wwPDB EM Validation Summary Report (i)

Apr 1, 2025 – 06:02 pm BST

PDB ID	:	6ZWM / pdb_00006zwm
EMDB ID	:	EMD-11488
Title	:	cryo-EM structure of human mTOR complex 2, overall refinement
Authors	:	Scaiola, A.; Mangia, F.; Imseng, S.; Boehringer, D.; Ban, N.; Maier, T.
Deposited on	:	2020-07-28
Resolution	:	3.20 Å(reported)

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

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

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

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

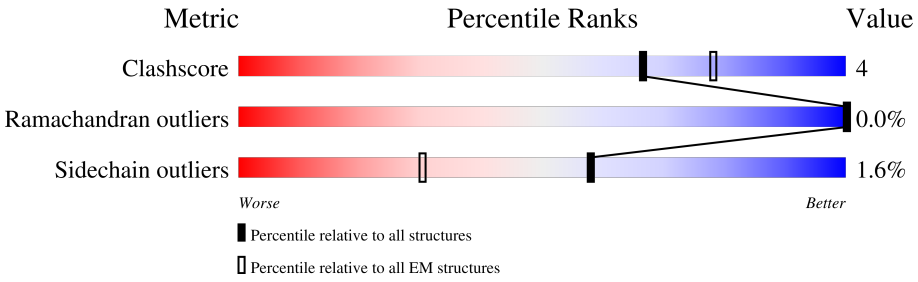
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 3.20 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	2549	15% 78% 8% 14%
1	B	2549	17% 79% 7% 14%
2	C	326	17% 79% 19%
2	D	326	9% 81% 17%
3	E	1708	15% 57% 8% 35%
3	F	1708	58% 7% 35%
4	G	522	10% 18% 81%
4	H	522	5% 17% 81%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 56947 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 Serine/threonine-protein kinase mTOR.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2184	Total	C	N	O	S	0	0
			16337	10356	2906	2977	98		
1	B	2185	Total	C	N	O	S	0	0
			16304	10330	2904	2972	98		

- Molecule 2 is a protein called Target of rapamycin complex subunit LST8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	319	Total	C	N	O	S	0	0
			2465	1533	437	477	18		
2	D	319	Total	C	N	O	S	0	0
			2465	1533	437	477	18		

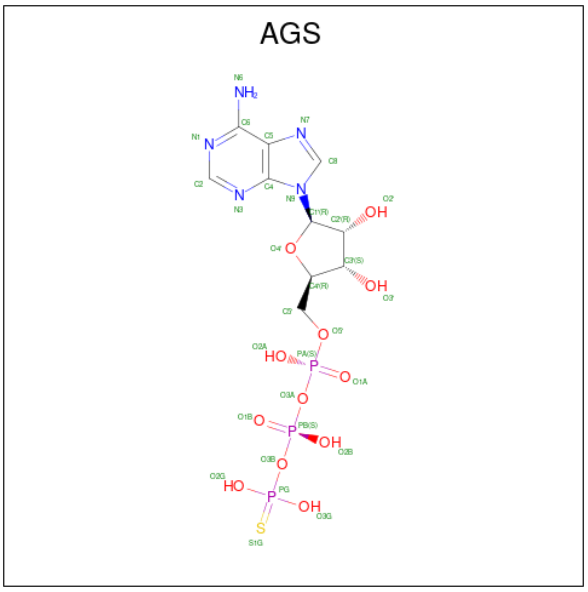
- Molecule 3 is a protein called Rapamycin-insensitive companion of mTOR.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	1117	Total	C	N	O	S	0	0
			8931	5689	1584	1611	47		
3	F	1117	Total	C	N	O	S	0	0
			8931	5689	1584	1611	47		

- Molecule 4 is a protein called Target of rapamycin complex 2 subunit MAPKAP1.

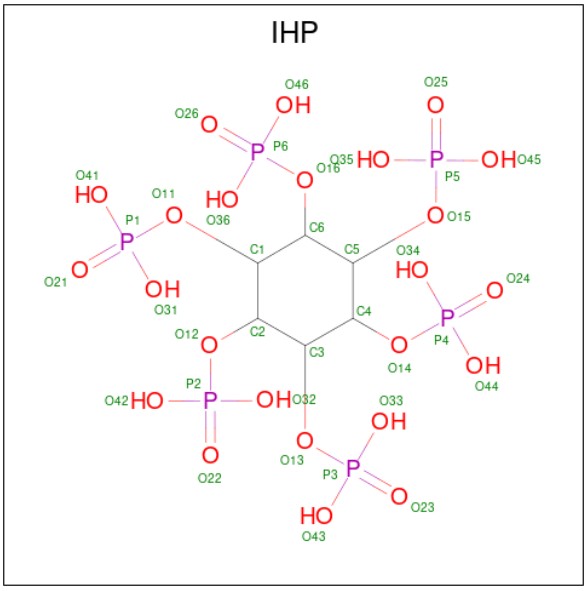
Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	98	Total	C	N	O	S	0	0
			655	399	125	127	4		
4	H	98	Total	C	N	O	S	0	0
			655	399	125	127	4		

- Molecule 5 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
5	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
5	B	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
5	E	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
5	F	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

- Molecule 6 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).

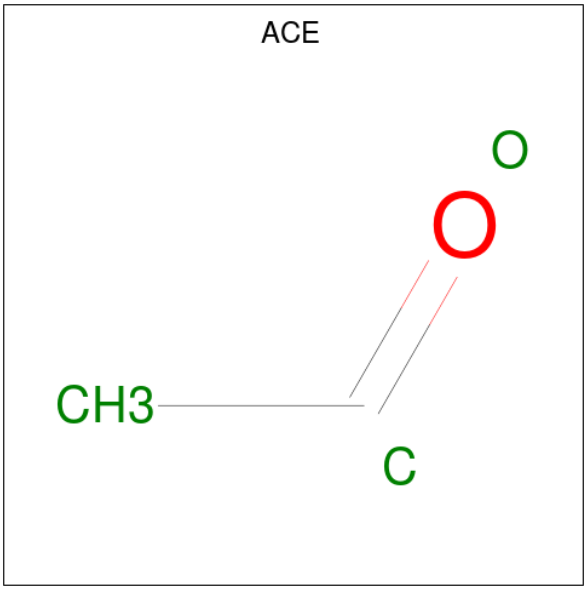


Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	O	P	0
			36	6	24	6	
6	B	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
7	E	1	Total	Zn	0
			1	1	
7	F	1	Total	Zn	0
			1	1	

- Molecule 8 is ACETYL GROUP (CCD ID: ACE) (formula: C_2H_4O).



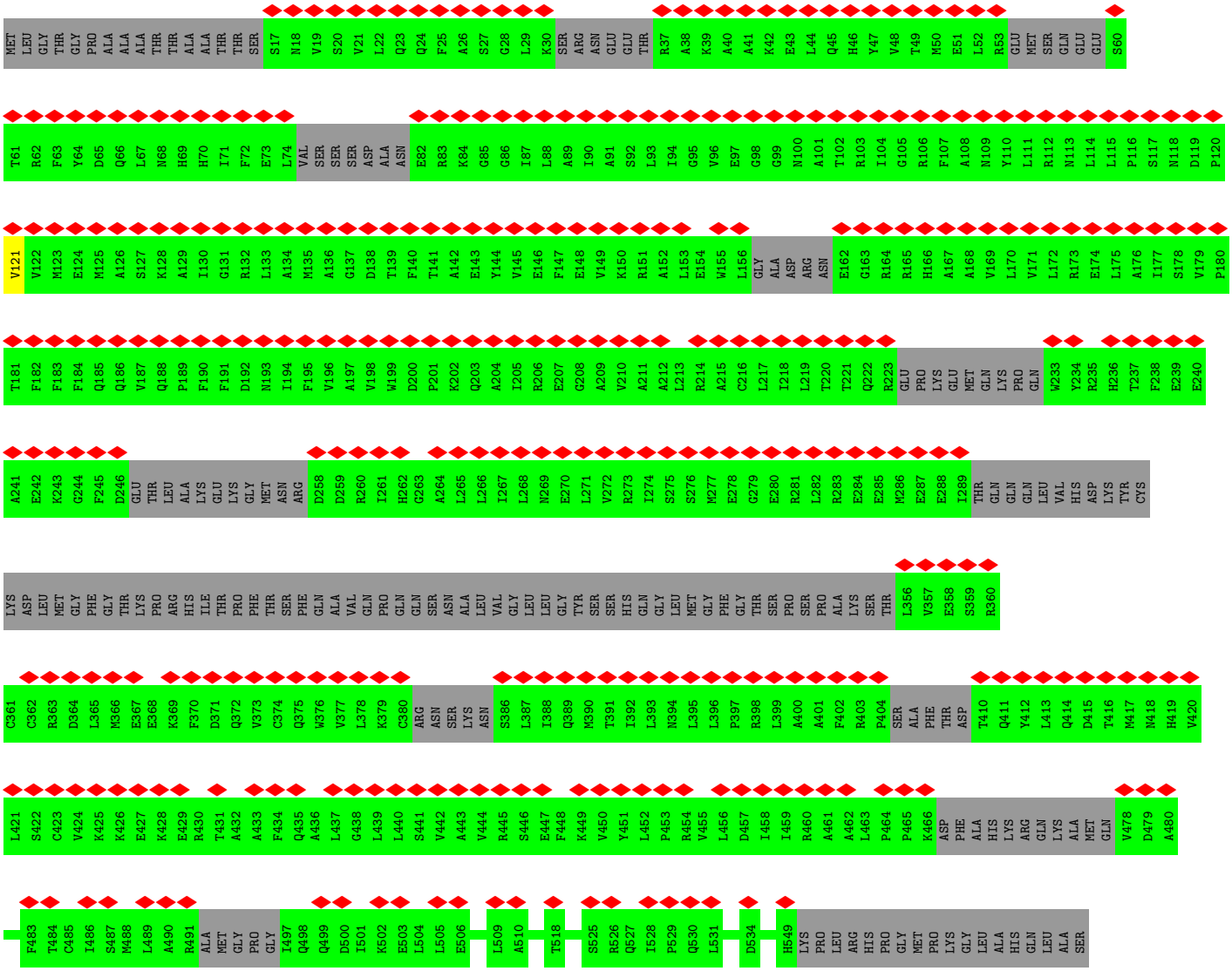
Mol	Chain	Residues	Atoms			AltConf
8	G	1	Total	C	O	0
			3	2	1	
8	H	1	Total	C	O	0
			3	2	1	

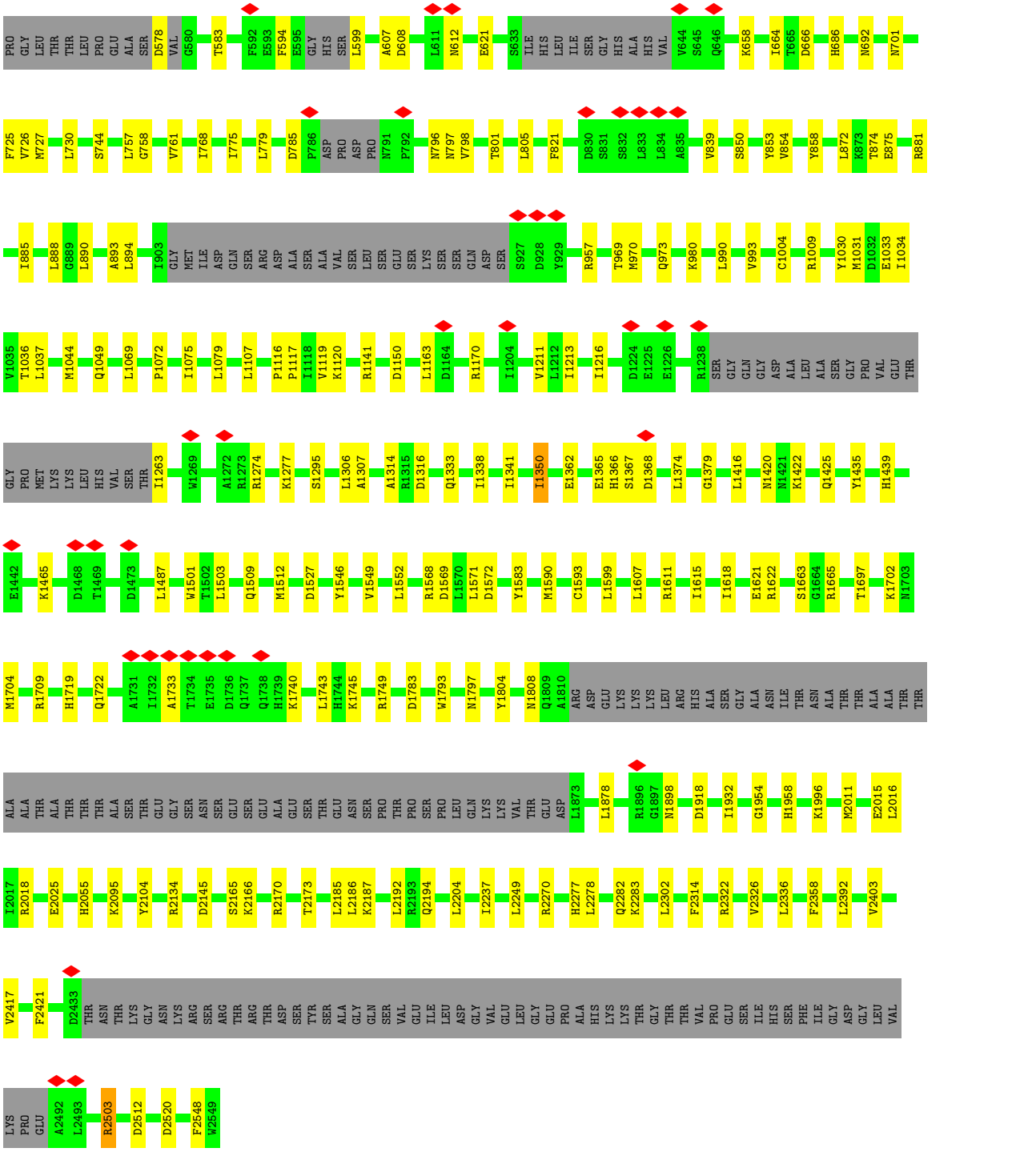
3 Residue-property plots (i)

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: Serine/threonine-protein kinase mTOR

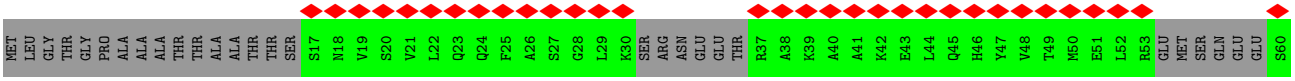
Chain A:

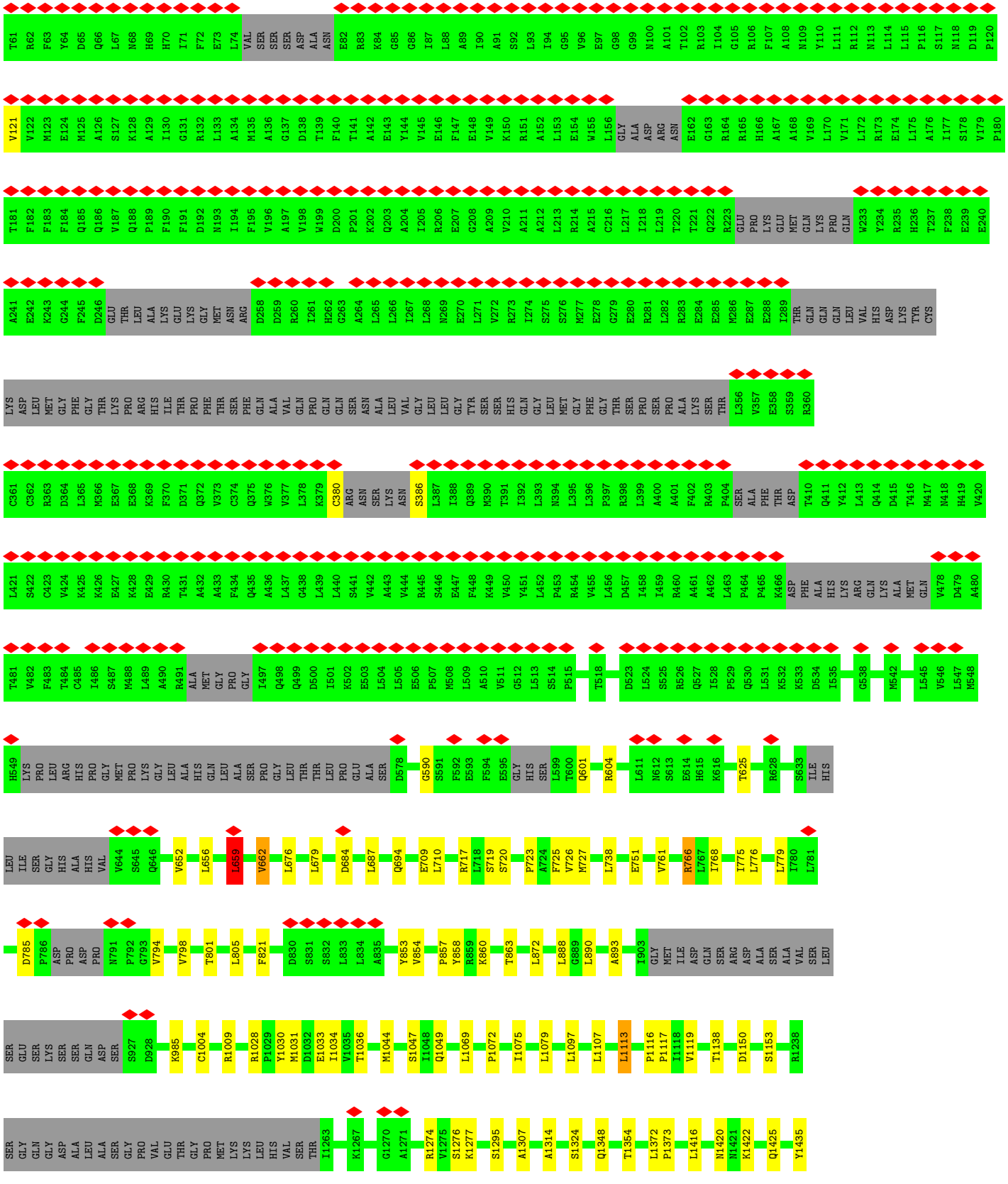


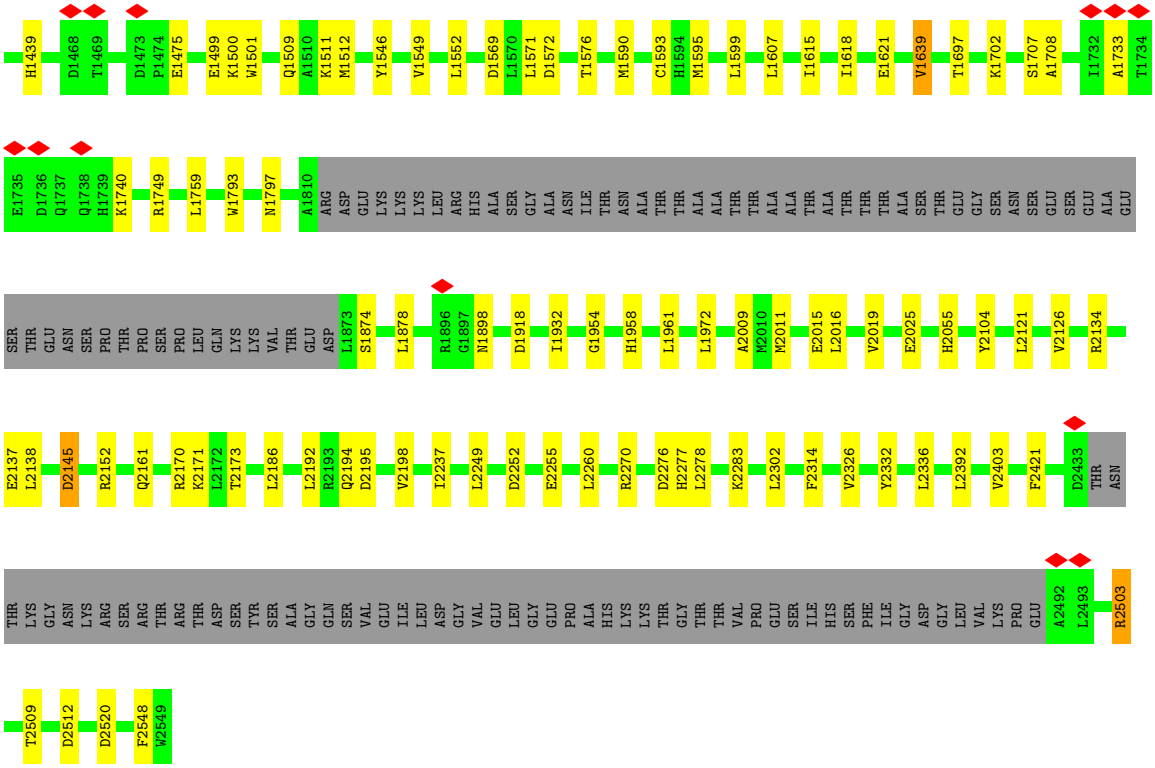


• Molecule 1: Serine/threonine-protein kinase mTOR

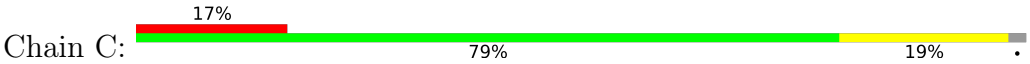
Chain B:

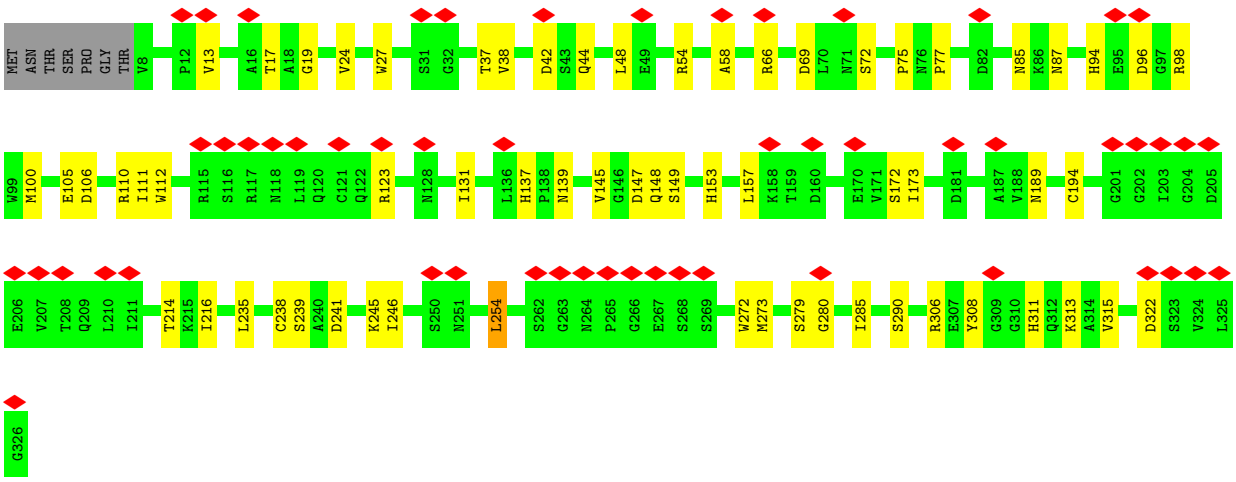



T61 R62 F63 Y64 D65 Q66 L67 N68 H69 H70 I71 F72 E73 L74 VAL SER SER SER ASP ALA ASN E82 R83 K84 G85 G86 I87 L88 A89 I90 A91 S92 L93 I94 G95 V96 E97 G98 G99 N100 A101 T102 R103 I104 G105 R106 F107 A108 N109 Y110 L111 R112 N113 L114 L115 P116 S117 N118 D119 P120
V121 V122 M123 E124 M125 A126 S127 K128 A129 I130 G131 R132 L133 A134 M135 A136 G137 D138 T139 F140 T141 A142 E143 Y144 V145 E146 F147 E148 V149 K150 R151 A152 L153 E154 W155 L156 GLY ALA ASP ARG ASN E162 G163 R164 R165 H166 A167 A168 V169 L170 V171 L172 R173 E174 L175 A176 I177 S178 V179 P180
T181 F182 F183 F184 Q185 Q186 V187 Q188 P189 F190 F191 D192 N193 I194 F195 V196 A197 V198 W199 D200 P201 K202 Q203 A204 I205 R206 E207 G208 A209 V210 A211 A212 L213 R214 A215 C216 L217 I218 L219 T220 T221 Q222 R223 GLU PRO LYS GLU MET GLN LYS PRO GLN W233 Y234 R235 H236 T237 F238 E239 E240
A241 E242 K243 G244 F245 D246 GLU THR LEU ALA LYS GLU LYS GLY MET ASN ARG D258 D259 R260 I261 H262 G263 A264 L265 L266 I267 L268 N269 E270 L271 V272 R273 I274 S275 S276 M277 E278 G279 E280 R281 L282 R283 E284 E285 M286 E287 E288 I289 THR GLN GLN GLN LEU VAL HIS ASP LYS TYR CYS
LYS ASP LEU MET GLY PHE GLY THR LYS PRO ARG HIS ILE THR PRO PHE THR SER PHE GLN ALA VAL GLN PRO GLN GLN SER ASN ALA LEU VAL GLY LEU LEU GLY TYR SER SER HIS GLN GLY LEU MET GLY PHE GLY THR SER PRO SER PRO ALA LYS SER THR L356 V357 E358 S359 R360
C361 C362 R363 D364 L365 M366 E367 E368 K369 F370 D371 Q372 V373 C374 Q375 W376 V377 L378 K379 C380 ARG ASN SER LYS ASN S386 L387 I388 Q389 M390 T391 I392 L393 N394 L395 L396 P397 R398 L399 A400 A401 F402 R403 P404 SER ALA PHE THR ASP T410 Q411 Y412 L413 Q414 D415 T416 M417 N418 H419 V420
L421 S422 C423 V424 K425 K426 E427 K428 E429 R430 T431 A432 A433 F434 Q435 A436 L437 G438 L439 L440 S441 V442 A443 V444 R445 S446 E447 F448 K449 V450 Y451 L452 P453 R454 V455 L456 D457 I458 I459 R460 A461 A462 L463 P464 P465 K466 ASP PHE ALA HIS LYS ARG GLN LYS ALA MET GLN V478 D479 A480
T481 V482 F483 T484 C485 I486 S487 M488 L489 A490 R491 ALA MET GLY PRO GLY I497 Q498 Q499 D500 I501 K502 E503 L504 L505 E506 P507 M508 L509 A510 V511 G512 L513 S514 P515 T518 D523 L524 S525 R526 Q527 I528 P529 Q530 L531 K532 K533 D534 I535 G538 M542 L545 V546 L547 M548
H549 LYS PRO LEU ARG HIS PRO GLY MET PRO LYS GLY LEU ALA HIS GLN LEU ALA SER PRO GLY LEU THR THR LEU PRO GLU ALA SER D578 G590 S591 F592 E593 F594 E595 GLY HIS SER L599 T600 Q601 R604 L611 N612 S613 E614 H615 K616 T625 R628 S633 ILE HIS
LEU ILE SER GLY HIS ALA HIS VAL V644 S645 Q646 V652 L656 L659 V662 L676 L679 D684 L687 Q694 E709 L710 R717 L718 S719 S720 P723 A724 F725 V726 M727 L738 E751 V761 R766 L767 I768 I775 L776 L779 I780 L781
D785 P786 ASP PRO ASP PRO N791 P792 G793 V794 V798 T801 L805 F821 D830 S831 S832 L833 L834 A835 Y853 V854 P857 Y858 R859 K860 T863 L872 L888 G889 L890 A893 I903 GLY MET ILE ASP GLN SER ARG ASP ALA SER ALA VAL SER LEU
SER GLU SER LYS SER SER GLN ASP SER S927 D928 K985 C1004 R1009 R1028 P1029 Y1030 M1031 D1032 E1033 I1034 V1035 T1036 M1044 S1047 I1048 Q1049 L1069 P1072 I1075 L1079 L1097 L1107 L1113 P1116 P1117 I1118 V1119 T1138 D1150 S1153 R1238
SER GLY GLN GLY ASP ALA LEU ALA SER GLY PRO VAL GLU THR GLY PRO MET LYS LYS LEU HIS VAL SER THR I1263 K1267 G1270 A1271 R1274 V1275 S1276 K1277 S1295 A1307 A1314 S1324 Q1348 T1354 L1372 P1373 L1416 N1420 N1421 K1422 Q1425 Y1435

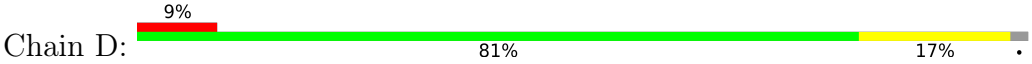


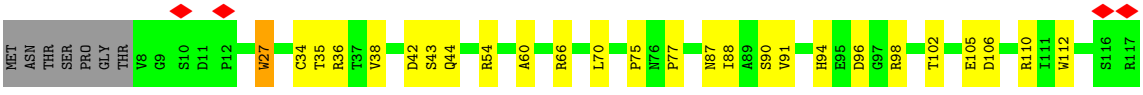
• Molecule 2: Target of rapamycin complex subunit LST8

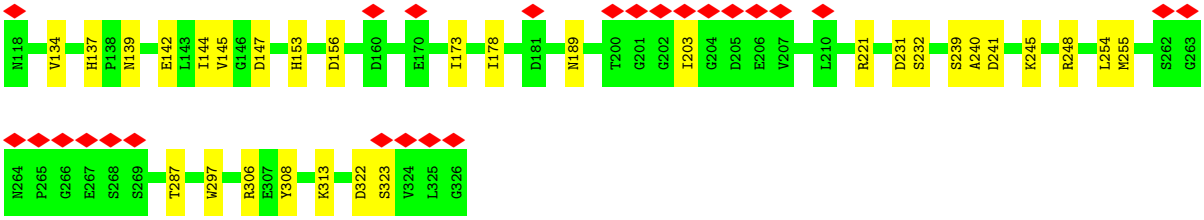




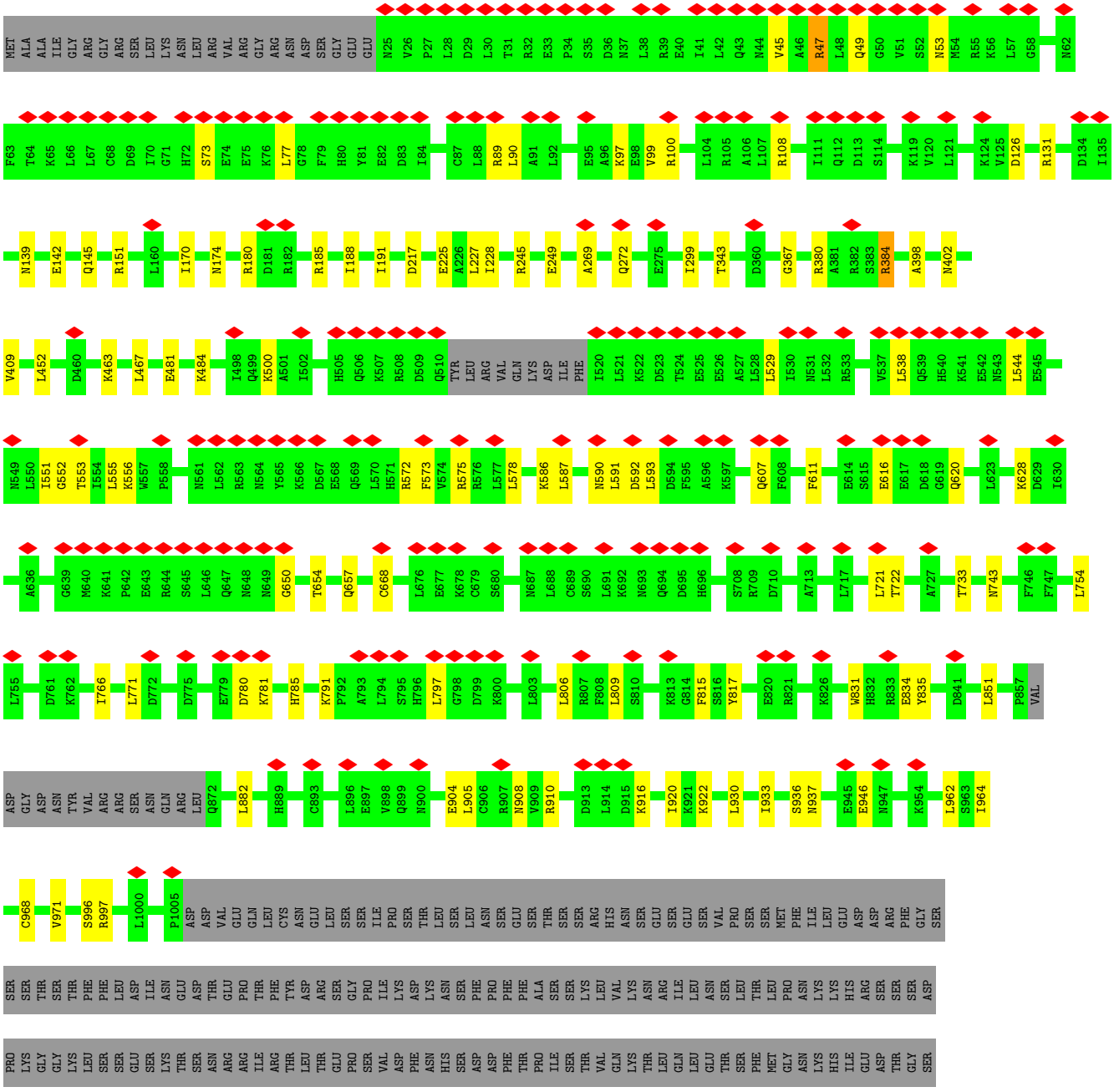
• Molecule 2: Target of rapamycin complex subunit LST8

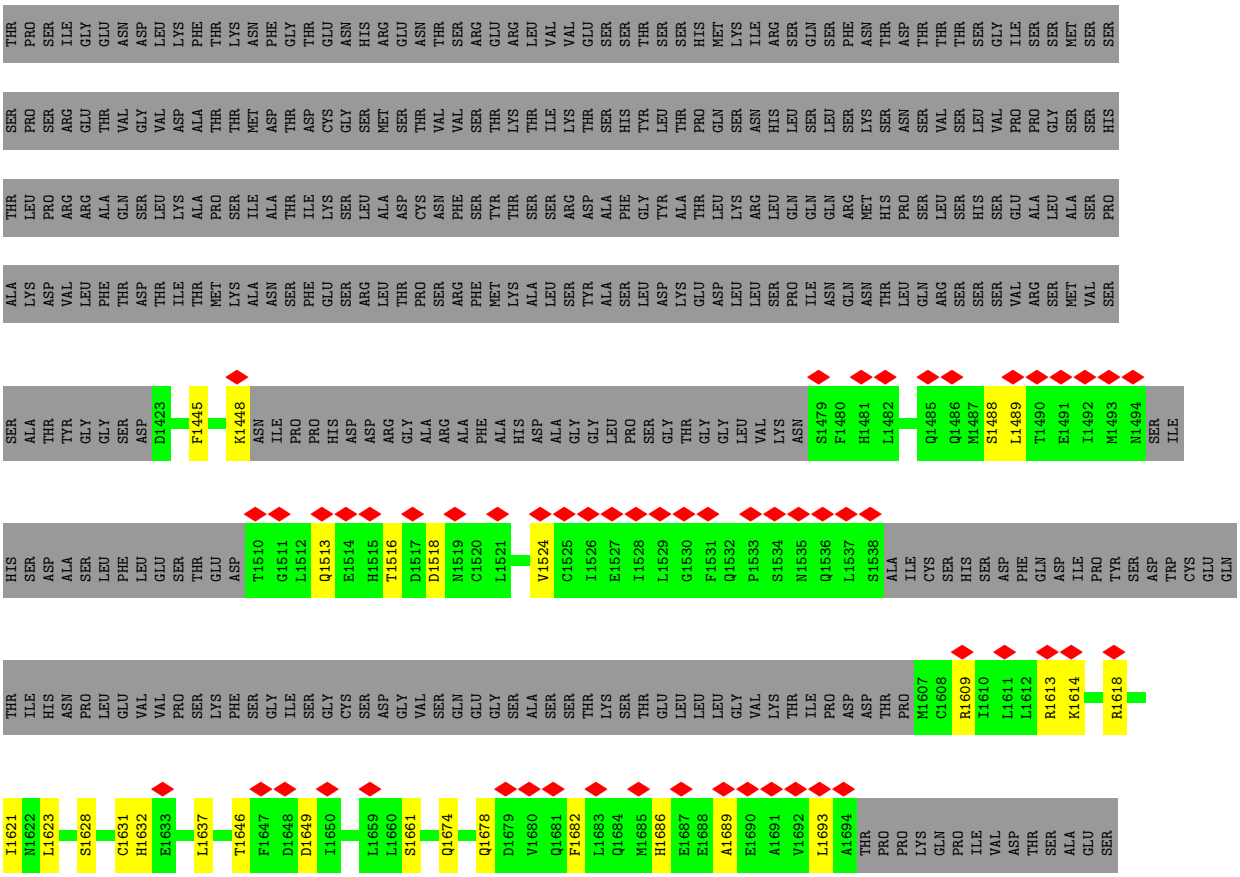






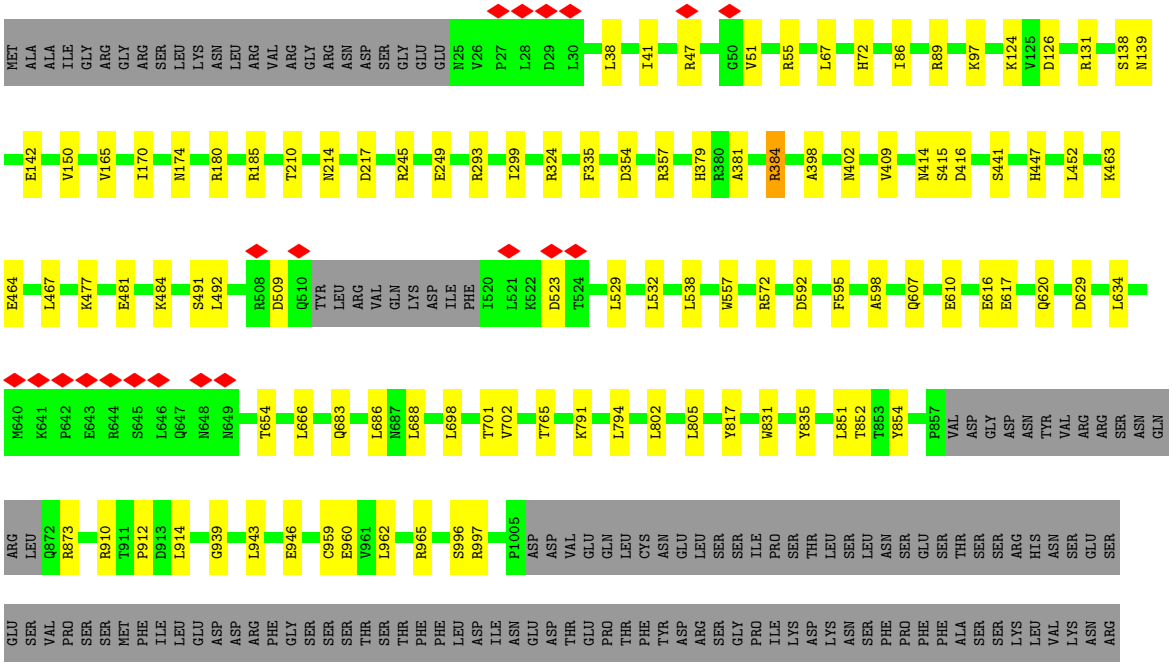
• Molecule 3: Rapamycin-insensitive companion of mTOR

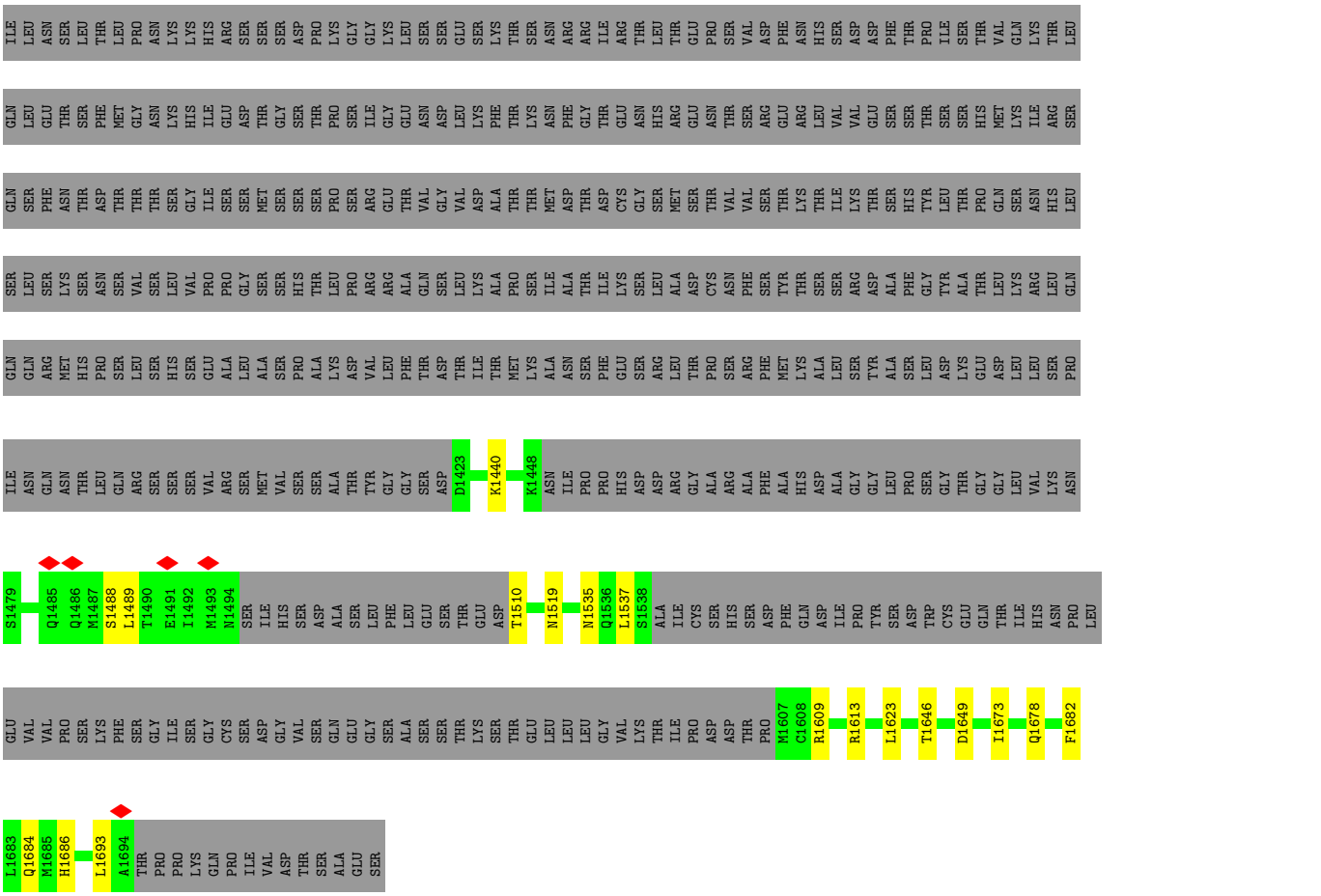




• Molecule 3: Rapamycin-insensitive companion of mTOR

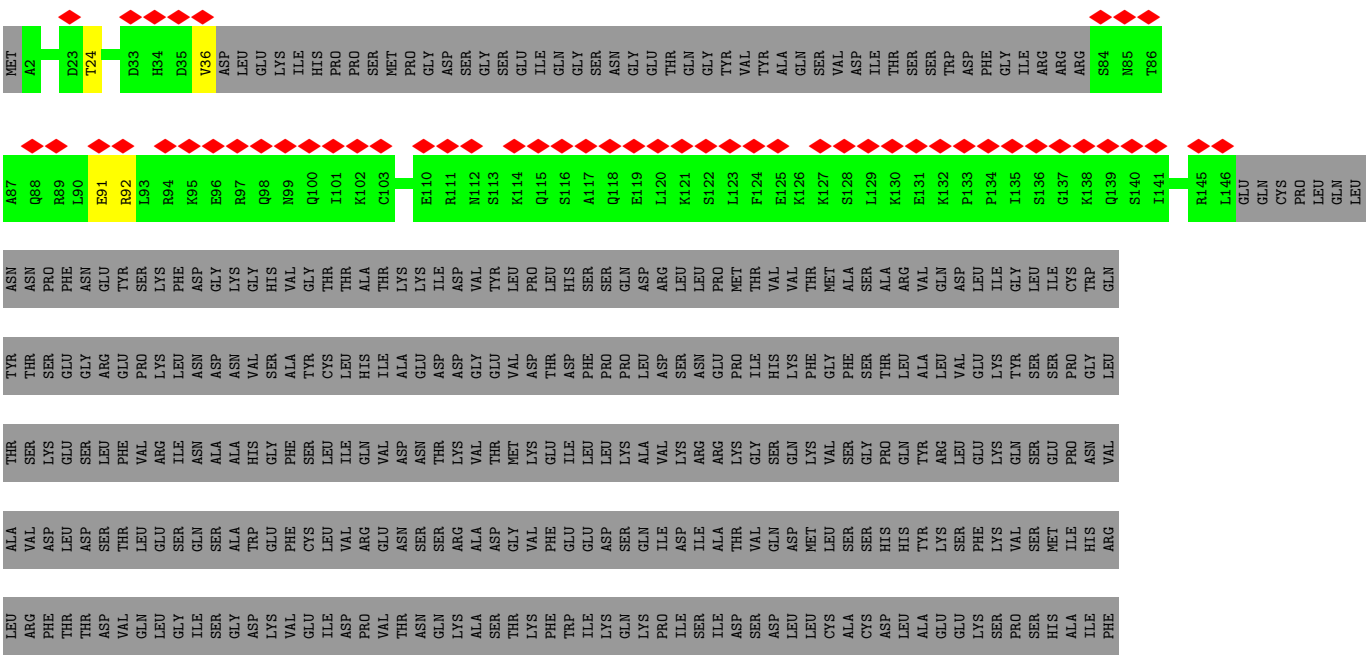
Chain F:

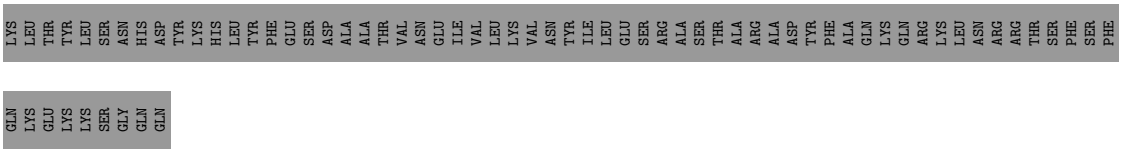




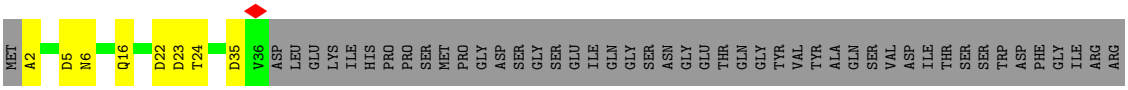
• Molecule 4: Target of rapamycin complex 2 subunit MAPKAP1

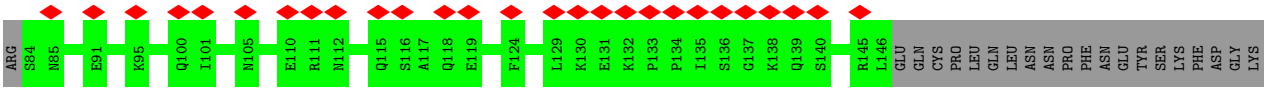
Chain G:

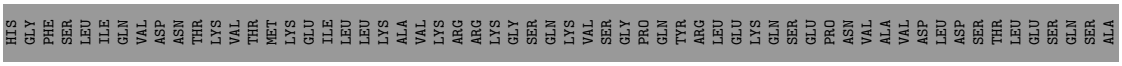




• Molecule 4: Target of rapamycin complex 2 subunit MAPKAP1







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	293038	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 ($e^-/Å^2$)	70	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.323	Depositor
Minimum map value	-1.756	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.077	Depositor
Recommended contour level	0.375	Depositor
Map size (Å)	430.08, 430.08, 430.08	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.344, 1.344, 1.344	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IHP, ACE, ZN, AGS

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	0/16632	0.49	3/22593 (0.0%)
1	B	0.26	0/16598	0.47	3/22552 (0.0%)
2	C	0.28	0/2523	0.58	0/3438
2	D	0.27	0/2523	0.58	0/3438
3	E	0.28	0/9092	0.53	1/12300 (0.0%)
3	F	0.26	0/9092	0.50	1/12300 (0.0%)
4	G	0.27	0/660	0.54	0/900
4	H	0.25	0/660	0.50	0/900
All	All	0.27	0/57780	0.50	8/78421 (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
3	E	0	1

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1107	LEU	CA-CB-CG	6.75	130.82	115.30
1	A	1107	LEU	CA-CB-CG	6.75	130.82	115.30
3	F	38	LEU	CA-CB-CG	6.51	130.28	115.30
3	E	529	LEU	CA-CB-CG	6.08	129.28	115.30
1	B	659	LEU	CA-CB-CG	5.74	128.49	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	367	GLY	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	16337	0	15369	110	0
1	B	16304	0	15298	97	0
2	C	2465	0	2351	33	0
2	D	2465	0	2351	33	0
3	E	8931	0	9080	80	0
3	F	8931	0	9080	69	0
4	G	655	0	519	2	0
4	H	655	0	519	6	0
5	A	31	0	12	1	0
5	B	31	0	12	0	0
5	E	31	0	12	1	0
5	F	31	0	12	1	0
6	A	36	0	6	2	0
6	B	36	0	6	2	0
7	E	1	0	0	0	0
7	F	1	0	0	0	0
8	G	3	0	3	0	0
8	H	3	0	3	0	0
All	All	56947	0	54633	413	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 4.

The worst 5 of 413 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:552:GLY:O	3:E:556:LYS:HB2	1.75	0.87
3:E:920:ILE:HG23	3:E:964:ILE:HD11	1.75	0.69
1:A:1211:VAL:HA	3:E:553:THR:HG21	1.75	0.67
3:E:555:LEU:HD11	3:E:607:GLN:HG3	1.76	0.66
2:D:134:VAL:HG12	2:D:145:VAL:HG12	1.82	0.62

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	2143/2549 (84%)	2080 (97%)	62 (3%)	1 (0%)	100	100
1	B	2145/2549 (84%)	2071 (97%)	73 (3%)	1 (0%)	100	100
2	C	317/326 (97%)	299 (94%)	18 (6%)	0	100	100
2	D	317/326 (97%)	291 (92%)	26 (8%)	0	100	100
3	E	1103/1708 (65%)	1066 (97%)	37 (3%)	0	100	100
3	F	1103/1708 (65%)	1067 (97%)	36 (3%)	0	100	100
4	G	94/522 (18%)	86 (92%)	8 (8%)	0	100	100
4	H	94/522 (18%)	85 (90%)	9 (10%)	0	100	100
All	All	7316/10210 (72%)	7045 (96%)	269 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	121	VAL
1	A	121	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1563/2220 (70%)	1541 (99%)	22 (1%)	62	82

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	1552/2220 (70%)	1524 (98%)	28 (2%)	54 77
2	C	269/276 (98%)	260 (97%)	9 (3%)	33 64
2	D	269/276 (98%)	262 (97%)	7 (3%)	41 70
3	E	987/1539 (64%)	977 (99%)	10 (1%)	73 87
3	F	987/1539 (64%)	976 (99%)	11 (1%)	70 86
4	G	50/471 (11%)	49 (98%)	1 (2%)	50 75
4	H	50/471 (11%)	48 (96%)	2 (4%)	27 59
All	All	5727/9012 (64%)	5637 (98%)	90 (2%)	58 79

5 of 90 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	306	ARG
3	E	611	PHE
2	D	27	TRP
2	D	308	TYR
3	E	1516	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	41	GLN
3	F	848	ASN
3	E	219	GLN
3	F	539	GLN
4	G	107	GLN

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)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	AGS	B	2601	-	26,33,33	1.85	6 (23%)	26,52,52	2.03	7 (26%)
5	AGS	A	2601	-	26,33,33	1.84	6 (23%)	26,52,52	2.05	7 (26%)
5	AGS	E	4802	-	26,33,33	1.89	6 (23%)	26,52,52	2.07	7 (26%)
6	IHP	B	2602	-	36,36,36	1.47	3 (8%)	54,60,60	1.03	5 (9%)
8	ACE	H	601	4	1,2,2	0.70	0	1,1,1	0.30	0
8	ACE	G	601	4	1,2,2	0.79	0	1,1,1	0.23	0
5	AGS	F	4802	-	26,33,33	1.89	6 (23%)	26,52,52	2.11	7 (26%)
6	IHP	A	2602	-	36,36,36	1.47	3 (8%)	54,60,60	1.04	5 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	AGS	B	2601	-	-	5/17/38/38	0/3/3/3
5	AGS	A	2601	-	-	5/17/38/38	0/3/3/3
5	AGS	E	4802	-	-	1/17/38/38	0/3/3/3
6	IHP	B	2602	-	-	8/30/54/54	0/1/1/1
5	AGS	F	4802	-	-	1/17/38/38	0/3/3/3
6	IHP	A	2602	-	-	8/30/54/54	0/1/1/1

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	4802	AGS	C2-N3	5.06	1.40	1.32
5	F	4802	AGS	C2-N3	5.04	1.40	1.32
5	A	2601	AGS	C2-N3	5.01	1.40	1.32
5	B	2601	AGS	C2-N3	4.96	1.40	1.32
5	E	4802	AGS	O4'-C1'	4.45	1.47	1.41

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	2601	AGS	N3-C2-N1	-6.93	117.85	128.68
5	F	4802	AGS	N3-C2-N1	-6.92	117.86	128.68
5	B	2601	AGS	N3-C2-N1	-6.92	117.87	128.68
5	E	4802	AGS	N3-C2-N1	-6.88	117.93	128.68
5	F	4802	AGS	PA-O3A-PB	-3.45	120.98	132.83

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2601	AGS	PB-O3B-PG-O3G
5	B	2601	AGS	PB-O3B-PG-O3G
5	E	4802	AGS	C5'-O5'-PA-O1A
5	F	4802	AGS	C5'-O5'-PA-O1A
5	A	2601	AGS	PA-O3A-PB-O3B

There are no ring outliers.

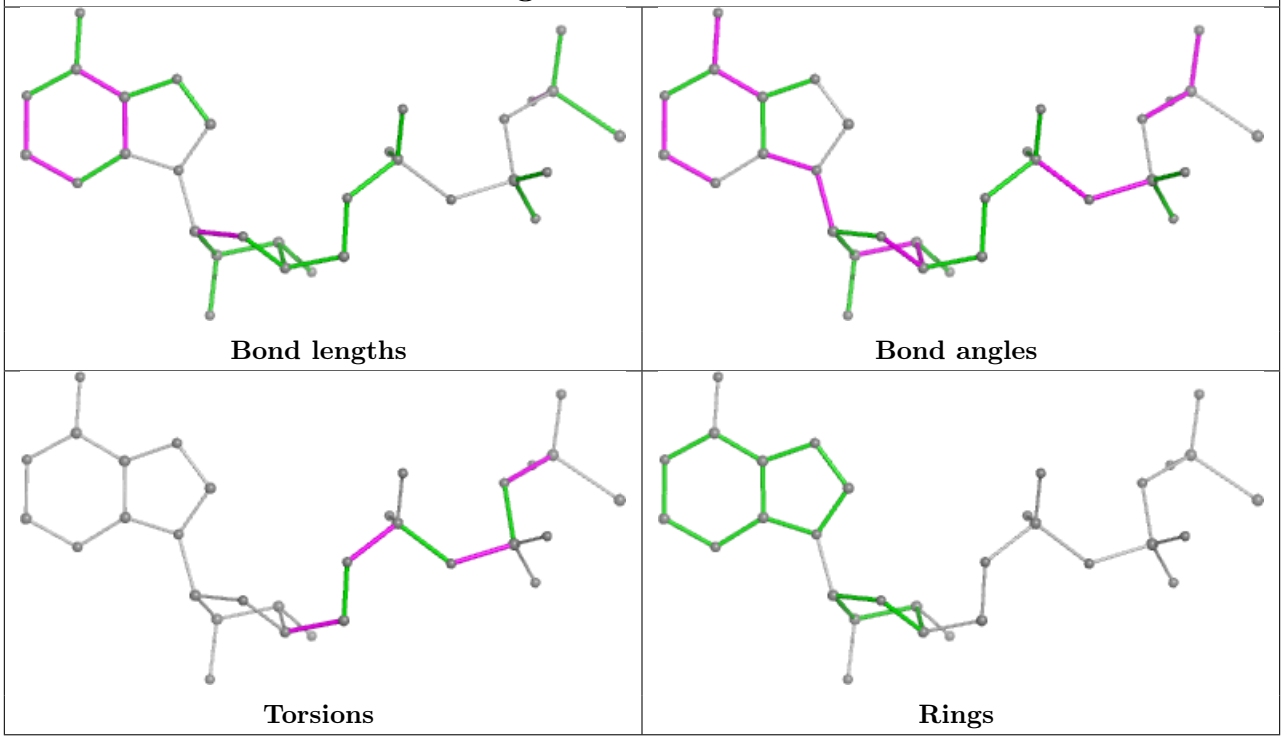
5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2601	AGS	1	0
5	E	4802	AGS	1	0
6	B	2602	IHP	2	0
5	F	4802	AGS	1	0
6	A	2602	IHP	2	0

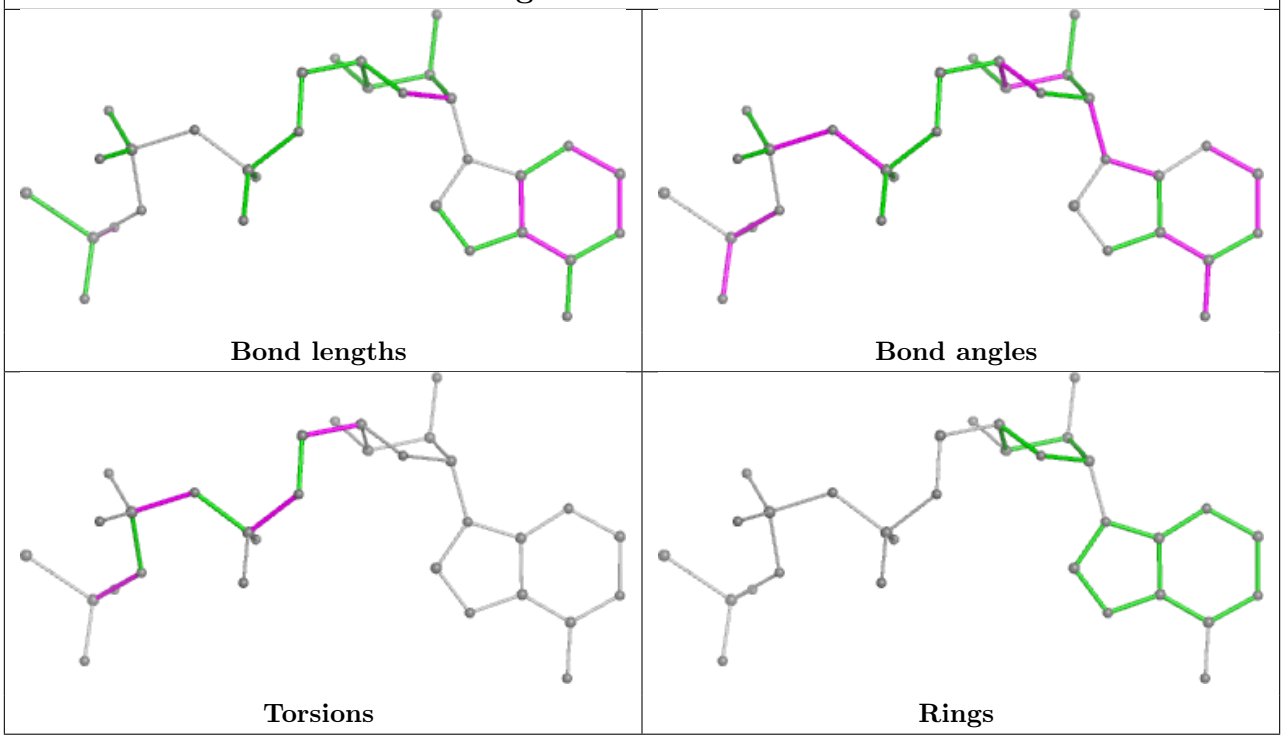
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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

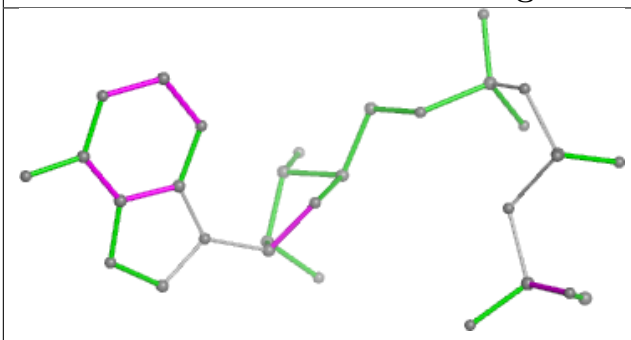
Ligand AGS B 2601



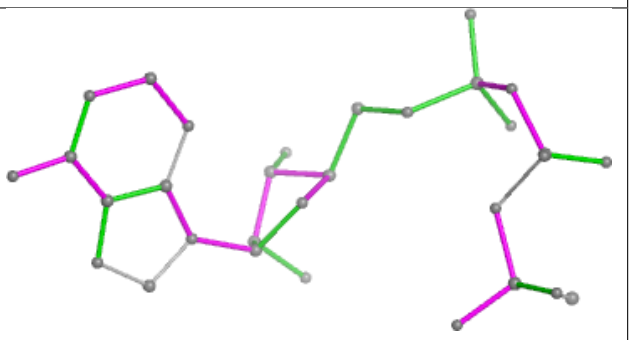
Ligand AGS A 2601



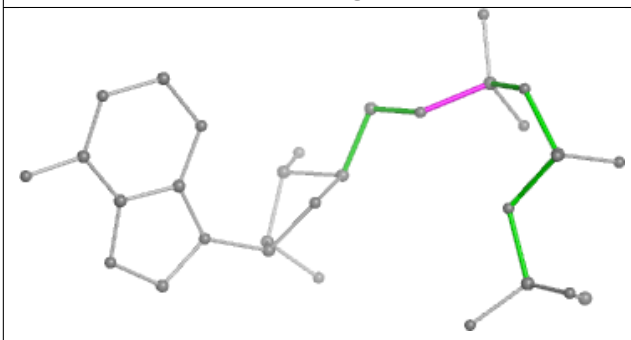
Ligand AGS E 4802



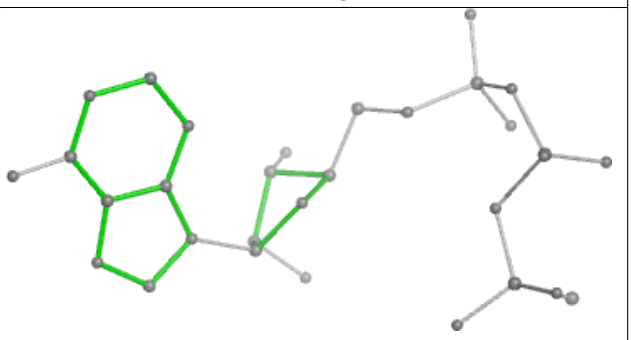
Bond lengths



Bond angles

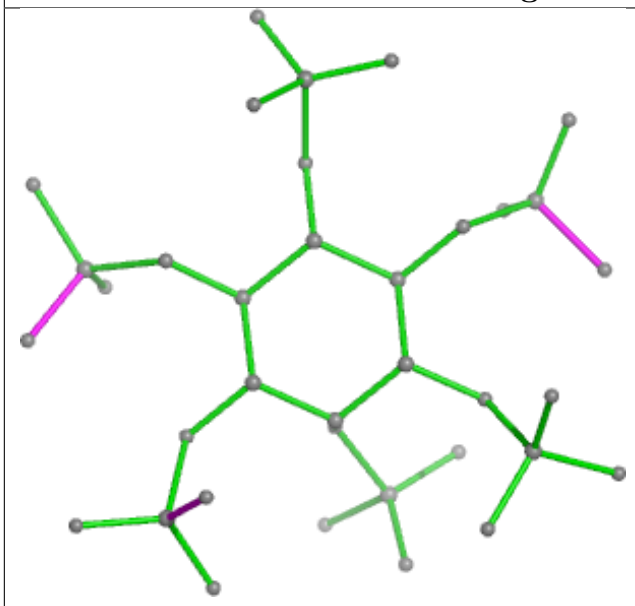


Torsions

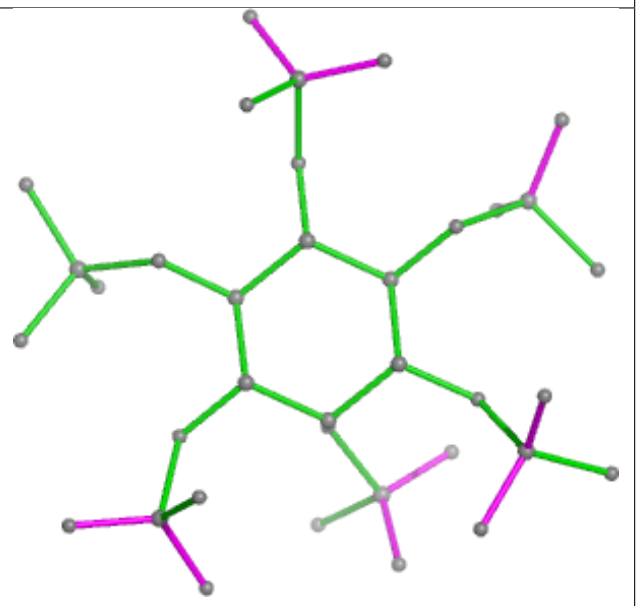


Rings

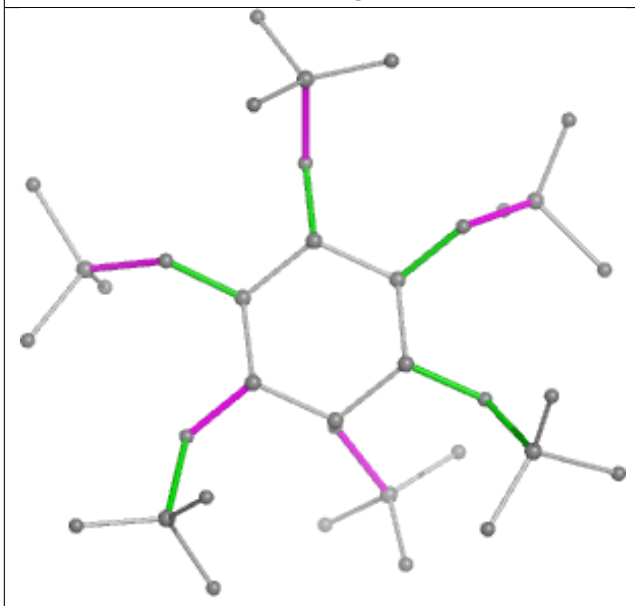
Ligand IHP B 2602



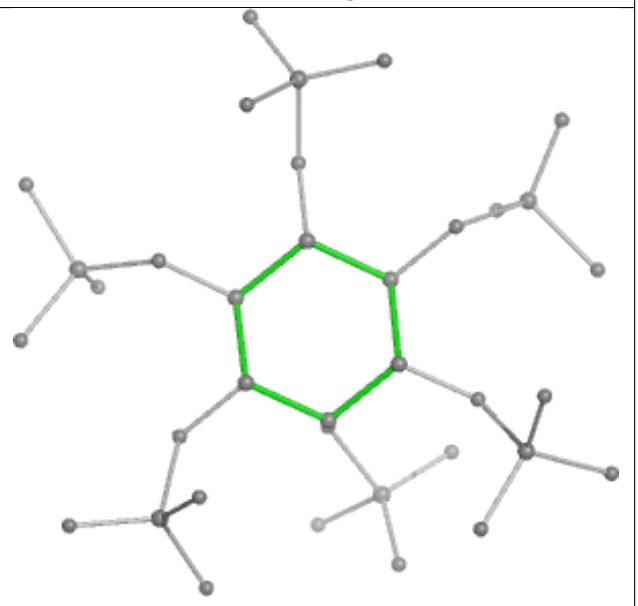
Bond lengths



Bond angles

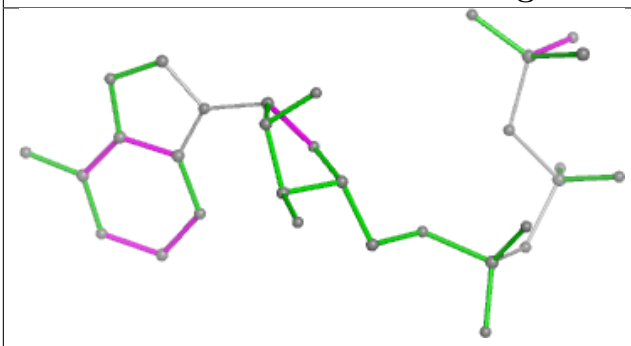


Torsions

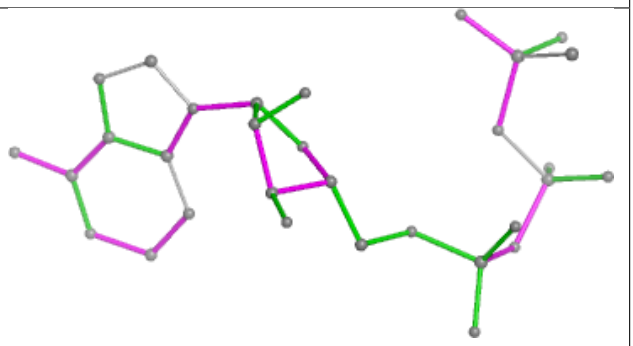


Rings

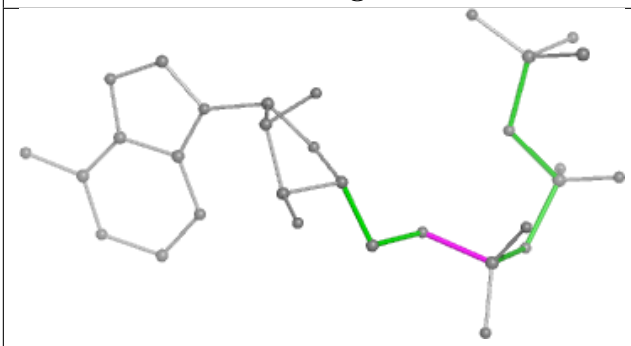
Ligand AGS F 4802



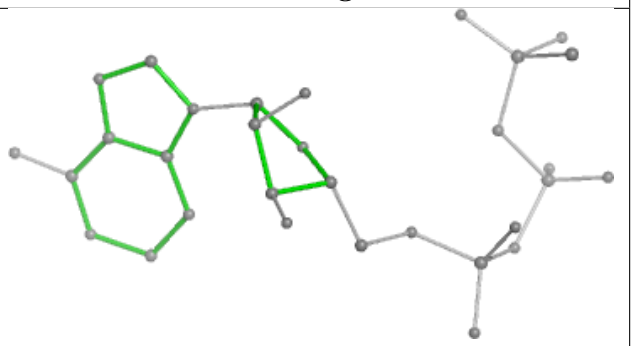
Bond lengths



Bond angles

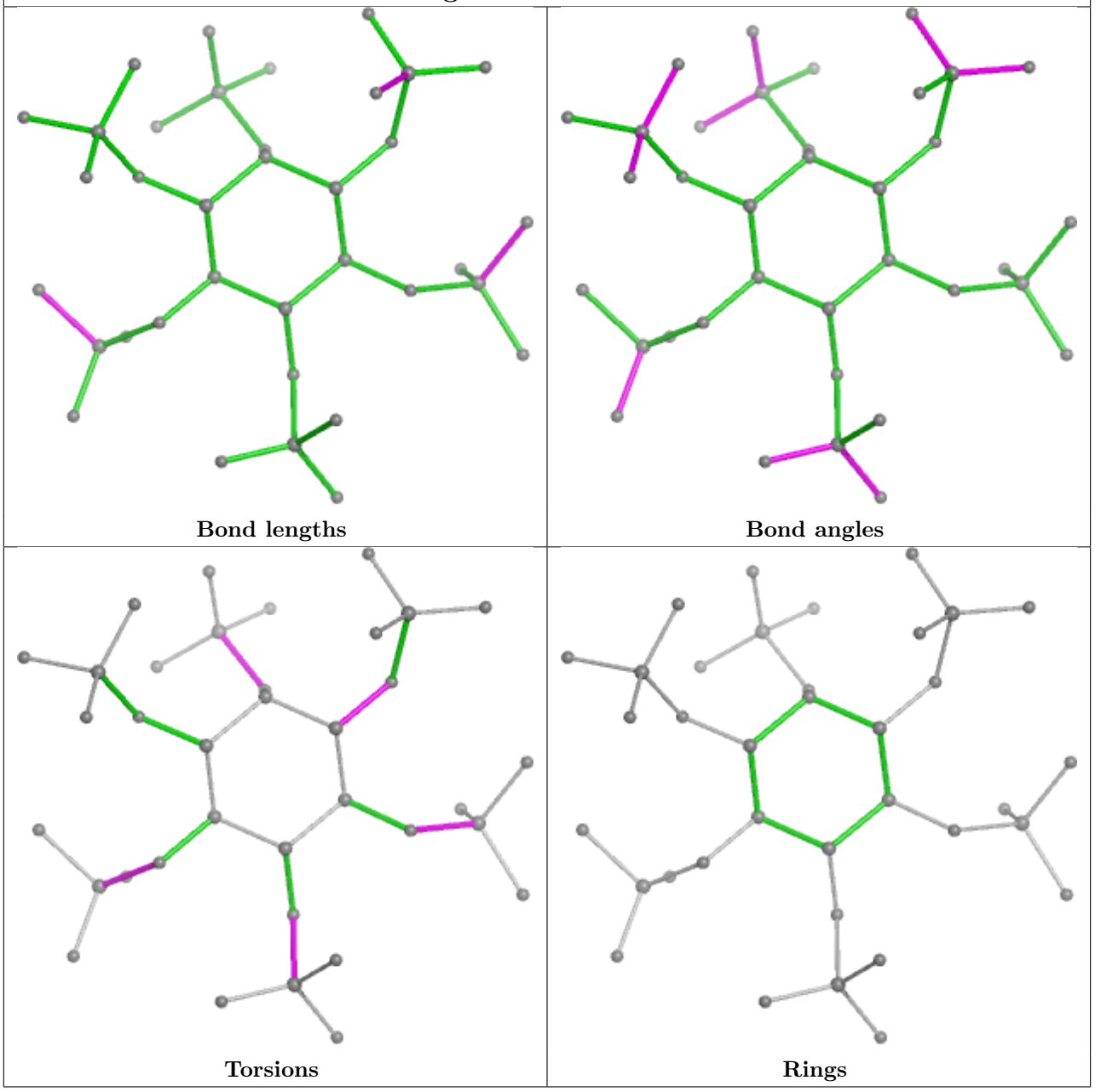


Torsions



Rings

Ligand IHP A 2602



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.

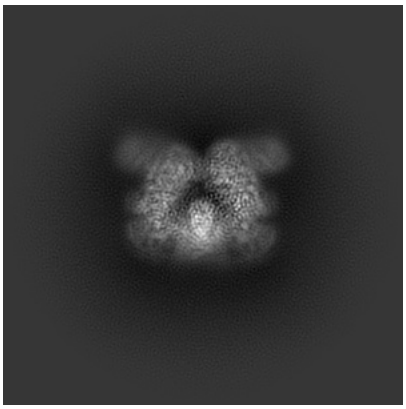
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11488. These allow visual inspection of the internal detail of the map and identification of artifacts.

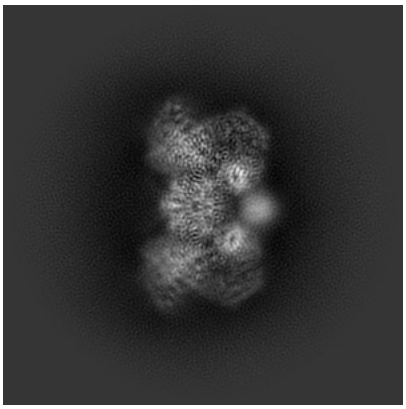
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

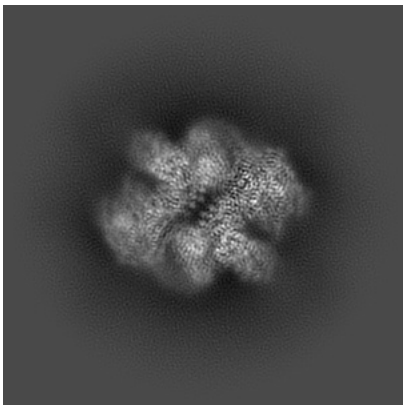
6.1.1 Primary map



X



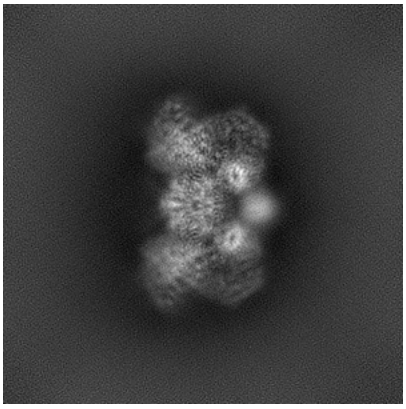
Y



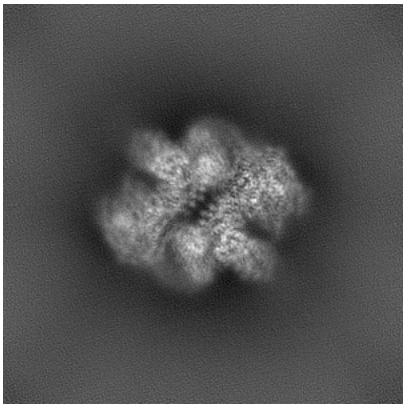
Z

6.1.2 Raw map

X



Y

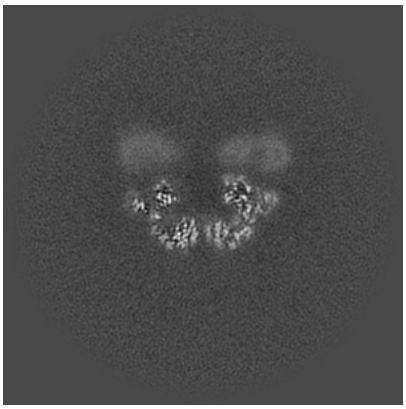


Z

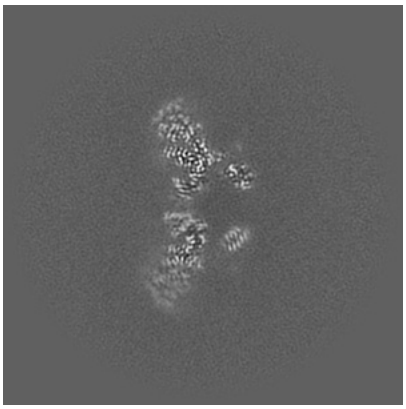
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

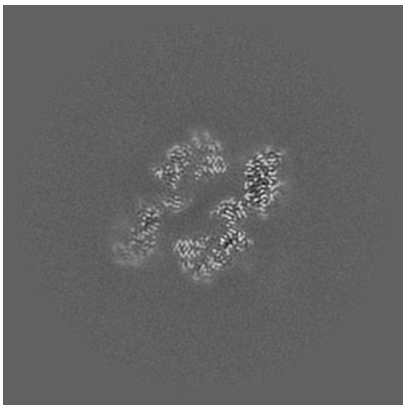
6.2.1 Primary map



X Index: 160

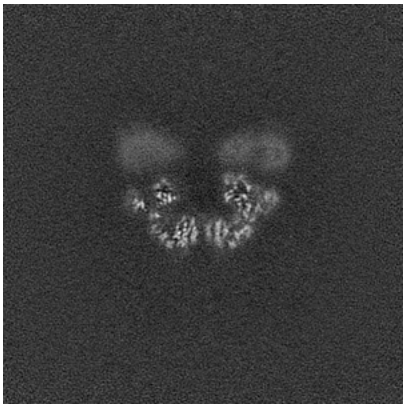


Y Index: 160



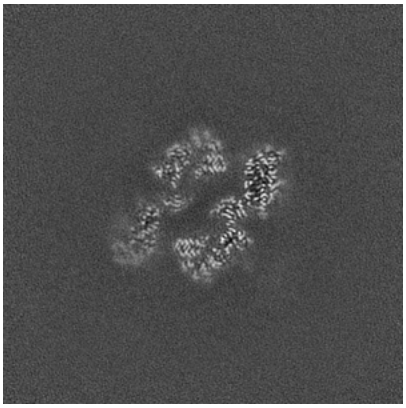
Z Index: 160

6.2.2 Raw map



X Index: 160

Y Index: 160

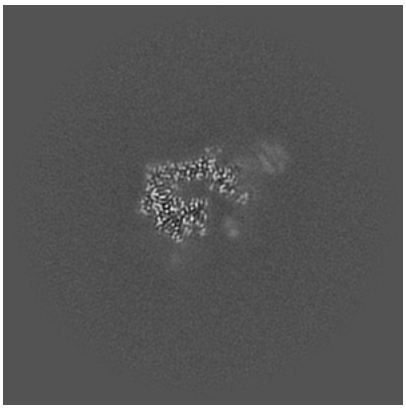


Z Index: 160

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

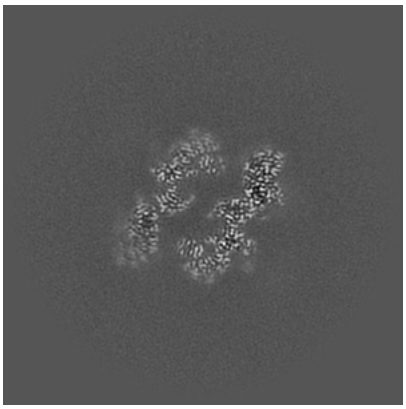
6.3 Largest variance slices (i)

6.3.1 Primary map



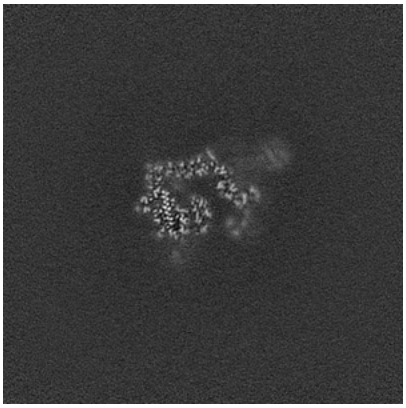
X Index: 179

Y Index: 182

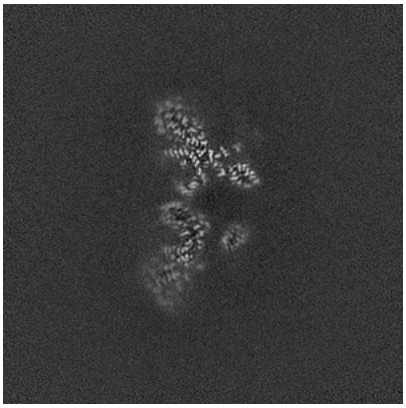


Z Index: 157

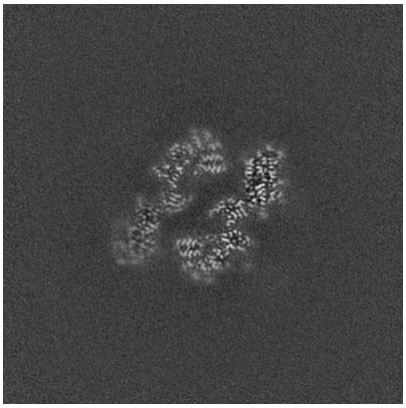
6.3.2 Raw map



X Index: 176



Y Index: 163

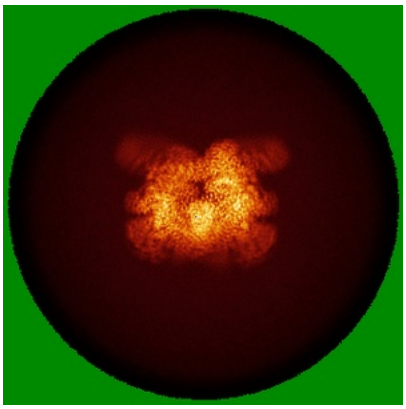


Z Index: 159

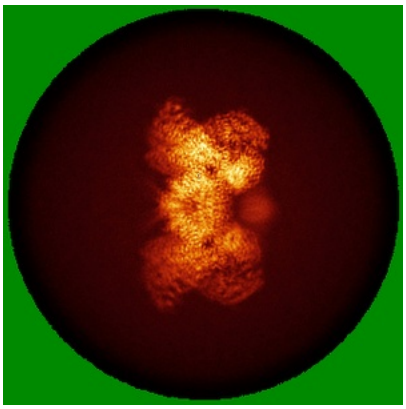
The images above show the largest variance slices of the map in three orthogonal directions.

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

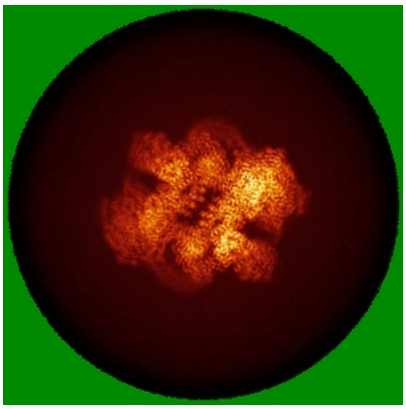
6.4.1 Primary map



X

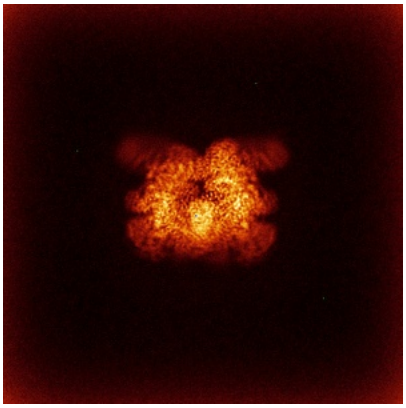


Y

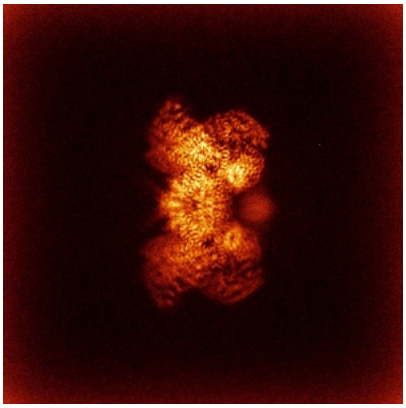


Z

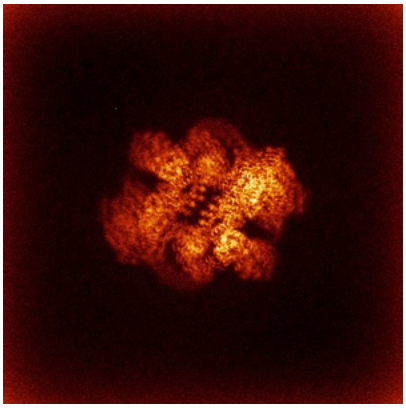
6.4.2 Raw map



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 0.375. 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.

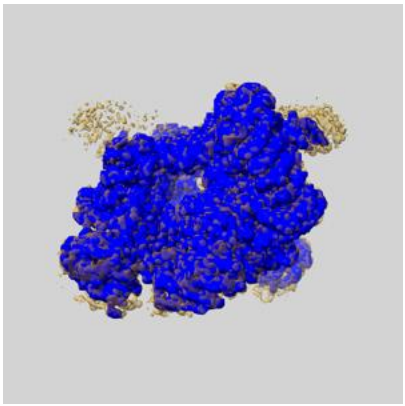
6.6 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

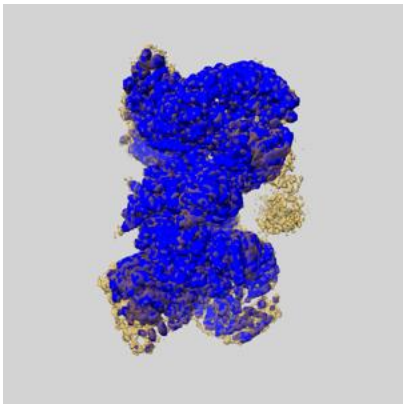
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

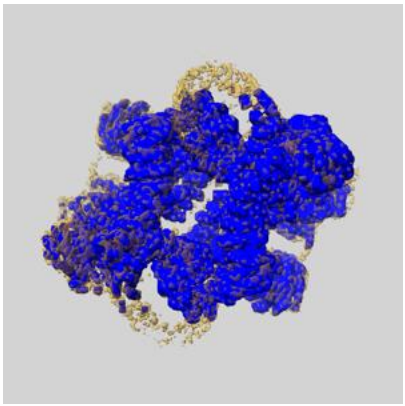
6.6.1 emd_11488_msk_2.map



X

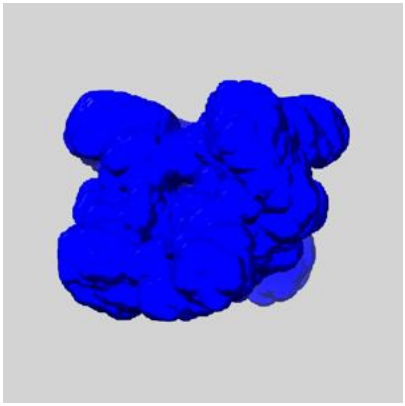


Y

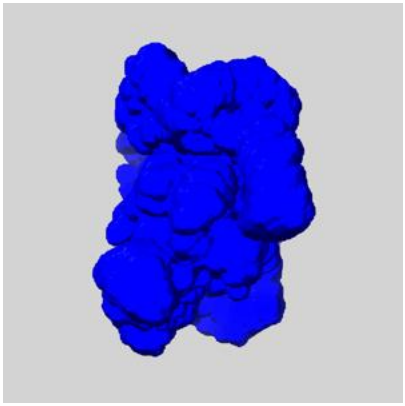


Z

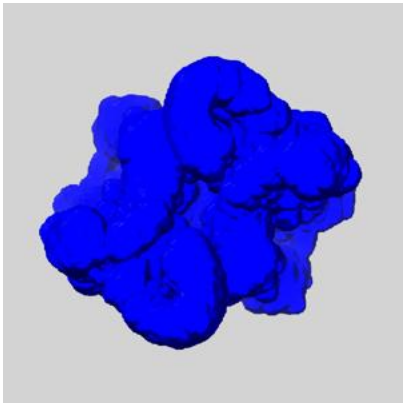
6.6.2 emd_11488_msk_1.map



X



Y

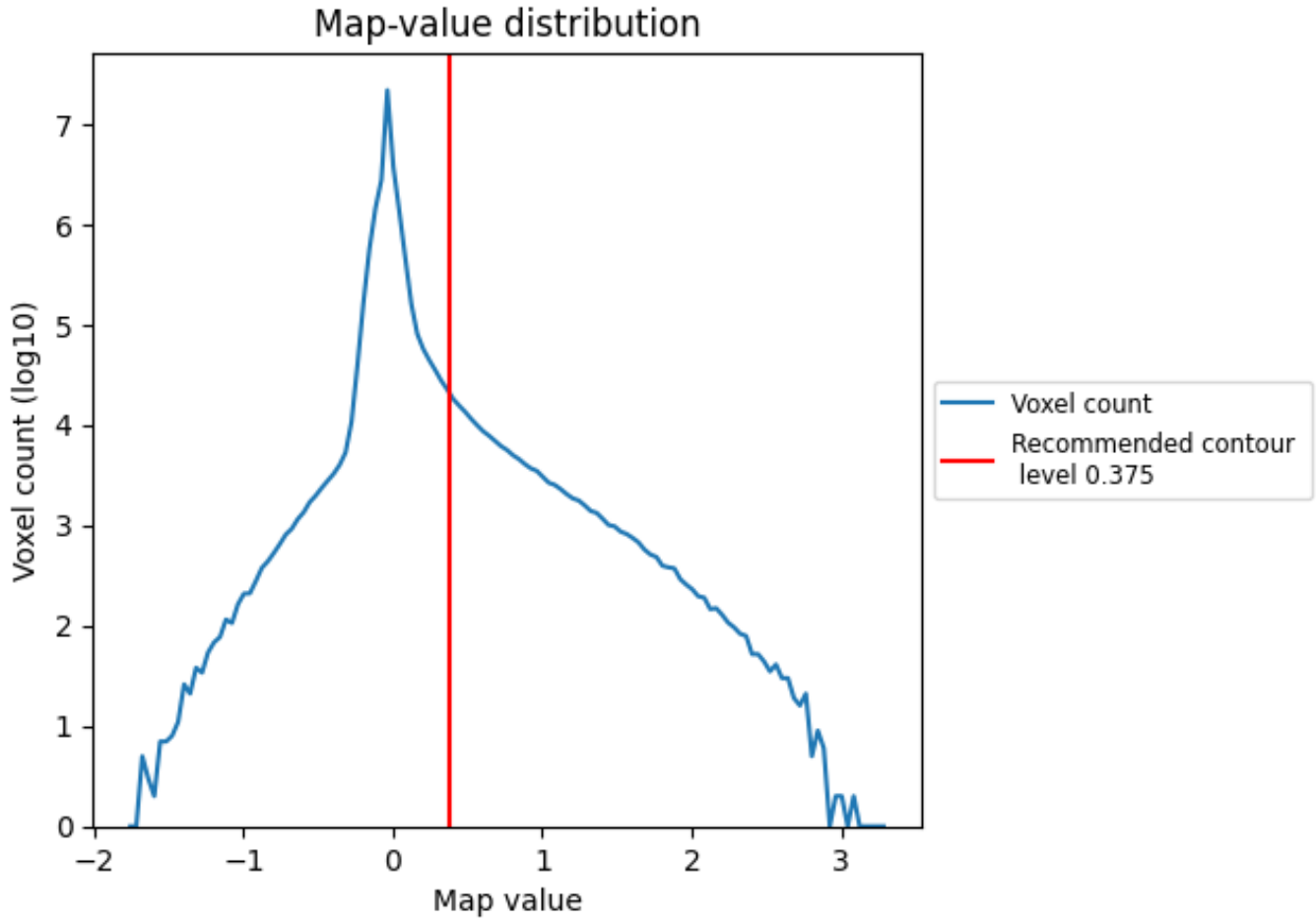


Z

7 Map analysis

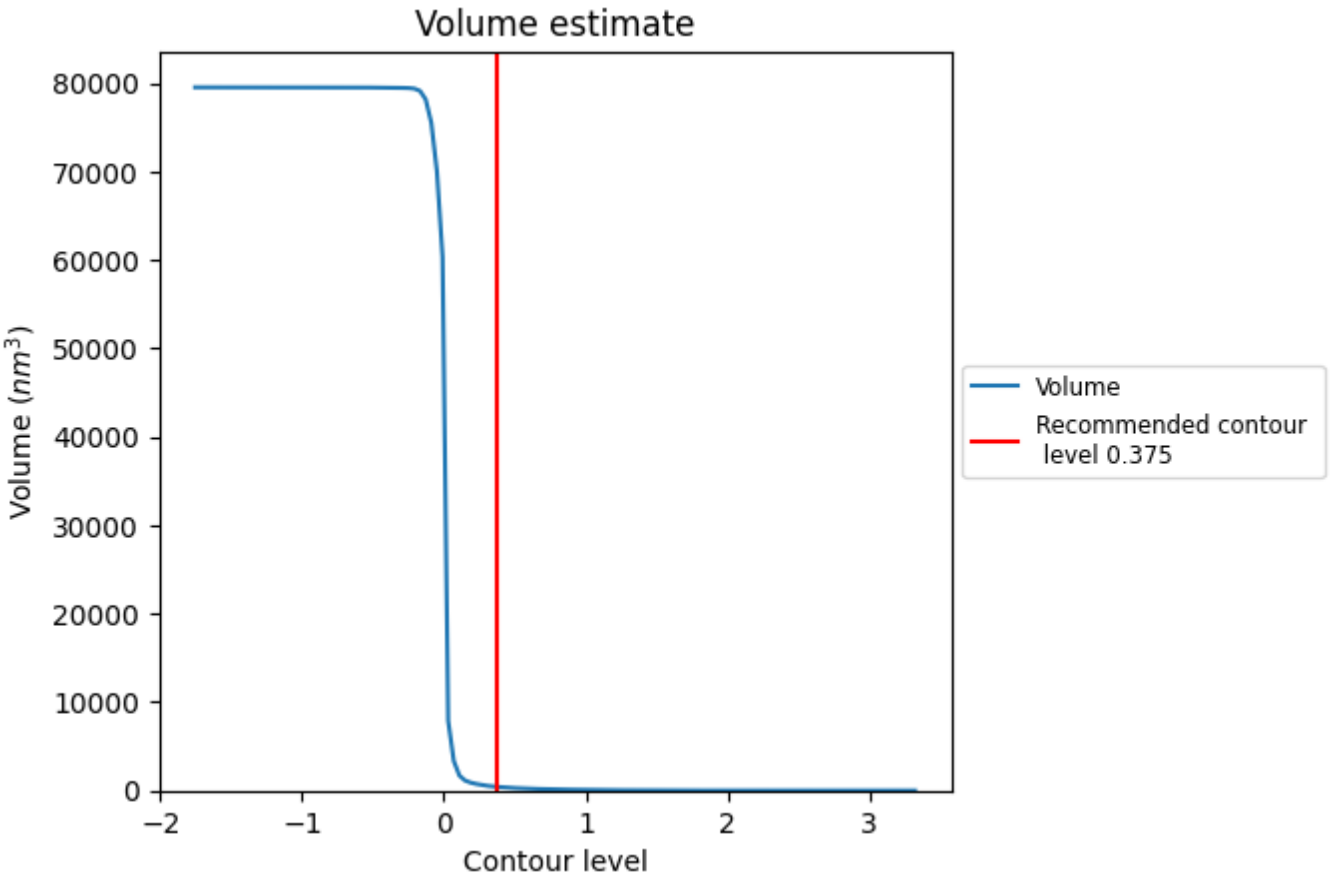
This section contains the results of statistical analysis of the map.

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.

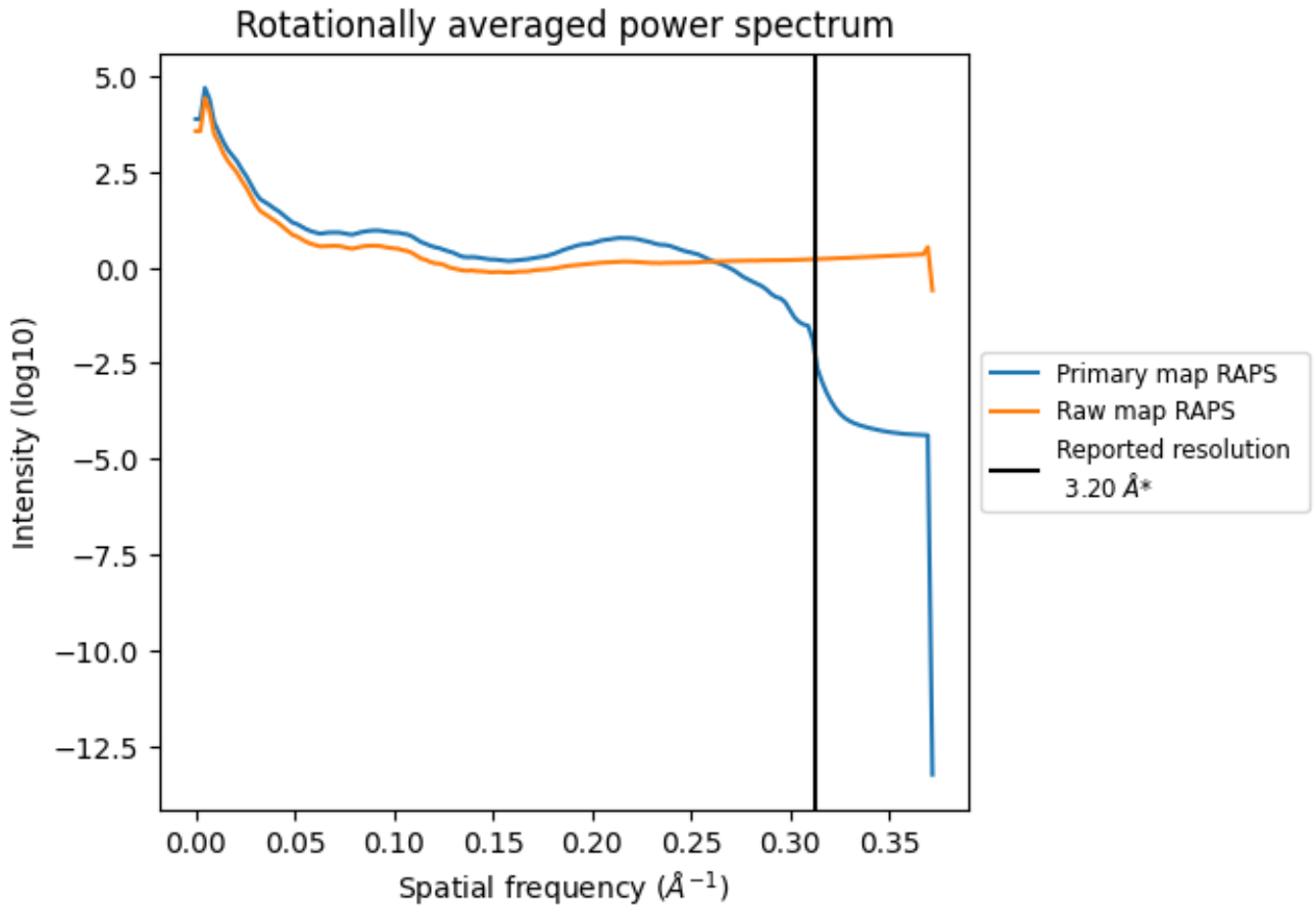
7.2 Volume estimate (i)



The volume at the recommended contour level is 419 nm^3; this corresponds to an approximate mass of 379 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)

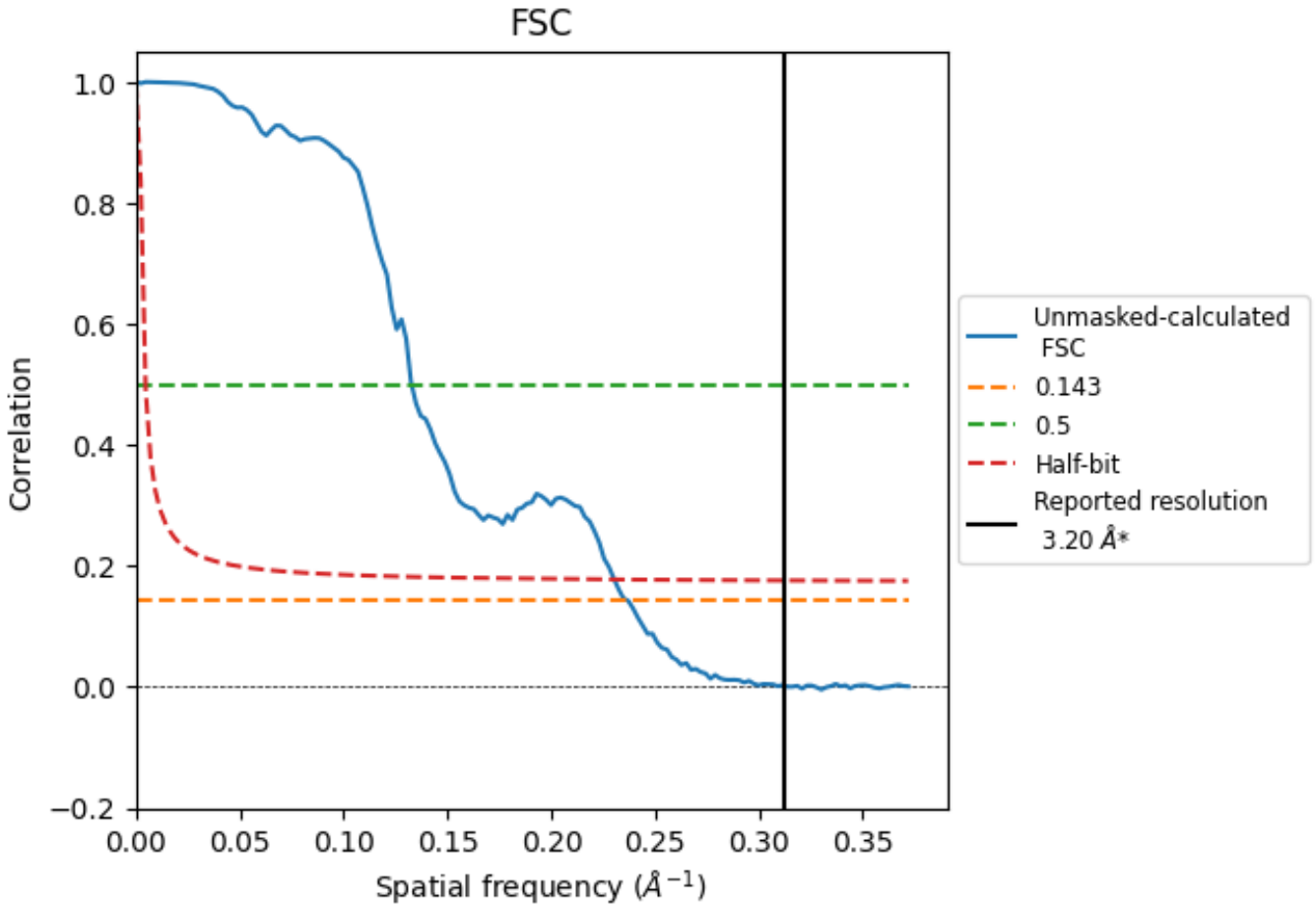


*Reported resolution corresponds to spatial frequency of 0.312 $Å^{-1}$

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 0.312 Å^{-1}

8.2 Resolution estimates (i)

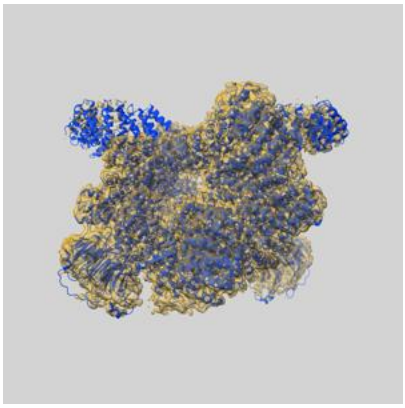
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.22	7.53	4.34

*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 4.22 differs from the reported value 3.2 by more than 10 %

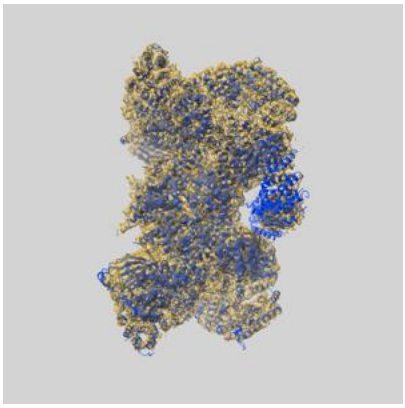
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11488 and PDB model 6ZWM. Per-residue inclusion information can be found in section 3 on page 6.

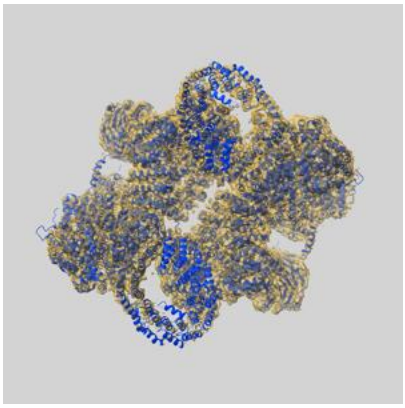
9.1 Map-model overlay



X



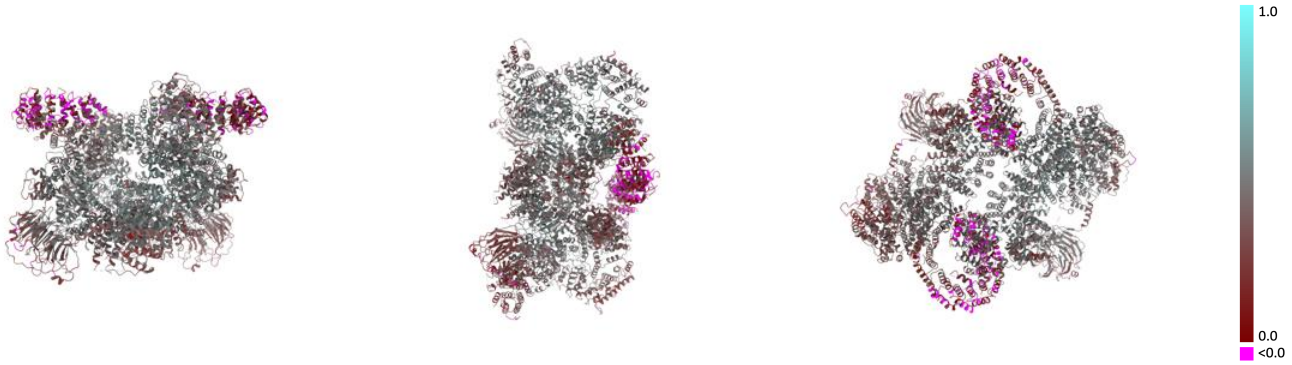
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.375 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

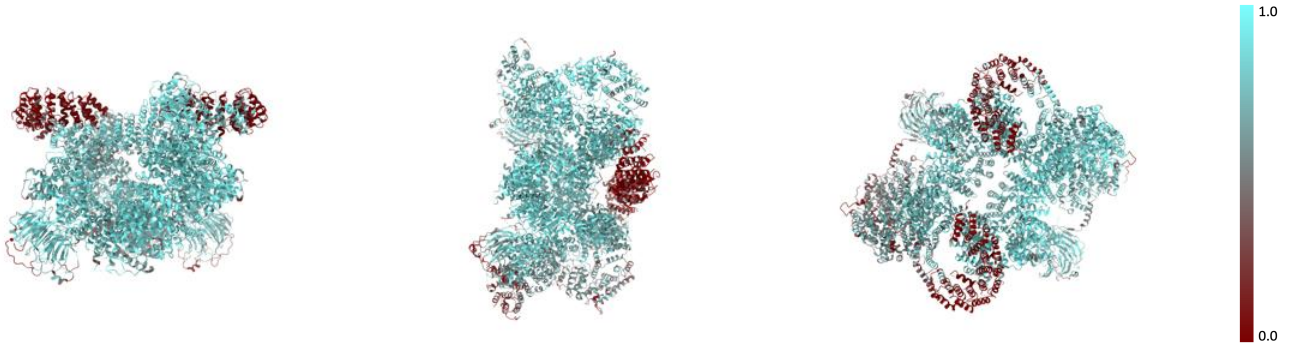
9.2 Q-score mapped to coordinate model



X Y Z

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

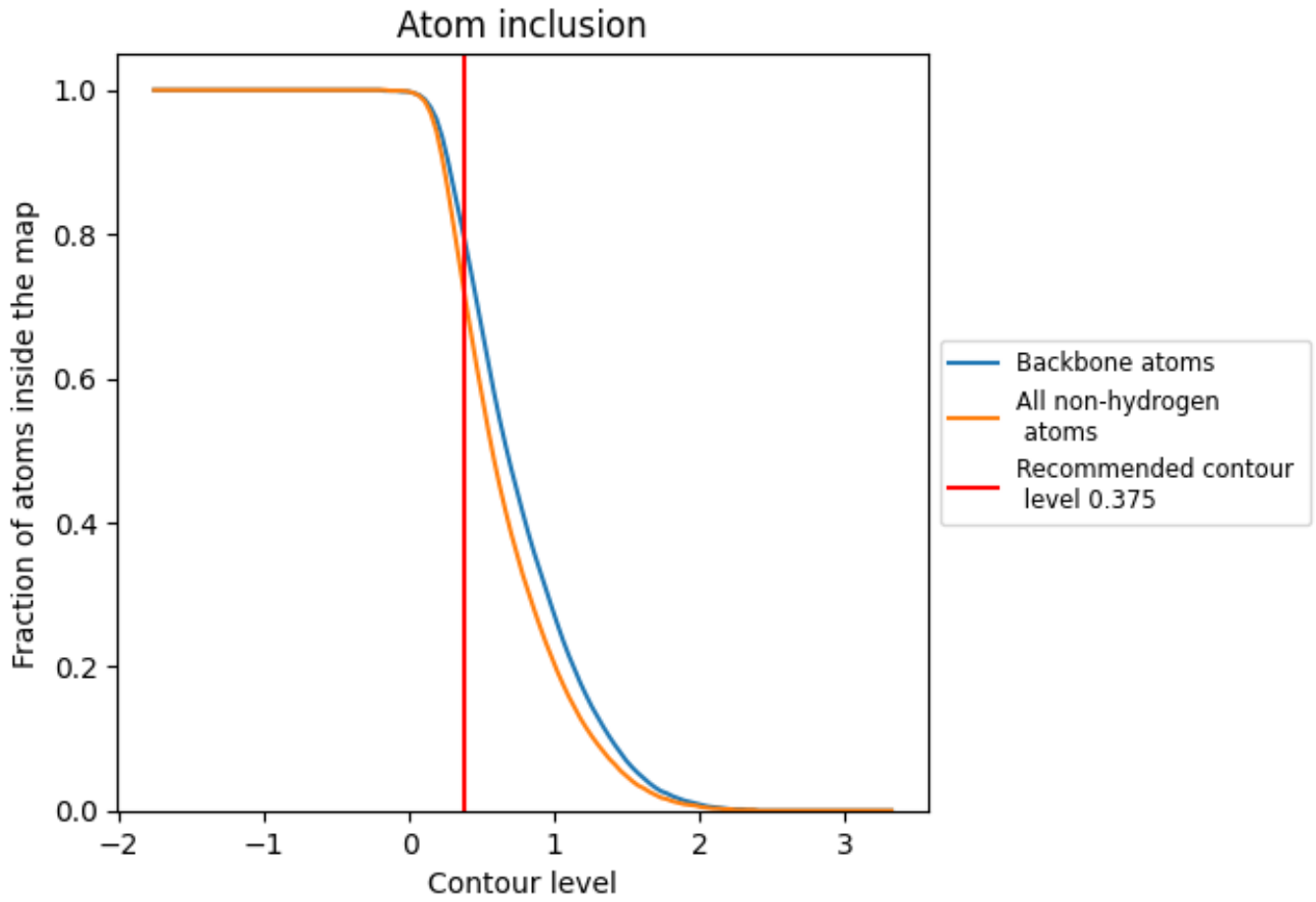
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.375).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 72% 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 (0.375) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7250	0.3960
A	0.7370	0.3860
B	0.7520	0.4130
C	0.6640	0.3020
D	0.7610	0.3740
E	0.5830	0.3580
F	0.8290	0.4600
G	0.4070	0.3060
H	0.6470	0.3700