Full wwPDB EM Validation Report

Mar 10, 2026 – 12:40 AM UTC

PDB ID	:	5JUY / pdb_00005juy
EMDB ID	:	EMD-8178
Title	:	Active human apoptosome with procaspase-9
Authors	:	Cheng, T.C.; Hong, C.; Akey, I.V.; Yuan, S.; Akey, C.W.
Deposited on	:	2016-05-10
Resolution	:	4.10 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:

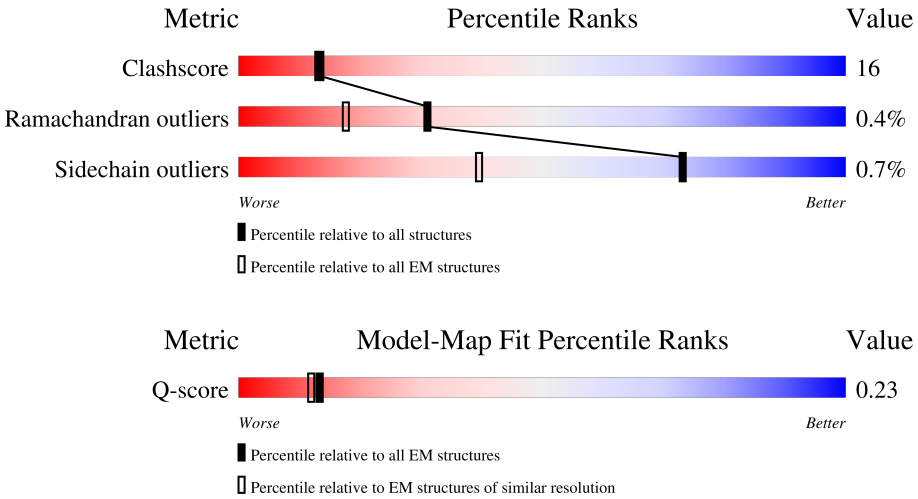
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.10 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6458 (3.60 - 4.60)

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	1248	39% 63% 27% • 9%
1	B	1248	46% 70% 28% ••
1	C	1248	39% 63% 27% • 9%
1	D	1248	46% 70% 28% ••

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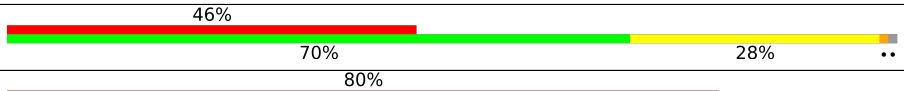
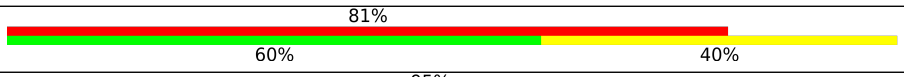
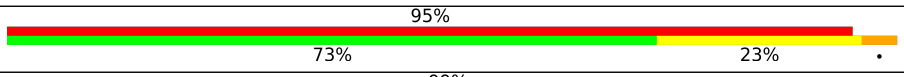
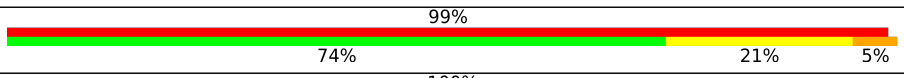
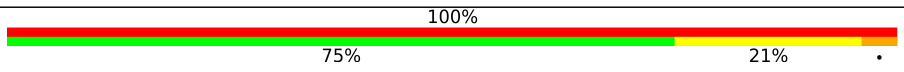
Mol	Chain	Length	Quality of chain
1	E	1248	
1	F	1248	
1	G	1248	
2	H	104	
2	I	104	
2	J	104	
2	K	104	
2	L	104	
2	M	104	
2	N	104	
3	O	95	
3	P	95	
3	Q	95	
3	R	95	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 76058 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 Apoptotic protease-activating factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1139	Total	C	N	O	S	0	0
			9099	5764	1563	1711	61		
1	B	1234	Total	C	N	O	S	0	0
			9861	6243	1694	1857	67		
1	C	1139	Total	C	N	O	S	0	0
			9099	5764	1563	1711	61		
1	D	1234	Total	C	N	O	S	0	0
			9861	6243	1694	1857	67		
1	E	1234	Total	C	N	O	S	0	0
			9861	6243	1694	1857	67		
1	F	1139	Total	C	N	O	S	0	0
			9099	5764	1563	1711	61		
1	G	1234	Total	C	N	O	S	0	0
			9861	6243	1694	1857	67		

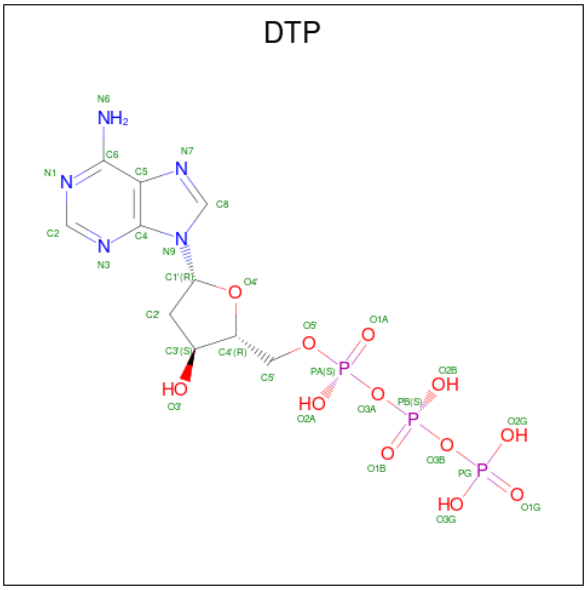
- Molecule 2 is a protein called Cytochrome c.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	104	Total	C	N	O	S	0	0
			814	517	143	150	4		
2	I	104	Total	C	N	O	S	0	0
			814	517	143	150	4		
2	J	104	Total	C	N	O	S	0	0
			814	517	143	150	4		
2	K	104	Total	C	N	O	S	0	0
			814	517	143	150	4		
2	L	104	Total	C	N	O	S	0	0
			814	517	143	150	4		
2	M	104	Total	C	N	O	S	0	0
			814	517	143	150	4		
2	N	104	Total	C	N	O	S	0	0
			814	517	143	150	4		

- Molecule 3 is a protein called Caspase-9.

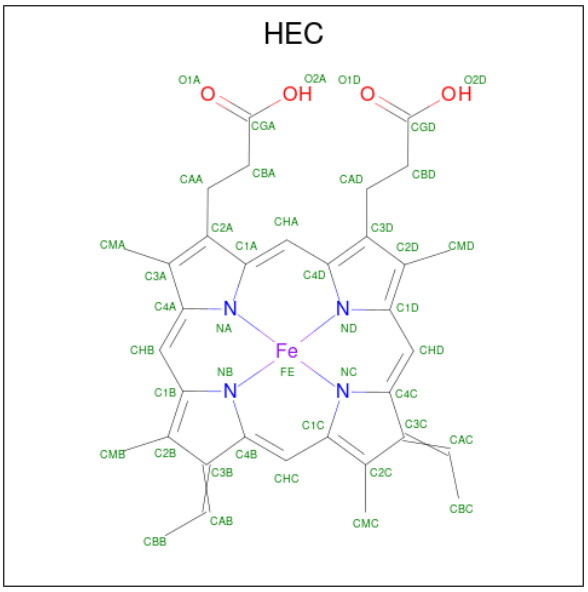
Mol	Chain	Residues	Atoms					AltConf	Trace
3	O	95	Total	C	N	O	S	0	0
			777	475	152	145	5		
3	P	95	Total	C	N	O	S	0	0
			777	475	152	145	5		
3	Q	95	Total	C	N	O	S	0	0
			777	475	152	145	5		
3	R	95	Total	C	N	O	S	0	0
			777	475	152	145	5		

- Molecule 4 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (CCD ID: DTP) (formula: $C_{10}H_{16}N_5O_{12}P_3$)



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			30	10	5	12	3	
4	B	1	Total	C	N	O	P	0
			30	10	5	12	3	
4	C	1	Total	C	N	O	P	0
			30	10	5	12	3	
4	D	1	Total	C	N	O	P	0
			30	10	5	12	3	
4	E	1	Total	C	N	O	P	0
			30	10	5	12	3	
4	F	1	Total	C	N	O	P	0
			30	10	5	12	3	
4	G	1	Total	C	N	O	P	0
			30	10	5	12	3	

- Molecule 5 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



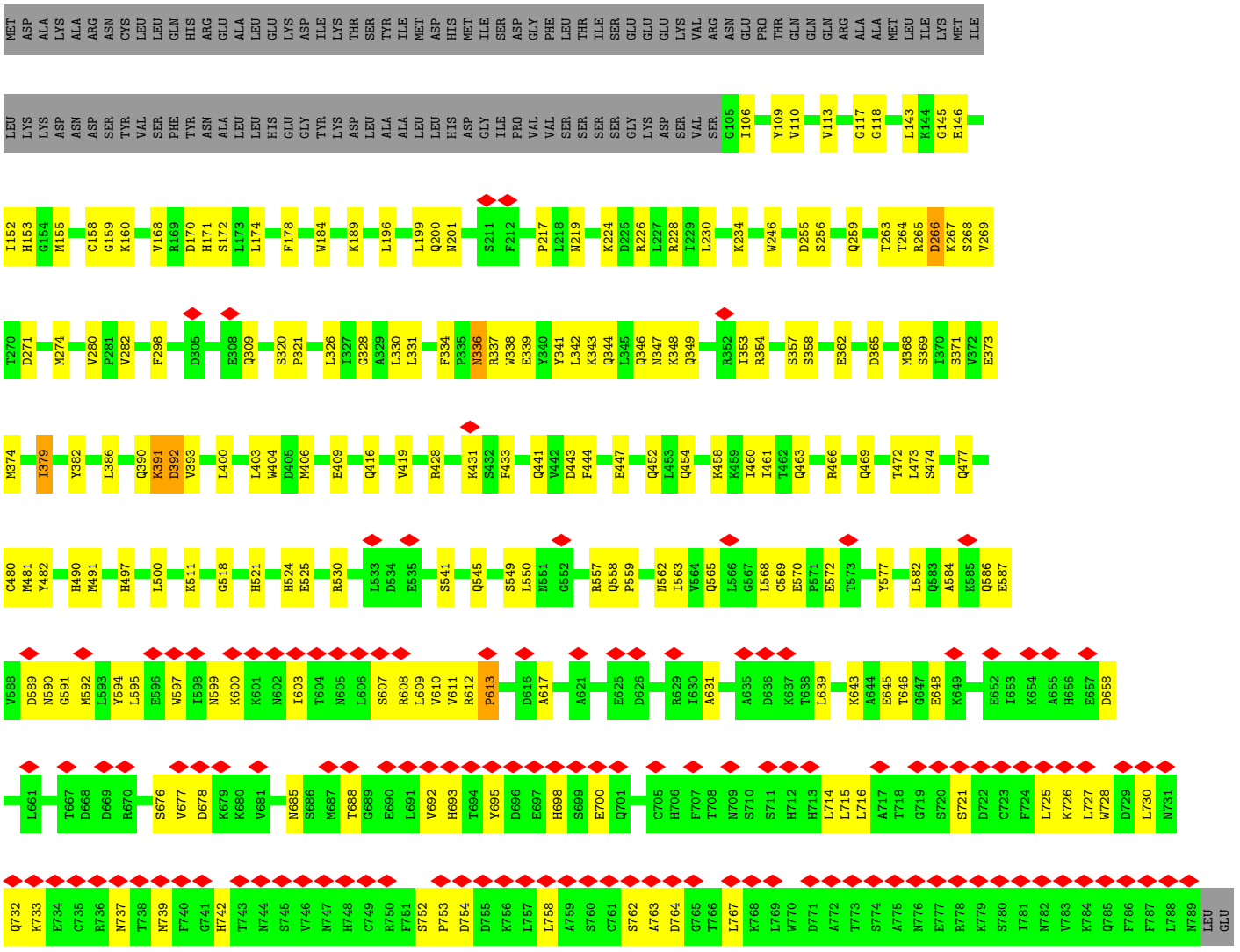
Mol	Chain	Residues	Atoms					AltConf
5	H	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
5	I	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
5	J	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
5	K	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
5	L	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
5	M	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
5	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

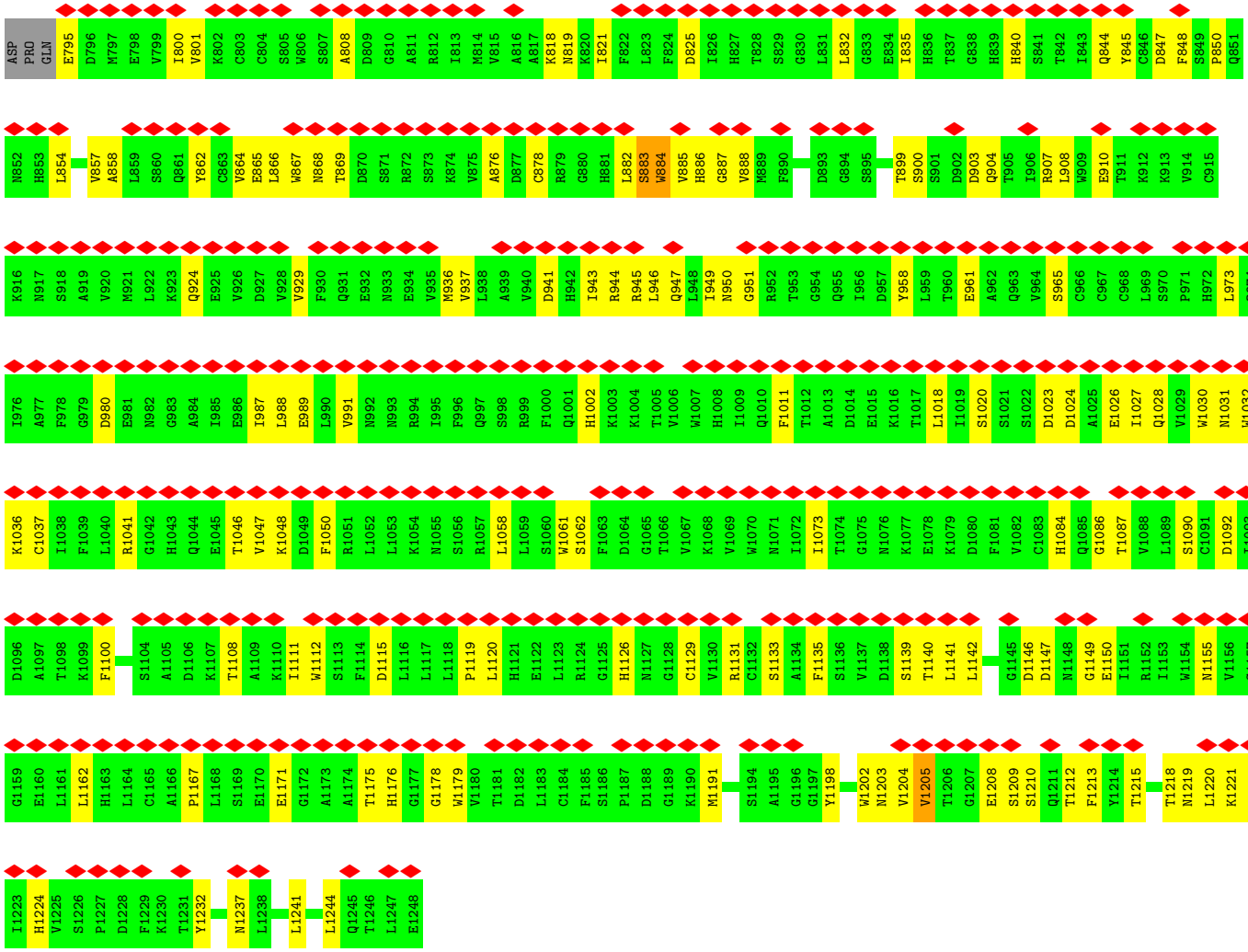
3 Residue-property plots (i)

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: Apoptotic protease-activating factor 1

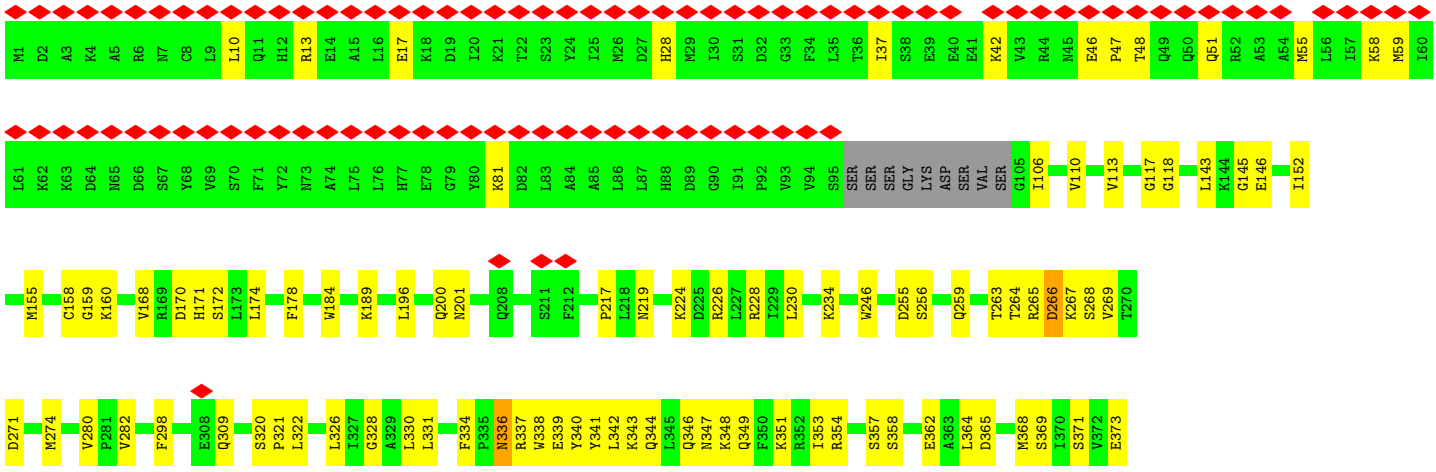
Chain A:

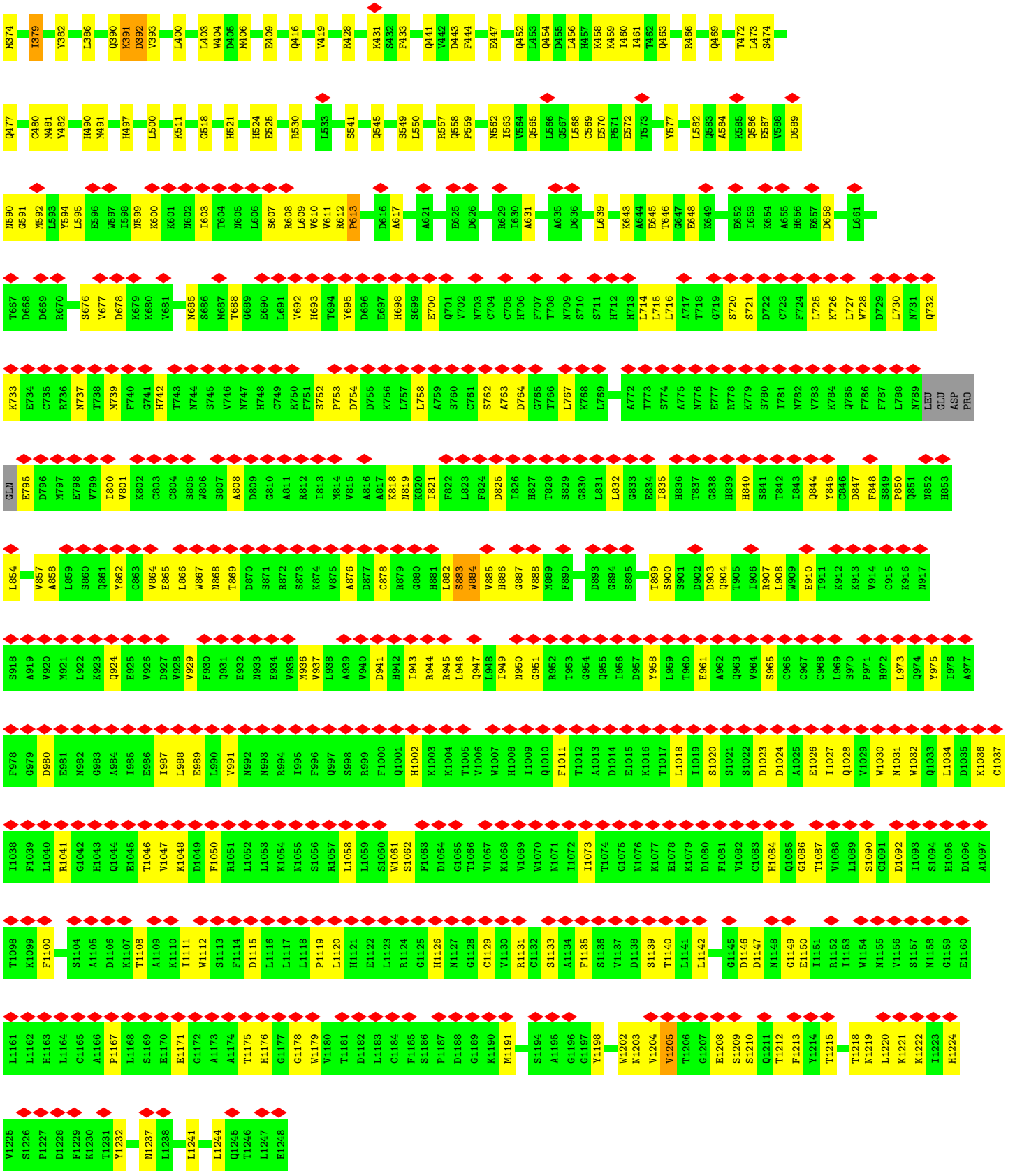




• Molecule 1: Apoptotic protease-activating factor 1

Chain B:

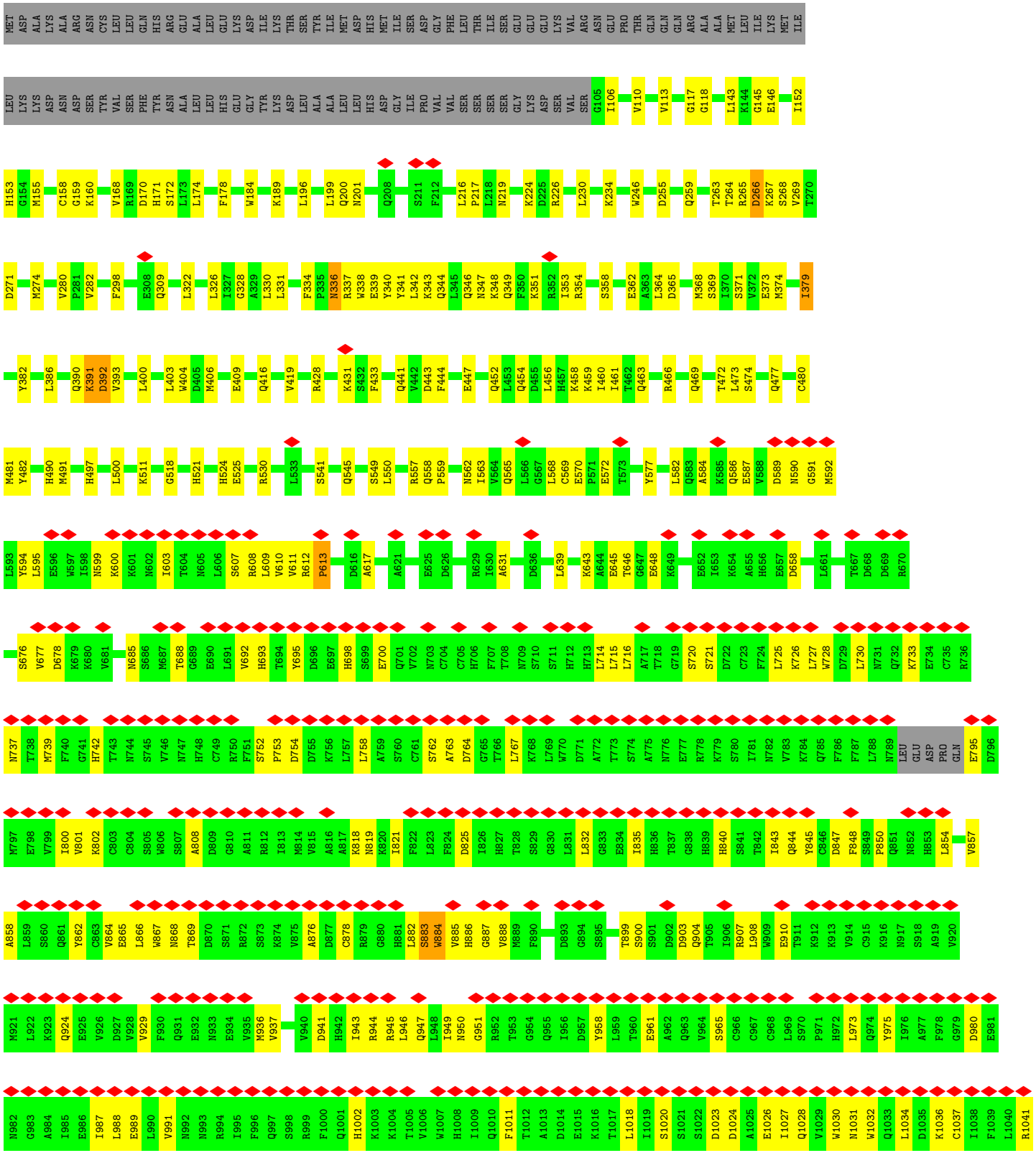


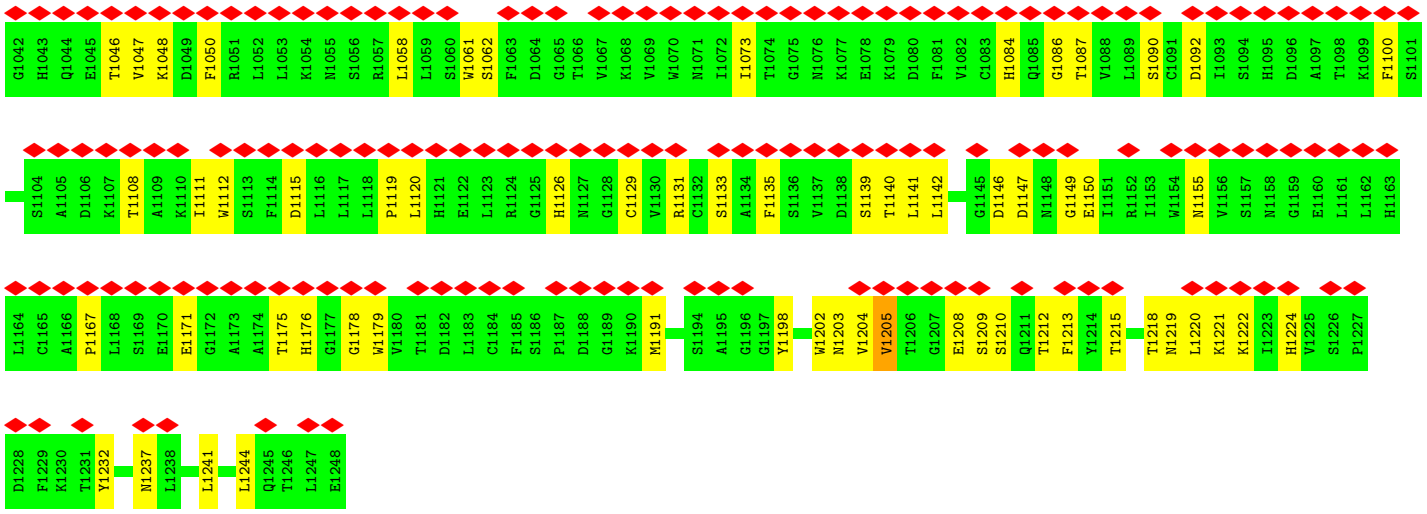


• Molecule 1: Apoptotic protease-activating factor 1

Chain C:

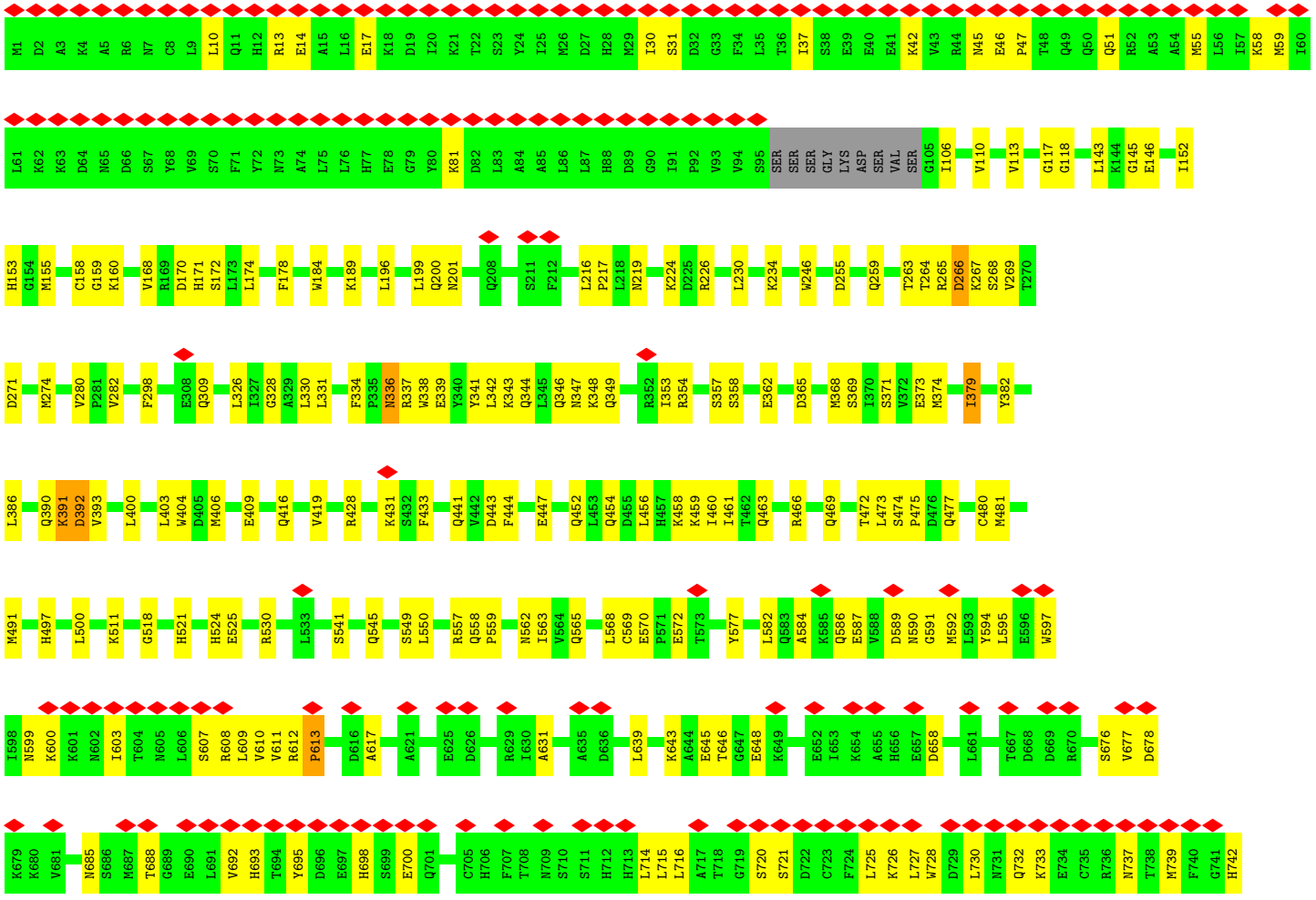
39%
63%
27%
9%

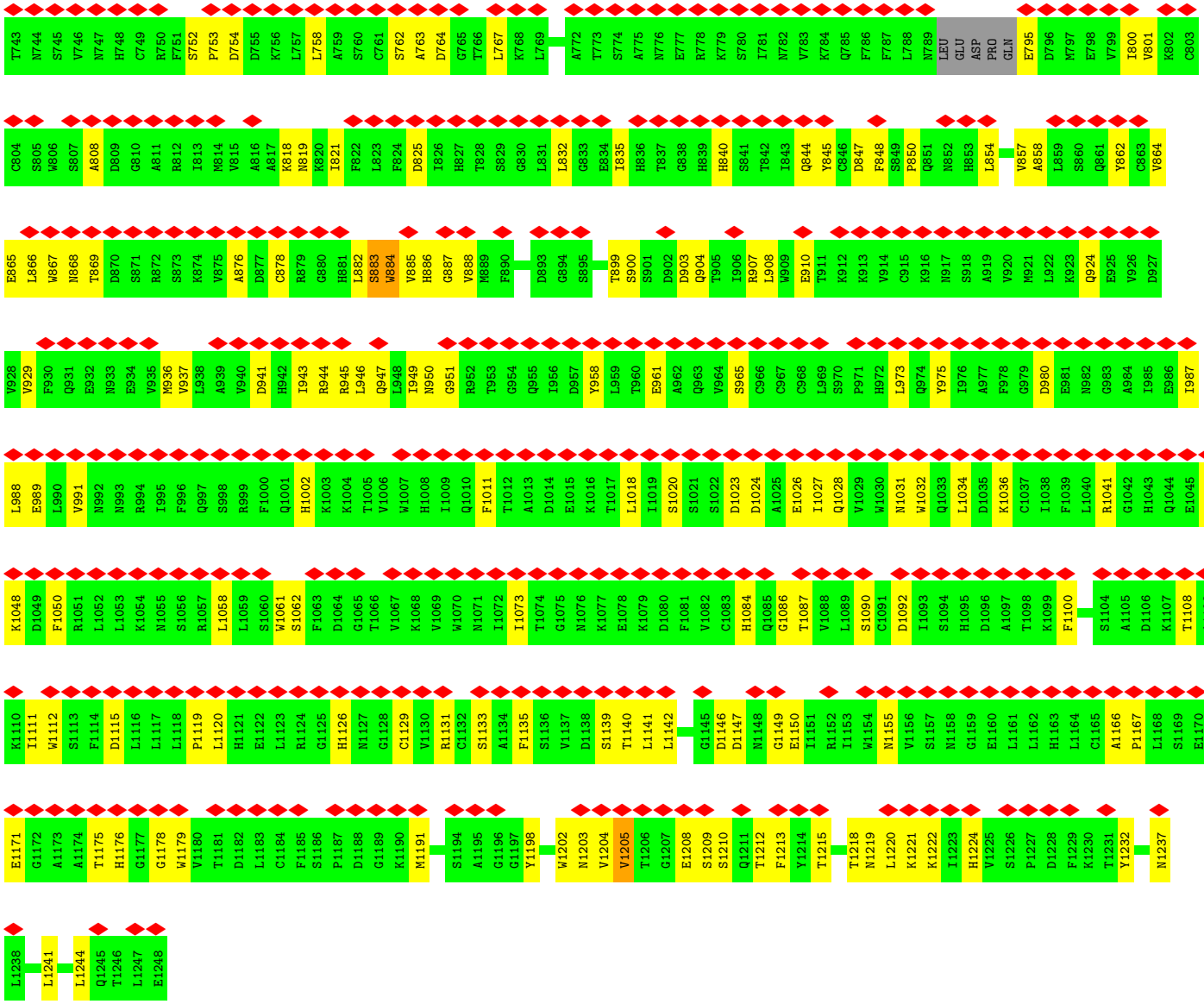

MET ASP ALA LYS ALA ARG ASN CYS LEU LEU GLN HIS ARG GLU ALA ALA LEU GLU LYS ASP ILE LYS THR SER TYR ILE MET ASP HIS MET ILE SER ASP GLY PHE LEU THR ILE SER GLU GLU GLU LYS VAL ARG ASN GLU PRO THR GLN GLN GLN ARG ALA ALA MET LEU ILE LYS MET ILE
LEU LYS LYS ASP ASN ASP SER TYR VAL SER PHE TYR ASN ALA LEU LEU HIS GLU GLY TYR LYS ASP LEU ALA ALA LEU LEU HIS ASP GLY ILE PRO VAL VAL SER SER SER SER GLY LYS ASP SER VAL SER G105 I106 V110 V113 G117 G118 L143 K144 G145 E146 I152
H153 G154 M155 C158 G159 K160 V168 R169 D170 H171 S172 L173 L174 F178 W184 K189 L196 L199 Q200 N201 Q208 S211 F212 L216 P217 L218 N219 K224 D225 R226 L230 K234 W246 D255 Q259 T263 T264 R265 D266 K267 S268 V269 T270
D271 M274 V280 P281 V282 F298 E308 Q309 L322 L326 I327 G328 A329 L330 L331 F334 P335 N336 R337 W338 E339 Y340 Y341 L342 K343 Q344 L345 Q346 N347 K348 Q349 F350 K351 R352 I353 R354 S358 E362 A363 L364 D365 M368 S369 I370 S371 V372 E373 M374 I379
Y382 L386 Q390 K391 D392 V393 L400 L403 W404 D405 M406 E409 Q416 V419 R428 K431 S432 F433 Q441 V442 D443 F444 E447 Q452 L453 Q454 D455 L456 H457 K458 K459 I460 I461 T462 Q463 R466 Q469 T472 L473 S474 Q477 C480
M481 Y482 H490 M491 H497 L500 K511 G518 H521 H524 E525 R530 L533 S541 Q545 S549 L550 R557 Q558 P559 N562 I563 V564 Q565 L566 G567 L568 C569 E570 F571 E572 T573 Y577 L582 Q583 A584 K585 Q586 E587 V588 D589 N590 G591 M592
L593 Y594 L595 E596 W597 I598 N599 K600 K601 N602 I603 T604 N605 L606 S607 R608 L609 V610 V611 R612 P613 D616 A617 A621 E625 D626 R629 I630 A631 D636 L639 K643 A644 E645 T646 G647 E648 K649 E652 I653 K654 A655 H656 E657 D658 L661 T667 D668 D669 R670
S676 V677 D678 K679 K680 V681 N685 S686 M687 T688 G689 E690 L691 V692 H693 T694 Y695 D696 E697 H698 S699 E700 Q701 V702 N703 C704 C705 H706 F707 T708 N709 S710 S711 H712 H713 L714 L715 L716 A717 T718 G719 S720 S721 D722 C723 F724 L725 K726 L727 W728 D729 L730 N731 Q732 K733 E734 C735 R736
N737 T738 M739 F740 G741 H742 T743 N744 S745 V746 N747 H748 C749 R750 F751 S752 P753 D754 D755 K756 L757 L758 A759 S760 C761 S762 A763 D764 G765 T766 L767 K768 L769 W770 D771 A772 T773 S774 A775 N776 E777 R778 K779 S780 I781 N782 V783 K784 Q785 F786 F787 L788 N789 LEU GLU ASP PRO GLN E795 D796
M797 E798 V799 I800 V801 K802 C803 C804 S805 W806 S807 A808 D809 G810 A811 R812 I813 N814 V815 A816 A817 K818 N819 K820 I821 F822 L823 F824 D825 I826 H827 T828 S829 G830 L831 L832 G833 E834 I835 H836 T837 G838 H839 H840 S841 T842 I843 Q844 Y845 C846 D847 F848 S849 P850 Q851 N852 H853 L854 V857
A858 L859 S860 Q861 Y862 C863 V864 E865 L866 W867 N868 T869 D870 S871 R872 S873 K874 V875 A876 D877 C878 R879 G880 H881 L882 S883 W884 V885 H886 G887 V888 M889 F890 D893 G894 S895 T899 S900 S901 D902 D903 Q904 T905 I906 R907 L908 W909 E910 T911 K912 K913 V914 C915 K916 N917 S918 A919 V920
M921 L922 K923 Q924 E925 V926 D927 V928 V929 F930 Q931 E932 N933 E934 V935 M936 V937 V940 D941 H942 I943 R944 R945 L946 Q947 L948 I949 N950 G951 R952 T953 G954 Q955 I956 D957 Y958 L959 T960 E961 A962 Q963 V964 S965 C966 C967 C968 L969 S970 P971 H972 L973 Q974 Y975 I976 A977 F978 G979 D980 E981
N982 G983 A984 I985 E986 I987 L988 E989 L990 V991 N992 N993 R994 I995 F996 Q997 S998 R999 F1000 Q1001 H1002 K1003 K1004 T1005 V1006 W1007 H1008 I1009 Q1010 F1011 T1012 A1013 D1014 E1015 K1016 T1017 L1018 L1019 S1020 S1021 S1022 D1023 D1024 A1025 E1026 I1027 Q1028 V1029 W1030 N1031 W1032 Q1033 L1034 D1035 K1036 C1037 I1038 F1039 L1040 R1041



• Molecule 1: Apoptotic protease-activating factor 1

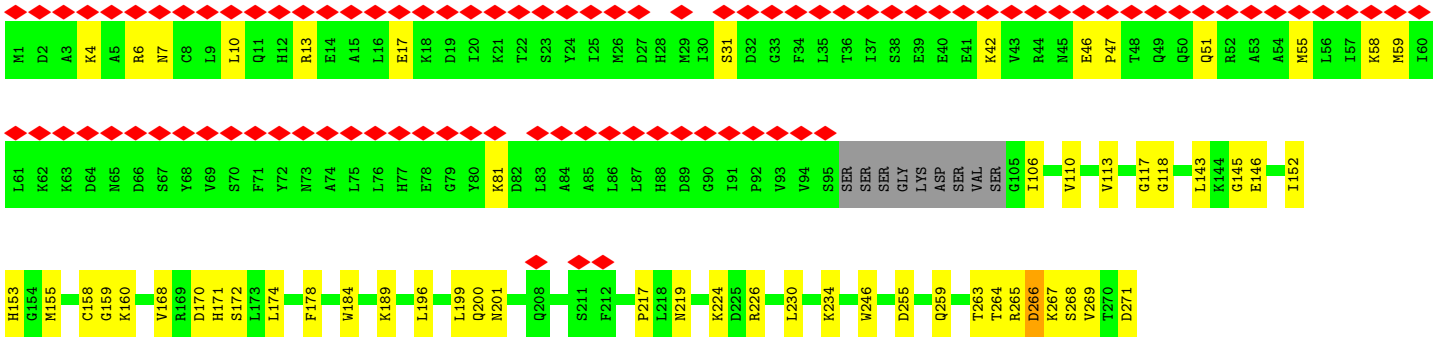
Chain D:

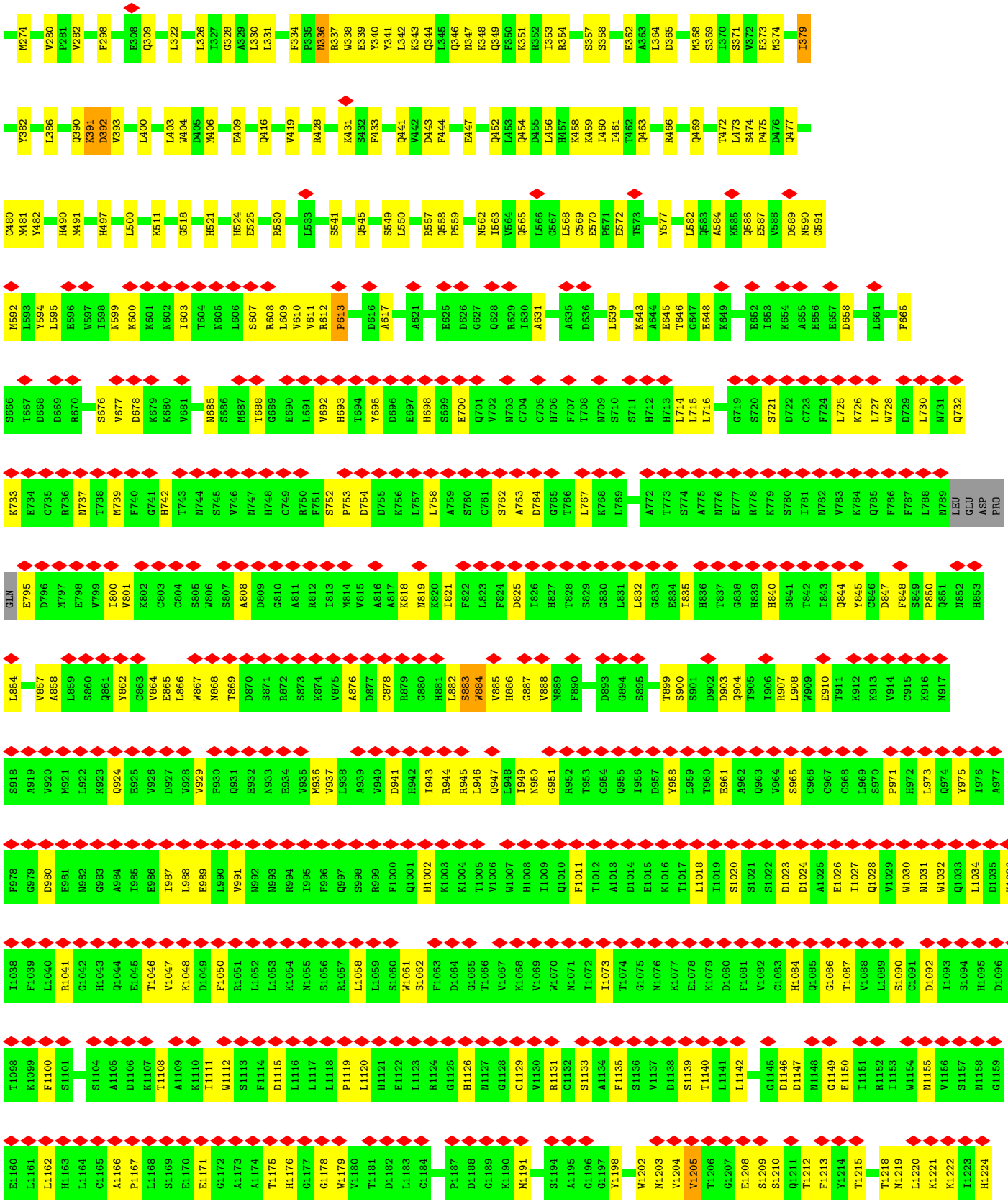




• Molecule 1: Apoptotic protease-activating factor 1

Chain E:

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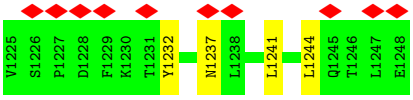
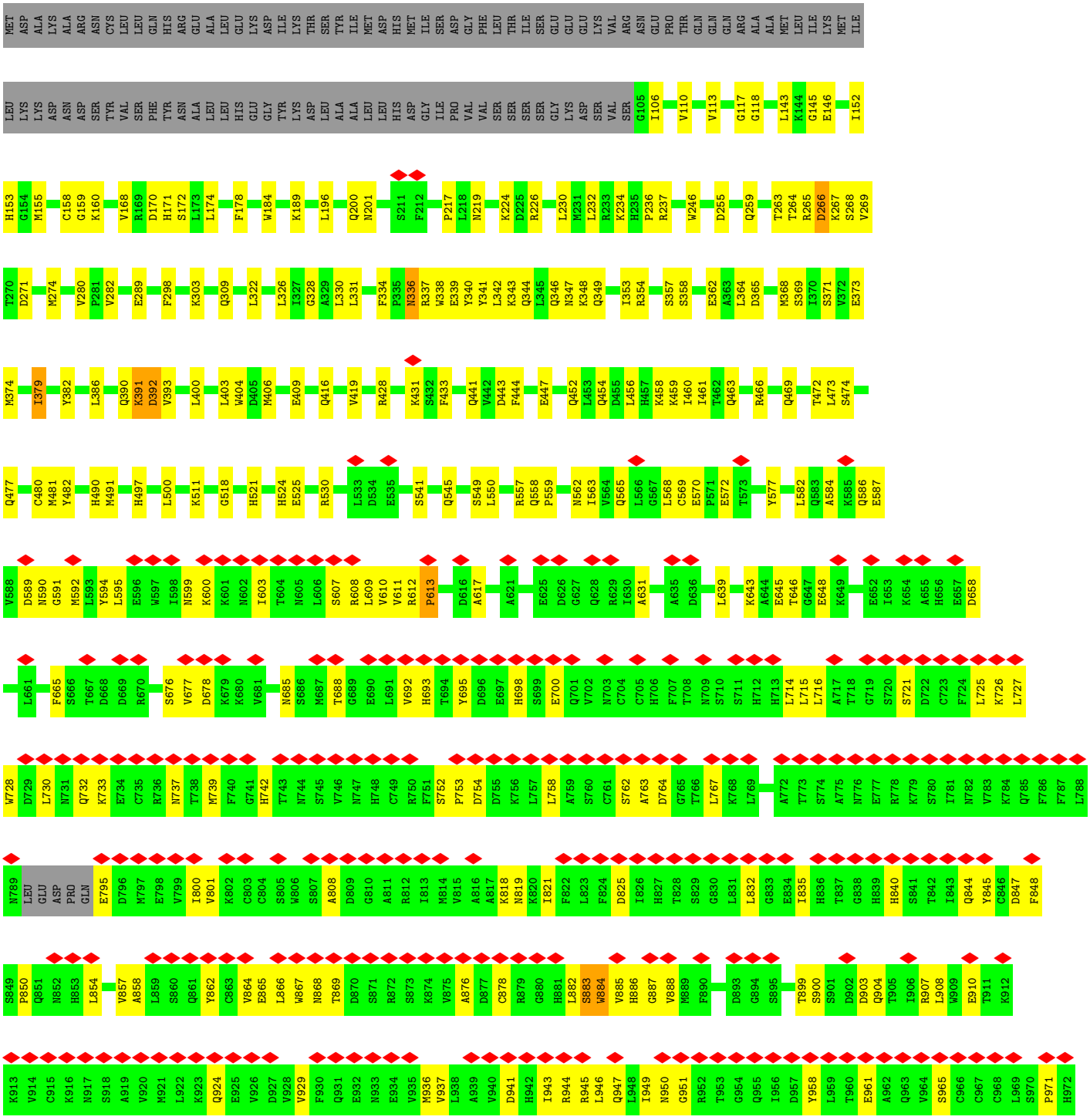
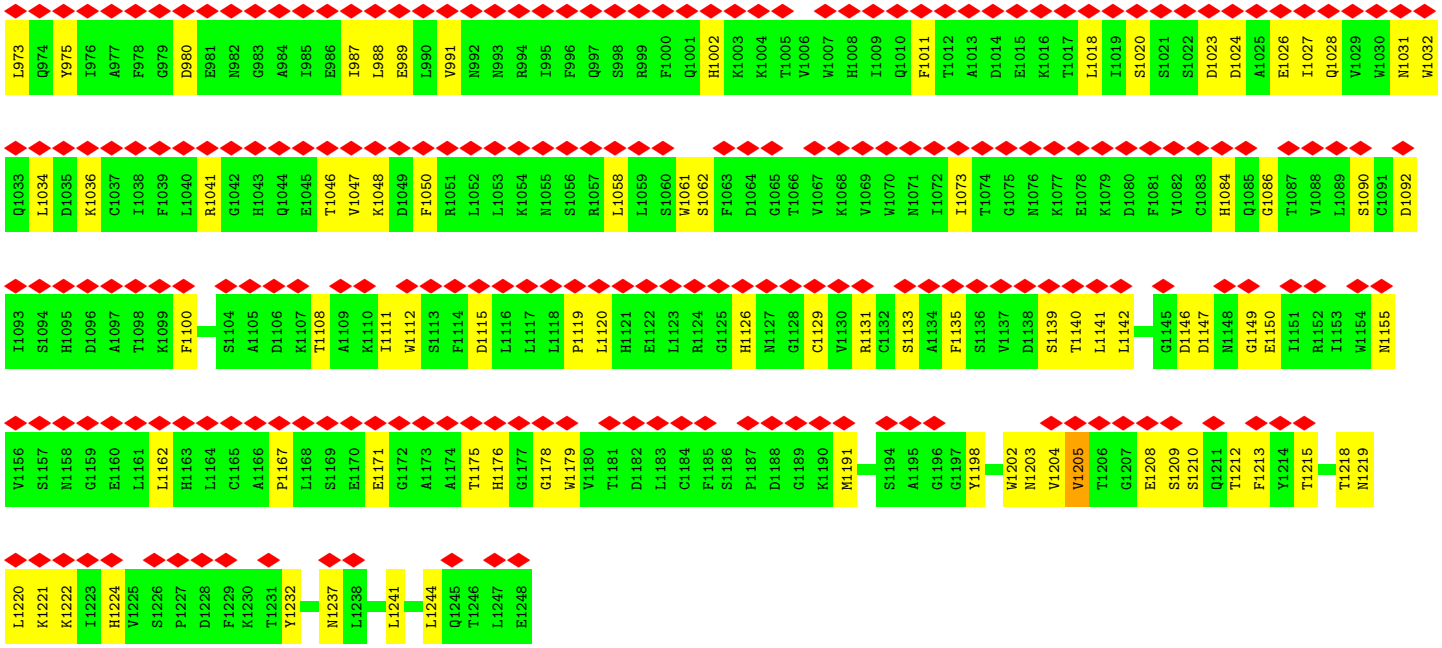
Y382 L386 Q390 K391 D392 V393 L400 L403 W404 D405 M406 E409 Q416 V419 R428 K431 S432 F433 Q441 V442 D443 F444 E447 Q452 L453 Q454 D455 L456 H457 K458 K459 I460 I461 T462 Q463 R466 Q469 T472 L473 S474 P475 D476 Q477
C480 M481 Y482 H490 M491 H497 L500 K511 G518 H521 H524 E525 R530 L533 S541 Q545 S549 L550 R557 Q558 P559 N562 I563 V564 Q565 L566 G567 L568 C569 E570 P571 E572 T573 Y577 L582 Q583 A584 K585 Q586 E587 V588 D589 N590 G591
M592 L593 Y594 L595 E596 W597 I598 N599 K600 K601 N602 I603 T604 N605 L606 S607 R608 L609 V610 V611 R612 P613 D616 A617 A621 E625 D626 G627 Q628 R629 I630 A631 A635 D636 L639 K643 A644 E645 T646 G647 E648 K649 E652 I653 K654 A655 H656 E657 D658 L661 F665
S666 T667 D668 D669 R670 S676 V677 D678 K679 K680 V681 N685 S686 M687 T688 G689 E690 L691 V692 H693 T694 Y695 D696 E697 H698 S699 E700 Q701 V702 N703 C704 C705 H706 F707 T708 N709 S710 S711 H712 H713 L714 L715 L716 G719 S720 S721 D722 C723 F724 L725 K726 L727 W728 D729 L730 N731 Q732
K733 E734 C735 R736 N737 T738 M739 F740 G741 H742 T743 N744 S745 V746 N747 H748 C749 R750 F751 S752 P753 D754 D755 K756 L757 L758 A759 S760 C761 S762 A763 D764 G765 T766 L767 K768 L769 A772 T773 S774 A775 N776 E777 R778 K779 S780 I781 N782 V783 K784 Q785 F786 F787 L788 N789 LEU GLU ASP PRO
GLN E795 D796 M797 E798 V799 I800 V801 K802 C803 C804 S805 W806 S807 A808 D809 C810 A811 R812 I813 M814 V815 A816 A817 K818 N819 K820 I821 F822 L823 F824 D825 I826 H827 T828 S829 G830 L831 L832 G833 E834 I835 H836 T837 G838 H839 H840 S841 T842 I843 Q844 Y845 C846 D847 F848 S849 P850 Q851 N852 H853
L854 V857 A858 L859 S860 Q861 Y862 C863 V864 E865 L866 W867 N868 T869 D870 S871 R872 S873 K874 V875 A876 D877 C878 R879 G880 H881 L882 S883 W884 V885 H886 G887 V888 M889 F890 D893 G894 S895 T899 S900 S901 D902 D903 Q904 T905 I906 R907 L908 W909 E910 T911 K912 K913 V914 C915 K916 N917
S918 A919 V920 M921 L922 K923 Q924 E925 V926 D927 V928 V929 F930 Q931 E932 N933 E934 V935 M936 V937 L938 A939 V940 D941 H942 I943 R944 R945 L946 Q947 L948 I949 N950 G951 R952 T953 G954 Q955 I956 D957 Y958 L959 T960 E961 A962 Q963 V964 S965 C966 C967 C968 L969 S970 P971 H972 L973 Q974 Y975 I976 A977
F978 G979 D980 E981 N982 G983 A984 I985 E986 I987 L988 E989 L990 V991 N992 N993 R994 I995 F996 Q997 S998 R999 F1000 Q1001 H1002 K1003 K1004 T1005 V1006 W1007 H1008 I1009 Q1010 F1011 T1012 A1013 D1014 E1015 K1016 T1017 L1018 I1019 S1020 S1021 S1022 D1023 D1024 A1025 E1026 I1027 Q1028 V1029 W1030 N1031 W1032 Q1033 L1034 D1035 K1036 C1037
I1038 F1039 L1040 R1041 G1042 H1043 Q1044 E1045 T1046 V1047 K1048 D1049 F1050 R1051 L1052 L1053 K1054 N1055 S1056 R1057 L1058 L1059 S1060 W1061 S1062 F1063 D1064 G1065 T1066 V1067 K1068 V1069 W1070 N1071 I1072 I1073 T1074 G1075 N1076 K1077 E1078 K1079 D1080 F1081 V1082 C1083 H1084 Q1085 G1086 T1087 V1088 L1089 S1090 C1091 D1092 I1093 S1094 H1095 D1096 A1097
T1098 K1099 F1100 S1101 S1104 A1105 D1106 K1107 T1108 A1109 K1110 I1111 W1112 S1113 F1114 D1115 L1116 L1117 L1118 P1119 L1120 H1121 E1122 L1123 R1124 G1125 H1126 N1127 G1128 C1129 V1130 R1131 C1132 S1133 A1134 F1135 S1136 V1137 D1138 S1139 T1140 L1141 L1142 G1145 D1146 D1147 N1148 G1149 E1150 I1151 R1152 I1153 W1154 N1155 V1156 S1157 N1158 G1159
E1160 L1161 L1162 H1163 L1164 C1165 A1166 P1167 L1168 S1169 E1170 E1171 G1172 A1173 A1174 T1175 H1176 G1177 G1178 W1179 V1180 T1181 D1182 L1183 C1184 P1187 D1188 G1189 K1190 M1191 S1194 A1195 G1196 G1197 Y1198 W1202 N1203 V1204 V1205 T1206 G1207 E1208 S1209 S1210 Q1211 T1212 F1213 Y1214 T1215 T1218 N1219 L1220 K1221 K1222 I1223 H1224



• Molecule 1: Apoptotic protease-activating factor 1

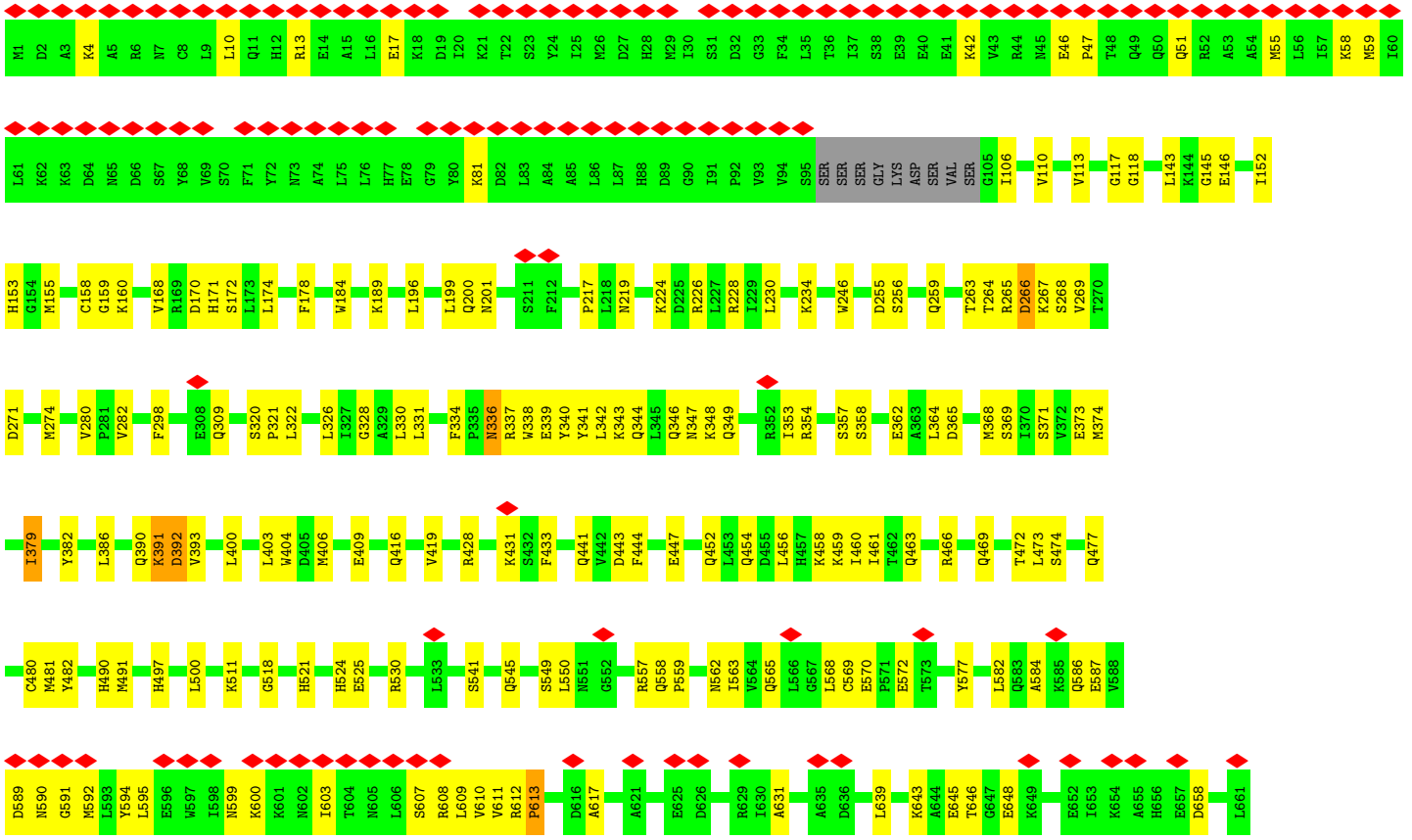
Chain F:

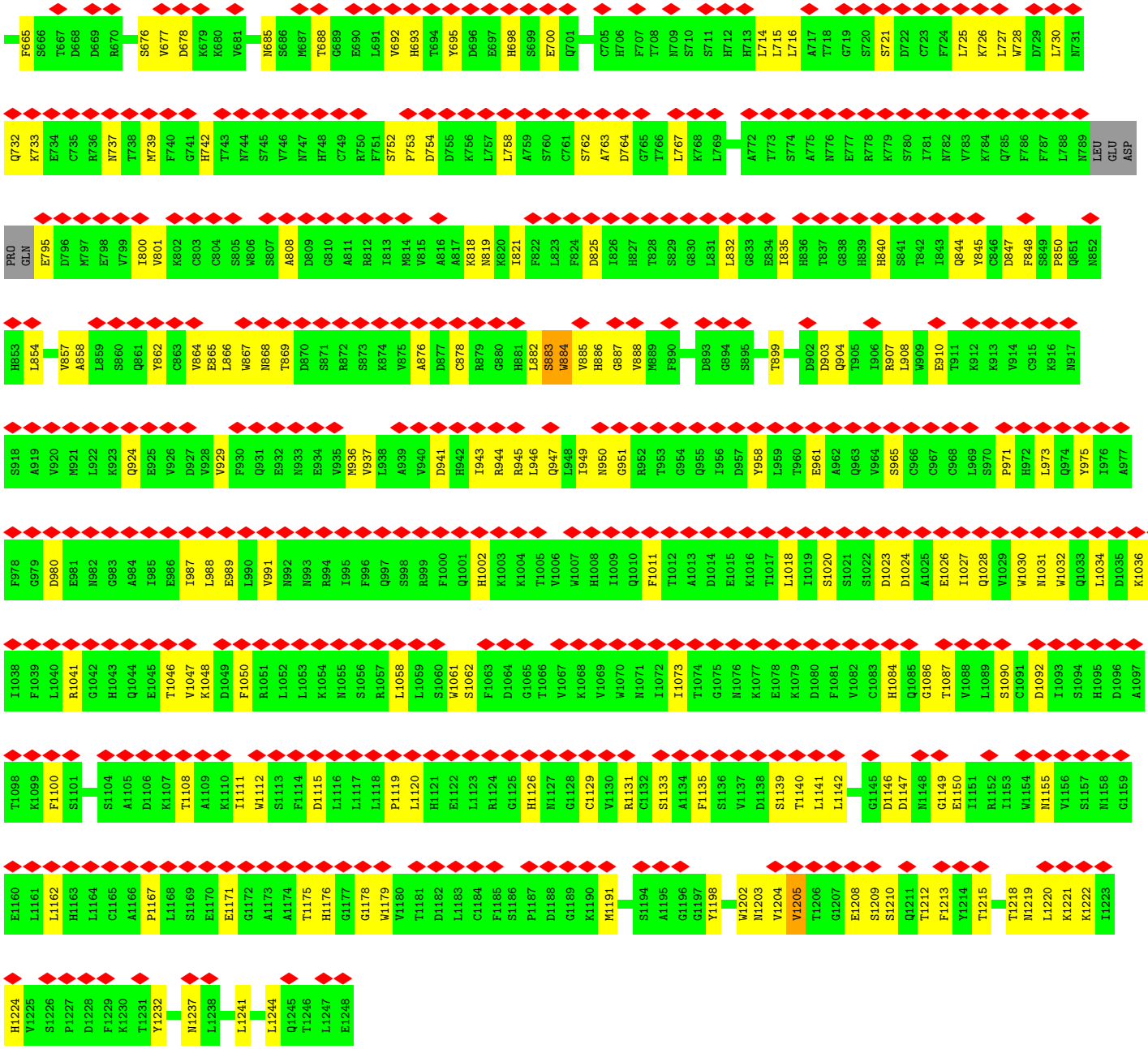




• Molecule 1: Apoptotic protease-activating factor 1

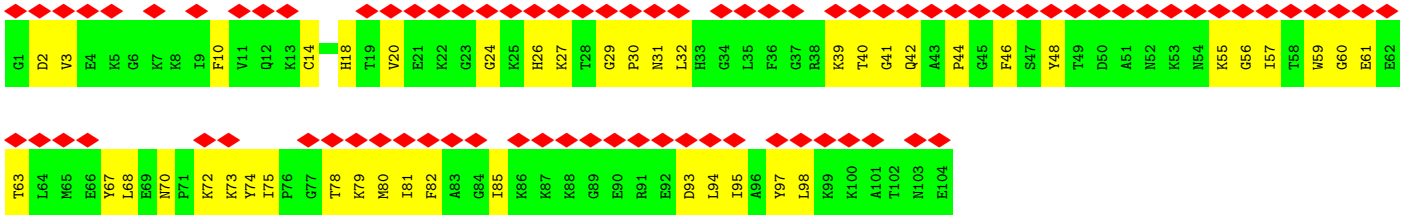
Chain G:





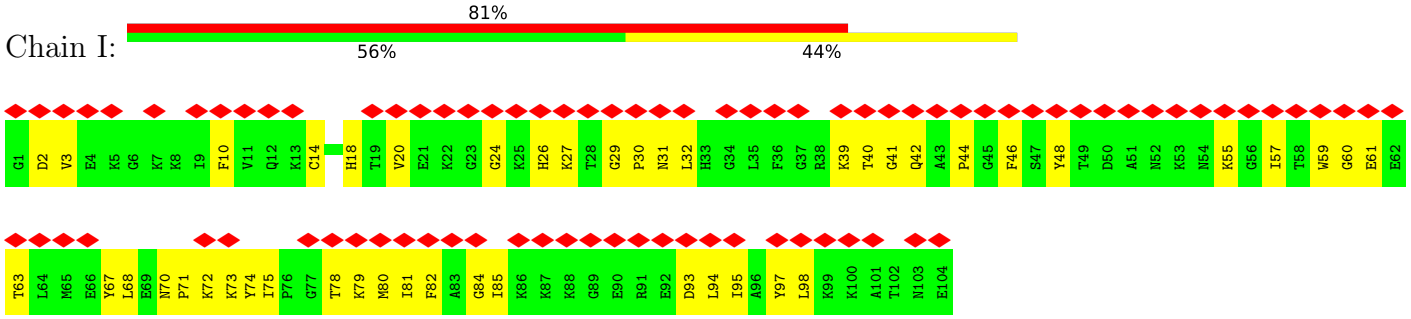
• Molecule 2: Cytochrome c

Chain H:



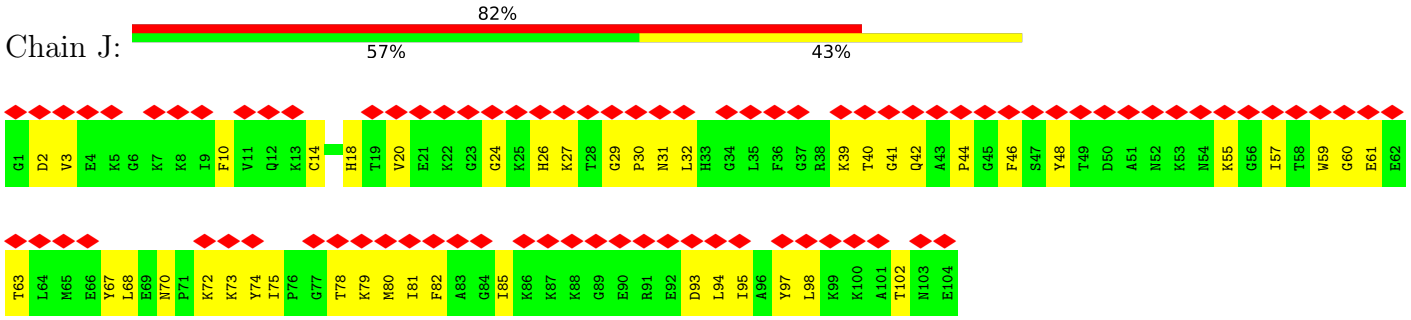
• Molecule 2: Cytochrome c

Chain I:



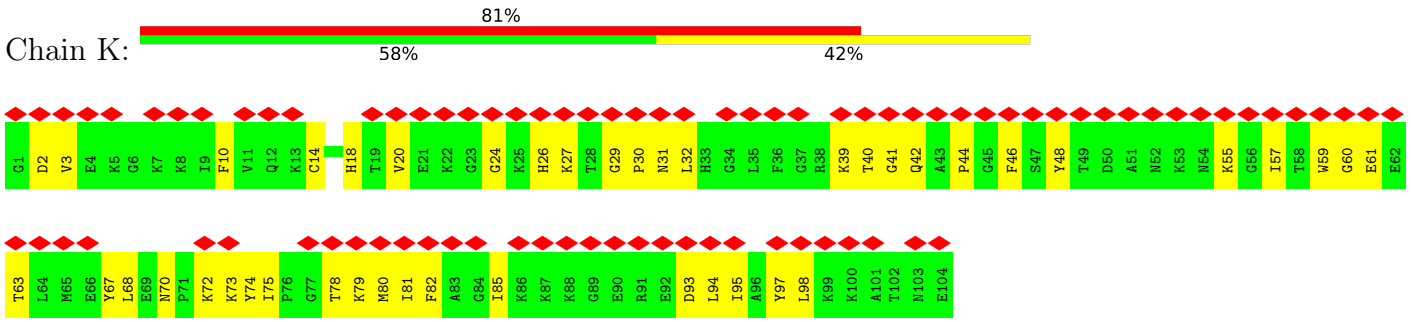
• Molecule 2: Cytochrome c

Chain J:



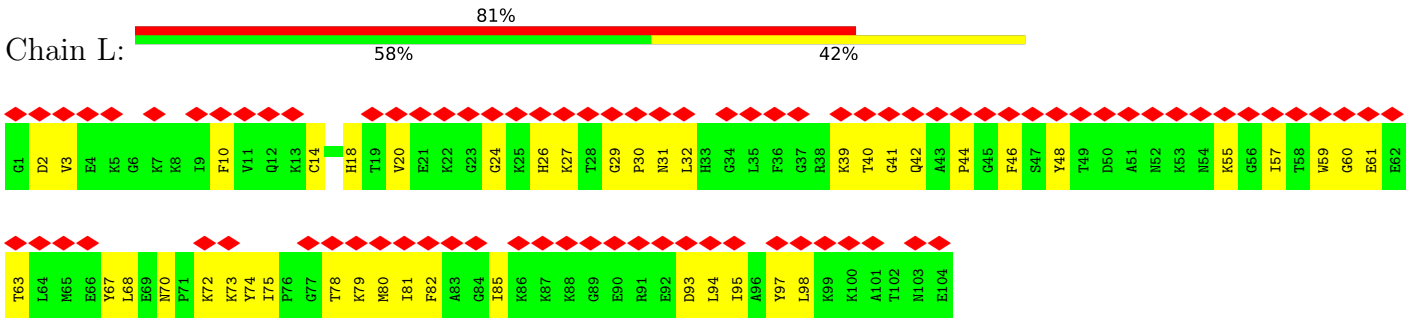
• Molecule 2: Cytochrome c

Chain K:



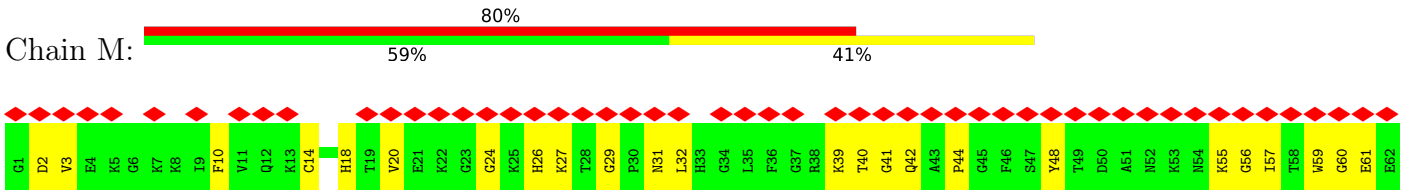
• Molecule 2: Cytochrome c

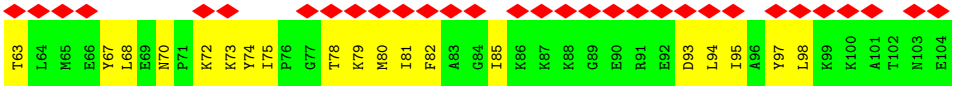
Chain L:



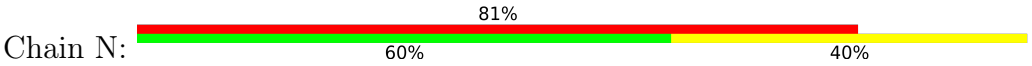
• Molecule 2: Cytochrome c

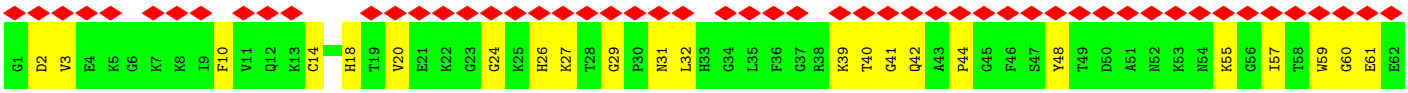
Chain M:

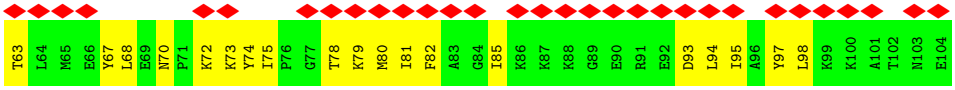




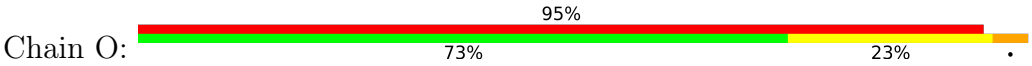
• Molecule 2: Cytochrome c

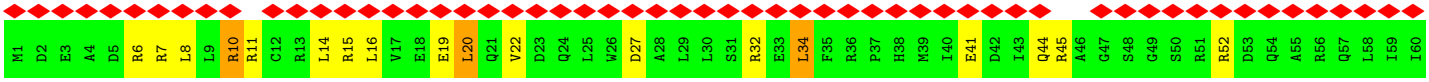




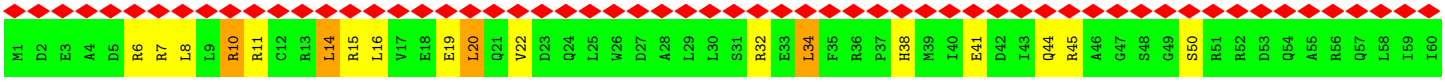


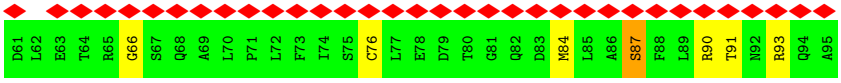
• Molecule 3: Caspase-9



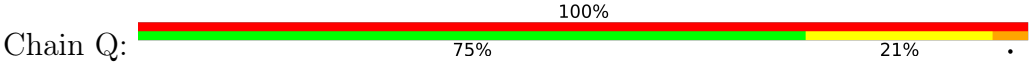


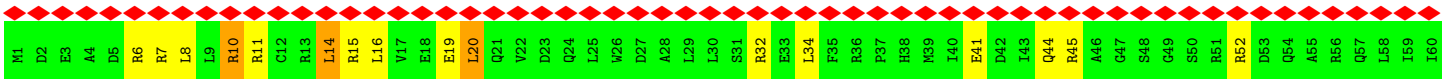
• Molecule 3: Caspase-9

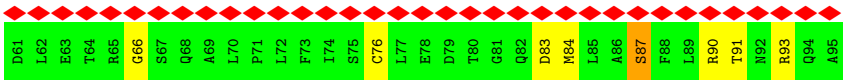




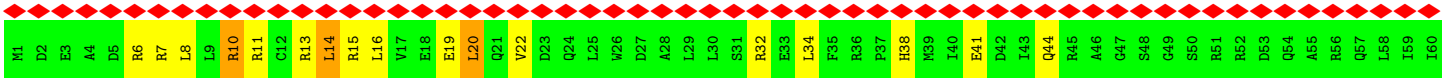
• Molecule 3: Caspase-9







• Molecule 3: Caspase-9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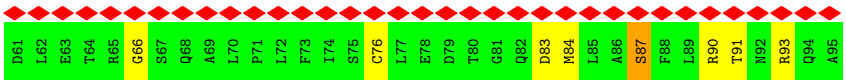
D61 L62 E63 T64 R65 G66 S67 Q68 A69 L70 P71 L72 F73 I74 S75 C76 L77 E78 D79 T80 G81 Q82 D83 M84 L85 A86 S87 F88 L89 R90 T91 N92 R93 Q94 A95

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C7	Depositor
Number of particles used	92867	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 ($e^-/Å^2$)	1.8	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	81000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.198	Depositor
Minimum map value	-0.084	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	437.76, 437.76, 437.76	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.368, 1.368, 1.368	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.42	1/9295 (0.0%)	0.80	14/12575 (0.1%)
1	B	0.49	1/10068 (0.0%)	0.80	14/13613 (0.1%)
1	C	0.42	1/9295 (0.0%)	0.80	14/12575 (0.1%)
1	D	0.48	1/10068 (0.0%)	0.80	14/13613 (0.1%)
1	E	0.49	1/10068 (0.0%)	0.80	14/13613 (0.1%)
1	F	0.42	1/9295 (0.0%)	0.80	14/12575 (0.1%)
1	G	0.49	1/10068 (0.0%)	0.80	14/13613 (0.1%)
2	H	0.31	0/830	0.73	0/1105
2	I	0.31	0/830	0.73	0/1105
2	J	0.31	0/830	0.73	0/1105
2	K	0.31	0/830	0.73	0/1105
2	L	0.31	0/830	0.73	0/1105
2	M	0.31	0/830	0.73	0/1105
2	N	0.31	0/830	0.73	0/1105
3	O	0.87	0/784	0.88	2/1051 (0.2%)
3	P	0.87	0/784	0.88	2/1051 (0.2%)
3	Q	0.87	0/784	0.88	1/1051 (0.1%)
3	R	0.87	0/784	0.88	2/1051 (0.2%)
All	All	0.47	7/77103 (0.0%)	0.80	105/104116 (0.1%)

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
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1
1	G	0	1
All	All	0	7

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	168	VAL	C-N	11.07	1.50	1.33
1	B	168	VAL	C-N	11.04	1.50	1.33
1	A	168	VAL	C-N	11.04	1.50	1.33
1	E	168	VAL	C-N	11.04	1.50	1.33
1	D	168	VAL	C-N	11.02	1.50	1.33
1	G	168	VAL	C-N	11.00	1.50	1.33
1	C	168	VAL	C-N	10.99	1.50	1.33

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	178	PHE	CA-C-N	-8.62	112.95	121.65
1	G	178	PHE	C-N-CA	-8.62	112.95	121.65
1	E	178	PHE	CA-C-N	-8.60	112.97	121.65
1	E	178	PHE	C-N-CA	-8.60	112.97	121.65
1	B	178	PHE	CA-C-N	-8.58	112.98	121.65
1	B	178	PHE	C-N-CA	-8.58	112.98	121.65
1	A	178	PHE	CA-C-N	-8.55	113.01	121.65
1	A	178	PHE	C-N-CA	-8.55	113.01	121.65
1	C	178	PHE	CA-C-N	-8.54	113.02	121.65
1	C	178	PHE	C-N-CA	-8.54	113.02	121.65
1	F	178	PHE	CA-C-N	-8.54	113.03	121.65
1	F	178	PHE	C-N-CA	-8.54	113.03	121.65
1	D	178	PHE	CA-C-N	-8.52	113.04	121.65
1	D	178	PHE	C-N-CA	-8.52	113.04	121.65
1	G	146	GLU	CA-C-N	-8.40	111.37	119.85
1	G	146	GLU	C-N-CA	-8.40	111.37	119.85
1	F	146	GLU	CA-C-N	-8.39	111.38	119.85
1	F	146	GLU	C-N-CA	-8.39	111.38	119.85
1	E	146	GLU	CA-C-N	-8.38	111.38	119.85
1	E	146	GLU	C-N-CA	-8.38	111.38	119.85
1	B	146	GLU	CA-C-N	-8.34	111.42	119.85
1	B	146	GLU	C-N-CA	-8.34	111.42	119.85
1	A	146	GLU	CA-C-N	-8.34	111.43	119.85
1	A	146	GLU	C-N-CA	-8.34	111.43	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	146	GLU	CA-C-N	-8.30	111.46	119.85
1	C	146	GLU	C-N-CA	-8.30	111.46	119.85
1	D	146	GLU	CA-C-N	-8.29	111.48	119.85
1	D	146	GLU	C-N-CA	-8.29	111.48	119.85
1	D	117	GLY	N-CA-C	-6.58	105.44	114.64
1	C	117	GLY	N-CA-C	-6.57	105.44	114.64
1	G	117	GLY	N-CA-C	-6.57	105.44	114.64
1	A	117	GLY	N-CA-C	-6.56	105.45	114.64
1	B	117	GLY	N-CA-C	-6.55	105.47	114.64
1	E	117	GLY	N-CA-C	-6.55	105.47	114.64
1	F	117	GLY	N-CA-C	-6.54	105.48	114.64
1	E	883	SER	N-CA-C	6.28	118.49	109.14
1	G	883	SER	N-CA-C	6.26	118.47	109.14
1	D	883	SER	N-CA-C	6.25	118.46	109.14
1	A	883	SER	N-CA-C	6.25	118.45	109.14
1	B	883	SER	N-CA-C	6.25	118.45	109.14
1	C	883	SER	N-CA-C	6.23	118.43	109.14
1	F	883	SER	N-CA-C	6.22	118.41	109.14
1	F	518	GLY	CA-C-N	6.20	125.61	118.85
1	F	518	GLY	C-N-CA	6.20	125.61	118.85
1	E	518	GLY	CA-C-N	6.20	125.61	118.85
1	E	518	GLY	C-N-CA	6.20	125.61	118.85
1	D	518	GLY	CA-C-N	6.19	125.60	118.85
1	D	518	GLY	C-N-CA	6.19	125.60	118.85
1	G	518	GLY	CA-C-N	6.18	125.58	118.85
1	G	518	GLY	C-N-CA	6.18	125.58	118.85
1	A	518	GLY	CA-C-N	6.17	125.58	118.85
1	A	518	GLY	C-N-CA	6.17	125.58	118.85
1	B	518	GLY	CA-C-N	6.14	125.54	118.85
1	B	518	GLY	C-N-CA	6.14	125.54	118.85
1	C	518	GLY	CA-C-N	6.14	125.54	118.85
1	C	518	GLY	C-N-CA	6.14	125.54	118.85
1	C	246	TRP	N-CA-C	6.01	119.09	111.69
1	F	246	TRP	N-CA-C	6.01	119.09	111.69
1	B	246	TRP	N-CA-C	6.00	119.07	111.69
1	A	246	TRP	N-CA-C	5.99	119.05	111.69
1	D	246	TRP	N-CA-C	5.99	119.05	111.69
1	G	246	TRP	N-CA-C	5.97	119.03	111.69
1	E	246	TRP	N-CA-C	5.97	119.03	111.69
3	R	66	GLY	N-CA-C	5.65	117.84	111.85
1	D	168	VAL	O-C-N	-5.64	115.52	122.57
1	C	886	HIS	N-CA-C	-5.64	105.21	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	886	HIS	N-CA-C	-5.64	105.22	111.36
1	A	886	HIS	N-CA-C	-5.63	105.23	111.36
1	F	886	HIS	N-CA-C	-5.63	105.23	111.36
1	A	168	VAL	O-C-N	-5.62	115.55	122.57
1	E	168	VAL	O-C-N	-5.62	115.55	122.57
1	F	168	VAL	O-C-N	-5.62	115.55	122.57
1	E	886	HIS	N-CA-C	-5.62	105.24	111.36
1	B	168	VAL	O-C-N	-5.62	115.55	122.57
1	B	886	HIS	N-CA-C	-5.62	105.24	111.36
1	G	168	VAL	O-C-N	-5.62	115.55	122.57
3	O	66	GLY	N-CA-C	5.60	117.79	111.85
1	C	168	VAL	O-C-N	-5.59	115.58	122.57
1	D	886	HIS	N-CA-C	-5.58	105.27	111.36
3	Q	66	GLY	N-CA-C	5.57	117.76	111.85
3	P	66	GLY	N-CA-C	5.54	117.72	111.85
1	G	589	ASP	N-CA-C	-5.30	105.45	112.24
1	F	589	ASP	N-CA-C	-5.29	105.46	112.24
1	B	589	ASP	N-CA-C	-5.29	105.46	112.24
1	C	589	ASP	N-CA-C	-5.29	105.47	112.24
1	A	589	ASP	N-CA-C	-5.29	105.47	112.24
1	E	589	ASP	N-CA-C	-5.29	105.47	112.24
1	D	589	ASP	N-CA-C	-5.26	105.51	112.24
3	O	22	VAL	N-CA-C	5.23	116.31	111.81
3	R	22	VAL	N-CA-C	5.23	116.31	111.81
3	P	22	VAL	N-CA-C	5.18	116.27	111.81
1	G	379	ILE	CA-C-N	5.13	127.87	120.38
1	G	379	ILE	C-N-CA	5.13	127.87	120.38
1	D	379	ILE	CA-C-N	5.13	127.86	120.38
1	D	379	ILE	C-N-CA	5.13	127.86	120.38
1	E	379	ILE	CA-C-N	5.12	127.86	120.38
1	E	379	ILE	C-N-CA	5.12	127.86	120.38
1	A	379	ILE	CA-C-N	5.12	127.85	120.38
1	A	379	ILE	C-N-CA	5.12	127.85	120.38
1	C	379	ILE	CA-C-N	5.11	127.84	120.38
1	C	379	ILE	C-N-CA	5.11	127.84	120.38
1	B	379	ILE	CA-C-N	5.11	127.84	120.38
1	B	379	ILE	C-N-CA	5.11	127.84	120.38
1	F	379	ILE	CA-C-N	5.10	127.83	120.38
1	F	379	ILE	C-N-CA	5.10	127.83	120.38

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	336	ASN	Peptide
1	B	336	ASN	Peptide
1	C	336	ASN	Peptide
1	D	336	ASN	Peptide
1	E	336	ASN	Peptide
1	F	336	ASN	Peptide
1	G	336	ASN	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	9099	0	8967	309	0
1	B	9861	0	9736	317	0
1	C	9099	0	8968	306	0
1	D	9861	0	9736	324	0
1	E	9861	0	9736	329	0
1	F	9099	0	8968	317	0
1	G	9861	0	9736	319	0
2	H	814	0	833	58	0
2	I	814	0	833	58	0
2	J	814	0	833	59	0
2	K	814	0	833	56	0
2	L	814	0	833	57	0
2	M	814	0	833	58	0
2	N	814	0	833	55	0
3	O	777	0	787	21	0
3	P	777	0	787	28	0
3	Q	777	0	786	39	0
3	R	777	0	787	29	0
4	A	30	0	9	3	0
4	B	30	0	9	3	0
4	C	30	0	9	3	0
4	D	30	0	9	3	0
4	E	30	0	9	3	0
4	F	30	0	9	3	0
4	G	30	0	9	3	0
5	H	43	0	32	2	0
5	I	43	0	32	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	J	43	0	32	2	0
5	K	43	0	32	2	0
5	L	43	0	32	2	0
5	M	43	0	32	2	0
5	N	43	0	32	2	0
All	All	76058	0	75112	2427	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 16.

All (2427) 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:Q:52:ARG:HD3	3:R:38:HIS:CE1	1.20	1.66
3:Q:52:ARG:CD	3:R:38:HIS:CE1	2.01	1.40
1:E:884:TRP:CH2	2:L:79:LYS:HA	1.68	1.28
1:D:884:TRP:CH2	2:K:79:LYS:HA	1.68	1.28
1:G:884:TRP:CH2	2:N:79:LYS:HA	1.68	1.28
1:A:884:TRP:CH2	2:H:79:LYS:HA	1.68	1.27
1:E:7:ASN:HB2	1:F:236:PRO:CG	1.63	1.26
1:C:884:TRP:CH2	2:J:79:LYS:HA	1.68	1.26
1:F:884:TRP:CH2	2:M:79:LYS:HA	1.68	1.26
1:B:884:TRP:CH2	2:I:79:LYS:HA	1.68	1.26
1:C:884:TRP:CZ3	2:J:79:LYS:HD2	1.74	1.22
1:B:884:TRP:CZ3	2:I:79:LYS:HD2	1.74	1.22
1:D:884:TRP:CZ3	2:K:79:LYS:HD2	1.74	1.21
1:A:884:TRP:CZ3	2:H:79:LYS:HD2	1.74	1.21
1:E:884:TRP:CZ3	2:L:79:LYS:HD2	1.74	1.21
1:F:884:TRP:CZ3	2:M:79:LYS:HD2	1.74	1.21
1:G:884:TRP:CZ3	2:N:79:LYS:HD2	1.74	1.21
1:B:884:TRP:CZ3	2:I:79:LYS:HA	1.82	1.15
1:A:884:TRP:CZ3	2:H:79:LYS:HA	1.82	1.15
1:C:884:TRP:CZ3	2:J:79:LYS:HA	1.82	1.15
1:G:884:TRP:CZ3	2:N:79:LYS:HA	1.81	1.14
1:D:884:TRP:CZ3	2:K:79:LYS:HA	1.82	1.14
1:E:884:TRP:CZ3	2:L:79:LYS:HA	1.82	1.14
1:F:884:TRP:CZ3	2:M:79:LYS:HA	1.82	1.13
1:F:1086:GLY:HA2	2:M:39:LYS:HZ1	1.16	1.11
1:E:7:ASN:HB2	1:F:236:PRO:HG3	1.28	1.10
1:G:1086:GLY:HA2	2:N:39:LYS:HZ1	1.22	1.04
1:E:7:ASN:HB2	1:F:236:PRO:HG2	1.36	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1086:GLY:HA2	2:L:39:LYS:HZ1	1.20	1.01
1:G:569:CYS:SG	1:G:1213:PHE:HE1	1.85	0.99
1:A:565:GLN:NE2	1:A:1213:PHE:H	1.60	0.99
1:F:569:CYS:SG	1:F:1213:PHE:CE1	2.56	0.99
1:B:569:CYS:SG	1:B:600:LYS:NZ	2.36	0.99
1:C:565:GLN:NE2	1:C:1213:PHE:H	1.60	0.99
1:G:569:CYS:SG	1:G:1213:PHE:CE1	2.56	0.99
1:D:569:CYS:SG	1:D:1213:PHE:HE1	1.85	0.99
1:E:569:CYS:SG	1:E:600:LYS:NZ	2.36	0.99
1:F:569:CYS:SG	1:F:600:LYS:NZ	2.36	0.99
1:B:569:CYS:SG	1:B:1213:PHE:HE1	1.85	0.99
1:B:569:CYS:SG	1:B:1213:PHE:CE1	2.56	0.99
1:E:565:GLN:CD	1:E:1213:PHE:H	1.71	0.99
1:F:565:GLN:CD	1:F:1213:PHE:H	1.71	0.99
1:C:569:CYS:SG	1:C:600:LYS:NZ	2.36	0.99
1:C:569:CYS:SG	1:C:1213:PHE:CE1	2.56	0.99
1:C:569:CYS:SG	1:C:1213:PHE:HE1	1.85	0.99
1:E:569:CYS:SG	1:E:1213:PHE:CE1	2.56	0.99
1:G:569:CYS:SG	1:G:600:LYS:NZ	2.36	0.99
1:A:569:CYS:SG	1:A:1213:PHE:CE1	2.56	0.99
1:B:565:GLN:NE2	1:B:1213:PHE:H	1.60	0.99
1:D:565:GLN:CD	1:D:1213:PHE:H	1.71	0.99
1:F:569:CYS:SG	1:F:1213:PHE:HE1	1.85	0.99
1:G:565:GLN:CD	1:G:1213:PHE:H	1.71	0.98
1:E:569:CYS:SG	1:E:1213:PHE:HE1	1.85	0.98
1:G:565:GLN:NE2	1:G:1213:PHE:H	1.60	0.98
1:G:884:TRP:HH2	2:N:79:LYS:HA	1.28	0.98
1:D:569:CYS:SG	1:D:1213:PHE:CE1	2.56	0.98
1:C:565:GLN:CD	1:C:1213:PHE:H	1.71	0.98
1:A:569:CYS:SG	1:A:600:LYS:NZ	2.36	0.98
1:A:569:CYS:SG	1:A:1213:PHE:HE1	1.85	0.98
1:C:1086:GLY:HA2	2:J:39:LYS:HZ1	1.27	0.98
1:A:565:GLN:CD	1:A:1213:PHE:H	1.71	0.98
1:B:565:GLN:CD	1:B:1213:PHE:H	1.71	0.97
1:E:565:GLN:NE2	1:E:1213:PHE:H	1.60	0.97
1:D:569:CYS:SG	1:D:600:LYS:NZ	2.36	0.97
1:F:565:GLN:NE2	1:F:1213:PHE:H	1.60	0.97
1:A:109:TYR:HE1	1:G:4:LYS:NZ	1.34	0.97
1:A:884:TRP:HH2	2:H:79:LYS:HA	1.28	0.97
1:D:565:GLN:NE2	1:D:1213:PHE:H	1.60	0.97
3:O:52:ARG:CB	3:P:38:HIS:CE1	2.48	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:52:ARG:HD3	3:R:38:HIS:ND1	1.79	0.96
1:E:884:TRP:HH2	2:L:79:LYS:HA	1.28	0.95
1:E:7:ASN:CB	1:F:236:PRO:HG2	1.97	0.94
1:D:884:TRP:HH2	2:K:79:LYS:HA	1.28	0.93
1:C:884:TRP:HH2	2:J:79:LYS:HA	1.28	0.93
1:B:1086:GLY:HA2	2:I:39:LYS:HZ1	1.30	0.93
1:D:30:ILE:CG2	3:Q:10:ARG:HB3	1.97	0.93
1:F:884:TRP:HH2	2:M:79:LYS:HA	1.28	0.93
1:E:7:ASN:CB	1:F:236:PRO:CG	2.46	0.92
1:E:550:LEU:CD2	1:E:607:SER:HB2	2.00	0.92
1:G:550:LEU:CD2	1:G:607:SER:HB2	2.00	0.92
1:B:884:TRP:HH2	2:I:79:LYS:HA	1.28	0.92
1:B:550:LEU:CD2	1:B:607:SER:HB2	2.00	0.92
1:F:550:LEU:CD2	1:F:607:SER:HB2	2.00	0.92
1:D:1086:GLY:HA2	2:K:39:LYS:HZ1	1.32	0.92
1:A:550:LEU:CD2	1:A:607:SER:HB2	2.00	0.91
1:A:1086:GLY:HA2	2:H:39:LYS:HZ1	1.32	0.91
1:D:524:HIS:HB2	1:D:646:THR:HG21	1.52	0.91
1:C:550:LEU:CD2	1:C:607:SER:HB2	2.00	0.91
1:C:1086:GLY:HA2	2:J:39:LYS:NZ	1.85	0.91
1:B:1086:GLY:HA2	2:I:39:LYS:NZ	1.86	0.91
1:C:524:HIS:HB2	1:C:646:THR:HG21	1.52	0.91
1:D:1086:GLY:HA2	2:K:39:LYS:NZ	1.85	0.91
1:A:1086:GLY:HA2	2:H:39:LYS:NZ	1.86	0.90
3:O:52:ARG:HB2	3:P:38:HIS:CE1	2.06	0.90
1:E:524:HIS:HB2	1:E:646:THR:HG21	1.52	0.90
1:D:550:LEU:CD2	1:D:607:SER:HB2	2.00	0.90
3:O:52:ARG:HB3	3:P:38:HIS:CE1	2.07	0.90
1:B:524:HIS:HB2	1:B:646:THR:HG21	1.52	0.90
1:E:1086:GLY:HA2	2:L:39:LYS:NZ	1.85	0.90
1:G:1086:GLY:HA2	2:N:39:LYS:NZ	1.85	0.90
1:G:524:HIS:HB2	1:G:646:THR:HG21	1.52	0.89
1:F:1086:GLY:HA2	2:M:39:LYS:NZ	1.85	0.89
1:A:524:HIS:HB2	1:A:646:THR:HG21	1.52	0.89
1:F:524:HIS:HB2	1:F:646:THR:HG21	1.52	0.88
1:F:884:TRP:CZ3	2:M:79:LYS:CD	2.57	0.88
1:B:884:TRP:CZ3	2:I:79:LYS:CD	2.57	0.88
1:A:884:TRP:CZ3	2:H:79:LYS:CD	2.57	0.88
1:E:884:TRP:CZ3	2:L:79:LYS:CD	2.57	0.88
1:C:884:TRP:CZ3	2:J:79:LYS:CD	2.57	0.87
1:A:109:TYR:CE1	1:G:4:LYS:NZ	2.04	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:884:TRP:CZ3	2:K:79:LYS:CD	2.57	0.87
1:A:109:TYR:CE1	1:G:4:LYS:HD2	2.11	0.86
3:Q:52:ARG:CD	3:R:38:HIS:HE1	1.89	0.86
3:Q:52:ARG:CB	3:R:38:HIS:HE1	1.88	0.86
3:P:50:SER:CB	3:Q:45:ARG:HH12	1.89	0.85
1:A:884:TRP:CH2	2:H:79:LYS:CA	2.59	0.85
3:Q:52:ARG:HD3	3:R:38:HIS:NE2	1.88	0.85
1:B:884:TRP:CH2	2:I:79:LYS:CA	2.59	0.85
1:E:885:VAL:HG11	1:E:888:VAL:HG13	1.59	0.85
1:G:885:VAL:HG11	1:G:888:VAL:HG13	1.59	0.85
1:G:884:TRP:CH2	2:N:79:LYS:CA	2.59	0.85
1:G:884:TRP:CZ3	2:N:79:LYS:CD	2.57	0.85
1:A:885:VAL:HG11	1:A:888:VAL:HG13	1.59	0.85
1:D:885:VAL:HG11	1:D:888:VAL:HG13	1.59	0.85
1:F:885:VAL:HG11	1:F:888:VAL:HG13	1.59	0.85
1:B:882:LEU:HB2	1:B:903:ASP:HB3	1.59	0.84
1:A:882:LEU:HB2	1:A:903:ASP:HB3	1.59	0.84
1:B:885:VAL:HG11	1:B:888:VAL:HG13	1.59	0.84
1:C:884:TRP:CH2	2:J:79:LYS:CA	2.58	0.84
1:G:550:LEU:HD21	1:G:607:SER:HB2	1.60	0.84
1:C:885:VAL:HG11	1:C:888:VAL:HG13	1.59	0.84
1:A:550:LEU:HD21	1:A:607:SER:HB2	1.60	0.83
1:F:884:TRP:CH2	2:M:79:LYS:CA	2.59	0.83
1:F:550:LEU:HD21	1:F:607:SER:HB2	1.60	0.83
1:G:882:LEU:HB2	1:G:903:ASP:HB3	1.59	0.83
1:C:882:LEU:HB2	1:C:903:ASP:HB3	1.59	0.83
1:F:565:GLN:NE2	1:F:1213:PHE:N	2.27	0.82
1:C:550:LEU:HD21	1:C:607:SER:HB2	1.60	0.82
1:E:550:LEU:HD21	1:E:607:SER:HB2	1.60	0.82
1:B:565:GLN:NE2	1:B:1213:PHE:N	2.27	0.82
1:E:565:GLN:NE2	1:E:1213:PHE:N	2.27	0.82
1:E:882:LEU:HB2	1:E:903:ASP:HB3	1.59	0.82
1:B:550:LEU:HD21	1:B:607:SER:HB2	1.60	0.82
1:D:358:SER:HB3	1:E:274:MET:HE2	1.62	0.82
1:D:550:LEU:HD21	1:D:607:SER:HB2	1.60	0.82
1:A:565:GLN:NE2	1:A:1213:PHE:N	2.27	0.82
1:C:565:GLN:NE2	1:C:1213:PHE:N	2.27	0.82
1:F:882:LEU:HB2	1:F:903:ASP:HB3	1.59	0.82
1:D:565:GLN:NE2	1:D:1213:PHE:N	2.27	0.81
1:F:1086:GLY:CA	2:M:39:LYS:HZ1	1.91	0.81
1:D:884:TRP:CH2	2:K:79:LYS:CA	2.59	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:MET:HE2	1:G:358:SER:HB3	1.62	0.81
1:G:565:GLN:NE2	1:G:1213:PHE:N	2.27	0.81
1:G:584:ALA:HA	1:G:594:TYR:CE2	2.16	0.81
1:E:584:ALA:HA	1:E:594:TYR:CE2	2.16	0.81
1:D:882:LEU:HB2	1:D:903:ASP:HB3	1.59	0.81
1:D:584:ALA:HA	1:D:594:TYR:CE2	2.16	0.81
1:E:358:SER:HB3	1:F:274:MET:HE2	1.63	0.81
1:A:862:TYR:CA	1:A:884:TRP:HA	2.11	0.80
1:B:584:ALA:HA	1:B:594:TYR:CE2	2.16	0.80
1:F:584:ALA:HA	1:F:594:TYR:CE2	2.16	0.80
1:F:862:TYR:CA	1:F:884:TRP:HA	2.11	0.80
1:B:358:SER:HB3	1:C:274:MET:HE2	1.64	0.80
1:C:862:TYR:HA	1:C:884:TRP:HA	1.63	0.80
1:E:7:ASN:CG	1:F:236:PRO:HG2	2.06	0.80
1:E:862:TYR:CA	1:E:884:TRP:HA	2.11	0.80
1:E:884:TRP:CH2	2:L:79:LYS:CA	2.59	0.80
1:A:584:ALA:HA	1:A:594:TYR:CE2	2.16	0.80
1:B:862:TYR:HA	1:B:884:TRP:HA	1.63	0.80
1:D:862:TYR:HA	1:D:884:TRP:HA	1.63	0.80
1:E:862:TYR:HA	1:E:884:TRP:HA	1.63	0.80
1:C:358:SER:HB3	1:D:274:MET:HE2	1.64	0.80
1:E:7:ASN:CB	1:F:236:PRO:HG3	2.11	0.80
1:A:862:TYR:HA	1:A:884:TRP:HA	1.63	0.80
3:Q:52:ARG:CD	3:R:38:HIS:ND1	2.40	0.80
1:D:862:TYR:CA	1:D:884:TRP:HA	2.11	0.79
1:E:6:ARG:NH2	1:F:232:LEU:O	2.15	0.79
1:G:862:TYR:CA	1:G:884:TRP:HA	2.11	0.79
1:F:862:TYR:HA	1:F:884:TRP:HA	1.64	0.79
1:F:882:LEU:HD13	1:F:1176:HIS:NE2	1.98	0.79
3:O:15:ARG:CD	3:O:19:GLU:OE2	2.30	0.79
1:A:358:SER:HB3	1:B:274:MET:HE2	1.64	0.79
1:B:862:TYR:CA	1:B:884:TRP:HA	2.11	0.79
1:C:584:ALA:HA	1:C:594:TYR:CE2	2.16	0.79
1:B:882:LEU:HD13	1:B:1176:HIS:NE2	1.98	0.79
1:E:1084:HIS:HE2	1:E:1108:THR:HG1	1.30	0.79
1:G:862:TYR:HA	1:G:884:TRP:HA	1.63	0.79
3:Q:15:ARG:CD	3:Q:19:GLU:OE2	2.30	0.79
1:C:862:TYR:CA	1:C:884:TRP:HA	2.11	0.79
3:P:15:ARG:CD	3:P:19:GLU:OE2	2.30	0.79
3:R:15:ARG:CD	3:R:19:GLU:OE2	2.30	0.79
1:C:1084:HIS:HE2	1:C:1108:THR:HG1	1.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:882:LEU:HD13	1:D:1176:HIS:NE2	1.98	0.78
1:C:882:LEU:HD13	1:C:1176:HIS:NE2	1.98	0.78
1:E:1086:GLY:CA	2:L:39:LYS:HZ1	1.96	0.78
1:F:1084:HIS:HE2	1:F:1108:THR:HG1	1.30	0.78
1:A:882:LEU:HD13	1:A:1176:HIS:NE2	1.98	0.78
1:G:882:LEU:HD13	1:G:1176:HIS:NE2	1.98	0.78
1:E:882:LEU:HD13	1:E:1176:HIS:NE2	1.98	0.77
3:P:50:SER:HB2	3:Q:45:ARG:HH12	1.48	0.77
1:D:1084:HIS:HE2	1:D:1108:THR:HG1	1.30	0.77
1:A:565:GLN:HE22	1:A:1213:PHE:H	1.33	0.77
1:E:349:GLN:HA	1:E:447:GLU:OE2	1.86	0.76
1:A:349:GLN:HA	1:A:447:GLU:OE2	1.85	0.76
1:B:884:TRP:HH2	2:I:79:LYS:CA	1.97	0.76
1:B:349:GLN:HA	1:B:447:GLU:OE2	1.85	0.76
1:F:884:TRP:HH2	2:M:79:LYS:CA	1.97	0.76
1:G:47:PRO:HG2	1:G:51:GLN:HE22	1.51	0.76
1:G:1086:GLY:CA	2:N:39:LYS:HZ1	1.98	0.76
1:C:565:GLN:HE22	1:C:1213:PHE:H	1.33	0.76
1:G:884:TRP:HH2	2:N:79:LYS:CA	1.97	0.76
1:F:349:GLN:HA	1:F:447:GLU:OE2	1.85	0.76
1:E:47:PRO:HG2	1:E:51:GLN:HE22	1.51	0.76
1:B:565:GLN:HE22	1:B:1213:PHE:H	1.33	0.75
1:D:349:GLN:HA	1:D:447:GLU:OE2	1.85	0.75
1:C:1112:TRP:HB3	1:C:1119:PRO:HA	1.68	0.75
1:A:882:LEU:CD1	1:A:1176:HIS:NE2	2.50	0.75
3:Q:7:ARG:O	3:Q:11:ARG:HG3	1.87	0.75
1:A:557:ARG:NH2	1:A:1175:THR:HG23	2.02	0.75
1:E:882:LEU:CD1	1:E:1176:HIS:NE2	2.50	0.75
1:G:882:LEU:CD1	1:G:1176:HIS:NE2	2.50	0.75
1:A:1084:HIS:HE2	1:A:1108:THR:HG1	1.31	0.75
1:B:47:PRO:HG2	1:B:51:GLN:HE22	1.51	0.75
1:B:557:ARG:NH2	1:B:1175:THR:HG23	2.01	0.75
1:E:884:TRP:HH2	2:L:79:LYS:CA	1.97	0.75
1:C:349:GLN:HA	1:C:447:GLU:OE2	1.85	0.75
1:D:1112:TRP:HB3	1:D:1119:PRO:HA	1.68	0.75
1:F:358:SER:HB3	1:G:274:MET:HE2	1.69	0.75
3:R:7:ARG:O	3:R:11:ARG:HG3	1.87	0.75
1:B:882:LEU:CD1	1:B:1176:HIS:NE2	2.50	0.75
1:F:882:LEU:CD1	1:F:1176:HIS:NE2	2.50	0.75
2:N:24:GLY:O	2:N:31:ASN:ND2	2.20	0.75
1:D:404:TRP:HB3	1:D:406:MET:HE3	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1112:TRP:HB3	1:E:1119:PRO:HA	1.68	0.75
1:F:1112:TRP:HB3	1:F:1119:PRO:HA	1.68	0.74
1:G:565:GLN:HE22	1:G:1213:PHE:H	1.33	0.74
2:H:24:GLY:O	2:H:31:ASN:ND2	2.20	0.74
1:B:884:TRP:HZ3	2:I:79:LYS:HD2	1.51	0.74
1:D:309:GLN:NE2	1:D:339:GLU:OE1	2.21	0.74
1:E:309:GLN:NE2	1:E:339:GLU:OE1	2.21	0.74
1:F:557:ARG:NH2	1:F:1175:THR:HG23	2.01	0.74
1:G:349:GLN:HA	1:G:447:GLU:OE2	1.85	0.74
1:G:557:ARG:NH2	1:G:1175:THR:HG23	2.01	0.74
3:P:7:ARG:O	3:P:11:ARG:HG3	1.87	0.74
1:B:339:GLU:OE2	1:B:343:LYS:NZ	2.20	0.74
1:C:404:TRP:HB3	1:C:406:MET:HE3	1.69	0.74
1:F:941:ASP:H	1:F:946:LEU:HA	1.53	0.74
1:A:884:TRP:HH2	2:H:79:LYS:CA	1.97	0.74
1:C:309:GLN:NE2	1:C:339:GLU:OE1	2.21	0.74
1:D:882:LEU:CD1	1:D:1176:HIS:NE2	2.50	0.74
1:F:309:GLN:NE2	1:F:339:GLU:OE1	2.21	0.74
1:A:1112:TRP:HB3	1:A:1119:PRO:HA	1.68	0.74
1:C:339:GLU:OE2	1:C:343:LYS:NZ	2.20	0.74
1:E:404:TRP:HB3	1:E:406:MET:HE3	1.69	0.74
2:L:24:GLY:O	2:L:31:ASN:ND2	2.20	0.74
1:C:557:ARG:NH2	1:C:1175:THR:HG23	2.01	0.74
1:C:882:LEU:CD1	1:C:1176:HIS:NE2	2.50	0.74
1:D:47:PRO:HG2	1:D:51:GLN:HE22	1.51	0.74
1:D:557:ARG:NH2	1:D:1175:THR:HG23	2.01	0.74
1:D:941:ASP:H	1:D:946:LEU:HA	1.53	0.74
1:F:565:GLN:HE22	1:F:1213:PHE:H	1.33	0.74
2:I:24:GLY:O	2:I:31:ASN:ND2	2.20	0.74
1:C:884:TRP:HH2	2:J:79:LYS:CA	1.97	0.74
1:C:941:ASP:H	1:C:946:LEU:HA	1.53	0.74
1:E:565:GLN:HE22	1:E:1213:PHE:H	1.33	0.74
1:E:884:TRP:HZ3	2:L:79:LYS:HD2	1.51	0.74
1:G:1112:TRP:HB3	1:G:1119:PRO:HA	1.68	0.74
2:K:24:GLY:O	2:K:31:ASN:ND2	2.20	0.74
2:M:24:GLY:O	2:M:31:ASN:ND2	2.20	0.74
3:Q:52:ARG:HD2	3:R:38:HIS:CE1	2.17	0.74
1:A:274:MET:CE	1:G:358:SER:HB3	2.17	0.74
1:B:1112:TRP:HB3	1:B:1119:PRO:HA	1.68	0.74
1:D:339:GLU:OE2	1:D:343:LYS:NZ	2.20	0.73
1:G:941:ASP:H	1:G:946:LEU:HA	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:7:ARG:O	3:O:11:ARG:HG3	1.87	0.73
1:D:884:TRP:HH2	2:K:79:LYS:CA	1.97	0.73
1:E:557:ARG:NH2	1:E:1175:THR:HG23	2.01	0.73
2:J:24:GLY:O	2:J:31:ASN:ND2	2.20	0.73
1:A:309:GLN:NE2	1:A:339:GLU:OE1	2.21	0.73
1:C:590:ASN:C	1:C:592:MET:H	1.97	0.73
1:B:309:GLN:NE2	1:B:339:GLU:OE1	2.21	0.73
1:B:404:TRP:HB3	1:B:406:MET:HE3	1.69	0.73
1:C:884:TRP:HZ3	2:J:79:LYS:HD2	1.51	0.73
1:E:339:GLU:OE2	1:E:343:LYS:NZ	2.20	0.73
1:G:309:GLN:NE2	1:G:339:GLU:OE1	2.21	0.73
3:Q:52:ARG:CB	3:R:38:HIS:CE1	2.72	0.73
1:B:590:ASN:C	1:B:592:MET:H	1.97	0.73
1:A:339:GLU:OE2	1:A:343:LYS:NZ	2.20	0.73
1:D:590:ASN:C	1:D:592:MET:H	1.97	0.73
1:D:884:TRP:HZ3	2:K:79:LYS:HD2	1.52	0.73
3:R:87:SER:O	3:R:91:THR:HG23	1.89	0.73
1:B:1084:HIS:HE2	1:B:1108:THR:HG1	1.34	0.73
1:F:404:TRP:HB3	1:F:406:MET:HE3	1.69	0.72
3:Q:87:SER:O	3:Q:91:THR:HG23	1.89	0.72
1:A:404:TRP:HB3	1:A:406:MET:HE3	1.69	0.72
1:E:941:ASP:H	1:E:946:LEU:HA	1.53	0.72
1:G:339:GLU:OE2	1:G:343:LYS:NZ	2.20	0.72
1:A:941:ASP:H	1:A:946:LEU:HA	1.53	0.72
1:C:358:SER:HB3	1:D:274:MET:CE	2.19	0.72
1:B:941:ASP:H	1:B:946:LEU:HA	1.53	0.72
3:P:87:SER:O	3:P:91:THR:HG23	1.89	0.72
1:G:404:TRP:HB3	1:G:406:MET:HE3	1.69	0.72
1:B:609:LEU:HB3	1:B:908:LEU:HB2	1.71	0.72
1:C:609:LEU:HB3	1:C:908:LEU:HB2	1.71	0.72
1:D:565:GLN:HE22	1:D:1213:PHE:H	1.33	0.72
2:K:26:HIS:NE2	2:K:44:PRO:O	2.23	0.72
1:E:565:GLN:CD	1:E:1213:PHE:N	2.48	0.72
1:A:590:ASN:C	1:A:592:MET:H	1.97	0.71
1:B:882:LEU:HB2	1:B:903:ASP:CB	2.20	0.71
1:F:339:GLU:OE2	1:F:343:LYS:NZ	2.20	0.71
1:G:882:LEU:HB2	1:G:903:ASP:CB	2.20	0.71
1:G:1084:HIS:HE2	1:G:1108:THR:HG1	1.35	0.71
2:I:26:HIS:NE2	2:I:44:PRO:O	2.23	0.71
1:D:609:LEU:HB3	1:D:908:LEU:HB2	1.71	0.71
1:E:590:ASN:C	1:E:592:MET:H	1.97	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:26:HIS:NE2	2:H:44:PRO:O	2.23	0.71
2:J:26:HIS:NE2	2:J:44:PRO:O	2.23	0.71
2:L:26:HIS:NE2	2:L:44:PRO:O	2.23	0.71
1:D:565:GLN:CD	1:D:1213:PHE:N	2.48	0.71
1:D:1034:LEU:HB3	1:D:1036:LYS:HD3	1.73	0.71
1:E:609:LEU:HB3	1:E:908:LEU:HB2	1.71	0.71
3:O:87:SER:O	3:O:91:THR:HG23	1.89	0.71
1:C:1034:LEU:HB3	1:C:1036:LYS:HD3	1.73	0.71
1:D:358:SER:HB3	1:E:274:MET:CE	2.19	0.71
2:M:26:HIS:NE2	2:M:44:PRO:O	2.23	0.71
1:A:609:LEU:HB3	1:A:908:LEU:HB2	1.71	0.71
1:F:590:ASN:C	1:F:592:MET:H	1.97	0.71
1:G:565:GLN:HE22	1:G:1213:PHE:N	1.89	0.71
1:A:1034:LEU:HB3	1:A:1036:LYS:HD3	1.73	0.71
1:D:30:ILE:HG23	3:Q:10:ARG:HB3	1.73	0.71
1:G:549:SER:O	1:G:610:VAL:HB	1.91	0.71
1:A:549:SER:O	1:A:610:VAL:HB	1.91	0.71
1:D:882:LEU:HB2	1:D:903:ASP:CB	2.20	0.71
1:E:549:SER:O	1:E:610:VAL:HB	1.91	0.71
2:N:26:HIS:NE2	2:N:44:PRO:O	2.23	0.71
3:P:41:GLU:HB3	3:P:45:ARG:HH12	1.56	0.71
1:B:28:HIS:CE1	3:P:14:LEU:HD21	2.26	0.71
1:B:346:GLN:O	1:B:348:LYS:HG3	1.91	0.71
1:B:549:SER:O	1:B:610:VAL:HB	1.91	0.71
1:B:1034:LEU:HB3	1:B:1036:LYS:HD3	1.73	0.71
1:F:609:LEU:HB3	1:F:908:LEU:HB2	1.71	0.71
1:G:1034:LEU:HB3	1:G:1036:LYS:HD3	1.73	0.71
1:C:346:GLN:O	1:C:348:LYS:HG3	1.91	0.70
1:D:47:PRO:HG2	1:D:51:GLN:NE2	2.07	0.70
1:E:882:LEU:HB2	1:E:903:ASP:CB	2.20	0.70
1:F:346:GLN:O	1:F:348:LYS:HG3	1.91	0.70
1:C:565:GLN:CD	1:C:1213:PHE:N	2.48	0.70
1:G:609:LEU:HB3	1:G:908:LEU:HB2	1.71	0.70
1:A:882:LEU:HB2	1:A:903:ASP:CB	2.20	0.70
1:C:549:SER:O	1:C:610:VAL:HB	1.91	0.70
1:D:346:GLN:O	1:D:348:LYS:HG3	1.91	0.70
1:D:403:LEU:HD13	1:D:460:ILE:HG22	1.73	0.70
1:D:569:CYS:SG	1:D:1213:PHE:CZ	2.85	0.70
1:E:47:PRO:HG2	1:E:51:GLN:NE2	2.07	0.70
1:F:549:SER:O	1:F:610:VAL:HB	1.91	0.70
1:A:569:CYS:SG	1:A:1213:PHE:CZ	2.85	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:565:GLN:HE22	1:C:1213:PHE:N	1.89	0.70
1:E:884:TRP:CE3	2:L:79:LYS:HD2	2.27	0.70
1:A:358:SER:HB3	1:B:274:MET:CE	2.20	0.70
1:E:346:GLN:O	1:E:348:LYS:HG3	1.91	0.70
1:E:1034:LEU:HB3	1:E:1036:LYS:HD3	1.73	0.70
1:E:189:LYS:NZ	1:E:374:MET:SD	2.65	0.70
1:E:403:LEU:HD13	1:E:460:ILE:HG22	1.73	0.70
1:G:569:CYS:SG	1:G:1213:PHE:CZ	2.85	0.70
1:G:590:ASN:C	1:G:592:MET:H	1.97	0.70
1:B:358:SER:HB3	1:C:274:MET:CE	2.21	0.70
1:C:403:LEU:HD13	1:C:460:ILE:HG22	1.73	0.70
1:C:569:CYS:SG	1:C:1213:PHE:CZ	2.85	0.70
1:D:189:LYS:NZ	1:D:374:MET:SD	2.65	0.70
1:D:854:LEU:HB3	1:D:866:LEU:HD11	1.74	0.70
1:A:854:LEU:HB3	1:A:866:LEU:HD11	1.74	0.70
1:G:346:GLN:O	1:G:348:LYS:HG3	1.91	0.70
1:B:565:GLN:CD	1:B:1213:PHE:N	2.48	0.70
1:C:854:LEU:HB3	1:C:866:LEU:HD11	1.74	0.70
1:C:882:LEU:HB2	1:C:903:ASP:CB	2.21	0.70
1:D:884:TRP:CE3	2:K:79:LYS:HD2	2.27	0.70
1:E:569:CYS:SG	1:E:1213:PHE:CZ	2.85	0.70
1:B:565:GLN:HE22	1:B:1213:PHE:N	1.89	0.69
1:B:884:TRP:CE3	2:I:79:LYS:HD2	2.27	0.69
1:G:854:LEU:HB3	1:G:866:LEU:HD11	1.74	0.69
1:A:346:GLN:O	1:A:348:LYS:HG3	1.91	0.69
1:A:565:GLN:CD	1:A:1213:PHE:N	2.48	0.69
1:E:854:LEU:HB3	1:E:866:LEU:HD11	1.74	0.69
1:F:882:LEU:HB2	1:F:903:ASP:CB	2.20	0.69
1:F:1034:LEU:HB3	1:F:1036:LYS:HD3	1.73	0.69
1:G:884:TRP:CE3	2:N:79:LYS:HD2	2.27	0.69
3:P:15:ARG:HD3	3:P:19:GLU:OE2	1.92	0.69
1:E:358:SER:HB3	1:F:274:MET:CE	2.21	0.69
1:G:47:PRO:HG2	1:G:51:GLN:NE2	2.07	0.69
1:A:844:GLN:HE22	2:H:79:LYS:NZ	1.91	0.69
1:B:854:LEU:HB3	1:B:866:LEU:HD11	1.74	0.69
1:E:844:GLN:HE22	2:L:79:LYS:NZ	1.91	0.69
1:B:569:CYS:SG	1:B:1213:PHE:CZ	2.85	0.69
1:C:844:GLN:HE22	2:J:79:LYS:NZ	1.91	0.69
1:D:549:SER:O	1:D:610:VAL:HB	1.91	0.69
1:G:565:GLN:CD	1:G:1213:PHE:N	2.48	0.69
3:Q:15:ARG:HD3	3:Q:19:GLU:OE2	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:PRO:HG2	1:B:51:GLN:NE2	2.07	0.69
1:F:854:LEU:HB3	1:F:866:LEU:HD11	1.74	0.69
1:B:844:GLN:HE22	2:I:79:LYS:NZ	1.90	0.69
1:D:844:GLN:HE22	2:K:79:LYS:NZ	1.91	0.69
1:F:189:LYS:NZ	1:F:374:MET:SD	2.65	0.69
1:F:403:LEU:HD13	1:F:460:ILE:HG22	1.74	0.69
1:F:569:CYS:SG	1:F:1213:PHE:CZ	2.85	0.69
1:G:844:GLN:HE22	2:N:79:LYS:NZ	1.91	0.69
1:F:565:GLN:HE22	1:F:1213:PHE:N	1.89	0.68
1:B:403:LEU:HD13	1:B:460:ILE:HG22	1.73	0.68
1:F:844:GLN:HE22	2:M:79:LYS:NZ	1.91	0.68
1:A:403:LEU:HD13	1:A:460:ILE:HG22	1.73	0.68
1:B:37:ILE:HG13	3:P:10:ARG:NH1	2.08	0.68
1:C:189:LYS:NZ	1:C:374:MET:SD	2.65	0.68
1:G:403:LEU:HD13	1:G:460:ILE:HG22	1.74	0.68
2:I:61:GLU:HA	2:I:95:ILE:HG21	1.76	0.68
3:R:15:ARG:HD3	3:R:19:GLU:OE2	1.93	0.68
1:F:884:TRP:CE3	2:M:79:LYS:HD2	2.27	0.68
2:J:61:GLU:HA	2:J:95:ILE:HG21	1.76	0.68
1:B:611:VAL:HG12	1:B:613:PRO:HD3	1.75	0.68
2:H:61:GLU:HA	2:H:95:ILE:HG21	1.75	0.68
1:D:565:GLN:HE22	1:D:1213:PHE:N	1.89	0.68
1:F:611:VAL:HG12	1:F:613:PRO:HD3	1.75	0.68
1:G:611:VAL:HG12	1:G:613:PRO:HD3	1.75	0.68
1:D:1204:VAL:HG12	1:D:1205:VAL:HG23	1.76	0.68
1:F:565:GLN:CD	1:F:1213:PHE:N	2.48	0.68
1:G:189:LYS:NZ	1:G:374:MET:SD	2.65	0.68
1:E:565:GLN:HE22	1:E:1213:PHE:N	1.89	0.67
2:H:20:VAL:HG12	2:H:32:LEU:HB2	1.77	0.67
1:A:884:TRP:CE3	2:H:79:LYS:HD2	2.27	0.67
1:C:611:VAL:HG12	1:C:613:PRO:HD3	1.75	0.67
1:C:884:TRP:CE3	2:J:79:LYS:HD2	2.27	0.67
1:C:1204:VAL:HG12	1:C:1205:VAL:HG23	1.76	0.67
1:C:1086:GLY:HA2	2:J:39:LYS:CE	2.24	0.67
1:D:14:GLU:OE1	1:E:31:SER:OG	2.10	0.67
2:K:61:GLU:HA	2:K:95:ILE:HG21	1.75	0.67
2:N:61:GLU:HA	2:N:95:ILE:HG21	1.75	0.67
3:O:15:ARG:HD3	3:O:19:GLU:OE2	1.93	0.67
3:O:52:ARG:CB	3:P:38:HIS:HE1	2.07	0.67
2:I:20:VAL:HG12	2:I:32:LEU:HB2	1.77	0.67
1:E:1204:VAL:HG12	1:E:1205:VAL:HG23	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:20:VAL:HG12	2:N:32:LEU:HB2	1.77	0.67
1:B:1086:GLY:HA2	2:I:39:LYS:CE	2.24	0.67
1:A:189:LYS:NZ	1:A:374:MET:SD	2.65	0.67
2:J:18:HIS:NE2	5:J:500:HEC:NB	2.43	0.67
2:K:18:HIS:NE2	5:K:500:HEC:NB	2.43	0.67
2:M:61:GLU:HA	2:M:95:ILE:HG21	1.76	0.67
3:O:6:ARG:O	3:O:10:ARG:HG2	1.95	0.67
1:A:611:VAL:HG12	1:A:613:PRO:HD3	1.75	0.67
2:L:61:GLU:HA	2:L:95:ILE:HG21	1.75	0.67
1:B:189:LYS:NZ	1:B:374:MET:SD	2.65	0.67
2:L:18:HIS:NE2	5:L:500:HEC:NB	2.43	0.67
1:B:1204:VAL:HG12	1:B:1205:VAL:HG23	1.76	0.66
1:D:611:VAL:HG12	1:D:613:PRO:HD3	1.75	0.66
2:N:18:HIS:NE2	5:N:500:HEC:NB	2.43	0.66
1:A:569:CYS:HG	1:A:1213:PHE:HE1	1.43	0.66
1:E:611:VAL:HG12	1:E:613:PRO:HD3	1.75	0.66
1:E:1086:GLY:HA2	2:L:39:LYS:CE	2.24	0.66
3:Q:6:ARG:O	3:Q:10:ARG:HG2	1.95	0.66
1:B:474:SER:HB2	1:B:477:GLN:HG2	1.78	0.66
1:A:1086:GLY:HA2	2:H:39:LYS:CE	2.24	0.66
1:F:1086:GLY:HA2	2:M:39:LYS:CE	2.25	0.66
2:H:18:HIS:NE2	5:H:500:HEC:NB	2.43	0.66
1:D:1027:ILE:HD11	1:D:1047:VAL:HG11	1.78	0.66
1:E:1027:ILE:HD11	1:E:1047:VAL:HG11	1.78	0.66
1:F:1027:ILE:HD11	1:F:1047:VAL:HG11	1.78	0.66
1:G:1086:GLY:HA2	2:N:39:LYS:CE	2.24	0.66
1:C:1086:GLY:CA	2:J:39:LYS:HZ1	2.04	0.66
1:A:474:SER:HB2	1:A:477:GLN:HG2	1.78	0.66
2:I:18:HIS:NE2	5:I:500:HEC:NB	2.43	0.66
2:L:20:VAL:HG12	2:L:32:LEU:HB2	1.77	0.66
1:E:844:GLN:NE2	2:L:79:LYS:HE3	2.11	0.66
1:F:1204:VAL:HG12	1:F:1205:VAL:HG23	1.77	0.66
3:R:6:ARG:O	3:R:10:ARG:HG2	1.95	0.66
1:D:1086:GLY:HA2	2:K:39:LYS:CE	2.24	0.66
2:J:20:VAL:HG12	2:J:32:LEU:HB2	1.77	0.66
1:F:844:GLN:NE2	2:M:79:LYS:HE3	2.11	0.66
3:P:6:ARG:O	3:P:10:ARG:HG2	1.95	0.66
1:D:844:GLN:NE2	2:K:79:LYS:HE3	2.11	0.65
1:F:354:ARG:NH1	1:F:362:GLU:OE1	2.30	0.65
1:G:844:GLN:NE2	2:N:79:LYS:HE3	2.11	0.65
1:G:1027:ILE:HD11	1:G:1047:VAL:HG11	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:20:VAL:HG12	2:K:32:LEU:HB2	1.77	0.65
2:M:18:HIS:NE2	5:M:500:HEC:NB	2.43	0.65
1:E:391:LYS:O	1:E:392:ASP:HB2	1.96	0.65
1:F:391:LYS:O	1:F:392:ASP:HB2	1.96	0.65
1:A:1204:VAL:HG12	1:A:1205:VAL:HG23	1.76	0.65
1:B:354:ARG:NH1	1:B:362:GLU:OE1	2.30	0.65
1:C:474:SER:HB2	1:C:477:GLN:HG2	1.78	0.65
1:D:943:ILE:HG22	1:D:944:ARG:HG2	1.78	0.65
1:E:943:ILE:HG22	1:E:944:ARG:HG2	1.78	0.65
1:F:201:ASN:HD21	1:G:219:ASN:HD21	1.44	0.65
1:F:943:ILE:HG22	1:F:944:ARG:HG2	1.78	0.65
1:G:1204:VAL:HG12	1:G:1205:VAL:HG23	1.76	0.65
1:A:866:LEU:HB3	1:A:876:ALA:HB3	1.77	0.65
1:B:590:ASN:O	1:B:592:MET:N	2.30	0.65
1:C:1027:ILE:HD11	1:C:1047:VAL:HG11	1.78	0.65
1:E:569:CYS:HG	1:E:1213:PHE:HE1	1.42	0.65
1:C:590:ASN:O	1:C:592:MET:N	2.30	0.65
1:E:354:ARG:NH1	1:E:362:GLU:OE1	2.30	0.65
1:F:590:ASN:O	1:F:592:MET:N	2.30	0.65
1:G:354:ARG:NH1	1:G:362:GLU:OE1	2.30	0.65
1:C:844:GLN:NE2	2:J:79:LYS:HE3	2.11	0.65
1:C:943:ILE:HG22	1:C:944:ARG:HG2	1.78	0.65
1:G:866:LEU:HB3	1:G:876:ALA:HB3	1.77	0.65
1:G:943:ILE:HG22	1:G:944:ARG:HG2	1.78	0.65
1:F:358:SER:HB3	1:G:274:MET:CE	2.25	0.65
2:M:20:VAL:HG12	2:M:32:LEU:HB2	1.77	0.65
1:A:943:ILE:HG22	1:A:944:ARG:HG2	1.78	0.65
1:B:391:LYS:O	1:B:392:ASP:HB2	1.96	0.65
1:B:884:TRP:HZ3	2:I:79:LYS:HA	1.56	0.65
1:C:354:ARG:NH1	1:C:362:GLU:OE1	2.30	0.65
1:C:266:ASP:OD2	1:C:268:SER:OG	2.16	0.64
1:D:866:LEU:HB3	1:D:876:ALA:HB3	1.77	0.64
1:A:565:GLN:HE22	1:A:1213:PHE:N	1.89	0.64
1:B:943:ILE:HG22	1:B:944:ARG:HG2	1.78	0.64
1:D:160:LYS:N	4:D:1301:DTP:O1A	2.21	0.64
1:D:266:ASP:OD2	1:D:268:SER:OG	2.16	0.64
1:D:391:LYS:O	1:D:392:ASP:HB2	1.96	0.64
1:F:469:GLN:HB2	1:F:472:THR:HB	1.79	0.64
1:F:1133:SER:HB2	1:F:1142:LEU:HD11	1.79	0.64
1:G:474:SER:HB2	1:G:477:GLN:HG2	1.78	0.64
1:A:590:ASN:O	1:A:592:MET:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1133:SER:HB2	1:A:1142:LEU:HD11	1.79	0.64
1:C:866:LEU:HB3	1:C:876:ALA:HB3	1.77	0.64
1:D:643:LYS:HE3	1:D:645:GLU:HB3	1.79	0.64
1:D:715:LEU:HD13	1:D:727:LEU:HD21	1.79	0.64
1:G:1133:SER:HB2	1:G:1142:LEU:HD11	1.79	0.64
2:J:2:ASP:N	2:J:93:ASP:OD1	2.28	0.64
1:A:160:LYS:N	4:A:1301:DTP:O1A	2.21	0.64
1:A:643:LYS:HE3	1:A:645:GLU:HB3	1.79	0.64
1:B:266:ASP:OD2	1:B:268:SER:OG	2.16	0.64
1:D:590:ASN:O	1:D:592:MET:N	2.30	0.64
1:E:469:GLN:HB2	1:E:472:THR:HB	1.79	0.64
2:N:2:ASP:N	2:N:93:ASP:OD1	2.28	0.64
1:A:354:ARG:NH1	1:A:362:GLU:OE1	2.30	0.64
1:B:844:GLN:NE2	2:I:79:LYS:HE3	2.11	0.64
1:B:866:LEU:HB3	1:B:876:ALA:HB3	1.77	0.64
1:F:866:LEU:HB3	1:F:876:ALA:HB3	1.77	0.64
1:A:1027:ILE:HD11	1:A:1047:VAL:HG11	1.78	0.64
1:C:643:LYS:HE3	1:C:645:GLU:HB3	1.79	0.64
1:D:354:ARG:NH1	1:D:362:GLU:OE1	2.30	0.64
1:A:844:GLN:NE2	2:H:79:LYS:HE3	2.11	0.64
1:E:715:LEU:HD13	1:E:727:LEU:HD21	1.79	0.64
1:G:391:LYS:O	1:G:392:ASP:HB2	1.96	0.64
1:G:884:TRP:HZ3	2:N:79:LYS:HD2	1.52	0.64
1:A:884:TRP:HZ3	2:H:79:LYS:HA	1.56	0.64
1:A:1232:TYR:HB2	1:A:1244:LEU:HB2	1.80	0.64
1:B:1027:ILE:HD11	1:B:1047:VAL:HG11	1.78	0.64
1:B:1232:TYR:HB2	1:B:1244:LEU:HB2	1.80	0.64
1:C:1232:TYR:HB2	1:C:1244:LEU:HB2	1.80	0.64
1:E:160:LYS:N	4:E:1301:DTP:O1A	2.21	0.64
1:E:643:LYS:HE3	1:E:645:GLU:HB3	1.79	0.64
1:E:474:SER:HB2	1:E:477:GLN:HG2	1.78	0.64
2:I:2:ASP:N	2:I:93:ASP:OD1	2.28	0.64
1:B:643:LYS:HE3	1:B:645:GLU:HB3	1.79	0.64
1:D:474:SER:HB2	1:D:477:GLN:HG2	1.78	0.64
1:E:266:ASP:OD2	1:E:268:SER:OG	2.16	0.64
1:E:866:LEU:HB3	1:E:876:ALA:HB3	1.77	0.64
1:A:391:LYS:O	1:A:392:ASP:HB2	1.96	0.63
1:B:1133:SER:HB2	1:B:1142:LEU:HD11	1.79	0.63
1:C:715:LEU:HD13	1:C:727:LEU:HD21	1.79	0.63
1:G:469:GLN:HB2	1:G:472:THR:HB	1.79	0.63
1:G:643:LYS:HE3	1:G:645:GLU:HB3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1232:TYR:HB2	1:G:1244:LEU:HB2	1.80	0.63
1:D:469:GLN:HB2	1:D:472:THR:HB	1.79	0.63
1:E:945:ARG:HH22	1:E:988:LEU:HD22	1.64	0.63
1:E:1133:SER:HB2	1:E:1142:LEU:HD11	1.79	0.63
1:F:474:SER:HB2	1:F:477:GLN:HG2	1.78	0.63
1:C:391:LYS:O	1:C:392:ASP:HB2	1.96	0.63
1:C:1133:SER:HB2	1:C:1142:LEU:HD11	1.79	0.63
1:A:266:ASP:OD2	1:A:268:SER:OG	2.16	0.63
1:C:884:TRP:HZ3	2:J:79:LYS:HA	1.56	0.63
1:G:715:LEU:HD13	1:G:727:LEU:HD21	1.79	0.63
1:D:1133:SER:HB2	1:D:1142:LEU:HD11	1.79	0.63
1:D:1232:TYR:HB2	1:D:1244:LEU:HB2	1.80	0.63
1:A:109:TYR:HE1	1:G:4:LYS:HZ3	0.70	0.63
1:F:565:GLN:OE1	1:F:1213:PHE:N	2.32	0.63
1:F:715:LEU:HD13	1:F:727:LEU:HD21	1.79	0.63
1:F:1232:TYR:HB2	1:F:1244:LEU:HB2	1.80	0.63
1:G:565:GLN:OE1	1:G:1213:PHE:N	2.32	0.63
1:D:565:GLN:OE1	1:D:1213:PHE:N	2.32	0.63
1:A:715:LEU:HD13	1:A:727:LEU:HD21	1.79	0.62
1:D:945:ARG:HH22	1:D:988:LEU:HD22	1.64	0.62
1:E:590:ASN:O	1:E:592:MET:N	2.30	0.62
1:F:643:LYS:HE3	1:F:645:GLU:HB3	1.79	0.62
1:G:945:ARG:HH22	1:G:988:LEU:HD22	1.64	0.62
1:B:715:LEU:HD13	1:B:727:LEU:HD21	1.79	0.62
1:C:903:ASP:OD2	1:C:907:ARG:NH1	2.28	0.62
1:D:587:GLU:OE1	1:D:594:TYR:OH	2.18	0.62
1:E:1232:TYR:HB2	1:E:1244:LEU:HB2	1.80	0.62
1:G:590:ASN:O	1:G:592:MET:N	2.30	0.62
3:O:52:ARG:HB2	3:P:38:HIS:HE1	1.61	0.62
1:A:945:ARG:HH22	1:A:988:LEU:HD22	1.64	0.62
1:B:469:GLN:HB2	1:B:472:THR:HB	1.79	0.62
1:B:945:ARG:HH22	1:B:988:LEU:HD22	1.64	0.62
1:G:160:LYS:N	4:G:1301:DTP:O1A	2.21	0.62
2:K:2:ASP:N	2:K:93:ASP:OD1	2.28	0.62
1:A:565:GLN:OE1	1:A:1213:PHE:N	2.32	0.62
1:A:1031:ASN:HB2	1:A:1036:LYS:HB2	1.82	0.62
1:C:945:ARG:HH22	1:C:988:LEU:HD22	1.64	0.62
1:F:266:ASP:OD2	1:F:268:SER:OG	2.16	0.62
1:F:569:CYS:HG	1:F:1213:PHE:HE1	1.47	0.62
1:A:557:ARG:HH22	1:A:1175:THR:HG23	1.64	0.62
1:C:565:GLN:OE1	1:C:1213:PHE:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:945:ARG:HH22	1:F:988:LEU:HD22	1.64	0.62
2:M:2:ASP:N	2:M:93:ASP:OD1	2.28	0.62
1:A:469:GLN:HB2	1:A:472:THR:HB	1.79	0.62
1:B:924:GLN:NE2	1:B:965:SER:O	2.33	0.62
1:B:1031:ASN:HB2	1:B:1036:LYS:HB2	1.82	0.62
1:C:469:GLN:HB2	1:C:472:THR:HB	1.79	0.62
1:G:569:CYS:HG	1:G:1213:PHE:HE1	1.44	0.62
1:G:1031:ASN:HB2	1:G:1036:LYS:HB2	1.82	0.62
1:B:557:ARG:HH22	1:B:1175:THR:HG23	1.64	0.62
1:A:1086:GLY:CA	2:H:39:LYS:HZ1	2.10	0.62
1:B:565:GLN:OE1	1:B:1213:PHE:N	2.32	0.62
1:C:924:GLN:NE2	1:C:965:SER:O	2.33	0.62
1:D:862:TYR:HB3	1:D:884:TRP:HA	1.82	0.62
1:F:924:GLN:NE2	1:F:965:SER:O	2.33	0.62
1:A:924:GLN:NE2	1:A:965:SER:O	2.33	0.62
1:E:924:GLN:NE2	1:E:965:SER:O	2.33	0.62
1:E:587:GLU:OE1	1:E:594:TYR:OH	2.18	0.62
1:G:559:PRO:HD3	1:G:1171:GLU:OE1	2.00	0.62
1:G:714:LEU:HB3	1:G:730:LEU:HD12	1.82	0.62
1:A:145:GLY:HA2	1:A:259:GLN:NE2	2.15	0.61
1:D:569:CYS:HG	1:D:1213:PHE:HE1	1.48	0.61
1:E:565:GLN:OE1	1:E:1213:PHE:N	2.32	0.61
1:G:266:ASP:OD2	1:G:268:SER:OG	2.16	0.61
1:G:587:GLU:OE1	1:G:594:TYR:OH	2.17	0.61
1:C:1031:ASN:HB2	1:C:1036:LYS:HB2	1.82	0.61
1:G:557:ARG:HH22	1:G:1175:THR:HG23	1.64	0.61
1:D:559:PRO:HD3	1:D:1171:GLU:OE1	2.00	0.61
1:F:714:LEU:HB3	1:F:730:LEU:HD12	1.82	0.61
1:G:884:TRP:HZ3	2:N:79:LYS:HA	1.56	0.61
1:G:924:GLN:NE2	1:G:965:SER:O	2.33	0.61
2:L:2:ASP:N	2:L:93:ASP:OD1	2.28	0.61
1:A:274:MET:HG2	1:G:358:SER:OG	2.00	0.61
1:C:559:PRO:HD3	1:C:1171:GLU:OE1	2.00	0.61
1:C:862:TYR:HB3	1:C:884:TRP:HA	1.82	0.61
1:D:924:GLN:NE2	1:D:965:SER:O	2.33	0.61
1:E:145:GLY:HA2	1:E:259:GLN:NE2	2.15	0.61
1:F:559:PRO:HD3	1:F:1171:GLU:OE1	2.00	0.61
1:A:587:GLU:OE1	1:A:594:TYR:OH	2.18	0.61
1:A:884:TRP:HZ3	2:H:79:LYS:HD2	1.52	0.61
1:D:145:GLY:HA2	1:D:259:GLN:NE2	2.15	0.61
1:E:862:TYR:HB3	1:E:884:TRP:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:882:LEU:HD12	1:F:903:ASP:HB2	1.83	0.61
1:F:1031:ASN:HB2	1:F:1036:LYS:HB2	1.82	0.61
2:H:2:ASP:N	2:H:93:ASP:OD1	2.28	0.61
2:J:67:TYR:OH	2:J:80:MET:SD	2.57	0.61
1:A:862:TYR:HB3	1:A:884:TRP:HA	1.82	0.61
1:B:160:LYS:N	4:B:1301:DTP:O1A	2.21	0.61
1:B:882:LEU:HD13	1:B:1176:HIS:CE1	2.36	0.61
1:A:882:LEU:HD13	1:A:1176:HIS:CE1	2.36	0.61
1:A:882:LEU:HD12	1:A:903:ASP:HB2	1.83	0.61
1:D:599:ASN:ND2	1:D:1241:LEU:O	2.34	0.61
1:D:882:LEU:HD13	1:D:1176:HIS:CE1	2.36	0.61
1:E:714:LEU:HB3	1:E:730:LEU:HD12	1.82	0.61
1:E:882:LEU:HD12	1:E:903:ASP:HB2	1.83	0.61
1:F:145:GLY:HA2	1:F:259:GLN:NE2	2.15	0.61
1:F:862:TYR:CB	1:F:884:TRP:HA	2.31	0.61
1:F:1092:ASP:OD2	1:F:1133:SER:OG	2.17	0.61
1:G:145:GLY:HA2	1:G:259:GLN:NE2	2.16	0.61
1:A:752:SER:OG	1:A:754:ASP:O	2.19	0.61
1:B:145:GLY:HA2	1:B:259:GLN:NE2	2.16	0.61
1:B:599:ASN:ND2	1:B:1241:LEU:O	2.34	0.61
1:E:559:PRO:HD3	1:E:1171:GLU:OE1	2.00	0.61
1:G:599:ASN:ND2	1:G:1241:LEU:O	2.34	0.61
1:A:714:LEU:HB3	1:A:730:LEU:HD12	1.82	0.61
1:B:882:LEU:HD12	1:B:903:ASP:HB2	1.83	0.61
1:C:265:ARG:NH2	4:C:1301:DTP:O2G	2.31	0.61
1:F:844:GLN:HE22	2:M:79:LYS:CE	2.14	0.61
1:G:862:TYR:HB3	1:G:884:TRP:HA	1.82	0.61
1:B:844:GLN:HE22	2:I:79:LYS:CE	2.14	0.61
1:C:557:ARG:HH22	1:C:1175:THR:HG23	1.64	0.61
1:C:714:LEU:HB3	1:C:730:LEU:HD12	1.82	0.61
1:C:882:LEU:HD13	1:C:1176:HIS:CE1	2.36	0.61
1:D:844:GLN:HE22	2:K:79:LYS:CE	2.14	0.61
3:Q:52:ARG:HB2	3:R:38:HIS:HE1	1.65	0.61
1:C:160:LYS:N	4:C:1301:DTP:O1A	2.21	0.60
1:D:1031:ASN:HB2	1:D:1036:LYS:HB2	1.82	0.60
1:G:752:SER:OG	1:G:754:ASP:O	2.19	0.60
1:G:882:LEU:HD12	1:G:903:ASP:HB2	1.83	0.60
1:A:559:PRO:HD3	1:A:1171:GLU:OE1	2.00	0.60
1:B:714:LEU:HB3	1:B:730:LEU:HD12	1.82	0.60
1:D:844:GLN:NE2	2:K:79:LYS:CE	2.64	0.60
1:D:882:LEU:HD12	1:D:903:ASP:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1086:GLY:CA	2:K:39:LYS:HZ1	2.10	0.60
1:E:201:ASN:HD21	1:F:219:ASN:HD21	1.49	0.60
1:E:557:ARG:HH22	1:E:1175:THR:HG23	1.64	0.60
1:E:752:SER:OG	1:E:754:ASP:O	2.19	0.60
1:E:844:GLN:NE2	2:L:79:LYS:CE	2.64	0.60
1:E:1031:ASN:HB2	1:E:1036:LYS:HB2	1.82	0.60
1:G:265:ARG:NH2	4:G:1301:DTP:O2G	2.31	0.60
1:B:903:ASP:OD2	1:B:907:ARG:NH1	2.28	0.60
1:B:1086:GLY:CA	2:I:39:LYS:HZ1	2.07	0.60
1:D:1092:ASP:OD2	1:D:1133:SER:OG	2.17	0.60
1:E:143:LEU:C	1:E:145:GLY:H	2.09	0.60
1:E:844:GLN:HE22	2:L:79:LYS:CE	2.14	0.60
1:F:599:ASN:ND2	1:F:1241:LEU:O	2.34	0.60
1:G:844:GLN:HE22	2:N:79:LYS:CE	2.14	0.60
1:C:844:GLN:NE2	2:J:79:LYS:CE	2.65	0.60
1:C:862:TYR:CB	1:C:884:TRP:HA	2.31	0.60
1:C:882:LEU:HD12	1:C:903:ASP:HB2	1.83	0.60
1:D:884:TRP:HZ3	2:K:79:LYS:HA	1.56	0.60
1:F:143:LEU:C	1:F:145:GLY:H	2.09	0.60
1:G:844:GLN:NE2	2:N:79:LYS:CE	2.65	0.60
1:B:559:PRO:HD3	1:B:1171:GLU:OE1	2.00	0.60
1:B:862:TYR:HB3	1:B:884:TRP:HA	1.82	0.60
1:D:714:LEU:HB3	1:D:730:LEU:HD12	1.82	0.60
1:D:752:SER:OG	1:D:754:ASP:O	2.19	0.60
1:E:862:TYR:CB	1:E:884:TRP:HA	2.31	0.60
1:F:557:ARG:HH22	1:F:1175:THR:HG23	1.64	0.60
1:F:1210:SER:HB2	1:F:1212:THR:HG23	1.84	0.60
1:A:599:ASN:ND2	1:A:1241:LEU:O	2.34	0.60
1:B:569:CYS:HG	1:B:1213:PHE:HE1	1.50	0.60
1:B:862:TYR:CB	1:B:884:TRP:HA	2.31	0.60
1:C:145:GLY:HA2	1:C:259:GLN:NE2	2.15	0.60
1:D:557:ARG:HH22	1:D:1175:THR:HG23	1.64	0.60
1:E:882:LEU:HD13	1:E:1176:HIS:CE1	2.36	0.60
1:F:862:TYR:HB3	1:F:884:TRP:HA	1.82	0.60
1:F:884:TRP:HZ3	2:M:79:LYS:HD2	1.51	0.60
1:B:587:GLU:OE1	1:B:594:TYR:OH	2.18	0.60
1:B:752:SER:OG	1:B:754:ASP:O	2.19	0.60
1:D:862:TYR:CB	1:D:884:TRP:HA	2.31	0.60
1:A:844:GLN:HE22	2:H:79:LYS:CE	2.14	0.60
1:A:844:GLN:NE2	2:H:79:LYS:CE	2.65	0.60
1:A:862:TYR:CB	1:A:884:TRP:HA	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:844:GLN:NE2	2:I:79:LYS:CE	2.65	0.60
1:G:1210:SER:HB2	1:G:1212:THR:HG23	1.84	0.60
1:E:265:ARG:NH2	4:E:1301:DTP:O2G	2.31	0.60
1:F:882:LEU:HD13	1:F:1176:HIS:CE1	2.36	0.60
1:G:862:TYR:CB	1:G:884:TRP:HA	2.31	0.60
1:G:882:LEU:HD13	1:G:1176:HIS:CE1	2.36	0.60
1:C:358:SER:OG	1:D:274:MET:HG2	2.02	0.60
1:D:1210:SER:HB2	1:D:1212:THR:HG23	1.84	0.60
1:E:599:ASN:ND2	1:E:1241:LEU:O	2.34	0.60
1:F:844:GLN:NE2	2:M:79:LYS:CE	2.64	0.60
1:C:599:ASN:ND2	1:C:1241:LEU:O	2.34	0.59
1:E:1115:ASP:HB2	1:E:1120:LEU:HD11	1.84	0.59
1:F:882:LEU:HD13	1:F:1176:HIS:CD2	2.37	0.59
1:A:903:ASP:OD2	1:A:907:ARG:NH1	2.28	0.59
1:A:1115:ASP:HB2	1:A:1120:LEU:HD11	1.84	0.59
1:B:201:ASN:HD21	1:C:219:ASN:HD21	1.50	0.59
1:E:1210:SER:HB2	1:E:1212:THR:HG23	1.84	0.59
1:F:752:SER:OG	1:F:754:ASP:O	2.19	0.59
1:F:903:ASP:OD2	1:F:907:ARG:NH1	2.28	0.59
3:R:8:LEU:HD23	3:R:8:LEU:C	2.27	0.59
1:B:1115:ASP:HB2	1:B:1120:LEU:HD11	1.84	0.59
1:G:903:ASP:OD2	1:G:907:ARG:NH1	2.28	0.59
3:P:8:LEU:C	3:P:8:LEU:HD23	2.27	0.59
1:A:201:ASN:HD21	1:B:219:ASN:HD21	1.50	0.59
1:A:882:LEU:HD13	1:A:1176:HIS:CD2	2.38	0.59
1:B:143:LEU:C	1:B:145:GLY:H	2.09	0.59
1:C:844:GLN:HE22	2:J:79:LYS:CE	2.14	0.59
1:D:143:LEU:C	1:D:145:GLY:H	2.09	0.59
1:F:587:GLU:OE1	1:F:594:TYR:OH	2.18	0.59
1:D:1115:ASP:HB2	1:D:1120:LEU:HD11	1.84	0.59
1:E:715:LEU:HB3	1:E:727:LEU:HD11	1.85	0.59
1:B:882:LEU:HD13	1:B:1176:HIS:CD2	2.38	0.59
1:C:143:LEU:C	1:C:145:GLY:H	2.09	0.59
1:C:752:SER:OG	1:C:754:ASP:O	2.19	0.59
1:C:1210:SER:HB2	1:C:1212:THR:HG23	1.84	0.59
1:D:715:LEU:HB3	1:D:727:LEU:HD11	1.85	0.59
1:D:1131:ARG:NH2	1:D:1147:ASP:OD1	2.36	0.59
1:E:903:ASP:OD2	1:E:907:ARG:NH1	2.28	0.59
1:F:1115:ASP:HB2	1:F:1120:LEU:HD11	1.84	0.59
2:N:67:TYR:OH	2:N:80:MET:SD	2.57	0.59
3:Q:52:ARG:CG	3:R:38:HIS:CE1	2.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:715:LEU:HB3	1:F:727:LEU:HD11	1.85	0.59
1:A:143:LEU:C	1:A:145:GLY:H	2.09	0.59
1:A:1210:SER:HB2	1:A:1212:THR:HG23	1.84	0.59
1:C:1131:ARG:NH2	1:C:1147:ASP:OD1	2.36	0.59
1:E:1131:ARG:NH2	1:E:1147:ASP:OD1	2.36	0.59
1:G:1115:ASP:HB2	1:G:1120:LEU:HD11	1.84	0.59
3:P:41:GLU:HB3	3:P:45:ARG:NH1	2.17	0.59
3:Q:8:LEU:HD23	3:Q:8:LEU:C	2.27	0.59
1:D:882:LEU:HD13	1:D:1176:HIS:CD2	2.37	0.59
1:C:521:HIS:NE2	1:C:525:GLU:OE2	2.36	0.59
1:C:1031:ASN:HB3	1:C:1034:LEU:HD12	1.85	0.59
1:E:882:LEU:HD13	1:E:1176:HIS:CD2	2.37	0.59
1:G:463:GLN:OE1	1:G:466:ARG:NH2	2.28	0.59
1:A:521:HIS:NE2	1:A:525:GLU:OE2	2.36	0.58
1:D:558:GLN:HA	1:D:559:PRO:C	2.28	0.58
1:F:160:LYS:N	4:F:1301:DTP:O1A	2.20	0.58
1:G:143:LEU:C	1:G:145:GLY:H	2.09	0.58
1:G:882:LEU:HD13	1:G:1176:HIS:CD2	2.38	0.58
1:D:358:SER:OG	1:E:274:MET:HG2	2.03	0.58
1:E:1202:TRP:HA	1:E:1208:GLU:HB2	1.85	0.58
1:F:482:TYR:OH	1:F:490:HIS:NE2	2.35	0.58
1:F:1202:TRP:HA	1:F:1208:GLU:HB2	1.85	0.58
1:A:558:GLN:HA	1:A:559:PRO:C	2.28	0.58
1:B:48:THR:HG22	1:D:45:ASN:OD1	2.04	0.58
1:B:1031:ASN:HB3	1:B:1034:LEU:HD12	1.85	0.58
1:B:1210:SER:HB2	1:B:1212:THR:HG23	1.84	0.58
1:C:201:ASN:HD21	1:D:219:ASN:HD21	1.51	0.58
1:C:715:LEU:HB3	1:C:727:LEU:HD11	1.85	0.58
1:C:1092:ASP:OD2	1:C:1133:SER:OG	2.17	0.58
1:C:1115:ASP:HB2	1:C:1120:LEU:HD11	1.84	0.58
1:D:903:ASP:OD2	1:D:907:ARG:NH1	2.28	0.58
1:E:4:LYS:HA	1:F:237:ARG:HH21	1.68	0.58
1:F:558:GLN:HA	1:F:559:PRO:C	2.28	0.58
1:F:884:TRP:HZ3	2:M:79:LYS:HA	1.56	0.58
3:Q:52:ARG:HB3	3:R:38:HIS:CE1	2.37	0.58
1:C:882:LEU:HD13	1:C:1176:HIS:CD2	2.38	0.58
1:C:1202:TRP:HA	1:C:1208:GLU:HB2	1.85	0.58
1:D:1202:TRP:HA	1:D:1208:GLU:HB2	1.85	0.58
1:B:1131:ARG:NH2	1:B:1147:ASP:OD1	2.36	0.58
1:C:558:GLN:HA	1:C:559:PRO:C	2.28	0.58
3:O:8:LEU:HD23	3:O:8:LEU:C	2.27	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:884:TRP:HZ3	2:L:79:LYS:HA	1.56	0.58
1:F:1131:ARG:NH2	1:F:1147:ASP:OD1	2.36	0.58
1:G:884:TRP:CZ3	2:N:79:LYS:CA	2.74	0.58
1:A:1031:ASN:HB3	1:A:1034:LEU:HD12	1.85	0.58
1:B:265:ARG:NH2	4:B:1301:DTP:O2G	2.31	0.58
1:B:482:TYR:HH	1:B:490:HIS:HE2	1.50	0.58
1:D:265:ARG:NH2	4:D:1301:DTP:O2G	2.31	0.58
1:E:558:GLN:HA	1:E:559:PRO:C	2.28	0.58
1:F:1031:ASN:HB3	1:F:1034:LEU:HD12	1.85	0.58
1:G:558:GLN:HA	1:G:559:PRO:C	2.28	0.58
1:G:1131:ARG:NH2	1:G:1147:ASP:OD1	2.36	0.58
1:A:1131:ARG:NH2	1:A:1147:ASP:OD1	2.36	0.58
1:C:884:TRP:CH2	2:J:78:THR:O	2.57	0.58
1:D:1031:ASN:HB3	1:D:1034:LEU:HD12	1.85	0.58
1:G:1048:LYS:H	1:G:1062:SER:HA	1.69	0.58
1:B:42:LYS:HB3	1:B:59:MET:HE1	1.86	0.58
1:B:1202:TRP:HA	1:B:1208:GLU:HB2	1.85	0.58
1:C:587:GLU:OE1	1:C:594:TYR:OH	2.18	0.58
1:F:1048:LYS:H	1:F:1062:SER:HA	1.69	0.58
1:G:715:LEU:HB3	1:G:727:LEU:HD11	1.85	0.58
1:B:521:HIS:NE2	1:B:525:GLU:OE2	2.36	0.57
1:D:521:HIS:NE2	1:D:525:GLU:OE2	2.36	0.57
1:F:521:HIS:NE2	1:F:525:GLU:OE2	2.36	0.57
1:G:482:TYR:OH	1:G:490:HIS:NE2	2.36	0.57
1:A:715:LEU:HB3	1:A:727:LEU:HD11	1.85	0.57
1:B:558:GLN:HA	1:B:559:PRO:C	2.28	0.57
1:B:884:TRP:CH2	2:I:78:THR:O	2.57	0.57
1:D:884:TRP:CH2	2:K:78:THR:O	2.57	0.57
1:G:1202:TRP:HA	1:G:1208:GLU:HB2	1.86	0.57
1:B:715:LEU:HB3	1:B:727:LEU:HD11	1.85	0.57
1:D:201:ASN:HD21	1:E:219:ASN:HD21	1.52	0.57
1:B:454:GLN:OE1	1:B:458:LYS:NZ	2.38	0.57
1:D:454:GLN:OE1	1:D:458:LYS:NZ	2.38	0.57
1:E:358:SER:OG	1:F:274:MET:HG2	2.04	0.57
1:E:521:HIS:NE2	1:E:525:GLU:OE2	2.36	0.57
1:B:1048:LYS:H	1:B:1062:SER:HA	1.69	0.57
1:C:454:GLN:OE1	1:C:458:LYS:NZ	2.38	0.57
1:E:454:GLN:OE1	1:E:458:LYS:NZ	2.38	0.57
1:F:884:TRP:CH2	2:M:78:THR:O	2.57	0.57
1:G:521:HIS:NE2	1:G:525:GLU:OE2	2.36	0.57
1:A:454:GLN:OE1	1:A:458:LYS:NZ	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:884:TRP:CZ3	2:I:79:LYS:CA	2.74	0.57
1:D:1048:LYS:H	1:D:1062:SER:HA	1.69	0.57
1:E:1048:LYS:H	1:E:1062:SER:HA	1.69	0.57
1:G:42:LYS:HB3	1:G:59:MET:HE1	1.86	0.57
1:G:884:TRP:CH2	2:N:78:THR:O	2.57	0.57
1:G:1031:ASN:HB3	1:G:1034:LEU:HD12	1.85	0.57
1:A:1202:TRP:HA	1:A:1208:GLU:HB2	1.85	0.57
1:B:358:SER:OG	1:C:274:MET:HG2	2.04	0.57
1:D:42:LYS:HB3	1:D:59:MET:HE1	1.86	0.57
1:G:454:GLN:OE1	1:G:458:LYS:NZ	2.38	0.57
1:A:884:TRP:CH2	2:H:78:THR:O	2.57	0.57
1:D:1139:SER:O	1:D:1140:THR:HG22	2.05	0.57
1:G:264:THR:OG1	1:G:265:ARG:N	2.37	0.57
1:A:358:SER:OG	1:B:274:MET:HG2	2.04	0.57
1:C:763:ALA:HA	1:C:801:VAL:H	1.70	0.57
1:C:1048:LYS:H	1:C:1062:SER:HA	1.69	0.57
1:D:264:THR:OG1	1:D:265:ARG:N	2.37	0.57
1:E:763:ALA:HA	1:E:801:VAL:H	1.70	0.57
1:E:1031:ASN:HB3	1:E:1034:LEU:HD12	1.85	0.57
1:F:265:ARG:NH2	4:F:1301:DTP:O2G	2.31	0.57
1:F:454:GLN:OE1	1:F:458:LYS:NZ	2.38	0.57
1:G:1092:ASP:OD2	1:G:1133:SER:OG	2.17	0.57
1:G:1139:SER:O	1:G:1140:THR:HG22	2.05	0.57
1:B:264:THR:OG1	1:B:265:ARG:N	2.37	0.56
1:B:524:HIS:HB2	1:B:646:THR:CG2	2.32	0.56
1:F:264:THR:OG1	1:F:265:ARG:N	2.38	0.56
1:A:1139:SER:O	1:A:1140:THR:HG22	2.05	0.56
1:C:1139:SER:O	1:C:1140:THR:HG22	2.05	0.56
1:E:1092:ASP:OD2	1:E:1133:SER:OG	2.17	0.56
1:B:1139:SER:O	1:B:1140:THR:HG22	2.05	0.56
1:E:524:HIS:HB2	1:E:646:THR:CG2	2.32	0.56
1:B:1023:ASP:OD1	1:B:1046:THR:OG1	2.24	0.56
1:C:590:ASN:C	1:C:592:MET:N	2.64	0.56
1:C:884:TRP:CZ3	2:J:79:LYS:CA	2.74	0.56
1:D:569:CYS:HB3	1:D:600:LYS:HZ3	1.71	0.56
1:E:42:LYS:HB3	1:E:59:MET:HE1	1.86	0.56
1:E:884:TRP:CH2	2:L:78:THR:O	2.57	0.56
1:A:264:THR:OG1	1:A:265:ARG:N	2.37	0.56
1:C:716:LEU:HB3	1:C:728:TRP:HB2	1.87	0.56
1:D:463:GLN:OE1	1:D:466:ARG:NH2	2.28	0.56
1:E:264:THR:OG1	1:E:265:ARG:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:HIS:HB2	1:A:646:THR:CG2	2.32	0.56
1:A:565:GLN:NE2	1:A:1213:PHE:CA	2.69	0.56
1:A:1048:LYS:H	1:A:1062:SER:HA	1.69	0.56
1:F:1139:SER:O	1:F:1140:THR:HG22	2.05	0.56
2:L:67:TYR:OH	2:L:80:MET:SD	2.57	0.56
1:C:1086:GLY:CA	2:J:39:LYS:NZ	2.66	0.56
1:G:565:GLN:NE2	1:G:1213:PHE:CA	2.69	0.56
1:G:716:LEU:HB3	1:G:728:TRP:HB2	1.87	0.56
1:A:844:GLN:HE22	2:H:79:LYS:HE3	1.71	0.56
1:A:1023:ASP:OD1	1:A:1046:THR:OG1	2.24	0.56
1:B:763:ALA:HA	1:B:801:VAL:H	1.70	0.56
1:D:716:LEU:HB3	1:D:728:TRP:HB2	1.87	0.56
1:E:1139:SER:O	1:E:1140:THR:HG22	2.05	0.56
2:M:67:TYR:OH	2:M:80:MET:SD	2.57	0.56
1:A:170:ASP:OD1	1:A:171:HIS:N	2.39	0.56
1:B:844:GLN:HE22	2:I:79:LYS:HE3	1.71	0.56
1:C:264:THR:OG1	1:C:265:ARG:N	2.37	0.56
1:C:326:LEU:HD13	1:C:353:ILE:CG2	2.37	0.56
1:D:326:LEU:HD13	1:D:353:ILE:CG2	2.36	0.56
3:P:50:SER:CB	3:Q:45:ARG:NH1	2.64	0.56
1:C:1023:ASP:OD1	1:C:1046:THR:OG1	2.24	0.55
1:D:884:TRP:CZ3	2:K:79:LYS:CA	2.74	0.55
1:E:326:LEU:HD13	1:E:353:ILE:CG2	2.36	0.55
1:F:336:ASN:HB2	1:G:431:LYS:HE3	1.87	0.55
1:G:844:GLN:HE22	2:N:79:LYS:HE3	1.71	0.55
1:A:463:GLN:OE1	1:A:466:ARG:NH2	2.28	0.55
1:B:170:ASP:OD1	1:B:171:HIS:N	2.39	0.55
1:B:326:LEU:HD13	1:B:353:ILE:CG2	2.37	0.55
1:B:1092:ASP:OD2	1:B:1133:SER:OG	2.17	0.55
1:G:170:ASP:OD1	1:G:171:HIS:N	2.39	0.55
1:A:326:LEU:HD13	1:A:353:ILE:CG2	2.37	0.55
1:A:716:LEU:HB3	1:A:728:TRP:HB2	1.87	0.55
1:A:884:TRP:CZ3	2:H:79:LYS:CA	2.74	0.55
1:B:845:TYR:HB3	1:B:858:ALA:HB3	1.89	0.55
1:C:217:PRO:HG3	1:C:226:ARG:HH12	1.72	0.55
1:C:844:GLN:HE22	2:J:79:LYS:HE3	1.71	0.55
1:D:217:PRO:HG3	1:D:226:ARG:HH12	1.71	0.55
1:A:763:ALA:HA	1:A:801:VAL:H	1.70	0.55
1:C:617:ALA:HA	1:C:904:GLN:HG2	1.89	0.55
1:C:845:TYR:HB3	1:C:858:ALA:HB3	1.89	0.55
1:D:572:GLU:HA	1:D:577:TYR:CD2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:884:TRP:N	1:E:884:TRP:CD1	2.73	0.55
1:F:572:GLU:HA	1:F:577:TYR:CD2	2.42	0.55
1:F:716:LEU:HB3	1:F:728:TRP:HB2	1.87	0.55
1:F:763:ALA:HA	1:F:801:VAL:H	1.70	0.55
1:G:590:ASN:C	1:G:592:MET:N	2.64	0.55
1:G:763:ALA:HA	1:G:801:VAL:H	1.70	0.55
1:A:845:TYR:HB3	1:A:858:ALA:HB3	1.89	0.55
1:B:572:GLU:HA	1:B:577:TYR:CD2	2.42	0.55
1:C:170:ASP:OD1	1:C:171:HIS:N	2.39	0.55
1:C:463:GLN:OE1	1:C:466:ARG:NH2	2.28	0.55
1:C:572:GLU:HA	1:C:577:TYR:CD2	2.42	0.55
1:D:763:ALA:HA	1:D:801:VAL:H	1.70	0.55
1:E:572:GLU:HA	1:E:577:TYR:CD2	2.42	0.55
1:F:326:LEU:HD13	1:F:353:ILE:CG2	2.36	0.55
1:A:572:GLU:HA	1:A:577:TYR:CD2	2.42	0.55
1:B:28:HIS:CE1	3:P:14:LEU:CD2	2.90	0.55
1:B:565:GLN:NE2	1:B:1213:PHE:CA	2.69	0.55
1:B:1086:GLY:CA	2:I:39:LYS:NZ	2.66	0.55
1:C:565:GLN:NE2	1:C:1213:PHE:CA	2.69	0.55
1:D:617:ALA:HA	1:D:904:GLN:HG2	1.89	0.55
1:D:844:GLN:HE22	2:K:79:LYS:HE3	1.71	0.55
1:F:217:PRO:HG3	1:F:226:ARG:HH12	1.71	0.55
1:G:326:LEU:HD13	1:G:353:ILE:CG2	2.36	0.55
1:G:572:GLU:HA	1:G:577:TYR:CD2	2.42	0.55
1:E:716:LEU:HB3	1:E:728:TRP:HB2	1.87	0.55
3:O:27:ASP:OD1	3:R:13:ARG:HG2	2.06	0.55
1:A:1092:ASP:OD2	1:A:1133:SER:OG	2.17	0.55
1:D:170:ASP:OD1	1:D:171:HIS:N	2.39	0.55
1:D:565:GLN:NE2	1:D:1213:PHE:CA	2.69	0.55
1:E:565:GLN:NE2	1:E:1213:PHE:CA	2.69	0.55
1:F:844:GLN:HE22	2:M:79:LYS:HE3	1.71	0.55
1:G:845:TYR:HB3	1:G:858:ALA:HB3	1.89	0.55
3:R:15:ARG:HD2	3:R:19:GLU:OE2	2.07	0.55
1:D:1086:GLY:CA	2:K:39:LYS:NZ	2.66	0.55
1:F:170:ASP:OD1	1:F:171:HIS:N	2.39	0.55
2:N:60:GLY:N	2:N:63:THR:OG1	2.34	0.55
1:B:617:ALA:HA	1:B:904:GLN:HG2	1.89	0.55
1:D:845:TYR:HB3	1:D:858:ALA:HB3	1.89	0.55
1:D:884:TRP:N	1:D:884:TRP:CD1	2.73	0.55
1:F:524:HIS:HB2	1:F:646:THR:CG2	2.32	0.55
1:A:482:TYR:HH	1:A:490:HIS:HE2	1.47	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:565:GLN:NE2	1:F:1213:PHE:CA	2.69	0.54
1:A:550:LEU:HD21	1:A:607:SER:CB	2.35	0.54
1:B:716:LEU:HB3	1:B:728:TRP:HB2	1.87	0.54
1:B:1219:ASN:HB2	1:B:1237:ASN:HB3	1.89	0.54
1:E:170:ASP:OD1	1:E:171:HIS:N	2.39	0.54
1:E:844:GLN:HE22	2:L:79:LYS:HE3	1.71	0.54
1:G:265:ARG:HH11	1:G:371:SER:HG	1.52	0.54
1:G:1023:ASP:OD1	1:G:1046:THR:OG1	2.24	0.54
1:C:1219:ASN:HB2	1:C:1237:ASN:HB3	1.89	0.54
1:F:550:LEU:HD21	1:F:607:SER:CB	2.35	0.54
1:F:590:ASN:C	1:F:592:MET:N	2.64	0.54
1:F:884:TRP:N	1:F:884:TRP:CD1	2.73	0.54
1:B:482:TYR:OH	1:B:490:HIS:NE2	2.35	0.54
1:C:727:LEU:HB3	1:C:737:ASN:HB2	1.90	0.54
1:D:800:ILE:H	1:D:818:LYS:HE2	1.73	0.54
1:D:1087:THR:N	2:K:39:LYS:HZ3	2.06	0.54
1:E:217:PRO:HG3	1:E:226:ARG:HH12	1.71	0.54
1:E:617:ALA:HA	1:E:904:GLN:HG2	1.89	0.54
1:A:217:PRO:HG3	1:A:226:ARG:HH12	1.71	0.54
1:A:219:ASN:HD21	1:G:201:ASN:HD21	1.54	0.54
1:D:727:LEU:HB3	1:D:737:ASN:HB2	1.90	0.54
1:D:1023:ASP:OD1	1:D:1046:THR:OG1	2.24	0.54
1:F:800:ILE:H	1:F:818:LYS:HE2	1.73	0.54
1:B:800:ILE:H	1:B:818:LYS:HE2	1.73	0.54
1:C:1030:TRP:CD1	1:C:1037:CYS:HG	2.26	0.54
1:E:884:TRP:CZ3	2:L:79:LYS:CA	2.74	0.54
3:O:15:ARG:HD2	3:O:19:GLU:OE2	2.07	0.54
1:B:217:PRO:HG3	1:B:226:ARG:HH12	1.72	0.54
1:B:727:LEU:HB3	1:B:737:ASN:HB2	1.90	0.54
1:C:800:ILE:H	1:C:818:LYS:HE2	1.73	0.54
1:C:884:TRP:H	1:C:884:TRP:CD1	2.25	0.54
1:D:612:ARG:NH2	1:D:903:ASP:O	2.41	0.54
1:E:727:LEU:HB3	1:E:737:ASN:HB2	1.90	0.54
1:F:612:ARG:NH2	1:F:903:ASP:O	2.41	0.54
1:F:845:TYR:HB3	1:F:858:ALA:HB3	1.89	0.54
2:I:40:THR:HA	2:I:59:TRP:HE1	1.73	0.54
2:I:67:TYR:OH	2:I:80:MET:SD	2.57	0.54
1:A:800:ILE:H	1:A:818:LYS:HE2	1.73	0.54
1:A:1219:ASN:HB2	1:A:1237:ASN:HB3	1.89	0.54
1:C:265:ARG:NH1	1:C:371:SER:OG	2.37	0.54
1:D:30:ILE:CG2	3:Q:10:ARG:CB	2.80	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:266:ASP:CG	1:E:268:SER:HG	2.16	0.54
1:F:266:ASP:CG	1:F:268:SER:HG	2.15	0.54
1:A:265:ARG:HH11	1:A:371:SER:HG	1.56	0.54
1:A:266:ASP:CG	1:A:268:SER:HG	2.15	0.54
1:G:482:TYR:HH	1:G:490:HIS:HE2	1.52	0.54
1:G:550:LEU:HD21	1:G:607:SER:CB	2.35	0.54
2:L:40:THR:HA	2:L:59:TRP:HE1	1.73	0.54
1:A:617:ALA:HA	1:A:904:GLN:HG2	1.89	0.54
1:A:864:VAL:CG2	1:A:885:VAL:HG21	2.38	0.54
1:B:336:ASN:HB2	1:C:431:LYS:HE3	1.90	0.54
1:D:884:TRP:CD1	1:D:884:TRP:H	2.25	0.54
1:D:1219:ASN:HB2	1:D:1237:ASN:HB3	1.89	0.54
1:F:265:ARG:HH11	1:F:371:SER:HG	1.55	0.54
1:F:987:ILE:HD11	1:F:1018:LEU:HD22	1.90	0.54
1:F:1219:ASN:HB2	1:F:1237:ASN:HB3	1.89	0.54
1:G:217:PRO:HG3	1:G:226:ARG:HH12	1.72	0.54
1:G:612:ARG:NH2	1:G:903:ASP:O	2.41	0.54
3:Q:15:ARG:HD2	3:Q:19:GLU:OE2	2.07	0.54
1:B:13:ARG:O	1:B:17:GLU:HG3	2.09	0.53
1:B:612:ARG:NH2	1:B:903:ASP:O	2.41	0.53
1:F:727:LEU:HB3	1:F:737:ASN:HB2	1.90	0.53
1:F:884:TRP:CD1	1:F:884:TRP:H	2.26	0.53
1:A:844:GLN:HE22	2:H:79:LYS:HZ2	1.55	0.53
1:D:524:HIS:HB2	1:D:646:THR:CG2	2.32	0.53
1:E:845:TYR:HB3	1:E:858:ALA:HB3	1.89	0.53
1:E:884:TRP:CD1	1:E:884:TRP:H	2.25	0.53
1:E:987:ILE:HD11	1:E:1018:LEU:HD22	1.90	0.53
1:F:266:ASP:OD1	1:F:267:LYS:N	2.41	0.53
1:G:800:ILE:H	1:G:818:LYS:HE2	1.73	0.53
1:A:266:ASP:OD1	1:A:267:LYS:N	2.41	0.53
1:B:884:TRP:CD1	1:B:884:TRP:H	2.25	0.53
1:C:266:ASP:OD1	1:C:267:LYS:N	2.42	0.53
1:C:1061:TRP:CE2	1:C:1090:SER:HA	2.43	0.53
1:E:266:ASP:OD1	1:E:267:LYS:N	2.42	0.53
1:E:612:ARG:NH2	1:E:903:ASP:O	2.41	0.53
1:E:1023:ASP:OD1	1:E:1046:THR:OG1	2.24	0.53
1:F:1023:ASP:OD1	1:F:1046:THR:OG1	2.24	0.53
2:K:40:THR:HA	2:K:59:TRP:HE1	1.73	0.53
2:N:40:THR:HA	2:N:59:TRP:HE1	1.73	0.53
1:C:864:VAL:CG2	1:C:885:VAL:HG21	2.38	0.53
1:D:13:ARG:O	1:D:17:GLU:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1061:TRP:CE2	1:D:1090:SER:HA	2.43	0.53
1:E:698:HIS:CE1	1:E:726:LYS:HD2	2.44	0.53
1:E:864:VAL:CG2	1:E:885:VAL:HG21	2.38	0.53
1:E:1061:TRP:CE2	1:E:1090:SER:HA	2.43	0.53
1:F:358:SER:OG	1:G:274:MET:HG2	2.09	0.53
1:G:266:ASP:OD1	1:G:267:LYS:N	2.41	0.53
1:G:864:VAL:CG2	1:G:885:VAL:HG21	2.38	0.53
1:G:987:ILE:HD11	1:G:1018:LEU:HD22	1.91	0.53
1:A:612:ARG:NH2	1:A:903:ASP:O	2.41	0.53
1:A:884:TRP:N	1:A:884:TRP:CD1	2.73	0.53
1:B:1061:TRP:CE2	1:B:1090:SER:HA	2.43	0.53
1:E:13:ARG:O	1:E:17:GLU:HG3	2.09	0.53
1:E:800:ILE:H	1:E:818:LYS:HE2	1.73	0.53
1:F:617:ALA:HA	1:F:904:GLN:HG2	1.89	0.53
1:G:1030:TRP:CD1	1:G:1037:CYS:HG	2.27	0.53
1:B:584:ALA:HB1	1:B:594:TYR:CD2	2.44	0.53
1:B:884:TRP:CD1	1:B:884:TRP:N	2.73	0.53
1:C:612:ARG:NH2	1:C:903:ASP:O	2.41	0.53
1:D:1149:GLY:HA3	1:D:1178:GLY:HA2	1.91	0.53
1:E:1149:GLY:HA3	1:E:1178:GLY:HA2	1.91	0.53
1:G:884:TRP:CD1	1:G:884:TRP:H	2.25	0.53
2:M:40:THR:HA	2:M:59:TRP:HE1	1.73	0.53
1:A:698:HIS:CE1	1:A:726:LYS:HD2	2.44	0.53
1:A:1086:GLY:CA	2:H:39:LYS:NZ	2.66	0.53
1:A:1087:THR:N	2:H:39:LYS:HZ3	2.06	0.53
1:B:463:GLN:OE1	1:B:466:ARG:NH2	2.28	0.53
1:C:884:TRP:CD1	1:C:884:TRP:N	2.73	0.53
1:D:864:VAL:CG2	1:D:885:VAL:HG21	2.38	0.53
1:D:987:ILE:HD11	1:D:1018:LEU:HD22	1.90	0.53
1:G:727:LEU:HB3	1:G:737:ASN:HB2	1.90	0.53
1:G:1149:GLY:HA3	1:G:1178:GLY:HA2	1.91	0.53
2:J:40:THR:HA	2:J:59:TRP:HE1	1.73	0.53
1:A:336:ASN:HB2	1:B:431:LYS:HE3	1.90	0.53
1:A:1149:GLY:HA3	1:A:1178:GLY:HA2	1.91	0.53
1:B:266:ASP:OD1	1:B:267:LYS:N	2.41	0.53
1:B:864:VAL:CG2	1:B:885:VAL:HG21	2.38	0.53
1:C:267:LYS:HZ1	1:C:419:VAL:HG12	1.74	0.53
1:F:864:VAL:CG2	1:F:885:VAL:HG21	2.38	0.53
1:G:524:HIS:HB2	1:G:646:THR:CG2	2.32	0.53
1:A:267:LYS:HZ1	1:A:419:VAL:HG12	1.74	0.53
1:A:727:LEU:HB3	1:A:737:ASN:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:584:ALA:HB1	1:D:594:TYR:CD2	2.44	0.53
1:F:698:HIS:CE1	1:F:726:LYS:HD2	2.44	0.53
1:G:617:ALA:HA	1:G:904:GLN:HG2	1.89	0.53
1:G:698:HIS:CE1	1:G:726:LYS:HD2	2.44	0.53
1:G:1219:ASN:HB2	1:G:1237:ASN:HB3	1.90	0.53
1:C:524:HIS:HB2	1:C:646:THR:CG2	2.32	0.53
1:C:584:ALA:HB1	1:C:594:TYR:CD2	2.44	0.53
1:D:698:HIS:CE1	1:D:726:LYS:HD2	2.44	0.53
1:F:631:ALA:HB1	1:F:639:LEU:HD11	1.91	0.53
1:F:1061:TRP:CE2	1:F:1090:SER:HA	2.43	0.53
1:F:1149:GLY:HA3	1:F:1178:GLY:HA2	1.91	0.53
1:F:1191:MET:SD	1:F:1209:SER:OG	2.63	0.53
2:H:40:THR:HA	2:H:59:TRP:HE1	1.73	0.53
1:D:266:ASP:OD1	1:D:267:LYS:N	2.41	0.52
1:D:267:LYS:HZ1	1:D:419:VAL:HG12	1.74	0.52
1:E:1219:ASN:HB2	1:E:1237:ASN:HB3	1.89	0.52
1:G:13:ARG:O	1:G:17:GLU:HG3	2.08	0.52
1:G:884:TRP:CD1	1:G:884:TRP:N	2.73	0.52
1:A:884:TRP:CD1	1:A:884:TRP:H	2.25	0.52
1:A:1061:TRP:CE2	1:A:1090:SER:HA	2.43	0.52
1:C:1149:GLY:HA3	1:C:1178:GLY:HA2	1.91	0.52
1:D:609:LEU:HD23	1:D:908:LEU:HD13	1.91	0.52
1:E:336:ASN:HB2	1:F:431:LYS:HE3	1.91	0.52
1:G:584:ALA:HB1	1:G:594:TYR:CD2	2.44	0.52
1:A:987:ILE:HD11	1:A:1018:LEU:HD22	1.90	0.52
1:B:326:LEU:HD13	1:B:353:ILE:HG22	1.92	0.52
1:B:1126:HIS:CE1	1:B:1129:CYS:H	2.28	0.52
1:B:1149:GLY:HA3	1:B:1178:GLY:HA2	1.91	0.52
1:C:698:HIS:CE1	1:C:726:LYS:HD2	2.44	0.52
1:E:631:ALA:HB1	1:E:639:LEU:HD11	1.91	0.52
1:G:945:ARG:HD2	1:G:961:GLU:HB2	1.92	0.52
1:G:1061:TRP:CE2	1:G:1090:SER:HA	2.43	0.52
2:K:67:TYR:OH	2:K:80:MET:SD	2.57	0.52
1:A:365:ASP:OD1	1:A:444:PHE:CE1	2.63	0.52
1:B:265:ARG:HH11	1:B:371:SER:HG	1.55	0.52
1:B:1087:THR:N	2:I:39:LYS:HZ3	2.07	0.52
1:C:265:ARG:HH11	1:C:371:SER:HG	1.57	0.52
1:E:267:LYS:HZ1	1:E:419:VAL:HG12	1.74	0.52
1:E:609:LEU:HD23	1:E:908:LEU:HD13	1.91	0.52
1:G:365:ASP:OD1	1:G:444:PHE:CE1	2.63	0.52
3:P:50:SER:HB3	3:Q:45:ARG:NH1	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:584:ALA:HB1	1:A:594:TYR:CD2	2.44	0.52
1:C:336:ASN:HB2	1:D:431:LYS:HE3	1.91	0.52
1:D:326:LEU:HD13	1:D:353:ILE:HG22	1.92	0.52
1:F:267:LYS:HZ1	1:F:419:VAL:HG12	1.74	0.52
1:F:945:ARG:HD2	1:F:961:GLU:HB2	1.92	0.52
2:M:60:GLY:N	2:M:63:THR:OG1	2.34	0.52
1:A:945:ARG:HD2	1:A:961:GLU:HB2	1.92	0.52
1:C:326:LEU:HD13	1:C:353:ILE:HG22	1.92	0.52
1:E:326:LEU:HD13	1:E:353:ILE:HG22	1.92	0.52
1:E:584:ALA:HB1	1:E:594:TYR:CD2	2.44	0.52
1:G:631:ALA:HB1	1:G:639:LEU:HD11	1.91	0.52
1:G:844:GLN:NE2	2:N:79:LYS:NZ	2.58	0.52
2:H:67:TYR:OH	2:H:80:MET:SD	2.57	0.52
1:B:267:LYS:HZ1	1:B:419:VAL:HG12	1.75	0.52
1:B:987:ILE:HD11	1:B:1018:LEU:HD22	1.90	0.52
1:C:987:ILE:HD11	1:C:1018:LEU:HD22	1.90	0.52
1:D:37:ILE:HG12	3:Q:10:ARG:CD	2.40	0.52
1:D:725:LEU:HB2	1:D:739:MET:HB2	1.92	0.52
1:F:365:ASP:OD1	1:F:444:PHE:CE1	2.63	0.52
1:A:326:LEU:HD13	1:A:353:ILE:HG22	1.92	0.52
1:A:609:LEU:HD23	1:A:908:LEU:HD13	1.91	0.52
1:A:882:LEU:HD12	1:A:1176:HIS:NE2	2.25	0.52
1:B:550:LEU:HD21	1:B:607:SER:CB	2.35	0.52
1:C:1126:HIS:CE1	1:C:1129:CYS:H	2.28	0.52
1:D:14:GLU:HB2	1:E:31:SER:OG	2.09	0.52
1:D:864:VAL:HG23	1:D:885:VAL:HG21	1.92	0.52
1:E:945:ARG:HD2	1:E:961:GLU:HB2	1.92	0.52
1:A:1126:HIS:CE1	1:A:1129:CYS:H	2.28	0.52
1:B:365:ASP:OD1	1:B:444:PHE:CE1	2.63	0.52
1:E:365:ASP:OD1	1:E:444:PHE:CE1	2.63	0.52
1:F:326:LEU:HD13	1:F:353:ILE:HG22	1.92	0.52
1:A:265:ARG:NH2	4:A:1301:DTP:O2G	2.31	0.52
1:A:416:GLN:HE21	1:G:334:PHE:HE1	1.57	0.52
1:A:530:ARG:HD2	1:A:545:GLN:HE22	1.75	0.52
1:B:698:HIS:CE1	1:B:726:LYS:HD2	2.44	0.52
1:B:945:ARG:HD2	1:B:961:GLU:HB2	1.92	0.52
1:C:864:VAL:HG23	1:C:885:VAL:HG21	1.92	0.52
1:D:844:GLN:NE2	2:K:79:LYS:NZ	2.57	0.52
1:D:882:LEU:HD12	1:D:1176:HIS:NE2	2.25	0.52
1:D:1126:HIS:CE1	1:D:1129:CYS:H	2.28	0.52
1:E:864:VAL:HG23	1:E:885:VAL:HG21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:584:ALA:HB1	1:F:594:TYR:CD2	2.44	0.52
1:G:609:LEU:HD23	1:G:908:LEU:HD13	1.91	0.52
1:B:844:GLN:NE2	2:I:79:LYS:NZ	2.57	0.51
1:C:609:LEU:HD23	1:C:908:LEU:HD13	1.91	0.51
1:E:550:LEU:HD21	1:E:607:SER:CB	2.35	0.51
1:E:600:LYS:HZ1	1:E:1213:PHE:HZ	1.58	0.51
1:G:265:ARG:NH1	1:G:371:SER:OG	2.37	0.51
1:A:844:GLN:NE2	2:H:79:LYS:NZ	2.58	0.51
1:E:725:LEU:HB2	1:E:739:MET:HB2	1.92	0.51
1:F:882:LEU:HD12	1:F:1176:HIS:NE2	2.25	0.51
1:G:267:LYS:HZ1	1:G:419:VAL:HG12	1.74	0.51
2:J:60:GLY:N	2:J:63:THR:OG1	2.34	0.51
1:A:1030:TRP:CD1	1:A:1037:CYS:HG	2.28	0.51
1:C:550:LEU:HD21	1:C:607:SER:CB	2.35	0.51
1:C:725:LEU:HB2	1:C:739:MET:HB2	1.92	0.51
1:F:337:ARG:NH1	1:G:409:GLU:OE2	2.44	0.51
1:G:326:LEU:HD13	1:G:353:ILE:HG22	1.92	0.51
1:B:400:LEU:HB3	1:B:404:TRP:CZ3	2.46	0.51
1:C:334:PHE:HE1	1:D:416:GLN:HE21	1.57	0.51
1:C:400:LEU:HB3	1:C:404:TRP:CZ3	2.46	0.51
1:D:365:ASP:OD1	1:D:444:PHE:CE1	2.63	0.51
1:D:530:ARG:HD2	1:D:545:GLN:HE22	1.75	0.51
1:D:550:LEU:HD21	1:D:607:SER:CB	2.35	0.51
1:D:631:ALA:HB1	1:D:639:LEU:HD11	1.91	0.51
1:E:530:ARG:HD2	1:E:545:GLN:HE22	1.76	0.51
1:F:609:LEU:HD23	1:F:908:LEU:HD13	1.91	0.51
1:F:692:VAL:HG12	1:F:693:HIS:ND1	2.26	0.51
1:F:884:TRP:CZ3	2:M:79:LYS:CA	2.74	0.51
1:G:864:VAL:HG23	1:G:885:VAL:HG21	1.92	0.51
1:A:692:VAL:HG12	1:A:693:HIS:ND1	2.25	0.51
1:A:725:LEU:HB2	1:A:739:MET:HB2	1.92	0.51
1:B:609:LEU:HD23	1:B:908:LEU:HD13	1.91	0.51
1:B:762:SER:OG	1:B:764:ASP:OD1	2.26	0.51
1:D:1191:MET:SD	1:D:1209:SER:OG	2.63	0.51
1:E:882:LEU:HD12	1:E:1176:HIS:NE2	2.25	0.51
1:F:844:GLN:NE2	2:M:79:LYS:NZ	2.57	0.51
2:K:60:GLY:N	2:K:63:THR:OG1	2.34	0.51
3:P:50:SER:HB3	3:Q:45:ARG:HH12	1.74	0.51
1:B:692:VAL:HG12	1:B:693:HIS:ND1	2.26	0.51
1:B:1030:TRP:CD1	1:B:1037:CYS:HG	2.28	0.51
1:C:692:VAL:HG12	1:C:693:HIS:ND1	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1086:GLY:HA2	2:L:39:LYS:HE2	1.92	0.51
1:F:530:ARG:HD2	1:F:545:GLN:HE22	1.75	0.51
1:F:1126:HIS:CE1	1:F:1129:CYS:H	2.28	0.51
1:C:365:ASP:OD1	1:C:444:PHE:CE1	2.63	0.51
1:G:1086:GLY:HA2	2:N:39:LYS:HE2	1.92	0.51
1:G:1086:GLY:CA	2:N:39:LYS:NZ	2.66	0.51
1:G:1126:HIS:CE1	1:G:1129:CYS:H	2.28	0.51
2:L:60:GLY:N	2:L:63:THR:OG1	2.34	0.51
1:A:400:LEU:HB3	1:A:404:TRP:CZ3	2.46	0.51
1:A:631:ALA:HB1	1:A:639:LEU:HD11	1.91	0.51
1:B:725:LEU:HB2	1:B:739:MET:HB2	1.92	0.51
1:B:864:VAL:HG23	1:B:885:VAL:HG21	1.92	0.51
1:C:945:ARG:HD2	1:C:961:GLU:HB2	1.92	0.51
1:D:336:ASN:HB2	1:E:431:LYS:HE3	1.93	0.51
1:D:400:LEU:HB3	1:D:404:TRP:CZ3	2.46	0.51
1:F:265:ARG:NH1	1:F:371:SER:OG	2.37	0.51
1:F:762:SER:OG	1:F:764:ASP:OD1	2.26	0.51
2:H:60:GLY:N	2:H:63:THR:OG1	2.34	0.51
1:C:530:ARG:HD2	1:C:545:GLN:HE22	1.76	0.51
1:E:1126:HIS:CE1	1:E:1129:CYS:H	2.28	0.51
1:G:152:ILE:HD11	1:G:263:THR:HG22	1.92	0.51
3:P:32:ARG:HD2	3:P:76:CYS:SG	2.51	0.51
1:B:530:ARG:HD2	1:B:545:GLN:HE22	1.76	0.51
1:B:1002:HIS:ND1	1:B:1024:ASP:OD2	2.44	0.51
1:C:562:ASN:HB2	1:C:565:GLN:HG2	1.93	0.51
1:C:762:SER:OG	1:C:764:ASP:OD1	2.26	0.51
1:F:334:PHE:HE1	1:G:416:GLN:HE21	1.58	0.51
1:F:725:LEU:HB2	1:F:739:MET:HB2	1.92	0.51
1:G:530:ARG:HD2	1:G:545:GLN:HE22	1.76	0.51
1:G:725:LEU:HB2	1:G:739:MET:HB2	1.92	0.51
1:G:882:LEU:HD12	1:G:1176:HIS:NE2	2.25	0.51
1:A:152:ILE:HD11	1:A:263:THR:HG22	1.92	0.50
1:A:864:VAL:HG23	1:A:885:VAL:HG21	1.92	0.50
1:B:608:ARG:HD2	1:B:910:GLU:HB2	1.94	0.50
1:C:844:GLN:NE2	2:J:79:LYS:NZ	2.57	0.50
1:D:562:ASN:HB2	1:D:565:GLN:HG2	1.94	0.50
1:D:945:ARG:HD2	1:D:961:GLU:HB2	1.92	0.50
1:E:692:VAL:HG12	1:E:693:HIS:ND1	2.26	0.50
1:F:864:VAL:HG23	1:F:885:VAL:HG21	1.92	0.50
2:I:60:GLY:N	2:I:63:THR:OG1	2.34	0.50
3:O:32:ARG:HD2	3:O:76:CYS:SG	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:700:GLU:HG3	1:B:721:SER:HB2	1.94	0.50
1:C:1002:HIS:ND1	1:C:1024:ASP:OD2	2.45	0.50
1:D:1002:HIS:ND1	1:D:1024:ASP:OD2	2.44	0.50
1:E:400:LEU:HB3	1:E:404:TRP:CZ3	2.46	0.50
1:E:844:GLN:HE22	2:L:79:LYS:HZ2	1.59	0.50
1:F:862:TYR:HB3	1:F:884:TRP:CA	2.42	0.50
1:F:1002:HIS:ND1	1:F:1024:ASP:OD2	2.44	0.50
1:A:334:PHE:HE1	1:B:416:GLN:HE21	1.58	0.50
1:A:608:ARG:HD2	1:A:910:GLU:HB2	1.94	0.50
1:A:1002:HIS:ND1	1:A:1024:ASP:OD2	2.44	0.50
1:B:344:GLN:OE1	1:B:349:GLN:NE2	2.44	0.50
1:B:562:ASN:HB2	1:B:565:GLN:HG2	1.94	0.50
1:C:1086:GLY:HA2	2:J:39:LYS:HE2	1.92	0.50
1:G:819:ASN:ND2	1:G:840:HIS:O	2.45	0.50
1:C:348:LYS:NZ	1:C:443:ASP:OD1	2.45	0.50
1:G:692:VAL:HG12	1:G:693:HIS:ND1	2.26	0.50
1:G:1002:HIS:ND1	1:G:1024:ASP:OD2	2.44	0.50
3:P:15:ARG:HD2	3:P:19:GLU:OE2	2.07	0.50
1:A:431:LYS:HE3	1:G:336:ASN:HB2	1.92	0.50
1:A:482:TYR:OH	1:A:490:HIS:NE2	2.35	0.50
1:A:762:SER:OG	1:A:764:ASP:OD1	2.26	0.50
1:B:631:ALA:HB1	1:B:639:LEU:HD11	1.91	0.50
1:D:155:MET:HE1	1:D:441:GLN:HG3	1.92	0.50
1:E:562:ASN:HB2	1:E:565:GLN:HG2	1.94	0.50
1:E:862:TYR:HB3	1:E:884:TRP:CA	2.42	0.50
1:E:1030:TRP:CD1	1:E:1037:CYS:HG	2.28	0.50
1:F:152:ILE:HD11	1:F:263:THR:HG22	1.92	0.50
1:G:400:LEU:HB3	1:G:404:TRP:CZ3	2.46	0.50
3:Q:52:ARG:HD2	3:R:38:HIS:ND1	2.22	0.50
1:B:152:ILE:HD11	1:B:263:THR:HG22	1.92	0.50
1:B:348:LYS:NZ	1:B:443:ASP:OD1	2.45	0.50
1:C:882:LEU:HD12	1:C:1176:HIS:NE2	2.25	0.50
1:D:265:ARG:NH1	1:D:371:SER:OG	2.37	0.50
1:D:348:LYS:NZ	1:D:443:ASP:OD1	2.45	0.50
1:E:463:GLN:OE1	1:E:466:ARG:NH2	2.28	0.50
1:F:562:ASN:HB2	1:F:565:GLN:HG2	1.93	0.50
1:F:819:ASN:ND2	1:F:840:HIS:O	2.45	0.50
1:G:646:THR:HG23	1:G:648:GLU:HG3	1.94	0.50
1:A:700:GLU:HG3	1:A:721:SER:HB2	1.94	0.50
1:A:819:ASN:ND2	1:A:840:HIS:O	2.45	0.50
1:C:631:ALA:HB1	1:C:639:LEU:HD11	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:700:GLU:HG3	1:C:721:SER:HB2	1.94	0.50
1:D:692:VAL:HG12	1:D:693:HIS:ND1	2.26	0.50
1:E:155:MET:HE1	1:E:441:GLN:HG3	1.92	0.50
1:F:862:TYR:OH	1:F:1237:ASN:O	2.30	0.50
3:R:32:ARG:HD2	3:R:76:CYS:SG	2.51	0.50
1:A:155:MET:HE1	1:A:441:GLN:HG3	1.92	0.50
1:C:152:ILE:HD11	1:C:263:THR:HG22	1.92	0.50
1:C:825:ASP:HB2	1:C:832:LEU:HD22	1.93	0.50
1:D:1086:GLY:HA2	2:K:39:LYS:HE2	1.92	0.50
1:D:1222:LYS:HB3	1:D:1224:HIS:HE1	1.77	0.50
1:E:1002:HIS:ND1	1:E:1024:ASP:OD2	2.44	0.50
1:F:400:LEU:HB3	1:F:404:TRP:CZ3	2.46	0.50
1:A:298:PHE:HD2	1:A:328:GLY:HA3	1.77	0.50
1:A:562:ASN:HB2	1:A:565:GLN:HG2	1.93	0.50
1:B:825:ASP:HB2	1:B:832:LEU:HD22	1.93	0.50
1:C:155:MET:HE1	1:C:441:GLN:HG3	1.92	0.50
1:C:608:ARG:HD2	1:C:910:GLU:HB2	1.94	0.50
1:C:819:ASN:ND2	1:C:840:HIS:O	2.45	0.50
1:D:819:ASN:ND2	1:D:840:HIS:O	2.45	0.50
1:E:348:LYS:NZ	1:E:443:ASP:OD1	2.45	0.50
1:E:862:TYR:OH	1:E:1237:ASN:O	2.30	0.50
1:A:365:ASP:OD1	1:A:444:PHE:HE1	1.95	0.49
1:A:646:THR:HG23	1:A:648:GLU:HG3	1.94	0.49
1:A:1222:LYS:HB3	1:A:1224:HIS:HE1	1.77	0.49
1:B:819:ASN:ND2	1:B:840:HIS:O	2.45	0.49
1:D:152:ILE:HD11	1:D:263:THR:HG22	1.92	0.49
1:D:365:ASP:OD1	1:D:444:PHE:HE1	1.95	0.49
1:F:646:THR:HG23	1:F:648:GLU:HG3	1.94	0.49
1:G:298:PHE:HD2	1:G:328:GLY:HA3	1.77	0.49
1:G:862:TYR:HB3	1:G:884:TRP:CA	2.42	0.49
1:G:862:TYR:OH	1:G:1237:ASN:O	2.30	0.49
2:I:41:GLY:HA2	2:I:48:TYR:CE1	2.47	0.49
2:J:41:GLY:HA2	2:J:48:TYR:CE1	2.47	0.49
3:Q:16:LEU:O	3:Q:20:LEU:HB2	2.12	0.49
1:A:1086:GLY:HA2	2:H:39:LYS:HE2	1.92	0.49
1:B:155:MET:HE1	1:B:441:GLN:HG3	1.92	0.49
1:B:1222:LYS:HB3	1:B:1224:HIS:HE1	1.77	0.49
1:E:819:ASN:ND2	1:E:840:HIS:O	2.45	0.49
1:E:884:TRP:CE3	2:L:81:ILE:HD11	2.48	0.49
1:F:155:MET:HE1	1:F:441:GLN:HG3	1.92	0.49
1:F:298:PHE:HD2	1:F:328:GLY:HA3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:463:GLN:OE1	1:F:466:ARG:NH2	2.28	0.49
1:F:1222:LYS:HB3	1:F:1224:HIS:HE1	1.77	0.49
1:G:155:MET:HE1	1:G:441:GLN:HG3	1.92	0.49
1:G:562:ASN:HB2	1:G:565:GLN:HG2	1.94	0.49
2:H:41:GLY:HA2	2:H:48:TYR:CE1	2.47	0.49
3:R:16:LEU:O	3:R:20:LEU:HB2	2.12	0.49
1:C:365:ASP:OD1	1:C:444:PHE:HE1	1.96	0.49
1:C:862:TYR:HB3	1:C:884:TRP:CA	2.42	0.49
1:C:884:TRP:CE3	2:J:81:ILE:HD11	2.48	0.49
1:D:762:SER:OG	1:D:764:ASP:OD1	2.26	0.49
1:E:762:SER:OG	1:E:764:ASP:OD1	2.26	0.49
1:F:884:TRP:CE3	2:M:81:ILE:HD11	2.47	0.49
1:G:1020:SER:HB2	1:G:1028:GLN:HE21	1.77	0.49
2:K:41:GLY:HA2	2:K:48:TYR:CE1	2.47	0.49
1:A:265:ARG:NH1	1:A:371:SER:OG	2.37	0.49
1:A:331:LEU:HD13	1:A:338:TRP:CH2	2.48	0.49
1:A:348:LYS:NZ	1:A:443:ASP:OD1	2.45	0.49
1:C:1087:THR:N	2:J:39:LYS:HZ3	2.10	0.49
1:C:1222:LYS:HB3	1:C:1224:HIS:HE1	1.77	0.49
1:D:825:ASP:HB2	1:D:832:LEU:HD22	1.93	0.49
1:E:152:ILE:HD11	1:E:263:THR:HG22	1.92	0.49
1:F:365:ASP:OD1	1:F:444:PHE:HE1	1.96	0.49
1:F:700:GLU:HG3	1:F:721:SER:HB2	1.94	0.49
2:N:41:GLY:HA2	2:N:48:TYR:CE1	2.47	0.49
3:Q:32:ARG:HD2	3:Q:76:CYS:SG	2.52	0.49
1:A:825:ASP:HB2	1:A:832:LEU:HD22	1.93	0.49
1:B:298:PHE:HD2	1:B:328:GLY:HA3	1.77	0.49
1:B:885:VAL:HG12	1:B:887:GLY:N	2.28	0.49
1:B:1086:GLY:HA2	2:I:39:LYS:HE2	1.92	0.49
1:D:646:THR:HG23	1:D:648:GLU:HG3	1.94	0.49
1:D:700:GLU:HG3	1:D:721:SER:HB2	1.94	0.49
1:D:862:TYR:OH	1:D:1237:ASN:O	2.30	0.49
1:D:884:TRP:CE3	2:K:81:ILE:HD11	2.47	0.49
1:E:700:GLU:HG3	1:E:721:SER:HB2	1.94	0.49
2:I:40:THR:HG22	2:I:59:TRP:CE2	2.48	0.49
1:B:118:GLY:O	1:B:184:TRP:HB2	2.13	0.49
1:B:862:TYR:HB3	1:B:884:TRP:CA	2.42	0.49
1:D:31:SER:HA	3:Q:11:ARG:HA	1.95	0.49
1:D:334:PHE:HE1	1:E:416:GLN:HE21	1.60	0.49
1:E:885:VAL:HG12	1:E:887:GLY:N	2.28	0.49
1:F:118:GLY:O	1:F:184:TRP:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:348:LYS:NZ	1:F:443:ASP:OD1	2.45	0.49
1:F:825:ASP:HB2	1:F:832:LEU:HD22	1.93	0.49
1:G:608:ARG:HD2	1:G:910:GLU:HB2	1.94	0.49
1:A:862:TYR:HB3	1:A:884:TRP:CA	2.42	0.49
1:B:334:PHE:HE1	1:C:416:GLN:HE21	1.60	0.49
1:B:884:TRP:CE3	2:I:81:ILE:HD11	2.48	0.49
1:D:118:GLY:O	1:D:184:TRP:HB2	2.13	0.49
1:D:565:GLN:NE2	1:D:1213:PHE:HA	2.28	0.49
1:E:265:ARG:NH1	1:E:371:SER:OG	2.37	0.49
1:E:365:ASP:OD1	1:E:444:PHE:HE1	1.95	0.49
1:E:844:GLN:NE2	2:L:79:LYS:NZ	2.57	0.49
1:F:608:ARG:HD2	1:F:910:GLU:HB2	1.94	0.49
1:G:346:GLN:C	1:G:348:LYS:N	2.71	0.49
1:G:825:ASP:HB2	1:G:832:LEU:HD22	1.93	0.49
1:G:1222:LYS:HB3	1:G:1224:HIS:HE1	1.76	0.49
1:A:862:TYR:OH	1:A:1237:ASN:O	2.30	0.49
1:C:118:GLY:O	1:C:184:TRP:HB2	2.13	0.49
1:C:885:VAL:HG12	1:C:887:GLY:N	2.28	0.49
1:C:1020:SER:HB2	1:C:1028:GLN:HE21	1.77	0.49
1:D:1020:SER:HB2	1:D:1028:GLN:HE21	1.77	0.49
1:E:331:LEU:HD13	1:E:338:TRP:CH2	2.48	0.49
1:E:825:ASP:HB2	1:E:832:LEU:HD22	1.93	0.49
2:L:41:GLY:HA2	2:L:48:TYR:CE1	2.47	0.49
2:M:40:THR:HG22	2:M:59:TRP:CE2	2.48	0.49
3:O:16:LEU:O	3:O:20:LEU:HB2	2.12	0.49
1:B:365:ASP:OD1	1:B:444:PHE:HE1	1.96	0.49
1:B:929:VAL:HB	1:B:936:MET:HB2	1.95	0.49
1:D:569:CYS:CB	1:D:600:LYS:HZ3	2.25	0.49
1:D:862:TYR:HB3	1:D:884:TRP:CA	2.42	0.49
1:E:298:PHE:HD2	1:E:328:GLY:HA3	1.77	0.49
1:E:608:ARG:HD2	1:E:910:GLU:HB2	1.94	0.49
1:F:331:LEU:HD13	1:F:338:TRP:CH2	2.47	0.49
1:F:565:GLN:NE2	1:F:1213:PHE:HA	2.28	0.49
2:H:40:THR:HG22	2:H:59:TRP:CE2	2.48	0.49
2:J:40:THR:HG22	2:J:59:TRP:CE2	2.48	0.49
2:L:40:THR:HG22	2:L:59:TRP:CE2	2.48	0.49
1:A:885:VAL:HG12	1:A:887:GLY:N	2.28	0.49
1:B:265:ARG:NH1	1:B:371:SER:OG	2.37	0.49
1:B:1203:ASN:OD1	1:B:1204:VAL:N	2.46	0.49
1:C:331:LEU:HD13	1:C:338:TRP:CH2	2.47	0.49
1:C:646:THR:HG23	1:C:648:GLU:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1086:GLY:HA2	2:M:39:LYS:HE2	1.92	0.49
1:G:700:GLU:HG3	1:G:721:SER:HB2	1.94	0.49
1:B:646:THR:HG23	1:B:648:GLU:HG3	1.94	0.48
1:C:565:GLN:NE2	1:C:1213:PHE:HA	2.28	0.48
1:D:608:ARG:HD2	1:D:910:GLU:HB2	1.94	0.48
1:D:1026:GLU:HG3	1:D:1041:ARG:HG2	1.95	0.48
1:D:1203:ASN:OD1	1:D:1204:VAL:N	2.46	0.48
1:E:646:THR:HG23	1:E:648:GLU:HG3	1.94	0.48
1:E:1203:ASN:OD1	1:E:1204:VAL:N	2.46	0.48
1:G:118:GLY:O	1:G:184:TRP:HB2	2.13	0.48
1:G:565:GLN:NE2	1:G:1213:PHE:HA	2.28	0.48
1:G:884:TRP:CE3	2:N:81:ILE:HD11	2.47	0.48
1:A:346:GLN:C	1:A:348:LYS:N	2.71	0.48
1:A:565:GLN:NE2	1:A:1213:PHE:HA	2.28	0.48
1:A:884:TRP:CE3	2:H:81:ILE:HD11	2.47	0.48
1:B:346:GLN:C	1:B:348:LYS:N	2.71	0.48
1:B:565:GLN:NE2	1:B:1213:PHE:HA	2.28	0.48
1:B:862:TYR:OH	1:B:1237:ASN:O	2.30	0.48
1:D:113:VAL:HG11	1:D:174:LEU:HD21	1.95	0.48
1:D:885:VAL:HG12	1:D:887:GLY:N	2.28	0.48
1:E:568:LEU:HD13	1:E:595:LEU:O	2.13	0.48
1:E:1026:GLU:HG3	1:E:1041:ARG:HG2	1.95	0.48
1:E:1222:LYS:HB3	1:E:1224:HIS:HE1	1.77	0.48
1:F:752:SER:HB2	1:F:753:PRO:HD2	1.95	0.48
1:G:1026:GLU:HG3	1:G:1041:ARG:HG2	1.95	0.48
1:G:1203:ASN:OD1	1:G:1204:VAL:N	2.46	0.48
2:K:40:THR:HG22	2:K:59:TRP:CE2	2.48	0.48
2:M:41:GLY:HA2	2:M:48:TYR:CE1	2.47	0.48
3:P:16:LEU:O	3:P:20:LEU:HB2	2.12	0.48
1:A:118:GLY:O	1:A:184:TRP:HB2	2.13	0.48
1:A:568:LEU:HD13	1:A:595:LEU:O	2.13	0.48
1:A:929:VAL:HB	1:A:936:MET:HB2	1.95	0.48
1:C:346:GLN:C	1:C:348:LYS:N	2.71	0.48
1:E:113:VAL:HG11	1:E:174:LEU:HD21	1.95	0.48
1:E:1020:SER:HB2	1:E:1028:GLN:HE21	1.77	0.48
1:F:885:VAL:HG12	1:F:887:GLY:N	2.28	0.48
1:F:1179:TRP:NE1	1:F:1220:LEU:H	2.12	0.48
1:G:752:SER:HB2	1:G:753:PRO:HD2	1.95	0.48
1:A:196:LEU:HG	1:A:200:GLN:HE22	1.78	0.48
1:A:1026:GLU:HG3	1:A:1041:ARG:HG2	1.95	0.48
1:B:1198:TYR:HA	1:B:1215:THR:HB	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:568:LEU:HD13	1:D:595:LEU:O	2.13	0.48
1:E:230:LEU:O	1:E:234:LYS:N	2.41	0.48
1:E:565:GLN:NE2	1:E:1213:PHE:HA	2.28	0.48
1:F:344:GLN:OE1	1:F:349:GLN:NE2	2.44	0.48
1:F:1026:GLU:HG3	1:F:1041:ARG:HG2	1.95	0.48
1:G:550:LEU:HD23	1:G:607:SER:HB2	1.91	0.48
1:B:331:LEU:HD13	1:B:338:TRP:CH2	2.48	0.48
1:B:1191:MET:SD	1:B:1209:SER:OG	2.63	0.48
1:C:113:VAL:HG11	1:C:174:LEU:HD21	1.95	0.48
1:C:862:TYR:OH	1:C:1237:ASN:O	2.30	0.48
1:C:929:VAL:HB	1:C:936:MET:HB2	1.95	0.48
1:C:1026:GLU:HG3	1:C:1041:ARG:HG2	1.95	0.48
1:C:1198:TYR:HA	1:C:1215:THR:HB	1.96	0.48
1:D:1198:TYR:HA	1:D:1215:THR:HB	1.96	0.48
1:E:1179:TRP:NE1	1:E:1220:LEU:H	2.12	0.48
1:F:569:CYS:HB3	1:F:600:LYS:HZ3	1.78	0.48
1:F:884:TRP:HH2	2:M:78:THR:C	2.22	0.48
1:G:331:LEU:HD13	1:G:338:TRP:CH2	2.48	0.48
1:G:885:VAL:HG12	1:G:887:GLY:N	2.28	0.48
2:N:40:THR:HG22	2:N:59:TRP:CE2	2.48	0.48
1:B:1020:SER:HB2	1:B:1028:GLN:HE21	1.77	0.48
1:C:298:PHE:HD2	1:C:328:GLY:HA3	1.77	0.48
1:D:298:PHE:HD2	1:D:328:GLY:HA3	1.77	0.48
1:F:196:LEU:HG	1:F:200:GLN:HE22	1.78	0.48
1:G:884:TRP:HH2	2:N:78:THR:C	2.22	0.48
1:A:113:VAL:HG11	1:A:174:LEU:HD21	1.95	0.48
1:A:1203:ASN:OD1	1:A:1204:VAL:N	2.46	0.48
1:B:113:VAL:HG11	1:B:174:LEU:HD21	1.95	0.48
1:B:752:SER:HB2	1:B:753:PRO:HD2	1.95	0.48
1:C:569:CYS:HB3	1:C:600:LYS:HZ3	1.78	0.48
1:D:331:LEU:HD13	1:D:338:TRP:CH2	2.48	0.48
1:D:752:SER:HB2	1:D:753:PRO:HD2	1.95	0.48
1:E:1198:TYR:HA	1:E:1215:THR:HB	1.96	0.48
1:F:1203:ASN:OD1	1:F:1204:VAL:N	2.46	0.48
1:A:266:ASP:CG	1:A:268:SER:H	2.20	0.48
1:C:170:ASP:OD2	1:C:172:SER:OG	2.32	0.48
1:D:326:LEU:HA	1:D:326:LEU:HD23	1.44	0.48
1:E:265:ARG:HH11	1:E:371:SER:HG	1.57	0.48
1:E:497:HIS:HA	1:E:500:LEU:HB3	1.96	0.48
1:F:113:VAL:HG11	1:F:174:LEU:HD21	1.95	0.48
1:F:497:HIS:HA	1:F:500:LEU:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1020:SER:HB2	1:F:1028:GLN:HE21	1.77	0.48
1:G:541:SER:O	1:G:545:GLN:HG3	2.14	0.48
1:G:929:VAL:HB	1:G:936:MET:HB2	1.95	0.48
1:A:884:TRP:HH2	2:H:78:THR:C	2.22	0.48
1:A:1198:TYR:HA	1:A:1215:THR:HB	1.96	0.48
1:B:497:HIS:HA	1:B:500:LEU:HB3	1.95	0.48
1:B:882:LEU:HD12	1:B:1176:HIS:NE2	2.25	0.48
1:B:1026:GLU:HG3	1:B:1041:ARG:HG2	1.95	0.48
1:D:14:GLU:OE1	1:E:31:SER:CB	2.62	0.48
1:D:929:VAL:HB	1:D:936:MET:HB2	1.95	0.48
1:E:118:GLY:O	1:E:184:TRP:HB2	2.13	0.48
1:E:170:ASP:OD2	1:E:172:SER:OG	2.32	0.48
1:E:346:GLN:C	1:E:348:LYS:N	2.71	0.48
1:E:884:TRP:HH2	2:L:78:THR:C	2.22	0.48
1:G:113:VAL:HG11	1:G:174:LEU:HD21	1.95	0.48
1:G:196:LEU:HG	1:G:200:GLN:HE22	1.78	0.48
1:G:568:LEU:HD13	1:G:595:LEU:O	2.13	0.48
1:G:762:SER:OG	1:G:764:ASP:OD1	2.26	0.48
1:G:1179:TRP:NE1	1:G:1220:LEU:H	2.12	0.48
1:A:330:LEU:HD13	1:A:341:TYR:OH	2.14	0.48
1:B:196:LEU:HG	1:B:200:GLN:HE22	1.78	0.48
1:C:541:SER:O	1:C:545:GLN:HG3	2.14	0.48
1:C:568:LEU:HD13	1:C:595:LEU:O	2.13	0.48
1:D:541:SER:O	1:D:545:GLN:HG3	2.14	0.48
1:D:550:LEU:HD23	1:D:607:SER:HB2	1.91	0.48
1:D:1179:TRP:NE1	1:D:1220:LEU:H	2.12	0.48
1:E:158:CYS:SG	1:E:159:GLY:N	2.87	0.48
1:E:196:LEU:HG	1:E:200:GLN:HE22	1.78	0.48
1:E:929:VAL:HB	1:E:936:MET:HB2	1.95	0.48
1:F:158:CYS:SG	1:F:159:GLY:N	2.87	0.48
1:F:346:GLN:C	1:F:348:LYS:N	2.71	0.48
1:F:550:LEU:HD23	1:F:607:SER:HB2	1.91	0.48
1:F:568:LEU:HD13	1:F:595:LEU:O	2.13	0.48
1:G:266:ASP:CG	1:G:268:SER:H	2.20	0.48
1:G:348:LYS:NZ	1:G:443:ASP:OD1	2.45	0.48
1:A:1179:TRP:NE1	1:A:1220:LEU:H	2.12	0.47
1:B:569:CYS:HB3	1:B:600:LYS:HZ3	1.79	0.47
1:D:330:LEU:HD13	1:D:341:TYR:OH	2.14	0.47
1:E:752:SER:HB2	1:E:753:PRO:HD2	1.95	0.47
1:G:365:ASP:OD1	1:G:444:PHE:HE1	1.95	0.47
1:A:344:GLN:OE1	1:A:349:GLN:NE2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:752:SER:HB2	1:A:753:PRO:HD2	1.95	0.47
1:B:568:LEU:HD13	1:B:595:LEU:O	2.13	0.47
1:C:330:LEU:HD13	1:C:341:TYR:OH	2.14	0.47
1:C:884:TRP:HH2	2:J:78:THR:C	2.22	0.47
1:D:884:TRP:HH2	2:K:78:THR:C	2.22	0.47
1:A:541:SER:O	1:A:545:GLN:HG3	2.14	0.47
1:A:1020:SER:HB2	1:A:1028:GLN:HE21	1.77	0.47
1:B:884:TRP:HH2	2:I:78:THR:C	2.22	0.47
1:C:497:HIS:HA	1:C:500:LEU:HB3	1.96	0.47
1:C:1203:ASN:OD1	1:C:1204:VAL:N	2.46	0.47
1:D:344:GLN:OE1	1:D:349:GLN:NE2	2.44	0.47
1:F:330:LEU:HD13	1:F:341:TYR:OH	2.14	0.47
1:F:844:GLN:HE22	2:M:79:LYS:HZ2	1.61	0.47
1:F:1198:TYR:HA	1:F:1215:THR:HB	1.96	0.47
1:A:109:TYR:CE1	1:G:4:LYS:CD	2.58	0.47
1:B:821:ILE:HB	1:B:835:ILE:HB	1.97	0.47
1:C:155:MET:HE3	1:C:368:MET:HE1	1.97	0.47
1:C:344:GLN:OE1	1:C:349:GLN:NE2	2.44	0.47
1:D:196:LEU:HG	1:D:200:GLN:HE22	1.78	0.47
1:E:1131:ARG:H	1:E:1146:ASP:HA	1.80	0.47
1:G:158:CYS:SG	1:G:159:GLY:N	2.87	0.47
1:A:106:ILE:HA	1:A:110:VAL:HG21	1.97	0.47
1:A:155:MET:HE3	1:A:368:MET:HE1	1.97	0.47
1:B:155:MET:HE3	1:B:368:MET:HE1	1.97	0.47
1:B:170:ASP:OD2	1:B:172:SER:OG	2.32	0.47
1:B:266:ASP:CG	1:B:268:SER:H	2.20	0.47
1:C:752:SER:HB2	1:C:753:PRO:HD2	1.95	0.47
1:C:821:ILE:HB	1:C:835:ILE:HB	1.97	0.47
1:D:155:MET:HE3	1:D:368:MET:HE1	1.97	0.47
1:E:330:LEU:HD13	1:E:341:TYR:OH	2.14	0.47
1:F:541:SER:O	1:F:545:GLN:HG3	2.14	0.47
1:B:230:LEU:O	1:B:234:LYS:N	2.41	0.47
1:C:1131:ARG:H	1:C:1146:ASP:HA	1.80	0.47
1:C:1179:TRP:NE1	1:C:1220:LEU:H	2.12	0.47
1:E:160:LYS:HB3	4:E:1301:DTP:O1B	2.15	0.47
1:F:266:ASP:CG	1:F:268:SER:H	2.20	0.47
1:G:600:LYS:HZ1	1:G:1213:PHE:HZ	1.63	0.47
2:K:39:LYS:HB2	2:K:42:GLN:HG3	1.97	0.47
2:L:39:LYS:HB2	2:L:42:GLN:HG3	1.97	0.47
1:A:230:LEU:O	1:A:234:LYS:N	2.41	0.47
1:A:337:ARG:NH1	1:B:409:GLU:OE2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:HIS:HA	1:A:500:LEU:HB3	1.96	0.47
1:A:550:LEU:HD23	1:A:607:SER:HB2	1.91	0.47
1:A:600:LYS:HZ1	1:A:1213:PHE:HZ	1.63	0.47
1:A:1032:TRP:C	1:A:1034:LEU:H	2.23	0.47
1:B:158:CYS:SG	1:B:159:GLY:N	2.87	0.47
1:B:330:LEU:HD13	1:B:341:TYR:OH	2.14	0.47
1:B:1179:TRP:NE1	1:B:1220:LEU:H	2.12	0.47
1:B:1221:LYS:HE3	1:B:1222:LYS:HE3	1.97	0.47
1:D:346:GLN:C	1:D:348:LYS:N	2.71	0.47
1:D:497:HIS:HA	1:D:500:LEU:HB3	1.96	0.47
1:D:821:ILE:HB	1:D:835:ILE:HB	1.97	0.47
1:D:1131:ARG:H	1:D:1146:ASP:HA	1.80	0.47
1:E:344:GLN:OE1	1:E:349:GLN:NE2	2.44	0.47
1:E:541:SER:O	1:E:545:GLN:HG3	2.14	0.47
1:F:106:ILE:HA	1:F:110:VAL:HG21	1.97	0.47
1:F:160:LYS:HB3	4:F:1301:DTP:O1B	2.15	0.47
1:F:1131:ARG:H	1:F:1146:ASP:HA	1.80	0.47
1:G:106:ILE:HA	1:G:110:VAL:HG21	1.97	0.47
1:G:497:HIS:HA	1:G:500:LEU:HB3	1.96	0.47
1:G:1198:TYR:HA	1:G:1215:THR:HB	1.96	0.47
2:I:39:LYS:HB2	2:I:42:GLN:HG3	1.97	0.47
1:A:158:CYS:SG	1:A:159:GLY:N	2.87	0.47
1:A:170:ASP:OD2	1:A:172:SER:OG	2.32	0.47
1:A:1221:LYS:HE3	1:A:1222:LYS:HE3	1.97	0.47
1:B:337:ARG:NH1	1:C:409:GLU:OE2	2.48	0.47
1:B:541:SER:O	1:B:545:GLN:HG3	2.14	0.47
1:C:158:CYS:SG	1:C:159:GLY:N	2.87	0.47
1:C:196:LEU:HG	1:C:200:GLN:HE22	1.78	0.47
1:D:158:CYS:SG	1:D:159:GLY:N	2.87	0.47
1:A:821:ILE:HB	1:A:835:ILE:HB	1.97	0.47
1:B:106:ILE:HA	1:B:110:VAL:HG21	1.97	0.47
1:B:1222:LYS:HB3	1:B:1224:HIS:CE1	2.50	0.47
1:D:170:ASP:OD2	1:D:172:SER:OG	2.32	0.47
1:D:230:LEU:O	1:D:234:LYS:N	2.41	0.47
1:F:929:VAL:HB	1:F:936:MET:HB2	1.95	0.47
1:A:1131:ARG:H	1:A:1146:ASP:HA	1.80	0.47
1:A:1222:LYS:HB3	1:A:1224:HIS:CE1	2.50	0.47
1:B:570:GLU:HB2	1:B:577:TYR:HB2	1.97	0.47
1:C:266:ASP:CG	1:C:268:SER:H	2.20	0.47
1:C:1222:LYS:HB3	1:C:1224:HIS:CE1	2.50	0.47
1:D:337:ARG:NH1	1:E:409:GLU:OE2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1222:LYS:HB3	1:D:1224:HIS:CE1	2.50	0.47
1:E:155:MET:HE3	1:E:368:MET:HE1	1.97	0.47
1:E:1222:LYS:HB3	1:E:1224:HIS:CE1	2.50	0.47
2:J:39:LYS:HB2	2:J:42:GLN:HG3	1.97	0.47
1:A:570:GLU:HB2	1:A:577:TYR:HB2	1.97	0.46
1:B:844:GLN:HE22	2:I:79:LYS:HZ2	1.60	0.46
1:C:230:LEU:O	1:C:234:LYS:N	2.41	0.46
1:E:266:ASP:CG	1:E:268:SER:H	2.20	0.46
1:C:612:ARG:HG3	1:C:904:GLN:O	2.16	0.46
1:C:1221:LYS:HE3	1:C:1222:LYS:HE3	1.97	0.46
1:D:160:LYS:HB3	4:D:1301:DTP:O1B	2.15	0.46
1:E:152:ILE:HG22	1:E:280:VAL:HB	1.97	0.46
1:G:155:MET:HE3	1:G:368:MET:HE1	1.97	0.46
1:G:330:LEU:HD13	1:G:341:TYR:OH	2.14	0.46
2:H:39:LYS:HB2	2:H:42:GLN:HG3	1.97	0.46
1:A:862:TYR:HB3	1:A:883:SER:C	2.41	0.46
1:B:160:LYS:HB3	4:B:1301:DTP:O1B	2.15	0.46
1:C:337:ARG:NH1	1:D:409:GLU:OE2	2.49	0.46
1:E:524:HIS:CB	1:E:646:THR:HG21	2.36	0.46
1:E:612:ARG:HG3	1:E:904:GLN:O	2.16	0.46
1:E:1221:LYS:HE3	1:E:1222:LYS:HE3	1.97	0.46
1:F:862:TYR:HB3	1:F:883:SER:C	2.41	0.46
1:G:1222:LYS:HB3	1:G:1224:HIS:CE1	2.50	0.46
2:I:70:ASN:HD22	2:I:73:LYS:HB2	1.81	0.46
2:M:39:LYS:HB2	2:M:42:GLN:HG3	1.97	0.46
1:A:160:LYS:HB3	4:A:1301:DTP:O1B	2.15	0.46
1:B:695:TYR:OH	1:B:732:GLN:O	2.31	0.46
1:B:862:TYR:HB3	1:B:884:TRP:N	2.31	0.46
1:B:1032:TRP:C	1:B:1034:LEU:H	2.23	0.46
1:D:266:ASP:CG	1:D:268:SER:H	2.20	0.46
1:E:106:ILE:HA	1:E:110:VAL:HG21	1.97	0.46
1:E:862:TYR:HB3	1:E:884:TRP:N	2.31	0.46
1:F:152:ILE:HG22	1:F:280:VAL:HB	1.97	0.46
1:G:1131:ARG:H	1:G:1146:ASP:HA	1.80	0.46
2:L:70:ASN:HD22	2:L:73:LYS:HB2	1.81	0.46
1:A:472:THR:O	1:A:473:LEU:HD12	2.16	0.46
1:A:888:VAL:HG12	1:A:899:THR:HA	1.98	0.46
1:C:524:HIS:CB	1:C:646:THR:HG21	2.36	0.46
1:D:152:ILE:HG22	1:D:280:VAL:HB	1.97	0.46
1:D:265:ARG:HH11	1:D:371:SER:HG	1.57	0.46
1:D:862:TYR:HB3	1:D:884:TRP:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:337:ARG:NH1	1:F:409:GLU:OE2	2.48	0.46
1:E:472:THR:O	1:E:473:LEU:HD12	2.16	0.46
1:E:821:ILE:HB	1:E:835:ILE:HB	1.97	0.46
1:G:160:LYS:HB3	4:G:1301:DTP:O1B	2.15	0.46
1:B:269:VAL:C	1:B:271:ASP:H	2.24	0.46
1:C:950:ASN:OD1	1:C:951:GLY:N	2.49	0.46
1:D:950:ASN:OD1	1:D:951:GLY:N	2.49	0.46
1:F:155:MET:HE3	1:F:368:MET:HE1	1.97	0.46
1:G:821:ILE:HB	1:G:835:ILE:HB	1.97	0.46
1:G:888:VAL:HG12	1:G:899:THR:HA	1.98	0.46
2:H:10:PHE:HA	2:H:14:CYS:HB2	1.98	0.46
1:B:862:TYR:HB3	1:B:883:SER:C	2.41	0.46
1:C:570:GLU:HB2	1:C:577:TYR:HB2	1.97	0.46
1:C:862:TYR:HB3	1:C:884:TRP:N	2.31	0.46
1:D:14:GLU:HB2	1:E:31:SER:HG	1.81	0.46
1:E:862:TYR:HB3	1:E:883:SER:C	2.41	0.46
1:F:170:ASP:OD2	1:F:172:SER:OG	2.32	0.46
1:F:1221:LYS:HE3	1:F:1222:LYS:HE3	1.97	0.46
1:G:152:ILE:HG22	1:G:280:VAL:HB	1.97	0.46
1:G:170:ASP:OD2	1:G:172:SER:OG	2.32	0.46
1:G:1011:PHE:HE1	1:G:1018:LEU:HD13	1.81	0.46
2:N:39:LYS:HB2	2:N:42:GLN:HG3	1.97	0.46
1:A:643:LYS:HD3	1:A:646:THR:HG22	1.98	0.46
1:A:1011:PHE:HE1	1:A:1018:LEU:HD13	1.81	0.46
1:B:590:ASN:C	1:B:592:MET:N	2.64	0.46
1:B:888:VAL:HG12	1:B:899:THR:HA	1.98	0.46
1:B:950:ASN:OD1	1:B:951:GLY:N	2.49	0.46
1:D:1011:PHE:HE1	1:D:1018:LEU:HD13	1.81	0.46
1:G:862:TYR:HB3	1:G:883:SER:C	2.41	0.46
1:G:1191:MET:SD	1:G:1209:SER:OG	2.63	0.46
2:J:98:LEU:O	2:J:102:THR:OG1	2.30	0.46
1:B:472:THR:O	1:B:473:LEU:HD12	2.16	0.46
1:B:643:LYS:HD3	1:B:646:THR:HG22	1.98	0.46
1:C:862:TYR:HB3	1:C:883:SER:C	2.41	0.46
1:D:106:ILE:HA	1:D:110:VAL:HG21	1.97	0.46
1:E:950:ASN:OD1	1:E:951:GLY:N	2.49	0.46
1:F:269:VAL:C	1:F:271:ASP:H	2.24	0.46
1:F:570:GLU:HB2	1:F:577:TYR:HB2	1.97	0.46
1:F:821:ILE:HB	1:F:835:ILE:HB	1.97	0.46
1:F:1222:LYS:HB3	1:F:1224:HIS:CE1	2.50	0.46
1:G:570:GLU:HB2	1:G:577:TYR:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:862:TYR:HB3	1:G:884:TRP:N	2.31	0.46
1:G:1032:TRP:C	1:G:1034:LEU:H	2.23	0.46
2:M:10:PHE:HA	2:M:14:CYS:HB2	1.98	0.46
2:M:70:ASN:HD22	2:M:73:LYS:HB2	1.81	0.46
2:N:10:PHE:HA	2:N:14:CYS:HB2	1.98	0.46
3:R:90:ARG:NH2	3:R:90:ARG:HG2	2.31	0.46
1:A:612:ARG:HG3	1:A:904:GLN:O	2.16	0.46
1:B:152:ILE:HG22	1:B:280:VAL:HB	1.97	0.46
1:F:950:ASN:OD1	1:F:951:GLY:N	2.49	0.46
1:F:1215:THR:HG21	1:F:1220:LEU:HD21	1.98	0.46
1:G:1215:THR:HG21	1:G:1220:LEU:HD21	1.98	0.46
2:H:70:ASN:HD22	2:H:73:LYS:HB2	1.81	0.46
1:A:950:ASN:OD1	1:A:951:GLY:N	2.49	0.45
1:A:1215:THR:HG21	1:A:1220:LEU:HD21	1.98	0.45
1:B:1215:THR:HG21	1:B:1220:LEU:HD21	1.99	0.45
1:C:160:LYS:HB3	4:C:1301:DTP:O1B	2.15	0.45
1:C:269:VAL:C	1:C:271:ASP:H	2.24	0.45
1:C:472:THR:O	1:C:473:LEU:HD12	2.16	0.45
1:C:1215:THR:HG21	1:C:1220:LEU:HD21	1.98	0.45
1:D:862:TYR:HB3	1:D:883:SER:C	2.41	0.45
1:D:1221:LYS:HE3	1:D:1222:LYS:HE3	1.97	0.45
1:E:550:LEU:HD23	1:E:607:SER:HB2	1.91	0.45
1:E:1011:PHE:HE1	1:E:1018:LEU:HD13	1.81	0.45
1:E:1032:TRP:C	1:E:1034:LEU:H	2.23	0.45
1:F:862:TYR:HB3	1:F:884:TRP:N	2.31	0.45
1:G:266:ASP:CG	1:G:268:SER:HG	2.22	0.45
1:G:472:THR:O	1:G:473:LEU:HD12	2.16	0.45
1:C:106:ILE:HA	1:C:110:VAL:HG21	1.97	0.45
1:C:844:GLN:HE22	2:J:79:LYS:HZ2	1.62	0.45
1:C:1011:PHE:HE1	1:C:1018:LEU:HD13	1.81	0.45
1:D:472:THR:O	1:D:473:LEU:HD12	2.16	0.45
1:D:570:GLU:HB2	1:D:577:TYR:HB2	1.97	0.45
1:D:1032:TRP:C	1:D:1034:LEU:H	2.23	0.45
1:G:269:VAL:C	1:G:271:ASP:H	2.24	0.45
1:G:1221:LYS:HE3	1:G:1222:LYS:HE3	1.97	0.45
2:J:68:LEU:HB3	2:J:85:ILE:HD12	1.98	0.45
2:K:68:LEU:HB3	2:K:85:ILE:HD12	1.98	0.45
3:O:90:ARG:NH2	3:O:90:ARG:HG2	2.31	0.45
3:Q:90:ARG:NH2	3:Q:90:ARG:HG2	2.31	0.45
1:A:298:PHE:CD2	1:A:328:GLY:HA3	2.52	0.45
1:A:461:ILE:HD11	1:A:491:MET:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:THR:CG2	1:D:45:ASN:OD1	2.64	0.45
1:C:152:ILE:HG22	1:C:280:VAL:HB	1.97	0.45
1:F:1011:PHE:HE1	1:F:1018:LEU:HD13	1.81	0.45
2:I:10:PHE:HA	2:I:14:CYS:HB2	1.98	0.45
1:A:862:TYR:HB3	1:A:884:TRP:N	2.31	0.45
1:D:1215:THR:HG21	1:D:1220:LEU:HD21	1.98	0.45
1:E:1215:THR:HG21	1:E:1220:LEU:HD21	1.99	0.45
1:F:612:ARG:HG3	1:F:904:GLN:O	2.16	0.45
1:F:1086:GLY:C	2:M:39:LYS:HZ1	2.24	0.45
1:G:612:ARG:HG3	1:G:904:GLN:O	2.16	0.45
2:H:68:LEU:HB3	2:H:85:ILE:HD12	1.98	0.45
1:A:1150:GLU:HB2	1:A:1167:PRO:HG2	1.99	0.45
1:B:461:ILE:HD11	1:B:491:MET:HA	1.99	0.45
1:C:482:TYR:OH	1:C:490:HIS:NE2	2.35	0.45
1:E:334:PHE:HE1	1:F:416:GLN:HE21	1.63	0.45
1:E:570:GLU:HB2	1:E:577:TYR:HB2	1.97	0.45
1:F:472:THR:O	1:F:473:LEU:HD12	2.16	0.45
1:F:1150:GLU:HB2	1:F:1167:PRO:HG2	1.99	0.45
1:G:950:ASN:OD1	1:G:951:GLY:N	2.49	0.45
1:G:1150:GLU:HB2	1:G:1167:PRO:HG2	1.99	0.45
2:J:70:ASN:HD22	2:J:73:LYS:HB2	1.81	0.45
2:L:10:PHE:HA	2:L:14:CYS:HB2	1.98	0.45
1:A:152:ILE:HG22	1:A:280:VAL:HB	1.97	0.45
1:B:1131:ARG:H	1:B:1146:ASP:HA	1.80	0.45
1:B:1150:GLU:HB2	1:B:1167:PRO:HG2	1.99	0.45
1:C:643:LYS:HD3	1:C:646:THR:HG22	1.98	0.45
1:C:1191:MET:SD	1:C:1209:SER:OG	2.63	0.45
1:D:612:ARG:HG3	1:D:904:GLN:O	2.16	0.45
1:F:461:ILE:HD11	1:F:491:MET:HA	1.99	0.45
1:G:461:ILE:HD11	1:G:491:MET:HA	1.99	0.45
1:B:266:ASP:CG	1:B:268:SER:HG	2.23	0.45
1:B:298:PHE:CD2	1:B:328:GLY:HA3	2.52	0.45
1:B:612:ARG:HG3	1:B:904:GLN:O	2.16	0.45
1:B:821:ILE:HD11	1:B:857:VAL:HG21	1.99	0.45
1:C:888:VAL:HG12	1:C:899:THR:HA	1.98	0.45
1:E:821:ILE:HD11	1:E:857:VAL:HG21	1.99	0.45
1:F:888:VAL:HG12	1:F:899:THR:HA	1.98	0.45
2:K:10:PHE:HA	2:K:14:CYS:HB2	1.98	0.45
1:C:216:LEU:HA	1:C:217:PRO:HD2	1.84	0.45
1:C:821:ILE:HD11	1:C:857:VAL:HG21	1.99	0.45
1:C:1032:TRP:C	1:C:1034:LEU:H	2.23	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:695:TYR:OH	1:D:732:GLN:O	2.30	0.45
1:D:868:ASN:OD1	1:D:869:THR:N	2.50	0.45
1:E:269:VAL:C	1:E:271:ASP:H	2.24	0.45
1:F:326:LEU:HD23	1:F:326:LEU:HA	1.44	0.45
1:F:821:ILE:HD11	1:F:857:VAL:HG21	1.99	0.45
1:A:868:ASN:OD1	1:A:869:THR:N	2.50	0.45
1:B:868:ASN:OD1	1:B:869:THR:N	2.50	0.45
1:E:326:LEU:HD23	1:E:326:LEU:HA	1.44	0.45
1:E:590:ASN:C	1:E:592:MET:N	2.64	0.45
1:E:1150:GLU:HB2	1:E:1167:PRO:HG2	1.99	0.45
1:F:868:ASN:OD1	1:F:869:THR:N	2.50	0.45
1:G:143:LEU:C	1:G:145:GLY:N	2.75	0.45
1:G:298:PHE:CD2	1:G:328:GLY:HA3	2.52	0.45
2:J:10:PHE:HA	2:J:14:CYS:HB2	1.98	0.45
2:K:70:ASN:HD22	2:K:73:LYS:HB2	1.81	0.45
2:N:68:LEU:HB3	2:N:85:ILE:HD12	1.98	0.45
3:P:90:ARG:NH2	3:P:90:ARG:HG2	2.31	0.45
1:A:409:GLU:OE2	1:G:337:ARG:NH1	2.49	0.45
1:A:480:CYS:SG	1:A:481:MET:N	2.90	0.45
1:B:1011:PHE:HE1	1:B:1018:LEU:HD13	1.81	0.45
1:C:1150:GLU:HB2	1:C:1167:PRO:HG2	1.99	0.45
1:E:390:GLN:HB2	1:E:393:VAL:HG21	1.99	0.45
1:E:461:ILE:HD11	1:E:491:MET:HA	1.99	0.45
1:G:643:LYS:HD3	1:G:646:THR:HG22	1.98	0.45
1:G:868:ASN:OD1	1:G:869:THR:N	2.50	0.45
2:N:70:ASN:HD22	2:N:73:LYS:HB2	1.81	0.45
1:A:269:VAL:C	1:A:271:ASP:H	2.24	0.44
1:B:600:LYS:HA	1:B:603:ILE:HG13	2.00	0.44
1:D:266:ASP:CG	1:D:268:SER:HG	2.23	0.44
1:D:821:ILE:HD11	1:D:857:VAL:HG21	1.99	0.44
1:E:643:LYS:HD3	1:E:646:THR:HG22	1.98	0.44
2:I:72:LYS:NZ	2:I:78:THR:O	2.51	0.44
3:Q:41:GLU:HA	3:Q:44:GLN:HE21	1.83	0.44
1:A:821:ILE:HD11	1:A:857:VAL:HG21	1.99	0.44
1:C:868:ASN:OD1	1:C:869:THR:N	2.50	0.44
1:D:357:SER:OG	1:D:358:SER:N	2.50	0.44
1:D:888:VAL:HG12	1:D:899:THR:HA	1.98	0.44
1:D:1150:GLU:HB2	1:D:1167:PRO:HG2	1.99	0.44
1:E:7:ASN:CG	1:F:236:PRO:CG	2.81	0.44
1:E:480:CYS:SG	1:E:481:MET:N	2.90	0.44
1:F:230:LEU:O	1:F:234:LYS:N	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:643:LYS:HD3	1:F:646:THR:HG22	1.98	0.44
1:F:1032:TRP:C	1:F:1034:LEU:H	2.23	0.44
1:G:1087:THR:N	2:N:39:LYS:HZ3	2.15	0.44
2:L:68:LEU:HB3	2:L:85:ILE:HD12	1.98	0.44
3:O:45:ARG:O	3:O:45:ARG:HG2	2.17	0.44
1:A:569:CYS:HB3	1:A:600:LYS:HZ3	1.82	0.44
1:B:357:SER:OG	1:B:358:SER:N	2.50	0.44
1:B:480:CYS:SG	1:B:481:MET:N	2.90	0.44
1:C:480:CYS:SG	1:C:481:MET:N	2.90	0.44
1:C:600:LYS:HA	1:C:603:ILE:HG13	2.00	0.44
1:D:143:LEU:C	1:D:145:GLY:N	2.75	0.44
1:D:298:PHE:CD2	1:D:328:GLY:HA3	2.52	0.44
1:D:643:LYS:HD3	1:D:646:THR:HG22	1.98	0.44
1:E:888:VAL:HG12	1:E:899:THR:HA	1.98	0.44
2:M:68:LEU:HB3	2:M:85:ILE:HD12	1.98	0.44
2:M:72:LYS:NZ	2:M:78:THR:O	2.51	0.44
1:A:600:LYS:HA	1:A:603:ILE:HG13	2.00	0.44
1:C:461:ILE:HD11	1:C:491:MET:HA	1.99	0.44
1:D:342:LEU:O	1:D:346:GLN:CG	2.66	0.44
1:D:480:CYS:SG	1:D:481:MET:N	2.90	0.44
1:E:530:ARG:NH1	1:E:545:GLN:OE1	2.51	0.44
1:E:1191:MET:SD	1:E:1209:SER:OG	2.63	0.44
1:F:342:LEU:O	1:F:346:GLN:CG	2.66	0.44
2:J:72:LYS:NZ	2:J:78:THR:O	2.51	0.44
3:R:10:ARG:HG2	3:R:10:ARG:H	1.60	0.44
1:A:357:SER:OG	1:A:358:SER:N	2.50	0.44
1:C:342:LEU:O	1:C:346:GLN:CG	2.66	0.44
1:D:269:VAL:C	1:D:271:ASP:H	2.24	0.44
1:D:390:GLN:HB2	1:D:393:VAL:HG21	1.99	0.44
1:E:357:SER:OG	1:E:358:SER:N	2.50	0.44
1:F:390:GLN:HB2	1:F:393:VAL:HG21	1.99	0.44
1:F:600:LYS:HA	1:F:603:ILE:HG13	2.00	0.44
1:F:600:LYS:HZ1	1:F:1213:PHE:HZ	1.66	0.44
1:G:342:LEU:O	1:G:346:GLN:CG	2.66	0.44
1:G:600:LYS:HA	1:G:603:ILE:HG13	2.00	0.44
1:G:695:TYR:HE1	1:G:733:LYS:HD2	1.83	0.44
1:G:821:ILE:HD11	1:G:857:VAL:HG21	1.99	0.44
2:I:68:LEU:HB3	2:I:85:ILE:HD12	1.98	0.44
2:J:3:VAL:O	2:J:97:TYR:HB2	2.18	0.44
2:N:3:VAL:O	2:N:97:TYR:HB2	2.18	0.44
1:A:143:LEU:C	1:A:145:GLY:N	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:GLN:HB2	1:B:393:VAL:HG21	1.99	0.44
1:B:550:LEU:HD23	1:B:607:SER:HB2	1.91	0.44
1:C:695:TYR:HE1	1:C:733:LYS:HD2	1.82	0.44
1:E:600:LYS:HA	1:E:603:ILE:HG13	2.00	0.44
1:E:868:ASN:OD1	1:E:869:THR:N	2.50	0.44
1:G:230:LEU:O	1:G:234:LYS:N	2.41	0.44
1:G:530:ARG:NH1	1:G:545:GLN:OE1	2.51	0.44
1:G:795:GLU:HG3	1:G:795:GLU:O	2.18	0.44
1:A:530:ARG:NH1	1:A:545:GLN:OE1	2.51	0.44
1:B:695:TYR:HE1	1:B:733:LYS:HD2	1.83	0.44
1:C:143:LEU:C	1:C:145:GLY:N	2.75	0.44
1:C:298:PHE:CD2	1:C:328:GLY:HA3	2.52	0.44
1:C:795:GLU:HG3	1:C:795:GLU:O	2.18	0.44
1:C:1135:PHE:CE1	1:C:1142:LEU:HD13	2.53	0.44
1:D:461:ILE:HD11	1:D:491:MET:HA	1.99	0.44
1:D:600:LYS:HA	1:D:603:ILE:HG13	2.00	0.44
1:D:685:ASN:HB3	1:D:688:THR:HB	1.99	0.44
1:F:143:LEU:C	1:F:145:GLY:N	2.75	0.44
1:F:298:PHE:CD2	1:F:328:GLY:HA3	2.52	0.44
1:G:344:GLN:OE1	1:G:349:GLN:NE2	2.44	0.44
1:G:390:GLN:HB2	1:G:393:VAL:HG21	1.99	0.44
2:K:3:VAL:O	2:K:97:TYR:HB2	2.18	0.44
2:L:3:VAL:O	2:L:97:TYR:HB2	2.18	0.44
2:M:70:ASN:ND2	2:M:73:LYS:HB2	2.33	0.44
1:A:342:LEU:O	1:A:346:GLN:CG	2.66	0.44
1:A:685:ASN:HB3	1:A:688:THR:HB	1.99	0.44
1:B:391:LYS:H	1:B:391:LYS:HG2	1.62	0.44
1:B:600:LYS:HZ1	1:B:1213:PHE:HZ	1.65	0.44
1:B:1135:PHE:CE1	1:B:1142:LEU:HD13	2.53	0.44
1:D:524:HIS:N	1:D:646:THR:OG1	2.51	0.44
2:K:72:LYS:NZ	2:K:78:THR:O	2.51	0.44
2:N:70:ASN:ND2	2:N:73:LYS:HB2	2.33	0.44
1:A:695:TYR:OH	1:A:732:GLN:O	2.31	0.44
1:B:685:ASN:HB3	1:B:688:THR:HB	1.99	0.44
1:C:530:ARG:NH1	1:C:545:GLN:OE1	2.51	0.44
1:C:847:ASP:OD1	1:C:848:PHE:N	2.51	0.44
1:D:530:ARG:NH1	1:D:545:GLN:OE1	2.51	0.44
1:D:695:TYR:HE1	1:D:733:LYS:HD2	1.83	0.44
1:D:847:ASP:OD1	1:D:848:PHE:N	2.51	0.44
1:E:685:ASN:HB3	1:E:688:THR:HB	2.00	0.44
1:G:480:CYS:SG	1:G:481:MET:N	2.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:72:LYS:NZ	2:H:78:THR:O	2.51	0.44
3:O:41:GLU:HA	3:O:44:GLN:HE21	1.83	0.44
1:A:795:GLU:HG3	1:A:795:GLU:O	2.18	0.43
1:B:326:LEU:HD23	1:B:326:LEU:HA	1.44	0.43
1:B:524:HIS:N	1:B:646:THR:OG1	2.51	0.43
1:C:390:GLN:HB2	1:C:393:VAL:HG21	1.99	0.43
1:E:342:LEU:O	1:E:346:GLN:CG	2.66	0.43
1:E:695:TYR:HE1	1:E:733:LYS:HD2	1.83	0.43
1:E:795:GLU:HG3	1:E:795:GLU:O	2.18	0.43
1:F:524:HIS:N	1:F:646:THR:OG1	2.51	0.43
1:F:795:GLU:HG3	1:F:795:GLU:O	2.18	0.43
1:G:685:ASN:HB3	1:G:688:THR:HB	1.99	0.43
2:L:18:HIS:CE1	2:L:29:GLY:HA3	2.53	0.43
2:L:72:LYS:NZ	2:L:78:THR:O	2.51	0.43
2:N:18:HIS:CE1	2:N:29:GLY:HA3	2.53	0.43
1:B:224:LYS:HE3	1:B:255:ASP:O	2.18	0.43
1:B:342:LEU:O	1:B:346:GLN:CG	2.66	0.43
1:B:530:ARG:NH1	1:B:545:GLN:OE1	2.51	0.43
1:B:795:GLU:HG3	1:B:795:GLU:O	2.18	0.43
1:C:334:PHE:HD2	1:C:337:ARG:HH11	1.66	0.43
1:E:298:PHE:CD2	1:E:328:GLY:HA3	2.52	0.43
1:F:480:CYS:SG	1:F:481:MET:N	2.90	0.43
1:G:224:LYS:HE3	1:G:255:ASP:O	2.18	0.43
1:G:357:SER:OG	1:G:358:SER:N	2.50	0.43
1:G:524:HIS:N	1:G:646:THR:OG1	2.51	0.43
2:H:18:HIS:CE1	2:H:29:GLY:HA3	2.53	0.43
2:J:70:ASN:ND2	2:J:73:LYS:HB2	2.33	0.43
1:A:524:HIS:N	1:A:646:THR:OG1	2.51	0.43
1:A:695:TYR:HE1	1:A:733:LYS:HD2	1.83	0.43
1:A:847:ASP:OD1	1:A:848:PHE:N	2.51	0.43
1:A:1135:PHE:CE1	1:A:1142:LEU:HD13	2.53	0.43
1:B:428:ARG:HG2	1:B:433:PHE:CE1	2.54	0.43
1:E:524:HIS:N	1:E:646:THR:OG1	2.51	0.43
1:F:357:SER:OG	1:F:358:SER:N	2.50	0.43
1:F:973:LEU:C	1:F:975:TYR:H	2.27	0.43
1:G:268:SER:O	1:G:271:ASP:N	2.51	0.43
1:G:844:GLN:HE22	2:N:79:LYS:HZ2	1.63	0.43
2:N:72:LYS:NZ	2:N:78:THR:O	2.51	0.43
3:R:41:GLU:HA	3:R:44:GLN:HE21	1.83	0.43
1:A:386:LEU:O	1:A:386:LEU:HD23	2.19	0.43
1:A:390:GLN:HB2	1:A:393:VAL:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:965:SER:H	1:A:980:ASP:HA	1.84	0.43
1:B:937:VAL:HB	1:B:949:ILE:HB	2.00	0.43
1:C:685:ASN:HB3	1:C:688:THR:HB	2.00	0.43
1:C:937:VAL:HB	1:C:949:ILE:HB	2.00	0.43
1:C:965:SER:H	1:C:980:ASP:HA	1.84	0.43
1:D:582:LEU:O	1:D:586:GLN:HG3	2.19	0.43
1:E:143:LEU:C	1:E:145:GLY:N	2.75	0.43
1:F:530:ARG:NH1	1:F:545:GLN:OE1	2.51	0.43
1:G:386:LEU:O	1:G:386:LEU:HD23	2.19	0.43
1:G:569:CYS:HB3	1:G:600:LYS:HZ3	1.83	0.43
2:H:70:ASN:ND2	2:H:73:LYS:HB2	2.33	0.43
2:M:26:HIS:O	2:M:27:LYS:HD2	2.19	0.43
1:A:224:LYS:HE3	1:A:255:ASP:O	2.18	0.43
1:B:334:PHE:HD2	1:B:337:ARG:HH11	1.66	0.43
1:B:582:LEU:O	1:B:586:GLN:HG3	2.19	0.43
1:E:973:LEU:C	1:E:975:TYR:H	2.27	0.43
1:E:1135:PHE:CE1	1:E:1142:LEU:HD13	2.53	0.43
1:F:965:SER:H	1:F:980:ASP:HA	1.84	0.43
1:G:1218:THR:H	1:G:1237:ASN:ND2	2.17	0.43
2:J:18:HIS:CE1	2:J:29:GLY:HA3	2.53	0.43
2:N:26:HIS:O	2:N:27:LYS:HD2	2.19	0.43
1:A:346:GLN:O	1:A:348:LYS:N	2.52	0.43
1:A:739:MET:HE1	1:A:758:LEU:HD23	2.00	0.43
1:C:428:ARG:HG2	1:C:433:PHE:CE1	2.54	0.43
1:C:524:HIS:N	1:C:646:THR:OG1	2.51	0.43
1:C:802:LYS:NZ	1:C:843:ILE:O	2.50	0.43
1:C:884:TRP:HH2	2:J:78:THR:O	2.02	0.43
1:D:224:LYS:HE3	1:D:255:ASP:O	2.18	0.43
1:D:386:LEU:O	1:D:386:LEU:HD23	2.19	0.43
1:D:937:VAL:HB	1:D:949:ILE:HB	2.00	0.43
1:E:224:LYS:HE3	1:E:255:ASP:O	2.18	0.43
1:E:428:ARG:HG2	1:E:433:PHE:CE1	2.54	0.43
1:E:1166:ALA:HA	1:E:1167:PRO:HD2	1.93	0.43
2:I:26:HIS:O	2:I:27:LYS:HD2	2.19	0.43
2:J:26:HIS:O	2:J:27:LYS:HD2	2.19	0.43
2:M:18:HIS:CE1	2:M:29:GLY:HA3	2.53	0.43
2:N:82:PHE:HE2	2:N:85:ILE:HG13	1.84	0.43
1:A:379:ILE:O	1:A:382:TYR:N	2.52	0.43
1:B:346:GLN:O	1:B:348:LYS:N	2.52	0.43
1:B:386:LEU:O	1:B:386:LEU:HD23	2.19	0.43
1:D:965:SER:H	1:D:980:ASP:HA	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:268:SER:O	1:E:271:ASP:N	2.51	0.43
1:E:1100:PHE:HB3	1:E:1111:ILE:HD11	2.00	0.43
1:F:224:LYS:HE3	1:F:255:ASP:O	2.18	0.43
1:F:386:LEU:HD23	1:F:386:LEU:O	2.19	0.43
1:F:685:ASN:HB3	1:F:688:THR:HB	1.99	0.43
1:F:695:TYR:HE1	1:F:733:LYS:HD2	1.83	0.43
1:F:847:ASP:OD1	1:F:848:PHE:N	2.51	0.43
1:G:379:ILE:O	1:G:382:TYR:N	2.52	0.43
1:G:973:LEU:C	1:G:975:TYR:H	2.27	0.43
2:H:3:VAL:O	2:H:97:TYR:HB2	2.18	0.43
2:I:18:HIS:CE1	2:I:29:GLY:HA3	2.53	0.43
1:A:326:LEU:HA	1:A:326:LEU:HD23	1.44	0.43
1:A:973:LEU:C	1:A:975:TYR:H	2.27	0.43
1:B:973:LEU:C	1:B:975:TYR:H	2.27	0.43
1:C:379:ILE:O	1:C:382:TYR:N	2.52	0.43
1:D:428:ARG:HG2	1:D:433:PHE:CE1	2.54	0.43
1:E:695:TYR:OH	1:E:732:GLN:O	2.31	0.43
1:F:582:LEU:O	1:F:586:GLN:HG3	2.19	0.43
1:F:937:VAL:HB	1:F:949:ILE:HB	2.00	0.43
1:G:847:ASP:OD1	1:G:848:PHE:N	2.51	0.43
2:I:3:VAL:O	2:I:97:TYR:HB2	2.18	0.43
2:I:70:ASN:ND2	2:I:73:LYS:HB2	2.33	0.43
2:K:26:HIS:O	2:K:27:LYS:HD2	2.19	0.43
2:L:41:GLY:HA2	2:L:48:TYR:CZ	2.54	0.43
1:A:524:HIS:CB	1:A:646:THR:HG21	2.36	0.43
1:B:379:ILE:O	1:B:382:TYR:N	2.52	0.43
1:B:767:LEU:HD21	1:B:801:VAL:HG11	2.01	0.43
1:B:1100:PHE:HB3	1:B:1111:ILE:HD11	2.00	0.43
1:C:224:LYS:HE3	1:C:255:ASP:O	2.18	0.43
1:C:346:GLN:O	1:C:348:LYS:N	2.52	0.43
1:D:725:LEU:HD11	1:D:742:HIS:CD2	2.54	0.43
1:D:1100:PHE:HB3	1:D:1111:ILE:HD11	2.00	0.43
1:E:725:LEU:HD11	1:E:742:HIS:CD2	2.54	0.43
1:E:739:MET:HE1	1:E:758:LEU:HD23	2.00	0.43
1:E:847:ASP:OD1	1:E:848:PHE:N	2.51	0.43
1:E:965:SER:H	1:E:980:ASP:HA	1.84	0.43
1:F:379:ILE:O	1:F:382:TYR:N	2.52	0.43
1:G:428:ARG:HG2	1:G:433:PHE:CE1	2.54	0.43
1:G:739:MET:HE1	1:G:758:LEU:HD23	2.00	0.43
2:H:41:GLY:HA2	2:H:48:TYR:CZ	2.54	0.43
2:H:82:PHE:HE2	2:H:85:ILE:HG13	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:18:HIS:CE1	2:K:29:GLY:HA3	2.53	0.43
2:K:70:ASN:ND2	2:K:73:LYS:HB2	2.33	0.43
2:M:3:VAL:O	2:M:97:TYR:HB2	2.18	0.43
1:B:739:MET:HE1	1:B:758:LEU:HD23	2.00	0.43
1:B:965:SER:H	1:B:980:ASP:HA	1.84	0.43
1:C:582:LEU:O	1:C:586:GLN:HG3	2.19	0.43
1:C:767:LEU:HD21	1:C:801:VAL:HG11	2.01	0.43
1:D:334:PHE:HD2	1:D:337:ARG:HH11	1.66	0.43
1:D:795:GLU:O	1:D:795:GLU:HG3	2.18	0.43
1:D:973:LEU:C	1:D:975:TYR:H	2.27	0.43
1:D:1135:PHE:CE1	1:D:1142:LEU:HD13	2.53	0.43
1:E:1218:THR:H	1:E:1237:ASN:ND2	2.17	0.43
1:F:201:ASN:ND2	1:G:219:ASN:HD21	2.14	0.43
1:F:346:GLN:O	1:F:348:LYS:N	2.52	0.43
1:F:1100:PHE:HB3	1:F:1111:ILE:HD11	2.00	0.43
1:G:346:GLN:O	1:G:348:LYS:N	2.52	0.43
1:G:1050:PHE:CD1	1:G:1058:LEU:HD11	2.54	0.43
2:H:67:TYR:HD1	2:H:74:TYR:HB3	1.84	0.43
2:L:26:HIS:O	2:L:27:LYS:HD2	2.19	0.43
2:L:70:ASN:ND2	2:L:73:LYS:HB2	2.33	0.43
2:L:82:PHE:HE2	2:L:85:ILE:HG13	1.84	0.43
3:P:41:GLU:HA	3:P:44:GLN:HE21	1.83	0.43
1:C:676:SER:OG	1:C:678:ASP:OD1	2.37	0.42
1:D:767:LEU:HD21	1:D:801:VAL:HG11	2.01	0.42
1:E:658:ASP:HB3	1:E:677:VAL:HB	2.00	0.42
1:F:1135:PHE:CE1	1:F:1142:LEU:HD13	2.53	0.42
1:G:658:ASP:HB3	1:G:677:VAL:HB	2.00	0.42
1:G:937:VAL:HB	1:G:949:ILE:HB	2.00	0.42
2:I:82:PHE:HE2	2:I:85:ILE:HG13	1.84	0.42
2:N:41:GLY:HA2	2:N:48:TYR:CZ	2.54	0.42
3:P:90:ARG:HG2	3:P:90:ARG:HH21	1.84	0.42
1:A:658:ASP:HB3	1:A:677:VAL:HB	2.00	0.42
1:A:1050:PHE:CD1	1:A:1058:LEU:HD11	2.54	0.42
1:C:550:LEU:HD23	1:C:607:SER:HB2	1.91	0.42
1:C:1100:PHE:HB3	1:C:1111:ILE:HD11	2.00	0.42
1:D:658:ASP:HB3	1:D:677:VAL:HB	2.00	0.42
1:E:482:TYR:OH	1:E:490:HIS:NE2	2.35	0.42
1:E:767:LEU:HD21	1:E:801:VAL:HG11	2.01	0.42
1:F:569:CYS:CB	1:F:600:LYS:HZ3	2.32	0.42
1:F:808:ALA:HB2	1:F:850:PRO:HA	2.01	0.42
1:G:1135:PHE:CE1	1:G:1142:LEU:HD13	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:82:PHE:HE2	2:M:85:ILE:HG13	1.84	0.42
3:R:90:ARG:HG2	3:R:90:ARG:HH21	1.85	0.42
1:A:511:LYS:HB2	1:A:563:ILE:HG13	2.02	0.42
1:A:767:LEU:HD21	1:A:801:VAL:HG11	2.01	0.42
1:B:658:ASP:HB3	1:B:677:VAL:HB	2.00	0.42
1:B:1218:THR:H	1:B:1237:ASN:ND2	2.17	0.42
1:C:973:LEU:C	1:C:975:TYR:H	2.27	0.42
1:D:524:HIS:CB	1:D:646:THR:HG21	2.36	0.42
1:G:808:ALA:HB2	1:G:850:PRO:HA	2.02	0.42
2:J:14:CYS:SG	5:J:500:HEC:HBB3	2.59	0.42
2:J:82:PHE:HE2	2:J:85:ILE:HG13	1.84	0.42
2:N:14:CYS:SG	5:N:500:HEC:HBB3	2.59	0.42
3:O:90:ARG:HG2	3:O:90:ARG:HH21	1.85	0.42
1:A:428:ARG:HG2	1:A:433:PHE:CE1	2.54	0.42
1:A:865:GLU:CD	1:A:867:TRP:HE1	2.27	0.42
1:A:937:VAL:HB	1:A:949:ILE:HB	2.00	0.42
1:A:1100:PHE:HB3	1:A:1111:ILE:HD11	2.00	0.42
1:A:1218:THR:H	1:A:1237:ASN:ND2	2.17	0.42
1:D:739:MET:HE1	1:D:758:LEU:HD23	2.00	0.42
1:E:379:ILE:O	1:E:382:TYR:N	2.52	0.42
1:E:937:VAL:HB	1:E:949:ILE:HB	2.00	0.42
1:F:658:ASP:HB3	1:F:677:VAL:HB	2.00	0.42
1:F:725:LEU:HD11	1:F:742:HIS:CD2	2.54	0.42
1:F:739:MET:HE1	1:F:758:LEU:HD23	2.00	0.42
1:F:767:LEU:HD21	1:F:801:VAL:HG11	2.01	0.42
2:J:67:TYR:HD1	2:J:74:TYR:HB3	1.84	0.42
2:K:14:CYS:SG	5:K:500:HEC:HBB3	2.59	0.42
3:O:34:LEU:HD12	3:O:34:LEU:HA	1.93	0.42
3:Q:90:ARG:HG2	3:Q:90:ARG:HH21	1.84	0.42
1:B:511:LYS:HB2	1:B:563:ILE:HG13	2.02	0.42
1:B:847:ASP:OD1	1:B:848:PHE:N	2.51	0.42
1:B:865:GLU:CD	1:B:867:TRP:HE1	2.27	0.42
1:B:989:GLU:HG2	1:B:991:VAL:H	1.85	0.42
1:C:725:LEU:HD11	1:C:742:HIS:CD2	2.54	0.42
1:C:1135:PHE:HE1	1:C:1142:LEU:HD13	1.85	0.42
1:D:676:SER:OG	1:D:678:ASP:OD1	2.37	0.42
1:D:1218:THR:H	1:D:1237:ASN:ND2	2.17	0.42
1:E:346:GLN:O	1:E:348:LYS:N	2.52	0.42
1:E:808:ALA:HB2	1:E:850:PRO:HA	2.01	0.42
1:F:482:TYR:HH	1:F:490:HIS:HE2	1.55	0.42
1:G:145:GLY:HA2	1:G:259:GLN:HE21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:26:HIS:O	2:H:27:LYS:HD2	2.19	0.42
2:I:14:CYS:SG	5:I:500:HEC:HBB3	2.59	0.42
2:K:41:GLY:HA2	2:K:48:TYR:CZ	2.54	0.42
3:R:7:ARG:HA	3:R:10:ARG:HG3	2.02	0.42
1:A:344:GLN:CD	1:A:349:GLN:HE21	2.28	0.42
1:A:808:ALA:HB2	1:A:850:PRO:HA	2.01	0.42
1:C:658:ASP:HB3	1:C:677:VAL:HB	2.00	0.42
1:D:452:GLN:N	1:D:452:GLN:OE1	2.53	0.42
1:E:386:LEU:HD23	1:E:386:LEU:O	2.19	0.42
1:E:582:LEU:O	1:E:586:GLN:HG3	2.19	0.42
1:F:334:PHE:HD2	1:F:337:ARG:HH11	1.66	0.42
1:F:865:GLU:CD	1:F:867:TRP:HE1	2.27	0.42
1:F:1050:PHE:CD1	1:F:1058:LEU:HD11	2.54	0.42
1:G:865:GLU:CD	1:G:867:TRP:HE1	2.27	0.42
2:H:40:THR:HG23	2:H:57:ILE:HG13	2.02	0.42
2:K:82:PHE:HE2	2:K:85:ILE:HG13	1.84	0.42
2:N:67:TYR:HD1	2:N:74:TYR:HB3	1.84	0.42
1:A:320:SER:HA	1:A:321:PRO:HD3	1.87	0.42
1:C:386:LEU:HD23	1:C:386:LEU:O	2.19	0.42
1:C:400:LEU:HB3	1:C:404:TRP:HZ3	1.84	0.42
1:C:1050:PHE:CD1	1:C:1058:LEU:HD11	2.54	0.42
1:D:884:TRP:HH2	2:K:78:THR:O	2.02	0.42
1:G:10:LEU:CD2	1:G:13:ARG:NH2	2.83	0.42
1:G:170:ASP:CG	1:G:172:SER:HG	2.26	0.42
1:G:320:SER:HA	1:G:321:PRO:HD3	1.87	0.42
1:G:344:GLN:CD	1:G:349:GLN:HE21	2.28	0.42
1:G:511:LYS:HB2	1:G:563:ILE:HG13	2.02	0.42
1:G:582:LEU:O	1:G:586:GLN:HG3	2.19	0.42
2:I:94:LEU:O	2:I:98:LEU:HG	2.20	0.42
2:J:41:GLY:HA2	2:J:48:TYR:CZ	2.54	0.42
2:M:41:GLY:HA2	2:M:48:TYR:CZ	2.54	0.42
1:B:265:ARG:HG3	1:B:265:ARG:O	2.20	0.42
1:B:320:SER:HA	1:B:321:PRO:HD3	1.87	0.42
1:B:1050:PHE:CD1	1:B:1058:LEU:HD11	2.54	0.42
1:B:1135:PHE:HE1	1:B:1142:LEU:HD13	1.85	0.42
1:C:145:GLY:HA2	1:C:259:GLN:HE21	1.85	0.42
1:C:600:LYS:HZ1	1:C:1213:PHE:HZ	1.66	0.42
1:C:1218:THR:H	1:C:1237:ASN:ND2	2.17	0.42
1:D:10:LEU:CD2	1:D:13:ARG:NH2	2.83	0.42
1:D:265:ARG:HG3	1:D:265:ARG:O	2.20	0.42
1:D:379:ILE:O	1:D:382:TYR:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1218:THR:H	1:F:1237:ASN:ND2	2.17	0.42
1:G:400:LEU:HB3	1:G:404:TRP:HZ3	1.85	0.42
1:G:767:LEU:HD21	1:G:801:VAL:HG11	2.01	0.42
1:G:1135:PHE:HE1	1:G:1142:LEU:HD13	1.85	0.42
2:H:14:CYS:SG	5:H:500:HEC:HBB3	2.59	0.42
2:L:14:CYS:SG	5:L:500:HEC:HBB3	2.59	0.42
2:N:40:THR:HG23	2:N:57:ILE:HG13	2.02	0.42
3:O:7:ARG:HA	3:O:10:ARG:HG3	2.02	0.42
1:A:265:ARG:HG3	1:A:265:ARG:O	2.20	0.42
1:B:268:SER:O	1:B:271:ASP:N	2.51	0.42
1:C:865:GLU:CD	1:C:867:TRP:HE1	2.27	0.42
1:D:346:GLN:O	1:D:348:LYS:N	2.52	0.42
1:D:865:GLU:CD	1:D:867:TRP:HE1	2.27	0.42
1:E:452:GLN:OE1	1:E:452:GLN:N	2.53	0.42
1:E:1050:PHE:CD1	1:E:1058:LEU:HD11	2.54	0.42
1:F:428:ARG:HG2	1:F:433:PHE:CE1	2.54	0.42
1:G:452:GLN:OE1	1:G:452:GLN:N	2.53	0.42
2:H:94:LEU:O	2:H:98:LEU:HG	2.20	0.42
2:M:40:THR:HG23	2:M:57:ILE:HG13	2.02	0.42
2:M:67:TYR:HD1	2:M:74:TYR:HB3	1.84	0.42
1:A:582:LEU:O	1:A:586:GLN:HG3	2.19	0.42
1:A:864:VAL:HB	1:A:878:CYS:HB2	2.02	0.42
1:B:10:LEU:CD2	1:B:13:ARG:NH2	2.83	0.42
1:B:452:GLN:OE1	1:B:452:GLN:N	2.53	0.42
1:C:265:ARG:O	1:C:265:ARG:HG3	2.20	0.42
1:C:268:SER:O	1:C:271:ASP:N	2.51	0.42
1:C:452:GLN:OE1	1:C:452:GLN:N	2.53	0.42
1:C:864:VAL:HB	1:C:878:CYS:HB2	2.02	0.42
1:D:346:GLN:C	1:D:348:LYS:H	2.28	0.42
1:D:864:VAL:HB	1:D:878:CYS:HB2	2.02	0.42
1:D:989:GLU:HG2	1:D:991:VAL:H	1.85	0.42
1:E:265:ARG:HG3	1:E:265:ARG:O	2.20	0.42
1:F:989:GLU:HG2	1:F:991:VAL:H	1.85	0.42
1:G:334:PHE:HD2	1:G:337:ARG:HH11	1.66	0.42
1:G:346:GLN:C	1:G:348:LYS:H	2.28	0.42
1:G:676:SER:OG	1:G:678:ASP:OD1	2.37	0.42
1:G:725:LEU:HD11	1:G:742:HIS:CD2	2.54	0.42
1:G:965:SER:H	1:G:980:ASP:HA	1.84	0.42
2:J:94:LEU:O	2:J:98:LEU:HG	2.20	0.42
2:L:67:TYR:HD1	2:L:74:TYR:HB3	1.84	0.42
2:M:14:CYS:SG	5:M:500:HEC:HBB3	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:GLN:N	1:A:452:GLN:OE1	2.53	0.41
1:A:989:GLU:HG2	1:A:991:VAL:H	1.85	0.41
1:B:346:GLN:C	1:B:348:LYS:H	2.28	0.41
1:F:947:GLN:HG2	1:F:958:TYR:HD1	1.85	0.41
1:B:456:LEU:O	1:B:459:LYS:HB3	2.20	0.41
1:D:1050:PHE:CD1	1:D:1058:LEU:HD11	2.54	0.41
1:E:865:GLU:CD	1:E:867:TRP:HE1	2.27	0.41
1:F:369:SER:O	1:F:373:GLU:HG2	2.21	0.41
1:F:511:LYS:HB2	1:F:563:ILE:HG13	2.01	0.41
1:F:864:VAL:HB	1:F:878:CYS:HB2	2.02	0.41
2:K:67:TYR:HD1	2:K:74:TYR:HB3	1.84	0.41
2:K:94:LEU:O	2:K:98:LEU:HG	2.20	0.41
2:L:94:LEU:O	2:L:98:LEU:HG	2.20	0.41
1:A:145:GLY:HA2	1:A:259:GLN:HE21	1.85	0.41
1:A:1191:MET:SD	1:A:1209:SER:OG	2.63	0.41
1:G:282:VAL:O	1:G:282:VAL:HG12	2.21	0.41
1:G:947:GLN:HG2	1:G:958:TYR:HD1	1.85	0.41
1:G:1100:PHE:HB3	1:G:1111:ILE:HD11	2.00	0.41
2:I:41:GLY:HA2	2:I:48:TYR:CZ	2.54	0.41
1:A:334:PHE:HD2	1:A:337:ARG:HH11	1.66	0.41
1:B:725:LEU:HD11	1:B:742:HIS:CD2	2.54	0.41
1:C:346:GLN:C	1:C:348:LYS:H	2.28	0.41
1:C:511:LYS:HB2	1:C:563:ILE:HG13	2.02	0.41
1:D:342:LEU:O	1:D:346:GLN:HG3	2.21	0.41
1:D:456:LEU:O	1:D:459:LYS:HB3	2.21	0.41
1:D:808:ALA:HB2	1:D:850:PRO:HA	2.02	0.41
1:D:885:VAL:HG13	1:D:900:SER:O	2.21	0.41
1:E:282:VAL:O	1:E:282:VAL:HG12	2.20	0.41
1:E:1135:PHE:HE1	1:E:1142:LEU:HD13	1.85	0.41
1:F:265:ARG:HG3	1:F:265:ARG:O	2.20	0.41
1:F:337:ARG:O	1:F:340:TYR:N	2.54	0.41
1:G:265:ARG:HG3	1:G:265:ARG:O	2.20	0.41
1:G:369:SER:O	1:G:373:GLU:HG2	2.20	0.41
2:I:40:THR:HG23	2:I:57:ILE:HG13	2.02	0.41
2:K:40:THR:HG23	2:K:57:ILE:HG13	2.02	0.41
1:A:676:SER:OG	1:A:678:ASP:OD1	2.37	0.41
1:B:808:ALA:HB2	1:B:850:PRO:HA	2.01	0.41
1:C:456:LEU:O	1:C:459:LYS:HB3	2.21	0.41
1:C:739:MET:HE1	1:C:758:LEU:HD23	2.00	0.41
1:C:808:ALA:HB2	1:C:850:PRO:HA	2.01	0.41
1:D:30:ILE:HG21	3:Q:10:ARG:HB3	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:268:SER:O	1:D:271:ASP:N	2.51	0.41
1:D:565:GLN:CD	1:D:1213:PHE:CA	2.94	0.41
1:E:369:SER:O	1:E:373:GLU:HG2	2.20	0.41
1:E:474:SER:HA	1:E:475:PRO:HD2	1.91	0.41
1:F:452:GLN:OE1	1:F:452:GLN:N	2.53	0.41
2:N:94:LEU:O	2:N:98:LEU:HG	2.20	0.41
3:Q:7:ARG:HA	3:Q:10:ARG:HG3	2.02	0.41
1:A:884:TRP:HH2	2:H:78:THR:O	2.02	0.41
1:C:369:SER:O	1:C:373:GLU:HG2	2.20	0.41
1:D:14:GLU:CB	1:E:31:SER:HG	2.34	0.41
1:D:358:SER:CB	1:E:274:MET:HE2	2.44	0.41
1:D:400:LEU:HB3	1:D:404:TRP:HZ3	1.84	0.41
1:D:947:GLN:HG2	1:D:958:TYR:HD1	1.85	0.41
1:E:337:ARG:O	1:E:340:TYR:N	2.54	0.41
1:E:565:GLN:CD	1:E:1213:PHE:CA	2.94	0.41
1:E:1087:THR:N	2:L:39:LYS:HZ3	2.17	0.41
1:F:268:SER:O	1:F:271:ASP:N	2.51	0.41
1:F:282:VAL:O	1:F:282:VAL:HG12	2.20	0.41
1:F:456:LEU:O	1:F:459:LYS:HB3	2.21	0.41
1:F:695:TYR:OH	1:F:732:GLN:O	2.31	0.41
1:F:884:TRP:HH2	2:M:79:LYS:N	2.18	0.41
1:F:884:TRP:HH2	2:M:78:THR:O	2.02	0.41
1:G:337:ARG:O	1:G:340:TYR:N	2.54	0.41
1:G:695:TYR:OH	1:G:732:GLN:O	2.31	0.41
1:G:989:GLU:HG2	1:G:991:VAL:H	1.85	0.41
2:J:40:THR:HG23	2:J:57:ILE:HG13	2.02	0.41
2:L:40:THR:HG23	2:L:57:ILE:HG13	2.02	0.41
2:M:94:LEU:O	2:M:98:LEU:HG	2.20	0.41
1:A:342:LEU:O	1:A:346:GLN:HG3	2.21	0.41
1:A:947:GLN:HG2	1:A:958:TYR:HD1	1.85	0.41
1:B:282:VAL:O	1:B:282:VAL:HG12	2.21	0.41
1:C:569:CYS:CB	1:C:600:LYS:HZ3	2.32	0.41
1:C:700:GLU:HB2	1:C:720:SER:HB2	2.03	0.41
1:D:216:LEU:HA	1:D:217:PRO:HD2	1.84	0.41
1:E:344:GLN:CD	1:E:349:GLN:HE21	2.28	0.41
1:F:971:PRO:C	1:F:973:LEU:H	2.29	0.41
1:G:342:LEU:O	1:G:346:GLN:HG3	2.21	0.41
1:A:725:LEU:HD11	1:A:742:HIS:CD2	2.54	0.41
1:A:1135:PHE:HE1	1:A:1142:LEU:HD13	1.85	0.41
1:B:145:GLY:HA2	1:B:259:GLN:HE21	1.85	0.41
1:B:569:CYS:CB	1:B:600:LYS:HZ3	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:885:VAL:HG13	1:B:900:SER:O	2.21	0.41
1:C:153:HIS:HA	1:C:264:THR:O	2.21	0.41
1:C:344:GLN:CD	1:C:349:GLN:HE21	2.28	0.41
1:C:358:SER:HB3	1:D:274:MET:HE3	2.00	0.41
1:C:584:ALA:CA	1:C:594:TYR:CE2	2.98	0.41
1:D:46:GLU:OE2	1:D:55:MET:HE2	2.21	0.41
1:D:196:LEU:O	1:D:199:LEU:HB2	2.21	0.41
1:D:348:LYS:NZ	1:D:443:ASP:CG	2.79	0.41
1:E:334:PHE:HD2	1:E:337:ARG:HH11	1.66	0.41
1:E:864:VAL:HB	1:E:878:CYS:HB2	2.02	0.41
1:E:971:PRO:C	1:E:973:LEU:H	2.29	0.41
1:F:322:LEU:HD23	1:F:364:LEU:HD13	2.03	0.41
1:F:676:SER:OG	1:F:678:ASP:OD1	2.37	0.41
1:F:885:VAL:HG13	1:F:900:SER:O	2.21	0.41
1:G:864:VAL:HB	1:G:878:CYS:HB2	2.02	0.41
2:I:30:PRO:HB3	2:I:46:PHE:CD2	2.56	0.41
2:K:30:PRO:HB3	2:K:46:PHE:CD2	2.56	0.41
2:M:55:LYS:HG2	2:M:75:ILE:HG12	2.03	0.41
1:A:400:LEU:HB3	1:A:404:TRP:HZ3	1.84	0.41
1:A:565:GLN:CD	1:A:1213:PHE:CA	2.94	0.41
1:B:46:GLU:OE2	1:B:55:MET:HE2	2.21	0.41
1:B:143:LEU:C	1:B:145:GLY:N	2.75	0.41
1:B:369:SER:O	1:B:373:GLU:HG2	2.21	0.41
1:B:400:LEU:HB3	1:B:404:TRP:HZ3	1.84	0.41
1:B:700:GLU:HB2	1:B:720:SER:HB2	2.03	0.41
1:B:864:VAL:HB	1:B:878:CYS:HB2	2.02	0.41
1:C:196:LEU:O	1:C:199:LEU:HB2	2.21	0.41
1:C:282:VAL:O	1:C:282:VAL:HG12	2.21	0.41
1:C:342:LEU:O	1:C:346:GLN:HG3	2.21	0.41
1:C:348:LYS:NZ	1:C:443:ASP:CG	2.79	0.41
1:C:565:GLN:CD	1:C:1213:PHE:CA	2.94	0.41
1:D:282:VAL:O	1:D:282:VAL:HG12	2.20	0.41
1:D:369:SER:O	1:D:373:GLU:HG2	2.21	0.41
1:D:530:ARG:HD2	1:D:545:GLN:NE2	2.36	0.41
1:E:10:LEU:CD2	1:E:13:ARG:NH2	2.83	0.41
1:E:322:LEU:HD23	1:E:364:LEU:HD13	2.03	0.41
1:E:346:GLN:C	1:E:348:LYS:H	2.28	0.41
1:E:456:LEU:O	1:E:459:LYS:HB3	2.21	0.41
1:E:511:LYS:HB2	1:E:563:ILE:HG13	2.02	0.41
1:E:530:ARG:HD2	1:E:545:GLN:NE2	2.36	0.41
1:E:565:GLN:OE1	1:E:1212:THR:HB	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:884:TRP:HH2	2:L:78:THR:O	2.02	0.41
1:F:565:GLN:OE1	1:F:1212:THR:HB	2.21	0.41
1:F:1141:LEU:HG	1:F:1155:ASN:HA	2.03	0.41
1:G:46:GLU:OE2	1:G:55:MET:HE2	2.21	0.41
1:G:228:ARG:HD3	1:G:256:SER:HB3	2.03	0.41
1:G:326:LEU:HA	1:G:326:LEU:HD23	1.44	0.41
1:G:456:LEU:O	1:G:459:LYS:HB3	2.21	0.41
1:G:565:GLN:OE1	1:G:1212:THR:HB	2.21	0.41
2:I:67:TYR:HD1	2:I:74:TYR:HB3	1.84	0.41
2:L:30:PRO:HB3	2:L:46:PHE:CD2	2.56	0.41
2:L:55:LYS:HG2	2:L:75:ILE:HG12	2.03	0.41
1:A:153:HIS:HA	1:A:264:THR:O	2.21	0.41
1:A:348:LYS:NZ	1:A:443:ASP:CG	2.79	0.41
1:B:160:LYS:NZ	1:B:264:THR:O	2.53	0.41
1:B:337:ARG:O	1:B:340:TYR:N	2.54	0.41
1:B:342:LEU:O	1:B:346:GLN:HG3	2.21	0.41
1:B:348:LYS:NZ	1:B:443:ASP:CG	2.79	0.41
1:B:676:SER:OG	1:B:678:ASP:OD1	2.37	0.41
1:D:474:SER:HA	1:D:475:PRO:HD2	1.91	0.41
1:D:511:LYS:HB2	1:D:563:ILE:HG13	2.02	0.41
1:D:700:GLU:HB2	1:D:720:SER:HB2	2.03	0.41
1:E:342:LEU:O	1:E:346:GLN:HG3	2.21	0.41
1:E:676:SER:OG	1:E:678:ASP:OD1	2.37	0.41
1:E:947:GLN:HG2	1:E:958:TYR:HD1	1.85	0.41
1:F:153:HIS:HA	1:F:264:THR:O	2.21	0.41
1:F:346:GLN:C	1:F:348:LYS:H	2.28	0.41
1:F:400:LEU:HB3	1:F:404:TRP:HZ3	1.85	0.41
2:J:30:PRO:HB3	2:J:46:PHE:CD2	2.56	0.41
1:A:346:GLN:C	1:A:348:LYS:H	2.28	0.40
1:A:1155:ASN:HB3	1:A:1162:LEU:HB2	2.04	0.40
1:B:351:LYS:NZ	1:B:365:ASP:OD2	2.54	0.40
1:C:322:LEU:HD23	1:C:364:LEU:HD13	2.03	0.40
1:C:326:LEU:HD23	1:C:326:LEU:HA	1.44	0.40
1:C:885:VAL:HG13	1:C:900:SER:O	2.21	0.40
1:C:1141:LEU:HG	1:C:1155:ASN:HA	2.03	0.40
1:D:37:ILE:HG12	3:Q:10:ARG:HD2	2.03	0.40
1:D:1141:LEU:HG	1:D:1155:ASN:HA	2.03	0.40
1:D:1166:ALA:HA	1:D:1167:PRO:HD2	1.93	0.40
1:E:153:HIS:HA	1:E:264:THR:O	2.21	0.40
1:E:885:VAL:HG13	1:E:900:SER:O	2.21	0.40
1:E:1086:GLY:CA	2:L:39:LYS:NZ	2.66	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:348:LYS:NZ	1:F:443:ASP:CG	2.79	0.40
1:F:631:ALA:H	1:F:665:PHE:HZ	1.69	0.40
1:F:1155:ASN:HB3	1:F:1162:LEU:HB2	2.04	0.40
1:G:322:LEU:HD23	1:G:364:LEU:HD13	2.03	0.40
1:G:1141:LEU:HG	1:G:1155:ASN:HA	2.03	0.40
1:G:1155:ASN:HB3	1:G:1162:LEU:HB2	2.04	0.40
2:N:55:LYS:HG2	2:N:75:ILE:HG12	2.03	0.40
3:R:14:LEU:HD13	3:R:14:LEU:HA	1.97	0.40
1:A:228:ARG:HD3	1:A:256:SER:HB3	2.03	0.40
1:A:282:VAL:O	1:A:282:VAL:HG12	2.21	0.40
1:D:153:HIS:HA	1:D:264:THR:O	2.21	0.40
1:D:565:GLN:OE1	1:D:1212:THR:HB	2.21	0.40
1:D:1135:PHE:HE1	1:D:1142:LEU:HD13	1.85	0.40
1:E:196:LEU:O	1:E:199:LEU:HB2	2.21	0.40
1:E:1155:ASN:HB3	1:E:1162:LEU:HB2	2.04	0.40
1:F:344:GLN:CD	1:F:349:GLN:HE21	2.28	0.40
1:F:530:ARG:HD2	1:F:545:GLN:NE2	2.36	0.40
1:F:584:ALA:CA	1:F:594:TYR:CE2	2.98	0.40
1:G:196:LEU:O	1:G:199:LEU:HB2	2.21	0.40
2:H:30:PRO:HB3	2:H:46:PHE:CD2	2.56	0.40
3:P:34:LEU:HD12	3:P:34:LEU:HA	1.93	0.40
1:A:885:VAL:HG13	1:A:900:SER:O	2.21	0.40
1:B:884:TRP:HH2	2:I:79:LYS:N	2.18	0.40
1:B:947:GLN:HG2	1:B:958:TYR:HD1	1.85	0.40
1:C:947:GLN:HG2	1:C:958:TYR:HD1	1.85	0.40
1:E:351:LYS:NZ	1:E:365:ASP:OD2	2.54	0.40
1:E:989:GLU:HG2	1:E:991:VAL:H	1.85	0.40
1:F:565:GLN:CD	1:F:1213:PHE:CA	2.94	0.40
1:G:153:HIS:HA	1:G:264:THR:O	2.21	0.40
1:G:348:LYS:NZ	1:G:443:ASP:CG	2.79	0.40
1:G:631:ALA:H	1:G:665:PHE:HZ	1.69	0.40
1:G:971:PRO:C	1:G:973:LEU:H	2.29	0.40
2:K:55:LYS:HG2	2:K:75:ILE:HG12	2.03	0.40
3:Q:14:LEU:HD13	3:Q:14:LEU:HA	1.98	0.40
1:A:196:LEU:O	1:A:199:LEU:HB2	2.21	0.40
1:A:274:MET:HE2	1:G:358:SER:CB	2.43	0.40
1:A:1141:LEU:HG	1:A:1155:ASN:HA	2.03	0.40
1:B:228:ARG:HD3	1:B:256:SER:HB3	2.03	0.40
1:B:1146:ASP:HB2	1:B:1150:GLU:HG2	2.04	0.40
1:C:337:ARG:O	1:C:340:TYR:N	2.54	0.40
1:C:351:LYS:NZ	1:C:365:ASP:OD2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:884:TRP:HH2	2:J:79:LYS:N	2.18	0.40
1:C:989:GLU:HG2	1:C:991:VAL:H	1.85	0.40
1:D:597:TRP:CD2	1:D:600:LYS:HE3	2.57	0.40
1:E:46:GLU:OE2	1:E:55:MET:HE2	2.21	0.40
1:E:348:LYS:NZ	1:E:443:ASP:CG	2.79	0.40
1:E:631:ALA:H	1:E:665:PHE:HZ	1.69	0.40
1:F:289:GLU:OE2	1:F:303:LYS:NZ	2.43	0.40
2:H:39:LYS:HD2	2:H:56:GLY:O	2.22	0.40
2:H:55:LYS:HG2	2:H:75:ILE:HG12	2.03	0.40
2:I:71:PRO:CD	2:I:84:GLY:HA2	2.52	0.40
2:J:55:LYS:HG2	2:J:75:ILE:HG12	2.03	0.40
2:M:39:LYS:HD2	2:M:56:GLY:O	2.22	0.40
1:A:217:PRO:HG3	1:A:226:ARG:NH1	2.36	0.40
1:A:369:SER:O	1:A:373:GLU:HG2	2.21	0.40
1:A:597:TRP:CD2	1:A:600:LYS:HE3	2.57	0.40
1:B:322:LEU:HD23	1:B:364:LEU:HD13	2.02	0.40
1:B:344:GLN:CD	1:B:349:GLN:HE21	2.28	0.40
1:D:145:GLY:HA2	1:D:259:GLN:HE21	1.85	0.40
1:E:400:LEU:HB3	1:E:404:TRP:HZ3	1.84	0.40
1:F:1086:GLY:CA	2:M:39:LYS:NZ	2.66	0.40
2:I:55:LYS:HG2	2:I:75:ILE:HG12	2.03	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	1135/1248 (91%)	1045 (92%)	84 (7%)	6 (0%)	24	61
1	B	1228/1248 (98%)	1138 (93%)	84 (7%)	6 (0%)	24	61
1	C	1135/1248 (91%)	1045 (92%)	84 (7%)	6 (0%)	24	61
1	D	1228/1248 (98%)	1138 (93%)	84 (7%)	6 (0%)	24	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	1228/1248 (98%)	1138 (93%)	84 (7%)	6 (0%)	24	61
1	F	1135/1248 (91%)	1045 (92%)	84 (7%)	6 (0%)	24	61
1	G	1228/1248 (98%)	1138 (93%)	84 (7%)	6 (0%)	24	61
2	H	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
2	I	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
2	J	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
2	K	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
2	L	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
2	M	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
2	N	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
3	O	93/95 (98%)	92 (99%)	1 (1%)	0	100	100
3	P	93/95 (98%)	92 (99%)	1 (1%)	0	100	100
3	Q	93/95 (98%)	92 (99%)	1 (1%)	0	100	100
3	R	93/95 (98%)	92 (99%)	1 (1%)	0	100	100
All	All	9403/9844 (96%)	8741 (93%)	620 (7%)	42 (0%)	31	65

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1073	ILE
1	B	1073	ILE
1	C	1073	ILE
1	D	1073	ILE
1	E	1073	ILE
1	F	1073	ILE
1	G	1073	ILE
1	A	591	GLY
1	B	591	GLY
1	C	591	GLY
1	D	591	GLY
1	E	591	GLY
1	F	591	GLY
1	G	591	GLY
1	A	347	ASN
1	B	347	ASN
1	C	347	ASN
1	D	347	ASN

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Mol	Chain	Res	Type
1	E	347	ASN
1	F	347	ASN
1	G	347	ASN
1	A	266	ASP
1	B	266	ASP
1	C	266	ASP
1	D	266	ASP
1	E	266	ASP
1	F	266	ASP
1	G	266	ASP
1	A	613	PRO
1	B	613	PRO
1	C	613	PRO
1	D	613	PRO
1	E	613	PRO
1	F	613	PRO
1	G	613	PRO
1	A	1205	VAL
1	B	1205	VAL
1	C	1205	VAL
1	D	1205	VAL
1	E	1205	VAL
1	F	1205	VAL
1	G	1205	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	1022/1119 (91%)	1019 (100%)	3 (0%)	86	85
1	B	1106/1119 (99%)	1101 (100%)	5 (0%)	81	82
1	C	1022/1119 (91%)	1019 (100%)	3 (0%)	86	85
1	D	1106/1119 (99%)	1101 (100%)	5 (0%)	81	82
1	E	1106/1119 (99%)	1101 (100%)	5 (0%)	81	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	1022/1119 (91%)	1019 (100%)	3 (0%)	86 85
1	G	1106/1119 (99%)	1101 (100%)	5 (0%)	81 82
2	H	84/84 (100%)	84 (100%)	0	100 100
2	I	84/84 (100%)	84 (100%)	0	100 100
2	J	84/84 (100%)	84 (100%)	0	100 100
2	K	84/84 (100%)	84 (100%)	0	100 100
2	L	84/84 (100%)	84 (100%)	0	100 100
2	M	84/84 (100%)	84 (100%)	0	100 100
2	N	84/84 (100%)	84 (100%)	0	100 100
3	O	84/84 (100%)	76 (90%)	8 (10%)	8 27
3	P	84/84 (100%)	77 (92%)	7 (8%)	10 32
3	Q	84/84 (100%)	76 (90%)	8 (10%)	8 27
3	R	84/84 (100%)	76 (90%)	8 (10%)	8 27
All	All	8414/8757 (96%)	8354 (99%)	60 (1%)	73 79

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	391	LYS
1	A	392	ASP
1	A	884	TRP
1	B	58	LYS
1	B	81	LYS
1	B	391	LYS
1	B	392	ASP
1	B	884	TRP
1	C	391	LYS
1	C	392	ASP
1	C	884	TRP
1	D	58	LYS
1	D	81	LYS
1	D	391	LYS
1	D	392	ASP
1	D	884	TRP
1	E	58	LYS
1	E	81	LYS
1	E	391	LYS

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Mol	Chain	Res	Type
1	E	392	ASP
1	E	884	TRP
1	F	391	LYS
1	F	392	ASP
1	F	884	TRP
1	G	58	LYS
1	G	81	LYS
1	G	391	LYS
1	G	392	ASP
1	G	884	TRP
3	O	10	ARG
3	O	14	LEU
3	O	20	LEU
3	O	34	LEU
3	O	83	ASP
3	O	84	MET
3	O	87	SER
3	O	93	ARG
3	P	10	ARG
3	P	14	LEU
3	P	20	LEU
3	P	34	LEU
3	P	84	MET
3	P	87	SER
3	P	93	ARG
3	Q	10	ARG
3	Q	14	LEU
3	Q	20	LEU
3	Q	34	LEU
3	Q	83	ASP
3	Q	84	MET
3	Q	87	SER
3	Q	93	ARG
3	R	10	ARG
3	R	14	LEU
3	R	20	LEU
3	R	34	LEU
3	R	83	ASP
3	R	84	MET
3	R	87	SER
3	R	93	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (196)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	201	ASN
1	A	214	GLN
1	A	416	GLN
1	A	469	GLN
1	A	551	ASN
1	A	602	ASN
1	A	620	HIS
1	A	698	HIS
1	A	703	ASN
1	A	709	ASN
1	A	712	HIS
1	A	713	HIS
1	A	748	HIS
1	A	782	ASN
1	A	785	GLN
1	A	819	ASN
1	A	836	HIS
1	A	844	GLN
1	A	917	ASN
1	A	992	ASN
1	A	1076	ASN
1	A	1126	HIS
1	B	11	GLN
1	B	45	ASN
1	B	50	GLN
1	B	51	GLN
1	B	201	ASN
1	B	214	GLN
1	B	416	GLN
1	B	469	GLN
1	B	551	ASN
1	B	602	ASN
1	B	605	ASN
1	B	620	HIS
1	B	698	HIS
1	B	703	ASN
1	B	712	HIS
1	B	713	HIS
1	B	748	HIS
1	B	782	ASN
1	B	785	GLN
1	B	819	ASN

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Mol	Chain	Res	Type
1	B	827	HIS
1	B	836	HIS
1	B	844	GLN
1	B	917	ASN
1	B	963	GLN
1	B	992	ASN
1	B	1076	ASN
1	B	1126	HIS
1	C	121	GLN
1	C	201	ASN
1	C	214	GLN
1	C	416	GLN
1	C	469	GLN
1	C	551	ASN
1	C	602	ASN
1	C	620	HIS
1	C	703	ASN
1	C	709	ASN
1	C	712	HIS
1	C	713	HIS
1	C	748	HIS
1	C	782	ASN
1	C	785	GLN
1	C	819	ASN
1	C	827	HIS
1	C	836	HIS
1	C	844	GLN
1	C	917	ASN
1	C	992	ASN
1	C	1076	ASN
1	C	1126	HIS
1	D	11	GLN
1	D	51	GLN
1	D	201	ASN
1	D	214	GLN
1	D	416	GLN
1	D	469	GLN
1	D	551	ASN
1	D	602	ASN
1	D	605	ASN
1	D	620	HIS
1	D	698	HIS

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Mol	Chain	Res	Type
1	D	703	ASN
1	D	712	HIS
1	D	713	HIS
1	D	748	HIS
1	D	782	ASN
1	D	785	GLN
1	D	819	ASN
1	D	836	HIS
1	D	844	GLN
1	D	917	ASN
1	D	982	ASN
1	D	992	ASN
1	D	1076	ASN
1	D	1126	HIS
1	D	1158	ASN
1	E	11	GLN
1	E	45	ASN
1	E	51	GLN
1	E	201	ASN
1	E	214	GLN
1	E	416	GLN
1	E	469	GLN
1	E	551	ASN
1	E	602	ASN
1	E	620	HIS
1	E	703	ASN
1	E	709	ASN
1	E	712	HIS
1	E	713	HIS
1	E	748	HIS
1	E	782	ASN
1	E	785	GLN
1	E	819	ASN
1	E	827	HIS
1	E	836	HIS
1	E	844	GLN
1	E	917	ASN
1	E	963	GLN
1	E	982	ASN
1	E	992	ASN
1	E	1043	HIS
1	E	1076	ASN

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Mol	Chain	Res	Type
1	E	1126	HIS
1	F	201	ASN
1	F	214	GLN
1	F	416	GLN
1	F	469	GLN
1	F	551	ASN
1	F	602	ASN
1	F	605	ASN
1	F	620	HIS
1	F	703	ASN
1	F	709	ASN
1	F	712	HIS
1	F	713	HIS
1	F	748	HIS
1	F	782	ASN
1	F	785	GLN
1	F	819	ASN
1	F	827	HIS
1	F	836	HIS
1	F	844	GLN
1	F	886	HIS
1	F	917	ASN
1	F	992	ASN
1	F	1043	HIS
1	F	1076	ASN
1	F	1126	HIS
1	F	1158	ASN
1	G	11	GLN
1	G	45	ASN
1	G	51	GLN
1	G	121	GLN
1	G	201	ASN
1	G	214	GLN
1	G	416	GLN
1	G	469	GLN
1	G	551	ASN
1	G	602	ASN
1	G	605	ASN
1	G	620	HIS
1	G	703	ASN
1	G	712	HIS
1	G	713	HIS

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Mol	Chain	Res	Type
1	G	748	HIS
1	G	782	ASN
1	G	785	GLN
1	G	819	ASN
1	G	827	HIS
1	G	836	HIS
1	G	844	GLN
1	G	917	ASN
1	G	963	GLN
1	G	982	ASN
1	G	992	ASN
1	G	1043	HIS
1	G	1076	ASN
1	G	1126	HIS
2	I	70	ASN
2	J	70	ASN
2	K	70	ASN
2	M	70	ASN
2	N	70	ASN
3	O	44	GLN
3	O	92	ASN
3	P	44	GLN
3	P	92	ASN
3	Q	44	GLN
3	Q	92	ASN
3	R	38	HIS
3	R	44	GLN
3	R	92	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	DTP	A	1301	-	31,32,32	3.51	12 (38%)	46,50,50	2.02	11 (23%)
5	HEC	M	500	-	46,50,50	2.02	7 (15%)	58,82,82	1.13	2 (3%)
4	DTP	C	1301	-	31,32,32	3.51	12 (38%)	46,50,50	2.02	11 (23%)
5	HEC	K	500	-	46,50,50	2.02	7 (15%)	58,82,82	1.14	2 (3%)
5	HEC	J	500	-	46,50,50	2.01	7 (15%)	58,82,82	1.13	2 (3%)
4	DTP	F	1301	-	31,32,32	3.51	12 (38%)	46,50,50	2.02	11 (23%)
5	HEC	N	500	-	46,50,50	2.01	7 (15%)	58,82,82	1.14	2 (3%)
4	DTP	B	1301	-	31,32,32	3.50	12 (38%)	46,50,50	2.02	11 (23%)
5	HEC	L	500	-	46,50,50	2.01	7 (15%)	58,82,82	1.13	2 (3%)
5	HEC	I	500	-	46,50,50	2.01	7 (15%)	58,82,82	1.13	2 (3%)
5	HEC	H	500	-	46,50,50	2.02	7 (15%)	58,82,82	1.12	2 (3%)
4	DTP	G	1301	-	31,32,32	3.51	12 (38%)	46,50,50	2.02	11 (23%)
4	DTP	D	1301	-	31,32,32	3.52	12 (38%)	46,50,50	2.02	11 (23%)
4	DTP	E	1301	-	31,32,32	3.51	12 (38%)	46,50,50	2.03	11 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DTP	A	1301	-	-	8/22/34/34	0/3/3/3
5	HEC	M	500	-	-	1/14/54/54	-
4	DTP	C	1301	-	-	8/22/34/34	0/3/3/3
5	HEC	K	500	-	-	1/14/54/54	-
5	HEC	J	500	-	-	1/14/54/54	-
4	DTP	F	1301	-	-	8/22/34/34	0/3/3/3
5	HEC	N	500	-	-	1/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DTP	B	1301	-	-	8/22/34/34	0/3/3/3
5	HEC	L	500	-	-	1/14/54/54	-
5	HEC	I	500	-	-	1/14/54/54	-
5	HEC	H	500	-	-	1/14/54/54	-
4	DTP	G	1301	-	-	8/22/34/34	0/3/3/3
4	DTP	D	1301	-	-	8/22/34/34	0/3/3/3
4	DTP	E	1301	-	-	8/22/34/34	0/3/3/3

All (133) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1301	DTP	C2'-C3'	-12.34	1.21	1.52
4	G	1301	DTP	C2'-C3'	-12.33	1.21	1.52
4	F	1301	DTP	C2'-C3'	-12.33	1.21	1.52
4	A	1301	DTP	C2'-C3'	-12.31	1.21	1.52
4	E	1301	DTP	C2'-C3'	-12.31	1.21	1.52
4	C	1301	DTP	C2'-C3'	-12.31	1.21	1.52
4	B	1301	DTP	C2'-C3'	-12.29	1.21	1.52
4	G	1301	DTP	O4'-C4'	-8.29	1.26	1.45
4	D	1301	DTP	O4'-C4'	-8.28	1.26	1.45
4	F	1301	DTP	O4'-C4'	-8.27	1.26	1.45
4	A	1301	DTP	O4'-C4'	-8.27	1.26	1.45
4	E	1301	DTP	O4'-C4'	-8.27	1.26	1.45
4	C	1301	DTP	O4'-C4'	-8.27	1.26	1.45
4	B	1301	DTP	O4'-C4'	-8.25	1.26	1.45
4	E	1301	DTP	C1'-N9	-8.11	1.31	1.46
4	C	1301	DTP	C1'-N9	-8.09	1.31	1.46
4	F	1301	DTP	C1'-N9	-8.07	1.31	1.46
4	G	1301	DTP	C1'-N9	-8.07	1.31	1.46
4	B	1301	DTP	C1'-N9	-8.07	1.31	1.46
4	A	1301	DTP	C1'-N9	-8.07	1.31	1.46
4	D	1301	DTP	C1'-N9	-8.06	1.31	1.46
5	M	500	HEC	CAC-C3C	6.37	1.55	1.35
5	H	500	HEC	CAC-C3C	6.37	1.55	1.35
5	N	500	HEC	CAC-C3C	6.37	1.55	1.35
5	J	500	HEC	CAC-C3C	6.36	1.55	1.35
5	K	500	HEC	CAC-C3C	6.35	1.55	1.35
5	L	500	HEC	CAC-C3C	6.35	1.55	1.35
5	I	500	HEC	CAC-C3C	6.32	1.55	1.35
5	M	500	HEC	CAB-C3B	6.26	1.55	1.35
5	N	500	HEC	CAB-C3B	6.26	1.55	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	500	HEC	CAB-C3B	6.26	1.55	1.35
5	H	500	HEC	CAB-C3B	6.25	1.55	1.35
5	K	500	HEC	CAB-C3B	6.25	1.55	1.35
5	I	500	HEC	CAB-C3B	6.24	1.55	1.35
5	J	500	HEC	CAB-C3B	6.24	1.55	1.35
5	K	500	HEC	C3D-C2D	5.76	1.53	1.38
5	I	500	HEC	C3D-C2D	5.74	1.53	1.38
5	H	500	HEC	C3D-C2D	5.74	1.53	1.38
5	J	500	HEC	C3D-C2D	5.74	1.53	1.38
5	L	500	HEC	C3D-C2D	5.73	1.53	1.38
5	M	500	HEC	C3D-C2D	5.72	1.53	1.38
5	N	500	HEC	C3D-C2D	5.70	1.53	1.38
4	D	1301	DTP	C3'-C4'	4.23	1.64	1.53
4	E	1301	DTP	C3'-C4'	4.23	1.64	1.53
4	G	1301	DTP	C3'-C4'	4.20	1.64	1.53
4	C	1301	DTP	C3'-C4'	4.20	1.64	1.53
4	B	1301	DTP	C3'-C4'	4.20	1.64	1.53
4	A	1301	DTP	C3'-C4'	4.20	1.64	1.53
4	F	1301	DTP	C3'-C4'	4.19	1.64	1.53
5	N	500	HEC	CBB-CAB	-4.16	1.34	1.49
5	H	500	HEC	CBB-CAB	-4.15	1.34	1.49
5	M	500	HEC	CBB-CAB	-4.15	1.34	1.49
5	L	500	HEC	CBB-CAB	-4.15	1.34	1.49
5	J	500	HEC	CBB-CAB	-4.14	1.34	1.49
5	K	500	HEC	CBB-CAB	-4.14	1.34	1.49
5	I	500	HEC	CBB-CAB	-4.14	1.34	1.49
5	H	500	HEC	CBC-CAC	-4.09	1.34	1.49
5	J	500	HEC	CBC-CAC	-4.09	1.34	1.49
5	N	500	HEC	CBC-CAC	-4.09	1.34	1.49
5	L	500	HEC	CBC-CAC	-4.08	1.34	1.49
5	K	500	HEC	CBC-CAC	-4.07	1.34	1.49
5	I	500	HEC	CBC-CAC	-4.07	1.34	1.49
5	M	500	HEC	CBC-CAC	-4.07	1.34	1.49
4	E	1301	DTP	O4'-C1'	3.37	1.49	1.42
4	D	1301	DTP	O4'-C1'	3.36	1.49	1.42
4	A	1301	DTP	O4'-C1'	3.35	1.49	1.42
4	G	1301	DTP	O4'-C1'	3.34	1.49	1.42
4	C	1301	DTP	O4'-C1'	3.33	1.49	1.42
4	B	1301	DTP	O4'-C1'	3.32	1.49	1.42
4	F	1301	DTP	O4'-C1'	3.32	1.49	1.42
4	E	1301	DTP	C6-N6	2.87	1.41	1.34
4	G	1301	DTP	C6-N6	2.87	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1301	DTP	C6-N6	2.87	1.41	1.34
4	D	1301	DTP	C6-N6	2.87	1.41	1.34
4	B	1301	DTP	C6-N6	2.86	1.41	1.34
4	A	1301	DTP	C6-N6	2.86	1.41	1.34
4	F	1301	DTP	C6-N6	2.86	1.41	1.34
4	G	1301	DTP	O3'-C3'	2.80	1.49	1.43
4	F	1301	DTP	O3'-C3'	2.77	1.49	1.43
4	C	1301	DTP	C5-C4	-2.77	1.34	1.39
4	C	1301	DTP	O3'-C3'	2.76	1.49	1.43
4	A	1301	DTP	O3'-C3'	2.76	1.49	1.43
4	A	1301	DTP	C5-C4	-2.75	1.34	1.39
4	F	1301	DTP	C5-C4	-2.75	1.34	1.39
4	B	1301	DTP	C5-C4	-2.74	1.34	1.39
4	D	1301	DTP	C5-C4	-2.74	1.34	1.39
4	E	1301	DTP	C5-C4	-2.74	1.34	1.39
4	B	1301	DTP	O3'-C3'	2.74	1.49	1.43
4	D	1301	DTP	O3'-C3'	2.74	1.49	1.43
4	G	1301	DTP	C5-C4	-2.73	1.34	1.39
4	E	1301	DTP	O3'-C3'	2.73	1.49	1.43
4	C	1301	DTP	PB-O3B	-2.71	1.56	1.59
4	F	1301	DTP	PB-O3B	-2.66	1.56	1.59
4	G	1301	DTP	PB-O3B	-2.65	1.56	1.59
4	A	1301	DTP	PB-O3B	-2.63	1.56	1.59
4	D	1301	DTP	PB-O3B	-2.63	1.56	1.59
4	B	1301	DTP	PB-O3B	-2.62	1.56	1.59
4	E	1301	DTP	PB-O3B	-2.57	1.56	1.59
4	B	1301	DTP	PA-O3A	-2.41	1.56	1.59
4	D	1301	DTP	PA-O3A	-2.40	1.56	1.59
4	F	1301	DTP	PA-O3A	-2.39	1.56	1.59
4	A	1301	DTP	PA-O3A	-2.38	1.56	1.59
4	C	1301	DTP	PA-O3A	-2.37	1.56	1.59
4	E	1301	DTP	PA-O3A	-2.37	1.56	1.59
4	G	1301	DTP	PA-O3A	-2.36	1.57	1.59
4	D	1301	DTP	PB-O3A	-2.34	1.57	1.59
4	B	1301	DTP	PB-O3A	-2.28	1.57	1.59
4	G	1301	DTP	PB-O3A	-2.27	1.57	1.59
4	A	1301	DTP	PB-O3A	-2.25	1.57	1.59
4	C	1301	DTP	PB-O3A	-2.24	1.57	1.59
4	F	1301	DTP	PB-O3A	-2.19	1.57	1.59
4	D	1301	DTP	C5-N7	-2.18	1.35	1.39
4	E	1301	DTP	PB-O3A	-2.17	1.57	1.59
4	G	1301	DTP	C5-N7	-2.16	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1301	DTP	C5-N7	-2.16	1.35	1.39
4	A	1301	DTP	C5-N7	-2.15	1.35	1.39
4	B	1301	DTP	C5-N7	-2.15	1.35	1.39
4	C	1301	DTP	C5-N7	-2.15	1.35	1.39
4	F	1301	DTP	C5-N7	-2.14	1.35	1.39
5	I	500	HEC	CMC-C2C	2.11	1.55	1.50
5	K	500	HEC	CMC-C2C	2.11	1.55	1.50
5	L	500	HEC	CMC-C2C	2.11	1.55	1.50
5	H	500	HEC	CMC-C2C	2.11	1.55	1.50
5	J	500	HEC	CMC-C2C	2.09	1.55	1.50
5	M	500	HEC	CMC-C2C	2.09	1.55	1.50
5	N	500	HEC	CMC-C2C	2.08	1.55	1.50
5	I	500	HEC	CMA-C3A	2.05	1.55	1.50
5	K	500	HEC	CMA-C3A	2.05	1.55	1.50
5	H	500	HEC	CMA-C3A	2.04	1.55	1.50
5	L	500	HEC	CMA-C3A	2.02	1.54	1.50
5	J	500	HEC	CMA-C3A	2.01	1.54	1.50
5	M	500	HEC	CMA-C3A	2.01	1.54	1.50
5	N	500	HEC	CMA-C3A	2.01	1.54	1.50

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	1301	DTP	N3-C2-N1	-5.67	120.00	128.58
4	G	1301	DTP	N3-C2-N1	-5.67	120.01	128.58
4	E	1301	DTP	N3-C2-N1	-5.66	120.01	128.58
4	C	1301	DTP	N3-C2-N1	-5.64	120.04	128.58
4	A	1301	DTP	N3-C2-N1	-5.64	120.04	128.58
4	B	1301	DTP	N3-C2-N1	-5.62	120.07	128.58
4	F	1301	DTP	N3-C2-N1	-5.60	120.10	128.58
4	D	1301	DTP	N6-C6-N1	-5.45	106.23	118.38
4	G	1301	DTP	N6-C6-N1	-5.45	106.24	118.38
4	E	1301	DTP	N6-C6-N1	-5.45	106.24	118.38
4	F	1301	DTP	N6-C6-N1	-5.45	106.24	118.38
4	A	1301	DTP	N6-C6-N1	-5.44	106.25	118.38
4	B	1301	DTP	N6-C6-N1	-5.44	106.25	118.38
4	C	1301	DTP	N6-C6-N1	-5.43	106.28	118.38
4	C	1301	DTP	C5-C4-N3	-4.98	119.86	126.72
4	E	1301	DTP	C5-C4-N3	-4.98	119.86	126.72
4	D	1301	DTP	C5-C4-N3	-4.96	119.88	126.72
4	F	1301	DTP	C5-C4-N3	-4.96	119.89	126.72
4	B	1301	DTP	C5-C4-N3	-4.96	119.89	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1301	DTP	C5-C4-N3	-4.96	119.89	126.72
4	G	1301	DTP	C5-C4-N3	-4.93	119.93	126.72
4	E	1301	DTP	C5-C6-N6	4.34	134.02	123.29
4	F	1301	DTP	C5-C6-N6	4.32	133.98	123.29
4	B	1301	DTP	C5-C6-N6	4.32	133.98	123.29
4	A	1301	DTP	C5-C6-N6	4.31	133.97	123.29
4	C	1301	DTP	C5-C6-N6	4.30	133.94	123.29
4	D	1301	DTP	C5-C6-N6	4.30	133.93	123.29
4	G	1301	DTP	C5-C6-N6	4.29	133.92	123.29
4	C	1301	DTP	N9-C8-N7	-4.04	108.20	113.94
4	F	1301	DTP	N9-C8-N7	-4.04	108.21	113.94
4	E	1301	DTP	N9-C8-N7	-4.04	108.21	113.94
4	D	1301	DTP	N9-C8-N7	-4.04	108.21	113.94
4	A	1301	DTP	N9-C8-N7	-4.02	108.23	113.94
4	G	1301	DTP	N9-C8-N7	-4.01	108.25	113.94
4	B	1301	DTP	N9-C8-N7	-4.00	108.26	113.94
5	I	500	HEC	C4D-ND-C1D	3.71	111.87	105.82
5	M	500	HEC	C4D-ND-C1D	3.71	111.86	105.82
5	K	500	HEC	C4D-ND-C1D	3.70	111.86	105.82
5	N	500	HEC	C4D-ND-C1D	3.70	111.85	105.82
5	L	500	HEC	C4D-ND-C1D	3.67	111.81	105.82
5	J	500	HEC	C4D-ND-C1D	3.67	111.81	105.82
5	H	500	HEC	C4D-ND-C1D	3.66	111.78	105.82
4	D	1301	DTP	C2-N3-C4	3.30	119.89	111.83
4	E	1301	DTP	C2-N3-C4	3.29	119.87	111.83
4	C	1301	DTP	C2-N3-C4	3.28	119.84	111.83
4	G	1301	DTP	C2-N3-C4	3.28	119.84	111.83
4	A	1301	DTP	C2-N3-C4	3.28	119.84	111.83
4	B	1301	DTP	C2-N3-C4	3.27	119.83	111.83
4	F	1301	DTP	C2-N3-C4	3.26	119.80	111.83
4	D	1301	DTP	N3-C4-N9	2.77	131.88	127.17
4	B	1301	DTP	N3-C4-N9	2.76	131.86	127.17
4	E	1301	DTP	N3-C4-N9	2.75	131.85	127.17
4	A	1301	DTP	N3-C4-N9	2.74	131.83	127.17
4	C	1301	DTP	N3-C4-N9	2.74	131.83	127.17
4	F	1301	DTP	N3-C4-N9	2.74	131.83	127.17
4	G	1301	DTP	N3-C4-N9	2.73	131.81	127.17
4	C	1301	DTP	C5-N7-C8	2.70	107.70	103.45
4	G	1301	DTP	C5-N7-C8	2.70	107.69	103.45
4	F	1301	DTP	C5-N7-C8	2.70	107.69	103.45
4	E	1301	DTP	C5-N7-C8	2.70	107.69	103.45
4	D	1301	DTP	C5-N7-C8	2.69	107.68	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1301	DTP	C5-N7-C8	2.68	107.67	103.45
4	B	1301	DTP	C5-N7-C8	2.67	107.65	103.45
4	E	1301	DTP	C6-C5-C4	2.44	120.51	117.18
4	C	1301	DTP	C6-C5-C4	2.44	120.50	117.18
4	F	1301	DTP	C6-C5-C4	2.42	120.49	117.18
4	B	1301	DTP	C6-C5-C4	2.42	120.48	117.18
4	A	1301	DTP	C6-C5-C4	2.41	120.47	117.18
5	J	500	HEC	C2A-C1A-NA	-2.41	108.00	110.32
5	M	500	HEC	C2A-C1A-NA	-2.41	108.00	110.32
4	D	1301	DTP	C6-C5-C4	2.39	120.44	117.18
5	L	500	HEC	C2A-C1A-NA	-2.38	108.02	110.32
4	G	1301	DTP	C6-C5-C4	2.37	120.42	117.18
5	K	500	HEC	C2A-C1A-NA	-2.35	108.05	110.32
5	I	500	HEC	C2A-C1A-NA	-2.34	108.06	110.32
5	N	500	HEC	C2A-C1A-NA	-2.34	108.06	110.32
5	H	500	HEC	C2A-C1A-NA	-2.32	108.09	110.32
4	C	1301	DTP	C5-C4-N9	2.29	108.30	105.81
4	E	1301	DTP	C5-C4-N9	2.27	108.28	105.81
4	F	1301	DTP	C5-C4-N9	2.26	108.28	105.81
4	A	1301	DTP	C5-C4-N9	2.26	108.27	105.81
4	G	1301	DTP	C5-C4-N9	2.25	108.26	105.81
4	B	1301	DTP	C5-C4-N9	2.23	108.25	105.81
4	D	1301	DTP	C5-C4-N9	2.22	108.23	105.81
4	C	1301	DTP	C4-C5-N7	-2.07	108.22	110.58
4	F	1301	DTP	C4-C5-N7	-2.06	108.23	110.58
4	G	1301	DTP	C4-C5-N7	-2.05	108.24	110.58
4	A	1301	DTP	C4-C5-N7	-2.05	108.24	110.58
4	B	1301	DTP	C4-C5-N7	-2.05	108.24	110.58
4	E	1301	DTP	C4-C5-N7	-2.05	108.24	110.58
4	D	1301	DTP	C4-C5-N7	-2.02	108.27	110.58

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1301	DTP	C5'-O5'-PA-O1A
4	A	1301	DTP	C5'-O5'-PA-O2A
4	A	1301	DTP	C5'-O5'-PA-O3A
4	A	1301	DTP	O4'-C4'-C5'-O5'
4	B	1301	DTP	C5'-O5'-PA-O1A
4	B	1301	DTP	C5'-O5'-PA-O2A
4	B	1301	DTP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
4	B	1301	DTP	O4'-C4'-C5'-O5'
4	C	1301	DTP	C5'-O5'-PA-O1A
4	C	1301	DTP	C5'-O5'-PA-O2A
4	C	1301	DTP	C5'-O5'-PA-O3A
4	C	1301	DTP	O4'-C4'-C5'-O5'
4	D	1301	DTP	C5'-O5'-PA-O1A
4	D	1301	DTP	C5'-O5'-PA-O2A
4	D	1301	DTP	C5'-O5'-PA-O3A
4	D	1301	DTP	O4'-C4'-C5'-O5'
4	E	1301	DTP	C5'-O5'-PA-O1A
4	E	1301	DTP	C5'-O5'-PA-O2A
4	E	1301	DTP	C5'-O5'-PA-O3A
4	E	1301	DTP	O4'-C4'-C5'-O5'
4	F	1301	DTP	C5'-O5'-PA-O1A
4	F	1301	DTP	C5'-O5'-PA-O2A
4	F	1301	DTP	C5'-O5'-PA-O3A
4	F	1301	DTP	O4'-C4'-C5'-O5'
4	G	1301	DTP	C5'-O5'-PA-O1A
4	G	1301	DTP	C5'-O5'-PA-O2A
4	G	1301	DTP	C5'-O5'-PA-O3A
4	G	1301	DTP	O4'-C4'-C5'-O5'
4	A	1301	DTP	C3'-C4'-C5'-O5'
4	B	1301	DTP	C3'-C4'-C5'-O5'
4	C	1301	DTP	C3'-C4'-C5'-O5'
4	D	1301	DTP	C3'-C4'-C5'-O5'
4	E	1301	DTP	C3'-C4'-C5'-O5'
4	F	1301	DTP	C3'-C4'-C5'-O5'
4	G	1301	DTP	C3'-C4'-C5'-O5'
4	A	1301	DTP	O4'-C1'-N9-C8
4	B	1301	DTP	O4'-C1'-N9-C8
4	C	1301	DTP	O4'-C1'-N9-C8
4	D	1301	DTP	O4'-C1'-N9-C8
4	E	1301	DTP	O4'-C1'-N9-C8
4	F	1301	DTP	O4'-C1'-N9-C8
4	G	1301	DTP	O4'-C1'-N9-C8
4	A	1301	DTP	PG-O3B-PB-O2B
4	B	1301	DTP	PG-O3B-PB-O2B
4	C	1301	DTP	PG-O3B-PB-O2B
4	D	1301	DTP	PG-O3B-PB-O2B
4	E	1301	DTP	PG-O3B-PB-O2B
4	F	1301	DTP	PG-O3B-PB-O2B
4	G	1301	DTP	PG-O3B-PB-O2B

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Mol	Chain	Res	Type	Atoms
4	A	1301	DTP	O4'-C1'-N9-C4
4	B	1301	DTP	O4'-C1'-N9-C4
4	C	1301	DTP	O4'-C1'-N9-C4
4	D	1301	DTP	O4'-C1'-N9-C4
4	E	1301	DTP	O4'-C1'-N9-C4
4	F	1301	DTP	O4'-C1'-N9-C4
4	G	1301	DTP	O4'-C1'-N9-C4
5	N	500	HEC	CAD-CBD-CGD-O2D
5	H	500	HEC	CAD-CBD-CGD-O2D
5	I	500	HEC	CAD-CBD-CGD-O2D
5	J	500	HEC	CAD-CBD-CGD-O2D
5	K	500	HEC	CAD-CBD-CGD-O2D
5	L	500	HEC	CAD-CBD-CGD-O2D
5	M	500	HEC	CAD-CBD-CGD-O2D

There are no ring outliers.

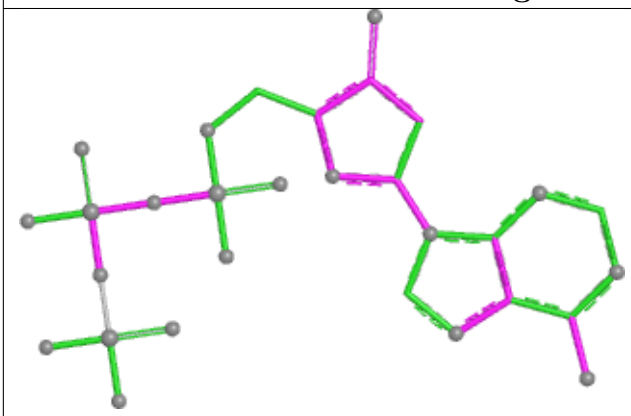
14 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1301	DTP	3	0
5	M	500	HEC	2	0
4	C	1301	DTP	3	0
5	K	500	HEC	2	0
5	J	500	HEC	2	0
4	F	1301	DTP	3	0
5	N	500	HEC	2	0
4	B	1301	DTP	3	0
5	L	500	HEC	2	0
5	I	500	HEC	2	0
5	H	500	HEC	2	0
4	G	1301	DTP	3	0
4	D	1301	DTP	3	0
4	E	1301	DTP	3	0

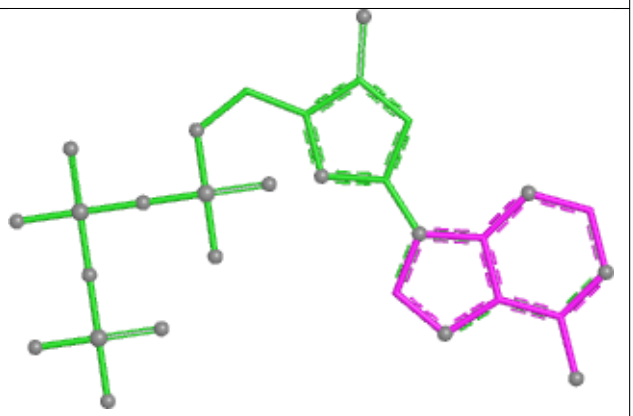
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

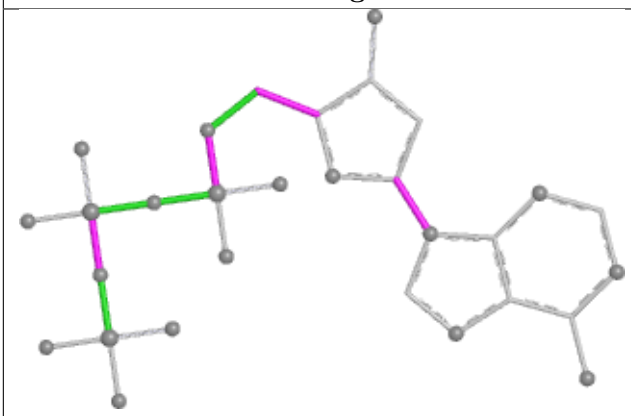
Ligand DTP A 1301



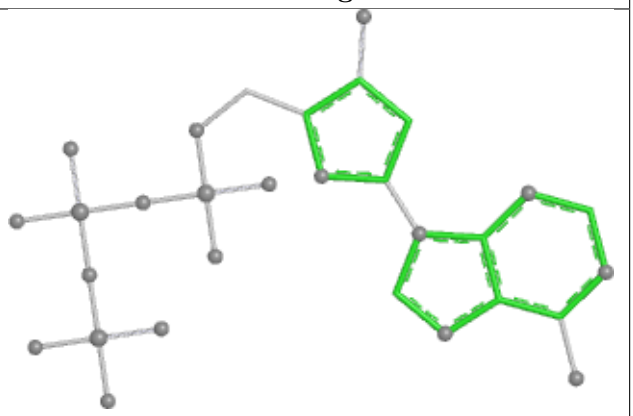
Bond lengths



Bond angles

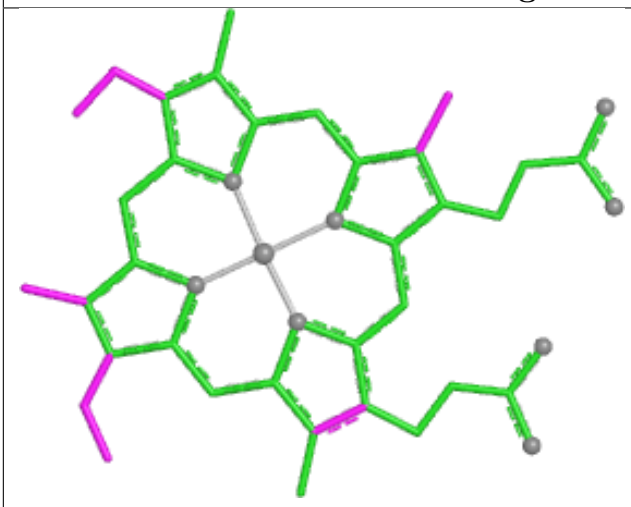


Torsions



Rings

Ligand HEC M 500



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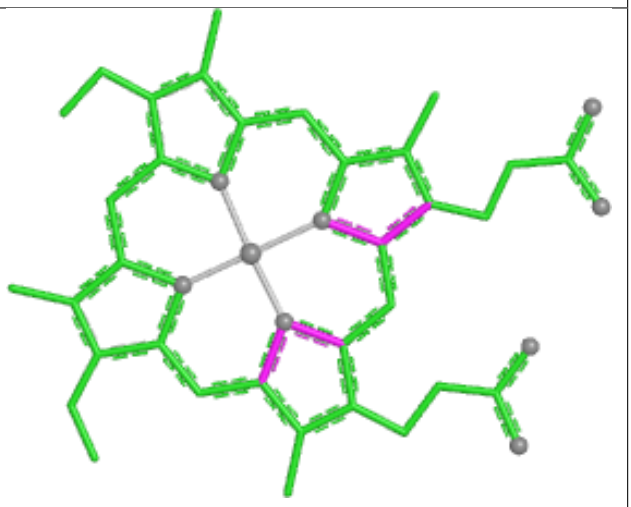
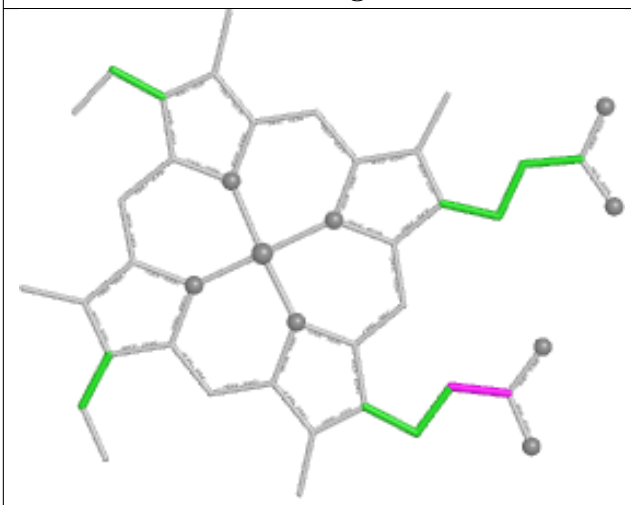


Bond angles



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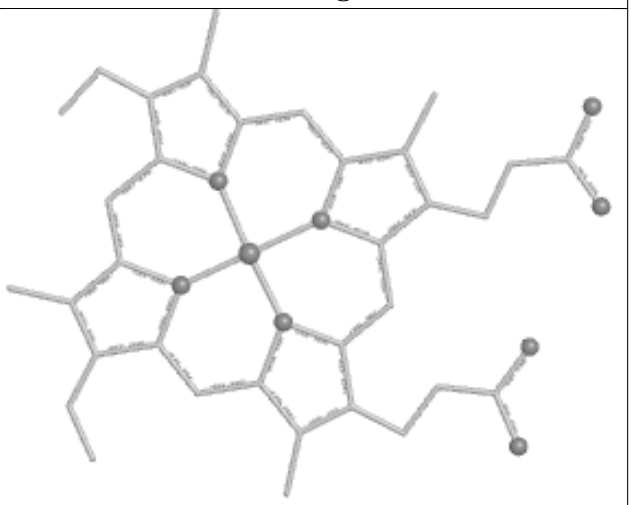
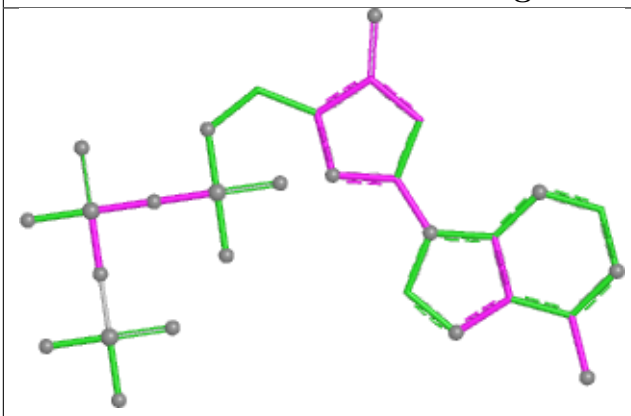
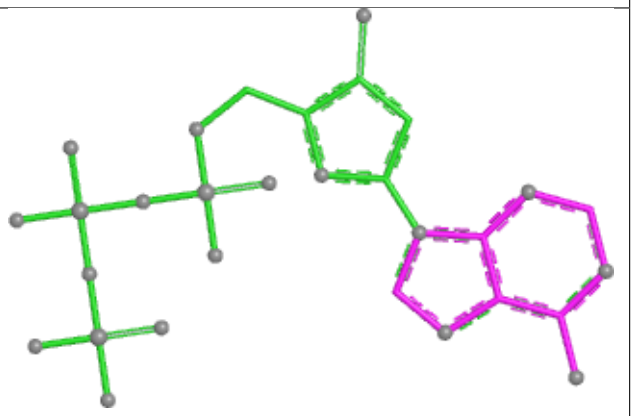


Rings

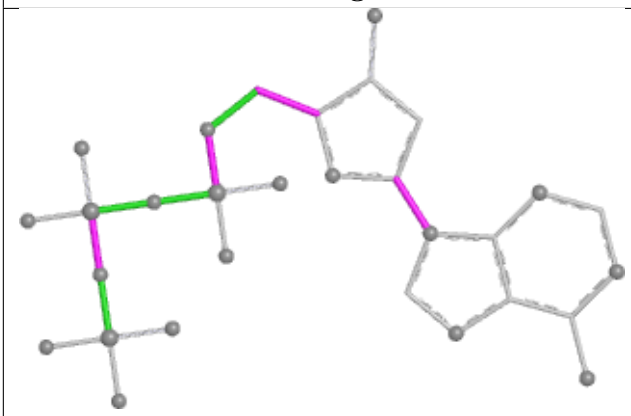
Ligand DTP C 1301



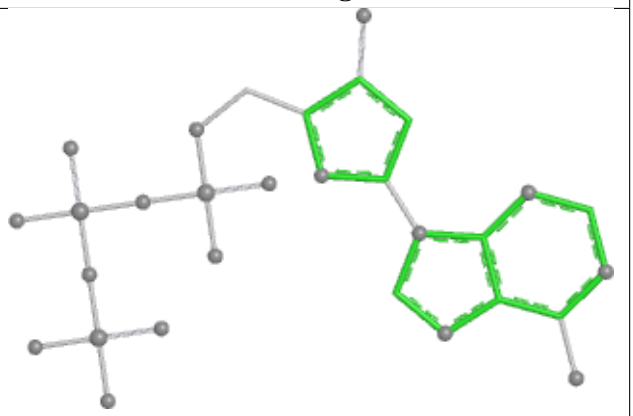
Bond lengths



Bond angles



Torsions



Rings

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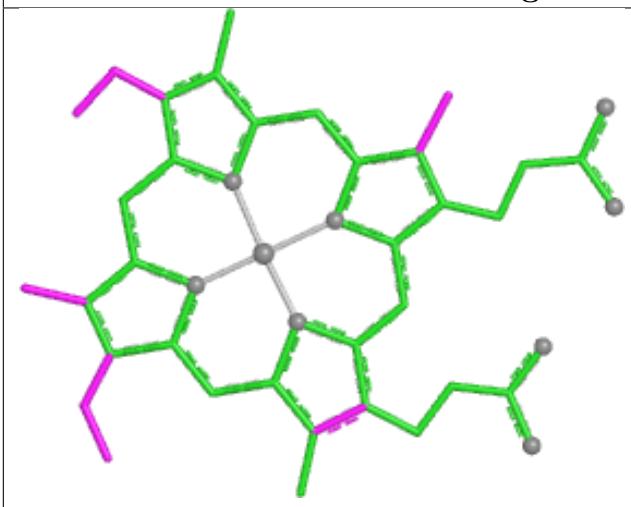

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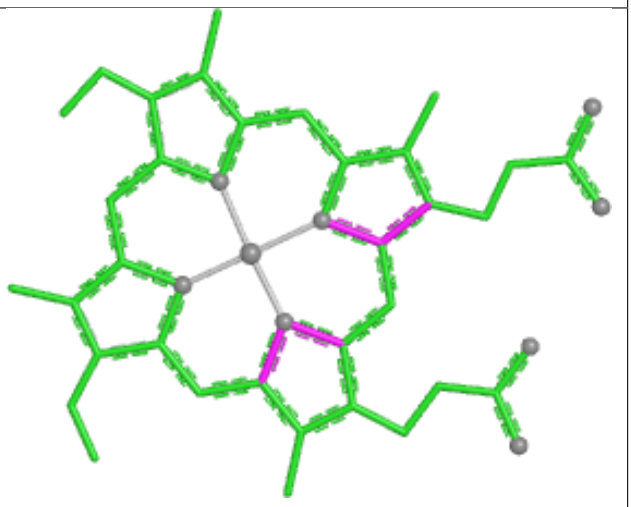

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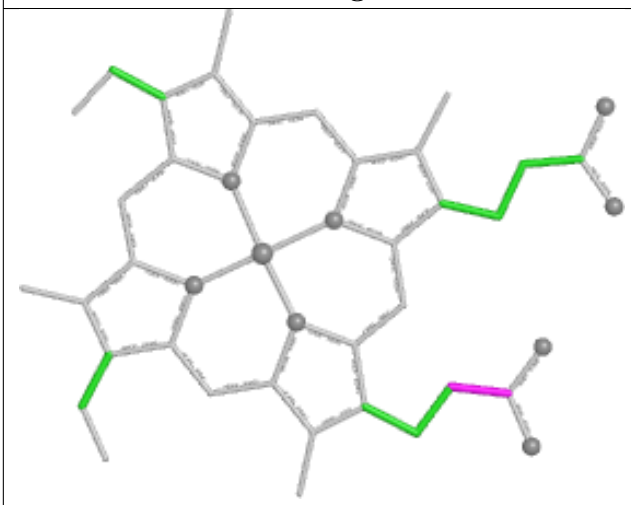

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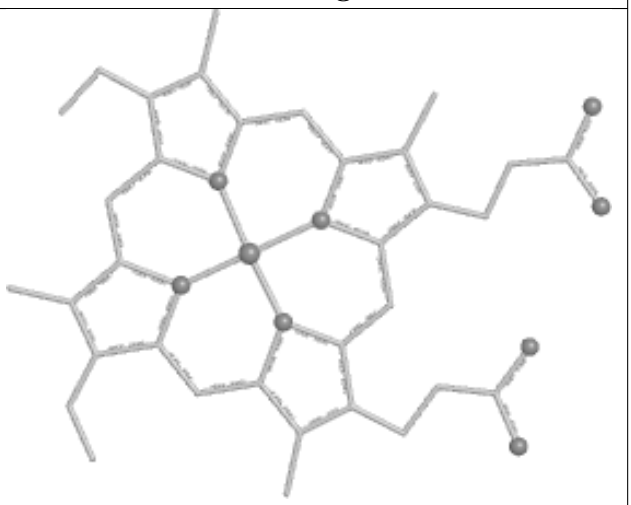
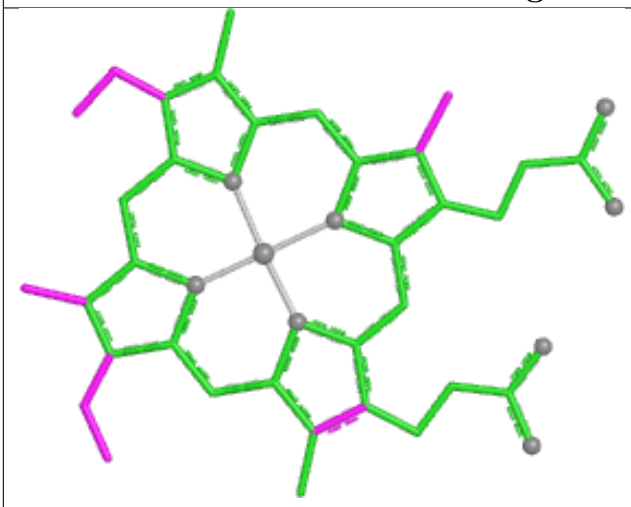


Rings

Ligand HEC J 500



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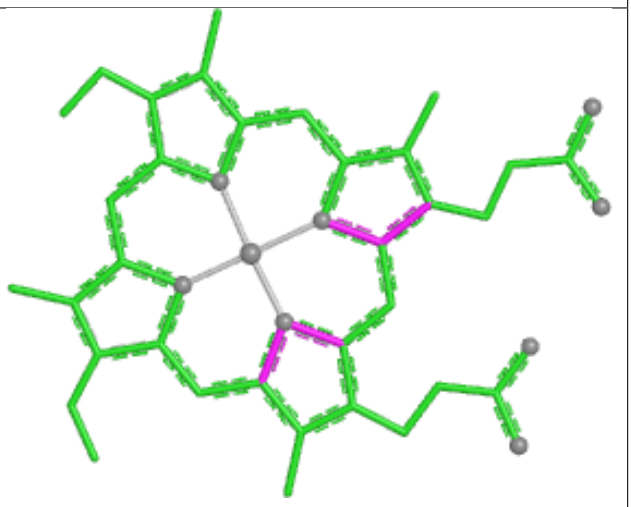

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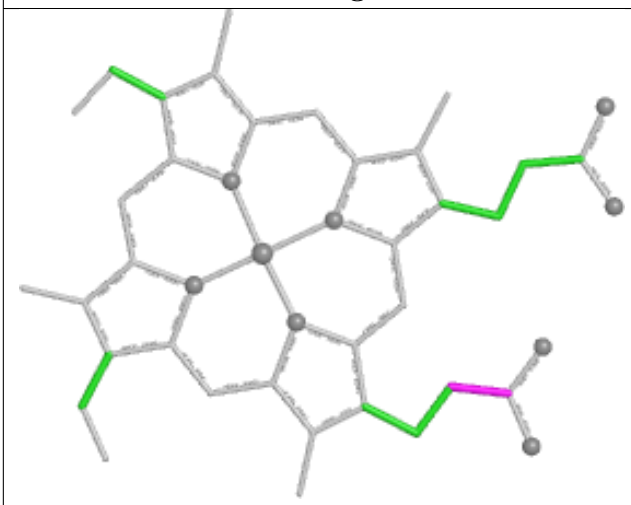

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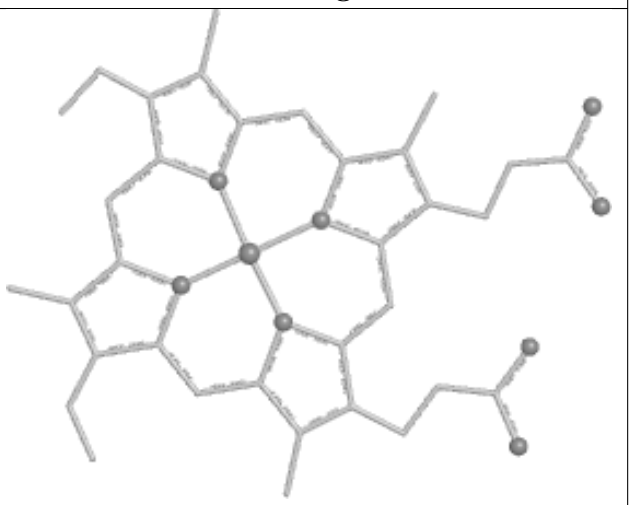
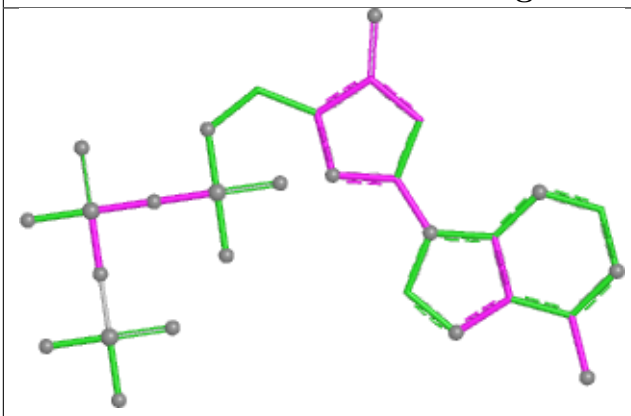


Rings

Ligand DTP F 1301



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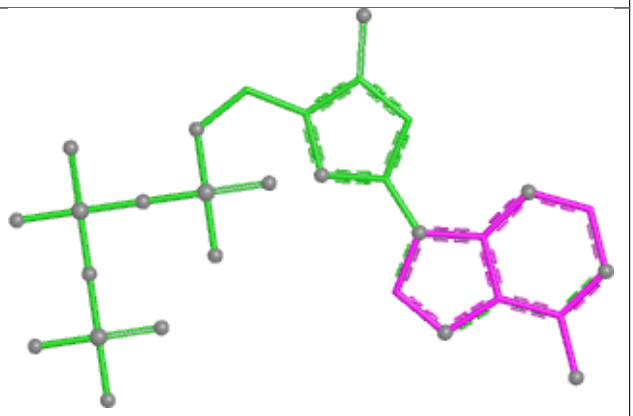

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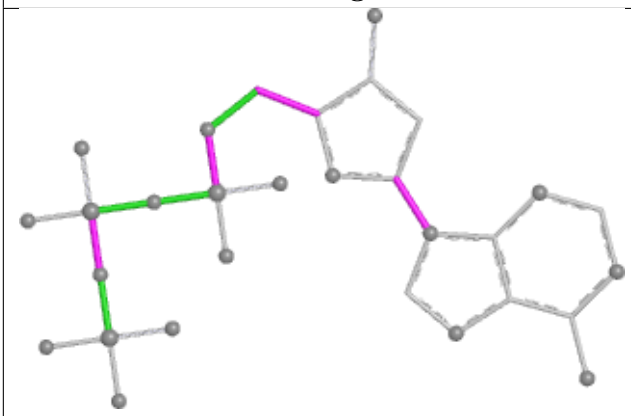

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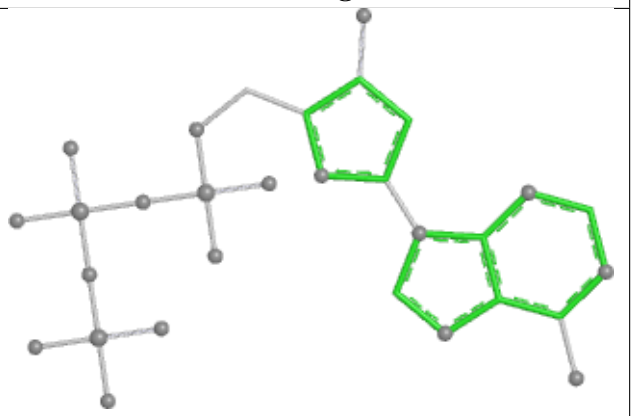

Rings

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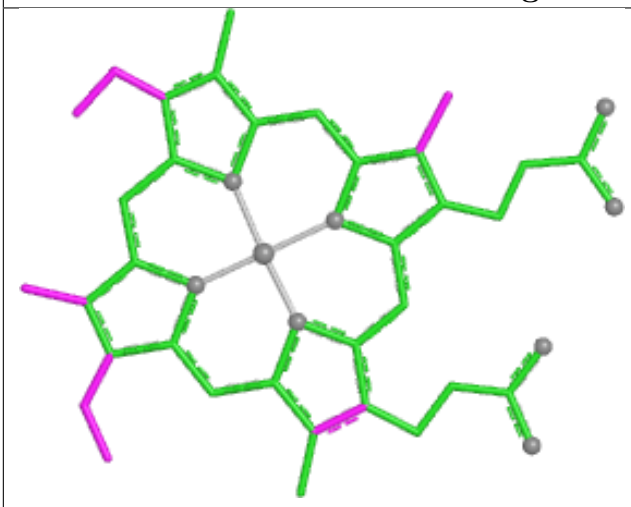

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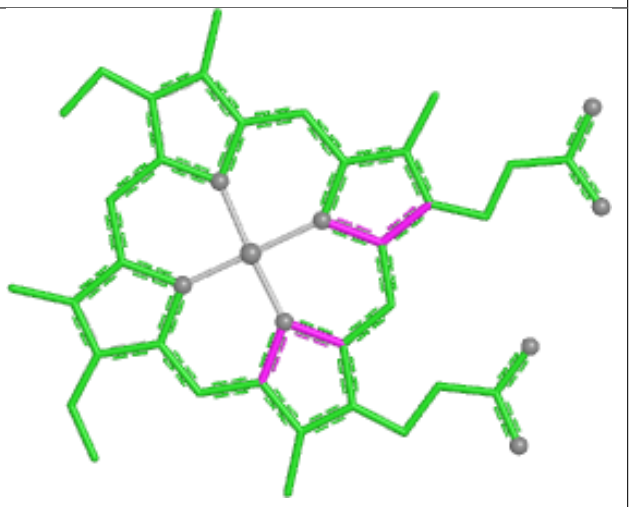

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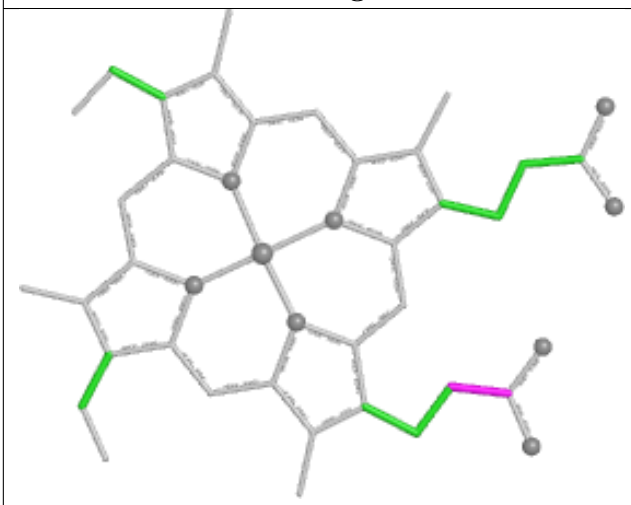

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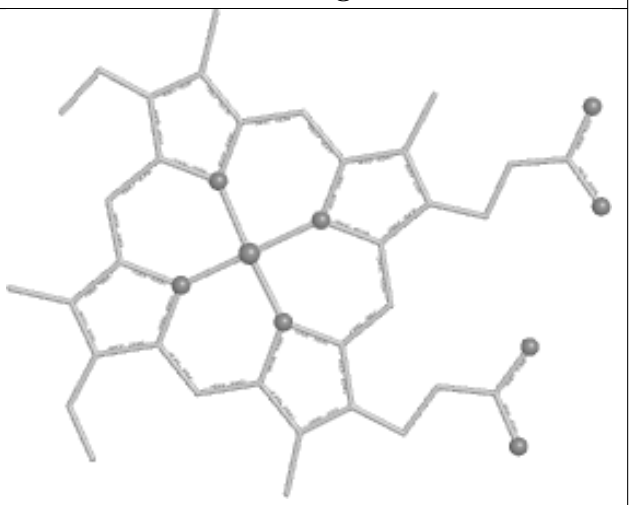

Rings

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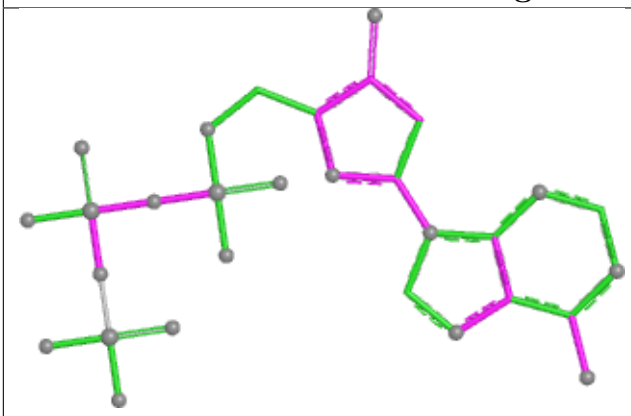

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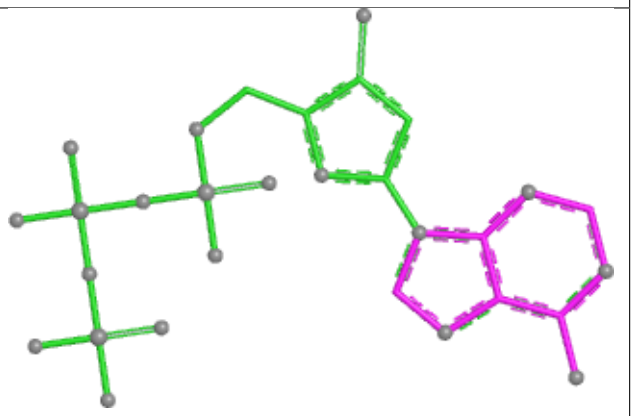

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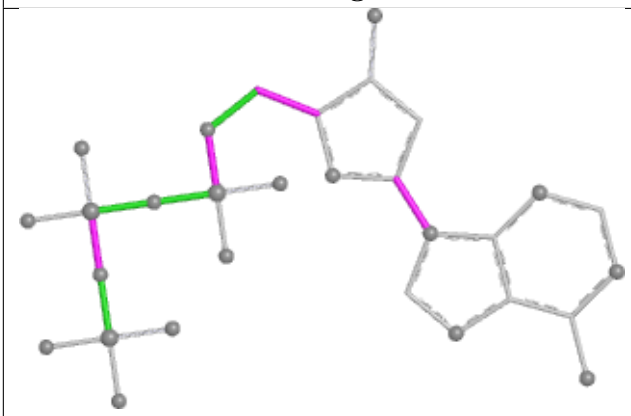

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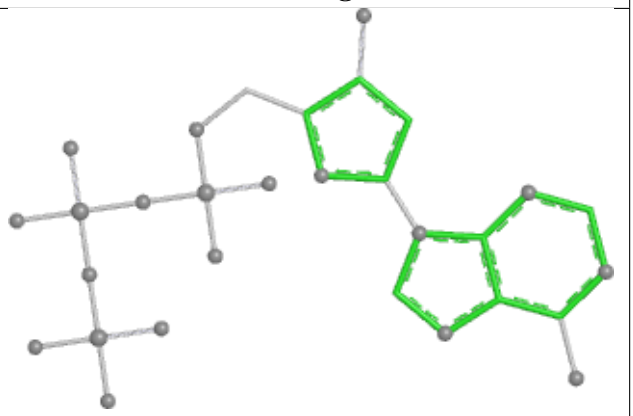
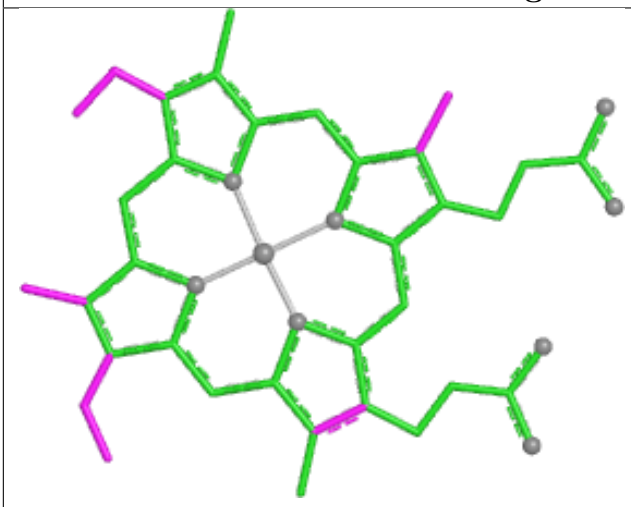


Rings

Ligand HEC L 500



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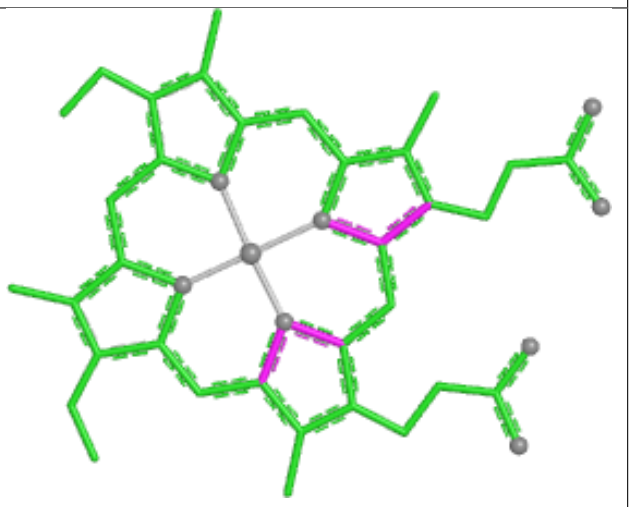
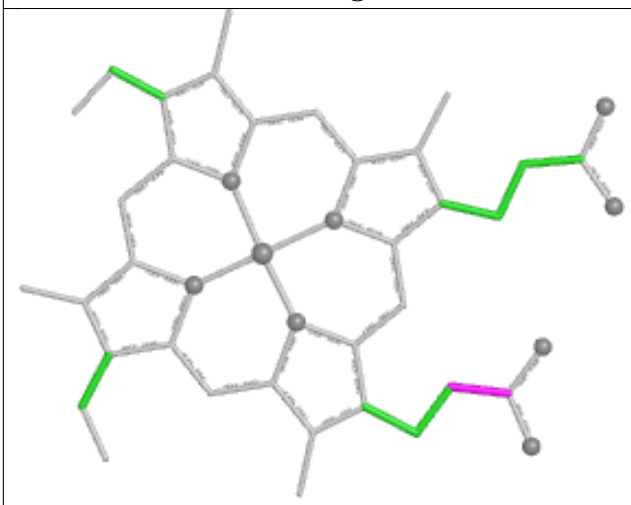


Bond angles



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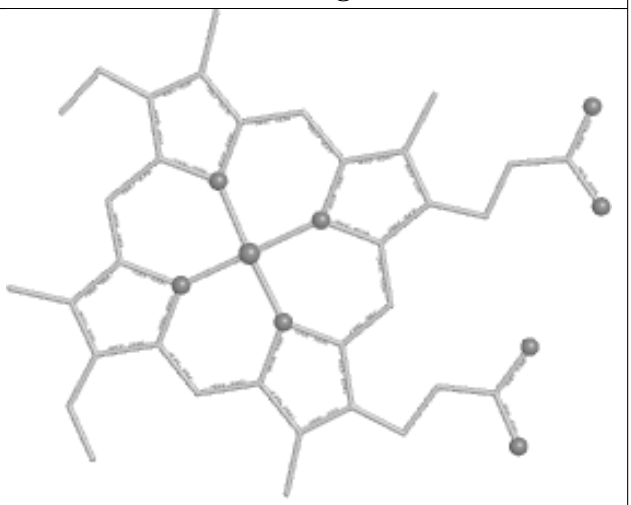
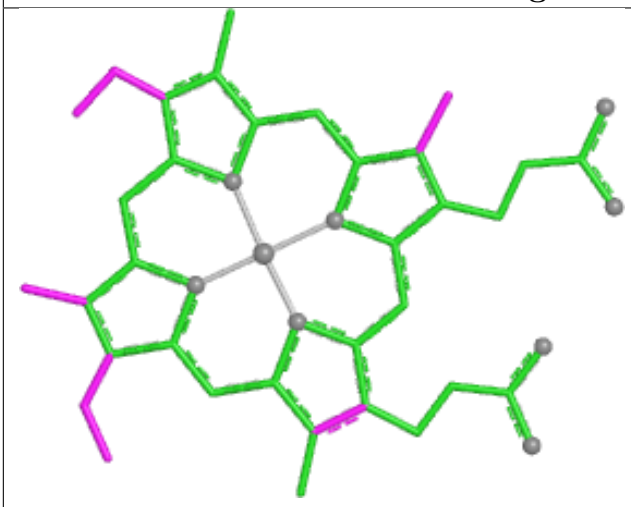


Rings

Ligand HEC I 500



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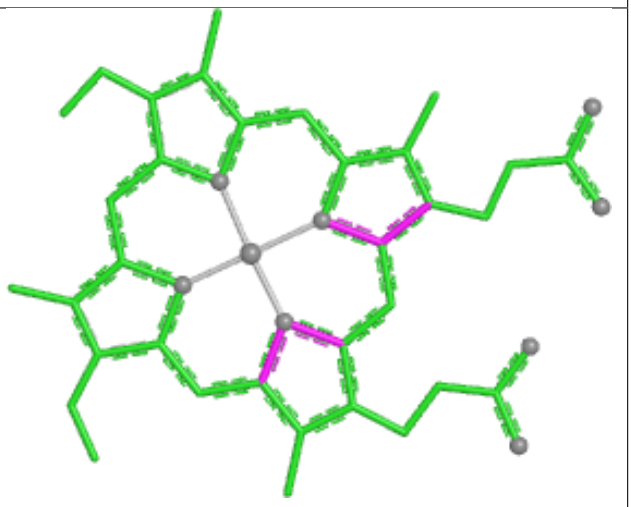

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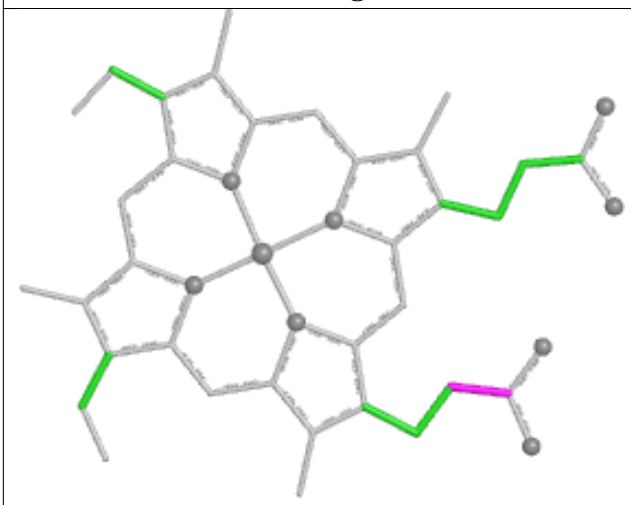

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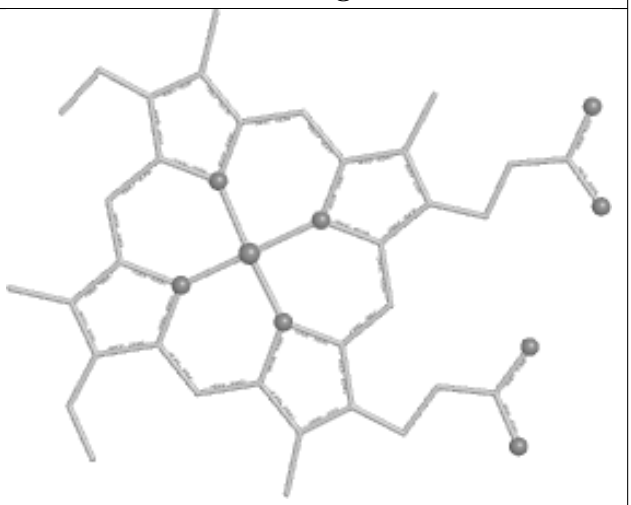

Rings

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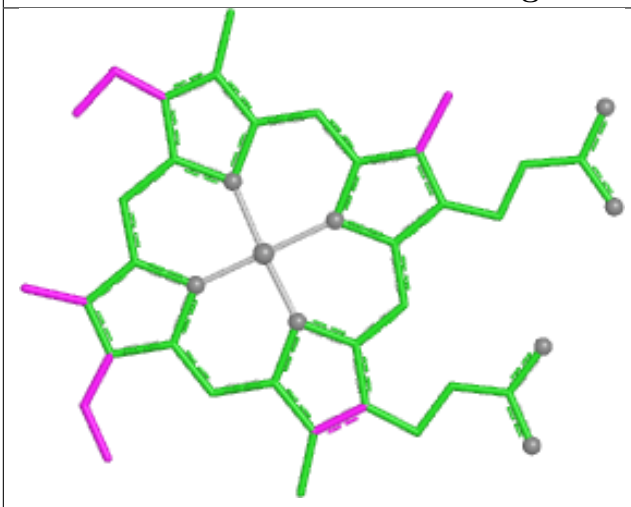

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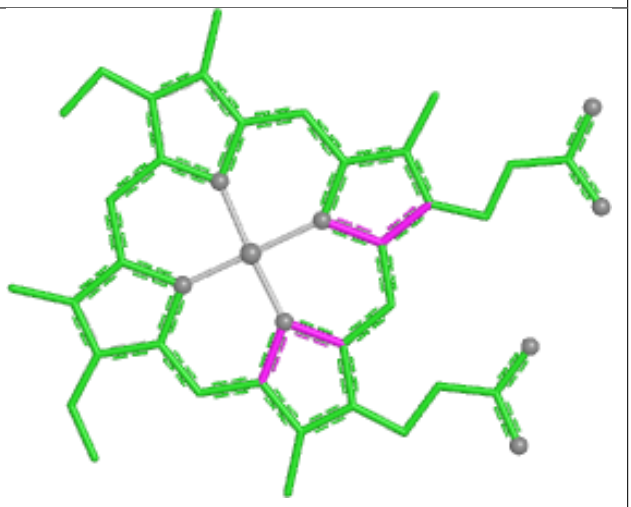
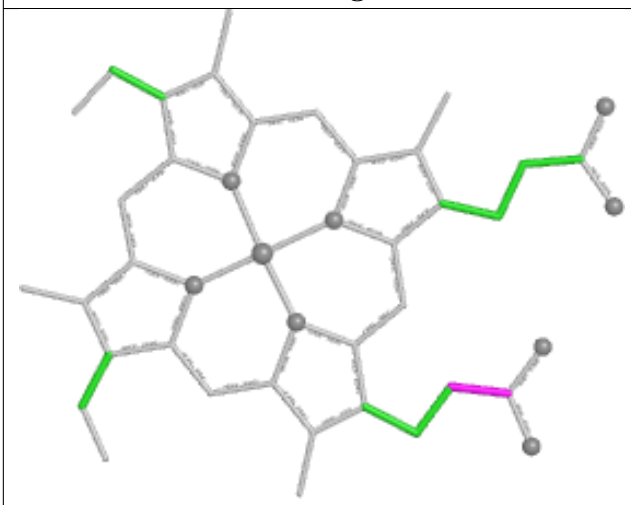


Bond angles



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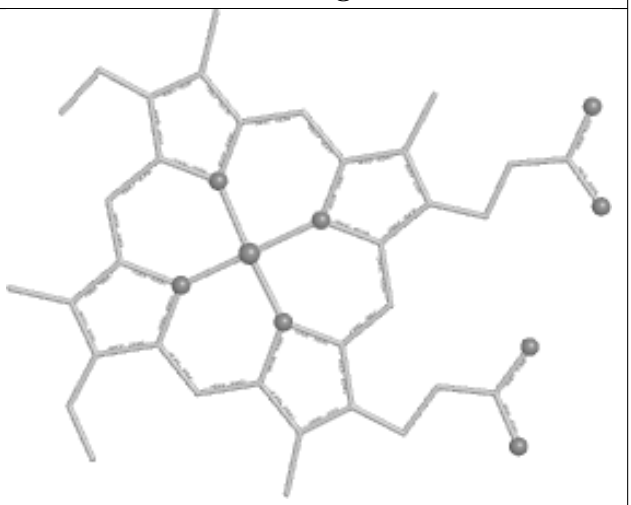
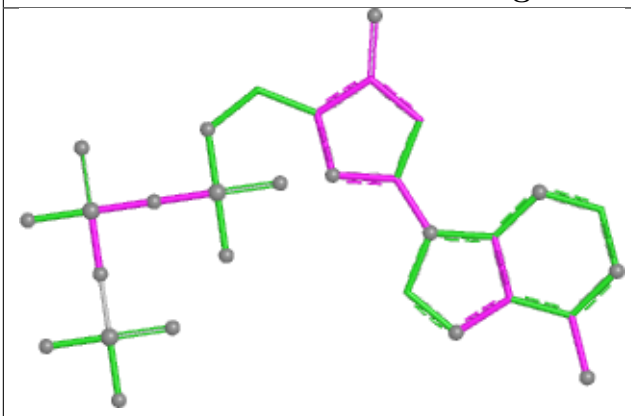


Rings

Ligand DTP G 1301



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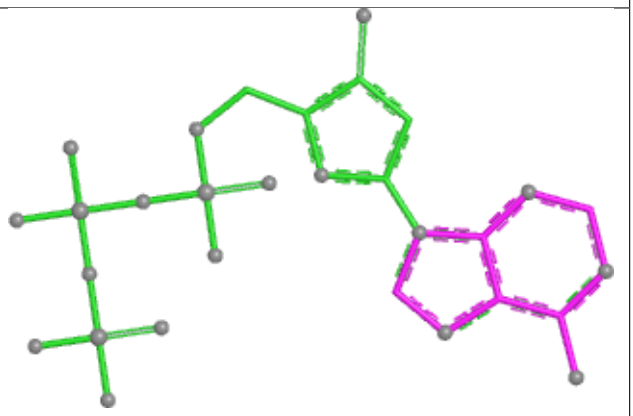
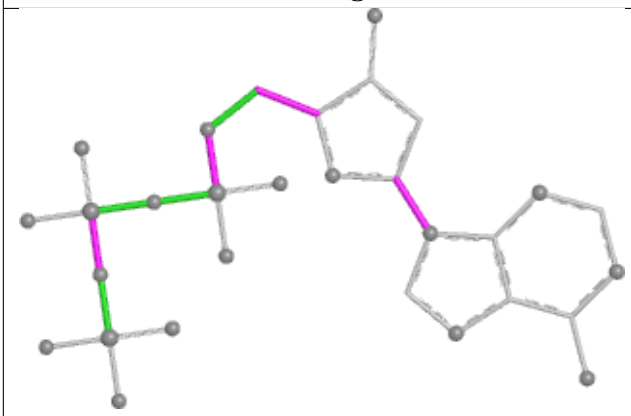
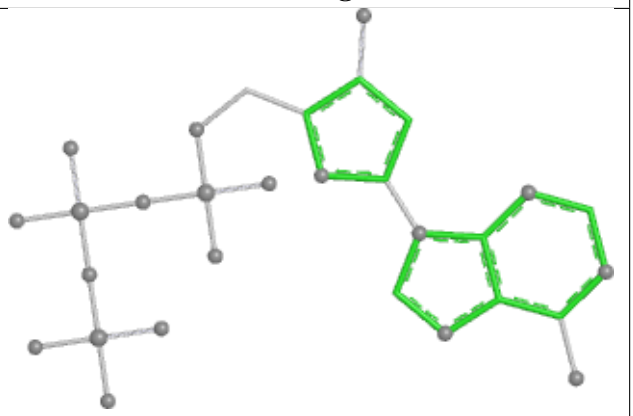


Bond angles



Torsions



Rings

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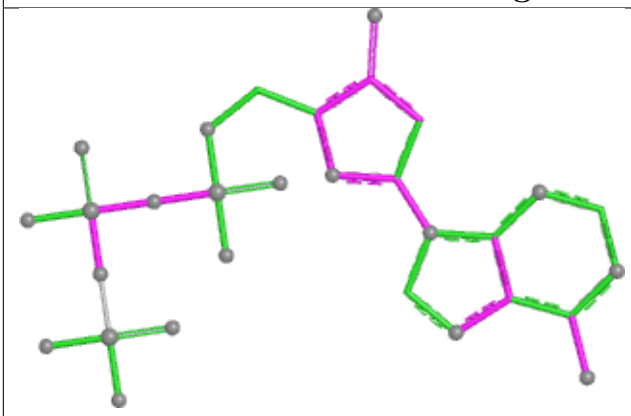

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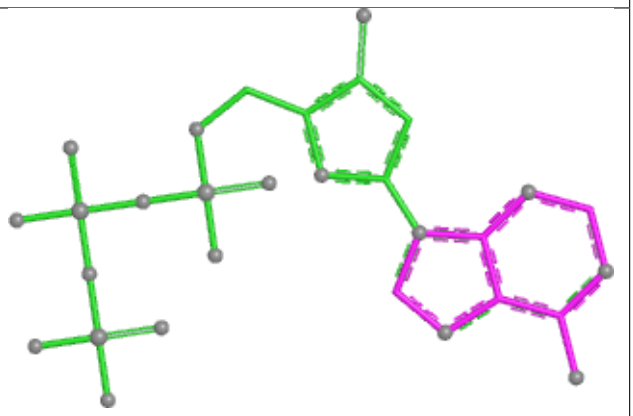
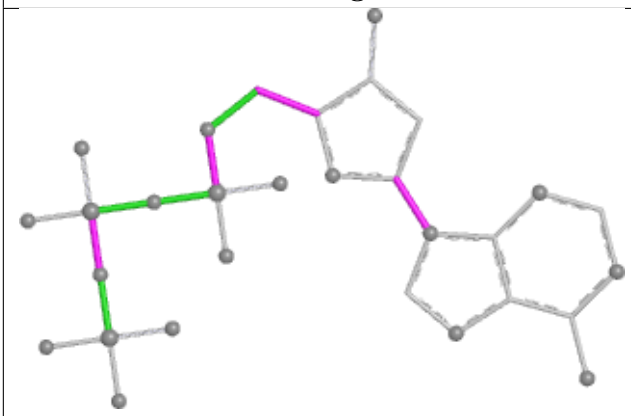
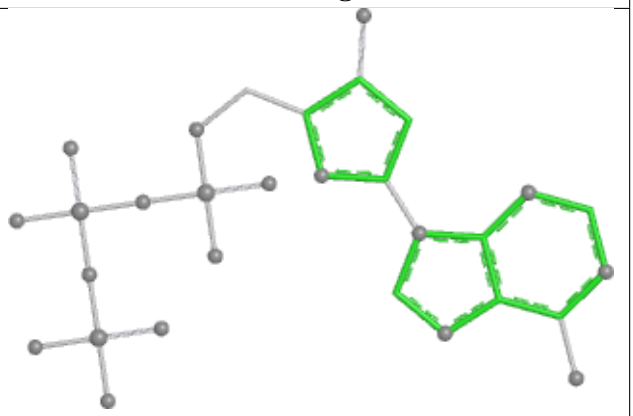


Bond angles

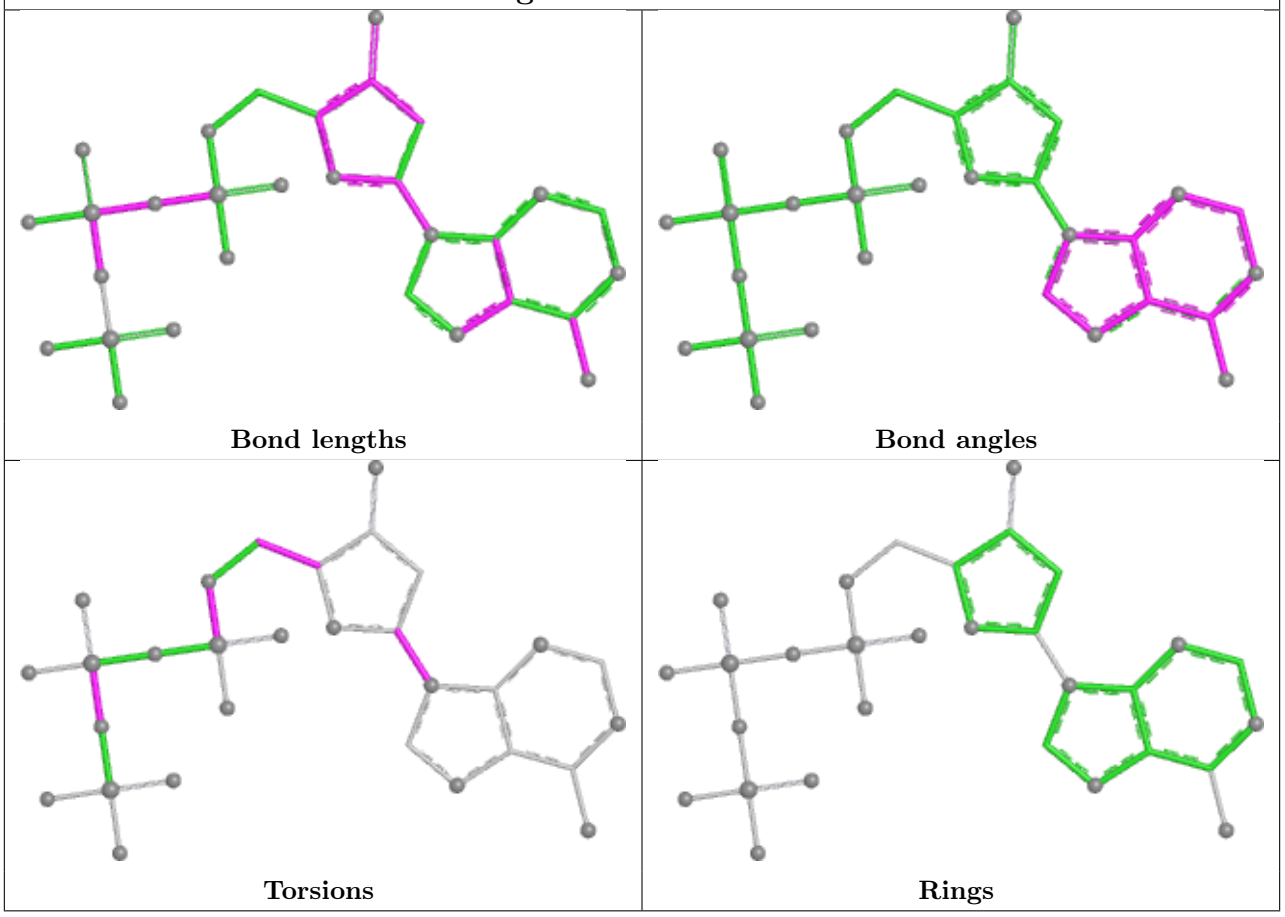


Torsions



Rings

Ligand DTP E 1301



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.

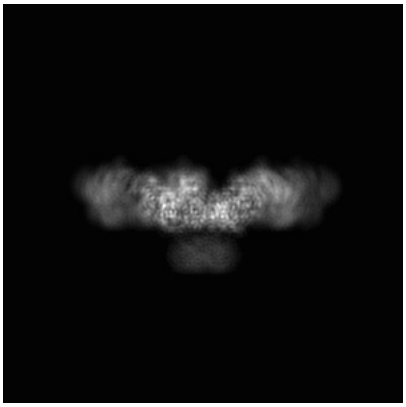
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8178. These allow visual inspection of the internal detail of the map and identification of artifacts.

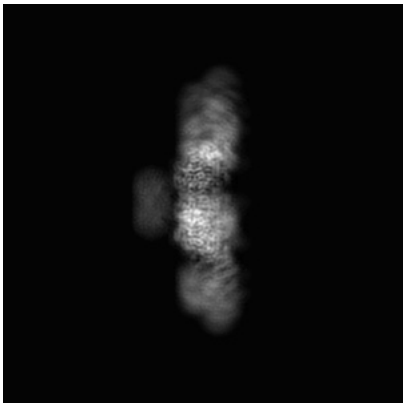
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

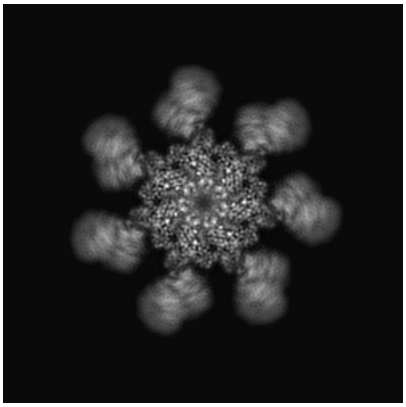
6.1.1 Primary map



X



Y

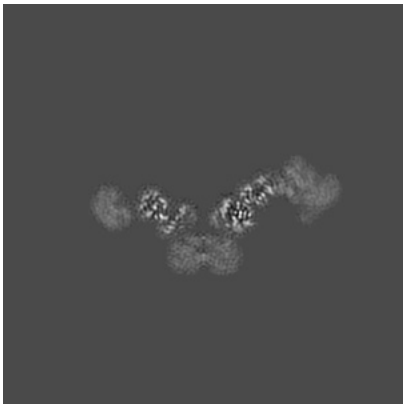


Z

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

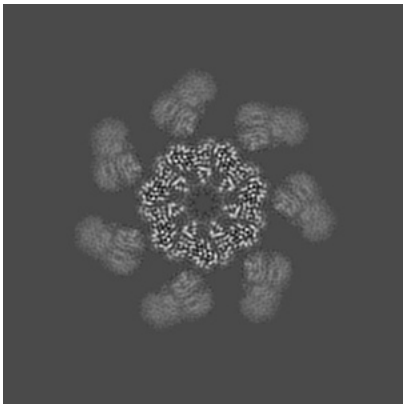
6.2 Central slices

6.2.1 Primary map



X Index: 160

Y Index: 160



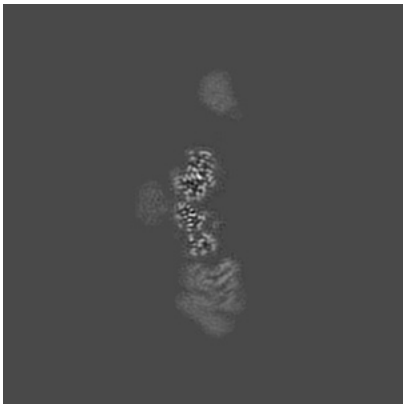
Z Index: 160

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

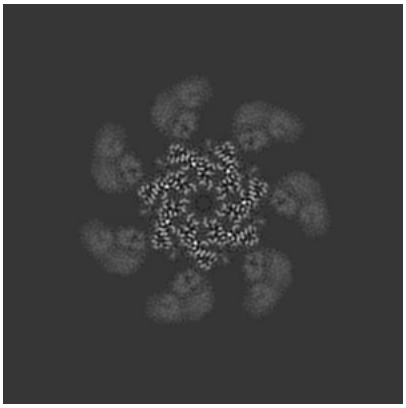
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 146



Y Index: 135

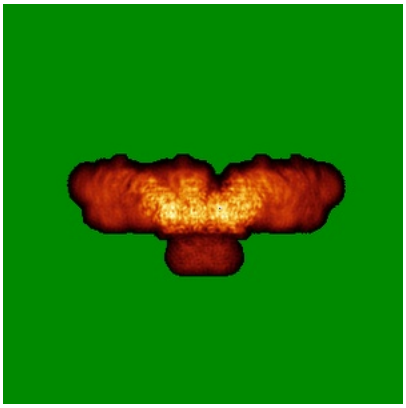


Z Index: 157

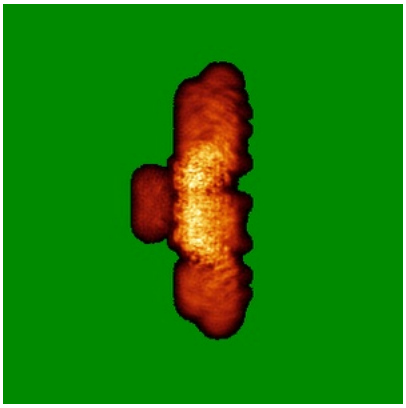
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

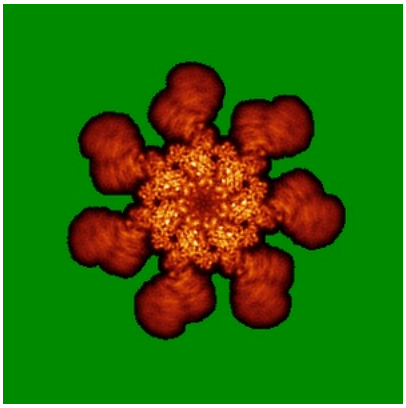
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

This section was not generated.

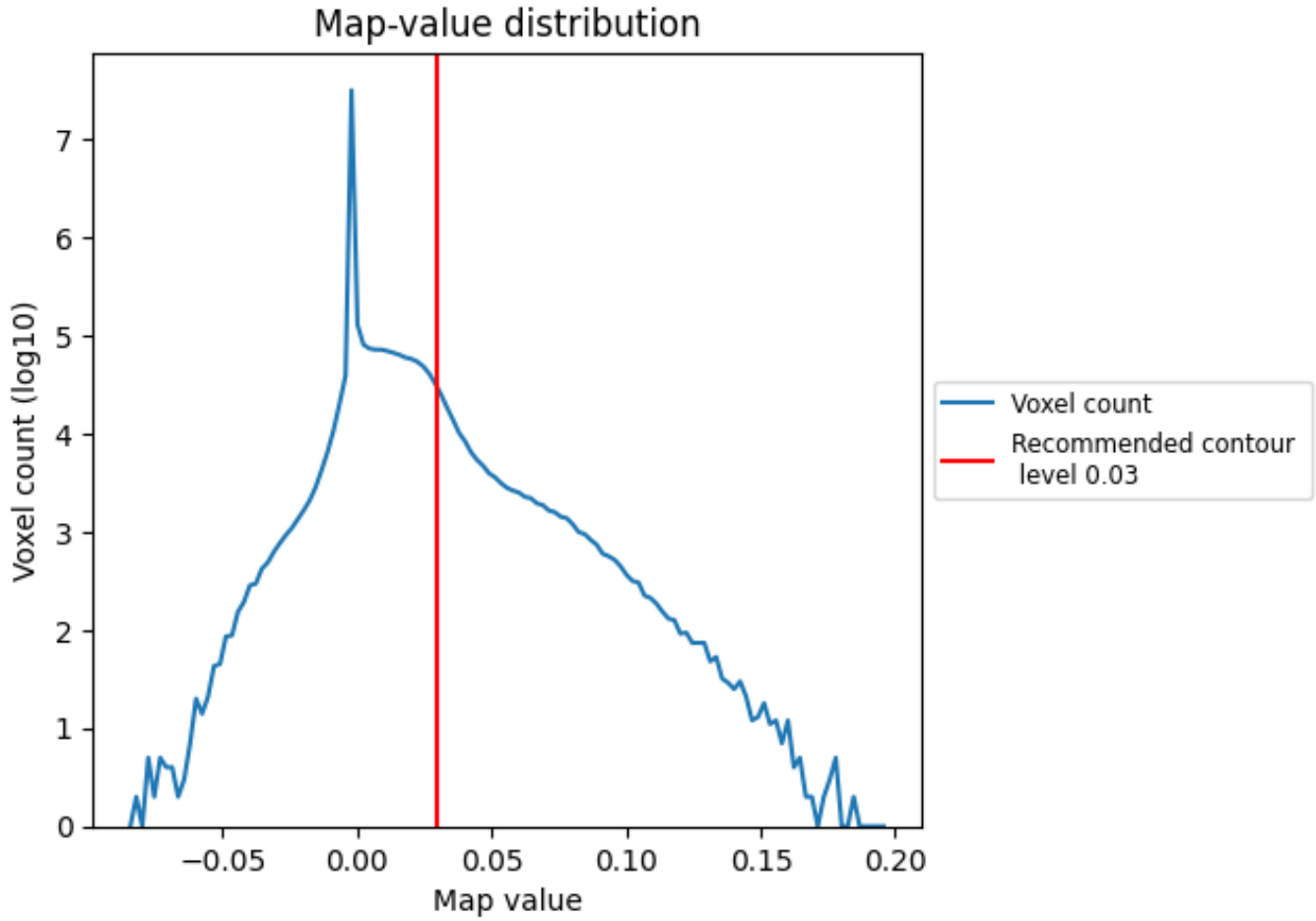
6.6 Mask visualisation (i)

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

7 Map analysis

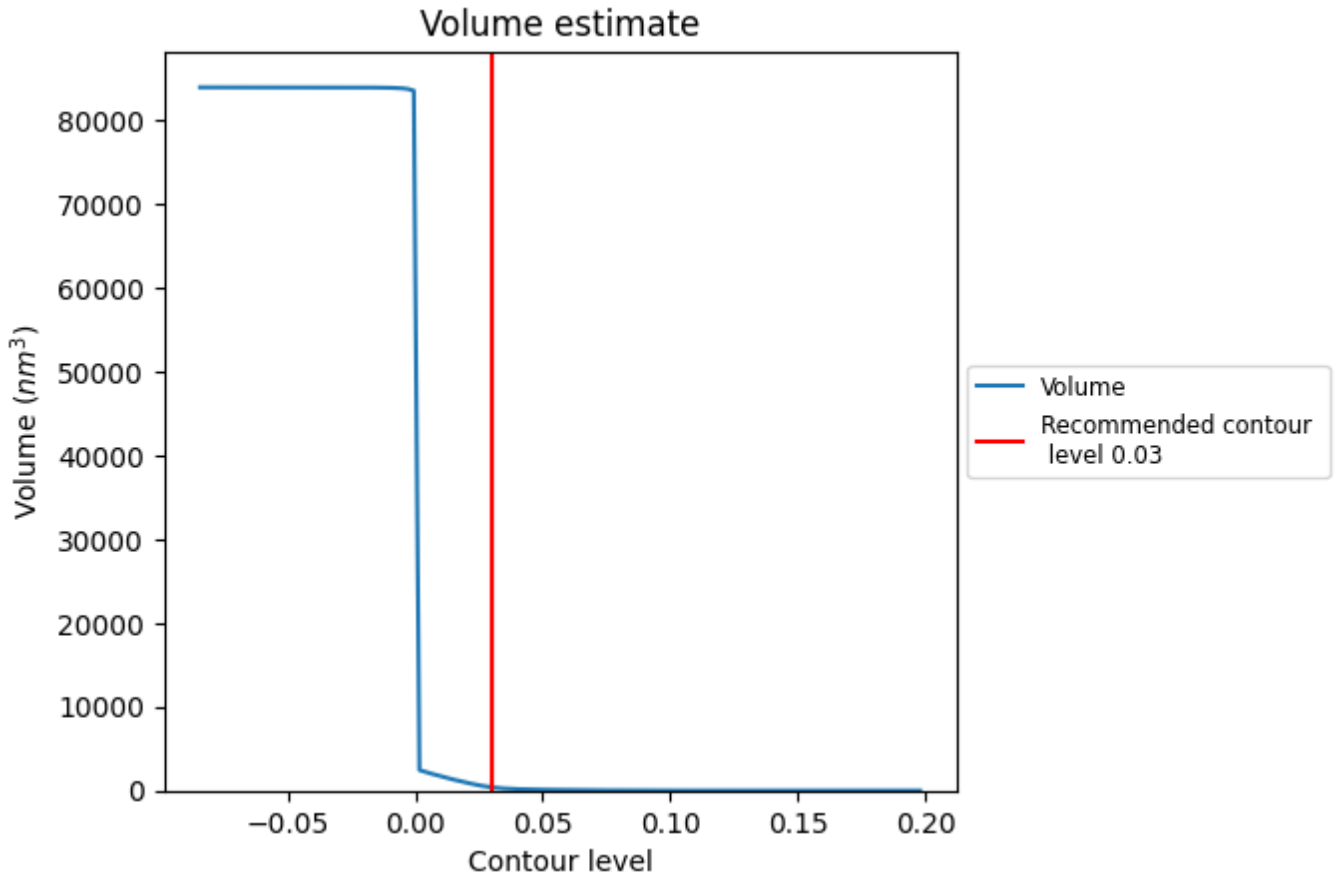
This section contains the results of statistical analysis of the map.

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.

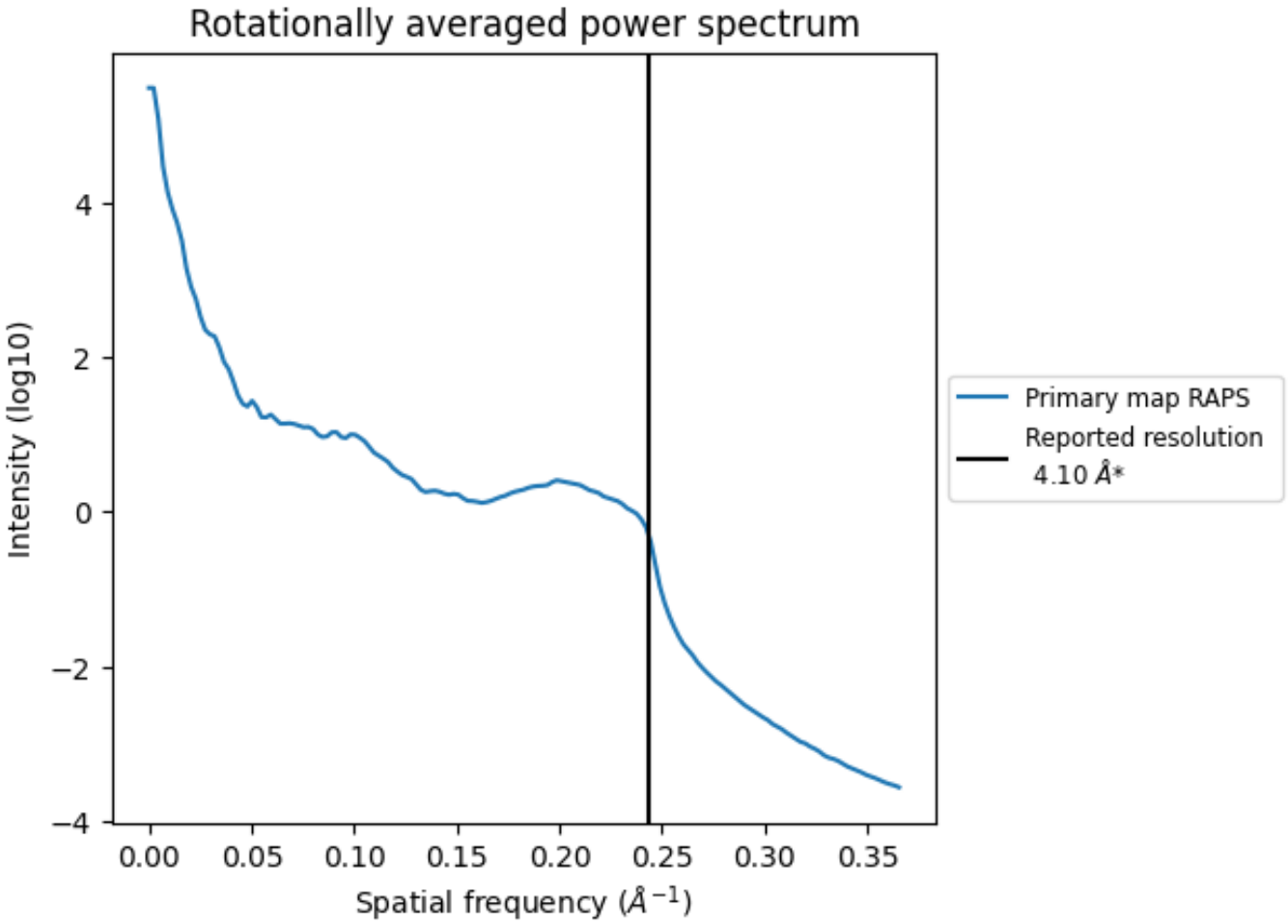
7.2 Volume estimate



The volume at the recommended contour level is 389 nm^3; this corresponds to an approximate mass of 352 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 0.244 Å^{-1}

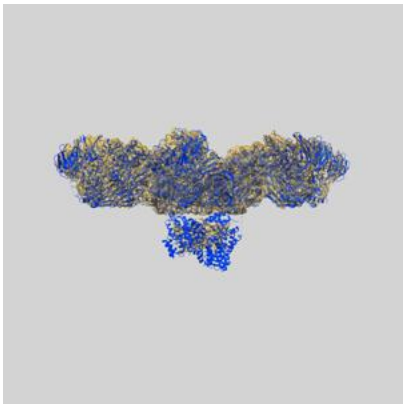
8 Fourier-Shell correlation

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

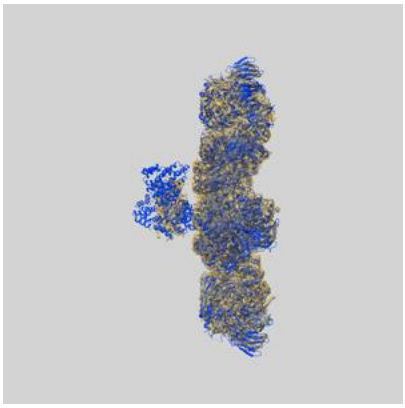
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8178 and PDB model 5JUY. Per-residue inclusion information can be found in section 3 on page 7.

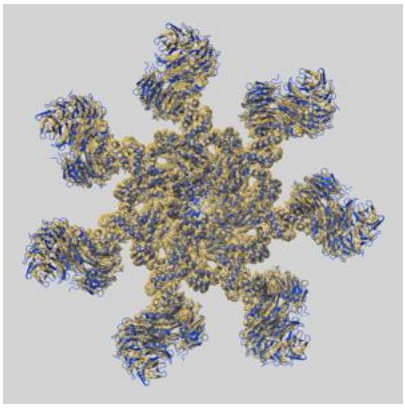
9.1 Map-model overlay



X



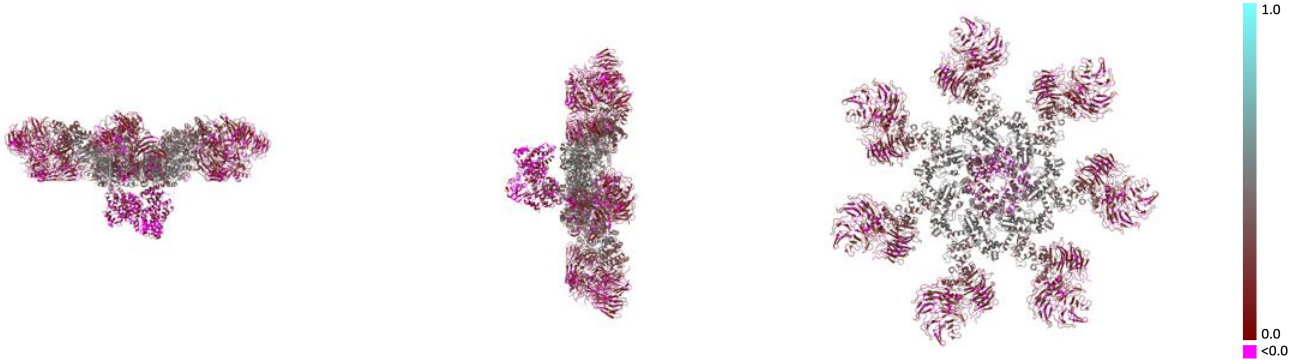
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 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.

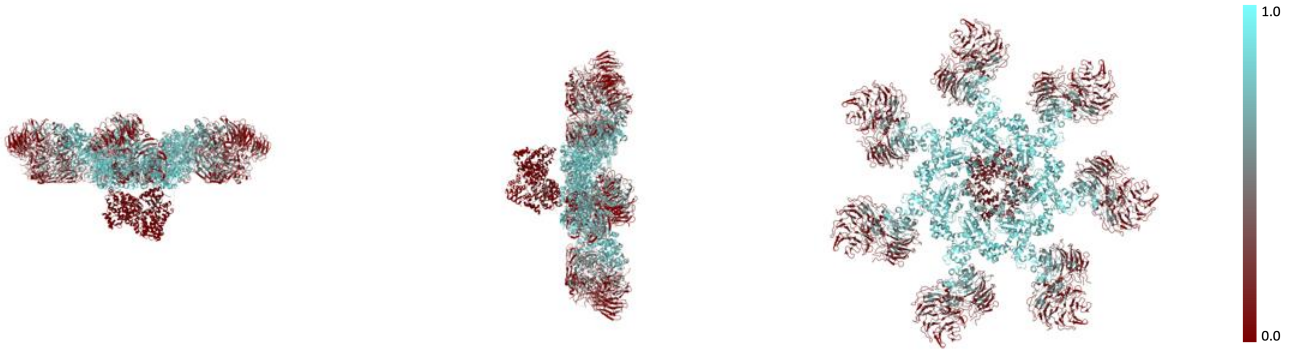
9.2 Q-score mapped to coordinate model (i)



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.

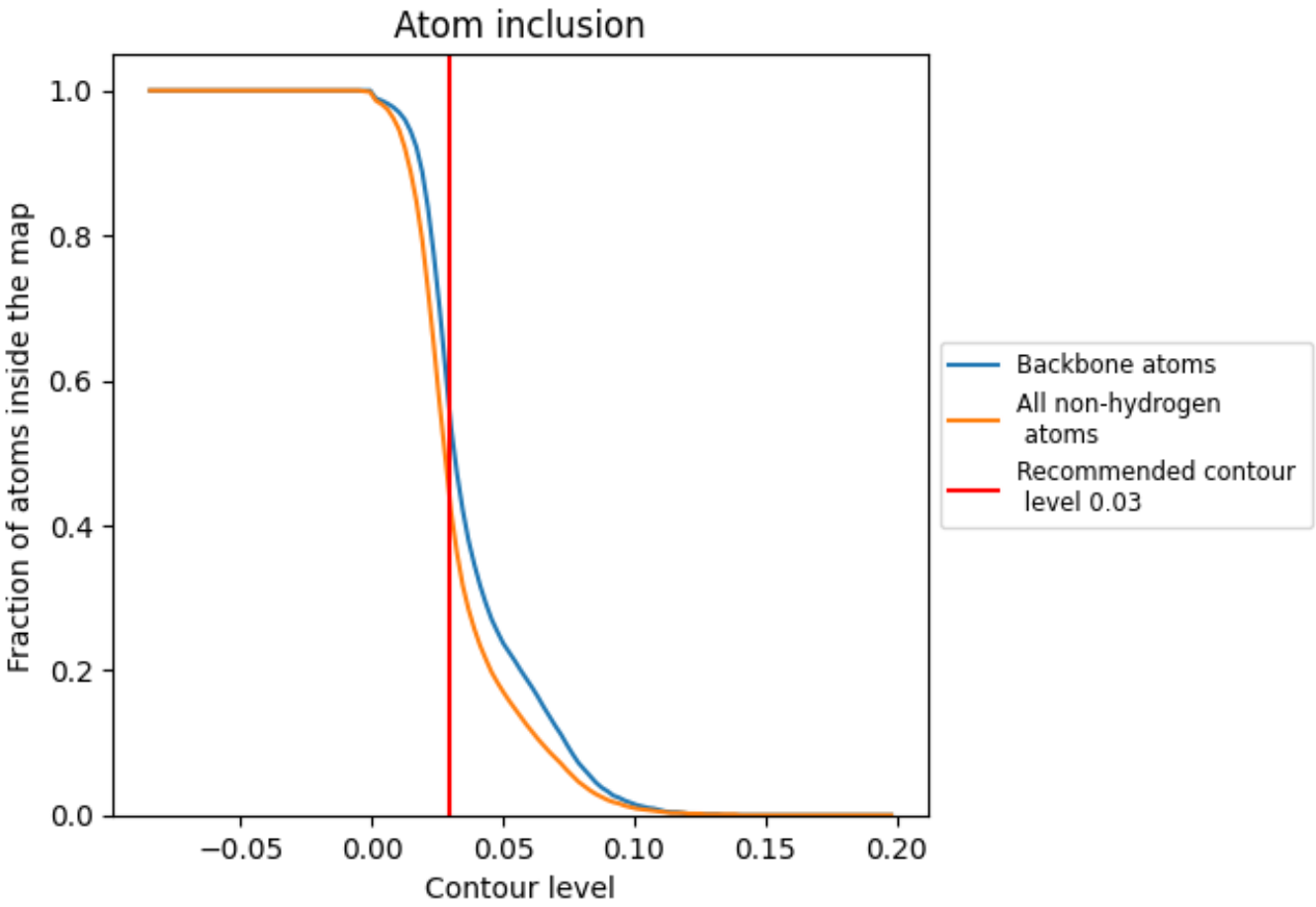
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 55% of all backbone atoms, 43% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4290	0.2300
A	0.4830	0.2610
B	0.4490	0.2420
C	0.4820	0.2620
D	0.4510	0.2410
E	0.4490	0.2460
F	0.4810	0.2590
G	0.4510	0.2500
H	0.2400	0.1010
I	0.2420	0.1010
J	0.2360	0.1010
K	0.2460	0.1060
L	0.2400	0.1040
M	0.2380	0.1050
N	0.2360	0.1030
O	0.1050	0.0880
P	0.0350	0.0600
Q	0.0040	-0.0120
R	0.0040	-0.0460