Full wwPDB EM Validation Report

Nov 16, 2022 – 04:09 PM JST

PDB ID	:	6M6G
EMDB ID	:	EMD-30123
Title	:	Structure of HSV2 viron capsid portal vertex
Authors	:	Wang, X.X.; Wang, N.
Deposited on	:	2020-03-14
Resolution	:	5.39 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 (i) 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 (i)) were used in the production of this report:

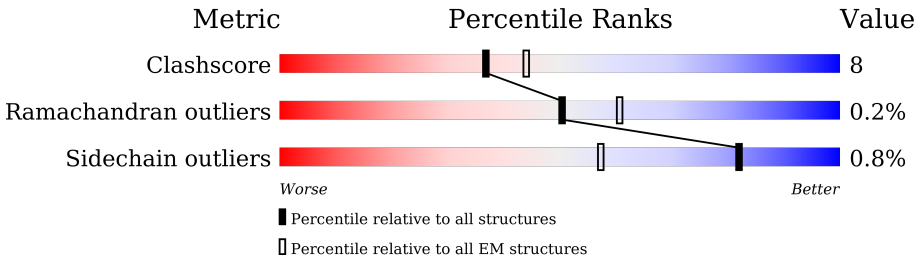
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 5.39 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	1374	25% 78% 21%
1	C	1374	31% 81% 18%
1	D	1374	26% 80% 19%
1	E	1374	20% 79% 19%
1	F	1374	22% 76% 21%
1	I	1374	22% 73% 22%
2	G	112	52% 75% 15% 10%
2	M	112	53% 81% 9% 10%

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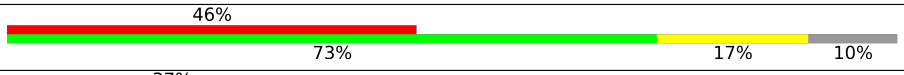
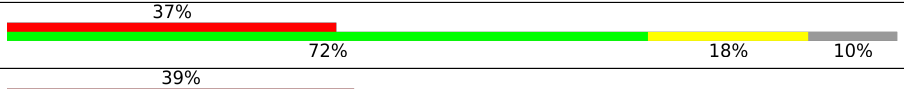
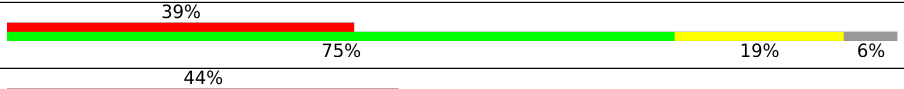
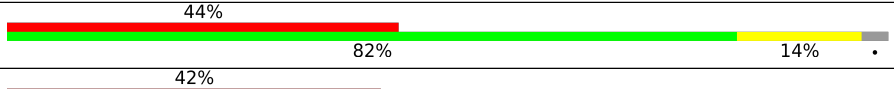
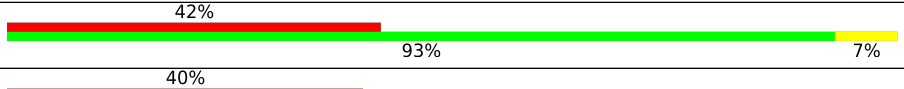
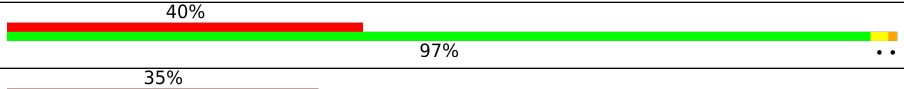
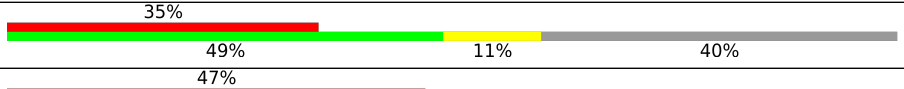
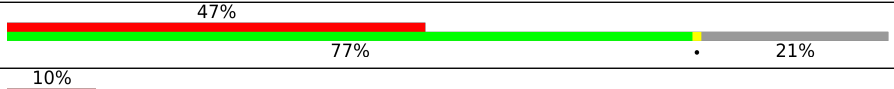
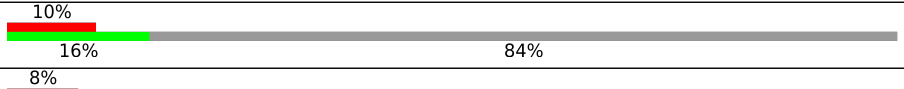
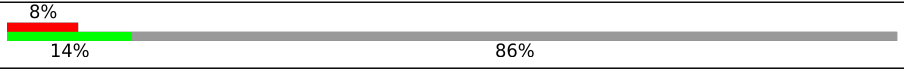
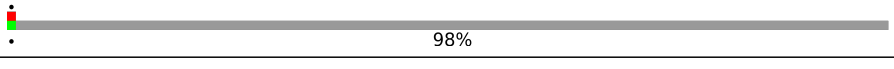
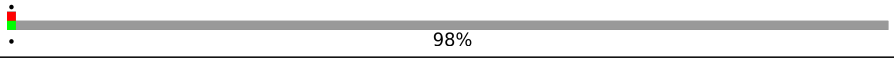
Mol	Chain	Length	Quality of chain
2	Q	112	
2	T	112	
2	U	112	
2	V	112	
3	K	318	
3	O	318	
4	L	84	
5	P	87	
6	S	466	
7	k	702	
8	l	585	
8	m	585	
9	n	3122	
9	o	3122	

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 78731 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 Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1362	Total	C	N	O	S	0	0
			10198	6475	1847	1821	55		
1	C	1362	Total	C	N	O	S	0	0
			10209	6479	1844	1831	55		
1	D	1362	Total	C	N	O	S	0	0
			10221	6485	1848	1833	55		
1	E	1351	Total	C	N	O	S	0	0
			10162	6452	1837	1818	55		
1	F	1351	Total	C	N	O	S	0	0
			9978	6343	1804	1779	52		
1	I	1319	Total	C	N	O	S	0	0
			9831	6234	1785	1758	54		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	17	MET	ILE	conflict	UNP P89442
B	18	VAL	LEU	conflict	UNP P89442
B	382	LYS	ARG	conflict	UNP P89442
B	986	HIS	ASP	conflict	UNP P89442
C	17	MET	ILE	conflict	UNP P89442
C	18	VAL	LEU	conflict	UNP P89442
C	382	LYS	ARG	conflict	UNP P89442
C	986	HIS	ASP	conflict	UNP P89442
D	17	MET	ILE	conflict	UNP P89442
D	18	VAL	LEU	conflict	UNP P89442
D	382	LYS	ARG	conflict	UNP P89442
D	986	HIS	ASP	conflict	UNP P89442
E	17	MET	ILE	conflict	UNP P89442
E	18	VAL	LEU	conflict	UNP P89442
E	382	LYS	ARG	conflict	UNP P89442
E	986	HIS	ASP	conflict	UNP P89442
F	17	MET	ILE	conflict	UNP P89442
F	18	VAL	LEU	conflict	UNP P89442

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Chain	Residue	Modelled	Actual	Comment	Reference
F	382	LYS	ARG	conflict	UNP P89442
F	986	HIS	ASP	conflict	UNP P89442
I	17	MET	ILE	conflict	UNP P89442
I	18	VAL	LEU	conflict	UNP P89442
I	382	LYS	ARG	conflict	UNP P89442
I	986	HIS	ASP	conflict	UNP P89442

- Molecule 2 is a protein called Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	101	Total	C	N	O	S	0	0
			772	488	143	139	2		
2	M	101	Total	C	N	O	S	0	0
			772	488	143	139	2		
2	Q	101	Total	C	N	O	S	0	0
			772	488	143	139	2		
2	T	101	Total	C	N	O	S	0	0
			772	488	143	139	2		
2	U	101	Total	C	N	O	S	0	0
			772	488	143	139	2		
2	V	101	Total	C	N	O	S	0	0
			772	488	143	139	2		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	22	THR	MET	conflict	UNP G9I257
M	22	THR	MET	conflict	UNP G9I257
Q	22	THR	MET	conflict	UNP G9I257
T	22	THR	MET	conflict	UNP G9I257
U	22	THR	MET	conflict	UNP G9I257
V	22	THR	MET	conflict	UNP G9I257

- Molecule 3 is a protein called Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	299	Total	C	N	O	S	0	0
			2078	1341	373	357	7		
3	O	307	Total	C	N	O	S	0	0
			2175	1405	392	370	8		

- Molecule 4 is a protein called coiled coils.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	L	84	Total	C	N	O	0	0
			420	252	84	84		

- Molecule 5 is a protein called Coiled coils.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	P	87	Total	C	N	O	0	0
			435	261	87	87		

- Molecule 6 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	S	279	Total	C	N	O	S	0	0
			1975	1264	354	341	16		

- Molecule 7 is a protein called Capsid vertex component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	k	553	Total	C	N	O	S	0	0
			4233	2695	773	748	17		

- Molecule 8 is a protein called Capsid vertex component 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	l	94	Total	C	N	O	S	0	0
			770	493	139	136	2		
8	m	80	Total	C	N	O		0	0
			648	411	123	114			

- Molecule 9 is a protein called Large tegument protein deneddylase.

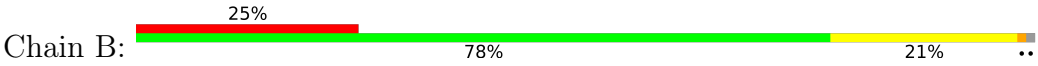
Mol	Chain	Residues	Atoms					AltConf	Trace
9	n	47	Total	C	N	O	S	0	0
			383	234	87	60	2		
9	o	47	Total	C	N	O	S	0	0
			383	234	87	60	2		

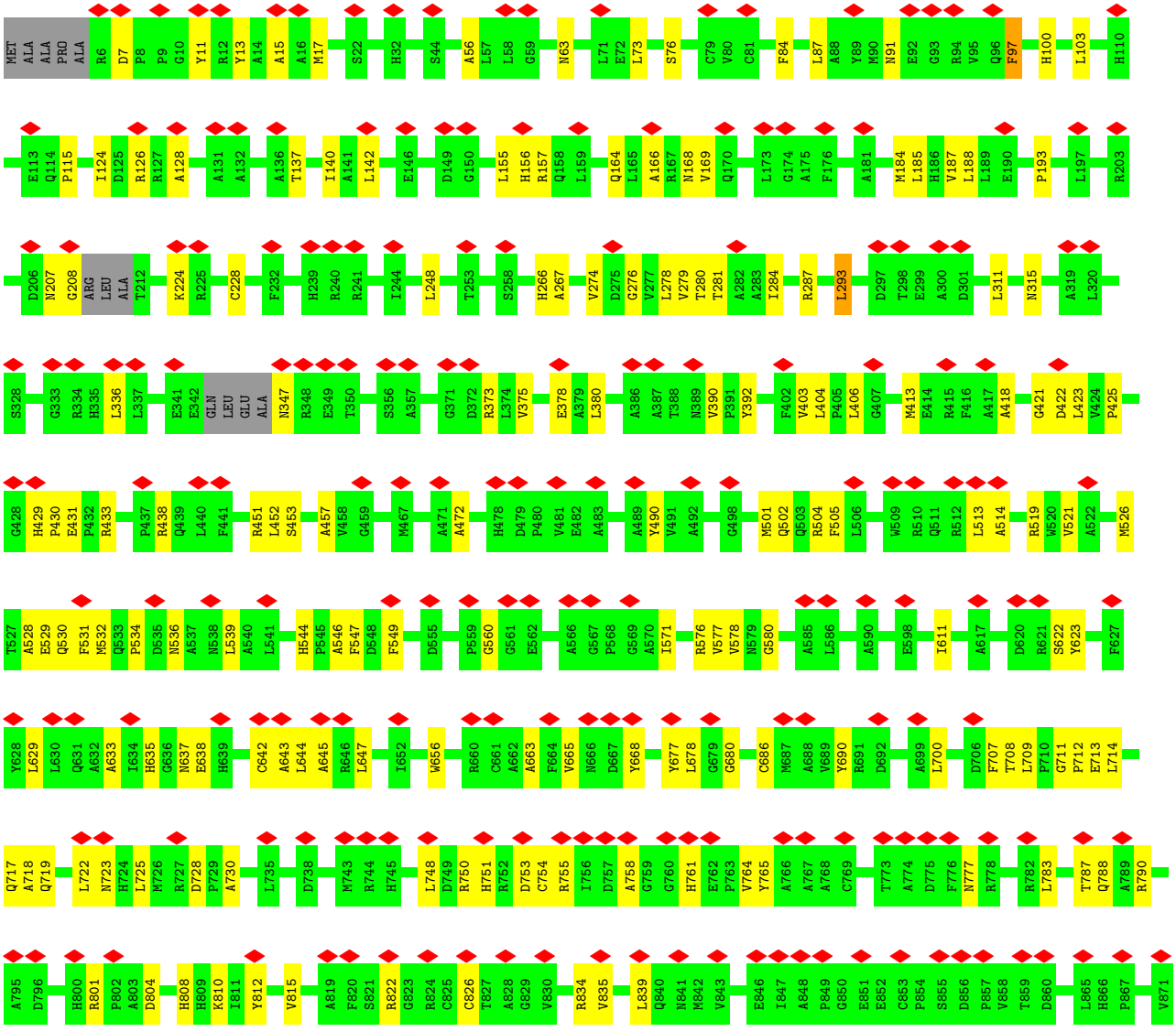
3 Residue-property plots (i)

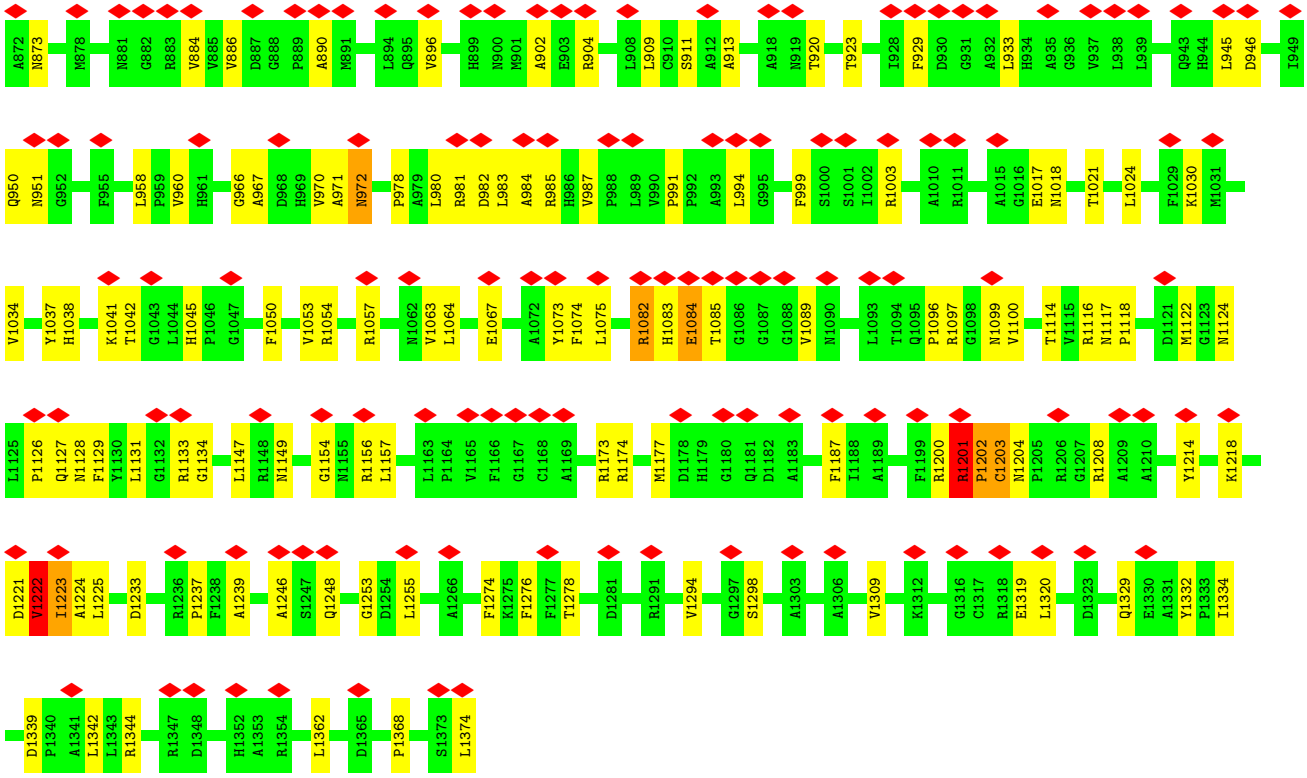
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

Chain B:

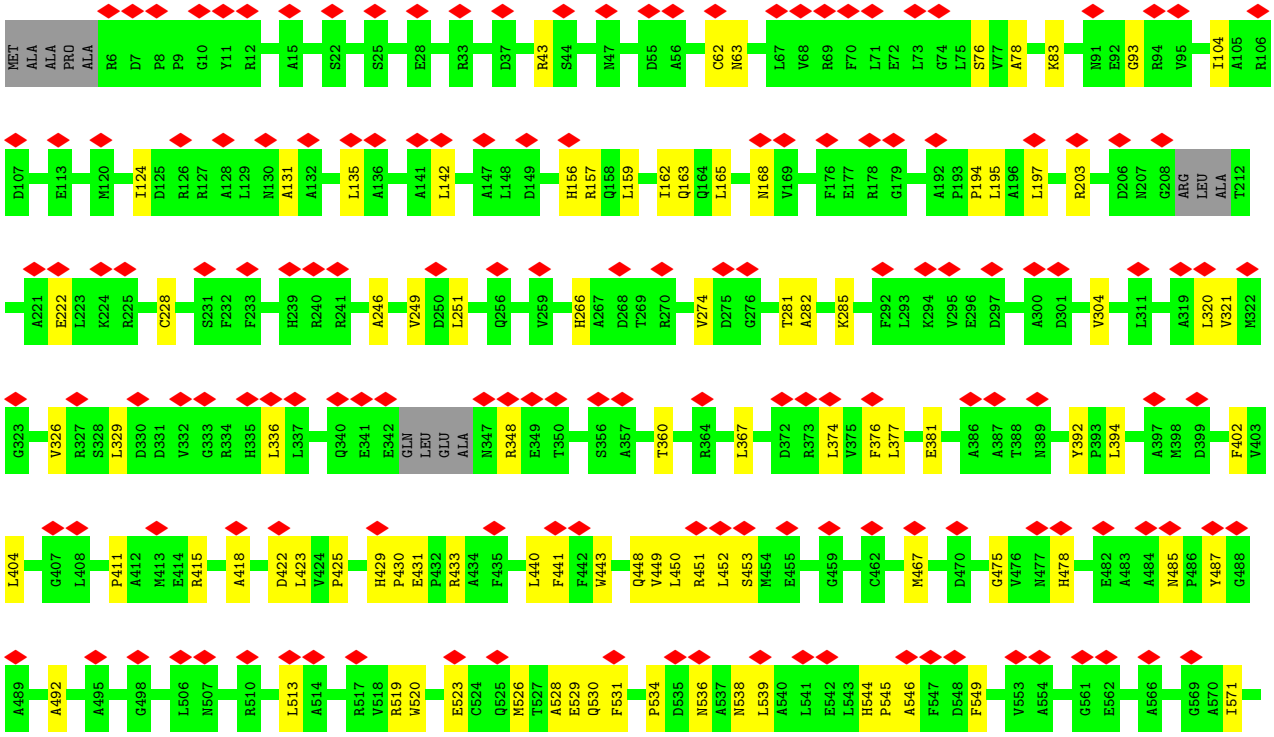


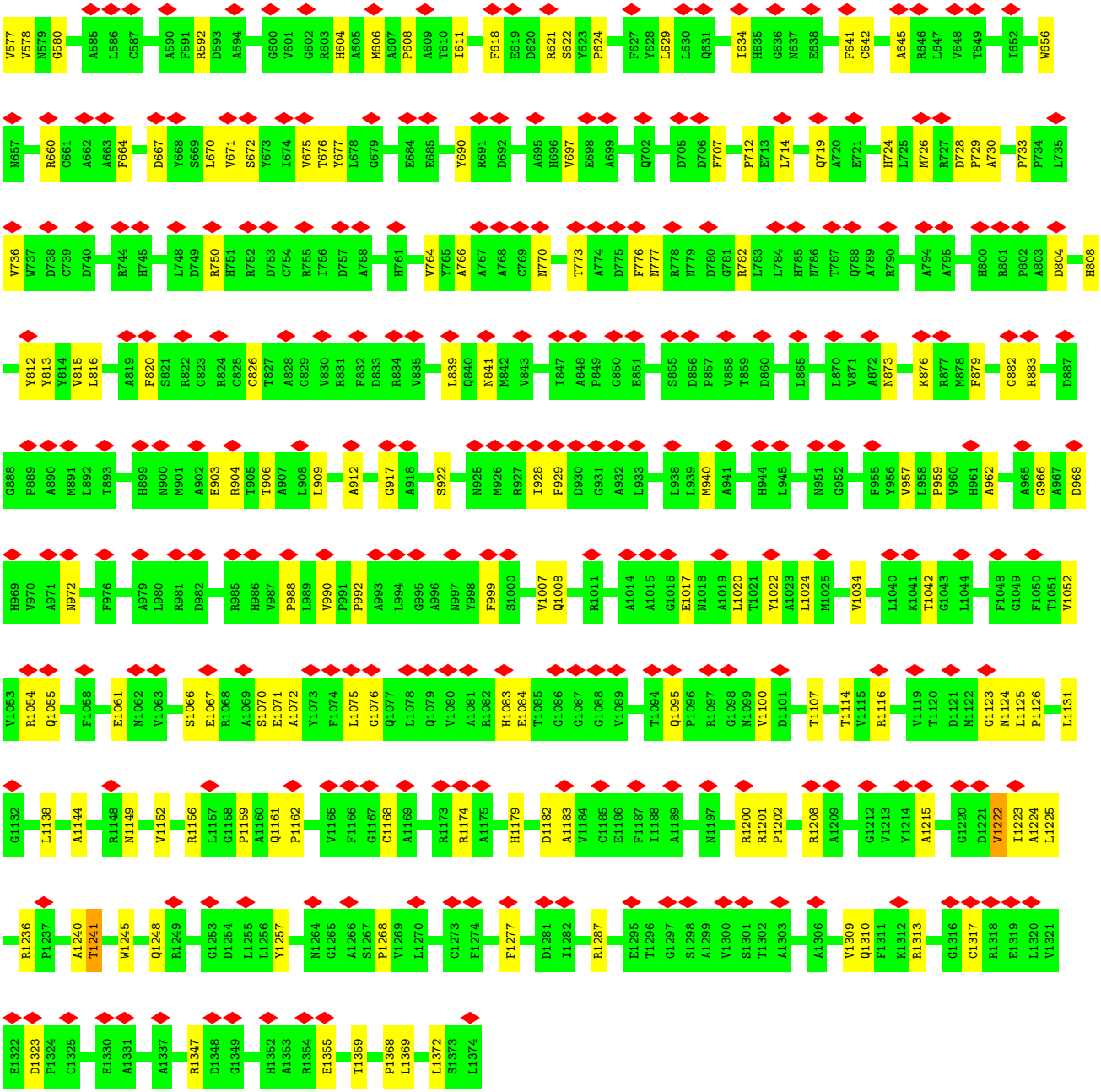




• Molecule 1: Major capsid protein

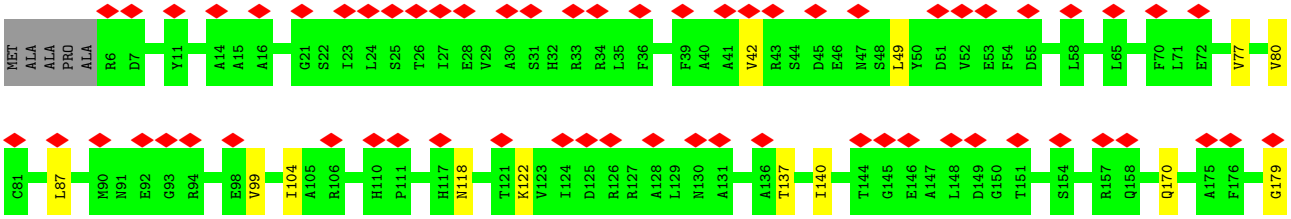
Chain C:

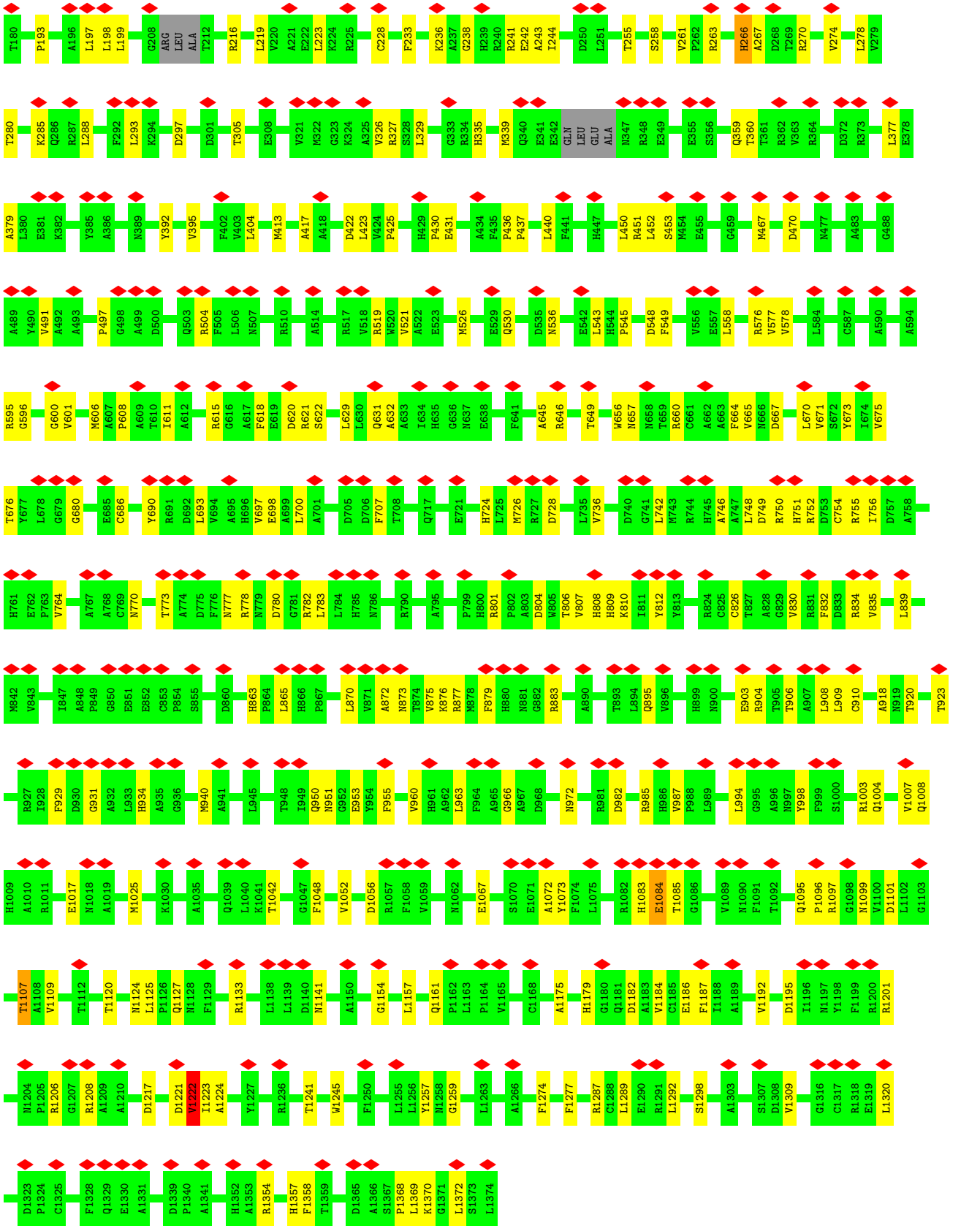




• Molecule 1: Major capsid protein

Chain D:

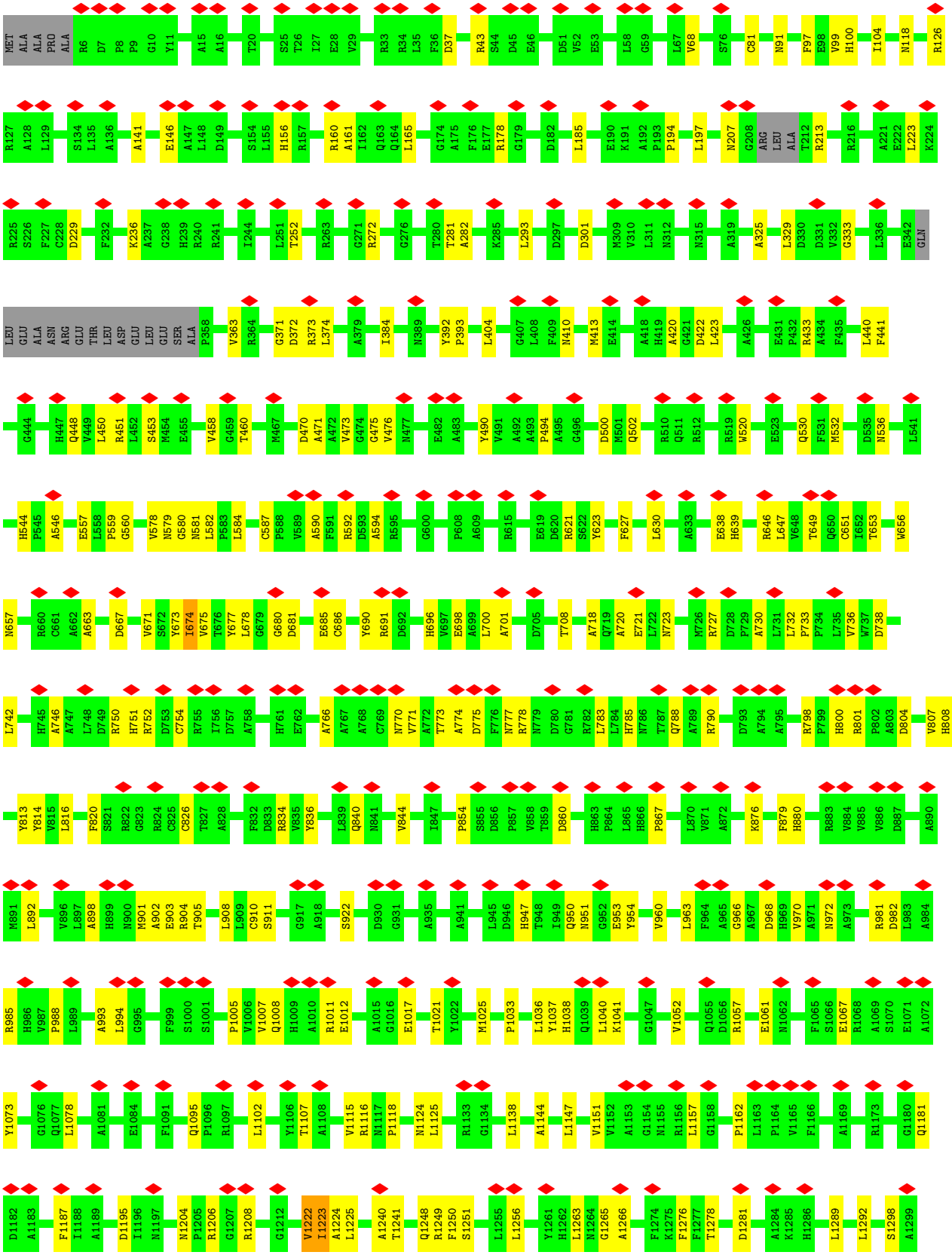


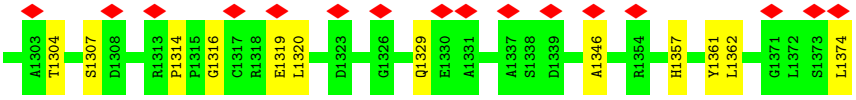


• Molecule 1: Major capsid protein

Chain E:

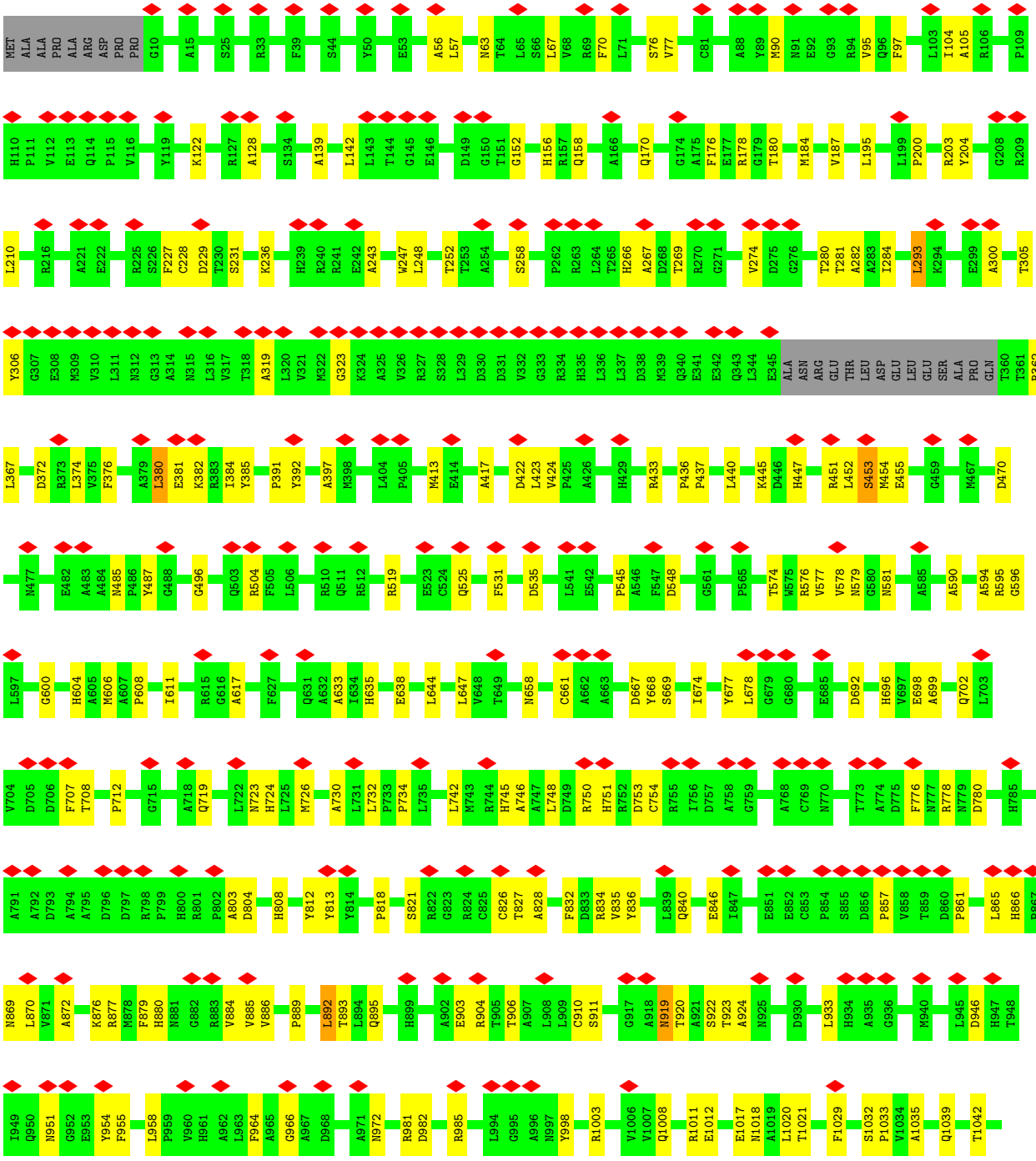

20%
79%
19%

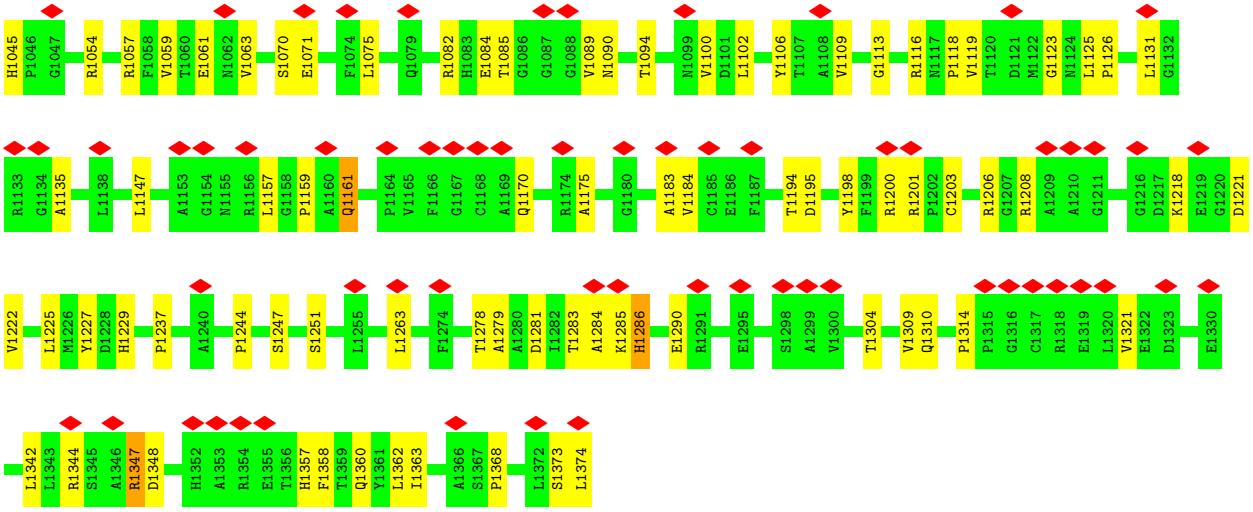

MET ALA ALA PRO ALA R6 D7 P8 P9 G10 Y11 A15 A16 T20 S25 T26 I27 E28 V29 R33 R34 L35 F36 D37 R43 S44 D45 E46 D51 V52 E53 L58 G59 L67 V68 S76 C81 N91 F97 E98 V99 H100 I104 N118 R126
R127 A128 L129 S134 L135 A136 A141 E146 A147 L148 D149 S154 L155 H156 R157 R160 A161 I162 Q163 Q164 L165 G174 A175 F176 E177 R178 G179 D182 L185 E190 K191 A192 P193 P194 L197 N207 G208 ARG LEU ALA T212 R213 R216 A221 E222 L223 K224
R225 S226 F227 C228 D229 F232 K236 A237 G238 H239 R240 R241 I244 L251 T252 R263 G271 R272 G276 T280 T281 A282 K285 L293 D297 D301 M309 V310 L311 N312 N315 A319 A325 L329 D330 D331 V332 G333 L336 E342 GLN
LEU GLU ALA ASN ARG GLU THR LEU ASP GLU LEU GLU SER ALA P358 V363 R364 G371 D372 R373 L374 A379 I384 N389 Y392 P393 L404 G407 L408 F409 N410 M413 E414 A418 H419 A420 G421 D422 L423 A426 E431 P432 R433 A434 F435 L440 F441
G444 H447 Q448 V449 L450 R451 L452 S453 H454 E455 V458 G459 T460 M467 D470 A471 A472 V473 G474 G475 V476 N477 E482 A483 Y490 V491 A492 A493 P494 A495 G496 D500 H501 Q502 R510 Q511 R512 R519 W520 E523 Q530 F531 M532 D535 N536 L541
H544 P545 A546 E557 L558 P559 G560 V578 N579 G580 N581 L582 P583 L584 C587 P588 V589 A590 F591 R592 D593 A594 R595 G600 P608 A609 R615 E619 D620 R621 S622 Y623 F627 L630 A633 E638 H639 R646 L647 V648 T649 Q650 C651 I652 T653 W656
N657 R660 C661 A662 A663 D667 V671 S672 Y673 I674 V675 T676 Y677 L678 G679 G680 D681 E685 C686 Y690 R691 D692 H696 V697 E698 A699 L700 A701 D705 T708 A718 Q719 A720 E721 L722 N723 M726 R727 D728 F729 A730 L731 L732 P733 P734 L735 V736 W737 D738
L742 H745 A746 A747 L748 D749 R750 H751 R752 D753 C754 R755 I756 D757 A758 H761 E762 A766 A767 A768 C769 N770 V771 A772 T773 A774 D775 F776 N777 R778 N779 D780 G781 R782 L783 L784 H785 N786 T787 Q788 A789 R790 D793 A794 A795 R798 P799 H800 R801 P802 A803 D804 V807 H808
Y813 Y814 V815 L816 F820 S821 R822 G823 R824 C825 C826 T827 A828 F832 D833 R834 V835 Y836 L839 Q840 N841 V844 I847 P854 S855 D856 P857 V858 T859 D860 H863 P864 L865 H866 P867 L870 V871 A872 K876 F879 H880 R883 V884 V885 V886 D887 A890
M891 L892 V896 L897 A898 H899 N900 M901 A902 E903 R904 T905 L908 L909 C910 S911 G917 A918 S922 D930 G931 A935 A941 L945 D946 H947 T948 I949 Q950 N951 G952 E953 Y954 V960 L963 F964 A965 G966 A967 D968 H969 V970 A971 N972 A973 R981 D982 L983 A984
R985 H986 V987 P988 L989 A993 L994 G995 F999 S1000 S1001 P1005 Y1006 V1007 Q1008 H1009 A1010 R1011 E1012 A1015 G1016 E1017 T1021 Y1022 M1025 P1033 L1036 Y1037 H1038 Q1039 L1040 K1041 G1047 V1052 Q1055 D1056 R1057 E1061 N1062 F1065 S1066 E1067 R1068 A1069 S1070 E1071 A1072
Y1073 G1076 Q1077 L1078 A1081 E1084 F1091 Q1095 P1096 R1097 L1102 Y1106 T1107 A1108 V1115 R1116 N1117 P1118 N1124 L1125 R1133 G1134 L1138 A1144 L1147 V1151 V1152 A1153 G1154 N1155 R1156 L1157 G1158 P1162 L1163 P1164 V1165 F1166 A1169 R1173 G1180 Q1181
D1182 A1183 F1187 I1188 A1189 D1195 I1196 N1197 N1204 P1205 R1206 G1207 R1208 G1212 V1222 I1223 A1224 L1225 A1240 T1241 Q1248 R1249 F1250 S1251 L1255 L1256 Y1261 H1262 L1263 N1264 G1265 A1266 F1274 K1275 F1276 F1277 T1278 D1281 A1284 K1285 H1286 L1289 L1292 S1298 A1299



• Molecule 1: Major capsid protein

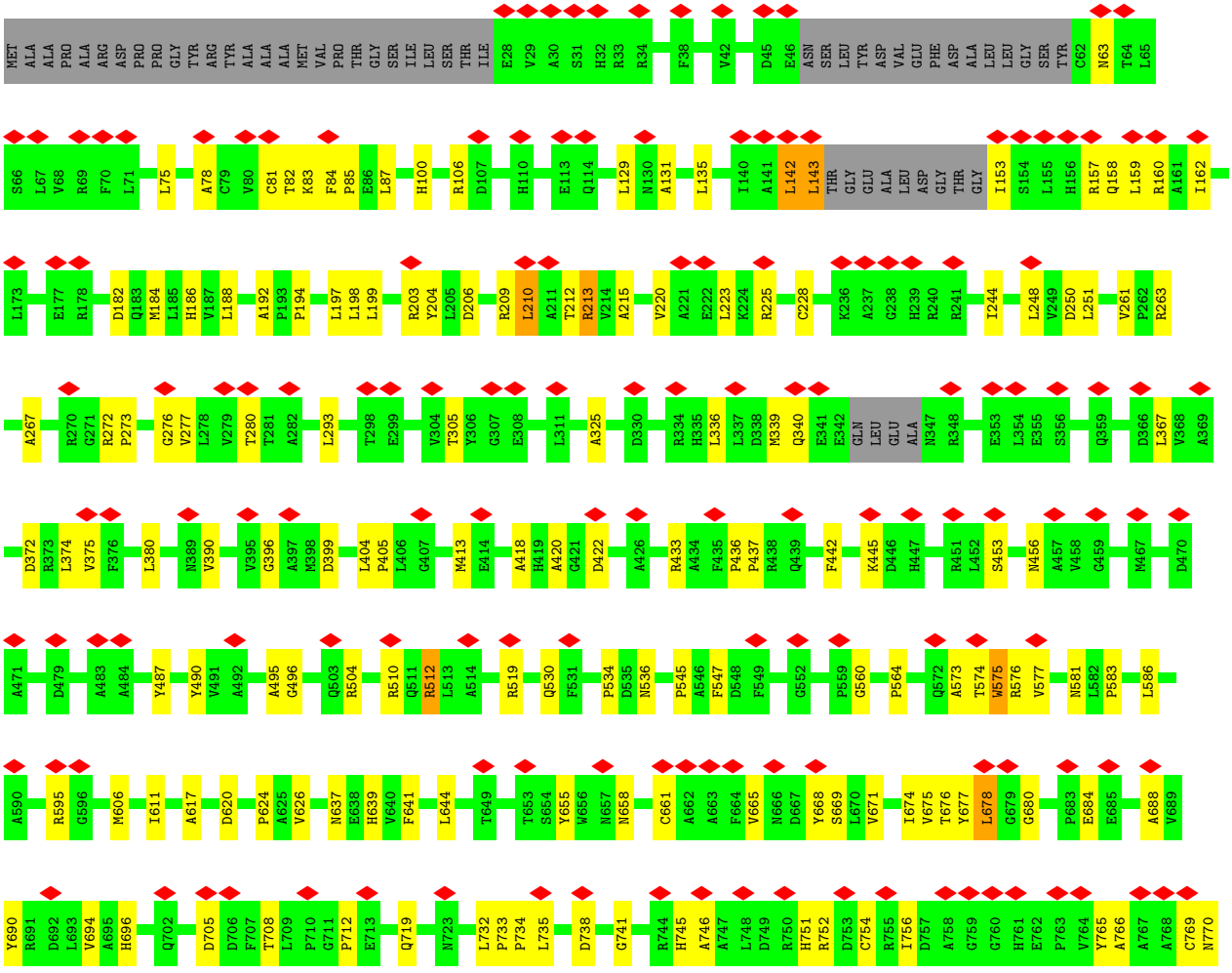
Chain F:

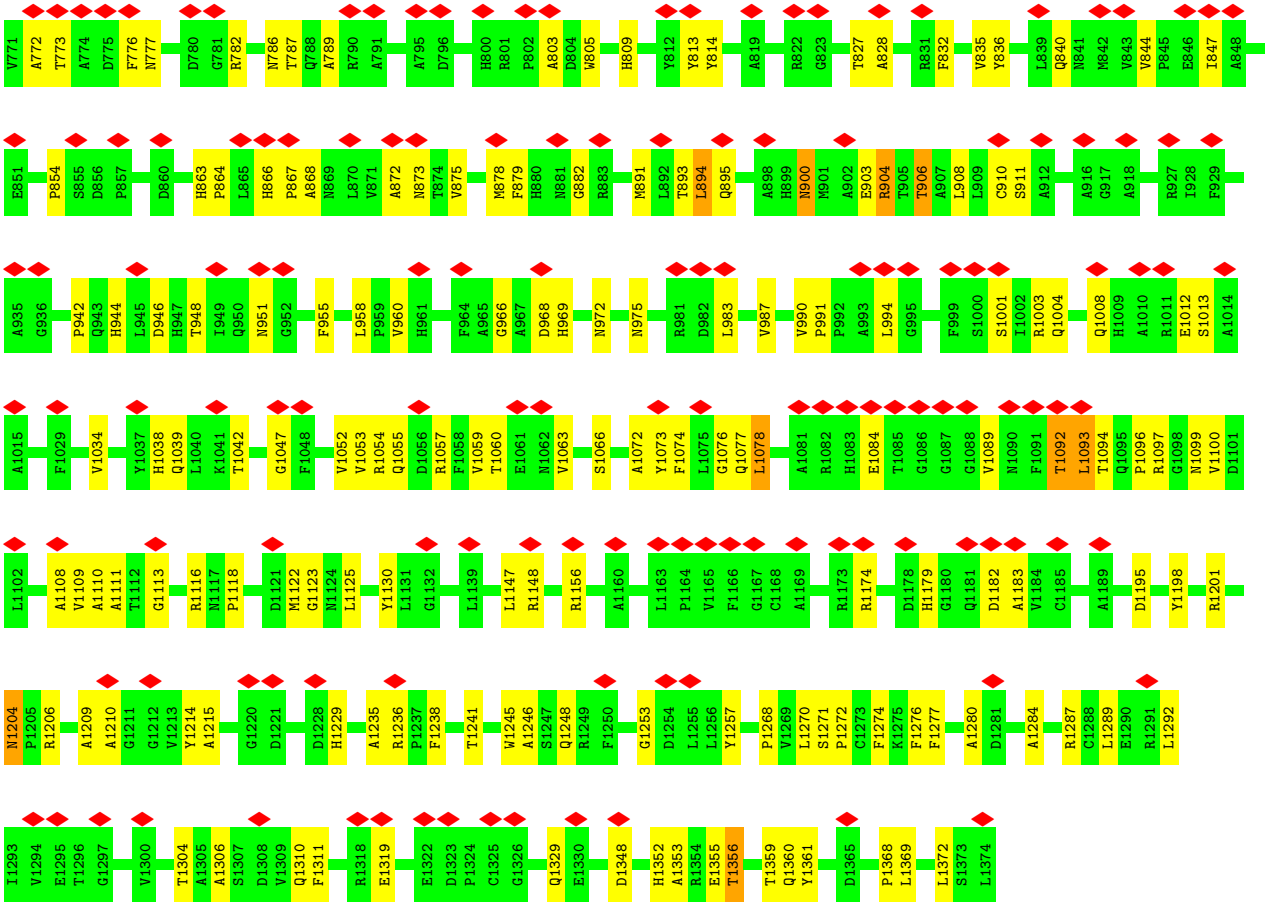




• Molecule 1: Major capsid protein

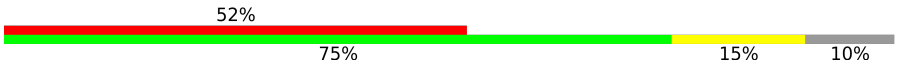
Chain I:

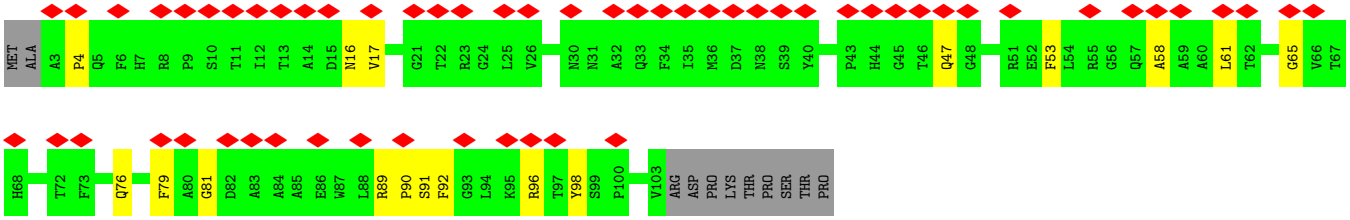




• Molecule 2: Small capsomere-interacting protein

Chain G:





• Molecule 2: Small capsomere-interacting protein

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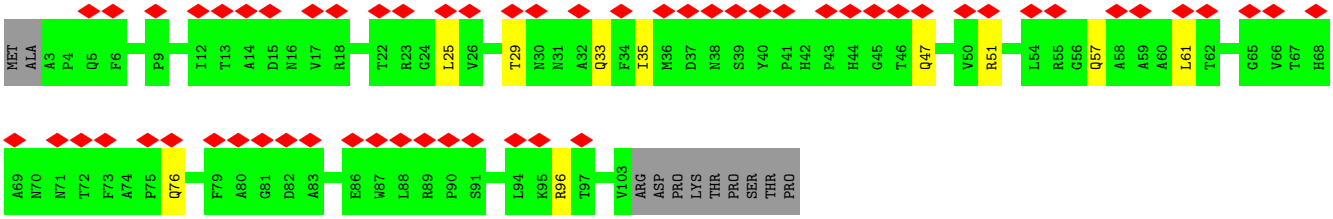

• Molecule 2: Small capsomere-interacting protein

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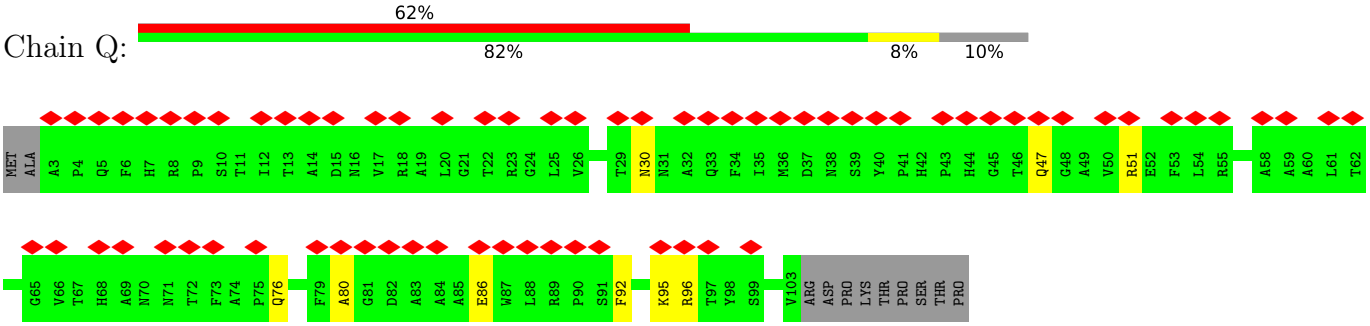

• Molecule 2: Small capsomere-interacting protein

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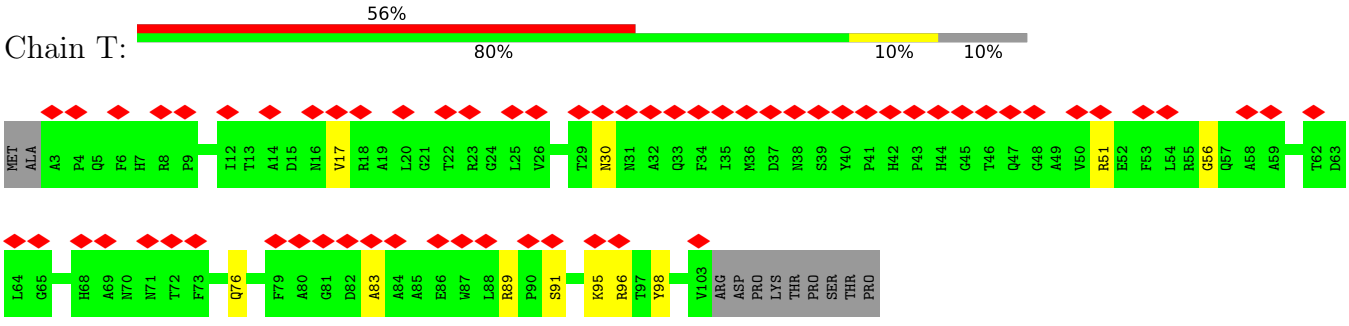

• Molecule 2: Small capsomere-interacting protein

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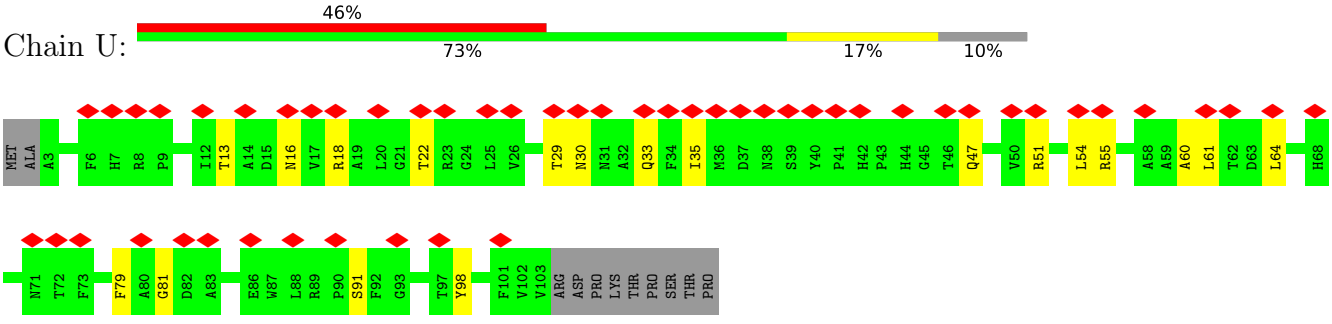

• Molecule 2: Small capsomere-interacting protein

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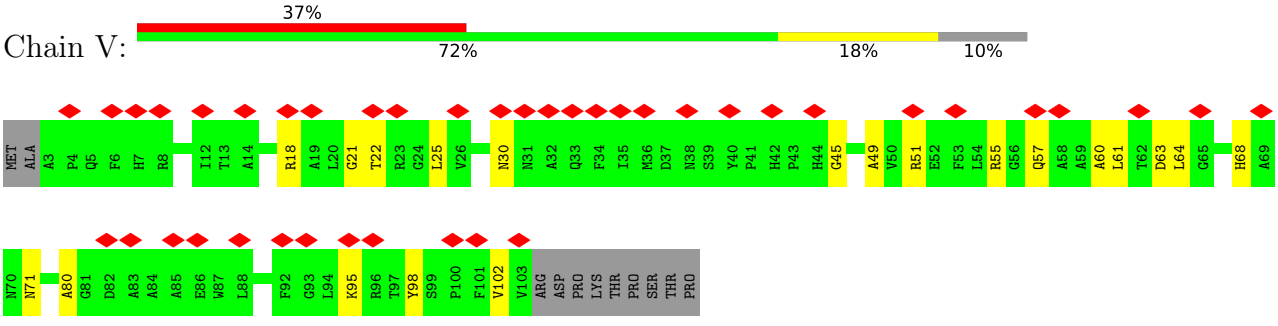
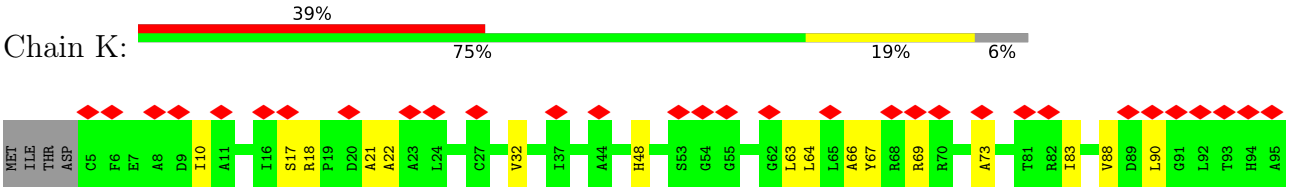
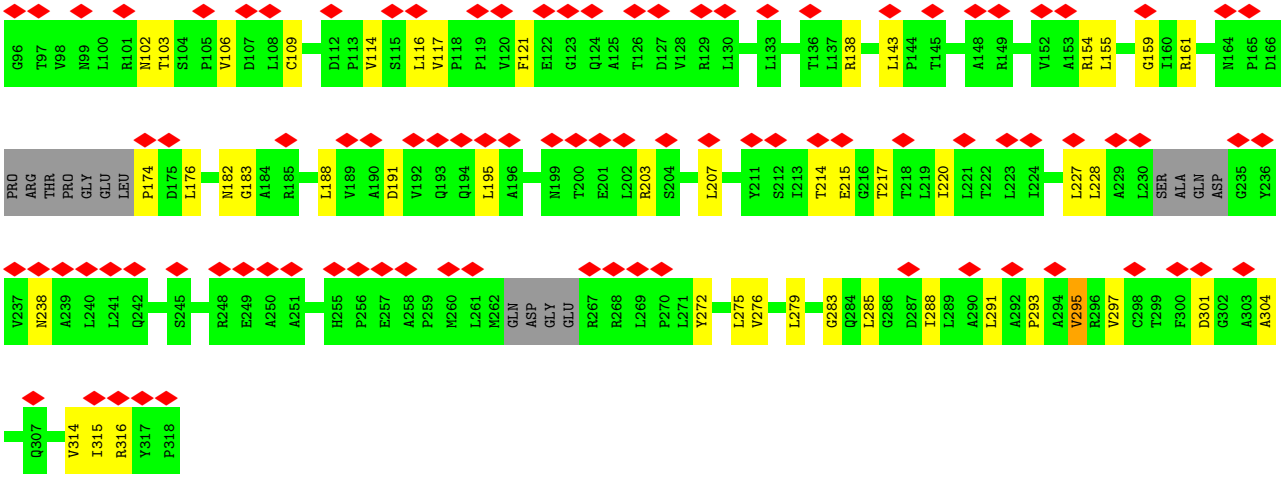


• Molecule 3: Triplex capsid protein 2

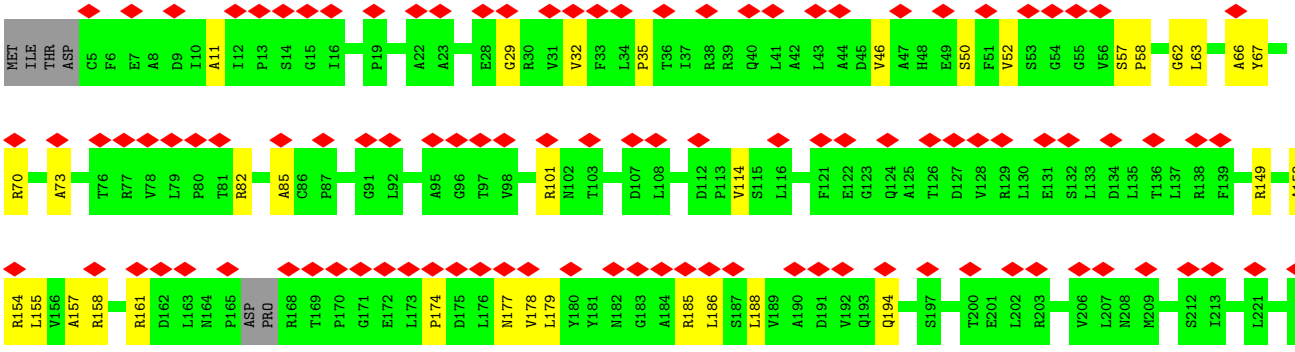
Chain K:





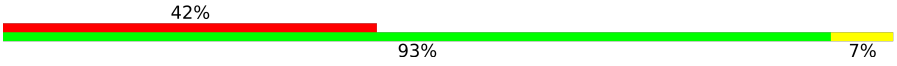
• Molecule 3: Triplex capsid protein 2

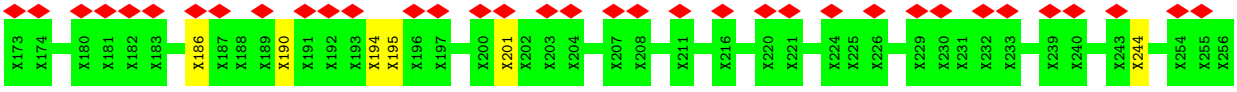
Chain O:



• Molecule 4: coiled coils

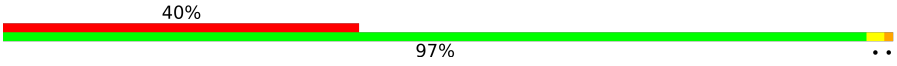
Chain L:

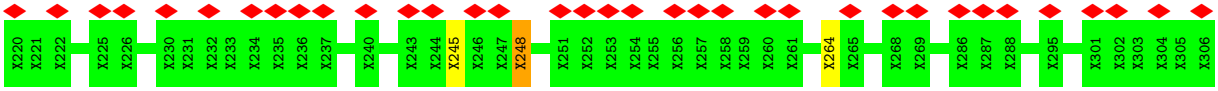




• Molecule 5: Coiled coils

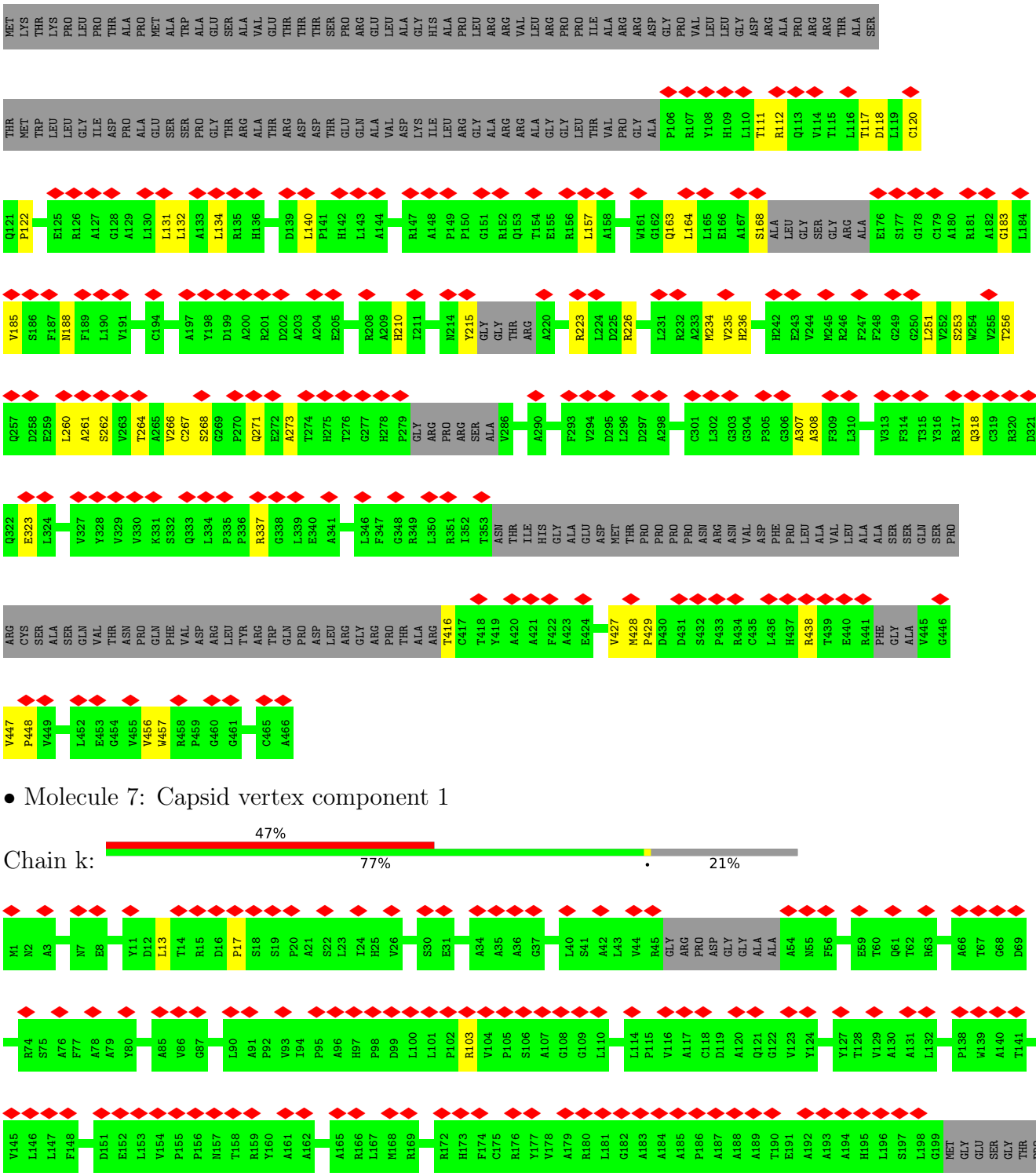
Chain P:





• Molecule 6: Triplex capsid protein 1

Chain S:



• Molecule 7: Capsid vertex component 1

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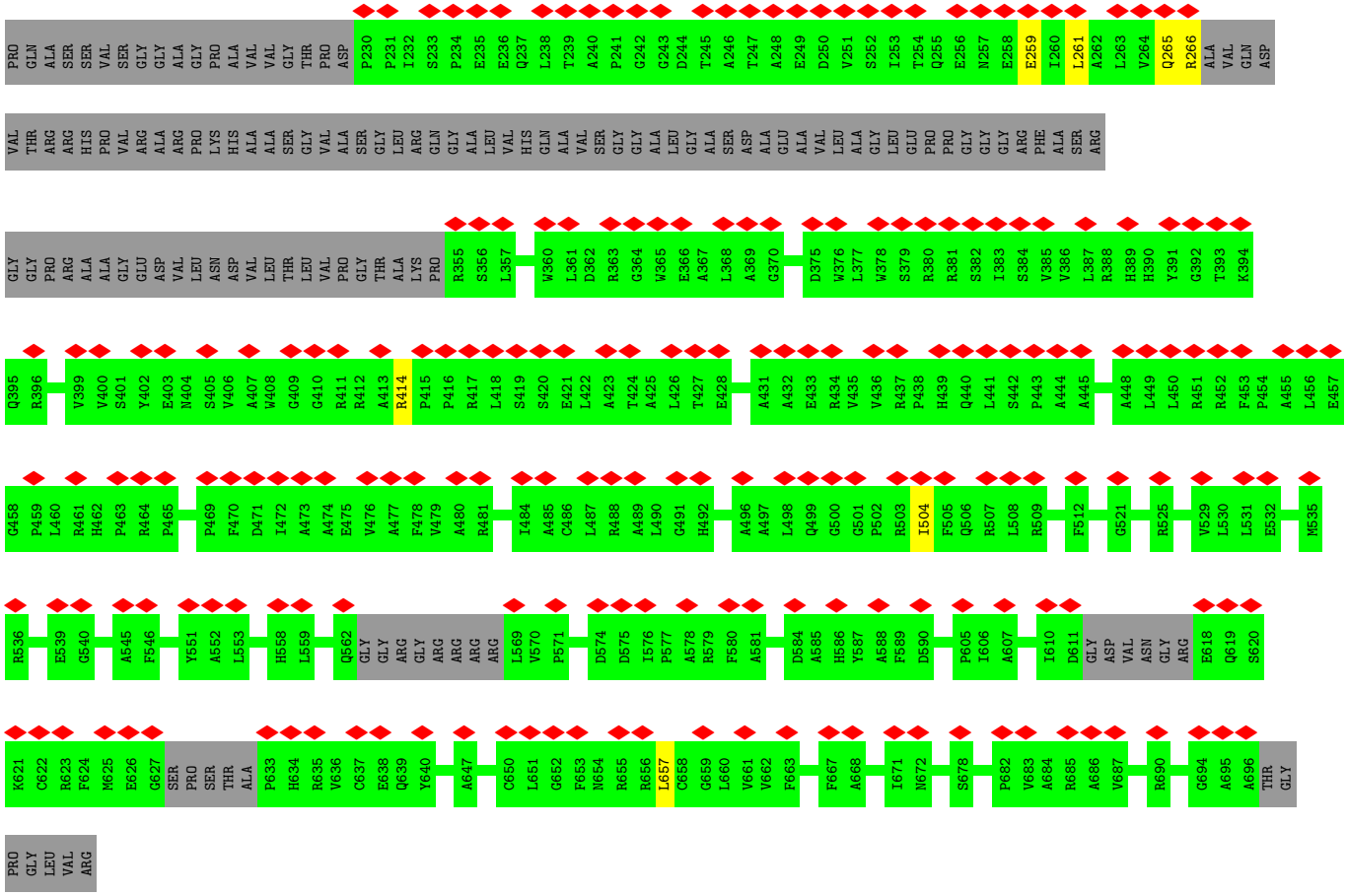

• Molecule 8: Capsid vertex component 2

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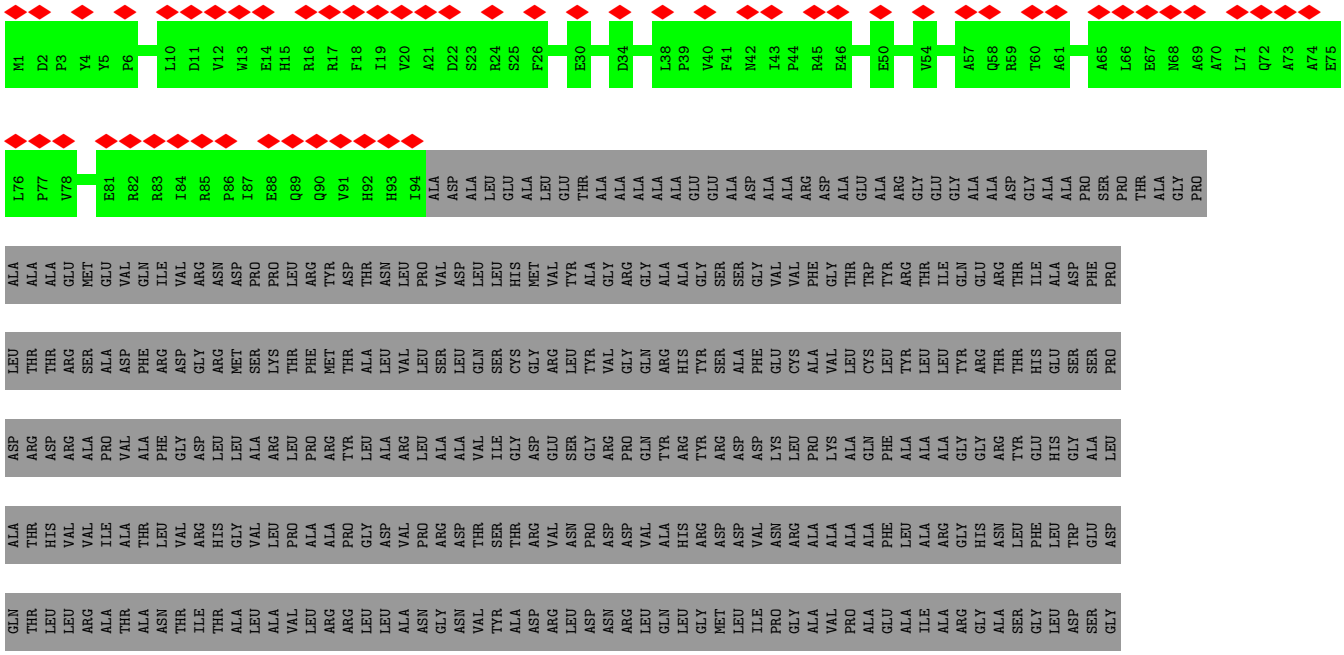
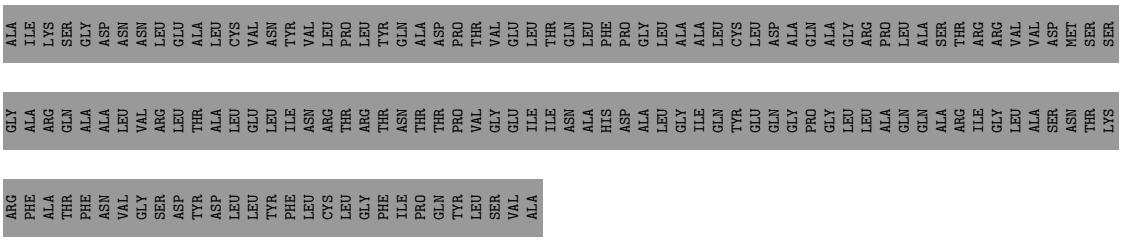
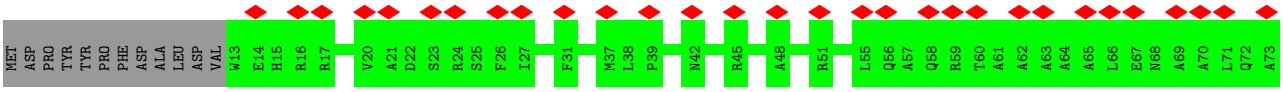
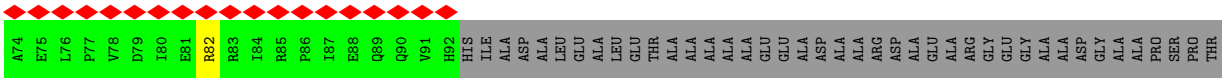


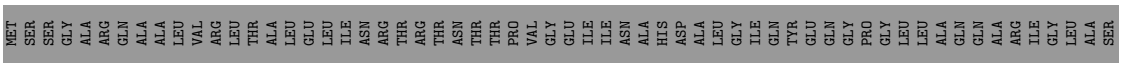


• Molecule 8: Capsid vertex component 2

Chain m:

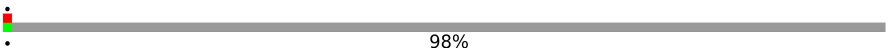






• Molecule 9: Large tegument protein deneddylase

Chain n:



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THR TYR LEU GLN ASP GLU PRO PHE VAL GLU ARG ARG VAL ALA ILE THR HIS PRO LEU ARG GLY GLU ILE GLY GLY LEU GLY ALA LEU PHE VAL GLY VAL VAL PRO ARG GLY ASP GLY GLU GLY SER GLY PRO VAL VAL PRO ALA LEU PRO ALA PRO THR HIS VAL GLN THR PRO GLY ALA

ASP ARG PRO PRO GLU ALA PRO ARG GLY ALA SER GLY PRO PRO ASP THR PRO GLN ALA GLY HIS PRO ASN ARG PRO PRO ASP ASP VAL TRP ALA ALA ALA LEU GLU GLY THR PRO PRO ALA LYS PRO SER ALA PRO ASP ALA ALA SER GLY PRO PRO HIS ALA ALA PRO PRO PRO GLN

THR PRO ALA GLY ASP ALA ALA GLU GLU ALA GLU ASP LEU ARG VAL LEU GLU VAL GLY ALA VAL PRO VAL GLY ARG HIS ARG ALA ARG TYR SER THR GLY LEU PRO LYS ARG ARG PRO THR TRP THR PRO PRO SER SER VAL GLU ASP LEU THR SER GLY GLU ARG PRO ALA PRO LYS

ALA PRO PRO ALA LYS ALA LYS LYS LYS SER ALA PRO LYS LYS LYS ALA PRO VAL ALA ALA GLU VAL PRO ALA SER SER PRO THR PRO ILE ALA ALA THR VAL PRO PRO ALA PRO ASP THR PRO PRO GLN SER GLY GLN GLY GLY GLY ASP ASP GLY PRO ALA SER PRO SER SER PRO SER

VAL LEU GLU THR LEU GLY ALA ARG ARG PRO PRO GLU PRO PRO GLY ALA ASP LEU ALA GLN LEU PHE GLU VAL HIS PRO ASN VAL ALA ALA THR ALA VAL ARG LEU ALA ALA ARG ASP ALA ALA LEU ALA ARG GLU VAL ALA ALA CYS SER GLN LEU THR ILE ASN ALA LEU ARG SER PRO

TYR PRO ALA HIS PRO GLY LEU LEU GLU LEU CYS VAL ILE PHE PHE PHE GLU ARG VAL LEU ALA PHE LEU ILE GLU ASN GLY ALA ARG THR HIS THR GLN ALA GLY VAL ALA GLY PRO ALA ALA ALA LEU LEU ASP PHE THR LEU ARG MET LEU PRO ARG LYS THR ALA VAL GLY ASP PHE

LEU ALA SER THR ARG MET SER LEU ALA ASP VAL ALA ALA HIS ARG PRO LEU ILE GLN HIS VAL LEU ASP GLU ASN SER GLN ILE GLY ARG LEU ALA LEU ALA LYS LEU VAL LEU VAL ALA ARG ASP VAL ILE ARG GLU THR ASP ALA PHE TYR GLY ASP LEU ALA ASP LEU ASP LEU GLN

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GLU ALA ARG GLU MET ARG GLU ALA LEU ASP ALA LEU ALA ARG GLY VAL ASP SER VAL SER GLN ARG ALA GLY PRO LEU THR VAL MET PRO VAL PRO ALA ALA PRO GLY ALA GLY GLY ARG ALA PRO CYS PRO PRO ALA LEU GLY PRO GLU ALA ILE GLN ALA ARG LEU GLU ASP VAL ARG

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LEU GLU GLU LEU ALA ARG SER ILE HIS GLY ILE ASN ASP GLN GLN ALA ARG ARG SER SER GLY LEU ALA GLU LEU GLN ARG PHE ASP ALA LEU ASP ALA ALA LEU ALA GLN GLN LEU ASP SER ASP ALA ALA PHE VAL PRO ALA THR GLY PRO ALA PRO TYR VAL ASP GLY GLY GLY LEU

SER PRO GLU ALA THR ARG MET ALA GLU ASP ALA LEU ARG GLN ALA ARG ALA MET GLU ALA ALA LYS MET THR ALA GLU LEU ALA PRO GLU ALA ARG SER ARG LEU ARG GLU ARG ALA HIS ALA LEU GLU ALA MET LEU ASN ASP ALA ARG GLU ARG ALA LYS VAL ALA HIS ASP ALA ARG

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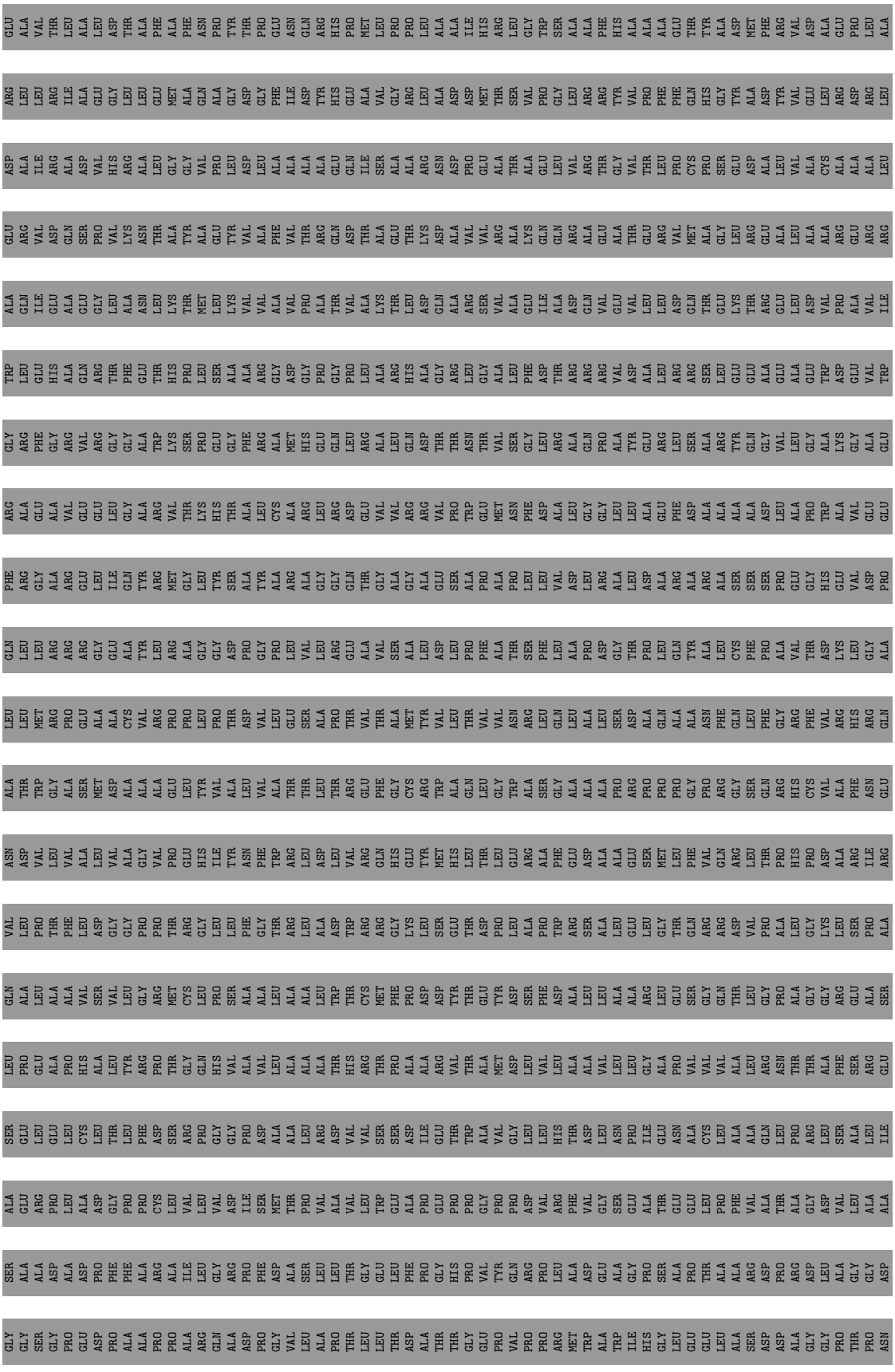
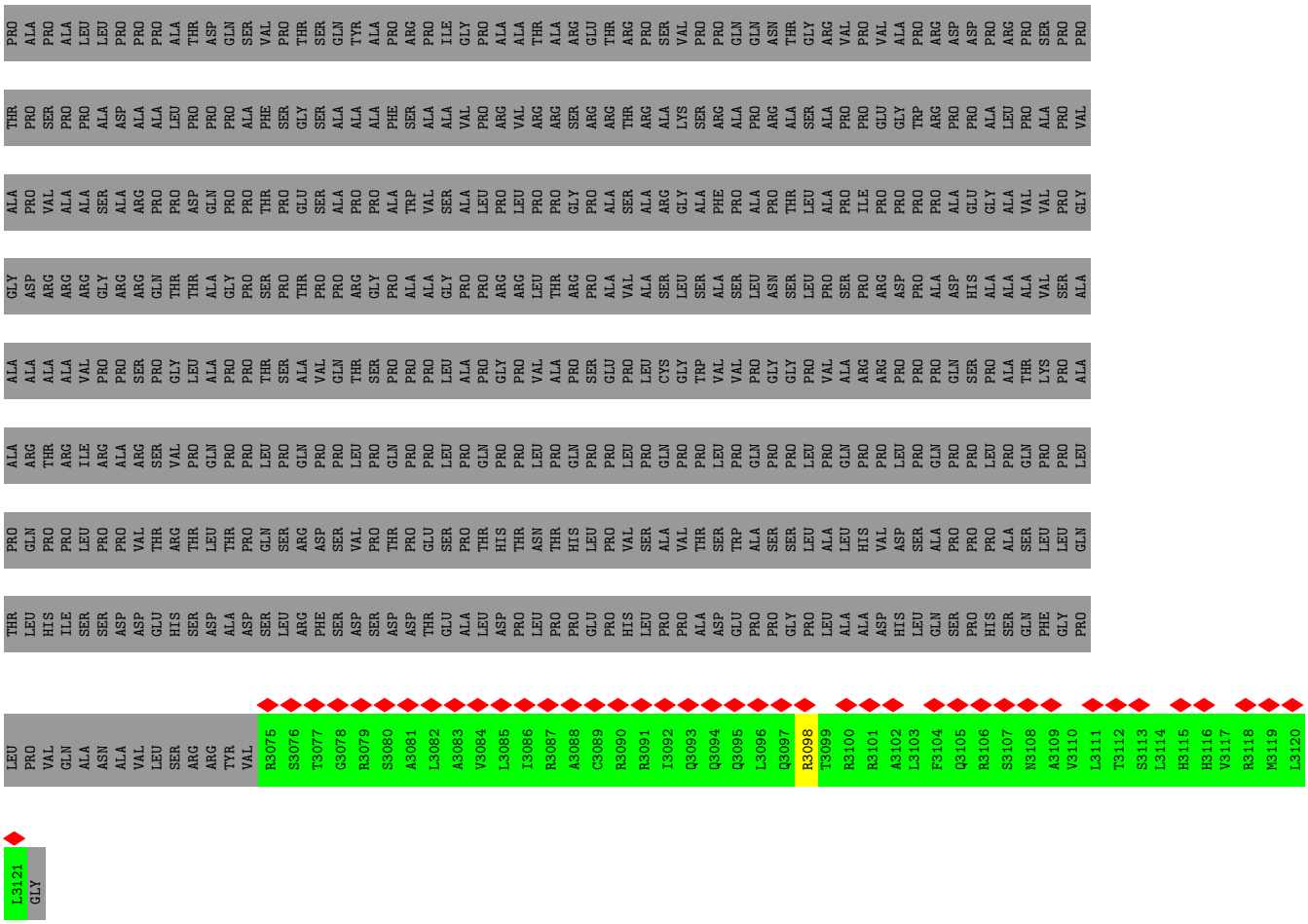
VAL SER ASN ALA ILE ASN ALA GLY SER ALA ALA VAL ALA THR ALA SER PRO ALA ALA THR VAL ASP ALA ALA VAL ARG ALA HIS GLY ALA LEU ALA ASP ALA VAL SER ALA LEU GLY ALA ALA ALA ARG ASP PRO ALA SER PRO LEU SER PHE LEU ALA VAL LEU ALA ASP SER ALA ALA

GLY TYR VAL LYS ALA THR ARG LEU ALA LEU GLU ALA ARG GLY ALA ILE ASP GLU LEU THR THR LEU GLY SER ALA ALA ALA ASP LEU VAL VAL GLN ALA ARG ARG ALA CYS ALA GLN PRO GLU GLY ASP HIS ALA ALA LEU ILE ASP ALA ALA ALA ARG ALA THR THR ALA ALA ARG GLU

SER LEU ALA GLY HIS GLU ALA GLY PHE GLY GLY LEU LEU HIS ALA GLU GLY THR ALA GLY ASP HIS SER PRO SER GLY ARG ALA LEU GLN GLU LEU GLY LYS VAL ILE GLY ALA THR ARG ARG ARG ALA ASP GLU LEU GLU ALA ALA VAL ALA ASP LEU THR ALA LYS MET ALA ALA GLN

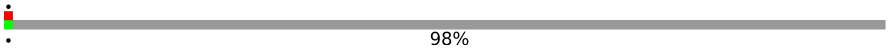
ARG ALA ARG GLY SER SER GLU ARG TRP ALA ALA GLY VAL GLU ALA ALA LEU ASP ARG VAL GLU ASN ARG ALA GLU PHE ASP VAL VAL GLU LEU ARG ARG LEU GLN ALA LEU ALA GLY THR HIS GLY TYR ASN PRO ARG ASP PHE ARG LYS ARG ALA GLU GLN ALA LEU ALA ALA ASN ALA

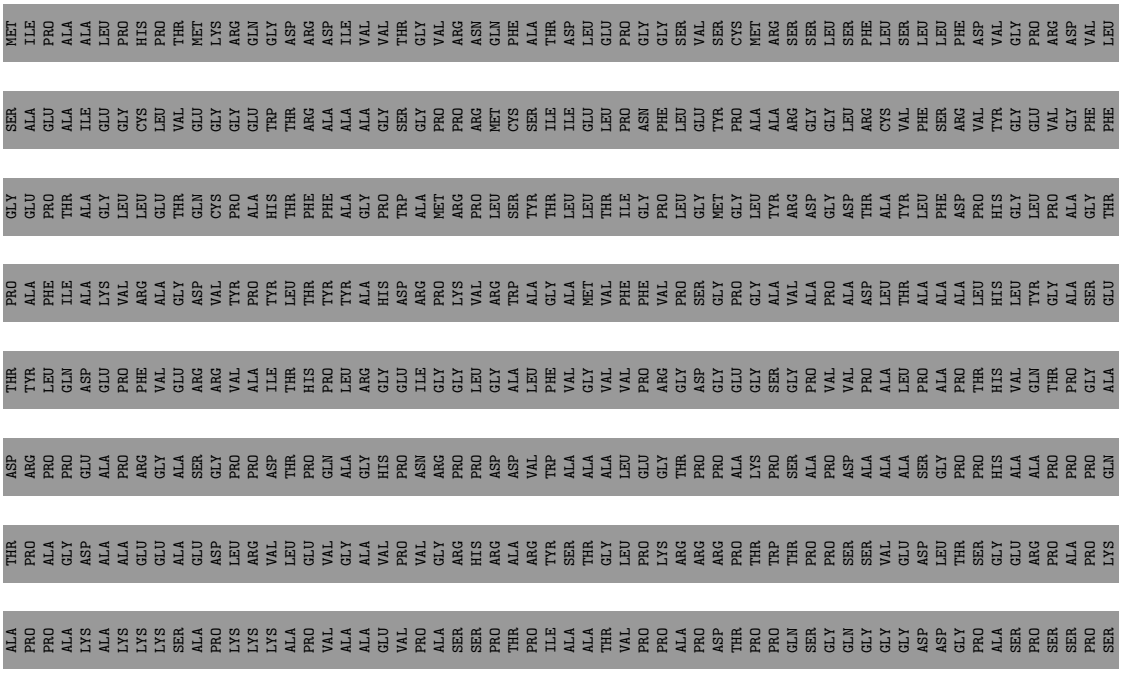




• Molecule 9: Large tegument protein deneddylase

Chain o:





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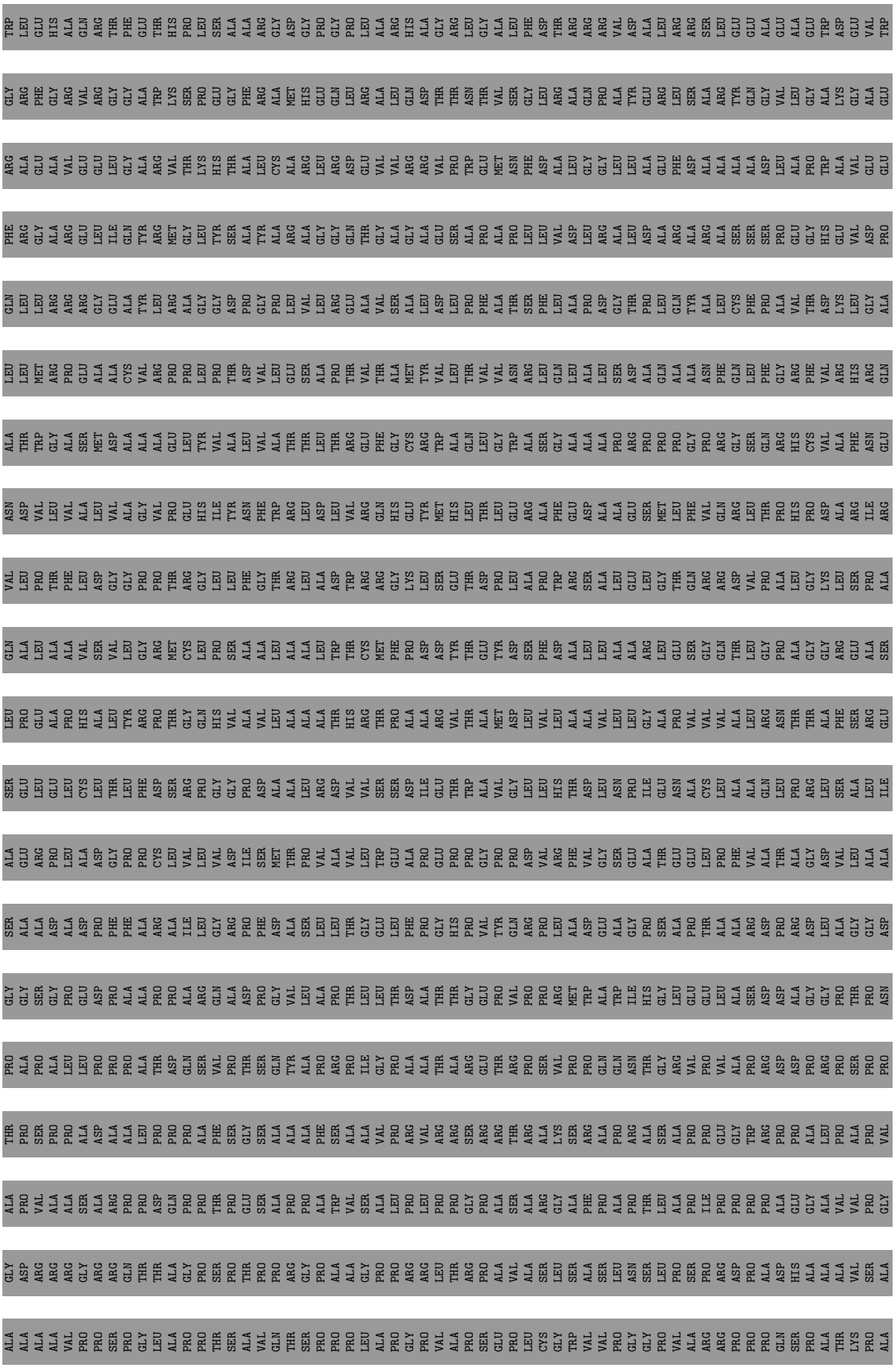

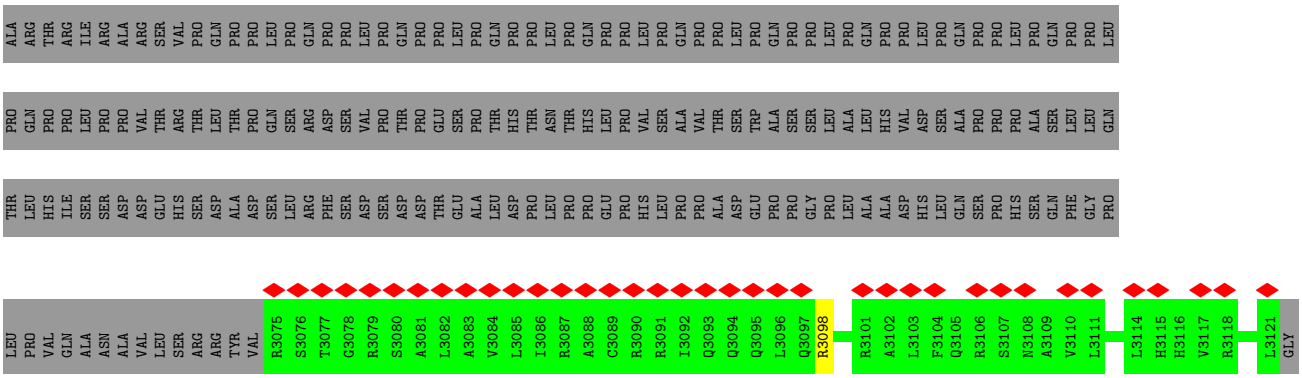
ALA ARG THR ARG ILE ARG ALA ARG SER VAL PRO GLN PRO PRO LEU PRO GLN PRO PRO LEU PRO GLN PRO PRO LEU PRO GLN PRO PRO LEU PRO GLN PRO PRO LEU PRO GLN PRO PRO LEU PRO GLN PRO PRO LEU PRO GLN PRO PRO LEU PRO GLN PRO PRO LEU
PRO GLN PRO PRO LEU PRO PRO VAL THR ARG THR LEU THR PRO GLN SER ARG ASP SER VAL PRO THR PRO GLU SER PRO THR HIS THR ASN THR HIS LEU PRO VAL SER ALA VAL THR SER TRP ALA SER SER LEU ALA LEU HIS VAL ASP SER ALA PRO PRO PRO ALA SER LEU LEU GLN
THR LEU HIS ILE SER SER ASP ASP GLU HIS SER ASP ALA ASP SER LEU ARG PHE SER ASP SER ASP ASP THR GLU ALA LEU ASP PRO LEU PRO PRO GLU HIS LEU PRO PRO ALA ASP GLU PRO PRO GLY PRO LEU ALA ALA ASP HIS LEU GLN GLN SER PRO HIS SER GLN GLY PHE GLY PRO
LEU PRO VAL GLN ALA ASN ALA VAL LEU SER ARG ARG TYR VAL R3075 S3076 T3077 G3078 R3079 S3080 A3081 L3082 A3083 V3084 L3085 I3086 R3087 A3088 C3089 R3090 R3091 I3092 Q3093 Q3094 Q3095 L3096 Q3097 R3098 R3101 A3102 L3103 F3104 Q3105 R3106 S3107 N3108 A3109 V3110 L3111 L3114 H3115 H3116 V3117 R3118 L3121 GLY

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	12001	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 ($e^-/Å^2$)	30.0, 30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k), FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.035	Depositor
Minimum map value	-0.025	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	472.5, 472.5, 472.5	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	B	0.39	0/10453	0.63	1/14290 (0.0%)
1	C	0.36	0/10464	0.59	0/14305
1	D	0.37	0/10475	0.61	3/14317 (0.0%)
1	E	0.39	0/10416	0.62	2/14233 (0.0%)
1	F	0.40	0/10227	0.65	8/13995 (0.1%)
1	I	0.41	0/10071	0.66	4/13769 (0.0%)
2	G	0.30	0/794	0.52	0/1084
2	M	0.26	0/794	0.47	0/1084
2	Q	0.26	0/794	0.49	0/1084
2	T	0.30	0/794	0.54	0/1084
2	U	0.32	0/794	0.56	0/1084
2	V	0.30	0/794	0.55	0/1084
3	K	0.32	0/2114	0.64	0/2909
3	O	0.30	0/2215	0.62	0/3047
6	S	0.32	0/2020	0.67	0/2768
7	k	0.32	0/4342	0.54	1/5924 (0.0%)
8	l	0.30	0/792	0.54	0/1081
8	m	0.30	0/664	0.54	0/905
9	n	0.23	0/385	0.50	0/514
9	o	0.29	0/385	0.49	0/514
All	All	0.37	0/79787	0.62	19/109075 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	5
1	C	0	8
1	D	0	6
1	E	0	6
1	F	0	7

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	0	7
3	K	0	2
3	O	0	1
5	P	0	1
6	S	0	1
7	k	0	1
All	All	0	45

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	293	LEU	CA-CB-CG	8.60	135.08	115.30
1	F	892	LEU	CA-CB-CG	6.93	131.23	115.30
1	I	678	LEU	CA-CB-CG	6.63	130.54	115.30
1	F	1348	ASP	CB-CG-OD1	6.50	124.15	118.30
7	k	657	LEU	CA-CB-CG	6.47	130.18	115.30
1	I	135	LEU	CA-CB-CG	6.32	129.83	115.30
1	F	1285	LYS	C-N-CA	6.26	137.35	121.70
1	B	513	LEU	CA-CB-CG	5.93	128.93	115.30
1	D	1084	GLU	C-N-CA	5.89	136.43	121.70
1	E	1266	ALA	C-N-CA	5.74	136.04	121.70
1	E	293	LEU	CA-CB-CG	5.70	128.42	115.30
1	D	199	LEU	CA-CB-CG	5.62	128.24	115.30
1	F	293	LEU	C-N-CA	5.53	135.51	121.70
1	F	892	LEU	CB-CG-CD1	-5.50	101.64	111.00
1	D	1083	HIS	C-N-CA	5.22	134.76	121.70
1	F	1347	ARG	C-N-CA	5.14	134.56	121.70
1	I	1078	LEU	CA-CB-CG	5.04	126.89	115.30
1	I	1092	THR	CA-CB-CG2	5.01	119.42	112.40
1	F	380	LEU	C-N-CA	5.01	134.22	121.70

There are no chirality outliers.

All (45) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1201	ARG	Peptide
1	B	1222	VAL	Peptide
1	B	534	PRO	Peptide
1	B	764	VAL	Peptide
1	B	972	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	C	1083	HIS	Peptide
1	C	1161	GLN	Peptide
1	C	1162	PRO	Peptide
1	C	1222	VAL	Peptide
1	C	1241	THR	Peptide
1	C	131	ALA	Peptide
1	C	411	PRO	Peptide
1	C	43	ARG	Peptide
1	D	1084	GLU	Peptide
1	D	1161	GLN	Peptide
1	D	1222	VAL	Peptide
1	D	258	SER	Peptide
1	D	266	HIS	Peptide
1	D	755	ARG	Peptide
1	E	1162	PRO	Peptide
1	E	1222	VAL	Peptide
1	E	1265	GLY	Peptide
1	E	1316	GLY	Peptide
1	E	371	GLY	Peptide
1	E	43	ARG	Peptide
1	F	105	ALA	Peptide
1	F	1113	GLY	Peptide
1	F	1161	GLN	Peptide
1	F	1222	VAL	Peptide
1	F	293	LEU	Peptide
1	F	447	HIS	Peptide
1	F	453	SER	Peptide
1	I	1012	GLU	Peptide
1	I	1113	GLY	Peptide
1	I	305	THR	Peptide
1	I	573	ALA	Peptide
1	I	665	VAL	Peptide
1	I	81	CYS	Peptide
1	I	975	ASN	Peptide
3	K	103	THR	Peptide
3	K	315	ILE	Peptide
3	O	260	MET	Peptide
5	P	248	UNK	Peptide
6	S	140	LEU	Peptide
7	k	504	ILE	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	B	10198	0	9937	189	0
1	C	10209	0	9940	149	0
1	D	10221	0	9963	161	0
1	E	10162	0	9939	163	0
1	F	9978	0	9630	190	0
1	I	9831	0	9549	204	0
2	G	772	0	746	15	0
2	M	772	0	746	7	0
2	Q	772	0	746	8	0
2	T	772	0	746	10	0
2	U	772	0	746	19	0
2	V	772	0	746	19	0
3	K	2078	0	2053	39	0
3	O	2175	0	2213	31	0
4	L	420	0	88	6	0
5	P	435	0	89	2	0
6	S	1975	0	1858	30	0
7	k	4233	0	4180	0	0
8	l	770	0	751	0	0
8	m	648	0	636	0	0
9	n	383	0	418	0	0
9	o	383	0	418	0	0
All	All	78731	0	76138	1121	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 8.

All (1121) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:244:UNK:CB	6:S:260:LEU:HD12	1.87	1.05
1:F:282:ALA:HB1	1:F:382:LYS:HE3	1.46	0.97
4:L:244:UNK:CB	6:S:260:LEU:CD1	2.42	0.96
5:P:245:UNK:O	5:P:248:UNK:O	1.85	0.93
4:L:201:UNK:CB	5:P:264:UNK:CB	2.49	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:22:THR:OG1	2:U:64:LEU:HD22	1.70	0.91
4:L:194:UNK:O	4:L:195:UNK:C	2.28	0.79
2:V:22:THR:CG2	2:V:60:ALA:HB1	2.14	0.77
1:B:826:CYS:HB2	1:B:966:GLY:H	1.52	0.74
1:F:895:GLN:HA	2:V:61:LEU:HB3	1.70	0.74
1:I:512:ARG:HH12	1:I:564:PRO:HD2	1.52	0.74
1:I:496:GLY:HA3	1:I:504:ARG:HH22	1.54	0.73
1:B:267:ALA:HB1	1:B:274:VAL:HB	1.71	0.72
4:L:244:UNK:CB	6:S:260:LEU:HD11	2.18	0.72
1:B:63:ASN:HD21	1:I:100:HIS:H	1.40	0.69
1:B:248:LEU:HD23	1:B:293:LEU:HD21	1.73	0.69
1:F:139:ALA:HA	1:F:142:LEU:HB2	1.75	0.69
2:V:22:THR:HG22	2:V:60:ALA:HB1	1.74	0.69
1:I:1073:TYR:OH	1:I:1097:ARG:NH1	2.26	0.68
6:S:267:CYS:O	6:S:271:GLN:NE2	2.27	0.67
1:I:836:TYR:O	1:I:840:GLN:NE2	2.26	0.67
1:E:530:GLN:O	1:E:536:ASN:ND2	2.26	0.66
3:O:70:ARG:O	6:S:337:ARG:NH2	2.28	0.66
1:D:425:PRO:HG3	1:D:431:GLU:HB2	1.78	0.66
1:D:267:ALA:HB1	1:D:274:VAL:H	1.59	0.66
1:B:281:THR:H	1:B:284:ILE:HD12	1.60	0.66
1:F:1342:LEU:HB3	1:F:1362:LEU:HD12	1.77	0.65
1:D:450:LEU:HB3	1:D:1124:ASN:HD21	1.60	0.65
1:F:1304:THR:HG21	1:F:1314:PRO:HD2	1.79	0.65
1:B:1117:ASN:ND2	1:I:204:TYR:OH	2.29	0.64
1:B:1124:ASN:O	1:B:1156:ARG:NH2	2.30	0.64
1:C:285:LYS:HE2	1:C:377:LEU:HB3	1.80	0.64
1:F:730:ALA:HB2	1:F:750:ARG:HH12	1.62	0.64
1:I:261:VAL:HG22	1:I:263:ARG:H	1.63	0.64
1:C:228:CYS:HA	1:C:1368:PRO:HG3	1.80	0.64
1:I:1304:THR:HG22	1:I:1306:ALA:H	1.63	0.64
1:D:417:ALA:O	1:D:1354:ARG:NH2	2.31	0.64
6:S:253:SER:HG	6:S:264:THR:HG1	1.44	0.64
6:S:118:ASP:O	6:S:223:ARG:NH1	2.31	0.63
1:B:960:VAL:HA	1:B:994:LEU:HD13	1.80	0.63
1:C:912:ALA:HB3	1:C:928:ILE:HB	1.81	0.63
1:D:193:PRO:HG2	1:D:198:LEU:HD12	1.81	0.63
1:E:252:THR:HG22	1:E:373:ARG:HD3	1.79	0.63
1:E:673:TYR:OH	1:E:801:ARG:NH2	2.32	0.63
1:C:523:GLU:HB3	1:C:1008:GLN:HG2	1.81	0.62
1:E:947:HIS:HB3	2:V:80:ALA:H	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:485:ASN:HD21	1:C:513:LEU:HA	1.64	0.62
1:B:336:LEU:HD22	1:C:156:HIS:HE1	1.65	0.62
1:B:576:ARG:HA	1:B:1003:ARG:HH12	1.64	0.62
1:D:707:PHE:HA	1:D:1042:THR:HG21	1.82	0.62
1:C:618:PHE:HA	1:C:940:MET:HB3	1.82	0.62
1:F:920:THR:H	1:F:923:THR:HG1	1.48	0.62
1:D:754:CYS:HA	1:D:910:CYS:HA	1.82	0.61
1:D:620:ASP:OD1	1:E:691:ARG:NH1	2.33	0.61
1:D:873:ASN:HA	2:G:92:PHE:HB2	1.82	0.61
1:B:707:PHE:HA	1:B:1042:THR:HG21	1.83	0.61
1:C:656:TRP:O	1:C:660:ARG:NH1	2.33	0.61
1:E:1276:PHE:HA	1:E:1329:GLN:HE22	1.65	0.61
1:D:982:ASP:OD1	1:D:985:ARG:NH1	2.33	0.61
1:I:182:ASP:O	1:I:186:HIS:ND1	2.33	0.61
1:C:957:VAL:HG22	1:C:959:PRO:HD3	1.82	0.61
1:E:557:GLU:HG3	1:E:559:PRO:HD2	1.80	0.61
1:B:530:GLN:O	1:B:536:ASN:ND2	2.33	0.61
1:D:530:GLN:O	1:D:536:ASN:ND2	2.33	0.61
1:E:982:ASP:OD1	1:E:985:ARG:NH1	2.33	0.61
1:B:1157:LEU:HD21	1:B:1309:VAL:HG11	1.82	0.61
1:D:629:LEU:HB3	1:D:839:LEU:HD21	1.82	0.61
1:D:1182:ASP:HB2	1:D:1309:VAL:HA	1.83	0.61
1:F:1085:THR:OG1	1:F:1090:ASN:ND2	2.34	0.61
1:C:1201:ARG:HH12	1:D:1179:HIS:HE1	1.48	0.60
1:D:236:LYS:NZ	1:D:1370:LYS:O	2.33	0.60
1:I:272:ARG:HE	1:I:374:LEU:HB2	1.65	0.60
1:B:76:SER:OG	1:B:266:HIS:NE2	2.32	0.60
1:D:326:VAL:HB	1:D:329:LEU:HD12	1.84	0.60
1:I:1130:TYR:HB3	1:I:1148:ARG:HH21	1.66	0.60
3:K:301:ASP:H	6:S:112:ARG:HB3	1.67	0.60
1:B:909:LEU:HD11	1:B:929:PHE:HB3	1.83	0.60
1:D:749:ASP:O	1:D:752:ARG:NH2	2.32	0.60
1:D:1257:TYR:HB2	1:D:1277:PHE:HD2	1.67	0.60
6:S:438:ARG:HA	6:S:448:PRO:HA	1.84	0.60
1:B:490:TYR:OH	1:B:560:GLY:O	2.19	0.60
1:D:834:ARG:HD3	2:G:90:PRO:HB3	1.83	0.60
1:B:712:PRO:O	1:B:719:GLN:NE2	2.35	0.60
1:I:891:MET:O	1:I:895:GLN:NE2	2.34	0.60
1:E:404:LEU:HB2	1:E:1052:VAL:HB	1.84	0.60
1:D:664:PHE:HB3	1:D:670:LEU:HD13	1.83	0.59
1:B:84:PHE:O	1:B:1097:ARG:NH2	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:674:ILE:HG23	1:I:678:LEU:HD12	1.83	0.59
1:E:785:HIS:NE2	1:E:798:ARG:O	2.35	0.59
1:I:828:ALA:HB1	1:I:955:PHE:HB3	1.84	0.59
1:B:728:ASP:O	1:B:810:LYS:NZ	2.35	0.59
1:E:674:ILE:HG13	1:E:678:LEU:HD12	1.85	0.59
1:F:826:CYS:SG	1:F:827:THR:N	2.76	0.59
1:I:87:LEU:H	1:I:1076:GLY:HA2	1.67	0.59
1:C:815:VAL:HA	1:C:1024:LEU:HD22	1.85	0.59
1:D:1206:ARG:HB3	1:D:1277:PHE:HE1	1.68	0.59
1:I:769:CYS:O	1:I:900:ASN:ND2	2.35	0.59
6:S:157:LEU:HD11	6:S:234:MET:HA	1.84	0.59
2:V:22:THR:HG22	2:V:60:ALA:CB	2.31	0.59
1:F:748:LEU:HD13	1:F:750:ARG:HB2	1.85	0.59
1:I:367:LEU:HD13	1:I:374:LEU:HD21	1.85	0.58
1:I:404:LEU:HB2	1:I:1052:VAL:HB	1.83	0.58
1:D:645:ALA:O	1:D:649:THR:N	2.33	0.58
1:F:707:PHE:HA	1:F:1042:THR:HG21	1.85	0.58
1:C:1236:ARG:NH2	1:C:1241:THR:O	2.36	0.58
1:F:872:ALA:O	2:V:30:ASN:ND2	2.36	0.58
3:K:161:ARG:NH1	3:K:174:PRO:O	2.36	0.58
1:B:276:GLY:HA3	1:B:375:VAL:HG22	1.86	0.58
1:B:406:LEU:HB2	1:B:1050:PHE:HB2	1.85	0.58
1:F:696:HIS:HE1	1:F:1021:THR:HG21	1.67	0.58
1:F:1082:ARG:NH2	1:F:1084:GLU:OE2	2.36	0.58
1:B:629:LEU:HB3	1:B:839:LEU:HD21	1.85	0.58
1:C:777:ASN:O	2:Q:51:ARG:NH2	2.37	0.58
1:B:278:LEU:HD13	1:B:375:VAL:HG11	1.86	0.58
1:B:1237:PRO:HB2	1:C:1156:ARG:HE	1.69	0.58
1:D:99:VAL:O	1:D:118:ASN:ND2	2.36	0.58
1:I:129:LEU:O	1:I:1094:THR:OG1	2.21	0.58
1:I:276:GLY:HA3	1:I:375:VAL:HG13	1.84	0.58
1:I:1004:GLN:O	1:I:1008:GLN:NE2	2.36	0.58
1:B:1118:PRO:HG3	1:B:1374:LEU:HD13	1.85	0.58
1:B:1118:PRO:HD3	1:B:1374:LEU:HD22	1.85	0.58
1:B:1233:ASP:O	1:C:1174:ARG:NH2	2.37	0.58
1:E:460:THR:HG21	1:E:1187:PHE:HB2	1.85	0.58
1:D:870:LEU:HD22	1:D:877:ARG:HA	1.86	0.58
1:D:909:LEU:HA	1:D:931:GLY:HA2	1.85	0.58
1:D:1052:VAL:HG22	1:D:1187:PHE:HE1	1.68	0.58
1:E:413:MET:O	1:F:433:ARG:NH1	2.32	0.58
2:G:76:GLN:O	2:G:96:ARG:NH2	2.30	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:717:GLN:HE21	1:B:748:LEU:HD22	1.69	0.58
1:C:730:ALA:HB2	1:C:750:ARG:HH12	1.69	0.58
1:D:497:PRO:HD2	1:D:504:ARG:HH12	1.69	0.58
1:F:381:GLU:HA	1:F:385:TYR:HB2	1.84	0.58
1:B:677:TYR:HD1	2:T:95:LYS:HG2	1.69	0.57
1:C:826:CYS:HB2	1:C:966:GLY:H	1.68	0.57
1:E:638:GLU:OE1	1:E:801:ARG:NH2	2.36	0.57
1:F:1008:GLN:HE22	1:F:1011:ARG:HH11	1.52	0.57
1:F:413:MET:O	1:I:433:ARG:NH1	2.35	0.57
1:I:960:VAL:HA	1:I:994:LEU:HD13	1.86	0.57
1:B:502:GLN:HA	1:B:505:PHE:HB3	1.86	0.57
1:F:595:ARG:NH1	1:F:1045:HIS:O	2.38	0.57
1:B:425:PRO:HG3	1:B:431:GLU:HB2	1.85	0.57
1:D:137:THR:HA	1:D:140:ILE:HD12	1.86	0.57
1:E:646:ARG:HA	1:E:649:THR:HG22	1.86	0.57
1:E:544:HIS:CD2	1:E:546:ALA:H	2.22	0.57
1:D:413:MET:O	1:E:433:ARG:NH1	2.38	0.57
1:F:204:TYR:OH	1:F:210:LEU:O	2.22	0.57
1:F:1161:GLN:NE2	1:F:1170:GLN:OE1	2.37	0.57
1:E:708:THR:HA	1:E:1038:HIS:HB3	1.86	0.57
3:K:275:LEU:HD22	3:O:157:ALA:HB2	1.86	0.57
1:B:373:ARG:NH2	1:B:1067:GLU:OE1	2.38	0.56
1:E:730:ALA:HB2	1:E:750:ARG:HH12	1.70	0.56
1:E:1208:ARG:NH2	1:E:1240:ALA:O	2.38	0.56
1:F:982:ASP:OD1	1:F:985:ARG:NH1	2.38	0.56
3:O:57:SER:O	3:O:194:GLN:NE2	2.37	0.56
1:F:67:LEU:HD21	1:F:170:GLN:HB3	1.87	0.56
1:C:1076:GLY:H	1:C:1095:GLN:HE21	1.53	0.56
1:D:42:VAL:HG21	1:D:49:LEU:HD21	1.87	0.56
1:B:528:ALA:HA	1:B:531:PHE:HB2	1.87	0.56
1:B:1246:ALA:HA	1:B:1253:GLY:HA3	1.86	0.56
1:I:272:ARG:NH2	1:I:372:ASP:O	2.38	0.56
1:D:697:VAL:HG12	1:D:808:HIS:HD2	1.71	0.56
1:F:946:ASP:HB3	1:I:676:THR:HG21	1.88	0.56
1:I:904:ARG:NH1	1:I:906:THR:OG1	2.36	0.56
1:C:159:LEU:O	1:C:163:GLN:NE2	2.38	0.56
1:E:742:LEU:HD21	1:E:908:LEU:HD21	1.87	0.56
3:K:10:ILE:HB	3:K:83:ILE:HB	1.88	0.56
1:C:804:ASP:O	1:C:808:HIS:ND1	2.37	0.56
1:F:95:VAL:HG13	1:I:63:ASN:HB3	1.87	0.56
1:D:875:VAL:O	1:D:879:PHE:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1074:PHE:HB3	1:B:1097:ARG:HH11	1.71	0.56
1:D:99:VAL:HG13	1:D:118:ASN:HD22	1.70	0.56
1:D:359:GLN:NE2	1:D:360:THR:O	2.39	0.56
1:I:1276:PHE:HA	1:I:1329:GLN:HE22	1.70	0.56
3:K:161:ARG:HE	3:O:271:LEU:HD12	1.71	0.56
1:C:544:HIS:CD2	1:C:546:ALA:H	2.24	0.56
1:D:618:PHE:HA	1:D:940:MET:HB3	1.88	0.56
3:O:179:LEU:HB2	3:O:186:LEU:HB2	1.87	0.56
1:F:981:ARG:HH22	1:I:803:ALA:H	1.53	0.55
1:I:1215:ALA:O	1:I:1287:ARG:NH1	2.39	0.55
1:B:665:VAL:O	1:B:812:TYR:OH	2.22	0.55
1:D:742:LEU:HD12	1:D:908:LEU:HD21	1.87	0.55
1:I:617:ALA:HB2	1:I:661:CYS:HB3	1.86	0.55
1:C:104:ILE:HG23	1:D:179:GLY:HA2	1.88	0.55
1:D:228:CYS:HA	1:D:1368:PRO:HG3	1.88	0.55
1:E:450:LEU:HD22	1:E:1124:ASN:HD22	1.71	0.55
1:F:754:CYS:HA	1:F:910:CYS:HA	1.89	0.55
1:B:1298:SER:HB2	1:B:1320:LEU:HD22	1.89	0.55
1:I:951:ASN:ND2	1:I:972:ASN:O	2.37	0.55
1:C:667:ASP:OD1	1:C:813:TYR:OH	2.25	0.55
1:E:590:ALA:O	1:E:594:ALA:N	2.39	0.55
1:E:738:ASP:OD1	1:E:738:ASP:N	2.37	0.55
1:E:1298:SER:HB2	1:E:1320:LEU:HD22	1.88	0.55
1:F:708:THR:OG1	1:F:723:ASN:ND2	2.40	0.55
1:D:255:THR:OG1	1:D:1067:GLU:OE2	2.25	0.55
1:E:951:ASN:ND2	1:E:972:ASN:O	2.39	0.55
1:F:229:ASP:O	1:F:236:LYS:NZ	2.39	0.55
1:F:445:LYS:NZ	1:F:1118:PRO:O	2.39	0.55
3:K:276:VAL:HG21	3:O:154:ARG:HD3	1.88	0.55
1:C:968:ASP:O	1:C:972:ASN:ND2	2.36	0.55
3:O:230:LEU:HA	3:O:233:GLN:HE21	1.71	0.55
2:V:51:ARG:HB3	2:V:55:ARG:HH12	1.72	0.55
1:D:1289:LEU:HD13	1:D:1292:LEU:HB2	1.89	0.55
1:E:1181:GLN:NE2	1:E:1307:SER:O	2.40	0.55
1:I:445:LYS:HE2	1:I:1118:PRO:HG2	1.89	0.55
1:B:711:GLY:H	1:B:719:GLN:HG3	1.70	0.55
1:B:1126:PRO:HG2	1:B:1129:PHE:HZ	1.72	0.55
1:C:712:PRO:O	1:C:719:GLN:NE2	2.34	0.55
1:D:451:ARG:NH2	1:D:453:SER:OG	2.40	0.55
1:D:951:ASN:ND2	1:D:972:ASN:O	2.33	0.55
1:F:284:ILE:HD11	1:F:1061:GLU:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:638:GLU:OE2	1:F:677:TYR:OH	2.25	0.54
3:O:306:VAL:HG11	3:O:312:ALA:HB2	1.89	0.54
1:B:1218:LYS:N	1:B:1221:ASP:OD2	2.40	0.54
1:C:1061:GLU:OE1	1:C:1114:THR:OG1	2.25	0.54
1:F:248:LEU:O	1:F:252:THR:N	2.39	0.54
2:G:17:VAL:HG21	2:G:53:PHE:HA	1.89	0.54
1:I:495:ALA:O	1:I:504:ARG:NH1	2.37	0.54
1:I:777:ASN:O	2:U:51:ARG:NH2	2.40	0.54
1:C:281:THR:OG1	1:C:381:GLU:OE2	2.26	0.54
1:I:197:LEU:HA	1:I:223:LEU:HD11	1.89	0.54
6:S:256:THR:HG22	6:S:262:SER:H	1.73	0.54
1:B:1200:ARG:NH2	1:B:1362:LEU:O	2.41	0.54
1:C:62:CYS:SG	1:C:63:ASN:N	2.81	0.54
1:C:76:SER:OG	1:C:266:HIS:NE2	2.40	0.54
3:K:283:GLY:O	3:O:149:ARG:NH1	2.40	0.54
2:U:18:ARG:HA	2:U:60:ALA:HB2	1.89	0.54
1:D:261:VAL:HG12	1:D:263:ARG:H	1.73	0.54
1:D:673:TYR:OH	1:D:801:ARG:NH2	2.40	0.54
1:D:777:ASN:ND2	2:M:47:GLN:OE1	2.40	0.54
1:E:104:ILE:HG12	1:F:178:ARG:HB3	1.88	0.54
1:I:194:PRO:HD2	1:I:197:LEU:HD12	1.90	0.54
1:I:1359:THR:OG1	1:I:1360:GLN:NE2	2.40	0.54
1:D:631:GLN:HG3	1:D:670:LEU:HD11	1.90	0.54
1:D:1298:SER:HB2	1:D:1320:LEU:HD22	1.90	0.54
1:F:604:HIS:NE2	1:F:692:ASP:OD1	2.37	0.54
1:B:100:HIS:O	1:C:63:ASN:ND2	2.41	0.54
1:B:451:ARG:NH2	1:B:453:SER:OG	2.40	0.54
1:E:81:CYS:HA	1:E:1073:TYR:HB3	1.89	0.54
1:E:229:ASP:O	1:E:236:LYS:NZ	2.37	0.54
1:E:700:LEU:HD22	1:E:1025:MET:HG2	1.90	0.54
1:F:545:PRO:O	1:F:576:ARG:NH1	2.41	0.54
1:C:1208:ARG:NH2	1:C:1240:ALA:O	2.41	0.53
1:D:392:TYR:HD2	1:D:395:VAL:HG12	1.74	0.53
1:I:777:ASN:ND2	2:U:47:GLN:OE1	2.39	0.53
1:I:944:HIS:HE1	1:I:968:ASP:HB3	1.73	0.53
1:C:621:ARG:NH2	1:D:698:GLU:OE2	2.42	0.53
1:C:1124:ASN:O	1:C:1156:ARG:NH1	2.40	0.53
1:D:906:THR:HB	1:D:934:HIS:HB3	1.90	0.53
1:B:193:PRO:HD3	1:B:1294:VAL:HG12	1.91	0.53
1:B:403:VAL:HG22	1:B:1053:VAL:HG22	1.90	0.53
1:B:1276:PHE:HA	1:B:1329:GLN:HE22	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:418:ALA:HA	1:D:423:LEU:HD23	1.91	0.53
1:F:440:LEU:HD23	1:F:452:LEU:HD12	1.90	0.53
1:F:577:VAL:HG12	1:F:578:VAL:HG13	1.91	0.53
1:I:1054:ARG:HH22	1:I:1122:MET:HA	1.74	0.53
1:I:1236:ARG:NH2	1:I:1241:THR:O	2.41	0.53
6:S:122:PRO:HB3	6:S:251:LEU:HD11	1.90	0.53
1:B:713:GLU:HG2	1:B:718:ALA:HA	1.91	0.53
1:B:777:ASN:O	2:T:51:ARG:NH2	2.37	0.53
1:F:861:PRO:O	1:F:869:ASN:ND2	2.42	0.53
1:C:1123:GLY:H	1:C:1183:ALA:HB3	1.74	0.53
1:C:1200:ARG:NH2	1:C:1355:GLU:OE2	2.41	0.53
1:F:548:ASP:OD1	1:F:576:ARG:NE	2.37	0.53
1:B:623:TYR:OH	1:B:663:ALA:O	2.23	0.53
1:B:663:ALA:N	1:B:690:TYR:OH	2.36	0.53
1:C:530:GLN:HG3	1:C:536:ASN:HD22	1.74	0.53
1:D:122:LYS:NZ	1:D:1101:ASP:O	2.34	0.53
1:E:708:THR:OG1	1:E:723:ASN:ND2	2.39	0.53
1:I:1059:VAL:HG12	1:I:1116:ARG:HD3	1.90	0.53
1:I:1348:ASP:OD2	1:I:1352:HIS:NE2	2.42	0.53
6:S:163:GLN:HB3	6:S:226:ARG:HD2	1.90	0.53
1:B:11:TYR:O	1:B:15:ALA:N	2.40	0.53
1:B:978:PRO:HA	1:B:981:ARG:HG2	1.90	0.53
1:B:982:ASP:OD1	1:B:985:ARG:NH2	2.38	0.53
1:D:80:VAL:HB	1:D:1072:ALA:HA	1.91	0.53
1:D:241:ARG:NH1	1:D:242:GLU:OE2	2.41	0.53
1:I:225:ARG:HH12	1:I:1201:ARG:HH12	1.57	0.53
1:D:198:LEU:HD13	1:D:1109:VAL:HG23	1.91	0.53
1:E:1222:VAL:O	1:E:1224:ALA:N	2.42	0.53
1:F:778:ARG:O	1:F:904:ARG:NE	2.42	0.53
3:K:161:ARG:HH22	3:K:174:PRO:HD2	1.73	0.53
1:B:709:LEU:H	1:B:1038:HIS:HD2	1.55	0.53
1:F:574:THR:OG1	1:F:1003:ARG:NH2	2.41	0.53
1:F:712:PRO:O	1:F:719:GLN:NE2	2.35	0.53
1:I:712:PRO:O	1:I:719:GLN:NE2	2.40	0.53
3:O:11:ALA:HA	3:O:82:ARG:HA	1.91	0.53
6:S:308:ALA:HB3	6:S:428:MET:HB3	1.91	0.53
1:B:873:ASN:ND2	2:T:30:ASN:OD1	2.38	0.52
1:C:203:ARG:NH2	1:C:222:GLU:OE2	2.42	0.52
1:F:832:PHE:HA	1:F:835:VAL:HB	1.90	0.52
1:B:532:MET:HA	1:B:1239:ALA:HA	1.91	0.52
1:B:680:GLY:O	1:I:658:ASN:ND2	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1037:TYR:O	1:E:1041:LYS:N	2.37	0.52
1:F:152:GLY:O	1:F:156:HIS:N	2.38	0.52
1:F:267:ALA:HB3	1:F:300:ALA:HB3	1.90	0.52
1:D:960:VAL:HG12	1:D:994:LEU:HD22	1.91	0.52
1:C:487:TYR:OH	1:C:990:VAL:N	2.43	0.52
1:C:677:TYR:HD1	2:Q:95:LYS:HG2	1.73	0.52
1:D:288:LEU:HB3	1:D:293:LEU:HD13	1.91	0.52
1:F:865:LEU:HD21	1:F:879:PHE:HB3	1.91	0.52
1:I:445:LYS:HD3	1:I:1179:HIS:HB3	1.92	0.52
6:S:427:VAL:O	6:S:456:VAL:N	2.43	0.52
3:K:215:GLU:OE1	3:O:245:SER:OG	2.27	0.52
1:B:187:VAL:HG11	1:B:1099:ASN:HD21	1.73	0.52
1:B:544:HIS:HD2	1:B:546:ALA:H	1.58	0.52
1:C:1313:ARG:NH1	1:C:1317:CYS:O	2.42	0.52
1:I:1369:LEU:HA	1:I:1372:LEU:HD12	1.91	0.52
1:B:951:ASN:ND2	1:B:972:ASN:O	2.40	0.52
1:D:826:CYS:HB2	1:D:966:GLY:H	1.75	0.52
1:E:470:ASP:HB3	1:E:922:SER:HB3	1.92	0.52
1:I:641:PHE:HE2	1:I:677:TYR:HB2	1.75	0.52
1:C:1071:GLU:OE2	1:C:1100:VAL:N	2.41	0.52
1:E:621:ARG:NH2	1:F:698:GLU:OE2	2.43	0.52
1:I:583:PRO:HG2	1:I:586:LEU:HD13	1.91	0.52
1:B:1075:LEU:O	1:B:1097:ARG:NH1	2.42	0.52
1:D:777:ASN:O	2:M:51:ARG:NH2	2.42	0.52
1:D:804:ASP:HA	1:D:807:VAL:HB	1.91	0.52
1:D:903:GLU:HG2	1:D:904:ARG:HG2	1.92	0.52
1:D:1222:VAL:O	1:D:1224:ALA:N	2.43	0.52
1:E:1061:GLU:OE2	1:E:1116:ARG:NH2	2.42	0.52
1:F:1084:GLU:HG3	1:F:1089:VAL:HG12	1.92	0.52
3:O:230:LEU:HD23	3:O:233:GLN:HE21	1.75	0.52
1:D:430:PRO:HB3	1:D:601:VAL:HG11	1.93	0.52
1:E:1225:LEU:HD23	1:F:1175:ALA:HB3	1.92	0.52
1:F:1017:GLU:HA	1:F:1020:LEU:HB3	1.92	0.52
1:I:752:ARG:O	1:I:911:SER:OG	2.28	0.52
3:K:114:VAL:HG11	3:K:291:LEU:HB3	1.92	0.52
1:B:1037:TYR:OH	1:B:1041:LYS:NZ	2.41	0.51
1:C:124:ILE:HG12	1:C:1100:VAL:HG22	1.92	0.51
1:F:804:ASP:O	1:F:808:HIS:ND1	2.38	0.51
1:F:1118:PRO:HD3	1:F:1374:LEU:HD13	1.92	0.51
1:F:1221:ASP:N	1:F:1221:ASP:OD1	2.41	0.51
1:D:491:VAL:HB	1:D:558:LEU:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1195:ASP:OD1	1:D:1195:ASP:N	2.42	0.51
1:D:1217:ASP:N	1:D:1221:ASP:OD2	2.44	0.51
1:E:1256:LEU:HA	1:E:1263:LEU:HD12	1.91	0.51
1:I:754:CYS:HA	1:I:910:CYS:HA	1.92	0.51
1:C:443:TRP:HH2	1:C:1347:ARG:HB3	1.75	0.51
1:E:1037:TYR:OH	1:E:1147:LEU:O	2.28	0.51
1:F:300:ALA:HA	1:F:362:ARG:HG2	1.92	0.51
1:I:575:TRP:O	1:I:1003:ARG:NH2	2.29	0.51
2:V:22:THR:OG1	2:V:64:LEU:HD13	2.10	0.51
1:B:933:LEU:HD11	1:B:958:LEU:HD23	1.92	0.51
1:F:104:ILE:HD12	1:I:390:VAL:HB	1.93	0.51
1:I:405:PRO:O	1:I:1361:TYR:OH	2.27	0.51
1:I:948:THR:HG21	2:T:95:LYS:HE3	1.93	0.51
1:B:103:LEU:HD11	1:B:115:PRO:HA	1.92	0.51
1:B:164:GLN:O	1:B:168:ASN:N	2.43	0.51
1:B:980:LEU:HD22	1:B:983:LEU:HD22	1.93	0.51
1:C:672:SER:O	1:C:676:THR:OG1	2.22	0.51
1:D:216:ARG:NH2	1:D:1287:ARG:O	2.41	0.51
1:E:141:ALA:HB1	1:E:146:GLU:HB3	1.92	0.51
1:E:372:ASP:OD1	1:E:372:ASP:N	2.43	0.51
1:F:1227:TYR:O	1:F:1229:HIS:ND1	2.44	0.51
1:B:1204:ASN:ND2	1:B:1208:ARG:O	2.44	0.51
1:C:1125:LEU:HD13	1:C:1156:ARG:HD2	1.93	0.51
1:F:451:ARG:NH2	1:F:453:SER:OG	2.44	0.51
6:S:210:HIS:HB2	6:S:447:VAL:HG21	1.93	0.51
1:D:656:TRP:CE2	1:D:686:CYS:HB3	2.46	0.51
1:E:410:ASN:HD21	1:E:1361:TYR:HB3	1.75	0.51
1:E:458:VAL:HG22	1:E:1151:VAL:HG22	1.92	0.51
1:F:104:ILE:HB	1:I:390:VAL:HG21	1.92	0.51
1:B:635:HIS:HB2	1:B:902:ALA:HB2	1.92	0.51
1:B:1201:ARG:HH12	1:C:1179:HIS:HE1	1.58	0.51
1:C:1225:LEU:HD23	1:D:1175:ALA:HB3	1.92	0.51
1:B:422:ASP:OD1	1:B:422:ASP:N	2.42	0.51
1:C:451:ARG:NH2	1:C:453:SER:OG	2.44	0.51
1:C:1149:ASN:HA	1:C:1152:VAL:HB	1.91	0.51
1:D:596:GLY:O	1:D:600:GLY:N	2.44	0.51
1:D:872:ALA:HB2	2:G:76:GLN:HB3	1.92	0.51
1:B:188:LEU:HD23	1:B:1064:LEU:HD21	1.93	0.51
1:B:753:ASP:OD1	1:B:911:SER:OG	2.28	0.51
1:B:755:ARG:HG3	1:B:761:HIS:HA	1.93	0.51
1:B:1208:ARG:NE	1:B:1225:LEU:O	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:804:ASP:HB3	1:C:808:HIS:CE1	2.46	0.51
1:C:1066:SER:OG	1:C:1067:GLU:N	2.43	0.51
1:I:244:ILE:O	1:I:248:LEU:N	2.42	0.51
3:K:121:PHE:HE2	3:K:143:LEU:HD11	1.75	0.51
3:O:35:PRO:HB3	3:O:70:ARG:HG2	1.92	0.51
1:D:895:GLN:HA	2:M:61:LEU:HD13	1.93	0.50
2:V:22:THR:HG23	2:V:60:ALA:HB1	1.91	0.50
1:E:1346:ALA:HB2	1:E:1362:LEU:HD11	1.93	0.50
1:F:496:GLY:HA3	1:F:504:ARG:HH22	1.76	0.50
4:L:186:UNK:O	4:L:190:UNK:CB	2.60	0.50
1:D:42:VAL:HG11	1:D:49:LEU:HD11	1.92	0.50
1:C:195:LEU:HD22	1:C:251:LEU:HD12	1.94	0.50
1:D:521:VAL:HG21	1:D:987:VAL:HG22	1.94	0.50
1:D:728:ASP:O	1:D:810:LYS:NZ	2.45	0.50
3:K:102:ASN:ND2	3:K:106:VAL:O	2.44	0.50
3:K:114:VAL:HG22	3:K:293:PRO:HA	1.94	0.50
1:B:228:CYS:HA	1:B:1368:PRO:HG3	1.92	0.50
1:C:608:PRO:HA	1:C:611:ILE:HD12	1.93	0.50
3:O:62:GLY:O	3:O:66:ALA:N	2.44	0.50
1:B:643:ALA:HB1	1:B:896:VAL:HG21	1.93	0.50
1:C:611:ILE:HG23	1:C:820:PHE:HE1	1.75	0.50
1:C:1257:TYR:HB2	1:C:1277:PHE:HD2	1.76	0.50
3:K:279:LEU:HD22	3:O:153:ALA:HB2	1.94	0.50
2:M:76:GLN:O	2:M:96:ARG:NH2	2.41	0.50
6:S:132:LEU:O	6:S:185:VAL:N	2.44	0.50
1:B:758:ALA:HB2	1:B:904:ARG:HH12	1.76	0.50
1:C:959:PRO:HB2	1:C:990:VAL:HG22	1.92	0.50
1:D:467:MET:HG3	1:D:918:ALA:HA	1.93	0.50
1:F:876:LYS:HA	1:F:879:PHE:HB2	1.94	0.50
1:B:433:ARG:NH1	1:I:413:MET:O	2.41	0.50
1:B:980:LEU:O	1:B:984:ALA:N	2.40	0.50
1:C:93:GLY:HA3	1:C:124:ILE:HD12	1.93	0.50
1:C:733:PRO:HG2	1:C:736:VAL:HG22	1.93	0.50
1:D:631:GLN:HE21	1:D:667:ASP:HB2	1.77	0.50
1:D:736:VAL:O	1:D:934:HIS:ND1	2.45	0.50
1:E:281:THR:OG1	1:E:282:ALA:N	2.43	0.50
1:E:963:LEU:HD23	1:E:1007:VAL:HG22	1.94	0.50
1:F:258:SER:OG	1:F:1102:LEU:O	2.29	0.50
1:F:1195:ASP:OD1	1:F:1195:ASP:N	2.45	0.50
1:I:873:ASN:HB2	2:U:30:ASN:HD21	1.76	0.50
1:I:1174:ARG:NH1	1:I:1182:ASP:OD2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:730:ALA:HB2	1:B:750:ARG:HH12	1.77	0.50
1:D:883:ARG:HB2	1:E:680:GLY:HA3	1.94	0.50
1:D:1201:ARG:NH1	1:E:448:GLN:OE1	2.45	0.50
2:G:89:ARG:NH2	2:M:29:THR:O	2.45	0.50
1:I:867:PRO:HG3	2:T:98:TYR:HB2	1.93	0.50
1:B:224:LYS:NZ	1:B:1214:TYR:OH	2.41	0.49
1:C:909:LEU:HD11	1:C:929:PHE:HB3	1.93	0.49
1:I:453:SER:OG	1:I:456:ASN:N	2.41	0.49
1:I:844:VAL:HG22	1:I:864:PRO:HB3	1.93	0.49
1:I:1057:ARG:NH2	1:I:1319:GLU:OE2	2.45	0.49
2:Q:76:GLN:O	2:Q:96:ARG:NH2	2.42	0.49
1:C:804:ASP:HB3	1:C:808:HIS:HE1	1.77	0.49
1:D:876:LYS:HA	1:D:879:PHE:HD2	1.76	0.49
1:F:422:ASP:N	1:F:422:ASP:OD1	2.45	0.49
1:I:1280:ALA:O	1:I:1284:ALA:N	2.44	0.49
1:C:664:PHE:HB3	1:C:670:LEU:HD13	1.93	0.49
1:C:1222:VAL:O	1:C:1224:ALA:N	2.44	0.49
1:D:621:ARG:NH2	1:E:698:GLU:OE2	2.45	0.49
1:E:161:ALA:O	1:E:165:LEU:N	2.41	0.49
1:F:453:SER:O	1:F:455:GLU:N	2.45	0.49
1:C:766:ALA:HB2	1:C:782:ARG:HD2	1.94	0.49
1:E:207:ASN:HB2	1:F:391:PRO:HA	1.94	0.49
1:C:1125:LEU:HD12	1:C:1126:PRO:HD2	1.93	0.49
1:D:436:PRO:HG2	1:D:595:ARG:HB3	1.95	0.49
1:E:1278:THR:HG22	1:E:1281:ASP:H	1.76	0.49
1:F:834:ARG:HD2	1:F:954:TYR:HA	1.94	0.49
1:F:1278:THR:HG22	1:F:1281:ASP:H	1.78	0.49
1:I:159:LEU:HD12	1:I:162:ILE:HB	1.94	0.49
1:C:404:LEU:HB2	1:C:1052:VAL:HB	1.95	0.49
1:D:440:LEU:HB3	1:D:452:LEU:HB2	1.95	0.49
1:E:1195:ASP:N	1:E:1195:ASP:OD1	2.46	0.49
1:E:1248:GLN:HB2	1:E:1251:SER:HB3	1.94	0.49
1:F:1206:ARG:NH1	1:F:1247:SER:O	2.46	0.49
1:C:1182:ASP:HB2	1:C:1309:VAL:HA	1.94	0.49
1:D:285:LYS:HE2	1:D:377:LEU:HB3	1.93	0.49
1:F:1284:ALA:O	1:F:1286:HIS:N	2.43	0.49
1:I:840:GLN:HB2	2:U:61:LEU:HD21	1.94	0.49
1:B:404:LEU:HD21	1:B:1334:ILE:HD11	1.95	0.49
1:C:671:VAL:HG13	1:C:690:TYR:HD1	1.78	0.49
1:C:1017:GLU:HA	1:C:1020:LEU:HB3	1.95	0.49
1:D:724:HIS:CD2	1:D:726:MET:H	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:100:HIS:H	1:F:63:ASN:HD21	1.61	0.49
1:E:325:ALA:H	1:F:56:ALA:HA	1.77	0.49
1:E:836:TYR:CZ	1:E:901:MET:HB2	2.48	0.49
1:E:867:PRO:HG3	2:V:98:TYR:HB2	1.93	0.49
1:I:827:THR:OG1	1:I:958:LEU:O	2.30	0.49
3:K:64:LEU:HA	3:K:67:TYR:HB2	1.94	0.49
1:D:77:VAL:HG23	1:D:266:HIS:HB3	1.95	0.49
1:D:622:SER:OG	1:E:675:VAL:O	2.25	0.49
1:F:97:PHE:HE1	1:F:122:LYS:HG2	1.78	0.49
1:I:991:PRO:HG2	1:I:994:LEU:HD12	1.95	0.49
3:K:182:ASN:OD1	3:K:183:GLY:N	2.45	0.49
3:O:67:TYR:HB3	3:O:291:LEU:HD21	1.94	0.49
1:D:270:ARG:NH1	1:D:297:ASP:OD1	2.44	0.48
1:E:790:ARG:HH11	2:G:79:PHE:HB2	1.77	0.48
1:F:470:ASP:N	1:F:470:ASP:OD1	2.46	0.48
1:I:396:GLY:N	1:I:1060:THR:O	2.42	0.48
1:B:1124:ASN:HD21	1:I:1238:PHE:HB3	1.77	0.48
1:C:841:ASN:ND2	1:C:873:ASN:O	2.46	0.48
1:F:734:PRO:HD2	1:F:813:TYR:HD2	1.78	0.48
1:I:624:PRO:HB3	1:I:882:GLY:HA3	1.93	0.48
3:K:154:ARG:HD2	3:K:176:LEU:HB3	1.94	0.48
3:O:114:VAL:N	3:O:295:VAL:O	2.41	0.48
1:B:73:LEU:HD21	1:B:380:LEU:HD21	1.94	0.48
1:B:629:LEU:O	1:B:633:ALA:N	2.46	0.48
1:F:1070:SER:OG	1:F:1071:GLU:N	2.46	0.48
1:I:708:THR:HG22	1:I:1038:HIS:HE1	1.79	0.48
1:B:142:LEU:HD21	1:B:157:ARG:HB3	1.95	0.48
1:C:549:PHE:HB3	1:C:571:ILE:HD11	1.95	0.48
1:D:285:LYS:HD3	1:D:379:ALA:HB2	1.95	0.48
1:D:1095:GLN:OE1	1:D:1097:ARG:NH2	2.47	0.48
1:F:658:ASN:ND2	1:I:680:GLY:O	2.47	0.48
1:I:84:PHE:HB2	1:I:1074:PHE:HB3	1.93	0.48
1:I:772:ALA:HA	2:U:55:ARG:HH21	1.78	0.48
1:I:1348:ASP:OD1	1:I:1348:ASP:N	2.45	0.48
3:K:116:LEU:HD21	3:K:143:LEU:HB2	1.95	0.48
1:B:184:MET:O	1:B:1073:TYR:OH	2.31	0.48
1:B:521:VAL:HG11	1:B:987:VAL:HG13	1.95	0.48
1:B:611:ILE:HD11	1:B:1018:ASN:HD21	1.79	0.48
1:B:1222:VAL:O	1:B:1224:ALA:N	2.46	0.48
1:C:135:LEU:HD21	1:C:165:LEU:HD13	1.96	0.48
1:I:228:CYS:HA	1:I:1368:PRO:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:832:PHE:HA	1:I:835:VAL:HB	1.95	0.48
1:I:1063:VAL:HB	1:I:1111:ALA:HB3	1.94	0.48
1:B:622:SER:OG	1:C:675:VAL:O	2.21	0.48
1:C:776:PHE:HA	1:C:903:GLU:HB2	1.96	0.48
1:F:846:GLU:HA	2:V:68:HIS:CE1	2.48	0.48
1:B:128:ALA:HA	1:B:1096:PRO:HA	1.95	0.48
1:C:78:ALA:O	1:C:1070:SER:OG	2.28	0.48
1:C:326:VAL:HB	1:C:329:LEU:HB2	1.95	0.48
1:E:981:ARG:HH22	1:F:803:ALA:H	1.61	0.48
1:F:1218:LYS:HB3	1:F:1221:ASP:HB3	1.96	0.48
1:B:544:HIS:CD2	1:B:546:ALA:H	2.31	0.48
1:C:724:HIS:CD2	1:C:726:MET:H	2.32	0.48
1:C:812:TYR:HA	1:C:816:LEU:HD13	1.95	0.48
1:F:753:ASP:OD1	1:F:911:SER:OG	2.25	0.48
1:F:857:PRO:HG3	1:F:885:VAL:HG22	1.96	0.48
3:K:297:VAL:HG22	3:K:314:VAL:HG22	1.96	0.48
1:D:963:LEU:HG	1:D:1007:VAL:HG22	1.94	0.48
1:I:766:ALA:HB2	1:I:782:ARG:HD3	1.96	0.48
1:I:1099:ASN:OD1	1:I:1099:ASN:N	2.47	0.48
2:V:71:ASN:HA	2:V:102:VAL:HB	1.96	0.48
1:B:390:VAL:HG22	1:I:106:ARG:HH21	1.79	0.48
1:B:421:GLY:HA3	1:I:420:ALA:HB2	1.95	0.48
1:B:438:ARG:HD3	1:B:1045:HIS:HB2	1.94	0.48
1:B:539:LEU:O	1:B:1248:GLN:NE2	2.43	0.48
1:D:1099:ASN:OD1	1:D:1099:ASN:N	2.47	0.48
1:E:854:PRO:HB3	1:E:860:ASP:HB3	1.95	0.48
1:E:1008:GLN:HE21	1:E:1012:GLU:HB2	1.79	0.48
1:F:281:THR:HG22	1:F:392:TYR:HE2	1.79	0.48
1:E:667:ASP:OD1	1:E:813:TYR:OH	2.32	0.47
1:I:192:ALA:HB1	1:I:1110:ALA:HB2	1.96	0.47
1:B:87:LEU:HD22	1:B:1097:ARG:HA	1.96	0.47
1:F:1106:TYR:OH	1:F:1290:GLU:O	2.32	0.47
1:B:87:LEU:HD22	1:B:1097:ARG:HE	1.79	0.47
1:D:632:ALA:HB1	1:D:832:PHE:HE1	1.79	0.47
1:E:301:ASP:N	1:E:363:VAL:O	2.42	0.47
1:E:754:CYS:HA	1:E:910:CYS:HA	1.95	0.47
1:E:1057:ARG:NH2	1:E:1319:GLU:OE2	2.47	0.47
1:I:225:ARG:NH1	1:I:1201:ARG:HH12	2.13	0.47
1:I:442:PHE:HE2	1:I:1122:MET:HB3	1.79	0.47
1:I:577:VAL:HG21	1:I:1001:SER:HA	1.95	0.47
1:I:746:ALA:HA	1:I:751:HIS:CG	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:894:LEU:HB2	2:U:61:LEU:HB3	1.95	0.47
2:V:18:ARG:NH2	2:V:63:ASP:OD2	2.36	0.47
1:C:1138:LEU:HB2	1:C:1144:ALA:HB2	1.94	0.47
1:D:548:ASP:OD1	1:D:576:ARG:NE	2.39	0.47
1:E:1017:GLU:O	1:E:1021:THR:OG1	2.24	0.47
1:F:919:ASN:HD21	1:F:924:ALA:HA	1.79	0.47
1:I:966:GLY:HA3	1:I:969:HIS:HB2	1.96	0.47
1:I:1078:LEU:HD12	1:I:1093:LEU:HD13	1.95	0.47
3:O:296:ARG:HB3	3:O:315:ILE:HG13	1.96	0.47
1:B:311:LEU:HD12	1:B:315:ASN:HB3	1.96	0.47
1:C:304:VAL:HG12	1:C:360:THR:HG22	1.95	0.47
1:C:526:MET:N	1:C:529:GLU:OE1	2.48	0.47
1:C:622:SER:OG	1:D:675:VAL:O	2.25	0.47
1:C:777:ASN:ND2	2:Q:47:GLN:OE1	2.47	0.47
1:D:646:ARG:HA	1:D:649:THR:HG22	1.97	0.47
1:E:840:GLN:HE22	2:G:58:ALA:HB2	1.80	0.47
1:I:1198:TYR:OH	1:I:1204:ASN:O	2.31	0.47
1:B:1274:PHE:O	1:B:1278:THR:OG1	2.32	0.47
1:E:156:HIS:CE1	1:E:160:ARG:HE	2.33	0.47
1:E:653:THR:O	1:E:657:ASN:ND2	2.48	0.47
1:E:1033:PRO:HA	1:E:1036:LEU:HB2	1.96	0.47
1:F:836:TYR:O	1:F:840:GLN:NE2	2.46	0.47
1:F:889:PRO:HA	1:F:892:LEU:HB3	1.97	0.47
1:B:1344:ARG:NH2	1:I:1353:ALA:O	2.43	0.47
1:D:526:MET:O	1:D:530:GLN:N	2.45	0.47
1:D:909:LEU:HD11	1:D:929:PHE:HB3	1.97	0.47
1:E:329:LEU:O	1:E:333:GLY:N	2.44	0.47
1:F:184:MET:HA	1:F:187:VAL:HG22	1.96	0.47
1:F:280:THR:HG23	1:F:1063:VAL:HG22	1.96	0.47
1:F:372:ASP:N	1:F:372:ASP:OD1	2.44	0.47
1:F:674:ILE:HG23	1:F:678:LEU:HD12	1.97	0.47
1:F:699:ALA:HA	1:F:702:GLN:HE21	1.79	0.47
1:F:828:ALA:HB1	1:F:955:PHE:HB3	1.95	0.47
1:I:277:VAL:HB	1:I:1066:SER:HB3	1.96	0.47
1:I:671:VAL:HG13	1:I:690:TYR:HD1	1.79	0.47
1:I:1077:GLN:H	1:I:1096:PRO:HD2	1.80	0.47
3:K:214:THR:HG21	3:O:227:LEU:HD11	1.96	0.47
1:B:642:CYS:HA	1:B:645:ALA:HB2	1.96	0.47
1:E:450:LEU:HD13	1:E:1124:ASN:HB2	1.96	0.47
1:E:579:ASN:N	1:E:579:ASN:OD1	2.47	0.47
1:I:639:HIS:HA	2:U:79:PHE:HE2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:770:ASN:H	1:I:773:THR:HB	1.79	0.47
1:I:854:PRO:HB3	1:I:863:HIS:HA	1.97	0.47
1:I:1289:LEU:HA	1:I:1292:LEU:HD12	1.95	0.47
6:S:131:LEU:HD21	6:S:251:LEU:HD12	1.96	0.47
6:S:134:LEU:HB3	6:S:183:GLY:HA2	1.97	0.47
1:F:305:THR:OG1	1:F:306:TYR:N	2.48	0.47
1:F:525:GLN:NE2	1:F:535:ASP:O	2.48	0.47
1:F:826:CYS:HA	1:F:964:PHE:HB3	1.97	0.47
1:F:1344:ARG:HG2	1:F:1347:ARG:HH12	1.79	0.47
1:I:83:LYS:HE3	1:I:85:PRO:HD3	1.97	0.47
2:U:13:THR:OG1	2:U:16:ASN:ND2	2.48	0.47
1:C:1055:GLN:HB3	1:C:1310:GLN:HE22	1.80	0.47
1:E:778:ARG:O	1:E:904:ARG:NE	2.48	0.47
1:I:248:LEU:HD12	1:I:251:LEU:HD13	1.96	0.47
1:I:267:ALA:HA	1:I:273:PRO:HA	1.97	0.47
1:B:452:LEU:HD21	1:B:1124:ASN:HA	1.97	0.46
1:D:606:MET:HE3	1:D:611:ILE:HG12	1.97	0.46
1:I:248:LEU:HA	1:I:251:LEU:HD13	1.97	0.46
1:I:1257:TYR:HB2	1:I:1277:PHE:HD2	1.80	0.46
1:B:577:VAL:HG12	1:B:578:VAL:HG13	1.97	0.46
1:B:884:VAL:HG12	1:B:886:VAL:HG23	1.98	0.46
1:F:1279:ALA:O	1:F:1283:THR:OG1	2.25	0.46
1:I:1066:SER:HA	1:I:1108:ALA:HA	1.97	0.46
1:I:1270:LEU:HB3	1:I:1310:GLN:HB3	1.97	0.46
6:S:273:ALA:HB2	6:S:457:TRP:HE1	1.79	0.46
1:C:929:PHE:N	1:C:999:PHE:O	2.48	0.46
1:F:70:PHE:O	1:F:76:SER:OG	2.33	0.46
1:F:742:LEU:HA	1:F:745:HIS:HB3	1.98	0.46
2:G:81:GLY:N	2:G:91:SER:OG	2.42	0.46
1:I:1125:LEU:HD11	1:I:1156:ARG:HB3	1.96	0.46
1:F:677:TYR:HD1	2:V:95:LYS:HG2	1.79	0.46
2:G:4:PRO:HB3	2:G:16:ASN:HB3	1.97	0.46
1:I:75:LEU:HD12	1:I:78:ALA:HB3	1.97	0.46
3:K:48:HIS:CD2	3:K:138:ARG:HD3	2.51	0.46
3:K:155:LEU:O	3:K:159:GLY:N	2.48	0.46
1:B:578:VAL:HG23	1:B:580:GLY:H	1.81	0.46
1:C:425:PRO:HG3	1:C:431:GLU:HB2	1.98	0.46
1:C:467:MET:O	1:C:922:SER:OG	2.33	0.46
1:F:668:TYR:HB2	1:F:812:TYR:CG	2.51	0.46
1:E:520:TRP:HH2	1:E:988:PRO:HD2	1.80	0.46
1:E:578:VAL:N	1:E:581:ASN:OD1	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:766:ALA:N	1:E:783:LEU:O	2.39	0.46
1:I:626:VAL:HG13	1:I:878:MET:HG3	1.97	0.46
1:I:675:VAL:HG21	1:I:694:VAL:HG21	1.96	0.46
1:B:822:ARG:NH2	1:B:1017:GLU:OE2	2.47	0.46
1:E:451:ARG:NH2	1:E:453:SER:OG	2.49	0.46
1:F:606:MET:HB2	1:F:1018:ASN:HD21	1.80	0.46
1:I:248:LEU:HD23	1:I:293:LEU:HD21	1.97	0.46
1:I:873:ASN:ND2	2:U:30:ASN:OD1	2.38	0.46
3:O:155:LEU:HD22	3:O:158:ARG:HH11	1.80	0.46
1:C:764:VAL:HG13	1:C:782:ARG:HE	1.81	0.46
1:D:335:HIS:O	1:D:339:MET:N	2.48	0.46
1:D:697:VAL:HG12	1:D:808:HIS:CD2	2.51	0.46
1:F:866:HIS:CD2	1:F:868:ALA:H	2.34	0.46
1:F:870:LEU:HD22	1:F:877:ARG:HA	1.98	0.46
3:K:285:LEU:HD23	3:K:288:ILE:HD12	1.97	0.46
6:S:307:ALA:HB1	6:S:429:PRO:HA	1.96	0.46
1:B:644:LEU:HD23	1:B:647:LEU:HD23	1.98	0.46
1:C:873:ASN:ND2	2:Q:30:ASN:OD1	2.43	0.46
1:E:422:ASP:OD1	1:E:422:ASP:N	2.48	0.46
1:E:494:PRO:HG3	1:E:993:ALA:HB1	1.98	0.46
1:E:844:VAL:HG11	1:E:892:LEU:HD12	1.96	0.46
1:E:950:GLN:HB3	1:E:953:GLU:HB2	1.97	0.46
1:E:968:ASP:O	1:E:972:ASN:ND2	2.38	0.46
1:F:274:VAL:HG11	1:F:376:PHE:CD2	2.51	0.46
1:F:724:HIS:CD2	1:F:726:MET:H	2.33	0.46
1:F:1237:PRO:HB3	1:I:1156:ARG:HH12	1.81	0.46
1:I:220:VAL:HG11	1:I:1214:TYR:HE1	1.80	0.46
1:I:1206:ARG:HD3	1:I:1210:ALA:HB2	1.97	0.46
3:K:109:CYS:HB2	3:K:304:ALA:HB1	1.97	0.46
3:K:272:TYR:HD2	3:O:161:ARG:HE	1.64	0.46
1:B:423:LEU:H	1:I:418:ALA:HA	1.81	0.46
1:B:717:GLN:HE22	1:B:750:ARG:HD3	1.81	0.46
1:D:417:ALA:HB2	1:D:1358:PHE:HE1	1.81	0.46
1:F:247:TRP:HE3	1:F:248:LEU:HD12	1.80	0.46
1:I:487:TYR:OH	1:I:990:VAL:N	2.49	0.46
2:V:21:GLY:O	2:V:25:LEU:N	2.49	0.46
1:B:1156:ARG:HD2	1:B:1174:ARG:HH22	1.81	0.45
1:B:1174:ARG:HD2	1:B:1177:MET:HB3	1.98	0.45
1:D:87:LEU:HD22	1:D:1096:PRO:HB2	1.98	0.45
1:E:584:LEU:HG	1:E:1005:PRO:HB3	1.99	0.45
3:K:155:LEU:HD11	3:K:188:LEU:HD11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:ASP:O	1:B:11:TYR:N	2.37	0.45
1:B:637:ASN:HA	1:B:787:THR:HA	1.98	0.45
1:C:1369:LEU:HA	1:C:1372:LEU:HD12	1.97	0.45
1:D:422:ASP:N	1:D:422:ASP:OD1	2.48	0.45
1:D:1073:TYR:HD1	1:D:1099:ASN:HB3	1.82	0.45
1:E:775:ASP:HB3	1:E:778:ARG:HD2	1.99	0.45
1:E:788:GLN:HB3	1:E:800:HIS:CG	2.51	0.45
1:F:892:LEU:HD11	2:V:68:HIS:CG	2.51	0.45
1:F:1008:GLN:NE2	1:F:1012:GLU:OE1	2.41	0.45
1:F:1054:ARG:HH11	1:F:1123:GLY:HA3	1.81	0.45
1:I:199:LEU:HD21	1:I:250:ASP:HB3	1.97	0.45
1:I:620:ASP:OD2	1:I:655:TYR:OH	2.32	0.45
1:I:1054:ARG:HH12	1:I:1123:GLY:H	1.64	0.45
1:I:1182:ASP:O	1:I:1310:GLN:NE2	2.49	0.45
1:B:155:LEU:HB2	1:I:340:GLN:HE22	1.81	0.45
1:E:532:MET:HA	1:E:1240:ALA:H	1.81	0.45
1:E:656:TRP:CD2	1:E:686:CYS:HB3	2.51	0.45
1:E:834:ARG:HD2	1:E:954:TYR:HA	1.98	0.45
6:S:188:ASN:ND2	6:S:215:TYR:OH	2.38	0.45
1:B:1116:ARG:HH21	1:I:203:ARG:HD3	1.80	0.45
1:C:539:LEU:O	1:C:1248:GLN:NE2	2.48	0.45
1:D:832:PHE:HA	1:D:835:VAL:HB	1.97	0.45
1:E:638:GLU:OE2	1:E:677:TYR:OH	2.23	0.45
1:I:280:THR:HG22	1:I:1063:VAL:HG13	1.98	0.45
1:B:804:ASP:O	1:B:808:HIS:ND1	2.43	0.45
1:C:1215:ALA:O	1:C:1287:ARG:NH1	2.35	0.45
1:D:665:VAL:O	1:D:812:TYR:OH	2.28	0.45
1:E:213:ARG:NH1	1:F:1175:ALA:O	2.50	0.45
1:F:195:LEU:HB2	1:F:1109:VAL:HB	1.99	0.45
1:F:1208:ARG:NE	1:F:1225:LEU:O	2.47	0.45
1:I:576:ARG:NH1	1:I:581:ASN:O	2.49	0.45
1:I:741:GLY:O	1:I:745:HIS:N	2.39	0.45
1:B:166:ALA:HA	1:B:169:VAL:HG12	1.99	0.45
1:D:1127:GLN:HB2	1:D:1186:GLU:HG2	1.99	0.45
1:E:647:LEU:O	1:E:651:CYS:N	2.47	0.45
1:B:834:ARG:NH1	2:Q:86:GLU:O	2.47	0.45
1:C:580:GLY:HA2	1:C:592:ARG:HH12	1.81	0.45
1:E:777:ASN:ND2	2:G:47:GLN:OE1	2.49	0.45
1:F:176:PHE:O	1:F:180:THR:N	2.49	0.45
1:F:753:ASP:OD1	1:F:753:ASP:N	2.50	0.45
1:F:998:TYR:O	1:F:1003:ARG:NH2	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:61:LEU:O	2:G:65:GLY:N	2.50	0.45
1:I:1355:GLU:HB3	1:I:1356:THR:HG22	1.99	0.45
3:O:52:VAL:HA	3:O:58:PRO:HD3	1.98	0.45
1:C:392:TYR:CZ	1:C:394:LEU:HB2	2.51	0.45
1:D:764:VAL:HG13	1:D:782:ARG:HE	1.81	0.45
1:E:502:GLN:HE22	1:E:970:VAL:HG22	1.82	0.45
1:E:1304:THR:HG21	1:E:1314:PRO:HD2	1.98	0.45
1:F:243:ALA:O	1:F:247:TRP:N	2.50	0.45
1:F:644:LEU:HD23	1:F:647:LEU:HD23	1.98	0.45
1:F:1184:VAL:HG23	1:F:1310:GLN:HE21	1.82	0.45
1:I:184:MET:O	1:I:188:LEU:N	2.45	0.45
1:I:805:TRP:CE2	1:I:809:HIS:HE1	2.35	0.45
3:K:88:VAL:HG11	3:K:295:VAL:HG22	1.98	0.45
6:S:271:GLN:H	6:S:271:GLN:HG3	1.58	0.45
1:B:647:LEU:HA	1:B:890:ALA:HB1	1.98	0.45
1:B:1131:LEU:HD12	1:B:1131:LEU:HA	1.82	0.45
1:C:142:LEU:HD21	1:C:157:ARG:HG3	1.98	0.45
1:D:778:ARG:NH2	1:D:780:ASP:OD2	2.42	0.45
1:D:873:ASN:OD1	2:G:92:PHE:N	2.48	0.45
1:F:590:ALA:O	1:F:594:ALA:N	2.49	0.45
1:F:633:ALA:O	1:F:635:HIS:ND1	2.39	0.45
1:F:751:HIS:NE2	1:F:754:CYS:HB2	2.32	0.45
1:F:1200:ARG:HG2	1:F:1363:ILE:HG23	1.98	0.45
1:I:422:ASP:N	1:I:422:ASP:OD1	2.50	0.45
1:C:642:CYS:HA	1:C:645:ALA:HB2	1.98	0.44
1:D:783:LEU:HD21	1:D:908:LEU:HD13	1.99	0.44
1:F:1157:LEU:HD21	1:F:1309:VAL:HG11	1.99	0.44
3:O:29:GLY:O	3:O:101:ARG:N	2.40	0.44
6:S:164:LEU:O	6:S:168:SER:N	2.43	0.44
2:V:25:LEU:HD21	2:V:57:GLN:HG2	1.98	0.44
1:B:287:ARG:HH12	1:B:1114:THR:HG21	1.82	0.44
1:D:404:LEU:HB2	1:D:1052:VAL:HB	1.99	0.44
1:D:1004:GLN:HE21	1:D:1008:GLN:HB2	1.82	0.44
1:E:804:ASP:HA	1:E:807:VAL:HB	1.99	0.44
1:F:200:PRO:HA	1:F:203:ARG:HG2	1.99	0.44
1:F:667:ASP:OD2	1:F:669:SER:OG	2.31	0.44
1:I:336:LEU:HA	1:I:339:MET:HG3	1.99	0.44
1:I:1183:ALA:HA	1:I:1310:GLN:HE22	1.82	0.44
3:K:66:ALA:HA	3:K:69:ARG:HB3	2.00	0.44
3:O:161:ARG:HH12	3:O:174:PRO:HG2	1.81	0.44
1:B:501:MET:HA	1:B:504:ARG:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:THR:OG1	1:C:282:ALA:N	2.51	0.44
1:D:238:GLY:HA2	1:D:244:ILE:HD11	2.00	0.44
1:E:156:HIS:HE1	1:E:160:ARG:HE	1.65	0.44
1:E:904:ARG:NH1	1:E:905:THR:O	2.50	0.44
1:F:228:CYS:HA	1:F:1368:PRO:HG3	1.99	0.44
1:I:131:ALA:HB3	1:I:1092:THR:HG23	1.97	0.44
1:D:280:THR:O	1:D:392:TYR:OH	2.25	0.44
1:D:748:LEU:HD13	1:D:750:ARG:HB2	1.99	0.44
1:D:770:ASN:H	1:D:773:THR:HB	1.83	0.44
1:D:1125:LEU:HD11	1:D:1157:LEU:HG	1.99	0.44
1:E:1078:LEU:HD23	1:E:1095:GLN:HB2	2.00	0.44
1:F:269:THR:HG22	1:F:362:ARG:HH12	1.83	0.44
1:F:893:THR:HA	1:F:895:GLN:HG2	2.00	0.44
1:I:545:PRO:HG3	1:I:1245:TRP:CD2	2.52	0.44
1:B:472:ALA:HB2	1:B:1255:LEU:HD11	2.00	0.44
1:B:549:PHE:HB3	1:B:571:ILE:HD11	1.99	0.44
1:C:697:VAL:HG12	1:C:808:HIS:HD2	1.82	0.44
1:D:1208:ARG:HB2	1:D:1241:THR:HG22	1.98	0.44
1:E:99:VAL:HG23	1:E:118:ASN:HD22	1.83	0.44
1:F:1059:VAL:HG11	1:F:1116:ARG:HD2	2.00	0.44
1:I:210:LEU:HD23	1:I:210:LEU:HA	1.83	0.44
1:I:891:MET:HA	1:I:894:LEU:HD21	1.98	0.44
1:B:750:ARG:HA	1:B:913:ALA:HB3	1.99	0.44
1:B:1034:VAL:HG22	1:B:1147:LEU:HD13	1.99	0.44
1:C:904:ARG:NH1	1:C:906:THR:OG1	2.50	0.44
1:D:1259:GLY:HA3	1:D:1274:PHE:HE1	1.83	0.44
1:F:203:ARG:HB2	1:I:1116:ARG:HH12	1.83	0.44
1:I:576:ARG:HA	1:I:1003:ARG:HH12	1.82	0.44
1:B:280:THR:HG22	1:B:1063:VAL:HG12	1.99	0.44
1:C:320:LEU:HD12	1:C:321:VAL:HG23	2.00	0.44
1:C:440:LEU:HB3	1:C:452:LEU:HB2	2.00	0.44
1:C:634:ILE:HD13	1:C:641:PHE:HD1	1.83	0.44
1:D:577:VAL:HG12	1:D:578:VAL:HG13	1.99	0.44
1:E:701:ALA:O	1:E:727:ARG:NH2	2.50	0.44
1:F:128:ALA:O	1:F:1094:THR:OG1	2.35	0.44
1:F:319:ALA:O	1:F:323:GLY:N	2.50	0.44
1:F:436:PRO:HA	1:F:437:PRO:HD3	1.77	0.44
1:I:946:ASP:OD1	1:I:946:ASP:N	2.50	0.44
1:I:1054:ARG:NH2	1:I:1122:MET:HA	2.33	0.44
1:C:429:HIS:HA	1:C:430:PRO:HD3	1.73	0.44
1:E:804:ASP:HB3	1:E:808:HIS:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:724:HIS:HD2	1:F:726:MET:H	1.64	0.44
1:F:1033:PRO:HB2	1:F:1147:LEU:HD21	1.99	0.44
1:I:751:HIS:NE2	1:I:754:CYS:HB2	2.33	0.44
6:S:111:THR:HG23	6:S:266:VAL:HG23	1.99	0.44
1:B:418:ALA:HA	1:C:423:LEU:H	1.82	0.44
1:D:1206:ARG:NH2	1:D:1208:ARG:O	2.50	0.44
1:E:718:ALA:H	1:E:721:GLU:HB2	1.82	0.44
1:E:1208:ARG:HB2	1:E:1241:THR:HG22	2.00	0.44
1:F:397:ALA:HB3	1:F:1321:VAL:HG13	1.99	0.44
1:F:608:PRO:HA	1:F:611:ILE:HD12	2.00	0.44
1:I:82:THR:OG1	1:I:83:LYS:N	2.51	0.44
1:I:738:ASP:OD1	1:I:738:ASP:N	2.47	0.44
1:I:875:VAL:O	1:I:879:PHE:N	2.48	0.44
1:I:1034:VAL:HG22	1:I:1147:LEU:HD22	2.00	0.44
1:C:883:ARG:HG3	1:D:680:GLY:HA3	2.00	0.43
1:E:582:LEU:HD11	1:E:587:CYS:HB2	2.00	0.43
1:F:1029:PHE:HB3	1:F:1039:GLN:NE2	2.33	0.43
6:S:117:THR:HG23	6:S:261:ALA:HB2	2.00	0.43
1:D:197:LEU:HA	1:D:223:LEU:HD11	2.01	0.43
1:I:1004:GLN:NE2	1:I:1008:GLN:OE1	2.51	0.43
1:B:645:ALA:HB1	1:B:678:LEU:HD21	1.99	0.43
1:C:876:LYS:HA	1:C:879:PHE:HD2	1.82	0.43
1:C:1131:LEU:HD23	1:C:1159:PRO:HG3	2.00	0.43
1:C:1168:CYS:HB2	1:C:1268:PRO:HD3	2.00	0.43
1:D:629:LEU:HG	1:D:835:VAL:HG13	2.00	0.43
1:D:1369:LEU:HA	1:D:1372:LEU:HD12	2.00	0.43
1:E:752:ARG:O	1:E:911:SER:OG	2.30	0.43
1:F:904:ARG:NH1	1:F:906:THR:OG1	2.51	0.43
1:F:1198:TYR:CZ	1:F:1203:CYS:HB2	2.53	0.43
1:I:1195:ASP:OD1	1:I:1195:ASP:N	2.46	0.43
1:B:56:ALA:HA	1:I:325:ALA:HB3	2.01	0.43
1:B:668:TYR:HB2	1:B:812:TYR:CG	2.54	0.43
1:B:765:TYR:HE1	1:B:783:LEU:HD13	1.83	0.43
1:B:967:ALA:O	1:B:971:ALA:N	2.48	0.43
1:B:1344:ARG:CZ	1:I:1355:GLU:HB2	2.48	0.43
1:C:492:ALA:H	1:C:992:PRO:HB2	1.82	0.43
1:C:1323:ASP:OD1	1:C:1323:ASP:N	2.51	0.43
1:D:233:PHE:HZ	1:D:243:ALA:HB1	1.84	0.43
1:D:950:GLN:HB3	1:D:953:GLU:HG3	2.01	0.43
1:E:272:ARG:HH11	1:E:374:LEU:HD12	1.83	0.43
1:E:392:TYR:HA	1:E:393:PRO:HD3	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1032:SER:OG	1:F:1035:ALA:N	2.43	0.43
1:F:1131:LEU:HD23	1:F:1159:PRO:HG3	2.01	0.43
1:F:1135:ALA:HA	1:F:1263:LEU:HD22	1.98	0.43
1:I:1054:ARG:HH22	1:I:1123:GLY:H	1.66	0.43
3:K:228:LEU:HG	3:K:238:ASN:HA	2.00	0.43
2:U:33:GLN:HE21	2:U:35:ILE:HD13	1.83	0.43
1:D:219:LEU:O	1:D:223:LEU:N	2.50	0.43
1:D:305:THR:OG1	1:D:359:GLN:OE1	2.34	0.43
1:D:423:LEU:HD12	1:D:1357:HIS:NE2	2.34	0.43
1:D:615:ARG:NH1	1:D:1017:GLU:OE2	2.51	0.43
1:D:806:THR:HA	1:D:809:HIS:HB2	2.00	0.43
1:F:857:PRO:HD3	1:F:885:VAL:HG13	2.00	0.43
1:I:733:PRO:HA	1:I:814:TYR:HE2	1.84	0.43
1:I:1209:ALA:HB2	1:I:1235:ALA:HB2	2.01	0.43
1:B:886:VAL:HG13	1:B:890:ALA:HB3	2.00	0.43
1:D:830:VAL:HG22	1:D:955:PHE:HD1	1.84	0.43
1:D:1048:PHE:HA	1:D:1192:VAL:HG13	1.99	0.43
1:E:420:ALA:HB2	1:F:424:VAL:HG21	1.99	0.43
1:E:696:HIS:HE1	1:E:1021:THR:HG21	1.84	0.43
1:E:751:HIS:CE1	1:E:754:CYS:HB2	2.53	0.43
1:F:440:LEU:HA	1:F:440:LEU:HD12	1.86	0.43
1:F:1125:LEU:HD12	1:F:1126:PRO:HD2	1.99	0.43
3:O:50:SER:O	3:O:70:ARG:NH2	2.50	0.43
1:C:629:LEU:HB3	1:C:839:LEU:HD21	2.00	0.43
1:D:1369:LEU:HD13	1:D:1372:LEU:HD12	1.99	0.43
1:E:99:VAL:O	1:E:118:ASN:ND2	2.46	0.43
1:E:774:ALA:HA	1:E:903:GLU:HB3	2.01	0.43
1:I:639:HIS:HA	2:U:79:PHE:CE2	2.53	0.43
3:K:217:THR:HA	3:K:220:ILE:HG22	2.01	0.43
1:B:1339:ASP:HB2	1:B:1342:LEU:HG	2.01	0.43
1:C:83:LYS:HE2	1:C:1075:LEU:HD22	1.99	0.43
1:C:402:PHE:HB2	1:C:1054:ARG:HG2	2.01	0.43
1:E:816:LEU:HD23	1:E:820:PHE:HE2	1.83	0.43
2:G:76:GLN:OE1	2:G:98:TYR:OH	2.25	0.43
1:I:436:PRO:HA	1:I:437:PRO:HD3	1.80	0.43
1:I:611:ILE:H	1:I:611:ILE:HG13	1.65	0.43
1:I:637:ASN:HA	1:I:787:THR:HA	2.00	0.43
1:I:1246:ALA:HA	1:I:1253:GLY:HA3	2.00	0.43
1:B:457:ALA:HA	1:B:1187:PHE:CE2	2.54	0.43
1:B:1154:GLY:H	1:I:534:PRO:HB3	1.83	0.43
1:E:771:VAL:HG13	1:E:898:ALA:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:579:ASN:OD1	1:F:579:ASN:N	2.52	0.43
1:F:920:THR:N	1:F:923:THR:OG1	2.39	0.43
1:F:933:LEU:HD11	1:F:958:LEU:HD23	2.00	0.43
1:F:1373:SER:OG	1:F:1374:LEU:N	2.52	0.43
6:S:318:GLN:OE1	6:S:416:THR:N	2.51	0.43
1:B:97:PHE:HD1	1:B:97:PHE:HA	1.72	0.43
1:B:629:LEU:HG	1:B:835:VAL:HG13	2.01	0.43
1:B:929:PHE:N	1:B:999:PHE:O	2.48	0.43
1:D:804:ASP:O	1:D:808:HIS:ND1	2.42	0.43
1:I:157:ARG:HA	1:I:160:ARG:HE	1.84	0.43
2:T:17:VAL:HB	2:T:56:GLY:HA3	2.01	0.43
1:B:13:TYR:O	1:B:17:MET:HG2	2.18	0.42
1:B:629:LEU:HD23	1:B:839:LEU:HG	2.01	0.42
1:C:1072:ALA:HB3	1:C:1100:VAL:HB	2.01	0.42
1:E:37:ASP:OD1	1:E:37:ASP:N	2.51	0.42
1:E:876:LYS:HA	1:E:879:PHE:HB2	2.00	0.42
1:F:380:LEU:HD13	1:F:384:ILE:HD11	2.01	0.42
1:F:1357:HIS:O	1:F:1360:GLN:N	2.52	0.42
3:K:203:ARG:HH22	3:K:207:LEU:HD11	1.84	0.42
6:S:267:CYS:SG	6:S:268:SER:N	2.92	0.42
1:B:725:LEU:HA	1:B:1030:LYS:HE3	2.01	0.42
1:C:448:GLN:NE2	1:C:449:VAL:O	2.48	0.42
1:C:450:LEU:HD13	1:C:1124:ASN:HB2	2.01	0.42
1:D:863:HIS:CE1	1:D:865:LEU:HB2	2.54	0.42
1:E:441:PHE:HE1	1:E:451:ARG:HG3	1.84	0.42
1:F:77:VAL:HG22	1:F:266:HIS:CD2	2.54	0.42
1:F:485:ASN:O	1:F:487:TYR:N	2.48	0.42
3:K:272:TYR:HB2	3:O:161:ARG:HH21	1.83	0.42
1:B:137:THR:HA	1:B:140:ILE:HD12	2.01	0.42
1:B:708:THR:OG1	1:B:723:ASN:ND2	2.50	0.42
1:C:157:ARG:HD2	1:C:157:ARG:HA	1.84	0.42
1:C:433:ARG:O	1:C:1359:THR:OG1	2.34	0.42
1:D:543:LEU:HB2	1:D:549:PHE:CE2	2.55	0.42
1:E:471:ALA:O	1:E:475:GLY:N	2.53	0.42
1:E:500:ASP:OD1	1:E:500:ASP:N	2.51	0.42
1:E:1115:VAL:HG11	1:E:1374:LEU:HD11	2.01	0.42
1:F:142:LEU:HD23	1:F:158:GLN:HA	2.01	0.42
1:F:578:VAL:N	1:F:581:ASN:OD1	2.42	0.42
1:F:1100:VAL:HG13	1:F:1102:LEU:HB2	2.01	0.42
1:I:756:ILE:HB	1:I:908:LEU:HD12	2.00	0.42
1:I:789:ALA:HB1	2:U:79:PHE:CG	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:63:LEU:O	3:K:67:TYR:N	2.44	0.42
2:M:33:GLN:HG2	2:M:35:ILE:H	1.84	0.42
1:B:946:ASP:HB3	1:C:676:THR:HG22	2.01	0.42
1:E:627:PHE:HD1	1:E:630:LEU:HD12	1.84	0.42
1:E:1138:LEU:HD12	1:E:1144:ALA:HA	2.00	0.42
1:F:470:ASP:HB3	1:F:922:SER:HB3	2.00	0.42
1:I:669:SER:OG	1:I:809:HIS:NE2	2.36	0.42
2:V:45:GLY:O	2:V:49:ALA:N	2.52	0.42
1:B:751:HIS:CE1	1:B:754:CYS:HB2	2.54	0.42
1:E:880:HIS:NE2	2:V:98:TYR:HB3	2.33	0.42
1:E:1040:LEU:HD23	1:E:1040:LEU:HA	1.84	0.42
1:F:840:GLN:H	1:F:840:GLN:HG2	1.51	0.42
1:F:1123:GLY:HA2	1:F:1183:ALA:HB3	2.02	0.42
1:I:198:LEU:HD22	1:I:1109:VAL:HG21	2.01	0.42
1:I:668:TYR:HB3	1:I:809:HIS:CD2	2.54	0.42
1:I:983:LEU:HD12	1:I:987:VAL:HG11	2.01	0.42
1:B:815:VAL:HA	1:B:1024:LEU:HD22	2.01	0.42
1:C:714:LEU:HD13	1:C:719:GLN:HE22	1.85	0.42
1:D:804:ASP:HB3	1:D:808:HIS:CE1	2.54	0.42
1:E:68:VAL:HG21	1:E:384:ILE:HG22	2.02	0.42
1:E:656:TRP:HZ2	1:E:685:GLU:HG2	1.85	0.42
1:F:880:HIS:HE1	2:U:98:TYR:HB3	1.84	0.42
1:I:143:LEU:HD21	1:I:153:ILE:CG2	2.50	0.42
1:I:547:PHE:O	1:I:576:ARG:NE	2.53	0.42
1:I:595:ARG:HH22	1:I:1047:GLY:HA2	1.84	0.42
1:I:893:THR:OG1	1:I:894:LEU:N	2.52	0.42
3:K:17:SER:O	3:K:21:ALA:N	2.49	0.42
3:K:67:TYR:HE2	3:K:117:VAL:HA	1.83	0.42
6:S:235:VAL:HB	6:S:323:GLU:HB3	2.02	0.42
1:B:124:ILE:HB	1:B:1100:VAL:HG22	2.01	0.42
1:B:185:LEU:HD21	1:B:279:VAL:HG11	2.01	0.42
1:B:1054:ARG:HH11	1:B:1122:MET:HB3	1.83	0.42
1:C:367:LEU:HD23	1:C:376:PHE:HA	2.00	0.42
1:E:623:TYR:OH	1:E:663:ALA:O	2.25	0.42
1:F:282:ALA:CB	1:F:382:LYS:HE3	2.34	0.42
1:F:780:ASP:N	1:F:780:ASP:OD1	2.53	0.42
1:F:884:VAL:HG12	1:F:886:VAL:HG23	2.01	0.42
1:F:1057:ARG:HB3	1:F:1119:VAL:HB	2.01	0.42
1:I:530:GLN:HG3	1:I:536:ASN:ND2	2.34	0.42
1:I:769:CYS:HB3	1:I:786:ASN:HD22	1.85	0.42
1:B:544:HIS:CD2	1:B:547:PHE:HD2	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1082:ARG:HE	1:B:1082:ARG:HB3	1.49	0.42
1:C:622:SER:OG	1:D:676:THR:O	2.38	0.42
1:D:700:LEU:HD22	1:D:1025:MET:HG2	2.01	0.42
1:D:1206:ARG:HH12	1:D:1208:ARG:HD3	1.83	0.42
1:E:732:LEU:O	1:E:814:TYR:OH	2.30	0.42
1:E:1067:GLU:HB2	1:E:1107:THR:HG23	2.02	0.42
1:C:475:GLY:O	1:C:478:HIS:NE2	2.53	0.42
1:E:751:HIS:NE2	1:E:754:CYS:HB2	2.35	0.42
1:E:836:TYR:OH	1:E:902:ALA:N	2.51	0.42
1:F:367:LEU:HB3	1:F:374:LEU:HD11	2.02	0.42
1:F:417:ALA:HB2	1:F:1358:PHE:CE1	2.55	0.42
1:I:684:GLU:O	1:I:688:ALA:N	2.48	0.42
1:I:708:THR:HA	1:I:1038:HIS:CE1	2.55	0.42
2:T:89:ARG:HE	2:U:29:THR:HB	1.85	0.42
2:U:81:GLY:N	2:U:91:SER:OG	2.39	0.42
1:B:514:ALA:HB2	1:B:980:LEU:HD21	2.01	0.42
1:B:945:LEU:HD23	1:B:945:LEU:HA	1.83	0.42
1:B:950:GLN:HB2	2:Q:80:ALA:HB1	2.02	0.42
1:B:1057:ARG:HH22	1:B:1319:GLU:HB3	1.84	0.42
1:B:1201:ARG:O	1:B:1203:CYS:N	2.38	0.42
1:C:728:ASP:HA	1:C:729:PRO:HD3	1.88	0.42
1:C:962:ALA:HB3	1:C:1007:VAL:HG21	2.02	0.42
1:D:671:VAL:HG13	1:D:690:TYR:HD1	1.85	0.42
1:E:1289:LEU:HD13	1:E:1292:LEU:HB2	2.02	0.42
1:I:272:ARG:HA	1:I:273:PRO:HD3	1.92	0.42
1:I:1072:ALA:HB3	1:I:1100:VAL:H	1.84	0.42
1:B:156:HIS:NE2	1:I:340:GLN:HB2	2.34	0.41
1:B:750:ARG:HD3	1:B:750:ARG:HH11	1.73	0.41
1:C:917:GLY:HA3	1:C:1034:VAL:HG23	2.02	0.41
1:E:1118:PRO:HG3	1:E:1374:LEU:HD13	2.02	0.41
3:K:18:ARG:O	3:K:22:ALA:N	2.45	0.41
1:B:293:LEU:H	1:B:293:LEU:HG	1.48	0.41
1:B:530:GLN:HG3	1:B:536:ASN:HD21	1.84	0.41
1:C:83:LYS:HG2	1:C:1075:LEU:HB2	2.03	0.41
1:C:528:ALA:HA	1:C:531:PHE:HB2	2.03	0.41
1:C:604:HIS:O	1:C:1022:TYR:OH	2.36	0.41
1:E:272:ARG:NH1	1:E:374:LEU:HB2	2.35	0.41
1:E:1125:LEU:HD11	1:E:1157:LEU:HG	2.02	0.41
1:F:1075:LEU:HD13	1:F:1075:LEU:HA	1.92	0.41
2:U:22:THR:HG1	2:U:64:LEU:HD22	1.79	0.41
1:B:87:LEU:HB2	1:B:1097:ARG:HH21	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:HIS:HA	1:B:430:PRO:HD3	1.77	0.41
1:B:920:THR:N	1:B:923:THR:OG1	2.42	0.41
1:B:991:PRO:HG2	1:B:994:LEU:HD12	2.01	0.41
1:B:1054:ARG:NH1	1:B:1122:MET:HB3	2.36	0.41
1:D:657:ASN:HA	1:D:660:ARG:HH12	1.85	0.41
3:O:178:VAL:HG13	3:O:185:ARG:HG2	2.00	0.41
1:B:1221:ASP:O	1:B:1225:LEU:HB2	2.20	0.41
1:C:606:MET:HB2	1:C:611:ILE:HD11	2.02	0.41
1:C:1125:LEU:HD13	1:C:1156:ARG:HH11	1.85	0.41
1:D:278:LEU:HD23	1:D:278:LEU:HA	1.90	0.41
1:E:733:PRO:HG2	1:E:736:VAL:HG22	2.02	0.41
1:F:531:PHE:HE2	1:F:1194:THR:HG22	1.85	0.41
1:F:596:GLY:O	1:F:600:GLY:N	2.54	0.41
1:F:1244:PRO:O	1:F:1251:SER:OG	2.31	0.41
1:I:212:THR:O	1:I:215:ALA:N	2.36	0.41
1:I:606:MET:HG3	1:I:696:HIS:CG	2.56	0.41
1:B:638:GLU:OE1	1:B:801:ARG:NH2	2.53	0.41
1:B:873:ASN:HA	2:Q:92:PHE:CD2	2.56	0.41
1:B:1202:PRO:HB3	1:B:1332:TYR:HA	2.02	0.41
1:C:274:VAL:HG22	1:C:374:LEU:HD22	2.02	0.41
1:C:422:ASP:OD1	1:C:422:ASP:N	2.52	0.41
1:C:534:PRO:HB3	1:D:1154:GLY:HA3	2.02	0.41
1:C:770:ASN:H	1:C:773:THR:HB	1.85	0.41
1:D:470:ASP:OD1	1:D:470:ASP:N	2.51	0.41
1:D:918:ALA:O	1:D:923:THR:OG1	2.24	0.41
1:D:1056:ASP:HA	1:D:1120:THR:HG21	2.03	0.41
1:E:423:LEU:HD12	1:E:1357:HIS:CE1	2.55	0.41
1:E:770:ASN:H	1:E:773:THR:HB	1.84	0.41
1:E:1223:ILE:H	1:E:1223:ILE:HG13	1.63	0.41
1:F:231:SER:H	1:F:236:LYS:HZ2	1.68	0.41
1:F:826:CYS:HB2	1:F:966:GLY:H	1.85	0.41
1:F:946:ASP:N	1:F:946:ASP:OD1	2.53	0.41
1:F:951:ASN:ND2	1:F:972:ASN:O	2.54	0.41
1:I:872:ALA:H	2:T:76:GLN:HG2	1.85	0.41
1:I:1039:GLN:O	1:I:1042:THR:OG1	2.39	0.41
1:B:278:LEU:O	1:B:378:GLU:N	2.53	0.41
1:C:450:LEU:HD23	1:C:450:LEU:HA	1.90	0.41
1:C:624:PRO:HB3	1:C:882:GLY:HA3	2.01	0.41
1:E:490:TYR:OH	1:E:560:GLY:O	2.29	0.41
1:E:1008:GLN:HA	1:E:1011:ARG:HG2	2.03	0.41
1:I:143:LEU:H	1:I:143:LEU:HG	1.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:866:HIS:CD2	1:I:868:ALA:H	2.39	0.41
1:I:903:GLU:HG2	1:I:904:ARG:H	1.85	0.41
1:I:1084:GLU:HA	1:I:1089:VAL:HB	2.03	0.41
3:K:32:VAL:O	3:K:73:ALA:N	2.51	0.41
1:B:413:MET:O	1:C:433:ARG:NH1	2.45	0.41
1:E:404:LEU:HD23	1:E:440:LEU:HD23	2.03	0.41
1:F:1374:LEU:H	1:F:1374:LEU:HG	1.68	0.41
3:K:191:ASP:HA	3:K:195:LEU:HD13	2.02	0.41
1:B:526:MET:N	1:B:529:GLU:OE1	2.50	0.41
1:B:788:GLN:HG2	1:B:790:ARG:H	1.86	0.41
1:B:1083:HIS:HB2	1:B:1084:GLU:H	1.72	0.41
1:C:336:LEU:HD23	1:C:336:LEU:HA	1.90	0.41
1:C:441:PHE:HE1	1:C:451:ARG:HG3	1.85	0.41
1:D:436:PRO:HA	1:D:437:PRO:HD3	1.92	0.41
1:D:746:ALA:HA	1:D:751:HIS:CD2	2.56	0.41
1:E:185:LEU:HD12	1:E:185:LEU:HA	1.90	0.41
1:F:269:THR:HG22	1:F:300:ALA:HB2	2.01	0.41
1:I:142:LEU:HD13	1:I:142:LEU:HA	1.74	0.41
1:I:735:LEU:HD12	1:I:813:TYR:CZ	2.56	0.41
1:B:91:ASN:H	1:B:126:ARG:HH22	1.69	0.41
1:C:348:ARG:NE	1:D:170:GLN:OE1	2.54	0.41
1:C:519:ARG:HG3	1:C:538:ASN:ND2	2.36	0.41
1:C:520:TRP:HZ3	1:C:988:PRO:HD2	1.85	0.41
1:C:545:PRO:HG3	1:C:1245:TRP:CD2	2.56	0.41
1:D:104:ILE:HG12	1:E:178:ARG:HB3	2.03	0.41
1:E:91:ASN:O	1:E:126:ARG:NH2	2.54	0.41
1:E:197:LEU:HA	1:E:223:LEU:HD11	2.02	0.41
1:E:720:ALA:HB1	1:E:727:ARG:HG3	2.02	0.41
1:E:746:ALA:HA	1:E:751:HIS:CD2	2.56	0.41
1:E:826:CYS:HB2	1:E:966:GLY:H	1.86	0.41
1:E:960:VAL:HA	1:E:994:LEU:HD13	2.03	0.41
1:F:776:PHE:HD1	1:F:903:GLU:HA	1.85	0.41
1:I:942:PRO:HB3	1:I:969:HIS:CD2	2.56	0.41
1:I:1271:SER:HB3	1:I:1274:PHE:HB2	2.03	0.41
2:M:25:LEU:HD21	2:M:57:GLN:HG2	2.03	0.41
2:U:54:LEU:HD23	2:U:54:LEU:HA	1.94	0.41
1:B:280:THR:O	1:B:392:TYR:OH	2.34	0.41
1:B:656:TRP:CD2	1:B:686:CYS:HB3	2.56	0.41
1:B:714:LEU:HB2	1:B:722:LEU:HD11	2.02	0.41
1:B:1223:ILE:H	1:B:1223:ILE:HG13	1.50	0.41
1:D:608:PRO:HA	1:D:611:ILE:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1125:LEU:HD23	1:D:1184:VAL:HG22	2.03	0.41
1:E:639:HIS:HA	2:G:79:PHE:HE2	1.86	0.41
1:E:1204:ASN:HB3	1:E:1206:ARG:HG2	2.02	0.41
1:F:617:ALA:HB2	1:F:661:CYS:HB3	2.01	0.41
1:F:985:ARG:NH1	1:I:705:ASP:OD2	2.54	0.41
1:I:776:PHE:HD1	1:I:903:GLU:HA	1.85	0.41
3:K:90:LEU:O	3:K:316:ARG:NE	2.54	0.41
2:T:76:GLN:O	2:T:96:ARG:NH2	2.43	0.41
1:C:577:VAL:HG12	1:C:578:VAL:HG13	2.03	0.40
1:F:742:LEU:O	1:F:746:ALA:N	2.47	0.40
1:I:644:LEU:HG	1:I:893:THR:HG22	2.03	0.40
1:I:746:ALA:HA	1:I:751:HIS:CD2	2.56	0.40
3:O:58:PRO:HB2	3:O:63:LEU:HG	2.04	0.40
1:D:998:TYR:O	1:D:1003:ARG:NH2	2.49	0.40
1:E:473:VAL:HA	1:E:476:VAL:HG12	2.03	0.40
1:E:580:GLY:HA2	1:E:592:ARG:HH12	1.86	0.40
1:E:1249:ARG:HG2	1:E:1250:PHE:CD2	2.56	0.40
1:F:57:LEU:HD22	1:F:57:LEU:HA	1.95	0.40
1:F:818:PRO:HA	1:F:821:SER:HB3	2.02	0.40
1:F:1017:GLU:O	1:F:1021:THR:OG1	2.30	0.40
1:I:490:TYR:OH	1:I:560:GLY:O	2.35	0.40
1:I:734:PRO:HB3	1:I:960:VAL:HG21	2.02	0.40
1:I:1053:VAL:HG12	1:I:1272:PRO:HB2	2.03	0.40
3:O:32:VAL:HG13	3:O:46:VAL:HG13	2.03	0.40
3:O:177:ASN:OD1	3:O:188:LEU:N	2.37	0.40
1:B:207:ASN:OD1	1:B:208:GLY:N	2.53	0.40
1:B:700:LEU:HD11	1:B:1021:THR:HG22	2.03	0.40
1:B:751:HIS:NE2	1:B:754:CYS:HB2	2.36	0.40
1:E:194:PRO:HD2	1:E:197:LEU:HD12	2.02	0.40
1:E:681:ASP:N	1:E:681:ASP:OD1	2.54	0.40
1:I:847:ILE:HD12	1:I:847:ILE:HA	1.98	0.40
1:I:1268:PRO:HB2	1:I:1311:PHE:HD1	1.86	0.40
1:B:502:GLN:HE22	1:B:970:VAL:HG22	1.85	0.40
1:C:194:PRO:HG2	1:C:197:LEU:HB2	2.04	0.40
1:C:246:ALA:HA	1:C:249:VAL:HG12	2.04	0.40
1:C:707:PHE:HA	1:C:1042:THR:HG21	2.04	0.40
1:C:1061:GLU:OE2	1:C:1116:ARG:NH1	2.54	0.40
1:F:227:PHE:O	1:F:231:SER:OG	2.35	0.40
1:F:423:LEU:HD12	1:F:1357:HIS:CD2	2.56	0.40
1:I:399:ASP:OD2	1:I:1055:GLN:NE2	2.52	0.40
1:I:765:TYR:HA	1:I:782:ARG:HG3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:236:HIS:HA	6:S:323:GLU:HG2	2.03	0.40
1:B:188:LEU:HD12	1:B:188:LEU:HA	1.90	0.40
1:D:545:PRO:HG3	1:D:1245:TRP:CD2	2.57	0.40
1:D:693:LEU:HD21	1:D:812:TYR:HE1	1.87	0.40
1:E:97:PHE:HZ	1:E:1102:LEU:HD12	1.86	0.40
1:E:671:VAL:HG13	1:E:690:TYR:HD1	1.87	0.40
1:I:1229:HIS:HE1	1:I:1248:GLN:HA	1.86	0.40
3:O:73:ALA:HB1	3:O:85:ALA:HB1	2.02	0.40
2:T:83:ALA:HB2	2:T:91:SER:HB3	2.04	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	B	1356/1374 (99%)	1200 (88%)	150 (11%)	6 (0%)	34 72
1	C	1356/1374 (99%)	1223 (90%)	130 (10%)	3 (0%)	47 81
1	D	1356/1374 (99%)	1205 (89%)	146 (11%)	5 (0%)	34 72
1	E	1345/1374 (98%)	1193 (89%)	151 (11%)	1 (0%)	51 85
1	F	1347/1374 (98%)	1162 (86%)	183 (14%)	2 (0%)	51 85
1	I	1311/1374 (95%)	1114 (85%)	193 (15%)	4 (0%)	41 76
2	G	99/112 (88%)	91 (92%)	8 (8%)	0	100 100
2	M	99/112 (88%)	93 (94%)	6 (6%)	0	100 100
2	Q	99/112 (88%)	96 (97%)	3 (3%)	0	100 100
2	T	99/112 (88%)	92 (93%)	7 (7%)	0	100 100
2	U	99/112 (88%)	89 (90%)	10 (10%)	0	100 100
2	V	99/112 (88%)	90 (91%)	9 (9%)	0	100 100
3	K	291/318 (92%)	253 (87%)	38 (13%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	O	301/318 (95%)	274 (91%)	27 (9%)	0	100 100
6	S	267/466 (57%)	216 (81%)	50 (19%)	1 (0%)	34 72
7	k	539/702 (77%)	506 (94%)	32 (6%)	1 (0%)	47 81
8	l	92/585 (16%)	84 (91%)	8 (9%)	0	100 100
8	m	78/585 (13%)	72 (92%)	6 (8%)	0	100 100
9	n	45/3122 (1%)	44 (98%)	1 (2%)	0	100 100
9	o	45/3122 (1%)	45 (100%)	0	0	100 100
All	All	10323/18134 (57%)	9142 (89%)	1158 (11%)	23 (0%)	50 81

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1223	ILE
1	C	1223	ILE
1	D	1085	THR
1	D	1223	ILE
1	E	1223	ILE
1	I	206	ASP
1	C	1084	GLU
1	F	454	MET
6	S	120	CYS
1	B	1202	PRO
1	D	1107	THR
1	B	1203	CYS
1	F	1286	HIS
1	I	213	ARG
1	I	1013	SER
1	B	1201	ARG
1	B	1222	VAL
1	C	1202	PRO
1	D	920	THR
1	I	575	TRP
1	D	1222	VAL
7	k	17	PRO
1	B	1134	GLY

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	B	1014/1080 (94%)	1000 (99%)	14 (1%)	67 81
1	C	1018/1080 (94%)	1014 (100%)	4 (0%)	91 94
1	D	1020/1080 (94%)	1014 (99%)	6 (1%)	86 91
1	E	1018/1080 (94%)	1017 (100%)	1 (0%)	93 97
1	F	968/1080 (90%)	963 (100%)	5 (0%)	88 93
1	I	970/1080 (90%)	951 (98%)	19 (2%)	55 73
2	G	78/88 (89%)	78 (100%)	0	100 100
2	M	78/88 (89%)	78 (100%)	0	100 100
2	Q	78/88 (89%)	78 (100%)	0	100 100
2	T	78/88 (89%)	78 (100%)	0	100 100
2	U	78/88 (89%)	78 (100%)	0	100 100
2	V	78/88 (89%)	78 (100%)	0	100 100
3	K	195/264 (74%)	193 (99%)	2 (1%)	76 86
3	O	214/264 (81%)	214 (100%)	0	100 100
6	S	181/365 (50%)	181 (100%)	0	100 100
7	k	426/529 (80%)	419 (98%)	7 (2%)	62 79
8	l	78/451 (17%)	78 (100%)	0	100 100
8	m	64/451 (14%)	63 (98%)	1 (2%)	62 79
9	n	41/2370 (2%)	40 (98%)	1 (2%)	49 69
9	o	41/2370 (2%)	40 (98%)	1 (2%)	49 69
All	All	7716/14072 (55%)	7655 (99%)	61 (1%)	82 89

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	97	PHE
1	B	293	LEU
1	B	347	ASN

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Mol	Chain	Res	Type
1	B	519	ARG
1	B	1082	ARG
1	B	1084	GLU
1	B	1085	THR
1	B	1089	VAL
1	B	1127	GLN
1	B	1128	ASN
1	B	1133	ARG
1	B	1149	ASN
1	B	1173	ARG
1	B	1201	ARG
1	C	162	ILE
1	C	168	ASN
1	C	415	ARG
1	C	1107	THR
1	D	327	ARG
1	D	519	ARG
1	D	756	ILE
1	D	1107	THR
1	D	1133	ARG
1	D	1141	ASN
1	E	674	ILE
1	F	90	MET
1	F	519	ARG
1	F	732	LEU
1	F	919	ASN
1	F	1201	ARG
1	I	142	LEU
1	I	143	LEU
1	I	158	GLN
1	I	209	ARG
1	I	210	LEU
1	I	213	ARG
1	I	380	LEU
1	I	510	ARG
1	I	512	ARG
1	I	519	ARG
1	I	574	THR
1	I	732	LEU
1	I	894	LEU
1	I	900	ASN
1	I	904	ARG

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Mol	Chain	Res	Type
1	I	906	THR
1	I	1093	LEU
1	I	1204	ASN
1	I	1356	THR
3	K	227	LEU
3	K	295	VAL
7	k	13	LEU
7	k	103	ARG
7	k	259	GLU
7	k	261	LEU
7	k	265	GLN
7	k	266	ARG
7	k	414	ARG
8	m	82	ARG
9	n	3098	ARG
9	o	3098	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (120) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	63	ASN
1	B	168	ASN
1	B	347	ASN
1	B	536	ASN
1	B	544	HIS
1	B	717	GLN
1	B	724	HIS
1	B	866	HIS
1	B	1008	GLN
1	B	1018	ASN
1	B	1038	HIS
1	B	1083	HIS
1	B	1090	ASN
1	B	1124	ASN
1	B	1128	ASN
1	B	1149	ASN
1	B	1161	GLN
1	B	1170	GLN
1	B	1329	GLN
1	C	163	GLN
1	C	168	ASN
1	C	485	ASN

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Mol	Chain	Res	Type
1	C	544	HIS
1	C	657	ASN
1	C	745	HIS
1	C	751	HIS
1	C	777	ASN
1	C	866	HIS
1	C	1008	GLN
1	C	1018	ASN
1	C	1179	HIS
1	C	1204	ASN
1	C	1310	GLN
1	C	1329	GLN
1	D	118	ASN
1	D	315	ASN
1	D	530	GLN
1	D	544	HIS
1	D	657	ASN
1	D	696	HIS
1	D	717	GLN
1	D	1004	GLN
1	D	1008	GLN
1	D	1009	HIS
1	D	1018	ASN
1	D	1124	ASN
1	D	1141	ASN
1	E	156	HIS
1	E	164	GLN
1	E	410	ASN
1	E	463	HIS
1	E	544	HIS
1	E	657	ASN
1	E	696	HIS
1	E	723	ASN
1	E	777	ASN
1	E	1018	ASN
1	E	1124	ASN
1	E	1329	GLN
1	F	100	HIS
1	F	544	HIS
1	F	658	ASN
1	F	696	HIS
1	F	702	GLN

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Mol	Chain	Res	Type
1	F	717	GLN
1	F	723	ASN
1	F	770	ASN
1	F	880	HIS
1	F	919	ASN
1	F	1004	GLN
1	F	1018	ASN
1	F	1039	GLN
1	F	1062	ASN
1	F	1090	ASN
1	F	1286	HIS
1	F	1310	GLN
2	G	7	HIS
2	G	16	ASN
2	G	42	HIS
2	G	47	GLN
1	I	118	ASN
1	I	266	HIS
1	I	419	HIS
1	I	502	GLN
1	I	507	ASN
1	I	544	HIS
1	I	604	HIS
1	I	696	HIS
1	I	724	HIS
1	I	777	ASN
1	I	880	HIS
1	I	900	ASN
1	I	1004	GLN
1	I	1008	GLN
1	I	1018	ASN
1	I	1204	ASN
1	I	1264	ASN
1	I	1329	GLN
3	K	48	HIS
3	K	208	ASN
2	M	7	HIS
2	M	16	ASN
2	M	44	HIS
3	O	233	GLN
2	Q	7	HIS
2	Q	16	ASN

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Mol	Chain	Res	Type
2	Q	47	GLN
6	S	123	ASN
6	S	188	ASN
6	S	210	HIS
2	T	16	ASN
2	U	16	ASN
2	U	33	GLN
2	U	68	HIS
7	k	61	GLN
7	k	506	GLN
7	k	533	ASN
7	k	619	GLN
8	l	93	HIS
8	m	68	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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

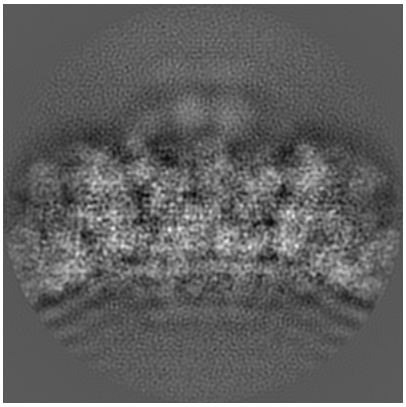
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30123. These allow visual inspection of the internal detail of the map and identification of artifacts.

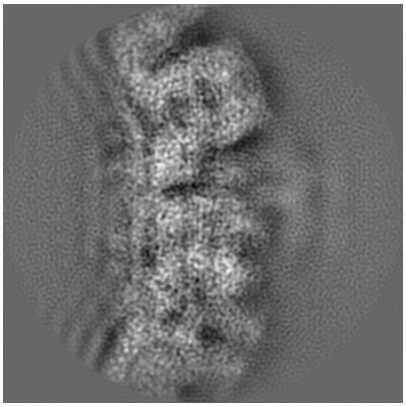
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

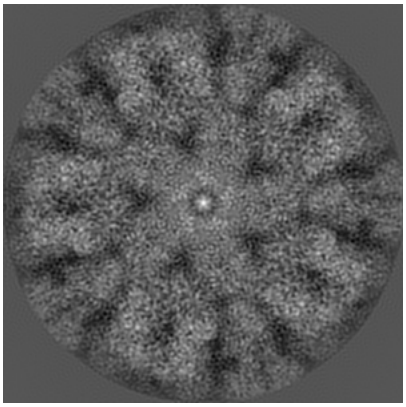
6.1.1 Primary map



X



Y

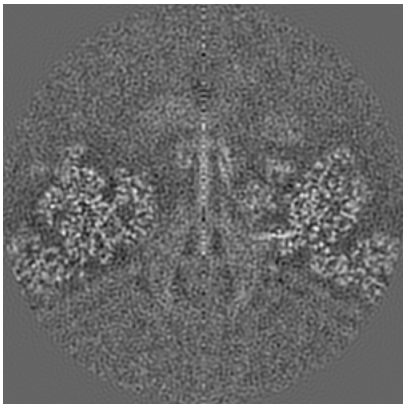


Z

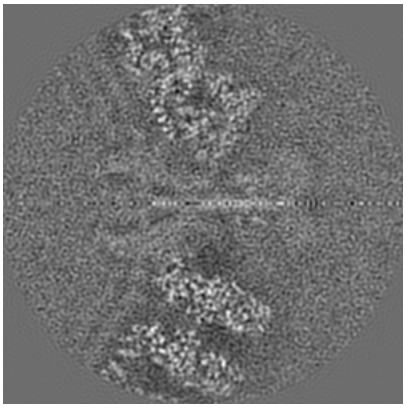
The images above show the map projected in three orthogonal directions.

6.2 Central slices

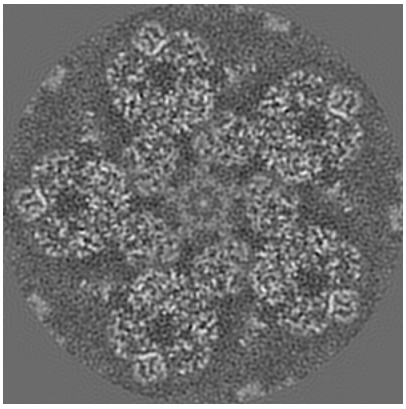
6.2.1 Primary map



X Index: 175



Y Index: 175

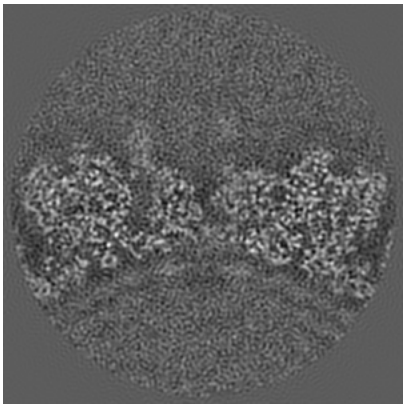


Z Index: 175

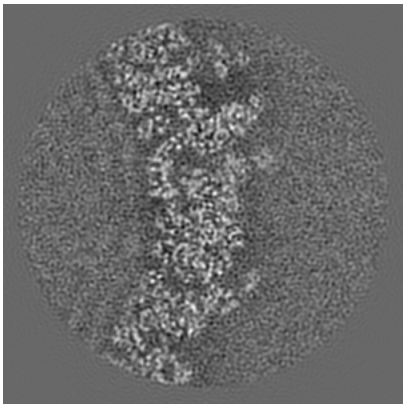
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

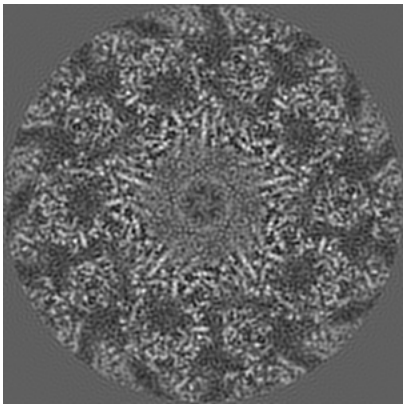
6.3.1 Primary map



X Index: 123



Y Index: 103

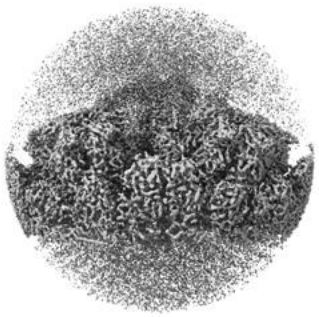


Z Index: 147

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

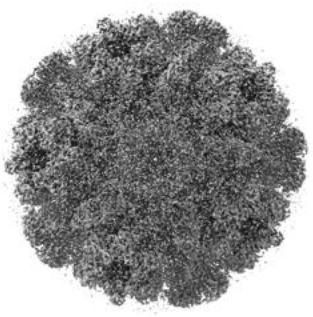
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

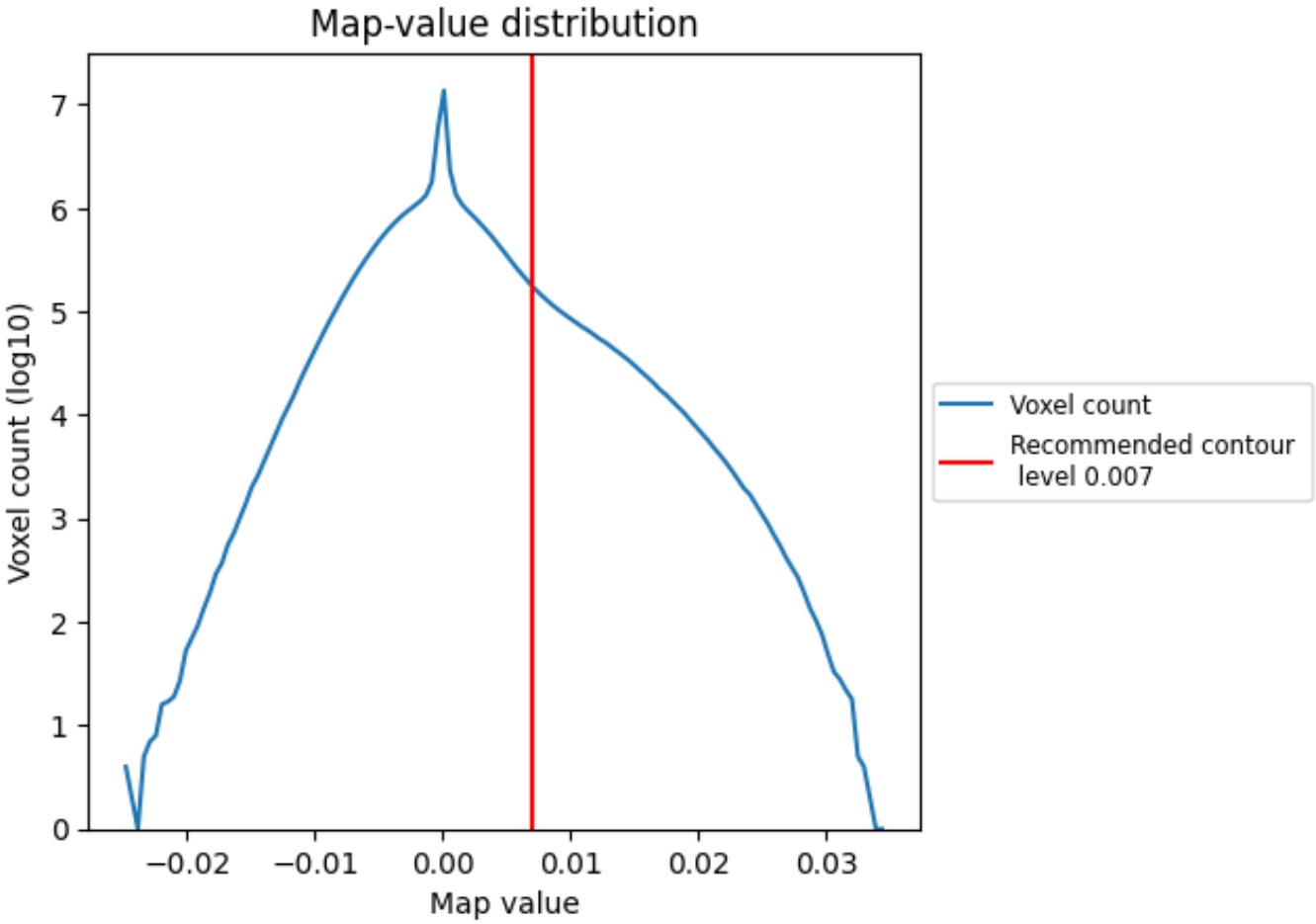
6.5 Mask visualisation (i)

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

7 Map analysis

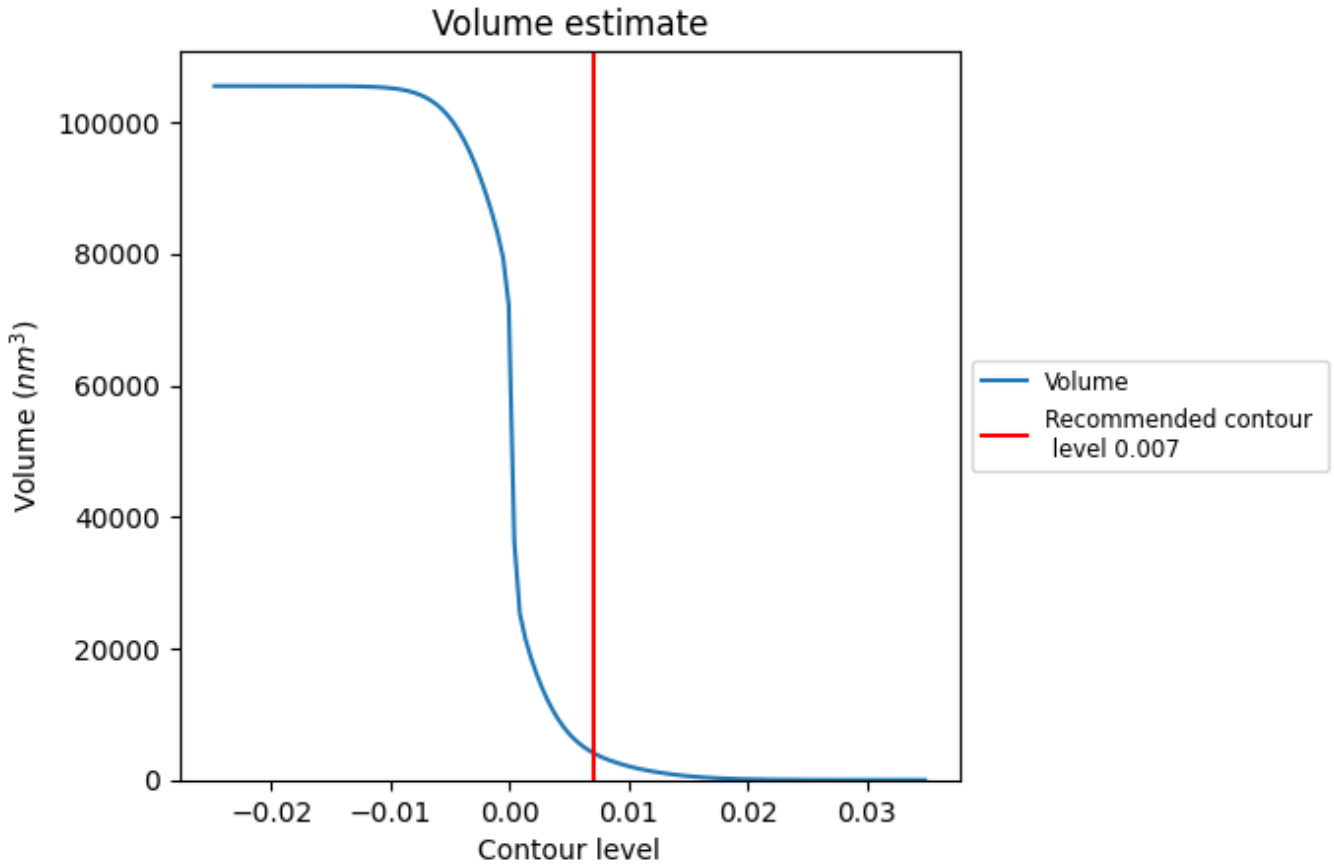
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

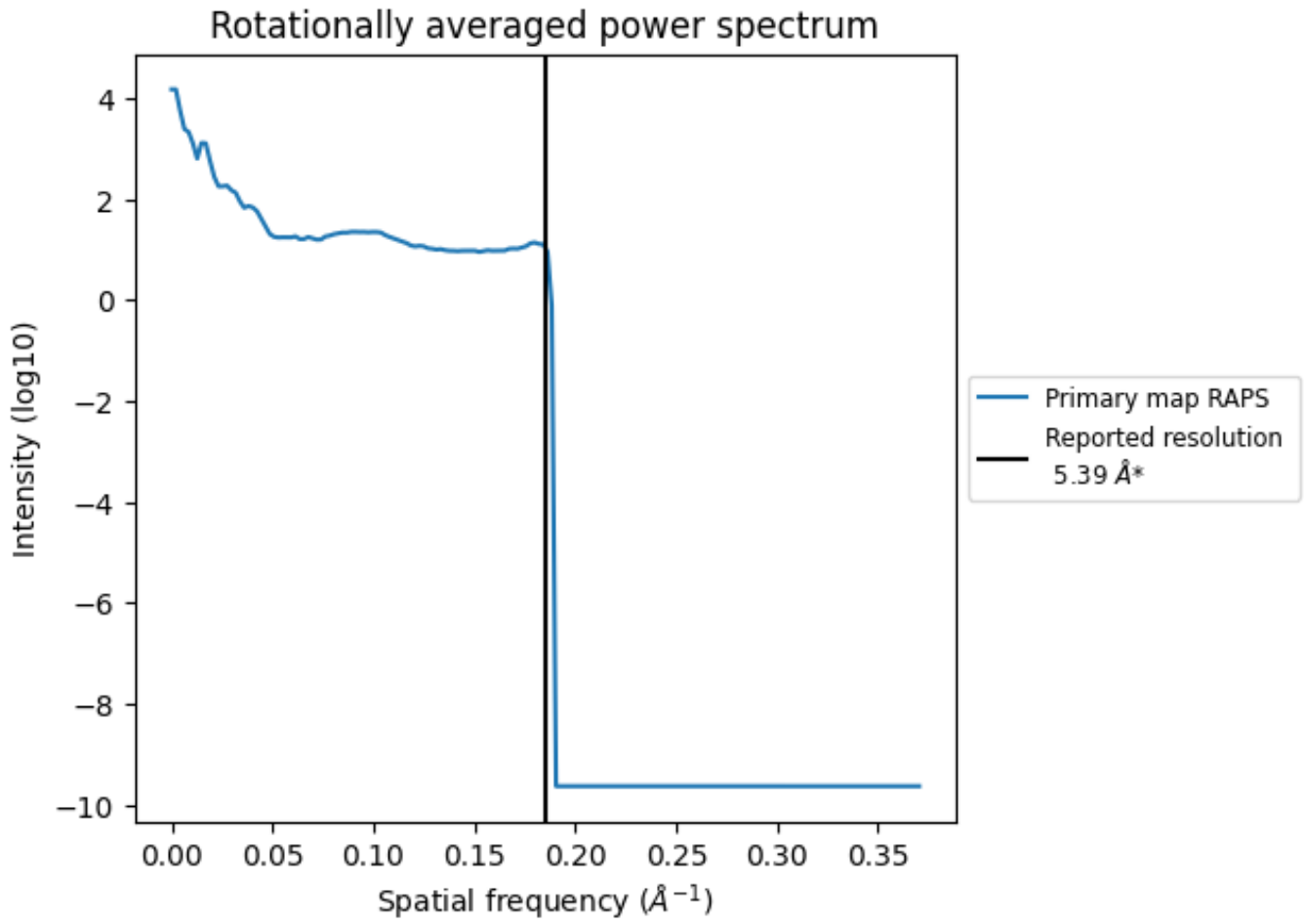
7.2 Volume estimate



The volume at the recommended contour level is 4131 nm^3; this corresponds to an approximate mass of 3731 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 0.186 Å^{-1}

8 Fourier-Shell correlation

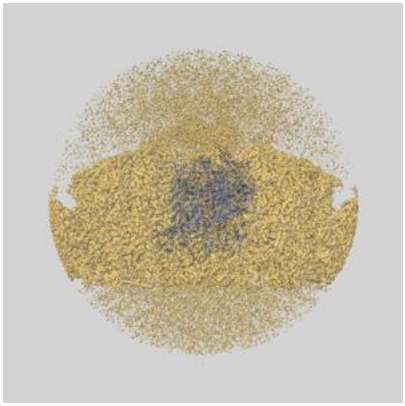
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

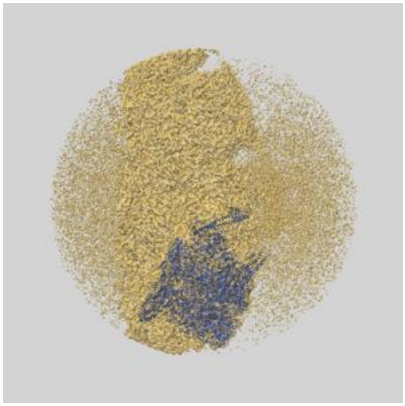
This section contains information regarding the fit between EMDB map EMD-30123 and PDB model 6M6G. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlays

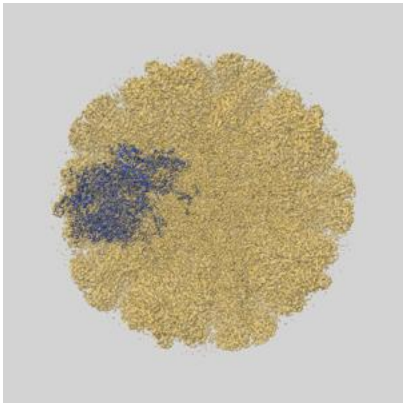
9.1.1 Map-model overlay



X

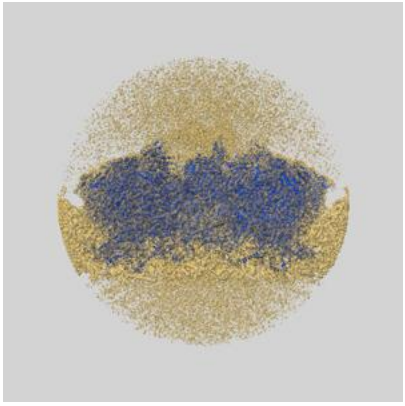


Y

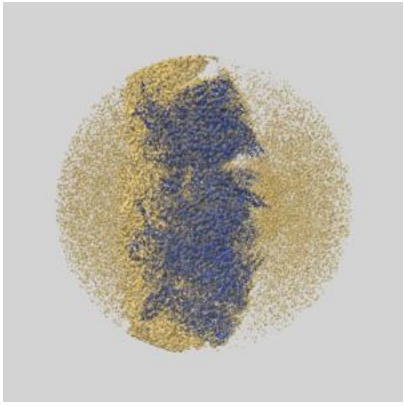


Z

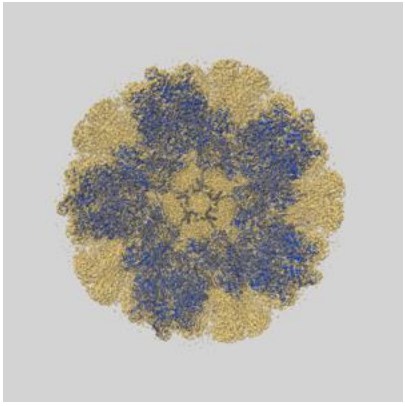
9.1.2 Map-model assembly overlay



X



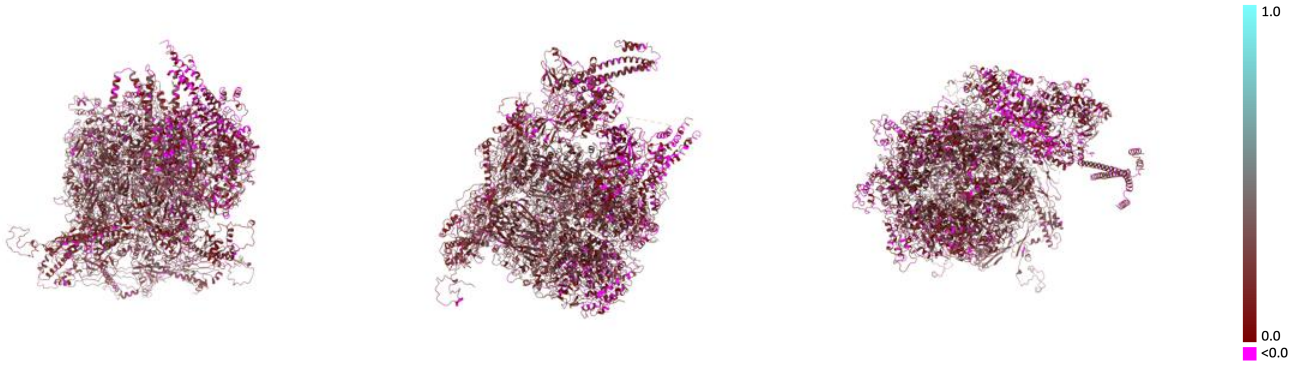
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.007 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.

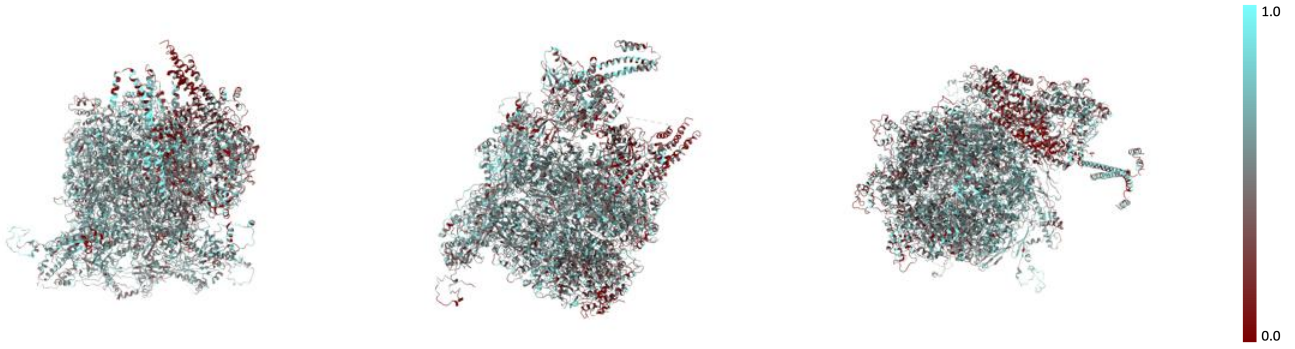
9.2 Q-score mapped to coordinate model (i)



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.

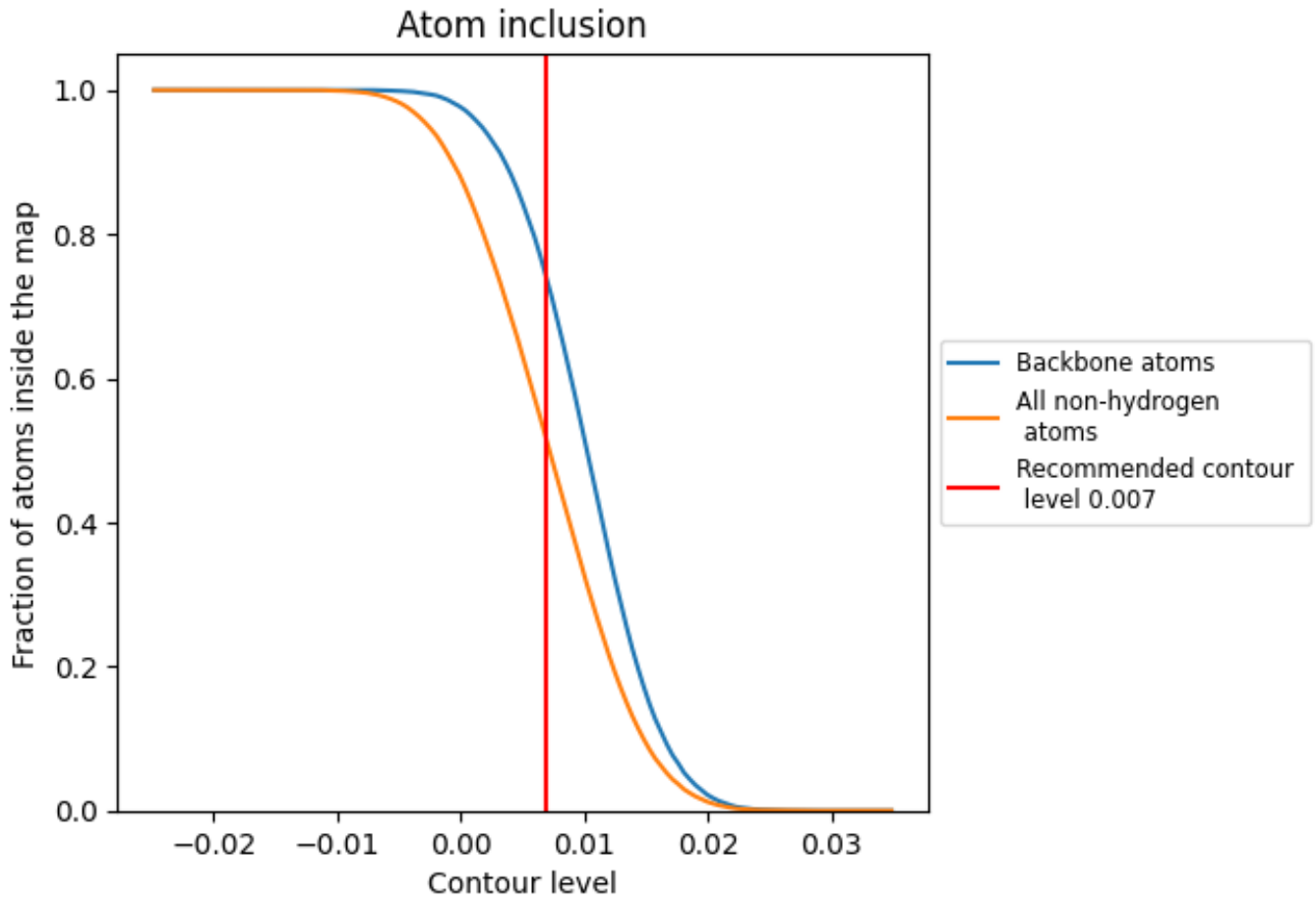
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.007).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 51% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5119	0.1880
B	0.5500	0.2060
C	0.5181	0.2010
D	0.5361	0.2040
E	0.5696	0.2130
F	0.5676	0.2140
G	0.3722	0.1420
I	0.5585	0.2110
K	0.4624	0.1560
L	0.5476	0.1710
M	0.3457	0.1140
O	0.4339	0.1720
P	0.5379	0.1790
Q	0.2808	0.0660
S	0.3839	0.1140
T	0.3205	0.0940
U	0.3775	0.1160
V	0.4517	0.1580
k	0.3670	0.0930
l	0.3539	0.1190
m	0.3514	0.1150
n	0.1295	0.0470
o	0.2066	0.0270