wwPDB EM Validation Summary Report (i)

Mar 5, 2026 – 07:45 PM UTC

PDB ID	:	7UXH / pdb_00007uxh
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 (i) symbol.

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

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

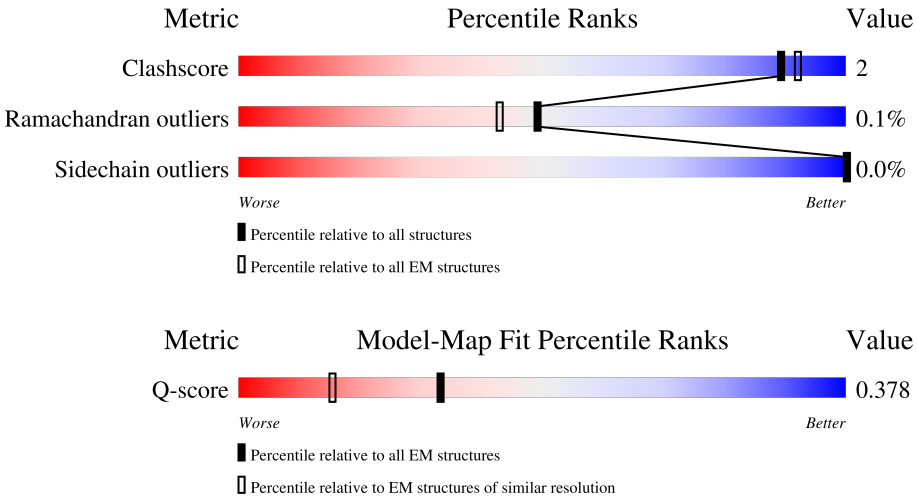
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 (i)

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2549	15% 83% · 14%
1	C	2549	19% 83% · 14%
2	B	326	19% 90% 7% ·
2	D	326	30% 91% 6% ·

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Mol	Chain	Length	Quality of chain
3	E	1335	80% 15%
3	U	1335	81% 15%
4	F	313	89% 6% 5%
4	M	313	89% 6% 5%
4	V	313	91% 5%
4	c	313	5% 85% 10% 5%
5	G	399	67% 30%
5	N	399	7% 64% 6% 31%
5	W	399	66% 30%
5	d	399	11% 64% 6% 31%
6	H	161	40% 65% 31%
6	O	161	27% 62% 9% 29%
6	X	161	50% 64% 5% 31%
6	e	161	41% 63% 8% 29%
7	I	125	14% 93% 6%
7	P	125	9% 91% 8%
7	Y	125	26% 91% 7%
7	f	125	14% 94% 6%
8	J	124	26% 88% 9%
8	Q	124	6% 90% 7%
8	Z	124	54% 88% 9%
8	g	124	13% 93%
9	K	99	77% 77% 7% 15%
9	R	99	32% 78% 7% 15%
9	a	99	84% 78% 6% 15%

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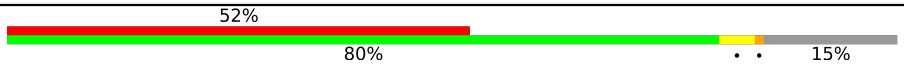
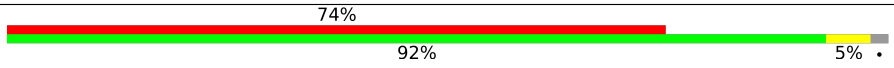
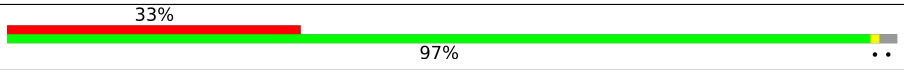
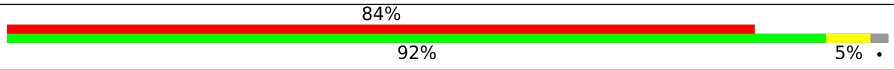
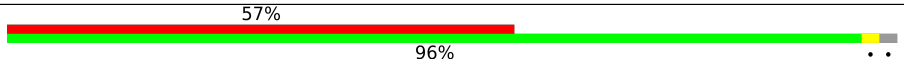
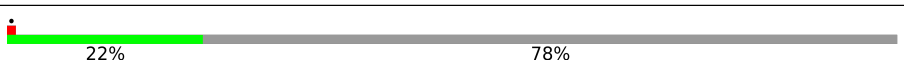
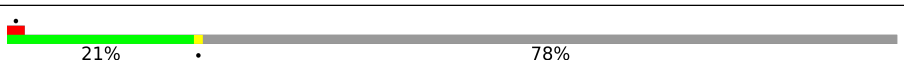
Mol	Chain	Length	Quality of chain
9	h	99	
10	L	91	
10	S	91	
10	b	91	
10	i	91	
11	T	476	
11	j	476	

2 Entry composition (i)

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 Ragulator 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 Ragulator complex protein LAMTOR2.

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

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

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

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

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

- Molecule 10 is a protein called Ragulator 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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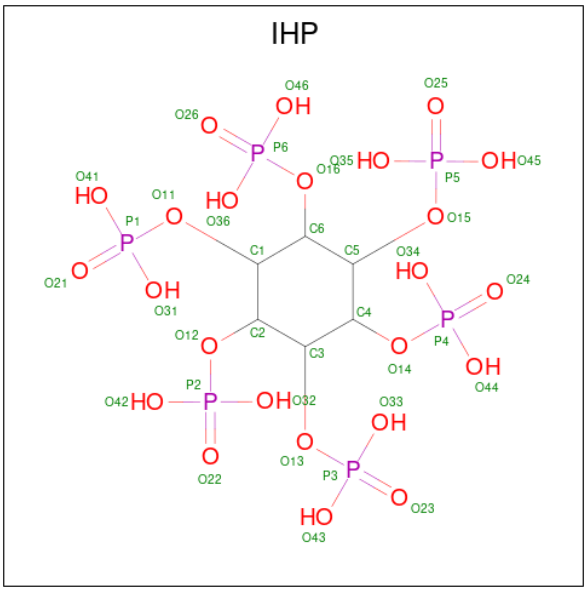
Mol	Chain	Residues	Atoms						AltConf	Trace
10	i	89	Total	C	H	N	O	S	0	0
			1311	400	656	113	135	7		

- Molecule 11 is a protein called Transcription factor EB.

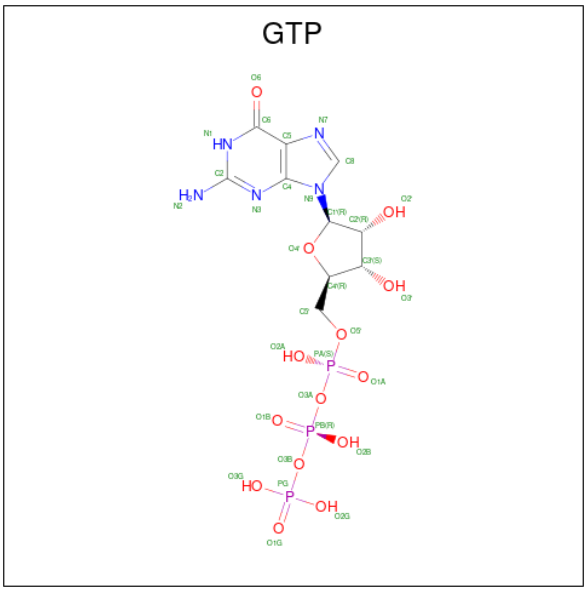
Mol	Chain	Residues	Atoms						AltConf	Trace
11	T	107	Total	C	H	N	O	S	0	0
			1723	541	847	165	165	5		
11	j	107	Total	C	H	N	O	S	0	0
			1724	541	848	165	165	5		

- Molecule 12 is INOSITOL HEXAKISPHOSPHATE (CCD ID: 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 (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

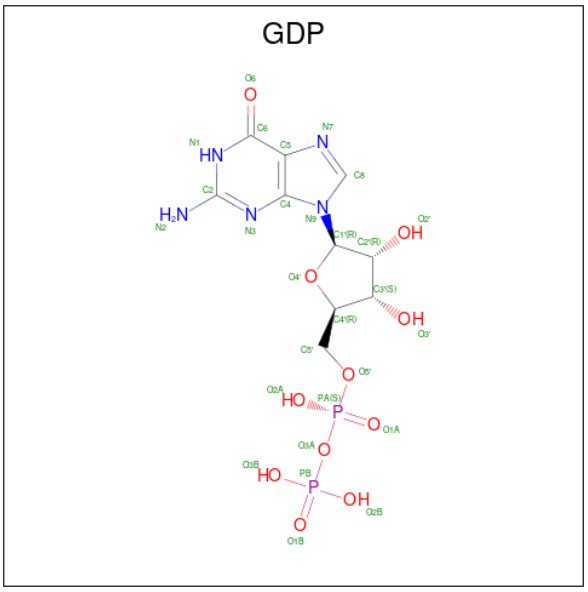


Mol	Chain	Residues	Atoms						AltConf
13	F	1	Total	C	H	N	O	P	0
			42	10	10	5	14	3	
13	M	1	Total	C	H	N	O	P	0
			42	10	10	5	14	3	
13	V	1	Total	C	H	N	O	P	0
			42	10	10	5	14	3	
13	c	1	Total	C	H	N	O	P	0
			42	10	10	5	14	3	

- Molecule 14 is MAGNESIUM ION (CCD ID: 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 (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



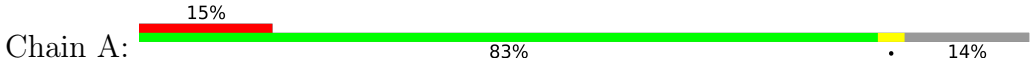
Mol	Chain	Residues	Atoms						AltConf
15	G	1	Total	C	H	N	O	P	0
			38	10	10	5	11	2	
15	N	1	Total	C	H	N	O	P	0
			38	10	10	5	11	2	
15	W	1	Total	C	H	N	O	P	0
			38	10	10	5	11	2	
15	d	1	Total	C	H	N	O	P	0
			38	10	10	5	11	2	

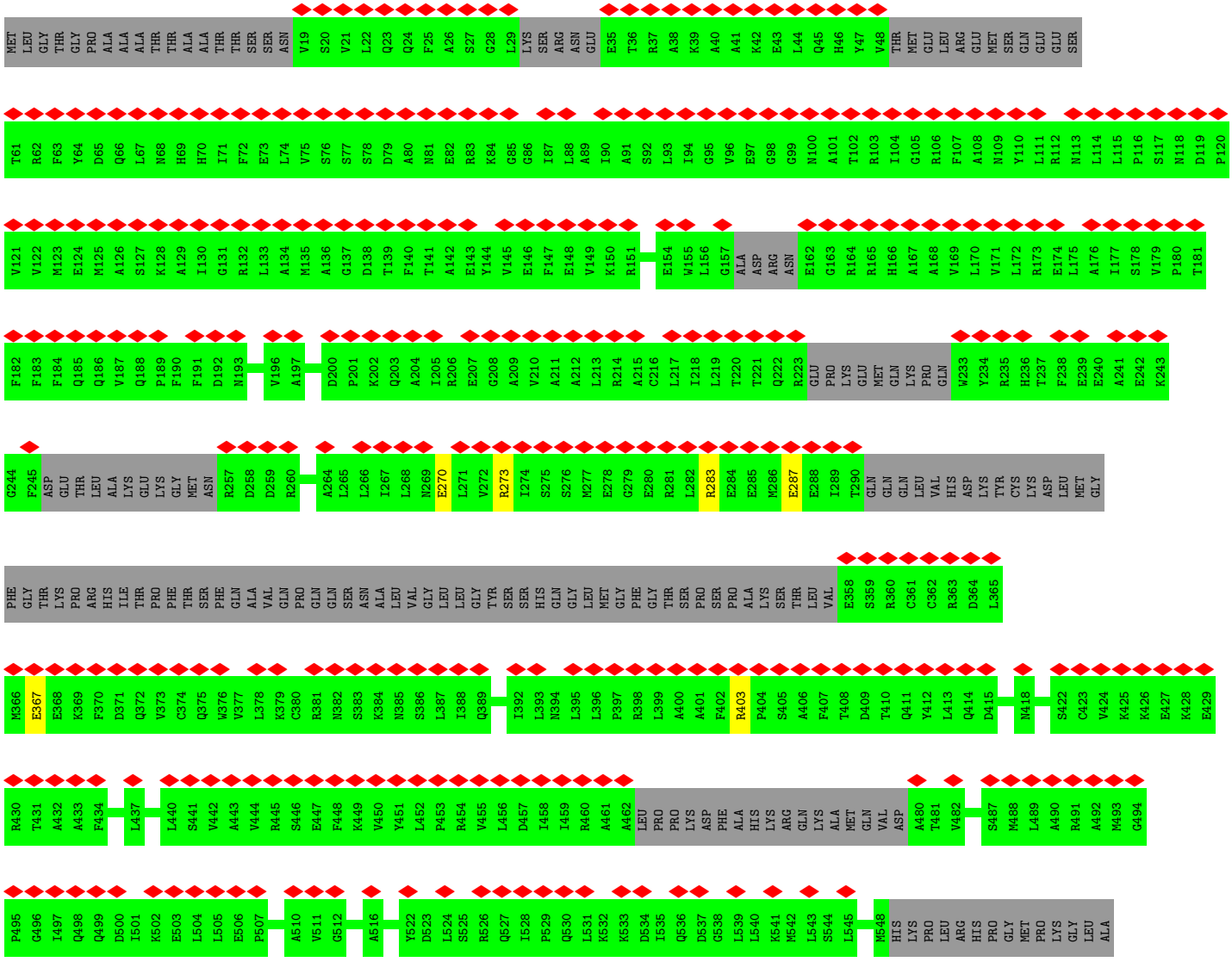
3 Residue-property plots (i)

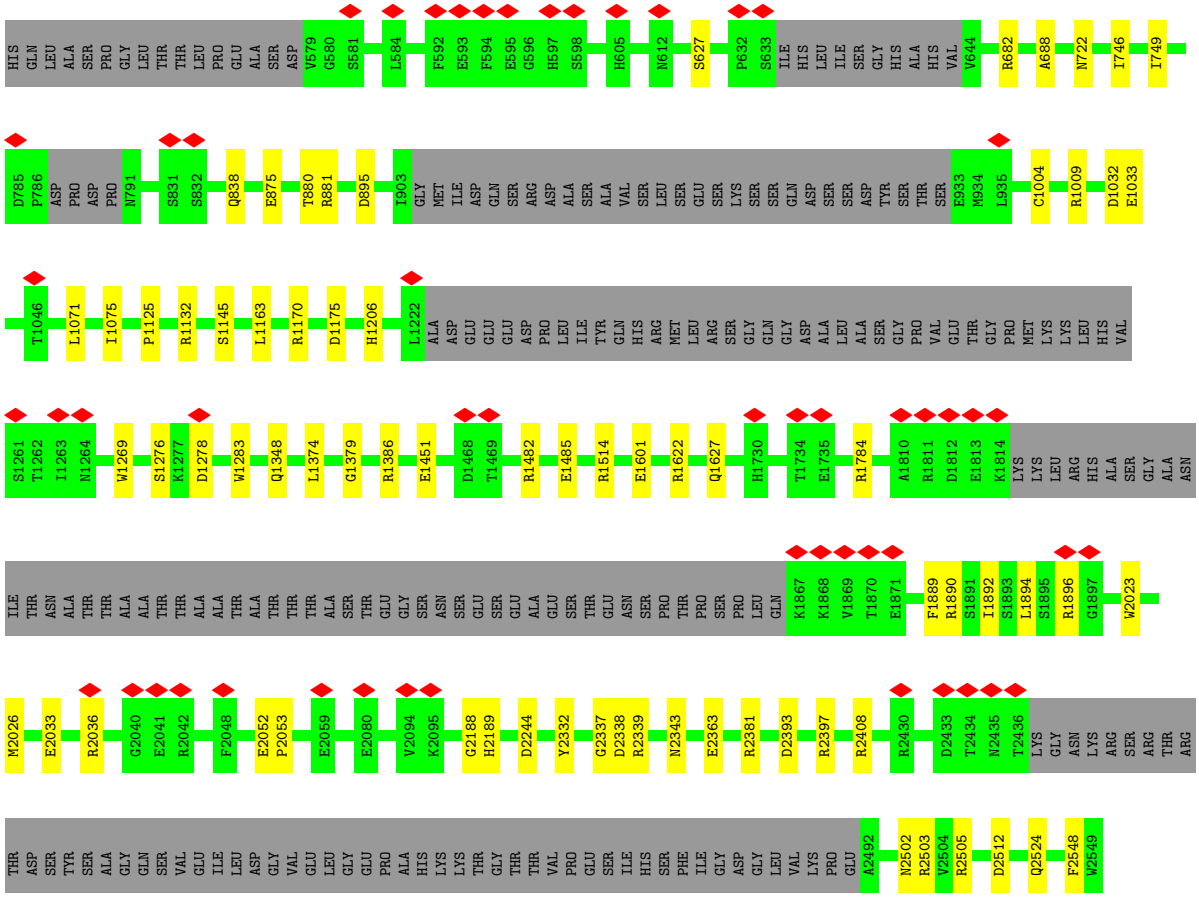
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Serine/threonine-protein kinase mTOR

Chain A:

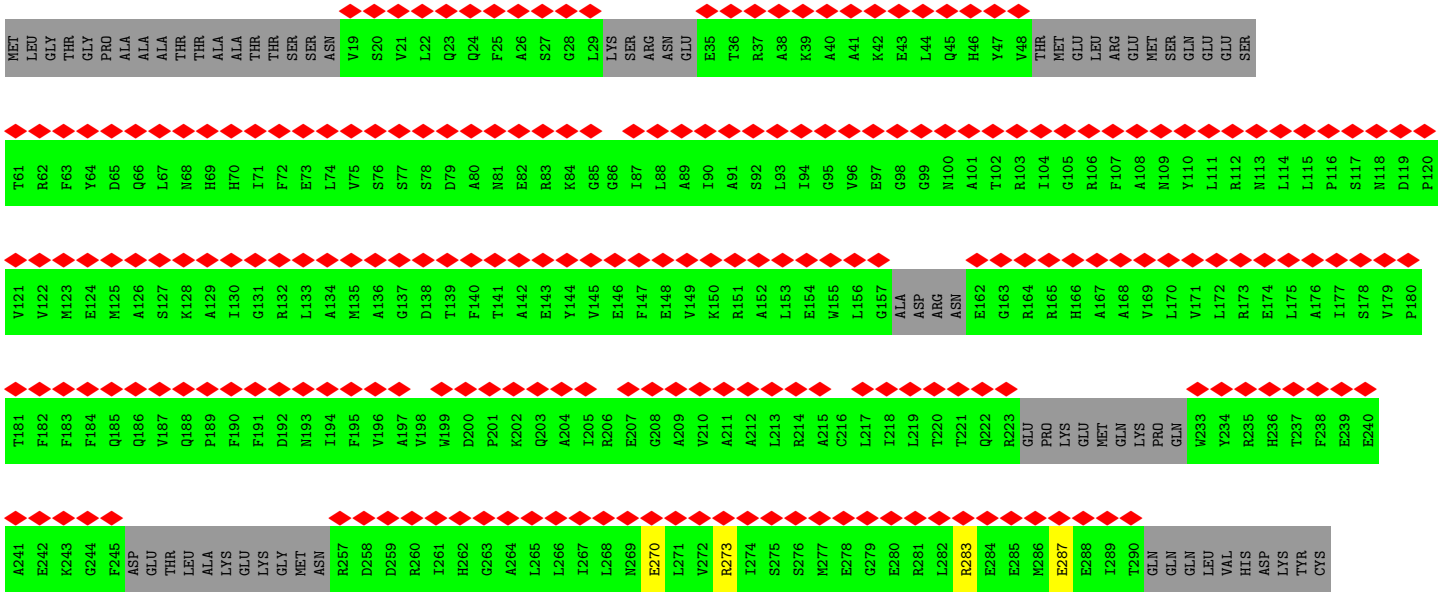


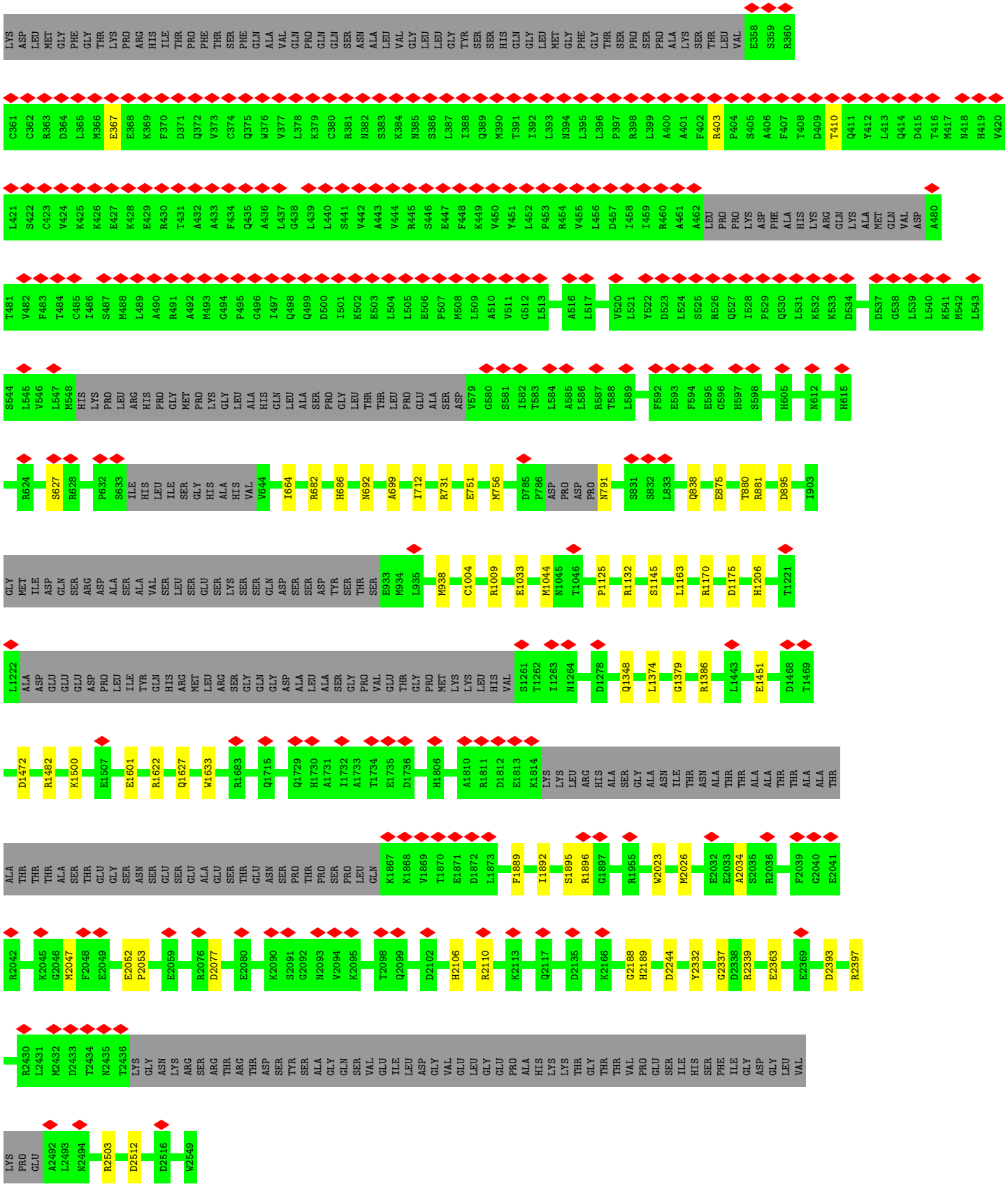




• Molecule 1: Serine/threonine-protein kinase mTOR

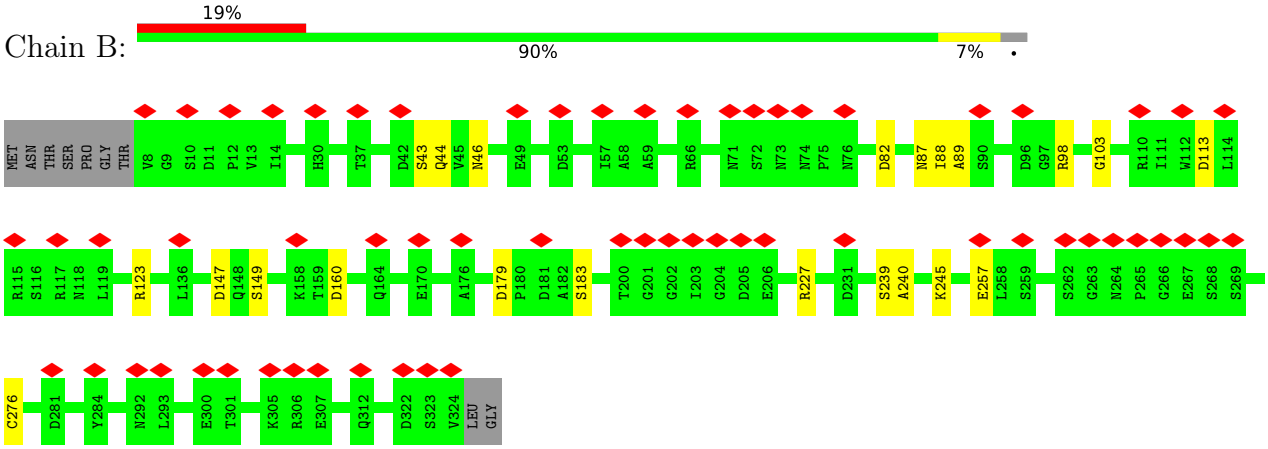
Chain C:





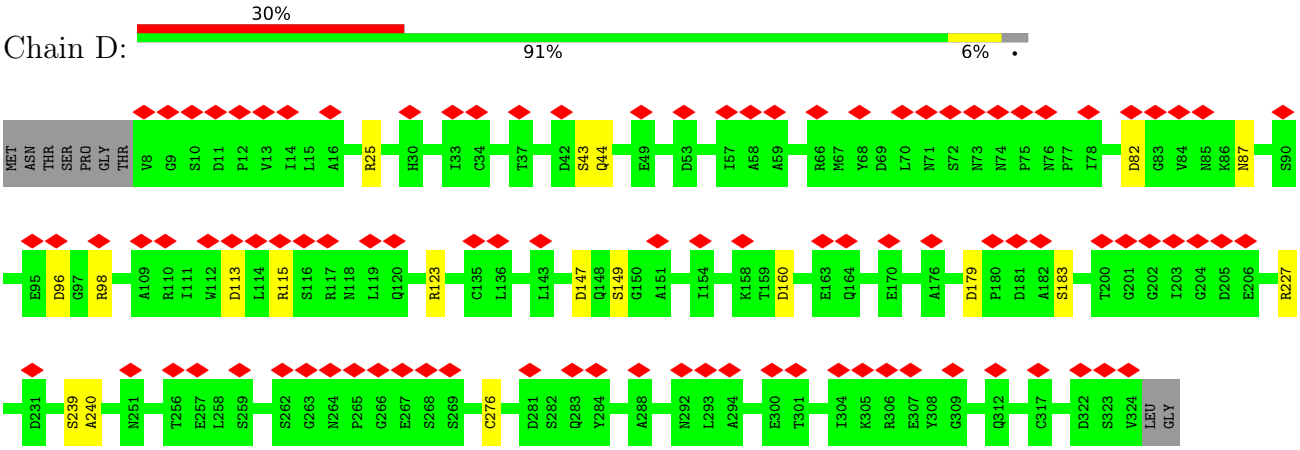
• Molecule 2: Target of rapamycin complex subunit LST8

Chain B:



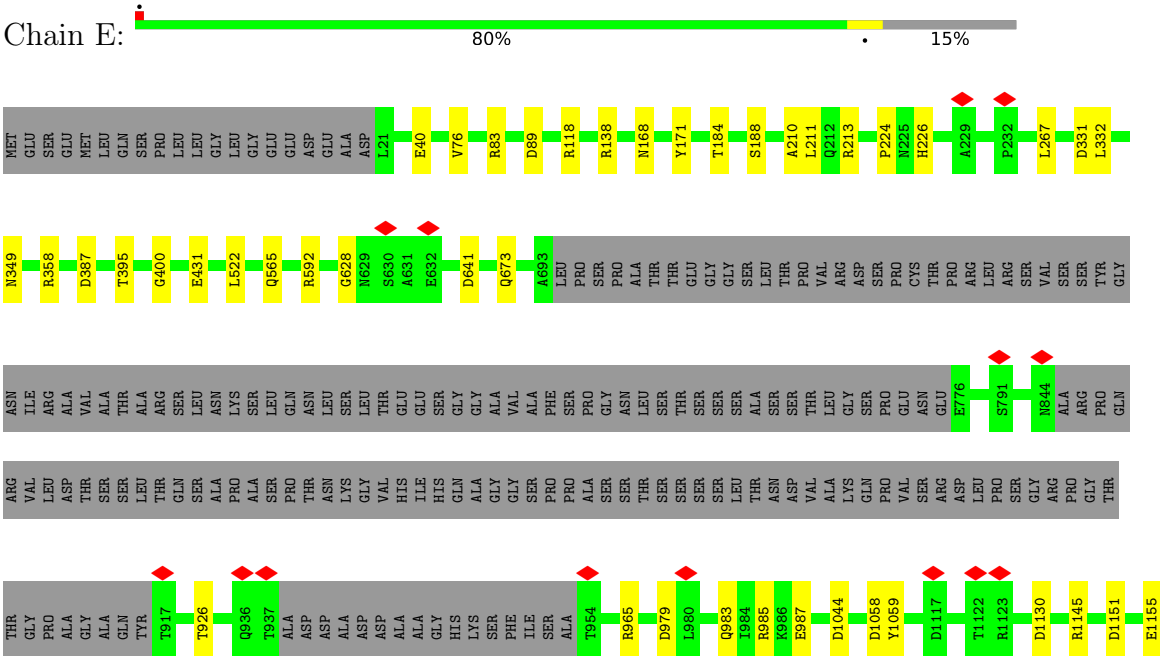
• Molecule 2: Target of rapamycin complex subunit LST8

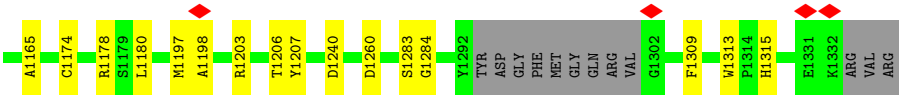
Chain D:



• Molecule 3: Regulatory-associated protein of mTOR

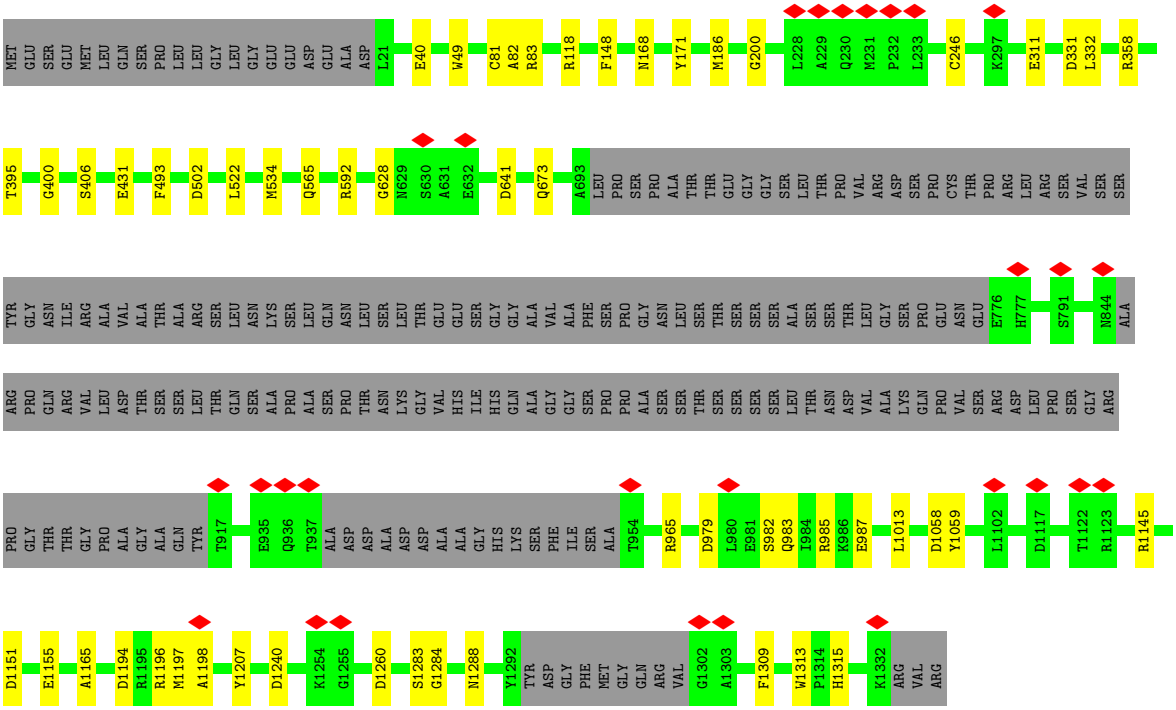
Chain E:





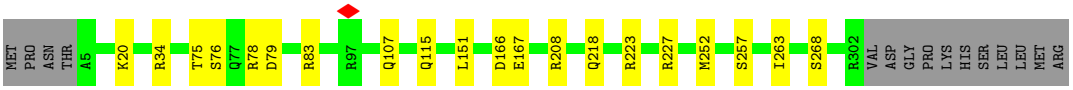
• Molecule 3: Regulatory-associated protein of mTOR

Chain U:



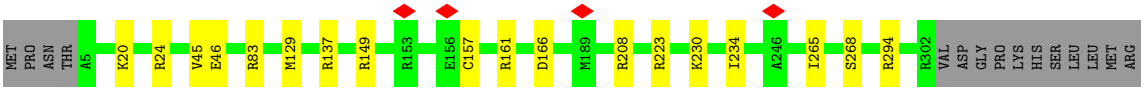
• Molecule 4: Ras-related GTP-binding protein A

Chain F:



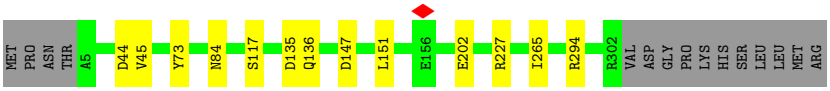
• Molecule 4: Ras-related GTP-binding protein A

Chain M:



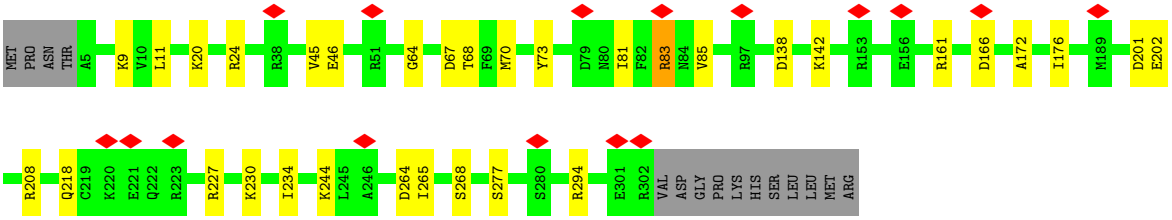
• Molecule 4: Ras-related GTP-binding protein A

Chain V:



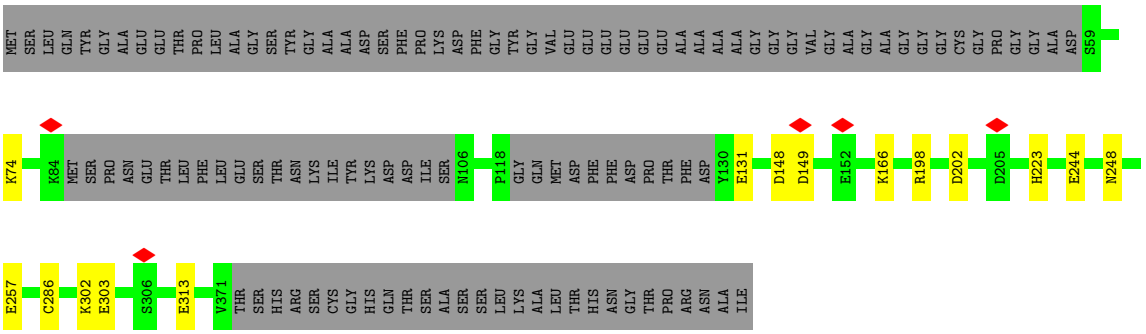
• Molecule 4: Ras-related GTP-binding protein A

Chain c:



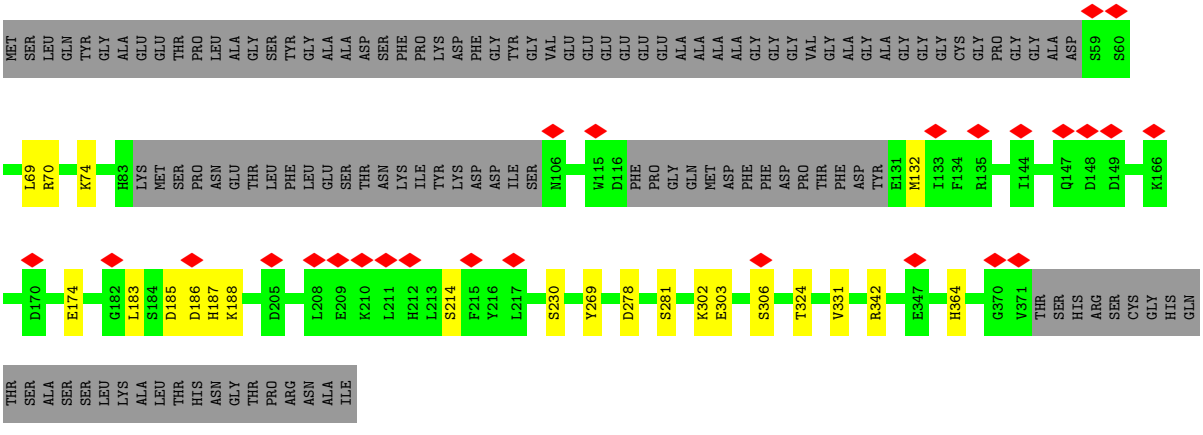
• Molecule 5: Ras-related GTP-binding protein C

Chain G:



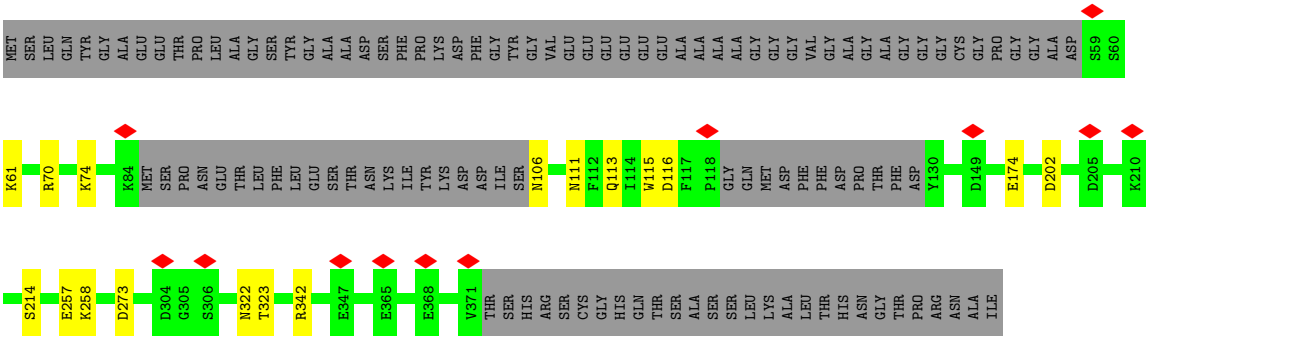
• Molecule 5: Ras-related GTP-binding protein C

Chain N:



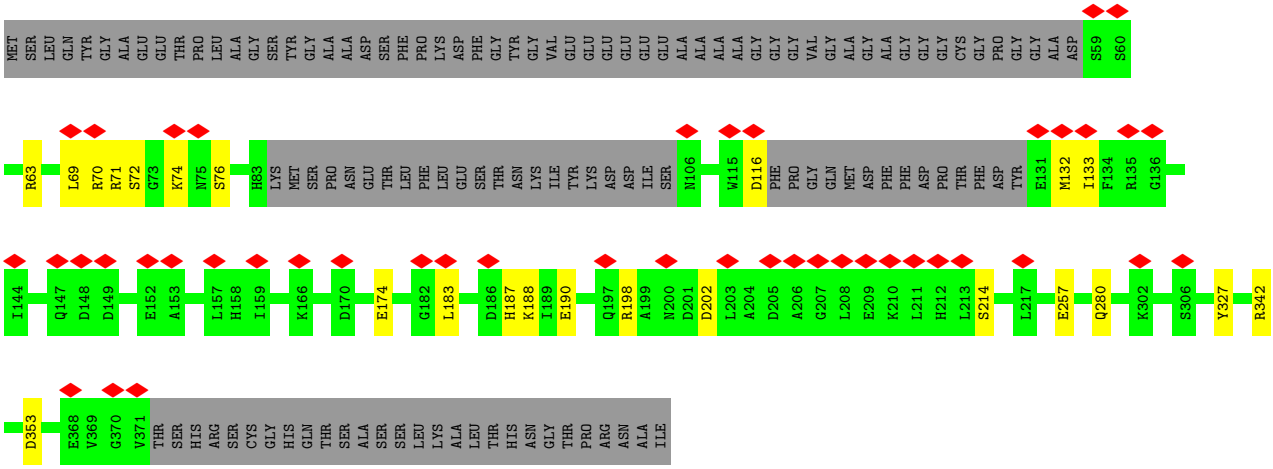
• Molecule 5: Ras-related GTP-binding protein C

Chain W:



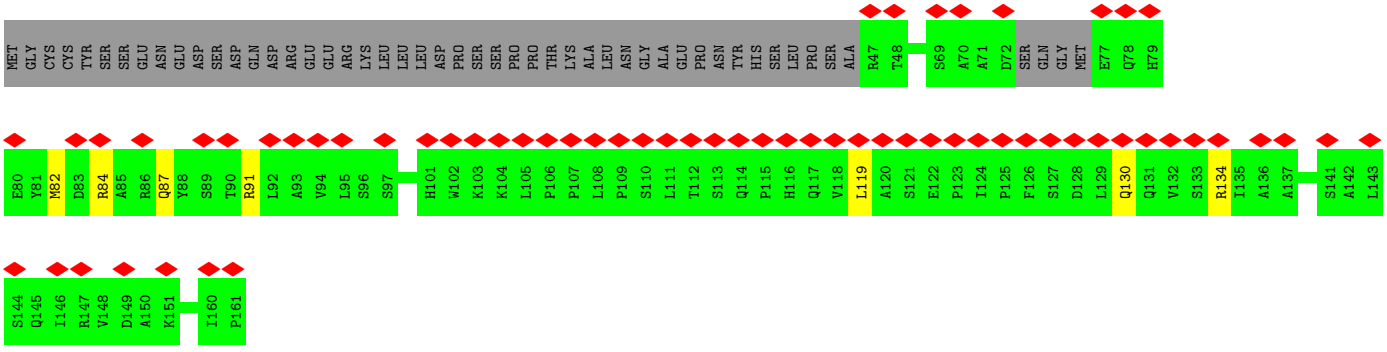
• Molecule 5: Ras-related GTP-binding protein C

Chain d:



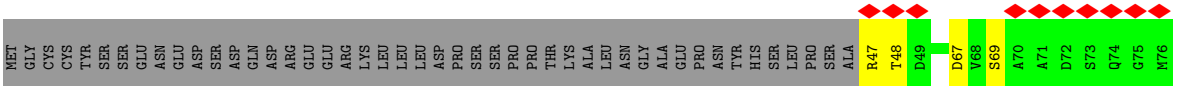
• Molecule 6: Ragulator complex protein LAMTOR1

Chain H:

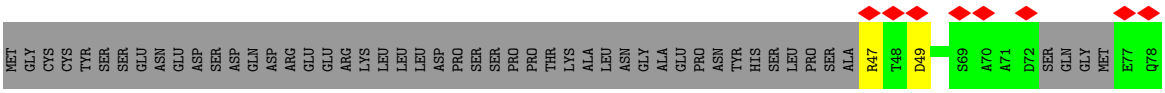


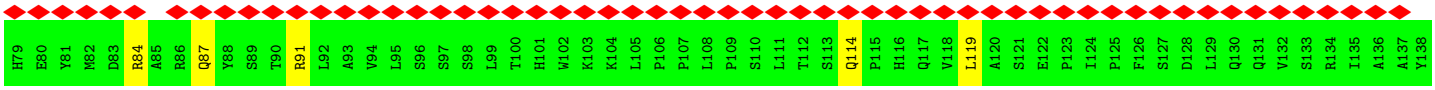
• Molecule 6: Ragulator complex protein LAMTOR1

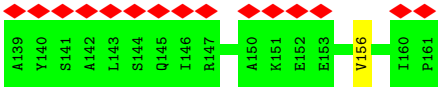
Chain O:



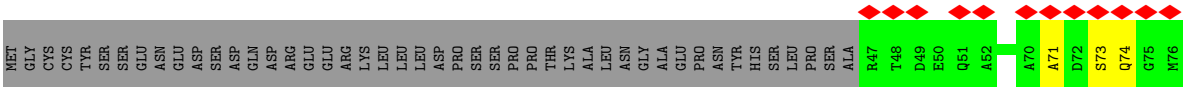
• Molecule 6: Ragulator complex protein LAMTOR1

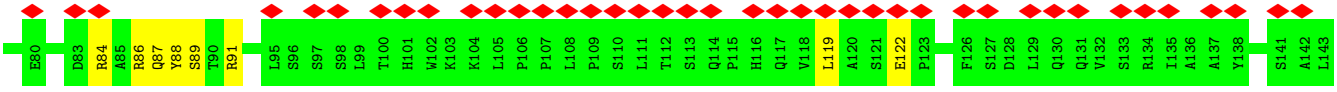


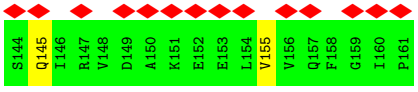




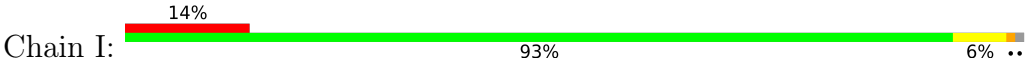
• Molecule 6: Ragulator complex protein LAMTOR1

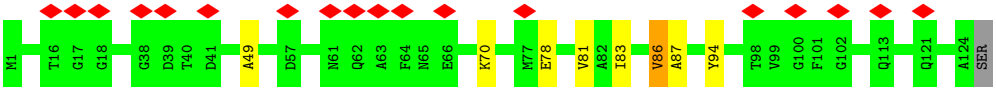




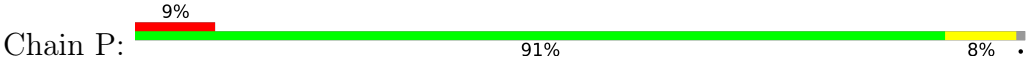


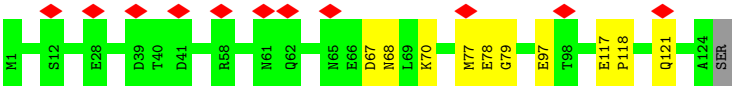
• Molecule 7: Ragulator complex protein LAMTOR2





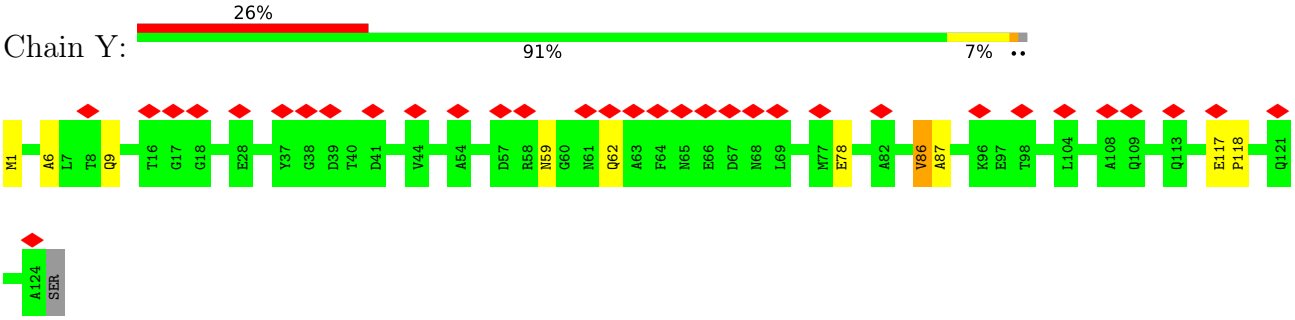
• Molecule 7: Ragulator complex protein LAMTOR2





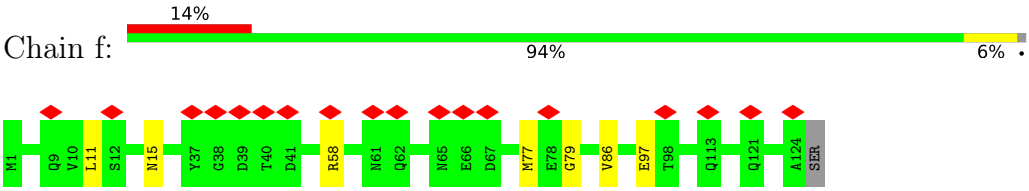
• Molecule 7: Ragulator complex protein LAMTOR2

Chain Y:



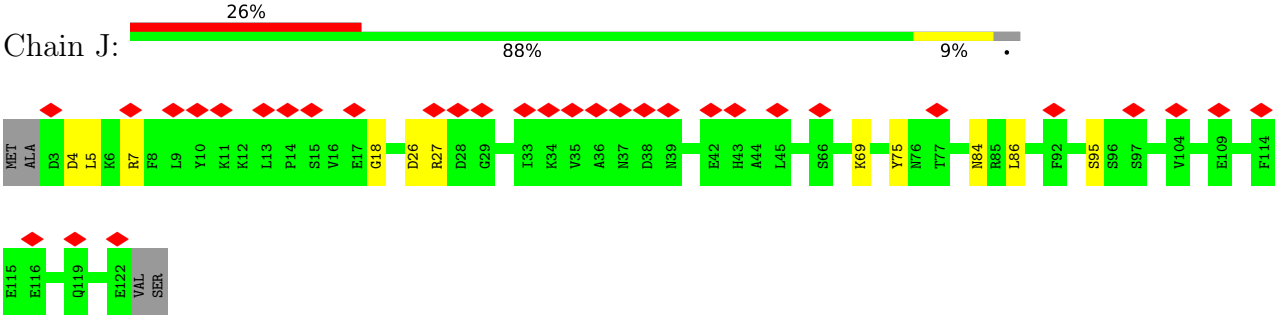
• Molecule 7: Ragulator complex protein LAMTOR2

Chain f:



• Molecule 8: Ragulator complex protein LAMTOR3

Chain J:



• Molecule 8: Ragulator complex protein LAMTOR3

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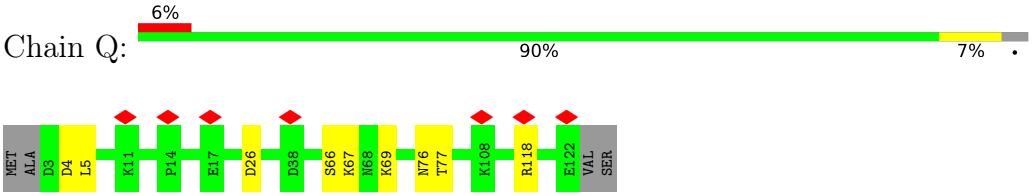
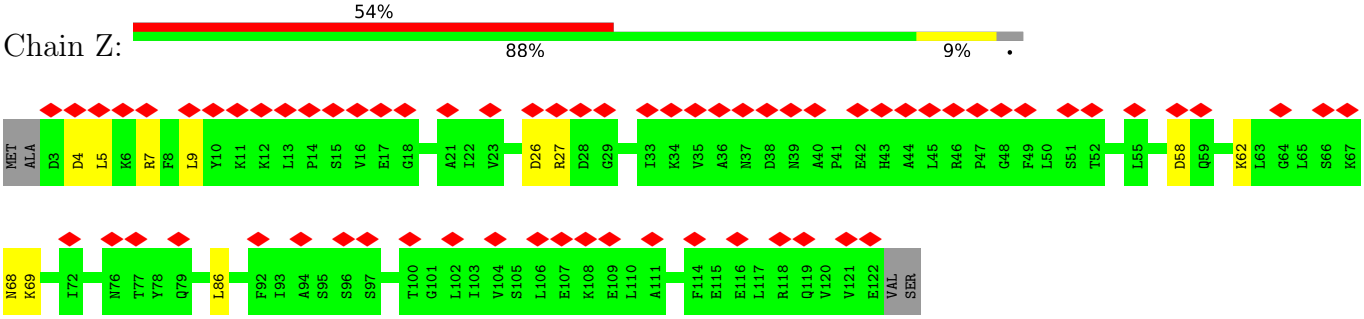


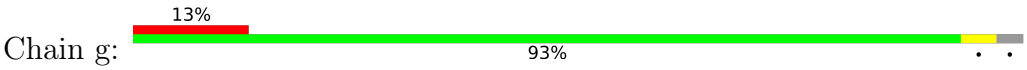
• Molecule 8: Ragulator complex protein LAMTOR3

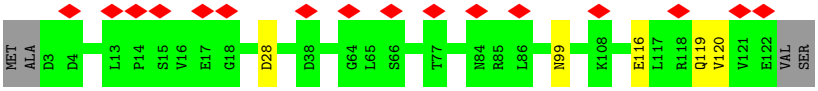
Chain Z:



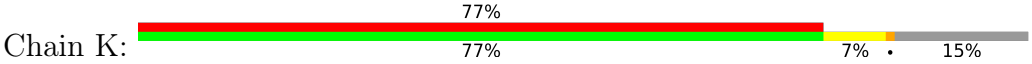
• Molecule 8: Ragulator complex protein LAMTOR3

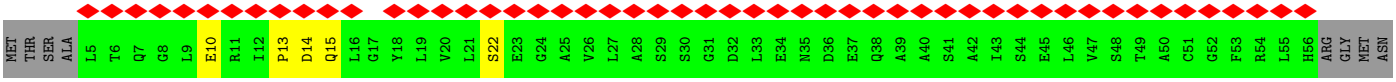
Chain g:

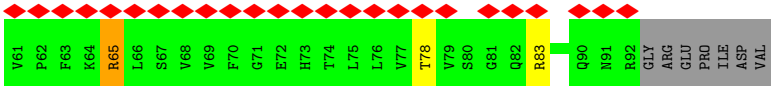




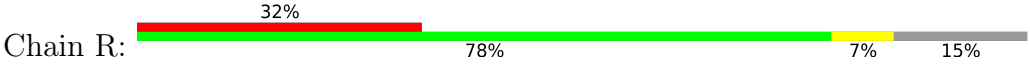
• Molecule 9: Ragulator complex protein LAMTOR4

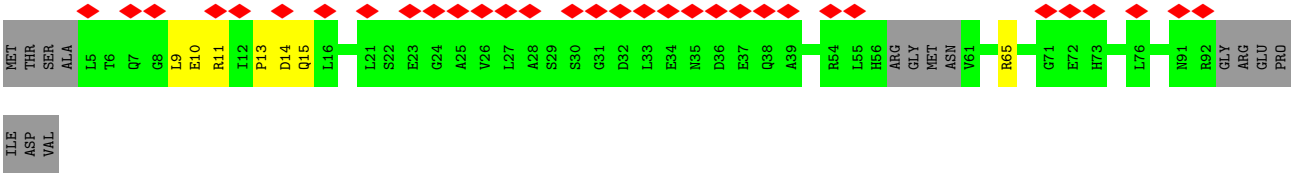




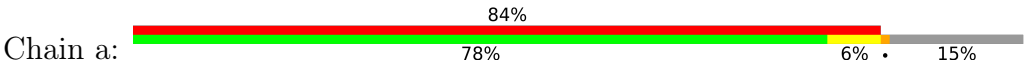


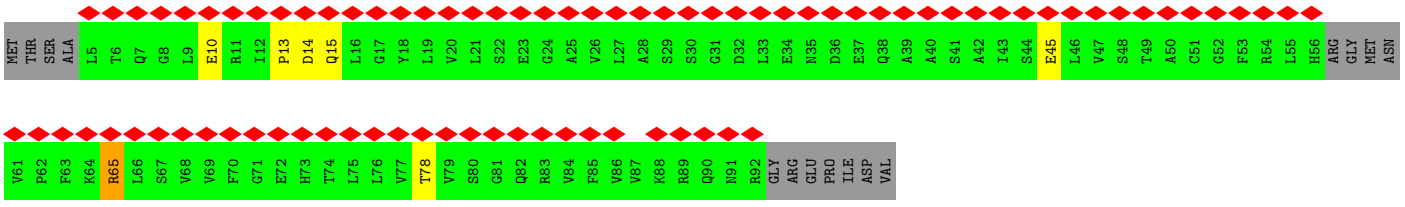
• Molecule 9: Ragulator complex protein LAMTOR4



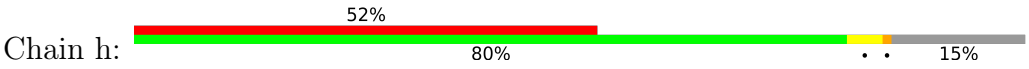


• Molecule 9: Ragulator complex protein LAMTOR4

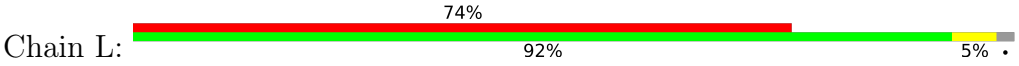


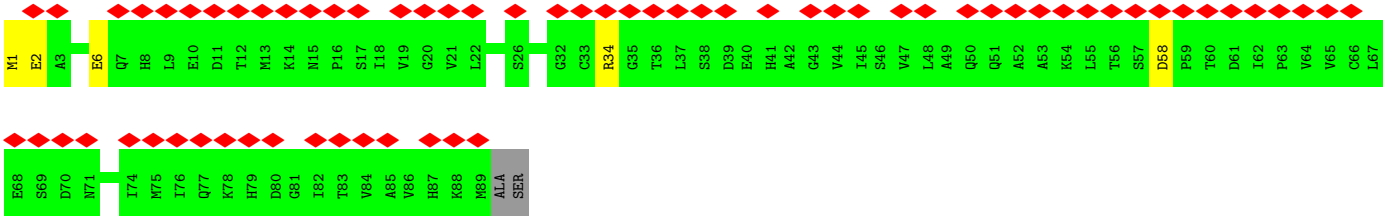


• Molecule 9: Ragulator complex protein LAMTOR4

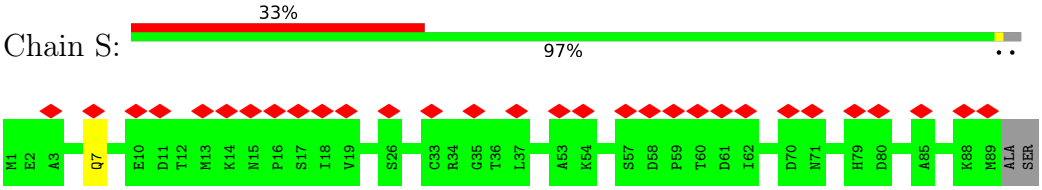


• Molecule 10: Ragulator complex protein LAMTOR5

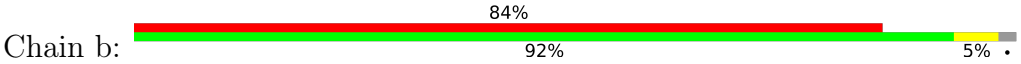


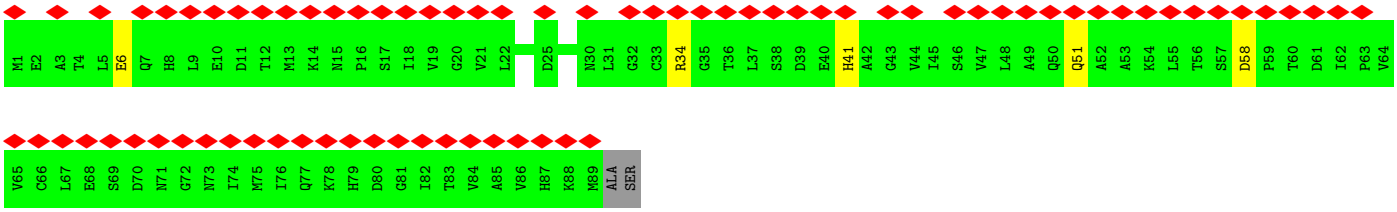


• Molecule 10: Ragulator complex protein LAMTOR5

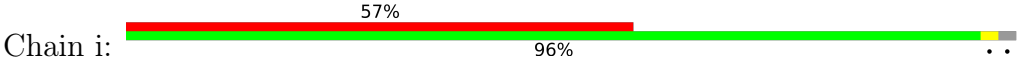


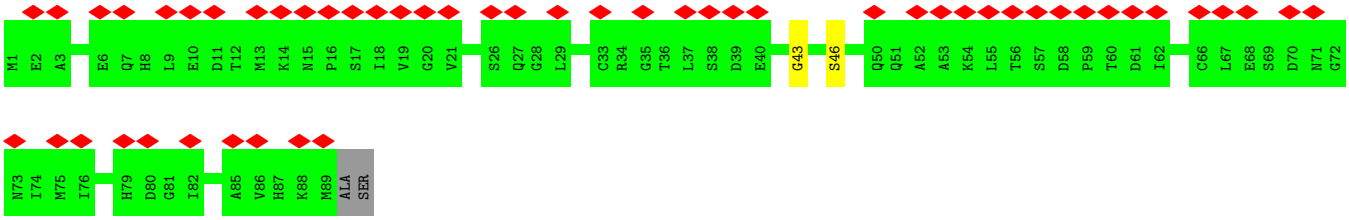
• Molecule 10: Ragulator complex protein LAMTOR5



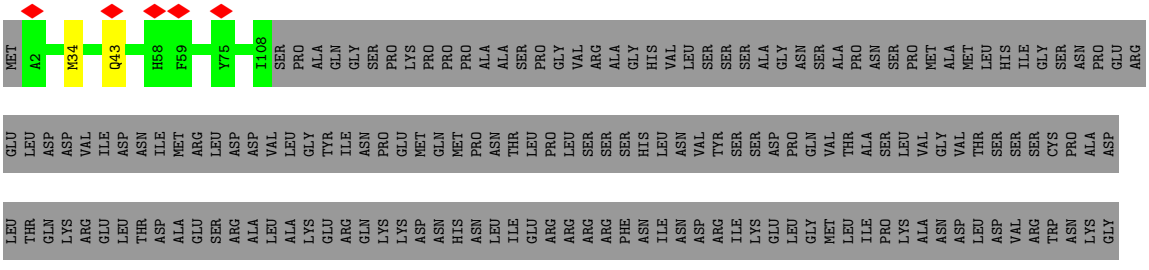


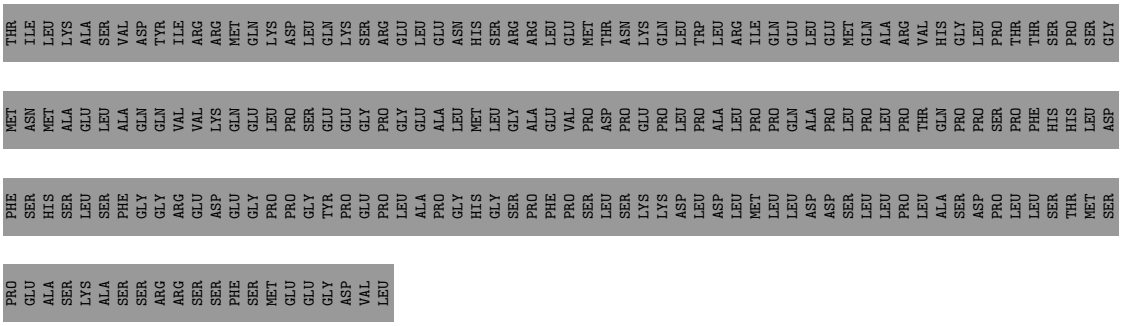
• Molecule 10: Ragulator complex protein LAMTOR5





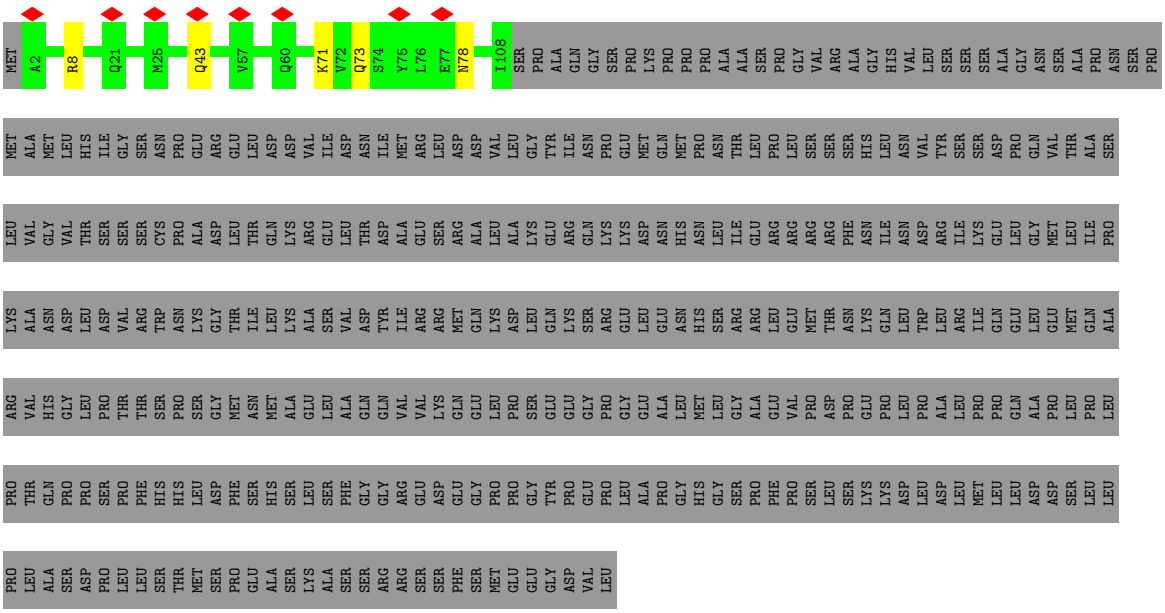
• Molecule 11: Transcription factor EB





• Molecule 11: Transcription factor EB

Chain j:



4 Experimental information (i)

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 ($e^-/Å^2$)	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	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: IHP, MG, GTP, GDP

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	0.19	0/17941	0.44	0/24276
1	C	0.19	0/17941	0.44	0/24276
2	B	0.17	0/2514	0.42	0/3426
2	D	0.16	0/2514	0.41	0/3426
3	E	0.23	0/9242	0.47	0/12573
3	U	0.22	0/9242	0.48	0/12573
4	F	0.22	0/2491	0.49	0/3353
4	M	0.21	0/2491	0.53	0/3353
4	V	0.21	0/2489	0.51	0/3350
4	c	0.25	0/2491	0.58	0/3353
5	G	0.23	0/2309	0.54	0/3114
5	N	0.22	0/2267	0.53	0/3057
5	W	0.22	0/2309	0.54	0/3114
5	d	0.22	0/2267	0.52	0/3057
6	H	0.20	0/884	0.49	0/1201
6	O	0.22	0/912	0.54	0/1239
6	X	0.19	0/884	0.48	0/1201
6	e	0.22	0/912	0.56	0/1239
7	I	0.23	0/949	0.59	0/1285
7	P	0.24	0/949	0.63	0/1285
7	Y	0.24	0/949	0.66	0/1285
7	f	0.24	0/949	0.63	0/1285
8	J	0.20	0/951	0.57	0/1290
8	Q	0.21	0/951	0.55	0/1290
8	Z	0.20	0/951	0.55	0/1290
8	g	0.26	0/951	0.63	0/1290
9	K	0.19	0/649	0.42	0/876
9	R	0.19	0/649	0.45	0/876
9	a	0.19	0/649	0.44	0/876
9	h	0.19	0/649	0.43	0/876
10	L	0.22	0/661	0.55	0/896
10	S	0.22	0/661	0.58	0/896

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
10	b	0.20	0/661	0.51	0/896
10	i	0.21	0/661	0.53	0/896
11	T	0.20	0/896	0.53	0/1211
11	j	0.22	0/896	0.52	0/1211
All	All	0.21	0/96732	0.49	0/130991

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.

There are no bond angle outliers.

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
9	K	65	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	A	17587	17819	17819	40	0
1	C	17587	17817	17819	42	0
2	B	2456	2341	2341	12	0
2	D	2456	2341	2341	10	0
3	E	9023	9002	9000	32	0
3	U	9023	9002	9000	29	0
4	F	2446	2443	2443	12	0
4	M	2446	2444	2443	9	0
4	V	2444	2438	2438	7	0
4	c	2446	2443	2443	19	0
5	G	2265	2258	2258	12	0
5	N	2226	2220	2220	15	0
5	W	2265	2258	2258	10	0
5	d	2226	2220	2220	14	0
6	H	868	870	870	5	0
6	O	895	896	896	12	0
6	X	868	870	870	5	0
6	e	895	896	896	11	0
7	I	938	950	950	5	0
7	P	938	950	950	8	0
7	Y	938	950	950	8	0
7	f	938	950	950	4	0
8	J	934	958	958	7	0
8	Q	934	958	958	8	0
8	Z	934	958	958	7	0
8	g	934	958	958	6	0
9	K	642	652	652	5	0
9	R	642	652	652	3	0
9	a	642	652	652	5	0
9	h	642	652	652	3	0
10	L	655	657	656	3	0
10	S	655	656	656	1	0
10	b	655	656	656	4	0
10	i	655	656	656	2	0
11	T	876	847	847	1	0
11	j	876	848	847	3	0
12	A	36	6	6	0	0
12	C	36	6	6	0	0
13	F	32	10	12	1	0
13	M	32	10	12	1	0
13	V	32	10	12	0	0
13	c	32	10	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	F	1	0	0	0	0
14	M	1	0	0	0	0
14	V	1	0	0	0	0
14	c	1	0	0	0	0
15	G	28	10	12	1	0
15	N	28	10	12	2	0
15	W	28	10	12	1	0
15	d	28	10	12	3	0
All	All	95166	95230	95241	348	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 2.

The worst 5 of 348 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:O:147:ARG:NH1	6:O:148:VAL:O	2.06	0.88
4:F:257:SER:OG	5:G:313:GLU:OE2	2.01	0.78
5:d:198:ARG:NH1	5:d:202:ASP:OD2	2.20	0.75
3:E:138:ARG:NH1	3:E:188:SER:OG	2.21	0.74
6:H:84:ARG:NH2	8:J:26:ASP:OD2	2.20	0.74

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	36	68
4	V	296/313 (95%)	283 (96%)	13 (4%)	0	100	100
4	c	296/313 (95%)	272 (92%)	23 (8%)	1 (0%)	36	68
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
6	e	113/161 (70%)	106 (94%)	7 (6%)	0	100	100
7	I	122/125 (98%)	118 (97%)	3 (2%)	1 (1%)	16	50
7	P	122/125 (98%)	107 (88%)	15 (12%)	0	100	100
7	Y	122/125 (98%)	117 (96%)	4 (3%)	1 (1%)	16	50
7	f	122/125 (98%)	115 (94%)	6 (5%)	1 (1%)	16	50
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%)	9	40
9	R	80/99 (81%)	70 (88%)	9 (11%)	1 (1%)	9	40
9	a	80/99 (81%)	69 (86%)	10 (12%)	1 (1%)	9	40
9	h	80/99 (81%)	69 (86%)	10 (12%)	1 (1%)	9	40
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
11	T	105/476 (22%)	96 (91%)	8 (8%)	1 (1%)	12 45
11	j	105/476 (22%)	97 (92%)	7 (7%)	1 (1%)	12 45
All	All	11746/14620 (80%)	11177 (95%)	558 (5%)	11 (0%)	49 79

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1919/2220 (86%)	1919 (100%)	0	100 100
1	C	1919/2220 (86%)	1919 (100%)	0	100 100
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%)	1000 (100%)	0	100 100
3	U	1000/1163 (86%)	1000 (100%)	0	100 100
4	F	272/287 (95%)	272 (100%)	0	100 100
4	M	272/287 (95%)	272 (100%)	0	100 100
4	V	271/287 (94%)	271 (100%)	0	100 100
4	c	272/287 (95%)	272 (100%)	0	100 100
5	G	255/340 (75%)	255 (100%)	0	100 100
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	H	97/141 (69%)	97 (100%)	0	100	100
6	O	100/141 (71%)	100 (100%)	0	100	100
6	X	97/141 (69%)	96 (99%)	1 (1%)	68	80
6	e	100/141 (71%)	99 (99%)	1 (1%)	68	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%)	105 (100%)	0	100	100
8	Q	105/108 (97%)	105 (100%)	0	100	100
8	Z	105/108 (97%)	105 (100%)	0	100	100
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%)	71 (100%)	0	100	100
9	a	71/83 (86%)	71 (100%)	0	100	100
9	h	71/83 (86%)	71 (100%)	0	100	100
10	L	76/77 (99%)	76 (100%)	0	100	100
10	S	76/77 (99%)	76 (100%)	0	100	100
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%)	96 (100%)	0	100	100
11	j	96/419 (23%)	96 (100%)	0	100	100
All	All	10457/12692 (82%)	10455 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	X	114	GLN
6	e	145	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 83 such sidechains are listed below:

Mol	Chain	Res	Type
11	T	37	GLN
6	X	157	GLN
3	U	212	GLN
3	U	1007	GLN
4	c	47	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
13	GTP	M	401	14	33,34,34	0.86	1 (3%)	50,54,54	1.56	8 (16%)
15	GDP	W	401	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	6 (13%)
13	GTP	V	401	14	33,34,34	0.85	1 (3%)	50,54,54	1.59	8 (16%)
15	GDP	N	401	-	29,30,30	1.16	3 (10%)	45,47,47	1.70	6 (13%)
15	GDP	d	401	-	29,30,30	1.20	3 (10%)	45,47,47	1.75	6 (13%)
12	IHP	A	2601	-	36,36,36	1.52	6 (16%)	60,60,60	0.97	4 (6%)
12	IHP	C	2601	-	36,36,36	1.52	6 (16%)	60,60,60	0.92	4 (6%)
15	GDP	G	401	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	GTP	F	401	14	33,34,34	0.85	1 (3%)	50,54,54	1.58	8 (16%)
13	GTP	c	401	14	33,34,34	0.87	1 (3%)	50,54,54	1.57	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
13	GTP	M	401	14	-	5/22/38/38	0/3/3/3
15	GDP	W	401	-	-	1/16/32/32	0/3/3/3
13	GTP	V	401	14	-	0/22/38/38	0/3/3/3
15	GDP	N	401	-	-	1/16/32/32	0/3/3/3
15	GDP	d	401	-	-	2/16/32/32	0/3/3/3
12	IHP	A	2601	-	-	7/30/54/54	0/1/1/1
12	IHP	C	2601	-	-	7/30/54/54	0/1/1/1
15	GDP	G	401	-	-	2/16/32/32	0/3/3/3
13	GTP	F	401	14	-	1/22/38/38	0/3/3/3
13	GTP	c	401	14	-	4/22/38/38	0/3/3/3

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	2601	IHP	P3-O13	3.88	1.66	1.59
12	A	2601	IHP	P3-O13	3.88	1.66	1.59
12	A	2601	IHP	P4-O14	3.19	1.65	1.59
12	C	2601	IHP	P4-O14	3.17	1.65	1.59
12	C	2601	IHP	P2-O12	3.16	1.65	1.59

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	d	401	GDP	C5-C4-N3	-6.05	118.76	128.39
15	N	401	GDP	C5-C4-N3	-6.04	118.77	128.39
15	G	401	GDP	C5-C4-N3	-5.90	119.00	128.39
15	W	401	GDP	C5-C4-N3	-5.88	119.03	128.39
13	M	401	GTP	C5-C4-N3	-5.09	120.29	128.39

There are no chirality outliers.

5 of 30 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

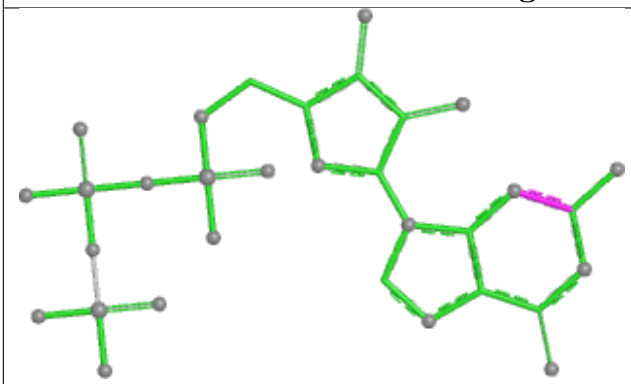
There are no ring outliers.

7 monomers are involved in 10 short contacts:

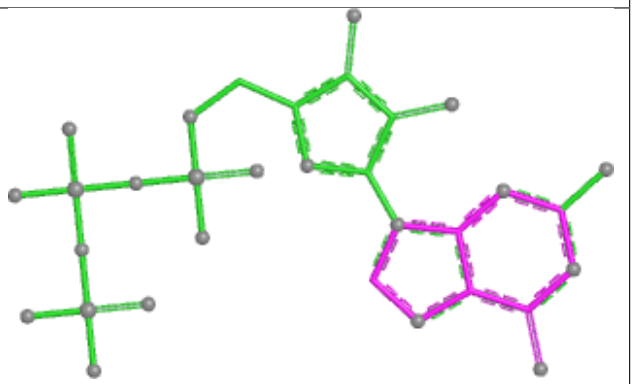
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	M	401	GTP	1	0
15	W	401	GDP	1	0
15	N	401	GDP	2	0
15	d	401	GDP	3	0
15	G	401	GDP	1	0
13	F	401	GTP	1	0
13	c	401	GTP	1	0

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 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.

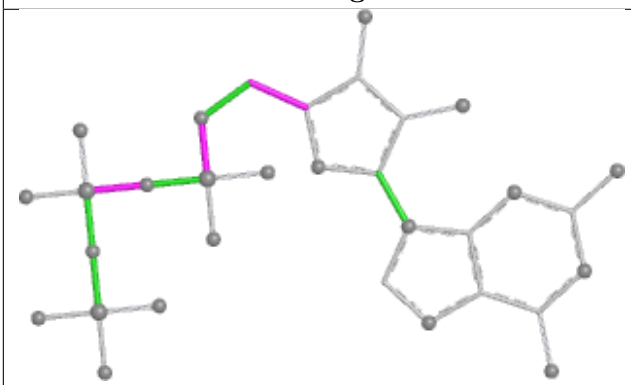
Ligand GTP M 401



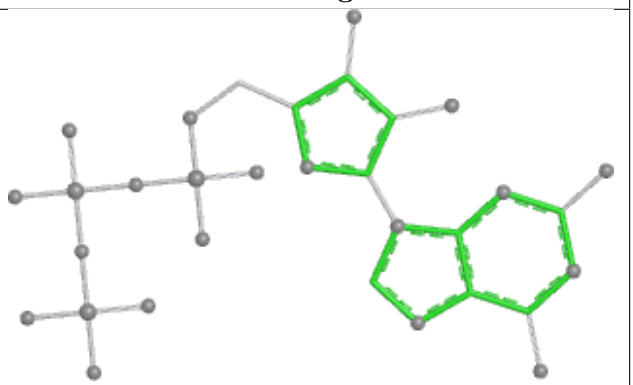
Bond lengths



Bond angles

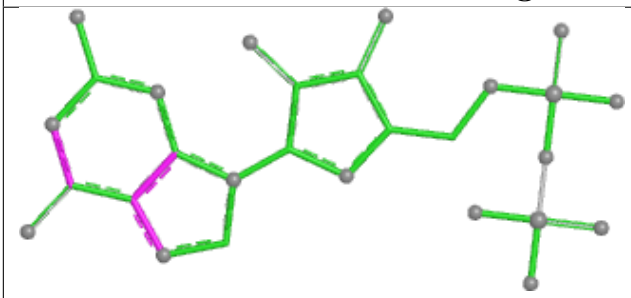


Torsions



Rings

Ligand GDP W 401



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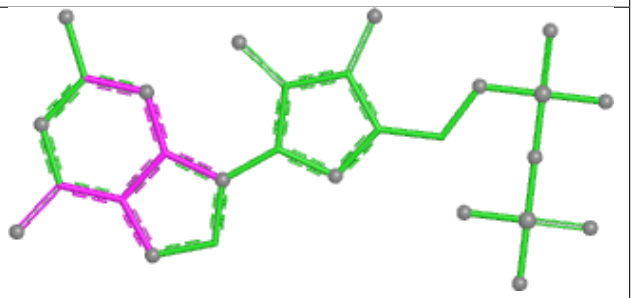

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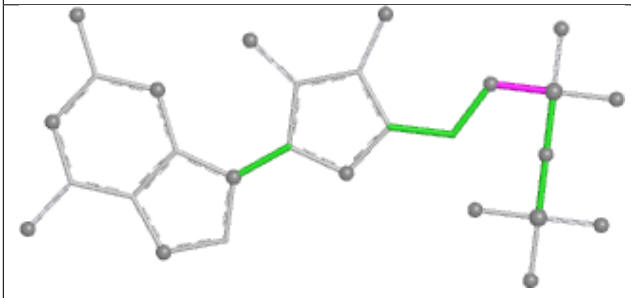

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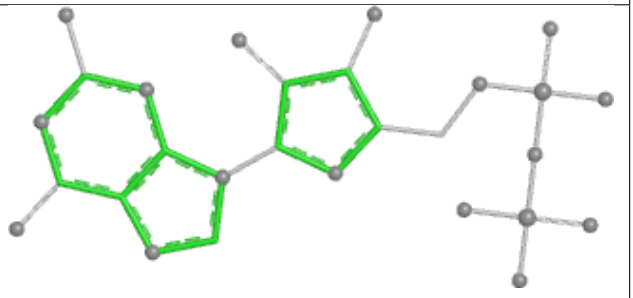
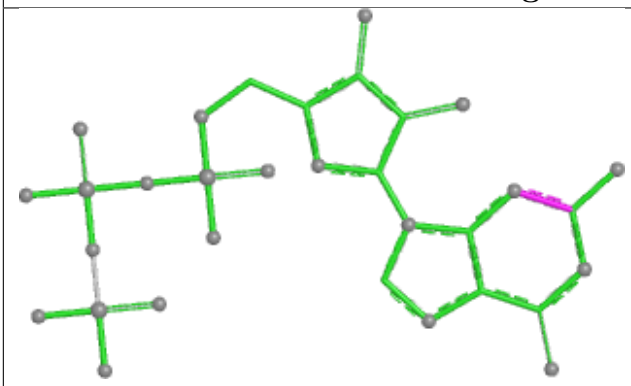
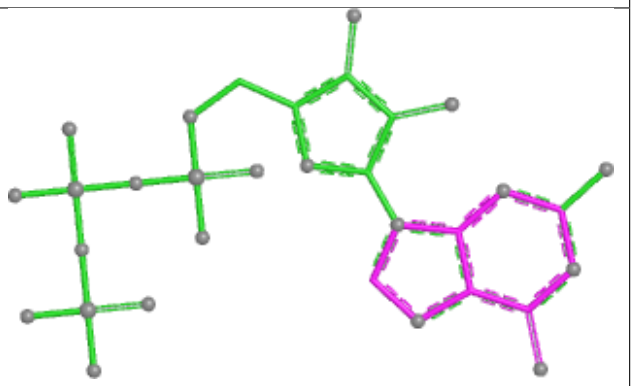


Rings

Ligand GTP V 401



Bond lengths



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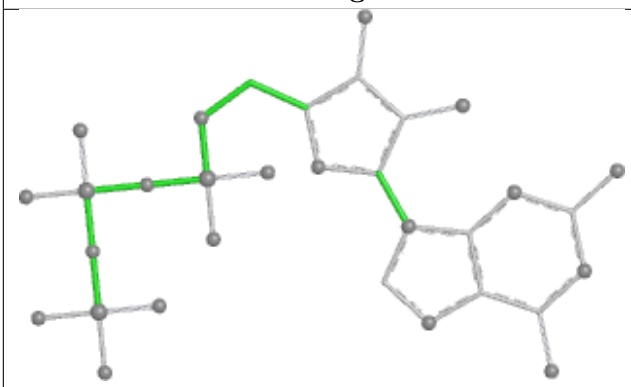

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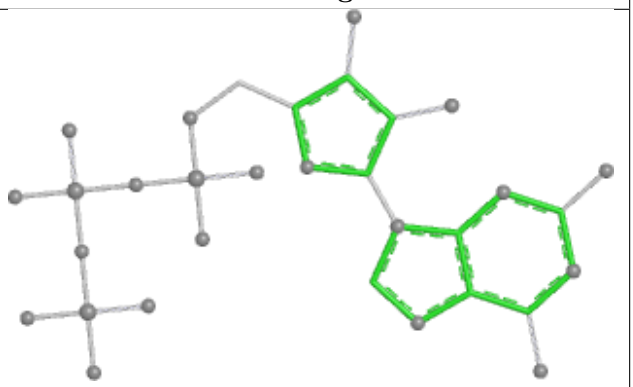
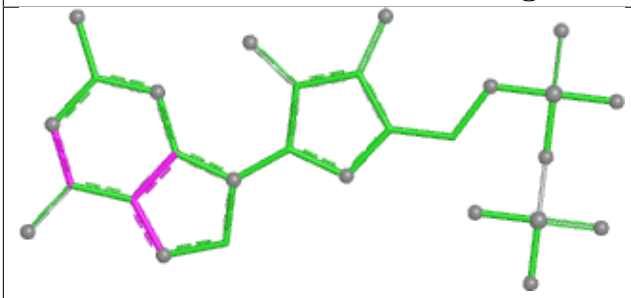


Rings

Ligand GDP N 401



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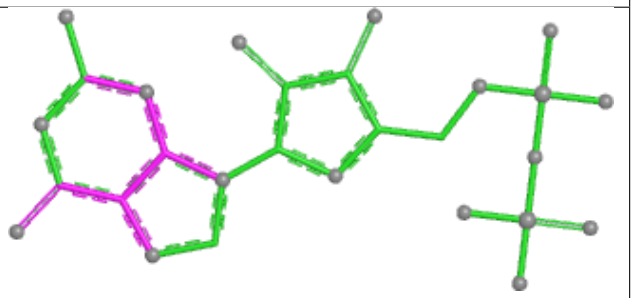

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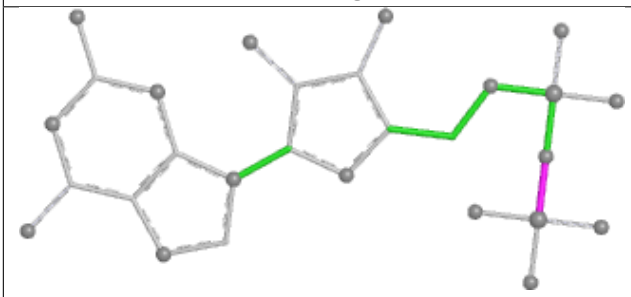
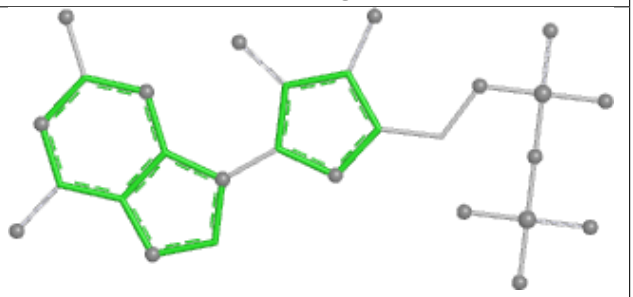
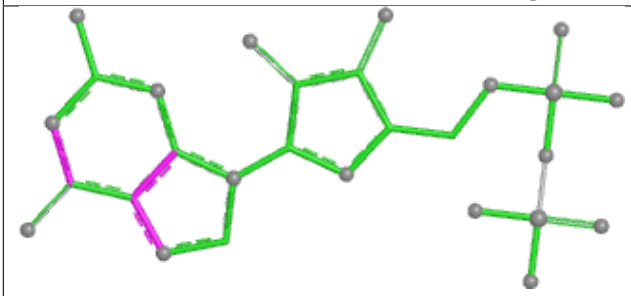


Torsions

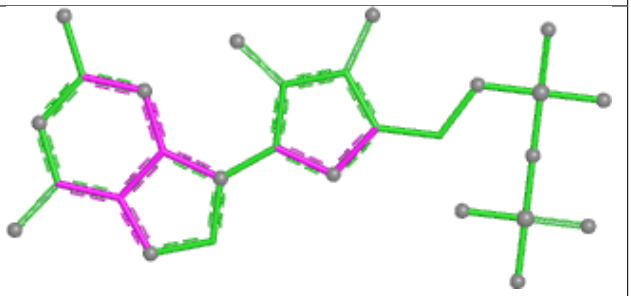


Rings

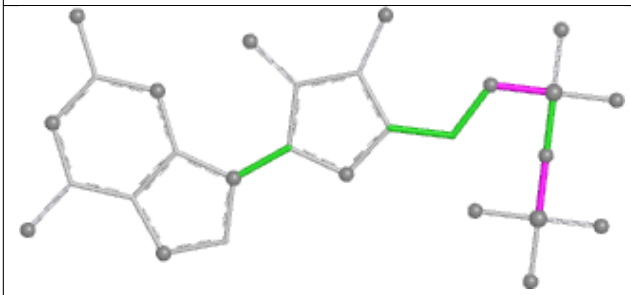
Ligand GDP d 401



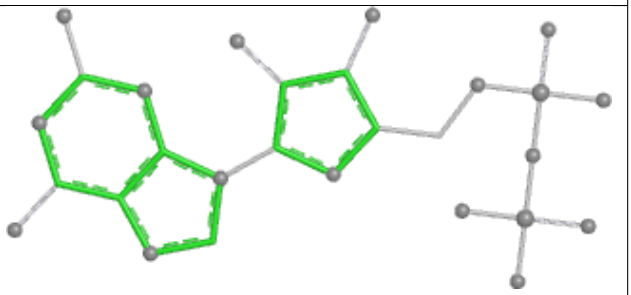
Bond lengths



Bond angles

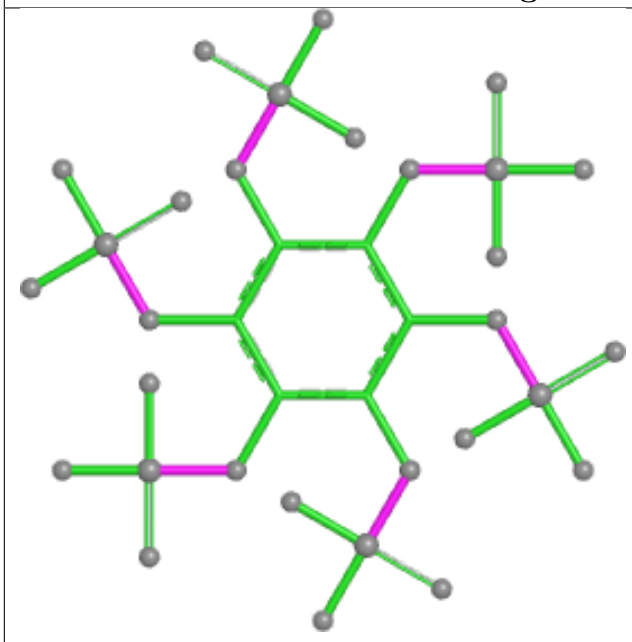


Torsions

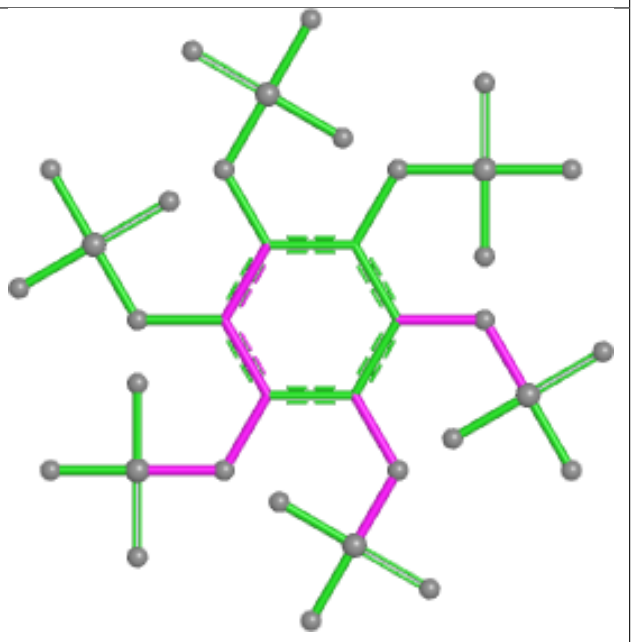


Rings

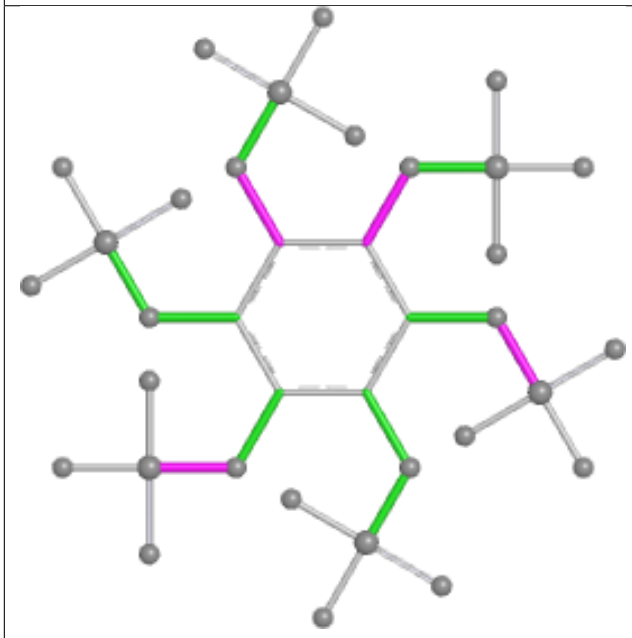
Ligand IHP A 2601



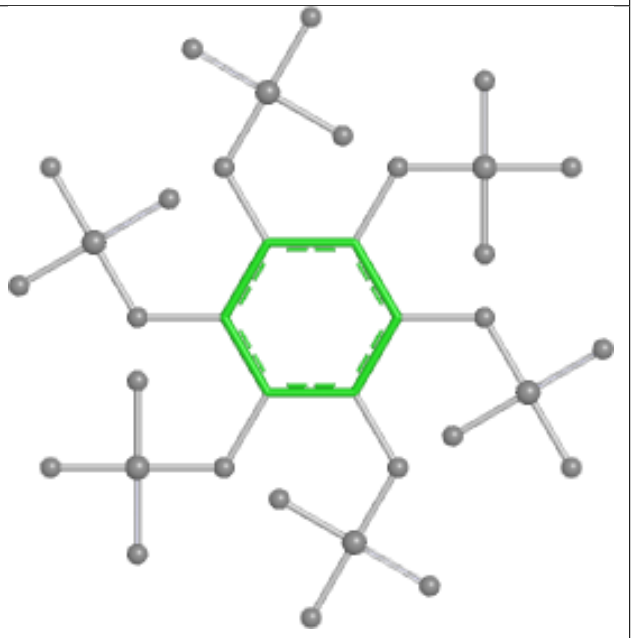
Bond lengths



Bond angles

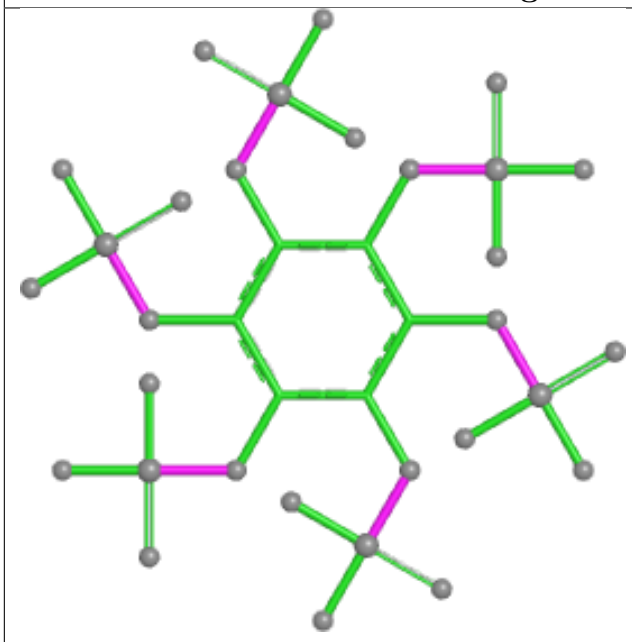


Torsions

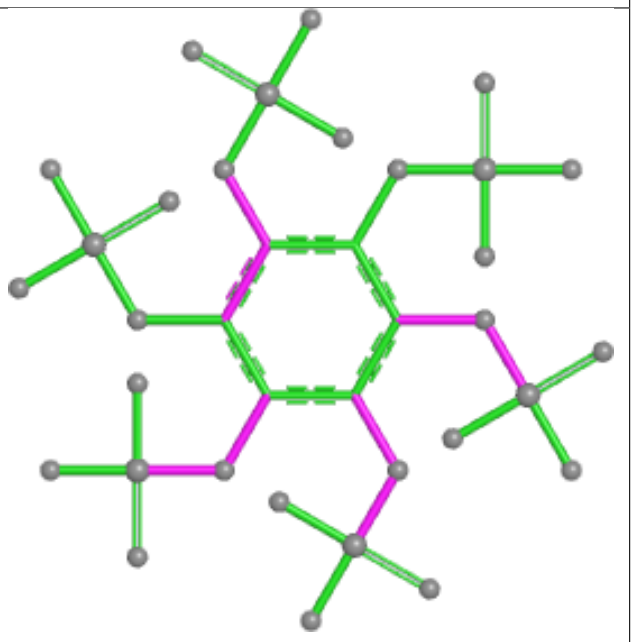


Rings

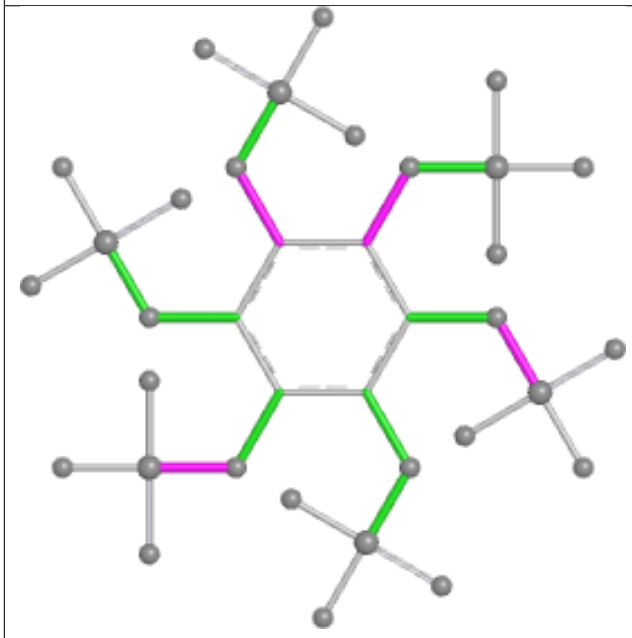
Ligand IHP C 2601



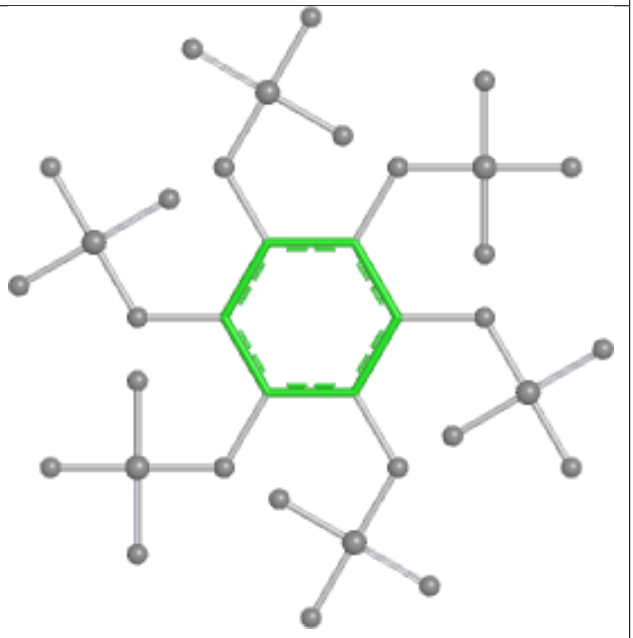
Bond lengths



Bond angles

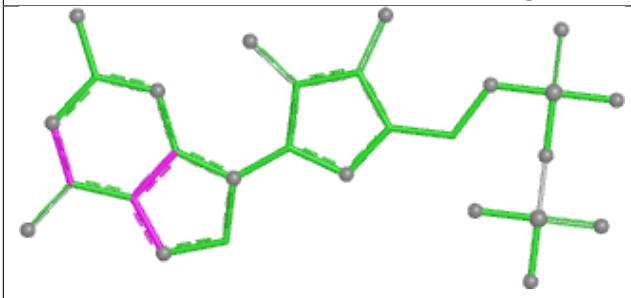


Torsions

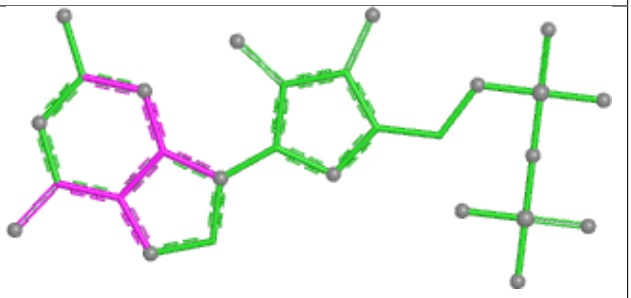


Rings

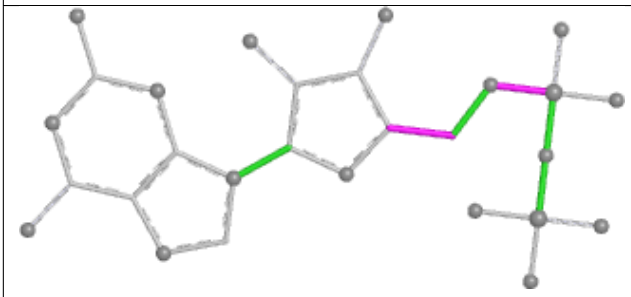
Ligand GDP G 401



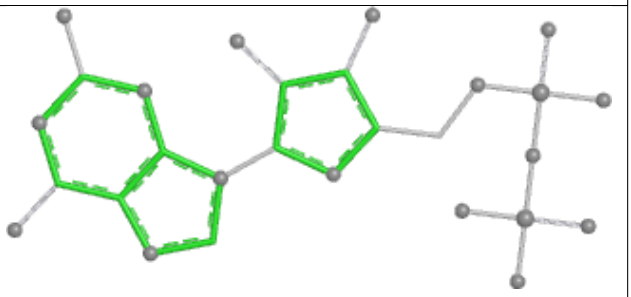
Bond lengths



Bond angles

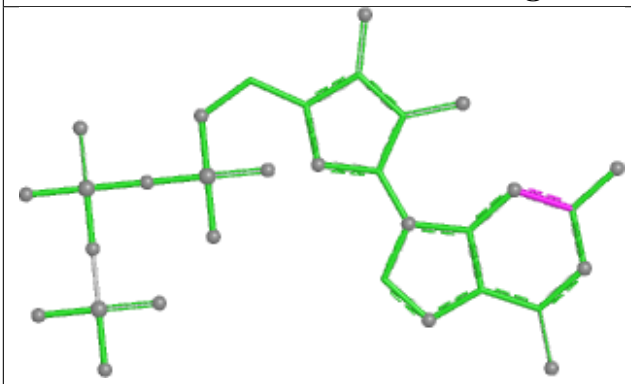


Torsions

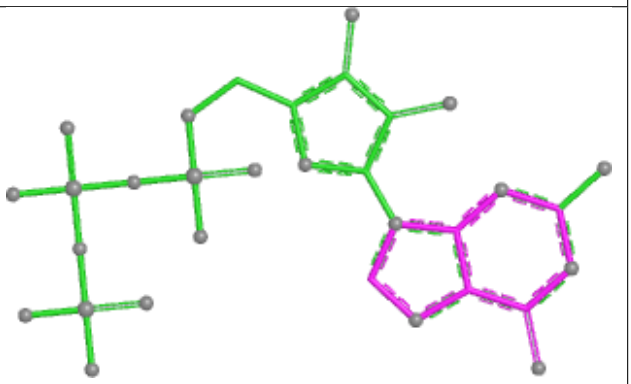


Rings

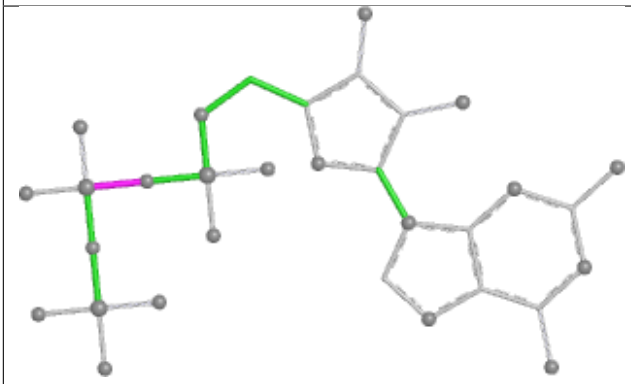
Ligand GTP F 401



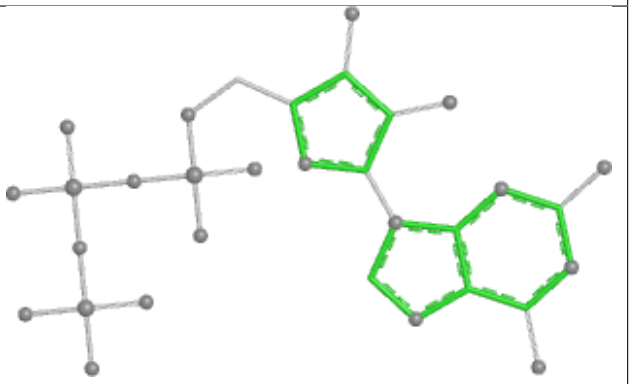
Bond lengths



Bond angles

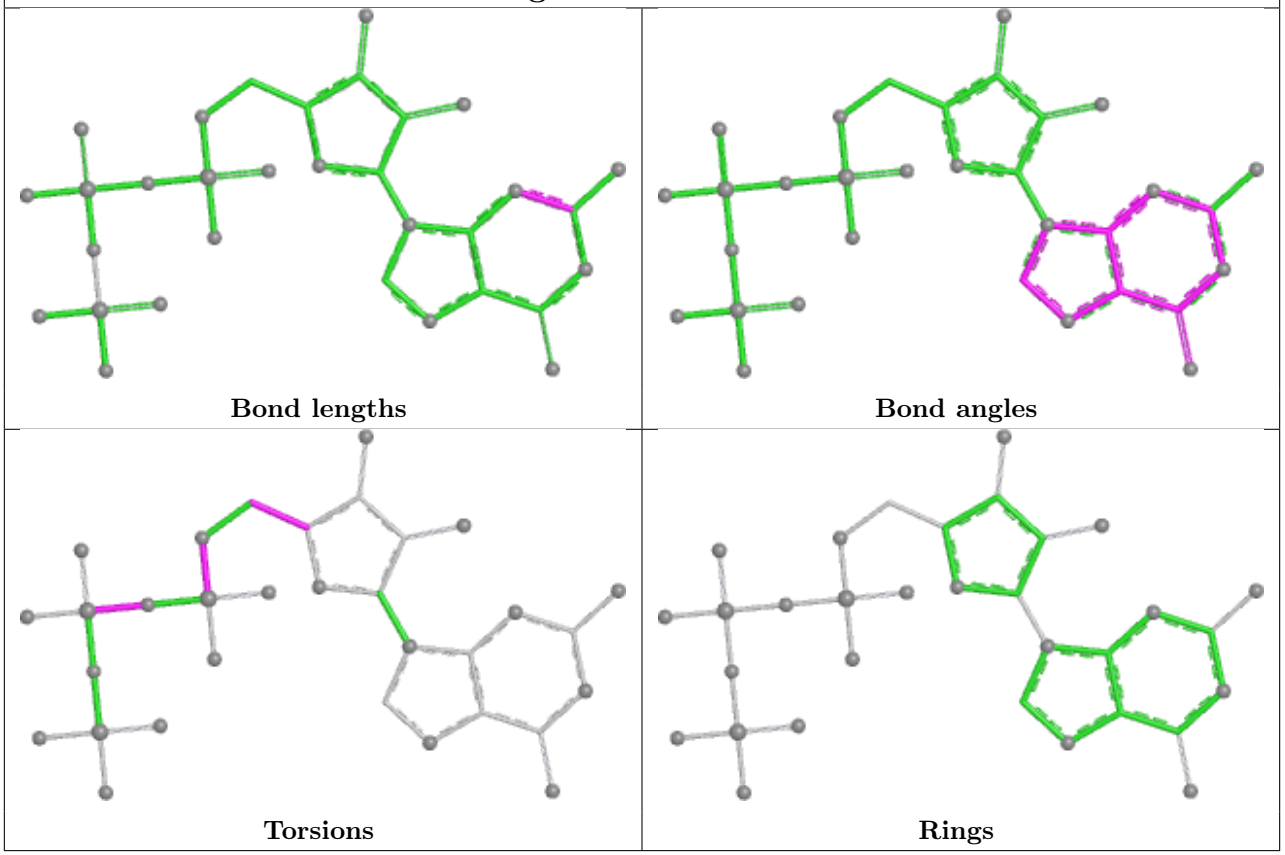


Torsions



Rings

Ligand GTP c 401



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

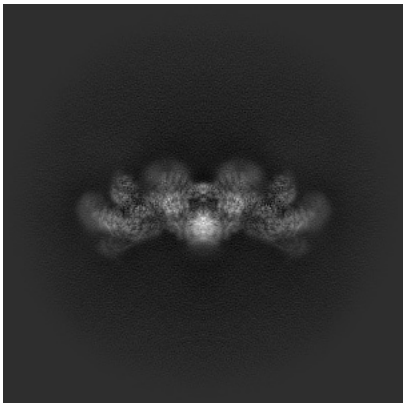
6 Map visualisation

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

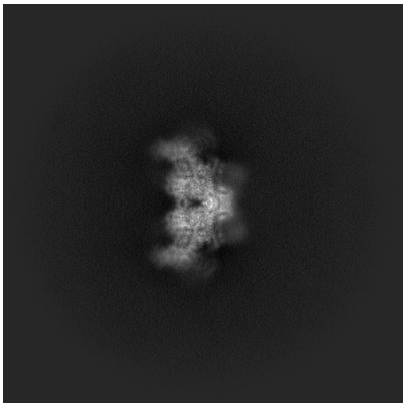
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

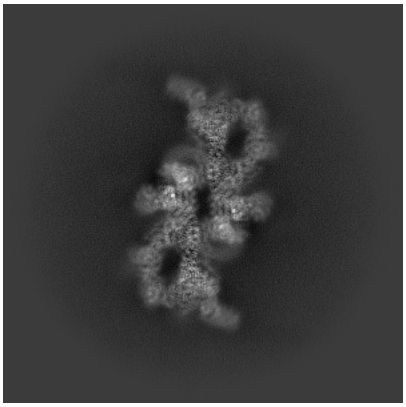
6.1.1 Primary map



X



Y

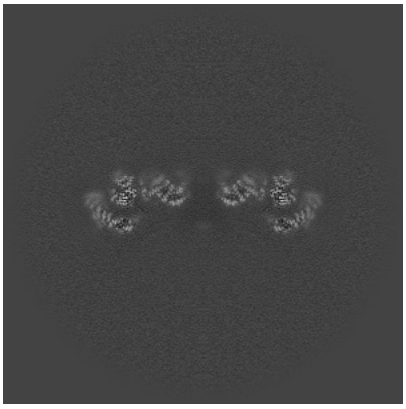


Z

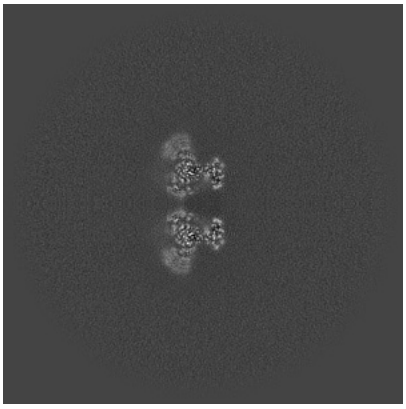
The images above show the map projected in three orthogonal directions.

6.2 Central slices

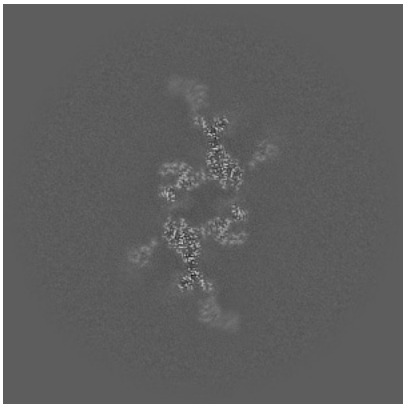
6.2.1 Primary map



X Index: 294



Y Index: 294

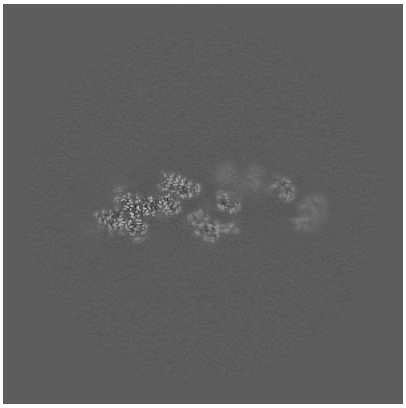


Z Index: 294

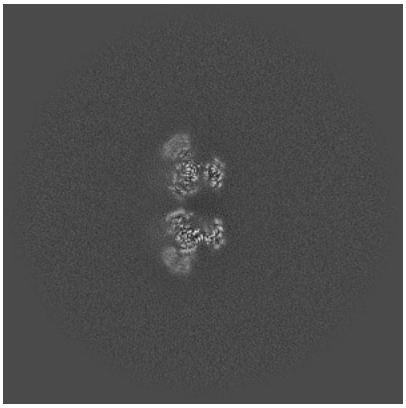
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

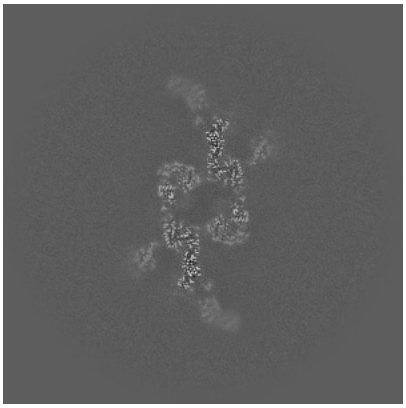
6.3.1 Primary map



X Index: 275



Y Index: 296

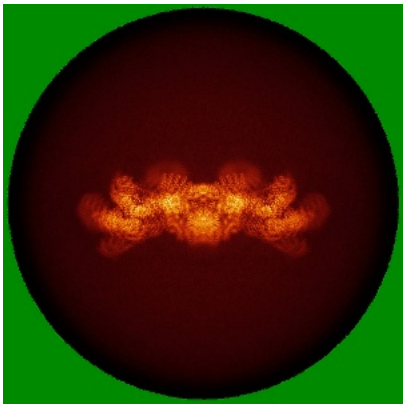


Z Index: 290

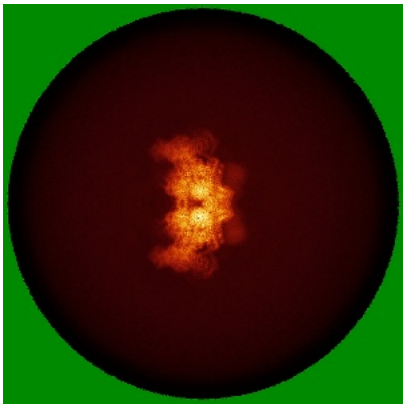
The images above show the largest variance slices of the map in three orthogonal directions.

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

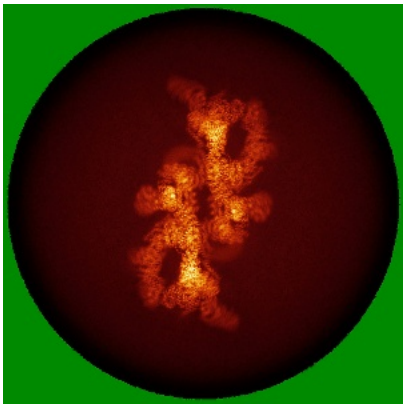
6.4.1 Primary map



X



Y

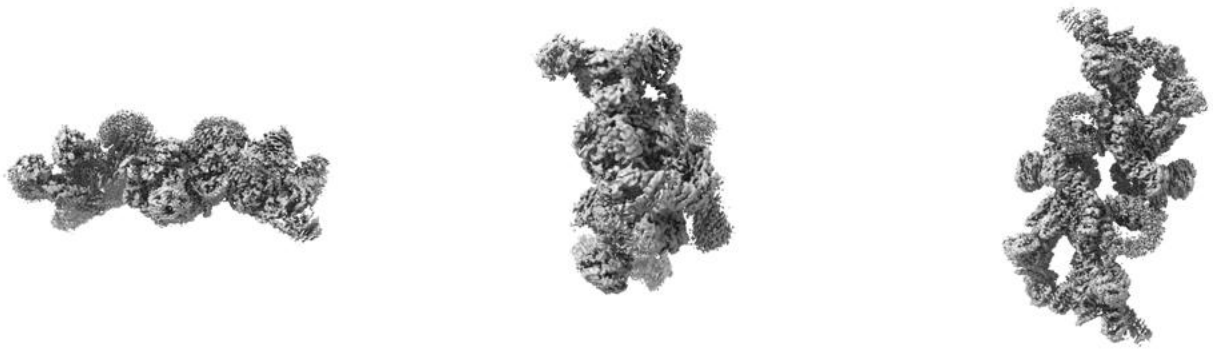


Z

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 (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 6.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

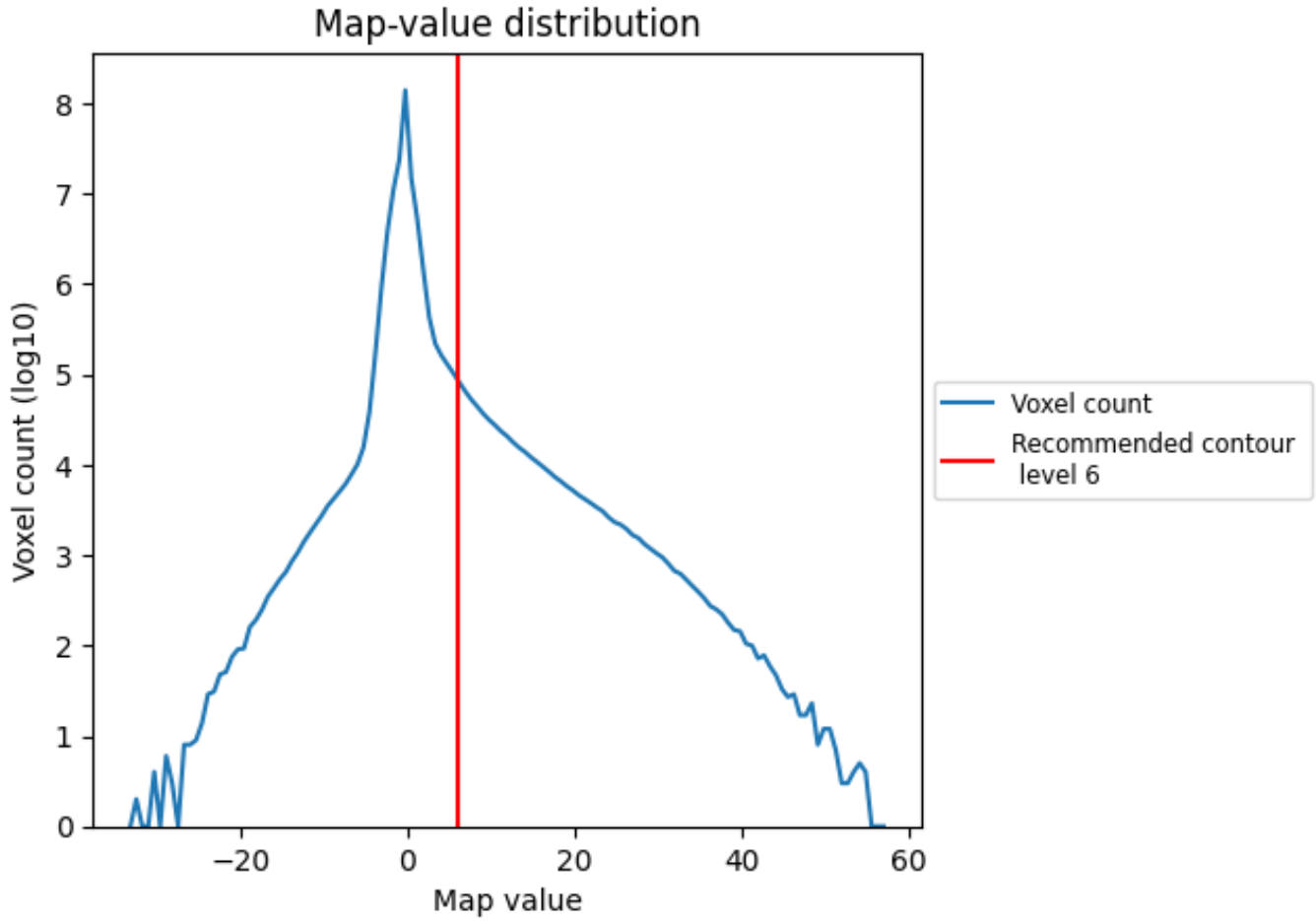
6.6 Mask visualisation (i)

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

7 Map analysis

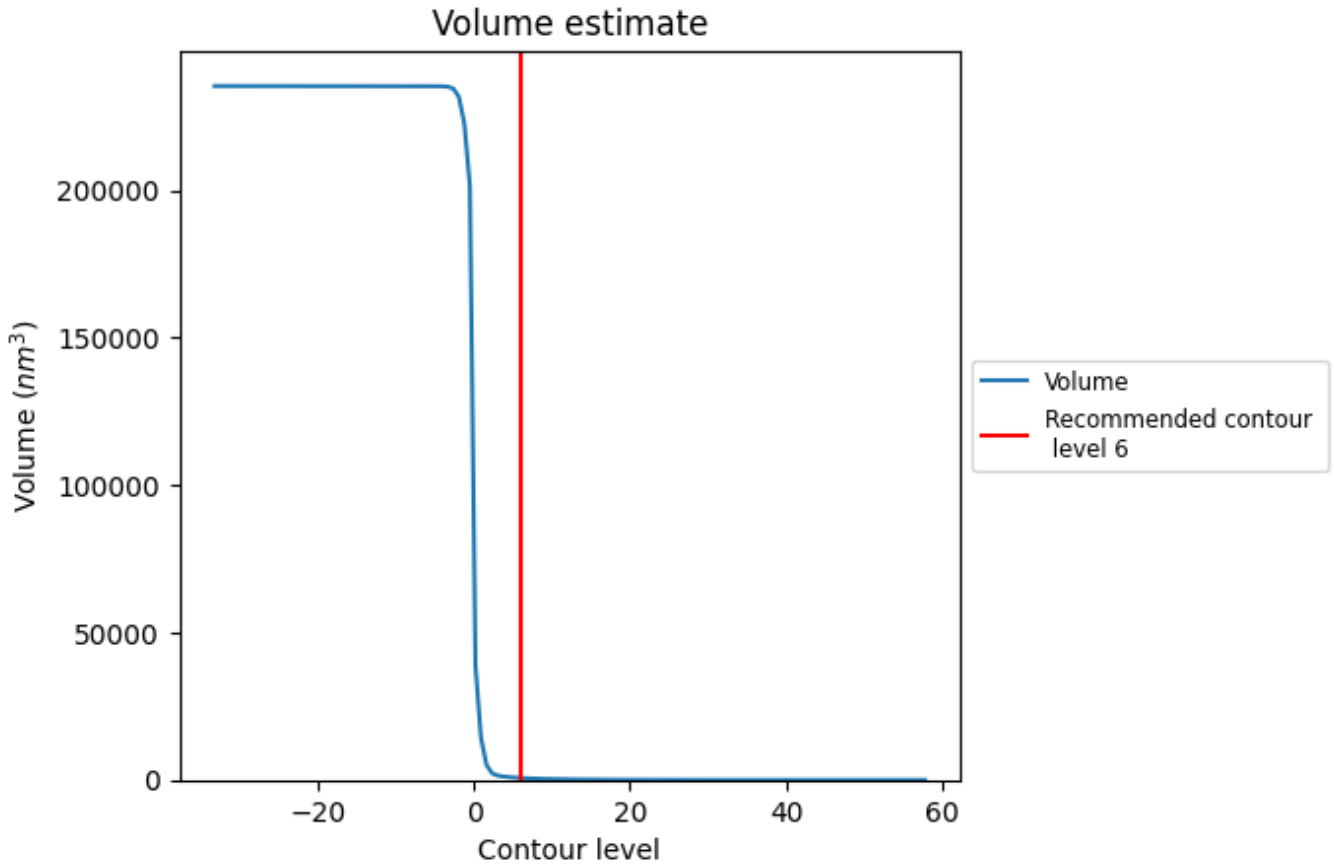
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

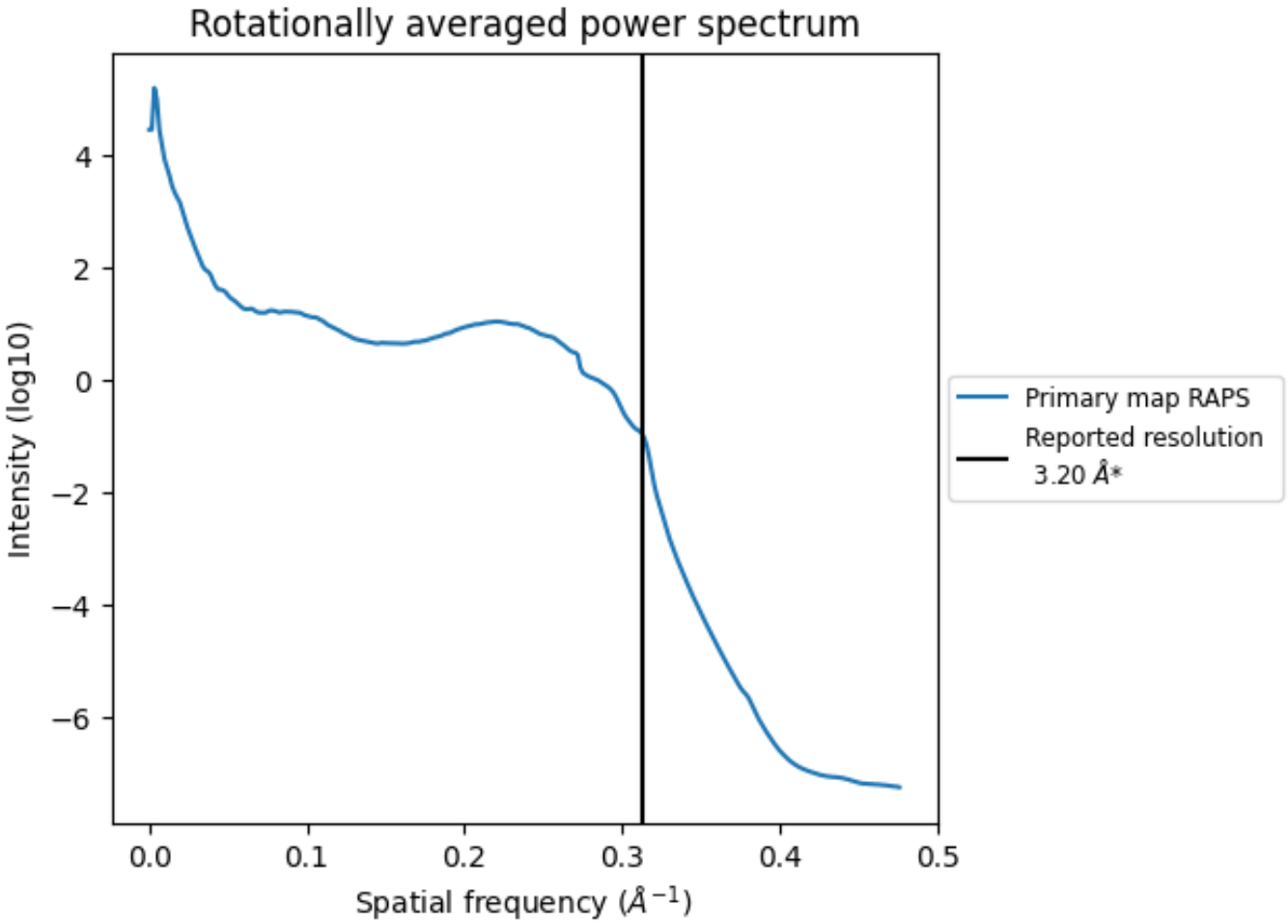
7.2 Volume estimate (i)



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 (i)



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

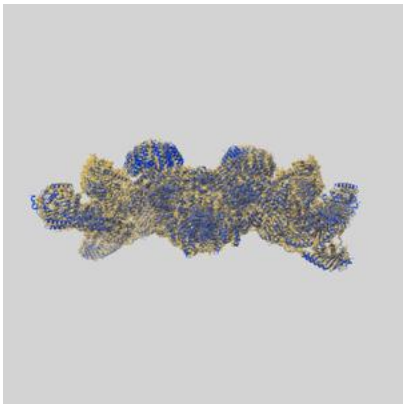
8 Fourier-Shell correlation

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

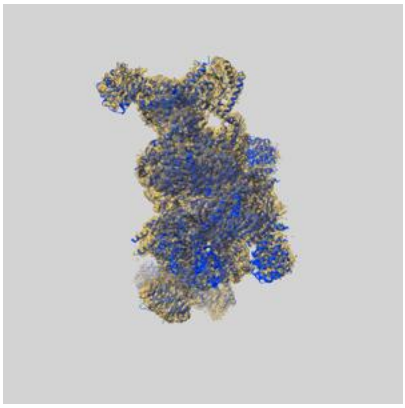
9 Map-model fit

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.

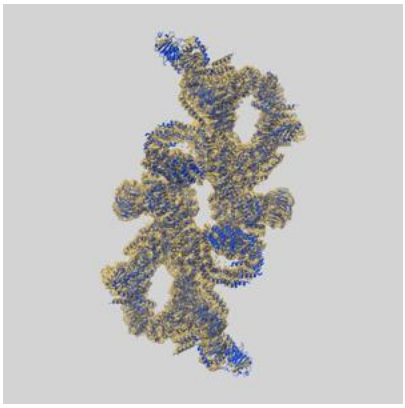
9.1 Map-model overlay



X



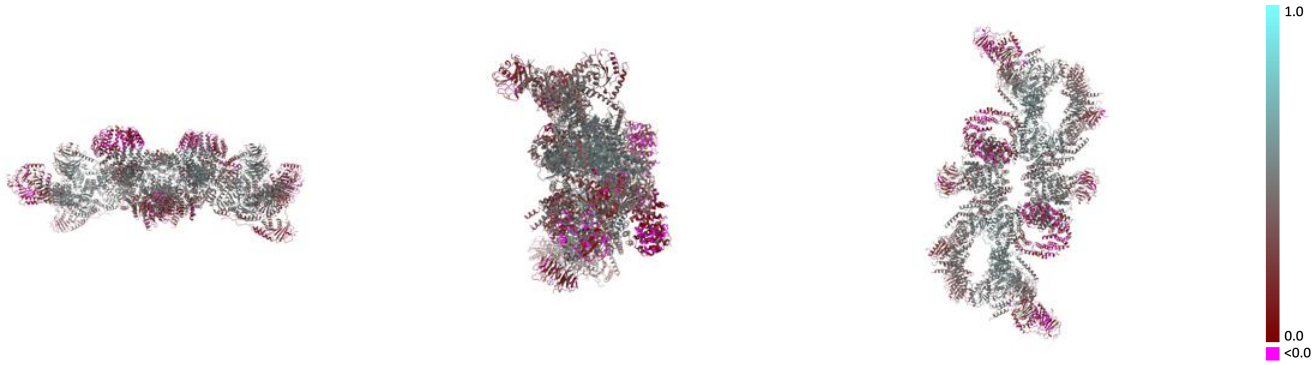
Y



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.

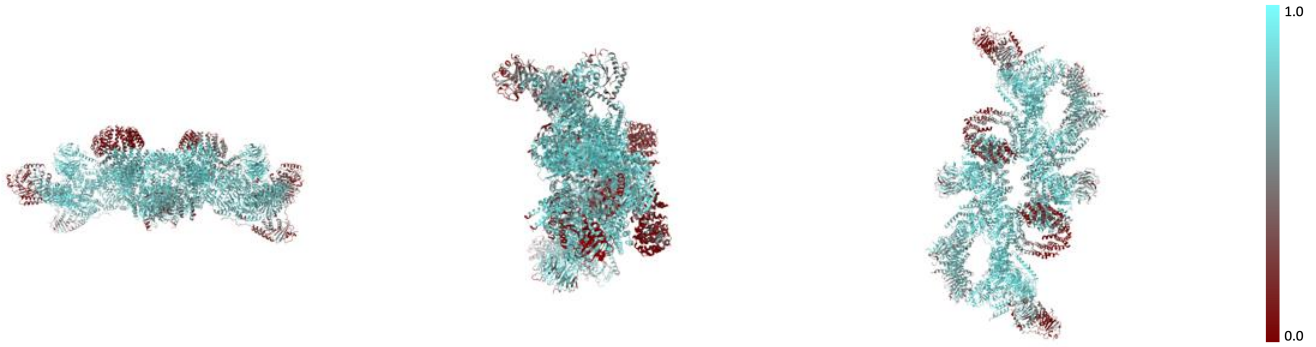
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

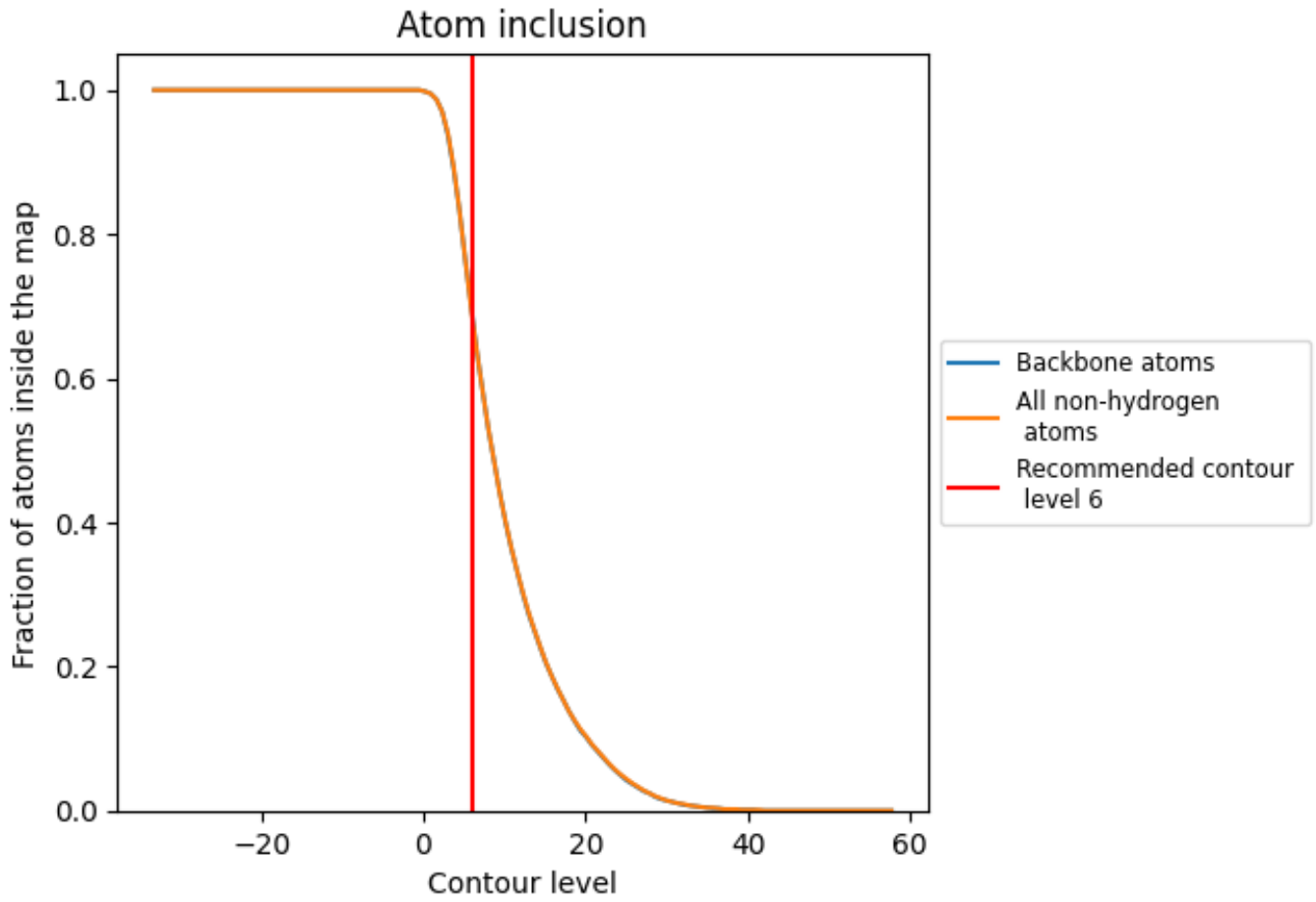
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (6).

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) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6880	0.3780
A	0.7190	0.3640
B	0.6610	0.2060
C	0.6670	0.3650
D	0.5550	0.2000
E	0.8820	0.4930
F	0.8880	0.4970
G	0.8500	0.4580
H	0.3520	0.2220
I	0.6470	0.3080
J	0.5470	0.2410
K	0.0910	0.1080
L	0.2050	0.0790
M	0.7870	0.4330
N	0.7030	0.3590
O	0.5090	0.2780
P	0.7190	0.3930
Q	0.7260	0.3850
R	0.4320	0.2090
S	0.4990	0.2580
T	0.7470	0.4180
U	0.8540	0.4940
V	0.8460	0.4920
W	0.7880	0.4530
X	0.2370	0.1730
Y	0.5560	0.3120
Z	0.3800	0.2230
a	0.0350	0.0810
b	0.1670	0.1190
c	0.7360	0.4280
d	0.6300	0.3660
e	0.3940	0.2690
f	0.6520	0.3960
g	0.6460	0.3740
h	0.3050	0.2060

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	0.3640	0.2510
j	0.6840	0.4100