Full wwPDB EM Validation Report ⓘ

Nov 26, 2024 – 06:37 PM JST

PDB ID	:	8XA2
EMDB ID	:	EMD-38192
Title	:	Penton capsomer of the VZV B-Capsid
Authors	:	Nan, W.; Lei, C.; Xiangxi, W.
Deposited on	:	2023-12-01
Resolution	:	4.00 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

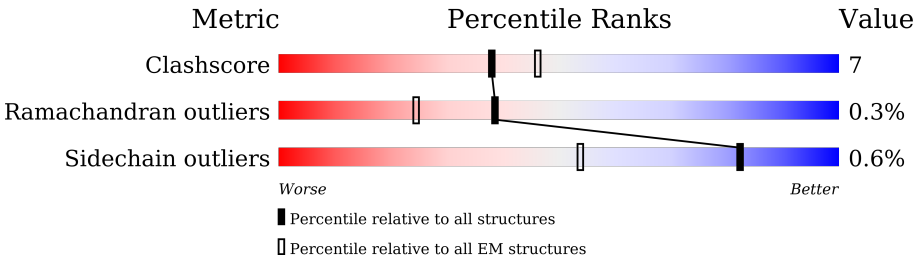
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.00 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	1370	39% 69% 15% 16%
1	C	1370	39% 68% 16% 16%
1	E	1370	40% 70% 14% 16%
1	F	1370	40% 68% 16% 16%
1	G	1370	39% 70% 14% 16%
2	R	256	29% 79% 21%
3	V	263	26% 81% 19%
4	Z	286	50% 73% 26%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 50633 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	A	1155	Total	C	N	O	S	0	0
			8918	5661	1575	1628	54		
1	C	1155	Total	C	N	O	S	0	0
			8918	5661	1575	1628	54		
1	E	1155	Total	C	N	O	S	0	0
			8918	5661	1575	1628	54		
1	F	1155	Total	C	N	O	S	0	0
			8918	5661	1575	1628	54		
1	G	1155	Total	C	N	O	S	0	0
			8918	5661	1575	1628	54		

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	43	ILE	ALA	conflict	UNP Q6QCL5
A	44	PHE	HIS	conflict	UNP Q6QCL5
A	45	PHE	ARG	conflict	UNP Q6QCL5
A	161	ALA	ASP	conflict	UNP Q6QCL5
A	162	ALA	GLY	conflict	UNP Q6QCL5
A	185	SER	LEU	conflict	UNP Q6QCL5
A	814	ALA	GLY	conflict	UNP Q6QCL5
C	43	ILE	ALA	conflict	UNP Q6QCL5
C	44	PHE	HIS	conflict	UNP Q6QCL5
C	45	PHE	ARG	conflict	UNP Q6QCL5
C	161	ALA	ASP	conflict	UNP Q6QCL5
C	162	ALA	GLY	conflict	UNP Q6QCL5
C	185	SER	LEU	conflict	UNP Q6QCL5
C	814	ALA	GLY	conflict	UNP Q6QCL5
E	43	ILE	ALA	conflict	UNP Q6QCL5
E	44	PHE	HIS	conflict	UNP Q6QCL5
E	45	PHE	ARG	conflict	UNP Q6QCL5
E	161	ALA	ASP	conflict	UNP Q6QCL5
E	162	ALA	GLY	conflict	UNP Q6QCL5
E	185	SER	LEU	conflict	UNP Q6QCL5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	814	ALA	GLY	conflict	UNP Q6QCL5
F	43	ILE	ALA	conflict	UNP Q6QCL5
F	44	PHE	HIS	conflict	UNP Q6QCL5
F	45	PHE	ARG	conflict	UNP Q6QCL5
F	161	ALA	ASP	conflict	UNP Q6QCL5
F	162	ALA	GLY	conflict	UNP Q6QCL5
F	185	SER	LEU	conflict	UNP Q6QCL5
F	814	ALA	GLY	conflict	UNP Q6QCL5
G	43	ILE	ALA	conflict	UNP Q6QCL5
G	44	PHE	HIS	conflict	UNP Q6QCL5
G	45	PHE	ARG	conflict	UNP Q6QCL5
G	161	ALA	ASP	conflict	UNP Q6QCL5
G	162	ALA	GLY	conflict	UNP Q6QCL5
G	185	SER	LEU	conflict	UNP Q6QCL5
G	814	ALA	GLY	conflict	UNP Q6QCL5

- Molecule 2 is a protein called Tri2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	R	256	Total	C	N	O	S	0	0
			1847	1191	315	333	8		

- Molecule 3 is a protein called Tri2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	V	263	Total	C	N	O	S	0	0
			1975	1269	339	358	9		

- Molecule 4 is a protein called Tri1.

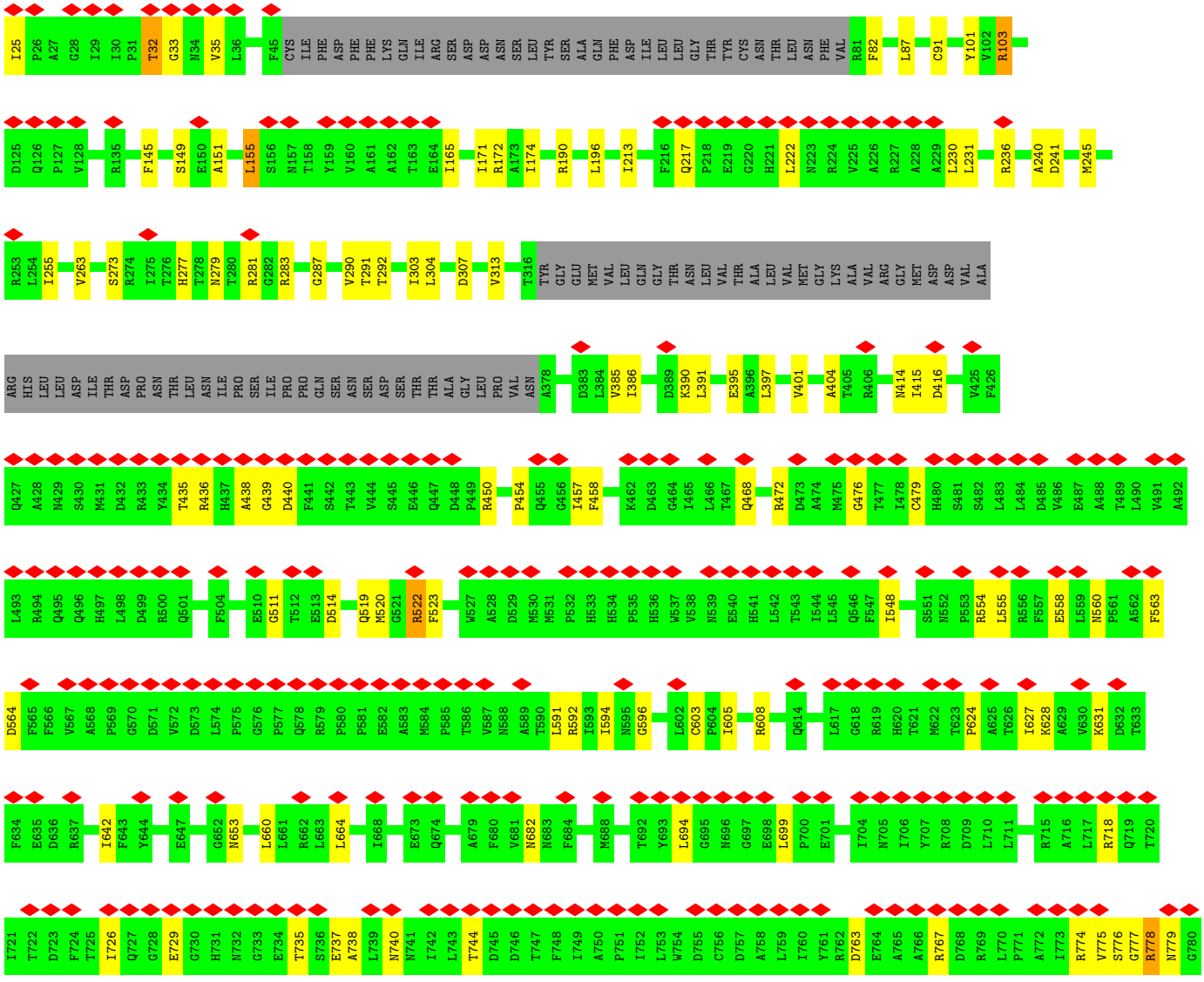
Mol	Chain	Residues	Atoms					AltConf	Trace
4	Z	286	Total	C	N	O	S	0	0
			2221	1408	411	389	13		

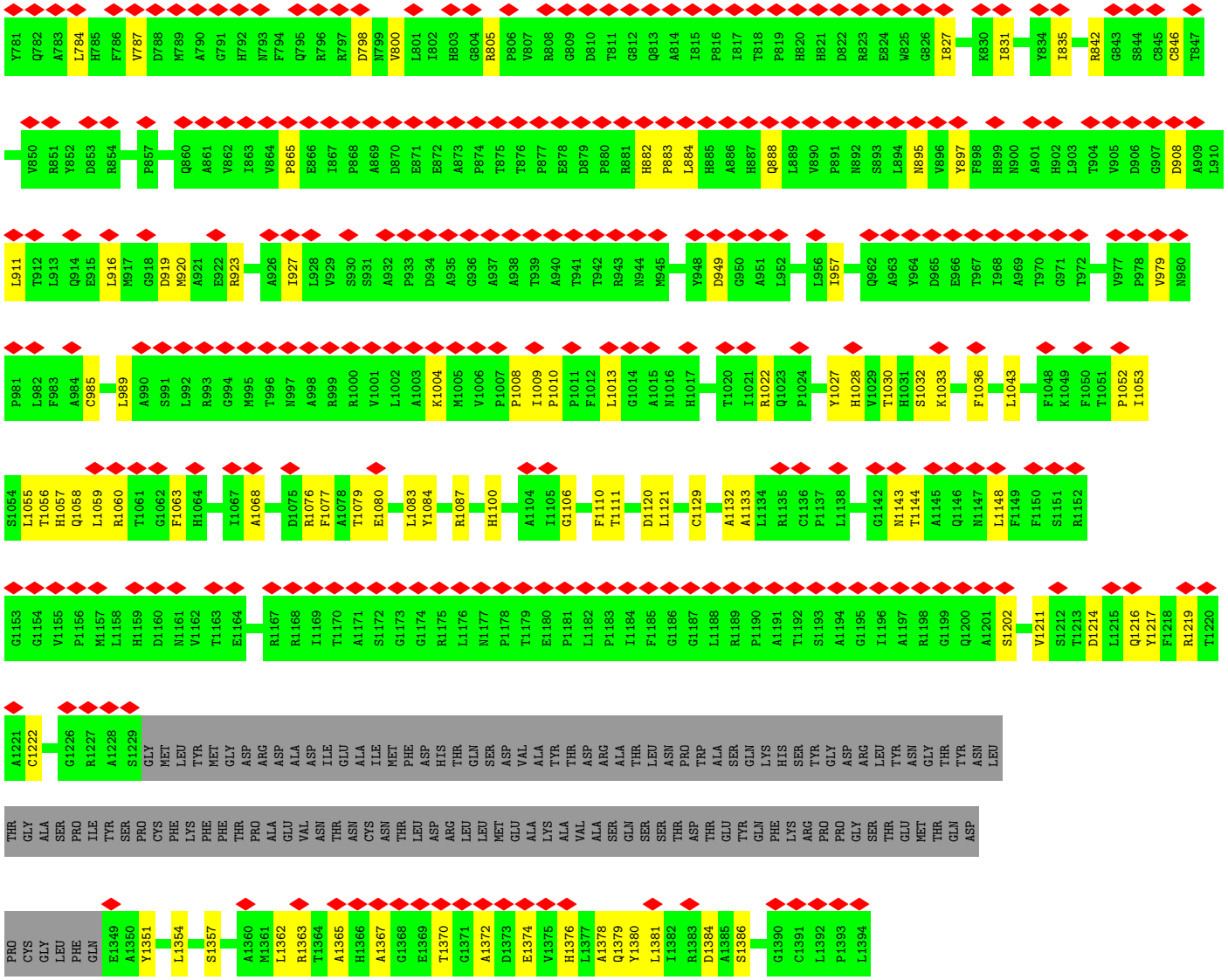
3 Residue-property plots (i)

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

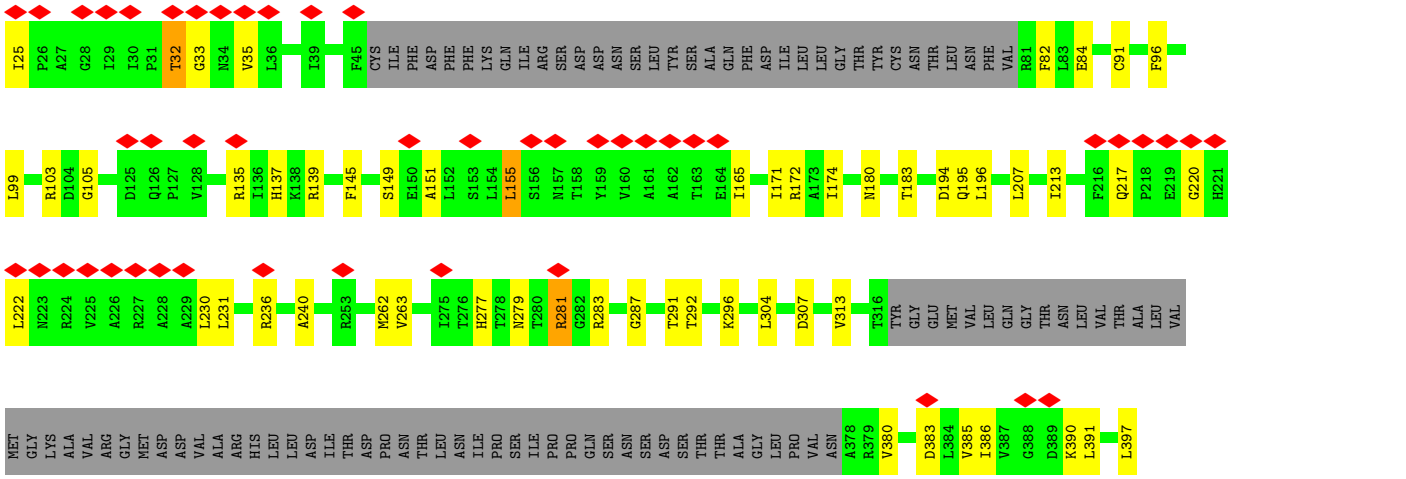
Chain A:

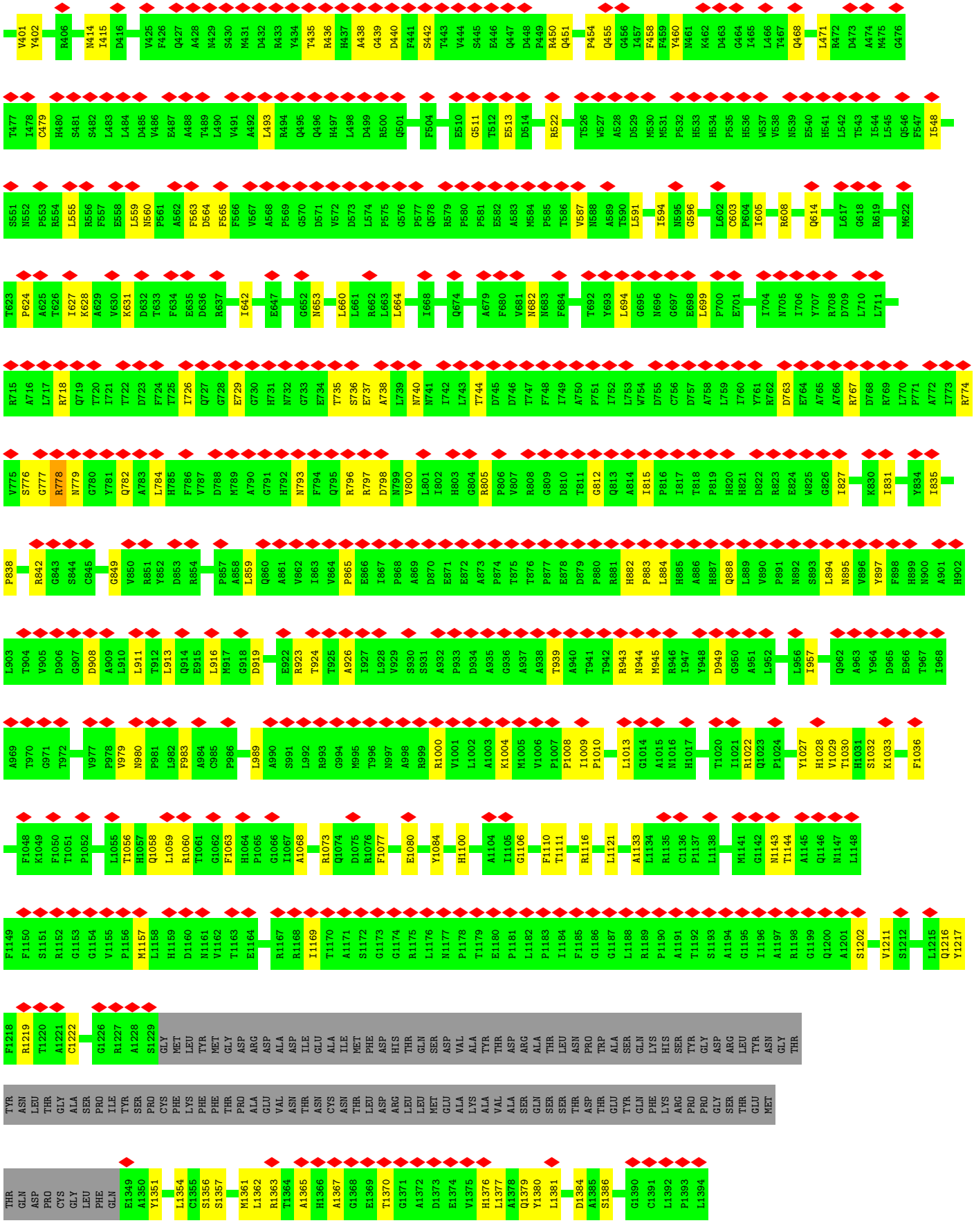




• Molecule 1: Major capsid protein

Chain C:

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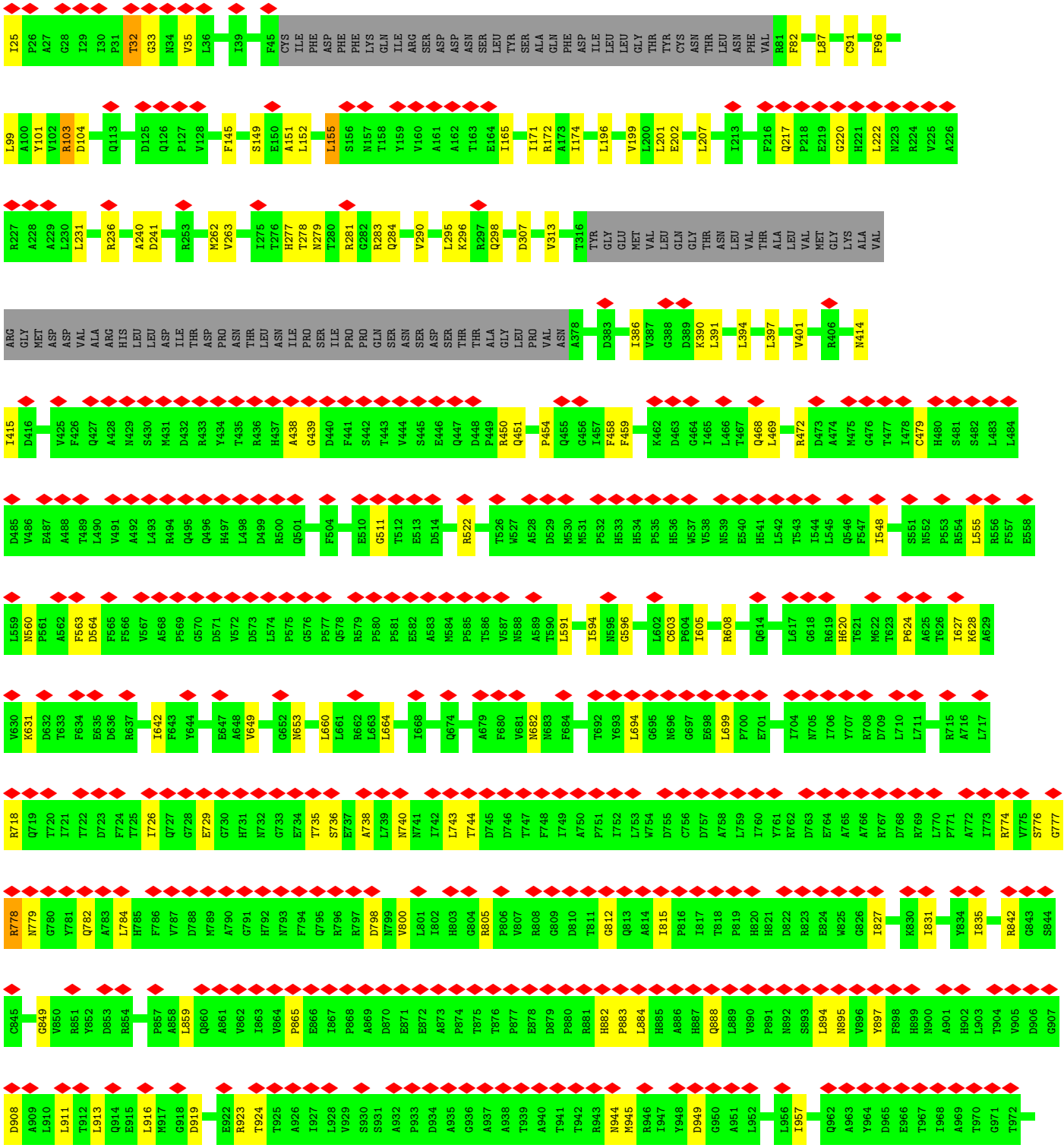
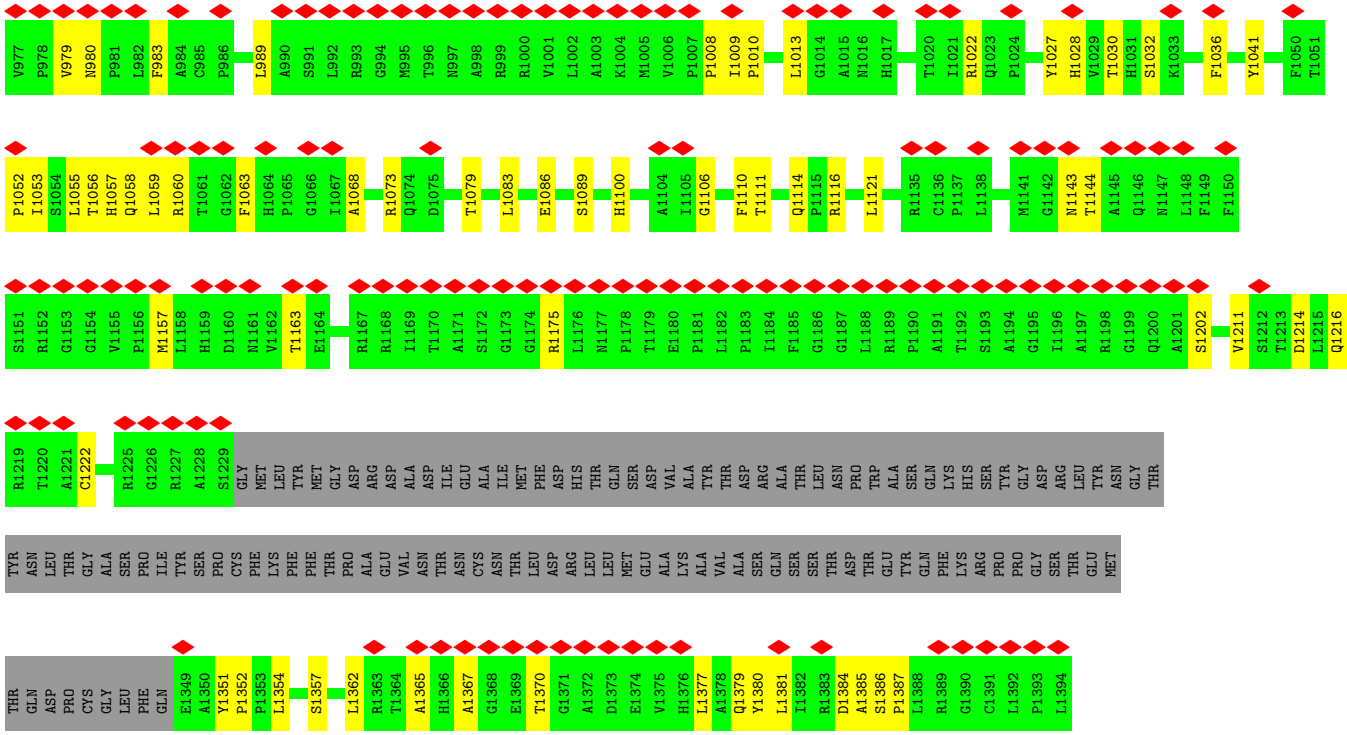
T477 I478 C479 H480 S481 S482 L483 L484 D485 V486 E487 A488 T489 L490 V491 A492 L493 R494 Q495 Q496 H497 L498 D499 R500 Q501 F504 E510 G511 T512 E513 D514 R522 T526 W527 A528 D529 M530 M531 P532 H533 H534 P535 H536 W537 V538 N539 E540 H541 L542 T543 I544 L545 Q546 F547 I548
S551 N552 P553 R554 L555 R556 F557 E558 L559 N560 P561 A562 F563 D564 F565 P566 V567 A568 P569 G570 D571 V572 D573 L574 P575 G576 P577 Q578 R579 P580 P581 E582 A583 M584 P585 T586 V587 N588 A589 T590 L591 I594 N595 Q596 L602 C603 P604 I605 R608 Q614 L617 G618 R619 M622
T623 P624 A625 T626 I627 K628 A629 V630 K631 D632 T633 F634 E635 D636 R637 I642 E647 G652 N653 L660 L661 R662 L663 L664 I668 Q674 A679 F680 V681 N682 N683 F684 T692 Y693 L694 G695 N696 G697 E698 L699 P700 E701 I704 N705 I706 Y707 R708 D709 L710 L711
R715 A716 L717 R718 Q719 T720 I721 T722 D723 F724 T725 I726 Q727 G728 E729 G730 H731 N732 G733 E734 T735 S736 E737 A738 L739 N740 N741 I742 L743 T744 D745 D746 T747 F748 I749 A750 P751 I752 L753 W754 D755 C756 D757 A758 L759 I760 Y761 R762 D763 E764 A765 A766 R767 D768 R769 L770 P771 A772 I773 R774
V775 S776 G777 R778 N779 G780 Y781 Q782 A783 L784 H785 F786 V787 D788 M789 A790 G791 H792 N793 F794 Q795 R796 R797 D798 N799 V800 L801 I802 H803 G804 R805 P806 V807 R808 G809 D810 T811 G812 Q813 A814 I815 P816 I817 T818 P819 H820 H821 D822 R823 E824 W825 G826 I827 K830 I831 Y834 I835
P838 R842 G843 S844 C845 G849 V850 R851 Y852 D853 R854 P857 A858 L859 Q860 A861 V862 I863 V864 P865 E866 I867 P868 A869 D870 E871 E872 A873 P874 T875 T876 P877 E878 D879 P880 R881 H882 P883 L884 H885 A886 H887 Q888 L889 V890 P891 N892 S893 L894 N895 V896 Y897 F898 H899 N900 A901 H902
L903 T904 V905 D906 G907 D908 A909 L910 L911 T912 L913 Q914 E915 L916 M917 G918 D919 E922 R923 T924 T925 A926 I927 L928 V929 S930 S931 A932 P933 D934 A935 G936 A937 A938 T939 A940 T941 T942 R943 N944 M945 R946 I947 Y948 D949 G950 A951 L952 L956 I957 Q962 A963 Y964 D965 E966 T967 I968
A969 T970 G971 T972 V977 P978 V979 N980 P981 L982 F983 A984 C985 P986 L989 A990 S991 L992 R993 G994 M995 T996 N997 A998 R999 R1000 V1001 L1002 A1003 K1004 M1005 V1006 P1007 P1008 I1009 P1010 L1013 G1014 A1015 N1016 H1017 T1020 I1021 R1022 Q1023 P1024 Y1027 H1028 V1029 T1030 H1031 S1032 K1033 F1036
F1048 K1049 F1050 T1051 P1052 L1055 T1056 H1057 Q1058 L1059 R1060 T1061 G1062 F1063 H1064 P1065 G1066 I1067 A1068 R1073 Q1074 D1075 R1076 F1077 E1080 Y1084 H1100 A1104 I1105 G1106 F1110 T1111 R1116 L1121 A1133 L1134 R1135 C1136 P1137 L1138 M1141 G1142 N1143 T1144 A1145 Q1146 N1147 L1148
F1149 F1150 S1151 R1152 G1153 G1154 V1155 P1156 M1157 L1158 H1159 D1160 N1161 V1162 T1163 E1164 R1167 R1168 I1169 T1170 A1171 S1172 G1173 G1174 R1175 L1176 N1177 P1178 T1179 E1180 P1181 L1182 P1183 I1184 F1185 G1186 G1187 L1188 R1189 P1190 A1191 T1192 S1193 A1194 G1195 I1196 A1197 R1198 G1199 Q1200 A1201 S1202 V1211 S1212 L1215 Q1216 Y1217
F1218 R1219 T1220 A1221 C1222 G1226 R1227 A1228 S1229 GLY MET LEU TYR MET GLY ASP ARG ASP ALA ASP ILE GLU ALA ILE MET PHE ASP HIS THR GLN SER ASP VAL ALA TYR THR ASP ARG ALA THR LEU ASN PRO TRP ALA SER GLN LYS HIS SER TYR GLY ASP ARG LEU TYR ASN GLY THR
TYR ASN LEU THR GLY ALA SER PRO ILE TYR SER PRO CYS PHE LYS PHE PHE THR PRO ALA GLU VAL ASN THR ASN CYS ASN THR LEU ASP ARG LEU LEU MET GLU ALA LYS ALA VAL ALA SER GLN SER SER THR ASP THR GLU TYR GLN PHE LYS ARG PRO PRO GLY SER THR GLU MET
THR GLN ASP PRO CYS GLY LEU PHE GLN E1349 A1350 Y1351 L1354 C1355 S1356 S1357 M1361 L1362 R1363 T1364 A1365 H1366 A1367 G1368 E1369 T1370 G1371 A1372 D1373 E1374 V1375 H1376 L1377 A1378 Q1379 Y1380 L1381 D1384 A1385 S1386 G1390 C1391 L1392 P1393 L1394

• Molecule 1: Major capsid protein

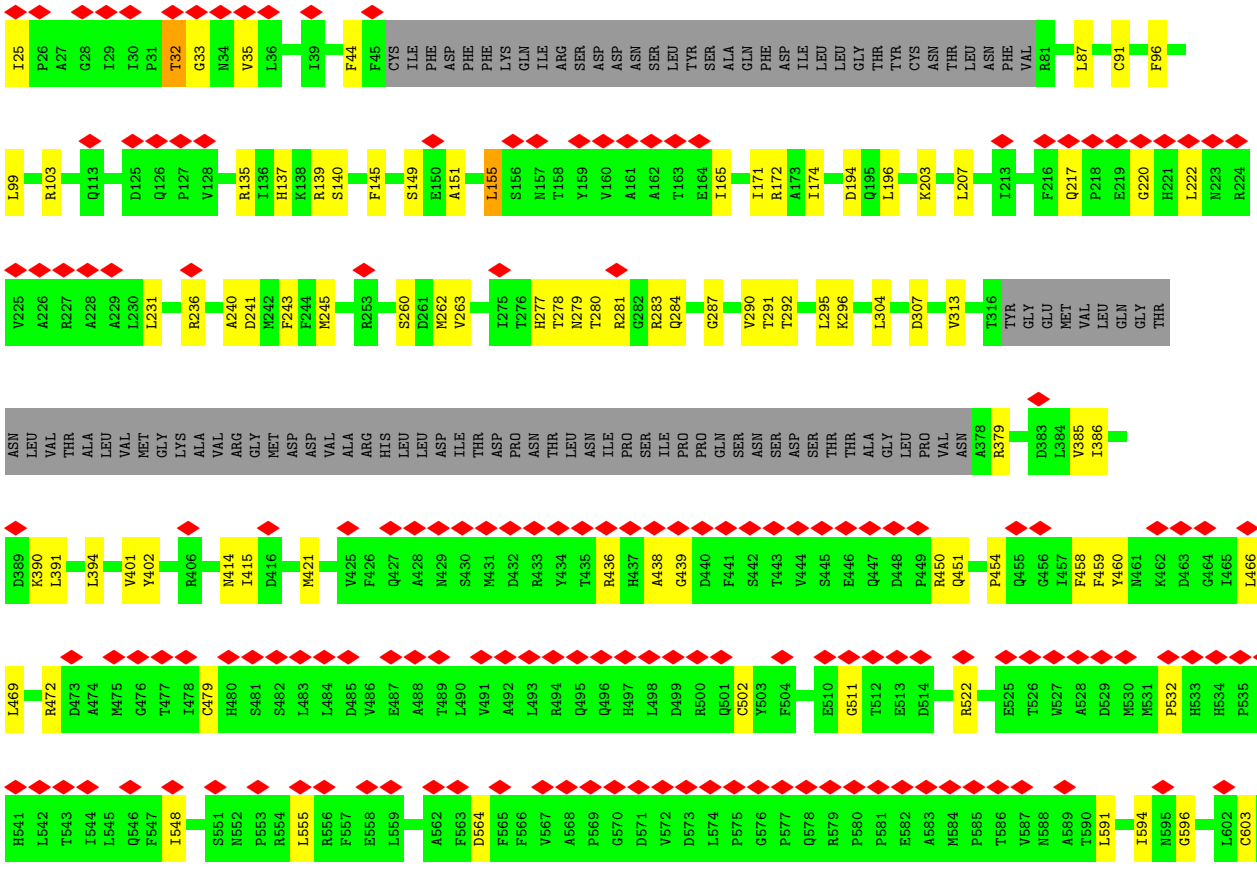
Chain E:

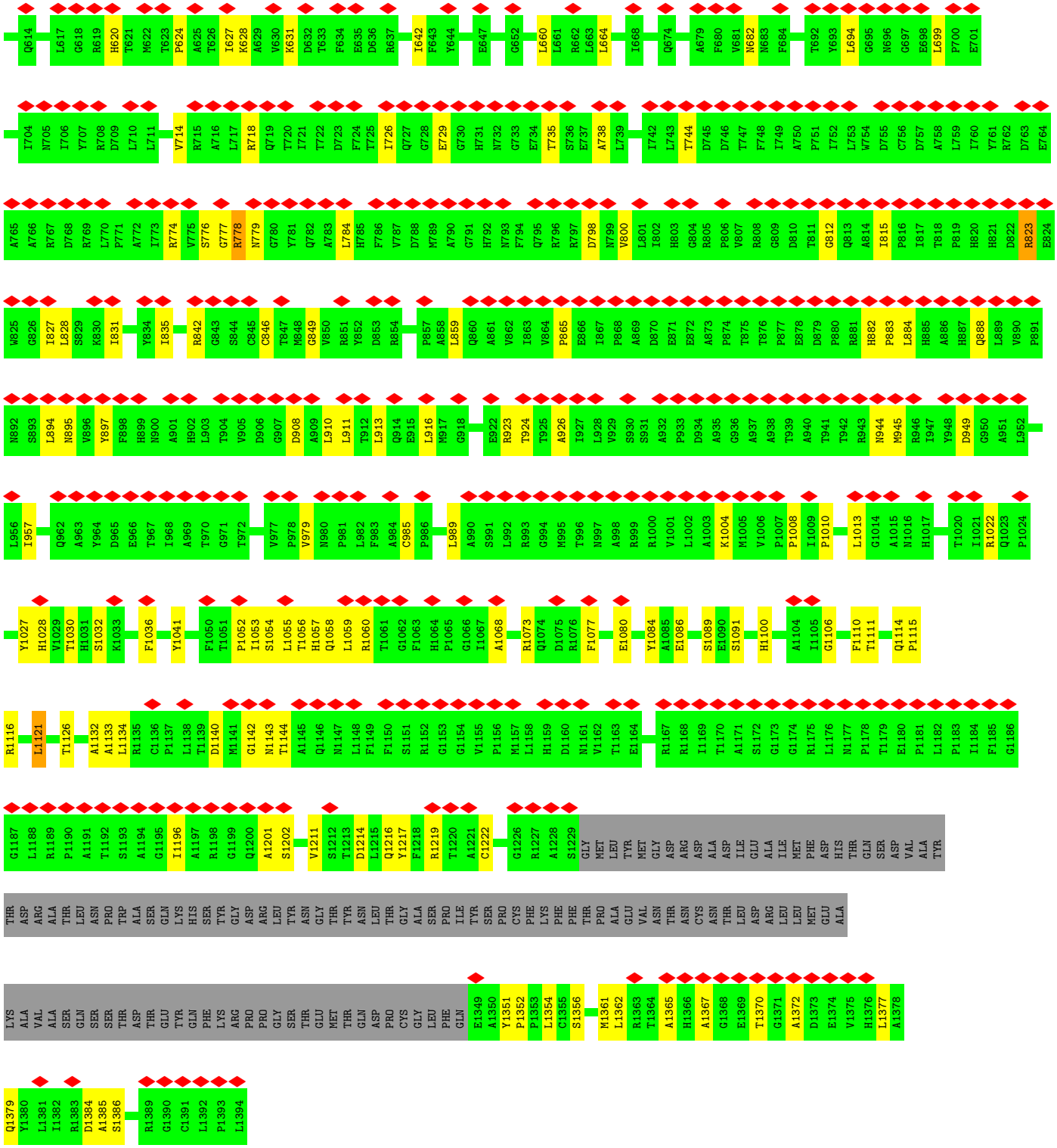




• Molecule 1: Major capsid protein

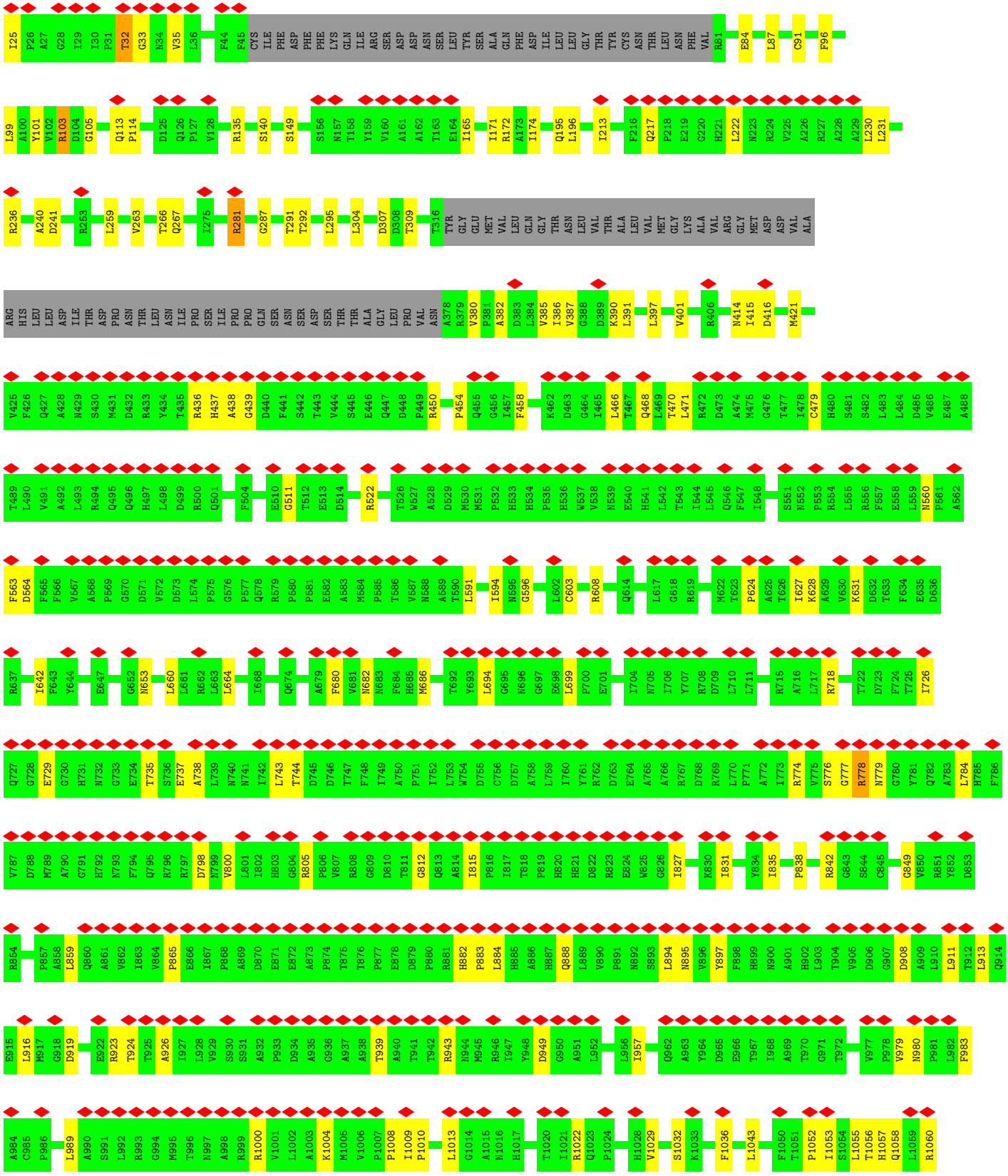
Chain F:





- Molecule 1: Major capsid protein

Chain G: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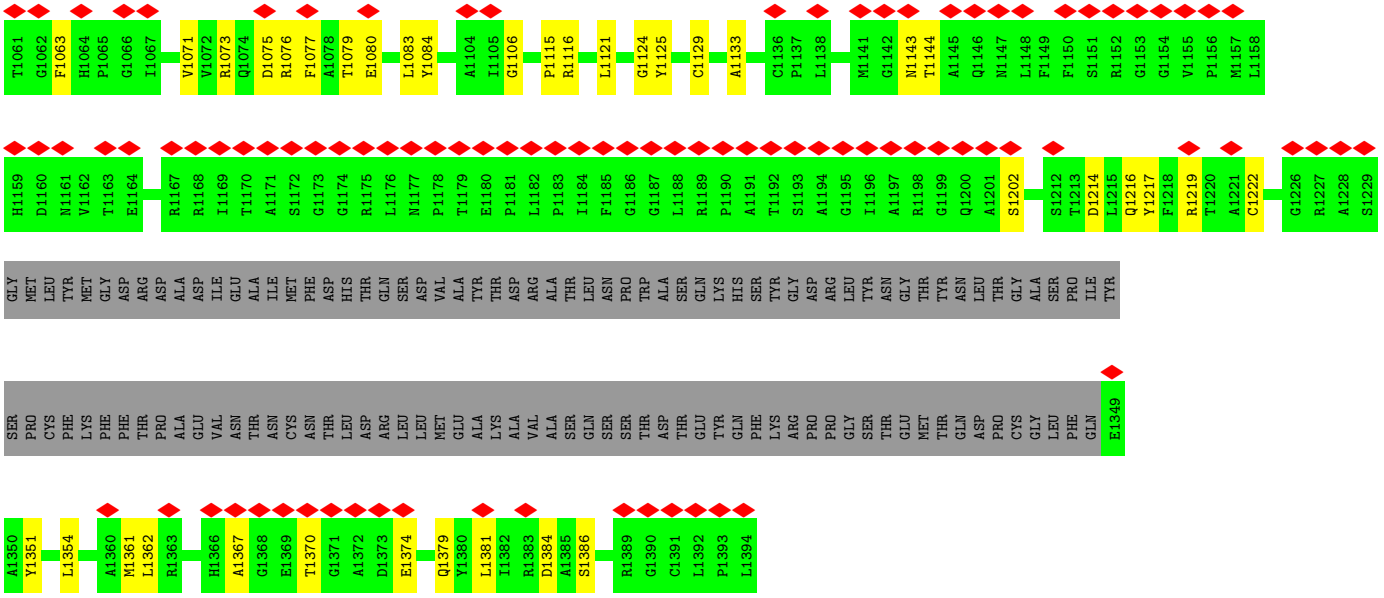
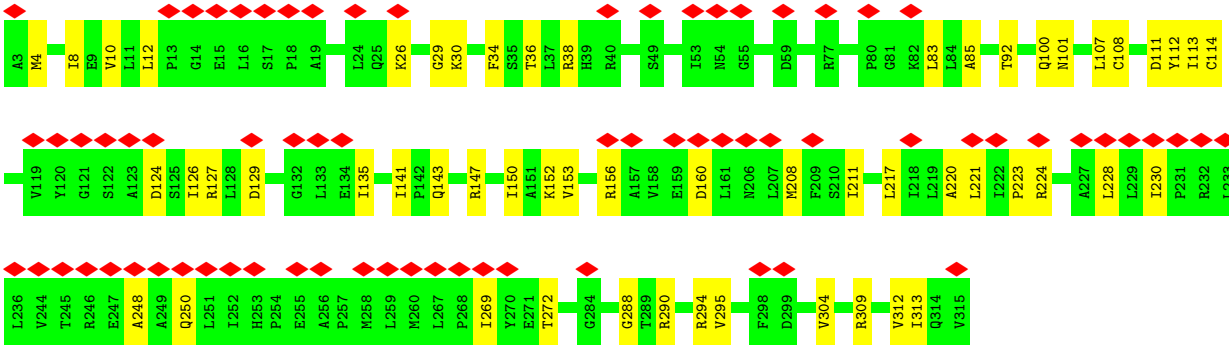
L99 A100 Y101 V102 R103 D104 G105 Q113 P114 D125 Q126 P127 V128 R135 S140 S149 S156 N157 T158 Y159 V160 A161 A162 T163 E164 I165 I171 R172 A173 I174 Q195 L196 I213 F216 Q217 P218 E219 G220 H221 L222 N223 R224 V225 A226 R227 A228 A229 L230 L231
R236 A240 D241 R253 L259 V263 T266 Q267 I275 R281 G287 T291 T292 L295 L304 D307 D308 T309 T316 TYR GLY GLU MET VAL LEU GLN GLY THR ASN LEU VAL THR ALA LEU VAL MET GLY LYS ALA VAL ARG GLY MET ASP ASP VAL ALA
ARG HIS LEU LEU ASP ILE THR ASP PRO ASN THR LEU ASN ILE PRO SER ILE PRO PRO GLN SER ASN SER ASP SER THR THR ALA GLY LEU PRO VAL ASN A378 R379 V380 P381 A382 D383 L384 V385 I386 V387 G388 D389 K390 L391 L397 V401 R406 N414 I415 D416 M421
V425 F426 Q427 A428 N429 S430 M431 D432 R433 Y434 T435 R436 H437 A438 G439 D440 F441 S442 T443 V444 S445 E446 Q447 D448 P449 R450 P454 Q455 G456 I457 F458 K462 D463 G464 I465 L466 T467 Q468 L469 T470 L471 R472 D473 A474 M475 G476 T477 I478 C479 H480 S481 S482 L483 L484 D485 V486 E487 A488
T489 L490 V491 A492 L493 R494 Q495 Q496 H497 L498 D499 R500 Q501 F504 E510 G511 T512 E513 D514 R522 T526 W527 A528 D529 N530 M531 P532 H533 H534 P535 H536 W537 V538 N539 E540 H541 L542 T543 I544 L545 Q546 F547 I548 S551 N552 P553 R554 L555 R556 F557 E558 L559 N560 P561 A562
F563 D564 F565 F566 V567 A568 P569 G570 D571 V572 D573 L574 P575 G576 P577 Q578 R579 P580 P581 E582 A583 M584 P585 T586 V587 N588 A589 T590 L591 I594 N595 G596 L602 C603 R608 Q614 L617 G618 R619 M622 T623 P624 A625 T626 I627 K628 A629 V630 K631 D632 T633 F634 E635 D636
R637 I642 F643 Y644 E647 G652 N653 L660 L661 R662 L663 L664 I668 Q674 A679 F680 V681 N682 N683 F684 H685 M686 T692 Y693 L694 G695 N696 G697 E698 L699 P700 E701 I704 N705 I706 Y707 R708 D709 L710 L711 R715 A716 L717 R718 T722 D723 F724 T725 I726
Q727 G728 E729 G730 H731 N732 G733 E734 T735 S736 E737 A738 L739 N740 N741 I742 L743 T744 D745 D746 T747 F748 I749 A750 P751 I752 L753 W754 D755 C756 D757 A758 L759 I760 Y761 R762 D763 E764 A765 A766 R767 D768 R769 L770 P771 A772 I773 R774 V775 S776 G777 R778 N779 G780 Y781 Q782 A783 L784 H785 F786
V787 D788 M789 A790 G791 H792 N793 F794 Q795 R796 R797 D798 W799 V800 L801 I802 H803 G804 R805 P806 V807 R808 G809 D810 T811 G812 Q813 A814 I815 P816 I817 T818 P819 H820 H821 D822 R823 E824 W825 G826 I827 K830 I831 Y834 I835 P838 R842 G843 S844 C845 G849 V850 R851 Y852 D853
R854 P857 A858 L859 Q860 A861 V862 I863 V864 P865 E866 I867 P868 A869 D870 E871 E872 A873 P874 T875 T876 P877 E878 D879 P880 R881 H882 P883 L884 H885 A886 H887 Q888 L889 V890 P891 N892 S893 L894 N895 V896 Y897 F898 H899 N900 A901 H902 L903 T904 V905 D906 G907 D908 A909 L910 L911 T912 L913 Q914
E915 L916 M917 G918 D919 E922 R923 T924 T925 A926 I927 L928 V929 S930 S931 A932 P933 D934 A935 G936 A937 A938 T939 A940 T941 T942 R943 N944 M945 R946 I947 Y948 D949 G950 A951 L952 L956 I957 Q962 A963 Y964 D965 E966 T967 I968 A969 T970 G971 T972 V977 P978 V979 N980 P981 L982 F983
A984 C985 P986 L989 A990 S991 L992 R993 G994 M995 T996 N997 A998 R999 R1000 V1001 L1002 A1003 K1004 M1005 V1006 P1007 P1008 I1009 P1010 L1013 G1014 A1015 N1016 H1017 T1020 I1021 R1022 Q1023 P1024 H1028 V1029 S1032 K1033 F1036 L1043 F1050 T1051 P1052 I1053 S1054 L1055 T1056 H1057 Q1058 L1059 R1060



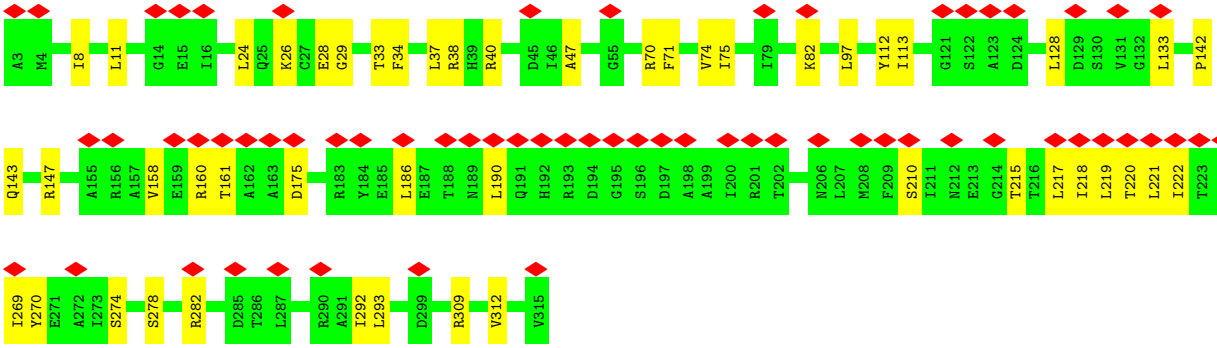
• Molecule 2: Tri2A

Chain R:



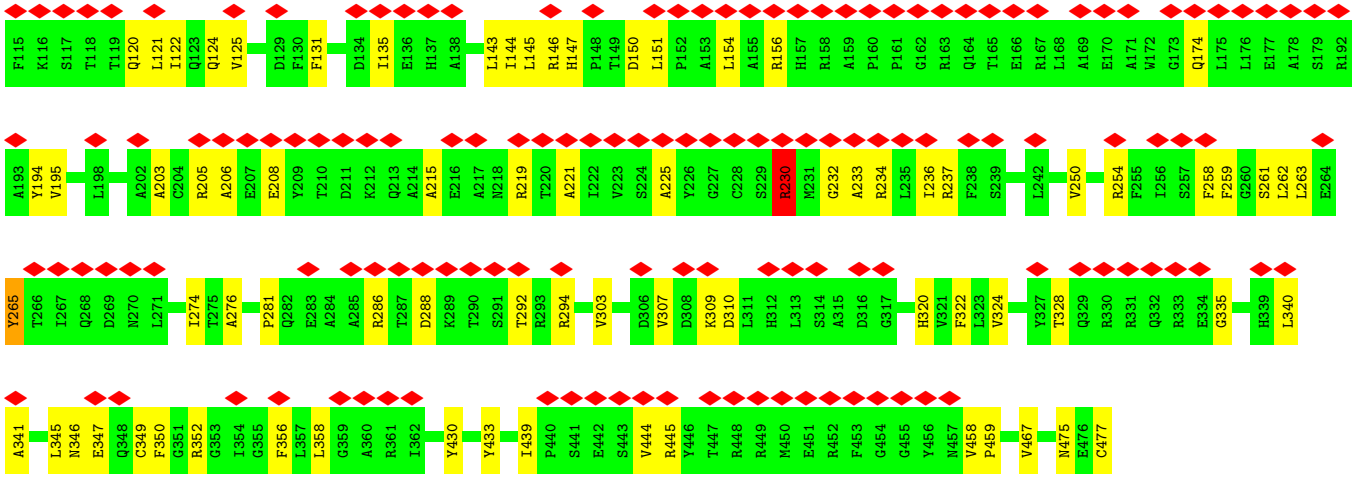
• Molecule 3: Tri2B

Chain V:



• Molecule 4: Tri1

Chain Z: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A193 Y194 V195 L198 A202 A203 C204 R205 A206 E207 E208 Y209 T210 D211 K212 Q213 A214 A215 E216 A217 N218 R219 T220 A221 I222 V223 S224 A225 Y226 G227 C228 S229 R230 M231 G232 A233 R234 L235 I236 R237 F238 S239 L242 V250 R254 F255 I256 S257 F258 F259 G260 S261 L262 L263 E264
Y265 T266 I267 Q268 D269 N270 L271 I274 T275 A276 P281 Q282 E283 A284 A285 R286 T287 D288 K289 T290 S291 T292 R293 R294 V303 D306 V307 D308 K309 D310 L311 H312 L313 S314 A315 D316 G317 H320 V321 F322 L323 V324 Y327 T328 Q329 R330 R331 Q332 R333 E334 G335 H339 L340
A341 L345 N346 E347 Q348 C349 F350 G351 R352 G353 I354 G355 F356 L357 L358 G359 A360 R361 I362 Y430 Y433 I439 P440 S441 E442 S443 V444 R445 Y446 T447 R448 R449 M450 E451 R452 F453 G454 G455 Y456 N457 V458 P459 V467 N475 E476 C477

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	267174	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	0.057	Depositor
Minimum map value	-0.029	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	418.5, 418.5, 418.5	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.27	0/9133	0.61	3/12454 (0.0%)
1	C	0.27	0/9133	0.62	3/12454 (0.0%)
1	E	0.27	0/9133	0.62	3/12454 (0.0%)
1	F	0.27	0/9133	0.62	4/12454 (0.0%)
1	G	0.27	0/9133	0.61	2/12454 (0.0%)
2	R	0.29	0/1878	0.67	0/2568
3	V	0.29	0/2010	0.66	0/2743
4	Z	0.30	0/2269	0.75	1/3078 (0.0%)
All	All	0.27	0/51822	0.63	16/70659 (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	F	0	2
3	V	0	1
4	Z	0	1
All	All	0	4

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	155	LEU	CA-CB-CG	8.21	134.18	115.30
1	F	155	LEU	CA-CB-CG	7.57	132.72	115.30
1	A	155	LEU	CA-CB-CG	7.54	132.63	115.30
4	Z	310	ASP	CB-CG-OD2	7.26	124.84	118.30
1	C	155	LEU	CA-CB-CG	6.62	130.54	115.30
1	G	231	LEU	CA-CB-CG	6.49	130.23	115.30
1	F	231	LEU	CA-CB-CG	6.45	130.13	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	231	LEU	CA-CB-CG	6.31	129.81	115.30
1	E	231	LEU	CA-CB-CG	6.19	129.53	115.30
1	C	231	LEU	CA-CB-CG	5.85	128.75	115.30
1	F	1121	LEU	CA-CB-CG	5.82	128.69	115.30
1	F	1134	LEU	CA-CB-CG	5.77	128.56	115.30
1	A	1121	LEU	CA-CB-CG	5.51	127.98	115.30
1	G	1121	LEU	CA-CB-CG	5.36	127.63	115.30
1	C	1121	LEU	CA-CB-CG	5.36	127.62	115.30
1	E	1121	LEU	CA-CB-CG	5.28	127.44	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	1196	ILE	Peptide
1	F	823	ARG	Sidechain
3	V	210	SER	Peptide
4	Z	230	ARG	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8918	0	8753	128	0
1	C	8918	0	8753	134	0
1	E	8918	0	8753	120	0
1	F	8918	0	8753	132	0
1	G	8918	0	8753	116	0
2	R	1847	0	1851	31	0
3	V	1975	0	2031	31	0
4	Z	2221	0	2184	44	0
All	All	50633	0	49831	719	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 7.

All (719) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1073:ARG:HE	1:C:1202:SER:HB2	1.50	0.77
1:F:1073:ARG:HE	1:F:1202:SER:HB2	1.50	0.75
1:E:1073:ARG:HE	1:E:1202:SER:HB2	1.52	0.74
1:E:25:ILE:HD12	1:E:174:ILE:HG13	1.70	0.74
1:G:1073:ARG:HE	1:G:1202:SER:HB2	1.55	0.71
2:R:113:ILE:HD11	2:R:295:VAL:HG13	1.75	0.69
1:C:468:GLN:H	1:C:1143:ASN:HD21	1.41	0.67
1:E:263:VAL:HG22	1:E:390:LYS:HE2	1.75	0.67
4:Z:120:GLN:HE22	4:Z:122:ILE:HG13	1.60	0.67
1:C:729:GLU:OE2	1:C:1060:ARG:NH2	2.23	0.66
1:C:653:ASN:HD21	1:C:805:ARG:H	1.44	0.66
1:E:458:PHE:HB3	1:E:1362:LEU:HD22	1.78	0.66
1:F:25:ILE:HD12	1:F:174:ILE:HG13	1.77	0.66
1:E:653:ASN:HD21	1:E:805:ARG:H	1.45	0.65
1:F:263:VAL:HG22	1:F:390:LYS:HE2	1.77	0.65
4:Z:143:LEU:HG	4:Z:258:PHE:HA	1.77	0.65
1:G:653:ASN:HD21	1:G:805:ARG:H	1.44	0.65
1:G:1354:LEU:HB2	1:G:1384:ASP:HB2	1.78	0.65
1:G:195:GLN:HE22	1:G:1116:ARG:HD2	1.61	0.65
1:G:450:ARG:HH12	1:G:1379:GLN:H	1.44	0.64
1:F:660:LEU:HD11	1:F:916:LEU:HB2	1.80	0.64
1:G:450:ARG:NH1	1:G:1379:GLN:OE1	2.30	0.64
4:Z:206:ALA:HB1	4:Z:215:ALA:HB1	1.79	0.64
1:C:450:ARG:HH12	1:C:1379:GLN:H	1.43	0.64
1:F:450:ARG:NH1	1:F:1379:GLN:OE1	2.32	0.63
1:C:776:SER:OG	1:C:778:ARG:NH1	2.32	0.63
1:E:415:ILE:HG23	1:E:1079:THR:HG21	1.81	0.63
1:C:1361:MET:O	1:C:1365:ALA:HB2	1.99	0.63
1:F:145:PHE:HB3	1:F:1110:PHE:HB2	1.81	0.63
1:E:454:PRO:HB3	1:E:1379:GLN:HG3	1.81	0.62
1:C:660:LEU:HD11	1:C:916:LEU:HB2	1.81	0.62
1:A:151:ALA:O	1:A:155:LEU:HB2	1.99	0.62
1:G:113:GLN:NE2	1:G:114:PRO:O	2.33	0.62
1:E:660:LEU:HD11	1:E:916:LEU:HB2	1.82	0.62
1:G:660:LEU:HD11	1:G:916:LEU:HB2	1.81	0.62
2:R:152:LYS:HE3	3:V:270:TYR:HD1	1.64	0.62
3:V:38:ARG:HD2	3:V:40:ARG:H	1.64	0.62
1:A:653:ASN:HD21	1:A:805:ARG:H	1.46	0.62
1:E:776:SER:OG	1:E:778:ARG:NH1	2.33	0.62
1:F:776:SER:OG	1:F:778:ARG:NH1	2.33	0.62
1:F:151:ALA:O	1:F:155:LEU:HB2	2.00	0.62
1:F:682:ASN:ND2	1:F:957:ILE:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:145:PHE:HB3	1:E:1110:PHE:HB2	1.82	0.61
1:A:989:LEU:HD11	1:A:1008:PRO:HG3	1.82	0.61
1:E:450:ARG:HH12	1:E:1379:GLN:H	1.48	0.61
3:V:292:ILE:HG13	3:V:293:LEU:HG	1.82	0.61
1:A:682:ASN:ND2	1:A:957:ILE:O	2.33	0.61
1:A:776:SER:OG	1:A:778:ARG:NH1	2.33	0.61
1:E:1357:SER:HG	1:E:1380:TYR:H	1.48	0.61
1:G:263:VAL:HG22	1:G:390:LYS:HD2	1.83	0.61
1:G:776:SER:OG	1:G:778:ARG:NH1	2.33	0.61
1:C:831:ILE:HG23	1:C:835:ILE:HD12	1.83	0.61
1:C:1080:GLU:HB2	1:C:1133:ALA:HB3	1.82	0.61
1:E:468:GLN:O	1:E:1143:ASN:ND2	2.34	0.61
1:E:450:ARG:NH1	1:E:1379:GLN:OE1	2.34	0.61
4:Z:233:ALA:O	4:Z:237:ARG:HB3	2.00	0.61
1:C:450:ARG:NH1	1:C:1379:GLN:OE1	2.33	0.61
3:V:215:THR:O	3:V:219:LEU:HB2	2.02	0.60
1:C:291:THR:HG22	1:C:292:THR:H	1.66	0.60
1:A:660:LEU:HD11	1:A:916:LEU:HB2	1.84	0.60
1:E:281:ARG:NH2	1:E:307:ASP:OD1	2.34	0.60
3:V:29:GLY:H	3:V:75:ILE:HG23	1.65	0.60
1:E:682:ASN:ND2	1:E:957:ILE:O	2.35	0.60
1:F:451:GLN:HA	1:F:1377:LEU:HD22	1.84	0.60
1:A:831:ILE:HG23	1:A:835:ILE:HD12	1.83	0.60
1:A:145:PHE:HB3	1:A:1110:PHE:HB2	1.83	0.60
1:G:458:PHE:HB3	1:G:1362:LEU:HD22	1.83	0.60
1:G:831:ILE:HG23	1:G:835:ILE:HD12	1.84	0.59
1:A:458:PHE:HB3	1:A:1362:LEU:HD22	1.84	0.59
1:C:458:PHE:HB3	1:C:1362:LEU:HD22	1.83	0.59
1:C:1354:LEU:HB2	1:C:1384:ASP:HB2	1.84	0.59
1:A:450:ARG:NH1	1:A:1379:GLN:OE1	2.34	0.59
1:F:281:ARG:NH2	1:F:307:ASP:OD1	2.34	0.59
1:C:151:ALA:O	1:C:155:LEU:HB2	2.03	0.59
1:G:682:ASN:ND2	1:G:957:ILE:O	2.35	0.59
1:G:281:ARG:NH2	1:G:307:ASP:OD1	2.35	0.59
1:G:989:LEU:HD11	1:G:1008:PRO:HG3	1.85	0.59
1:E:740:ASN:OD1	1:E:1058:GLN:NE2	2.35	0.59
1:F:1054:SER:O	1:F:1058:GLN:NE2	2.36	0.59
1:A:1354:LEU:HB2	1:A:1384:ASP:HB2	1.84	0.59
1:E:831:ILE:HG23	1:E:835:ILE:HD12	1.84	0.59
1:F:1351:TYR:HB3	1:F:1386:SER:HA	1.85	0.59
1:C:908:ASP:HA	1:C:911:LEU:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:THR:OG1	1:A:33:GLY:N	2.36	0.58
1:C:281:ARG:NH2	1:C:307:ASP:OD1	2.35	0.58
1:C:1357:SER:HG	1:C:1380:TYR:H	1.51	0.58
1:F:989:LEU:HD11	1:F:1008:PRO:HG3	1.85	0.58
1:G:564:ASP:OD2	1:G:1022:ARG:NH1	2.37	0.58
1:F:908:ASP:HA	1:F:911:LEU:HB2	1.85	0.58
1:G:32:THR:OG1	1:G:33:GLY:N	2.37	0.58
1:E:32:THR:OG1	1:E:33:GLY:N	2.37	0.58
1:F:831:ILE:HG23	1:F:835:ILE:HD12	1.84	0.58
1:G:784:LEU:HB3	1:G:800:VAL:HG13	1.85	0.58
1:A:279:ASN:HD21	1:A:283:ARG:HB3	1.69	0.58
1:A:1080:GLU:HB2	1:A:1133:ALA:HB3	1.86	0.58
1:E:564:ASP:OD2	1:E:1022:ARG:NH1	2.37	0.58
1:F:236:ARG:O	1:F:240:ALA:HB2	2.04	0.58
1:G:454:PRO:HB3	1:G:1379:GLN:HG3	1.85	0.58
2:R:147:ARG:NH1	3:V:274:SER:O	2.37	0.58
1:A:594:ILE:HG22	1:A:596:GLY:H	1.68	0.57
1:C:279:ASN:HD21	1:C:283:ARG:HB3	1.68	0.57
1:C:682:ASN:ND2	1:C:957:ILE:O	2.37	0.57
4:Z:265:TYR:HA	4:Z:274:ILE:HA	1.86	0.57
1:C:25:ILE:HG23	1:C:155:LEU:HG	1.86	0.57
1:C:454:PRO:HB3	1:C:1379:GLN:HG3	1.86	0.57
1:E:908:ASP:HA	1:E:911:LEU:HB2	1.85	0.57
1:A:653:ASN:ND2	1:A:919:ASP:OD2	2.37	0.57
1:E:774:ARG:NH2	1:E:777:GLY:O	2.38	0.57
1:C:989:LEU:HD11	1:C:1008:PRO:HG3	1.85	0.57
1:F:594:ILE:HG22	1:F:596:GLY:H	1.69	0.57
1:G:774:ARG:NH2	1:G:777:GLY:O	2.38	0.57
1:G:908:ASP:HA	1:G:911:LEU:HB2	1.85	0.57
1:F:32:THR:OG1	1:F:33:GLY:N	2.38	0.57
1:G:594:ILE:HG22	1:G:596:GLY:H	1.69	0.57
1:A:438:ALA:HB2	1:C:439:GLY:HA3	1.87	0.56
1:C:774:ARG:NH2	1:C:777:GLY:O	2.38	0.56
1:G:468:GLN:O	1:G:1143:ASN:ND2	2.38	0.56
1:G:171:ILE:HA	1:G:174:ILE:HG22	1.88	0.56
1:A:564:ASP:OD2	1:A:1022:ARG:NH1	2.37	0.56
1:A:1010:PRO:HG2	1:A:1013:LEU:HB2	1.86	0.56
1:C:438:ALA:HB2	1:E:439:GLY:HA3	1.87	0.56
1:C:564:ASP:OD2	1:C:1022:ARG:NH1	2.39	0.56
1:C:939:THR:O	1:C:943:ARG:NH1	2.38	0.56
1:C:1351:TYR:HB3	1:C:1386:SER:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:594:ILE:HG22	1:E:596:GLY:H	1.69	0.56
1:A:908:ASP:HA	1:A:911:LEU:HB2	1.87	0.56
1:E:199:VAL:HA	1:E:202:GLU:HG2	1.88	0.56
1:E:989:LEU:HD11	1:E:1008:PRO:HG3	1.87	0.56
1:G:101:TYR:O	1:G:103:ARG:NH1	2.38	0.56
4:Z:145:LEU:HD12	4:Z:194:TYR:HB2	1.86	0.56
1:C:1058:GLN:HB3	1:C:1063:PHE:HB3	1.86	0.56
1:F:591:LEU:O	1:F:1022:ARG:NH2	2.39	0.56
2:R:10:VAL:HB	2:R:83:LEU:HB3	1.87	0.56
1:F:454:PRO:HB3	1:F:1379:GLN:HG3	1.88	0.56
1:G:939:THR:O	1:G:943:ARG:NH1	2.38	0.56
4:Z:328:THR:OG1	4:Z:335:GLY:O	2.24	0.56
1:F:450:ARG:HH12	1:F:1379:GLN:H	1.53	0.56
1:F:1214:ASP:OD2	1:F:1216:GLN:NE2	2.39	0.56
1:A:740:ASN:OD1	1:A:1058:GLN:NE2	2.39	0.55
1:A:1100:HIS:HB3	1:A:1111:THR:HB	1.88	0.55
1:F:217:GLN:HE21	1:F:220:GLY:HA2	1.71	0.55
1:F:774:ARG:NH2	1:F:777:GLY:O	2.39	0.55
1:A:1058:GLN:HB3	1:A:1063:PHE:HB3	1.89	0.55
1:C:939:THR:HG22	1:C:1157:MET:HA	1.88	0.55
1:E:1351:TYR:HB3	1:E:1386:SER:HA	1.88	0.55
1:G:415:ILE:HD11	1:G:1077:PHE:HD2	1.72	0.55
1:C:32:THR:OG1	1:C:33:GLY:N	2.39	0.55
1:C:603:CYS:HB3	1:C:608:ARG:HH21	1.72	0.55
1:E:1100:HIS:HB3	1:E:1111:THR:HB	1.89	0.55
1:A:450:ARG:HH12	1:A:1378:ALA:H	1.54	0.55
1:A:511:GLY:HA3	1:A:776:SER:HA	1.88	0.55
1:E:217:GLN:HE21	1:E:220:GLY:HA2	1.71	0.55
1:A:404:ALA:O	1:G:113:GLN:NE2	2.34	0.55
1:F:564:ASP:OD2	1:F:1022:ARG:NH1	2.40	0.55
1:A:591:LEU:O	1:A:1022:ARG:NH2	2.40	0.54
1:F:438:ALA:HB2	1:G:439:GLY:HA3	1.89	0.54
1:G:591:LEU:O	1:G:1022:ARG:NH2	2.40	0.54
1:A:101:TYR:O	1:A:103:ARG:NH1	2.40	0.54
1:C:207:LEU:HD22	1:C:262:MET:HG3	1.89	0.54
1:G:479:CYS:SG	1:G:1056:THR:OG1	2.66	0.54
1:A:774:ARG:NH2	1:A:777:GLY:O	2.40	0.54
1:A:787:VAL:HG13	1:A:920:MET:HB2	1.88	0.54
1:C:263:VAL:HG22	1:C:390:LYS:HD2	1.88	0.54
1:C:1144:THR:OG1	1:C:1202:SER:O	2.25	0.54
1:A:472:ARG:HA	1:A:1059:LEU:HD13	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:458:PHE:N	1:C:1356:SER:O	2.35	0.54
1:E:1214:ASP:OD2	1:E:1216:GLN:NE2	2.40	0.54
1:G:603:CYS:HB3	1:G:608:ARG:HH21	1.72	0.54
1:C:91:CYS:HB3	1:C:196:LEU:HD11	1.89	0.54
1:C:511:GLY:HA3	1:C:776:SER:HA	1.90	0.54
1:E:591:LEU:O	1:E:1022:ARG:NH2	2.40	0.54
1:G:1058:GLN:HB3	1:G:1063:PHE:HB3	1.89	0.54
1:A:1351:TYR:HB3	1:A:1386:SER:HA	1.90	0.54
1:C:415:ILE:HG22	1:C:1077:PHE:H	1.73	0.54
1:C:594:ILE:HG22	1:C:596:GLY:H	1.71	0.54
1:F:472:ARG:HA	1:F:1059:LEU:HD13	1.90	0.54
1:F:415:ILE:HD11	1:F:1077:PHE:HD2	1.72	0.54
3:V:28:GLU:OE1	3:V:309:ARG:NH2	2.41	0.54
4:Z:281:PRO:HA	4:Z:467:VAL:HA	1.90	0.54
1:A:273:SER:OG	1:A:1087:ARG:NH2	2.41	0.54
1:A:842:ARG:NH1	1:A:1032:SER:O	2.41	0.54
2:R:127:ARG:NE	2:R:129:ASP:OD1	2.38	0.54
3:V:282:ARG:NH2	4:Z:475:ASN:OD1	2.40	0.54
1:A:1357:SER:HG	1:A:1380:TYR:H	1.56	0.54
1:E:295:LEU:HA	1:E:298:GLN:HB3	1.90	0.54
1:G:149:SER:OG	1:G:1106:GLY:O	2.26	0.54
1:G:778:ARG:NH2	1:G:798:ASP:O	2.41	0.54
1:C:560:ASN:HB3	1:C:563:PHE:HB2	1.90	0.53
1:E:979:VAL:HG23	1:E:1009:ILE:HG23	1.89	0.53
1:F:744:THR:HA	1:F:827:ILE:HD12	1.89	0.53
1:F:883:PRO:O	1:F:895:ASN:ND2	2.42	0.53
1:G:267:GLN:HE21	1:G:1124:GLY:HA3	1.73	0.53
1:A:744:THR:HA	1:A:827:ILE:HD12	1.90	0.53
1:F:458:PHE:HB3	1:F:1362:LEU:HD22	1.90	0.53
4:Z:146:ARG:HH22	4:Z:151:LEU:HD11	1.73	0.53
4:Z:205:ARG:NH1	4:Z:208:GLU:OE2	2.39	0.53
1:A:660:LEU:HD21	1:A:916:LEU:HD22	1.90	0.53
1:A:454:PRO:HB3	1:A:1379:GLN:HG3	1.89	0.53
1:C:145:PHE:HB3	1:C:1110:PHE:HB2	1.89	0.53
1:E:151:ALA:O	1:E:155:LEU:HB2	2.08	0.53
1:E:472:ARG:HA	1:E:1059:LEU:HD13	1.90	0.53
1:F:603:CYS:HB3	1:F:608:ARG:HH21	1.74	0.53
1:F:729:GLU:OE2	1:F:1060:ARG:NH2	2.41	0.53
1:G:979:VAL:HG23	1:G:1009:ILE:HG23	1.90	0.53
1:E:603:CYS:HB3	1:E:608:ARG:HH21	1.74	0.53
1:F:778:ARG:NH2	1:F:798:ASP:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:729:GLU:OE2	1:G:1060:ARG:NH2	2.42	0.53
1:C:842:ARG:NH1	1:C:1032:SER:O	2.42	0.53
1:E:778:ARG:NH2	1:E:798:ASP:O	2.42	0.53
1:E:1058:GLN:HB3	1:E:1063:PHE:HB3	1.91	0.53
1:G:84:GLU:HB2	1:G:380:VAL:HG11	1.89	0.53
1:E:883:PRO:O	1:E:895:ASN:ND2	2.42	0.53
1:F:436:ARG:NH2	1:F:1372:ALA:O	2.38	0.53
1:F:627:ILE:HD11	1:F:1036:PHE:HB2	1.91	0.53
1:F:1086:GLU:HB2	1:F:1089:SER:HB2	1.89	0.53
3:V:143:GLN:OE1	3:V:147:ARG:NH1	2.40	0.53
1:C:744:THR:HA	1:C:827:ILE:HD12	1.91	0.53
1:E:660:LEU:HD21	1:E:916:LEU:HD22	1.91	0.53
1:E:627:ILE:HD11	1:E:1036:PHE:HB2	1.91	0.52
1:G:627:ILE:HD11	1:G:1036:PHE:HB2	1.91	0.52
1:A:1363:ARG:NH2	1:G:1374:GLU:OE1	2.41	0.52
1:G:726:ILE:HB	1:G:1060:ARG:HH21	1.75	0.52
1:A:519:GLN:O	1:A:522:ARG:NH1	2.43	0.52
1:F:1010:PRO:HG2	1:F:1013:LEU:HB2	1.92	0.52
4:Z:286:ARG:NH1	4:Z:288:ASP:OD2	2.42	0.52
1:C:195:GLN:HE22	1:C:1116:ARG:HD2	1.74	0.52
1:F:511:GLY:HA3	1:F:776:SER:HA	1.92	0.52
1:G:883:PRO:O	1:G:895:ASN:ND2	2.42	0.52
1:A:1144:THR:OG1	1:A:1202:SER:O	2.27	0.52
1:E:1144:THR:OG1	1:E:1202:SER:O	2.26	0.52
1:A:415:ILE:HD11	1:A:1077:PHE:HD2	1.74	0.52
1:A:778:ARG:NH2	1:A:798:ASP:O	2.42	0.52
1:C:627:ILE:HD11	1:C:1036:PHE:HB2	1.92	0.52
1:E:479:CYS:SG	1:E:1056:THR:OG1	2.67	0.52
1:F:479:CYS:SG	1:F:1056:THR:OG1	2.67	0.52
1:F:660:LEU:HD21	1:F:916:LEU:HD22	1.92	0.52
1:G:744:THR:HA	1:G:827:ILE:HD12	1.92	0.52
1:C:1100:HIS:HB3	1:C:1111:THR:HB	1.92	0.52
1:E:1010:PRO:HG2	1:E:1013:LEU:HB2	1.91	0.52
1:G:1351:TYR:HB3	1:G:1386:SER:HA	1.91	0.52
1:E:660:LEU:HB3	1:E:664:LEU:HD23	1.92	0.52
1:E:1114:GLN:OE1	1:E:1116:ARG:NH2	2.43	0.52
1:F:1114:GLN:OE1	1:F:1116:ARG:NH2	2.43	0.52
1:G:660:LEU:HD21	1:G:916:LEU:HD22	1.92	0.52
1:F:1144:THR:OG1	1:F:1202:SER:O	2.29	0.51
1:A:660:LEU:HB3	1:A:664:LEU:HD23	1.92	0.51
1:C:1010:PRO:HG2	1:C:1013:LEU:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:386:ILE:HA	1:E:391:LEU:HA	1.91	0.51
1:E:653:ASN:ND2	1:E:919:ASP:OD2	2.43	0.51
1:G:511:GLY:HA3	1:G:776:SER:HA	1.92	0.51
1:A:149:SER:OG	1:A:1106:GLY:O	2.29	0.51
1:C:979:VAL:HG23	1:C:1009:ILE:HG23	1.91	0.51
1:G:217:GLN:HA	1:G:222:LEU:HD11	1.91	0.51
1:G:295:LEU:HD13	1:G:1080:GLU:HG2	1.93	0.51
1:G:653:ASN:ND2	1:G:919:ASP:OD2	2.43	0.51
4:Z:121:LEU:HD11	4:Z:263:LEU:HD22	1.93	0.51
1:A:1214:ASP:OD2	1:A:1216:GLN:NE2	2.42	0.51
1:C:660:LEU:HD21	1:C:916:LEU:HD22	1.91	0.51
1:F:735:THR:HG23	1:F:738:ALA:H	1.75	0.51
1:A:217:GLN:HA	1:A:222:LEU:HD11	1.93	0.51
2:R:36:THR:OG1	2:R:38:ARG:NH1	2.44	0.51
1:A:281:ARG:NH2	1:A:307:ASP:OD1	2.44	0.51
1:A:397:LEU:HG	1:A:401:VAL:HG12	1.93	0.51
1:A:729:GLU:OE2	1:A:1060:ARG:NH2	2.44	0.51
1:C:784:LEU:HB2	1:C:800:VAL:HG13	1.93	0.51
1:F:726:ILE:HB	1:F:1060:ARG:HH21	1.76	0.51
1:F:1080:GLU:HB3	1:F:1133:ALA:HB3	1.93	0.51
1:G:1010:PRO:HG2	1:G:1013:LEU:HB2	1.93	0.51
1:E:459:PHE:HE1	1:E:469:LEU:HD23	1.76	0.51
1:E:784:LEU:HB2	1:E:800:VAL:HG13	1.93	0.51
2:R:295:VAL:HA	2:R:312:VAL:HG12	1.93	0.51
4:Z:320:HIS:ND1	4:Z:345:LEU:O	2.42	0.51
1:E:842:ARG:NH1	1:E:1032:SER:O	2.44	0.51
1:A:603:CYS:HB3	1:A:608:ARG:HH21	1.76	0.51
1:E:1157:MET:SD	1:E:1163:THR:OG1	2.69	0.51
1:C:735:THR:HG23	1:C:738:ALA:H	1.76	0.51
1:G:660:LEU:HB3	1:G:664:LEU:HD23	1.92	0.51
2:R:4:MET:O	2:R:92:THR:OG1	2.29	0.51
3:V:158:VAL:HA	3:V:161:THR:HG22	1.93	0.51
1:E:729:GLU:OE2	1:E:1060:ARG:NH2	2.42	0.50
1:E:735:THR:HG23	1:E:738:ALA:H	1.77	0.50
1:E:1354:LEU:HB2	1:E:1384:ASP:HB2	1.93	0.50
1:F:842:ARG:NH1	1:F:1032:SER:O	2.44	0.50
1:E:217:GLN:HA	1:E:222:LEU:HD11	1.94	0.50
1:F:295:LEU:HD13	1:F:1080:GLU:HG2	1.93	0.50
1:C:883:PRO:O	1:C:895:ASN:ND2	2.44	0.50
1:F:1073:ARG:NH1	1:F:1142:GLY:O	2.41	0.50
1:A:726:ILE:HB	1:A:1060:ARG:HH21	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:386:ILE:HA	1:F:391:LEU:HA	1.92	0.50
1:E:91:CYS:HB3	1:E:196:LEU:HD11	1.92	0.50
1:F:1052:PRO:O	1:F:1056:THR:OG1	2.30	0.50
2:R:208:MET:HB2	2:R:211:ILE:HD12	1.93	0.50
1:C:149:SER:OG	1:C:1106:GLY:O	2.30	0.50
1:C:591:LEU:O	1:C:1022:ARG:NH2	2.44	0.50
1:C:660:LEU:HB3	1:C:664:LEU:HD23	1.92	0.50
1:E:511:GLY:HA3	1:E:776:SER:HA	1.93	0.50
1:E:1052:PRO:HA	1:E:1055:LEU:HG	1.94	0.50
1:F:135:ARG:NH1	1:F:135:ARG:HA	2.27	0.50
1:G:105:GLY:O	1:G:135:ARG:NH2	2.41	0.50
1:A:624:PRO:HA	1:A:627:ILE:HG22	1.94	0.50
1:C:96:PHE:HD2	1:C:99:LEU:HB2	1.77	0.50
1:C:778:ARG:NH2	1:C:798:ASP:O	2.45	0.50
1:G:1144:THR:OG1	1:G:1202:SER:O	2.30	0.50
1:A:468:GLN:O	1:A:1143:ASN:ND2	2.45	0.50
1:G:735:THR:HG23	1:G:738:ALA:H	1.76	0.50
1:G:849:GLY:HA3	1:G:924:THR:HG21	1.94	0.50
4:Z:322:PHE:O	4:Z:341:ALA:N	2.41	0.50
1:A:439:GLY:HA3	1:G:438:ALA:HB2	1.93	0.50
1:C:1216:GLN:HA	1:C:1219:ARG:HG3	1.94	0.50
1:G:415:ILE:HG23	1:G:1079:THR:HG21	1.94	0.50
1:A:735:THR:HG23	1:A:738:ALA:H	1.77	0.49
1:E:1367:ALA:HB1	1:E:1370:THR:HA	1.94	0.49
1:F:91:CYS:HB3	1:F:196:LEU:HD11	1.93	0.49
4:Z:144:ILE:HG23	4:Z:259:PHE:HB2	1.93	0.49
1:A:291:THR:HG22	1:A:292:THR:H	1.77	0.49
1:E:438:ALA:HB2	1:F:439:GLY:HA3	1.94	0.49
2:R:150:ILE:HA	2:R:153:VAL:HG22	1.94	0.49
3:V:34:PHE:HA	3:V:70:ARG:HH21	1.77	0.49
1:C:386:ILE:HA	1:C:391:LEU:HA	1.94	0.49
1:E:624:PRO:HA	1:E:627:ILE:HG22	1.94	0.49
1:E:744:THR:HA	1:E:827:ILE:HD12	1.93	0.49
1:F:217:GLN:HA	1:F:222:LEU:HD11	1.95	0.49
1:G:624:PRO:HA	1:G:627:ILE:HG22	1.94	0.49
1:G:980:ASN:HB3	1:G:983:PHE:H	1.77	0.49
1:E:1365:ALA:HB2	1:E:1381:LEU:HD11	1.95	0.49
3:V:160:ARG:NH1	3:V:190:LEU:O	2.45	0.49
1:A:25:ILE:HG23	1:A:155:LEU:HG	1.95	0.49
1:A:1365:ALA:HB2	1:A:1381:LEU:HD11	1.93	0.49
1:F:624:PRO:HA	1:F:627:ILE:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:842:ARG:NH1	1:G:1032:SER:O	2.45	0.49
3:V:219:LEU:HA	3:V:222:ILE:HG22	1.94	0.49
1:C:726:ILE:HD13	1:C:1060:ARG:HE	1.77	0.49
1:F:1367:ALA:HB1	1:F:1370:THR:HA	1.94	0.49
1:G:236:ARG:O	1:G:240:ALA:HB2	2.12	0.49
3:V:8:ILE:HD12	3:V:34:PHE:HE1	1.75	0.49
1:A:1052:PRO:HA	1:A:1055:LEU:HG	1.93	0.49
1:C:1367:ALA:HB1	1:C:1370:THR:HA	1.93	0.49
1:E:101:TYR:O	1:E:103:ARG:NH1	2.46	0.49
1:E:241:ASP:N	1:E:241:ASP:OD1	2.45	0.49
1:F:149:SER:OG	1:F:1106:GLY:O	2.30	0.49
1:F:908:ASP:OD1	1:F:908:ASP:N	2.45	0.49
1:G:416:ASP:OD1	1:G:1076:ARG:NH1	2.45	0.49
1:A:1216:GLN:HA	1:A:1219:ARG:HG3	1.95	0.49
1:F:25:ILE:HG23	1:F:155:LEU:HG	1.94	0.49
2:R:223:PRO:HA	2:R:228:LEU:HD13	1.94	0.49
1:A:416:ASP:OD1	1:A:1076:ARG:NH1	2.46	0.49
1:C:849:GLY:HA3	1:C:924:THR:HG21	1.95	0.49
1:E:908:ASP:OD1	1:E:908:ASP:N	2.46	0.49
1:C:236:ARG:O	1:C:240:ALA:HB2	2.13	0.48
1:F:171:ILE:HA	1:F:174:ILE:HG22	1.95	0.48
1:C:171:ILE:HA	1:C:174:ILE:HG22	1.95	0.48
1:C:624:PRO:HA	1:C:627:ILE:HG22	1.96	0.48
1:G:291:THR:HG22	1:G:292:THR:H	1.78	0.48
1:F:1052:PRO:HA	1:F:1055:LEU:HG	1.96	0.48
3:V:175:ASP:HB2	3:V:186:LEU:HB3	1.94	0.48
1:A:450:ARG:HH21	1:A:1376:HIS:HB3	1.77	0.48
1:A:642:ILE:HD11	1:A:897:TYR:HB3	1.96	0.48
1:E:1352:PRO:HG2	1:E:1385:ALA:HB3	1.95	0.48
1:F:96:PHE:HD2	1:F:99:LEU:HB2	1.78	0.48
1:C:812:GLY:HA3	1:C:815:ILE:HD12	1.95	0.48
2:R:147:ARG:HH12	3:V:278:SER:HB2	1.77	0.48
1:F:1100:HIS:HB3	1:F:1111:THR:HB	1.94	0.48
1:F:1354:LEU:HB2	1:F:1384:ASP:HB2	1.96	0.48
4:Z:144:ILE:HG22	4:Z:195:VAL:HG12	1.95	0.48
1:A:263:VAL:HG12	1:A:390:LYS:HE2	1.95	0.48
1:C:908:ASP:OD1	1:C:908:ASP:N	2.46	0.48
1:C:980:ASN:HB3	1:C:983:PHE:H	1.77	0.48
1:E:149:SER:OG	1:E:1106:GLY:O	2.31	0.48
1:F:241:ASP:OD1	1:F:241:ASP:N	2.46	0.48
1:F:660:LEU:HB3	1:F:664:LEU:HD23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:812:GLY:HA3	1:F:815:ILE:HD12	1.96	0.48
1:A:1057:HIS:CE1	1:A:1060:ARG:HH22	2.32	0.48
1:C:548:ILE:HA	1:C:555:LEU:HD13	1.96	0.48
1:F:304:LEU:HD13	1:F:385:VAL:HG11	1.96	0.48
1:G:1214:ASP:OD2	1:G:1216:GLN:NE2	2.46	0.48
2:R:217:LEU:HA	2:R:221:LEU:HD13	1.96	0.48
1:A:171:ILE:HA	1:A:174:ILE:HG22	1.96	0.48
1:A:440:ASP:HB2	1:A:1376:HIS:CE1	2.49	0.48
1:A:627:ILE:HD11	1:A:1036:PHE:HB2	1.96	0.48
1:A:763:ASP:O	1:A:767:ARG:NH1	2.47	0.48
1:A:883:PRO:O	1:A:895:ASN:ND2	2.47	0.48
1:C:740:ASN:OD1	1:C:1058:GLN:NE2	2.47	0.48
1:E:1057:HIS:CE1	1:E:1060:ARG:HH22	2.31	0.48
1:A:865:PRO:HB3	1:A:888:GLN:HE22	1.78	0.47
1:A:1367:ALA:HB1	1:A:1370:THR:HA	1.95	0.47
1:F:1053:ILE:O	1:F:1057:HIS:ND1	2.45	0.47
1:G:865:PRO:HB3	1:G:888:GLN:HE22	1.79	0.47
2:R:114:CYS:HB3	2:R:141:ILE:HG23	1.96	0.47
3:V:47:ALA:HB2	3:V:133:LEU:HD12	1.95	0.47
1:C:283:ARG:HH12	1:C:386:ILE:HD12	1.78	0.47
1:C:471:LEU:HB3	1:C:1059:LEU:HD22	1.96	0.47
1:G:1052:PRO:HA	1:G:1055:LEU:HG	1.95	0.47
2:R:288:GLY:O	2:R:290:ARG:NH1	2.47	0.47
1:A:560:ASN:HB3	1:A:563:PHE:HB2	1.94	0.47
1:E:980:ASN:HB3	1:E:983:PHE:H	1.78	0.47
1:E:1144:THR:HG22	1:E:1175:ARG:HB3	1.97	0.47
4:Z:221:ALA:O	4:Z:225:ALA:CB	2.62	0.47
1:F:291:THR:HG22	1:F:292:THR:H	1.79	0.47
1:F:865:PRO:HB3	1:F:888:GLN:HE22	1.78	0.47
1:G:91:CYS:HB3	1:G:196:LEU:HD11	1.96	0.47
1:F:1361:MET:O	1:F:1365:ALA:HB2	2.15	0.47
2:R:112:TYR:HB2	2:R:143:GLN:HG2	1.96	0.47
3:V:112:TYR:O	3:V:143:GLN:N	2.48	0.47
4:Z:430:TYR:HH	4:Z:477:CYS:HG	1.58	0.47
4:Z:346:ASN:OD1	4:Z:347:GLU:N	2.47	0.47
1:C:217:GLN:HA	1:C:222:LEU:HD11	1.95	0.47
1:C:397:LEU:HG	1:C:401:VAL:HG12	1.96	0.47
1:F:774:ARG:NH1	1:F:779:ASN:OD1	2.48	0.47
1:F:1091:SER:HB3	1:F:1121:LEU:HD23	1.97	0.47
1:G:812:GLY:HA3	1:G:815:ILE:HD12	1.96	0.47
1:G:1367:ALA:HB1	1:G:1370:THR:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Z:154:LEU:HG	4:Z:156:ARG:H	1.79	0.47
1:G:25:ILE:HD13	1:G:174:ILE:HD13	1.97	0.47
1:A:908:ASP:OD1	1:A:908:ASP:N	2.47	0.47
1:G:1057:HIS:CE1	1:G:1060:ARG:HH22	2.32	0.47
1:E:296:LYS:NZ	1:E:394:LEU:O	2.47	0.46
1:E:1053:ILE:O	1:E:1057:HIS:ND1	2.48	0.46
1:F:243:PHE:HZ	1:F:415:ILE:HD13	1.81	0.46
1:F:628:LYS:HA	1:F:631:LYS:HG2	1.98	0.46
4:Z:203:ALA:O	4:Z:219:ARG:NH1	2.48	0.46
4:Z:221:ALA:O	4:Z:225:ALA:HB2	2.15	0.46
1:C:479:CYS:SG	1:C:1056:THR:OG1	2.68	0.46
1:F:458:PHE:N	1:F:1356:SER:O	2.35	0.46
1:F:913:LEU:HD13	1:F:916:LEU:HD23	1.97	0.46
1:G:882:HIS:HE1	1:G:884:LEU:HD12	1.80	0.46
2:R:30:LYS:NZ	2:R:124:ASP:OD2	2.41	0.46
3:V:24:LEU:HD11	3:V:128:LEU:HD21	1.97	0.46
4:Z:131:PHE:HZ	4:Z:262:LEU:HD13	1.80	0.46
1:C:628:LYS:HA	1:C:631:LYS:HG2	1.97	0.46
1:E:171:ILE:HA	1:E:174:ILE:HG22	1.98	0.46
1:F:468:GLN:O	1:F:1143:ASN:ND2	2.48	0.46
4:Z:303:VAL:O	4:Z:340:LEU:N	2.42	0.46
1:C:287:GLY:HA3	1:C:1084:TYR:HE1	1.80	0.46
1:F:859:LEU:HA	1:F:894:LEU:HD21	1.98	0.46
1:A:32:THR:HB	1:A:35:VAL:HG23	1.98	0.46
1:A:172:ARG:HD2	1:A:172:ARG:HA	1.80	0.46
1:A:842:ARG:HH12	1:A:1033:LYS:HA	1.81	0.46
1:E:560:ASN:HB3	1:E:563:PHE:HB2	1.98	0.46
3:V:215:THR:O	3:V:219:LEU:CB	2.64	0.46
1:E:849:GLY:HA3	1:E:924:THR:HG21	1.98	0.46
1:F:245:MET:HG3	1:F:1132:ALA:HB1	1.98	0.46
1:C:304:LEU:HD13	1:C:385:VAL:HG11	1.98	0.46
1:F:1004:LYS:HD3	1:F:1004:LYS:HA	1.74	0.46
1:C:642:ILE:HD11	1:C:897:TYR:HB3	1.98	0.46
1:E:96:PHE:HD2	1:E:99:LEU:HB2	1.80	0.46
1:F:280:THR:HG22	1:F:379:ARG:HH21	1.81	0.46
2:R:156:ARG:O	2:R:160:ASP:CB	2.64	0.46
1:A:255:ILE:HG21	1:A:303:ILE:HD13	1.98	0.45
1:C:105:GLY:O	1:C:135:ARG:NH2	2.48	0.45
1:G:386:ILE:HA	1:G:391:LEU:HA	1.98	0.45
1:G:628:LYS:HA	1:G:631:LYS:HG2	1.99	0.45
1:A:236:ARG:O	1:A:240:ALA:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:32:THR:HB	1:E:35:VAL:HG23	1.97	0.45
1:G:213:ILE:HD13	1:G:230:LEU:HD11	1.98	0.45
2:R:294:ARG:HB2	2:R:313:ILE:HG13	1.98	0.45
1:A:213:ILE:HD13	1:A:230:LEU:HD11	1.98	0.45
1:E:82:PHE:HZ	1:E:196:LEU:HD13	1.81	0.45
1:E:628:LYS:HA	1:E:631:LYS:HG2	1.99	0.45
1:E:812:GLY:HA3	1:E:815:ILE:HD12	1.99	0.45
1:F:849:GLY:HA3	1:F:924:THR:HG21	1.97	0.45
1:G:1053:ILE:O	1:G:1057:HIS:ND1	2.50	0.45
1:C:213:ILE:HG13	1:C:230:LEU:HD21	1.99	0.45
1:C:913:LEU:HD13	1:C:916:LEU:HD23	1.98	0.45
1:G:1083:LEU:HD12	1:G:1129:CYS:HB3	1.97	0.45
2:R:269:ILE:HA	2:R:272:THR:HG22	1.99	0.45
1:C:774:ARG:NH1	1:C:779:ASN:OD1	2.50	0.45
1:E:1086:GLU:HB2	1:E:1089:SER:HB2	1.98	0.45
1:A:1053:ILE:O	1:A:1057:HIS:ND1	2.50	0.45
2:R:220:ALA:HA	3:V:215:THR:HG23	1.97	0.45
1:A:1217:TYR:CZ	1:A:1222:CYS:HB2	2.51	0.45
1:C:882:HIS:HE1	1:C:884:LEU:HD12	1.82	0.45
1:F:784:LEU:HB2	1:F:800:VAL:HG13	1.98	0.45
1:F:1057:HIS:CE1	1:F:1060:ARG:HH22	2.34	0.45
1:A:436:ARG:NH2	1:A:1372:ALA:O	2.49	0.45
1:E:279:ASN:OD1	1:E:283:ARG:N	2.50	0.45
1:E:548:ILE:HA	1:E:555:LEU:HD13	1.99	0.45
1:E:726:ILE:HB	1:E:1060:ARG:HH21	1.82	0.45
4:Z:292:THR:HG23	4:Z:294:ARG:H	1.81	0.45
1:C:84:GLU:HB2	1:C:380:VAL:HG11	1.98	0.45
1:C:729:GLU:O	1:C:736:SER:OG	2.35	0.45
1:G:287:GLY:HA3	1:G:1084:TYR:HE1	1.82	0.45
1:A:241:ASP:OD1	1:A:241:ASP:N	2.51	0.44
1:A:245:MET:HG3	1:A:1132:ALA:HB1	1.99	0.44
1:E:882:HIS:HE1	1:E:884:LEU:HD12	1.83	0.44
2:R:8:ILE:HB	2:R:85:ALA:HB3	1.99	0.44
1:A:386:ILE:HA	1:A:391:LEU:HA	1.99	0.44
1:C:296:LYS:NZ	1:C:383:ASP:OD1	2.50	0.44
1:E:865:PRO:HB3	1:E:888:GLN:HE22	1.81	0.44
1:G:421:MET:HB3	1:G:1071:VAL:HG23	1.97	0.44
2:R:108:CYS:HB2	4:Z:146:ARG:HE	1.82	0.44
1:A:415:ILE:HG23	1:A:1079:THR:HG21	1.98	0.44
1:A:548:ILE:HA	1:A:555:LEU:HD13	1.99	0.44
1:A:882:HIS:HE1	1:A:884:LEU:HD12	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:782:GLN:HB2	1:C:800:VAL:HA	1.99	0.44
1:F:548:ILE:HA	1:F:555:LEU:HD13	2.00	0.44
1:F:1352:PRO:HG2	1:F:1385:ALA:HB3	1.99	0.44
1:G:1361:MET:HB3	1:G:1381:LEU:HD12	1.98	0.44
1:A:628:LYS:HA	1:A:631:LYS:HG2	1.99	0.44
1:C:865:PRO:HB3	1:C:888:GLN:HE22	1.83	0.44
1:E:859:LEU:HA	1:E:894:LEU:HD21	2.00	0.44
1:F:172:ARG:HA	1:F:172:ARG:HD2	1.81	0.44
4:Z:324:VAL:HG23	4:Z:433:TYR:HB3	1.99	0.44
1:A:554:ARG:NH2	1:A:558:GLU:OE2	2.49	0.44
1:A:1004:LYS:HA	1:A:1004:LYS:HD3	1.73	0.44
1:C:435:THR:OG1	1:C:436:ARG:N	2.51	0.44
1:E:278:THR:HA	1:E:284:GLN:HA	1.99	0.44
1:G:859:LEU:HA	1:G:894:LEU:HD21	1.99	0.44
4:Z:356:PHE:O	4:Z:358:LEU:N	2.51	0.44
1:A:87:LEU:HD21	1:A:196:LEU:HD22	2.00	0.44
1:A:558:GLU:OE1	1:A:592:ARG:NH2	2.49	0.44
1:E:207:LEU:HD22	1:E:262:MET:HG3	2.00	0.44
1:F:1068:ALA:HB2	1:F:1211:VAL:HA	2.00	0.44
1:G:259:LEU:HG	1:G:387:VAL:HG11	1.99	0.44
4:Z:458:VAL:HA	4:Z:459:PRO:HD3	1.90	0.44
1:A:846:CYS:HB2	1:A:985:CYS:HB3	1.64	0.44
1:E:774:ARG:NH1	1:E:779:ASN:OD1	2.50	0.44
1:E:782:GLN:HB2	1:E:800:VAL:HA	2.00	0.44
1:G:908:ASP:N	1:G:908:ASP:OD1	2.47	0.44
3:V:267:PHE:HB2	3:V:270:TYR:HB3	2.00	0.44
4:Z:261:SER:H	4:Z:276:ALA:HB1	1.83	0.44
1:A:277:HIS:HD2	1:A:313:VAL:HG22	1.83	0.44
1:E:397:LEU:HG	1:E:401:VAL:HG12	2.00	0.44
1:F:137:HIS:CE1	1:F:139:ARG:HE	2.35	0.44
1:G:774:ARG:NH1	1:G:779:ASN:OD1	2.51	0.44
2:R:111:ASP:OD2	4:Z:146:ARG:NH2	2.47	0.44
4:Z:439:ILE:HG21	4:Z:444:VAL:HG12	2.00	0.44
1:C:194:ASP:OD1	1:C:402:TYR:OH	2.29	0.44
1:E:782:GLN:HB3	1:E:784:LEU:HD23	1.99	0.44
1:A:949:ASP:OD1	1:A:949:ASP:N	2.50	0.43
1:C:440:ASP:HB2	1:C:1376:HIS:CD2	2.53	0.43
1:C:1056:THR:O	1:C:1060:ARG:HG2	2.17	0.43
1:G:470:THR:HG22	1:G:471:LEU:H	1.83	0.43
1:G:1080:GLU:HB3	1:G:1133:ALA:HB3	1.98	0.43
1:C:949:ASP:N	1:C:949:ASP:OD1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:620:HIS:O	1:E:1041:TYR:OH	2.35	0.43
1:F:846:CYS:HB2	1:F:985:CYS:HB3	1.66	0.43
1:A:979:VAL:HG21	1:A:1013:LEU:HB3	2.00	0.43
1:C:82:PHE:HZ	1:C:196:LEU:HD13	1.84	0.43
1:F:279:ASN:OD1	1:F:283:ARG:N	2.52	0.43
1:F:949:ASP:OD1	1:F:949:ASP:N	2.51	0.43
3:V:293:LEU:HD13	3:V:312:VAL:HG11	2.00	0.43
1:C:137:HIS:CE1	1:C:139:ARG:HE	2.37	0.43
1:C:559:LEU:HB2	1:C:565:PHE:CE1	2.54	0.43
1:E:25:ILE:HG23	1:E:155:LEU:HG	1.99	0.43
1:F:468:GLN:NE2	1:F:469:LEU:O	2.52	0.43
1:F:1217:TYR:CZ	1:F:1222:CYS:HB2	2.54	0.43
1:G:241:ASP:N	1:G:241:ASP:OD1	2.49	0.43
1:G:266:THR:OG1	1:G:1125:TYR:O	2.33	0.43
2:R:126:ILE:HB	2:R:135:ILE:HB	1.99	0.43
1:F:823:ARG:HA	1:F:823:ARG:HD2	1.79	0.43
1:F:979:VAL:HG21	1:F:1013:LEU:HB3	2.00	0.43
1:G:32:THR:HB	1:G:35:VAL:HG23	2.00	0.43
1:G:87:LEU:HD21	1:G:196:LEU:HD22	2.01	0.43
1:A:283:ARG:HH12	1:A:386:ILE:HD12	1.84	0.43
1:E:913:LEU:HD13	1:E:916:LEU:HD23	2.00	0.43
1:F:882:HIS:HE1	1:F:884:LEU:HD12	1.83	0.43
1:G:304:LEU:HD13	1:G:385:VAL:HG11	2.01	0.43
1:G:949:ASP:OD1	1:G:949:ASP:N	2.51	0.43
1:E:277:HIS:HD2	1:E:313:VAL:HG22	1.84	0.43
1:F:642:ILE:HD11	1:F:897:TYR:HB3	1.99	0.43
1:F:1140:ASP:HB3	1:F:1201:ALA:HA	2.01	0.43
1:G:694:LEU:HB3	1:G:699:LEU:HD13	2.00	0.43
4:Z:147:HIS:CE1	4:Z:150:ASP:HB3	2.53	0.43
1:F:287:GLY:HA3	1:F:1084:TYR:HE1	1.84	0.43
1:C:513:GLU:O	1:C:797:ARG:NH2	2.52	0.43
1:E:104:ASP:HB3	1:F:44:PHE:HD2	1.83	0.43
1:G:466:LEU:HD22	1:G:1362:LEU:HD23	2.00	0.43
1:G:913:LEU:HD13	1:G:916:LEU:HD23	2.01	0.43
2:R:100:GLN:NE2	2:R:101:ASN:O	2.52	0.43
4:Z:230:ARG:O	4:Z:234:ARG:HB2	2.18	0.43
1:A:190:ARG:HG2	1:A:401:VAL:HG23	2.01	0.43
1:A:435:THR:HG22	1:C:442:SER:H	1.84	0.43
1:A:605:ILE:HG23	1:A:1028:HIS:HD1	1.84	0.43
2:R:8:ILE:HG12	2:R:34:PHE:HE2	1.84	0.43
2:R:107:LEU:O	2:R:304:VAL:N	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1068:ALA:HB2	1:A:1211:VAL:HA	2.01	0.42
1:E:949:ASP:OD1	1:E:949:ASP:N	2.52	0.42
1:E:1068:ALA:HB2	1:E:1211:VAL:HA	2.01	0.42
3:V:218:ILE:HA	3:V:221:LEU:HB2	2.01	0.42
1:A:304:LEU:HB3	1:A:385:VAL:HG11	2.01	0.42
1:A:479:CYS:SG	1:A:1056:THR:OG1	2.74	0.42
1:C:277:HIS:HD2	1:C:313:VAL:HG22	1.84	0.42
1:E:944:ASN:OD1	1:E:945:MET:N	2.52	0.42
1:G:560:ASN:HB3	1:G:563:PHE:HB2	2.01	0.42
1:A:25:ILE:HD12	1:A:174:ILE:HG13	2.00	0.42
1:C:1000:ARG:O	1:C:1004:LYS:HG2	2.20	0.42
1:E:743:LEU:HD13	1:E:831:ILE:HA	2.00	0.42
1:F:278:THR:HA	1:F:284:GLN:HA	2.01	0.42
1:F:694:LEU:HB3	1:F:699:LEU:HD13	2.01	0.42
4:Z:232:GLY:O	4:Z:236:ILE:HG12	2.20	0.42
4:Z:307:VAL:HG21	4:Z:350:PHE:HE1	1.83	0.42
1:E:694:LEU:HB3	1:E:699:LEU:HD13	2.02	0.42
1:G:642:ILE:HD11	1:G:897:TYR:HB3	2.00	0.42
1:A:91:CYS:HB3	1:A:196:LEU:HD11	2.02	0.42
1:C:793:ASN:HB3	1:C:796:ARG:HH21	1.84	0.42
1:G:468:GLN:OE1	1:G:470:THR:OG1	2.31	0.42
2:R:29:GLY:HA3	2:R:309:ARG:HH12	1.84	0.42
3:V:74:VAL:HG11	3:V:97:LEU:HD11	2.00	0.42
1:C:842:ARG:HH12	1:C:1033:LYS:HA	1.83	0.42
1:C:859:LEU:HA	1:C:894:LEU:HD21	2.01	0.42
1:E:87:LEU:HD12	1:E:290:VAL:HG11	2.01	0.42
1:G:140:SER:HA	1:G:1115:PRO:HA	2.02	0.42
4:Z:349:CYS:HA	4:Z:352:ARG:HH12	1.84	0.42
1:A:287:GLY:HA3	1:A:1084:TYR:HE1	1.84	0.42
1:A:774:ARG:NH1	1:A:779:ASN:OD1	2.52	0.42
1:F:620:HIS:O	1:F:1041:TYR:OH	2.37	0.42
1:F:714:VAL:HG12	1:F:828:LEU:HD22	2.02	0.42
1:F:926:ALA:HB1	1:F:1013:LEU:HD21	2.00	0.42
1:G:96:PHE:HD2	1:G:99:LEU:HB2	1.84	0.42
1:G:838:PRO:HB2	1:G:1029:VAL:HG21	2.00	0.42
1:G:1000:ARG:O	1:G:1004:LYS:HG2	2.19	0.42
1:C:460:TYR:OH	1:C:1362:LEU:O	2.33	0.42
1:C:1356:SER:HB2	1:C:1381:LEU:HD13	2.00	0.42
1:E:451:GLN:HA	1:E:1377:LEU:HD22	2.02	0.42
1:G:926:ALA:HB1	1:G:1013:LEU:HD21	2.02	0.42
1:C:737:GLU:O	1:C:744:THR:OG1	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:466:LEU:HD22	1:F:1362:LEU:HD23	2.01	0.42
2:R:12:LEU:HD23	2:R:12:LEU:HA	1.93	0.42
4:Z:135:ILE:HG21	4:Z:225:ALA:HB1	2.01	0.42
1:A:520:MET:HA	1:A:523:PHE:HB3	2.02	0.42
1:C:172:ARG:HD2	1:C:172:ARG:HA	1.82	0.42
1:E:152:LEU:HA	1:E:155:LEU:HD13	2.02	0.42
1:F:277:HIS:HD2	1:F:313:VAL:HG22	1.85	0.42
1:F:296:LYS:NZ	1:F:394:LEU:O	2.51	0.42
1:F:401:VAL:HG13	1:F:402:TYR:CD1	2.55	0.42
1:A:457:ILE:HA	1:A:1357:SER:HA	2.02	0.41
1:C:694:LEU:HB3	1:C:699:LEU:HD13	2.02	0.41
1:C:838:PRO:HB2	1:C:1029:VAL:HG21	2.02	0.41
1:E:283:ARG:HH12	1:E:386:ILE:HD12	1.85	0.41
1:C:217:GLN:HE21	1:C:220:GLY:HA2	1.85	0.41
1:F:207:LEU:HD22	1:F:262:MET:HG3	2.00	0.41
1:G:743:LEU:HD13	1:G:831:ILE:HA	2.02	0.41
3:V:11:LEU:HD23	3:V:82:LYS:HB3	2.02	0.41
4:Z:174:GLN:HB2	4:Z:237:ARG:HH12	1.83	0.41
1:A:979:VAL:HG23	1:A:1009:ILE:HG23	2.02	0.41
1:C:401:VAL:HG13	1:C:402:TYR:CD1	2.56	0.41
1:C:776:SER:HG	1:C:778:ARG:NH1	2.18	0.41
1:F:87:LEU:HD12	1:F:290:VAL:HG11	2.03	0.41
1:F:421:MET:HE1	1:F:459:PHE:HB3	2.02	0.41
1:F:944:ASN:OD1	1:F:945:MET:N	2.53	0.41
4:Z:250:VAL:HB	4:Z:254:ARG:HH22	1.85	0.41
1:A:290:VAL:HG12	1:A:395:GLU:HB3	2.01	0.41
1:C:1027:TYR:HA	1:C:1030:THR:HG22	2.03	0.41
1:E:605:ILE:HG23	1:E:1028:HIS:HD1	1.85	0.41
1:E:642:ILE:HD11	1:E:897:TYR:HB3	2.03	0.41
1:G:737:GLU:O	1:G:744:THR:OG1	2.36	0.41
1:G:172:ARG:HD2	1:G:172:ARG:HA	1.79	0.41
1:A:450:ARG:NH2	1:A:1376:HIS:HB3	2.35	0.41
1:C:782:GLN:HB3	1:C:784:LEU:HD23	2.01	0.41
1:E:87:LEU:HD21	1:E:196:LEU:HD22	2.03	0.41
3:V:217:LEU:O	3:V:220:THR:OG1	2.31	0.41
1:A:1083:LEU:HD12	1:A:1129:CYS:HB3	2.02	0.41
1:C:763:ASP:O	1:C:767:ARG:NH1	2.53	0.41
1:C:926:ALA:HB1	1:C:1013:LEU:HD21	2.03	0.41
1:E:201:LEU:HD22	1:E:1083:LEU:HD22	2.02	0.41
1:F:32:THR:HB	1:F:35:VAL:HG23	2.02	0.41
1:F:203:LYS:NZ	1:F:1126:THR:OG1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:910:LEU:HA	1:F:913:LEU:HD23	2.02	0.41
1:C:455:GLN:HE21	1:C:614:GLN:HE22	1.67	0.41
1:C:944:ASN:OD1	1:C:945:MET:N	2.54	0.41
1:E:172:ARG:HA	1:E:172:ARG:HD2	1.81	0.41
1:A:82:PHE:HZ	1:A:196:LEU:HD13	1.86	0.41
1:A:476:GLY:O	1:A:1148:LEU:N	2.53	0.41
1:A:520:MET:SD	1:A:520:MET:N	2.93	0.41
1:A:775:VAL:HG22	1:A:927:ILE:HG12	2.03	0.41
1:A:1027:TYR:HA	1:A:1030:THR:HG22	2.03	0.41
1:A:1120:ASP:OD1	1:A:1120:ASP:N	2.53	0.41
1:C:32:THR:HB	1:C:35:VAL:HG23	2.02	0.41
1:C:180:ASN:O	1:C:183:THR:OG1	2.31	0.41
1:C:726:ILE:HD13	1:C:1060:ARG:NE	2.36	0.41
1:C:979:VAL:HG21	1:C:1013:LEU:HB3	2.03	0.41
1:C:1056:THR:HG21	1:C:1169:ILE:HD13	2.02	0.41
1:C:1068:ALA:HB2	1:C:1211:VAL:HA	2.02	0.41
1:E:1217:TYR:CZ	1:E:1222:CYS:HB2	2.56	0.41
1:F:140:SER:HA	1:F:1115:PRO:HA	2.03	0.41
1:G:309:THR:O	1:G:382:ALA:N	2.53	0.41
1:G:1216:GLN:HA	1:G:1219:ARG:HG3	2.03	0.41
3:V:33:THR:O	3:V:70:ARG:NH2	2.53	0.41
1:A:514:ASP:HB2	1:A:519:GLN:HE21	1.86	0.41
1:A:737:GLU:O	1:A:744:THR:OG1	2.37	0.41
1:F:450:ARG:NH2	1:F:1379:GLN:HB2	2.36	0.41
1:F:1216:GLN:HA	1:F:1219:ARG:HG3	2.03	0.41
1:A:784:LEU:HB2	1:A:800:VAL:HG13	2.02	0.40
1:C:451:GLN:HA	1:C:1377:LEU:HD22	2.03	0.40
1:E:1027:TYR:HA	1:E:1030:THR:HG22	2.03	0.40
1:F:460:TYR:OH	1:F:1362:LEU:O	2.35	0.40
1:F:502:CYS:HB2	1:F:532:PRO:HD2	2.04	0.40
3:V:113:ILE:HA	3:V:142:PRO:HA	2.03	0.40
4:Z:124:GLN:NE2	4:Z:125:VAL:O	2.54	0.40
1:E:649:VAL:HG21	1:E:859:LEU:HD22	2.04	0.40
1:E:729:GLU:O	1:E:736:SER:OG	2.39	0.40
1:G:680:PHE:HB3	1:G:686:MET:HG2	2.03	0.40
3:V:8:ILE:HD12	3:V:34:PHE:CE1	2.55	0.40
4:Z:261:SER:N	4:Z:276:ALA:HB1	2.36	0.40
4:Z:352:ARG:O	4:Z:356:PHE:N	2.42	0.40
1:A:1374:GLU:HB3	1:C:1363:ARG:NH1	2.35	0.40
1:C:493:LEU:HG	1:C:587:VAL:HG11	2.03	0.40
1:C:605:ILE:HG23	1:C:1028:HIS:HD1	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1356:SER:HB3	1:C:1362:LEU:HB2	2.02	0.40
1:F:1053:ILE:HG22	1:F:1057:HIS:CE1	2.56	0.40
1:F:1089:SER:O	1:F:1089:SER:OG	2.39	0.40
1:G:397:LEU:HG	1:G:401:VAL:HG12	2.03	0.40
1:G:1043:LEU:HD23	1:G:1043:LEU:HA	1.94	0.40
2:R:248:ALA:O	2:R:250:GLN:N	2.55	0.40
3:V:37:LEU:HD11	3:V:71:PHE:HB2	2.03	0.40
1:A:694:LEU:HB3	1:A:699:LEU:HD13	2.04	0.40
1:F:260:SER:HA	1:F:263:VAL:HG12	2.03	0.40
1:F:605:ILE:HG23	1:F:1028:HIS:HD1	1.86	0.40
1:G:436:ARG:O	1:G:437:HIS:ND1	2.54	0.40
1:G:1075:ASP:OD1	1:G:1076:ARG:N	2.54	0.40
1:A:1043:LEU:HD23	1:A:1043:LEU:HA	1.94	0.40
1:C:653:ASN:ND2	1:C:919:ASP:OD2	2.54	0.40
1:C:1217:TYR:CZ	1:C:1222:CYS:HB2	2.55	0.40
1:E:236:ARG:O	1:E:240:ALA:HB2	2.22	0.40
1:E:1351:TYR:CG	1:E:1387:PRO:HD3	2.57	0.40
1:F:194:ASP:OD1	1:F:402:TYR:OH	2.27	0.40
1:F:1027:TYR:HA	1:F:1030:THR:HG22	2.03	0.40
1:G:979:VAL:HG21	1:G:1013:LEU:HB3	2.04	0.40
1:G:1217:TYR:CZ	1:G:1222:CYS:HB2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1145/1370 (84%)	1050 (92%)	92 (8%)	3 (0%)	37	71
1	C	1145/1370 (84%)	1057 (92%)	85 (7%)	3 (0%)	37	71
1	E	1145/1370 (84%)	1057 (92%)	85 (7%)	3 (0%)	37	71
1	F	1145/1370 (84%)	1060 (93%)	82 (7%)	3 (0%)	37	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	G	1145/1370 (84%)	1059 (92%)	83 (7%)	3 (0%)	37 71
2	R	248/256 (97%)	230 (93%)	17 (7%)	1 (0%)	30 66
3	V	257/263 (98%)	241 (94%)	15 (6%)	1 (0%)	30 66
4	Z	280/286 (98%)	242 (86%)	37 (13%)	1 (0%)	30 66
All	All	6510/7655 (85%)	5996 (92%)	496 (8%)	18 (0%)	38 71

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	414	ASN
1	C	414	ASN
1	E	414	ASN
1	F	414	ASN
1	G	414	ASN
3	V	269	ILE
2	R	230	ILE
4	Z	265	TYR
1	F	32	THR
1	A	32	THR
1	A	165	ILE
1	C	32	THR
1	C	165	ILE
1	E	32	THR
1	E	165	ILE
1	F	165	ILE
1	G	32	THR
1	G	165	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	947/1159 (82%)	942 (100%)	5 (0%)	86 89
1	C	947/1159 (82%)	941 (99%)	6 (1%)	84 88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	947/1159 (82%)	942 (100%)	5 (0%)	86 89
1	F	947/1159 (82%)	942 (100%)	5 (0%)	86 89
1	G	947/1159 (82%)	941 (99%)	6 (1%)	84 88
2	R	188/218 (86%)	186 (99%)	2 (1%)	70 80
3	V	214/224 (96%)	212 (99%)	2 (1%)	75 83
4	Z	225/238 (94%)	222 (99%)	3 (1%)	65 77
All	All	5362/6475 (83%)	5328 (99%)	34 (1%)	82 88

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	ARG
1	A	522	ARG
1	A	718	ARG
1	A	778	ARG
1	A	923	ARG
1	C	103	ARG
1	C	281	ARG
1	C	522	ARG
1	C	718	ARG
1	C	778	ARG
1	C	923	ARG
1	E	103	ARG
1	E	522	ARG
1	E	718	ARG
1	E	778	ARG
1	E	923	ARG
1	F	103	ARG
1	F	522	ARG
1	F	718	ARG
1	F	778	ARG
1	F	923	ARG
1	G	103	ARG
1	G	281	ARG
1	G	522	ARG
1	G	718	ARG
1	G	778	ARG
1	G	923	ARG
2	R	26	LYS
2	R	224	ARG

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Mol	Chain	Res	Type
3	V	26	LYS
3	V	266	ARG
4	Z	230	ARG
4	Z	309	LYS
4	Z	445	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	455	GLN
1	A	519	GLN
1	A	653	ASN
1	A	740	ASN
1	A	1058	GLN
1	C	195	GLN
1	C	614	GLN
1	C	653	ASN
1	C	988	HIS
1	C	1143	ASN
1	E	217	GLN
1	E	455	GLN
1	E	653	ASN
1	E	1081	GLN
1	F	217	GLN
1	F	988	HIS
1	F	1058	GLN
1	G	195	GLN
1	G	455	GLN
1	G	519	GLN
1	G	653	ASN
1	G	988	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	R	3
3	V	2
4	Z	2
1	E	1
1	G	1
1	C	1
1	F	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	V	226:LEU	C	266:ARG	N	28.94
1	R	236:LEU	C	244:VAL	N	20.66
1	R	260:MET	C	267:LEU	N	18.80
1	V	163:ALA	C	175:ASP	N	17.50
1	Z	362:ILE	C	428:CYS	N	12.71
1	R	161:LEU	C	206:ASN	N	12.60
1	Z	179:SER	C	192:ARG	N	11.14
1	E	103:ARG	C	104:ASP	N	3.56
1	G	103:ARG	C	104:ASP	N	3.33
1	C	103:ARG	C	104:ASP	N	3.26
1	F	103:ARG	C	104:ASP	N	3.26
1	A	103:ARG	C	104:ASP	N	3.24

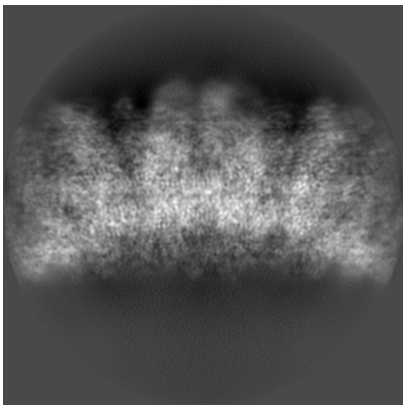
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-38192. These allow visual inspection of the internal detail of the map and identification of artifacts.

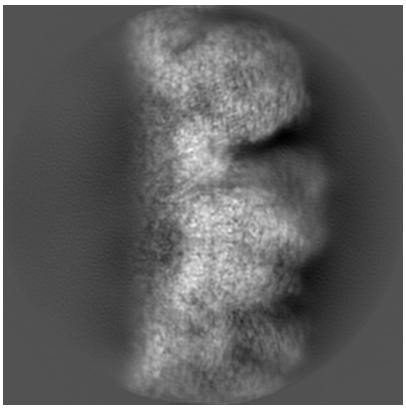
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

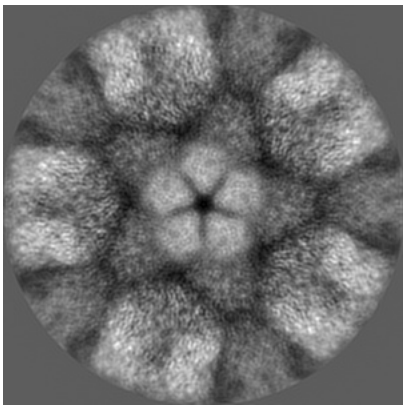
6.1.1 Primary map



X

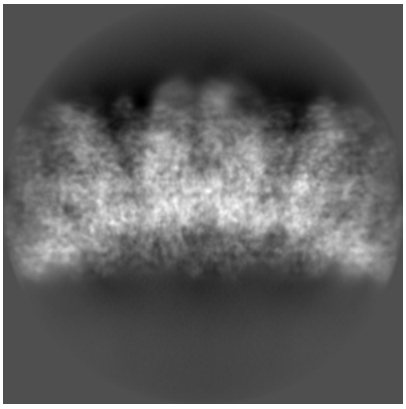


Y

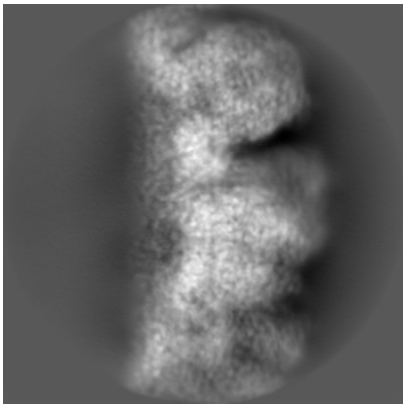


Z

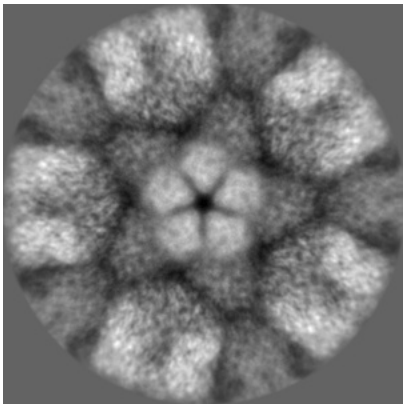
6.1.2 Raw map



X



Y

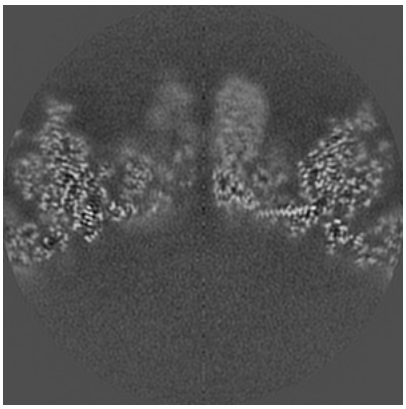


Z

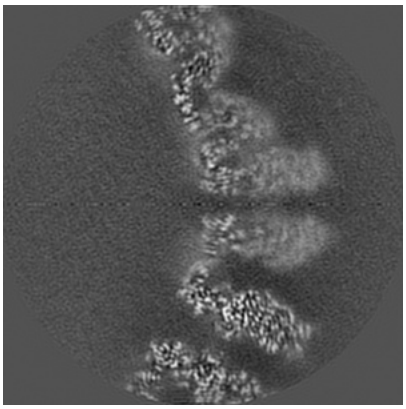
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

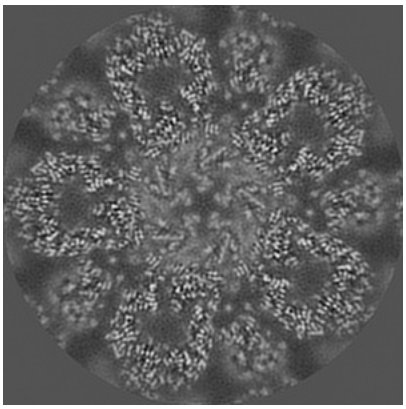
6.2.1 Primary map



X Index: 155

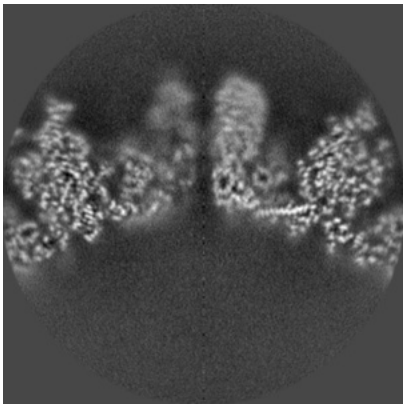


Y Index: 155

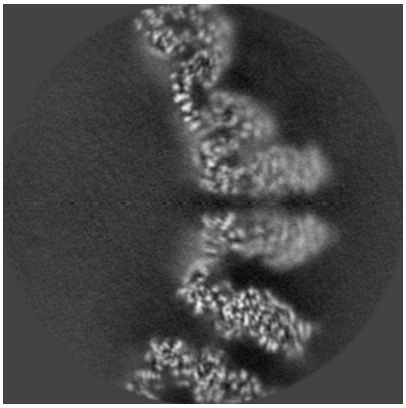


Z Index: 155

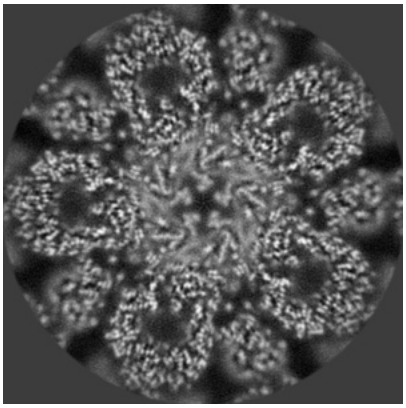
6.2.2 Raw map



X Index: 155



Y Index: 155

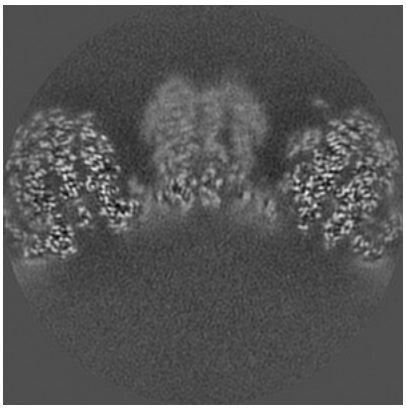


Z Index: 155

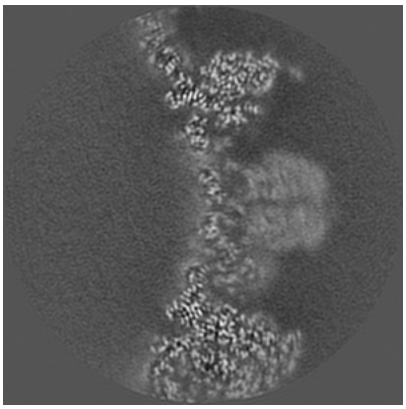
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

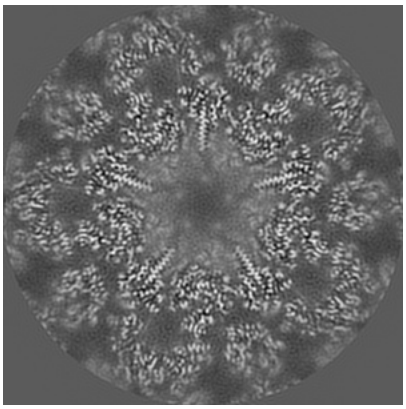
6.3.1 Primary map



X Index: 142

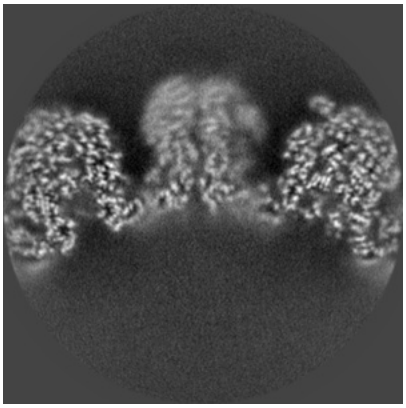


Y Index: 127

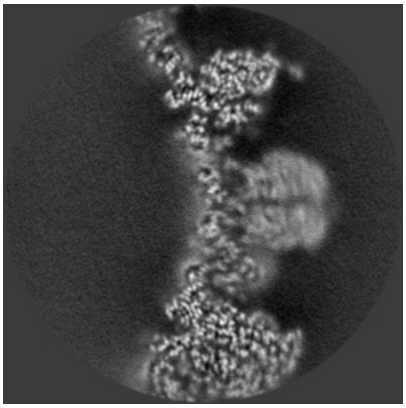


Z Index: 149

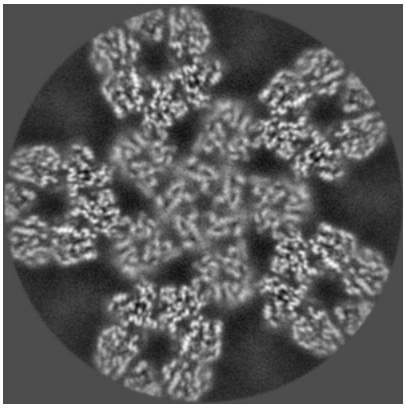
6.3.2 Raw map



X Index: 137



Y Index: 127

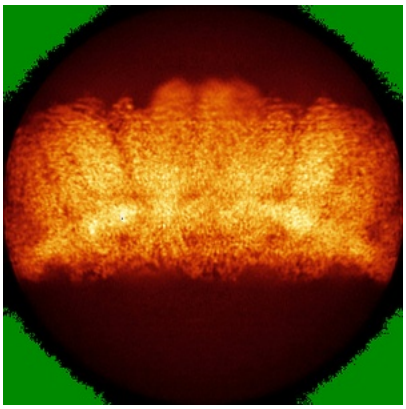


Z Index: 182

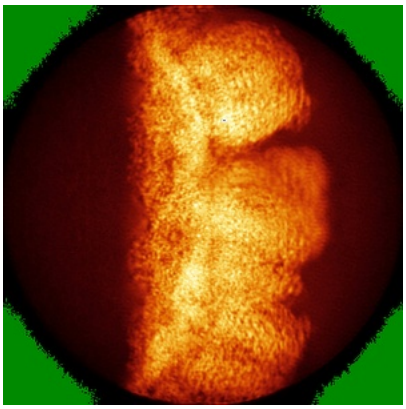
The images above show the largest variance slices of the map in three orthogonal directions.

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

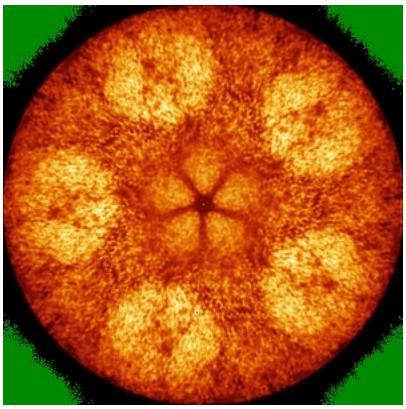
6.4.1 Primary map



X

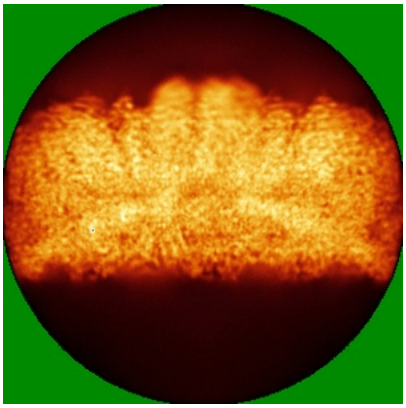


Y

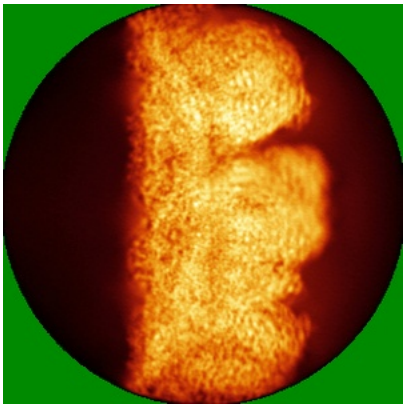


Z

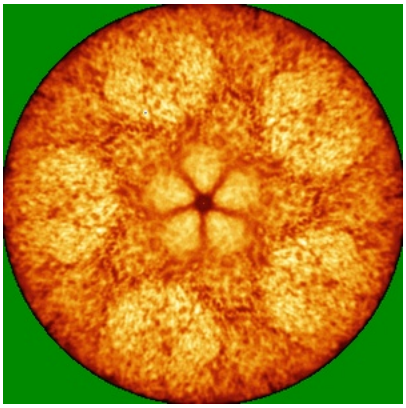
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

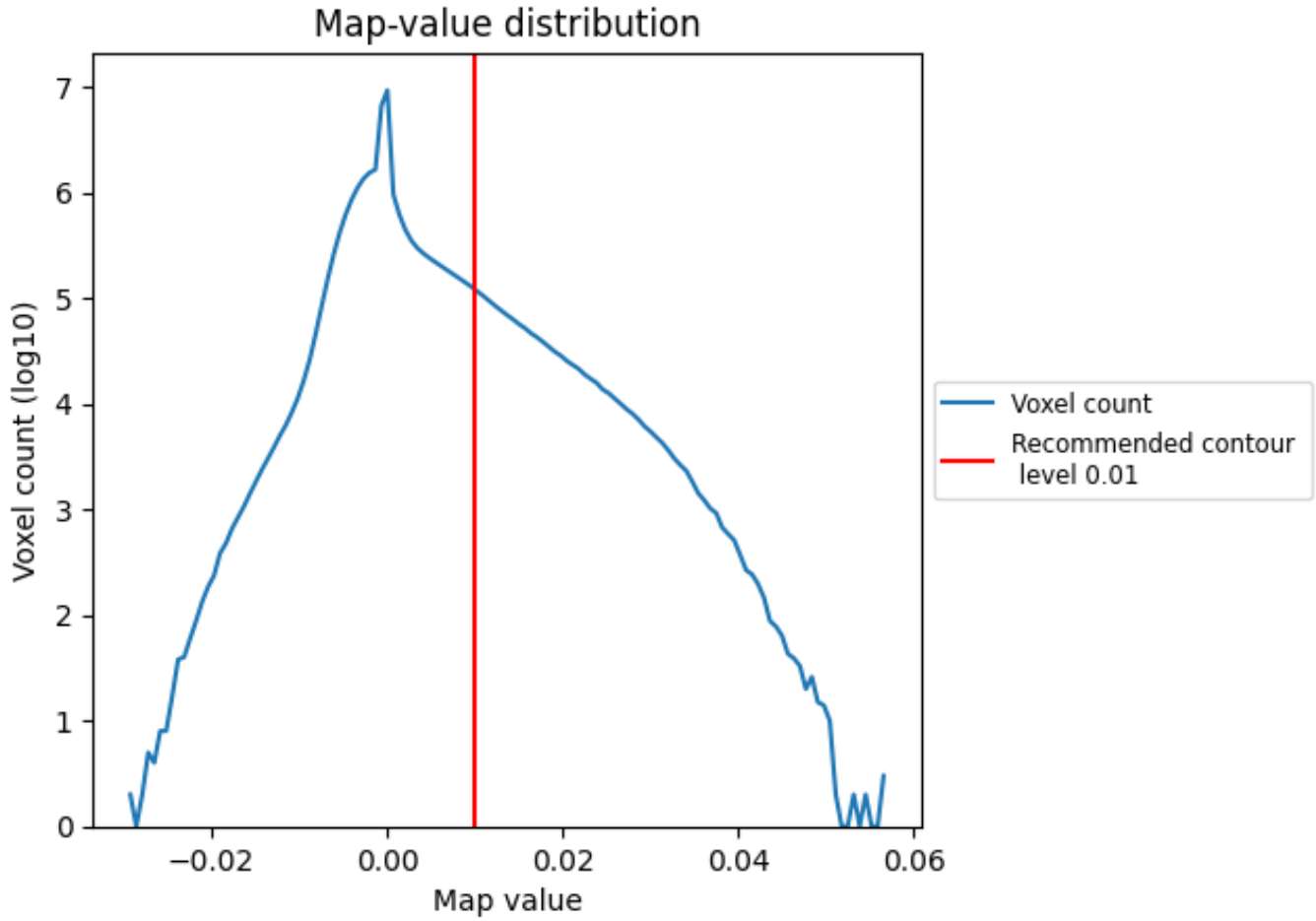
6.6 Mask visualisation (i)

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

7 Map analysis

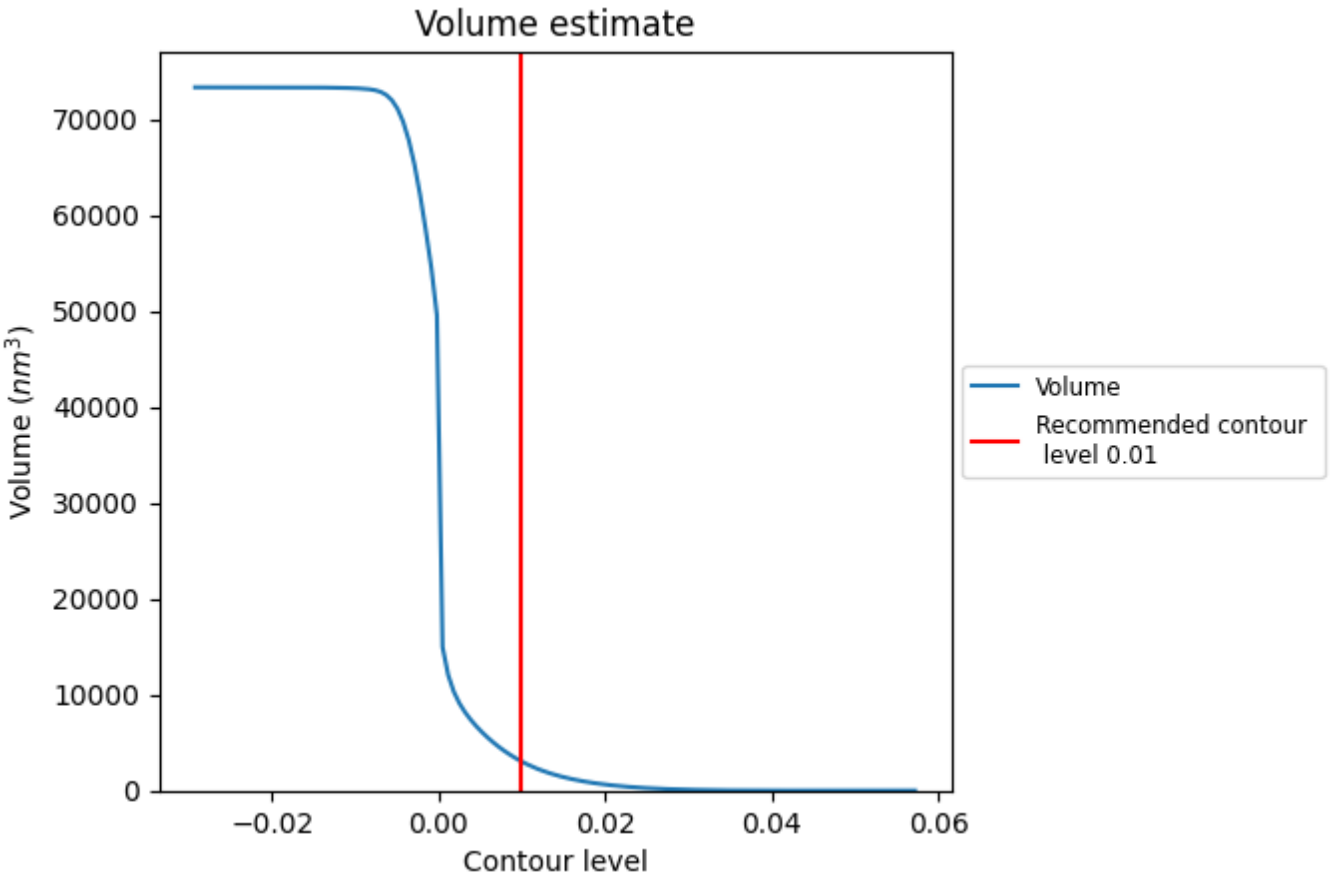
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

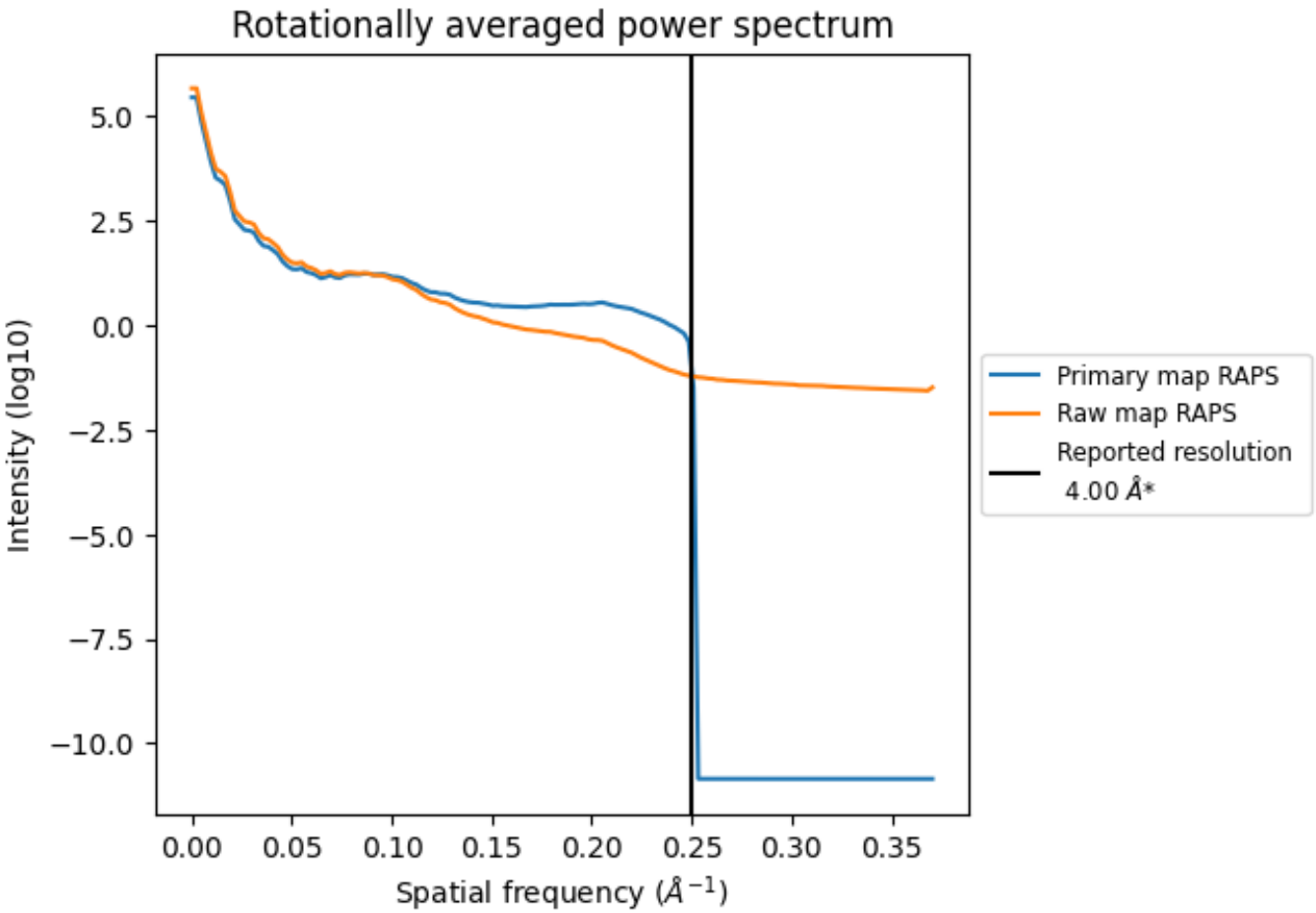
7.2 Volume estimate



The volume at the recommended contour level is 3021 nm^3; this corresponds to an approximate mass of 2729 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)

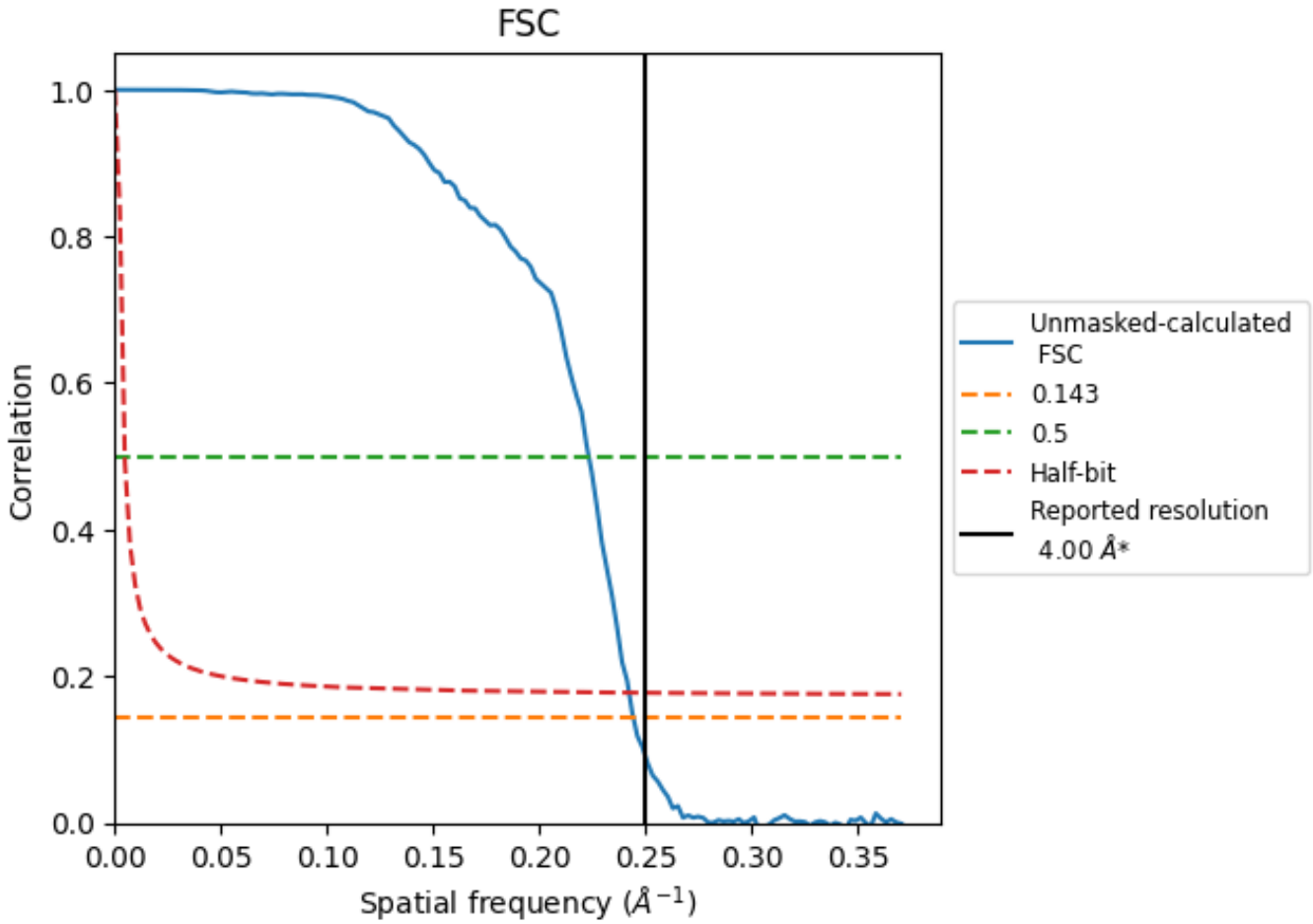


*Reported resolution corresponds to spatial frequency of 0.250 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.250 Å^{-1}

8.2 Resolution estimates (i)

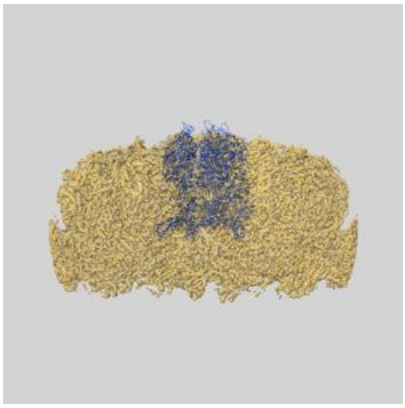
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.09	4.48	4.13

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

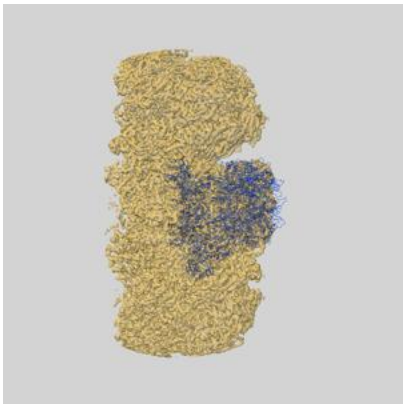
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-38192 and PDB model 8XA2. Per-residue inclusion information can be found in section 3 on page 5.

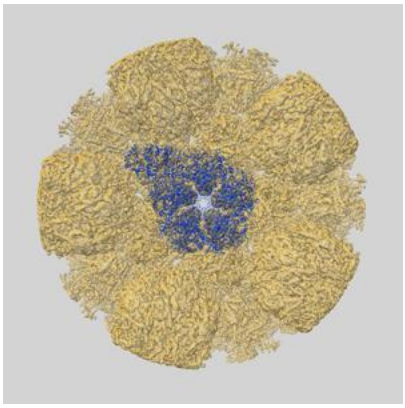
9.1 Map-model overlay



X



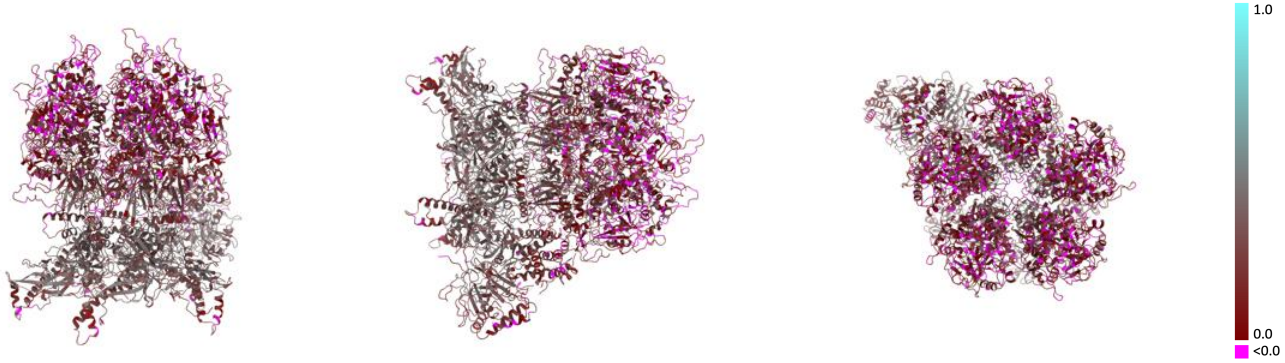
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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.

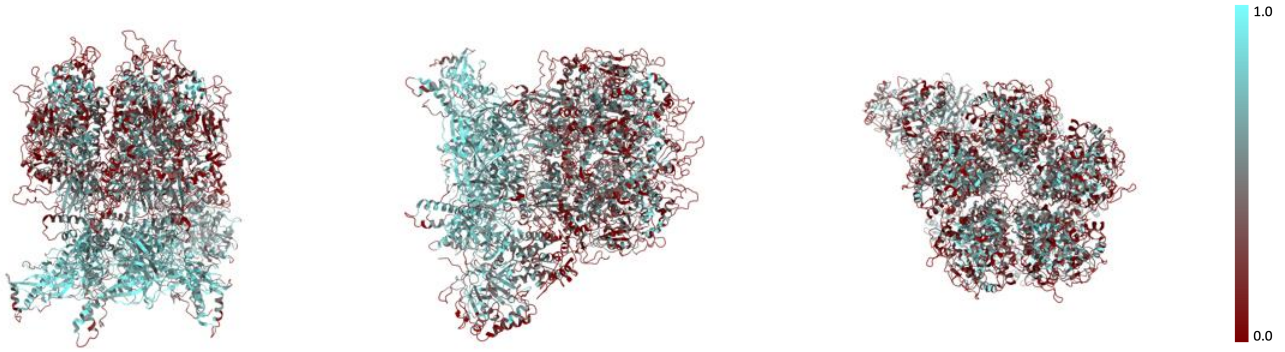
9.2 Q-score mapped to coordinate model (i)



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.

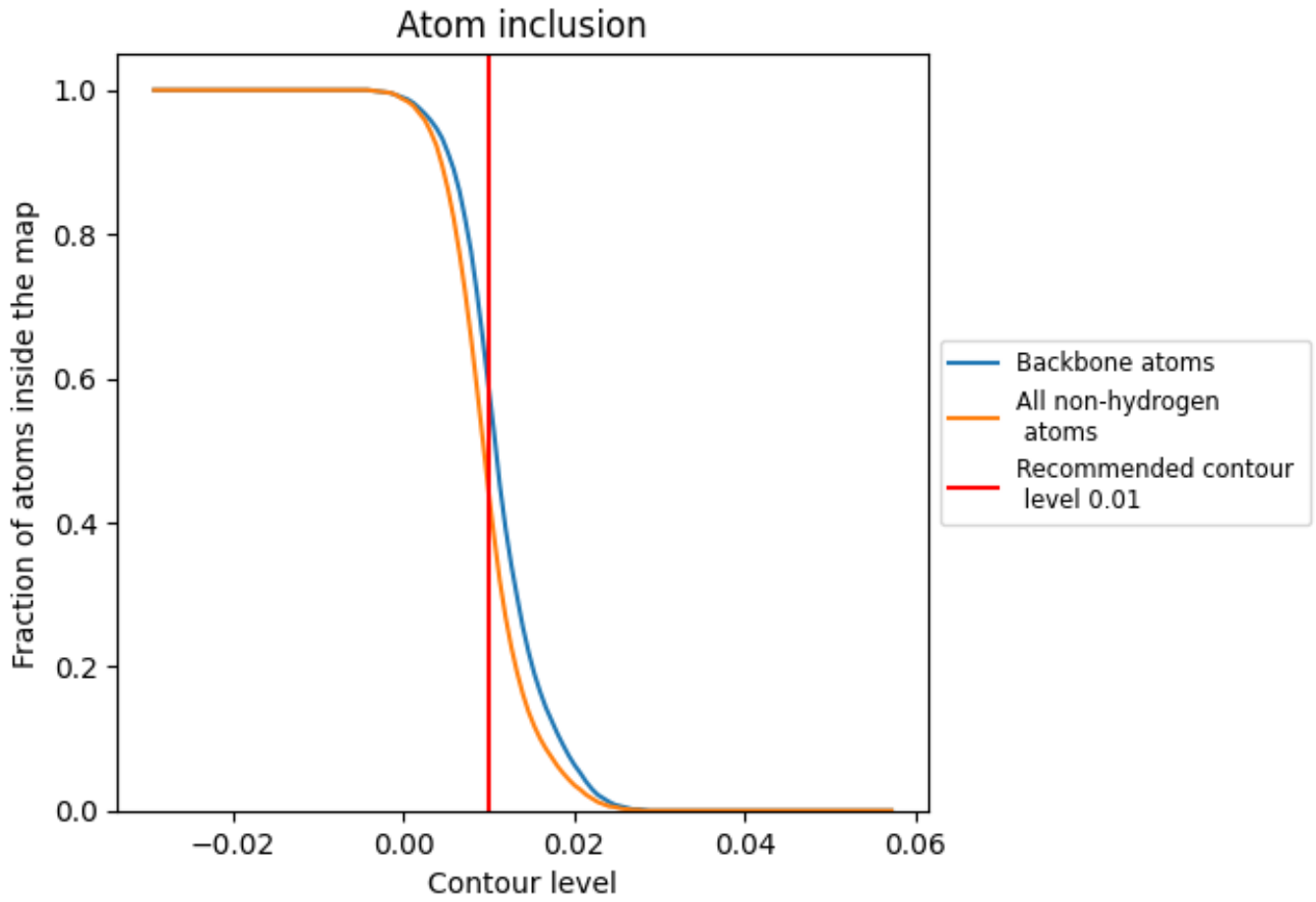
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 58% of all backbone atoms, 44% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4400	0.2170
A	0.4360	0.2060
C	0.4390	0.2080
E	0.4350	0.2050
F	0.4350	0.2050
G	0.4360	0.2060
R	0.5060	0.3140
V	0.5270	0.3320
Z	0.3920	0.2660