Full wwPDB EM Validation Report ⓘ

Oct 24, 2023 – 12:40 PM JST

PDB ID	:	8HEX
EMDB ID	:	EMD-34696
Title	:	C5 portal vertex in HCMV B-capsid
Authors	:	Li, Z.; Yu, X.
Deposited on	:	2022-11-08
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:

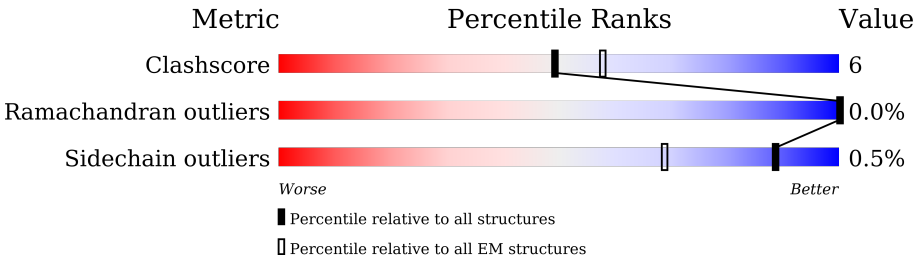
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 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	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	I	306	33% 80% 14% 6%
1	h	306	32% 93% · 6%
1	n	306	47% 96% ·
1	o	306	47% 94% 6%
2	g	290	46% 75% · 24%
2	m	290	41% 100%
3	M	594	37% 65% 13% 22%
4	N	642	8% 8% · 91%

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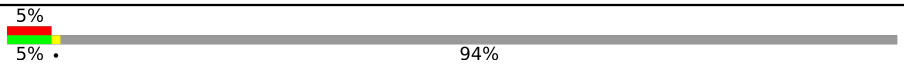
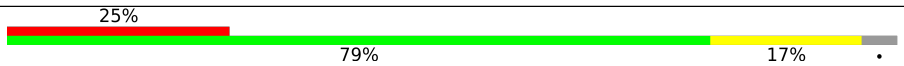
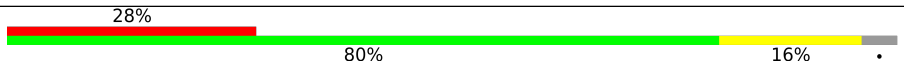
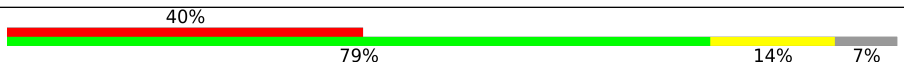
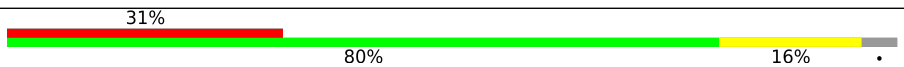
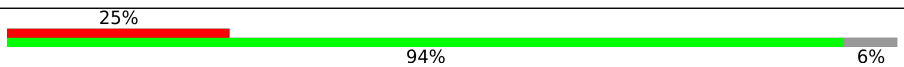
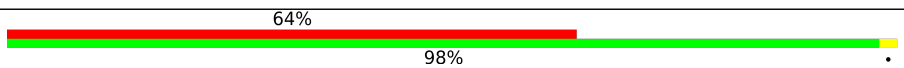
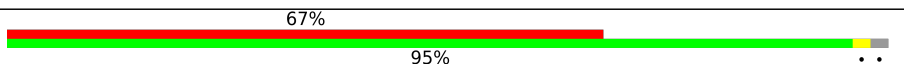
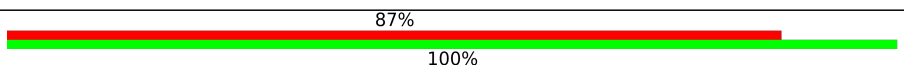
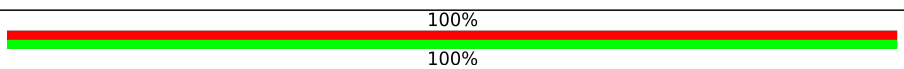
Mol	Chain	Length	Quality of chain
4	O	642	
5	R	75	
5	S	75	
5	i	75	
5	j	75	
6	B	1370	
6	C	1370	
6	D	1370	
6	Y	1370	
6	Z	1370	
6	a	1370	
7	A	42	
7	E	42	
8	F	15	
9	G	13	

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 82790 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 Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	h	288	Total	C	N	O	S	0	0
			2290	1473	394	406	17		
1	I	287	Total	C	N	O	S	0	0
			2282	1466	394	405	17		
1	n	295	Total	C	N	O	S	0	0
			2334	1501	402	412	19		
1	o	289	Total	C	N	O	S	0	0
			2291	1473	393	407	18		

- Molecule 2 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	g	219	Total	C	N	O	S	0	0
			1758	1129	311	307	11		
2	m	290	Total	C	N	O	S	0	0
			2325	1485	411	417	12		

- Molecule 3 is a protein called Capsid vertex component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	465	Total	C	N	O	S	0	0
			3820	2393	734	679	14		

- Molecule 4 is a protein called Capsid vertex component 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	60	Total	C	N	O	S	0	0
			509	325	98	83	3		
4	O	39	Total	C	N	O	S	0	0
			329	214	60	54	1		

- Molecule 5 is a protein called Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
5	S	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
5	i	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
5	j	63	Total	C	N	O	S	0	0
			513	321	97	91	4		

- Molecule 6 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	a	1286	Total	C	N	O	S	0	0
			10167	6466	1771	1871	59		
6	B	1311	Total	C	N	O	S	0	0
			10389	6624	1797	1909	59		
6	C	1316	Total	C	N	O	S	0	0
			10431	6646	1809	1916	60		
6	D	1278	Total	C	N	O	S	0	0
			10114	6443	1754	1860	57		
6	Y	1347	Total	C	N	O	S	0	0
			10676	6799	1850	1966	61		
6	Z	1322	Total	C	N	O	S	0	0
			10468	6672	1813	1925	58		

- Molecule 7 is a protein called portal protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	A	42	Total	C	N	O	0	0
			210	126	42	42		
7	E	41	Total	C	N	O	0	0
			205	123	41	41		

- Molecule 8 is a protein called portal protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	F	15	Total	C	N	O	0	0
			75	45	15	15		

- Molecule 9 is a protein called portal protein.

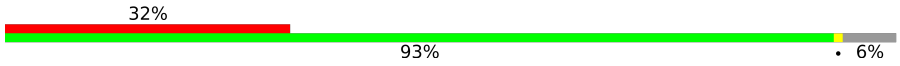
Mol	Chain	Residues	Atoms				AltConf	Trace
9	G	13	Total	C	N	O	0	0
			65	39	13	13		

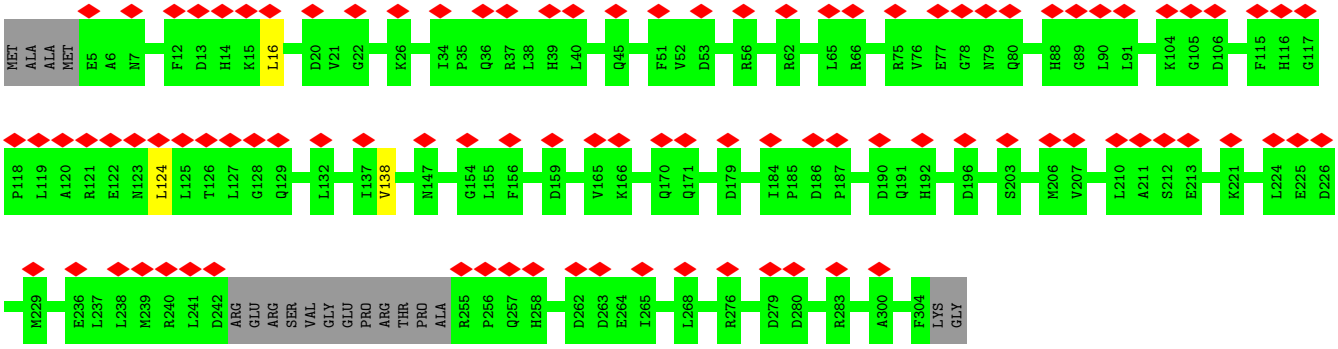
3 Residue-property plots (i)

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: Triplex capsid protein 2

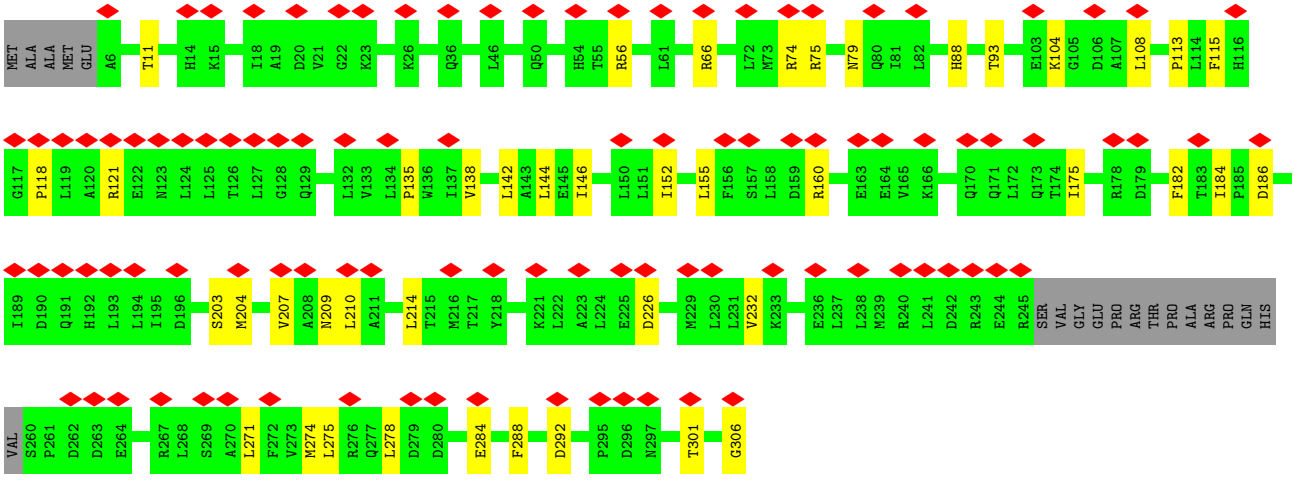
Chain h:





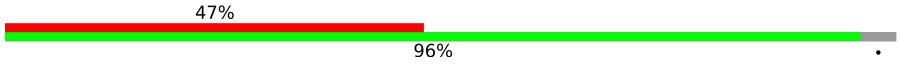
• Molecule 1: Triplex capsid protein 2

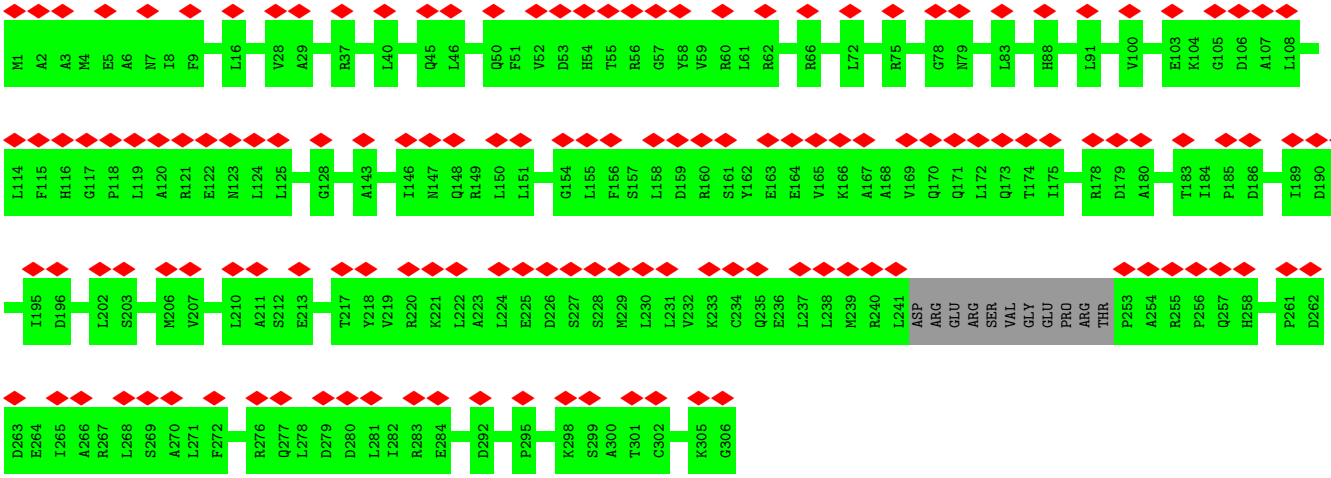
Chain I:



• Molecule 1: Triplex capsid protein 2

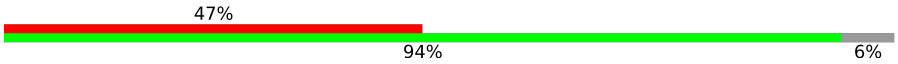
Chain n:

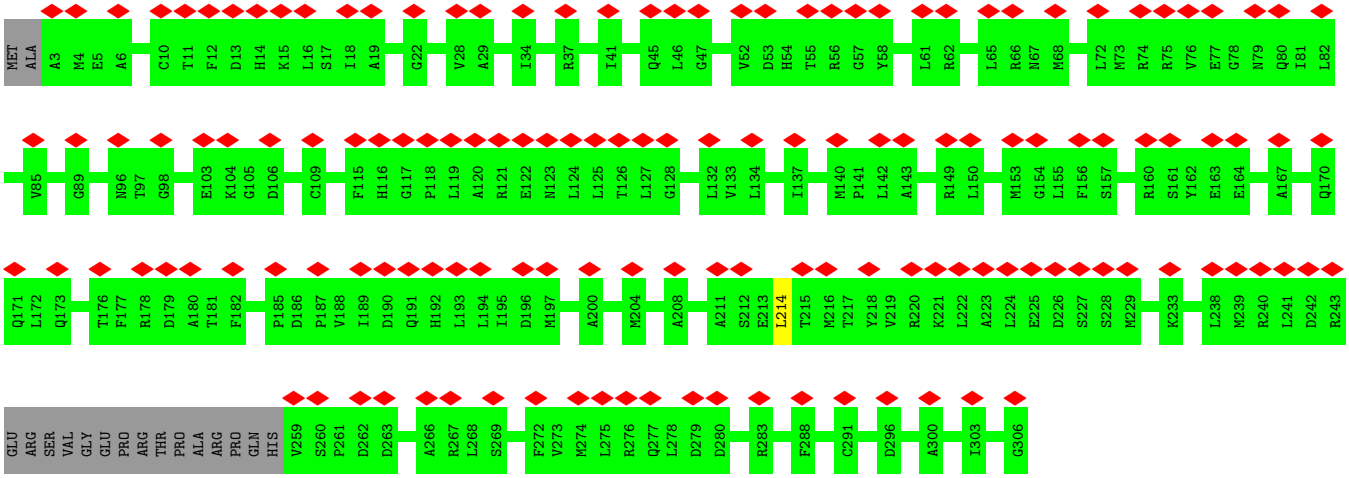




• Molecule 1: Triplex capsid protein 2

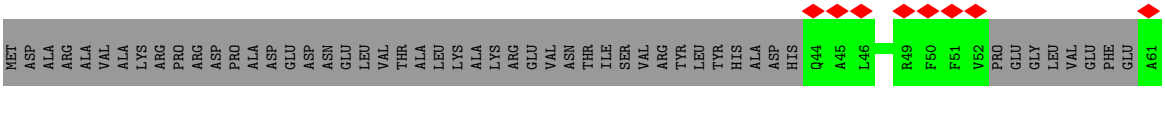
Chain o:

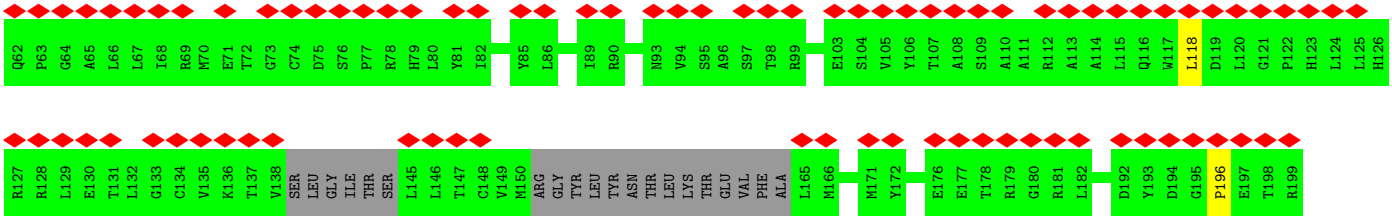


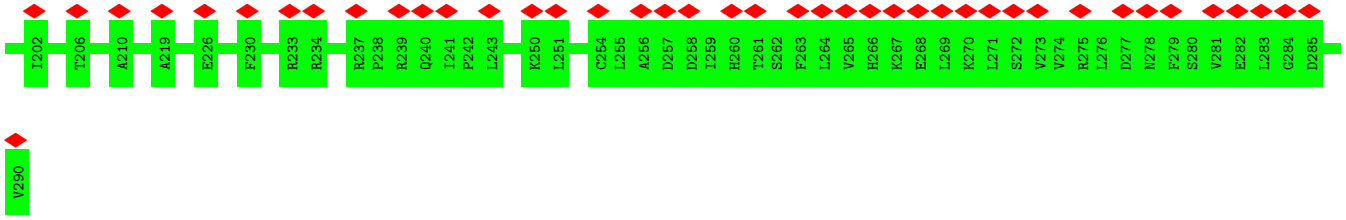


• Molecule 2: Triplex capsid protein 1

Chain g:

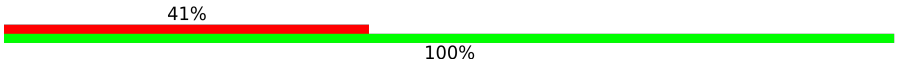


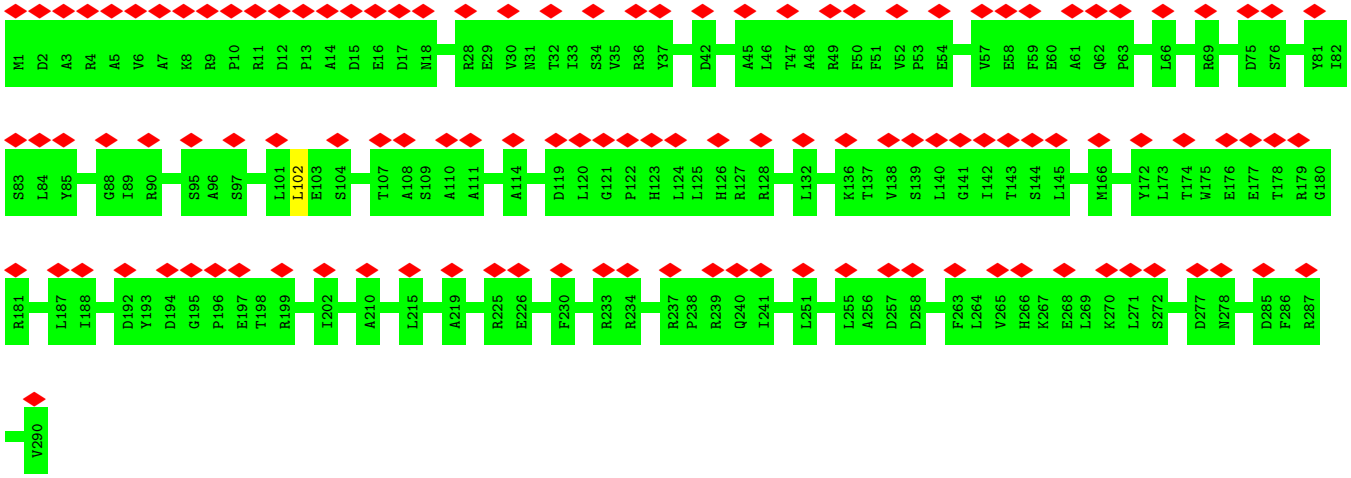




• Molecule 2: Triplex capsid protein 1

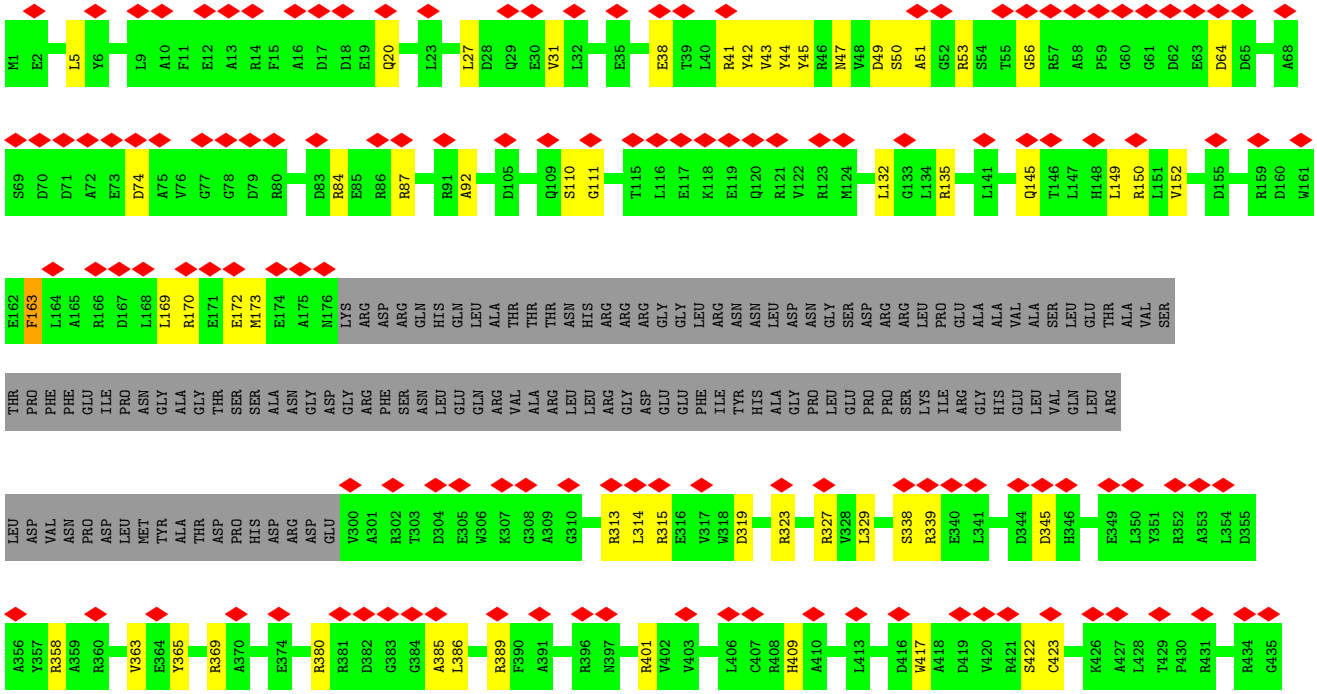
Chain m:

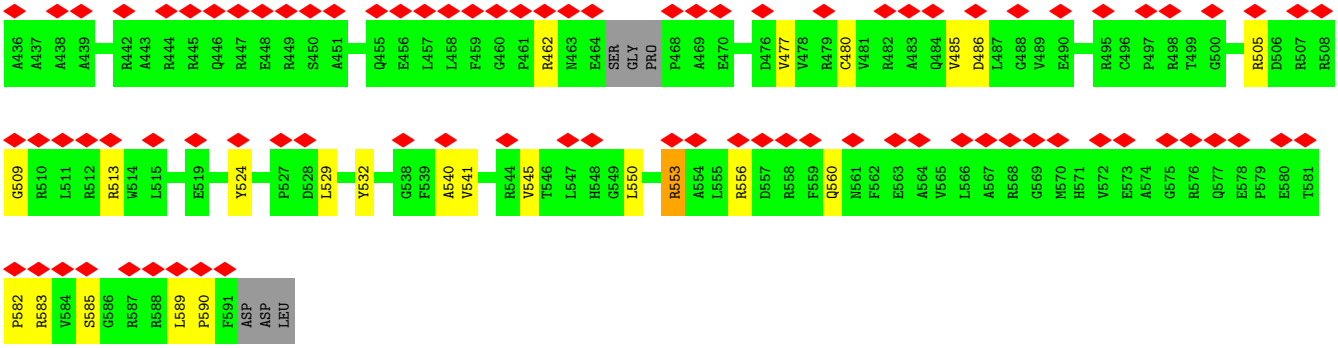




• Molecule 3: Capsid vertex component 1

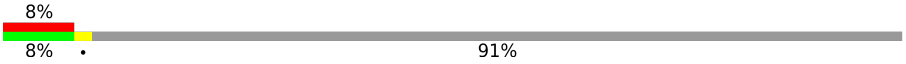
Chain M:

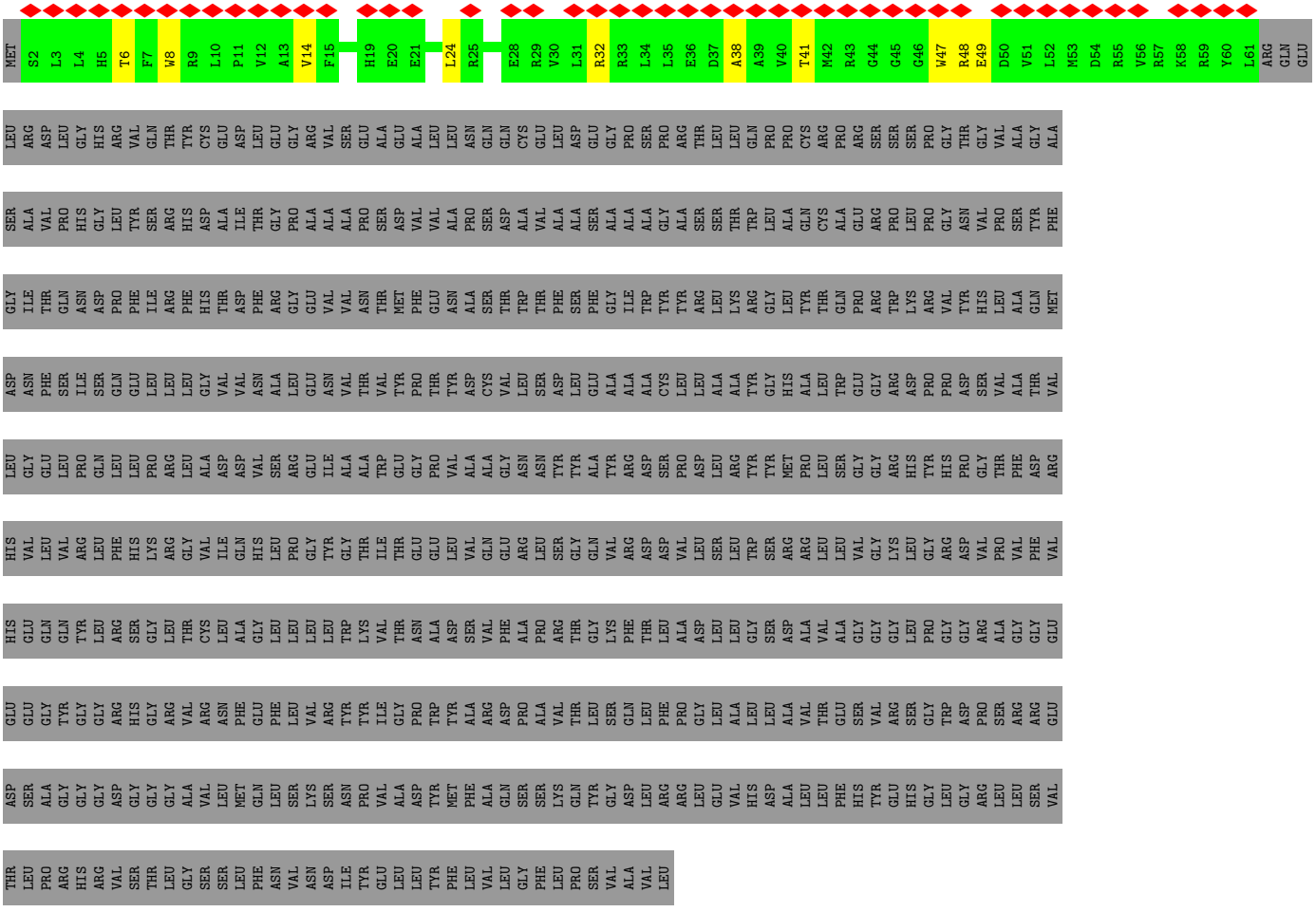




• Molecule 4: Capsid vertex component 2

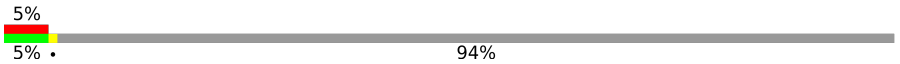
Chain N:

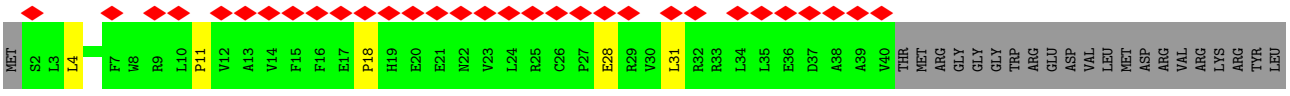


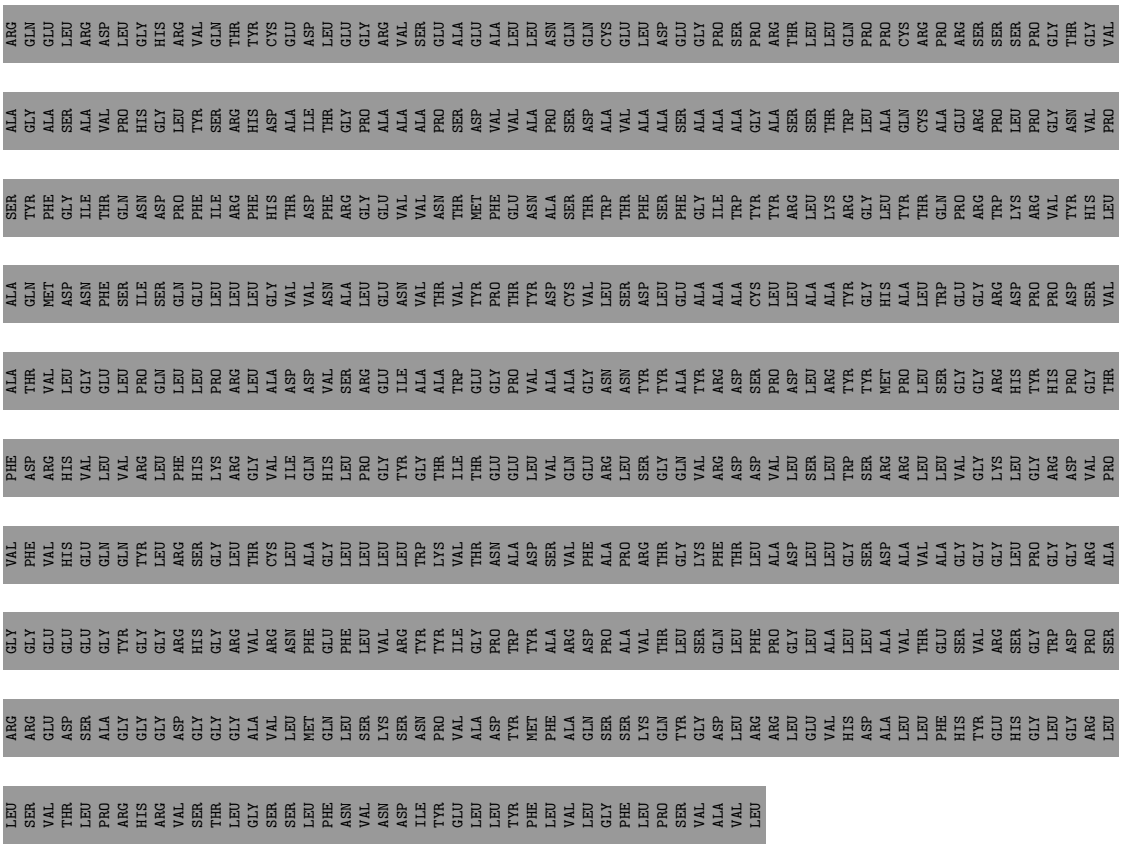


• Molecule 4: Capsid vertex component 2

Chain O:





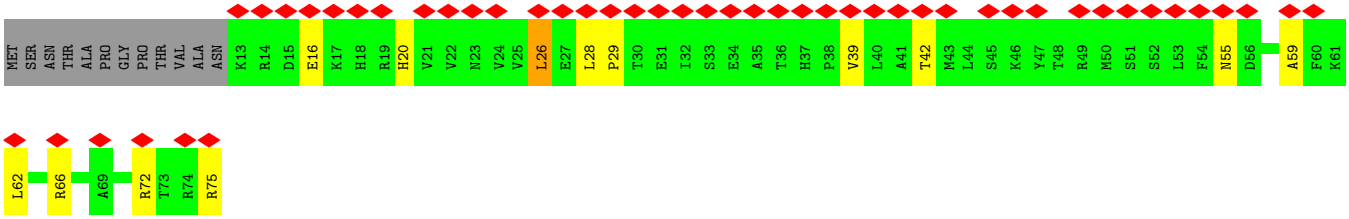


• Molecule 5: Small capsomere-interacting protein

Chain R:

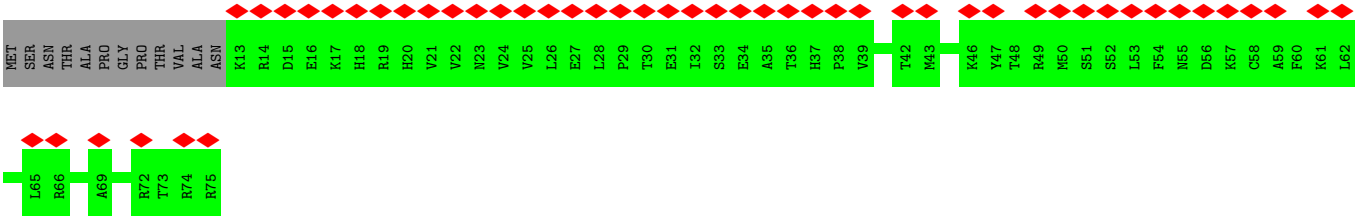
• Molecule 5: Small capsomere-interacting protein

Chain S:



• Molecule 5: Small capsomere-interacting protein

Chain i:

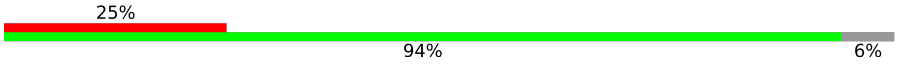


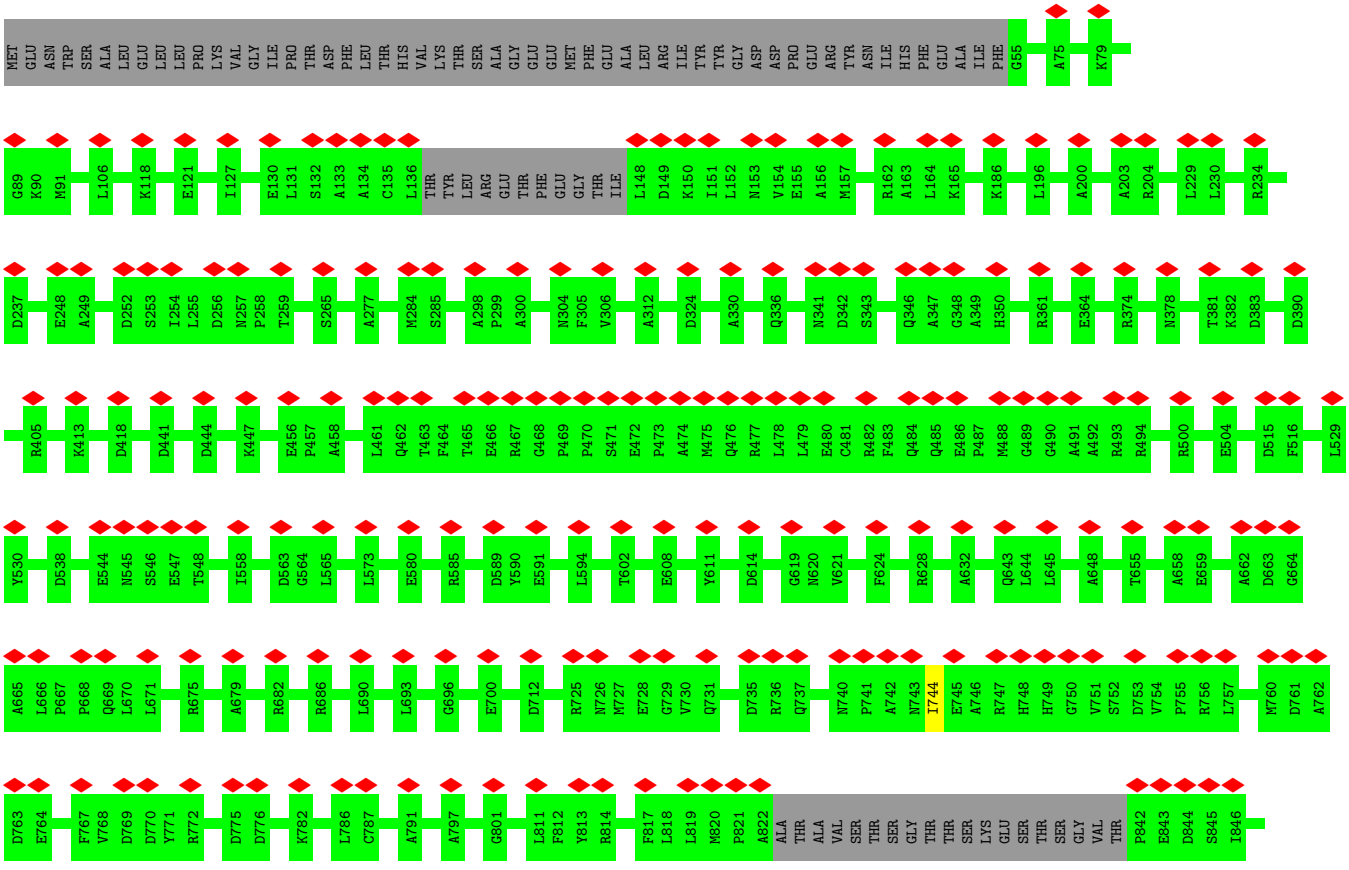
• Molecule 5: Small capsomere-interacting protein

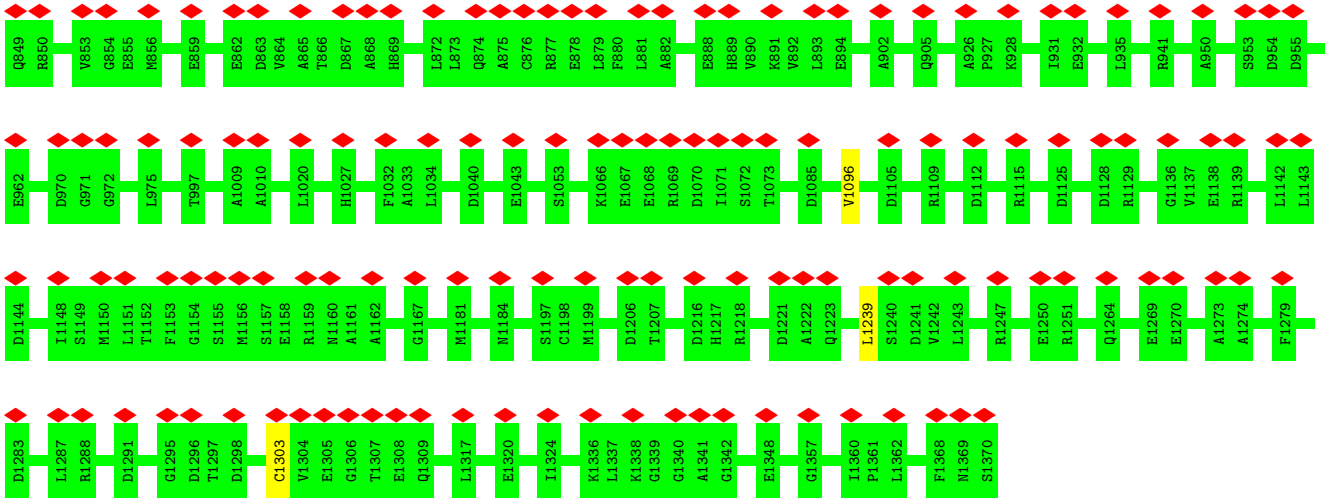
Chain j:

• Molecule 6: Major capsid protein

Chain a:

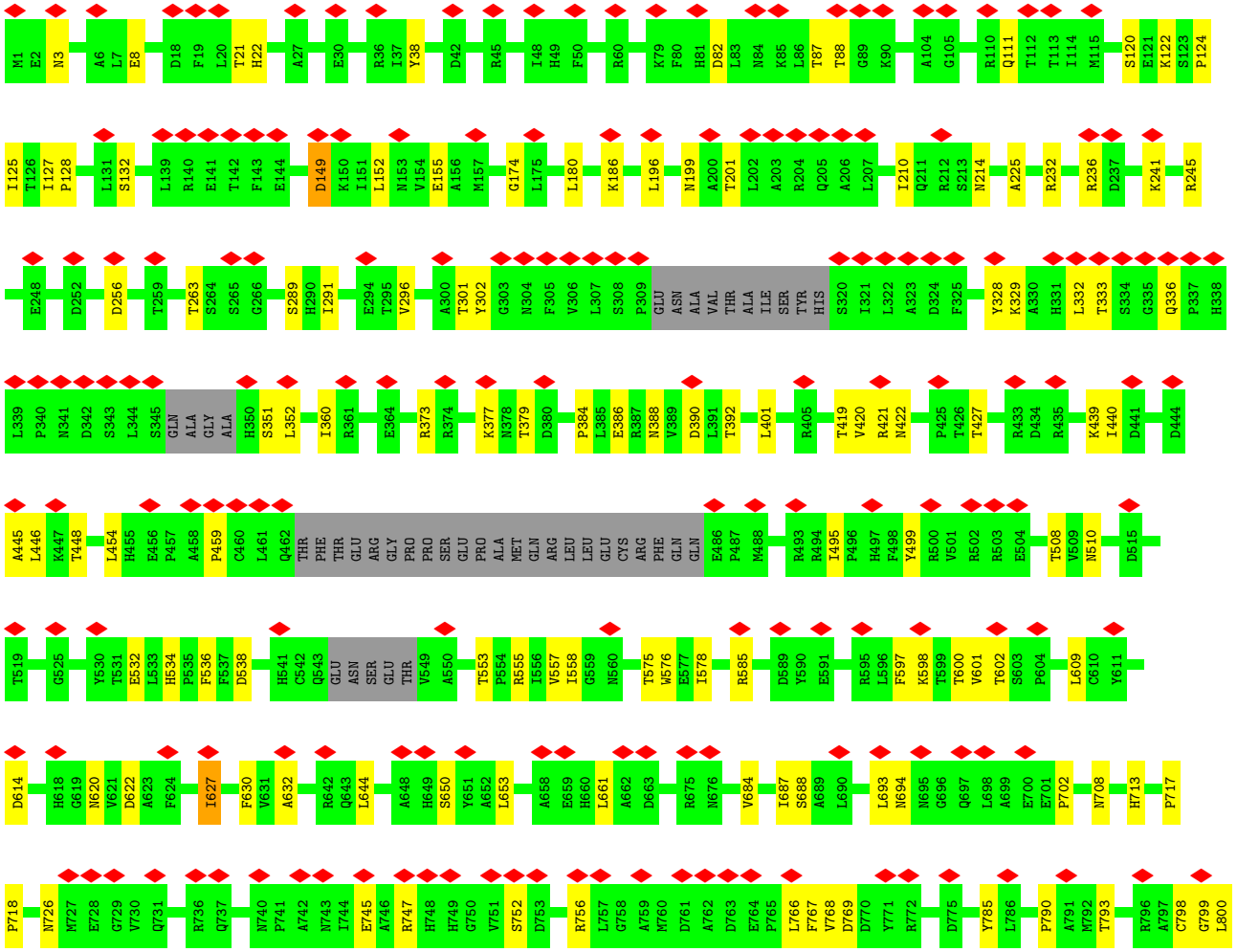


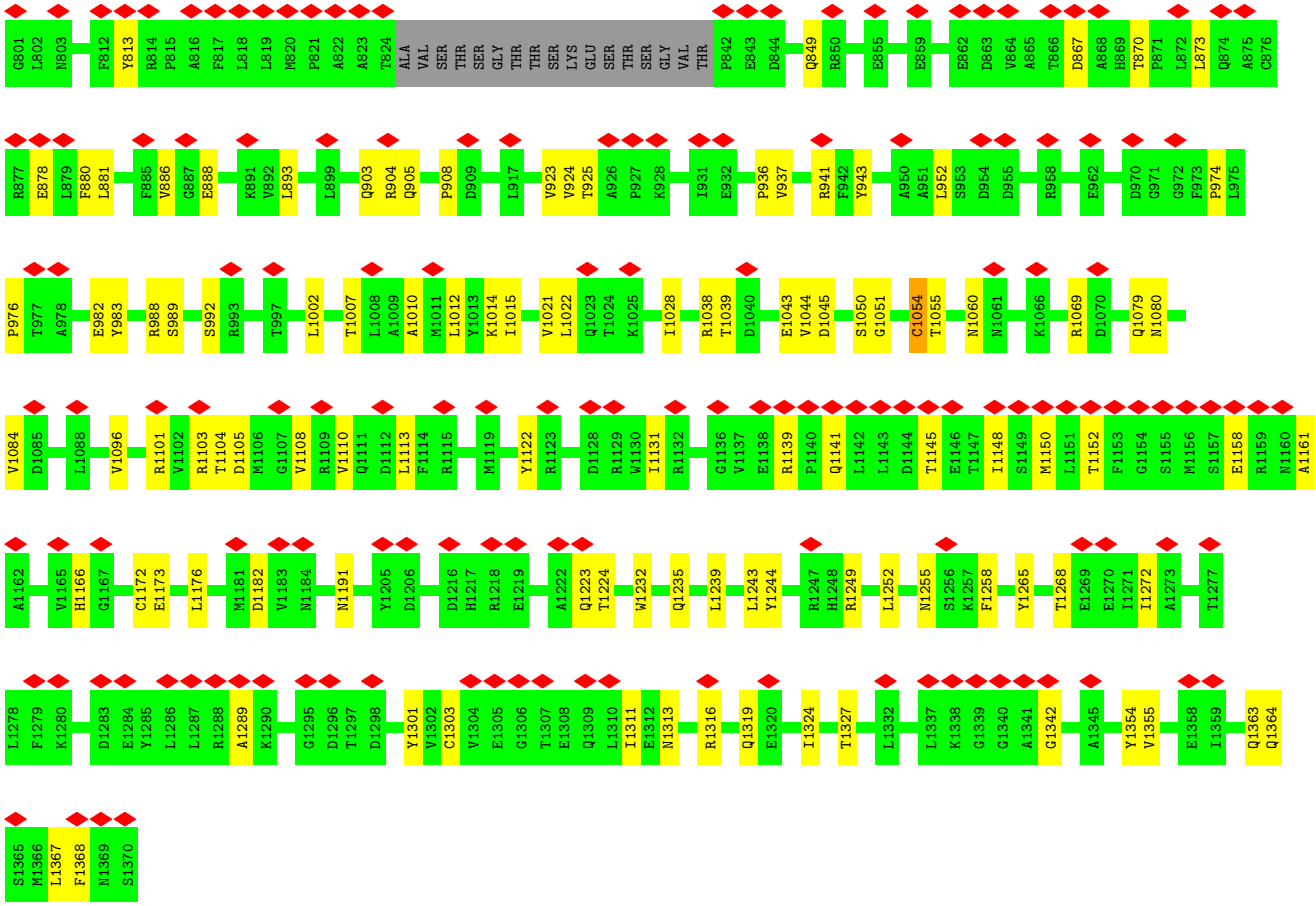




• Molecule 6: Major capsid protein

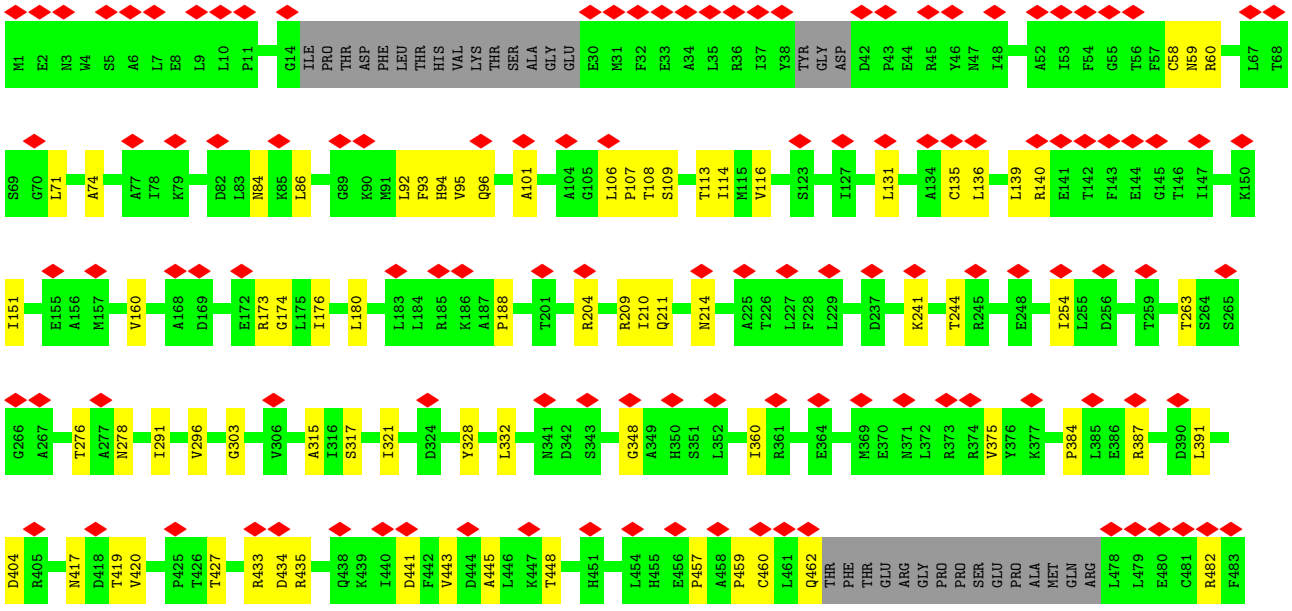
Chain B:

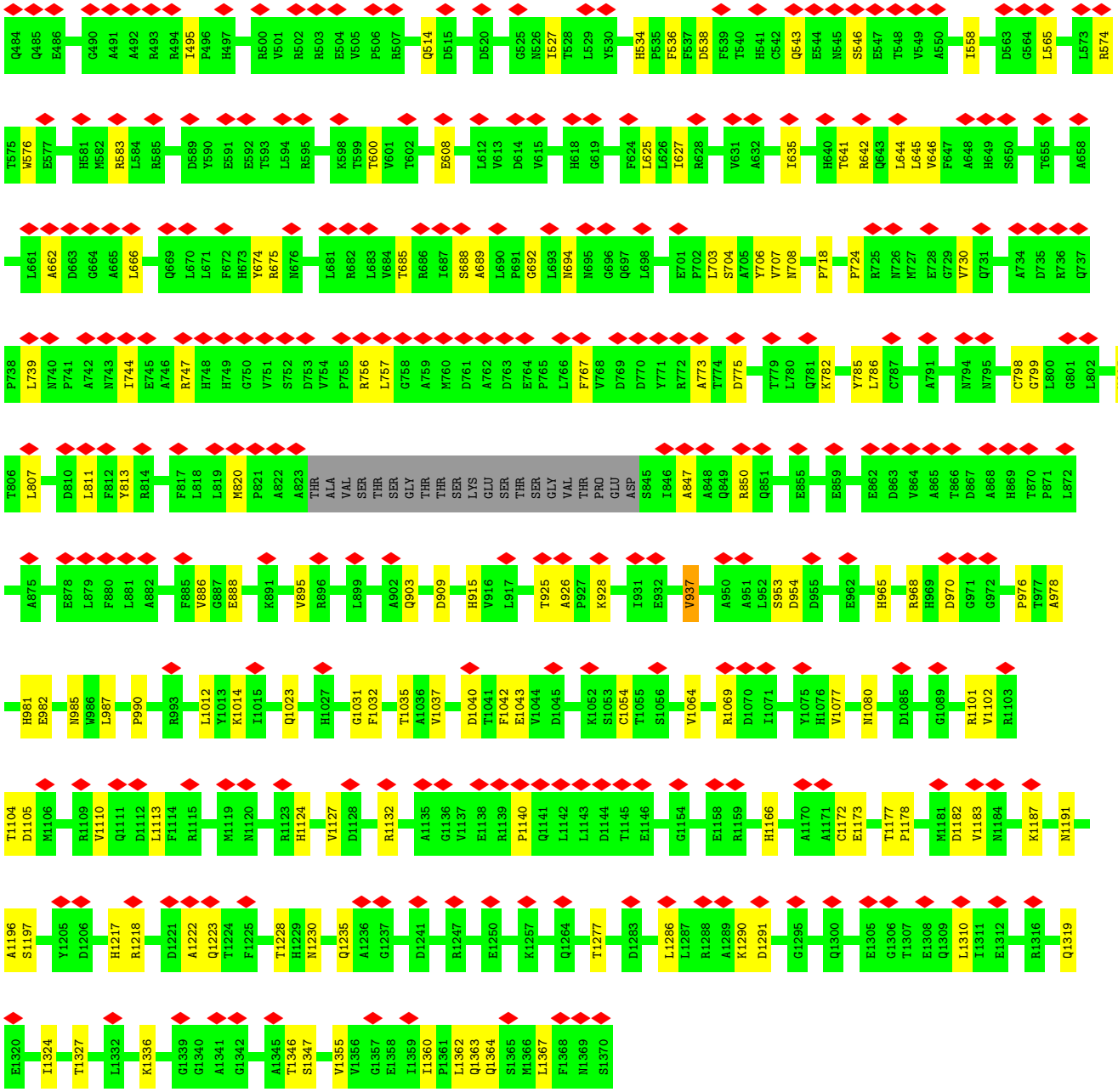




• Molecule 6: Major capsid protein

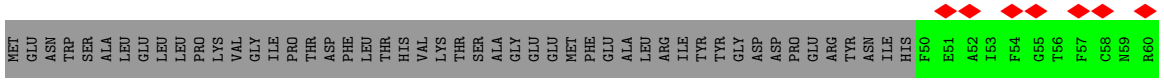
Chain C:

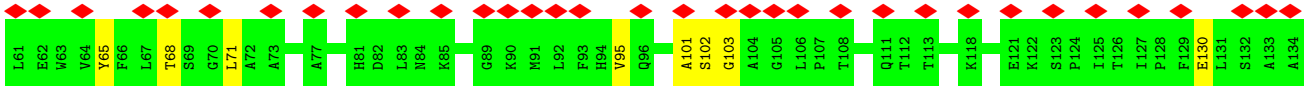


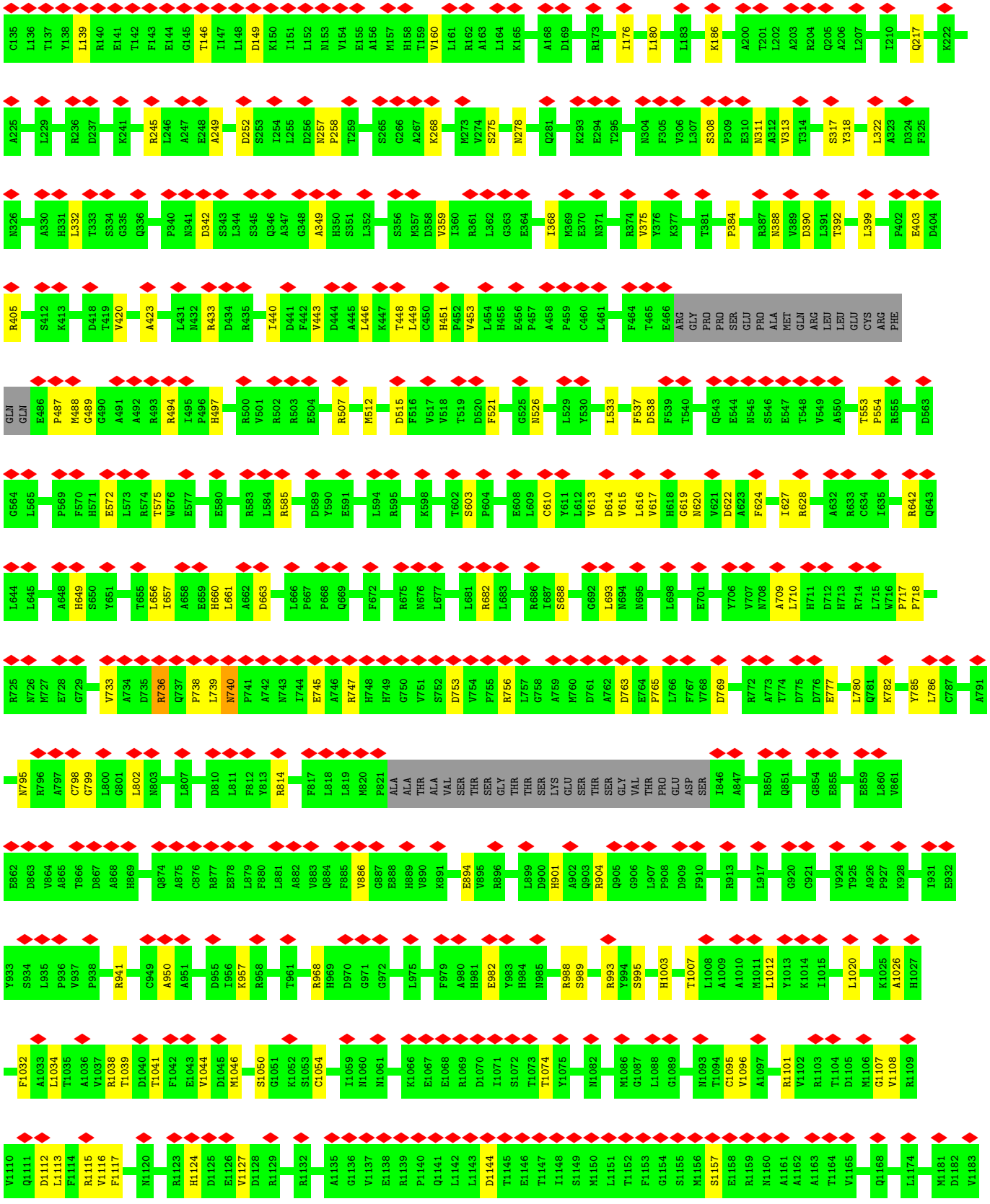


• Molecule 6: Major capsid protein

Chain D:



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N326 A330 H331 L332 T333 S334 G335 Q336 P340 N341 D342 S343 L344 S345 Q346 A347 G348 A349 H350 S351 L352 S356 M357 D358 V359 I360 R361 L362 G363 E364 I368 M369 E370 N371 R374 V375 Y376 K377 T381 P384 R387 N388 V389 D390 L391 T392 L399 P402 E403 D404
R405 S412 K413 D418 T419 V420 A423 L431 N432 R433 D434 R435 I440 D441 F442 V443 D444 A445 L446 K447 T448 L449 C450 H451 P452 V453 L454 H455 E456 P457 A458 P459 C460 L461 F464 T465 E466 ARG GLY PRO PRO SER GLU PRO ALA MET GLN ARG LEU LEU GLU CYS ARG PHE
GLN GLN E486 P487 M488 G489 G490 A491 A492 R493 R494 I495 P496 H497 R500 V501 R502 R503 E504 R507 M512 D515 F516 V517 V518 T519 D520 F521 G525 N526 L529 Y530 L533 F537 D538 F539 T540 Q543 E544 N545 S546 E547 T548 V549 A550 T553 P554 R555 D563
G564 L565 P569 F570 H571 E572 L573 R574 T575 W576 E577 E580 R583 L584 R585 D589 Y590 E591 L594 R595 K598 T602 S603 P604 E608 L609 C610 Y611 L612 V613 D614 V615 L616 V617 H618 G619 N620 V621 D622 A623 F624 I627 R628 A632 R633 C634 I635 R642 Q643
L644 L645 A648 H649 S650 Y651 T655 L656 I657 A658 E659 H660 L661 A662 D663 L666 P667 P668 Q669 F672 R675 N676 L677 L681 R682 L683 R686 I687 S688 G692 L693 N694 N695 L698 E701 Y706 V707 N708 A709 L710 H711 D712 H713 R714 L715 W716 P717 P718
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Y933 S934 L935 P936 V937 P938 R941 C949 A950 A951 D955 I956 K957 R958 T961 R968 H969 D970 G971 G972 L975 F979 A980 H981 E982 Y983 H984 N985 R988 S989 R993 Y994 S995 H1003 T1007 L1008 A1009 A1010 M1011 L1012 Y1013 K1014 I1015 L1020 K1025 A1026 H1027
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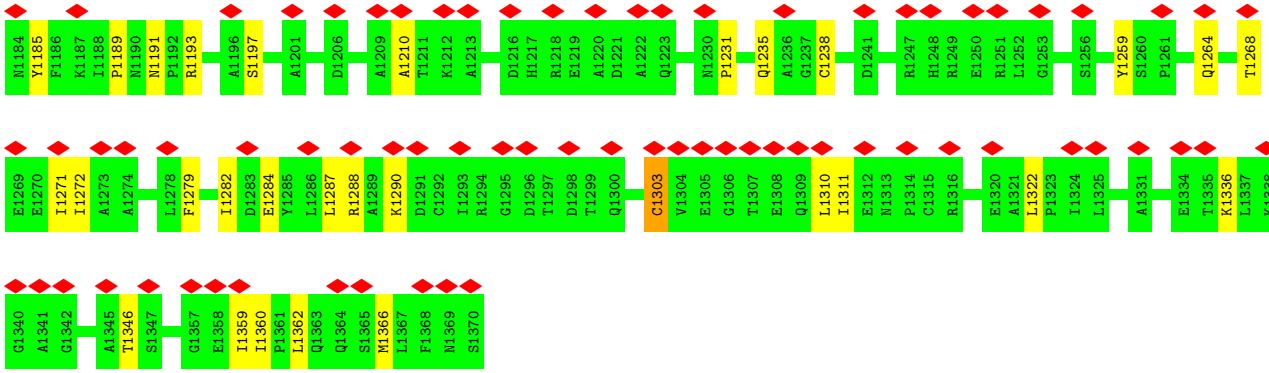
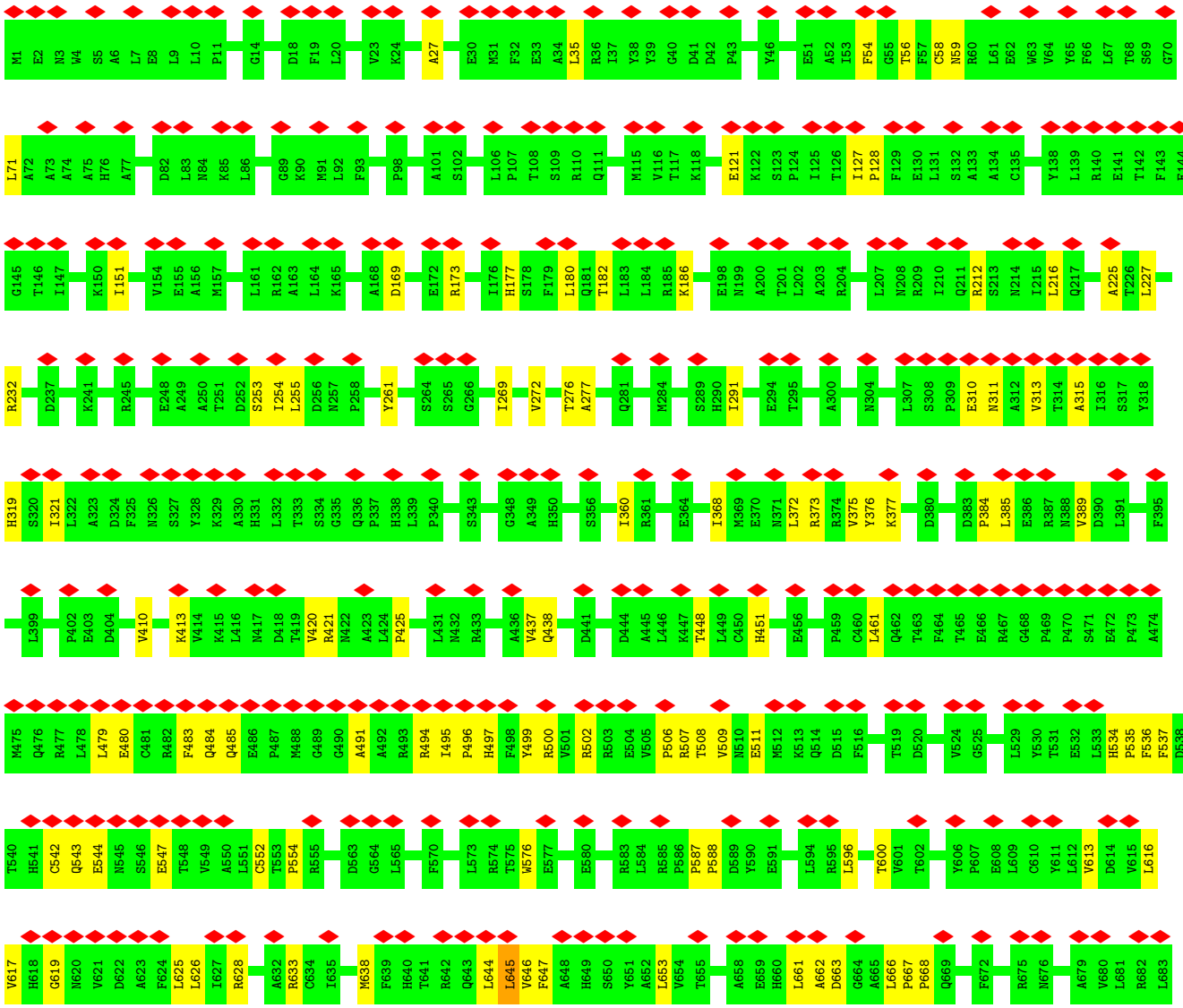
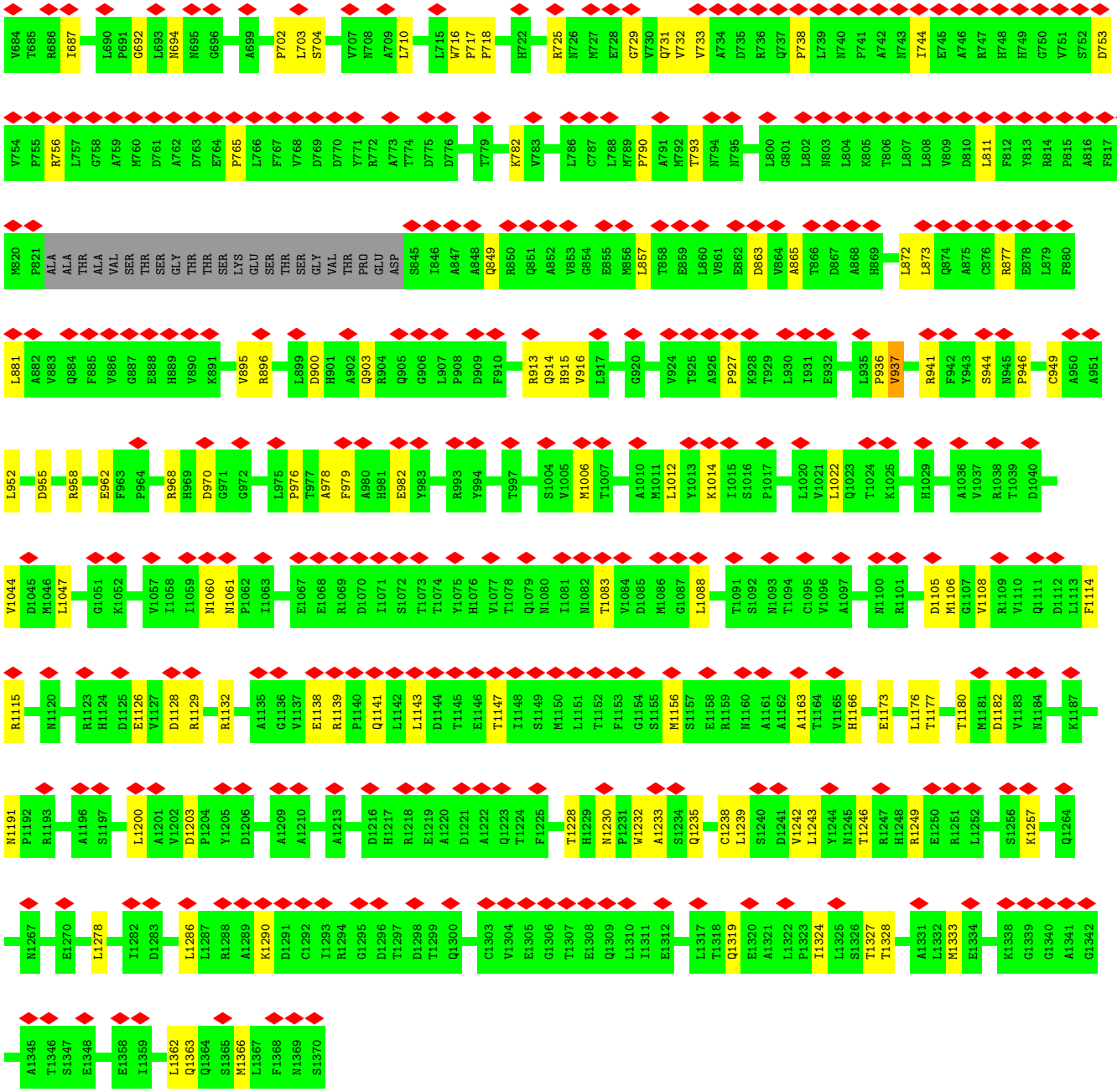
V1110 Q1111 D1112 L1113 F1114 R1115 V1116 F1117 N1120 R1123 H1124 D1125 E1126 V1127 D1128 R1129 R1132 A1135 G1136 V1137 E1138 R1139 P1140 Q1141 L1142 L1143 D1144 T1145 E1146 T1147 I1148 S1149 M1150 L1151 T1152 F1153 G1154 S1155 M1156 S1157 E1158 R1159 N1160 A1161 A1162 A1163 T1164 V1165 Q1168 L1174 M1181 D1182 V1183



• Molecule 6: Major capsid protein

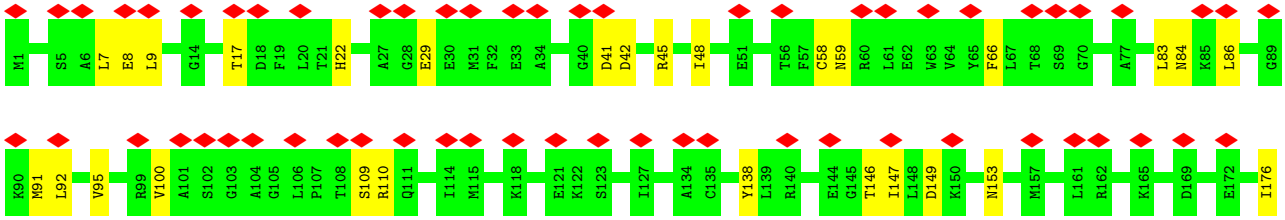
Chain Y:

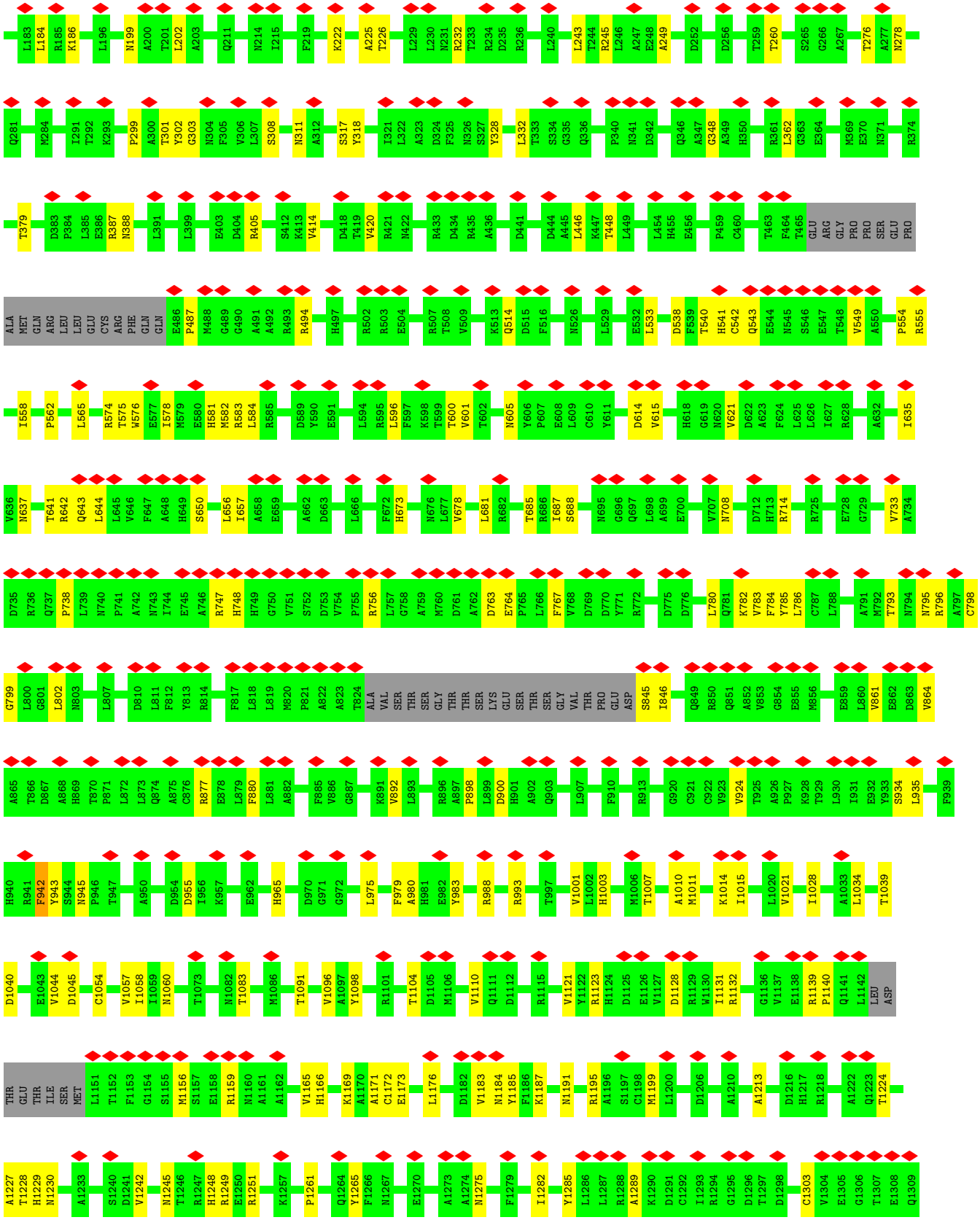




• Molecule 6: Major capsid protein

Chain Z:

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T379 D383 P384 L385 E386 R387 N388 L391 L399 E403 D404 R405 S412 K413 V414 D418 T419 V420 R421 N422 R433 D434 R435 A436 D441 D444 A445 L446 K447 T448 L449 L454 H455 E456 P459 C460 T463 F464 T465 GLU ARG GLY PRO PRO SER GLU PRO
ALA MET GLN ARG LEU LEU GLU CYS ARG PHE GLN GLN E486 P487 M488 G489 G490 A491 A492 R493 R494 H497 R502 R503 E504 R507 T508 V509 K513 Q514 D515 F516 N526 L529 E532 L533 D538 F539 T540 H541 C542 Q543 E544 N545 S546 E547 T548 V549 A550 P554 R555
I558 P562 L565 R574 T575 W576 E577 I578 M579 E580 H581 M582 R583 L584 R585 D589 Y590 E591 L594 R595 L596 F597 K598 T599 T600 V601 T602 N605 Y606 P607 E608 L609 C610 Y611 D614 V615 H618 G619 N620 V621 D622 A623 F624 L625 L626 I627 R628 A632 I635
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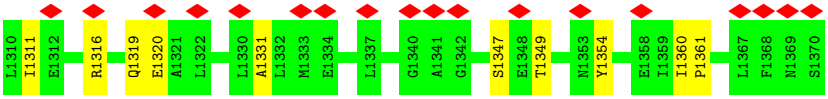
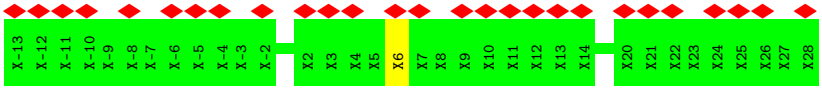
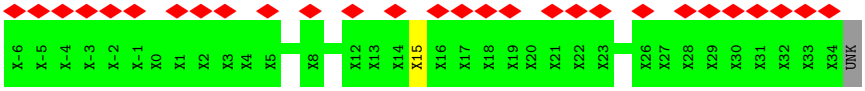
D1040 E1043 V1044 D1045 C1054 V1057 I1058 I1059 N1060 T1073 N1082 T1083 M1086 T1091 V1096 A1097 Y1098 R1101 T1104 D1105 M1106 V1110 Q1111 D1112 R1115 V1121 Y1122 R1123 H1124 D1125 E1126 V1127 D1128 R1129 W1130 I1131 R1132 G1136 V1137 E1138 R1139 P1140 Q1141 L1142 LEU ASP
THR GLU THR ILE SER MET L1151 T1152 F1153 G1154 S1155 M1156 S1157 E1158 R1159 N1160 A1161 A1162 V1165 H1166 K1169 A1170 A1171 C1172 E1173 L1176 D1182 V1183 N1184 Y1185 F1186 K1187 N1191 R1195 A1196 S1197 C1198 M1199 L1200 D1206 A1210 A1213 D1216 H1217 R1218 A1222 Q1223 T1224
A1227 T1228 H1229 N1230 A1233 S1240 D1241 V1242 N1245 T1246 R1247 H1248 R1249 E1250 R1251 K1257 P1261 Q1264 Y1265 F1266 N1267 E1270 A1273 A1274 N1275 F1279 I1282 Y1285 L1286 L1287 R1288 A1289 K1290 D1291 C1292 I1293 R1294 G1295 D1296 T1297 D1298 C1303 V1304 E1305 G1306 T1307 E1308 Q1309



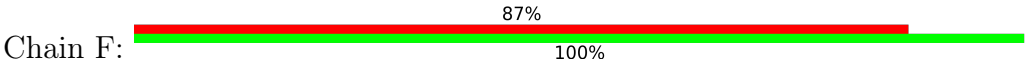
• Molecule 7: portal protein

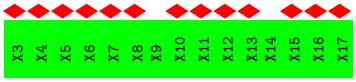


• Molecule 7: portal protein

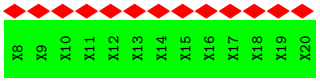


• Molecule 8: portal protein





• Molecule 9: portal protein



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	26181	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	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.066	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	416.0, 416.0, 416.0	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.625, 1.625, 1.625	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	I	0.31	0/2324	0.61	0/3154
1	h	0.31	0/2334	0.65	2/3173 (0.1%)
1	n	0.29	0/2379	0.58	0/3230
1	o	0.30	0/2333	0.56	0/3167
2	g	0.30	0/1793	0.58	1/2428 (0.0%)
2	m	0.31	0/2374	0.56	0/3221
3	M	0.31	0/3907	0.55	2/5294 (0.0%)
4	N	0.28	0/521	0.56	0/703
4	O	0.28	0/338	0.52	0/460
5	R	0.26	0/520	0.52	0/697
5	S	0.26	0/520	0.60	1/697 (0.1%)
5	i	0.28	0/520	0.53	0/697
5	j	0.27	0/520	0.57	0/697
6	B	0.33	0/10635	0.58	4/14483 (0.0%)
6	C	0.33	0/10676	0.56	2/14538 (0.0%)
6	D	0.32	0/10353	0.56	1/14105 (0.0%)
6	Y	0.31	0/10932	0.55	2/14892 (0.0%)
6	Z	0.32	0/10718	0.56	2/14601 (0.0%)
6	a	0.33	0/10407	0.56	1/14177 (0.0%)
All	All	0.32	0/84104	0.56	18/114414 (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
6	B	0	1
6	D	0	2
6	Y	0	1
6	Z	0	1
All	All	0	5

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	1002	LEU	CA-CB-CG	6.69	130.69	115.30
6	Z	86	LEU	CA-CB-CG	6.44	130.11	115.30
3	M	152	VAL	C-N-CA	6.13	137.02	121.70
5	S	26	LEU	CA-CB-CG	5.89	128.85	115.30
6	C	86	LEU	CA-CB-CG	5.85	128.75	115.30
6	D	1303	CYS	CA-CB-SG	5.77	124.38	114.00
6	B	627	ILE	CG1-CB-CG2	-5.71	98.84	111.40
1	h	124	LEU	CA-CB-CG	5.51	127.97	115.30
6	B	1176	LEU	CA-CB-CG	5.46	127.86	115.30
3	M	385	ALA	C-N-CA	5.42	135.26	121.70
6	B	352	LEU	CA-CB-CG	5.39	127.70	115.30
6	C	627	ILE	CG1-CB-CG2	-5.22	99.92	111.40
1	h	16	LEU	CA-CB-CG	5.19	127.24	115.30
2	g	118	LEU	CA-CB-CG	5.07	126.96	115.30
6	a	1239	LEU	CA-CB-CG	5.06	126.94	115.30
6	Z	1034	LEU	CA-CB-CG	5.06	126.94	115.30
6	Y	645	LEU	CA-CB-CG	5.02	126.85	115.30
6	Y	1047	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	B	585	ARG	Peptide
6	D	1303	CYS	Peptide
6	D	585	ARG	Peptide
6	Y	944	SER	Peptide
6	Z	764	GLU	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	I	2282	0	2373	28	0
1	h	2290	0	2375	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	n	2334	0	2431	0	0
1	o	2291	0	2383	0	0
2	g	1758	0	1797	0	0
2	m	2325	0	2363	0	0
3	M	3820	0	3750	50	0
4	N	509	0	515	10	0
4	O	329	0	330	4	0
5	R	513	0	539	5	0
5	S	513	0	539	11	0
5	i	513	0	539	0	0
5	j	513	0	539	0	0
6	B	10389	0	10345	138	0
6	C	10431	0	10386	137	0
6	D	10114	0	10074	113	0
6	Y	10676	0	10618	137	0
6	Z	10468	0	10413	140	0
6	a	10167	0	10125	0	0
7	A	210	0	44	1	0
7	E	205	0	43	1	0
8	F	75	0	17	0	0
9	G	65	0	15	0	0
All	All	82790	0	82553	711	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 6.

All (711) 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)
6:Y:1239:LEU:O	6:Y:1243:LEU:HB2	1.80	0.81
6:D:610:CYS:O	6:D:614:ASP:HB2	1.84	0.77
6:C:543:GLN:HE21	6:C:546:SER:H	1.37	0.71
6:C:92:LEU:HB3	6:Z:7:LEU:HD12	1.72	0.70
6:D:433:ARG:HH22	6:D:1101:ARG:HH21	1.40	0.68
6:Z:578:ILE:HG12	6:Z:1028:ILE:HD12	1.76	0.67
6:Y:694:ASN:HD22	6:Y:704:SER:HB2	1.59	0.66
6:Z:1176:LEU:HD22	6:Z:1230:ASN:HD22	1.61	0.66
6:B:575:THR:HG21	6:B:1007:THR:HA	1.79	0.65
6:Y:600:THR:HG22	6:Y:644:LEU:HB2	1.78	0.65
6:C:433:ARG:HE	6:D:217:GLN:HG2	1.62	0.65
6:Y:180:LEU:HD23	6:Y:384:PRO:HG2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Y:534:HIS:HD2	6:Y:536:PHE:H	1.44	0.64
1:I:74:ARG:HG2	1:I:75:ARG:HG3	1.78	0.64
6:D:1284:GLU:O	6:D:1288:ARG:HB2	1.97	0.63
5:S:16:GLU:O	5:S:20:HIS:HB2	1.98	0.63
6:B:553:THR:HG21	6:B:983:TYR:HB3	1.80	0.63
6:Y:716:TRP:H	6:Y:914:GLN:HE22	1.46	0.63
6:Z:1172:CYS:SG	6:Z:1173:GLU:N	2.72	0.63
6:Y:753:ASP:HB3	6:Y:756:ARG:HE	1.64	0.62
6:C:135:CYS:O	6:C:139:LEU:HB2	1.99	0.62
6:Z:414:VAL:HG21	6:Z:1331:ALA:HB1	1.81	0.62
6:Y:58:CYS:SG	6:Y:59:ASN:N	2.73	0.62
1:I:93:THR:HG22	1:I:301:THR:HG22	1.82	0.62
6:B:600:THR:HA	6:B:644:LEU:HD12	1.81	0.62
6:D:747:ARG:HD2	6:D:769:ASP:HB3	1.82	0.62
6:Y:272:VAL:HG12	6:Y:368:ILE:HB	1.81	0.61
3:M:44:TYR:HB2	3:M:150:ARG:HB2	1.82	0.61
6:C:782:LYS:O	6:C:786:LEU:HB2	2.00	0.61
6:D:448:THR:HG23	6:D:1113:LEU:HG	1.83	0.61
6:D:139:LEU:HD22	6:D:160:VAL:HG21	1.81	0.61
6:C:495:ILE:HG13	6:C:976:PRO:HG2	1.83	0.61
6:C:798:CYS:SG	6:C:799:GLY:N	2.74	0.61
6:D:901:HIS:HA	6:D:904:ARG:HB2	1.83	0.61
3:M:363:VAL:HG23	3:M:550:LEU:HD21	1.82	0.61
6:Y:502:ARG:NH2	6:Y:962:GLU:OE2	2.34	0.61
6:Y:542:CYS:SG	6:Y:543:GLN:N	2.74	0.61
6:B:941:ARG:HH11	6:B:992:SER:HB3	1.64	0.60
6:D:624:PHE:HA	6:D:627:ILE:HG22	1.82	0.60
6:Y:1106:MET:SD	6:Y:1363:GLN:NE2	2.74	0.60
6:B:1239:LEU:O	6:B:1243:LEU:HB2	2.01	0.60
6:Z:798:CYS:SG	6:Z:799:GLY:N	2.75	0.60
6:Y:311:ASN:HB3	6:Y:321:ILE:HG23	1.82	0.60
6:Y:495:ILE:HG23	6:Y:496:PRO:HD3	1.83	0.60
6:Z:575:THR:HG21	6:Z:1007:THR:HA	1.83	0.60
6:B:1150:MET:SD	6:B:1255:ASN:ND2	2.75	0.60
6:Z:600:THR:HG22	6:Z:644:LEU:HB2	1.84	0.60
1:I:160:ARG:NH2	1:I:186:ASP:OD2	2.34	0.59
6:B:1054:CYS:SG	6:B:1055:THR:N	2.75	0.59
6:B:386:GLU:HA	6:B:1045:ASP:HA	1.85	0.59
6:B:534:HIS:HD2	6:B:536:PHE:H	1.51	0.59
6:C:174:GLY:HA3	6:D:101:ALA:HB3	1.82	0.59
6:B:1060:ASN:O	6:B:1079:GLN:NE2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:578:ILE:HG22	6:B:1028:ILE:HD12	1.84	0.59
6:B:756:ARG:NH2	6:B:886:VAL:O	2.35	0.59
6:C:93:PHE:HB2	6:C:116:VAL:HB	1.84	0.59
6:Y:638:MET:HG2	6:Y:646:VAL:HG13	1.84	0.58
6:Z:58:CYS:SG	6:Z:59:ASN:N	2.76	0.58
6:Z:678:VAL:HA	6:Z:681:LEU:HD12	1.83	0.58
5:S:62:LEU:HB3	6:C:757:LEU:HD13	1.85	0.58
6:C:180:LEU:HD23	6:C:384:PRO:HG2	1.85	0.58
6:D:449:LEU:HD11	6:D:1034:LEU:HD21	1.85	0.58
6:B:1172:CYS:SG	6:B:1173:GLU:N	2.72	0.58
6:Y:692:GLY:HA2	6:Z:993:ARG:HH12	1.67	0.58
6:B:1044:VAL:HG11	6:B:1096:VAL:HG13	1.85	0.58
6:C:433:ARG:NH2	6:C:1102:VAL:O	2.36	0.58
6:Z:138:TYR:O	6:Z:153:ASN:ND2	2.37	0.58
6:B:149:ASP:OD1	6:B:149:ASP:N	2.37	0.57
6:B:22:HIS:NE2	6:Z:379:THR:O	2.33	0.57
6:Y:173:ARG:HB3	6:Z:100:VAL:HG12	1.86	0.57
6:Y:1235:GLN:HB2	6:Y:1238:CYS:HB3	1.85	0.57
6:Z:795:ASN:O	6:Z:945:ASN:ND2	2.35	0.57
6:Z:1199:MET:HB3	6:Z:1275:ASN:HB3	1.86	0.57
6:B:849:GLN:HB2	6:B:873:LEU:HD13	1.85	0.57
6:C:675:ARG:NH1	6:D:603:SER:OG	2.36	0.57
6:B:1043:GLU:OE1	6:B:1101:ARG:NH1	2.33	0.57
6:D:717:PRO:HB3	6:D:782:LYS:HA	1.86	0.57
6:Z:747:ARG:NH2	6:Z:767:PHE:O	2.38	0.57
1:I:115:PHE:HB3	1:I:118:PRO:HB3	1.86	0.57
6:B:1182:ASP:OD1	6:B:1182:ASP:N	2.38	0.57
6:D:1095:CYS:SG	6:D:1096:VAL:N	2.77	0.57
6:Y:687:ILE:HG21	6:Y:1006:MET:HG2	1.85	0.57
6:Z:601:VAL:HG11	6:Z:793:THR:HG22	1.86	0.57
1:I:56:ARG:NH1	6:B:1152:THR:O	2.38	0.56
3:M:47:ASN:HD21	3:M:135:ARG:HB3	1.70	0.56
3:M:409:HIS:ND1	3:M:480:CYS:SG	2.78	0.56
3:M:513:ARG:NH2	4:O:18:PRO:O	2.39	0.56
6:Z:1172:CYS:HB2	6:Z:1261:PRO:HD2	1.88	0.56
5:S:75:ARG:NH2	6:C:625:LEU:O	2.39	0.56
6:D:795:ASN:ND2	6:D:995:SER:OG	2.39	0.56
6:Y:941:ARG:HH12	6:Y:982:GLU:HA	1.70	0.56
6:C:482:ARG:HH22	6:C:982:GLU:H	1.51	0.56
6:C:600:THR:HG22	6:C:644:LEU:HB2	1.88	0.56
6:Z:581:HIS:ND1	6:Z:582:MET:SD	2.78	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Z:748:HIS:H	6:Z:756:ARG:HH22	1.54	0.56
6:Z:900:ASP:OD2	6:Z:1014:LYS:NZ	2.38	0.56
6:B:196:LEU:O	6:B:201:THR:OG1	2.24	0.56
6:Y:180:LEU:HD21	6:Y:385:LEU:HG	1.86	0.56
6:Z:955:ASP:OD1	6:Z:955:ASP:N	2.39	0.56
1:I:232:VAL:HG21	3:M:5:LEU:HB3	1.86	0.56
6:C:151:ILE:HD12	6:D:332:LEU:HG	1.88	0.56
3:M:386:LEU:HD22	3:M:541:VAL:HG22	1.88	0.55
1:I:118:PRO:HG2	1:I:121:ARG:H	1.71	0.55
3:M:339:ARG:O	3:M:339:ARG:NH1	2.39	0.55
6:B:510:ASN:ND2	6:B:538:ASP:OD1	2.39	0.55
6:C:315:ALA:HB2	6:C:321:ILE:HD11	1.88	0.55
1:I:207:VAL:HG21	1:I:275:LEU:HB3	1.87	0.55
1:I:210:LEU:O	1:I:214:LEU:HB2	2.06	0.55
6:Y:420:VAL:HG11	6:Y:576:TRP:HB3	1.89	0.55
6:B:924:VAL:HG23	6:B:925:THR:HG23	1.89	0.55
6:C:433:ARG:NH1	6:C:1166:HIS:O	2.40	0.55
6:D:740:ASN:OD1	6:D:740:ASN:N	2.36	0.55
6:Y:151:ILE:HD12	6:Z:332:LEU:HG	1.87	0.55
6:D:521:PHE:O	6:D:526:ASN:ND2	2.40	0.55
6:D:1113:LEU:HA	6:D:1116:VAL:HG12	1.88	0.55
6:Z:558:ILE:HG21	6:Z:574:ARG:HH22	1.70	0.55
6:C:688:SER:O	6:C:708:ASN:ND2	2.39	0.55
6:C:1191:ASN:ND2	6:C:1319:GLN:O	2.40	0.55
6:Y:666:LEU:HD12	6:Y:667:PRO:HD2	1.89	0.55
6:D:1112:ASP:OD1	6:D:1112:ASP:N	2.40	0.55
3:M:110:SER:OG	3:M:111:GLY:N	2.40	0.55
6:B:1223:GLN:HG3	6:B:1224:THR:HG23	1.89	0.55
6:Y:710:LEU:HD12	6:Y:782:LYS:HE2	1.88	0.55
6:Z:1183:VAL:HA	6:Z:1187:LYS:HE2	1.88	0.55
6:C:558:ILE:HD11	6:C:1031:GLY:HA3	1.89	0.55
6:C:724:PRO:HA	6:C:773:ALA:HB3	1.89	0.55
6:D:777:GLU:HA	6:D:780:LEU:HB2	1.88	0.55
1:I:66:ARG:NH2	1:I:284:GLU:OE1	2.40	0.54
6:Y:626:LEU:HD12	6:Y:881:LEU:HD13	1.90	0.54
6:C:417:ASN:ND2	6:D:403:GLU:O	2.40	0.54
6:Y:56:THR:HG22	6:Z:92:LEU:HB3	1.90	0.54
6:B:598:LYS:HE2	6:B:602:THR:HG21	1.89	0.54
6:D:515:ASP:OD1	6:D:515:ASP:N	2.39	0.54
6:D:756:ARG:NH2	6:D:886:VAL:O	2.36	0.54
6:Y:915:HIS:NE2	6:Y:978:ALA:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Y:662:ALA:HB1	6:Z:605:ASN:HD22	1.73	0.54
6:Y:1246:THR:HA	6:Y:1249:ARG:HB3	1.88	0.54
6:Z:621:VAL:HG12	6:Z:656:LEU:HD11	1.89	0.54
5:S:26:LEU:HD22	5:S:28:LEU:HB2	1.89	0.54
6:Y:729:GLY:O	6:Y:731:GLN:NE2	2.41	0.54
6:Y:946:PRO:HA	6:Y:949:CYS:HB3	1.89	0.54
6:Y:1139:ARG:HD3	6:Y:1141:GLN:HE22	1.72	0.54
6:Z:584:LEU:HD12	6:Z:687:ILE:HD11	1.89	0.54
6:Z:845:SER:OG	6:Z:846:ILE:N	2.41	0.54
6:B:1103:ARG:HD2	6:C:210:ILE:HD12	1.90	0.54
6:B:688:SER:OG	6:B:708:ASN:ND2	2.41	0.54
6:Z:8:GLU:OE2	6:Z:45:ARG:NH1	2.40	0.54
6:C:608:GLU:OE2	6:C:928:LYS:N	2.40	0.53
1:I:204:MET:HB3	1:I:278:LEU:HD21	1.89	0.53
6:B:558:ILE:HD13	6:B:1015:ILE:HD13	1.91	0.53
6:D:615:VAL:HG21	6:D:802:LEU:HD23	1.91	0.53
6:Y:495:ILE:HG21	6:Y:937:VAL:HG12	1.90	0.53
6:C:210:ILE:O	6:C:214:ASN:ND2	2.42	0.53
6:Y:1200:LEU:HD21	6:Y:1278:LEU:HD13	1.90	0.53
6:B:1191:ASN:ND2	6:B:1319:GLN:O	2.32	0.53
6:D:1290:LYS:HB2	6:D:1310:LEU:HD23	1.91	0.53
6:B:941:ARG:NH2	6:B:982:GLU:OE2	2.42	0.53
6:C:136:LEU:O	6:C:140:ARG:NH1	2.41	0.53
6:D:782:LYS:O	6:D:786:LEU:HB2	2.09	0.53
6:B:632:ALA:HB2	6:B:661:LEU:HD11	1.89	0.53
6:C:968:ARG:HD3	6:C:970:ASP:HB3	1.89	0.53
6:Z:276:THR:HG23	6:Z:278:ASN:H	1.74	0.53
6:D:1336:LYS:NZ	6:D:1346:THR:OG1	2.39	0.53
6:Z:487:PRO:HG2	6:Z:494:ARG:HH12	1.72	0.53
6:B:210:ILE:O	6:B:214:ASN:ND2	2.42	0.53
6:D:950:ALA:HB1	6:D:957:LYS:HD3	1.91	0.53
6:Y:732:VAL:HG22	6:Y:895:VAL:HG12	1.91	0.53
6:Y:1105:ASP:HB3	6:Y:1166:HIS:HB3	1.91	0.53
6:Y:483:PHE:HB3	6:Y:913:ARG:HH12	1.74	0.52
6:Z:782:LYS:O	6:Z:786:LEU:HB2	2.09	0.52
3:M:369:ARG:NH1	4:N:47:TRP:O	2.39	0.52
6:C:807:LEU:O	6:C:811:LEU:HB3	2.08	0.52
6:C:981:HIS:O	6:C:985:ASN:ND2	2.41	0.52
6:C:291:ILE:HA	6:C:360:ILE:HG22	1.91	0.52
6:D:1115:ARG:NH1	6:D:1157:SER:O	2.43	0.52
6:Z:1289:ALA:HB1	6:Z:1316:ARG:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:694:ASN:O	6:D:968:ARG:NH2	2.42	0.52
6:C:953:SER:OG	6:C:954:ASP:N	2.42	0.52
6:Z:733:VAL:HG12	6:Z:738:PRO:HA	1.92	0.52
6:Z:983:TYR:O	6:Z:988:ARG:NH1	2.41	0.52
1:I:138:VAL:HG11	1:I:142:LEU:HD22	1.90	0.52
6:B:575:THR:HG22	6:B:1010:ALA:HB3	1.90	0.52
6:Z:1054:CYS:SG	6:Z:1091:THR:OG1	2.64	0.52
6:D:537:PHE:HA	6:D:554:PRO:HA	1.92	0.52
6:D:1185:TYR:OH	6:D:1193:ARG:O	2.27	0.52
3:M:49:ASP:HA	3:M:145:GLN:HG2	1.91	0.52
3:M:50:SER:O	3:M:53:ARG:NH1	2.41	0.52
6:Y:169:ASP:OD2	6:Y:173:ARG:NH2	2.42	0.52
5:R:68:VAL:HG13	6:B:880:PHE:HZ	1.75	0.52
6:B:236:ARG:NH2	6:B:289:SER:OG	2.43	0.52
6:C:583:ARG:NH1	6:D:572:GLU:OE1	2.42	0.52
6:Y:216:LEU:HD21	6:Y:1200:LEU:HD22	1.92	0.52
6:Y:507:ARG:HH21	6:Y:968:ARG:HH12	1.56	0.52
6:C:420:VAL:HG21	6:C:576:TRP:HB3	1.91	0.52
6:C:1336:LYS:NZ	6:C:1346:THR:OG1	2.43	0.52
6:B:532:GLU:OE1	6:B:555:ARG:NH2	2.43	0.51
6:D:180:LEU:HD23	6:D:384:PRO:HG2	1.92	0.51
6:Y:480:GLU:HG2	6:Y:506:PRO:HD2	1.92	0.51
3:M:169:LEU:HB3	3:M:173:MET:HB2	1.92	0.51
6:D:488:MET:HG3	6:D:894:GLU:HG3	1.93	0.51
6:Y:373:ARG:HG3	6:Y:377:LYS:HD2	1.92	0.51
6:Z:225:ALA:O	6:Z:232:ARG:NH1	2.44	0.51
6:B:329:LYS:HE2	6:B:333:THR:HB	1.92	0.51
6:Y:1327:THR:HG21	6:Y:1333:MET:HB2	1.92	0.51
6:Z:186:LYS:NZ	6:Z:1054:CYS:SG	2.82	0.51
6:B:694:ASN:HB3	6:C:968:ARG:HH11	1.75	0.51
6:C:909:ASP:OD1	6:C:909:ASP:N	2.44	0.51
3:M:20:GLN:HA	3:M:135:ARG:HA	1.93	0.51
6:B:745:GLU:HB2	6:B:768:VAL:HG22	1.92	0.51
6:Z:514:GLN:HE21	6:Z:993:ARG:HD3	1.76	0.51
6:C:482:ARG:HA	6:C:981:HIS:HE1	1.74	0.51
6:C:574:ARG:HH11	6:C:1023:GLN:HE22	1.57	0.51
6:Y:182:THR:O	6:Y:186:LYS:NZ	2.37	0.51
6:Z:83:LEU:HD11	6:Z:1058:ILE:HG22	1.93	0.51
6:C:915:HIS:NE2	6:C:978:ALA:O	2.44	0.51
3:M:505:ARG:NH1	3:M:509:GLY:O	2.44	0.51
6:B:713:HIS:CG	6:B:726:ASN:HD21	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:427:THR:OG1	6:D:405:ARG:NH1	2.43	0.51
6:D:739:LEU:HD12	6:D:745:GLU:HG3	1.92	0.51
6:Y:495:ILE:HG13	6:Y:976:PRO:HG2	1.92	0.51
6:B:256:ASP:OD1	6:B:256:ASP:N	2.43	0.50
6:B:1327:THR:HG22	6:B:1355:VAL:HG22	1.91	0.50
6:Y:900:ASP:OD2	6:Y:1014:LYS:NZ	2.44	0.50
6:Z:109:SER:OG	6:Z:110:ARG:N	2.44	0.50
6:B:420:VAL:HG21	6:B:576:TRP:HB3	1.91	0.50
6:B:1289:ALA:HB1	6:B:1316:ARG:HG2	1.92	0.50
6:C:1228:THR:HG22	6:C:1230:ASN:H	1.76	0.50
6:Y:507:ARG:HD3	6:Y:511:GLU:HG3	1.92	0.50
6:Z:714:ARG:NE	6:Z:900:ASP:OD1	2.45	0.50
6:B:745:GLU:HA	6:B:767:PHE:HA	1.93	0.50
3:M:38:GLU:OE1	3:M:583:ARG:NE	2.45	0.50
6:B:1161:ALA:O	6:C:209:ARG:NH2	2.44	0.50
6:C:278:ASN:OD1	6:C:278:ASN:N	2.43	0.50
3:M:172:GLU:OE1	3:M:313:ARG:NE	2.40	0.50
3:M:389:ARG:HB2	3:M:540:ALA:HB3	1.94	0.50
6:B:225:ALA:O	6:B:232:ARG:NH1	2.44	0.50
6:C:59:ASN:HB2	6:D:95:VAL:HA	1.93	0.50
6:C:459:PRO:HA	6:C:462:GLN:HE21	1.77	0.50
6:Z:184:LEU:HD13	6:Z:387:ARG:HH21	1.76	0.50
6:Z:934:SER:OG	6:Z:935:LEU:N	2.44	0.50
6:Z:1007:THR:O	6:Z:1011:MET:HB2	2.12	0.50
6:Z:1349:THR:HA	6:Z:1354:TYR:HA	1.94	0.50
6:B:132:SER:OG	6:Z:41:ASP:O	2.29	0.50
6:Z:1195:ARG:NH1	6:Z:1227:ALA:O	2.44	0.50
6:C:756:ARG:NH1	6:C:886:VAL:O	2.44	0.49
6:D:275:SER:OG	6:D:1046:MET:O	2.30	0.49
6:D:710:LEU:HD22	6:D:1012:LEU:HD22	1.94	0.49
6:Z:420:VAL:HG21	6:Z:576:TRP:HB3	1.94	0.49
6:Z:1057:VAL:HG12	6:Z:1083:THR:HG22	1.94	0.49
3:M:56:GLY:O	3:M:87:ARG:NH2	2.40	0.49
6:C:419:THR:OG1	6:C:420:VAL:N	2.45	0.49
6:Z:42:ASP:OD1	6:Z:42:ASP:N	2.45	0.49
5:S:28:LEU:HD12	5:S:29:PRO:HD2	1.93	0.49
6:B:747:ARG:NH2	6:B:888:GLU:OE1	2.45	0.49
6:Z:681:LEU:HB3	6:Z:780:LEU:HD12	1.94	0.49
3:M:163:PHE:HB3	3:M:319:ASP:HA	1.94	0.49
3:M:422:SER:OG	3:M:423:CYS:N	2.45	0.49
6:B:798:CYS:SG	6:B:799:GLY:N	2.86	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:1158:GLU:O	6:B:1301:TYR:OH	2.30	0.49
6:D:718:PRO:HD2	6:D:785:TYR:HB3	1.93	0.49
6:B:903:GLN:HE22	6:B:1014:LYS:HB3	1.77	0.49
6:C:1124:HIS:HB3	6:C:1127:VAL:HG12	1.93	0.49
3:M:64:ASP:HB3	3:M:553:ARG:HB3	1.95	0.49
6:B:180:LEU:HD23	6:B:384:PRO:HG2	1.93	0.49
6:C:925:THR:OG1	6:C:926:ALA:N	2.44	0.49
1:I:226:ASP:OD1	1:I:226:ASP:N	2.46	0.49
6:D:130:GLU:HA	6:D:1074:THR:HA	1.94	0.49
6:D:620:ASN:HD21	6:D:622:ASP:HB2	1.77	0.49
6:Y:1126:GLU:HA	6:Y:1129:ARG:HD2	1.94	0.49
6:Z:146:THR:HG23	6:Z:149:ASP:H	1.77	0.49
6:Y:900:ASP:OD1	6:Y:900:ASP:N	2.40	0.49
6:B:684:VAL:HA	6:B:687:ILE:HG22	1.95	0.49
6:C:1182:ASP:OD1	6:C:1182:ASP:N	2.46	0.49
6:D:390:ASP:HB3	6:D:1041:THR:HG22	1.95	0.49
6:D:1116:VAL:HG13	6:D:1117:PHE:HD1	1.78	0.49
6:Y:484:GLN:O	6:Y:485:GLN:NE2	2.46	0.49
6:Z:748:HIS:O	6:Z:756:ARG:NH1	2.41	0.49
3:M:319:ASP:OD1	3:M:323:ARG:N	2.43	0.48
3:M:529:LEU:HD12	3:M:545:VAL:HG21	1.94	0.48
6:C:747:ARG:HB2	6:C:767:PHE:HB3	1.94	0.48
6:Y:310:GLU:HA	6:Y:313:VAL:HG22	1.95	0.48
6:Y:702:PRO:HB3	6:Z:965:HIS:HB3	1.95	0.48
6:Z:1139:ARG:HE	6:Z:1140:PRO:HD2	1.78	0.48
3:M:345:ASP:N	3:M:345:ASP:OD1	2.46	0.48
6:Y:485:GLN:OE1	6:Y:896:ARG:NH2	2.45	0.48
6:Z:388:ASN:HB2	6:Z:1311:ILE:HD12	1.94	0.48
6:Z:785:TYR:O	6:Z:943:TYR:OH	2.31	0.48
6:Z:861:VAL:HA	6:Z:864:VAL:HG22	1.94	0.48
6:B:401:LEU:HD11	6:B:1354:TYR:HB3	1.95	0.48
6:C:1064:VAL:HG22	6:C:1077:VAL:HG12	1.95	0.48
6:Y:596:LEU:HD23	6:Y:645:LEU:HD23	1.95	0.48
1:I:104:LYS:HE2	1:I:292:ASP:HA	1.94	0.48
3:M:589:LEU:HD12	3:M:590:PRO:HD2	1.95	0.48
6:B:82:ASP:OD1	6:B:82:ASP:N	2.46	0.48
6:D:614:ASP:OD2	6:D:649:HIS:NE2	2.46	0.48
6:D:1039:THR:HG21	6:D:1259:TYR:HE2	1.78	0.48
6:Y:1176:LEU:HD21	6:Y:1233:ALA:HB2	1.95	0.48
6:Z:260:THR:HB	6:Z:299:PRO:HD3	1.95	0.48
6:Z:448:THR:HG21	6:Z:1173:GLU:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Z:541:HIS:O	6:Z:543:GLN:NE2	2.46	0.48
6:Y:182:THR:HG21	6:Y:1083:THR:HG21	1.95	0.48
1:I:11:THR:HG21	6:B:124:PRO:HG3	1.94	0.48
6:C:1327:THR:HG23	6:C:1355:VAL:HG22	1.95	0.48
6:Y:253:SER:OG	6:Y:255:LEU:O	2.32	0.48
6:Y:863:ASP:OD1	6:Y:863:ASP:N	2.46	0.48
1:I:113:PRO:HD3	1:I:135:PRO:HA	1.95	0.48
3:M:27:LEU:HB3	3:M:31:VAL:HG11	1.96	0.48
6:Z:146:THR:OG1	6:Z:147:ILE:N	2.46	0.48
6:Z:317:SER:OG	6:Z:318:TYR:N	2.46	0.48
6:Z:555:ARG:HA	6:Z:988:ARG:HH21	1.79	0.48
6:B:614:ASP:HA	6:B:653:LEU:HD11	1.96	0.48
6:C:173:ARG:NH2	6:C:375:VAL:O	2.46	0.48
6:C:188:PRO:HA	6:C:1286:LEU:HD21	1.95	0.48
6:C:303:GLY:HA3	6:C:348:GLY:HA2	1.96	0.48
6:C:565:LEU:HD22	6:C:1177:THR:HG21	1.95	0.48
6:D:617:VAL:HG13	6:D:619:GLY:H	1.79	0.48
6:Y:744:ILE:HD12	6:Y:765:PRO:HA	1.96	0.48
6:Z:66:PHE:HA	6:Z:176:ILE:HD11	1.96	0.48
6:B:388:ASN:HB2	6:B:1311:ILE:HD12	1.96	0.48
6:Y:421:ARG:HE	6:Z:405:ARG:HD3	1.79	0.48
6:Z:685:THR:HB	6:Z:783:VAL:HG21	1.96	0.48
6:B:199:ASN:OD1	6:B:199:ASN:N	2.47	0.47
6:D:258:PRO:O	6:D:268:LYS:NZ	2.47	0.47
6:D:451:HIS:HD2	6:D:453:VAL:HG23	1.79	0.47
6:D:1144:ASP:OD1	6:D:1144:ASP:N	2.45	0.47
6:B:614:ASP:OD2	6:B:650:SER:OG	2.27	0.47
6:B:800:LEU:HD22	6:B:923:VAL:HB	1.95	0.47
6:B:1268:THR:O	6:B:1272:ILE:N	2.46	0.47
6:D:941:ARG:HD2	6:D:989:SER:HA	1.96	0.47
6:Y:225:ALA:O	6:Y:232:ARG:NH1	2.47	0.47
6:Y:733:VAL:HG12	6:Y:738:PRO:HA	1.95	0.47
6:Z:84:ASN:OD1	6:Z:84:ASN:N	2.47	0.47
4:O:28:GLU:HA	4:O:31:LEU:HD12	1.96	0.47
6:C:457:PRO:HA	6:C:460:CYS:HB3	1.97	0.47
6:Y:811:LEU:HB3	6:Y:857:LEU:HD11	1.97	0.47
6:B:532:GLU:OE2	6:B:1232:TRP:NE1	2.39	0.47
6:C:391:LEU:HD12	6:C:1042:PHE:HE2	1.80	0.47
6:Z:1110:VAL:HA	6:Z:1171:ALA:HB3	1.95	0.47
6:D:656:LEU:O	6:D:660:HIS:HB2	2.15	0.47
6:D:1231:PRO:O	6:D:1235:GLN:NE2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Z:892:VAL:HG11	6:Z:979:PHE:HE1	1.80	0.47
6:B:120:SER:HB2	6:B:1084:VAL:HG22	1.95	0.47
6:B:263:THR:HA	6:B:296:VAL:HA	1.95	0.47
6:C:538:ASP:N	6:C:538:ASP:OD1	2.41	0.47
6:C:685:THR:O	6:C:689:ALA:HB2	2.14	0.47
6:D:1124:HIS:HB3	6:D:1127:VAL:HG12	1.97	0.47
6:Y:1060:ASN:ND2	6:Y:1061:ASN:O	2.48	0.47
6:Z:1001:VAL:HG13	6:Z:1003:HIS:H	1.78	0.47
6:C:241:LYS:HA	6:C:244:THR:HG22	1.96	0.47
6:C:441:ASP:HB2	6:C:443:VAL:HG12	1.96	0.47
6:C:1132:ARG:HH22	6:C:1140:PRO:HD3	1.79	0.47
6:D:392:THR:HA	6:D:1039:THR:HA	1.97	0.47
6:Y:451:HIS:HE2	6:Y:1114:PHE:HA	1.77	0.47
6:Z:301:THR:OG1	6:Z:302:TYR:N	2.47	0.47
6:Z:554:PRO:O	6:Z:988:ARG:NH2	2.47	0.47
6:B:454:LEU:HD22	6:B:1239:LEU:HD12	1.96	0.47
6:C:435:ARG:HG2	6:C:1367:LEU:HD13	1.97	0.47
6:Z:975:LEU:HB2	6:Z:980:ALA:HB2	1.97	0.47
6:B:152:LEU:HD21	6:Z:48:ILE:HD11	1.97	0.47
6:B:867:ASP:OD1	6:B:870:THR:OG1	2.29	0.47
6:D:575:THR:HG21	6:D:1007:THR:HA	1.97	0.47
6:D:628:ARG:NH1	6:D:663:ASP:OD2	2.48	0.47
6:Y:59:ASN:HB2	6:Z:95:VAL:HA	1.96	0.47
6:Z:635:ILE:HD13	6:Z:657:ILE:HD11	1.97	0.47
5:S:55:ASN:OD1	5:S:55:ASN:N	2.48	0.47
6:B:769:ASP:N	6:B:769:ASP:OD1	2.45	0.47
6:B:1080:ASN:N	6:B:1080:ASN:OD1	2.47	0.47
6:D:538:ASP:N	6:D:553:THR:O	2.48	0.47
6:Y:121:GLU:OE2	6:Y:1083:THR:OG1	2.33	0.47
6:Y:535:PRO:HD3	6:Y:1232:TRP:CG	2.50	0.47
6:Y:955:ASP:HA	6:Y:958:ARG:HG2	1.97	0.47
6:Z:542:CYS:HB3	6:Z:549:VAL:HG23	1.97	0.47
3:M:313:ARG:HH22	3:M:315:ARG:HD2	1.80	0.46
6:B:8:GLU:OE2	6:B:38:TYR:OH	2.34	0.46
6:B:1342:GLY:H	6:B:1364:GLN:HE22	1.62	0.46
6:Y:227:LEU:H	6:Y:232:ARG:HH22	1.62	0.46
6:Z:637:ASN:O	6:Z:641:THR:OG1	2.31	0.46
3:M:365:TYR:O	3:M:369:ARG:NH2	2.48	0.46
5:S:66:ARG:HD2	6:C:757:LEU:HD11	1.97	0.46
6:B:905:GLN:HG3	6:B:1122:TYR:HD1	1.80	0.46
6:C:1105:ASP:HB2	6:C:1166:HIS:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:317:SER:OG	6:D:318:TYR:N	2.47	0.46
6:Y:71:LEU:HD22	6:Y:372:LEU:HD11	1.96	0.46
1:I:79:ASN:HD22	6:B:122:LYS:HG3	1.80	0.46
1:I:175:ILE:HG22	1:I:182:PHE:H	1.80	0.46
3:M:358:ARG:NH1	4:N:49:GLU:O	2.49	0.46
6:B:936:PRO:HB3	6:B:952:LEU:HD23	1.97	0.46
6:C:739:LEU:HD22	6:C:744:ILE:HD11	1.97	0.46
4:N:6:THR:HG21	6:Z:1123:ARG:HG2	1.98	0.46
6:C:775:ASP:OD1	6:C:775:ASP:N	2.46	0.46
6:Y:173:ARG:HG2	6:Y:375:VAL:HG13	1.97	0.46
6:Z:1121:VAL:HG12	6:Z:1132:ARG:HH11	1.80	0.46
3:M:132:LEU:HD11	3:M:149:LEU:HD13	1.97	0.46
5:S:39:VAL:HA	5:S:42:THR:HG22	1.96	0.46
6:B:941:ARG:HE	6:B:941:ARG:HB3	1.59	0.46
6:D:1038:ARG:NH1	6:D:1107:GLY:O	2.39	0.46
6:Z:540:THR:OG1	6:Z:541:HIS:N	2.48	0.46
1:I:146:ILE:HD11	1:I:184:ILE:HG12	1.96	0.46
3:M:313:ARG:HH12	3:M:315:ARG:HB3	1.80	0.46
6:B:557:VAL:HG11	6:B:1012:LEU:HD23	1.97	0.46
6:B:597:PHE:HA	6:B:600:THR:HG22	1.98	0.46
6:B:800:LEU:HA	6:B:936:PRO:HA	1.98	0.46
6:D:342:ASP:OD1	6:D:342:ASP:N	2.44	0.46
6:Z:199:ASN:HA	6:Z:202:LEU:HD23	1.97	0.46
6:Z:1040:ASP:OD1	6:Z:1104:THR:OG1	2.33	0.46
6:B:1045:ASP:OD1	6:B:1045:ASP:N	2.43	0.46
6:B:1139:ARG:O	6:B:1141:GLN:NE2	2.46	0.46
6:C:84:ASN:HB3	6:C:1080:ASN:HD21	1.80	0.46
6:D:311:ASN:ND2	6:D:322:LEU:O	2.42	0.46
6:D:443:VAL:HA	6:D:446:LEU:HD23	1.98	0.46
6:Y:27:ALA:HB1	6:Y:35:LEU:HD21	1.97	0.46
6:Y:790:PRO:HA	6:Y:793:THR:HG22	1.98	0.46
6:B:1235:GLN:H	6:B:1235:GLN:HG2	1.58	0.46
6:C:263:THR:HG22	6:C:296:VAL:HG12	1.97	0.46
6:C:1347:SER:O	6:C:1347:SER:OG	2.34	0.46
6:D:388:ASN:HB2	6:D:1311:ILE:HD12	1.98	0.46
6:D:487:PRO:HB3	6:D:736:ARG:HH11	1.81	0.46
6:B:241:LYS:HG2	6:B:245:ARG:HH21	1.79	0.46
6:C:58:CYS:SG	6:C:59:ASN:N	2.89	0.46
6:D:102:SER:OG	6:D:103:GLY:N	2.48	0.46
6:D:733:VAL:HG12	6:D:738:PRO:HA	1.98	0.46
6:Y:936:PRO:HB3	6:Y:952:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Z:243:LEU:HB3	6:Z:362:LEU:HD21	1.98	0.46
3:M:417:TRP:HE3	3:M:485:VAL:HG22	1.81	0.46
6:D:252:ASP:OD1	6:D:252:ASP:N	2.46	0.46
6:D:575:THR:HG1	6:D:1003:HIS:HE2	1.60	0.46
6:D:613:VAL:HA	6:D:616:LEU:HG	1.98	0.46
3:M:41:ARG:HH22	3:M:582:PRO:HG2	1.81	0.45
6:B:1104:THR:OG1	6:B:1105:ASP:N	2.48	0.45
6:C:434:ASP:OD1	6:D:217:GLN:NE2	2.49	0.45
6:Y:873:LEU:O	6:Y:877:ARG:NH1	2.49	0.45
6:Z:1045:ASP:HB2	6:Z:1098:TYR:HB3	1.97	0.45
3:M:314:LEU:HD21	3:M:327:ARG:HD3	1.97	0.45
6:D:507:ARG:HE	6:D:512:MET:HG3	1.80	0.45
6:Y:372:LEU:HD23	6:Y:372:LEU:HA	1.84	0.45
6:Z:83:LEU:HD12	6:Z:1060:ASN:HB3	1.98	0.45
3:M:369:ARG:HG3	4:N:47:TRP:CE2	2.52	0.45
6:C:1032:PHE:HA	6:C:1178:PRO:HD3	1.98	0.45
6:D:1191:ASN:HD22	6:D:1197:SER:H	1.62	0.45
6:Y:1128:ASP:OD2	6:Y:1132:ARG:NH2	2.50	0.45
3:M:524:TYR:HB2	3:M:532:TYR:HB2	1.98	0.45
6:C:94:HIS:HB2	6:Z:7:LEU:HD21	1.98	0.45
6:C:328:TYR:O	6:C:332:LEU:HB2	2.17	0.45
6:C:1037:VAL:HG23	6:C:1172:CYS:HB3	1.99	0.45
6:Y:127:ILE:HD12	6:Y:128:PRO:HD2	1.99	0.45
6:Y:315:ALA:HA	6:Y:319:HIS:HA	1.98	0.45
6:Y:437:VAL:HG13	6:Z:1184:ASN:HB3	1.97	0.45
6:Z:1316:ARG:O	6:Z:1319:GLN:NE2	2.46	0.45
1:I:108:LEU:HB2	1:I:288:PHE:HB2	1.99	0.45
6:C:558:ILE:HG21	6:C:574:ARG:HH12	1.82	0.45
6:Y:703:LEU:HD12	6:Y:1022:LEU:HD11	1.99	0.45
6:C:662:ALA:O	6:D:642:ARG:NH2	2.49	0.45
6:Y:410:VAL:HG22	6:Y:413:LYS:HB2	1.98	0.45
6:Z:303:GLY:HA2	6:Z:348:GLY:HA3	1.99	0.45
6:Z:877:ARG:HA	6:Z:880:PHE:HB3	1.98	0.45
3:M:556:ARG:HH21	3:M:560:GLN:HG3	1.82	0.45
6:B:124:PRO:HA	6:B:1080:ASN:HA	1.98	0.45
6:C:635:ILE:HD11	6:C:666:LEU:HD21	1.98	0.45
6:C:1277:THR:OG1	6:Z:29:GLU:OE2	2.27	0.45
6:D:753:ASP:OD1	6:D:753:ASP:N	2.49	0.45
4:N:14:VAL:HB	4:O:11:PRO:HB2	1.99	0.45
6:Y:461:LEU:HD13	6:Y:552:CYS:HB2	1.98	0.45
6:Z:538:ASP:OD1	6:Z:555:ARG:NH1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:59:ALA:HA	6:C:805:LYS:HZ1	1.81	0.45
6:C:445:ALA:HA	6:C:1110:VAL:HG21	1.97	0.45
6:D:1020:LEU:HD21	6:D:1032:PHE:HE2	1.82	0.45
3:M:51:ALA:O	3:M:53:ARG:NH2	2.50	0.44
3:M:329:LEU:HD23	3:M:329:LEU:HA	1.82	0.44
6:C:534:HIS:HD2	6:C:536:PHE:H	1.64	0.44
6:C:641:THR:HG23	6:C:642:ARG:HG3	1.98	0.44
6:Y:276:THR:OG1	6:Y:277:ALA:N	2.47	0.44
6:Y:438:GLN:HE21	6:Y:1108:VAL:HG13	1.83	0.44
6:Y:508:THR:OG1	6:Y:509:VAL:N	2.50	0.44
6:Y:1115:ARG:NH2	6:Y:1138:GLU:OE2	2.49	0.44
1:I:292:ASP:OD1	1:I:301:THR:OG1	2.35	0.44
6:C:106:LEU:HD12	6:C:107:PRO:HD2	1.99	0.44
6:C:131:LEU:HD11	6:C:160:VAL:HG23	1.98	0.44
6:Y:1327:THR:OG1	6:Y:1328:THR:N	2.50	0.44
6:C:448:THR:HG21	6:C:1173:GLU:HG2	1.98	0.44
6:C:703:LEU:HA	6:C:706:TYR:HD2	1.82	0.44
6:C:704:SER:HA	6:C:707:VAL:HG12	2.00	0.44
6:D:1189:PRO:HB3	6:D:1322:LEU:HD23	1.98	0.44
6:Y:613:VAL:HA	6:Y:616:LEU:HG	2.00	0.44
6:Y:955:ASP:N	6:Y:955:ASP:OD1	2.49	0.44
1:I:209:ASN:HD22	1:I:209:ASN:HA	1.62	0.44
6:B:392:THR:OG1	6:B:1265:TYR:OH	2.26	0.44
6:C:1172:CYS:SG	6:C:1173:GLU:N	2.89	0.44
6:Y:495:ILE:HD12	6:Y:979:PHE:HE2	1.83	0.44
6:Y:625:LEU:HA	6:Y:628:ARG:HG3	1.99	0.44
6:Z:614:ASP:OD1	6:Z:650:SER:OG	2.31	0.44
6:B:291:ILE:HG12	6:B:360:ILE:HG22	1.99	0.44
6:B:332:LEU:O	6:B:336:GLN:N	2.51	0.44
6:B:440:ILE:HD13	6:B:1108:VAL:HB	2.00	0.44
6:Z:795:ASN:HD21	6:Z:942:PHE:HD1	1.65	0.44
6:B:785:TYR:O	6:B:943:TYR:OH	2.29	0.44
6:D:1279:PHE:HA	6:D:1282:ILE:HG12	1.99	0.44
6:Z:763:ASP:OD1	6:Z:763:ASP:N	2.50	0.44
1:I:204:MET:HA	1:I:207:VAL:HG12	2.00	0.44
6:Y:1177:THR:HG1	6:Y:1180:THR:HG1	1.57	0.44
6:Z:1185:TYR:OH	6:Z:1191:ASN:O	2.29	0.44
6:B:379:THR:O	6:Z:22:HIS:NE2	2.43	0.44
6:C:495:ILE:HD13	6:C:937:VAL:HA	1.99	0.44
6:C:756:ARG:NE	6:C:888:GLU:OE2	2.50	0.44
6:D:657:ILE:HG23	6:D:661:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Y:177:HIS:ND1	6:Y:376:TYR:OH	2.38	0.44
6:B:127:ILE:HD12	6:B:128:PRO:HD2	1.99	0.43
6:B:174:GLY:HA3	6:C:101:ALA:HB3	2.00	0.43
6:B:351:SER:O	6:B:351:SER:OG	2.36	0.43
6:B:499:TYR:OH	6:B:974:PRO:O	2.34	0.43
6:C:254:ILE:HG22	6:Z:17:THR:HG22	1.99	0.43
6:C:387:ARG:HA	6:C:387:ARG:HD3	1.70	0.43
6:Y:448:THR:HG21	6:Y:1173:GLU:HG3	2.00	0.43
6:Z:446:LEU:HD22	6:Z:1021:VAL:HG22	2.00	0.43
6:Z:681:LEU:HD21	6:Z:784:PHE:HD1	1.83	0.43
6:B:495:ILE:HG13	6:B:976:PRO:HG2	2.00	0.43
6:B:1145:THR:HA	6:B:1148:ILE:HG12	1.99	0.43
6:C:646:VAL:O	6:C:674:TYR:OH	2.27	0.43
6:Z:1242:VAL:HA	6:Z:1248:HIS:CD2	2.53	0.43
6:D:65:TYR:HB2	6:D:68:THR:HG22	1.99	0.43
6:D:709:ALA:HB3	6:D:1012:LEU:HD23	2.01	0.43
6:C:71:LEU:HD23	6:C:176:ILE:HG23	2.00	0.43
6:C:805:LYS:HB3	6:C:805:LYS:HE2	1.79	0.43
6:C:1291:ASP:OD1	6:C:1291:ASP:N	2.51	0.43
6:D:278:ASN:N	6:D:278:ASN:OD1	2.51	0.43
6:D:420:VAL:HA	6:D:423:ALA:HB3	2.00	0.43
6:Z:1128:ASP:HA	6:Z:1131:ILE:HG22	2.00	0.43
1:I:152:ILE:HG22	1:I:155:LEU:HD12	2.00	0.43
5:S:26:LEU:O	6:C:813:TYR:OH	2.30	0.43
5:S:72:ARG:HG2	6:C:820:MET:HB3	2.00	0.43
6:B:373:ARG:HH12	6:B:377:LYS:HG3	1.83	0.43
6:C:730:VAL:HG13	6:C:895:VAL:HG13	2.00	0.43
6:Z:245:ARG:O	6:Z:249:ALA:HB2	2.18	0.43
6:Z:575:THR:HG22	6:Z:1010:ALA:HB3	2.00	0.43
4:N:8:TRP:HD1	6:Z:1121:VAL:HG21	1.83	0.43
6:B:459:PRO:HG2	6:B:1252:LEU:HD11	2.01	0.43
6:B:702:PRO:HB3	6:C:965:HIS:HB3	2.01	0.43
6:Y:717:PRO:HA	6:Y:718:PRO:HD3	1.79	0.43
6:Y:1143:LEU:O	6:Y:1147:THR:OG1	2.27	0.43
6:Z:1360:ILE:HD12	6:Z:1361:PRO:HD2	1.99	0.43
6:B:445:ALA:HA	6:B:1110:VAL:HG11	2.00	0.43
6:D:245:ARG:O	6:D:249:ALA:HB2	2.19	0.43
6:D:693:LEU:HD11	6:D:1026:ALA:HB2	2.01	0.43
6:Y:718:PRO:HA	6:Y:916:VAL:HG23	2.01	0.43
6:Z:1228:THR:OG1	6:Z:1229:HIS:N	2.52	0.43
5:R:13:LYS:HE3	5:R:15:ASP:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:1050:SER:OG	6:B:1051:GLY:N	2.51	0.43
6:C:276:THR:OG1	6:C:278:ASN:OD1	2.37	0.43
6:C:1324:ILE:HD11	6:C:1363:GLN:HE21	1.83	0.43
6:Y:291:ILE:HG12	6:Y:360:ILE:HB	2.01	0.43
6:Y:1115:ARG:HA	6:Y:1115:ARG:HD3	1.89	0.43
6:B:627:ILE:HG22	6:B:630:PHE:HB3	2.01	0.42
6:B:752:SER:O	6:B:752:SER:OG	2.34	0.42
6:B:1244:TYR:HA	6:B:1249:ARG:HD2	2.01	0.42
6:B:1364:GLN:O	6:B:1368:PHE:HB2	2.19	0.42
6:C:527:ILE:HG22	6:C:1218:ARG:HH12	1.83	0.42
6:C:847:ALA:HA	6:C:850:ARG:HB3	2.01	0.42
6:D:313:VAL:O	6:D:317:SER:HB3	2.18	0.42
6:D:1210:ALA:HB1	6:D:1272:ILE:HG12	2.00	0.42
6:Y:261:TYR:HB3	6:Y:269:ILE:HD12	2.00	0.42
6:B:155:GLU:HG3	6:Z:9:LEU:HD13	2.00	0.42
6:B:790:PRO:HA	6:B:793:THR:HG22	2.01	0.42
6:D:308:SER:OG	6:D:311:ASN:OD1	2.36	0.42
6:D:494:ARG:HG2	6:D:497:HIS:HD2	1.83	0.42
6:Y:502:ARG:HH21	6:Y:962:GLU:HB2	1.84	0.42
6:Z:615:VAL:HG21	6:Z:802:LEU:HD23	2.01	0.42
6:C:1183:VAL:HA	6:C:1187:LYS:HD2	2.00	0.42
6:Y:903:GLN:HE22	6:Y:1014:LYS:HB3	1.85	0.42
3:M:401:ARG:H	3:M:401:ARG:HG2	1.53	0.42
5:R:73:THR:HG22	5:R:75:ARG:H	1.85	0.42
6:B:620:ASN:HD21	6:B:622:ASP:HB2	1.83	0.42
6:Y:425:PRO:HB3	6:Y:1328:THR:HB	2.01	0.42
6:Y:537:PHE:HA	6:Y:554:PRO:HA	2.00	0.42
6:Y:903:GLN:HE22	6:Y:1014:LYS:HE2	1.84	0.42
6:Y:927:PRO:HD2	6:Y:952:LEU:HD21	2.01	0.42
6:Y:1191:ASN:ND2	6:Y:1319:GLN:O	2.53	0.42
6:Z:1156:MET:O	6:Z:1159:ARG:NH2	2.52	0.42
6:Z:1245:ASN:O	6:Z:1249:ARG:N	2.51	0.42
3:M:43:VAL:HG23	3:M:92:ALA:HB3	2.02	0.42
6:B:21:THR:OG1	6:B:22:HIS:N	2.52	0.42
6:B:601:VAL:HG13	6:B:924:VAL:HG11	2.01	0.42
6:C:74:ALA:O	6:C:1054:CYS:N	2.48	0.42
6:C:96:GLN:HG2	6:C:113:THR:HG22	2.01	0.42
6:C:718:PRO:HD2	6:C:785:TYR:HB3	2.01	0.42
6:C:1360:ILE:HG13	6:C:1362:LEU:HD22	2.02	0.42
6:D:533:LEU:HD12	6:D:1238:CYS:HA	2.01	0.42
6:Y:212:ARG:NH1	6:Y:1203:ASP:OD1	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Y:849:GLN:HG3	6:Y:872:LEU:HD12	2.00	0.42
6:Z:542:CYS:N	6:Z:549:VAL:O	2.53	0.42
1:I:203:SER:OG	1:I:274:MET:O	2.37	0.42
3:M:64:ASP:OD1	3:M:84:ARG:NH2	2.53	0.42
6:B:186:LYS:HD3	6:B:186:LYS:HA	1.84	0.42
6:B:766:LEU:HD11	6:B:893:LEU:HD21	2.02	0.42
6:Y:1362:LEU:HD12	6:Y:1366:MET:HB2	2.01	0.42
6:Z:714:ARG:NH1	6:Z:898:PRO:O	2.52	0.42
6:B:392:THR:OG1	6:B:392:THR:O	2.37	0.42
6:C:1040:ASP:HA	6:C:1104:THR:HG21	2.00	0.42
6:Y:491:ALA:HA	6:Y:494:ARG:HG3	2.00	0.42
6:Y:1324:ILE:HD12	6:Y:1324:ILE:HA	1.91	0.42
6:Z:1347:SER:O	6:Z:1347:SER:OG	2.37	0.42
3:M:45:TYR:HB3	3:M:132:LEU:HD22	2.01	0.42
5:R:26:LEU:O	6:B:813:TYR:OH	2.34	0.42
6:C:95:VAL:HG13	6:C:114:ILE:HB	2.01	0.42
6:D:982:GLU:HG2	6:D:988:ARG:HG3	2.02	0.42
6:D:1050:SER:HG	6:D:1054:CYS:HG	1.68	0.42
6:Y:668:PRO:HB2	6:Z:643:GLN:HB2	2.00	0.42
6:Z:222:LYS:O	6:Z:226:THR:OG1	2.33	0.42
6:D:146:THR:HB	6:D:149:ASP:HB2	2.02	0.42
6:D:392:THR:HG21	6:D:1264:GLN:HE22	1.85	0.42
6:Y:970:ASP:OD1	6:Y:970:ASP:N	2.50	0.42
6:Z:1044:VAL:HG11	6:Z:1096:VAL:HG13	2.02	0.42
6:Z:1230:ASN:OD1	6:Z:1230:ASN:N	2.53	0.42
3:M:380:ARG:HB2	4:N:32:ARG:HH11	1.84	0.42
6:C:987:LEU:HD11	6:C:1012:LEU:HD21	2.01	0.42
6:D:1268:THR:HA	6:D:1271:ILE:HG22	2.01	0.42
6:Y:663:ASP:O	6:Z:642:ARG:NH2	2.53	0.42
3:M:170:ARG:HB3	3:M:315:ARG:HH12	1.84	0.41
4:N:24:LEU:HA	4:O:4:LEU:HB2	2.02	0.41
6:B:125:ILE:HG13	6:B:1079:GLN:HB3	2.02	0.41
6:B:422:ASN:ND2	6:C:404:ASP:O	2.53	0.41
6:B:448:THR:HG23	6:B:1113:LEU:HG	2.02	0.41
6:C:211:GLN:HA	6:C:214:ASN:HD22	1.84	0.41
6:C:435:ARG:NH2	6:C:1364:GLN:OE1	2.53	0.41
6:D:440:ILE:HD12	6:D:1108:VAL:HB	2.02	0.41
7:A:6:UNK:CB	7:E:15:UNK:CB	2.98	0.41
3:M:74:ASP:OD1	3:M:74:ASP:N	2.49	0.41
6:B:609:LEU:HD11	6:B:630:PHE:HZ	1.85	0.41
6:B:904:ARG:HG2	6:B:908:PRO:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:692:GLY:HA2	6:D:993:ARG:HH12	1.85	0.41
6:C:448:THR:HA	6:C:1113:LEU:HB2	2.03	0.41
6:D:1287:LEU:HD12	6:D:1288:ARG:HG2	2.02	0.41
6:Y:1163:ALA:HB2	6:Z:1213:ALA:HB1	2.03	0.41
6:Y:544:GLU:HB2	6:Y:547:GLU:HG3	2.01	0.41
6:Y:633:ARG:HH21	6:Y:865:ALA:HB1	1.84	0.41
6:Z:596:LEU:HD12	6:Z:673:HIS:CD2	2.55	0.41
6:Z:688:SER:O	6:Z:708:ASN:ND2	2.46	0.41
6:Z:1165:VAL:HG12	6:Z:1166:HIS:HD2	1.86	0.41
6:B:693:LEU:HB3	6:B:1022:LEU:HD12	2.01	0.41
6:B:878:GLU:HA	6:B:881:LEU:HB2	2.02	0.41
6:D:941:ARG:HE	6:D:941:ARG:HB2	1.67	0.41
6:Y:497:HIS:HA	6:Y:500:ARG:HG2	2.01	0.41
6:Y:1286:LEU:O	6:Y:1290:LYS:NZ	2.52	0.41
4:N:48:ARG:HD3	4:N:48:ARG:HA	1.88	0.41
6:B:3:ASN:ND2	6:C:317:SER:O	2.53	0.41
6:B:152:LEU:HD23	6:B:152:LEU:HA	1.89	0.41
6:B:390:ASP:OD1	6:B:1039:THR:OG1	2.35	0.41
6:B:1166:HIS:NE2	6:C:1223:GLN:O	2.51	0.41
6:D:359:VAL:HG12	6:D:368:ILE:HD13	2.03	0.41
6:D:399:LEU:HD23	6:D:399:LEU:HA	1.84	0.41
6:Y:54:PHE:HB2	6:Z:91:MET:HG2	2.01	0.41
6:Y:647:PHE:HB3	6:Y:653:LEU:HB3	2.01	0.41
6:Z:601:VAL:HG13	6:Z:924:VAL:HG11	2.03	0.41
1:I:88:HIS:ND1	1:I:306:GLY:OXT	2.42	0.41
6:C:1290:LYS:HD3	6:C:1310:LEU:HB3	2.03	0.41
6:Y:496:PRO:HA	6:Y:499:TYR:HD2	1.86	0.41
6:Y:1228:THR:HG22	6:Y:1230:ASN:H	1.86	0.41
1:I:56:ARG:H	1:I:56:ARG:HG2	1.67	0.41
6:B:427:THR:HG21	6:B:439:LYS:HZ3	1.86	0.41
6:B:717:PRO:HA	6:B:718:PRO:HD3	1.91	0.41
6:C:514:GLN:HE22	6:C:990:PRO:HD3	1.85	0.41
6:C:1196:ALA:HB3	6:C:1222:ALA:HB3	2.03	0.41
6:D:176:ILE:HG21	6:D:375:VAL:HG21	2.03	0.41
6:Y:254:ILE:HD11	6:Y:1088:LEU:HB2	2.03	0.41
6:Z:1248:HIS:CE1	6:Z:1251:ARG:HH11	2.38	0.41
4:N:38:ALA:HA	4:N:41:THR:HG22	2.03	0.41
5:R:19:ARG:O	5:R:23:ASN:HB2	2.20	0.41
6:B:301:THR:OG1	6:B:302:TYR:N	2.54	0.41
6:B:446:LEU:HD22	6:B:1021:VAL:HG23	2.02	0.41
6:C:903:GLN:HE22	6:C:1014:LYS:HE2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:1197:SER:O	6:C:1197:SER:OG	2.30	0.41
6:D:71:LEU:HD21	6:D:180:LEU:HD13	2.02	0.41
6:Y:1239:LEU:HA	6:Y:1242:VAL:HG12	2.01	0.41
6:Z:533:LEU:HD23	6:Z:533:LEU:HA	1.91	0.41
6:Z:1265:TYR:OH	6:Z:1320:GLU:O	2.30	0.41
1:I:207:VAL:HG23	1:I:271:LEU:HD12	2.03	0.41
6:B:419:THR:HG22	6:B:421:ARG:H	1.86	0.41
6:B:1313:ASN:N	6:B:1313:ASN:OD1	2.54	0.41
6:C:645:LEU:HD12	6:C:674:TYR:CZ	2.56	0.41
6:D:1359:ILE:HG23	6:D:1360:ILE:HG13	2.03	0.41
6:Y:389:VAL:HG13	6:Y:1044:VAL:HG21	2.03	0.41
6:Z:562:PRO:HD2	6:Z:565:LEU:HD12	2.03	0.41
3:M:583:ARG:O	3:M:585:SER:OG	2.36	0.40
6:B:510:ASN:O	6:B:989:SER:OG	2.39	0.40
6:B:1131:ILE:HD13	6:B:1131:ILE:HA	1.93	0.40
6:B:1363:GLN:O	6:B:1367:LEU:HB2	2.22	0.40
6:C:108:THR:OG1	6:C:109:SER:N	2.54	0.40
6:D:663:ASP:OD1	6:D:663:ASP:N	2.53	0.40
6:Z:1282:ILE:HA	6:Z:1285:TYR:HB3	2.04	0.40
3:M:477:VAL:HG13	3:M:486:ASP:HB2	2.02	0.40
6:C:1043:GLU:OE2	6:C:1101:ARG:NH1	2.54	0.40
6:D:257:ASN:HD21	6:D:349:ALA:HB2	1.86	0.40
6:Y:710:LEU:HD13	6:Y:1012:LEU:HD22	2.03	0.40
6:Y:1182:ASP:OD1	6:Y:1182:ASP:N	2.39	0.40
3:M:338:SER:O	3:M:338:SER:OG	2.35	0.40
6:B:87:THR:HG22	6:B:88:THR:HG23	2.02	0.40
6:C:1217:HIS:CE1	6:C:1235:GLN:HG3	2.56	0.40
6:Y:479:LEU:HG	6:Y:543:GLN:HB2	2.03	0.40
6:Y:587:PRO:HA	6:Y:588:PRO:HD3	1.87	0.40
6:Y:617:VAL:HG23	6:Y:619:GLY:H	1.86	0.40
6:Z:308:SER:H	6:Z:311:ASN:HD22	1.69	0.40
6:Z:328:TYR:O	6:Z:332:LEU:HB2	2.21	0.40
6:Z:583:ARG:HE	6:Z:583:ARG:HB3	1.69	0.40
6:D:688:SER:O	6:D:688:SER:OG	2.34	0.40
6:Y:661:LEU:HD12	6:Y:661:LEU:HA	1.86	0.40
6:Z:83:LEU:HD23	6:Z:83:LEU:HA	1.92	0.40
6:B:1038:ARG:HH22	6:B:1324:ILE:HG21	1.87	0.40
6:C:321:ILE:HD13	6:C:321:ILE:HA	1.92	0.40
6:D:489:GLY:HA2	6:D:763:ASP:HB3	2.02	0.40
6:D:682:ARG:HA	6:D:682:ARG:HD2	1.89	0.40
6:D:798:CYS:SG	6:D:799:GLY:N	2.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:1362:LEU:HD13	6:D:1366:MET:HG3	2.03	0.40
6:Y:1156:MET:HG2	6:Y:1257:LYS:HZ1	1.87	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	I	283/306 (92%)	267 (94%)	16 (6%)	0	100	100
1	h	284/306 (93%)	263 (93%)	21 (7%)	0	100	100
1	n	291/306 (95%)	266 (91%)	25 (9%)	0	100	100
1	o	285/306 (93%)	270 (95%)	15 (5%)	0	100	100
2	g	211/290 (73%)	195 (92%)	15 (7%)	1 (0%)	29	67
2	m	288/290 (99%)	264 (92%)	24 (8%)	0	100	100
3	M	459/594 (77%)	431 (94%)	28 (6%)	0	100	100
4	N	58/642 (9%)	53 (91%)	5 (9%)	0	100	100
4	O	37/642 (6%)	33 (89%)	4 (11%)	0	100	100
5	R	61/75 (81%)	60 (98%)	1 (2%)	0	100	100
5	S	61/75 (81%)	57 (93%)	4 (7%)	0	100	100
5	i	61/75 (81%)	60 (98%)	1 (2%)	0	100	100
5	j	61/75 (81%)	59 (97%)	2 (3%)	0	100	100
6	B	1299/1370 (95%)	1202 (92%)	97 (8%)	0	100	100
6	C	1306/1370 (95%)	1229 (94%)	77 (6%)	0	100	100
6	D	1272/1370 (93%)	1193 (94%)	78 (6%)	1 (0%)	51	84
6	Y	1343/1370 (98%)	1271 (95%)	72 (5%)	0	100	100
6	Z	1314/1370 (96%)	1237 (94%)	77 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	a	1280/1370 (93%)	1214 (95%)	66 (5%)	0	100	100
All	All	10254/12202 (84%)	9624 (94%)	628 (6%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	g	196	PRO
6	D	765	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	258/273 (94%)	257 (100%)	1 (0%)	91	94
1	h	260/273 (95%)	259 (100%)	1 (0%)	91	94
1	n	263/273 (96%)	263 (100%)	0	100	100
1	o	259/273 (95%)	258 (100%)	1 (0%)	91	94
2	g	192/252 (76%)	192 (100%)	0	100	100
2	m	252/252 (100%)	251 (100%)	1 (0%)	91	94
3	M	392/500 (78%)	388 (99%)	4 (1%)	76	86
4	N	54/526 (10%)	54 (100%)	0	100	100
4	O	36/526 (7%)	36 (100%)	0	100	100
5	R	59/68 (87%)	59 (100%)	0	100	100
5	S	59/68 (87%)	59 (100%)	0	100	100
5	i	59/68 (87%)	59 (100%)	0	100	100
5	j	59/68 (87%)	58 (98%)	1 (2%)	60	78
6	B	1143/1192 (96%)	1133 (99%)	10 (1%)	78	88
6	C	1146/1192 (96%)	1141 (100%)	5 (0%)	91	94
6	D	1113/1192 (93%)	1108 (100%)	5 (0%)	91	94
6	Y	1174/1192 (98%)	1172 (100%)	2 (0%)	93	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	Z	1149/1192 (96%)	1142 (99%)	7 (1%)	86 92
6	a	1120/1192 (94%)	1117 (100%)	3 (0%)	92 95
All	All	9047/10572 (86%)	9006 (100%)	41 (0%)	89 93

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	h	138	VAL
1	I	144	LEU
1	o	214	LEU
2	m	102	LEU
3	M	42	TYR
3	M	163	PHE
3	M	462	ARG
3	M	553	ARG
5	j	75	ARG
6	a	744	ILE
6	a	1096	VAL
6	a	1303	CYS
6	B	111	GLN
6	B	149	ASP
6	B	328	TYR
6	B	508	THR
6	B	937	VAL
6	B	988	ARG
6	B	1054	CYS
6	B	1069	ARG
6	B	1258	PHE
6	B	1303	CYS
6	C	60	ARG
6	C	204	ARG
6	C	937	VAL
6	C	1035	THR
6	C	1069	ARG
6	D	186	LYS
6	D	736	ARG
6	D	740	ASN
6	D	814	ARG
6	D	1044	VAL
6	Y	725	ARG
6	Y	937	VAL

Continued on next page...

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Mol	Chain	Res	Type
6	Z	796	ARG
6	Z	942	PHE
6	Z	1015	ILE
6	Z	1039	THR
6	Z	1169	LYS
6	Z	1224	THR
6	Z	1303	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100) such sidechains are listed below:

Mol	Chain	Res	Type
1	h	50	GLN
1	h	80	GLN
1	h	88	HIS
1	h	129	GLN
1	h	277	GLN
1	I	209	ASN
1	n	277	GLN
1	o	36	GLN
2	m	43	HIS
2	m	211	HIS
3	M	148	HIS
3	M	176	ASN
6	a	81	HIS
6	a	111	GLN
6	a	205	GLN
6	a	208	ASN
6	a	438	GLN
6	a	484	GLN
6	a	534	HIS
6	a	676	ASN
6	a	726	ASN
6	a	749	HIS
6	a	781	GLN
6	a	965	HIS
6	a	1023	GLN
6	a	1076	HIS
6	a	1160	ASN
6	a	1235	GLN
6	a	1350	HIS
6	a	1364	GLN
6	B	214	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	B	231	ASN
6	B	388	ASN
6	B	422	ASN
6	B	534	HIS
6	B	620	ASN
6	B	726	ASN
6	B	781	GLN
6	B	1023	GLN
6	B	1061	ASN
6	B	1100	ASN
6	B	1229	HIS
6	B	1364	GLN
6	C	94	HIS
6	C	214	ASN
6	C	422	ASN
6	C	462	GLN
6	C	514	GLN
6	C	543	GLN
6	C	560	ASN
6	C	794	ASN
6	C	981	HIS
6	C	985	ASN
6	C	1000	ASN
6	C	1023	GLN
6	C	1079	GLN
6	C	1093	ASN
6	C	1124	HIS
6	C	1363	GLN
6	C	1369	ASN
6	D	214	ASN
6	D	217	GLN
6	D	438	GLN
6	D	451	HIS
6	D	618	HIS
6	D	620	ASN
6	D	673	HIS
6	D	795	ASN
6	D	969	HIS
6	D	985	ASN
6	D	1027	HIS
6	D	1168	GLN
6	D	1350	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	Y	47	ASN
6	Y	231	ASN
6	Y	534	HIS
6	Y	713	HIS
6	Y	731	GLN
6	Y	781	GLN
6	Y	794	ASN
6	Y	795	ASN
6	Y	903	GLN
6	Y	914	GLN
6	Y	981	HIS
6	Y	1061	ASN
6	Y	1093	ASN
6	Y	1141	GLN
6	Z	153	ASN
6	Z	181	GLN
6	Z	311	ASN
6	Z	497	HIS
6	Z	560	ASN
6	Z	676	ASN
6	Z	697	GLN
6	Z	905	GLN
6	Z	969	HIS
6	Z	1027	HIS
6	Z	1093	ASN
6	Z	1166	HIS
6	Z	1248	HIS

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 (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)

There are no chain breaks in this entry.

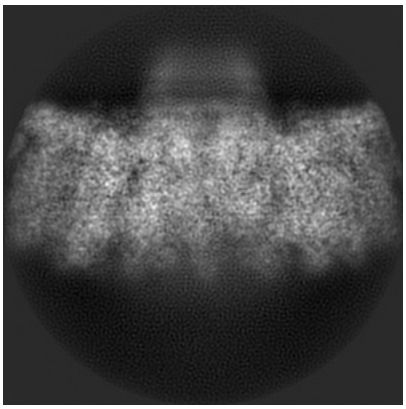
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-34696. These allow visual inspection of the internal detail of the map and identification of artifacts.

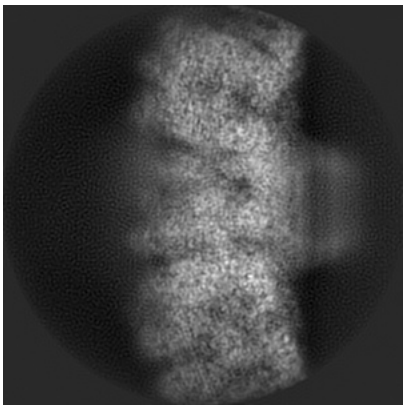
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

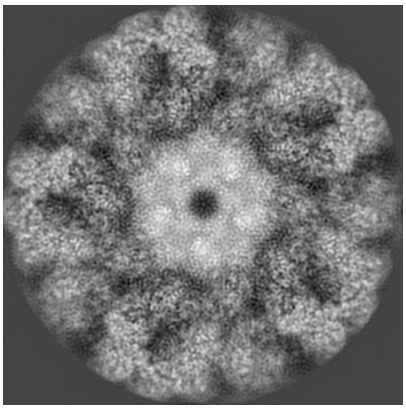
6.1.1 Primary map



X

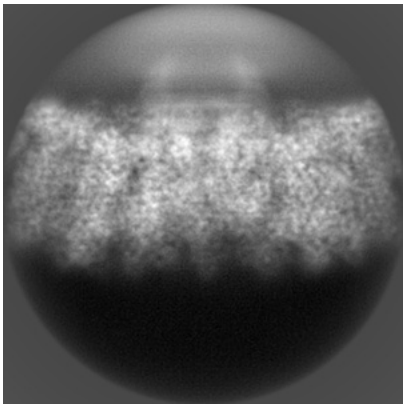


Y

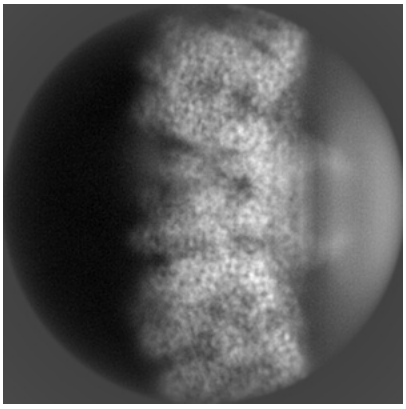


Z

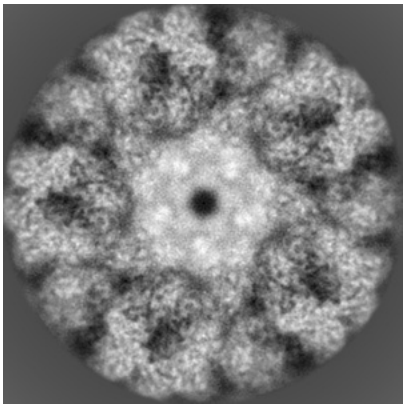
6.1.2 Raw map



X



Y

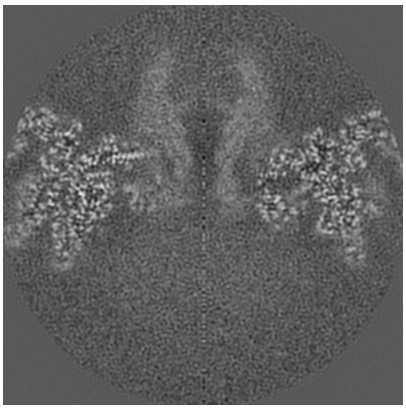


Z

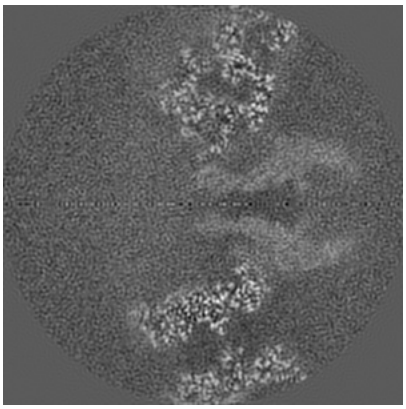
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

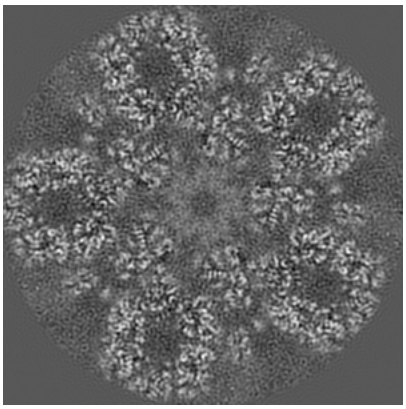
6.2.1 Primary map



X Index: 128

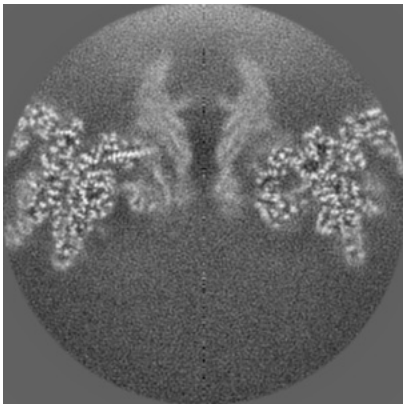


Y Index: 128

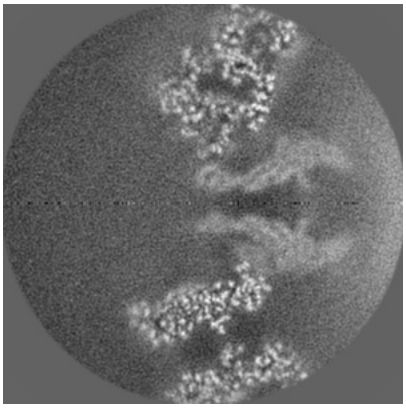


Z Index: 128

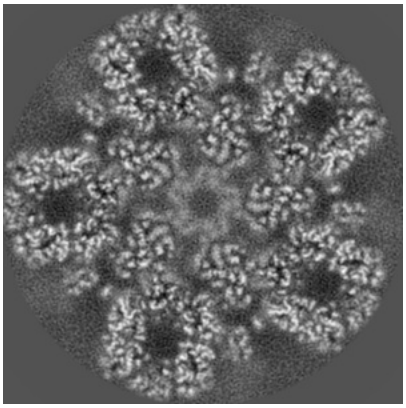
6.2.2 Raw map



X Index: 128



Y Index: 128

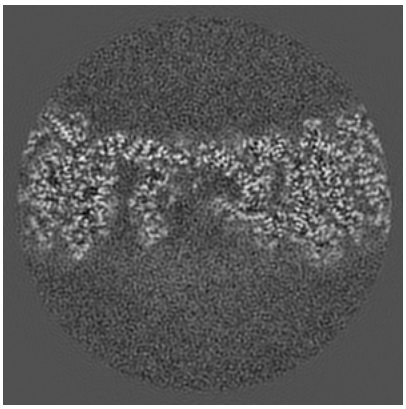


Z Index: 128

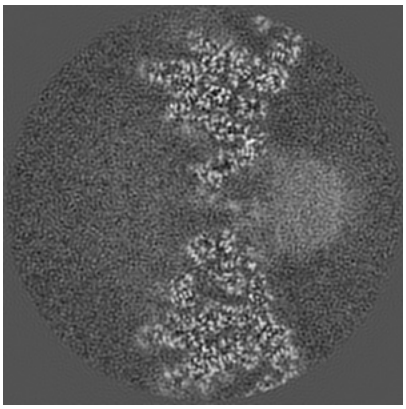
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

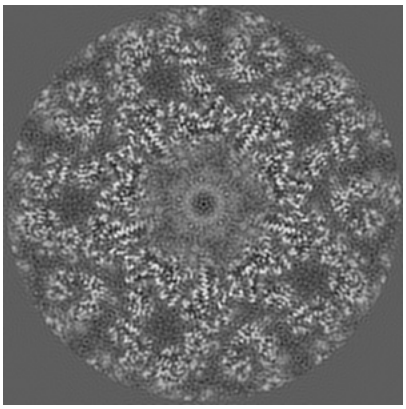
6.3.1 Primary map



X Index: 79

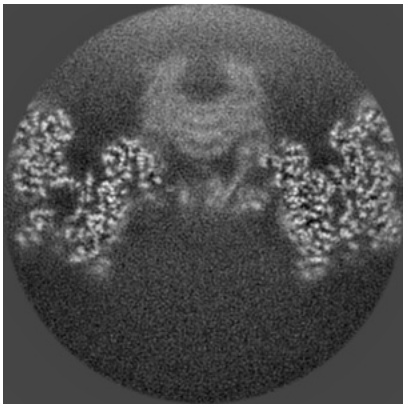


Y Index: 98

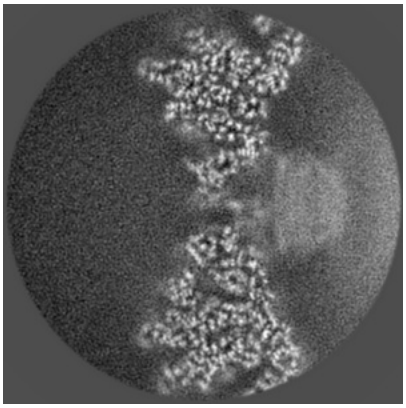


Z Index: 158

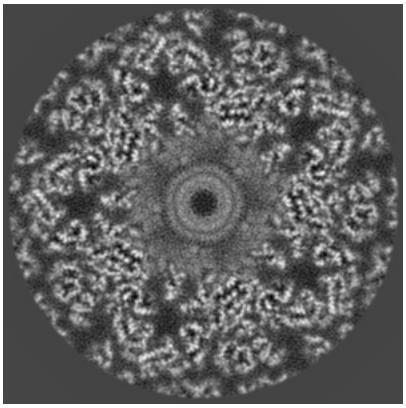
6.3.2 Raw map



X Index: 109



Y Index: 98

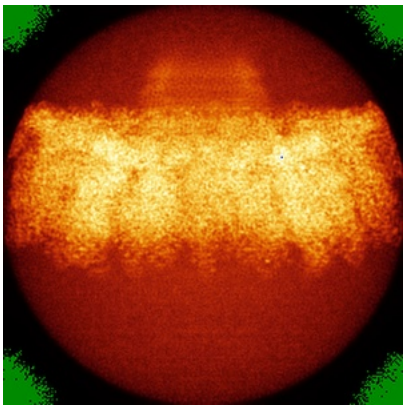


Z Index: 164

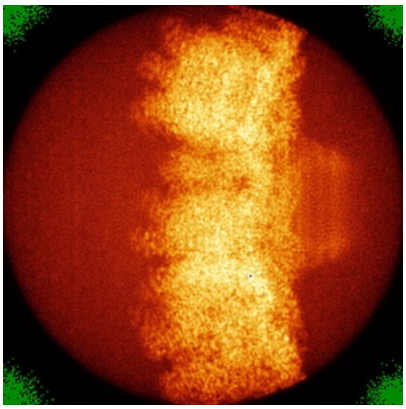
The images above show the largest variance slices of the map in three orthogonal directions.

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

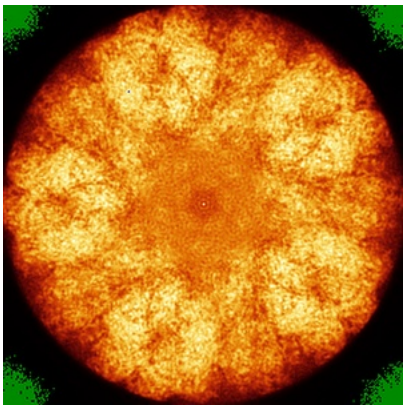
6.4.1 Primary map



X

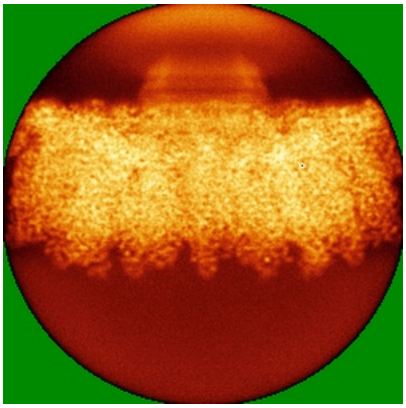


Y

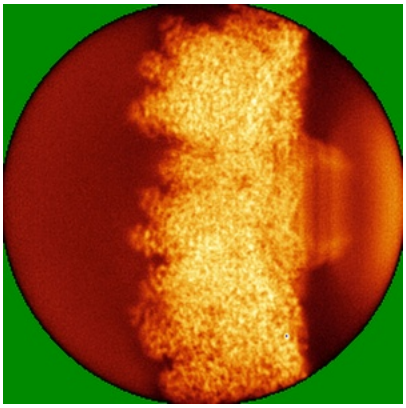


Z

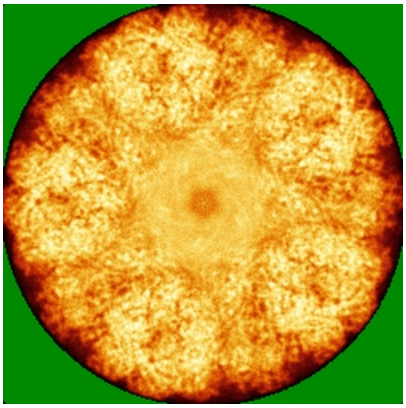
6.4.2 Raw map



X



Y

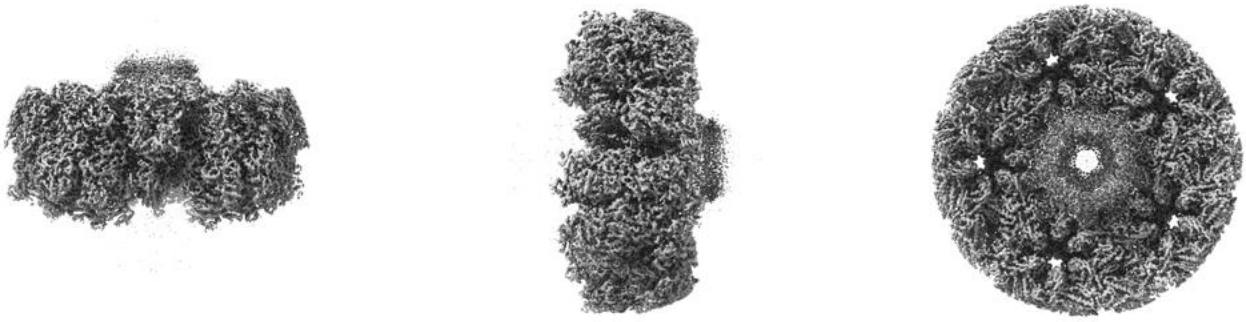


Z

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)

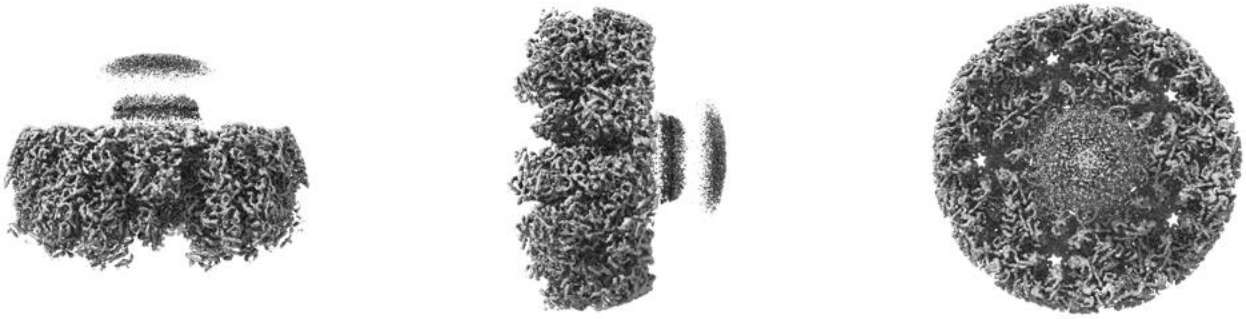
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.018. 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.

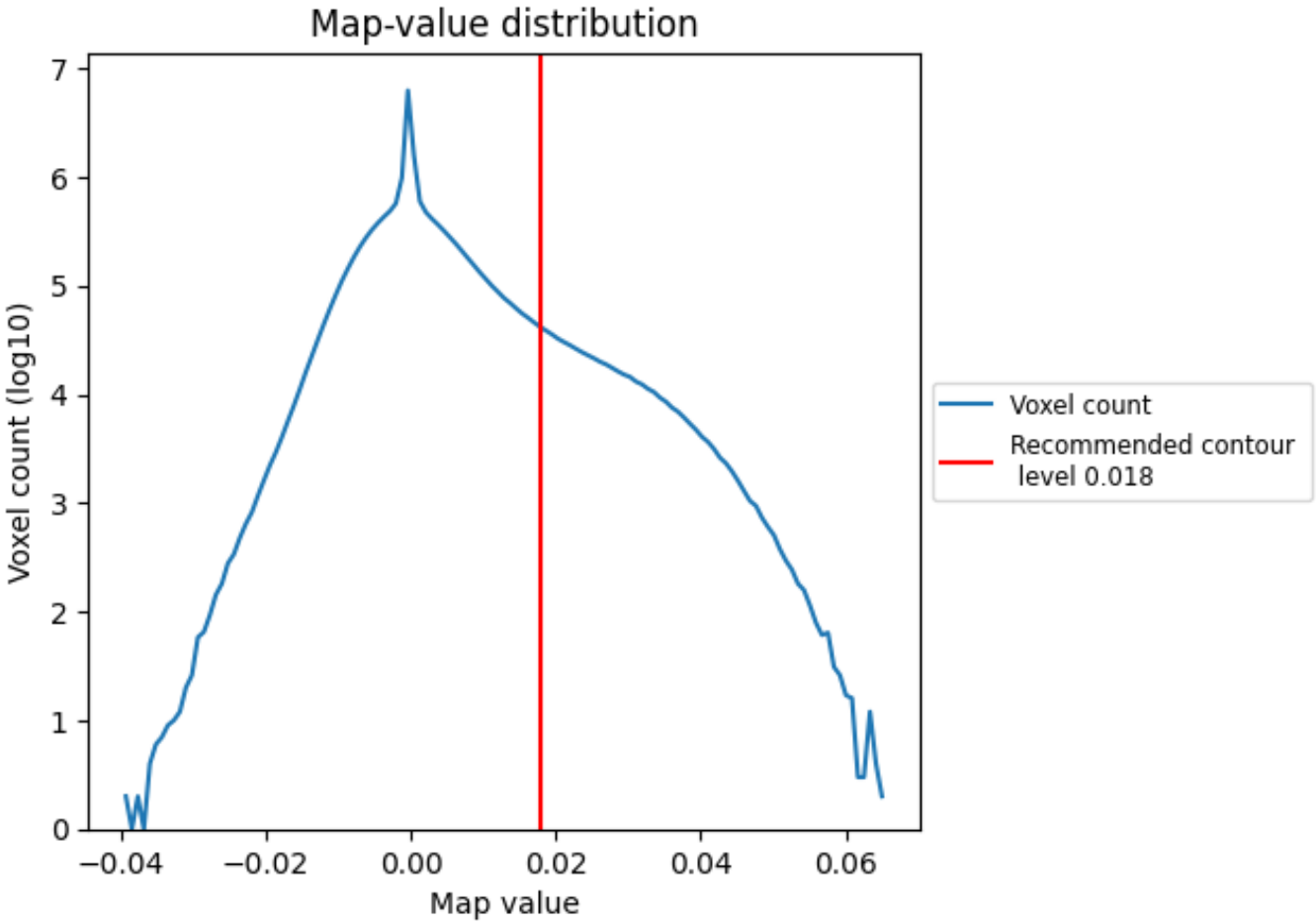
6.6 Mask visualisation (i)

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

7 Map analysis

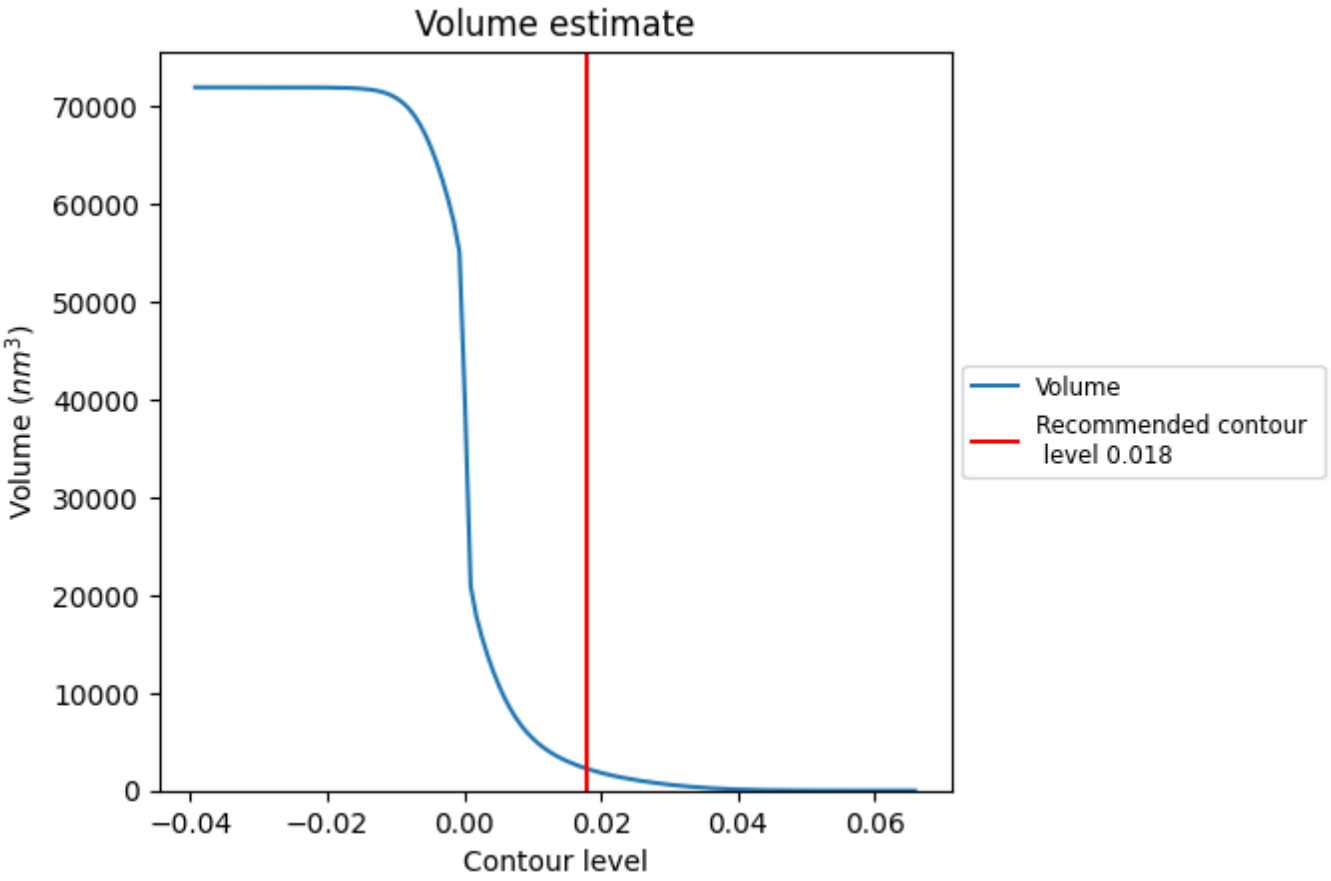
This section contains the results of statistical analysis of the map.

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.

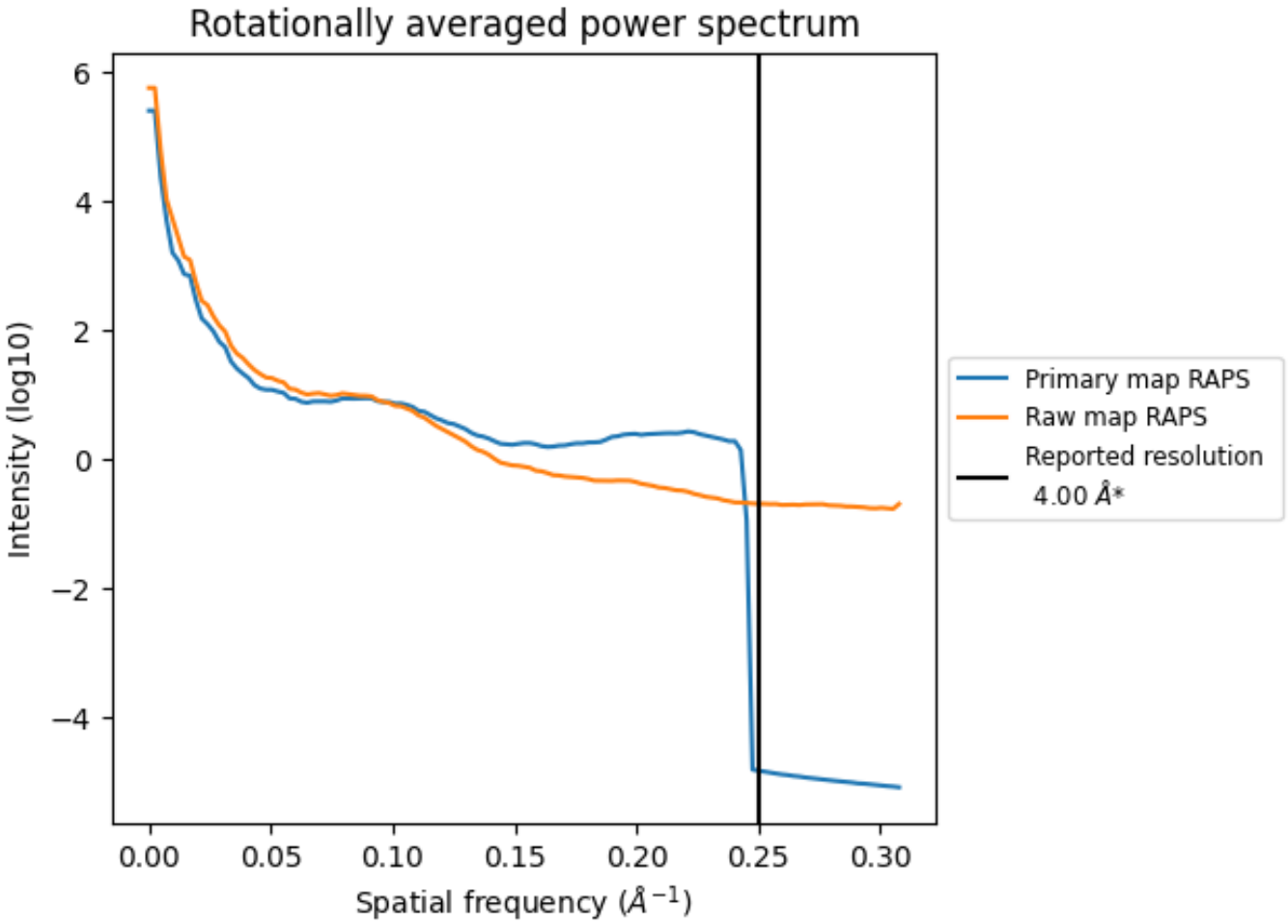
7.2 Volume estimate



The volume at the recommended contour level is 2218 nm^3; this corresponds to an approximate mass of 2004 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)

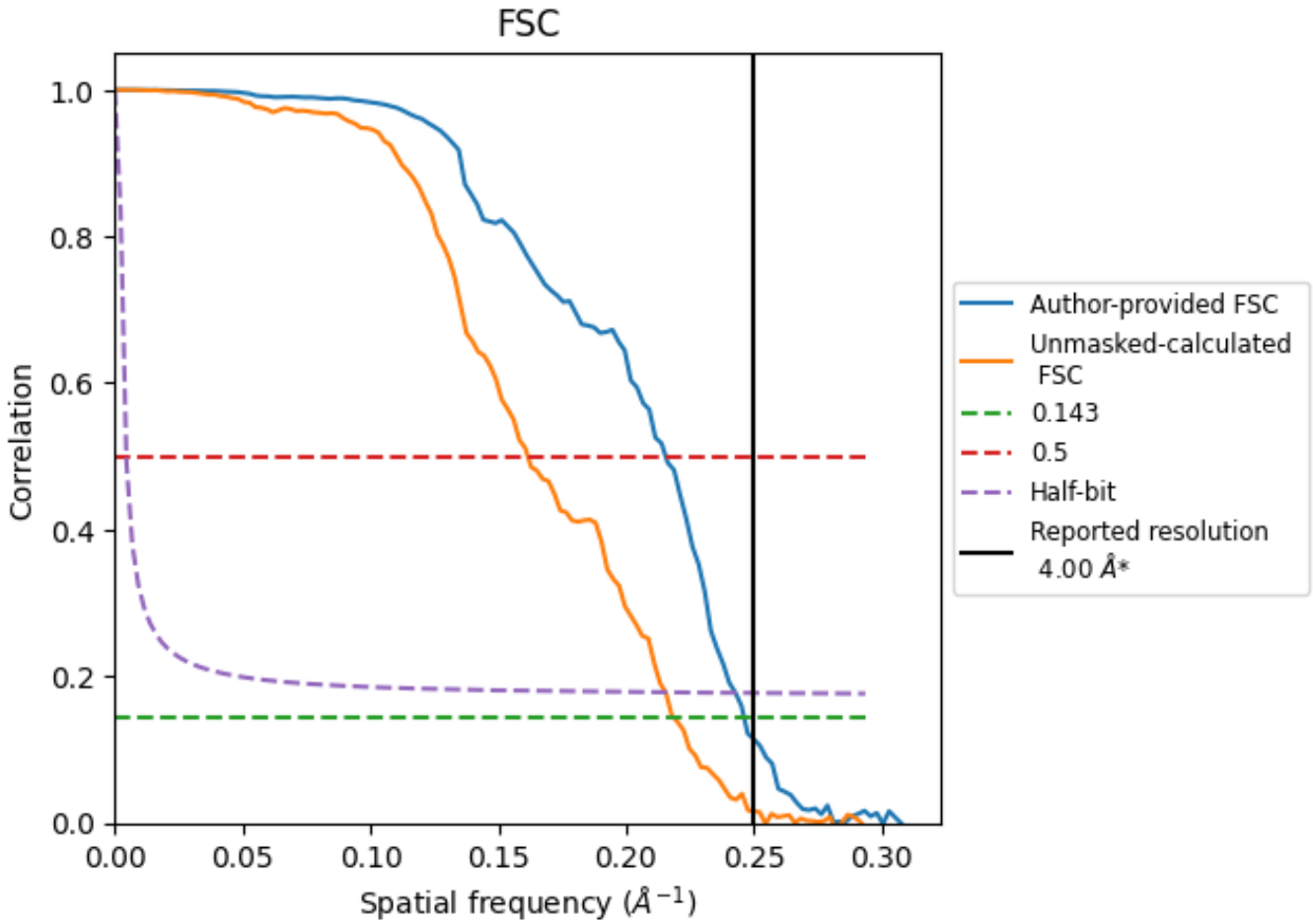


*Reported resolution corresponds to spatial frequency of 0.250 $Å^{-1}$

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	4.06	4.64	4.12
Unmasked-calculated*	4.57	6.19	4.64

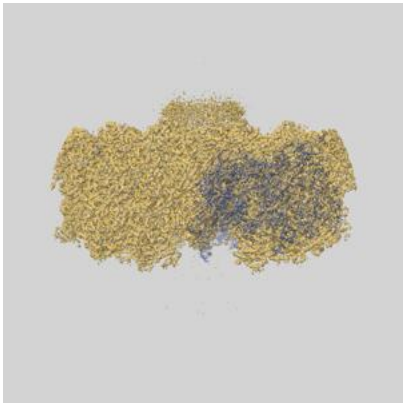
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.57 differs from the reported value 4.0 by more than 10 %

9 Map-model fit

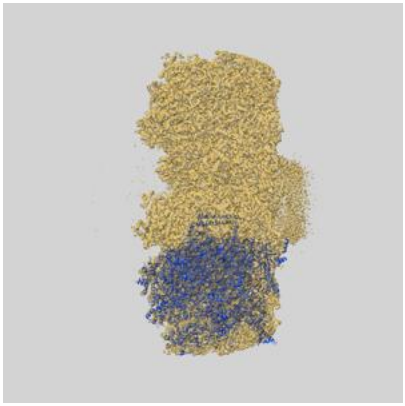
This section contains information regarding the fit between EMDB map EMD-34696 and PDB model 8HEX. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlays

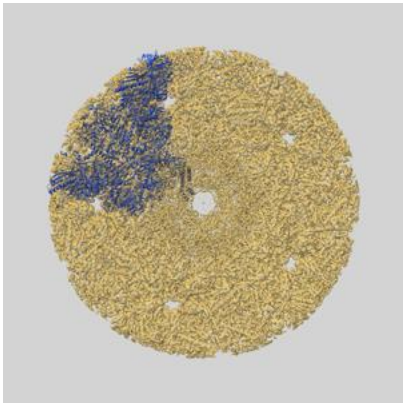
9.1.1 Map-model overlay



X

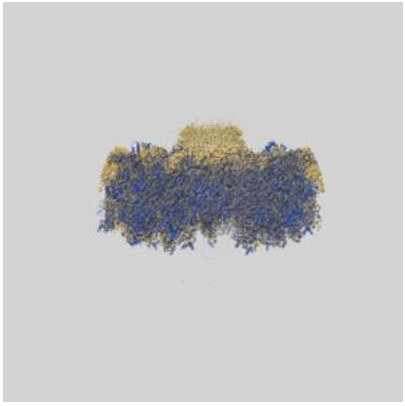


Y

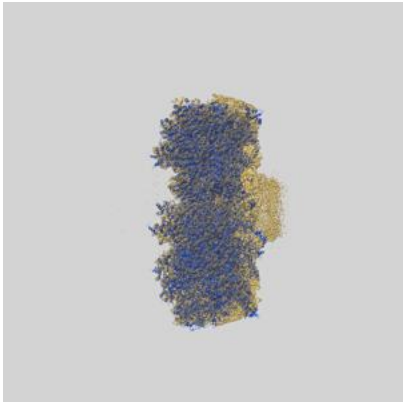


Z

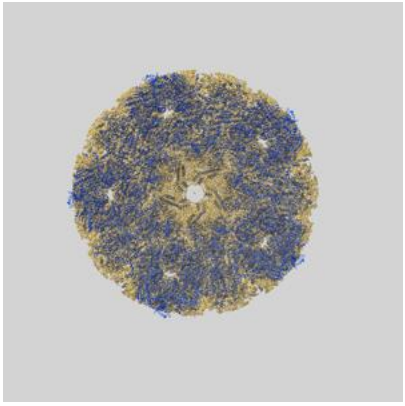
9.1.2 Map-model assembly overlay



X



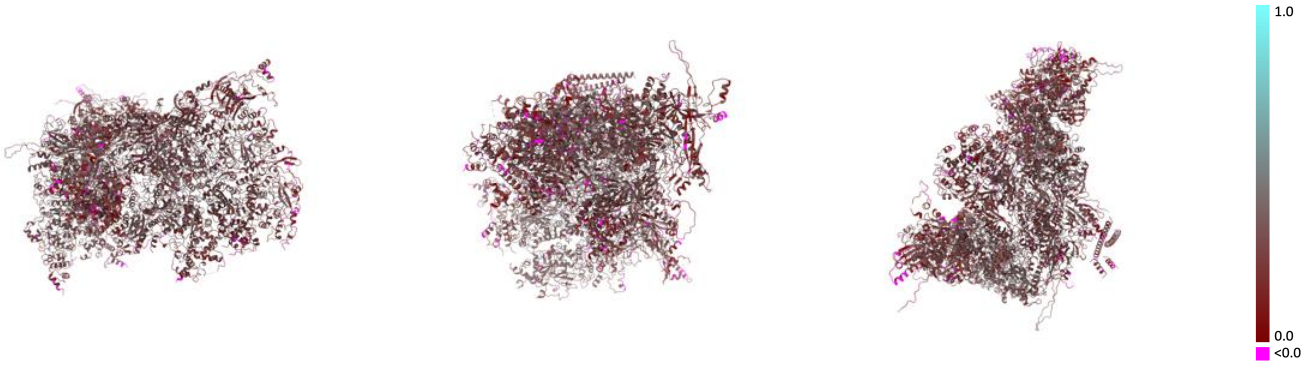
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.018 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.

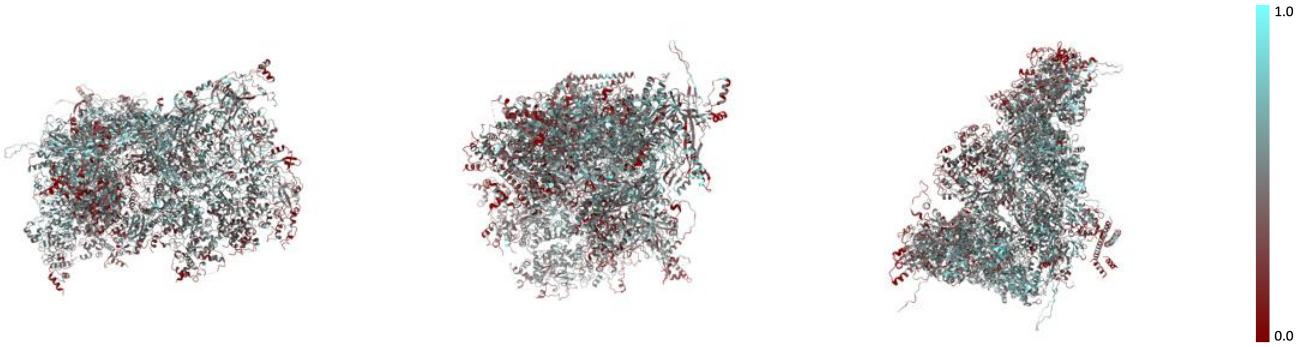
9.2 Q-score mapped to coordinate model (i)



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.

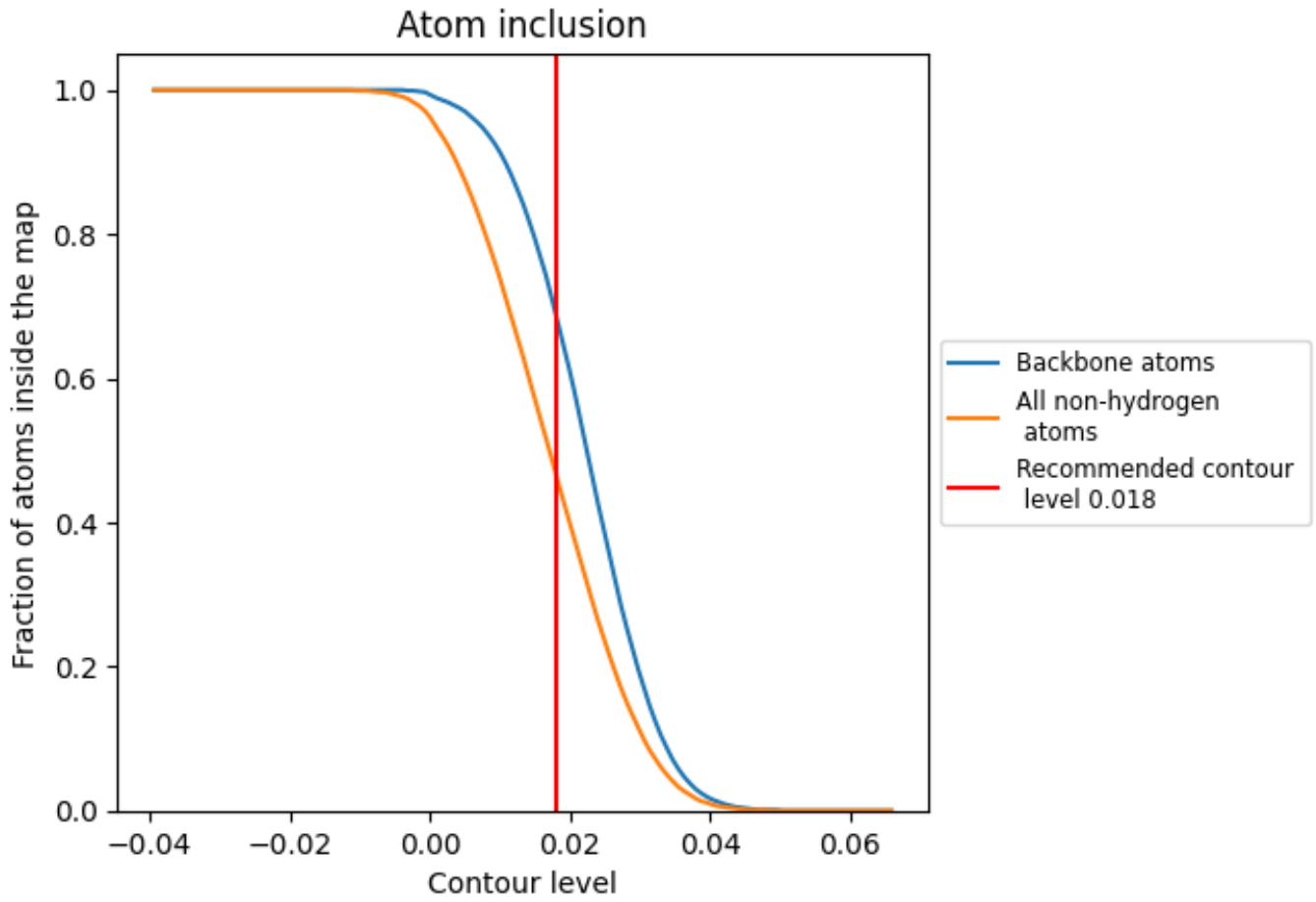
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.018).

9.4 Atom inclusion (i)



At the recommended contour level, 69% of all backbone atoms, 47% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4660	0.2830
A	0.3710	0.2410
B	0.5260	0.3210
C	0.5160	0.3070
D	0.4470	0.2660
E	0.3810	0.2480
F	0.2000	0.2240
G	0.0920	0.1340
I	0.4900	0.2800
M	0.4320	0.2920
N	0.2510	0.1960
O	0.2040	0.1650
R	0.2450	0.1830
S	0.2410	0.1390
Y	0.4230	0.2550
Z	0.5010	0.2950
a	0.5260	0.3200
g	0.3380	0.2070
h	0.4630	0.2890
i	0.1750	0.1630
j	0.2670	0.2110
m	0.4380	0.2620
n	0.3980	0.2480
o	0.3900	0.2340