



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 04:56 AM UTC

PDB ID : 7KZO / pdb_00007kzo
EMDB ID : EMD-23084
Title : Outer dynein arm docking complex bound to doublet microtubules from C. reinhardtii
Authors : Walton, T.; Wu, H.; Brown, A.B.
Deposited on : 2020-12-10
Resolution : 3.30 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 ⓘ 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

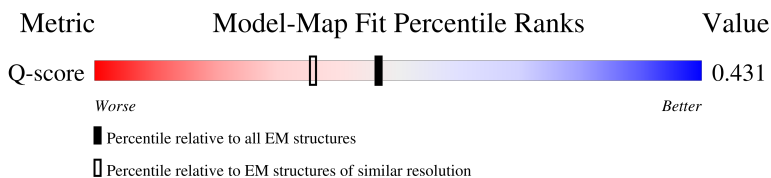
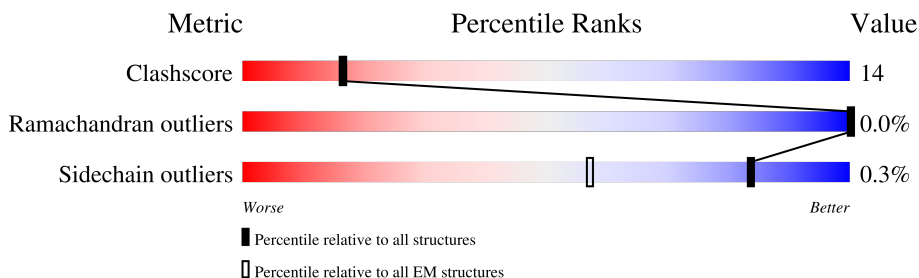
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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.



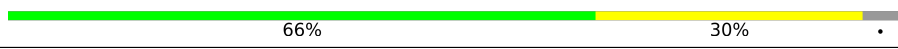
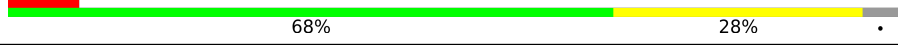
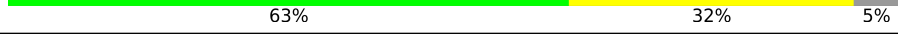
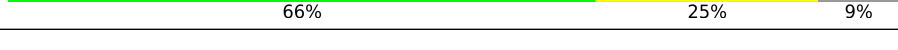
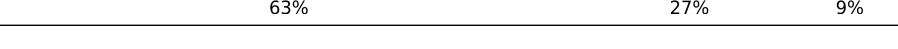
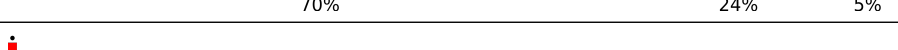
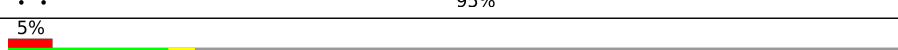
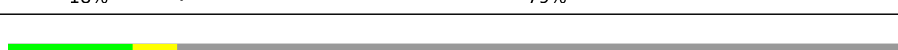
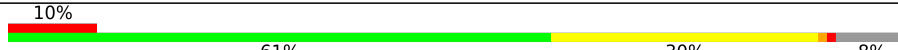
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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 $\leq 5\%$. 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	A1	443	
1	A3	443	
1	A5	443	
1	A7	443	

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Mol	Chain	Length	Quality of chain
1	B1	443	
1	B3	443	
1	B5	443	
1	B7	443	
2	A2	451	
2	A4	451	
2	A6	451	
2	B2	451	
2	B4	451	
2	B6	451	
3	C	4485	
4	X	749	
4	X1	749	
5	Y	552	
5	Y1	552	
6	Z	184	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 54110 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 Tubulin beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A1	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	A3	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	A5	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	A7	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	B1	419	Total	C	N	O	S	0	0
			3298	2077	563	628	30		
1	B3	410	Total	C	N	O	S	0	0
			3227	2030	553	614	30		
1	B5	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	B7	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		

- Molecule 2 is a protein called Tubulin alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A2	430	Total	C	N	O	S	0	0
			3339	2114	568	636	21		
2	A4	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	A6	429	Total	C	N	O	S	0	0
			3335	2112	567	635	21		
2	B2	411	Total	C	N	O	S	0	0
			3204	2035	544	605	20		
2	B4	409	Total	C	N	O	S	0	0
			3193	2028	542	603	20		
2	B6	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		

- Molecule 3 is a protein called Dynein gamma chain, flagellar outer arm.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	218	Total	C	N	O	S	0	0
			1771	1123	302	335	11		

- Molecule 4 is a protein called Outer dynein arm-docking complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	X	157	Total	C	N	O	S	0	0
			985	594	198	190	3		
4	X1	142	Total	C	N	O	S	0	0
			1178	715	223	235	5		

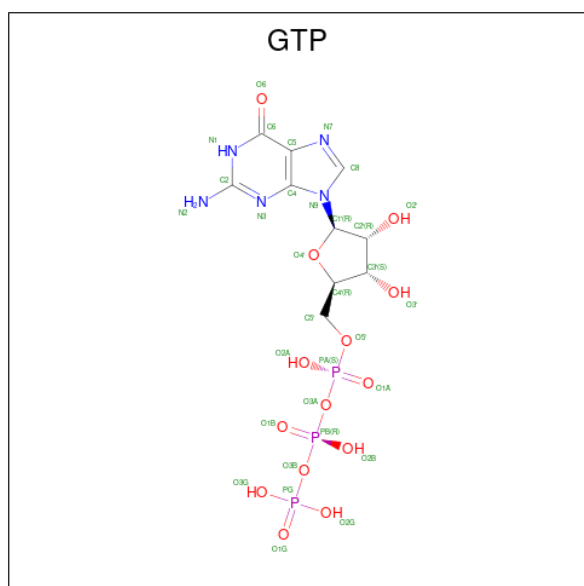
- Molecule 5 is a protein called Outer dynein arm protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Y	121	Total	C	N	O	S	0	0
			844	508	162	171	3		
5	Y1	147	Total	C	N	O	S	0	0
			1185	729	223	224	9		

- Molecule 6 is a protein called Outer dynein arm-docking complex protein DC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Z	170	Total	C	N	O	S	0	0
			1384	863	242	270	9		

- Molecule 7 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

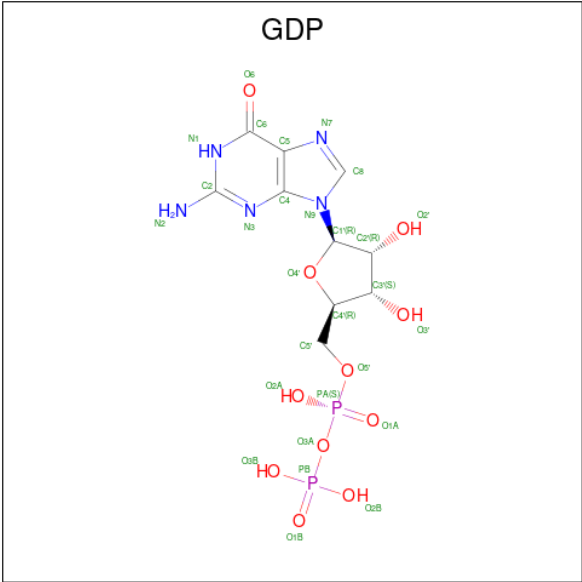


Mol	Chain	Residues	Atoms					AltConf
7	A1	1	Total	C	N	O	P	0
			32	10	5	14	3	
7	A3	1	Total	C	N	O	P	0
			32	10	5	14	3	
7	A5	1	Total	C	N	O	P	0
			32	10	5	14	3	
7	A7	1	Total	C	N	O	P	0
			32	10	5	14	3	
7	B2	1	Total	C	N	O	P	0
			32	10	5	14	3	
7	B5	1	Total	C	N	O	P	0
			32	10	5	14	3	
7	B7	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
8	A1	1	Total	Mg	0
			1	1	
8	A2	1	Total	Mg	0
			1	1	
8	A4	1	Total	Mg	0
			1	1	
8	A6	1	Total	Mg	0
			1	1	
8	B3	1	Total	Mg	0
			1	1	
8	B4	1	Total	Mg	0
			1	1	
8	B6	1	Total	Mg	0
			1	1	

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).

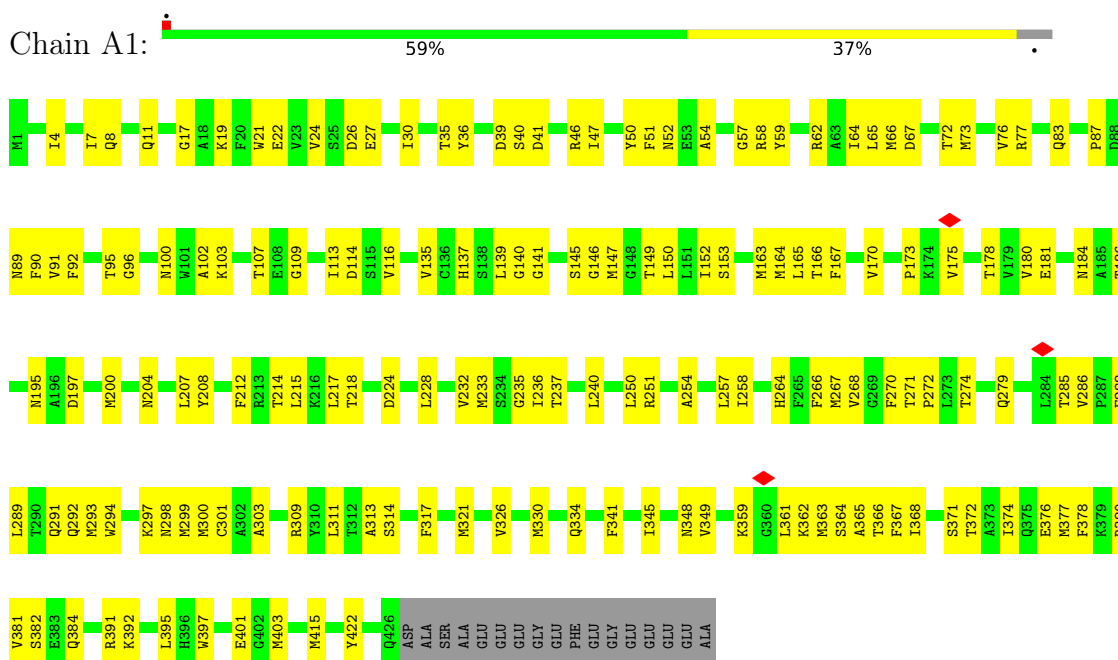


Mol	Chain	Residues	Atoms					AltConf
9	A1	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	A3	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	A5	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	A7	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	B1	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	B3	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	B5	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	B7	1	Total	C	N	O	P	0
			28	10	5	11	2	

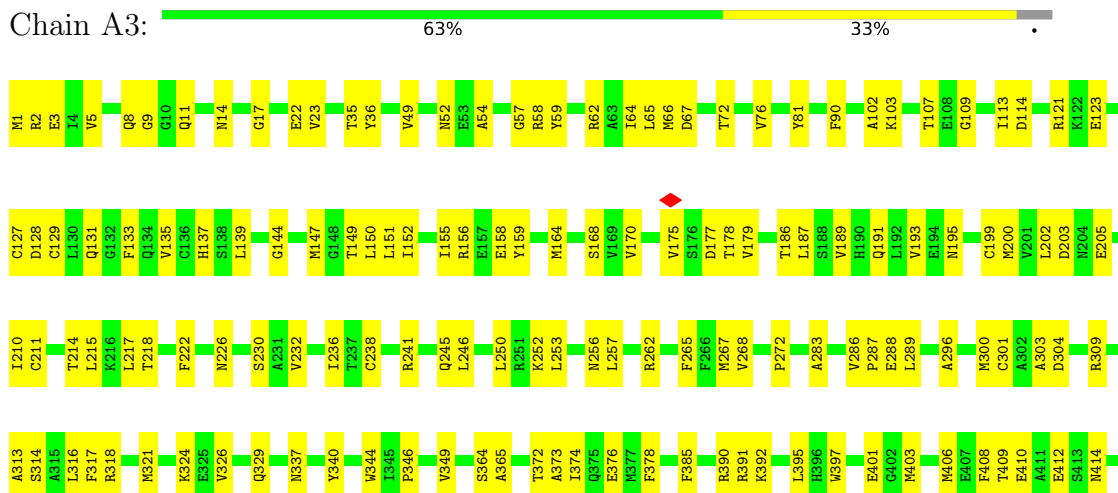
3 Residue-property plots

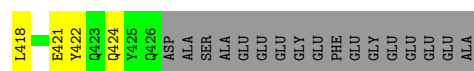
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



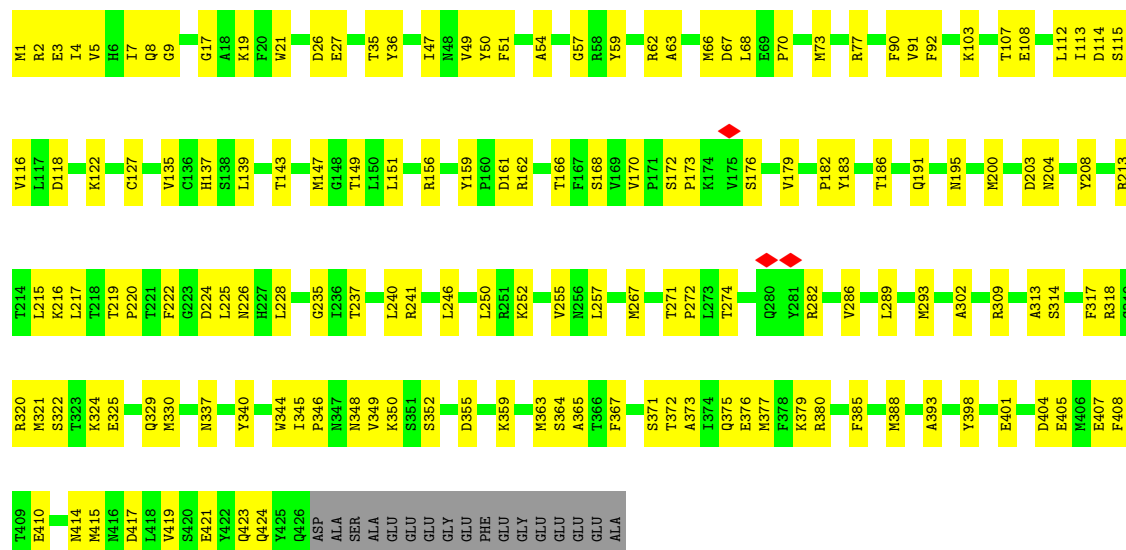
• Molecule 1: Tubulin beta





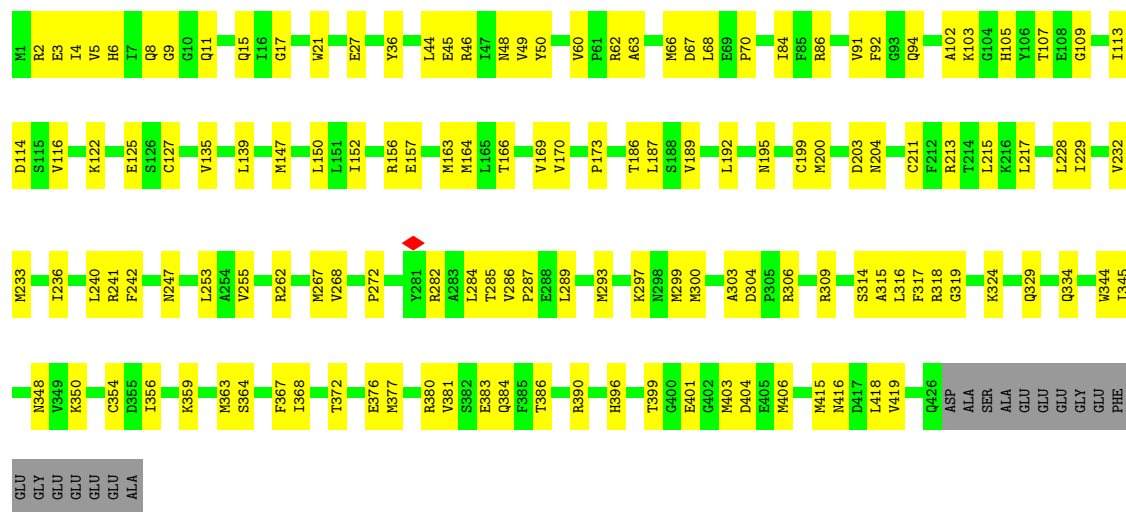
• Molecule 1: Tubulin beta

Chain A5: 62% 34%



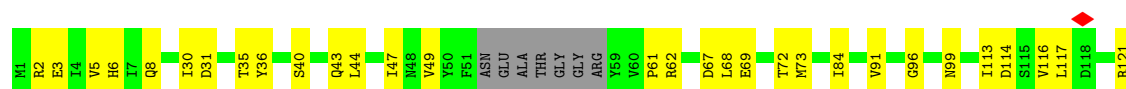
• Molecule 1: Tubulin beta

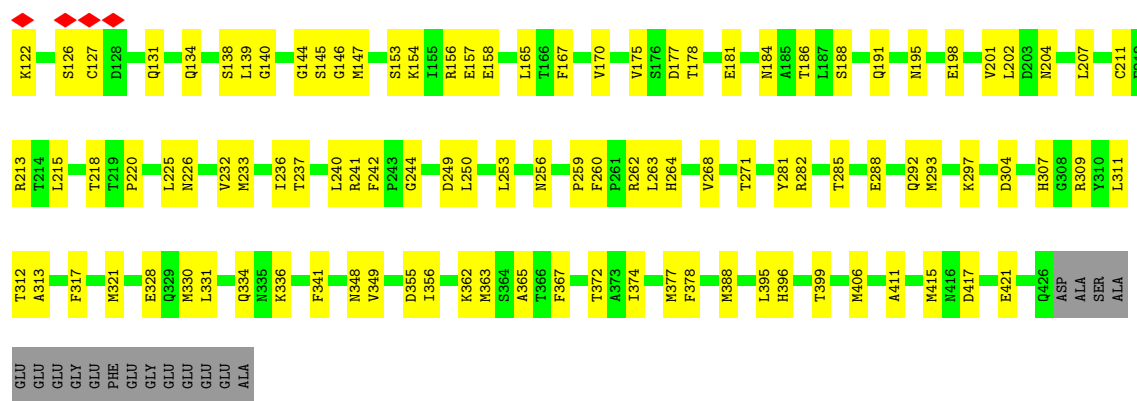
Chain A7: 65% 31%



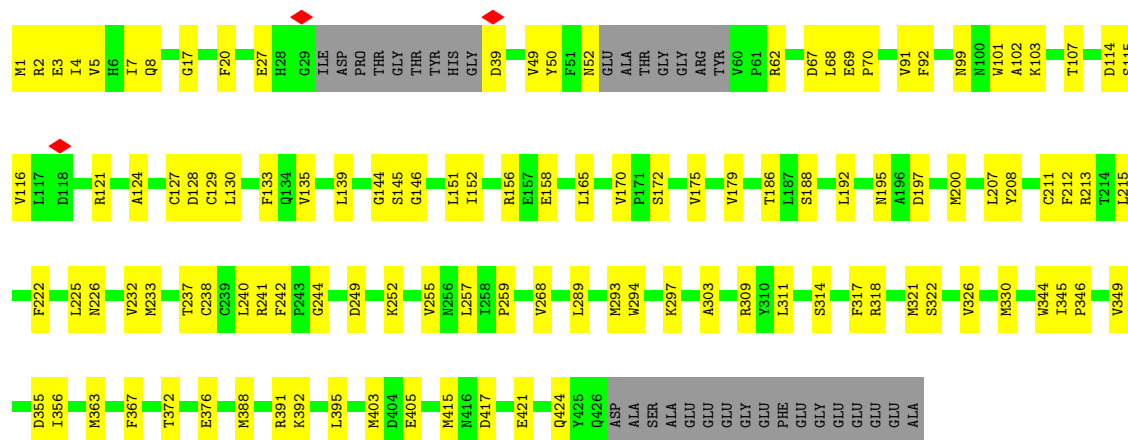
• Molecule 1: Tubulin beta

Chain B1: 65% 30% 5%

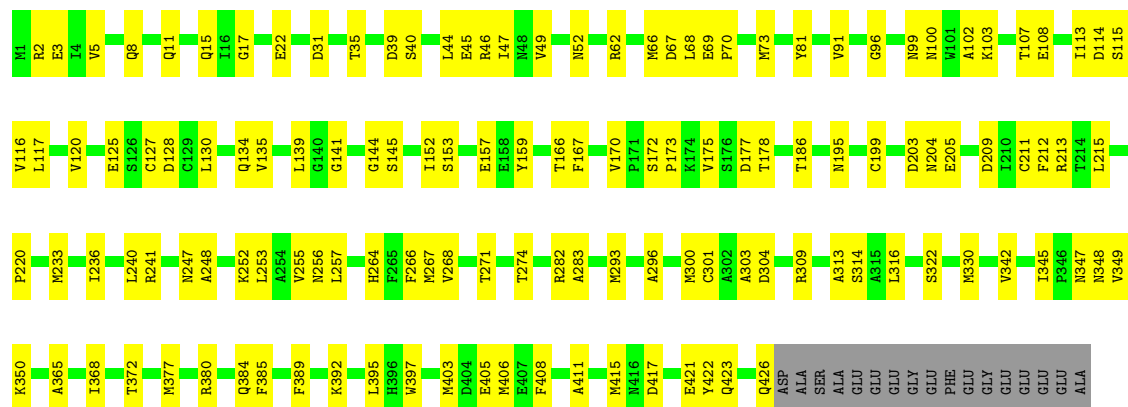




• Molecule 1: Tubulin beta

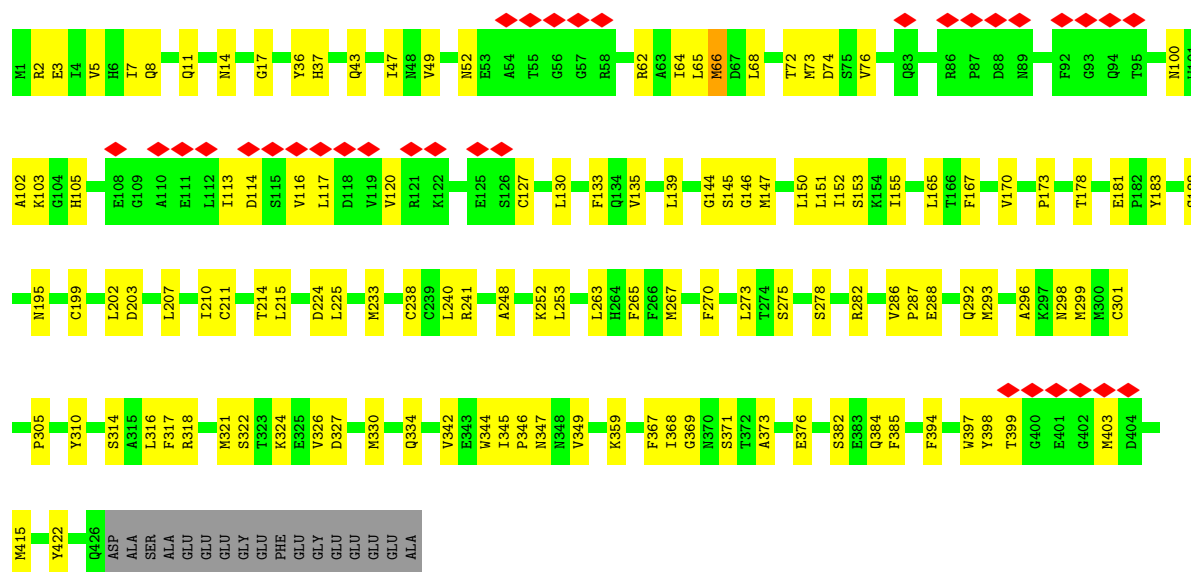


• Molecule 1: Tubulin beta



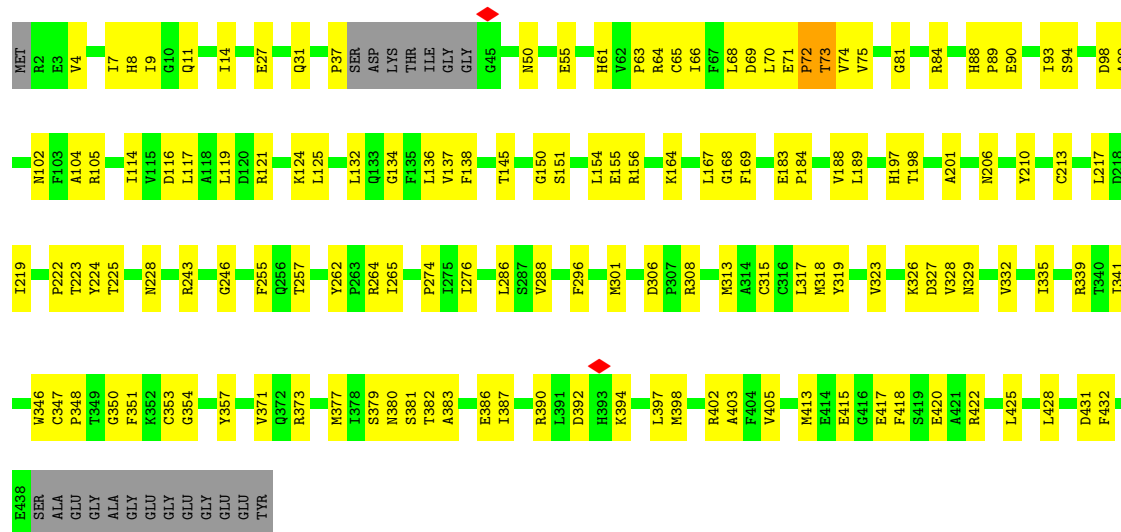
• Molecule 1: Tubulin beta





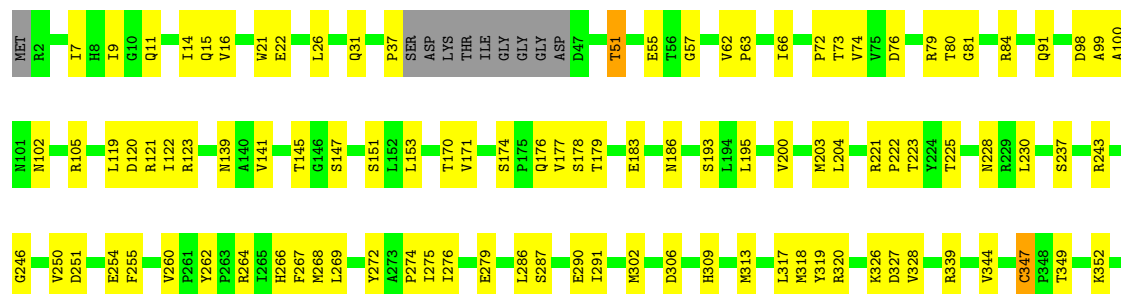
• Molecule 2: Tubulin alpha

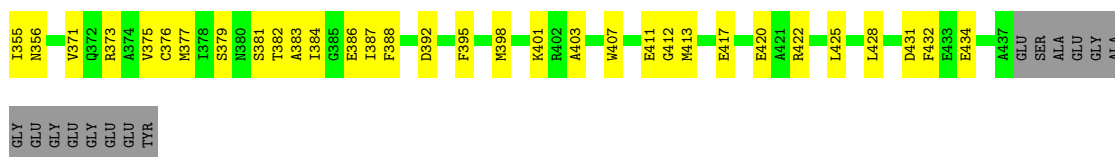
Chain A2:



• Molecule 2: Tubulin alpha

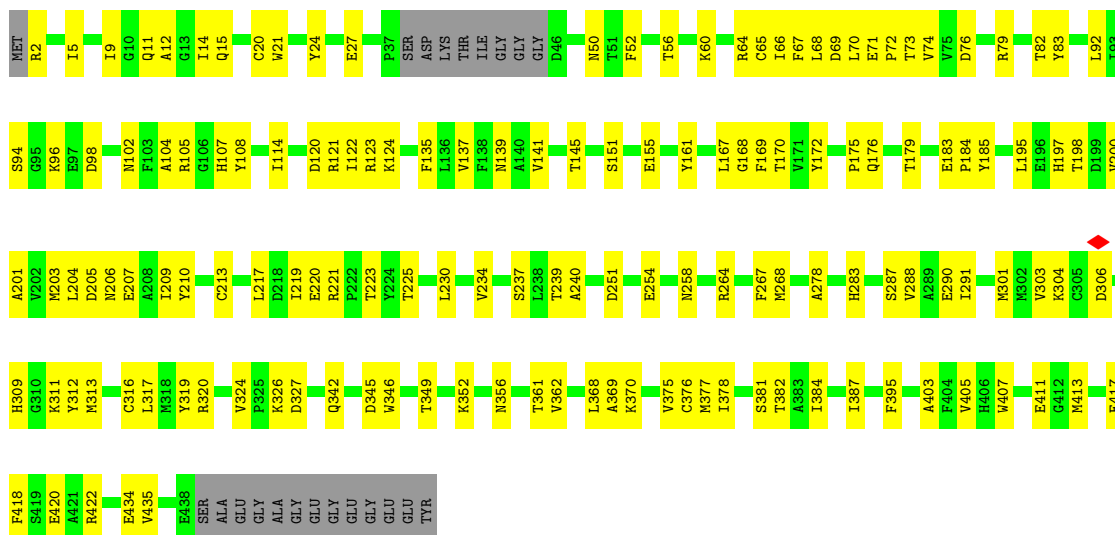
Chain A4:





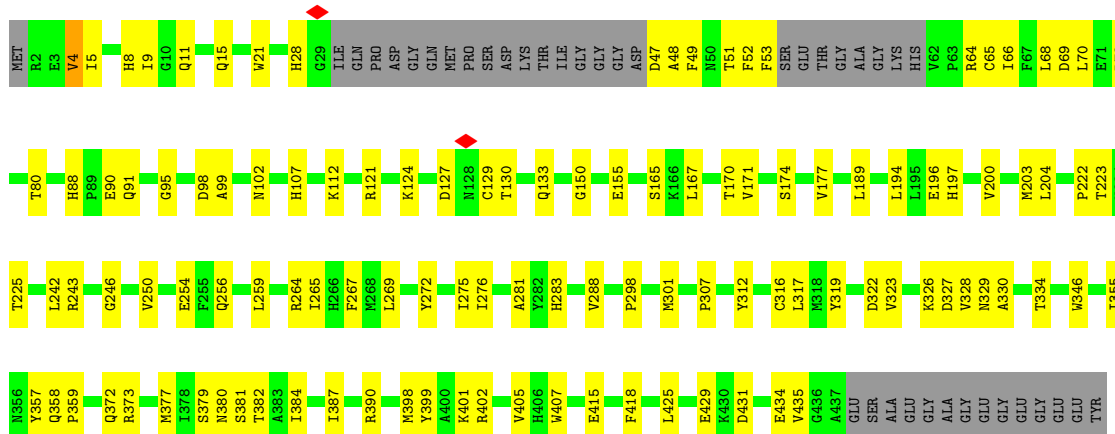
• Molecule 2: Tubulin alpha

Chain A6: 63% 32% 5%



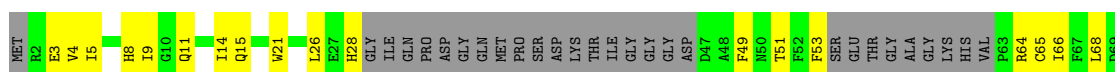
• Molecule 2: Tubulin alpha

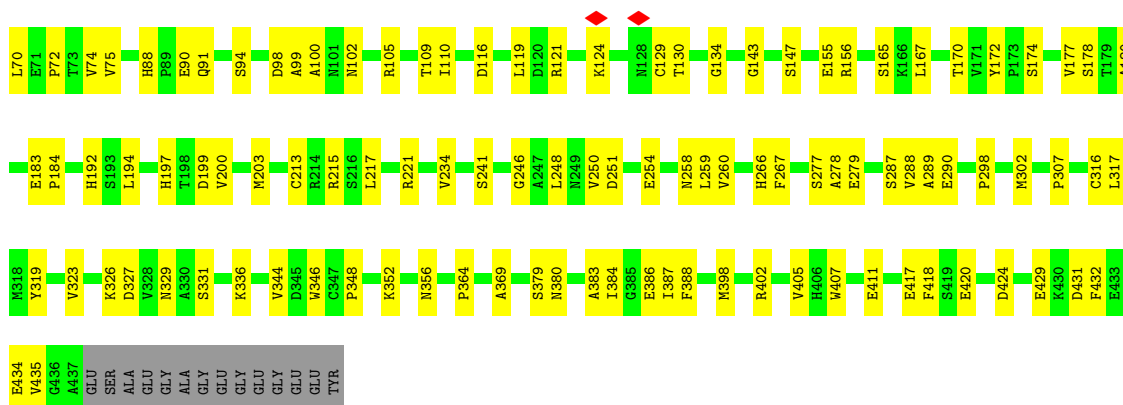
Chain B2: 66% 25% 9%



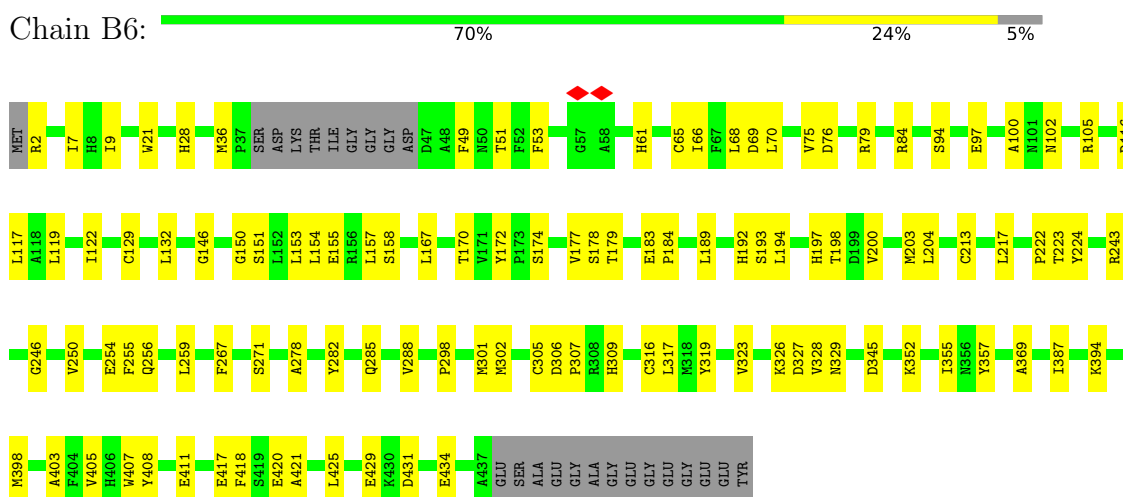
• Molecule 2: Tubulin alpha

Chain B4: 63% 27% 9%

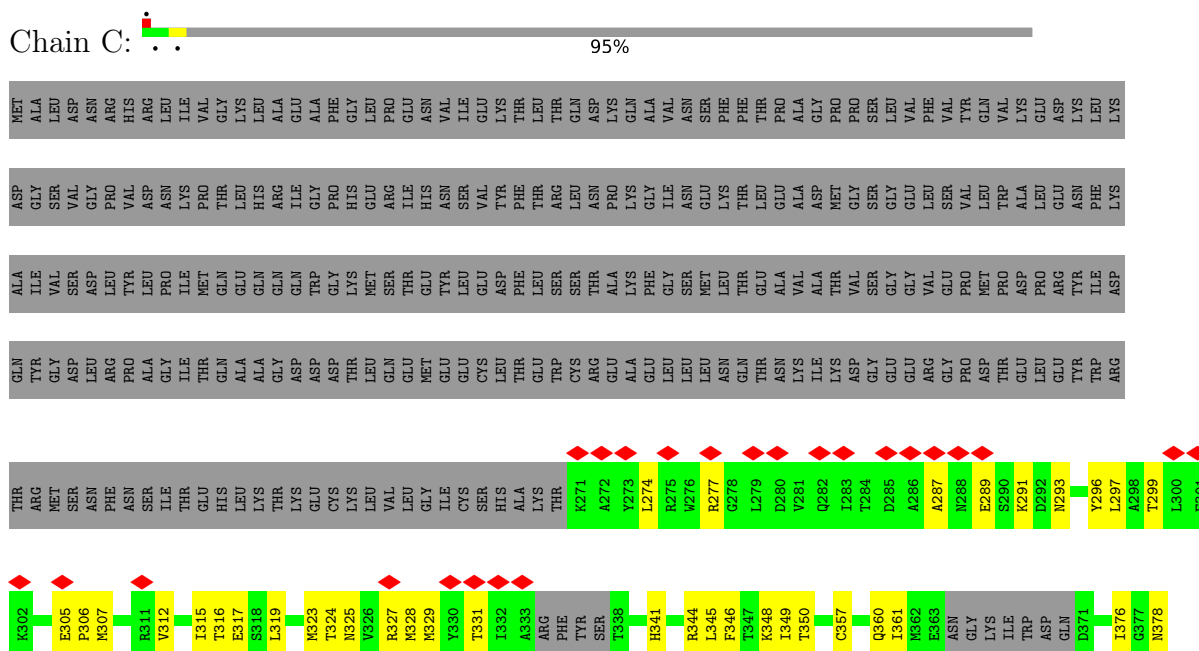




- Molecule 2: Tubulin alpha



- Molecule 3: Dynein gamma chain, flagellar outer arm









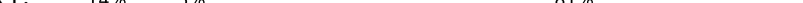
[illegible]

- Molecule 4: Outer dynein arm-docking complex subunit 1

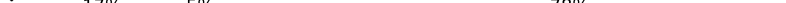


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PRO	PRO	PRO	ALA	ARG	ASP	ASN	GLU	W359	K248	GLN	ASP	THR	GLN	ALA
GLU	GLU	ALA	ASN	GLU	GLY	GLY	GLU	E360	E252	GLU	ASP	LYS	ASP	GLN
ALA	ALA	ALA	MET	GLU	GLY	GLY	GLU	G361	R253	LYS	MET	ILE	ALA	SER
GLU	GLU	GLU	GLY	GLY	GLY	GLY	GLU	L362	E254	GLN	LYS	THR	LYS	THR
GLU	GLU	ALA	ALA	ALA	ALA	ALA	ALA	K363	L255	ILE	GLY	LYS	LEU	LYS
LEU	LEU	ALA	ARG	ARG	LYS	LYS	LYS	A364	A256	ASP	ARG	PRO	PRO	LEU
ALA	ALA	ALA	ARG	GLY	GLY	GLY	LYS	K365	R257	GLU	ARG	GLY	PRO	PRO
GLY	GLY	GLY	GLY	LYS	LYS	LYS	LYS	E366	R260	GLU	GLU	MET	ARG	ARG
GLU	GLU	GLU	PHE	GLU	GLY	GLY	PHE			LEU	LEU	ASP	LEU	LEU
ALA	ALA	ALA	ALA	ALA	GLY	GLY	LYS	M369	E263	VAL	GLU	THR	ARG	ARG
GLU	GLU	GLU	HIS	GLY	GLY	GLY	LYS	R370		GLU	GLU	PRO	THR	THR
MET	MET	ALA	LYS	LEU	LEU	LEU	LEU		R266	ALA	LYS	LYS	LYS	LYS
VAL	VAL	VAL	HIS	ARG	GLY	GLY	ARG	V373	V267	GLU	LYS	GLY	GLU	GLU
SER	SER	SER	THR	SER	SER	SER	SER			ALA	ALA	LEU	GLU	GLU
PRO	PRO	PRO	PRO	VAL	VAL	VAL	VAL	E377	K271	LYS	LYS	GLY	GLY	LEU
LEU	LEU	LEU	GLY	ASP	GLY	GLY	CYS	K272	K272	ASN	ASN	GLU	GLU	LYS
GLY	GLY	GLY	ILE	ILE	ILE	ILE	ILE			ARG	ARG	GLY	GLY	LYS
ALA	ALA	ALA	ASN	GLY	GLY	GLY	GLY	E275		LEU	LEU	GLU	GLU	LYS
ASP	ASP	ASP	LYS	ALA	ALA	ALA	ALA	R379	R276	TYR	TYR	LEU	LEU	THR
GLY	GLY	GLY	ARG	GLU	GLU	GLU	GLU	E380	R277	LEU	LEU	GLY	GLY	SER
ASN	ASN	GLY	GLN	GLN	GLY	GLN	GLN	S381	R278	LEU	LEU	ASP	GLU	PRO
THR	THR	THR	PRO	GLY	GLY	GLY	GLY			GLY	VAL	GLU	GLU	LEU
ILE	ILE	ILE	ALA	LEU	LEU	LEU	LEU	S382	U280	GLY	VAL	GLU	CYS	LYS
ASP	ASP	ASP	THR	ARG	THR	THR	ARG			GLU	ARG	LEU	LEU	LEU
ASP	ASP	GLY	GLY	SER	GLY	SER	SER	L302		ARG	ARG	LEU	LEU	LEU
GLU	GLU	SER	SER	LEU	LEU	LEU	LEU			THR	THR	ARG	LEU	LEU
HIS	HIS	ARG	ARG	GLN	GLN	GLN	ILE	R306		ARG	ARG	GLU	GLY	GLY
PHE	PHE	SER	SER	GLU	GLU	GLU	GLU			GLU	VAL	VAL	LEU	ASP
PHE	PHE	GLN	GLN	ARG	ARG	ALA	ALA			HIS	LEU	LEU	SER	SER
PRO	PRO	SER	SER	LEU	LEU	LEU	LEU	M317		LEU	ASN	LYS	ASP	ASP
GLU	GLU	PRO	PRO	MET	MET	PRO	LEU			LEU	ASN	LYS	ASP	ASP
LEU	LEU	ALA	ALA	ILE	ILE	ALA	ILE			ALA	LYS	ILE	ASP	ASP
PRO	PRO	PRO	LEU	ALA	ALA	ALA	ALA	S321		ALA	LYS	LYS	GLY	GLY
GLU	GLU	GLU	VAL	LEU	LEU	LEU	LEU	Y322		MET	GLN	ASN	GLY	GLY
LEU	LEU	PRO	VAL	VAL	VAL	GLU	GLU	ARG		ASP	ARG	ASN	ARG	ARG
LEU	LEU	HIS	HIS	GLU	GLU	SER	SER	E323		MET	ASP	GLU	MET	SER
LEU	LEU	SER	SER	ILE	ILE	GLY	GLY	M324		LYS	ASP	ARG	MET	MET
THR	THR	SER	SER	PRO	PRO	MET	MET	R325		VAL	THR	GLN	SER	SER
VAL	VAL	ALA	ALA	HIS	HIS	THR	TYR	V326		ARG	ASP	VAL	PRO	PRO
THR	THR	GLY	GLY	ASP	ASP	GLU	GLU	A327		ALA	ALA	LEU	THR	THR
ASP	ASP	ASP	ASP	GLN	GLN	LYS	LYS	A328		S223	ALA	LEU	THR	THR
ARG	ARG	LYS	LYS	LEU	LEU	GLY	GLY			S223	ALA	LEU	THR	THR
LEU	LEU	PRO	PRO	ARG	ARG	SER	SER	P331		L226	ARG	SER	PRO	PRO
ASN	ASN	SER	SER	ALA	ALA	ALA	ALA	K332		L226	ARG	SER	PRO	PRO
ARG	ARG	SER	SER	SER	SER	SER	SER			D229	THR	ILE	PRO	PRO
VAL	VAL	PRO	PRO	HIS	HIS	PRO	PRO			S230	PRO	LEU	ALA	ALA
LEU	LEU	LEU	LEU	MET	MET	ALA	ALA				GLY	VAL	GLY	GLY
VAL	VAL	HIS	HIS	GLY	GLY	GLY	GLY	M336		Y235	GLU	LYS	THR	THR
VAL	VAL	HIS	HIS	VAL	VAL	ASP	ASP			T236	LEU	ALA	VAL	VAL
ALA	ALA	GLY	GLY	GLY	GLY	GLY	GLY	S339		L237	SER	GLN	LYS	LYS
ALA	ALA	THR	THR	GLY	GLY	GLY	GLY	W340		L237	SER	GLN	VAL	VAL
ALA	ALA	SER	SER	HIS	HIS	GLY	GLY			H240	GLU	ALA	THR	THR
GLU	GLU	PRO	PRO	ASP	ASP	ALA	ALA	N341		H240	GLU	ALA	THR	THR
LEU	LEU	GLU	GLU	ALA	ALA	SER	SER			F241	GLN	ALA	ALA	ARG
LEU	LEU	GLU	GLU	LYS	LYS	GLY	GLY	I346		F241	GLN	ALA	ALA	ARG
ASP	ASP	HIS	HIS	GLY	GLY	GLU	GLU	SER		E243	TYR	GLY	GLY	GLY
ALA	ALA	GLY	GLY	ALA	ALA	GLU	GLU			N244	ILE	ILE	GLY	GLY
GLN	GLN	HIS	HIS	ARG	ARG	ARG	ARG	A349		N244	ILE	ILE	GLY	GLY
GLU	GLU	GLY	GLY	ALA	ALA	THR	THR	D350		R245	GLN	ALA	PRO	PRO
								T351		R245	GLN	ALA	ALA	ALA
								P352		A246	GLN	ALA	ALA	ALA
								E353						

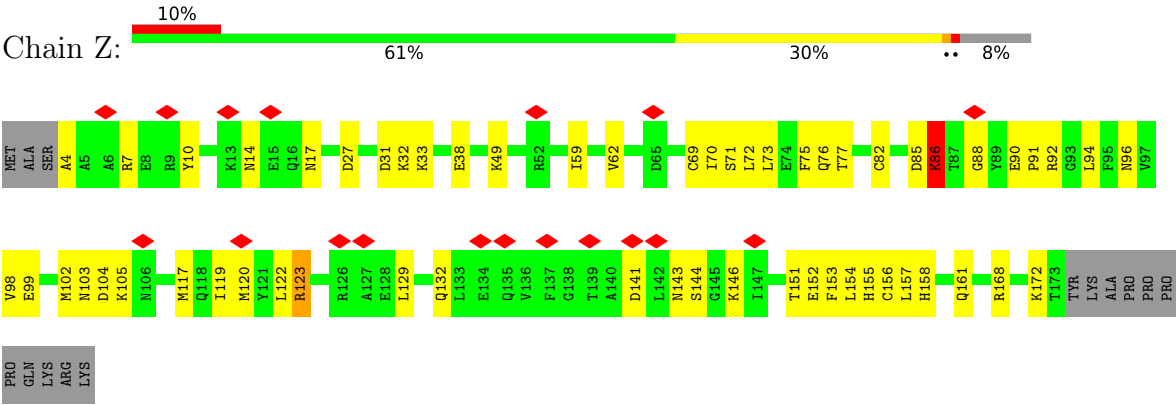
GLY	VAL	VAL	ASP	ASP	TYR	ILE	LYS	LEU	ARG	ALA	LEU	LYS	MET	SER	GLN	ARG	LEU	ALA	ASN	GLN	GLN	ARG	ALA	ILE	LYS	VAL
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

Chain X1:  14% 5% 81%

LEU
ARG
ALA
LEU
LYS
MET
SER
GLN
ARG
LEU
ALA
ASN
GLN
GLN
ARG
ALA
ILE
LYS
VAL

Chain Y: 

MET	PRO	SER	SER	ALA	ALA	ASP	THR	ARG	GLY	GLY	SER	ALA	GLY	LYS	THR	LEU	ALA	ALA	GLY	ASP	THR	LEU	GLY	HIS	LYS	SER	VAL	LEU	ASP	LYS	GLN	ARG	ALA	ALA	ILE	GLI	GLY	LYS	LEU	ARG	LYS	THR	GLY	LEU	LEU	ASN	GLI	GLN	LEU	LEU	LEU	GLY	ASN	LYS	THR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=0°, rise=82 Å, axial sym=C1	Depositor
Number of segments used	485694	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	61.48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.121	Depositor
Minimum map value	0.000	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	394.4, 394.4, 394.4	wwPDB
Map dimensions	290, 290, 290	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	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: GDP, GTP, MG

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	A1	0.17	0/3420	0.47	0/4628
1	A3	0.22	0/3420	0.50	0/4628
1	A5	0.20	0/3420	0.47	0/4628
1	A7	0.17	0/3420	0.46	0/4628
1	B1	0.19	0/3371	0.43	0/4561
1	B3	0.22	0/3295	0.44	0/4454
1	B5	0.22	0/3420	0.45	0/4628
1	B7	0.21	0/3420	0.45	0/4628
2	A2	0.22	0/3410	0.50	2/4623 (0.0%)
2	A4	0.32	0/3389	0.60	0/4595
2	A6	0.26	0/3406	0.53	0/4618
2	B2	0.22	0/3271	0.48	0/4434
2	B4	0.22	0/3260	0.47	0/4418
2	B6	0.21	0/3389	0.47	0/4595
3	C	0.18	0/1796	0.46	0/2418
4	X	0.19	0/987	0.56	2/1341 (0.1%)
4	X1	0.35	0/1186	0.66	2/1582 (0.1%)
5	Y	0.21	0/846	0.52	0/1132
5	Y1	0.27	0/1192	0.57	0/1585
6	Z	0.37	0/1403	0.89	2/1885 (0.1%)
All	All	0.23	0/54721	0.51	8/74009 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	86	LYS	CA-C-N	-6.78	111.91	122.08
6	Z	86	LYS	C-N-CA	-6.78	111.91	122.08
4	X	331	PRO	N-CA-CB	6.32	110.28	103.33
4	X	352	PRO	N-CA-CB	6.22	110.17	103.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X1	218	MET	N-CA-C	-5.54	105.40	111.82

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	A1	3346	0	3238	122	0
1	A3	3346	0	3238	115	0
1	A5	3346	0	3238	117	0
1	A7	3346	0	3238	99	0
1	B1	3298	0	3196	91	0
1	B3	3227	0	3134	85	0
1	B5	3346	0	3238	111	0
1	B7	3346	0	3238	102	0
2	A2	3339	0	3272	108	0
2	A4	3318	0	3259	102	0
2	A6	3335	0	3269	108	0
2	B2	3204	0	3152	86	0
2	B4	3193	0	3141	107	0
2	B6	3318	0	3259	85	0
3	C	1771	0	1781	49	0
4	X	985	0	714	20	0
4	X1	1178	0	1179	31	0
5	Y	844	0	735	24	0
5	Y1	1185	0	1230	38	0
6	Z	1384	0	1359	48	0
7	A1	32	0	12	0	0
7	A3	32	0	12	1	0
7	A5	32	0	12	1	0
7	A7	32	0	12	4	0
7	B2	32	0	12	1	0
7	B5	32	0	12	0	0
7	B7	32	0	12	0	0
8	A1	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A2	1	0	0	0	0
8	A4	1	0	0	0	0
8	A6	1	0	0	0	0
8	B3	1	0	0	0	0
8	B4	1	0	0	0	0
8	B6	1	0	0	0	0
9	A1	28	0	12	0	0
9	A3	28	0	12	2	0
9	A5	28	0	12	0	0
9	A7	28	0	12	2	0
9	B1	28	0	12	3	0
9	B3	28	0	12	2	0
9	B5	28	0	12	1	0
9	B7	28	0	12	2	0
All	All	54110	0	52288	1495	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 14.

The worst 5 of 1495 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A7:200:MET:HE1	1:A7:368:ILE:HD12	1.54	0.90
1:A3:215:LEU:HB3	1:A3:217:LEU:HD13	1.54	0.90
1:B5:175:VAL:HG22	2:B6:329:ASN:HD21	1.35	0.87
1:B5:102:ALA:HB2	1:B5:403:MET:HE1	1.57	0.86
1:B7:113:ILE:HD13	1:B7:150:LEU:HD11	1.55	0.85

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	A1	424/443 (96%)	399 (94%)	25 (6%)	0	100	100
1	A3	424/443 (96%)	405 (96%)	19 (4%)	0	100	100
1	A5	424/443 (96%)	407 (96%)	17 (4%)	0	100	100
1	A7	424/443 (96%)	405 (96%)	19 (4%)	0	100	100
1	B1	415/443 (94%)	396 (95%)	19 (5%)	0	100	100
1	B3	404/443 (91%)	392 (97%)	12 (3%)	0	100	100
1	B5	424/443 (96%)	403 (95%)	21 (5%)	0	100	100
1	B7	424/443 (96%)	405 (96%)	19 (4%)	0	100	100
2	A2	426/451 (94%)	402 (94%)	24 (6%)	0	100	100
2	A4	423/451 (94%)	409 (97%)	14 (3%)	0	100	100
2	A6	425/451 (94%)	408 (96%)	17 (4%)	0	100	100
2	B2	405/451 (90%)	391 (96%)	14 (4%)	0	100	100
2	B4	403/451 (89%)	385 (96%)	18 (4%)	0	100	100
2	B6	423/451 (94%)	407 (96%)	16 (4%)	0	100	100
3	C	210/4485 (5%)	204 (97%)	6 (3%)	0	100	100
4	X	151/749 (20%)	151 (100%)	0	0	100	100
4	X1	140/749 (19%)	140 (100%)	0	0	100	100
5	Y	117/552 (21%)	116 (99%)	1 (1%)	0	100	100
5	Y1	145/552 (26%)	145 (100%)	0	0	100	100
6	Z	168/184 (91%)	156 (93%)	10 (6%)	2 (1%)	10	37
All	All	6799/13521 (50%)	6526 (96%)	271 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	Z	86	LYS
6	Z	141	ASP

5.3.2 Protein sidechains ⓘ

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	A1	367/379 (97%)	367 (100%)	0	100	100
1	A3	367/379 (97%)	367 (100%)	0	100	100
1	A5	367/379 (97%)	367 (100%)	0	100	100
1	A7	367/379 (97%)	367 (100%)	0	100	100
1	B1	363/379 (96%)	363 (100%)	0	100	100
1	B3	356/379 (94%)	356 (100%)	0	100	100
1	B5	367/379 (97%)	367 (100%)	0	100	100
1	B7	367/379 (97%)	365 (100%)	2 (0%)	81	83
2	A2	361/374 (96%)	360 (100%)	1 (0%)	86	86
2	A4	359/374 (96%)	355 (99%)	4 (1%)	65	76
2	A6	361/374 (96%)	361 (100%)	0	100	100
2	B2	347/374 (93%)	346 (100%)	1 (0%)	86	86
2	B4	346/374 (92%)	346 (100%)	0	100	100
2	B6	359/374 (96%)	359 (100%)	0	100	100
3	C	197/3945 (5%)	197 (100%)	0	100	100
4	X	50/618 (8%)	50 (100%)	0	100	100
4	X1	125/618 (20%)	121 (97%)	4 (3%)	34	60
5	Y	63/462 (14%)	63 (100%)	0	100	100
5	Y1	128/462 (28%)	127 (99%)	1 (1%)	73	79
6	Z	150/162 (93%)	146 (97%)	4 (3%)	39	63
All	All	5767/11543 (50%)	5750 (100%)	17 (0%)	84	86

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	Z	122	LEU
6	Z	129	LEU
1	B7	72	THR
4	X1	204	LEU
4	X1	208	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 93 such sidechains are listed below:

Mol	Chain	Res	Type
2	B4	206	ASN

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Mol	Chain	Res	Type
1	B5	384	GLN
2	B4	329	ASN
1	B5	100	ASN
2	B6	101	ASN

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 22 ligands modelled in this entry, 7 are monoatomic - leaving 15 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$
9	GDP	A1	503	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	7 (15%)
9	GDP	B7	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.84	8 (17%)
9	GDP	B1	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.81	7 (15%)
9	GDP	B3	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	7 (15%)
7	GTP	A7	501	8	33,34,34	0.93	1 (3%)	50,54,54	1.55	8 (16%)
9	GDP	A5	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.81	8 (17%)
7	GTP	A3	501	8	33,34,34	0.88	1 (3%)	50,54,54	1.58	9 (18%)
9	GDP	A7	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GTP	B7	501	8	33,34,34	0.94	1 (3%)	50,54,54	1.59	8 (16%)
9	GDP	A3	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.81	8 (17%)
9	GDP	B5	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.79	6 (13%)
7	GTP	B2	501	8	33,34,34	0.84	1 (3%)	50,54,54	1.62	9 (18%)
7	GTP	A5	501	8	33,34,34	0.90	1 (3%)	50,54,54	1.56	8 (16%)
7	GTP	A1	501	8	33,34,34	0.93	1 (3%)	50,54,54	1.57	8 (16%)
7	GTP	B5	501	8	33,34,34	0.92	1 (3%)	50,54,54	1.58	8 (16%)

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
9	GDP	A1	503	-	-	3/16/32/32	0/3/3/3
9	GDP	B7	502	-	-	6/16/32/32	0/3/3/3
9	GDP	B1	501	-	-	2/16/32/32	0/3/3/3
9	GDP	B3	502	-	-	3/16/32/32	0/3/3/3
7	GTP	A7	501	8	-	8/22/38/38	0/3/3/3
9	GDP	A5	502	-	-	1/16/32/32	0/3/3/3
7	GTP	A3	501	8	-	8/22/38/38	0/3/3/3
9	GDP	A7	502	-	-	4/16/32/32	0/3/3/3
7	GTP	B7	501	8	-	6/22/38/38	0/3/3/3
9	GDP	A3	502	-	-	1/16/32/32	0/3/3/3
9	GDP	B5	502	-	-	3/16/32/32	0/3/3/3
7	GTP	B2	501	8	-	4/22/38/38	0/3/3/3
7	GTP	A5	501	8	-	6/22/38/38	0/3/3/3
7	GTP	A1	501	8	-	5/22/38/38	0/3/3/3
7	GTP	B5	501	8	-	7/22/38/38	0/3/3/3

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B7	502	GDP	C5-C4	3.11	1.47	1.38
9	A1	503	GDP	C5-C4	3.06	1.47	1.38
9	A7	502	GDP	C5-C4	3.06	1.47	1.38
9	A3	502	GDP	C5-C4	3.05	1.47	1.38
9	B1	501	GDP	C5-C4	3.03	1.47	1.38

The worst 5 of 117 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B7	502	GDP	C5-C4-N3	-6.26	118.43	128.39
9	B1	501	GDP	C5-C4-N3	-6.25	118.44	128.39
9	A1	503	GDP	C5-C4-N3	-6.18	118.55	128.39
9	A3	502	GDP	C5-C4-N3	-6.15	118.61	128.39
9	A5	502	GDP	C5-C4-N3	-6.08	118.72	128.39

There are no chirality outliers.

5 of 67 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A1	501	GTP	C5'-O5'-PA-O3A
7	A1	501	GTP	C5'-O5'-PA-O1A
7	A3	501	GTP	C5'-O5'-PA-O3A
7	A3	501	GTP	C5'-O5'-PA-O1A
7	A3	501	GTP	C5'-O5'-PA-O2A

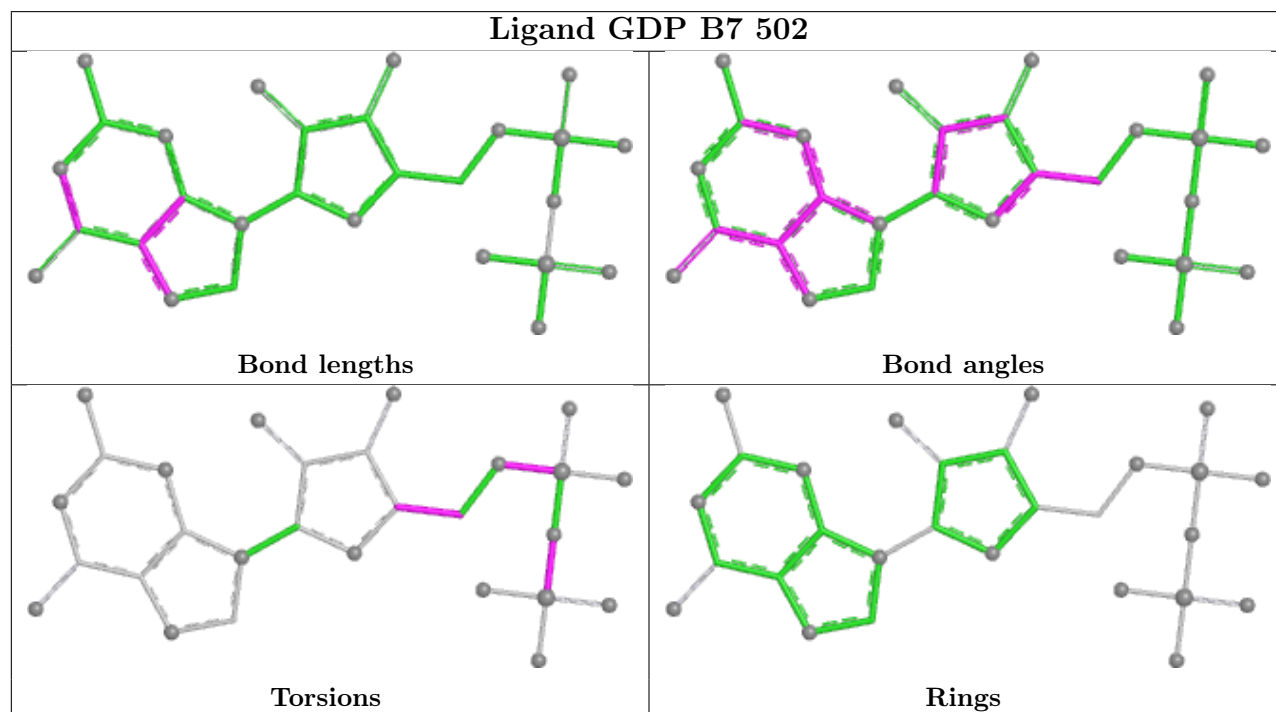
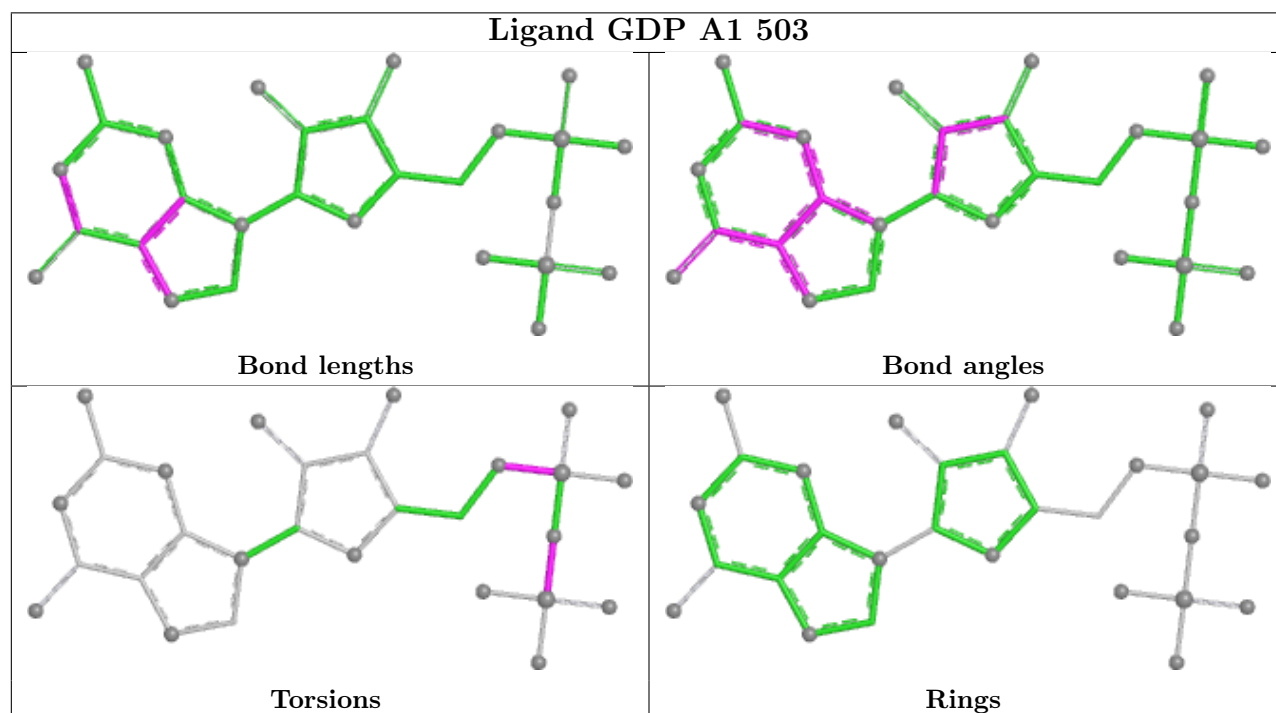
There are no ring outliers.

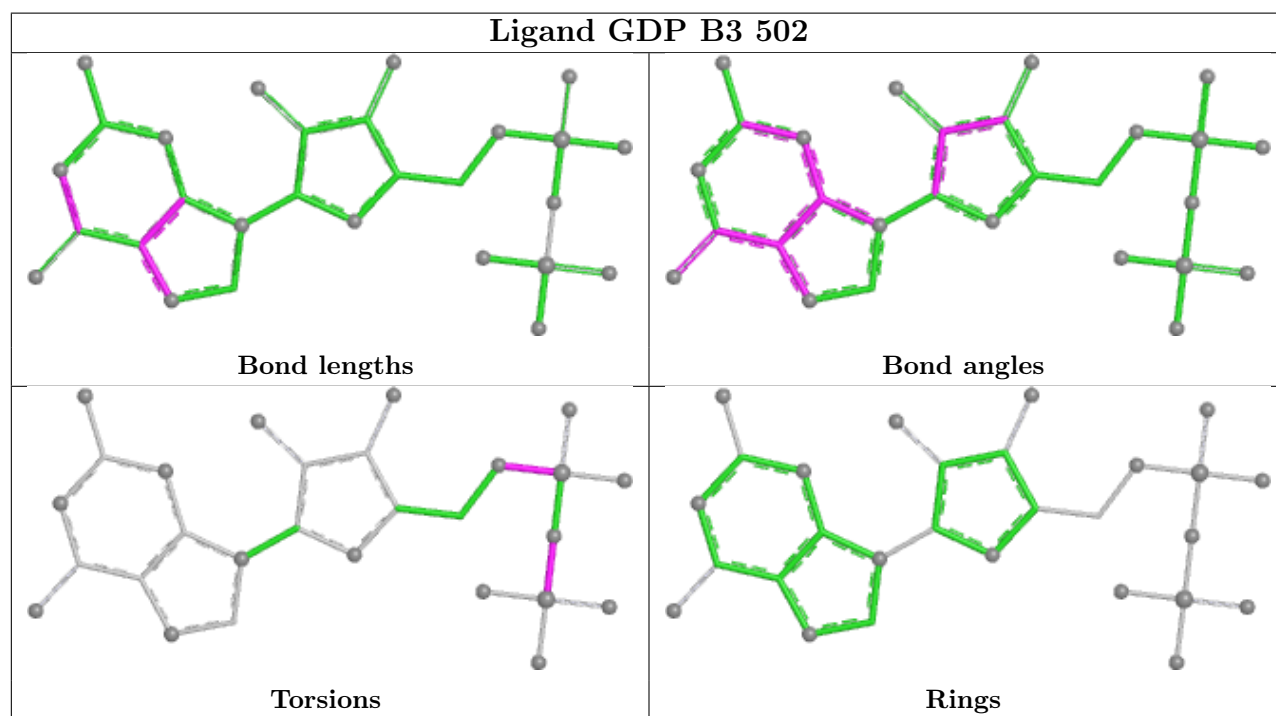
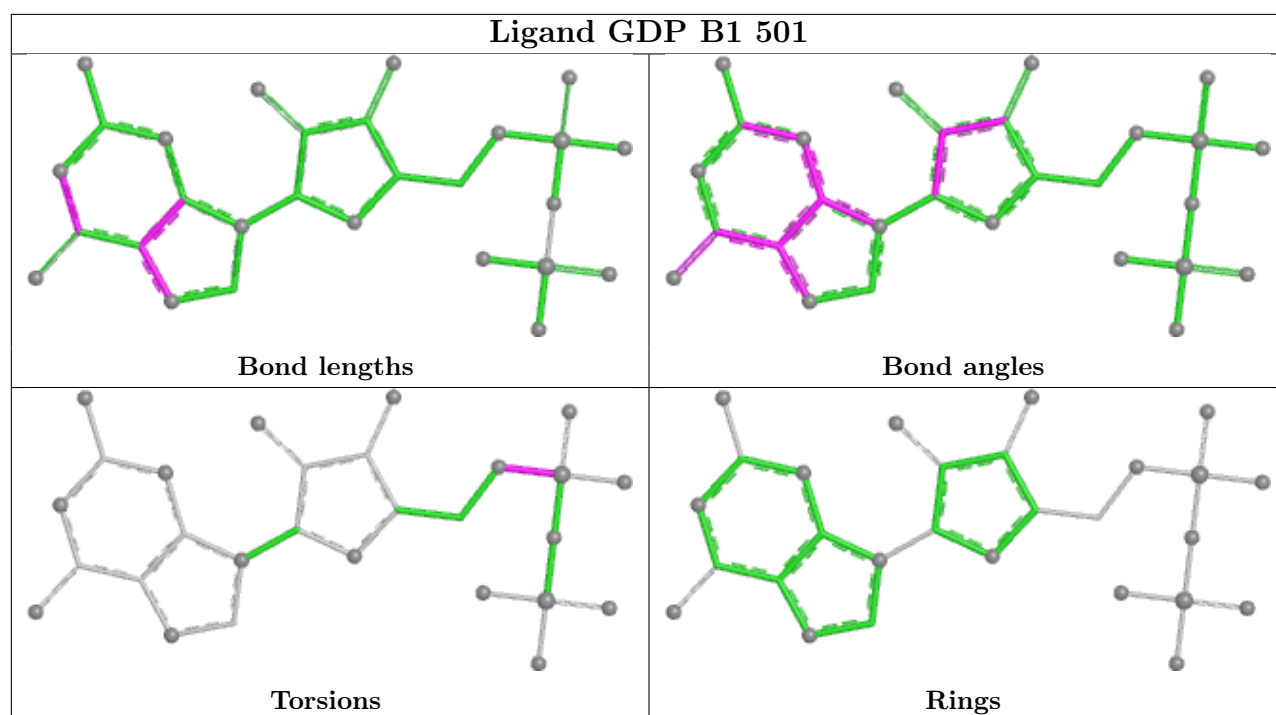
10 monomers are involved in 19 short contacts:

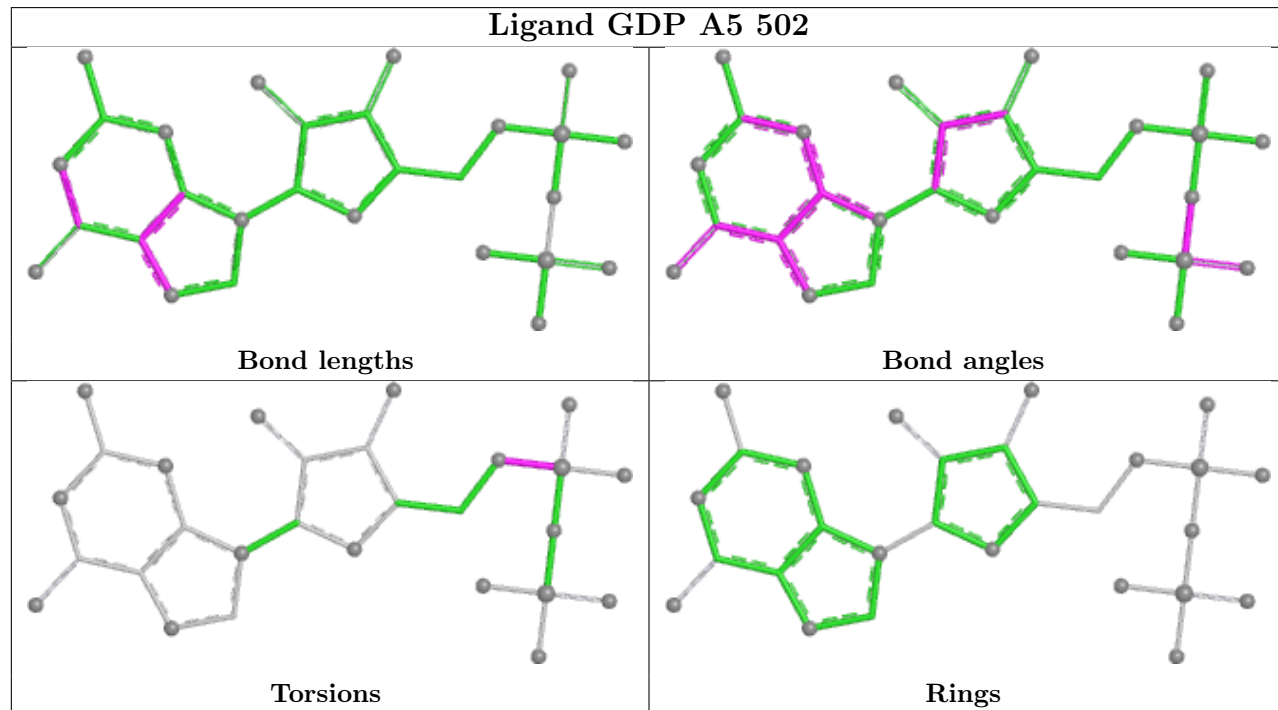
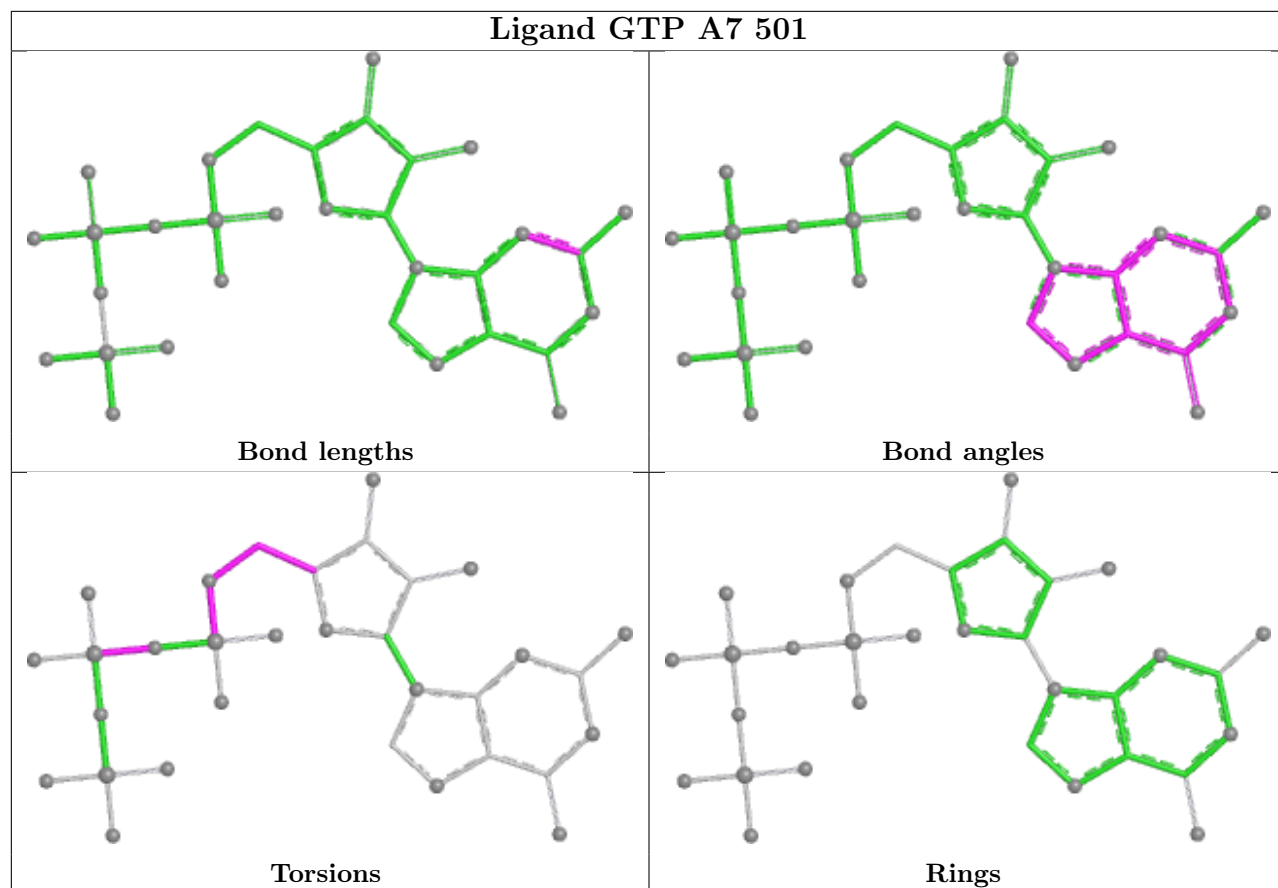
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B7	502	GDP	2	0
9	B1	501	GDP	3	0
9	B3	502	GDP	2	0
7	A7	501	GTP	4	0
7	A3	501	GTP	1	0
9	A7	502	GDP	2	0
9	A3	502	GDP	2	0
9	B5	502	GDP	1	0
7	B2	501	GTP	1	0
7	A5	501	GTP	1	0

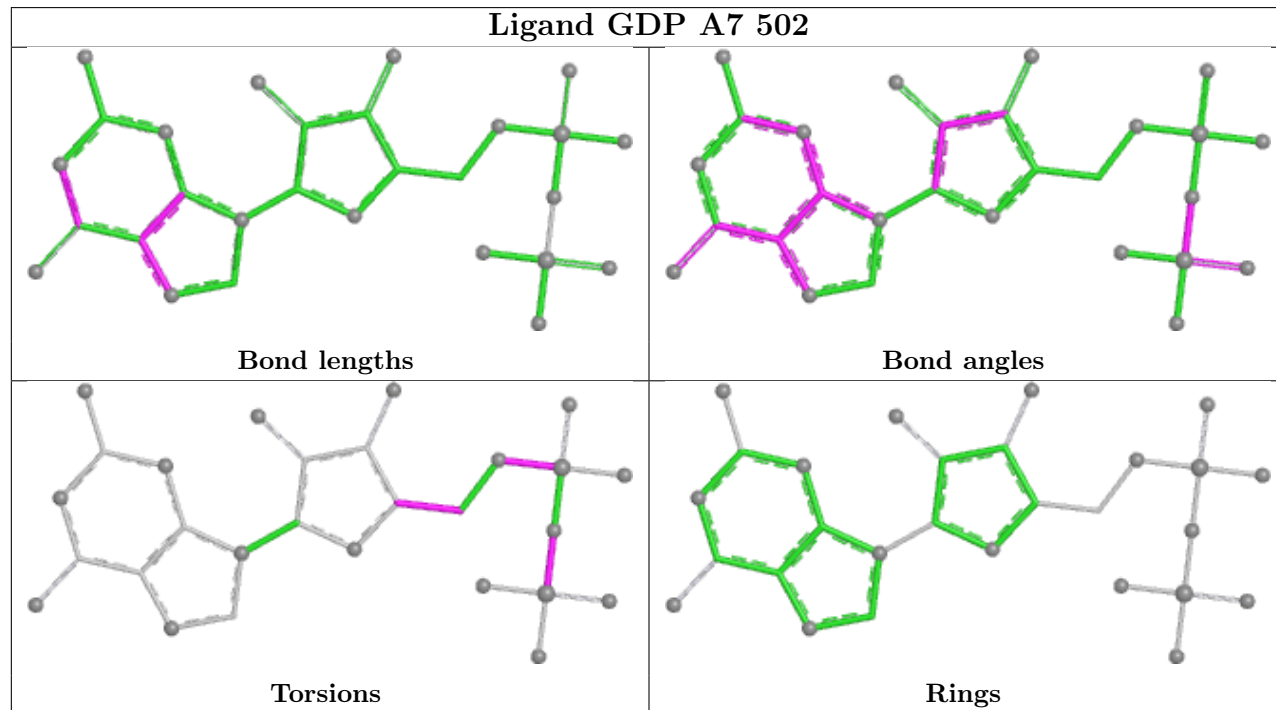
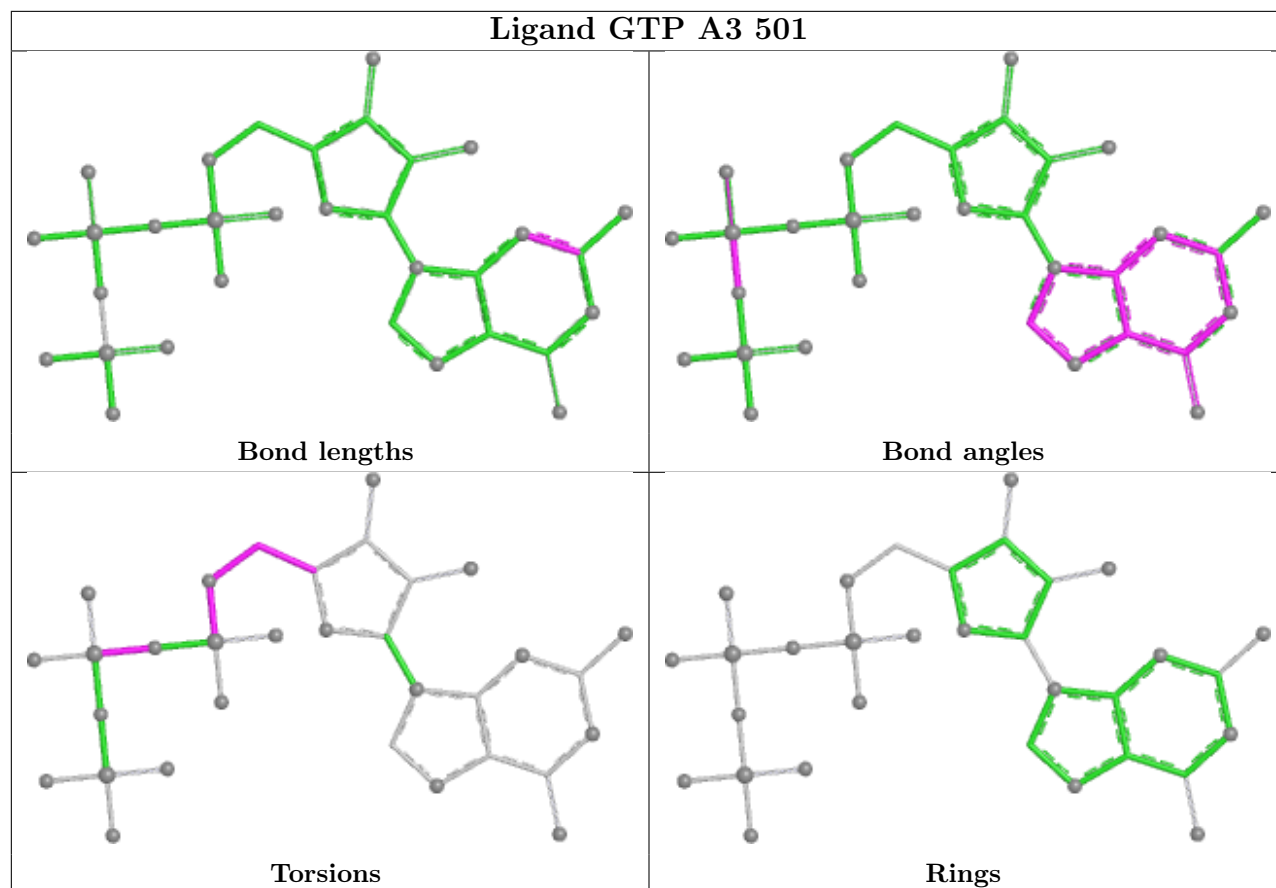
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

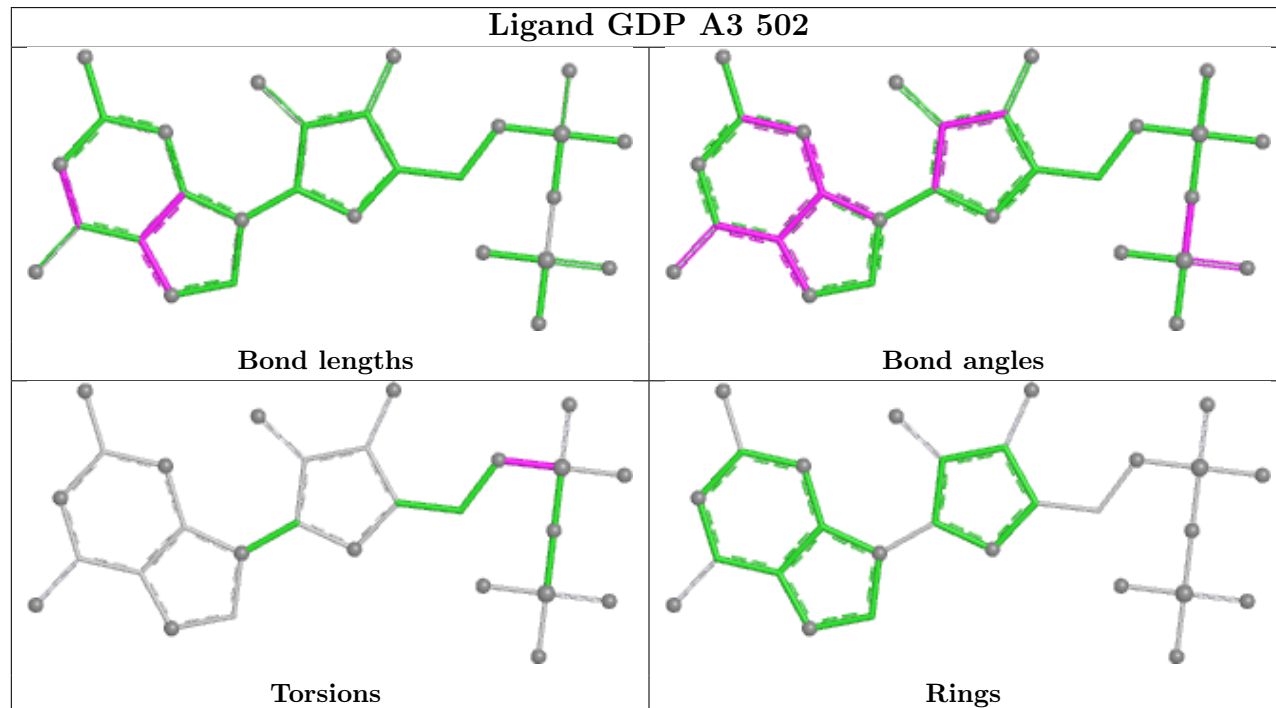
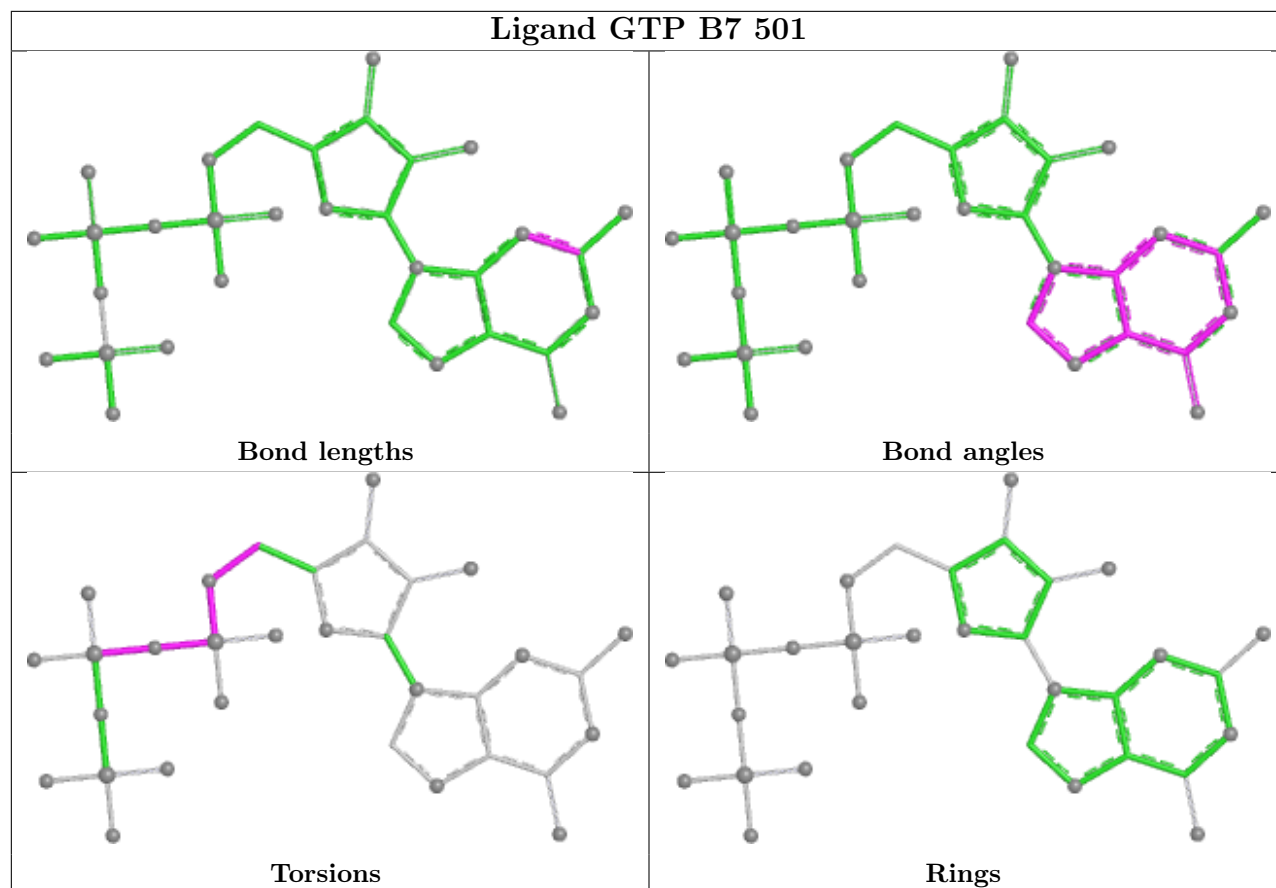
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

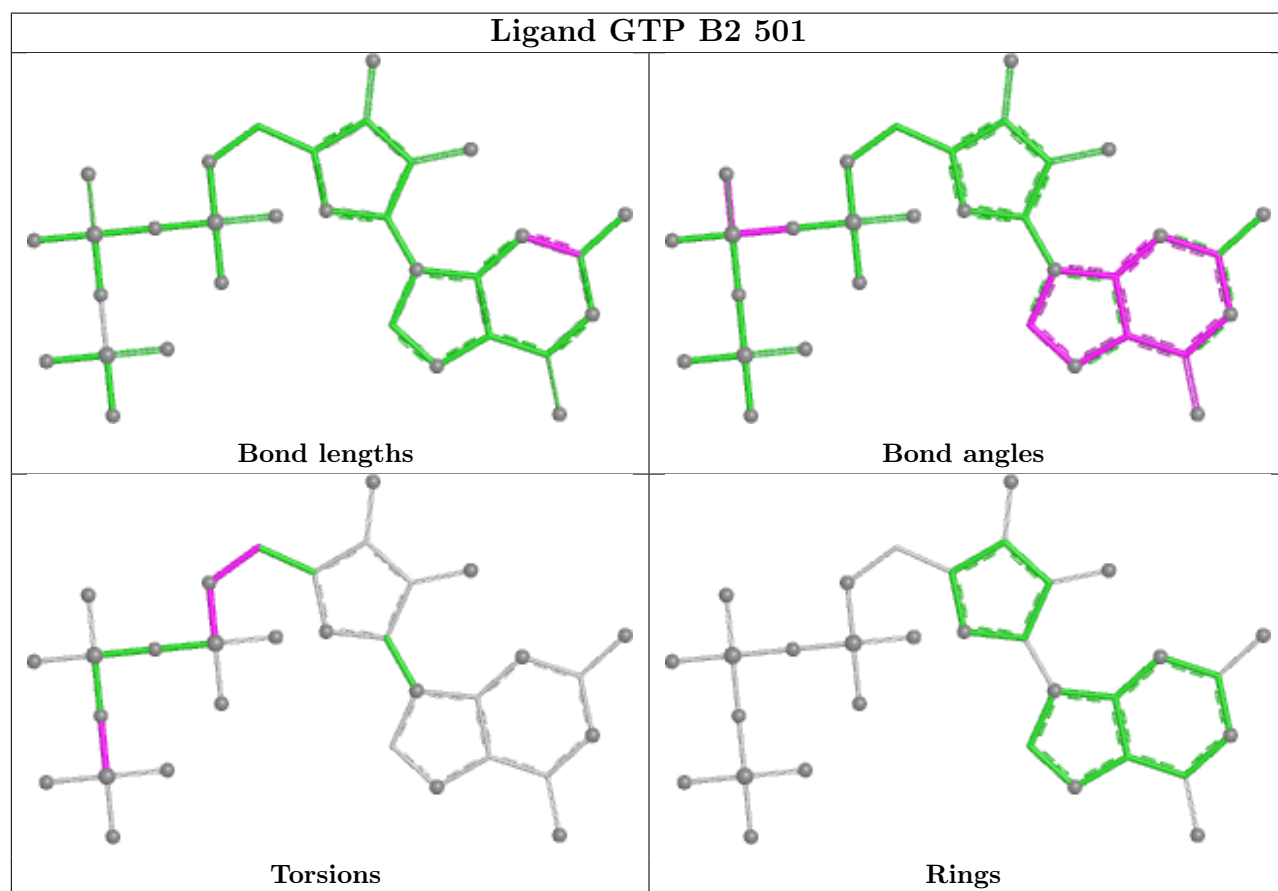
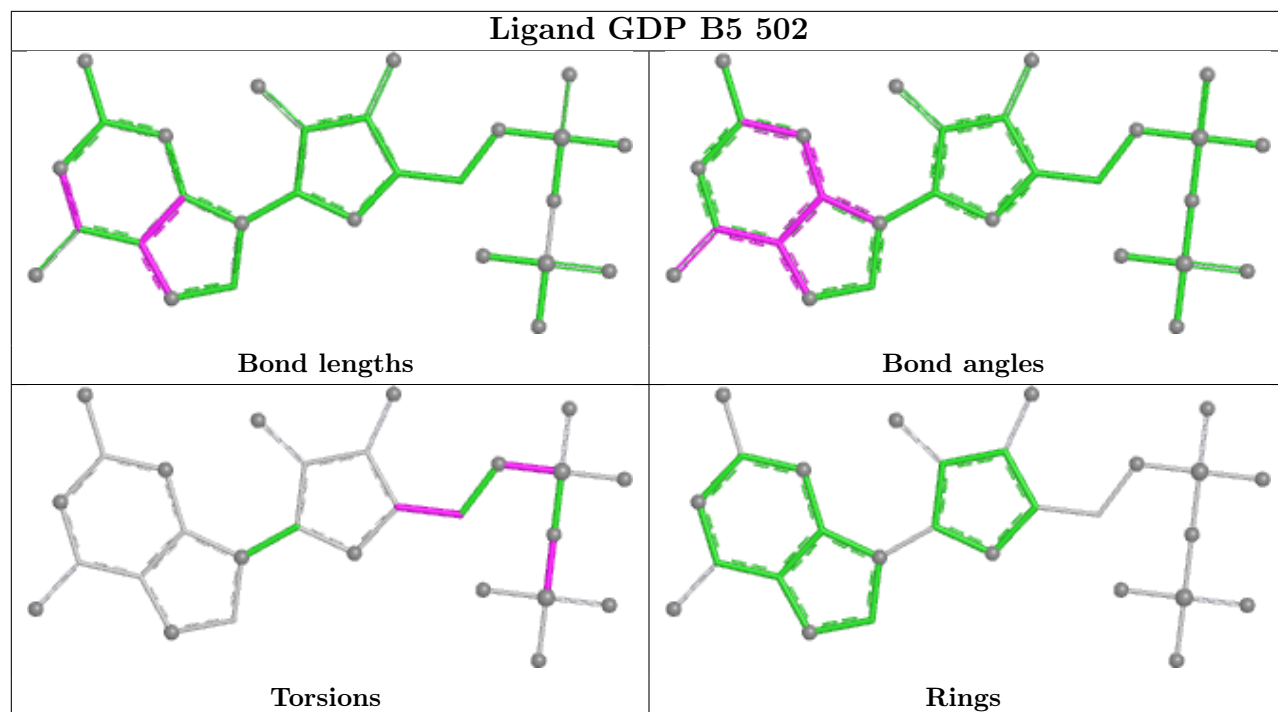


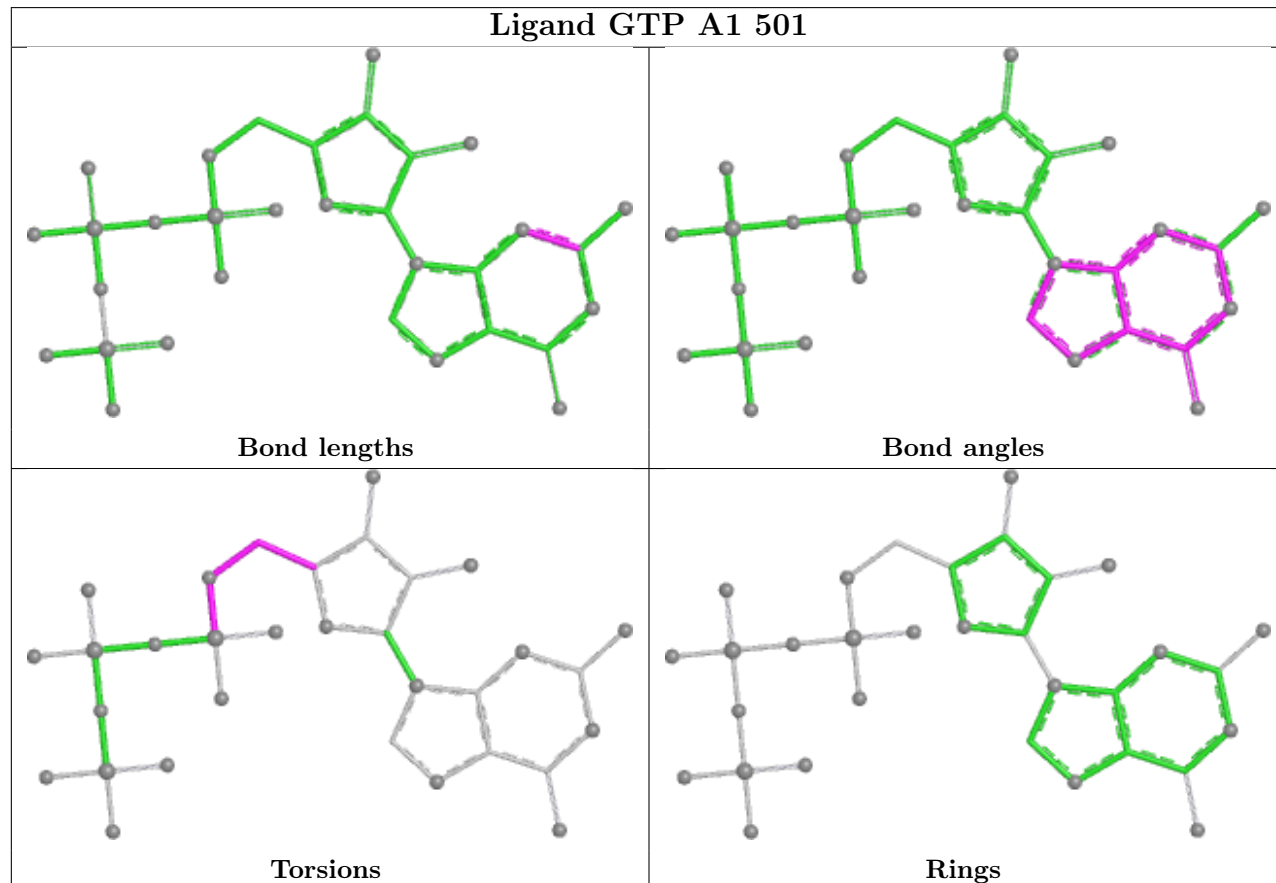
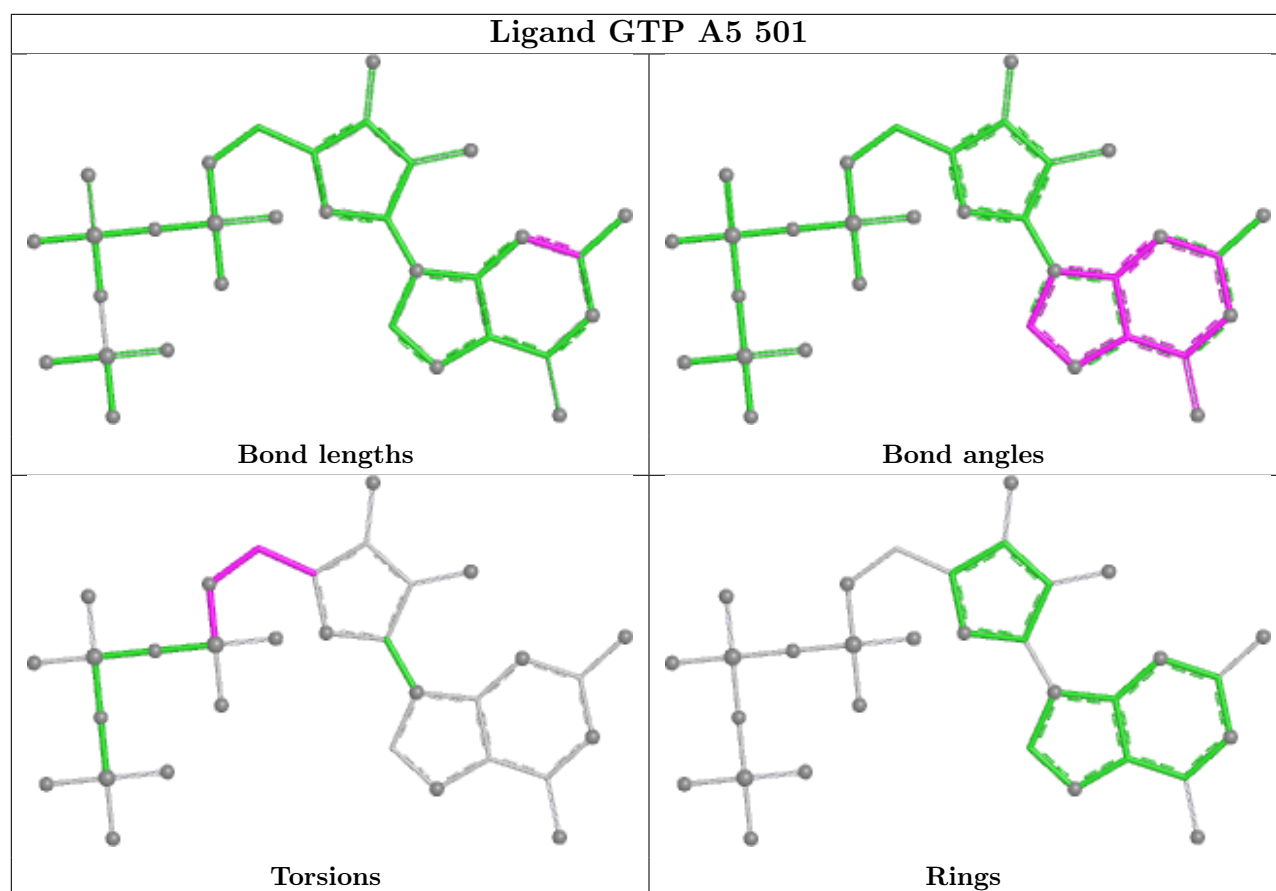


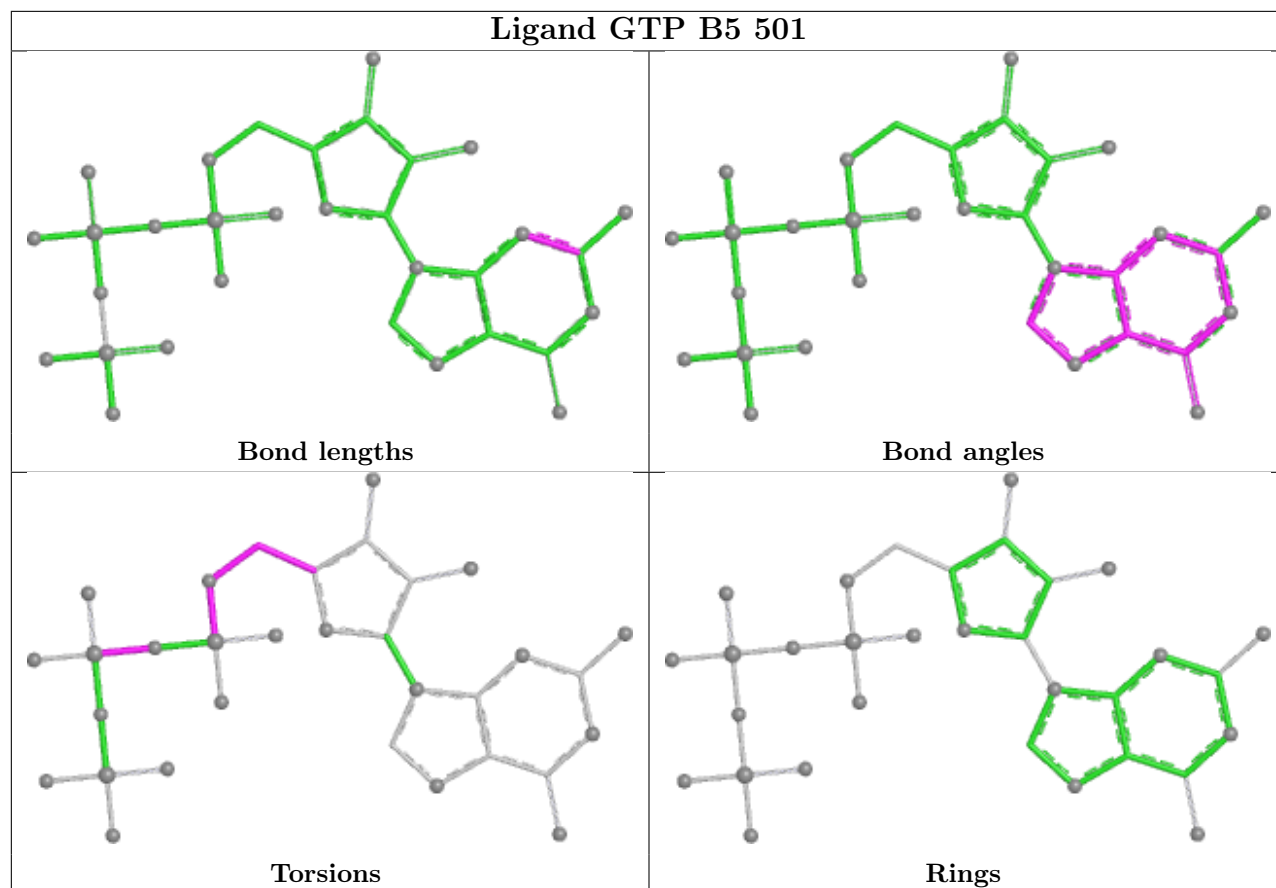












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

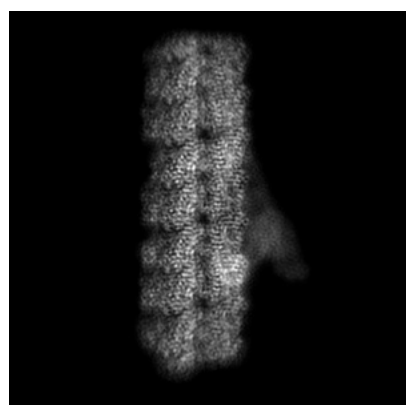
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23084. These allow visual inspection of the internal detail of the map and identification of artifacts.

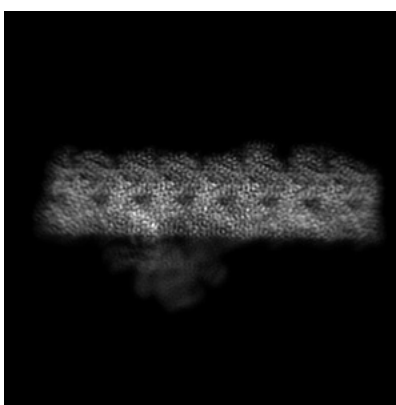
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

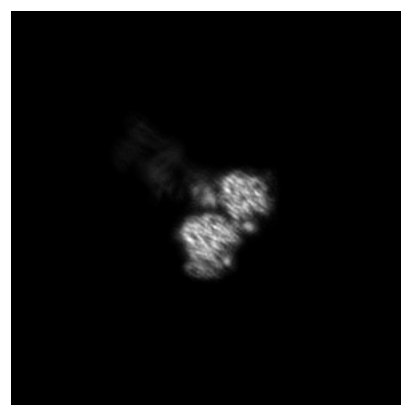
6.1.1 Primary map



X



Y

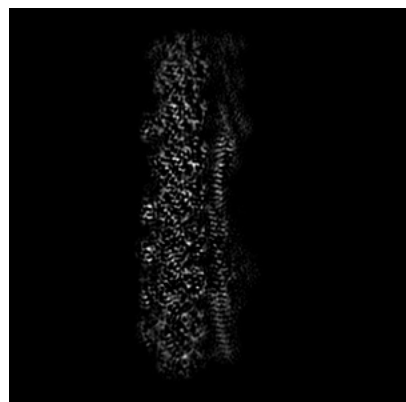


Z

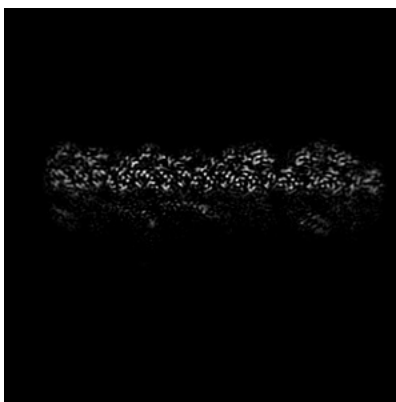
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

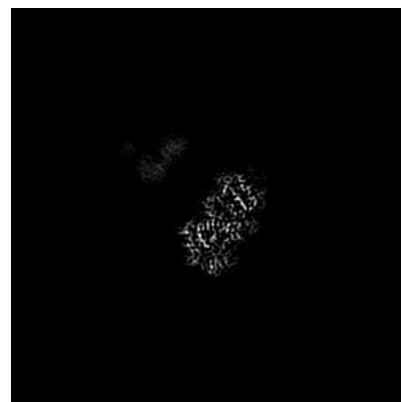
6.2.1 Primary map



X Index: 145



Y Index: 145



Z Index: 145

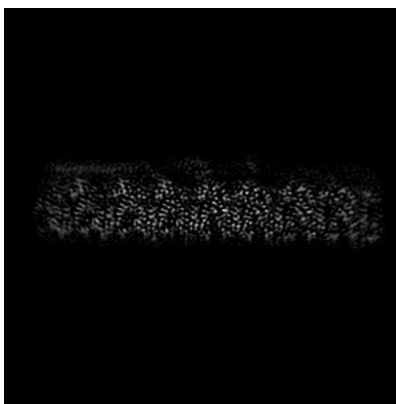
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

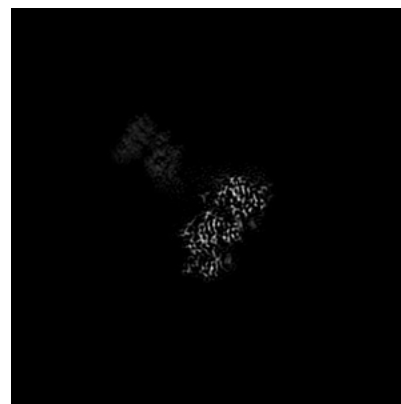
6.3.1 Primary map



X Index: 141



Y Index: 129

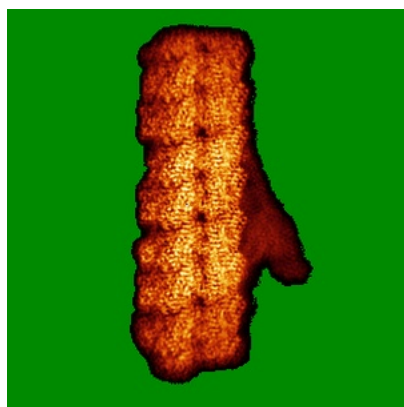


Z Index: 115

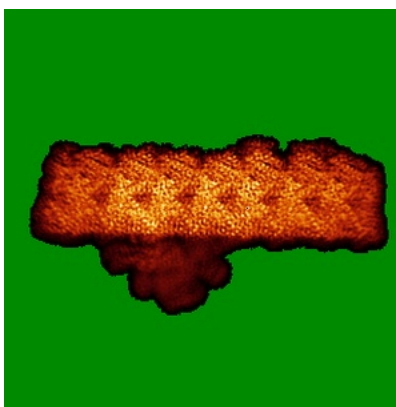
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

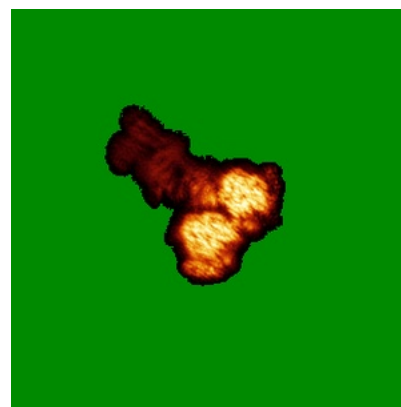
6.4.1 Primary map



X



Y



Z

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

This section was not generated.

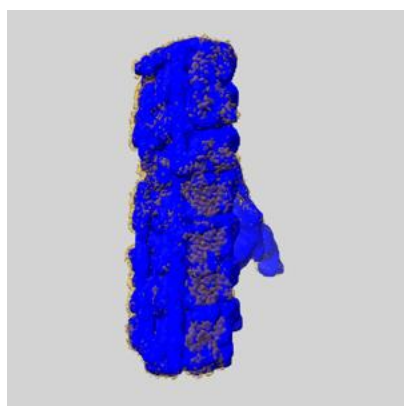
6.6 Mask visualisation [i](#)

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

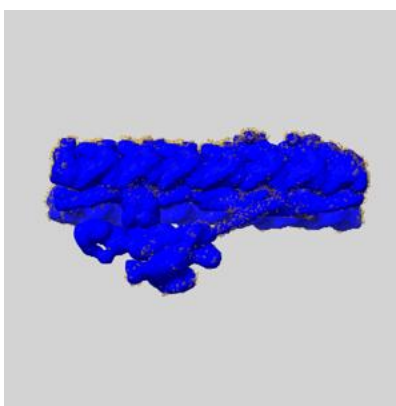
A mask typically either:

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

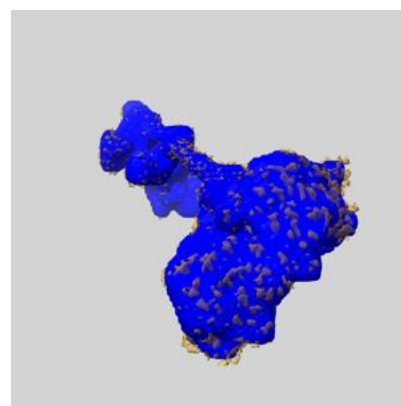
6.6.1 emd_23084_msk_1.map [i](#)



X



Y

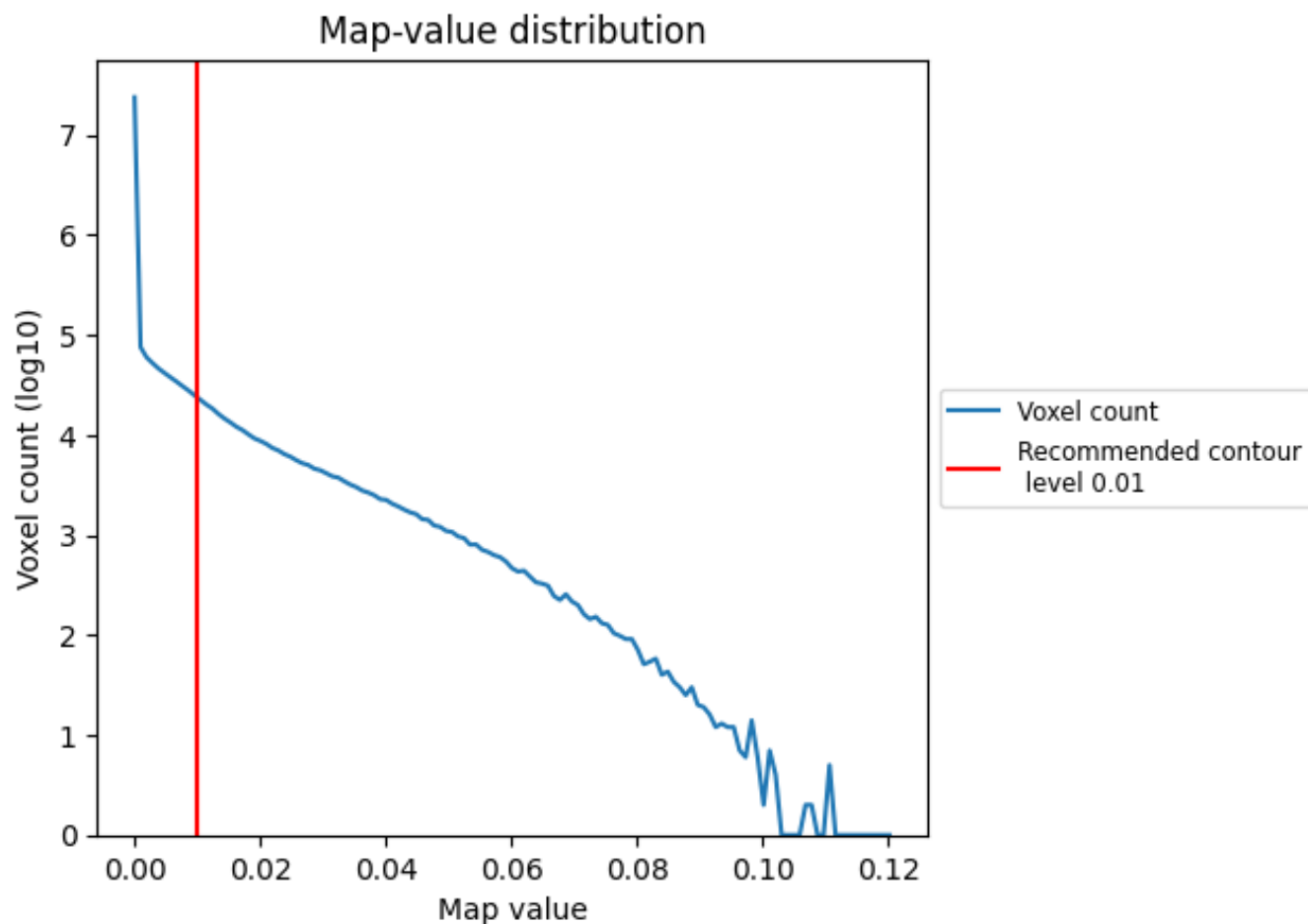


Z

7 Map analysis [i](#)

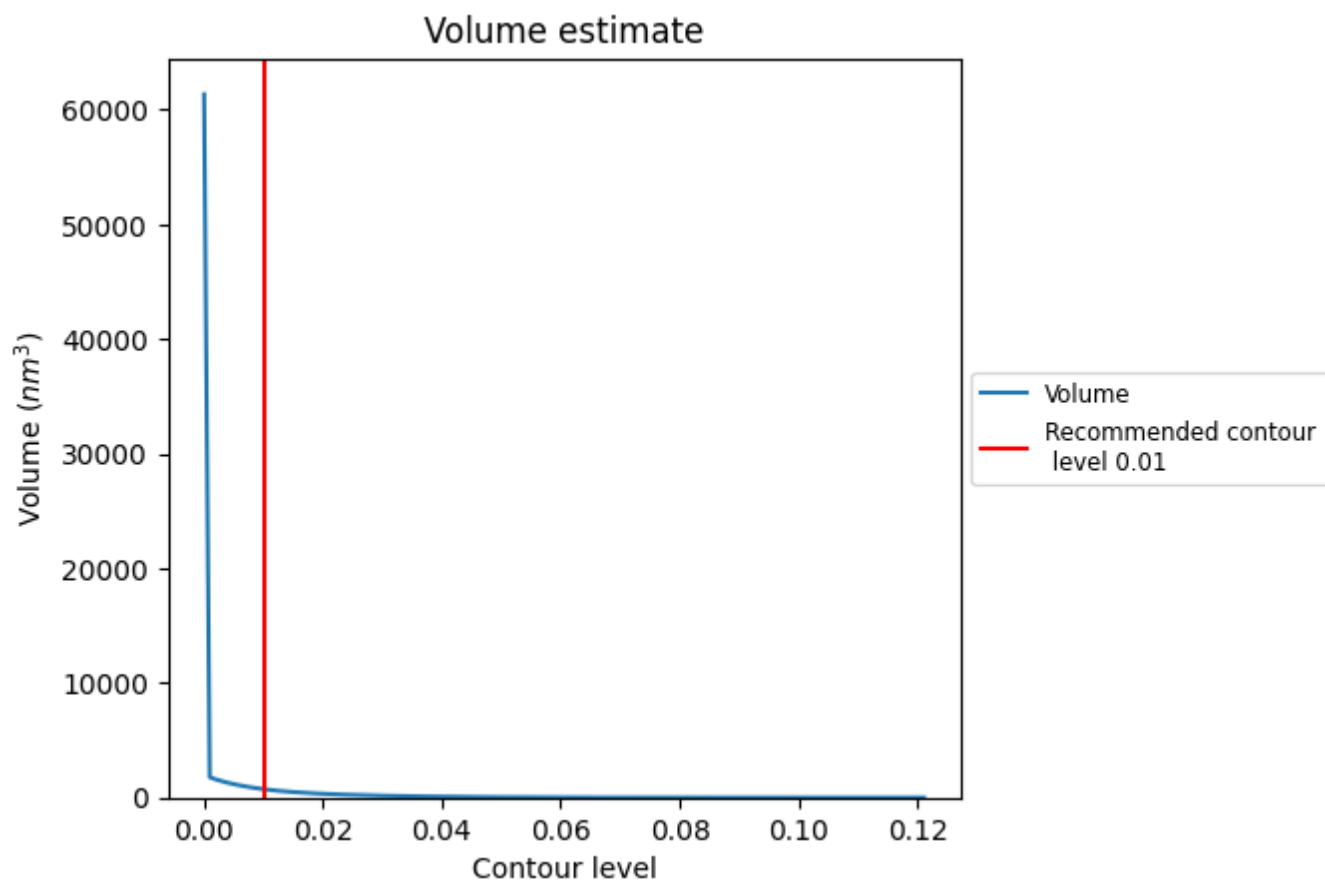
This section contains the results of statistical analysis of the map.

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.

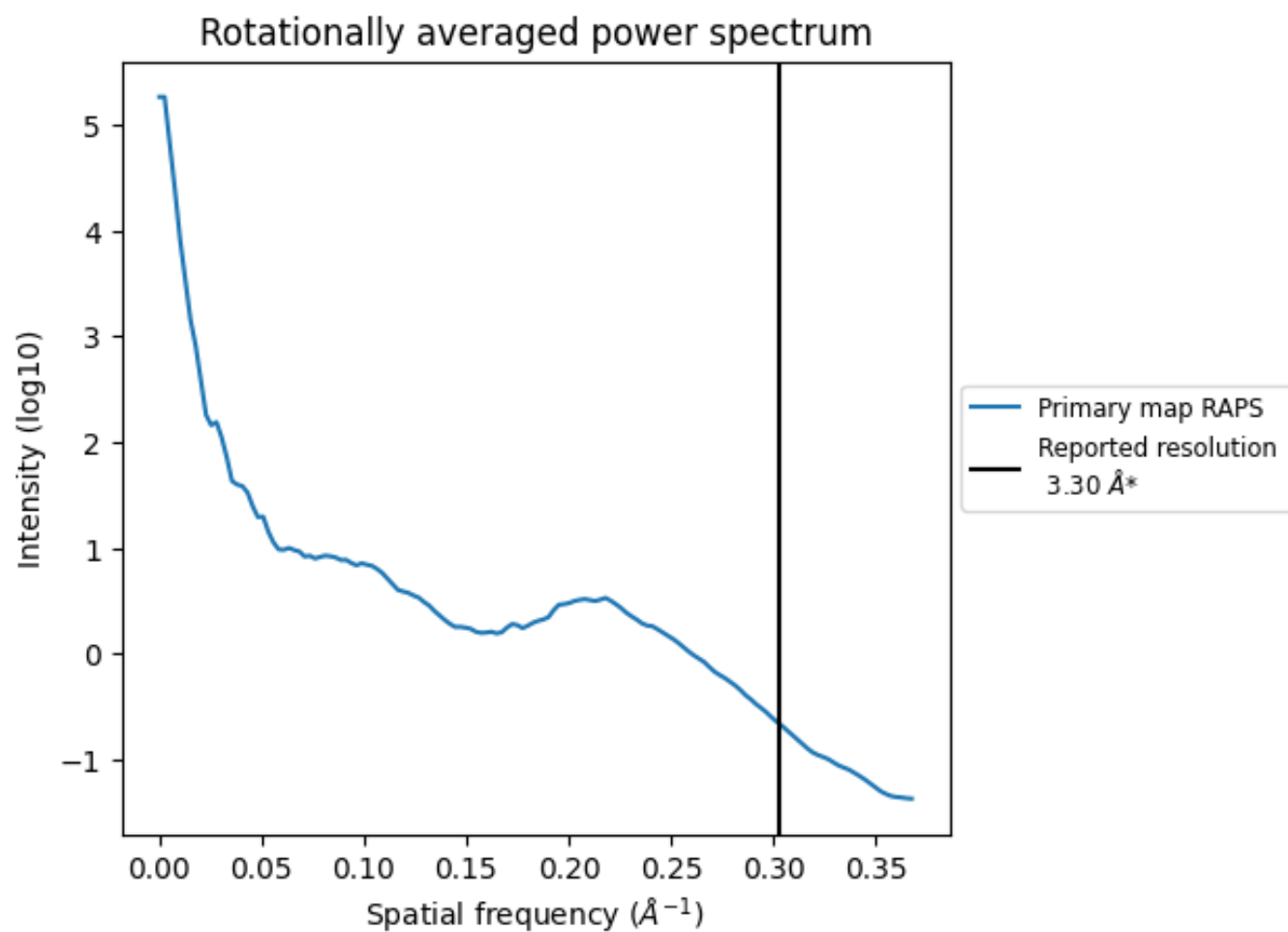
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 732 nm³; this corresponds to an approximate mass of 662 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

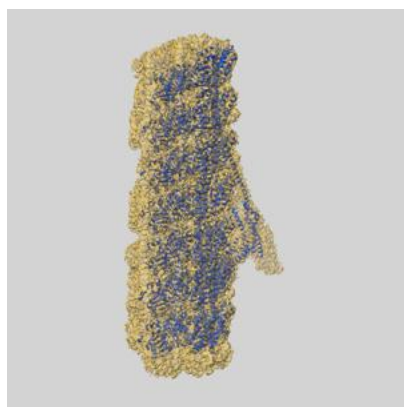
8 Fourier-Shell correlation ⓘ

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

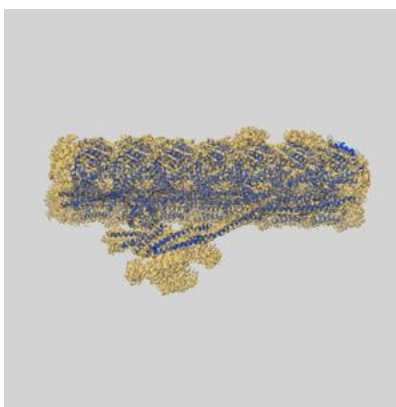
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23084 and PDB model 7KZO. Per-residue inclusion information can be found in section [3](#) on page [8](#).

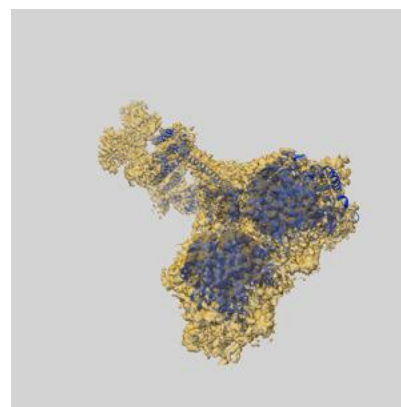
9.1 Map-model overlay [i](#)



X



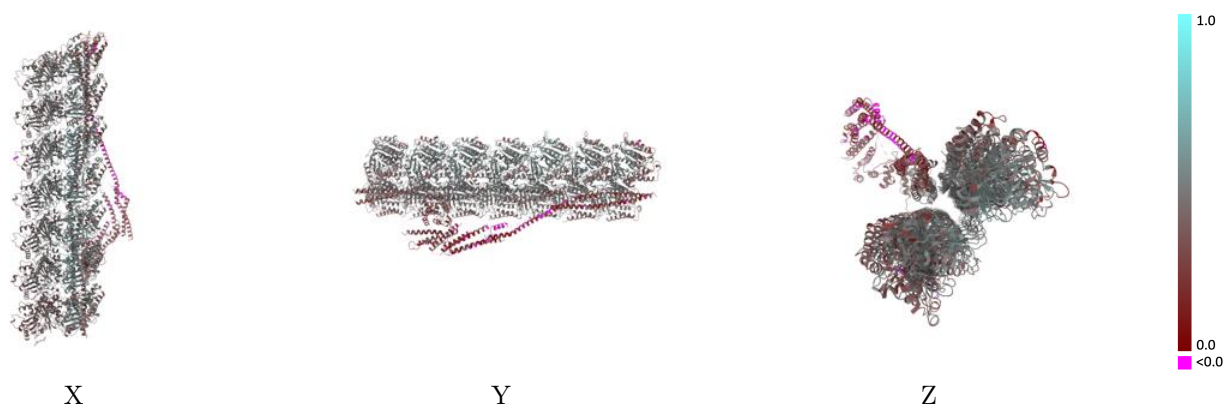
Y



Z

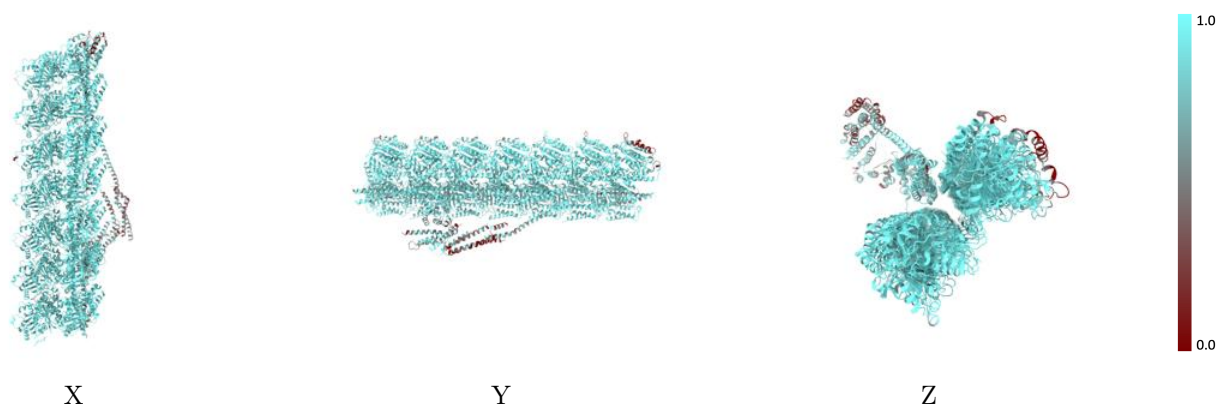
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



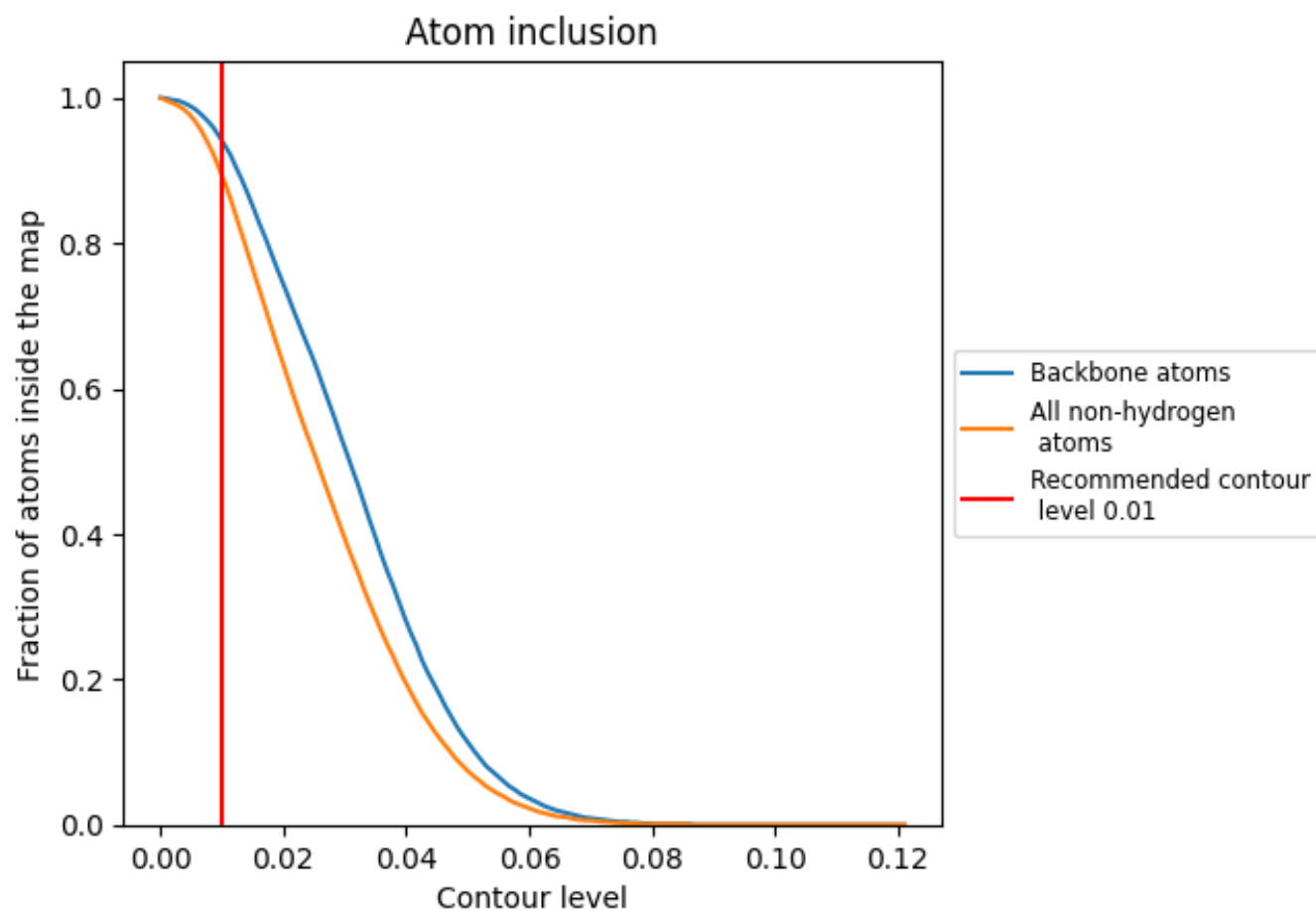
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8930	 0.4310
A1	 0.9070	 0.3880
A2	 0.9220	 0.4220
A3	 0.9280	 0.4350
A4	 0.9360	 0.4490
A5	 0.9310	 0.4500
A6	 0.9180	 0.4290
A7	 0.9180	 0.4230
B1	 0.9050	 0.4540
B2	 0.9220	 0.4920
B3	 0.9350	 0.5020
B4	 0.9290	 0.4950
B5	 0.9480	 0.5050
B6	 0.9200	 0.4760
B7	 0.8440	 0.4410
C	 0.6240	 0.2160
X	 0.6830	 0.1930
X1	 0.8400	 0.4150
Y	 0.6630	 0.2040
Y1	 0.8590	 0.4030
Z	 0.7190	 0.2770

