wwPDB EM Validation Summary Report (i)

Nov 19, 2022 – 03:33 pm GMT

PDB ID	:	5ND2
EMDB ID	:	EMD-3620
Title	:	Microtubule-bound MKLP2 motor domain in the presence of ADP
Authors	:	Atherton, J.; Yu, I.M.; Cook, A.; Muretta, J.M.; Joseph, A.P.; Major, J.; Sourigues, Y.; Clause, J.; Topf, M.; Rosenfeld, S.S.; Houdusse, A.; Moores, C.A.
Deposited on	:	2017-03-07
Resolution	:	5.80 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 (1)) were used in the production of this report:

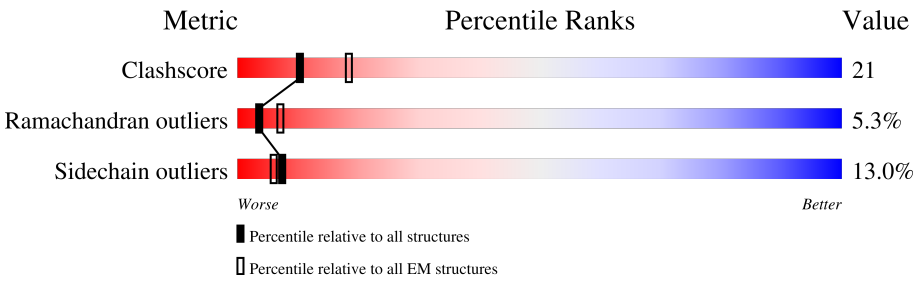
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 5.80 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	1-C	501	22%; 24%, 27%, 5%, 44%
1	2-C	501	24%, 27%, 5%, 44%
1	3-C	501	24%, 28%, 5%, 44%
1	4-C	501	24%, 27%, 5%, 44%
1	5-C	501	25%, 26%, 5%, 44%
2	1-A	451	15%; 52%, 34%, 5%, 9%
2	2-A	451	52%, 34%, 5%, 9%
2	3-A	451	52%, 34%, 5%, 9%

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Mol	Chain	Length	Quality of chain
2	4-A	451	52% 34% 5% 9%
2	5-A	451	52% 34% 5% 9%
3	1-B	445	13% 52% 38% 6% •
3	2-B	445	52% 38% 6% •
3	3-B	445	52% 38% 6% •
3	4-B	445	52% 38% 6% •
3	5-B	445	52% 38% 6% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ADP	1-C	601	-	-	X	-
4	ADP	2-C	601	-	-	X	-
4	ADP	3-C	601	-	-	X	-
4	ADP	4-C	601	-	-	X	-
4	ADP	5-C	601	-	-	X	-
6	GTP	1-A	500	-	-	X	-
6	GTP	2-A	500	-	-	X	-
6	GTP	3-A	500	-	-	X	-
6	GTP	4-A	500	-	-	X	-
6	GTP	5-A	500	-	-	X	-
7	GDP	1-B	600	-	-	X	-
7	GDP	2-B	600	-	-	X	-
7	GDP	3-B	600	-	-	X	-
7	GDP	4-B	600	-	-	X	-
7	GDP	5-B	600	-	-	X	-
8	TA1	1-B	601	-	-	X	-
8	TA1	2-B	601	-	-	X	-
8	TA1	3-B	601	-	-	X	-
8	TA1	4-B	601	-	-	X	-
8	TA1	5-B	601	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 44865 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 Kinesin-like protein KIF20A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1-C	280	2244	1432	391	411	10	0	0
1	2-C	280	2244	1432	391	411	10	0	0
1	3-C	280	2244	1432	391	411	10	0	0
1	4-C	280	2244	1432	391	411	10	0	0
1	5-C	280	2244	1432	391	411	10	0	0

- Molecule 2 is a protein called Tubulin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1-A	412	3227	2043	551	613	20	0	0
2	2-A	412	3227	2043	551	613	20	0	0
2	3-A	412	3227	2043	551	613	20	0	0
2	4-A	412	3227	2043	551	613	20	0	0
2	5-A	412	3227	2043	551	613	20	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	136	SER	LEU	conflict	UNP F2Z4C1
A	265	GLY	ILE	conflict	UNP F2Z4C1
A	358	GLU	GLN	conflict	UNP F2Z4C1

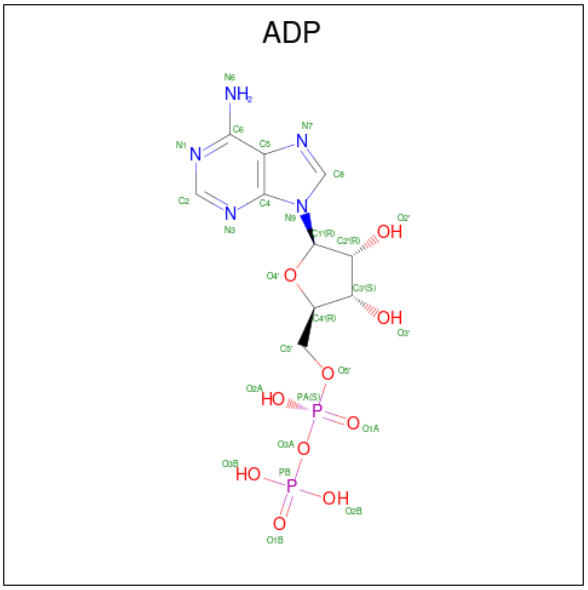
- Molecule 3 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	1-B	426	3351	2105	575	646	25	0	0
3	2-B	426	3351	2105	575	646	25	0	0
3	3-B	426	3351	2105	575	646	25	0	0
3	4-B	426	3351	2105	575	646	25	0	0
3	5-B	426	3351	2105	575	646	25	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	57	ALA	THR	conflict	UNP Q6B856
B	172	VAL	MET	conflict	UNP Q6B856
B	298	ALA	SER	conflict	UNP Q6B856
B	318	VAL	ILE	conflict	UNP Q6B856

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	1-C	1	27	10	5	10	2	0
4	2-C	1	27	10	5	10	2	0

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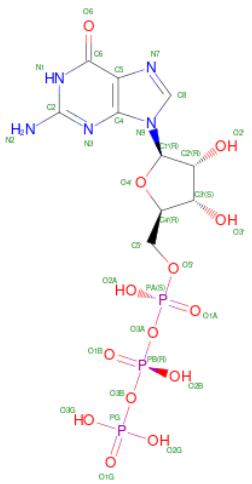
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	3-C	1	27	10	5	10	2	0
			Total	C	N	O	P	
4	4-C	1	27	10	5	10	2	0
			Total	C	N	O	P	
4	5-C	1	27	10	5	10	2	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
5	1-C	1	1	1	0
			Total	Mg	
5	2-C	1	1	1	0
			Total	Mg	
5	3-C	1	1	1	0
			Total	Mg	
5	4-C	1	1	1	0
			Total	Mg	
5	5-C	1	1	1	0
			Total	Mg	
5	1-A	1	1	1	0
			Total	Mg	
5	2-A	1	1	1	0
			Total	Mg	
5	3-A	1	1	1	0
			Total	Mg	
5	4-A	1	1	1	0
			Total	Mg	
5	5-A	1	1	1	0

- Molecule 6 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

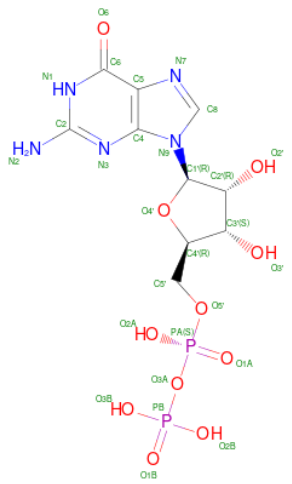
GTP



Mol	Chain	Residues	Atoms					AltConf
6	1-A	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	2-A	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	3-A	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	4-A	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	5-A	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 7 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

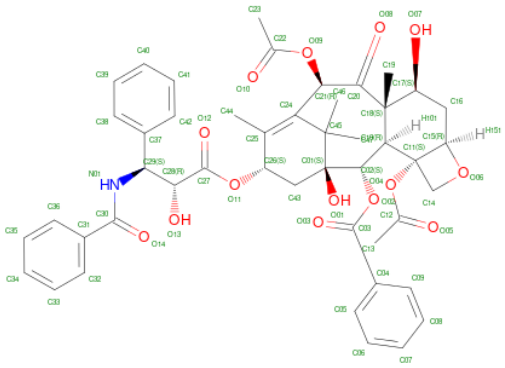
GDP



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
7	1-B	1	28	10	5	11	2	0
7	2-B	1	28	10	5	11	2	0
7	3-B	1	28	10	5	11	2	0
7	4-B	1	28	10	5	11	2	0
7	5-B	1	28	10	5	11	2	0

- Molecule 8 is TAXOL (three-letter code: TA1) (formula: $C_{47}H_{51}NO_{14}$).

TA1



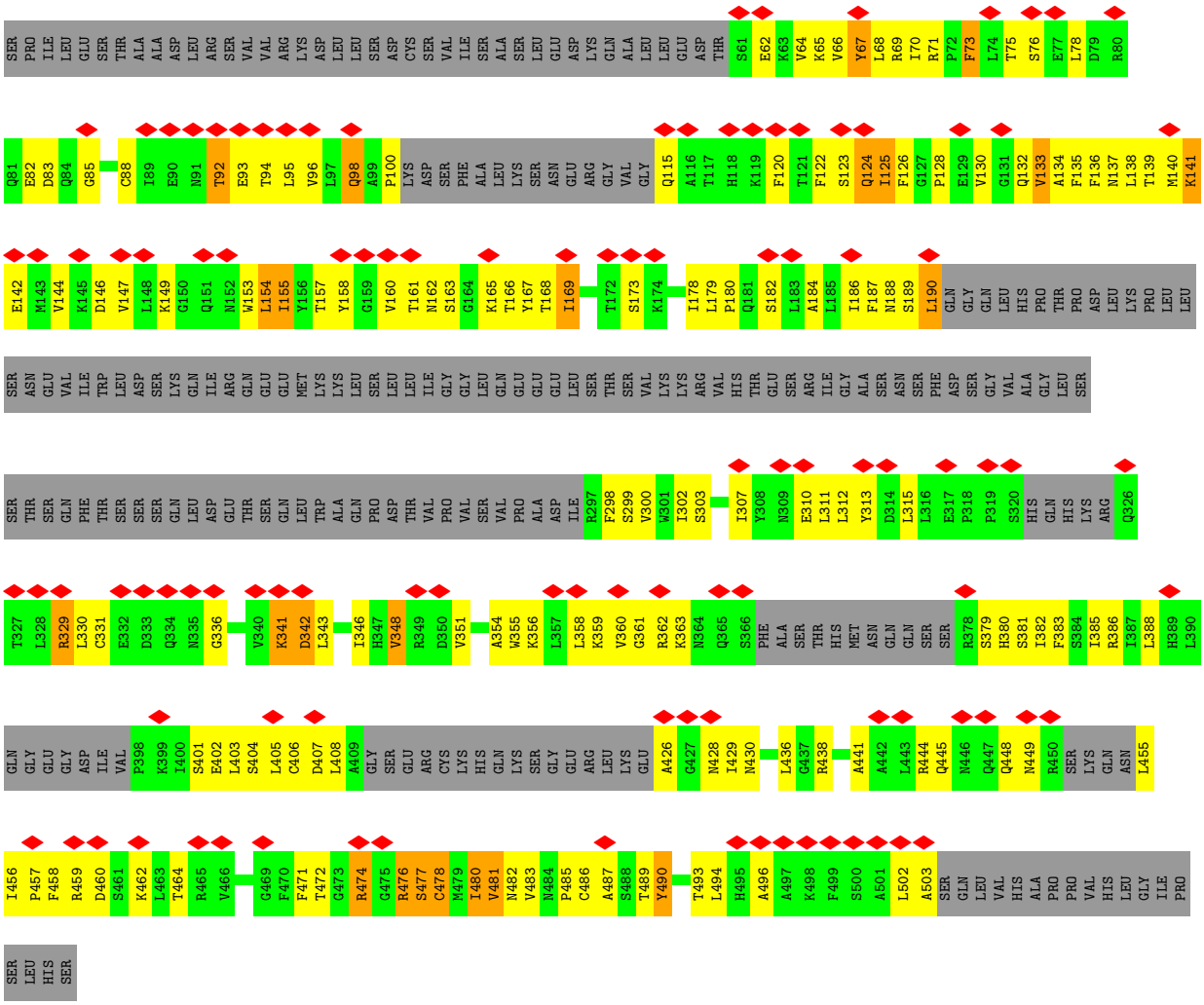
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
8	1-B	1	62	47	1	14	0
8	2-B	1	62	47	1	14	0
8	3-B	1	62	47	1	14	0
8	4-B	1	62	47	1	14	0
8	5-B	1	62	47	1	14	0

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.

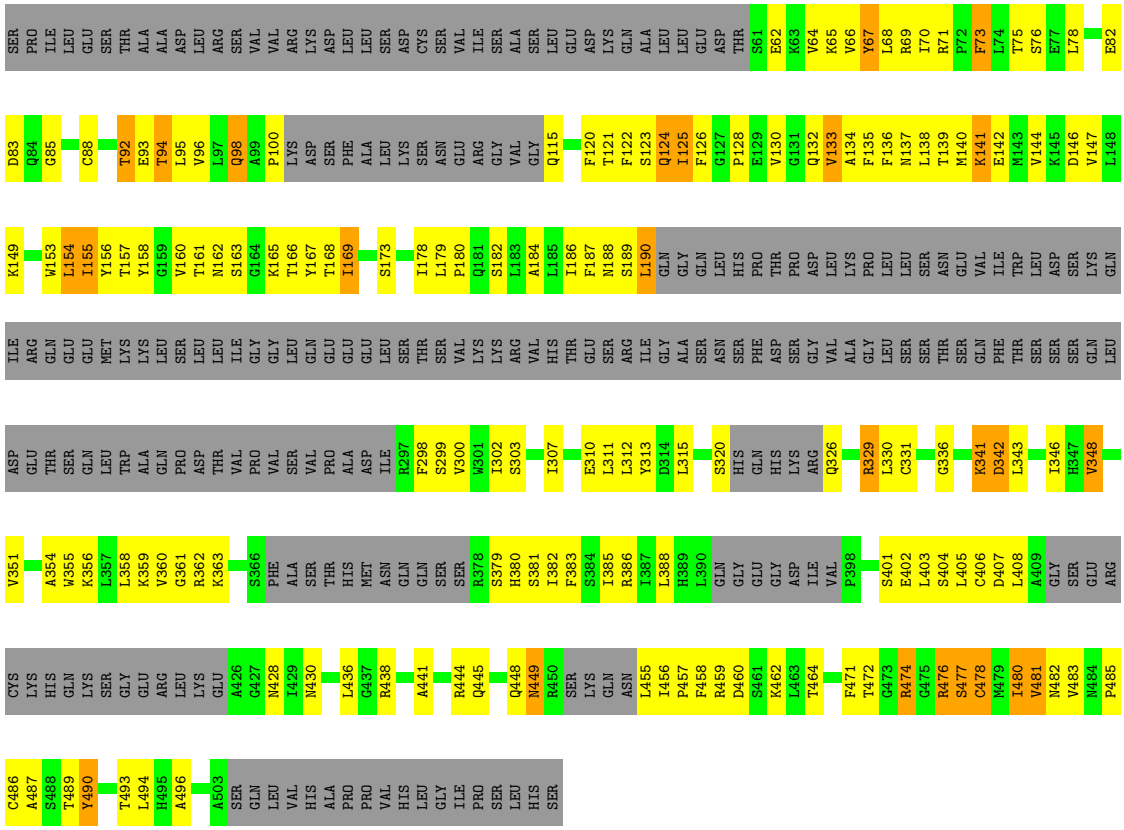
• Molecule 1: Kinesin-like protein KIF20A

Chain 1-C: 22% 24% 27% 5% 44%



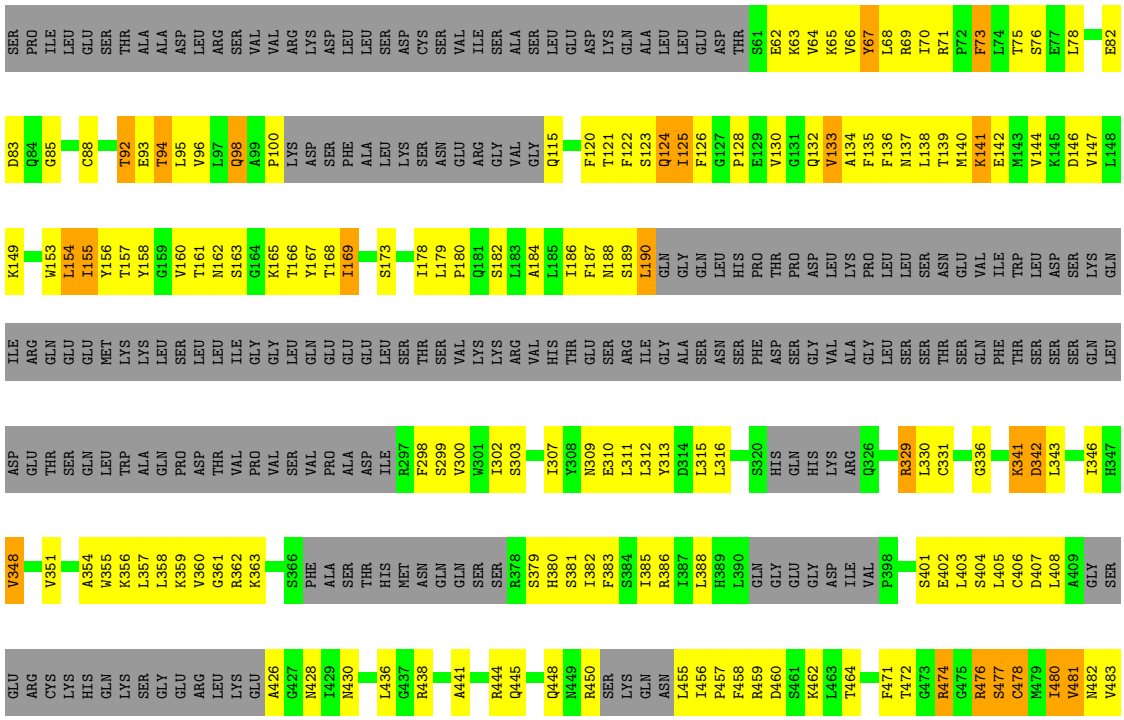
• Molecule 1: Kinesin-like protein KIF20A

Chain 2-C: 24% 27% 5% 44%



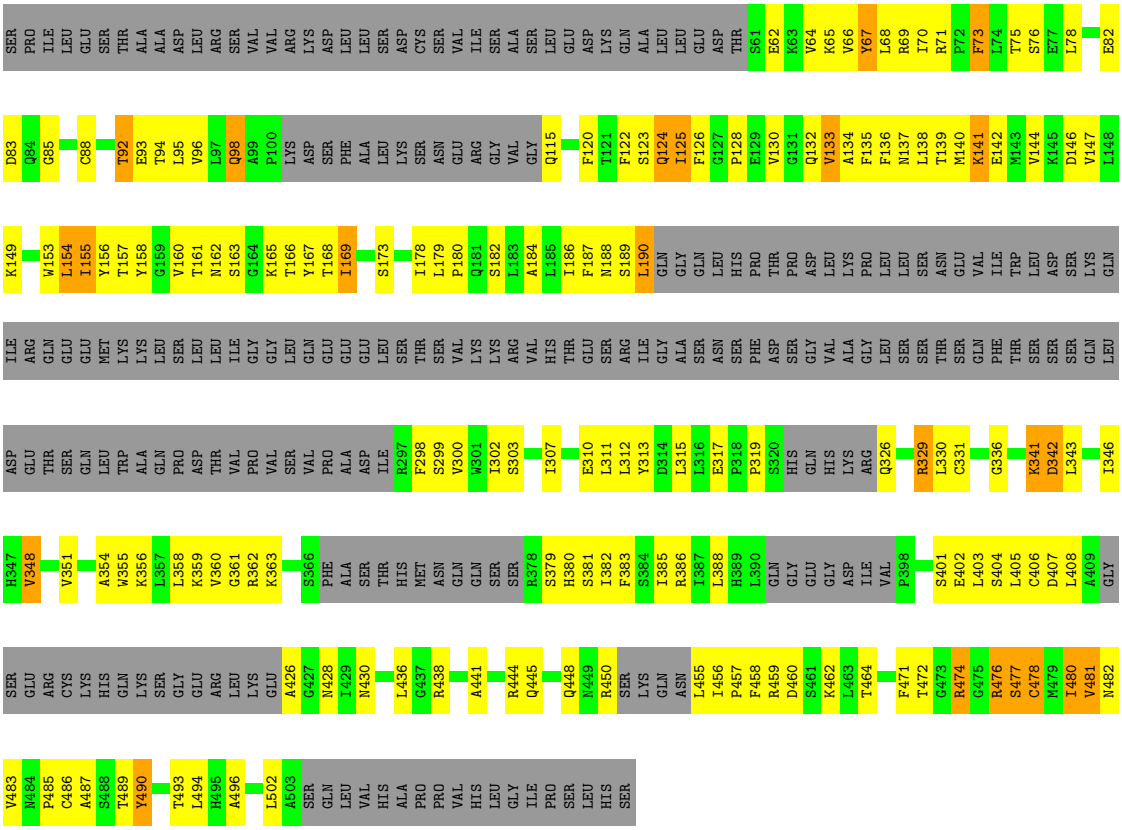
- Molecule 1: Kinesin-like protein KIF20A

Chain 3-C: 24% 28% 5% 44%



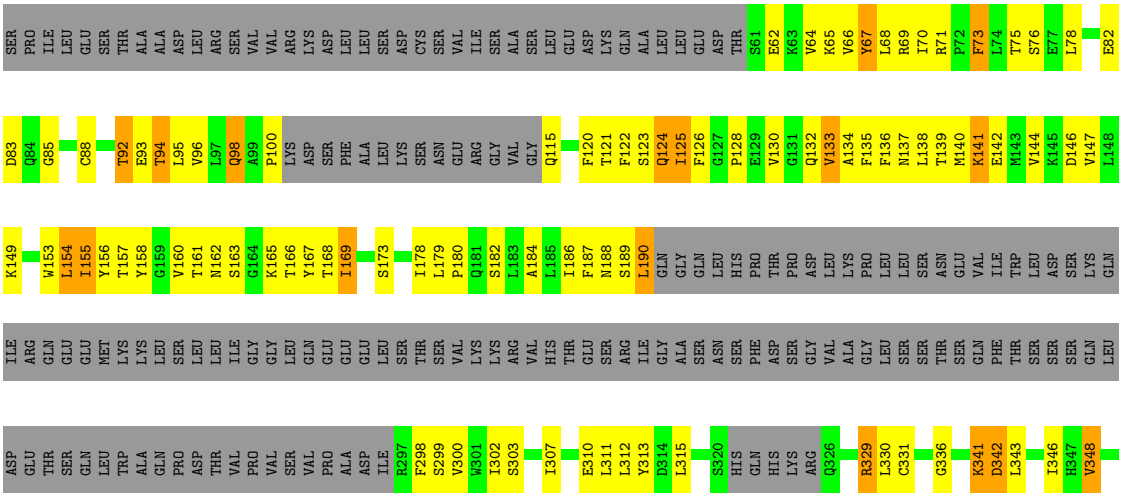
- Molecule 1: Kinesin-like protein KIF20A

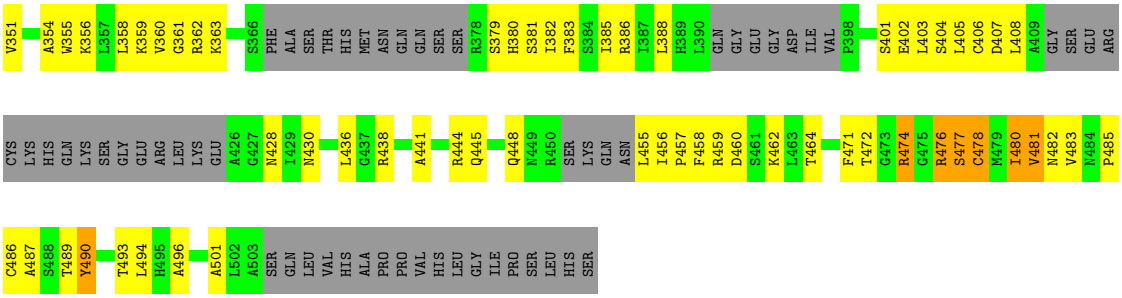
Chain 4-C: 24% 27% 5% 44%



- Molecule 1: Kinesin-like protein KIF20A

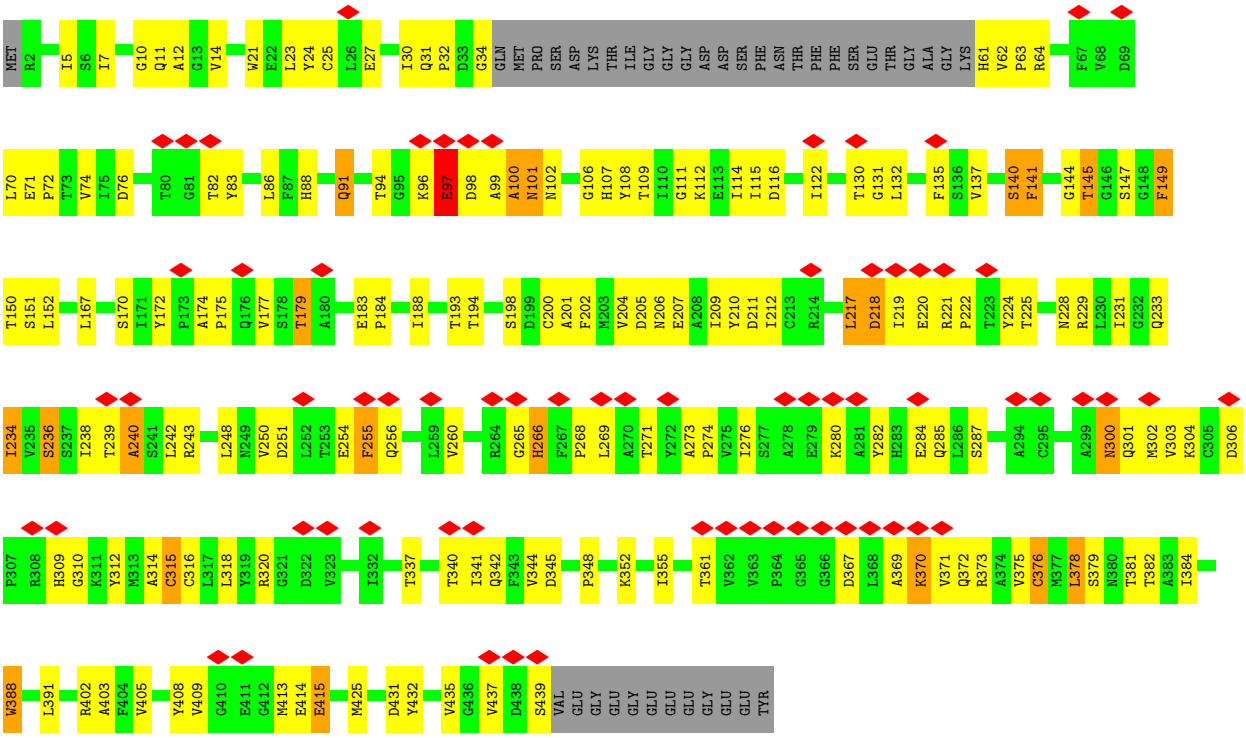
Chain 5-C: 25% 26% 5% 44%





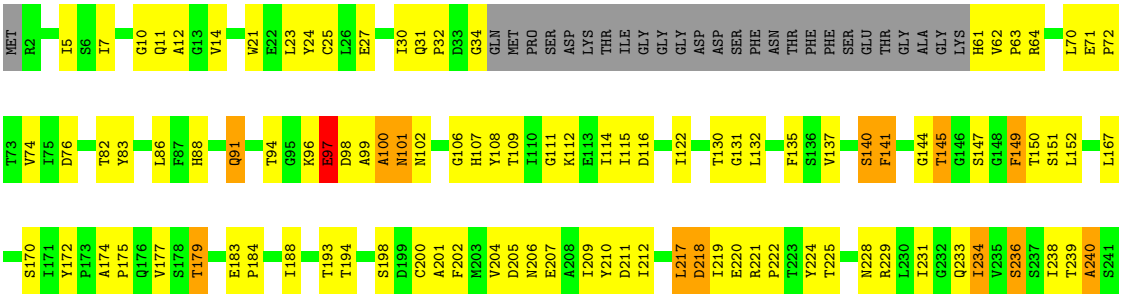
- Molecule 2: Tubulin alpha chain

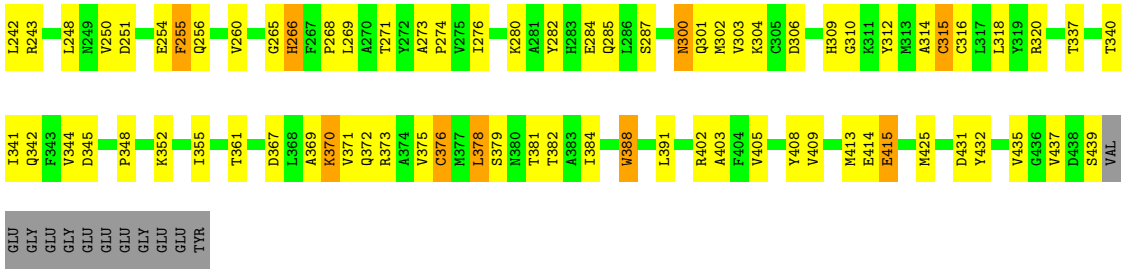
Chain 1-A:



- Molecule 2: Tubulin alpha chain

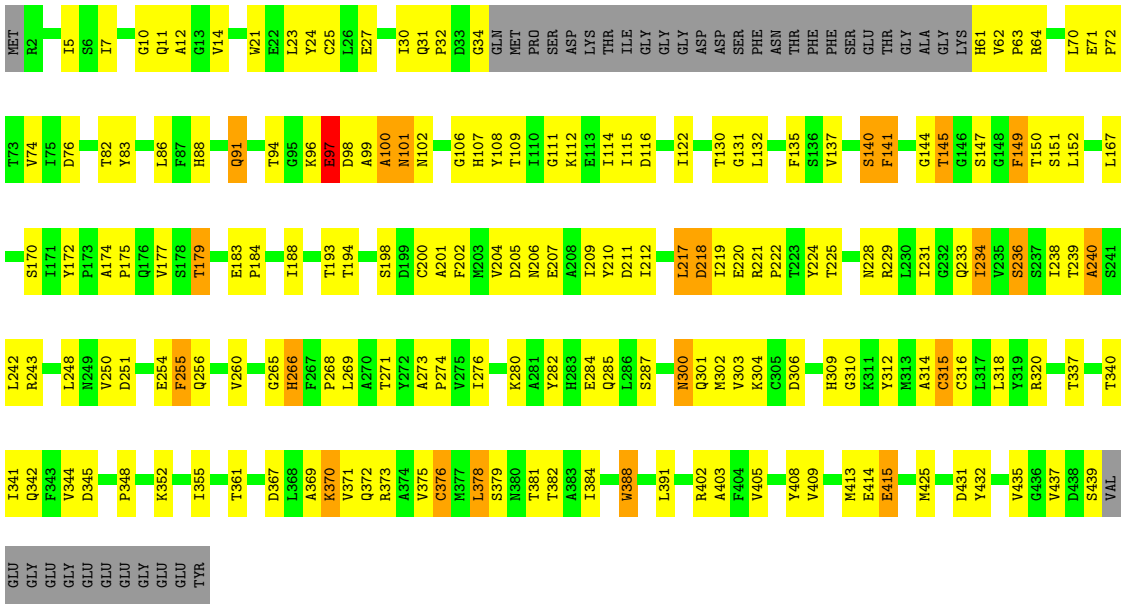
Chain 2-A:





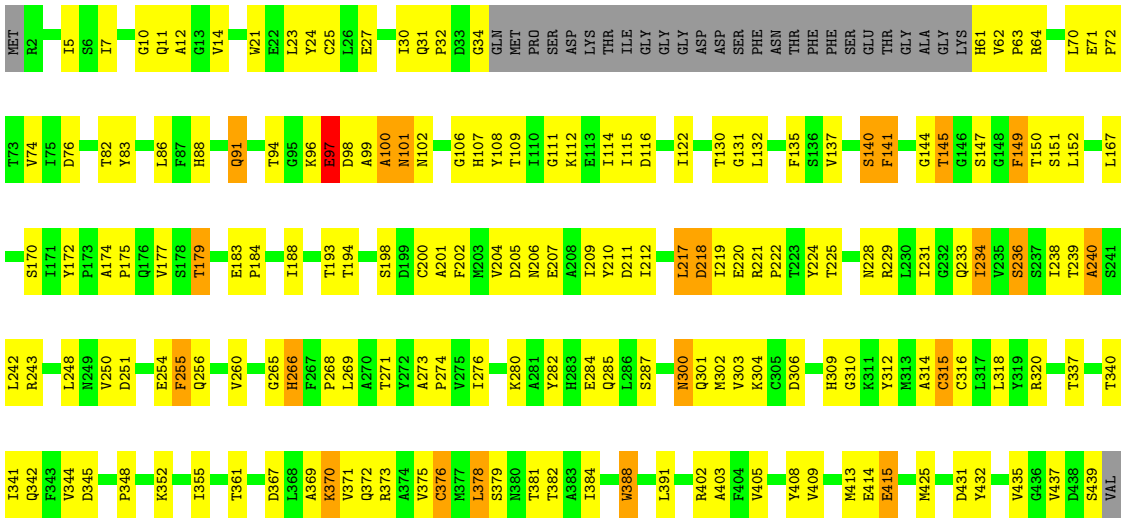
- Molecule 2: Tubulin alpha chain

Chain 3-A:



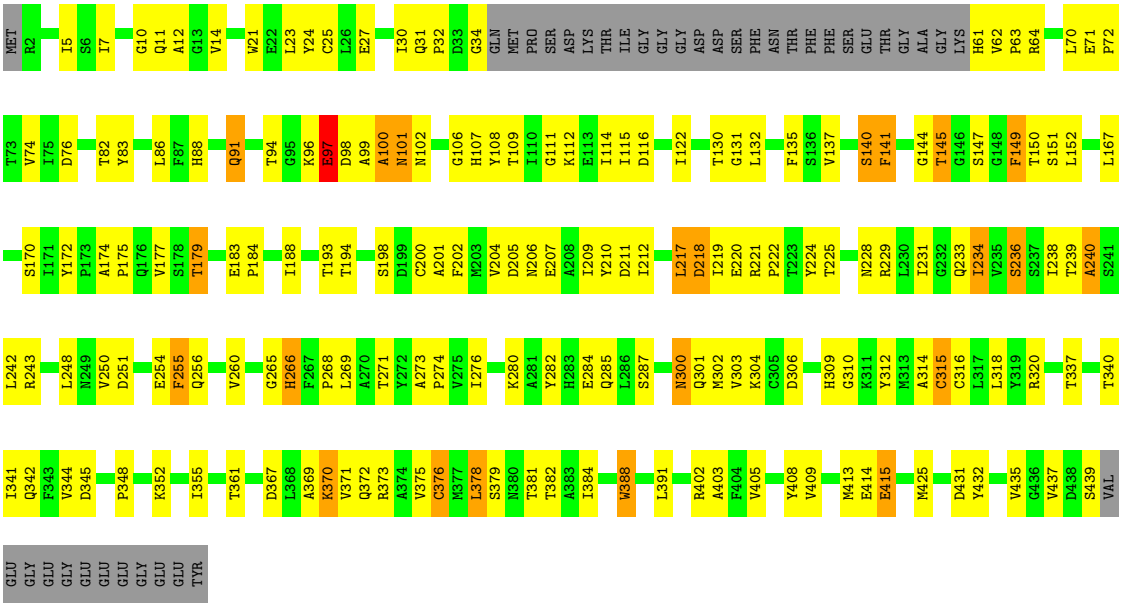
- Molecule 2: Tubulin alpha chain

Chain 4-A:



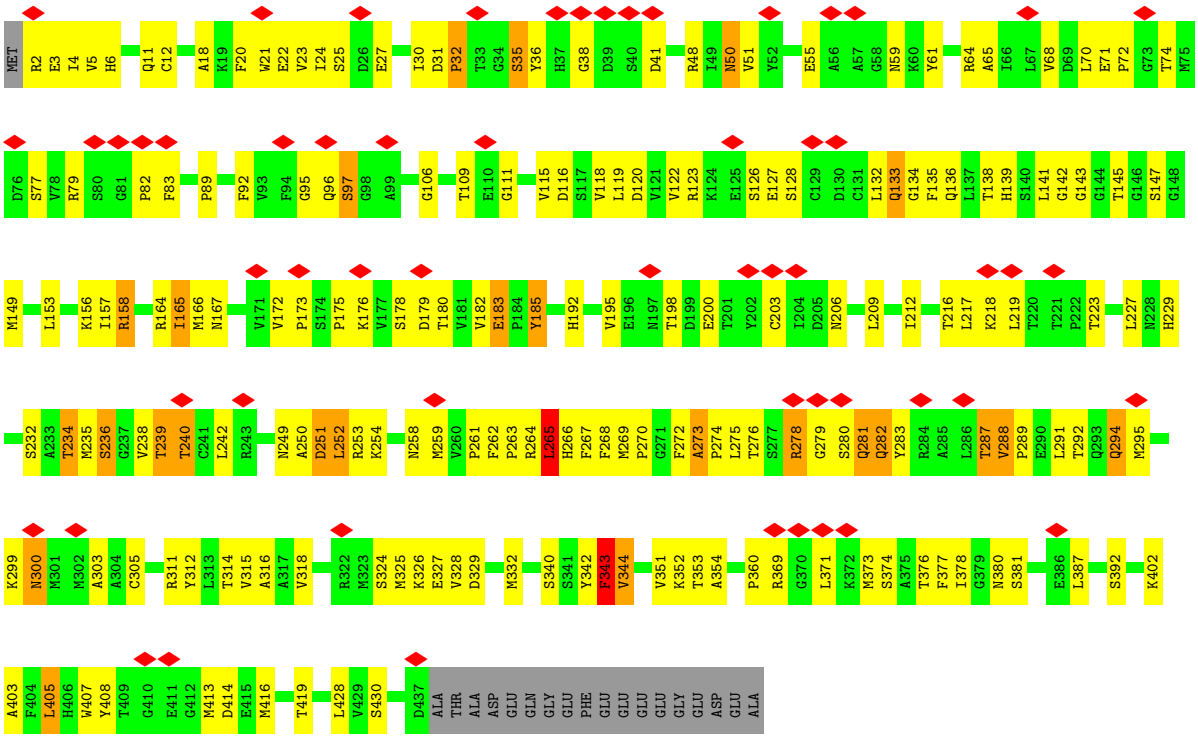
- Molecule 2: Tubulin alpha chain

Chain 5-A:



- Molecule 3: Tubulin beta-2B chain

Chain 1-B:



- Molecule 3: Tubulin beta-2B chain

Chain 2-B: 52% 38% 6% •

MET R2 E3 I4 V5 H6 Q11 C12 A18 K19 F20 W21 E22 V23 I24 S25 D26 E27 I30 D31 P32 S35 Y36 H37 G38 D41 R48 I49 N50 V51 E55 N59 K60 Y61 R64 A65 V68 D69 L70 E71 P72 G73 T74 S77 V78 R79 P82 F83

P89 F92 G95 Q96 S97 G106 T109 E110 G111 V115 D116 S117 V118 L119 D120 V121 V122 R123 S126 E127 S128 L132 Q133 G134 F135 Q136 L137 T138 H139 S140 L141 G142 G143 G144 T145 G146 S147 G148 M149 L153 K156 I157 R158 R164 I165 M166 N167 V172

P173 S174 P175 K176 V177 S178 D179 T180 V181 V182 E183 P184 Y185 H192 V195 T198 D199 E200 C203 N206 L209 I212 T216 L217 K218 L219 T223 L227 N228 H229 S232 A233 T234 M235 S236 G237 V238 T239 T240 C241 L242 N249 A250 D251 L252 R253 K254

N258 M259 V260 P261 F262 P263 R264 L265 H266 F267 F268 M269 P270 G271 F272 A273 P274 L275 T276 S277 R278 G279 S280 Q281 Q282 Y283 T287 V288 P289 E290 L291 T292 Q293 Q294 M295 K299 N300 A303 A304 C305 R311 Y312 L313 T314 V315 A316 A317 V318 S324 M325 K326 E327 V328 D329

M332 S340 S341 Y342 F343 V344 V351 K352 T353 A354 P360 R369 G370 L371 K372 M373 S374 A375 T376 F377 I378 G379 N380 S381 L387 S392 K402 A403 F404 L405 H406 W407 Y408 M413 D414 E415 M416 T419 L428 V429 S430 D437 ALA THR ALA ASP GLU GLN GLY GLU

PHE GLU GLU GLU GLU GLY GLU ASP GLU ALA

- Molecule 3: Tubulin beta-2B chain

Chain 3-B: 52% 38% 6% •

MET R2 E3 I4 V5 H6 Q11 C12 A18 K19 F20 W21 E22 V23 I24 S25 D26 E27 I30 D31 P32 S35 Y36 H37 G38 D41 R48 I49 N50 V51 E55 N59 K60 Y61 R64 A65 V68 D69 L70 E71 P72 G73 T74 S77 V78 R79 P82 F83

P89 F92 G95 Q96 S97 G106 T109 E110 G111 V115 D116 S117 V118 L119 D120 V121 V122 R123 S126 E127 S128 L132 Q133 G134 F135 Q136 L137 T138 H139 S140 L141 G142 G143 G144 T145 G146 S147 G148 M149 L153 K156 I157 R158 R164 I165 M166 N167 V172

P173 S174 P175 K176 V177 S178 D179 T180 V181 V182 E183 P184 Y185 H192 V195 T198 D199 E200 C203 N206 L209 I212 T216 L217 K218 L219 T223 L227 N228 H229 S232 A233 T234 M235 S236 G237 V238 T239 T240 C241 L242 N249 A250 D251 L252 R253 K254

N258 M259 V260 P261 F262 P263 R264 L265 H266 F267 F268 M269 P270 G271 F272 A273 P274 L275 T276 S277 R278 G279 S280 Q281 Q282 Y283 T287 V288 P289 E290 L291 T292 Q293 Q294 M295 K299 N300 A303 A304 C305 R311 Y312 L313 T314 V315 A316 A317 V318 S324 M325 K326 E327 V328 D329

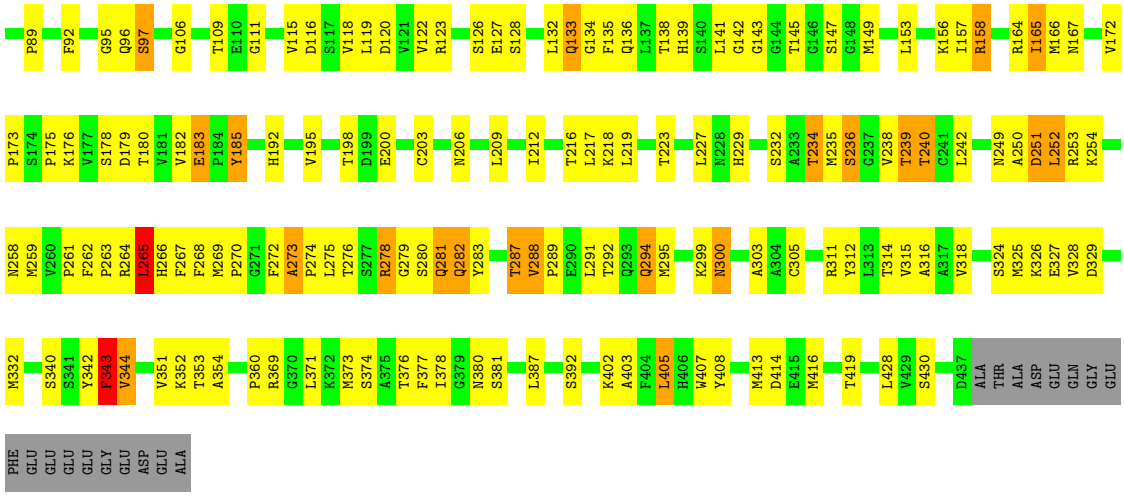
M332 S340 S341 Y342 F343 V344 V351 K352 T353 A354 P360 R369 G370 L371 K372 M373 S374 A375 T376 F377 I378 G379 N380 S381 L387 S392 K402 A403 F404 L405 H406 W407 Y408 M413 D414 E415 M416 T419 L428 V429 S430 D437 ALA THR ALA ASP GLU GLN GLY GLU

PHE GLU GLU GLU GLU GLY GLU ASP GLU ALA

- Molecule 3: Tubulin beta-2B chain

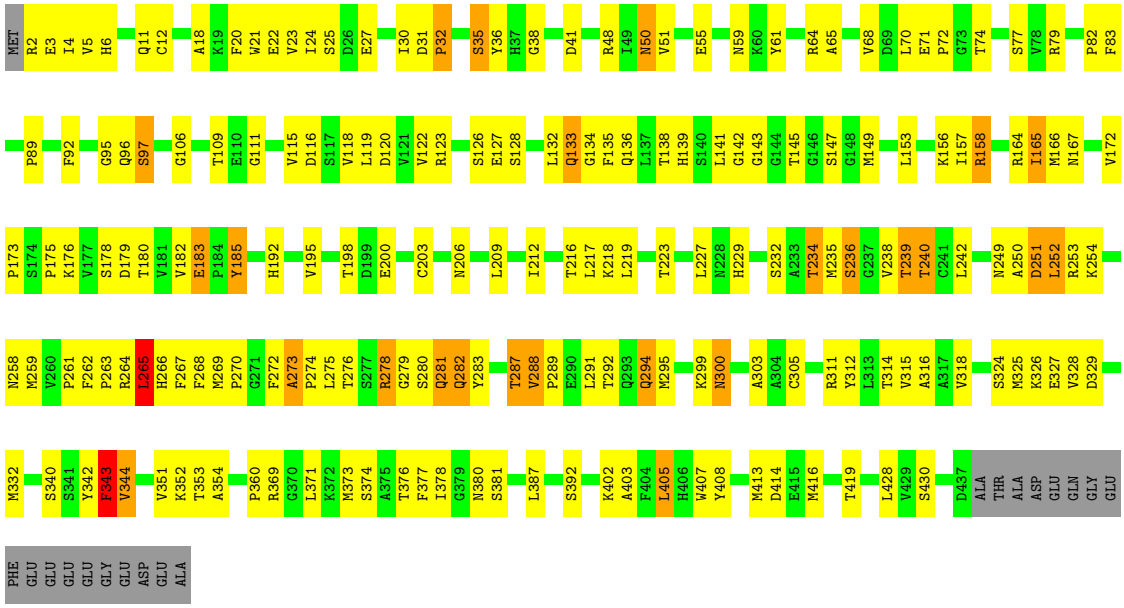
Chain 4-B: 52% 38% 6% •

MET R2 E3 I4 V5 H6 Q11 C12 A18 K19 F20 W21 E22 V23 I24 S25 D26 E27 I30 D31 P32 S35 Y36 H37 G38 D41 R48 I49 N50 V51 E55 N59 K60 Y61 R64 A65 V68 D69 L70 E71 P72 G73 T74 S77 V78 R79 P82 F83



- Molecule 3: Tubulin beta-2B chain

Chain 5-B:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	9842	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	DIRECT ELECTRON DE-20 (5k x 3k)	Depositor
Maximum map value	0.099	Depositor
Minimum map value	-0.029	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.027	Depositor
Map size (Å)	244.79999, 212.67, 246.33	wwPDB
Map dimensions	160, 139, 161	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.53, 1.53, 1.53	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, TA1, MG, GDP, ADP

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	1-C	0.46	0/2284	0.61	0/3080
1	2-C	0.46	0/2284	0.63	1/3080 (0.0%)
1	3-C	0.47	0/2284	0.62	0/3080
1	4-C	0.46	0/2284	0.64	1/3080 (0.0%)
1	5-C	0.45	0/2284	0.60	0/3080
2	1-A	0.30	0/3300	0.46	0/4482
2	2-A	0.30	0/3300	0.46	0/4482
2	3-A	0.30	0/3300	0.46	0/4482
2	4-A	0.30	0/3300	0.46	0/4482
2	5-A	0.30	0/3300	0.46	0/4482
3	1-B	0.30	0/3426	0.46	0/4642
3	2-B	0.30	0/3426	0.46	0/4642
3	3-B	0.30	0/3426	0.46	0/4642
3	4-B	0.30	0/3426	0.46	0/4642
3	5-B	0.30	0/3426	0.46	0/4642
All	All	0.35	0/45050	0.50	2/61020 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	4-C	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	4-C	426	ALA	C-N-CA	6.51	135.98	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2-C	449	ASN	CB-CA-C	-5.29	99.81	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	4-C	450	ARG	Sidechain

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	1-C	2244	0	2248	124	0
1	2-C	2244	0	2248	127	0
1	3-C	2244	0	2248	132	0
1	4-C	2244	0	2248	124	0
1	5-C	2244	0	2248	122	0
2	1-A	3227	0	3143	119	0
2	2-A	3227	0	3143	119	0
2	3-A	3227	0	3143	119	0
2	4-A	3227	0	3143	119	0
2	5-A	3227	0	3143	119	0
3	1-B	3351	0	3229	143	0
3	2-B	3351	0	3229	143	0
3	3-B	3351	0	3229	143	0
3	4-B	3351	0	3229	143	0
3	5-B	3351	0	3229	143	0
4	1-C	27	0	12	11	0
4	2-C	27	0	12	12	0
4	3-C	27	0	12	11	0
4	4-C	27	0	12	11	0
4	5-C	27	0	12	11	0
5	1-A	1	0	0	0	0
5	1-C	1	0	0	0	0
5	2-A	1	0	0	0	0
5	2-C	1	0	0	0	0
5	3-A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	3-C	1	0	0	0	0
5	4-A	1	0	0	0	0
5	4-C	1	0	0	0	0
5	5-A	1	0	0	0	0
5	5-C	1	0	0	0	0
6	1-A	32	0	12	12	0
6	2-A	32	0	12	12	0
6	3-A	32	0	12	12	0
6	4-A	32	0	12	12	0
6	5-A	32	0	12	12	0
7	1-B	28	0	12	13	0
7	2-B	28	0	12	13	0
7	3-B	28	0	12	13	0
7	4-B	28	0	12	13	0
7	5-B	28	0	12	13	0
8	1-B	62	0	51	24	0
8	2-B	62	0	51	24	0
8	3-B	62	0	51	24	0
8	4-B	62	0	51	24	0
8	5-B	62	0	51	24	0
All	All	44865	0	43535	1879	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 21.

The worst 5 of 1879 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:B:12:CYS:SG	7:B:600:GDP:C4	2.25	1.30
3:B:12:CYS:SG	7:B:600:GDP:C4	2.25	1.30
3:B:12:CYS:SG	7:B:600:GDP:C4	2.25	1.30
3:B:12:CYS:SG	7:B:600:GDP:C4	2.25	1.30
3:B:12:CYS:SG	7:B:600:GDP:C4	2.25	1.30

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	1-C	264/501 (53%)	256 (97%)	7 (3%)	1 (0%)	34	72
1	2-C	264/501 (53%)	257 (97%)	6 (2%)	1 (0%)	34	72
1	3-C	264/501 (53%)	256 (97%)	7 (3%)	1 (0%)	34	72
1	4-C	264/501 (53%)	258 (98%)	5 (2%)	1 (0%)	34	72
1	5-C	264/501 (53%)	257 (97%)	6 (2%)	1 (0%)	34	72
2	1-A	408/451 (90%)	328 (80%)	54 (13%)	26 (6%)	1	16
2	2-A	408/451 (90%)	328 (80%)	54 (13%)	26 (6%)	1	16
2	3-A	408/451 (90%)	328 (80%)	54 (13%)	26 (6%)	1	16
2	4-A	408/451 (90%)	328 (80%)	54 (13%)	26 (6%)	1	16
2	5-A	408/451 (90%)	328 (80%)	54 (13%)	26 (6%)	1	16
3	1-B	424/445 (95%)	345 (81%)	48 (11%)	31 (7%)	1	13
3	2-B	424/445 (95%)	345 (81%)	48 (11%)	31 (7%)	1	13
3	3-B	424/445 (95%)	345 (81%)	48 (11%)	31 (7%)	1	13
3	4-B	424/445 (95%)	345 (81%)	48 (11%)	31 (7%)	1	13
3	5-B	424/445 (95%)	345 (81%)	48 (11%)	31 (7%)	1	13
All	All	5480/6985 (78%)	4649 (85%)	541 (10%)	290 (5%)	3	19

5 of 290 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	1-A	97	GLU
2	1-A	109	THR
2	1-A	141	PHE
2	1-A	183	GLU
2	1-A	370	LYS

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	1-C	250/447 (56%)	206 (82%)	44 (18%)	2	11
1	2-C	250/447 (56%)	206 (82%)	44 (18%)	2	11
1	3-C	250/447 (56%)	206 (82%)	44 (18%)	2	11
1	4-C	250/447 (56%)	206 (82%)	44 (18%)	2	11
1	5-C	250/447 (56%)	206 (82%)	44 (18%)	2	11
2	1-A	347/377 (92%)	309 (89%)	38 (11%)	6	22
2	2-A	347/377 (92%)	309 (89%)	38 (11%)	6	22
2	3-A	347/377 (92%)	309 (89%)	38 (11%)	6	22
2	4-A	347/377 (92%)	309 (89%)	38 (11%)	6	22
2	5-A	347/377 (92%)	309 (89%)	38 (11%)	6	22
3	1-B	367/381 (96%)	324 (88%)	43 (12%)	5	21
3	2-B	367/381 (96%)	324 (88%)	43 (12%)	5	21
3	3-B	367/381 (96%)	324 (88%)	43 (12%)	5	21
3	4-B	367/381 (96%)	324 (88%)	43 (12%)	5	21
3	5-B	367/381 (96%)	324 (88%)	43 (12%)	5	21
All	All	4820/6025 (80%)	4195 (87%)	625 (13%)	7	18

5 of 625 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	4-B	79	ARG
2	5-A	352	LYS
3	4-B	216	THR
3	4-B	77	SER
1	5-C	189	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 72 such sidechains are listed below:

Mol	Chain	Res	Type
3	4-B	206	ASN
3	5-B	337	ASN
1	5-C	98	GLN
2	5-A	107	HIS
2	2-A	393	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 30 ligands modelled in this entry, 10 are monoatomic - leaving 20 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	$\#\|Z\| > 2$
8	TA1	1-B	601	-	68,68,68	2.01	19 (27%)	105,105,105	1.39	11 (10%)
6	GTP	3-A	500	5	26,34,34	1.32	4 (15%)	32,54,54	1.02	2 (6%)
7	GDP	5-B	600	-	24,30,30	2.60	9 (37%)	30,47,47	2.93	8 (26%)
7	GDP	4-B	600	-	24,30,30	2.60	9 (37%)	30,47,47	2.93	8 (26%)
6	GTP	4-A	500	5	26,34,34	1.32	4 (15%)	32,54,54	1.02	2 (6%)
7	GDP	3-B	600	-	24,30,30	2.60	9 (37%)	30,47,47	2.93	8 (26%)
8	TA1	3-B	601	-	68,68,68	2.01	19 (27%)	105,105,105	1.39	11 (10%)
8	TA1	5-B	601	-	68,68,68	2.01	19 (27%)	105,105,105	1.39	11 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	ADP	1-C	601	5	24,29,29	1.03	2 (8%)	29,45,45	1.33	3 (10%)
4	ADP	4-C	601	5	24,29,29	1.03	2 (8%)	29,45,45	1.33	3 (10%)
6	GTP	5-A	500	5	26,34,34	1.32	4 (15%)	32,54,54	1.02	2 (6%)
8	TA1	4-B	601	-	68,68,68	2.01	19 (27%)	105,105,105	1.39	11 (10%)
7	GDP	2-B	600	-	24,30,30	2.60	9 (37%)	30,47,47	2.93	8 (26%)
4	ADP	5-C	601	5	24,29,29	1.03	2 (8%)	29,45,45	1.33	3 (10%)
6	GTP	2-A	500	5	26,34,34	1.32	4 (15%)	32,54,54	1.02	2 (6%)
4	ADP	2-C	601	5	24,29,29	1.04	2 (8%)	29,45,45	1.34	3 (10%)
6	GTP	1-A	500	5	26,34,34	1.32	4 (15%)	32,54,54	1.02	2 (6%)
8	TA1	2-B	601	-	68,68,68	2.01	19 (27%)	105,105,105	1.39	11 (10%)
7	GDP	1-B	600	-	24,30,30	2.60	9 (37%)	30,47,47	2.93	8 (26%)
4	ADP	3-C	601	5	24,29,29	1.03	2 (8%)	29,45,45	1.33	3 (10%)

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
8	TA1	1-B	601	-	-	9/41/127/127	0/7/7/7
6	GTP	3-A	500	5	-	3/18/38/38	0/3/3/3
7	GDP	5-B	600	-	-	4/12/32/32	0/3/3/3
7	GDP	4-B	600	-	-	4/12/32/32	0/3/3/3
6	GTP	4-A	500	5	-	3/18/38/38	0/3/3/3
7	GDP	3-B	600	-	-	4/12/32/32	0/3/3/3
8	TA1	3-B	601	-	-	9/41/127/127	0/7/7/7
8	TA1	5-B	601	-	-	9/41/127/127	0/7/7/7
4	ADP	1-C	601	5	-	2/12/32/32	0/3/3/3
4	ADP	4-C	601	5	-	2/12/32/32	0/3/3/3
6	GTP	5-A	500	5	-	3/18/38/38	0/3/3/3
8	TA1	4-B	601	-	-	9/41/127/127	0/7/7/7
7	GDP	2-B	600	-	-	4/12/32/32	0/3/3/3
4	ADP	5-C	601	5	-	2/12/32/32	0/3/3/3
6	GTP	2-A	500	5	-	3/18/38/38	0/3/3/3
4	ADP	2-C	601	5	-	2/12/32/32	0/3/3/3
6	GTP	1-A	500	5	-	3/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	TA1	2-B	601	-	-	9/41/127/127	0/7/7/7
7	GDP	1-B	600	-	-	4/12/32/32	0/3/3/3
4	ADP	3-C	601	5	-	2/12/32/32	0/3/3/3

The worst 5 of 170 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	1-B	600	GDP	O4'-C1'	6.20	1.49	1.41
7	2-B	600	GDP	O4'-C1'	6.20	1.49	1.41
7	3-B	600	GDP	O4'-C1'	6.20	1.49	1.41
7	4-B	600	GDP	O4'-C1'	6.20	1.49	1.41
7	5-B	600	GDP	O4'-C1'	6.20	1.49	1.41

The worst 5 of 120 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	1-B	600	GDP	C8-N7-C5	9.28	120.66	102.99
7	2-B	600	GDP	C8-N7-C5	9.28	120.66	102.99
7	3-B	600	GDP	C8-N7-C5	9.28	120.66	102.99
7	4-B	600	GDP	C8-N7-C5	9.28	120.66	102.99
7	5-B	600	GDP	C8-N7-C5	9.28	120.66	102.99

There are no chirality outliers.

5 of 90 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	1-C	601	ADP	PA-O3A-PB-O3B
4	2-C	601	ADP	PA-O3A-PB-O3B
4	3-C	601	ADP	PA-O3A-PB-O3B
4	4-C	601	ADP	PA-O3A-PB-O3B
4	5-C	601	ADP	PA-O3A-PB-O3B

There are no ring outliers.

20 monomers are involved in 301 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	1-B	601	TA1	24	0
6	3-A	500	GTP	12	0
7	5-B	600	GDP	13	0
7	4-B	600	GDP	13	0

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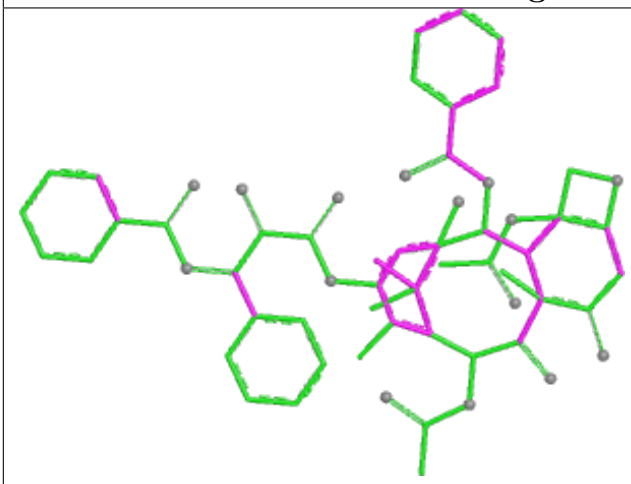
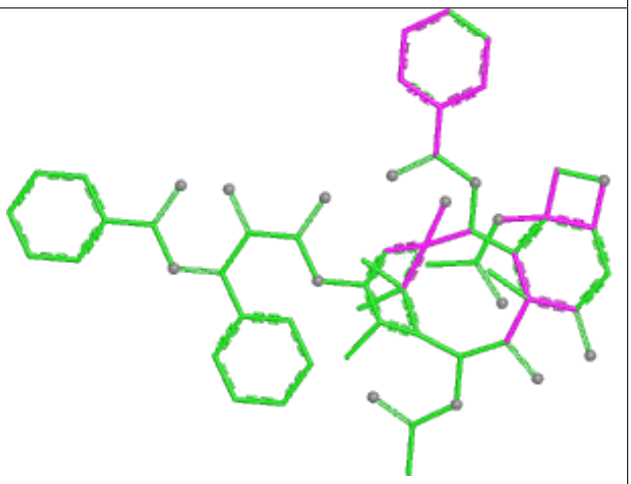
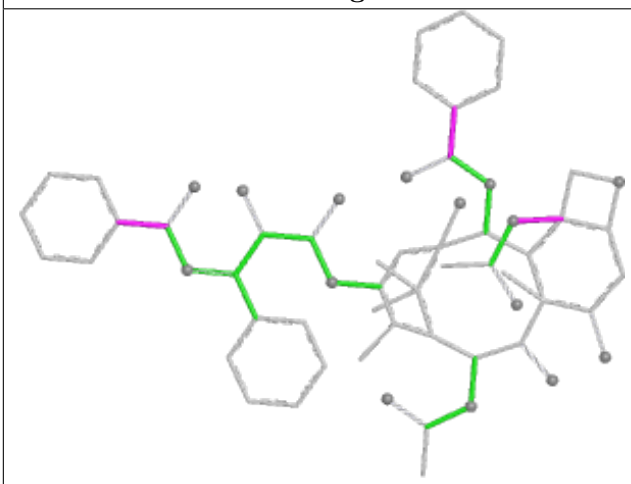
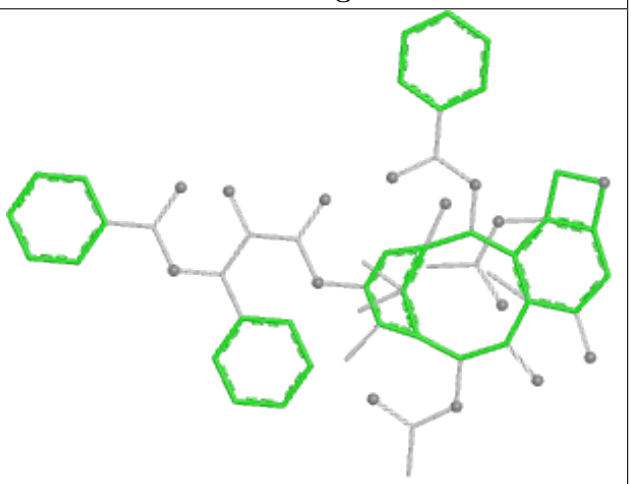
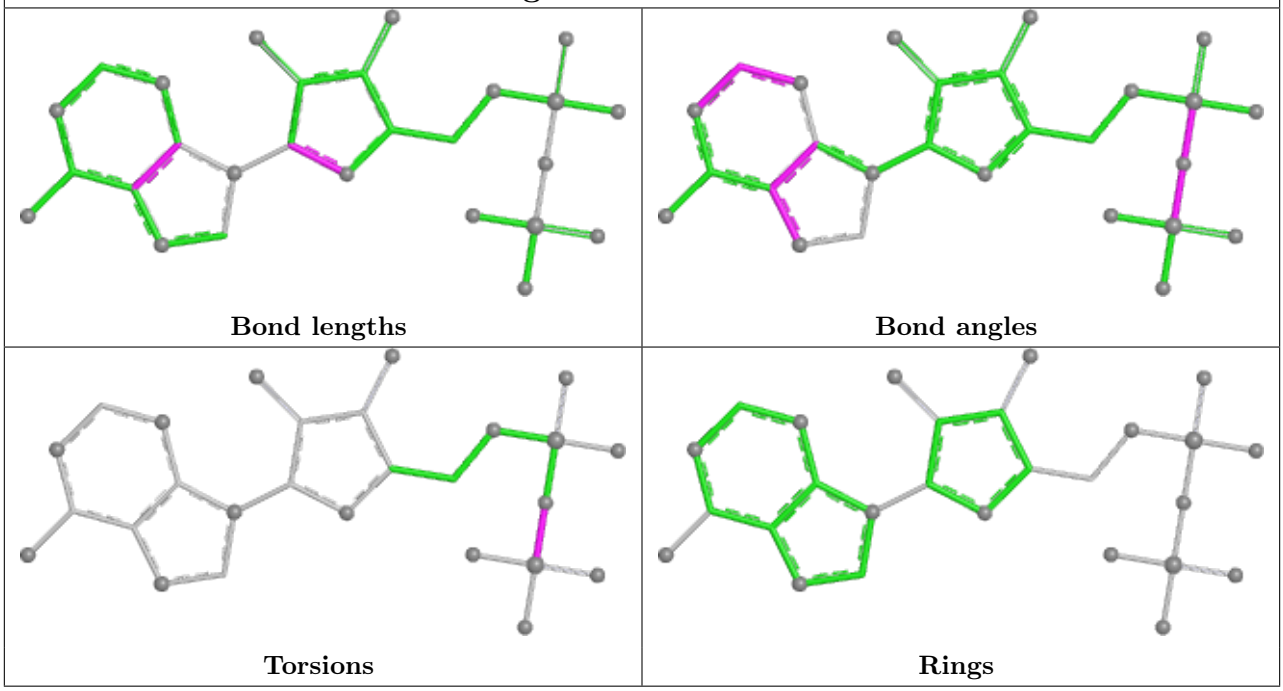
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	4-A	500	GTP	12	0
7	3-B	600	GDP	13	0
8	3-B	601	TA1	24	0
8	5-B	601	TA1	24	0
4	1-C	601	ADP	11	0
4	4-C	601	ADP	11	0
6	5-A	500	GTP	12	0
8	4-B	601	TA1	24	0
7	2-B	600	GDP	13	0
4	5-C	601	ADP	11	0
6	2-A	500	GTP	12	0
4	2-C	601	ADP	12	0
6	1-A	500	GTP	12	0
8	2-B	601	TA1	24	0
7	1-B	600	GDP	13	0
4	3-C	601	ADP	11	0

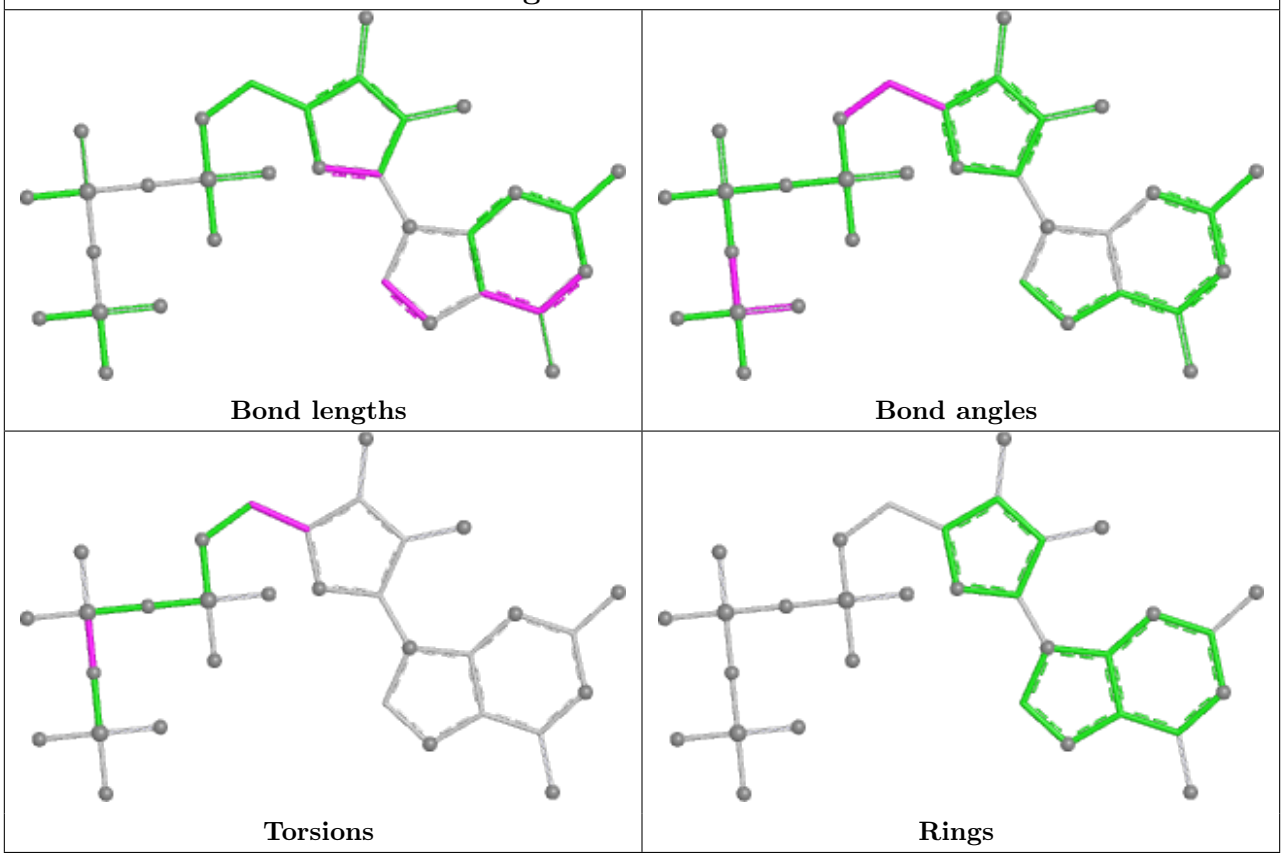
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

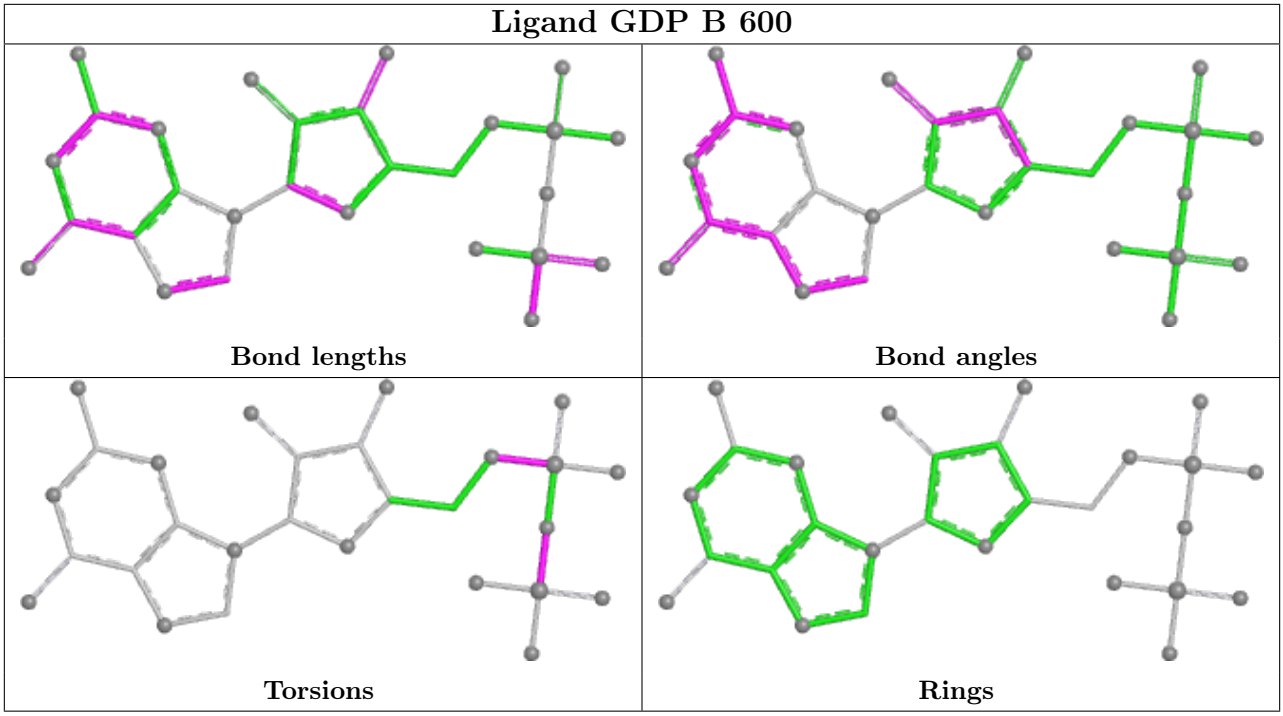
Ligand TA1 B 601	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand ADP C 601



Ligand GTP A 500





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.

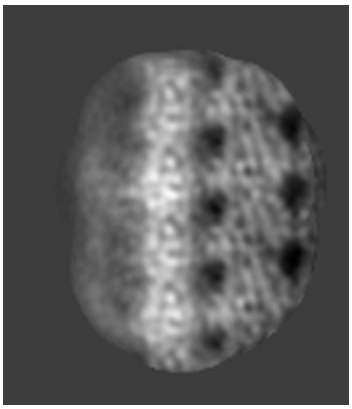
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-3620. These allow visual inspection of the internal detail of the map and identification of artifacts.

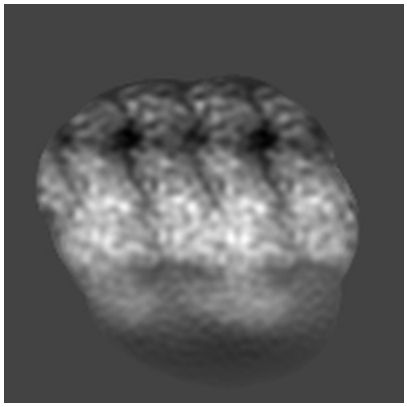
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

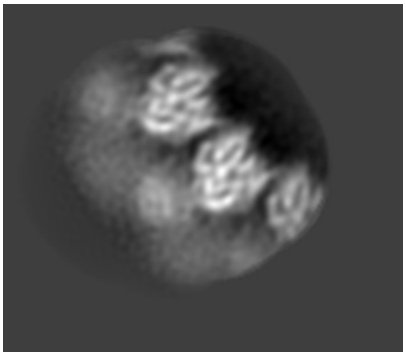
6.1.1 Primary map



X



Y

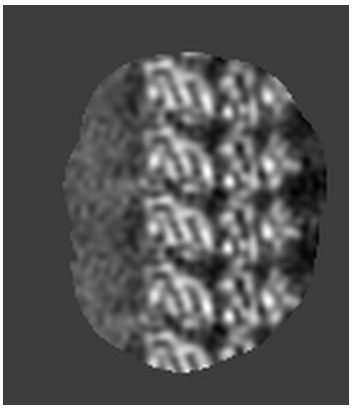


Z

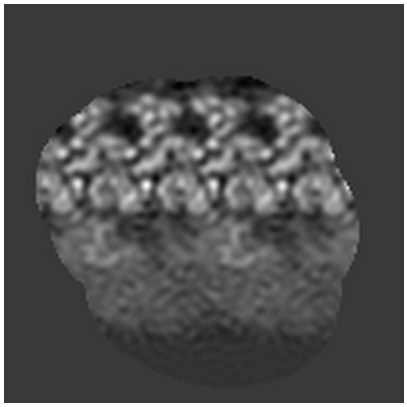
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

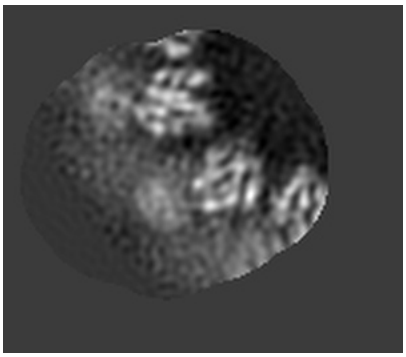
6.2.1 Primary map



X Index: 80



Y Index: 69

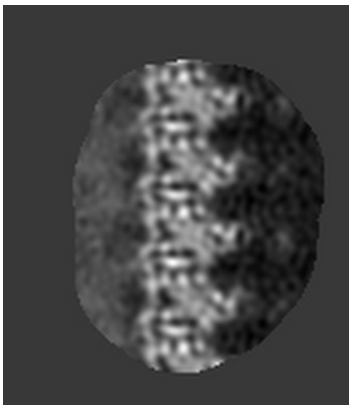


Z Index: 80

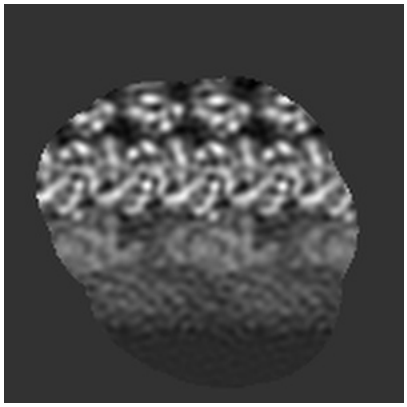
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

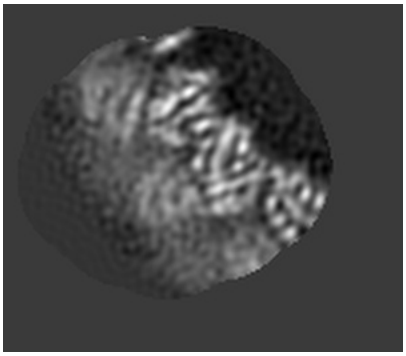
6.3.1 Primary map



X Index: 87



Y Index: 66

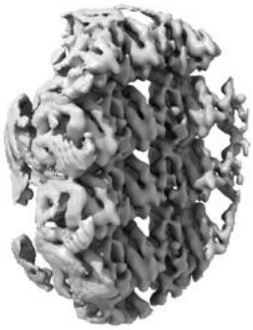


Z Index: 90

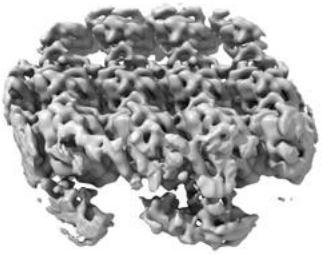
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.027. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

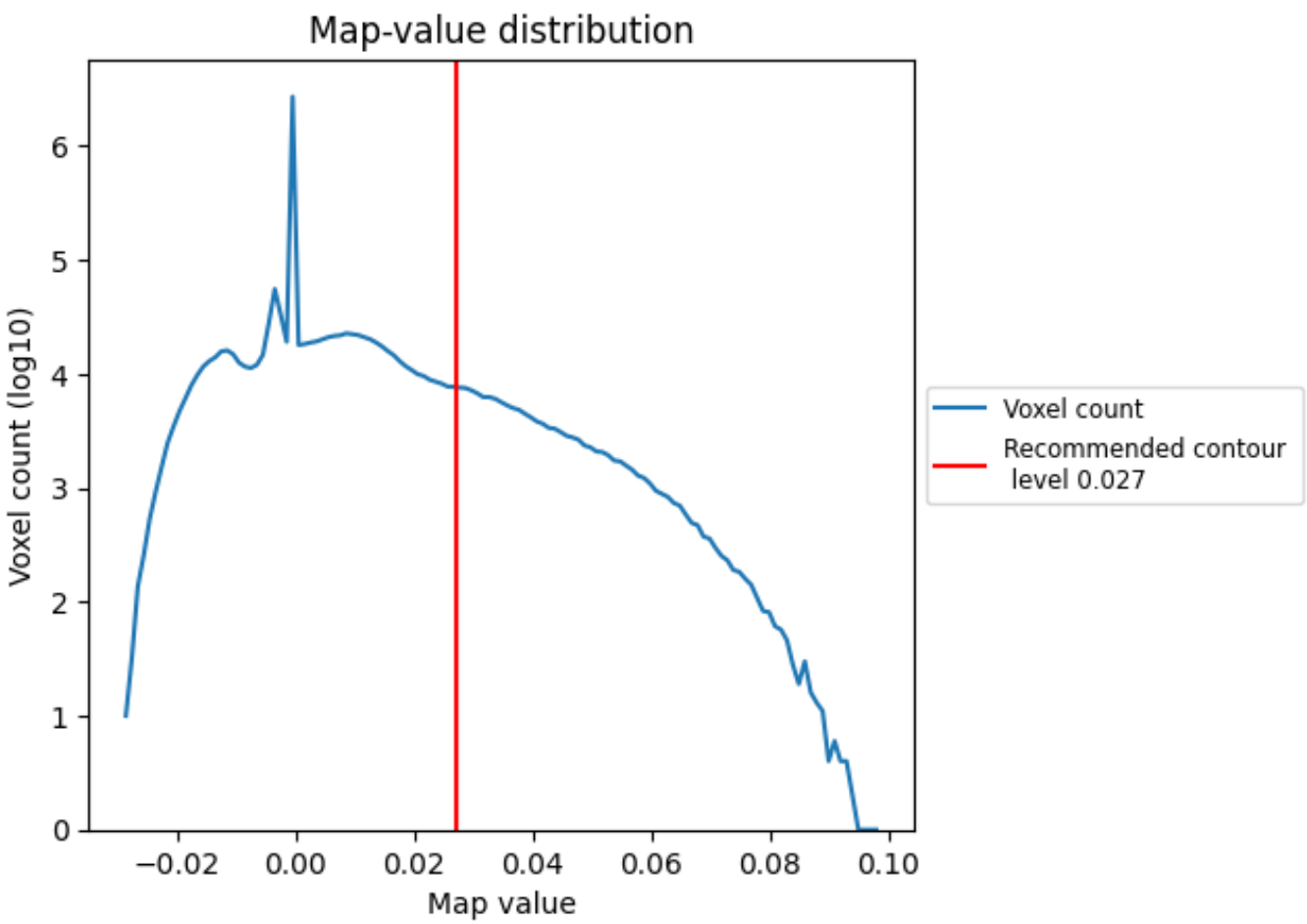
6.5 Mask visualisation (i)

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

7 Map analysis (i)

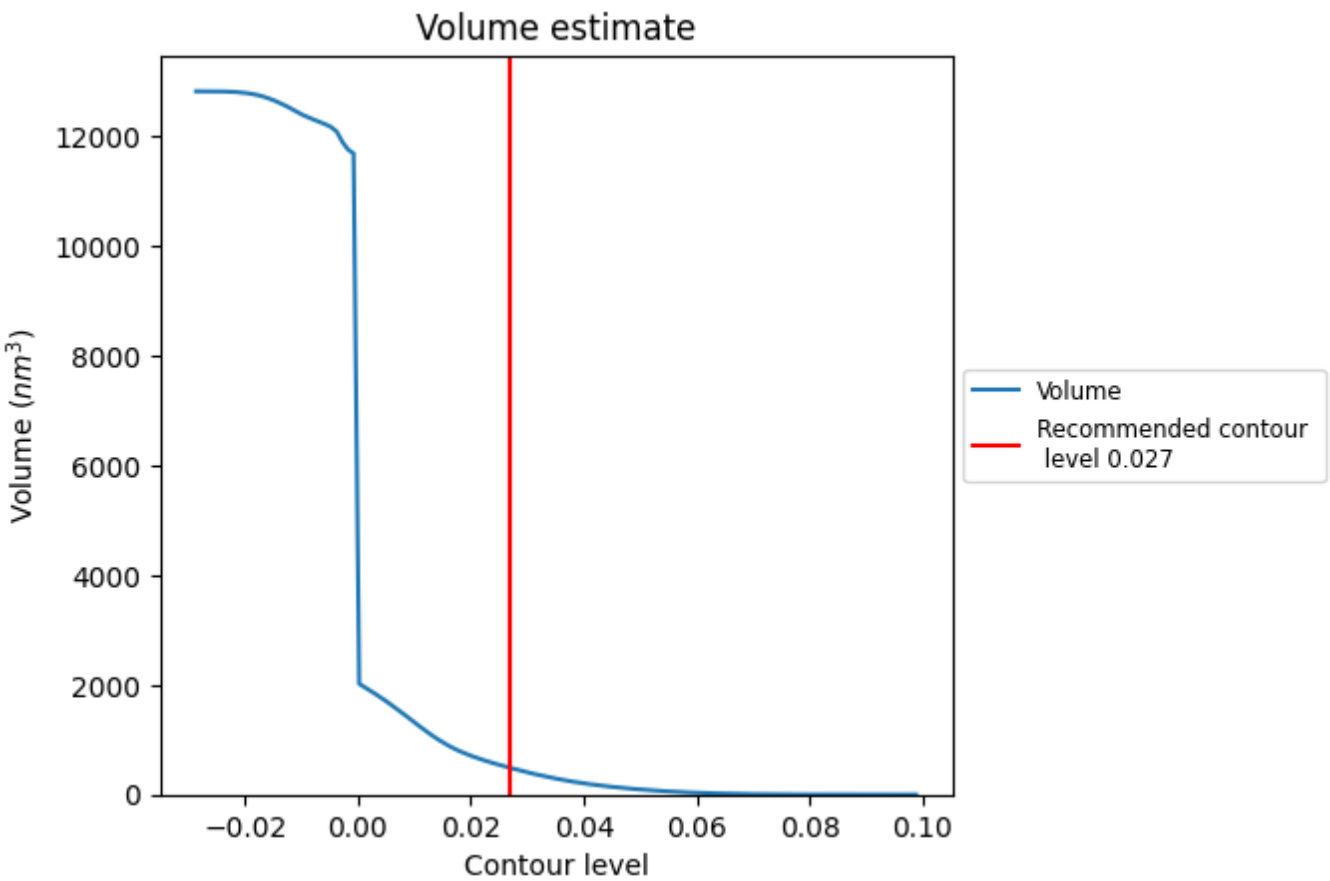
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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 487 nm^3; this corresponds to an approximate mass of 440 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)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

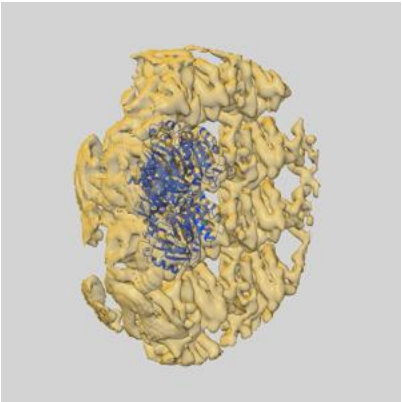
8 Fourier-Shell correlation (i)

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

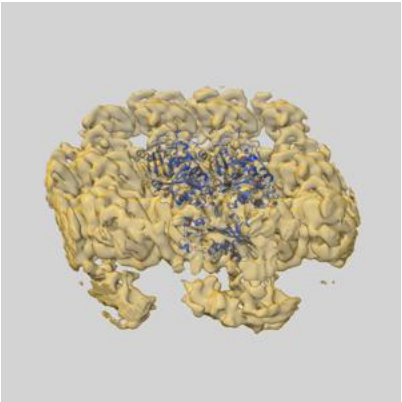
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-3620 and PDB model 5ND2. Per-residue inclusion information can be found in section 3 on page 10.

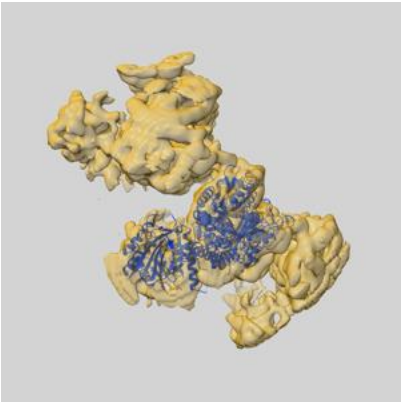
9.1 Map-model overlay (i)



X



Y



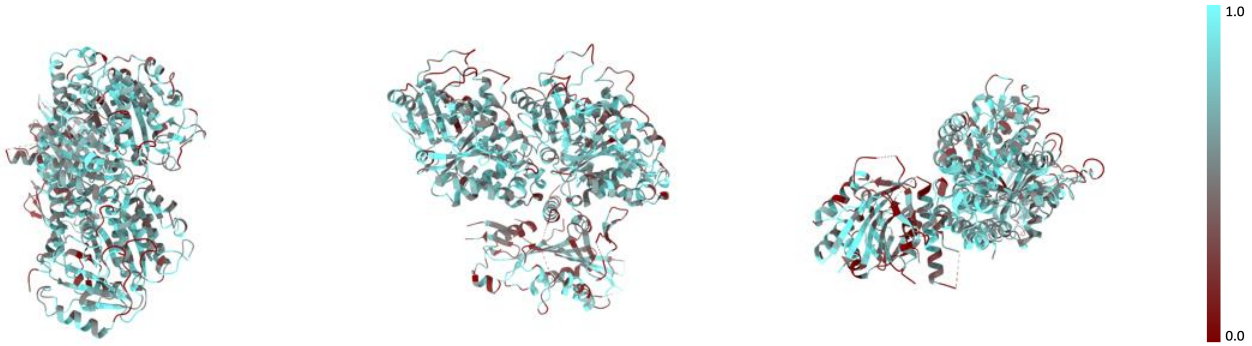
Z

The images above show the 3D surface view of the map at the recommended contour level 0.027 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)

This section was not generated.

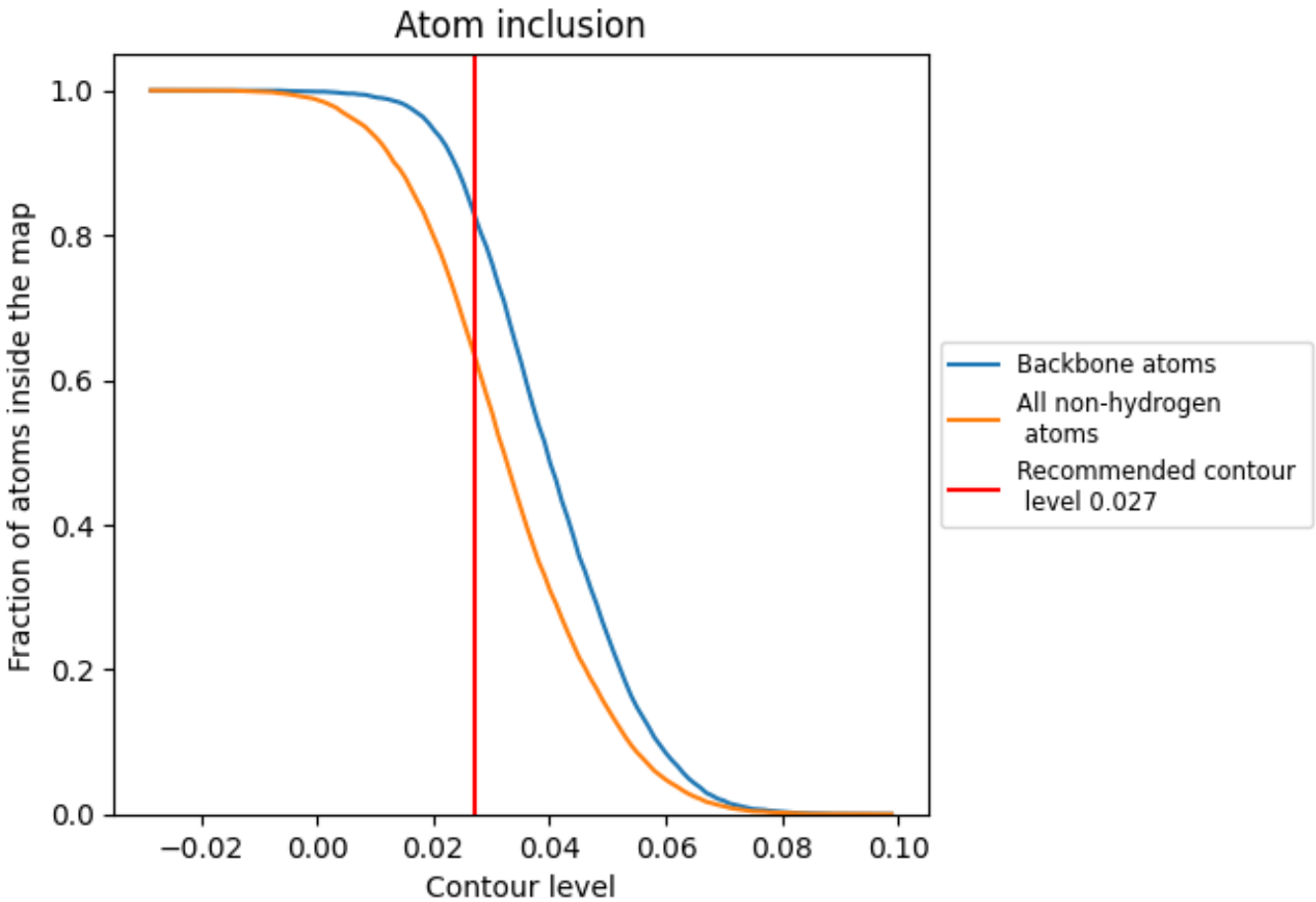
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.027).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.027) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	0.6358
A	0.6724
B	0.6624
C	0.5431