
7	Q	99	ASN

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Mol	Chain	Res	Type
7	Q	140	ASN
7	Q	153	ASN
7	Q	157	ASN
7	Q	161	ASN
7	Q	177	ASN
7	Q	195	HIS
7	Q	275	HIS
7	Q	281	HIS
7	Q	380	ASN
7	Q	450	GLN
7	Q	465	ASN
7	Q	482	ASN
7	Q	494	ASN
7	R	53	ASN
7	R	82	ASN
7	R	99	ASN
7	R	140	ASN
7	R	153	ASN
7	R	157	ASN
7	R	161	ASN
7	R	177	ASN
7	R	195	HIS
7	R	275	HIS
7	R	281	HIS
7	R	450	GLN
7	R	465	ASN
7	R	482	ASN
7	R	494	ASN
7	S	53	ASN
7	S	82	ASN
7	S	99	ASN
7	S	102	ASN
7	S	140	ASN
7	S	153	ASN
7	S	157	ASN
7	S	161	ASN
7	S	177	ASN
7	S	275	HIS
7	S	281	HIS
7	S	465	ASN
7	S	482	ASN
7	S	494	ASN

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Mol	Chain	Res	Type
7	T	53	ASN
7	T	82	ASN
7	T	99	ASN
7	T	140	ASN
7	T	153	ASN
7	T	157	ASN
7	T	161	ASN
7	T	177	ASN
7	T	275	HIS
7	T	281	HIS
7	T	450	GLN
7	T	465	ASN
7	T	482	ASN
7	T	494	ASN
7	U	53	ASN
7	U	82	ASN
7	U	99	ASN
7	U	140	ASN
7	U	153	ASN
7	U	157	ASN
7	U	161	ASN
7	U	177	ASN
7	U	195	HIS
7	U	208	GLN
7	U	275	HIS
7	U	281	HIS
7	U	450	GLN
7	U	465	ASN
7	U	482	ASN
7	U	494	ASN
7	V	39	GLN
7	V	53	ASN
7	V	82	ASN
7	V	99	ASN
7	V	140	ASN
7	V	153	ASN
7	V	157	ASN
7	V	161	ASN
7	V	177	ASN
7	V	208	GLN
7	V	275	HIS
7	V	281	HIS

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Mol	Chain	Res	Type
7	V	380	ASN
7	V	450	GLN
7	V	465	ASN
7	V	482	ASN
7	V	494	ASN
7	W	39	GLN
7	W	53	ASN
7	W	82	ASN
7	W	99	ASN
7	W	140	ASN
7	W	153	ASN
7	W	157	ASN
7	W	161	ASN
7	W	167	ASN
7	W	177	ASN
7	W	195	HIS
7	W	275	HIS
7	W	281	HIS
7	W	465	ASN
7	W	482	ASN
7	W	494	ASN
7	X	39	GLN
7	X	53	ASN
7	X	82	ASN
7	X	99	ASN
7	X	140	ASN
7	X	153	ASN
7	X	157	ASN
7	X	161	ASN
7	X	177	ASN
7	X	195	HIS
7	X	275	HIS
7	X	281	HIS
7	X	450	GLN
7	X	465	ASN
7	X	482	ASN
7	X	494	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

43 monosaccharides 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	$\#\|Z\| > 2$
8	NAG	Y	1	2,8	14,14,15	0.33	0	17,19,21	0.42	0
8	NAG	Y	2	8	14,14,15	0.31	0	17,19,21	0.62	0
8	BMA	Y	3	8	11,11,12	0.58	0	15,15,17	0.84	0
9	NAG	Z	1	3,9	14,14,15	0.57	0	17,19,21	1.69	4 (23%)
9	NAG	Z	2	9	14,14,15	0.42	0	17,19,21	0.52	0
9	NAG	a	1	9,6	14,14,15	0.52	0	17,19,21	1.16	1 (5%)
9	NAG	a	2	9	14,14,15	0.38	0	17,19,21	0.49	0
9	NAG	b	1	7,9	14,14,15	0.51	0	17,19,21	1.34	1 (5%)
9	NAG	b	2	9	14,14,15	0.50	0	17,19,21	0.52	0
9	NAG	c	1	7,9	14,14,15	0.56	0	17,19,21	0.94	1 (5%)
9	NAG	c	2	9	14,14,15	0.55	0	17,19,21	0.54	0
9	NAG	d	1	7,9	14,14,15	0.53	0	17,19,21	0.88	1 (5%)
9	NAG	d	2	9	14,14,15	0.54	0	17,19,21	0.53	0
9	NAG	e	1	7,9	14,14,15	0.53	0	17,19,21	0.89	1 (5%)
9	NAG	e	2	9	14,14,15	0.53	0	17,19,21	0.53	0
9	NAG	f	1	7,9	14,14,15	0.52	0	17,19,21	0.88	1 (5%)
9	NAG	f	2	9	14,14,15	0.56	0	17,19,21	0.51	0
9	NAG	g	1	7,9	14,14,15	0.52	0	17,19,21	0.88	1 (5%)
9	NAG	g	2	9	14,14,15	0.56	0	17,19,21	0.53	0
9	NAG	h	1	7,9	14,14,15	0.53	0	17,19,21	0.88	1 (5%)
9	NAG	h	2	9	14,14,15	0.57	0	17,19,21	0.53	0
9	NAG	i	1	7,9	14,14,15	0.53	0	17,19,21	0.89	1 (5%)
9	NAG	i	2	9	14,14,15	0.56	0	17,19,21	0.53	0
9	NAG	j	1	7,9	14,14,15	0.52	0	17,19,21	0.88	1 (5%)
9	NAG	j	2	9	14,14,15	0.55	0	17,19,21	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	NAG	k	1	7,9	14,14,15	0.52	0	17,19,21	0.89	1 (5%)
9	NAG	k	2	9	14,14,15	0.54	0	17,19,21	0.53	0
9	NAG	l	1	7,9	14,14,15	0.54	0	17,19,21	0.89	1 (5%)
9	NAG	l	2	9	14,14,15	0.55	0	17,19,21	0.54	0
9	NAG	m	1	7,9	14,14,15	0.52	0	17,19,21	0.88	1 (5%)
9	NAG	m	2	9	14,14,15	0.55	0	17,19,21	0.53	0
9	NAG	n	1	7,9	14,14,15	0.54	0	17,19,21	0.88	1 (5%)
9	NAG	n	2	9	14,14,15	0.55	0	17,19,21	0.53	0
9	NAG	o	1	7,9	14,14,15	0.53	0	17,19,21	0.90	1 (5%)
9	NAG	o	2	9	14,14,15	0.56	0	17,19,21	0.54	0
9	NAG	p	1	7,9	14,14,15	0.55	0	17,19,21	0.88	1 (5%)
9	NAG	p	2	9	14,14,15	0.56	0	17,19,21	0.53	0
9	NAG	q	1	7,9	14,14,15	0.53	0	17,19,21	0.88	1 (5%)
9	NAG	q	2	9	14,14,15	0.56	0	17,19,21	0.53	0
9	NAG	r	1	7,9	14,14,15	0.53	0	17,19,21	0.89	1 (5%)
9	NAG	r	2	9	14,14,15	0.55	0	17,19,21	0.53	0
9	NAG	s	1	7,9	14,14,15	0.53	0	17,19,21	0.88	1 (5%)
9	NAG	s	2	9	14,14,15	0.56	0	17,19,21	0.53	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
8	NAG	Y	1	2,8	-	0/6/23/26	0/1/1/1
8	NAG	Y	2	8	-	2/6/23/26	0/1/1/1
8	BMA	Y	3	8	-	0/2/19/22	0/1/1/1
9	NAG	Z	1	3,9	-	5/6/23/26	0/1/1/1
9	NAG	Z	2	9	-	3/6/23/26	0/1/1/1
9	NAG	a	1	9,6	-	3/6/23/26	0/1/1/1
9	NAG	a	2	9	-	2/6/23/26	0/1/1/1
9	NAG	b	1	7,9	-	5/6/23/26	0/1/1/1
9	NAG	b	2	9	-	0/6/23/26	0/1/1/1
9	NAG	c	1	7,9	-	3/6/23/26	0/1/1/1
9	NAG	c	2	9	-	2/6/23/26	0/1/1/1
9	NAG	d	1	7,9	-	3/6/23/26	0/1/1/1
9	NAG	d	2	9	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	e	1	7,9	-	3/6/23/26	0/1/1/1
9	NAG	e	2	9	-	2/6/23/26	0/1/1/1
9	NAG	f	1	7,9	-	3/6/23/26	0/1/1/1
9	NAG	f	2	9	-	2/6/23/26	0/1/1/1
9	NAG	g	1	7,9	-	3/6/23/26	0/1/1/1
9	NAG	g	2	9	-	2/6/23/26	0/1/1/1
9	NAG	h	1	7,9	-	3/6/23/26	0/1/1/1
9	NAG	h	2	9	-	2/6/23/26	0/1/1/1
9	NAG	i	1	7,9	-	3/6/23/26	0/1/1/1
9	NAG	i	2	9	-	2/6/23/26	0/1/1/1
9	NAG	j	1	7,9	-	3/6/23/26	0/1/1/1
9	NAG	j	2	9	-	2/6/23/26	0/1/1/1
9	NAG	k	1	7,9	-	3/6/23/26	0/1/1/1
9	NAG	k	2	9	-	2/6/23/26	0/1/1/1
9	NAG	l	1	7,9	-	3/6/23/26	0/1/1/1
9	NAG	l	2	9	-	2/6/23/26	0/1/1/1
9	NAG	m	1	7,9	-	3/6/23/26	0/1/1/1
9	NAG	m	2	9	-	2/6/23/26	0/1/1/1
9	NAG	n	1	7,9	-	3/6/23/26	0/1/1/1
9	NAG	n	2	9	-	2/6/23/26	0/1/1/1
9	NAG	o	1	7,9	-	3/6/23/26	0/1/1/1
9	NAG	o	2	9	-	2/6/23/26	0/1/1/1
9	NAG	p	1	7,9	-	3/6/23/26	0/1/1/1
9	NAG	p	2	9	-	2/6/23/26	0/1/1/1
9	NAG	q	1	7,9	-	3/6/23/26	0/1/1/1
9	NAG	q	2	9	-	2/6/23/26	0/1/1/1
9	NAG	r	1	7,9	-	3/6/23/26	0/1/1/1
9	NAG	r	2	9	-	2/6/23/26	0/1/1/1
9	NAG	s	1	7,9	-	3/6/23/26	0/1/1/1
9	NAG	s	2	9	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	Z	1	NAG	C2-N2-C7	4.57	129.41	122.90
9	b	1	NAG	C2-N2-C7	4.26	128.96	122.90
9	c	1	NAG	C1-O5-C5	2.94	116.18	112.19
9	o	1	NAG	C1-O5-C5	2.86	116.06	112.19
9	l	1	NAG	C1-O5-C5	2.83	116.02	112.19
9	e	1	NAG	C1-O5-C5	2.80	115.99	112.19
9	i	1	NAG	C1-O5-C5	2.80	115.99	112.19
9	k	1	NAG	C1-O5-C5	2.80	115.99	112.19
9	j	1	NAG	C1-O5-C5	2.80	115.98	112.19
9	p	1	NAG	C1-O5-C5	2.79	115.97	112.19
9	r	1	NAG	C1-O5-C5	2.78	115.96	112.19
9	d	1	NAG	C1-O5-C5	2.78	115.96	112.19
9	m	1	NAG	C1-O5-C5	2.77	115.95	112.19
9	f	1	NAG	C1-O5-C5	2.77	115.95	112.19
9	q	1	NAG	C1-O5-C5	2.77	115.94	112.19
9	s	1	NAG	C1-O5-C5	2.77	115.94	112.19
9	h	1	NAG	C1-O5-C5	2.77	115.94	112.19
9	g	1	NAG	C1-O5-C5	2.76	115.93	112.19
9	n	1	NAG	C1-O5-C5	2.75	115.92	112.19
9	a	1	NAG	C1-O5-C5	2.55	115.65	112.19
9	Z	1	NAG	C1-C2-N2	2.41	114.60	110.49
9	Z	1	NAG	C1-O5-C5	2.14	115.09	112.19
9	Z	1	NAG	C3-C4-C5	2.01	113.83	110.24

There are no chirality outliers.

All (105) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	Y	2	NAG	C4-C5-C6-O6
9	c	1	NAG	O5-C5-C6-O6
9	Z	1	NAG	C4-C5-C6-O6
9	Z	1	NAG	O5-C5-C6-O6
8	Y	2	NAG	O5-C5-C6-O6
9	Z	2	NAG	O5-C5-C6-O6
9	d	1	NAG	O5-C5-C6-O6
9	e	1	NAG	O5-C5-C6-O6
9	f	1	NAG	O5-C5-C6-O6
9	g	1	NAG	O5-C5-C6-O6
9	h	1	NAG	O5-C5-C6-O6
9	i	1	NAG	O5-C5-C6-O6
9	j	1	NAG	O5-C5-C6-O6
9	k	1	NAG	O5-C5-C6-O6
9	l	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	m	1	NAG	O5-C5-C6-O6
9	n	1	NAG	O5-C5-C6-O6
9	o	1	NAG	O5-C5-C6-O6
9	p	1	NAG	O5-C5-C6-O6
9	q	1	NAG	O5-C5-C6-O6
9	r	1	NAG	O5-C5-C6-O6
9	s	1	NAG	O5-C5-C6-O6
9	d	2	NAG	O5-C5-C6-O6
9	e	2	NAG	O5-C5-C6-O6
9	f	2	NAG	O5-C5-C6-O6
9	g	2	NAG	O5-C5-C6-O6
9	h	2	NAG	O5-C5-C6-O6
9	i	2	NAG	O5-C5-C6-O6
9	j	2	NAG	O5-C5-C6-O6
9	k	2	NAG	O5-C5-C6-O6
9	l	2	NAG	O5-C5-C6-O6
9	m	2	NAG	O5-C5-C6-O6
9	n	2	NAG	O5-C5-C6-O6
9	o	2	NAG	O5-C5-C6-O6
9	p	2	NAG	O5-C5-C6-O6
9	q	2	NAG	O5-C5-C6-O6
9	r	2	NAG	O5-C5-C6-O6
9	s	2	NAG	O5-C5-C6-O6
9	Z	1	NAG	C8-C7-N2-C2
9	Z	1	NAG	O7-C7-N2-C2
9	b	1	NAG	C8-C7-N2-C2
9	b	1	NAG	O7-C7-N2-C2
9	b	1	NAG	O5-C5-C6-O6
9	c	2	NAG	O5-C5-C6-O6
9	g	2	NAG	C4-C5-C6-O6
9	h	2	NAG	C4-C5-C6-O6
9	n	2	NAG	C4-C5-C6-O6
9	d	2	NAG	C4-C5-C6-O6
9	f	2	NAG	C4-C5-C6-O6
9	l	2	NAG	C4-C5-C6-O6
9	m	2	NAG	C4-C5-C6-O6
9	e	2	NAG	C4-C5-C6-O6
9	i	2	NAG	C4-C5-C6-O6
9	j	2	NAG	C4-C5-C6-O6
9	k	2	NAG	C4-C5-C6-O6
9	o	2	NAG	C4-C5-C6-O6
9	p	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	q	2	NAG	C4-C5-C6-O6
9	r	2	NAG	C4-C5-C6-O6
9	s	2	NAG	C4-C5-C6-O6
9	b	1	NAG	C4-C5-C6-O6
9	c	2	NAG	C4-C5-C6-O6
9	a	1	NAG	O5-C5-C6-O6
9	c	1	NAG	C4-C5-C6-O6
9	d	1	NAG	C4-C5-C6-O6
9	e	1	NAG	C4-C5-C6-O6
9	g	1	NAG	C4-C5-C6-O6
9	i	1	NAG	C4-C5-C6-O6
9	p	1	NAG	C4-C5-C6-O6
9	q	1	NAG	C4-C5-C6-O6
9	s	1	NAG	C4-C5-C6-O6
9	f	1	NAG	C4-C5-C6-O6
9	h	1	NAG	C4-C5-C6-O6
9	j	1	NAG	C4-C5-C6-O6
9	k	1	NAG	C4-C5-C6-O6
9	l	1	NAG	C4-C5-C6-O6
9	m	1	NAG	C4-C5-C6-O6
9	n	1	NAG	C4-C5-C6-O6
9	o	1	NAG	C4-C5-C6-O6
9	r	1	NAG	C4-C5-C6-O6
9	a	2	NAG	O5-C5-C6-O6
9	Z	2	NAG	C4-C5-C6-O6
9	a	1	NAG	C3-C2-N2-C7
9	c	1	NAG	C3-C2-N2-C7
9	d	1	NAG	C3-C2-N2-C7
9	e	1	NAG	C3-C2-N2-C7
9	f	1	NAG	C3-C2-N2-C7
9	g	1	NAG	C3-C2-N2-C7
9	h	1	NAG	C3-C2-N2-C7
9	i	1	NAG	C3-C2-N2-C7
9	j	1	NAG	C3-C2-N2-C7
9	k	1	NAG	C3-C2-N2-C7
9	l	1	NAG	C3-C2-N2-C7
9	m	1	NAG	C3-C2-N2-C7
9	n	1	NAG	C3-C2-N2-C7
9	o	1	NAG	C3-C2-N2-C7
9	p	1	NAG	C3-C2-N2-C7
9	q	1	NAG	C3-C2-N2-C7
9	r	1	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
9	s	1	NAG	C3-C2-N2-C7
9	a	2	NAG	C1-C2-N2-C7
9	Z	2	NAG	C1-C2-N2-C7
9	a	1	NAG	C4-C5-C6-O6
9	Z	1	NAG	C3-C2-N2-C7
9	b	1	NAG	C3-C2-N2-C7

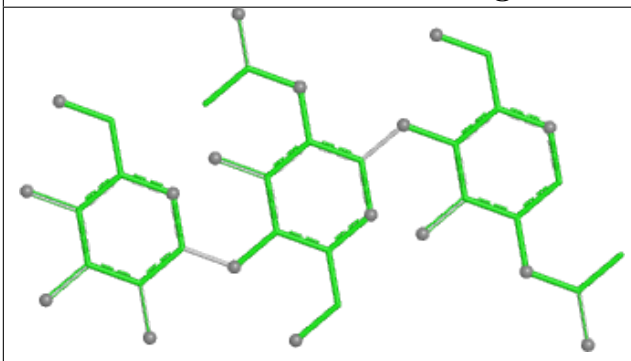
There are no ring outliers.

2 monomers are involved in 2 short contacts:

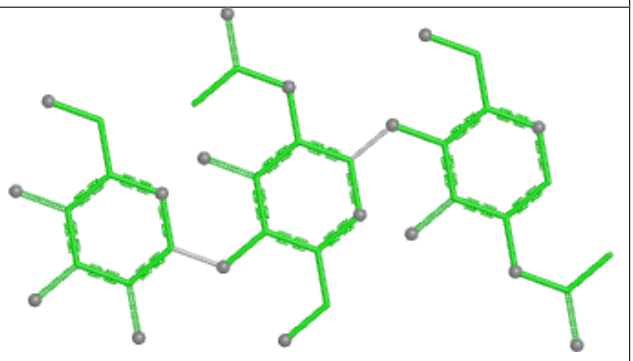
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	Z	1	NAG	2	0
9	Z	2	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

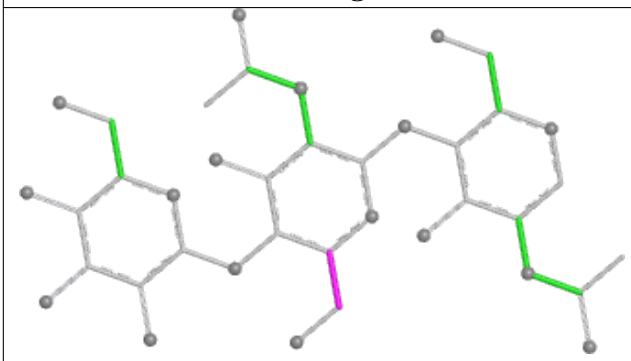
Oligosaccharide Chain Y



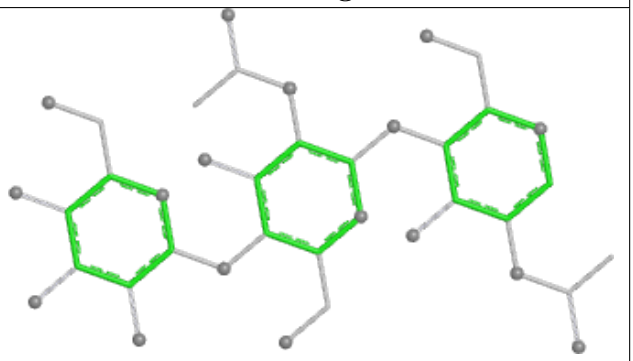
Bond lengths



Bond angles

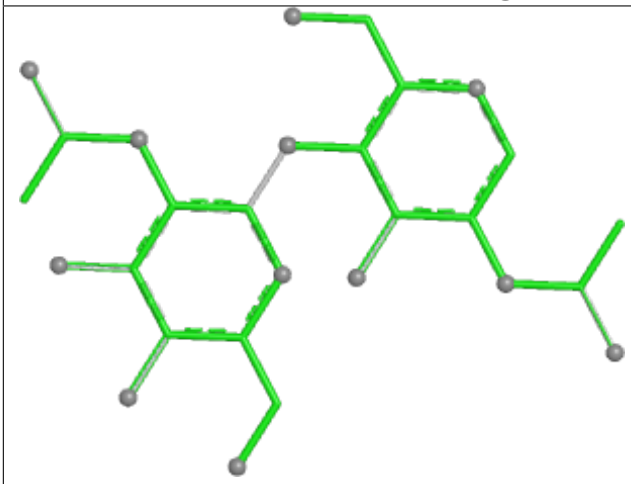


Torsions

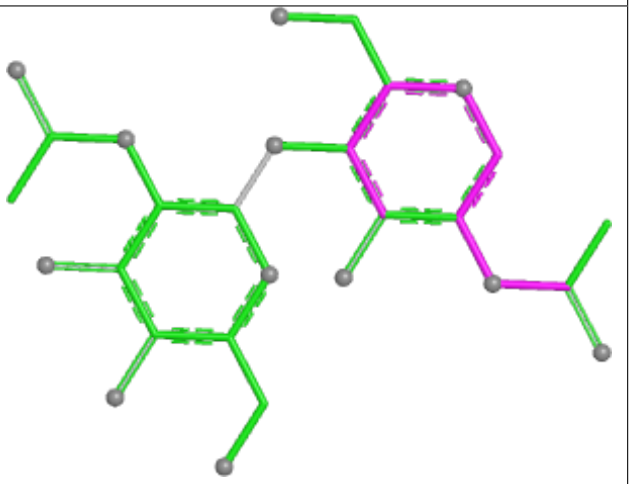


Rings

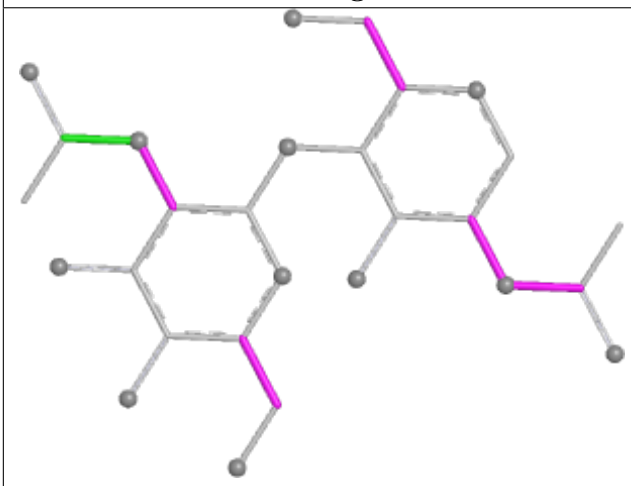
Oligosaccharide Chain Z



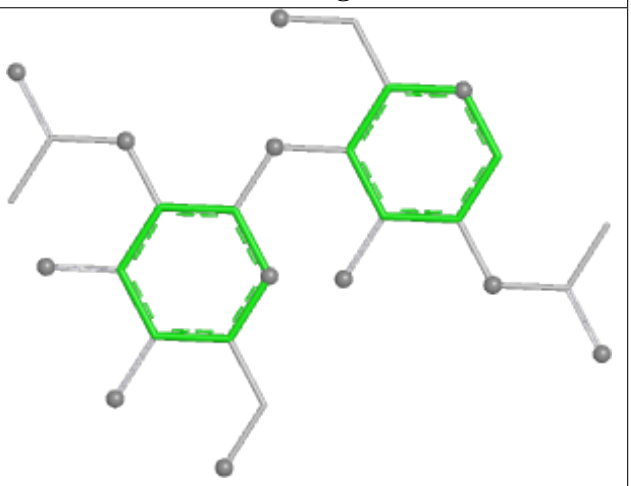
Bond lengths



Bond angles

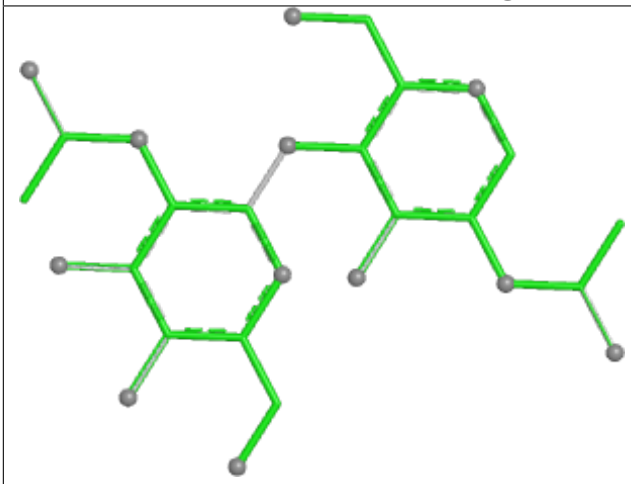


Torsions



Rings

Oligosaccharide Chain a



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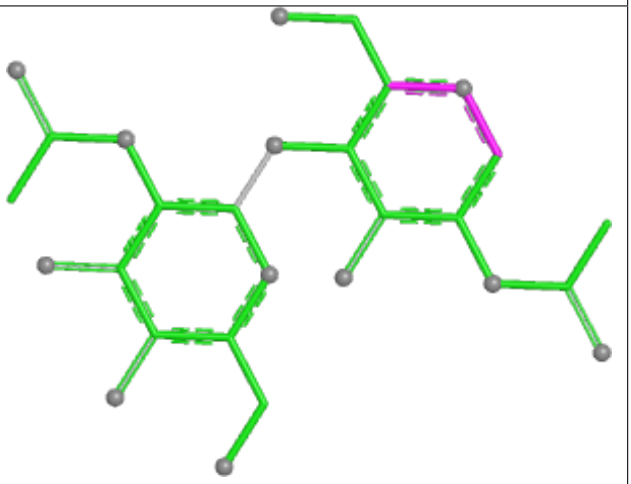
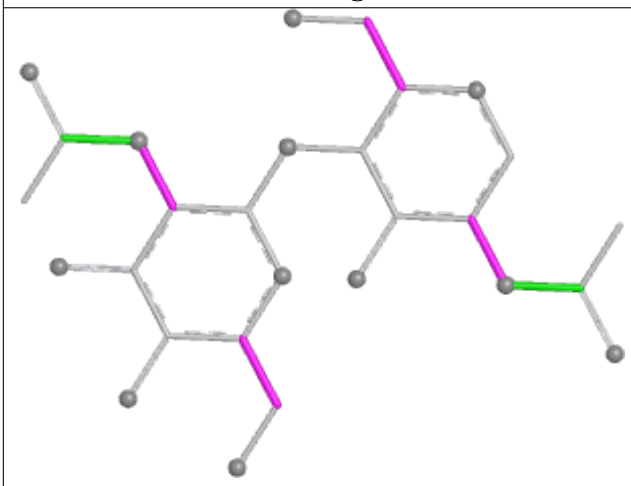
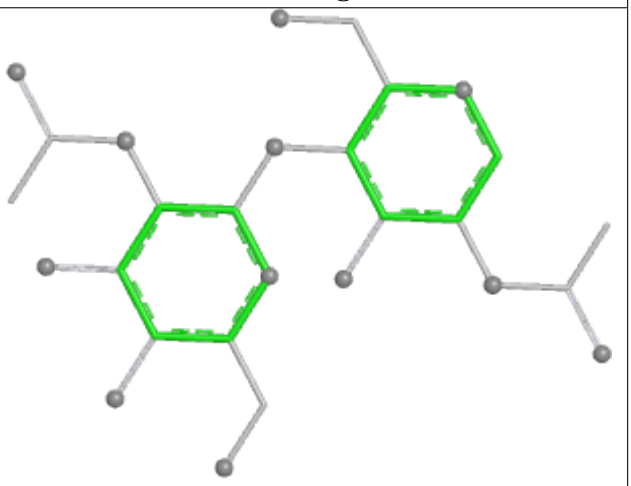


Bond angles

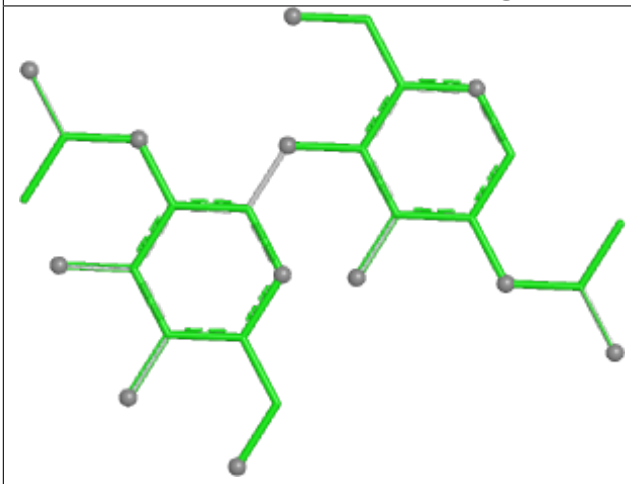


Torsions



Rings

Oligosaccharide Chain b



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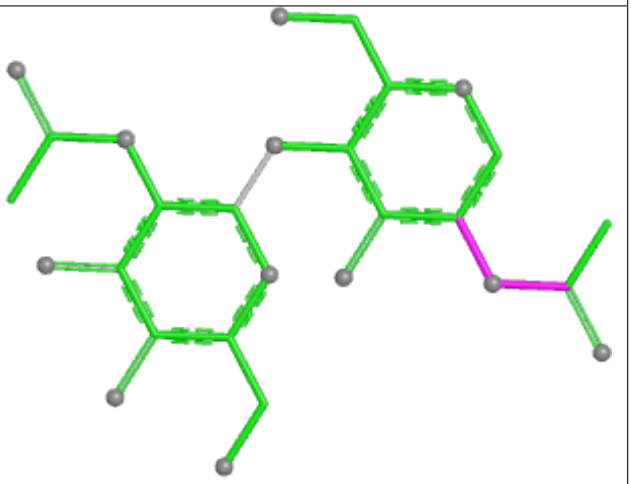
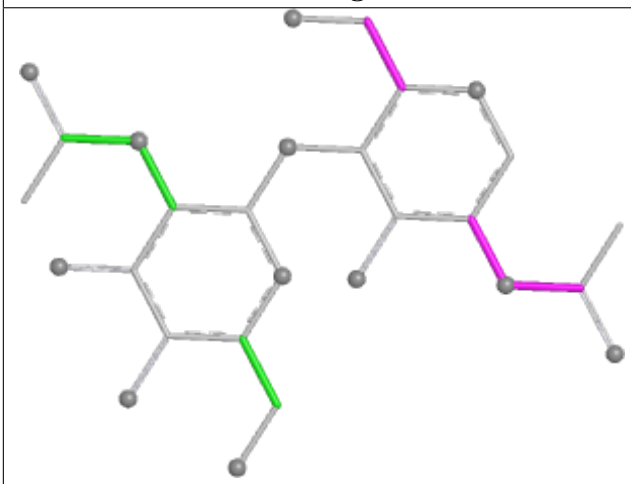


Bond angles



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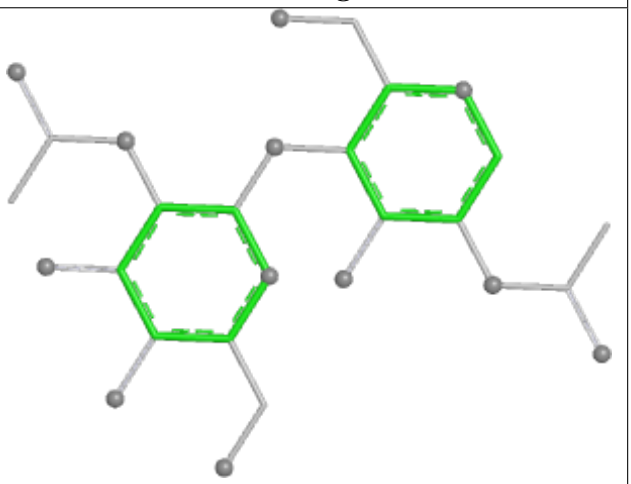
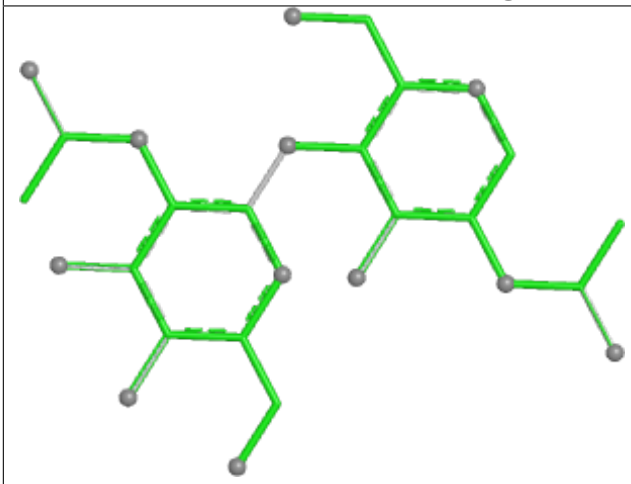


Rings

Oligosaccharide Chain c



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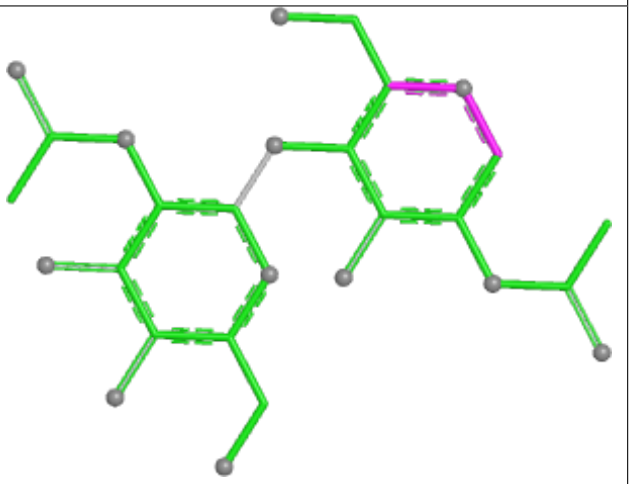
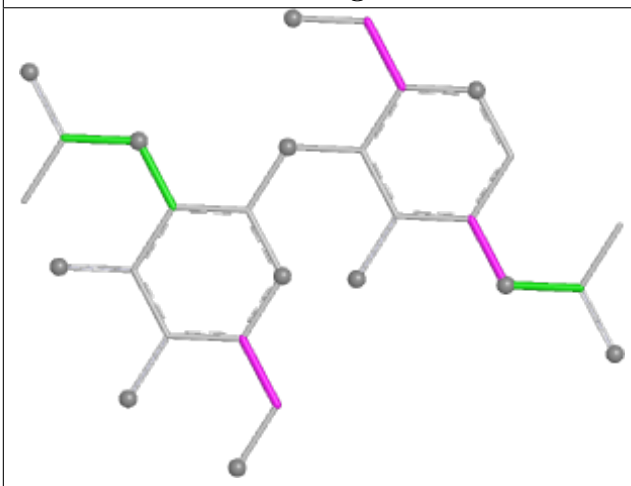
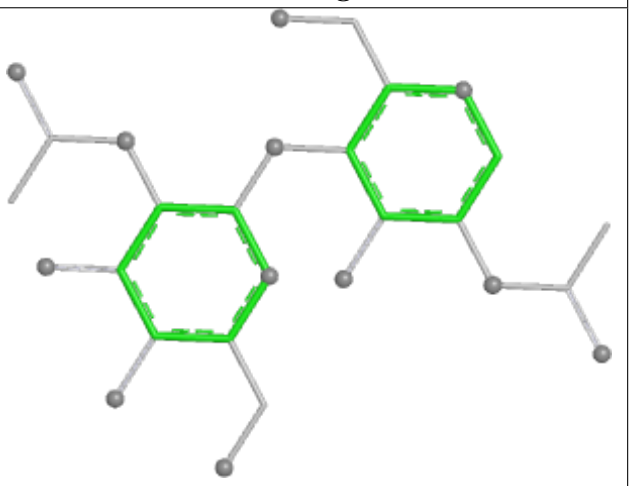


Bond angles

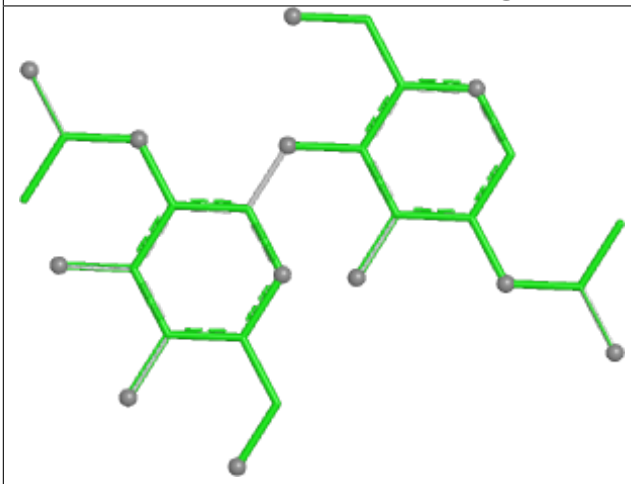


Torsions



Rings

Oligosaccharide Chain d



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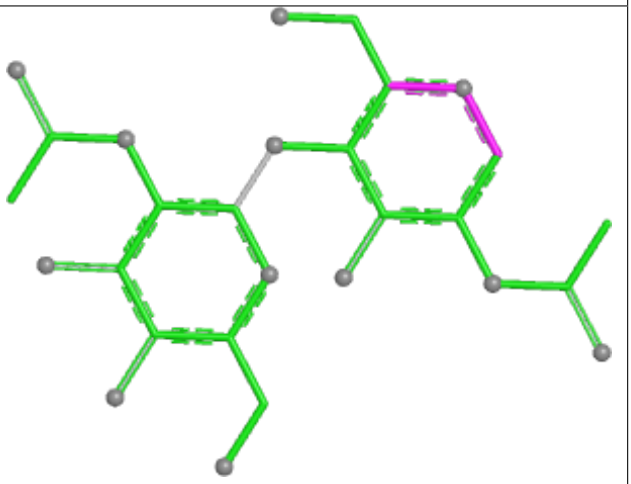
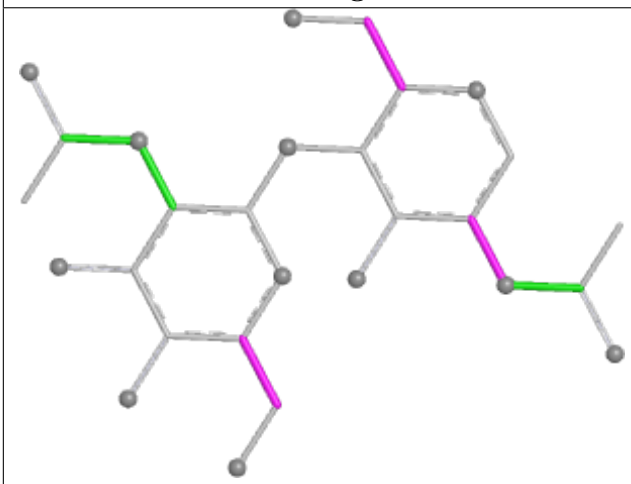


Bond angles



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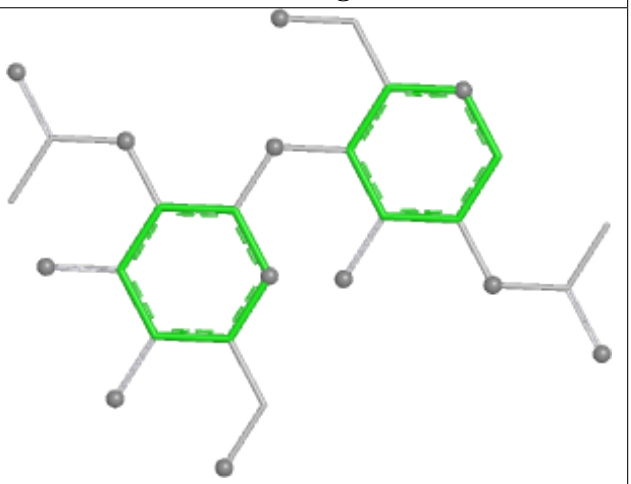
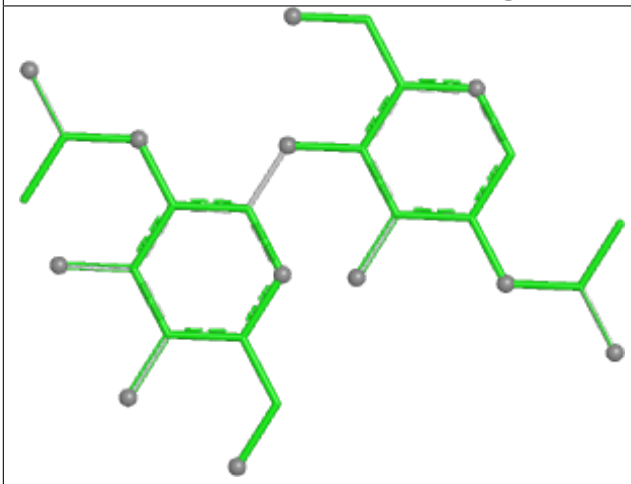


Rings

Oligosaccharide Chain e



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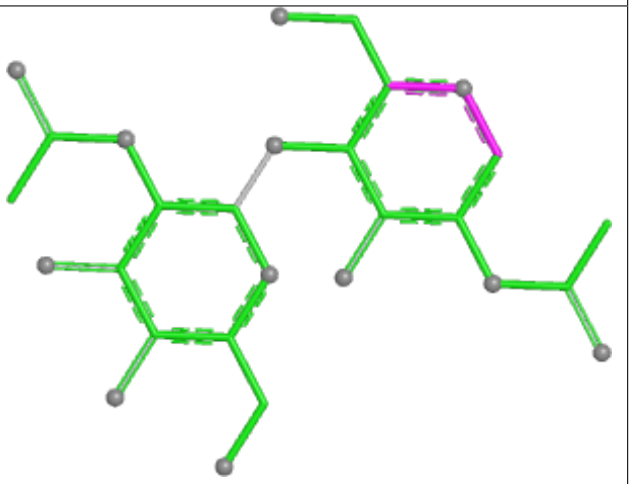
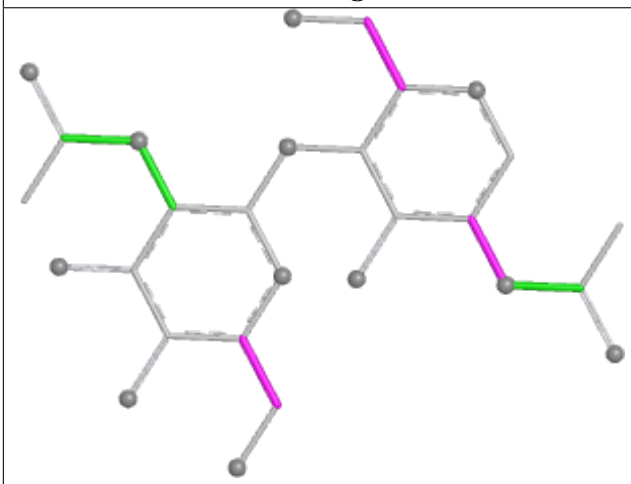


Bond angles



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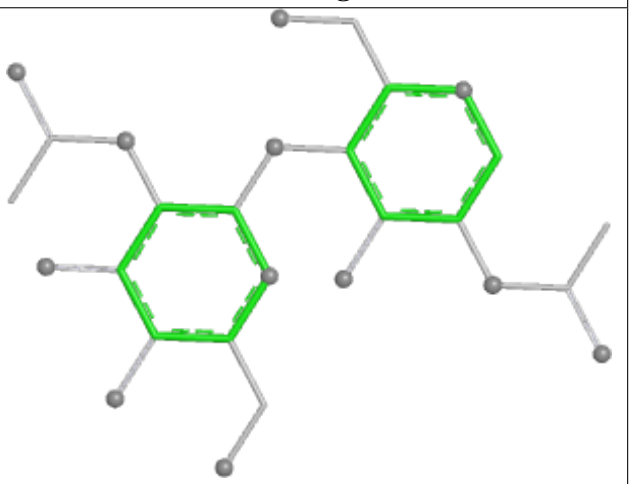
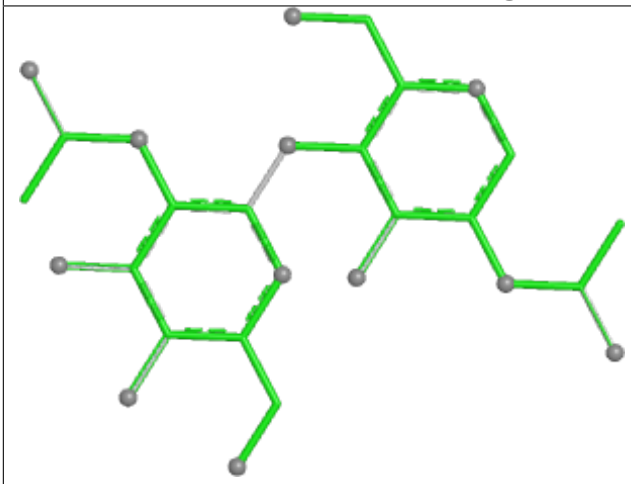


Rings

Oligosaccharide Chain f



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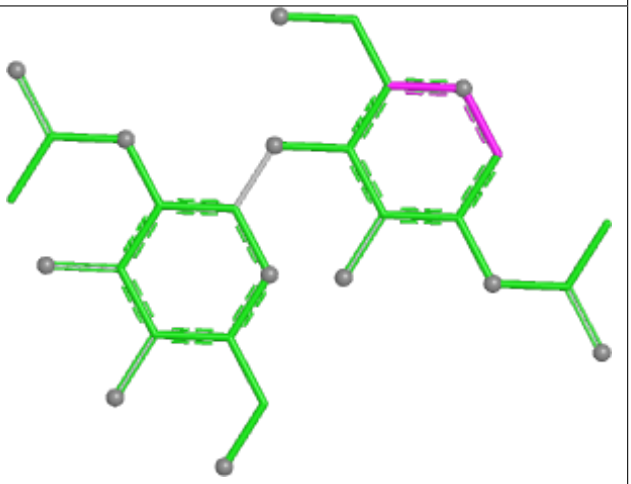
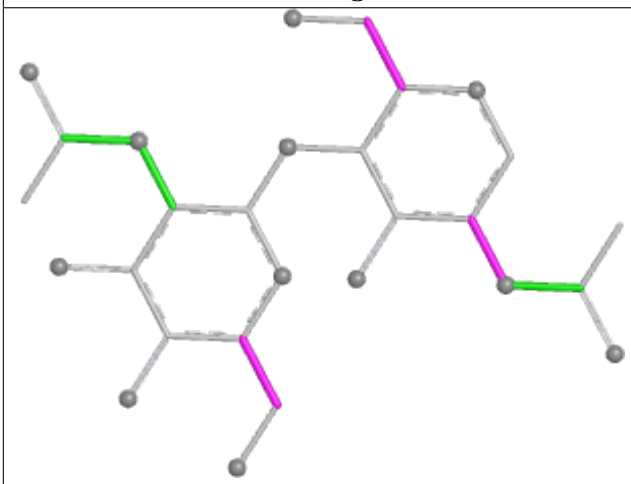


Bond angles



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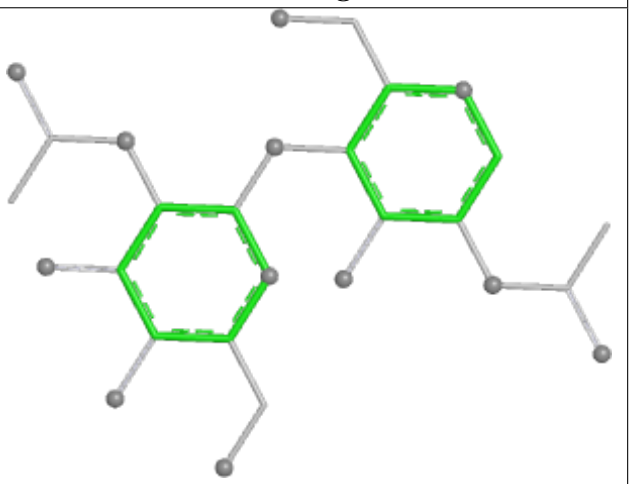
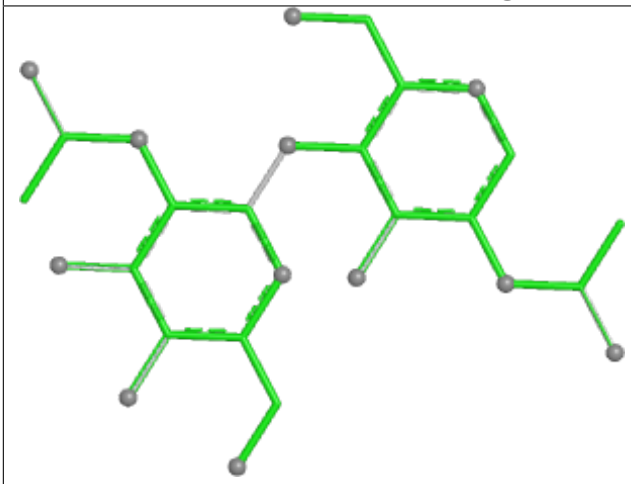


Rings

Oligosaccharide Chain g



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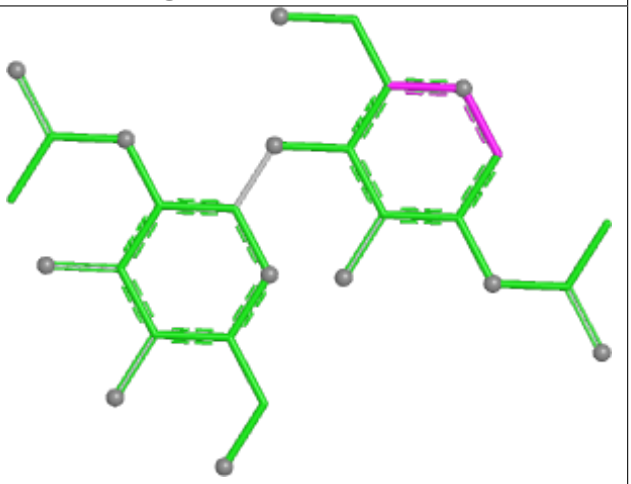
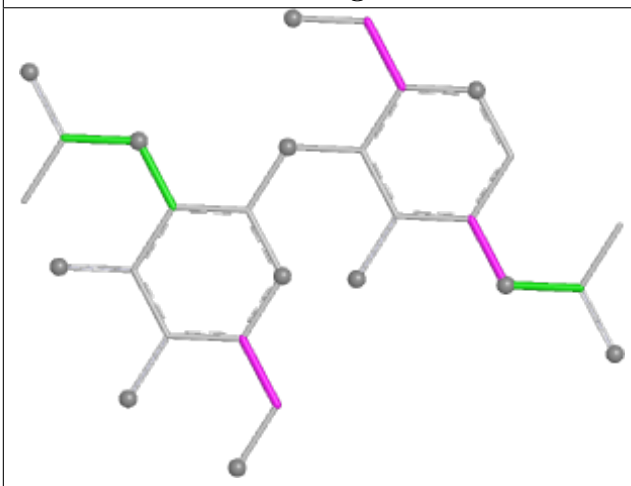


Bond angles



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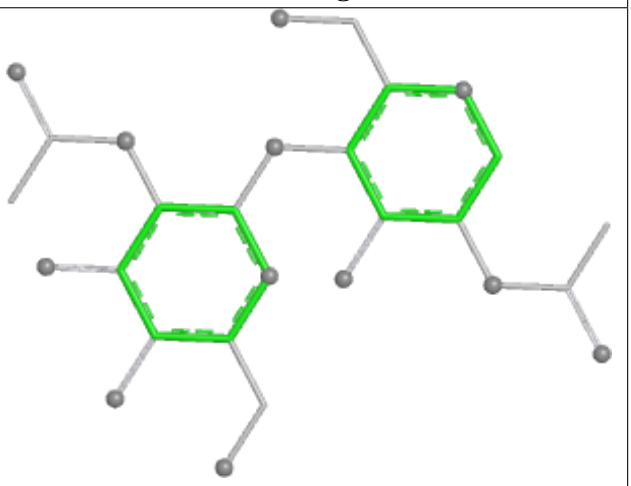
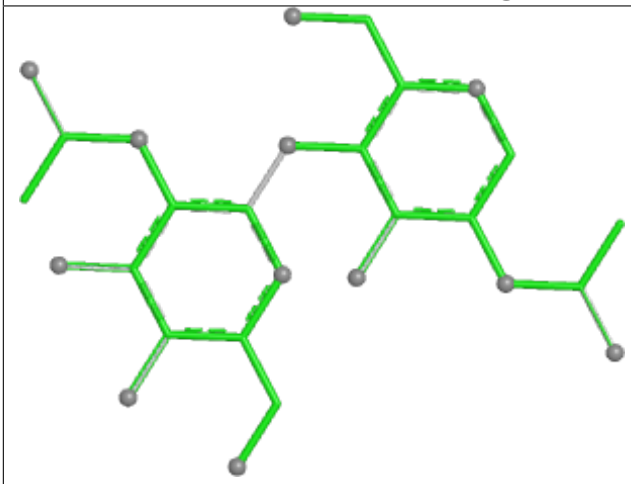


Rings

Oligosaccharide Chain h



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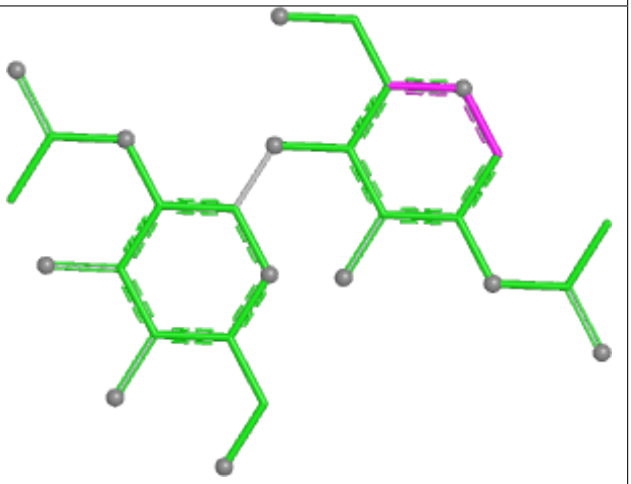
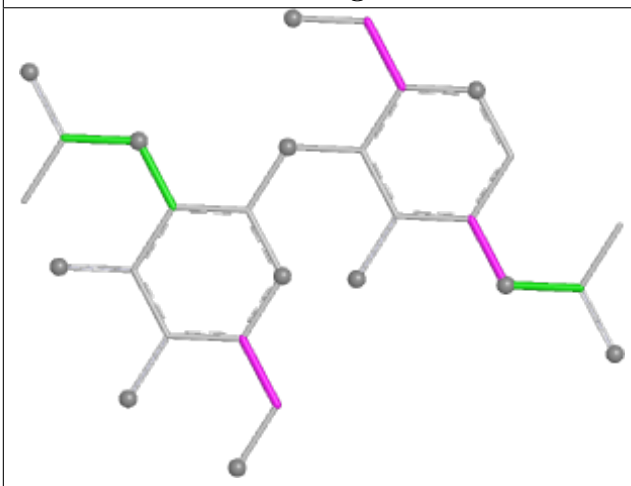


Bond angles



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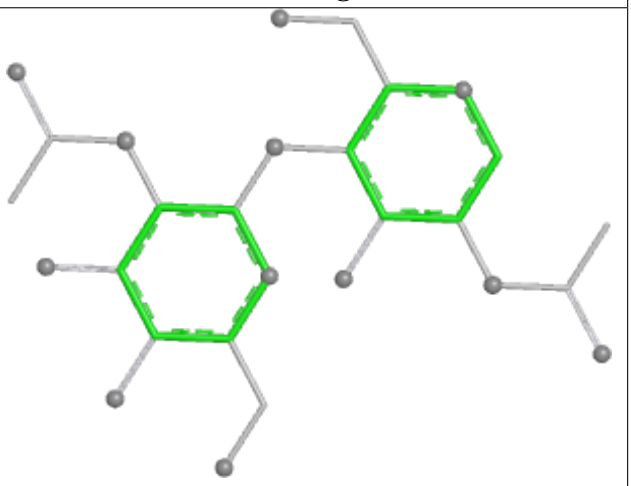
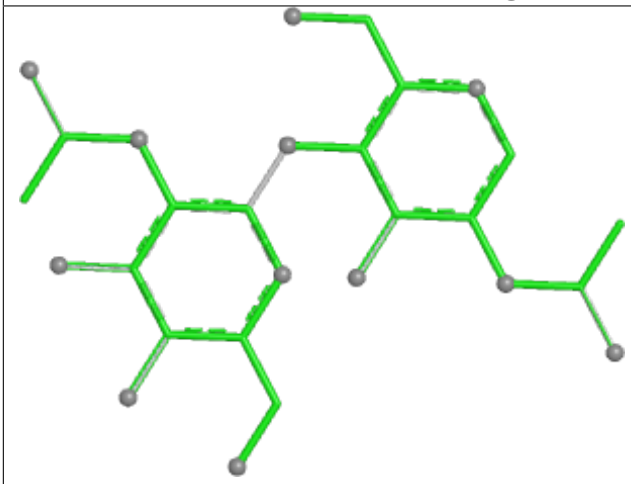


Rings

Oligosaccharide Chain i



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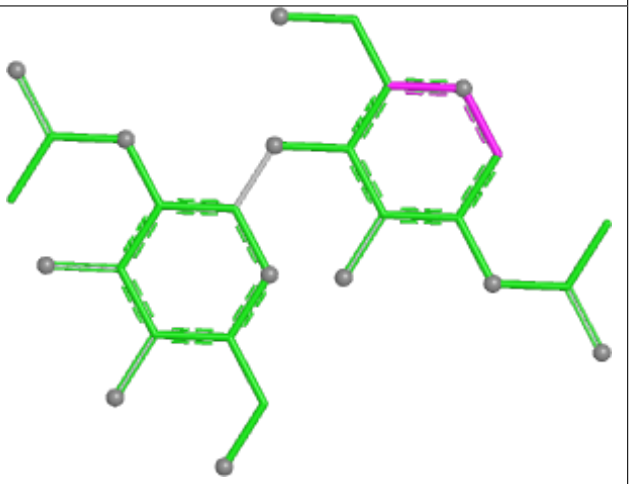
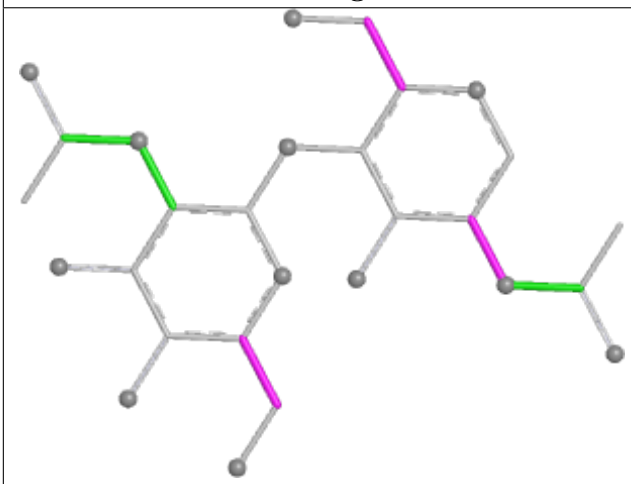
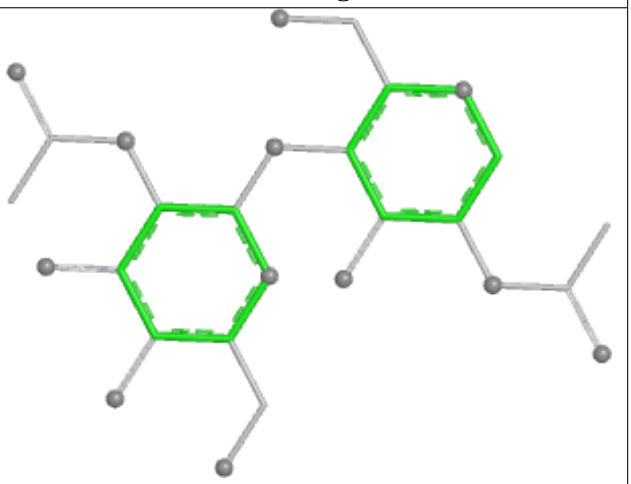


Bond angles

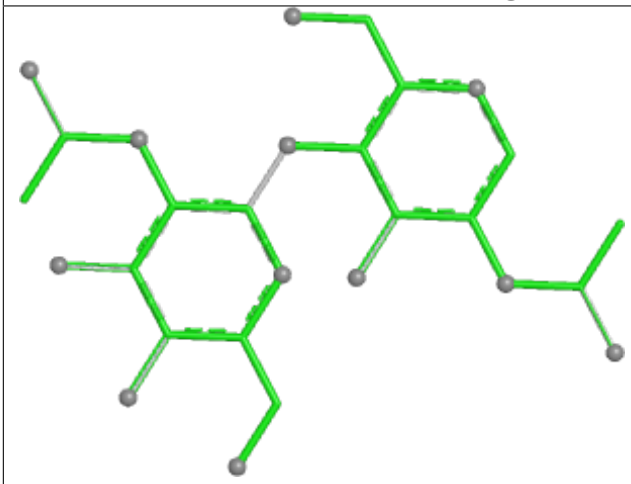


Torsions



Rings

Oligosaccharide Chain j



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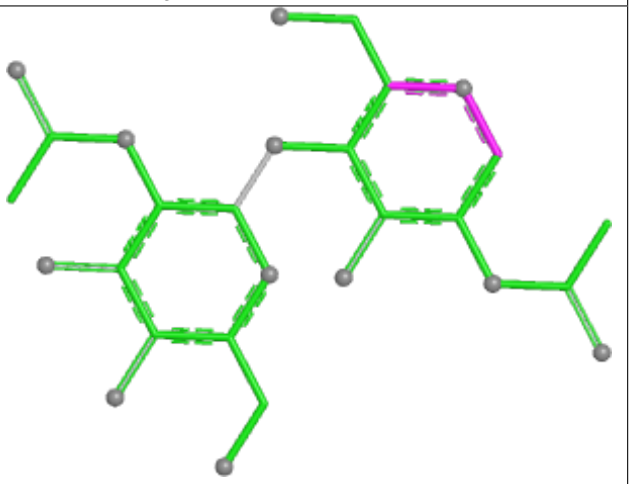
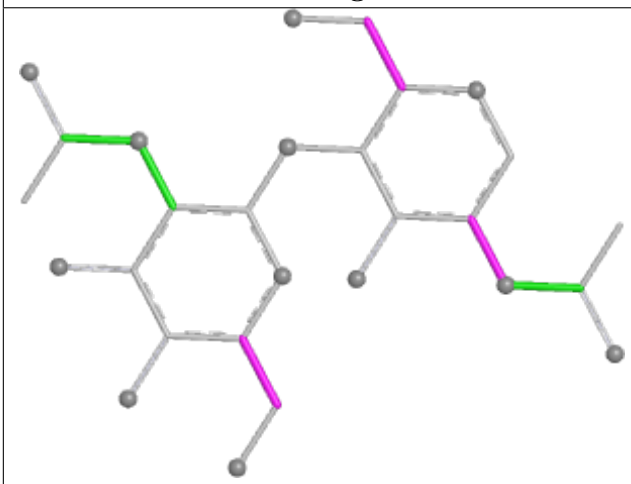
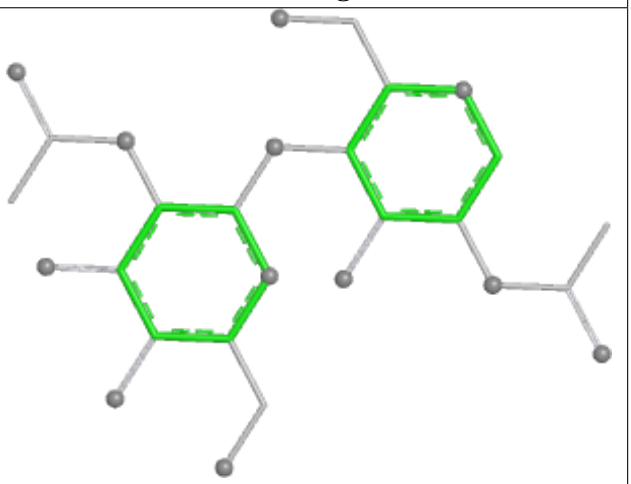


Bond angles

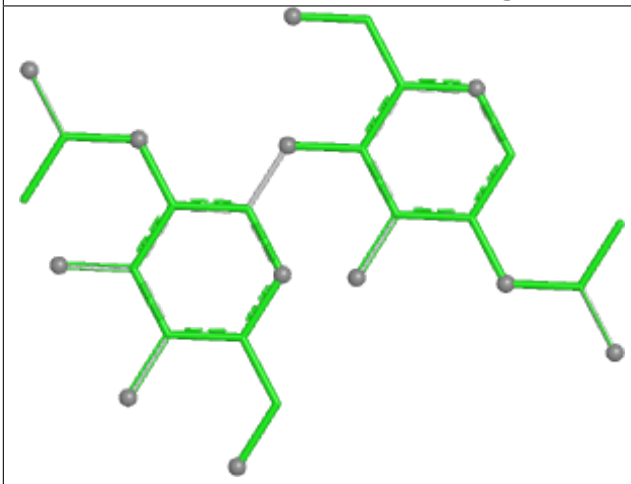


Torsions



Rings

Oligosaccharide Chain k



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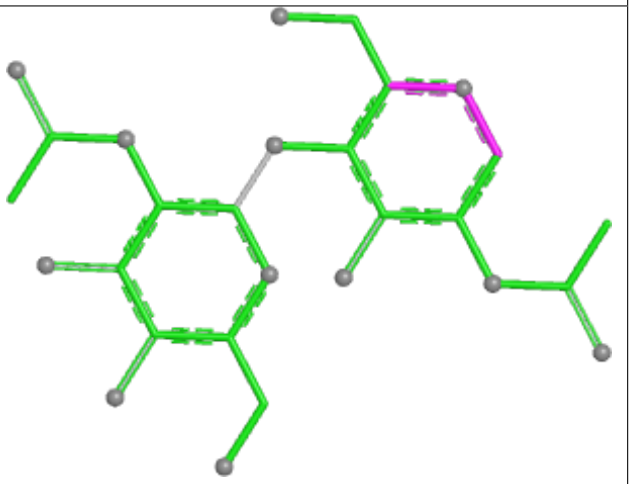
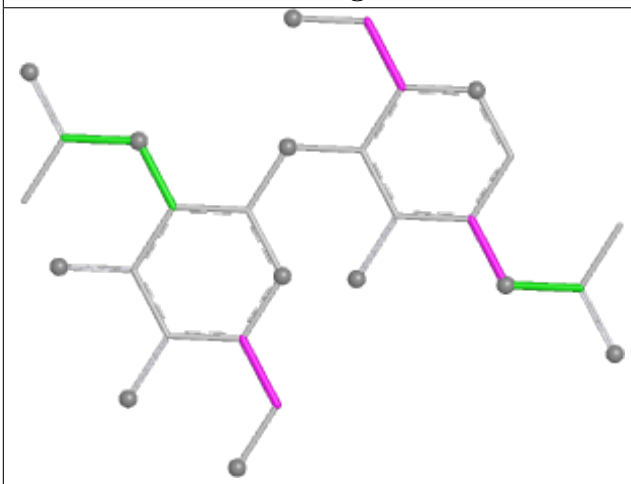


Bond angles



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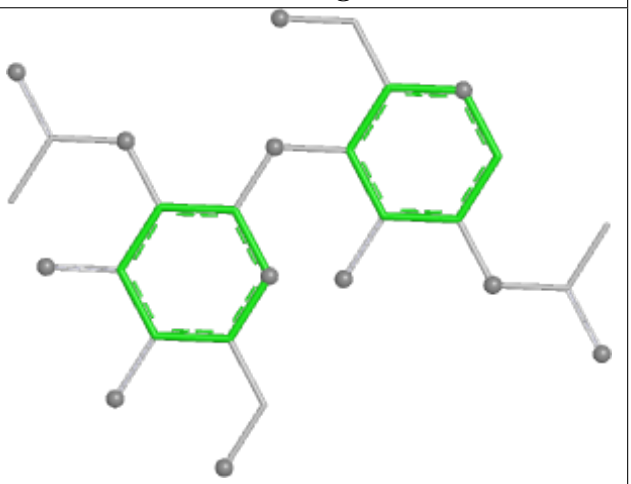
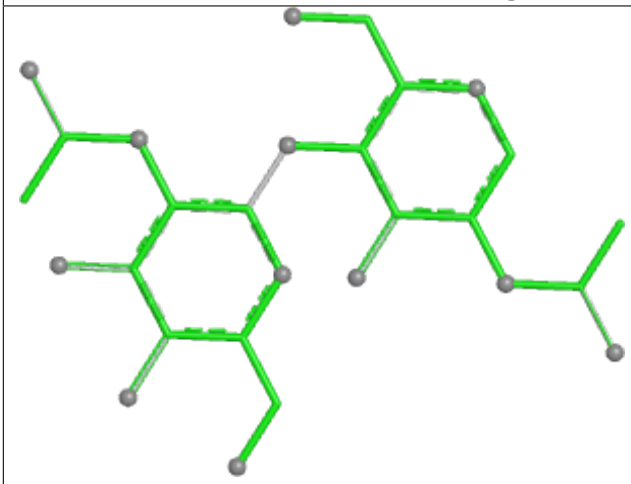
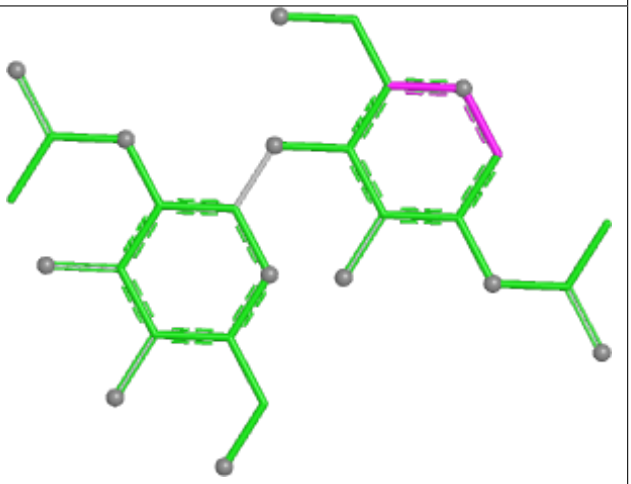


Rings

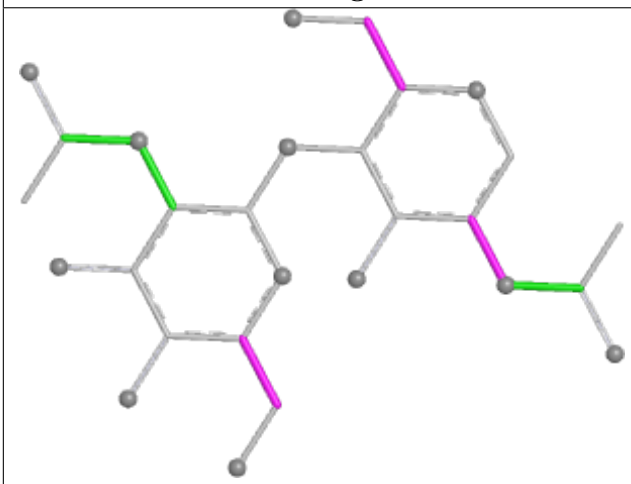
Oligosaccharide Chain l



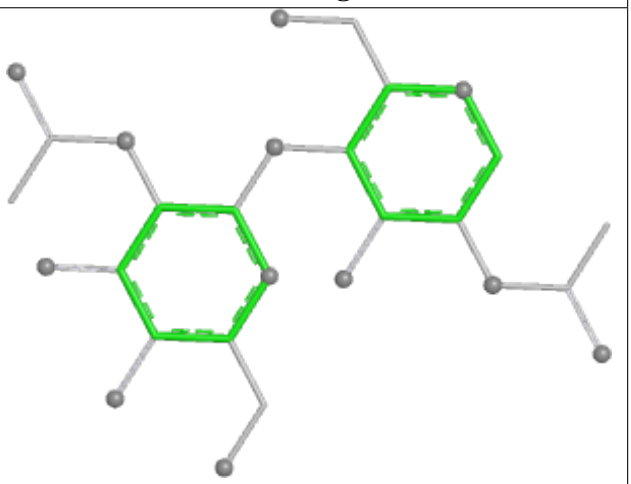
Bond lengths



Bond angles

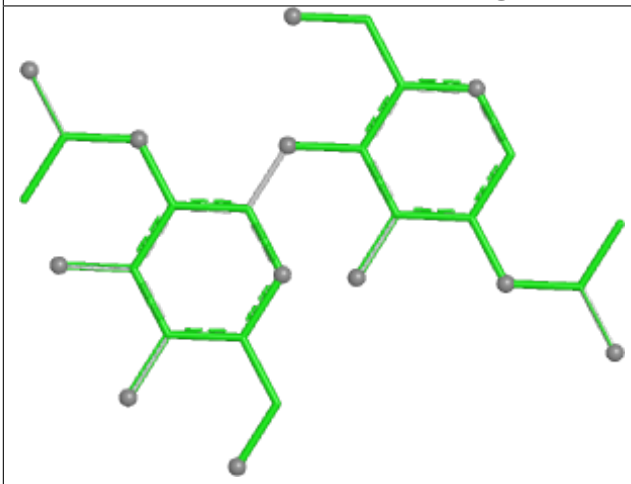


Torsions

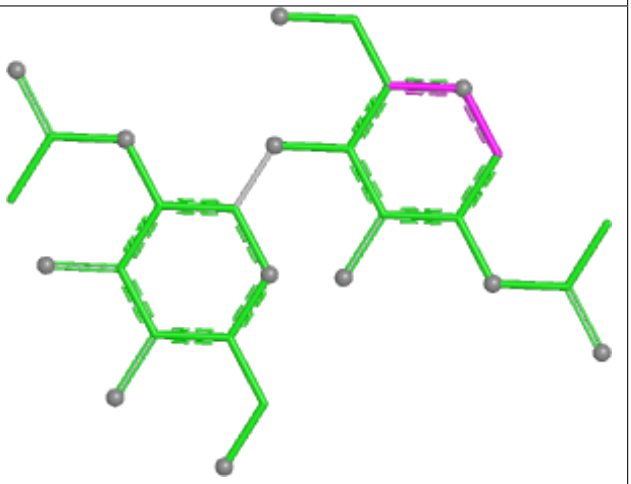


Rings

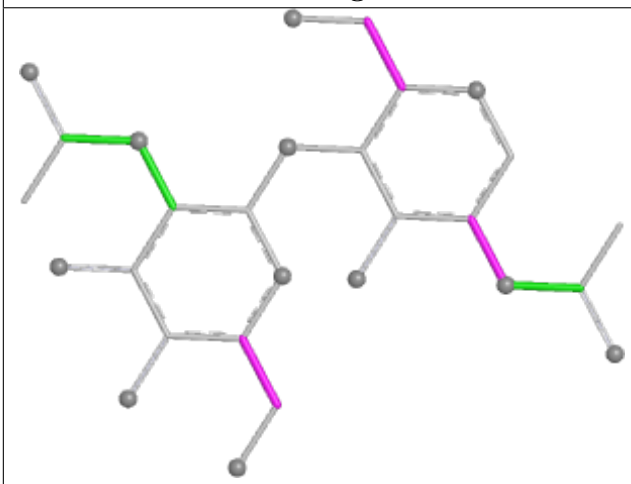
Oligosaccharide Chain m



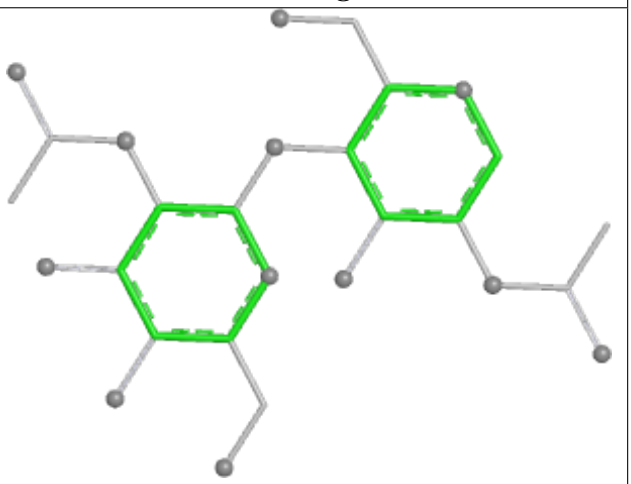
Bond lengths



Bond angles

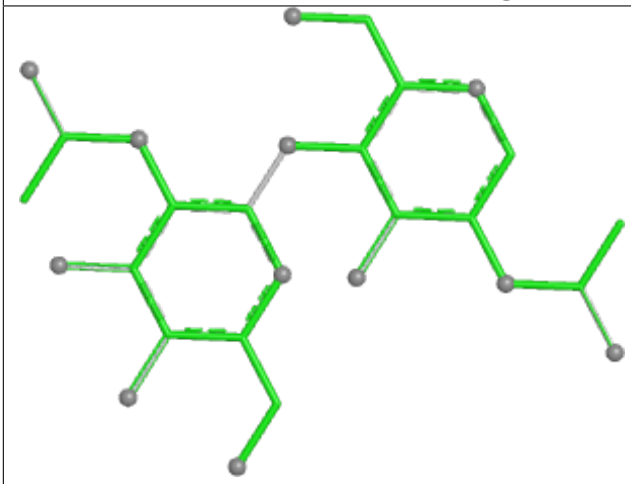


Torsions

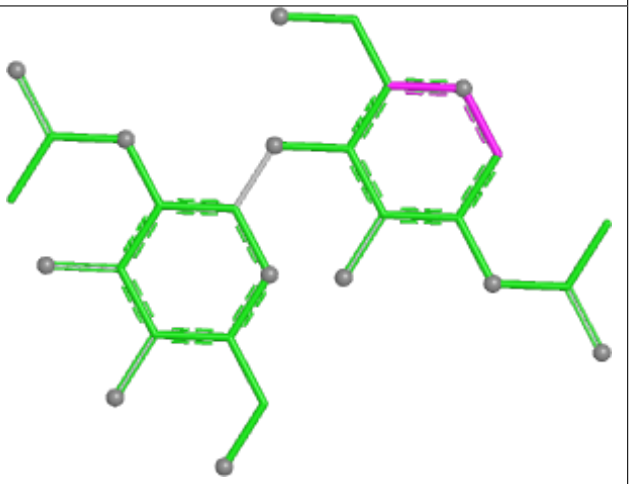


Rings

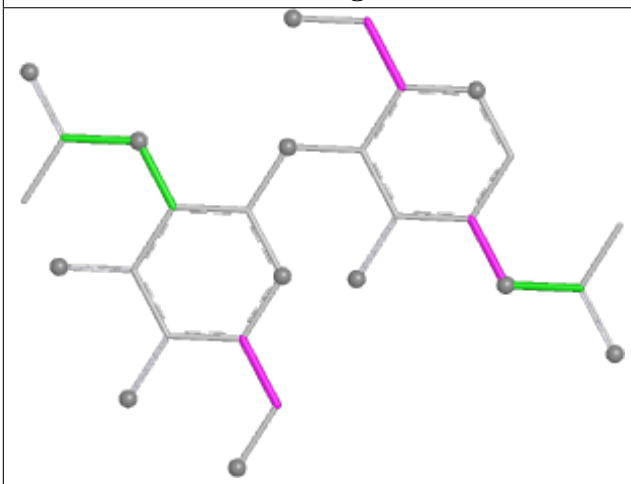
Oligosaccharide Chain n



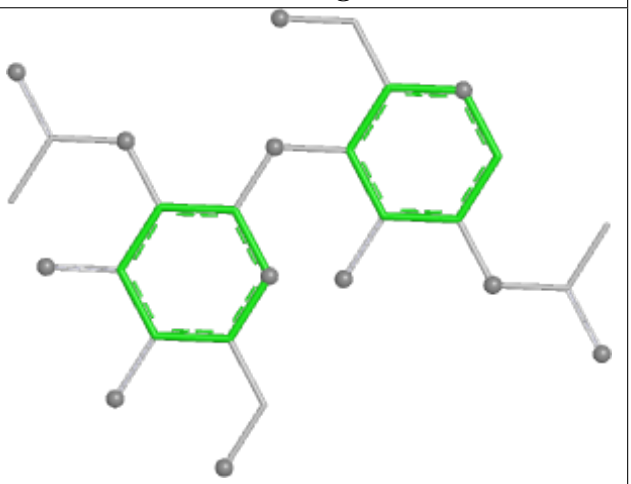
Bond lengths



Bond angles

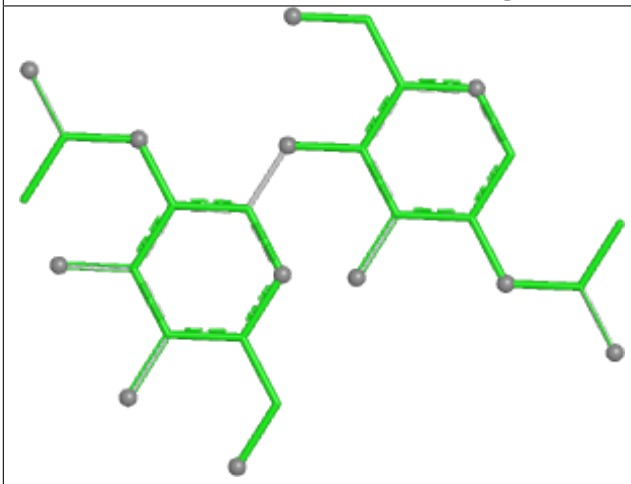


Torsions

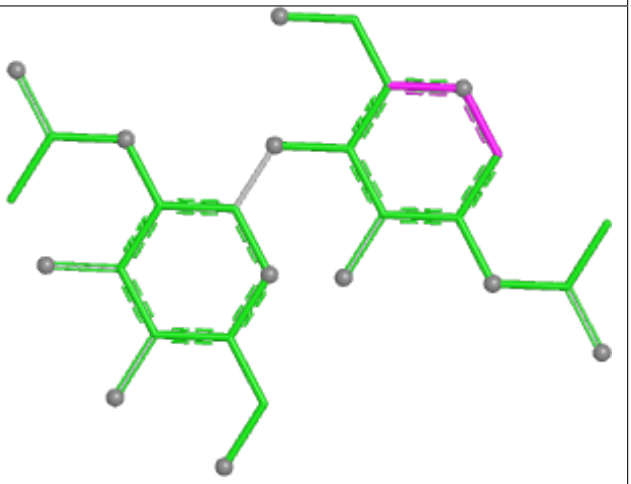


Rings

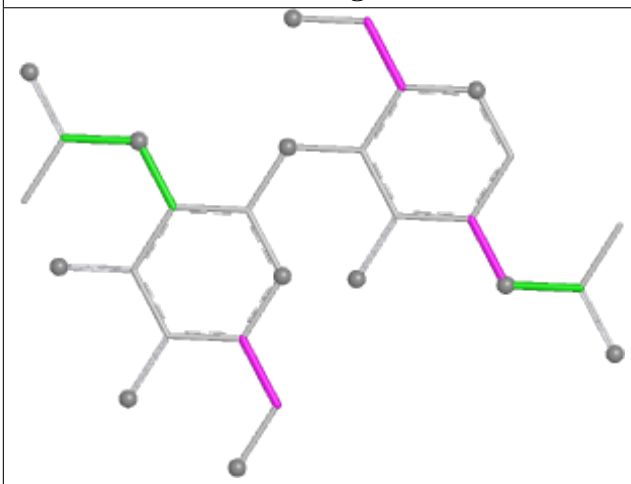
Oligosaccharide Chain o



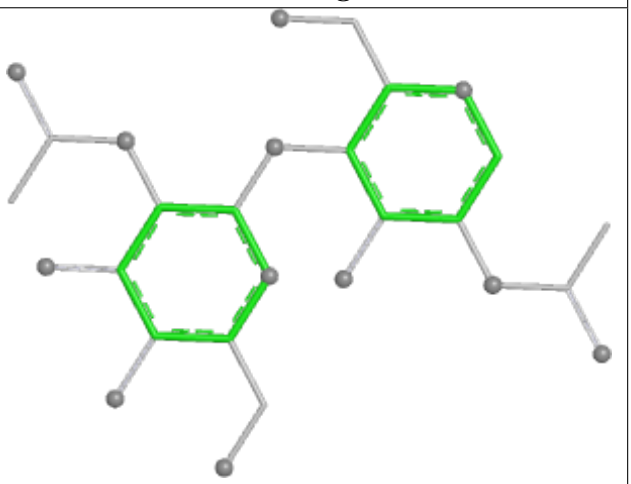
Bond lengths



Bond angles

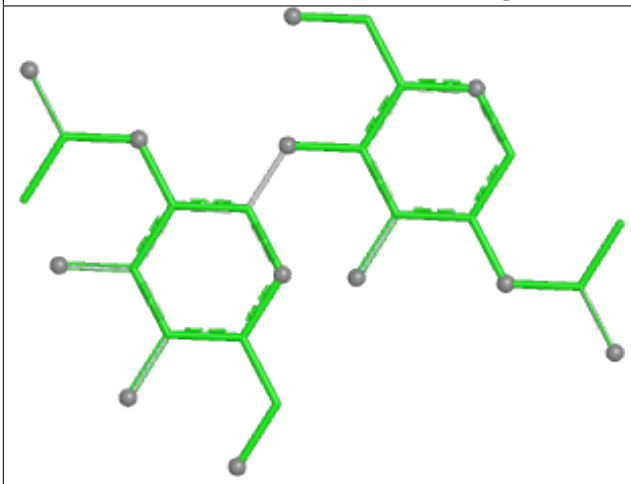


Torsions

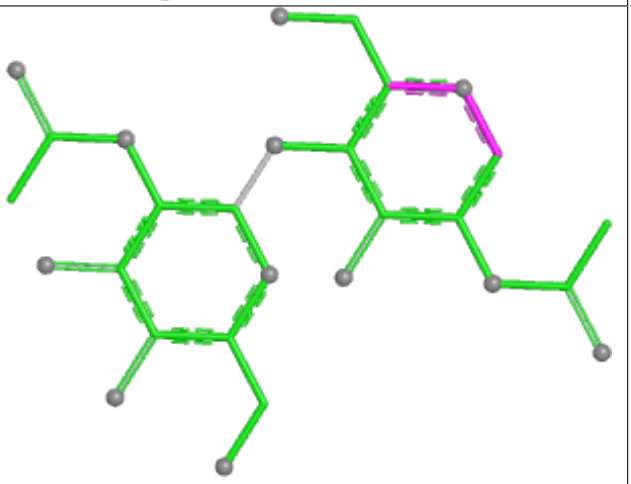


Rings

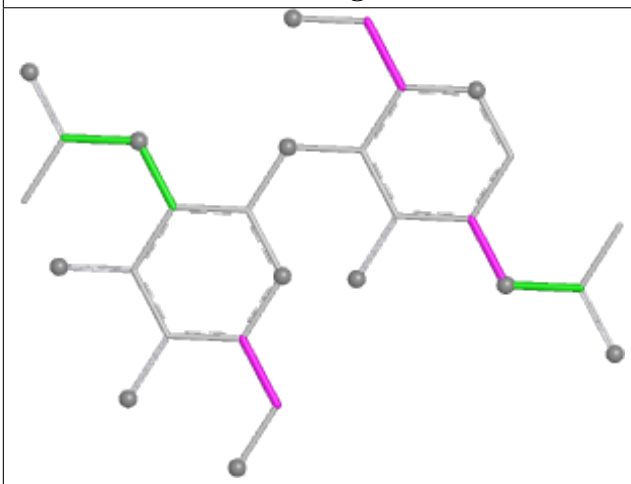
Oligosaccharide Chain p



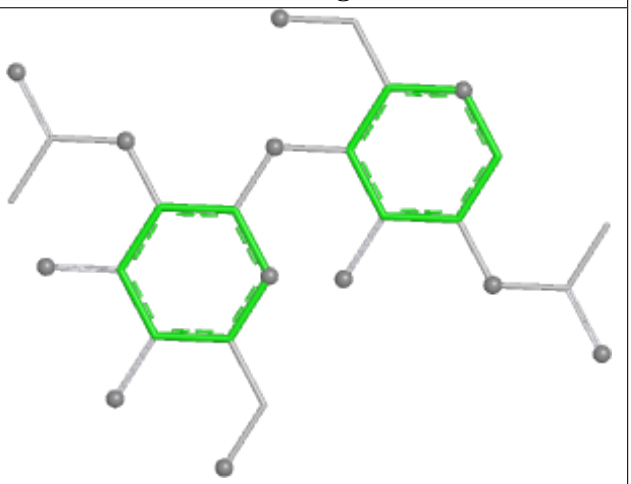
Bond lengths



Bond angles

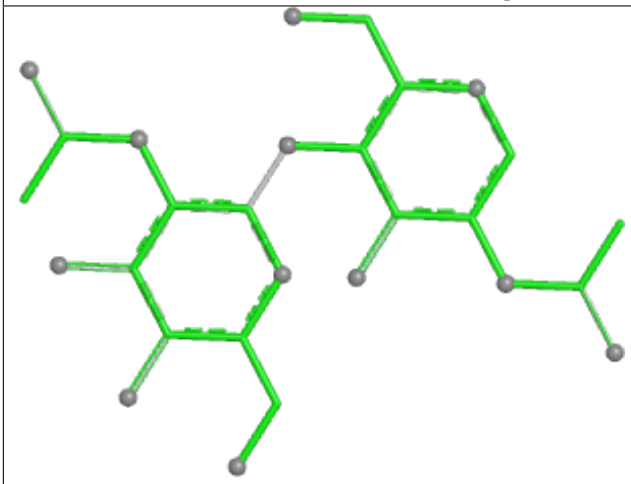


Torsions

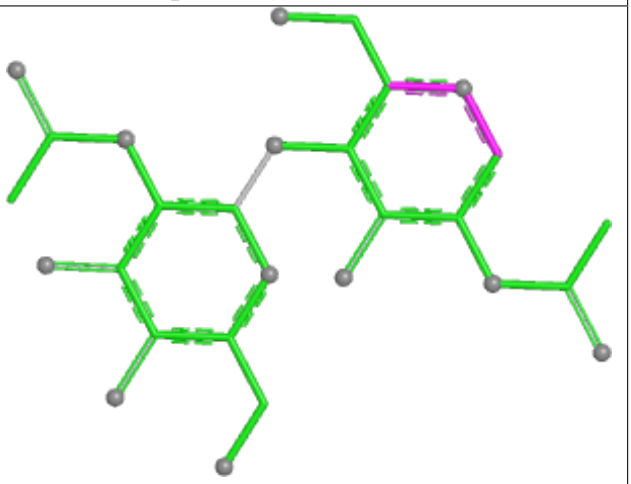


Rings

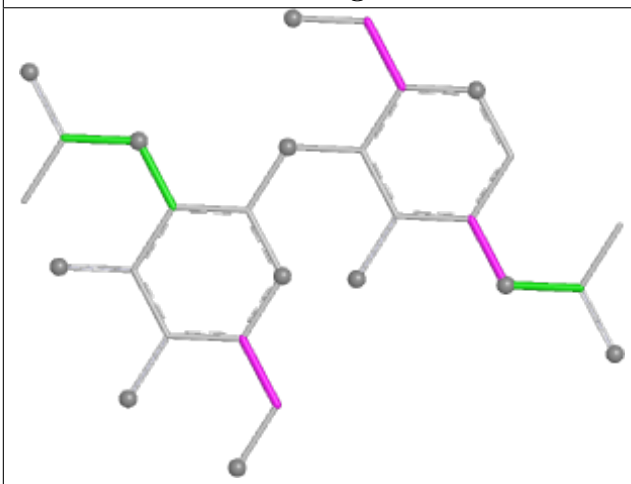
Oligosaccharide Chain q



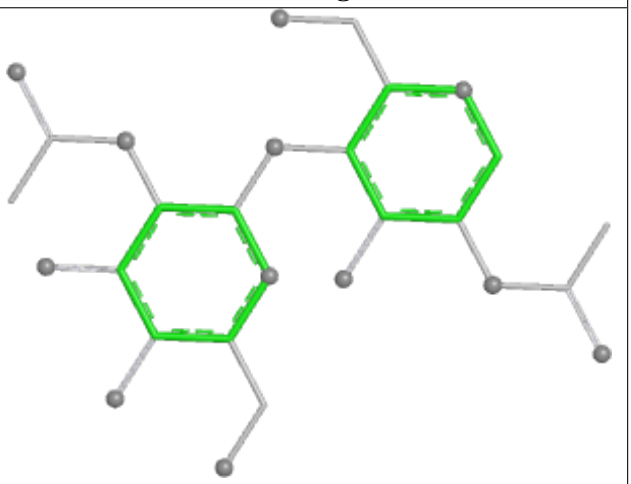
Bond lengths



Bond angles

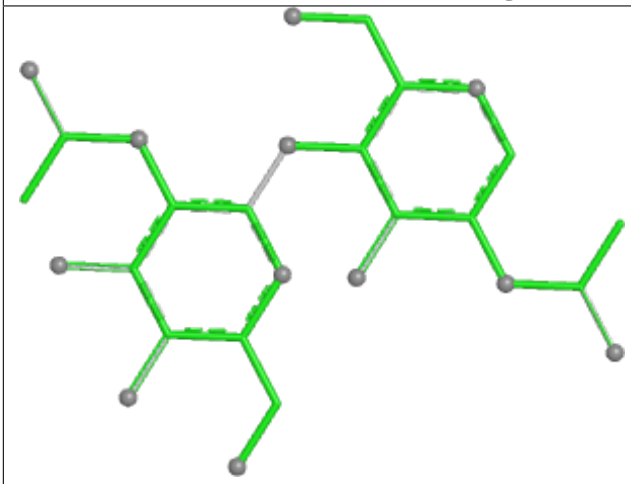


Torsions

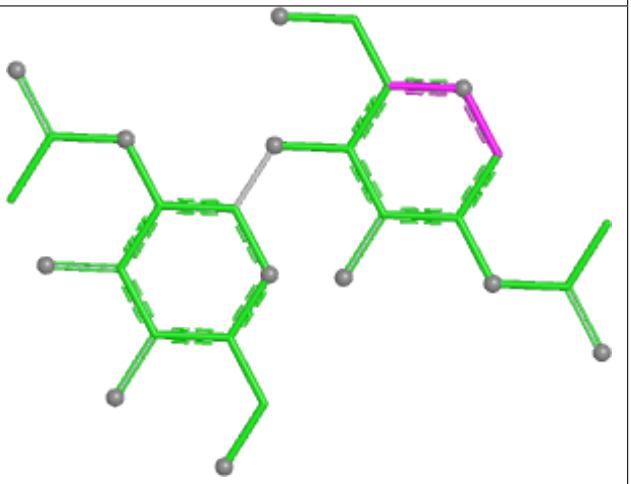


Rings

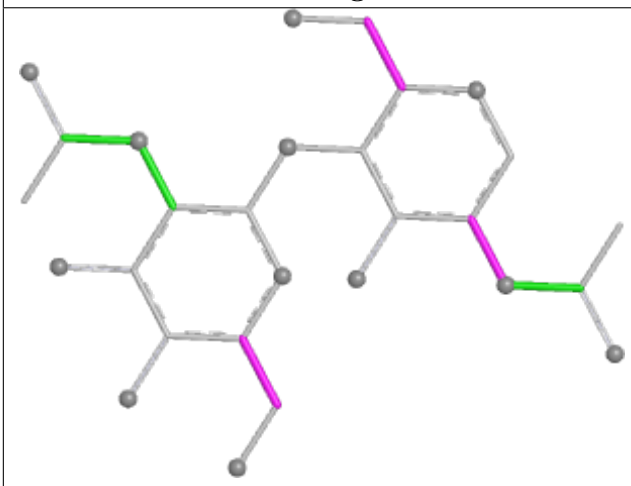
Oligosaccharide Chain r



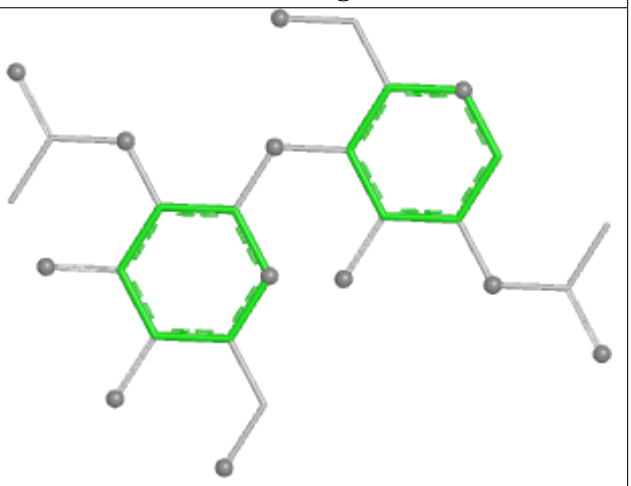
Bond lengths



Bond angles

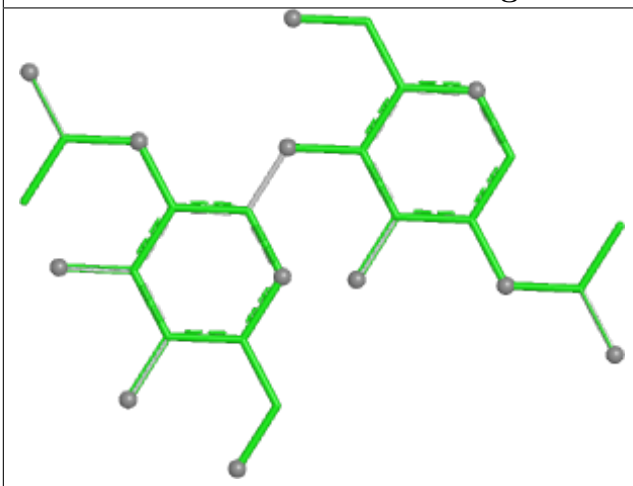


Torsions

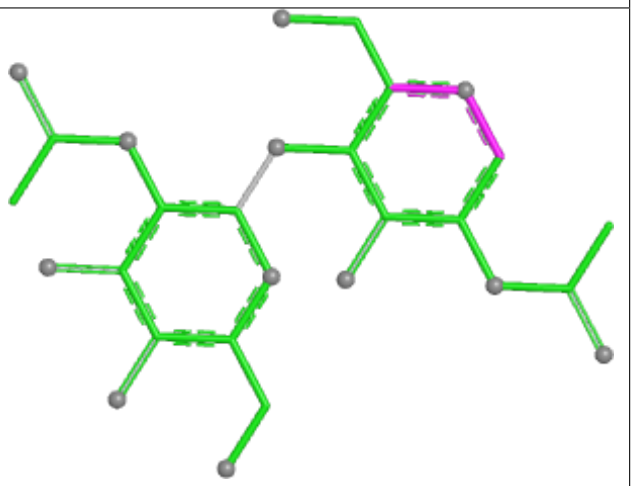


Rings

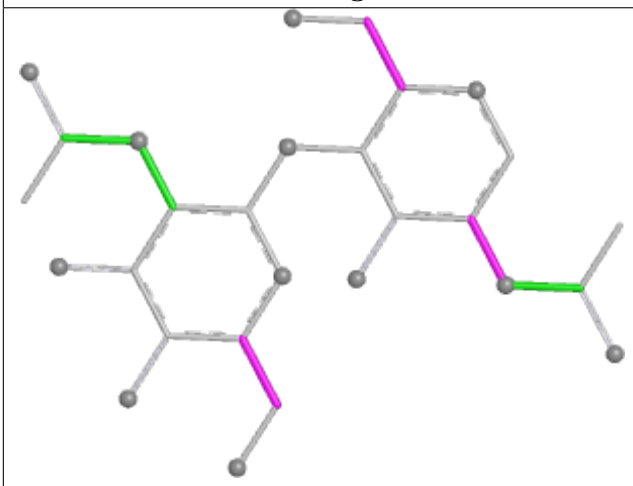
Oligosaccharide Chain s



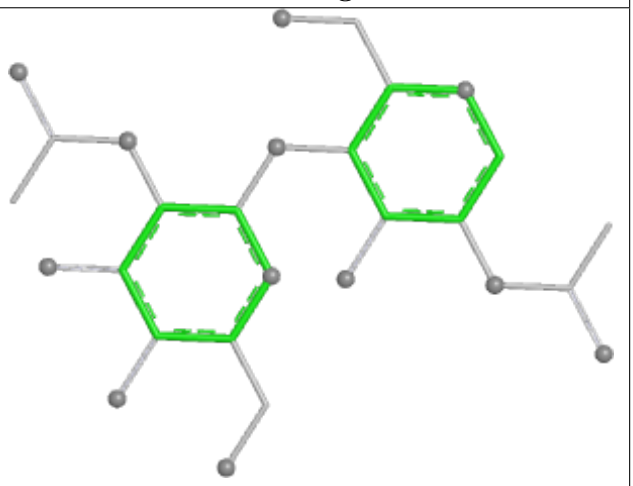
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

37 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	$\#\|Z\| > 2$
10	NAG	F	601	5	14,14,15	0.33	0	17,19,21	0.52	0
10	NAG	M	604	7	14,14,15	0.52	0	17,19,21	1.27	1 (5%)
10	NAG	T	603	7	14,14,15	0.24	0	17,19,21	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	NAG	U	603	7	14,14,15	0.25	0	17,19,21	0.34	0
10	NAG	R	604	7	14,14,15	0.51	0	17,19,21	1.27	1 (5%)
10	NAG	H	604	7	14,14,15	0.52	0	17,19,21	1.27	1 (5%)
10	NAG	V	604	7	14,14,15	0.51	0	17,19,21	1.26	1 (5%)
10	NAG	U	604	7	14,14,15	0.52	0	17,19,21	1.27	1 (5%)
10	NAG	X	603	7	14,14,15	0.24	0	17,19,21	0.35	0
10	NAG	M	603	7	14,14,15	0.23	0	17,19,21	0.36	0
10	NAG	O	604	7	14,14,15	0.52	0	17,19,21	1.26	1 (5%)
10	NAG	T	604	7	14,14,15	0.51	0	17,19,21	1.27	1 (5%)
10	NAG	V	603	7	14,14,15	0.23	0	17,19,21	0.36	0
10	NAG	W	603	7	14,14,15	0.24	0	17,19,21	0.35	0
10	NAG	R	603	7	14,14,15	0.23	0	17,19,21	0.35	0
10	NAG	N	603	7	14,14,15	0.23	0	17,19,21	0.35	0
10	NAG	S	603	7	14,14,15	0.24	0	17,19,21	0.35	0
10	NAG	W	604	7	14,14,15	0.51	0	17,19,21	1.27	1 (5%)
10	NAG	O	603	7	14,14,15	0.24	0	17,19,21	0.35	0
10	NAG	P	603	7	14,14,15	0.54	0	17,19,21	1.24	1 (5%)
10	NAG	K	603	7	14,14,15	0.24	0	17,19,21	0.35	0
10	NAG	L	604	7	14,14,15	0.51	0	17,19,21	1.27	1 (5%)
10	NAG	Q	604	7	14,14,15	0.52	0	17,19,21	1.27	1 (5%)
10	NAG	L	603	7	14,14,15	0.23	0	17,19,21	0.35	0
10	NAG	Q	603	7	14,14,15	0.22	0	17,19,21	0.35	0
10	NAG	J	603	7	14,14,15	0.23	0	17,19,21	0.34	0
10	NAG	S	604	7	14,14,15	0.51	0	17,19,21	1.27	1 (5%)
10	NAG	J	604	7	14,14,15	0.52	0	17,19,21	1.27	1 (5%)
10	NAG	N	604	7	14,14,15	0.50	0	17,19,21	1.26	1 (5%)
10	NAG	P	604	7	14,14,15	0.46	0	17,19,21	0.60	0
10	NAG	H	603	7	14,14,15	0.23	0	17,19,21	0.35	0
10	NAG	X	604	7	14,14,15	0.51	0	17,19,21	1.26	1 (5%)
10	NAG	K	604	7	14,14,15	0.52	0	17,19,21	1.26	1 (5%)
10	NAG	G	604	7	14,14,15	0.32	0	17,19,21	0.51	0
10	NAG	I	603	7	14,14,15	0.25	0	17,19,21	0.34	0
10	NAG	I	604	7	14,14,15	0.51	0	17,19,21	1.27	1 (5%)
10	NAG	G	603	7	14,14,15	0.29	0	17,19,21	0.35	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
10	NAG	F	601	5	-	2/6/23/26	0/1/1/1
10	NAG	M	604	7	-	3/6/23/26	0/1/1/1
10	NAG	T	603	7	-	2/6/23/26	0/1/1/1
10	NAG	U	603	7	-	2/6/23/26	0/1/1/1
10	NAG	R	604	7	-	3/6/23/26	0/1/1/1
10	NAG	H	604	7	-	3/6/23/26	0/1/1/1
10	NAG	V	604	7	-	3/6/23/26	0/1/1/1
10	NAG	U	604	7	-	3/6/23/26	0/1/1/1
10	NAG	X	603	7	-	2/6/23/26	0/1/1/1
10	NAG	M	603	7	-	2/6/23/26	0/1/1/1
10	NAG	O	604	7	-	3/6/23/26	0/1/1/1
10	NAG	T	604	7	-	3/6/23/26	0/1/1/1
10	NAG	V	603	7	-	2/6/23/26	0/1/1/1
10	NAG	W	603	7	-	2/6/23/26	0/1/1/1
10	NAG	R	603	7	-	2/6/23/26	0/1/1/1
10	NAG	N	603	7	-	2/6/23/26	0/1/1/1
10	NAG	S	603	7	-	2/6/23/26	0/1/1/1
10	NAG	W	604	7	-	3/6/23/26	0/1/1/1
10	NAG	O	603	7	-	2/6/23/26	0/1/1/1
10	NAG	P	603	7	-	5/6/23/26	0/1/1/1
10	NAG	K	603	7	-	2/6/23/26	0/1/1/1
10	NAG	L	604	7	-	3/6/23/26	0/1/1/1
10	NAG	Q	604	7	-	3/6/23/26	0/1/1/1
10	NAG	L	603	7	-	2/6/23/26	0/1/1/1
10	NAG	Q	603	7	-	2/6/23/26	0/1/1/1
10	NAG	J	603	7	-	2/6/23/26	0/1/1/1
10	NAG	S	604	7	-	3/6/23/26	0/1/1/1
10	NAG	J	604	7	-	3/6/23/26	0/1/1/1
10	NAG	N	604	7	-	3/6/23/26	0/1/1/1
10	NAG	P	604	7	-	0/6/23/26	0/1/1/1
10	NAG	H	603	7	-	2/6/23/26	0/1/1/1
10	NAG	X	604	7	-	3/6/23/26	0/1/1/1
10	NAG	K	604	7	-	3/6/23/26	0/1/1/1
10	NAG	G	604	7	-	2/6/23/26	0/1/1/1
10	NAG	I	603	7	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	I	604	7	-	3/6/23/26	0/1/1/1
10	NAG	G	603	7	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	U	604	NAG	C2-N2-C7	4.27	128.99	122.90
10	P	603	NAG	C2-N2-C7	4.27	128.98	122.90
10	I	604	NAG	C2-N2-C7	4.26	128.98	122.90
10	W	604	NAG	C2-N2-C7	4.26	128.97	122.90
10	J	604	NAG	C2-N2-C7	4.26	128.97	122.90
10	R	604	NAG	C2-N2-C7	4.25	128.96	122.90
10	V	604	NAG	C2-N2-C7	4.25	128.96	122.90
10	T	604	NAG	C2-N2-C7	4.25	128.95	122.90
10	L	604	NAG	C2-N2-C7	4.24	128.94	122.90
10	H	604	NAG	C2-N2-C7	4.24	128.94	122.90
10	K	604	NAG	C2-N2-C7	4.22	128.92	122.90
10	M	604	NAG	C2-N2-C7	4.22	128.91	122.90
10	X	604	NAG	C2-N2-C7	4.22	128.91	122.90
10	N	604	NAG	C2-N2-C7	4.21	128.89	122.90
10	Q	604	NAG	C2-N2-C7	4.21	128.89	122.90
10	S	604	NAG	C2-N2-C7	4.21	128.89	122.90
10	O	604	NAG	C2-N2-C7	4.19	128.87	122.90

There are no chirality outliers.

All (90) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	H	603	NAG	C4-C5-C6-O6
10	I	603	NAG	C4-C5-C6-O6
10	J	603	NAG	C4-C5-C6-O6
10	K	603	NAG	C4-C5-C6-O6
10	L	603	NAG	C4-C5-C6-O6
10	M	603	NAG	C4-C5-C6-O6
10	N	603	NAG	C4-C5-C6-O6
10	O	603	NAG	C4-C5-C6-O6
10	Q	603	NAG	C4-C5-C6-O6
10	R	603	NAG	C4-C5-C6-O6
10	S	603	NAG	C4-C5-C6-O6
10	T	603	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
10	U	603	NAG	C4-C5-C6-O6
10	V	603	NAG	C4-C5-C6-O6
10	W	603	NAG	C4-C5-C6-O6
10	X	603	NAG	C4-C5-C6-O6
10	P	603	NAG	O5-C5-C6-O6
10	H	603	NAG	O5-C5-C6-O6
10	I	603	NAG	O5-C5-C6-O6
10	J	603	NAG	O5-C5-C6-O6
10	K	603	NAG	O5-C5-C6-O6
10	L	603	NAG	O5-C5-C6-O6
10	M	603	NAG	O5-C5-C6-O6
10	N	603	NAG	O5-C5-C6-O6
10	O	603	NAG	O5-C5-C6-O6
10	Q	603	NAG	O5-C5-C6-O6
10	R	603	NAG	O5-C5-C6-O6
10	S	603	NAG	O5-C5-C6-O6
10	T	603	NAG	O5-C5-C6-O6
10	U	603	NAG	O5-C5-C6-O6
10	V	603	NAG	O5-C5-C6-O6
10	W	603	NAG	O5-C5-C6-O6
10	X	603	NAG	O5-C5-C6-O6
10	G	604	NAG	C4-C5-C6-O6
10	F	601	NAG	C8-C7-N2-C2
10	F	601	NAG	O7-C7-N2-C2
10	P	603	NAG	C8-C7-N2-C2
10	P	603	NAG	O7-C7-N2-C2
10	H	604	NAG	C8-C7-N2-C2
10	H	604	NAG	O7-C7-N2-C2
10	I	604	NAG	C8-C7-N2-C2
10	I	604	NAG	O7-C7-N2-C2
10	J	604	NAG	C8-C7-N2-C2
10	J	604	NAG	O7-C7-N2-C2
10	K	604	NAG	C8-C7-N2-C2
10	K	604	NAG	O7-C7-N2-C2
10	L	604	NAG	C8-C7-N2-C2
10	L	604	NAG	O7-C7-N2-C2
10	M	604	NAG	C8-C7-N2-C2
10	M	604	NAG	O7-C7-N2-C2
10	N	604	NAG	C8-C7-N2-C2
10	N	604	NAG	O7-C7-N2-C2
10	O	604	NAG	C8-C7-N2-C2
10	O	604	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
10	Q	604	NAG	C8-C7-N2-C2
10	Q	604	NAG	O7-C7-N2-C2
10	R	604	NAG	C8-C7-N2-C2
10	R	604	NAG	O7-C7-N2-C2
10	S	604	NAG	C8-C7-N2-C2
10	S	604	NAG	O7-C7-N2-C2
10	T	604	NAG	C8-C7-N2-C2
10	T	604	NAG	O7-C7-N2-C2
10	U	604	NAG	C8-C7-N2-C2
10	U	604	NAG	O7-C7-N2-C2
10	V	604	NAG	C8-C7-N2-C2
10	V	604	NAG	O7-C7-N2-C2
10	W	604	NAG	C8-C7-N2-C2
10	W	604	NAG	O7-C7-N2-C2
10	X	604	NAG	C8-C7-N2-C2
10	X	604	NAG	O7-C7-N2-C2
10	G	604	NAG	O5-C5-C6-O6
10	P	603	NAG	C4-C5-C6-O6
10	G	603	NAG	O5-C5-C6-O6
10	P	603	NAG	C3-C2-N2-C7
10	H	604	NAG	C3-C2-N2-C7
10	I	604	NAG	C3-C2-N2-C7
10	J	604	NAG	C3-C2-N2-C7
10	K	604	NAG	C3-C2-N2-C7
10	L	604	NAG	C3-C2-N2-C7
10	M	604	NAG	C3-C2-N2-C7
10	N	604	NAG	C3-C2-N2-C7
10	O	604	NAG	C3-C2-N2-C7
10	Q	604	NAG	C3-C2-N2-C7
10	R	604	NAG	C3-C2-N2-C7
10	S	604	NAG	C3-C2-N2-C7
10	T	604	NAG	C3-C2-N2-C7
10	U	604	NAG	C3-C2-N2-C7
10	V	604	NAG	C3-C2-N2-C7
10	W	604	NAG	C3-C2-N2-C7
10	X	604	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	F	601	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	P	603	NAG	1	0
10	P	604	NAG	1	0

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.

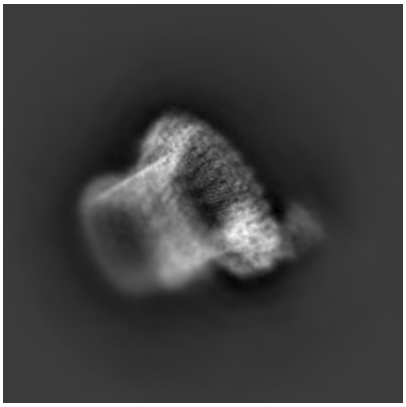
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0106. These allow visual inspection of the internal detail of the map and identification of artifacts.

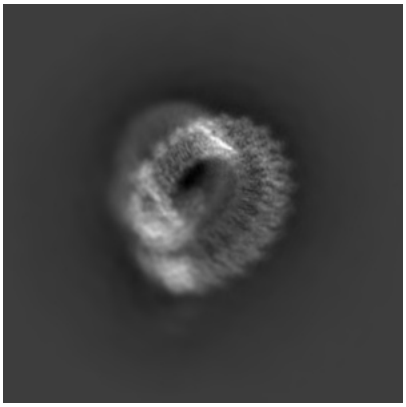
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

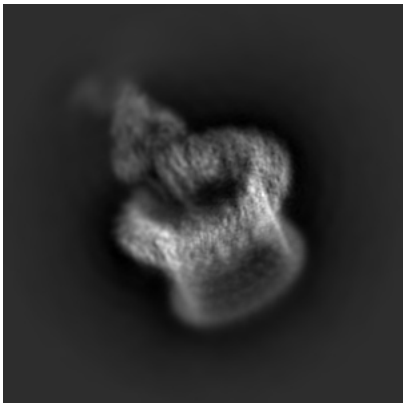
6.1.1 Primary map



X



Y

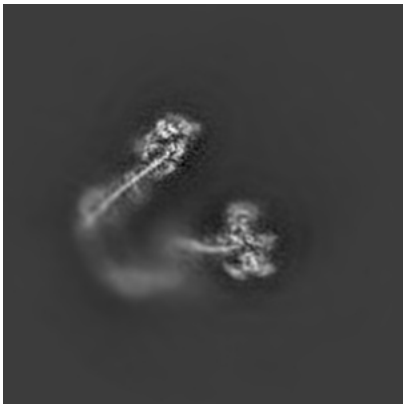


Z

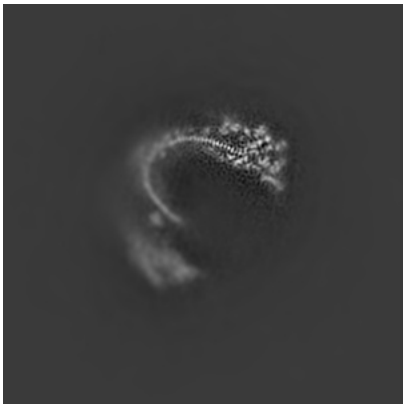
The images above show the map projected in three orthogonal directions.

6.2 Central slices

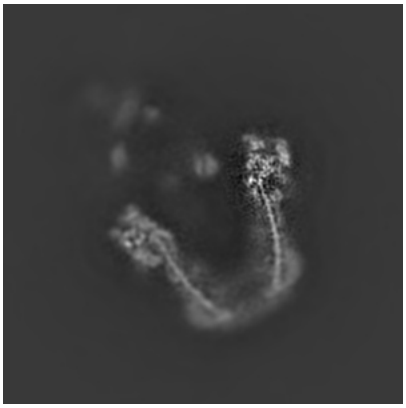
6.2.1 Primary map



X Index: 180



Y Index: 180



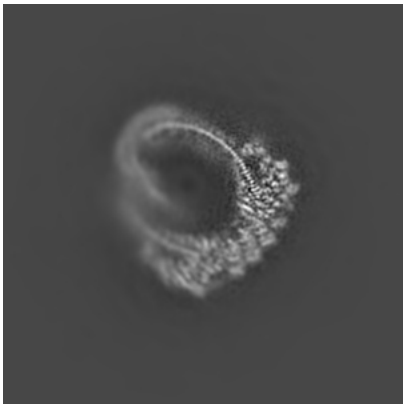
Z Index: 180

The images above show central slices of the map in three orthogonal directions.

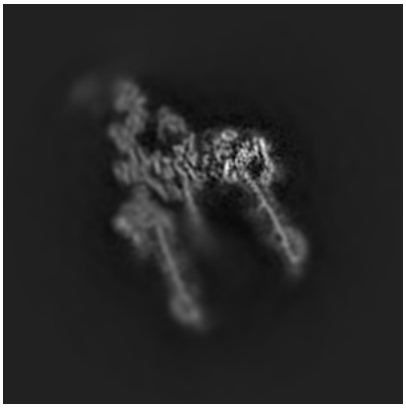
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 232



Y Index: 153

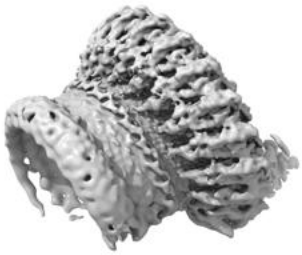


Z Index: 152

The images above show the largest variance slices of the map in three orthogonal directions.

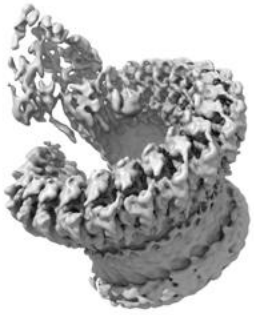
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

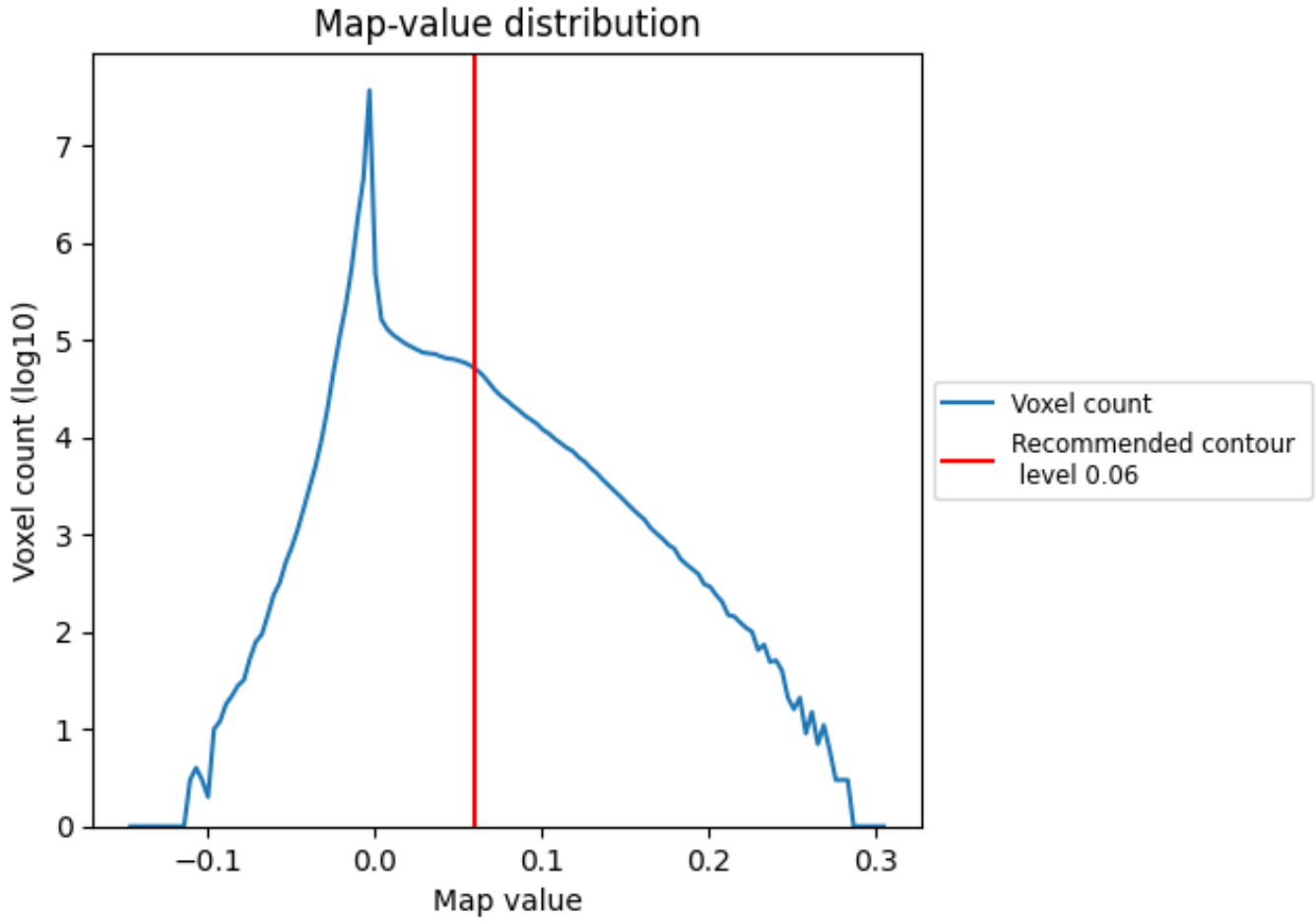
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

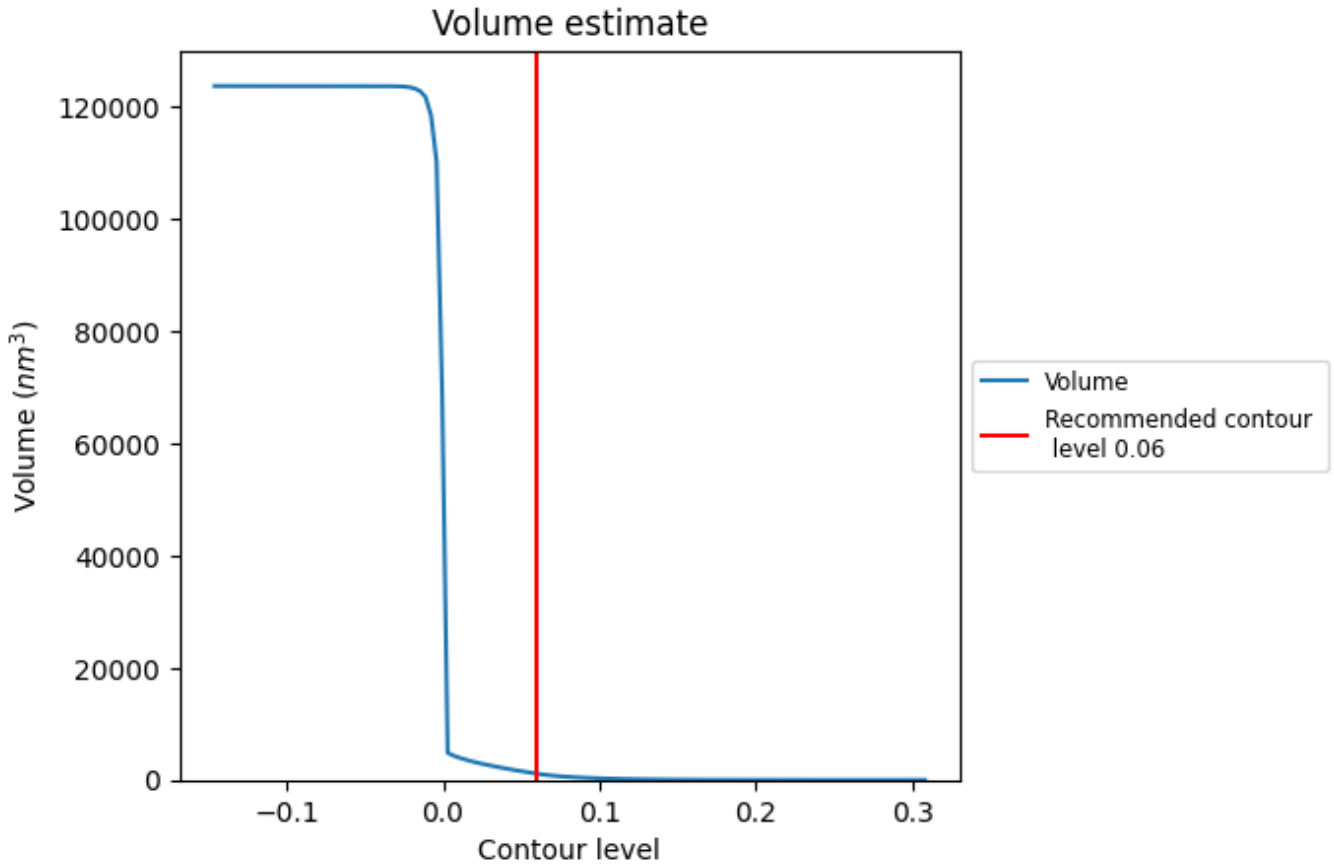
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

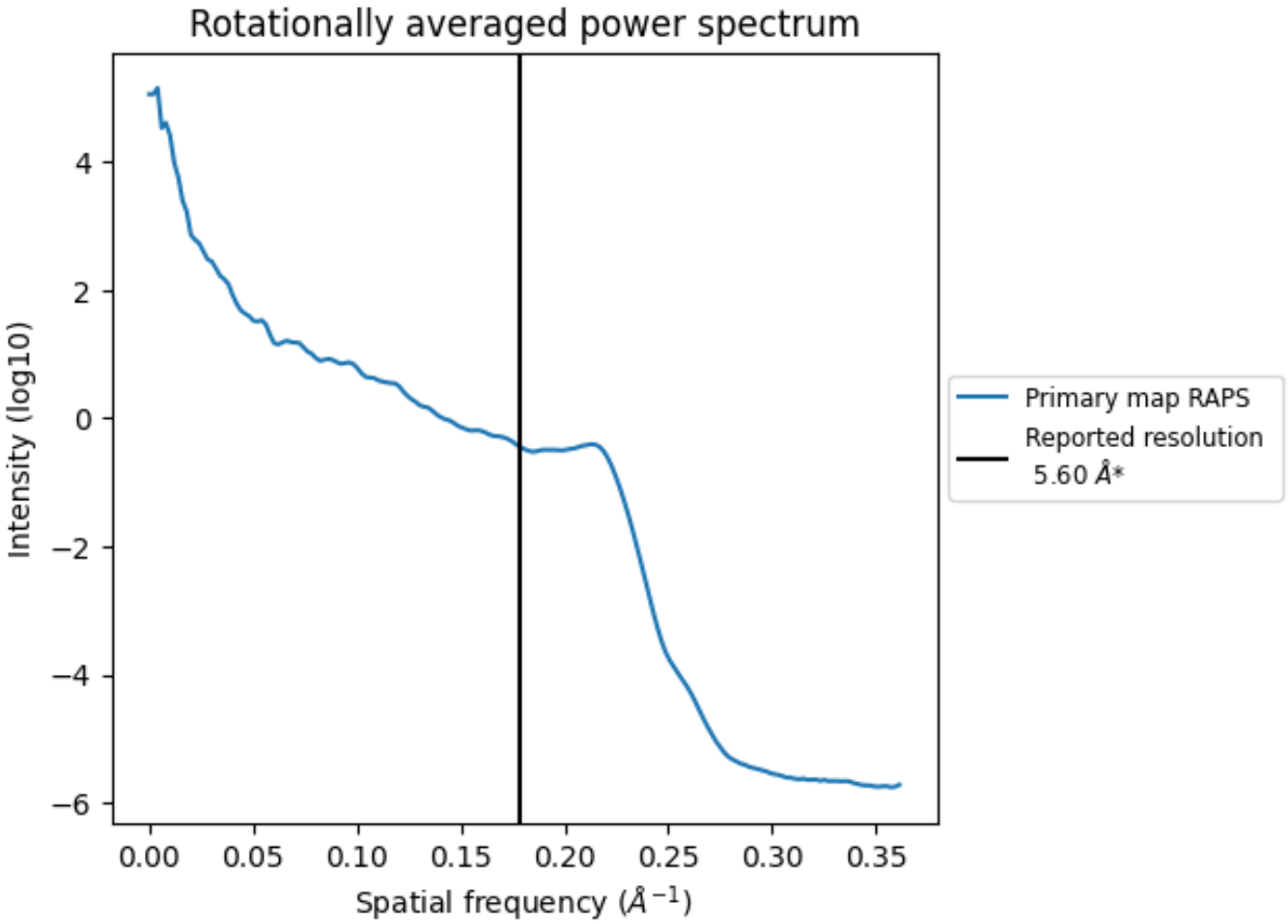
7.2 Volume estimate



The volume at the recommended contour level is 1116 nm^3; this corresponds to an approximate mass of 1008 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.179 Å^{-1}

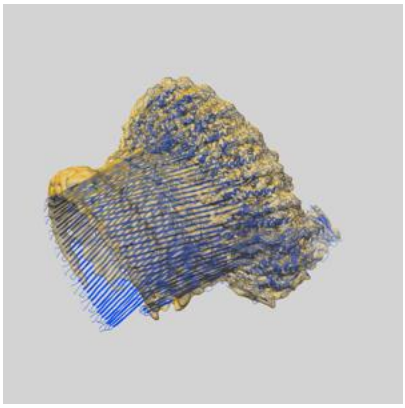
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

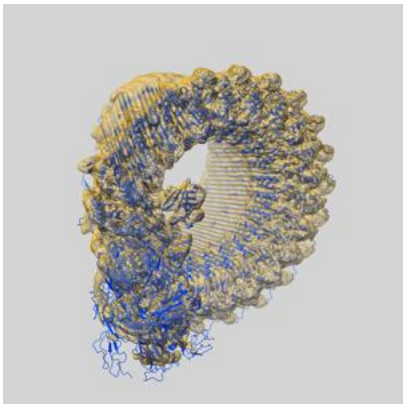
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0106 and PDB model 6H03. Per-residue inclusion information can be found in section 3 on page 11.

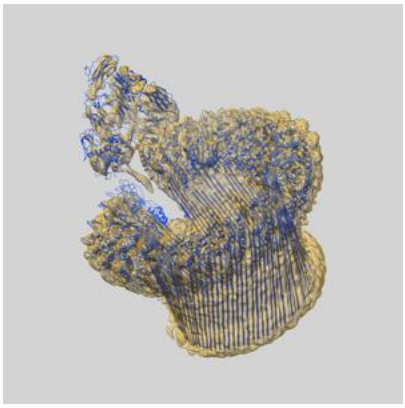
9.1 Map-model overlay



X



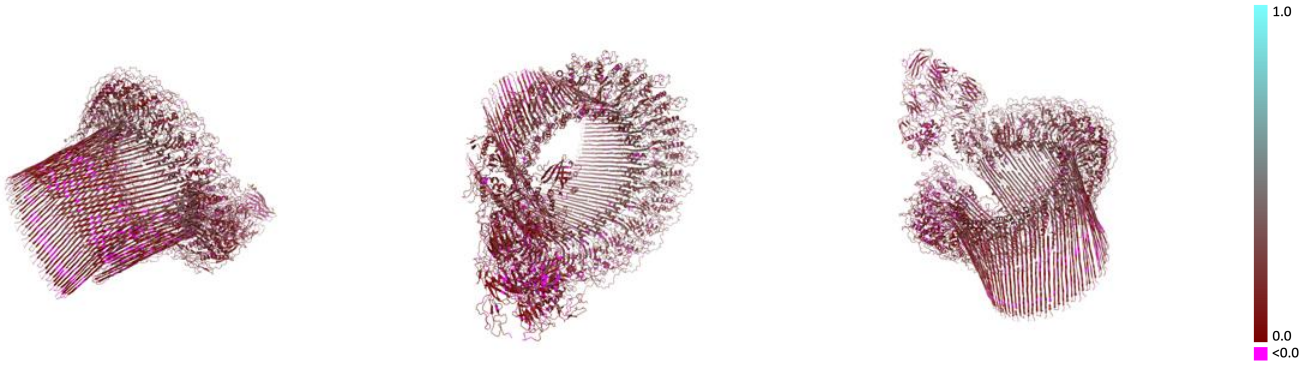
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

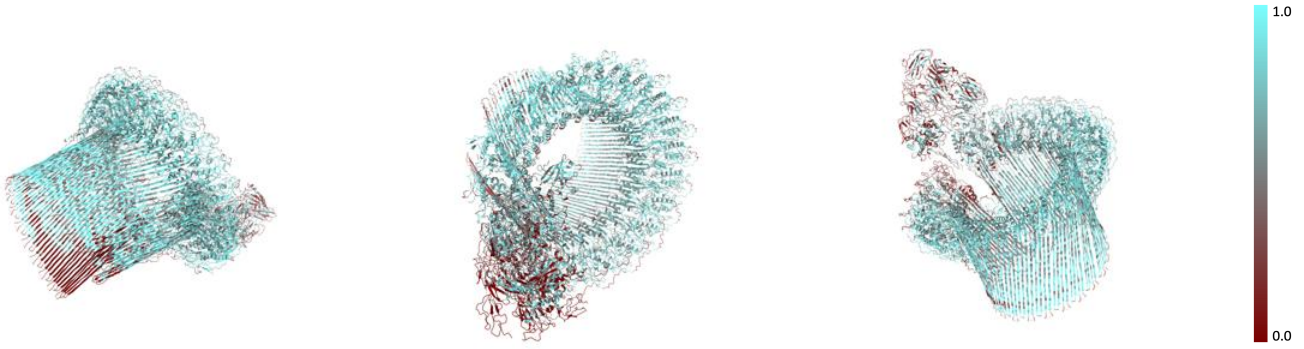
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

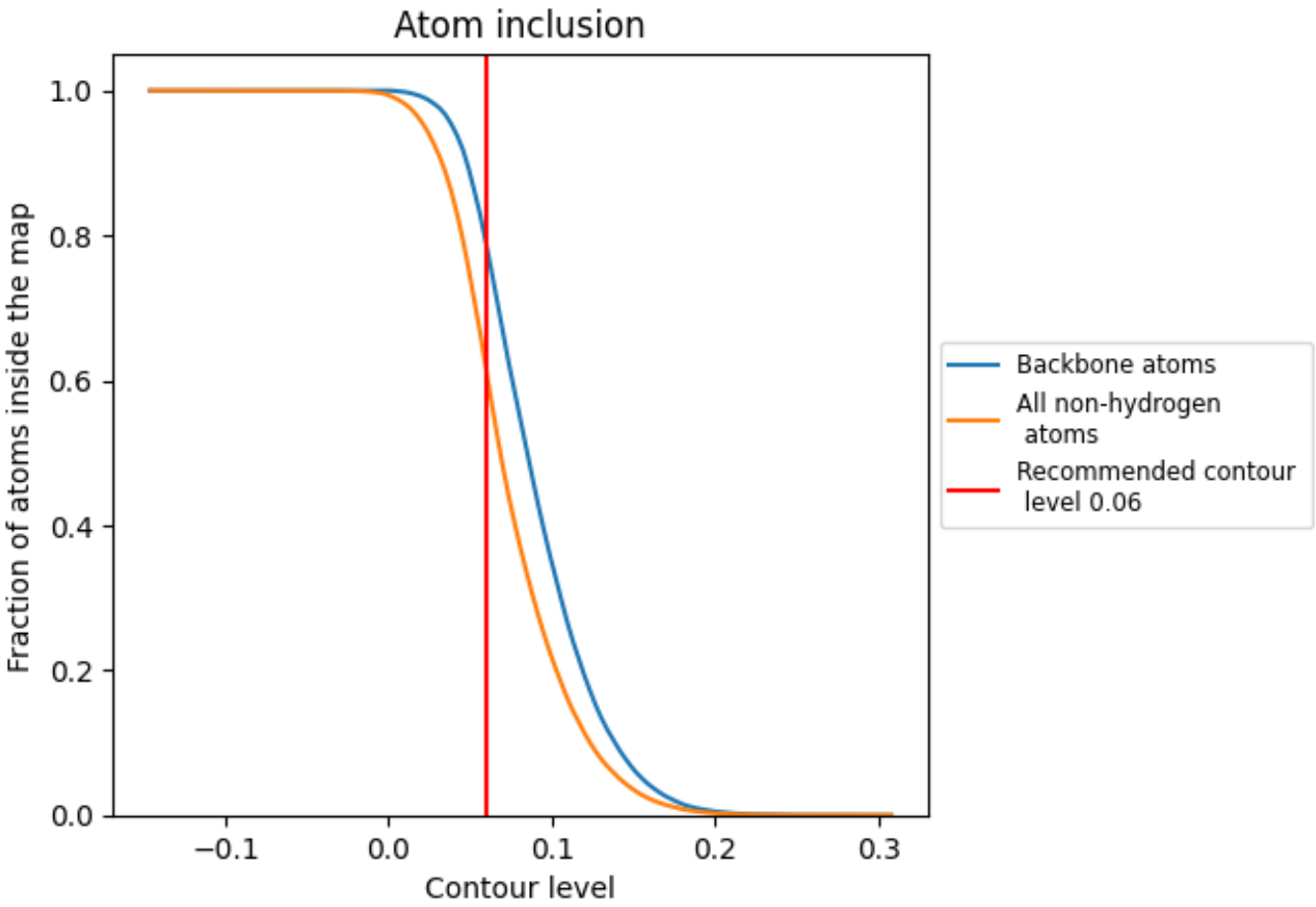
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6135	0.1560
A	0.3697	0.1050
B	0.4417	0.1270
C	0.6998	0.1720
D	0.5538	0.1350
E	0.5508	0.1650
F	0.7093	0.1630
G	0.6896	0.1610
H	0.7483	0.1980
I	0.7466	0.1930
J	0.7404	0.1980
K	0.7430	0.2070
L	0.7455	0.2070
M	0.7511	0.2170
N	0.7248	0.1850
O	0.7417	0.2020
P	0.7333	0.1810
Q	0.7289	0.1870
R	0.7172	0.1620
S	0.6924	0.1550
T	0.6506	0.1280
U	0.6248	0.1280
V	0.5419	0.1170
W	0.3947	0.0780
X	0.1108	0.0670
Y	0.1282	0.1780
Z	0.0000	0.0820
a	0.0000	-0.0210
b	0.3929	0.2130
c	0.4286	0.2220
d	0.3929	0.1300
e	0.3571	0.1020
f	0.4643	0.2440
g	0.3929	0.2000
h	0.6071	0.1970

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Chain	Atom inclusion	Q-score
i	0.5000	0.1720
j	0.6071	0.1800
k	0.4286	0.2100
l	0.4286	0.2300
m	0.5714	0.2100
n	0.2500	0.1690
o	0.1786	0.1800
p	0.1786	0.0630
q	0.1429	0.0170
r	0.0357	0.0560
s	0.0000	0.0610