



wwPDB EM Validation Summary Report ⓘ

Nov 22, 2022 – 01:05 PM EST

PDB ID : 7UXH
EMDB ID : EMD-26861
Title : cryo-EM structure of the mTORC1-TFEB-Rag-Ragulator complex
Authors : Cui, Z.; Hurley, J.
Deposited on : 2022-05-05
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 ⓘ 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:

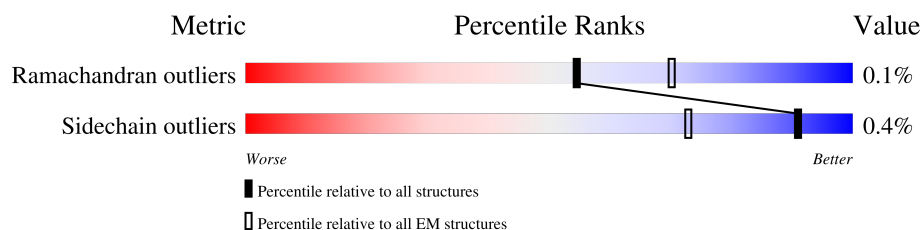
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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)
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 $\leq 5\%$. 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	A	2549	
1	C	2549	
2	B	326	
2	D	326	
3	E	1335	
3	U	1335	
4	F	313	
4	M	313	
4	V	313	



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Mol	Chain	Length	Quality of chain
4	c	313	
5	G	399	
5	N	399	
5	W	399	
5	d	399	
6	H	161	
6	O	161	
6	X	161	
6	e	161	
7	I	125	
7	P	125	
7	Y	125	
7	f	125	
8	J	124	
8	Q	124	
8	Z	124	
8	g	124	
9	K	99	
9	R	99	
9	a	99	
9	h	99	
10	L	91	
10	S	91	
10	b	91	
10	i	91	

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Mol	Chain	Length	Quality of chain
11	T	476	 22% 78%
11	j	476	 22% 78%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 190396 atoms, of which 95230 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	2188	Total	C	H	N	O	S	0	0
			35406	11226	17819	3080	3164	117		
1	C	2188	Total	C	H	N	O	S	0	0
			35404	11226	17817	3080	3164	117		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	317	Total	C	H	N	O	S	0	0
			4797	1526	2341	436	476	18		
2	D	317	Total	C	H	N	O	S	0	0
			4797	1526	2341	436	476	18		

- Molecule 3 is a protein called Regulatory-associated protein of mTOR.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	E	1133	Total	C	H	N	O	S	0	0
			18025	5757	9002	1568	1638	60		
3	U	1133	Total	C	H	N	O	S	0	0
			18025	5757	9002	1568	1638	60		

- Molecule 4 is a protein called Ras-related GTP-binding protein A.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	F	298	Total	C	H	N	O	S	0	0
			4889	1554	2443	427	448	17		
4	M	298	Total	C	H	N	O	S	0	0
			4890	1554	2444	427	448	17		
4	V	298	Total	C	H	N	O	S	0	0
			4882	1553	2438	427	447	17		
4	c	298	Total	C	H	N	O	S	0	0
			4889	1554	2443	427	448	17		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	66	LEU	GLN	conflict	UNP Q7L523
M	66	LEU	GLN	conflict	UNP Q7L523
V	66	LEU	GLN	conflict	UNP Q7L523
c	66	LEU	GLN	conflict	UNP Q7L523

- Molecule 5 is a protein called Ras-related GTP-binding protein C.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	G	281	Total	C	H	N	O	S	0	0
			4523	1459	2258	370	424	12		
5	N	277	Total	C	H	N	O	S	0	0
			4446	1430	2220	365	419	12		
5	W	281	Total	C	H	N	O	S	0	0
			4523	1459	2258	370	424	12		
5	d	277	Total	C	H	N	O	S	0	0
			4446	1430	2220	365	419	12		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	75	ASN	SER	engineered mutation	UNP Q9HB90
N	75	ASN	SER	engineered mutation	UNP Q9HB90
W	75	ASN	SER	engineered mutation	UNP Q9HB90
d	75	ASN	SER	engineered mutation	UNP Q9HB90

- Molecule 6 is a protein called Regulator complex protein LAMTOR1.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	H	111	Total	C	H	N	O	S	0	0
			1738	547	870	150	170	1		
6	O	115	Total	C	H	N	O	S	0	0
			1791	562	896	155	176	2		
6	X	111	Total	C	H	N	O	S	0	0
			1738	547	870	150	170	1		
6	e	115	Total	C	H	N	O	S	0	0
			1791	562	896	155	176	2		

- Molecule 7 is a protein called Regulator complex protein LAMTOR2.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	I	124	Total 1888	C 590	H 950	N 161	O 180	S 7	0	0
7	P	124	Total 1888	C 590	H 950	N 161	O 180	S 7	0	0
7	Y	124	Total 1888	C 590	H 950	N 161	O 180	S 7	0	0
7	f	124	Total 1888	C 590	H 950	N 161	O 180	S 7	0	0

- Molecule 8 is a protein called Regulator complex protein LAMTOR3.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	J	120	Total 1892	C 601	H 958	N 157	O 175	S 1	0	0
8	Q	120	Total 1892	C 601	H 958	N 157	O 175	S 1	0	0
8	Z	120	Total 1892	C 601	H 958	N 157	O 175	S 1	0	0
8	g	120	Total 1892	C 601	H 958	N 157	O 175	S 1	0	0

- Molecule 9 is a protein called Regulator complex protein LAMTOR4.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	K	84	Total 1294	C 404	H 652	N 115	O 122	S 1	0	0
9	R	84	Total 1294	C 404	H 652	N 115	O 122	S 1	0	0
9	a	84	Total 1294	C 404	H 652	N 115	O 122	S 1	0	0
9	h	84	Total 1294	C 404	H 652	N 115	O 122	S 1	0	0

- Molecule 10 is a protein called Regulator complex protein LAMTOR5.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	L	89	Total	C	H	N	O	S	0	0
			1312	400	657	113	135	7		
10	S	89	Total	C	H	N	O	S	0	0
			1311	400	656	113	135	7		
10	b	89	Total	C	H	N	O	S	0	0
			1311	400	656	113	135	7		

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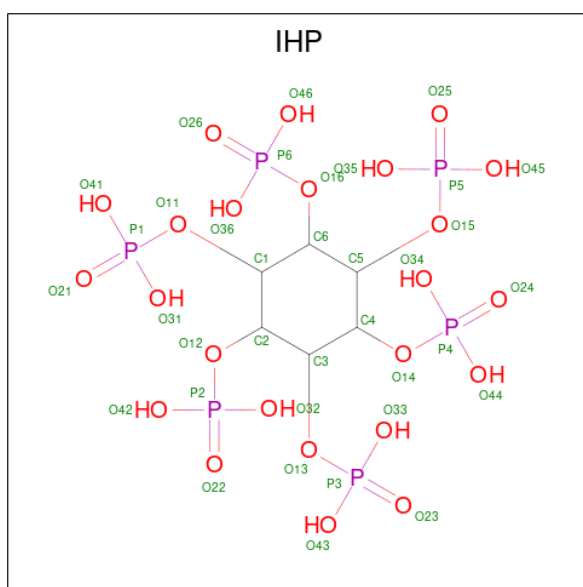
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Mol	Chain	Residues	Atoms						AltConf	Trace
10	i	89	Total	C	H	N	O	S	0	0
			1311	400	656	113	135	7		

- Molecule 11 is a protein called Transcription factor EB.

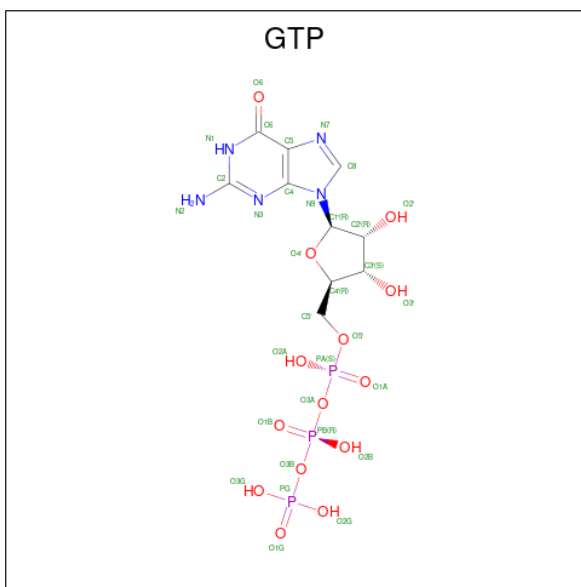
Mol	Chain	Residues	Atoms						AltConf	Trace
11	T	107	Total	C	H	N	O	S	0	0
			1723	541	847	165	165	5		
11	j	107	Total	C	H	N	O	S	0	0
			1724	541	848	165	165	5		

- Molecule 12 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total	C	H	O	P	0
			42	6	6	24	6	
12	C	1	Total	C	H	O	P	0
			42	6	6	24	6	

- Molecule 13 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

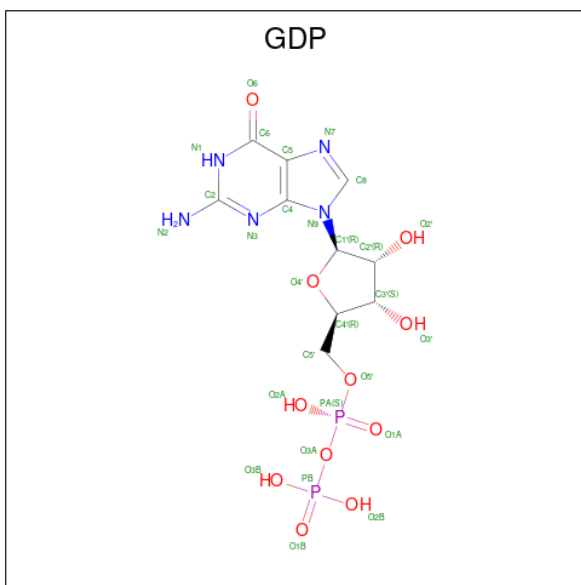


Mol	Chain	Residues	Atoms						AltConf
13	F	1	Total 42	C 10	H 10	N 5	O 14	P 3	0
13	M	1	Total 42	C 10	H 10	N 5	O 14	P 3	0
13	V	1	Total 42	C 10	H 10	N 5	O 14	P 3	0
13	c	1	Total 42	C 10	H 10	N 5	O 14	P 3	0

- Molecule 14 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

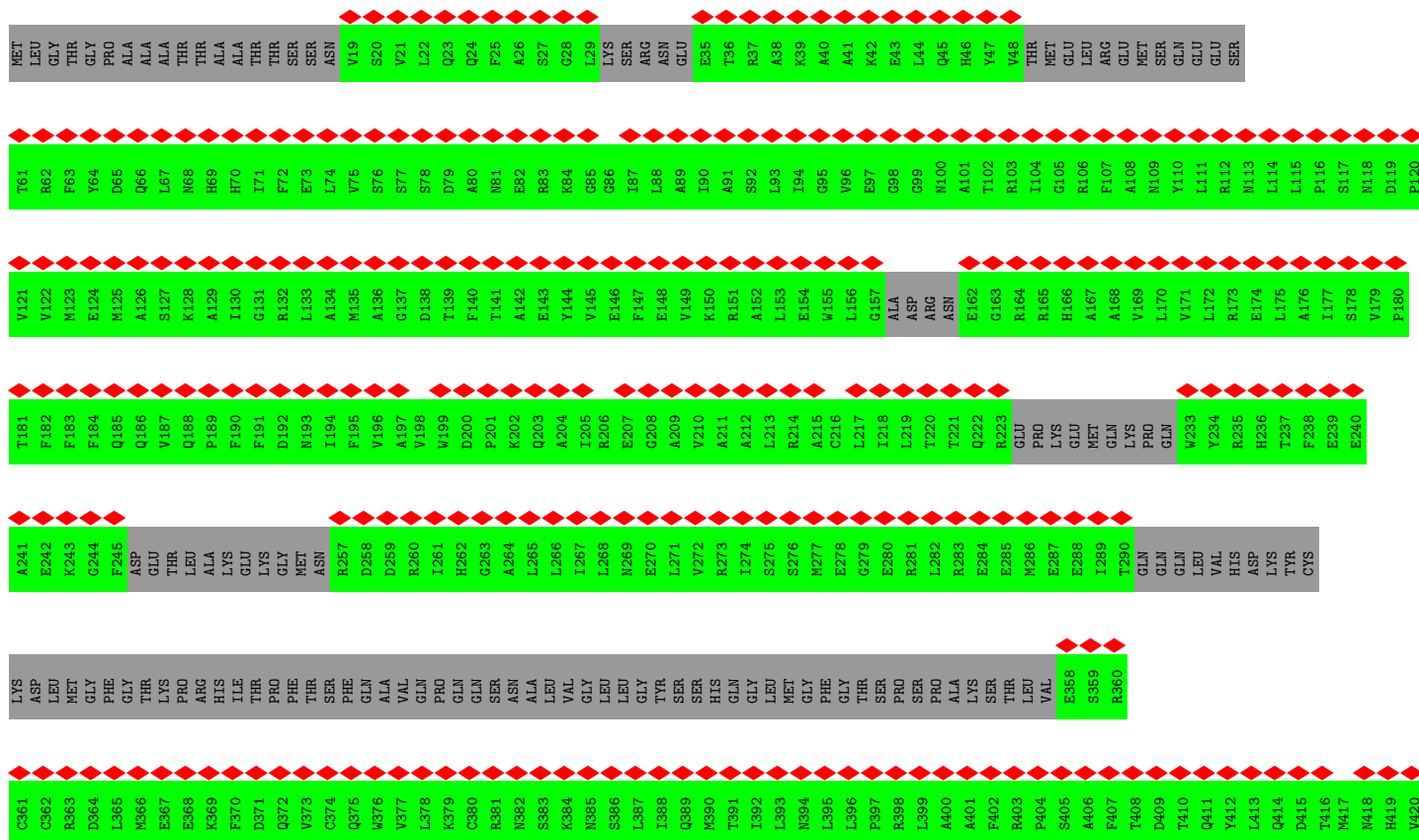
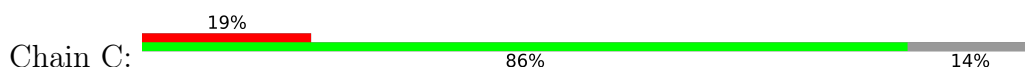
Mol	Chain	Residues	Atoms		AltConf
14	F	1	Total	Mg	0
			1	1	
14	M	1	Total	Mg	0
			1	1	
14	V	1	Total	Mg	0
			1	1	
14	c	1	Total	Mg	0
			1	1	

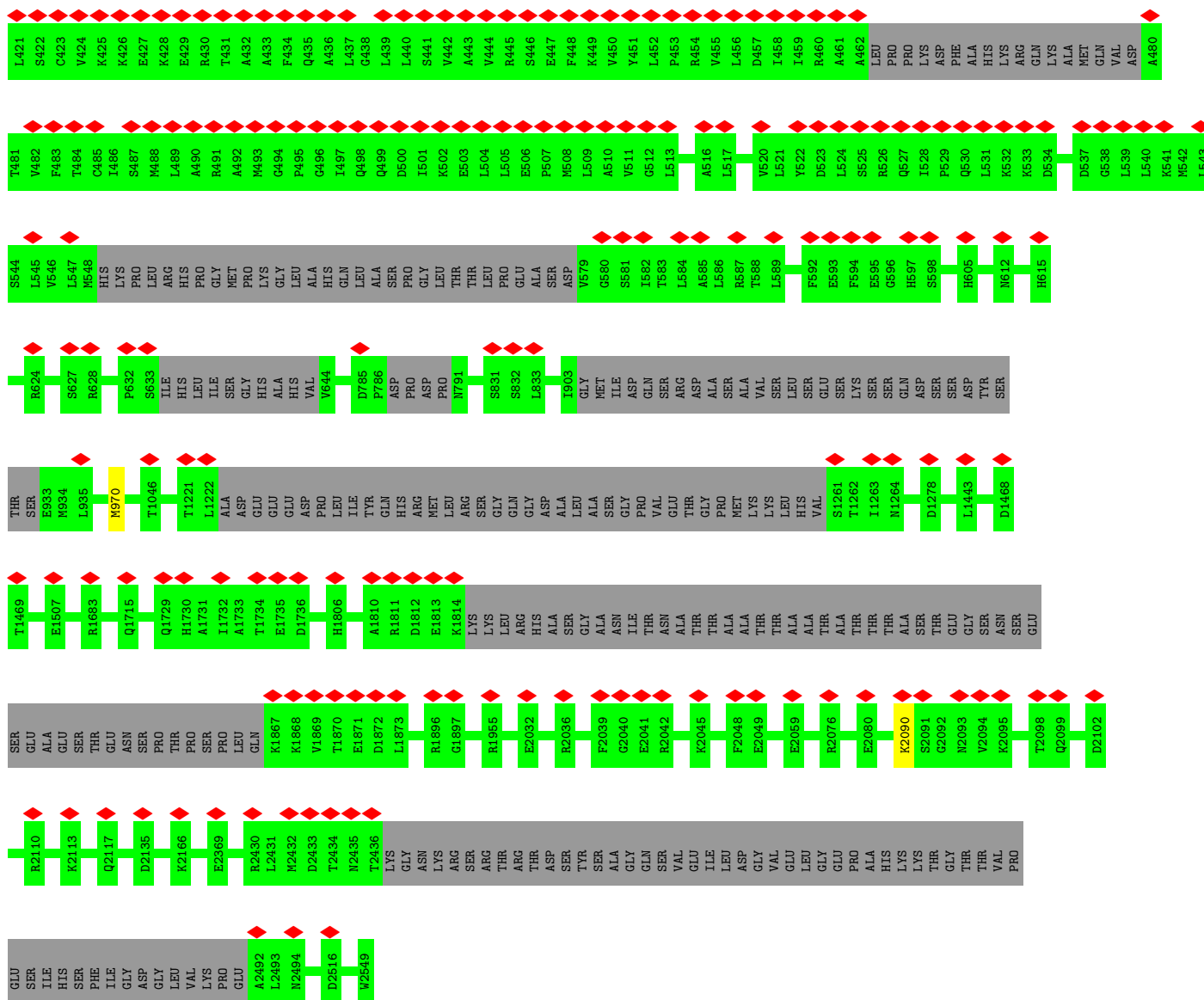
- Molecule 15 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



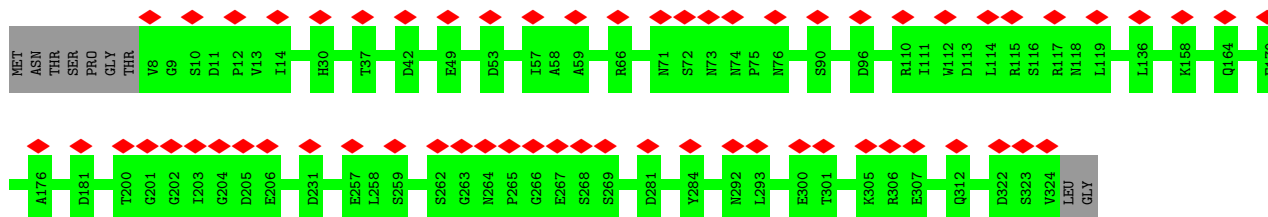
Mol	Chain	Residues	Atoms						AltConf
15	G	1	Total 38	C 10	H 10	N 5	O 11	P 2	0
15	N	1	Total 38	C 10	H 10	N 5	O 11	P 2	0
15	W	1	Total 38	C 10	H 10	N 5	O 11	P 2	0
15	d	1	Total 38	C 10	H 10	N 5	O 11	P 2	0

- Molecule 1: Serine/threonine-protein kinase mTOR



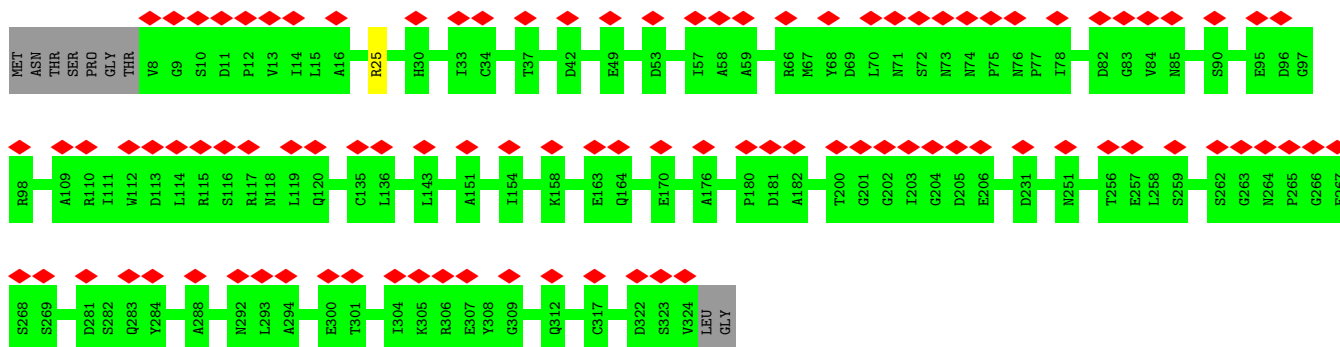


- Molecule 2: Target of rapamycin complex subunit LST8

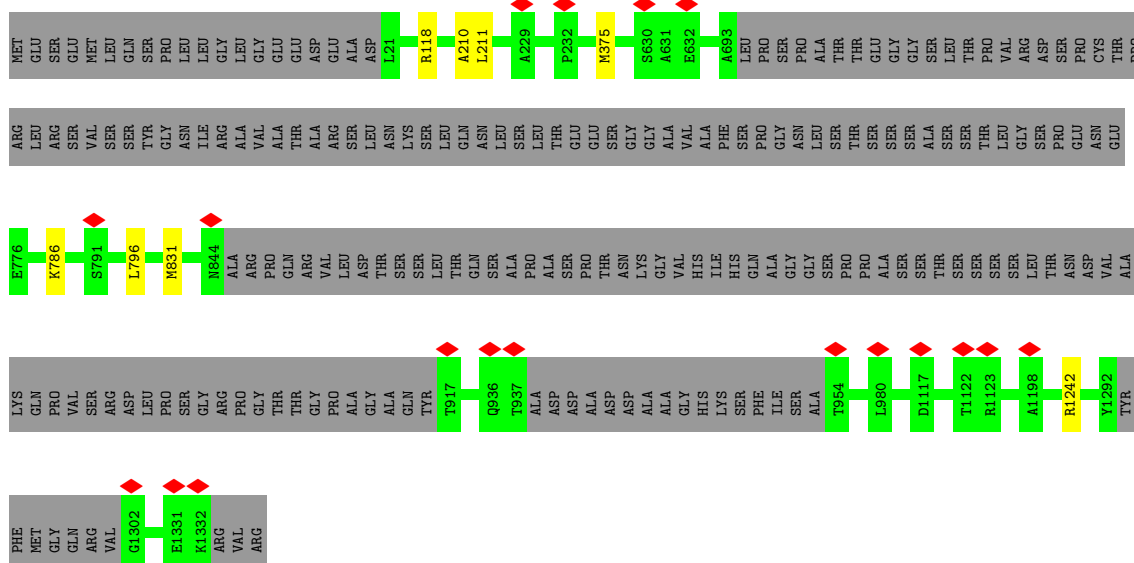
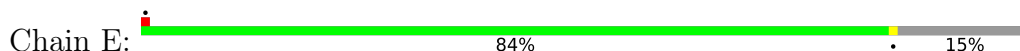


- Molecule 2: Target of rapamycin complex subunit LST8

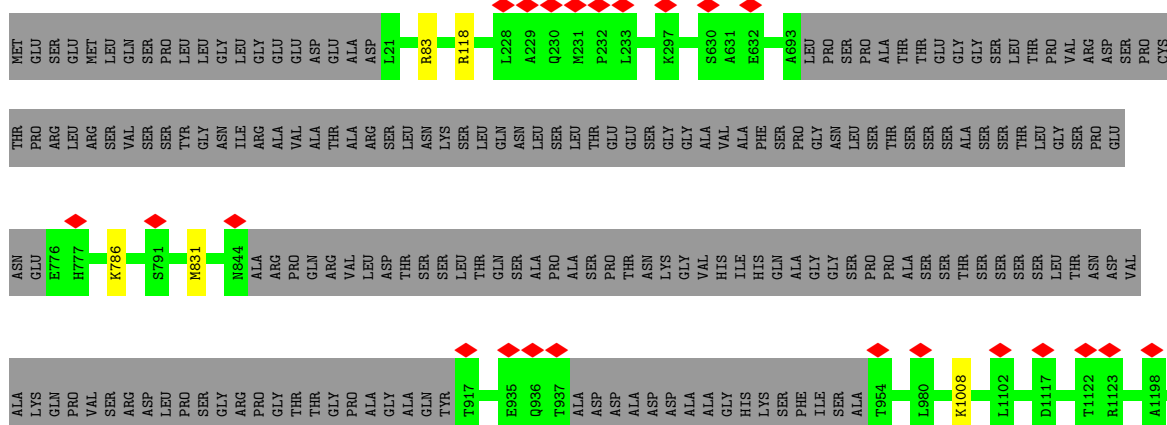
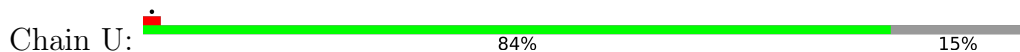


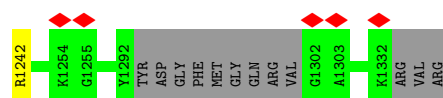


- Molecule 3: Regulatory-associated protein of mTOR



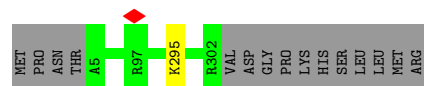
- Molecule 3: Regulatory-associated protein of mTOR





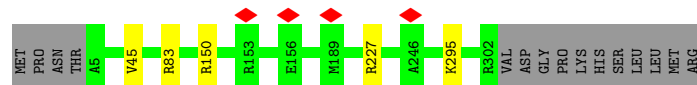
- Molecule 4: Ras-related GTP-binding protein A

Chain F: 95% 5%



- Molecule 4: Ras-related GTP-binding protein A

Chain M: 94% 5%



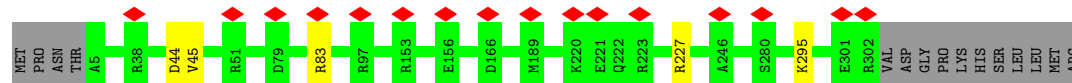
- Molecule 4: Ras-related GTP-binding protein A

Chain V: 94% 5%



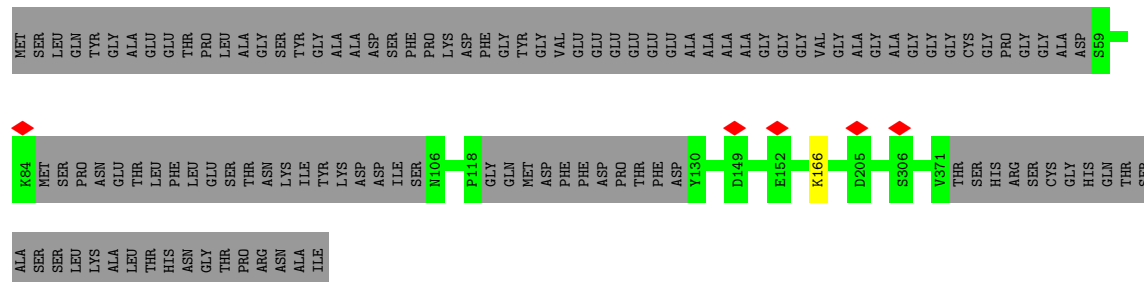
- Molecule 4: Ras-related GTP-binding protein A

Chain c: 94% 5% 5%



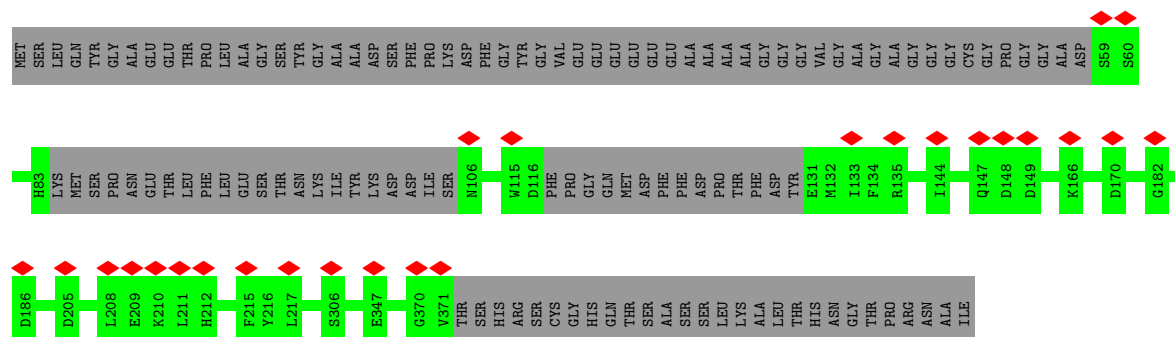
- Molecule 5: Ras-related GTP-binding protein C

Chain G: 70% 30% 5%

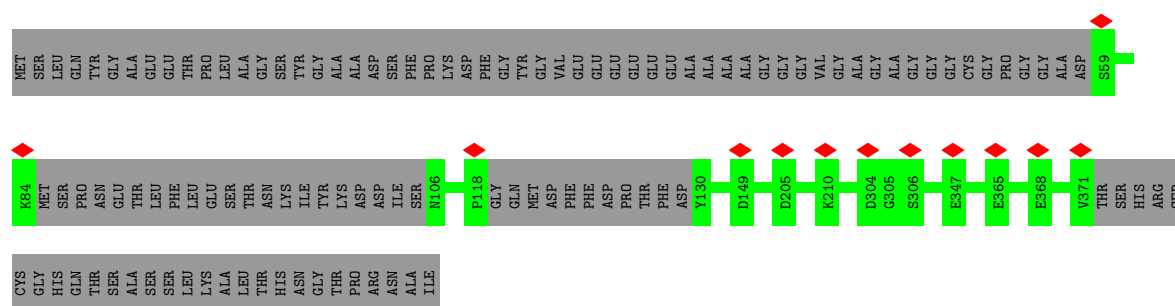


- Molecule 5: Ras-related GTP-binding protein C

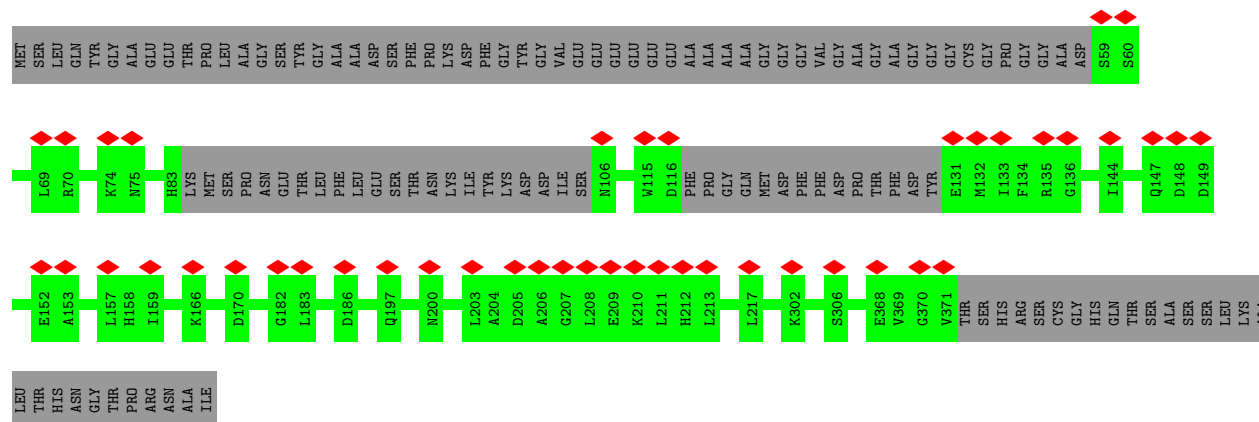
Chain N: 69% 31% 7%



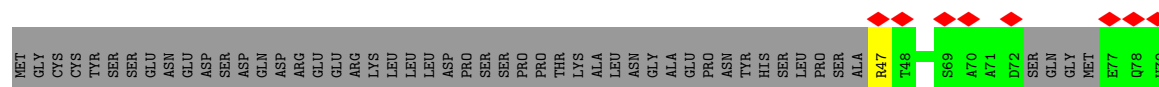
- Molecule 5: Ras-related GTP-binding protein C

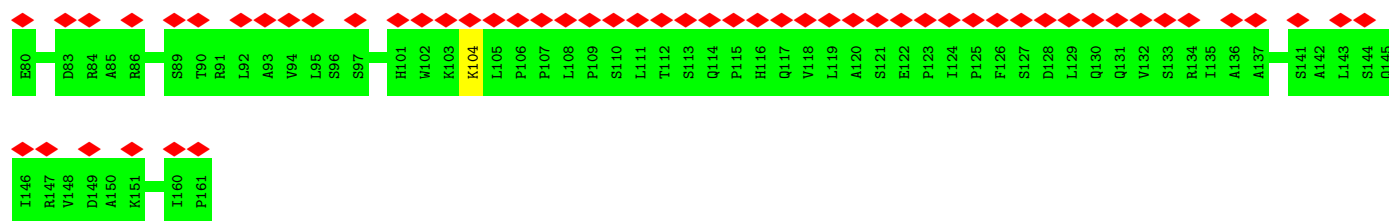


- Molecule 5: Ras-related GTP-binding protein C

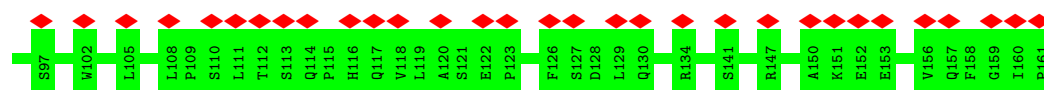
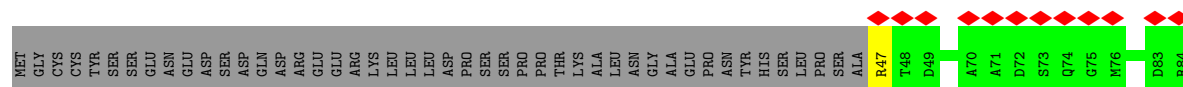


- Molecule 6: Regulator complex protein LAMTOR1

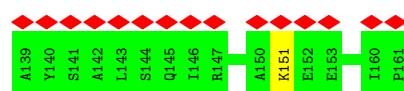
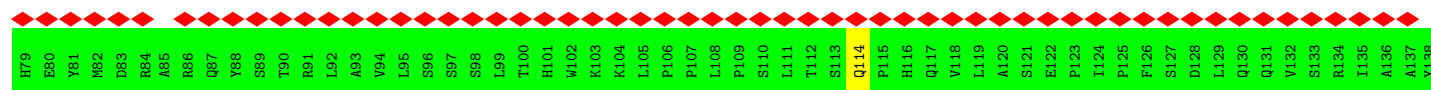
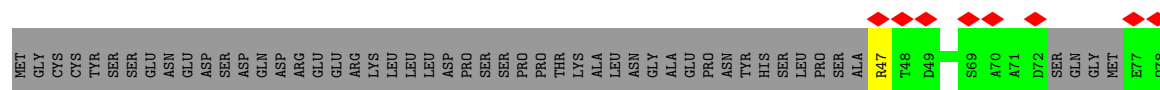




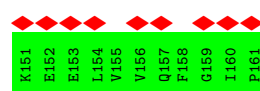
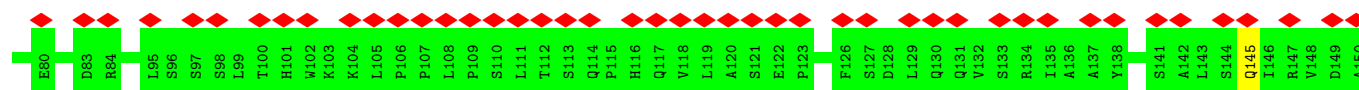
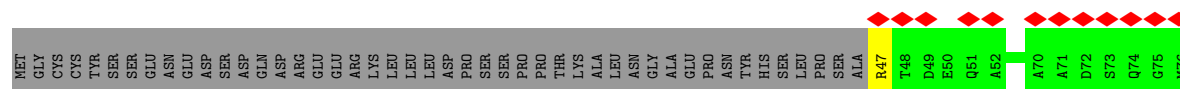
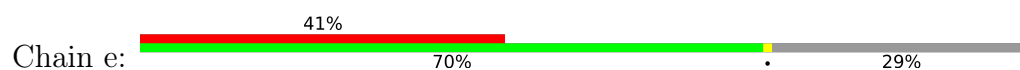
• Molecule 6: Regulator complex protein LAMTOR1



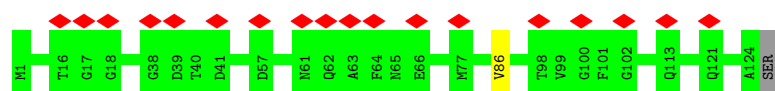
• Molecule 6: Regulator complex protein LAMTOR1



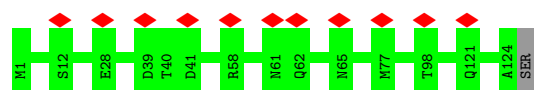
• Molecule 6: Regulator complex protein LAMTOR1



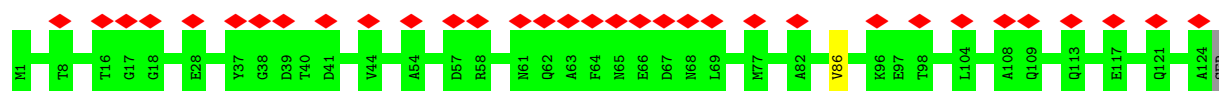
• Molecule 7: Regulator complex protein LAMTOR2



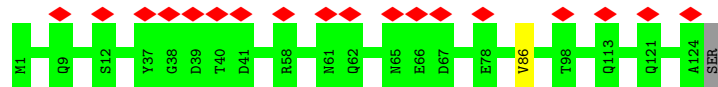
- Molecule 7: Regulator complex protein LAMTOR2



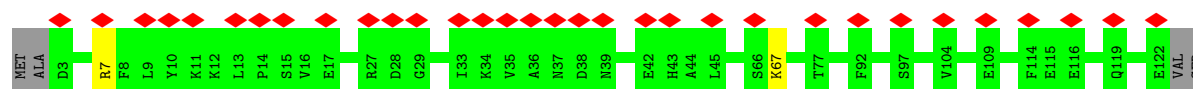
- Molecule 7: Regulator complex protein LAMTOR2



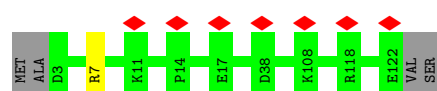
- Molecule 7: Regulator complex protein LAMTOR2



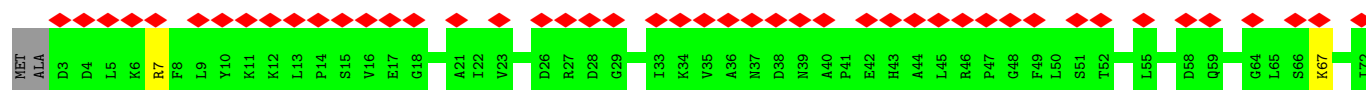
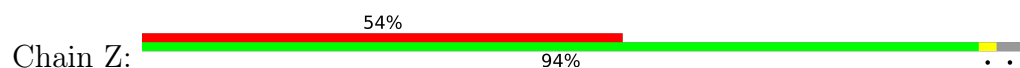
- Molecule 8: Regulator complex protein LAMTOR3

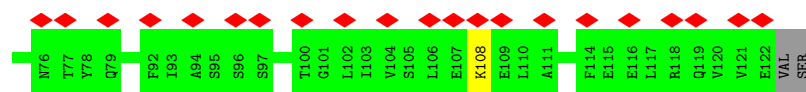


- Molecule 8: Regulator complex protein LAMTOR3

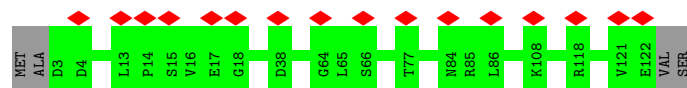


- Molecule 8: Regulator complex protein LAMTOR3

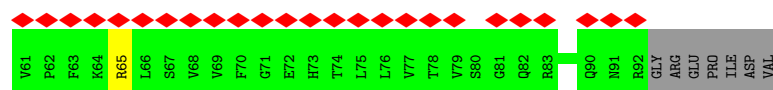
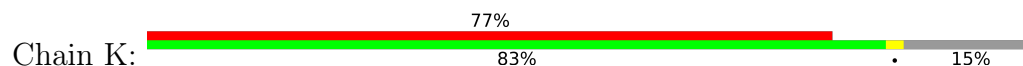




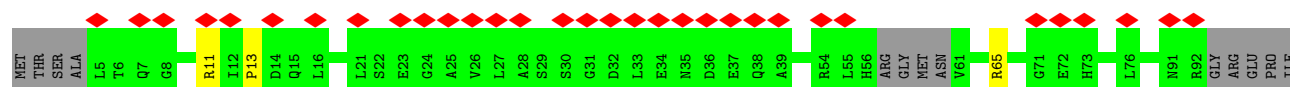
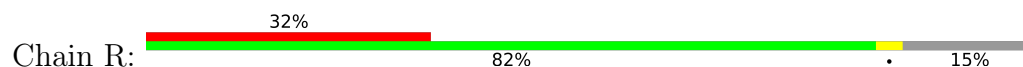
• Molecule 8: Regulator complex protein LAMTOR3



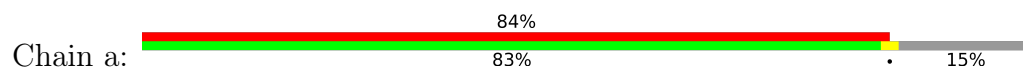
• Molecule 9: Regulator complex protein LAMTOR4



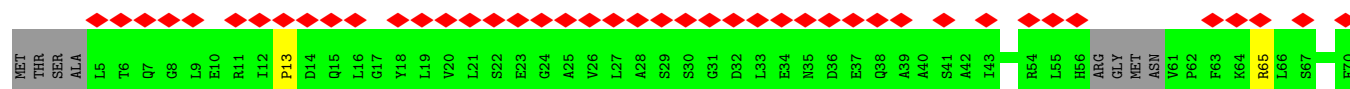
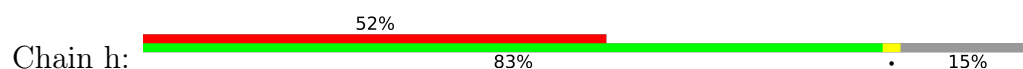
• Molecule 9: Regulator complex protein LAMTOR4

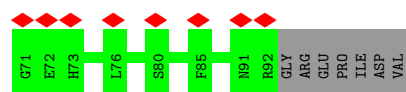


• Molecule 9: Regulator complex protein LAMTOR4

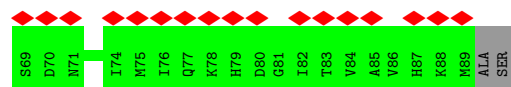
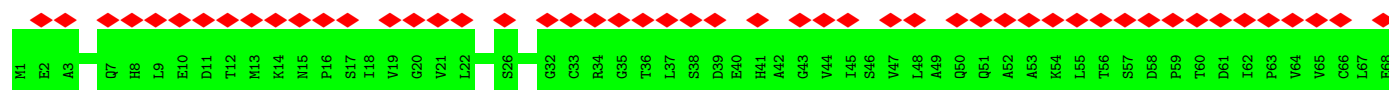
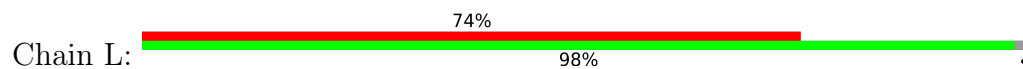


• Molecule 9: Regulator complex protein LAMTOR4

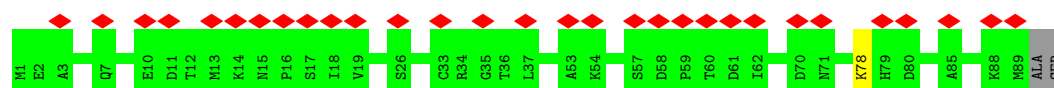




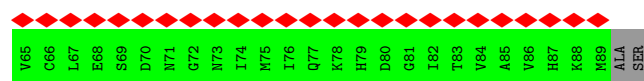
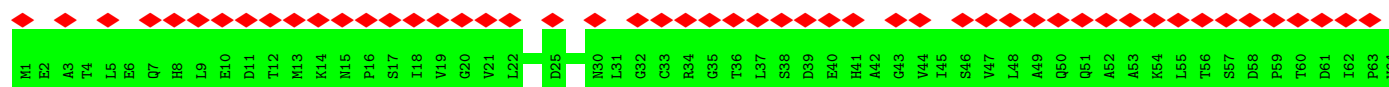
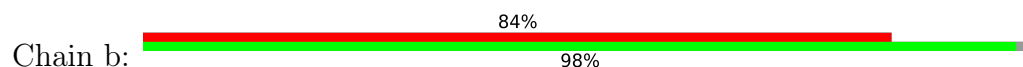
- Molecule 10: Regulator complex protein LAMTOR5



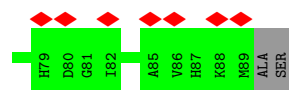
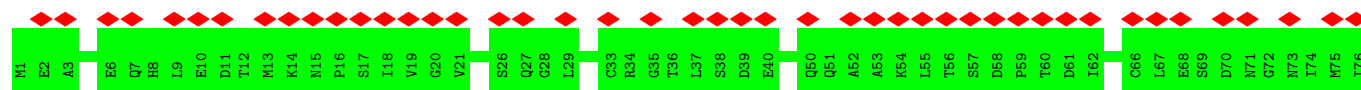
- Molecule 10: Regulator complex protein LAMTOR5



- Molecule 10: Regulator complex protein LAMTOR5



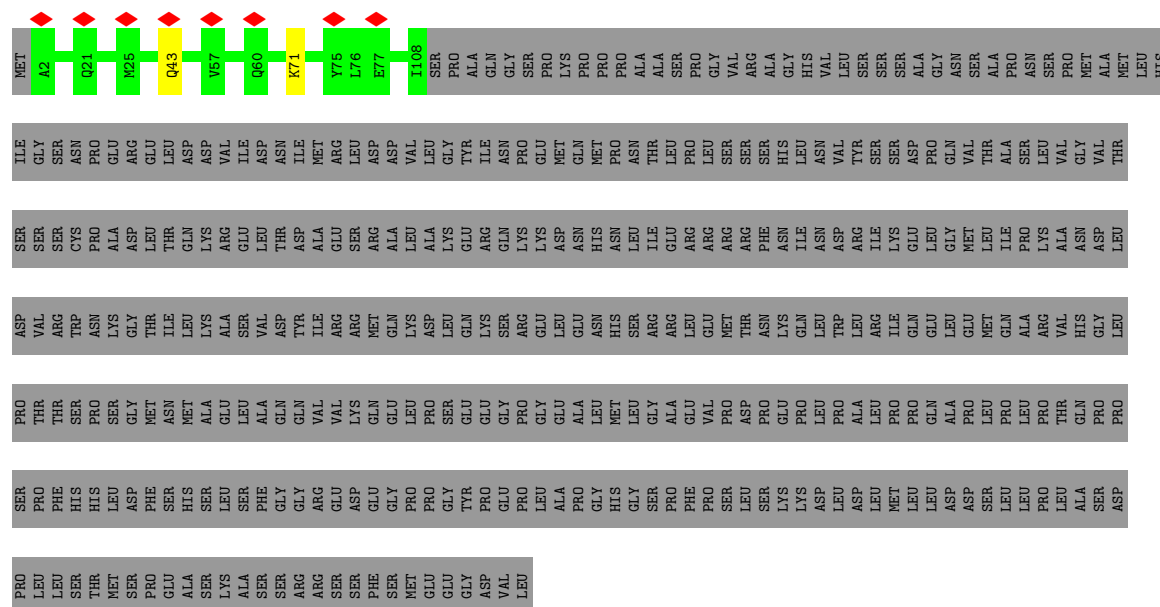
- Molecule 10: Regulator complex protein LAMTOR5



- Molecule 11: Transcription factor EB



- Molecule 11: Transcription factor EB



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	192332	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	57.773	Depositor
Minimum map value	-33.205	Depositor
Average map value	-0.015	Depositor
Map value standard deviation	0.964	Depositor
Recommended contour level	6.0	Depositor
Map size (Å)	617.39996, 617.39996, 617.39996	wwPDB
Map dimensions	588, 588, 588	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, IHP, 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	A	0.28	0/17941	0.60	0/24276
1	C	0.28	0/17941	0.60	0/24276
2	B	0.27	0/2514	0.57	0/3426
2	D	0.26	0/2514	0.57	0/3426
3	E	0.31	0/9242	0.61	2/12573 (0.0%)
3	U	0.31	0/9242	0.62	1/12573 (0.0%)
4	F	0.31	0/2491	0.65	0/3353
4	M	0.30	0/2491	0.65	0/3353
4	V	0.31	0/2489	0.65	1/3350 (0.0%)
4	c	0.33	0/2491	0.70	1/3353 (0.0%)
5	G	0.31	0/2309	0.62	0/3114
5	N	0.29	0/2267	0.62	0/3057
5	W	0.31	0/2309	0.63	0/3114
5	d	0.30	0/2267	0.61	0/3057
6	H	0.28	0/884	0.63	0/1201
6	O	0.29	0/912	0.64	0/1239
6	X	0.27	0/884	0.63	0/1201
6	e	0.30	0/912	0.68	0/1239
7	I	0.31	0/949	0.69	0/1285
7	P	0.32	0/949	0.69	0/1285
7	Y	0.32	0/949	0.74	0/1285
7	f	0.32	0/949	0.71	0/1285
8	J	0.29	0/951	0.64	0/1290
8	Q	0.29	0/951	0.68	0/1290
8	Z	0.29	0/951	0.67	0/1290
8	g	0.32	0/951	0.71	0/1290
9	K	0.28	0/649	0.64	0/876
9	R	0.27	0/649	0.66	0/876
9	a	0.27	0/649	0.65	0/876
9	h	0.27	0/649	0.66	0/876
10	L	0.30	0/661	0.64	0/896
10	S	0.29	0/661	0.66	0/896

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
10	b	0.27	0/661	0.60	0/896
10	i	0.29	0/661	0.64	0/896
11	T	0.28	0/896	0.63	0/1211
11	j	0.31	0/896	0.64	0/1211
All	All	0.29	0/96732	0.62	5/130991 (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
2	D	0	1
3	E	0	3
3	U	0	1
4	M	0	1
4	c	0	1
9	K	0	1
9	R	0	1
9	a	0	1
9	h	0	1
All	All	0	11

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	V	151	LEU	CA-CB-CG	5.77	128.58	115.30
4	c	44	ASP	CB-CG-OD1	5.32	123.09	118.30
3	U	831	MET	CA-CB-CG	5.13	122.02	113.30
3	E	796	LEU	CA-CB-CG	5.12	127.09	115.30
3	E	831	MET	CA-CB-CG	5.04	121.88	113.30

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	25	ARG	Sidechain
3	E	118	ARG	Sidechain
3	E	210	ALA	Mainchain
3	E	211	LEU	Peptide

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Mol	Chain	Res	Type	Group
9	K	65	ARG	Sidechain

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	2158/2549 (85%)	2108 (98%)	50 (2%)	0	100	100
1	C	2158/2549 (85%)	2108 (98%)	50 (2%)	0	100	100
2	B	315/326 (97%)	298 (95%)	17 (5%)	0	100	100
2	D	315/326 (97%)	298 (95%)	17 (5%)	0	100	100
3	E	1123/1335 (84%)	1046 (93%)	77 (7%)	0	100	100
3	U	1123/1335 (84%)	1048 (93%)	75 (7%)	0	100	100
4	F	296/313 (95%)	280 (95%)	16 (5%)	0	100	100
4	M	296/313 (95%)	277 (94%)	18 (6%)	1 (0%)	41	74
4	V	296/313 (95%)	283 (96%)	13 (4%)	0	100	100
4	c	296/313 (95%)	272 (92%)	23 (8%)	1 (0%)	41	74
5	G	275/399 (69%)	264 (96%)	11 (4%)	0	100	100
5	N	271/399 (68%)	258 (95%)	13 (5%)	0	100	100
5	W	275/399 (69%)	262 (95%)	13 (5%)	0	100	100
5	d	271/399 (68%)	259 (96%)	12 (4%)	0	100	100
6	H	107/161 (66%)	103 (96%)	4 (4%)	0	100	100
6	O	113/161 (70%)	106 (94%)	7 (6%)	0	100	100
6	X	107/161 (66%)	102 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	e	113/161 (70%)	106 (94%)	7 (6%)	0	100	100
7	I	122/125 (98%)	118 (97%)	3 (2%)	1 (1%)	19	58
7	P	122/125 (98%)	107 (88%)	15 (12%)	0	100	100
7	Y	122/125 (98%)	117 (96%)	4 (3%)	1 (1%)	19	58
7	f	122/125 (98%)	115 (94%)	6 (5%)	1 (1%)	19	58
8	J	118/124 (95%)	112 (95%)	6 (5%)	0	100	100
8	Q	118/124 (95%)	117 (99%)	1 (1%)	0	100	100
8	Z	118/124 (95%)	112 (95%)	6 (5%)	0	100	100
8	g	118/124 (95%)	114 (97%)	4 (3%)	0	100	100
9	K	80/99 (81%)	68 (85%)	11 (14%)	1 (1%)	12	47
9	R	80/99 (81%)	70 (88%)	9 (11%)	1 (1%)	12	47
9	a	80/99 (81%)	69 (86%)	10 (12%)	1 (1%)	12	47
9	h	80/99 (81%)	69 (86%)	10 (12%)	1 (1%)	12	47
10	L	87/91 (96%)	79 (91%)	8 (9%)	0	100	100
10	S	87/91 (96%)	79 (91%)	8 (9%)	0	100	100
10	b	87/91 (96%)	79 (91%)	8 (9%)	0	100	100
10	i	87/91 (96%)	81 (93%)	6 (7%)	0	100	100
11	T	105/476 (22%)	96 (91%)	8 (8%)	1 (1%)	15	54
11	j	105/476 (22%)	97 (92%)	7 (7%)	1 (1%)	15	54
All	All	11746/14620 (80%)	11177 (95%)	558 (5%)	11 (0%)	54	83

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	M	45	VAL
7	Y	86	VAL
7	f	86	VAL
11	T	43	GLN
11	j	43	GLN

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	A	1919/2220 (86%)	1918 (100%)	1 (0%)	93	98
1	C	1919/2220 (86%)	1917 (100%)	2 (0%)	93	98
2	B	269/276 (98%)	269 (100%)	0	100	100
2	D	269/276 (98%)	269 (100%)	0	100	100
3	E	1000/1163 (86%)	997 (100%)	3 (0%)	92	96
3	U	1000/1163 (86%)	996 (100%)	4 (0%)	91	95
4	F	272/287 (95%)	271 (100%)	1 (0%)	91	95
4	M	272/287 (95%)	269 (99%)	3 (1%)	73	88
4	V	271/287 (94%)	268 (99%)	3 (1%)	73	88
4	c	272/287 (95%)	270 (99%)	2 (1%)	84	94
5	G	255/340 (75%)	254 (100%)	1 (0%)	91	95
5	N	251/340 (74%)	251 (100%)	0	100	100
5	W	255/340 (75%)	255 (100%)	0	100	100
5	d	251/340 (74%)	251 (100%)	0	100	100
6	H	97/141 (69%)	95 (98%)	2 (2%)	53	79
6	O	100/141 (71%)	99 (99%)	1 (1%)	76	90
6	X	97/141 (69%)	94 (97%)	3 (3%)	40	72
6	e	100/141 (71%)	98 (98%)	2 (2%)	55	80
7	I	97/98 (99%)	97 (100%)	0	100	100
7	P	97/98 (99%)	97 (100%)	0	100	100
7	Y	97/98 (99%)	97 (100%)	0	100	100
7	f	97/98 (99%)	97 (100%)	0	100	100
8	J	105/108 (97%)	103 (98%)	2 (2%)	57	81
8	Q	105/108 (97%)	104 (99%)	1 (1%)	76	90
8	Z	105/108 (97%)	102 (97%)	3 (3%)	42	74
8	g	105/108 (97%)	105 (100%)	0	100	100
9	K	71/83 (86%)	71 (100%)	0	100	100
9	R	71/83 (86%)	70 (99%)	1 (1%)	67	86
9	a	71/83 (86%)	71 (100%)	0	100	100
9	h	71/83 (86%)	71 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	L	76/77 (99%)	76 (100%)	0	100	100
10	S	76/77 (99%)	75 (99%)	1 (1%)	69	87
10	b	76/77 (99%)	76 (100%)	0	100	100
10	i	76/77 (99%)	76 (100%)	0	100	100
11	T	96/419 (23%)	95 (99%)	1 (1%)	76	90
11	j	96/419 (23%)	95 (99%)	1 (1%)	76	90
All	All	10457/12692 (82%)	10419 (100%)	38 (0%)	91	95

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	X	114	GLN
6	e	47	ARG
6	X	151	LYS
8	Z	108	LYS
11	j	71	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	2106	HIS
7	P	121	GLN
11	T	28	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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$
12	IHP	A	2601	-	36,36,36	1.47	6 (16%)	54,60,60	0.73	1 (1%)
15	GDP	G	401	-	24,30,30	0.95	1 (4%)	30,47,47	1.20	3 (10%)
13	GTP	V	401	14	26,34,34	1.19	2 (7%)	32,54,54	1.63	6 (18%)
13	GTP	M	401	14	26,34,34	1.17	2 (7%)	32,54,54	1.55	6 (18%)
13	GTP	c	401	14	26,34,34	1.17	2 (7%)	32,54,54	1.59	6 (18%)
15	GDP	N	401	-	24,30,30	0.96	1 (4%)	30,47,47	1.16	3 (10%)
15	GDP	d	401	-	24,30,30	0.95	1 (4%)	30,47,47	1.24	4 (13%)
15	GDP	W	401	-	24,30,30	0.93	1 (4%)	30,47,47	1.20	3 (10%)
13	GTP	F	401	14	26,34,34	1.21	2 (7%)	32,54,54	1.64	6 (18%)
12	IHP	C	2601	-	36,36,36	1.47	6 (16%)	54,60,60	0.64	1 (1%)

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
12	IHP	A	2601	-	-	7/30/54/54	0/1/1/1
15	GDP	G	401	-	-	2/12/32/32	0/3/3/3
13	GTP	V	401	14	-	1/18/38/38	0/3/3/3
13	GTP	M	401	14	-	5/18/38/38	0/3/3/3
13	GTP	c	401	14	-	5/18/38/38	0/3/3/3
15	GDP	N	401	-	-	2/12/32/32	0/3/3/3
15	GDP	d	401	-	-	3/12/32/32	0/3/3/3
15	GDP	W	401	-	-	1/12/32/32	0/3/3/3
13	GTP	F	401	14	-	1/18/38/38	0/3/3/3
12	IHP	C	2601	-	-	7/30/54/54	0/1/1/1

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	F	401	GTP	C5-C6	-4.16	1.39	1.47
13	c	401	GTP	C5-C6	-4.13	1.39	1.47
13	M	401	GTP	C5-C6	-4.12	1.39	1.47
13	V	401	GTP	C5-C6	-4.12	1.39	1.47
12	C	2601	IHP	P3-O13	3.72	1.66	1.59

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	V	401	GTP	PB-O3B-PG	-4.34	117.94	132.83
13	F	401	GTP	PB-O3B-PG	-4.08	118.82	132.83
13	c	401	GTP	PB-O3B-PG	-4.07	118.87	132.83
13	F	401	GTP	PA-O3A-PB	-3.93	119.33	132.83
13	M	401	GTP	PB-O3B-PG	-3.79	119.82	132.83

There are no chirality outliers.

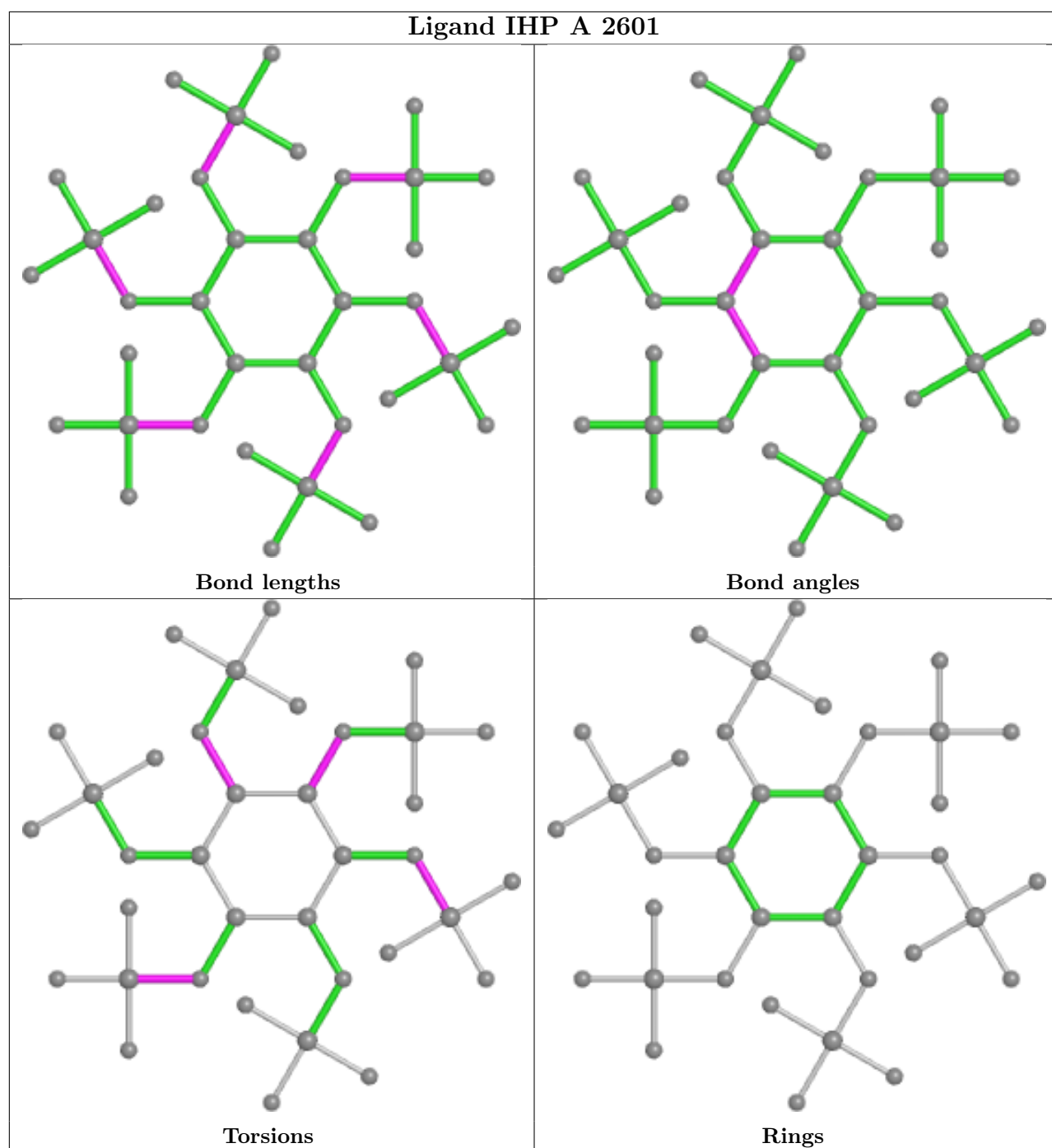
5 of 34 torsion outliers are listed below:

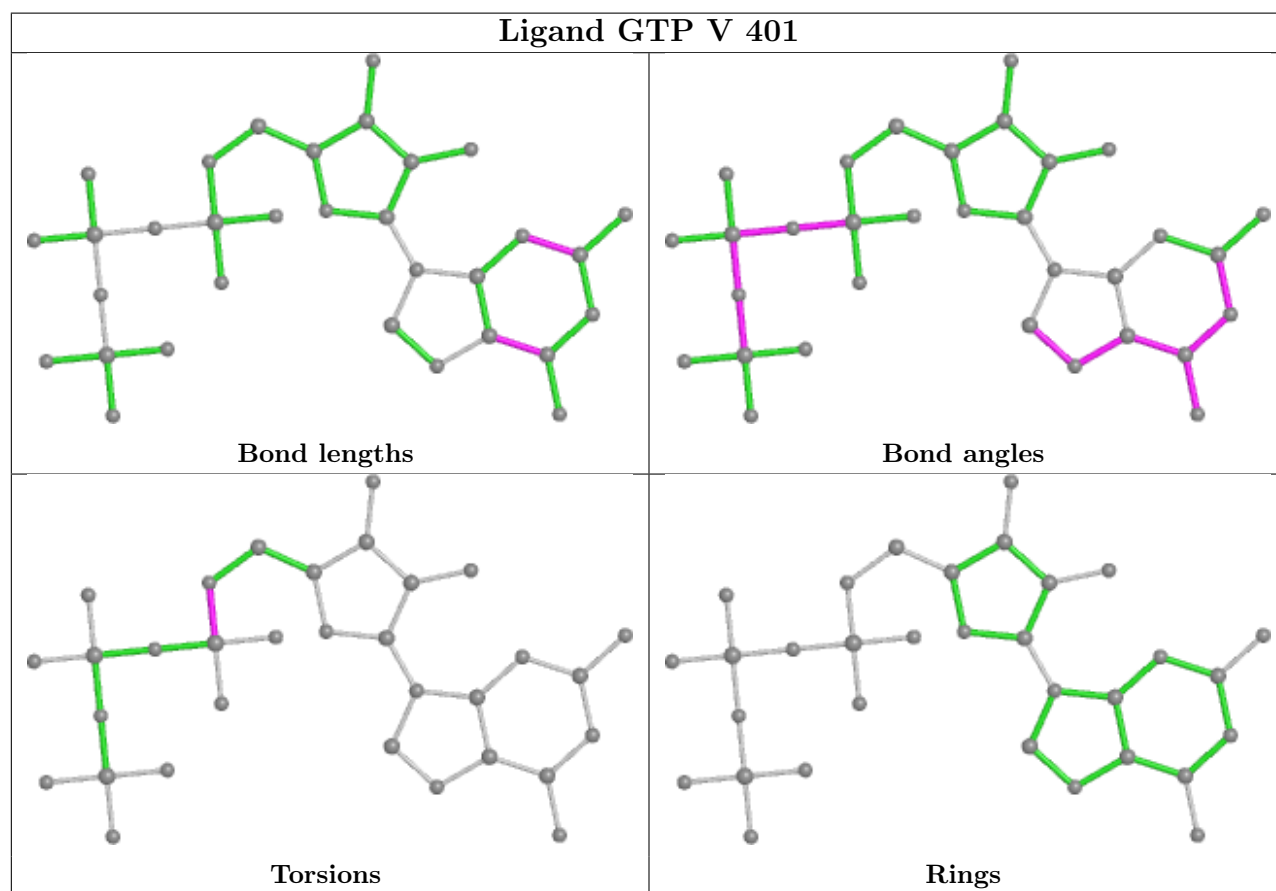
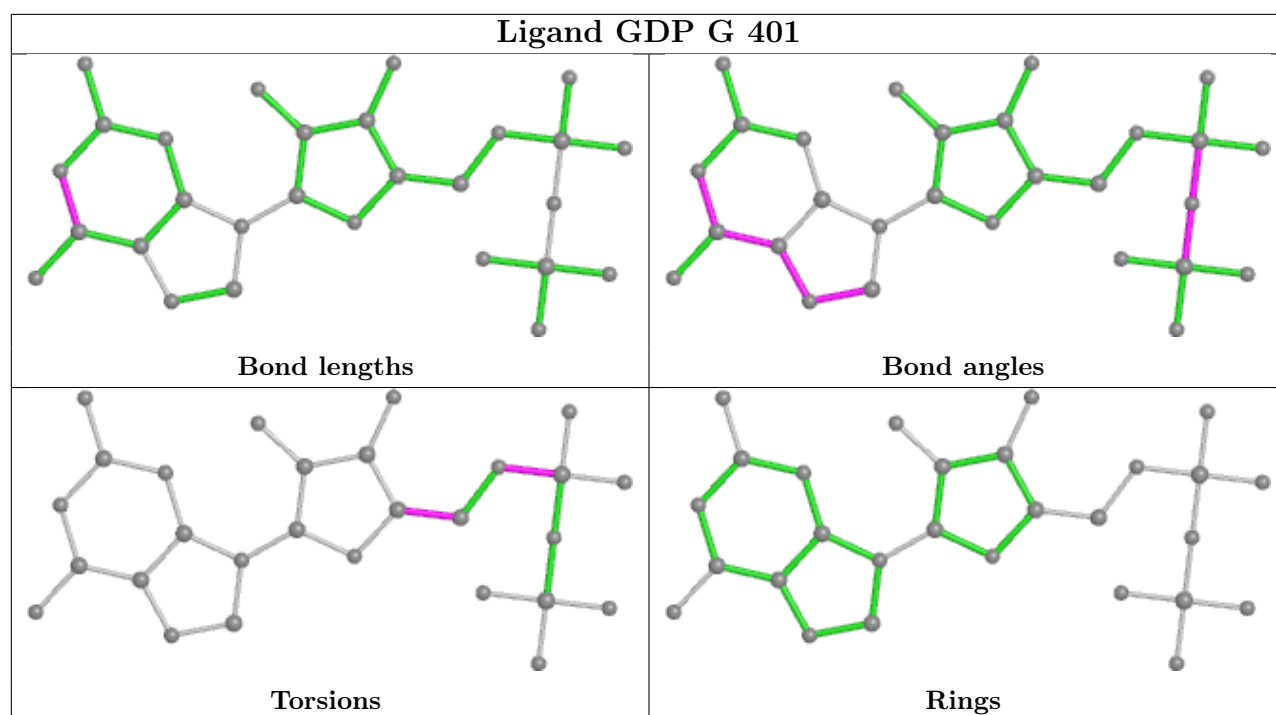
Mol	Chain	Res	Type	Atoms
12	A	2601	IHP	C2-C3-O13-P3
12	A	2601	IHP	C3-C4-O14-P4
12	A	2601	IHP	C5-C4-O14-P4
12	C	2601	IHP	C2-C3-O13-P3
12	C	2601	IHP	C3-C4-O14-P4

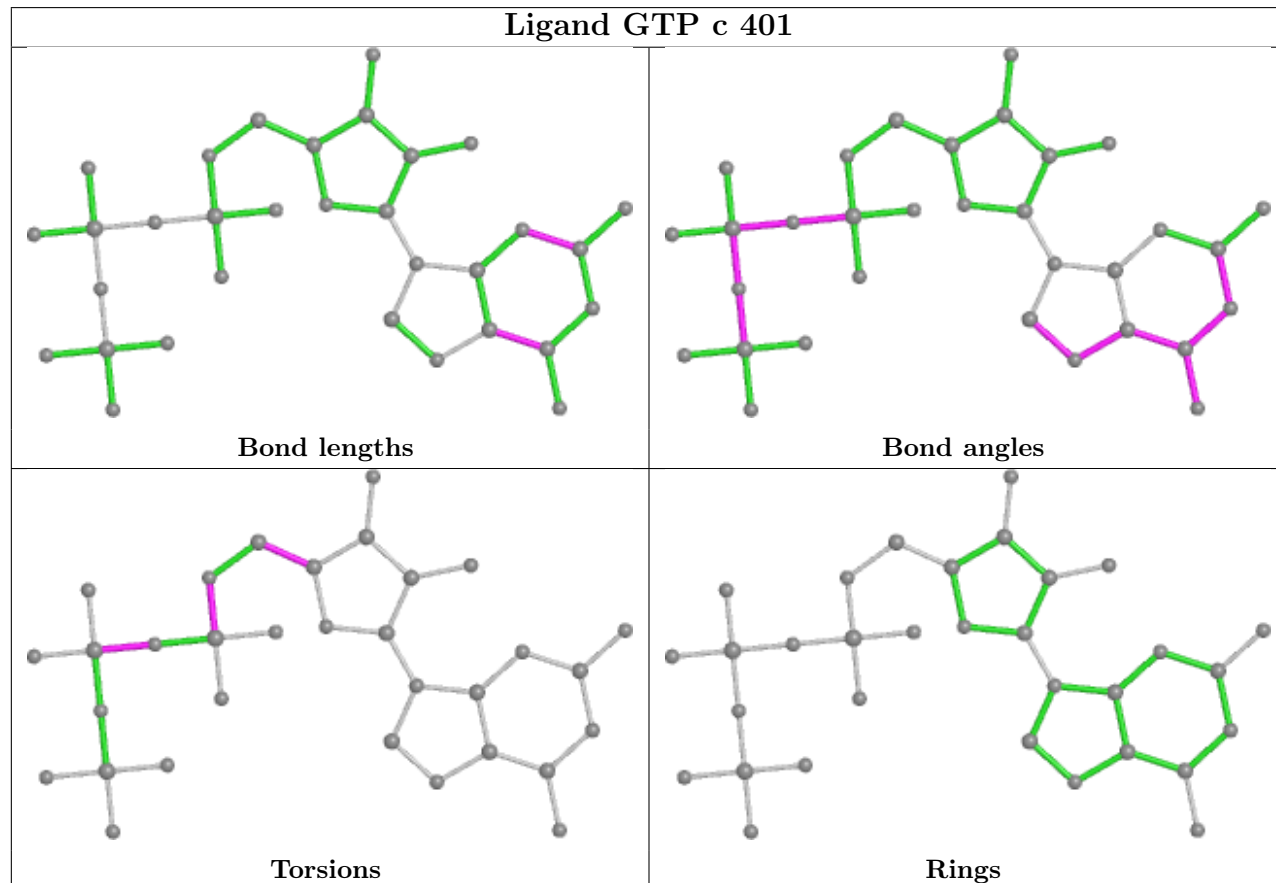
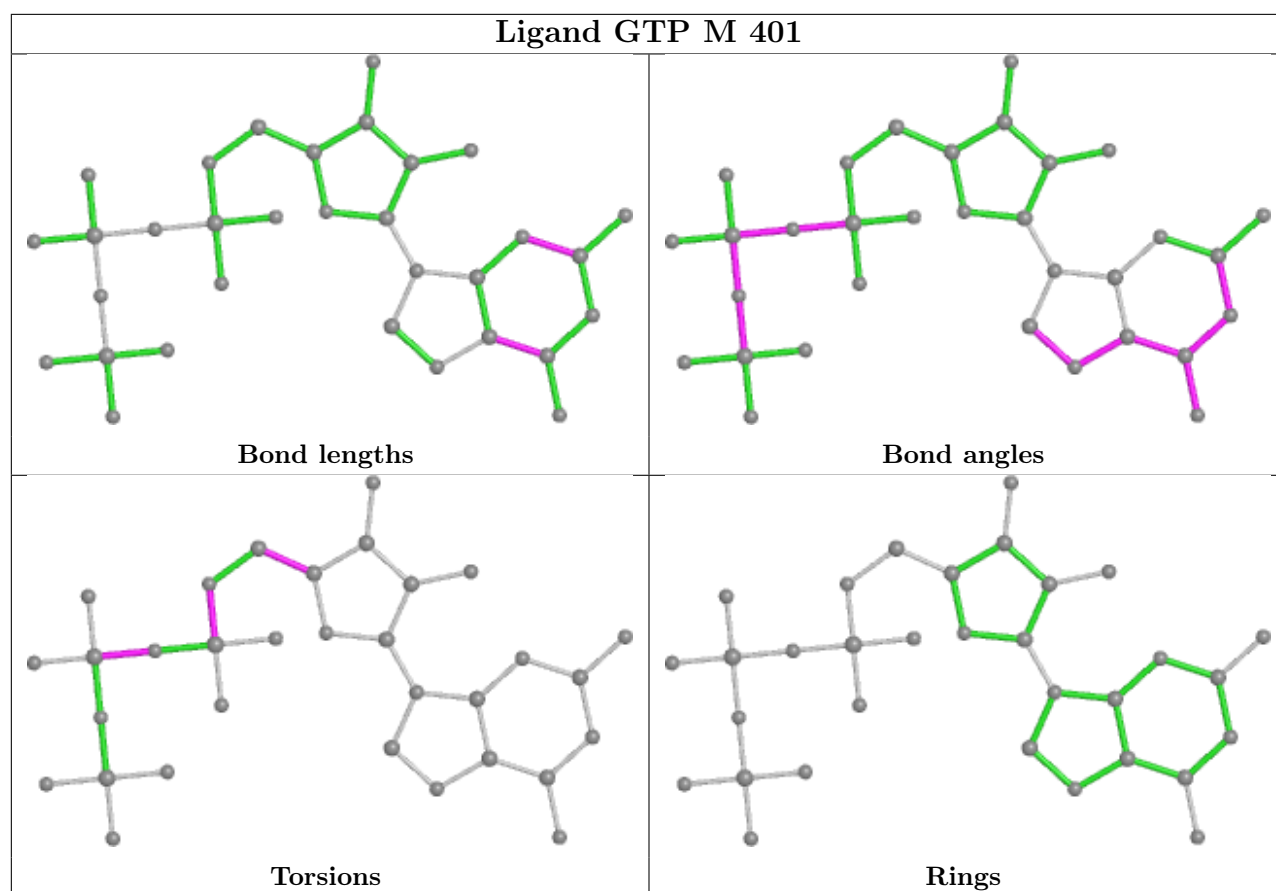
There are no ring outliers.

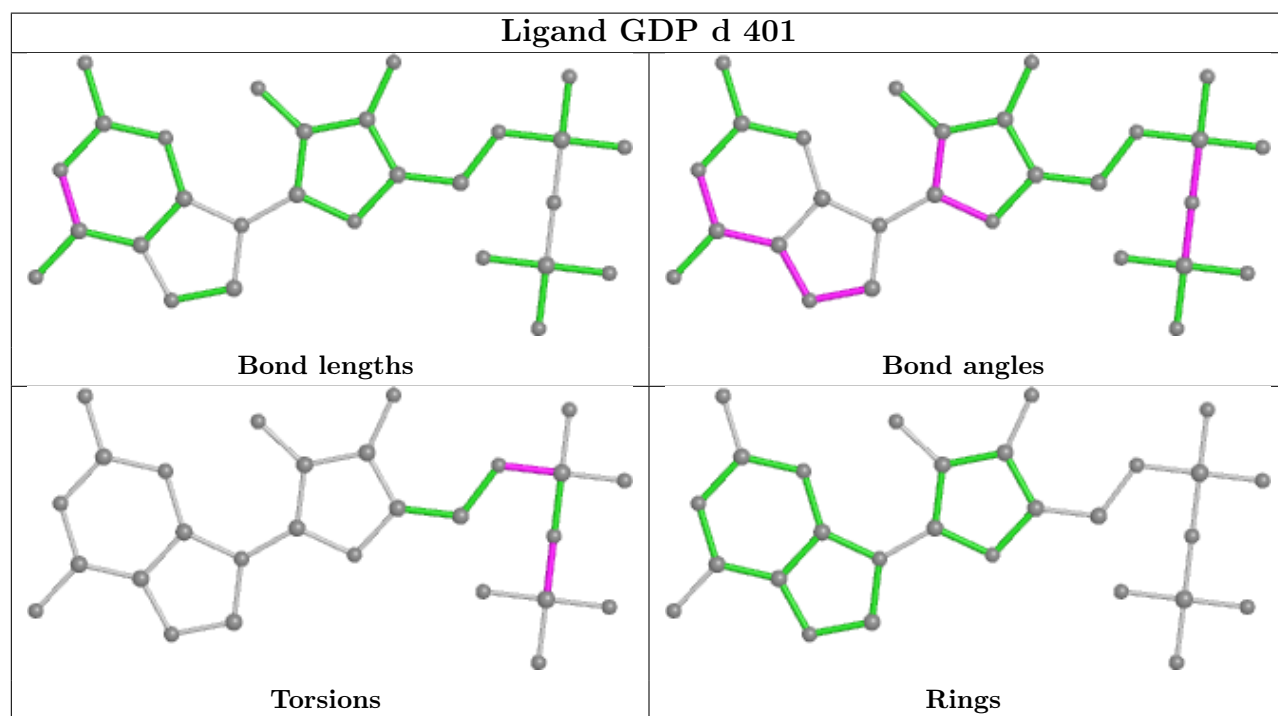
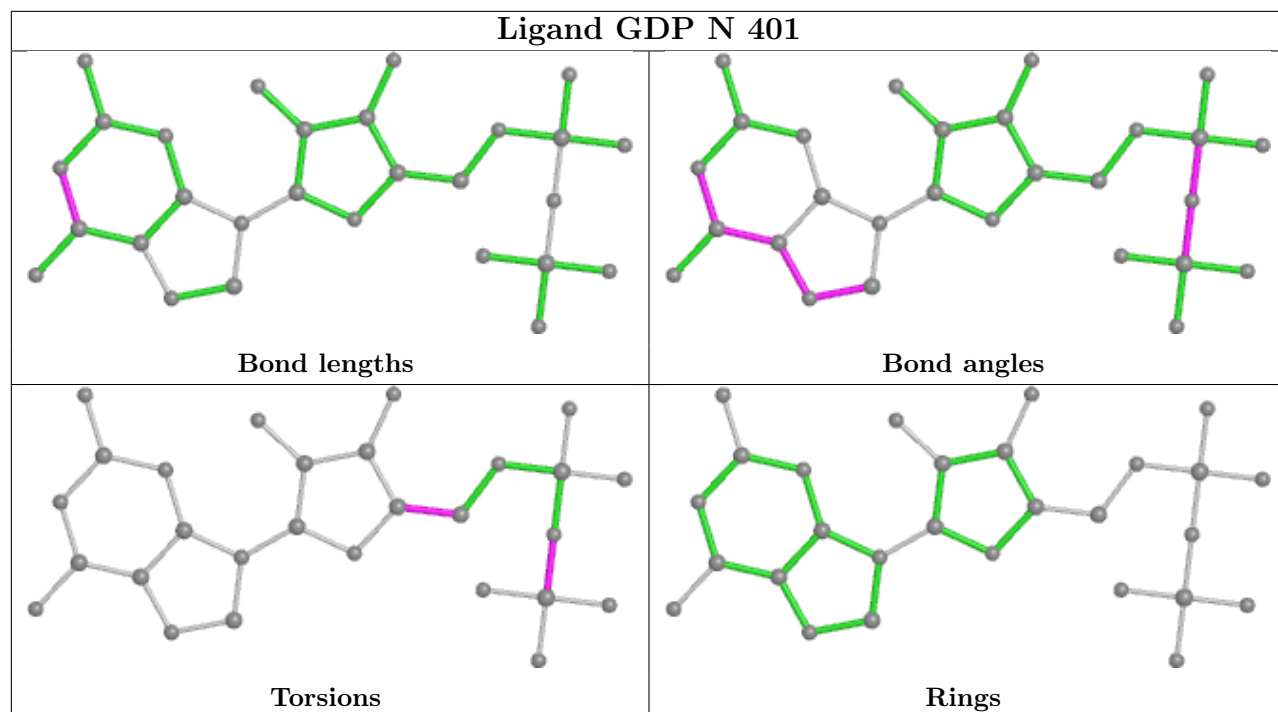
No monomer is involved in short contacts.

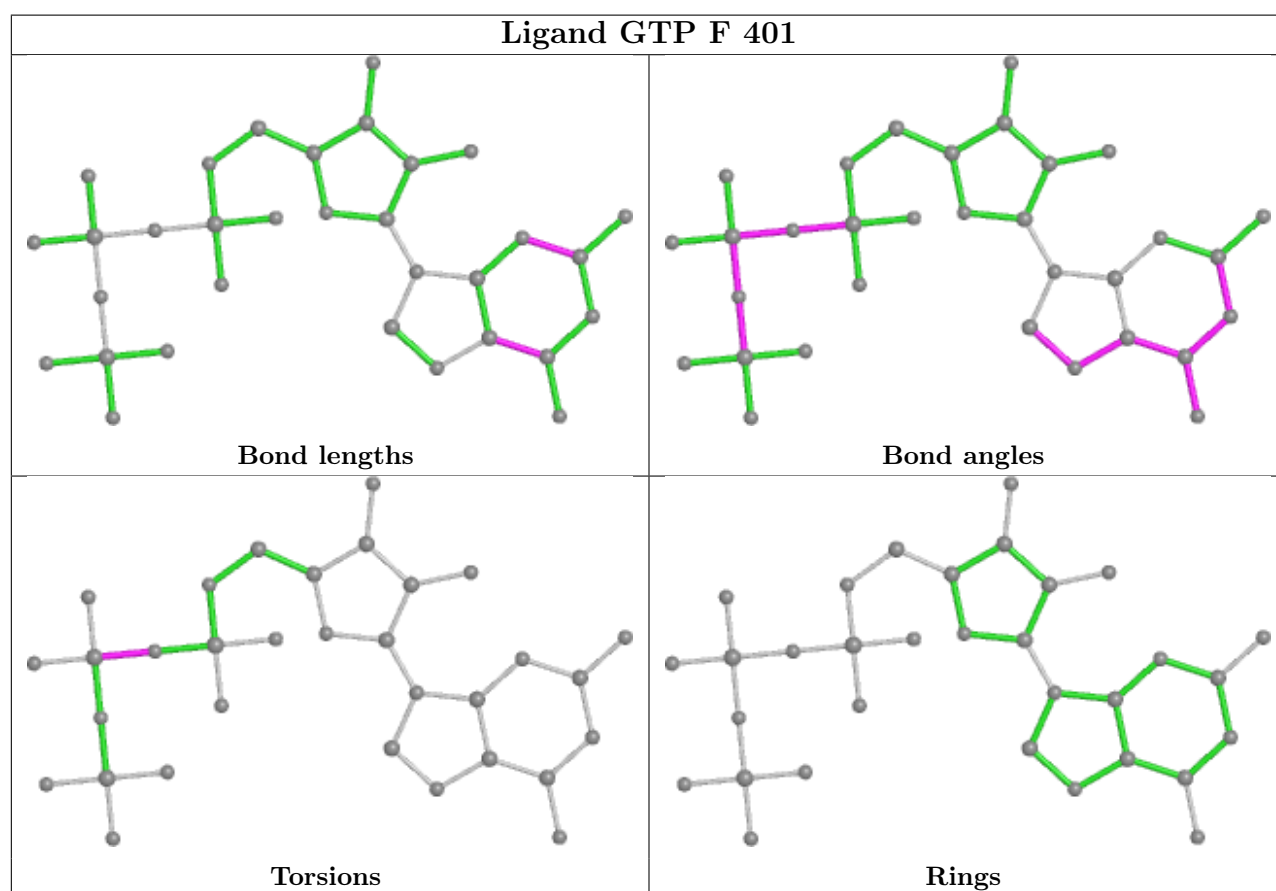
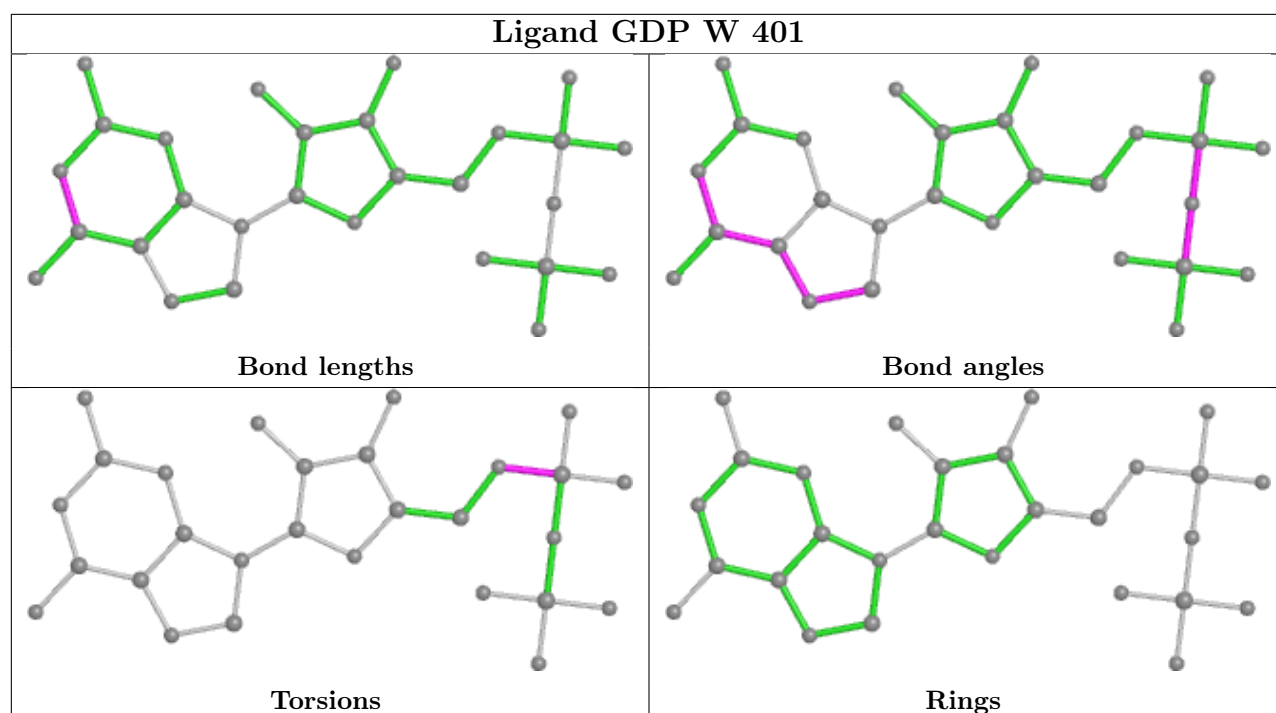
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

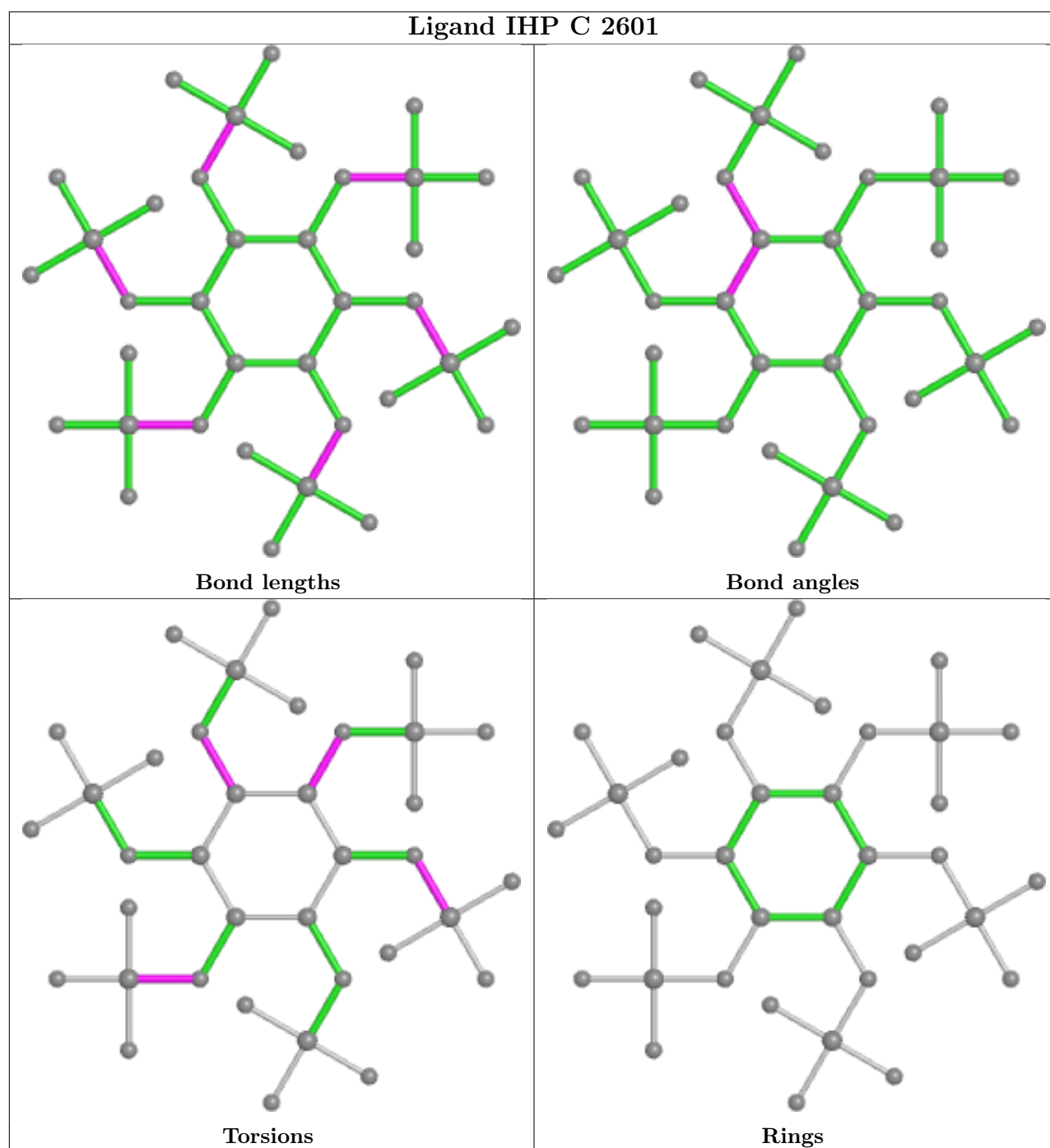












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

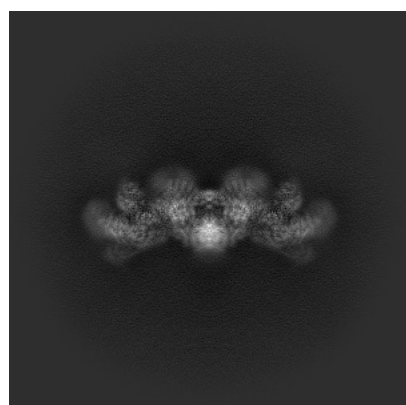
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26861. These allow visual inspection of the internal detail of the map and identification of artifacts.

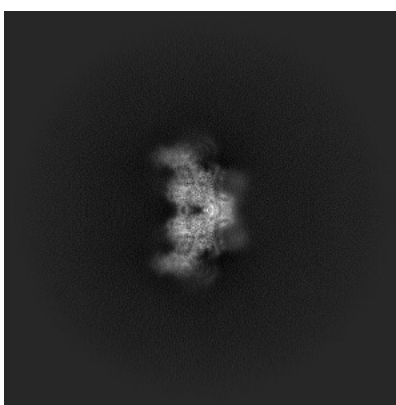
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

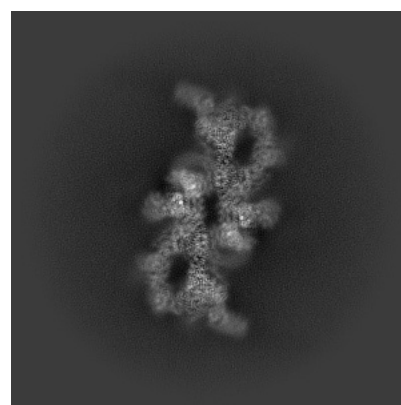
6.1.1 Primary map



X



Y



Z

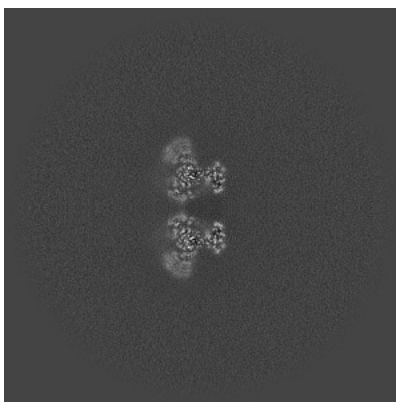
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

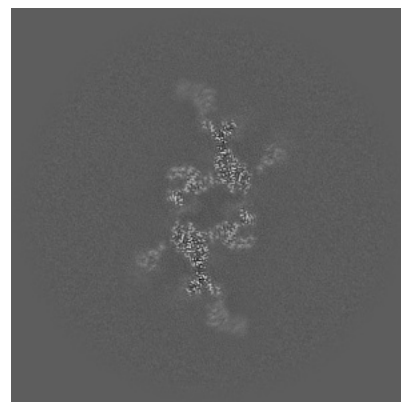
6.2.1 Primary map



X Index: 294



Y Index: 294

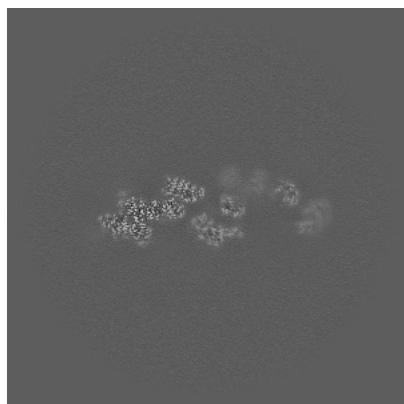


Z Index: 294

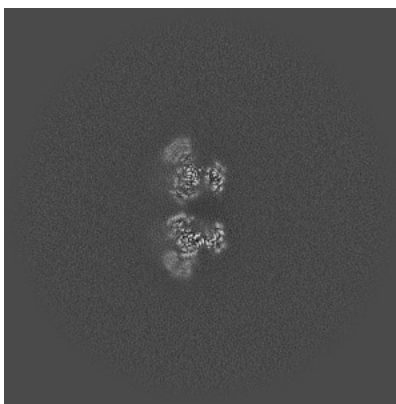
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

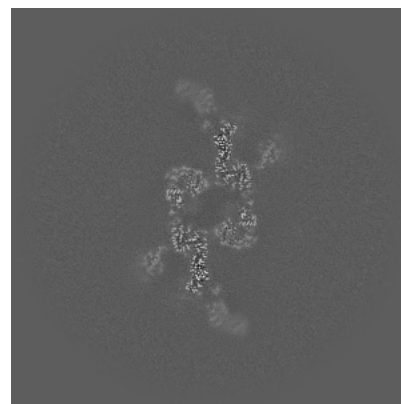
6.3.1 Primary map



X Index: 275



Y Index: 296

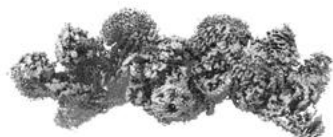


Z Index: 290

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 6.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

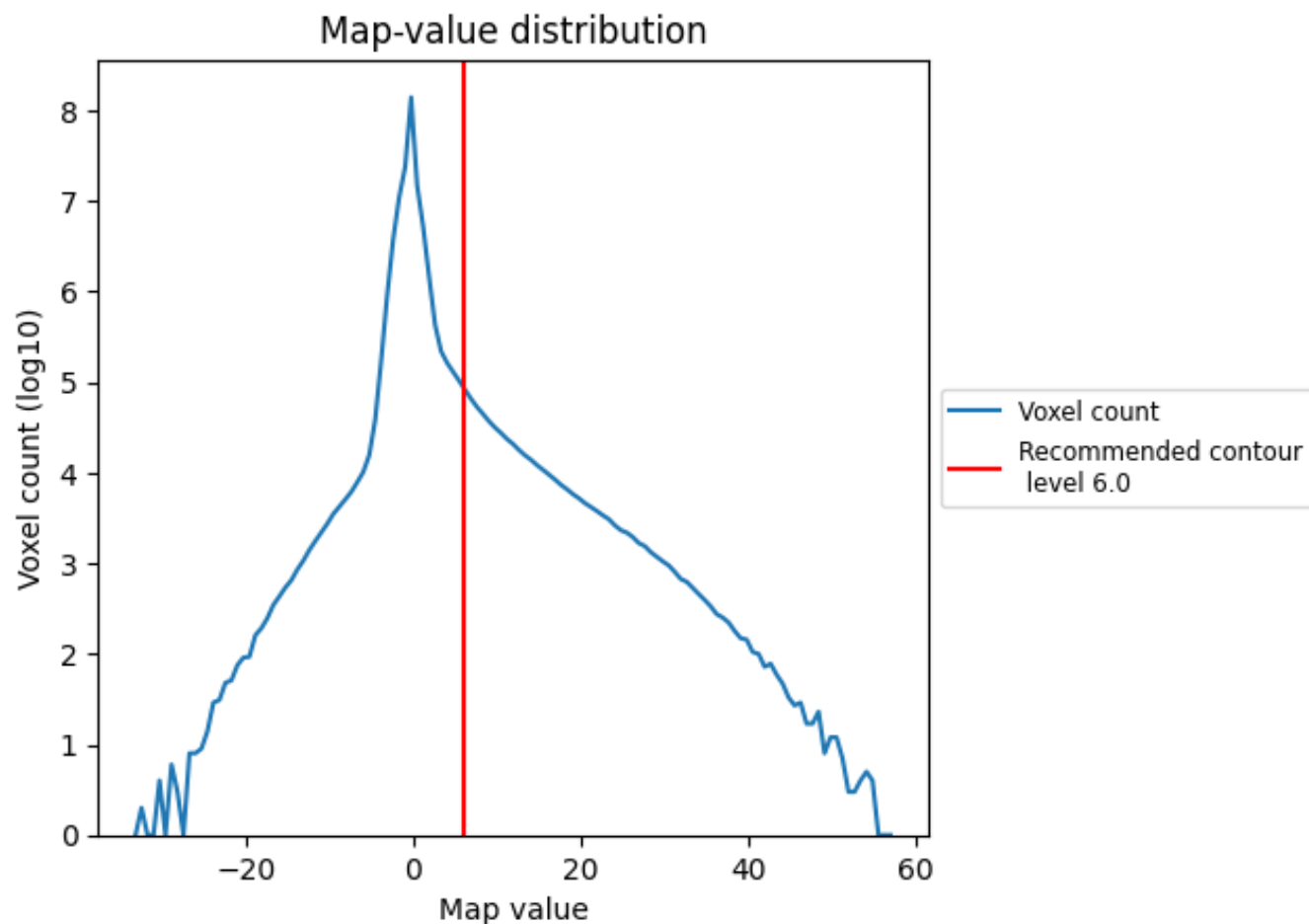
6.5 Mask visualisation

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

7 Map analysis [i](#)

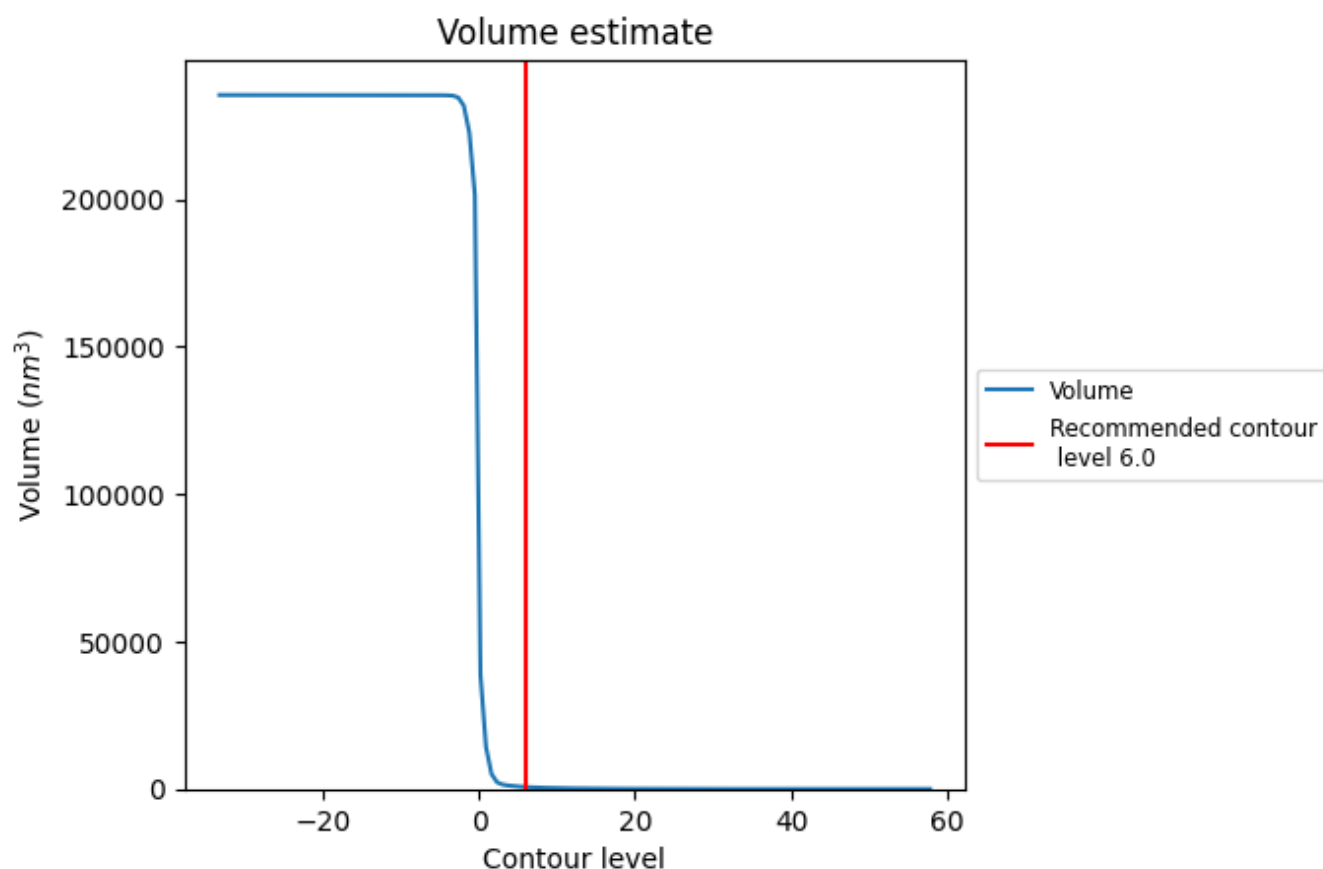
This section contains the results of statistical analysis of the map.

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.

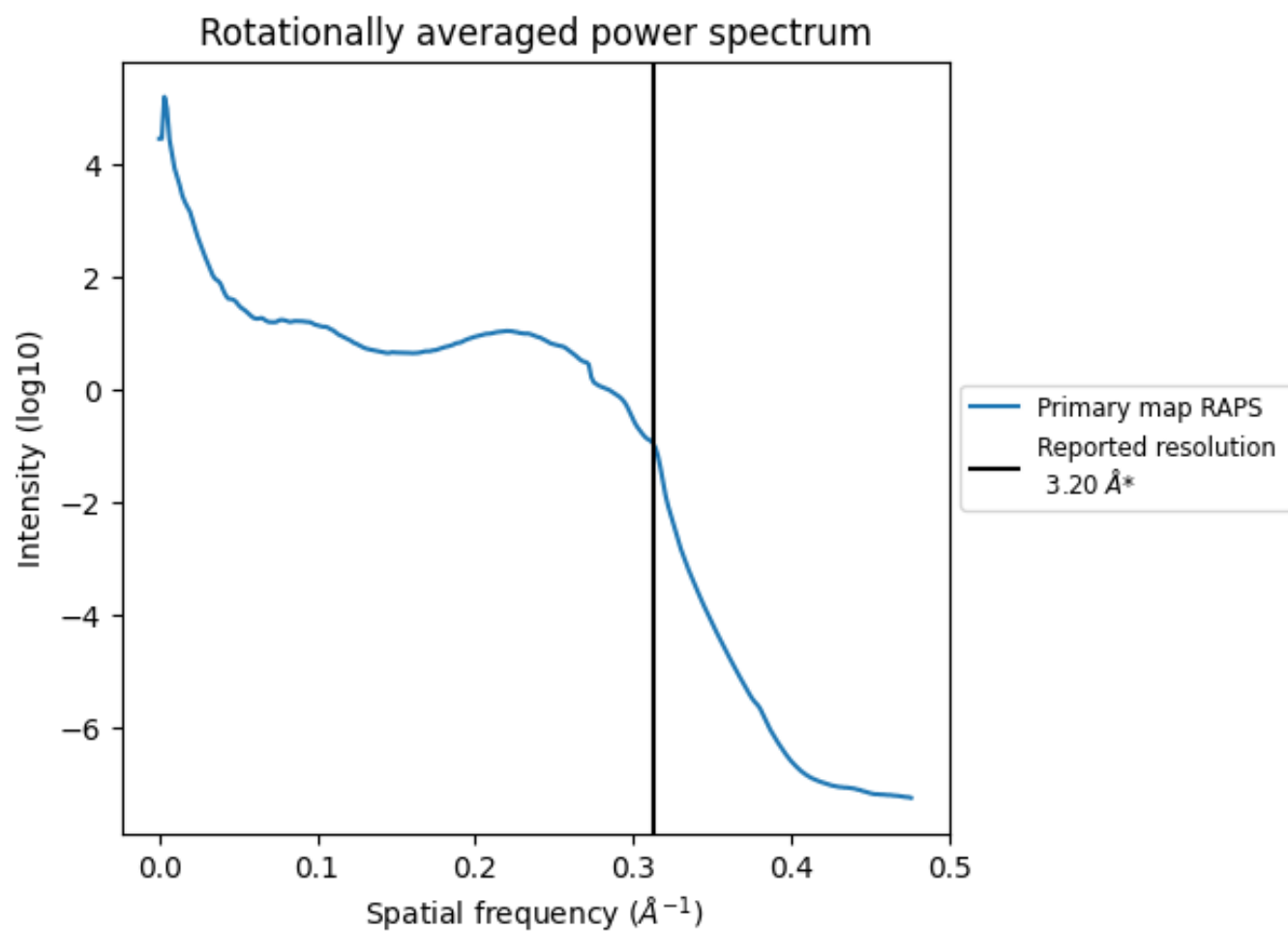
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 658 nm^3 ; this corresponds to an approximate mass of 595 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 0.312 Å⁻¹

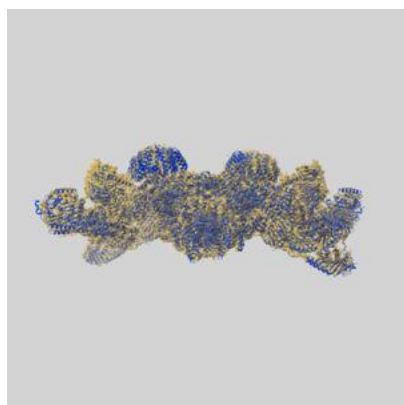
8 Fourier-Shell correlation

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

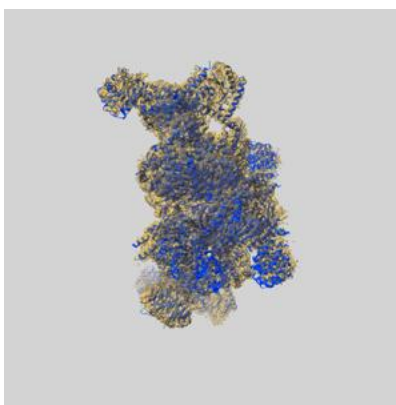
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26861 and PDB model 7UXH. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

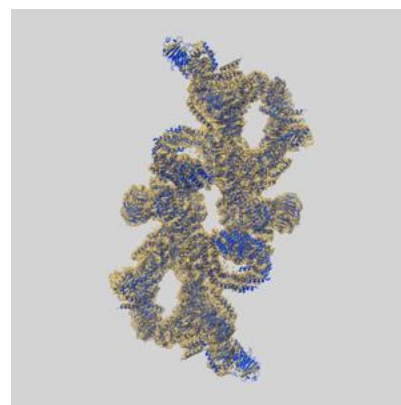
9.1 Map-model overlay [i](#)



X



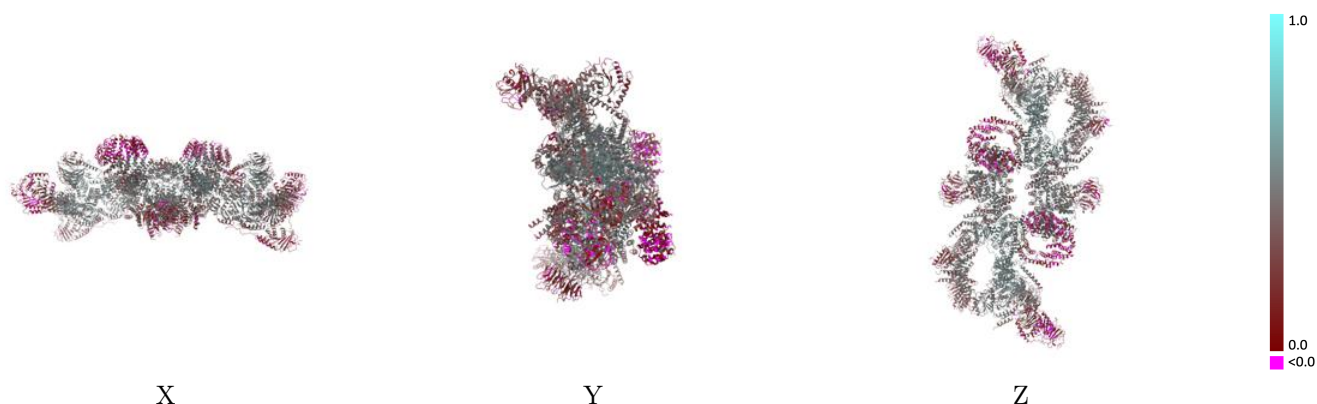
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.0 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](#)



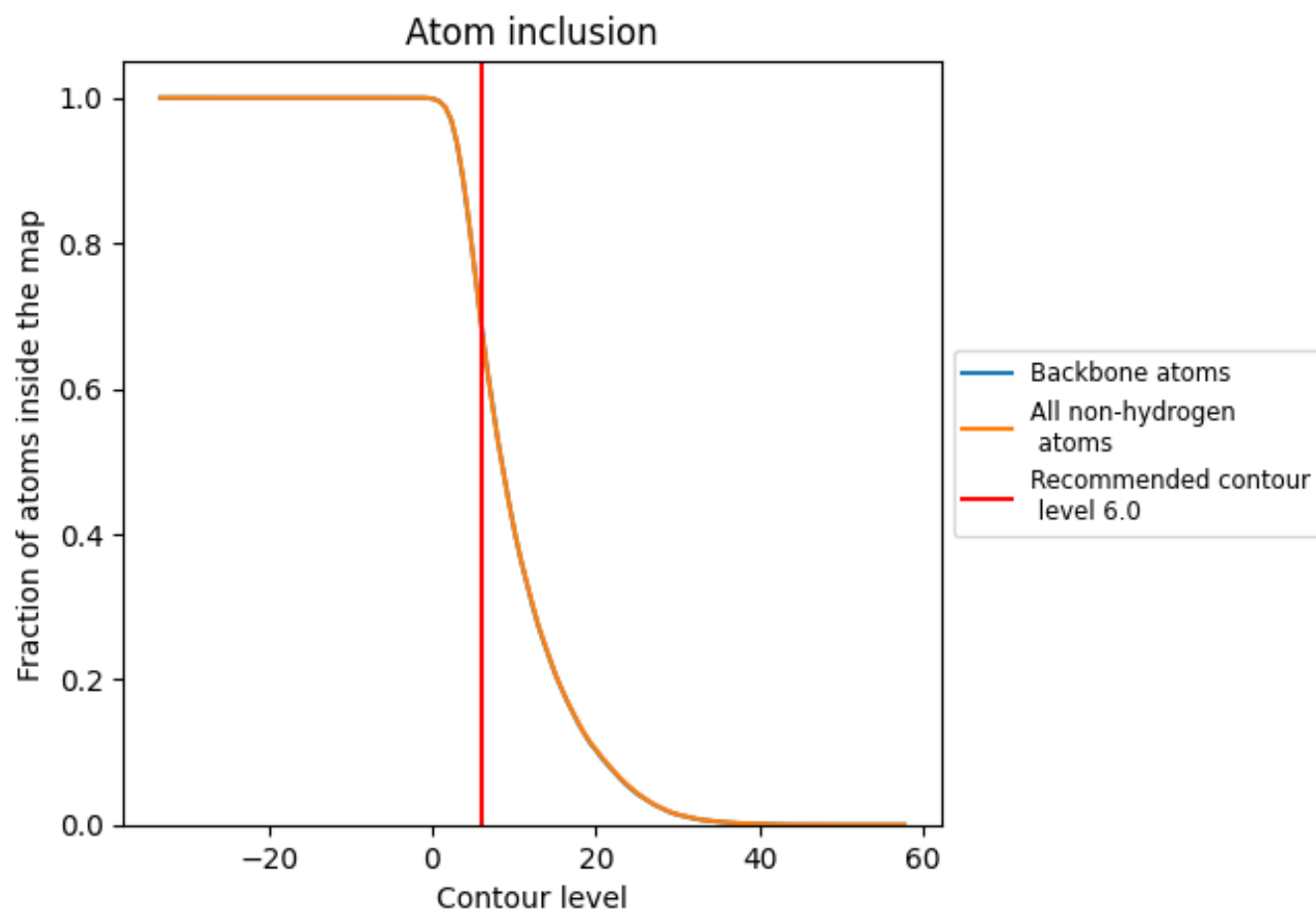
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (6.0).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 69% 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 (6.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6882	 0.3780
A	 0.7186	 0.3640
B	 0.6614	 0.2060
C	 0.6671	 0.3650
D	 0.5555	 0.2000
E	 0.8820	 0.4930
F	 0.8877	 0.4970
G	 0.8504	 0.4580
H	 0.3525	 0.2220
I	 0.6475	 0.3080
J	 0.5467	 0.2410
K	 0.0906	 0.1080
L	 0.2052	 0.0790
M	 0.7866	 0.4330
N	 0.7030	 0.3590
O	 0.5091	 0.2780
P	 0.7191	 0.3930
Q	 0.7261	 0.3850
R	 0.4324	 0.2090
S	 0.4992	 0.2580
T	 0.7474	 0.4180
U	 0.8539	 0.4940
V	 0.8463	 0.4920
W	 0.7885	 0.4530
X	 0.2374	 0.1730
Y	 0.5564	 0.3120
Z	 0.3804	 0.2230
a	 0.0350	 0.0810
b	 0.1669	 0.1190
c	 0.7359	 0.4280
d	 0.6305	 0.3660
e	 0.3941	 0.2690
f	 0.6518	 0.3960
g	 0.6457	 0.3740
h	 0.3052	 0.2060



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Chain	Atom inclusion	Q-score
i	 0.3645	 0.2510
j	 0.6845	 0.4100