



wwPDB EM Validation Summary Report ⓘ

Dec 29, 2024 – 10:16 AM EST

PDB ID : 7NZ2
EMDB ID : EMD-12662
Title : Cryo-EM structure of the MukBEF-MatP-DNA tetrad
Authors : Buermann, F.; Lowe, J.
Deposited on : 2021-03-23
Resolution : 11.00 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.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

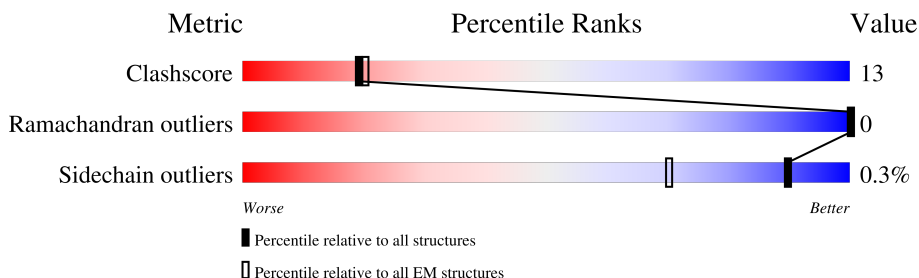
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 11.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




























Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A1	1482	
1	A2	1482	
1	A3	1482	
1	A4	1482	
1	B1	1482	
1	B2	1482	
1	B3	1482	
1	B4	1482	

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Mol	Chain	Length	Quality of chain
2	C1	440	
2	C2	440	
2	D1	440	
2	D2	440	
3	E1	240	
3	E2	240	
3	E3	240	
3	E4	240	
3	F1	240	
3	F2	240	
3	F3	240	
3	F4	240	
4	G1	78	
4	G2	78	
4	G3	78	
4	G4	78	
4	H1	78	
4	H2	78	
4	H3	78	
4	H4	78	
5	I1	151	
5	I2	151	
5	I3	151	
5	I4	151	
5	J1	151	

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Mol	Chain	Length	Quality of chain
5	J2	151	
5	J3	151	
5	J4	151	
6	K1	80	
6	K2	80	
6	N1	80	
6	N2	80	
7	L1	80	
7	L2	80	
7	M1	80	
7	M2	80	

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 289777 atoms, of which 141230 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 Chromosome partition protein MukB.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A1	1467	Total	C	H	N	O	S	0	0
			23548	7298	11708	2189	2313	40		
1	A2	1467	Total	C	H	N	O	S	0	0
			23548	7298	11708	2189	2313	40		
1	A3	1467	Total	C	H	N	O	S	0	0
			23548	7298	11708	2189	2313	40		
1	A4	1467	Total	C	H	N	O	S	0	0
			23548	7298	11708	2189	2313	40		
1	B1	1467	Total	C	H	N	O	S	0	0
			23549	7298	11709	2189	2313	40		
1	B2	1467	Total	C	H	N	O	S	0	0
			23549	7298	11709	2189	2313	40		
1	B3	1467	Total	C	H	N	O	S	0	0
			23549	7298	11709	2189	2313	40		
1	B4	1467	Total	C	H	N	O	S	0	0
			23549	7298	11709	2189	2313	40		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A1	1407	GLN	GLU	engineered mutation	UNP A0A0F7LRY2
A2	1407	GLN	GLU	engineered mutation	UNP A0A0F7LRY2
A3	1407	GLN	GLU	engineered mutation	UNP A0A0F7LRY2
A4	1407	GLN	GLU	engineered mutation	UNP A0A0F7LRY2
B1	1407	GLN	GLU	engineered mutation	UNP A0A0F7LRY2
B2	1407	GLN	GLU	engineered mutation	UNP A0A0F7LRY2
B3	1407	GLN	GLU	engineered mutation	UNP A0A0F7LRY2
B4	1407	GLN	GLU	engineered mutation	UNP A0A0F7LRY2

- Molecule 2 is a protein called Chromosome partition protein MukF.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C1	431	Total	C	H	N	O	S	0	0
			6844	2174	3384	604	670	12		

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Mol	Chain	Residues	Atoms						AltConf	Trace
2	C2	431	Total	C	H	N	O	S	0	0
			6844	2174	3384	604	670	12		
2	D1	431	Total	C	H	N	O	S	0	0
			6844	2174	3384	604	670	12		
2	D2	431	Total	C	H	N	O	S	0	0
			6844	2174	3384	604	670	12		

- Molecule 3 is a protein called Chromosome partition protein MukE.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	E1	212	Total	C	H	N	O	S	0	0
			3441	1090	1719	301	322	9		
3	E2	212	Total	C	H	N	O	S	0	0
			3441	1090	1719	301	322	9		
3	E3	212	Total	C	H	N	O	S	0	0
			3441	1090	1719	301	322	9		
3	E4	212	Total	C	H	N	O	S	0	0
			3441	1090	1719	301	322	9		
3	F1	198	Total	C	H	N	O	S	0	0
			3246	1029	1627	284	298	8		
3	F2	198	Total	C	H	N	O	S	0	0
			3246	1029	1627	284	298	8		
3	F3	198	Total	C	H	N	O	S	0	0
			3246	1029	1627	284	298	8		
3	F4	198	Total	C	H	N	O	S	0	0
			3246	1029	1627	284	298	8		

- Molecule 4 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	G1	72	Total	C	H	N	O	S	0	0
			1105	349	543	85	127	1		
4	G2	72	Total	C	H	N	O	S	0	0
			1105	349	543	85	127	1		
4	G3	72	Total	C	H	N	O	S	0	0
			1105	349	543	85	127	1		
4	G4	72	Total	C	H	N	O	S	0	0
			1105	349	543	85	127	1		
4	H1	72	Total	C	H	N	O	S	0	0
			1105	349	543	85	127	1		
4	H2	72	Total	C	H	N	O	S	0	0
			1105	349	543	85	127	1		

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Mol	Chain	Residues	Atoms						AltConf	Trace
4	H3	72	Total	C	H	N	O	S	0	0
			1105	349	543	85	127	1		
4	H4	72	Total	C	H	N	O	S	0	0
			1105	349	543	85	127	1		

- Molecule 5 is a protein called Macrodomein Ter protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	I1	134	Total	C	H	N	O	S	0	0
			2271	714	1136	215	202	4		
5	I2	134	Total	C	H	N	O	S	0	0
			2271	714	1136	215	202	4		
5	I3	134	Total	C	H	N	O	S	0	0
			2271	714	1136	215	202	4		
5	I4	134	Total	C	H	N	O	S	0	0
			2271	714	1136	215	202	4		
5	J1	135	Total	C	H	N	O	S	0	0
			2288	719	1144	217	204	4		
5	J2	135	Total	C	H	N	O	S	0	0
			2288	719	1144	217	204	4		
5	J3	135	Total	C	H	N	O	S	0	0
			2288	719	1144	217	204	4		
5	J4	135	Total	C	H	N	O	S	0	0
			2288	719	1144	217	204	4		

- Molecule 6 is a DNA chain called matS2 DNA 80 b, oligo FBA769.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	K1	77	Total	C	H	N	O	P	0	0
			2449	752	872	277	471	77		
6	K2	77	Total	C	H	N	O	P	0	0
			2449	752	872	277	471	77		
6	N1	77	Total	C	H	N	O	P	0	0
			2449	752	872	277	471	77		
6	N2	76	Total	C	H	N	O	P	0	0
			2416	742	861	272	465	76		

- Molecule 7 is a DNA chain called matS2 DNA 80 b, oligo FBA770.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	L1	77	Total	C	H	N	O	P	0	0
			2442	750	862	300	453	77		

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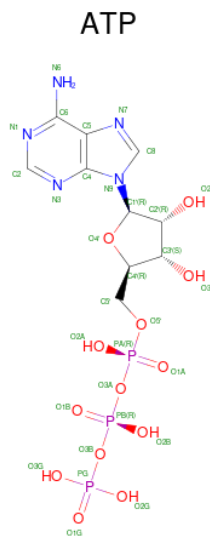
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Mol	Chain	Residues	Atoms						AltConf	Trace
7	L2	77	Total	C	H	N	O	P	0	0
			2442	750	862	300	453	77		
7	M1	77	Total	C	H	N	O	P	0	0
			2442	750	862	300	453	77		
7	M2	76	Total	C	H	N	O	P	0	0
			2412	741	851	297	447	76		

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

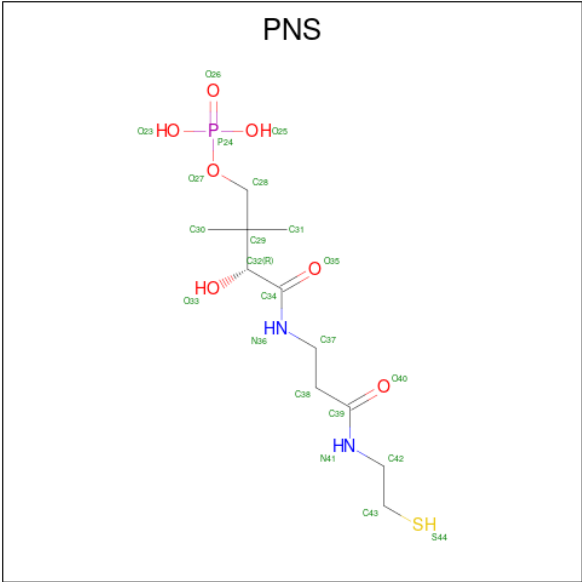
Mol	Chain	Residues	Atoms		AltConf
8	A1	1	Total	Mg	0
			1	1	
8	A2	1	Total	Mg	0
			1	1	
8	A3	1	Total	Mg	0
			1	1	
8	A4	1	Total	Mg	0
			1	1	
8	B1	1	Total	Mg	0
			1	1	
8	B2	1	Total	Mg	0
			1	1	
8	B3	1	Total	Mg	0
			1	1	
8	B4	1	Total	Mg	0
			1	1	

- Molecule 9 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms						AltConf
9	A1	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
9	A2	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
9	A3	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
9	A4	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
9	B1	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
9	B2	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
9	B3	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
9	B4	1	Total 43	C 10	H 12	N 5	O 13	P 3	0

- Molecule 10 is 4'-PHOSPHOPANTETHEINE (three-letter code: PNS) (formula: $C_{11}H_{23}N_2O_7PS$).

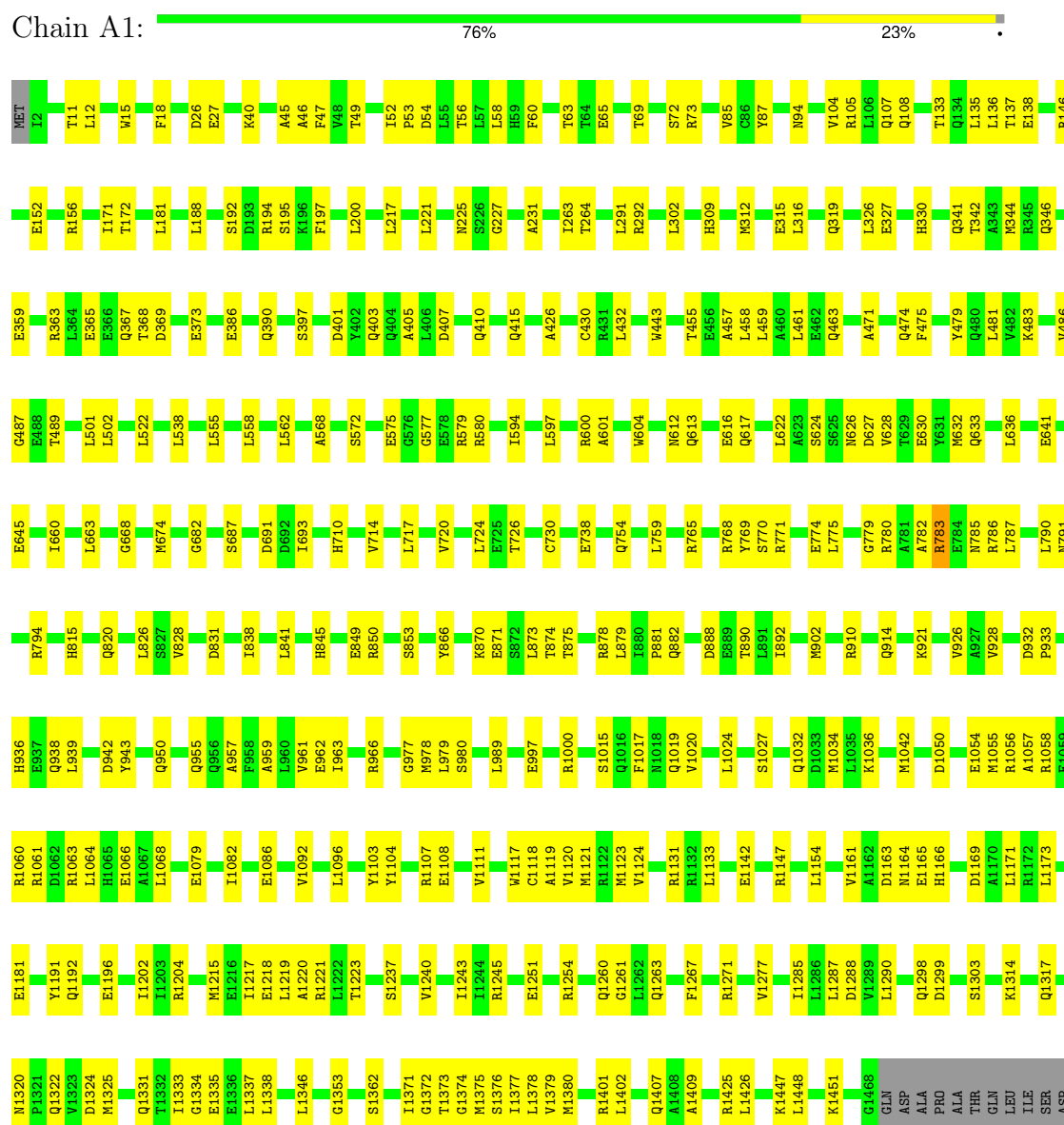


Mol	Chain	Residues	Atoms							AltConf
10	G1	1	Total	C	H	N	O	P	S	0
			42	11	21	2	6	1	1	
10	G2	1	Total	C	H	N	O	P	S	0
			42	11	21	2	6	1	1	
10	G3	1	Total	C	H	N	O	P	S	0
			42	11	21	2	6	1	1	
10	G4	1	Total	C	H	N	O	P	S	0
			42	11	21	2	6	1	1	
10	H1	1	Total	C	H	N	O	P	S	0
			42	11	21	2	6	1	1	
10	H2	1	Total	C	H	N	O	P	S	0
			42	11	21	2	6	1	1	
10	H3	1	Total	C	H	N	O	P	S	0
			42	11	21	2	6	1	1	
10	H4	1	Total	C	H	N	O	P	S	0
			42	11	21	2	6	1	1	

3 Residue-property plots

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

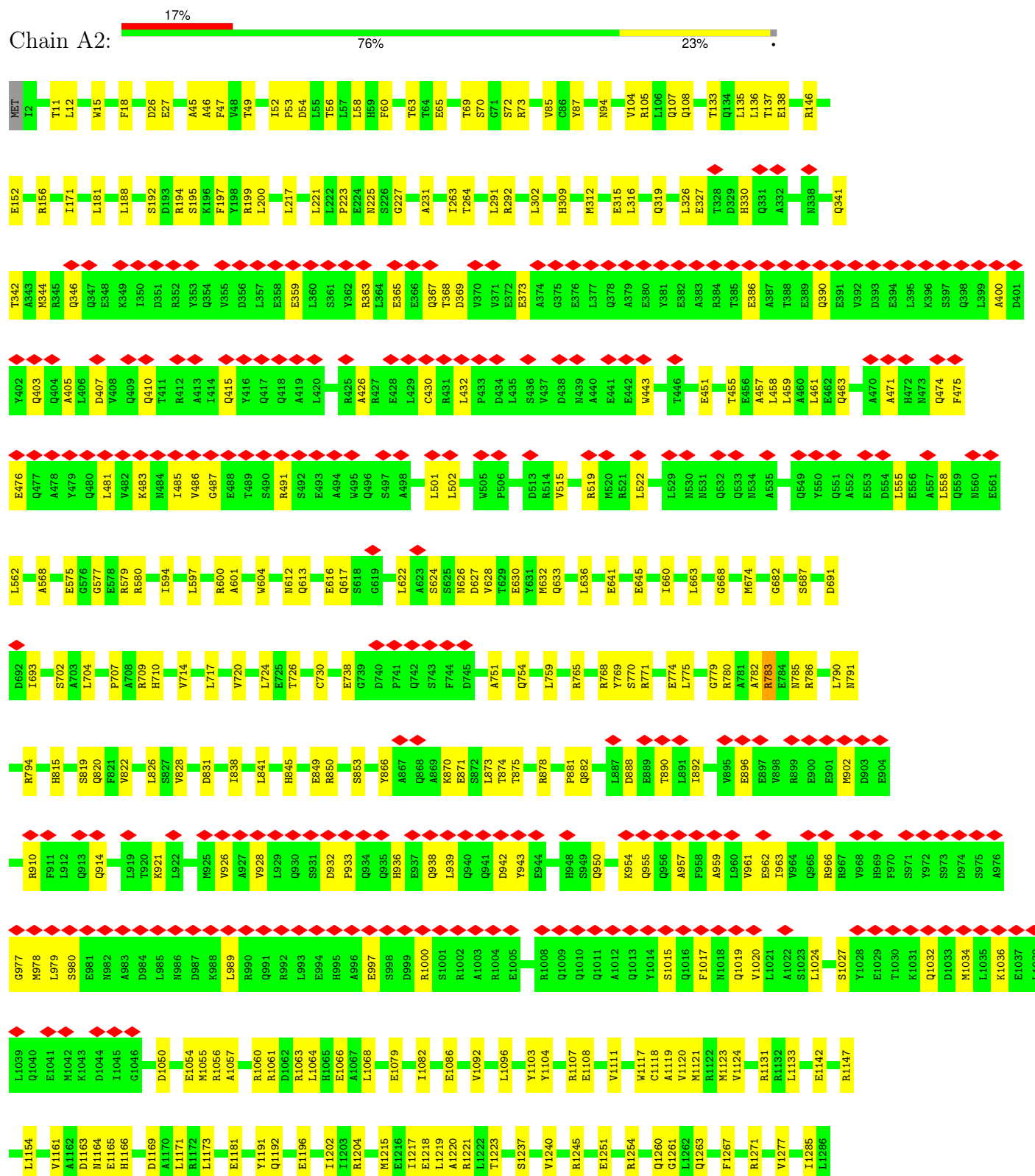
• Molecule 1: Chromosome partition protein MukB

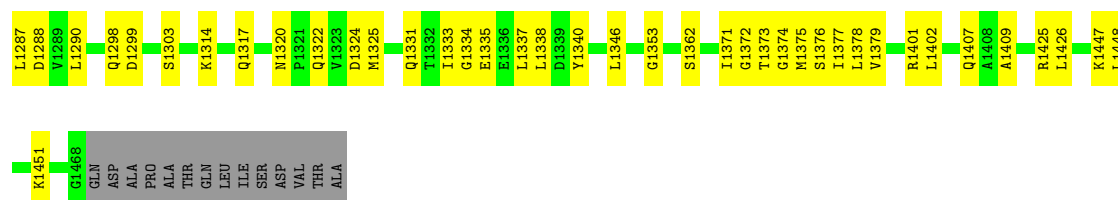


VAL
THR
ALA

● Molecule 1: Chromosome partition protein MukB

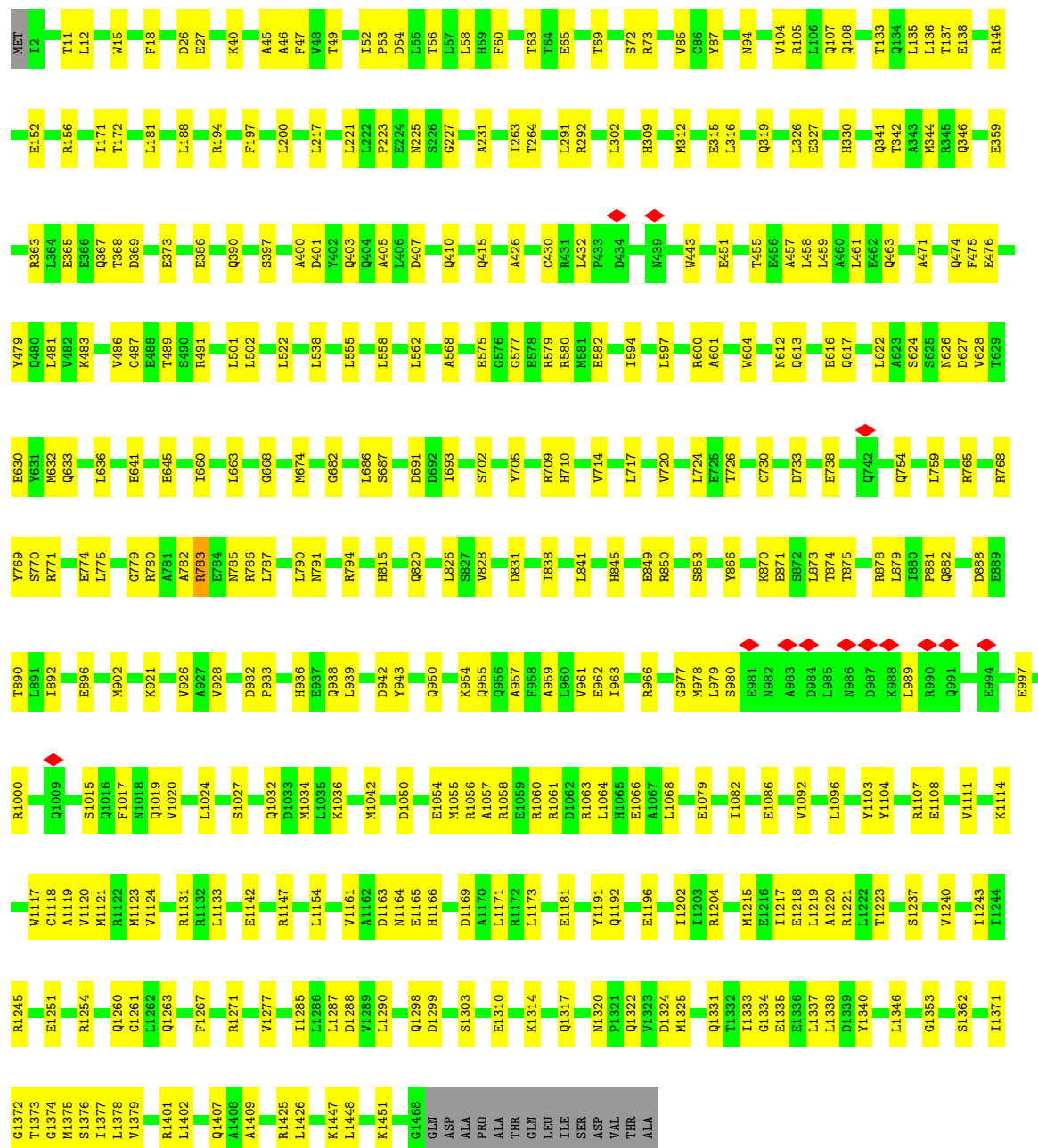
Chain A2:





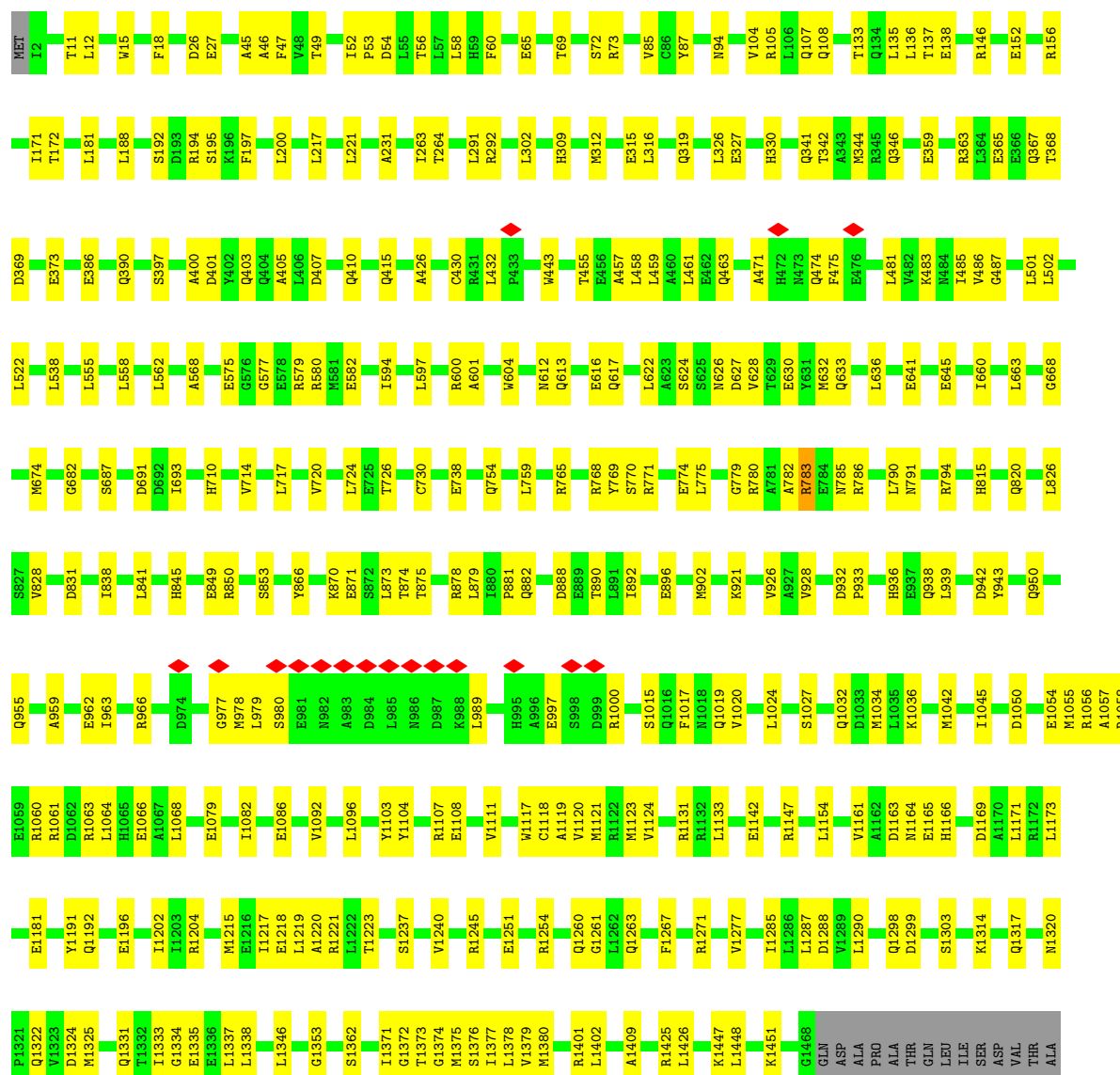
• Molecule 1: Chromosome partition protein MukB

Chain A3: 75% 24%

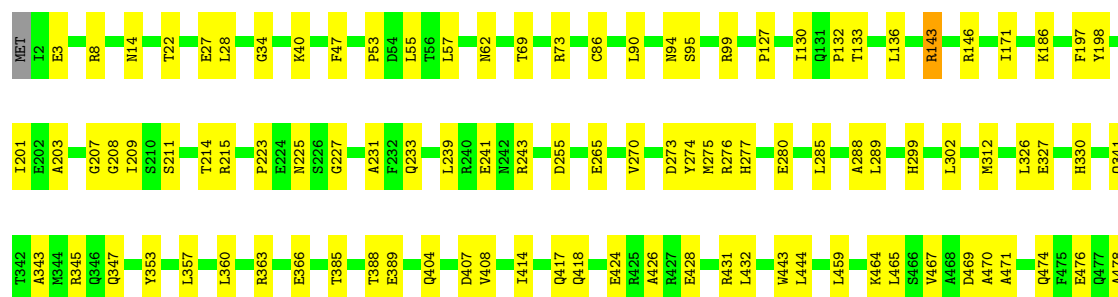


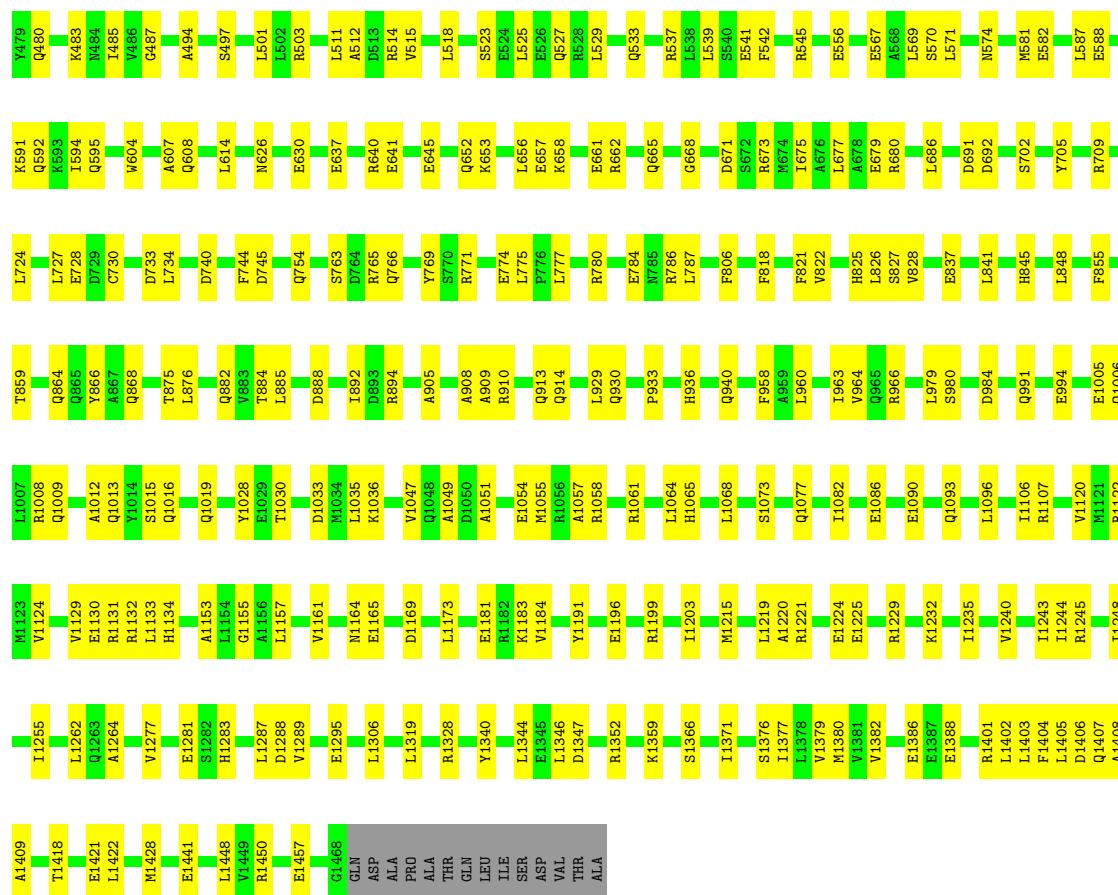
• Molecule 1: Chromosome partition protein MukB

Chain A4:

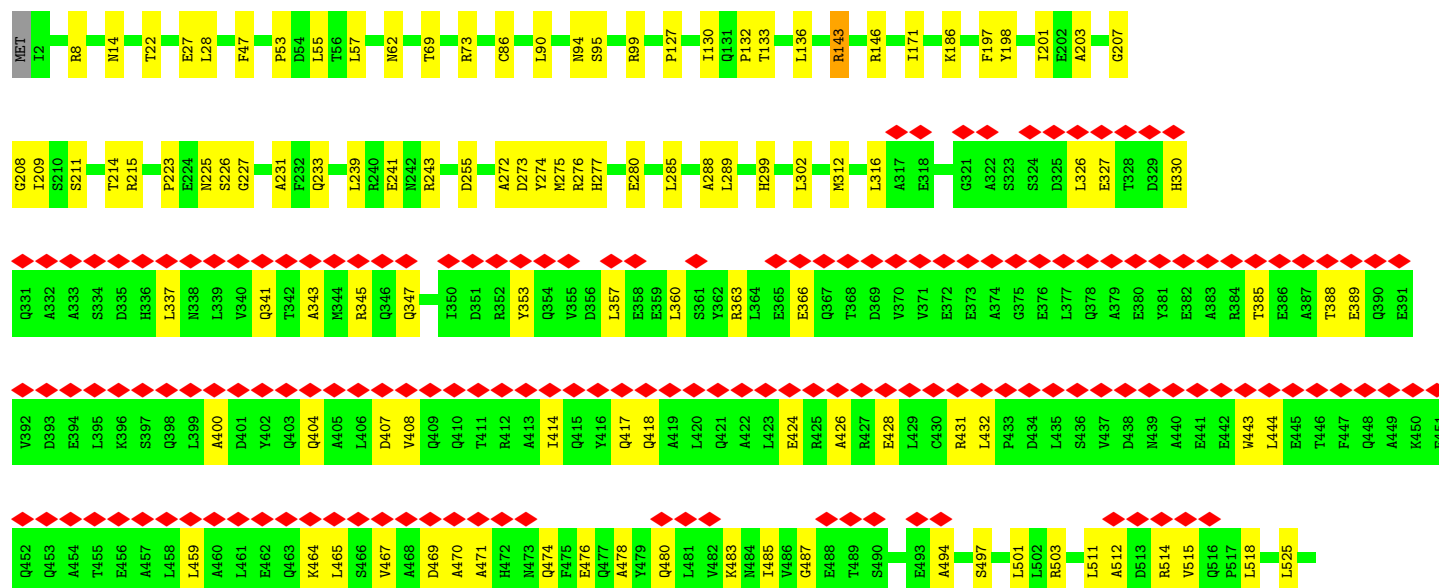
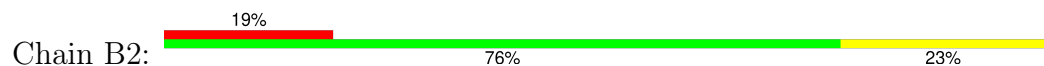


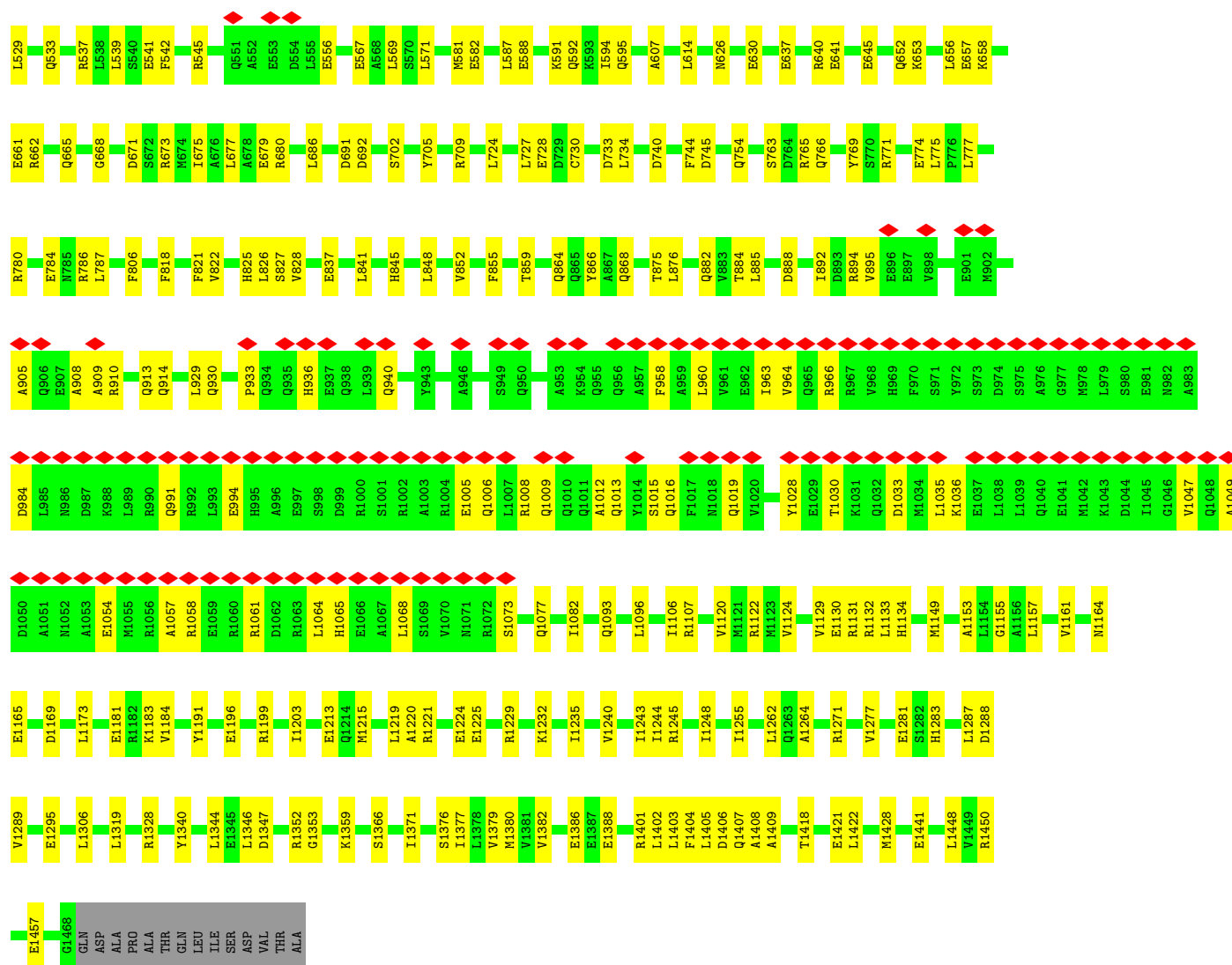
Chain B1: 75% 24%





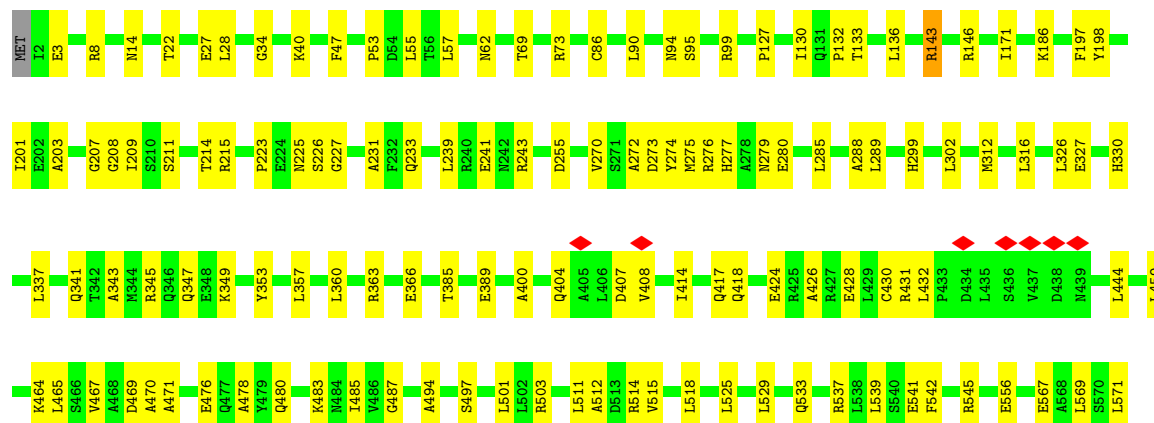
• Molecule 1: Chromosome partition protein MukB

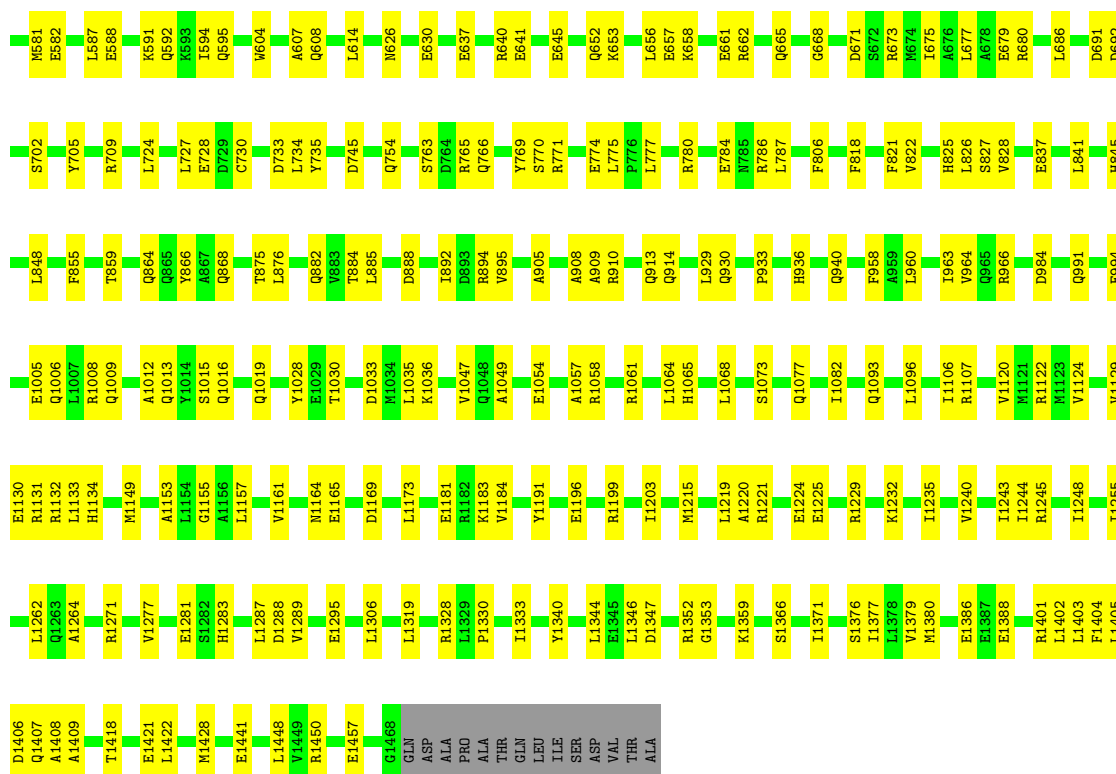




● Molecule 1: Chromosome partition protein MukB

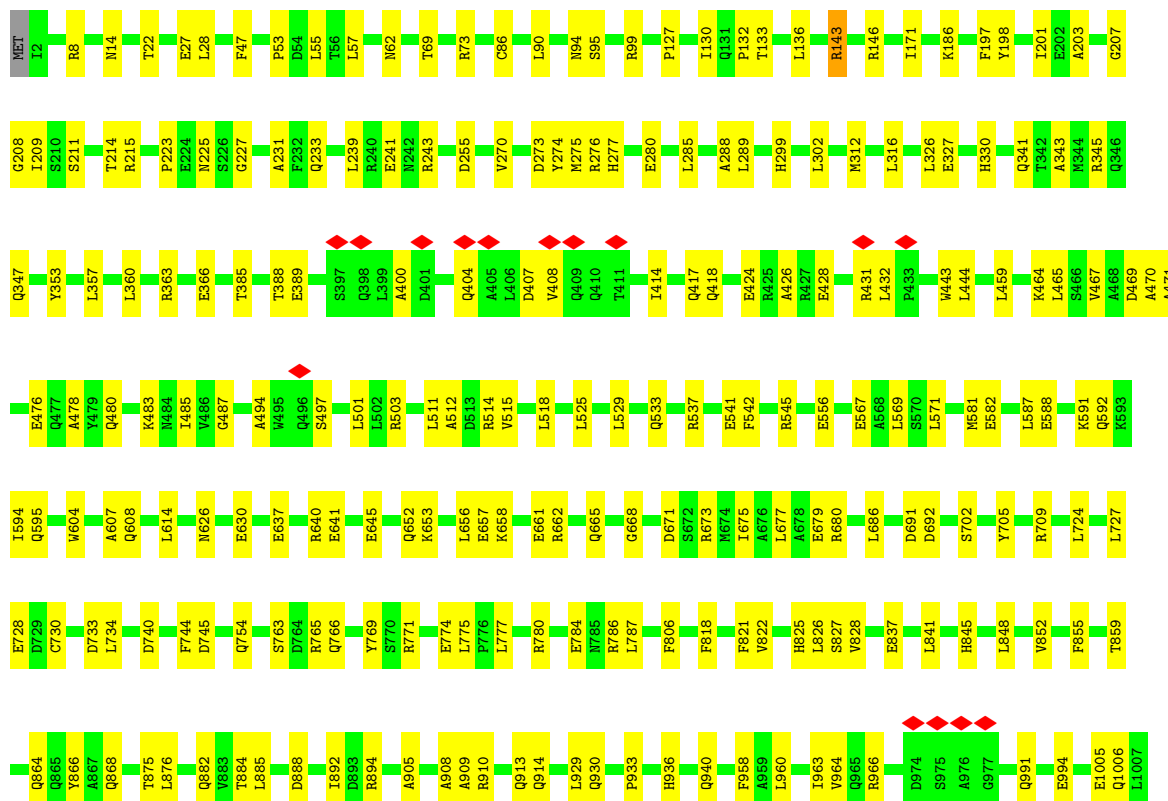
Chain B3: 75% 24%

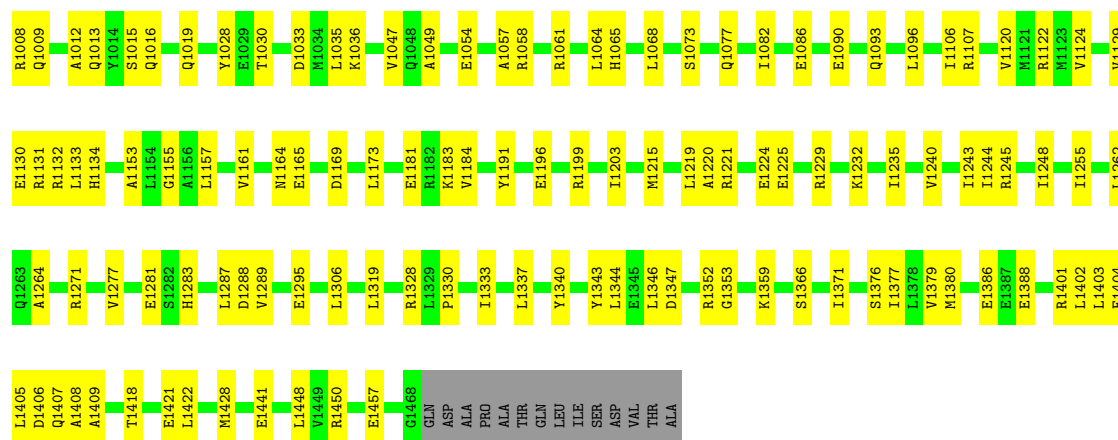




● Molecule 1: Chromosome partition protein MukB

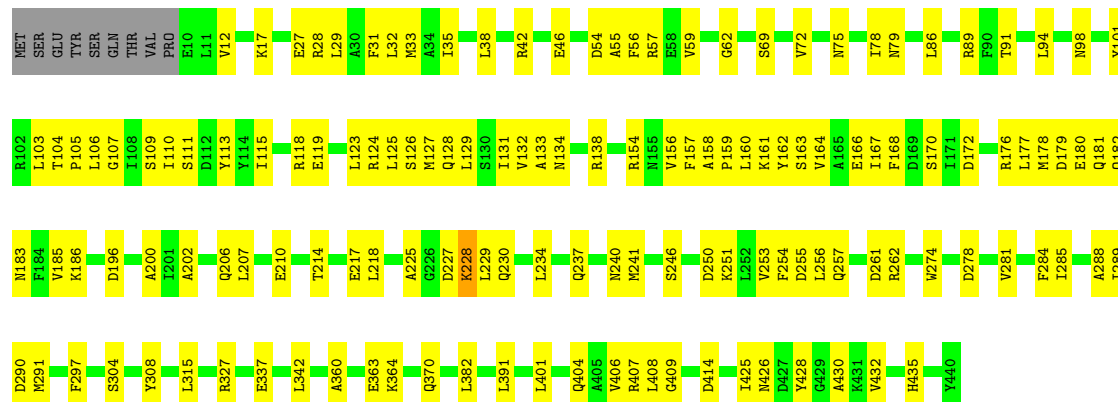
Chain B4: 76% 23%





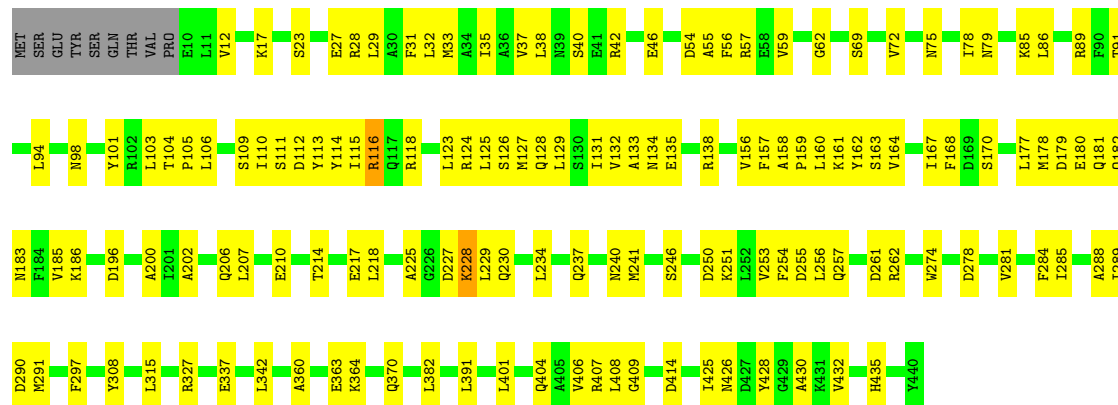
• Molecule 2: Chromosome partition protein MukF

Chain C1: 66% 32%



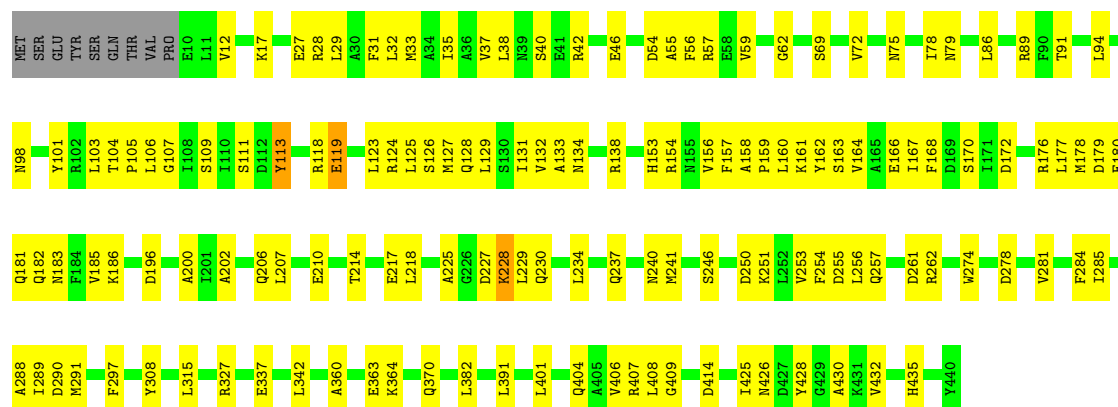
• Molecule 2: Chromosome partition protein MukF

Chain C2: 66% 32%



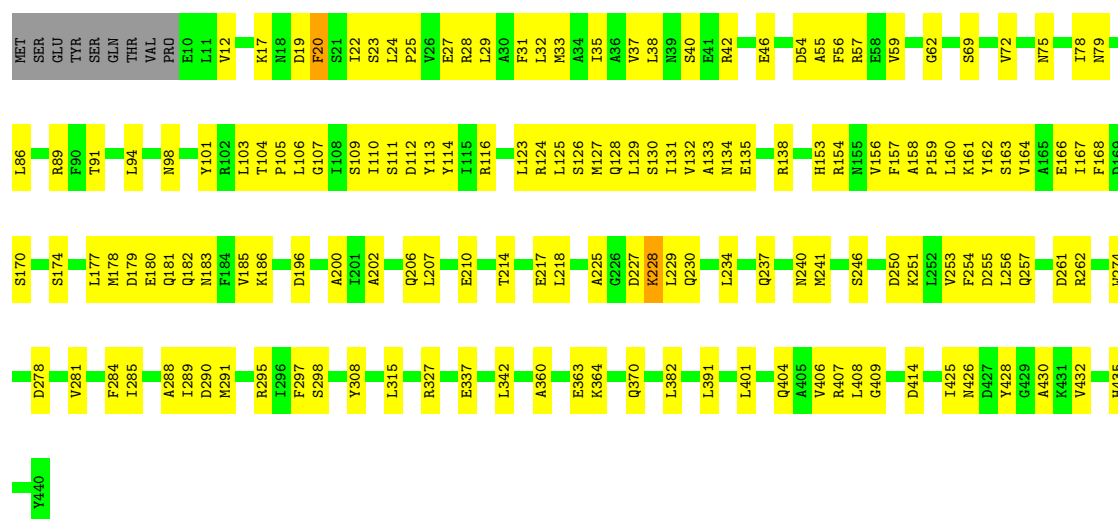
• Molecule 2: Chromosome partition protein MukF

Chain D1: 66% 31%



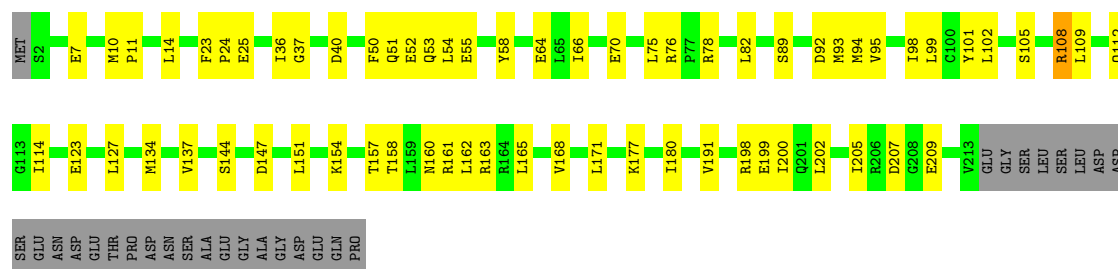
• Molecule 2: Chromosome partition protein MukF

Chain D2: 63% 34% .



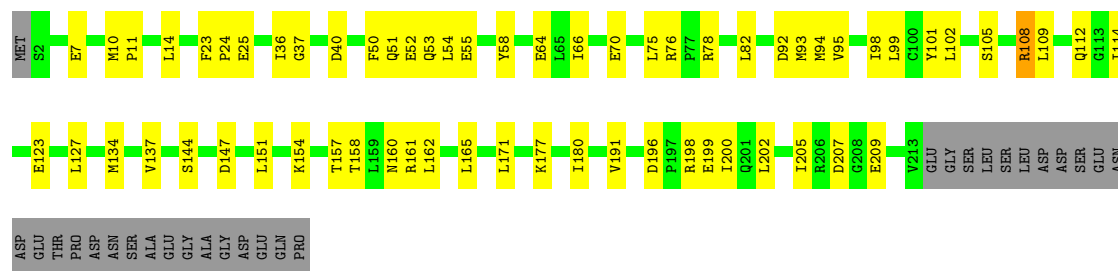
• Molecule 3: Chromosome partition protein MukE

Chain E1: 61% 27% 12%



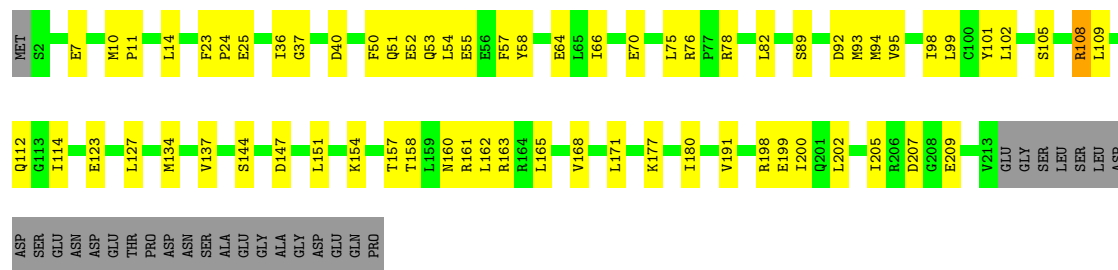
• Molecule 3: Chromosome partition protein MukE

Chain E2: 62% 26% 12%



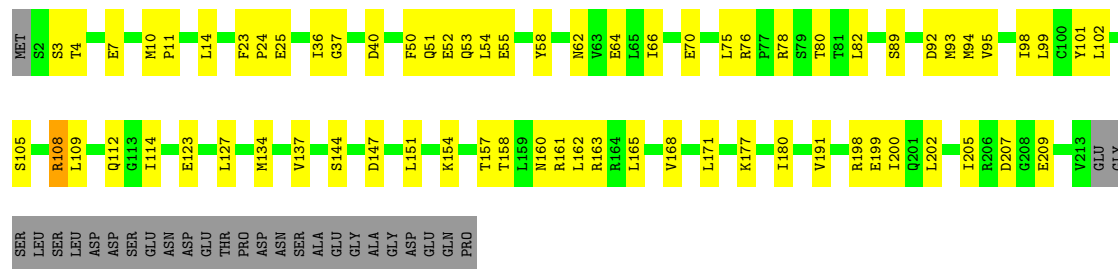
• Molecule 3: Chromosome partition protein MukE

Chain E3: 61% 27% 12%



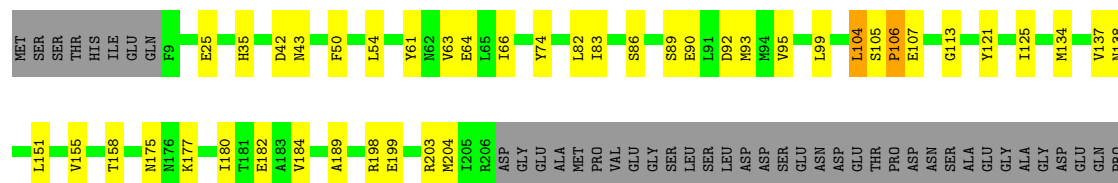
• Molecule 3: Chromosome partition protein MukE

Chain E4: 60% 28% 12%



• Molecule 3: Chromosome partition protein MukE

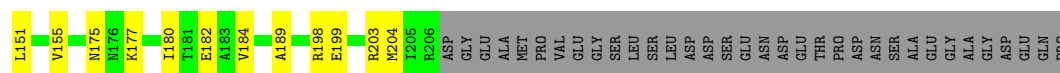
Chain F1: 65% 17% 18%



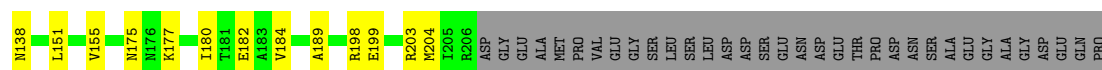
• Molecule 3: Chromosome partition protein MukE

Chain F2: 65% 16% 18%

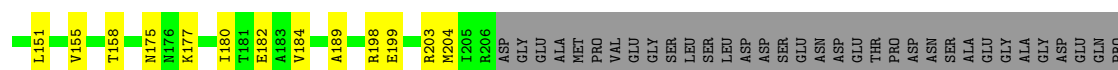




- Molecule 3: Chromosome partition protein MukE



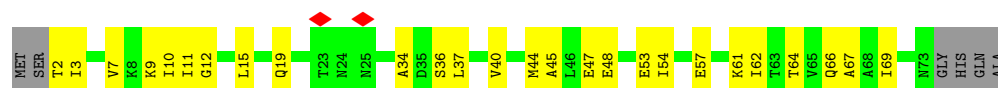
- Molecule 3: Chromosome partition protein MukE



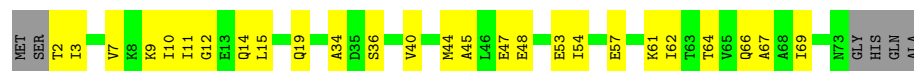
- Molecule 4: Acyl carrier protein



- Molecule 4: Acyl carrier protein

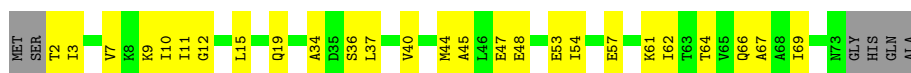


- Molecule 4: Acyl carrier protein



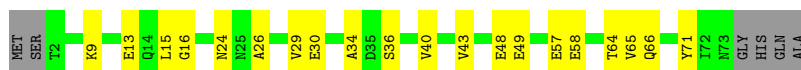
- Molecule 4: Acyl carrier protein





- Molecule 4: Acyl carrier protein

Chain H1: 67% 26% 8%



- Molecule 4: Acyl carrier protein

Chain H2: 64% 28% 8%



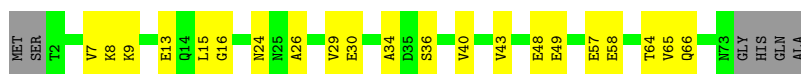
- Molecule 4: Acyl carrier protein

Chain H3: 67% 26% 8%



- Molecule 4: Acyl carrier protein

Chain H4: 65% 27% 8%



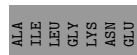
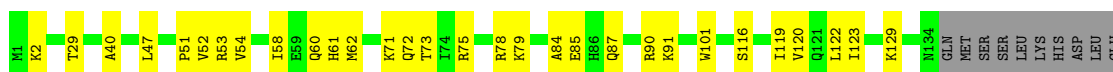
- Molecule 5: Macrodomain Ter protein

Chain I1: 70% 19% 11%

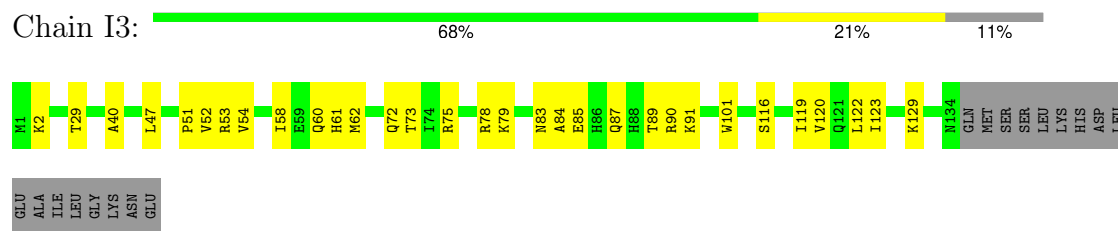


- Molecule 5: Macrodomain Ter protein

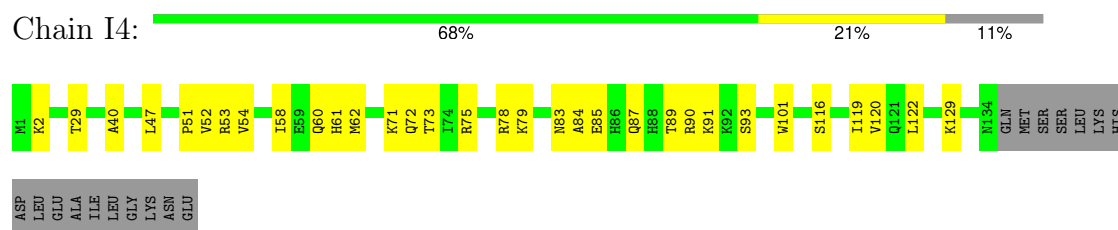
Chain I2: 69% 20% 11%



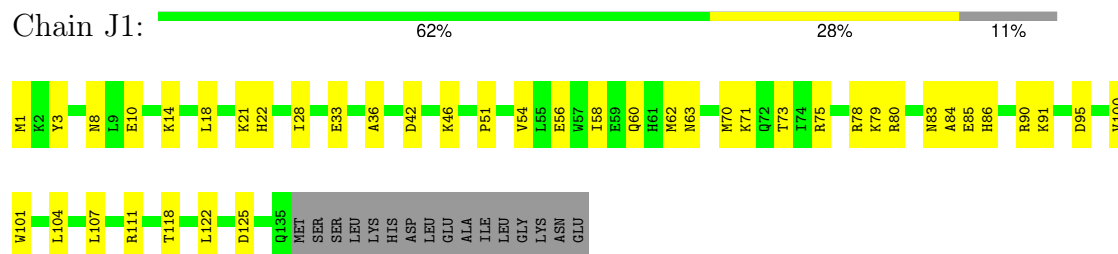
- Molecule 5: Macrodomain Ter protein



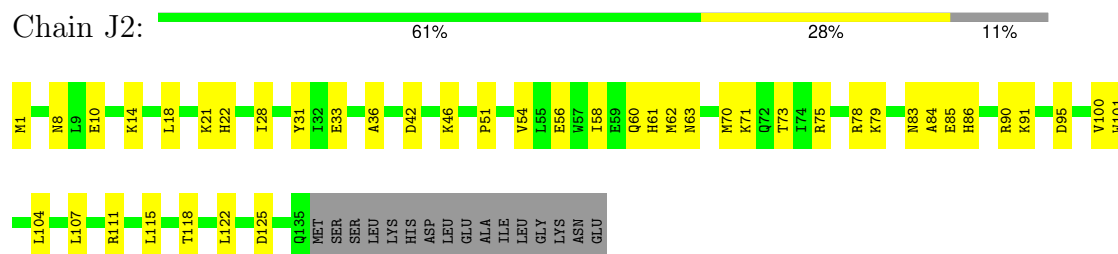
- Molecule 5: Macrodomain Ter protein



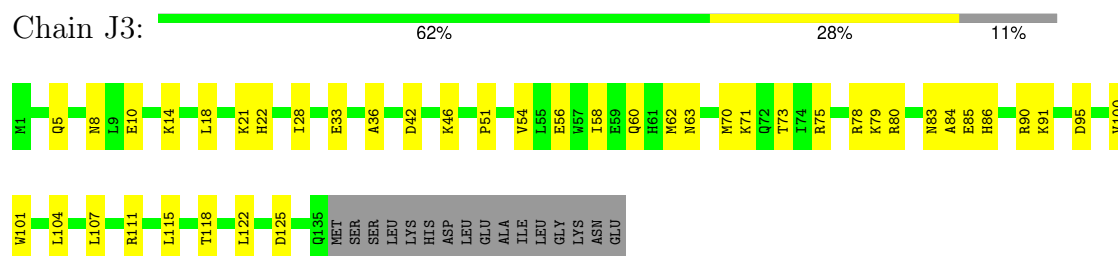
- Molecule 5: Macrodomain Ter protein



- Molecule 5: Macrodomain Ter protein

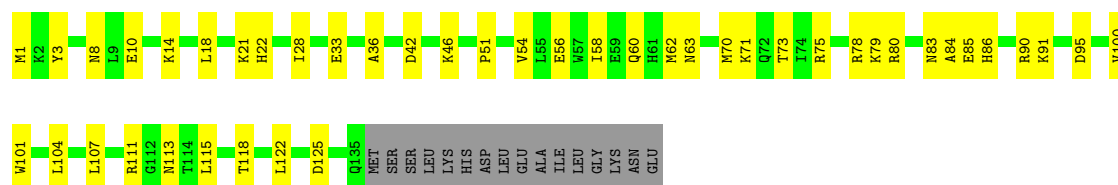


- Molecule 5: Macrodomain Ter protein

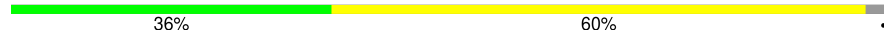


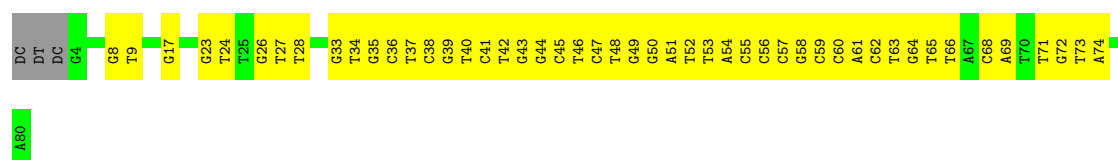
- Molecule 5: Macrodomain Ter protein

Chain J4: 



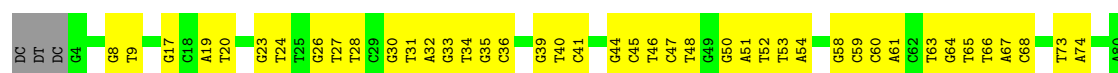
- Molecule 6: matS2 DNA 80 b, oligo FBA769

Chain K1: 



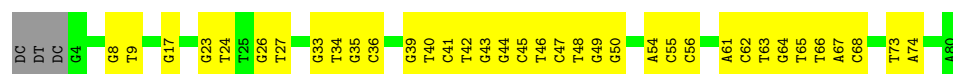
- Molecule 6: matS2 DNA 80 b, oligo FBA769

Chain K2: 



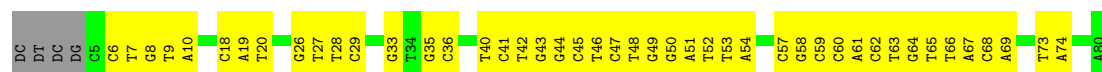
- Molecule 6: matS2 DNA 80 b, oligo FBA769

Chain N1: 



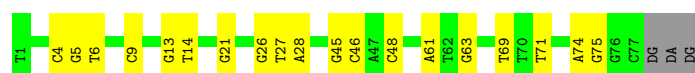
- Molecule 6: matS2 DNA 80 b, oligo FBA769

Chain N2: 



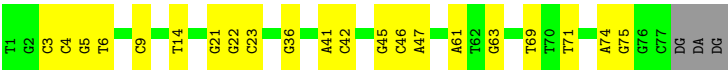
- Molecule 7: matS2 DNA 80 b, oligo FBA770

Chain L1: 

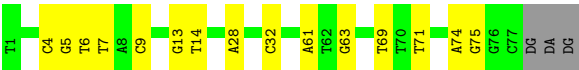
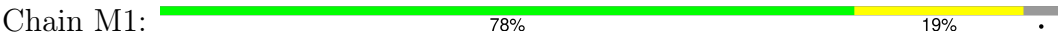


- Molecule 7: matS2 DNA 80 b, oligo FBA770

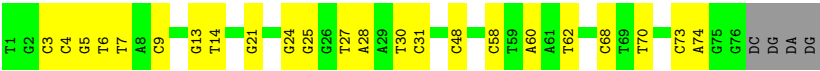
Chain L2: 



- Molecule 7: matS2 DNA 80 b, oligo FBA770



- Molecule 7: matS2 DNA 80 b, oligo FBA770



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	12010	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.248	Depositor
Minimum map value	-0.041	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.017	Depositor
Map size (\AA)	924.48004, 924.48004, 924.48004	wwPDB
Map dimensions	216, 216, 216	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	4.28, 4.28, 4.28	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PNS, MG, ATP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A1	0.25	0/11999	0.53	0/16166
1	A2	0.25	0/11999	0.53	0/16166
1	A3	0.25	0/11999	0.53	0/16166
1	A4	0.25	0/11999	0.53	0/16166
1	B1	0.26	0/11999	0.53	0/16166
1	B2	0.26	0/11999	0.53	0/16166
1	B3	0.26	0/11999	0.53	0/16166
1	B4	0.26	0/11999	0.53	0/16166
2	C1	0.26	0/3519	0.53	0/4762
2	C2	0.26	0/3519	0.53	0/4762
2	D1	0.38	1/3519 (0.0%)	0.57	1/4762 (0.0%)
2	D2	0.29	1/3519 (0.0%)	0.57	2/4762 (0.0%)
3	E1	0.30	0/1753	0.58	0/2361
3	E2	0.30	0/1753	0.58	0/2361
3	E3	0.30	0/1753	0.57	0/2361
3	E4	0.30	0/1753	0.58	0/2361
3	F1	0.27	0/1648	0.62	2/2218 (0.1%)
3	F2	0.28	0/1648	0.62	2/2218 (0.1%)
3	F3	0.27	0/1648	0.62	2/2218 (0.1%)
3	F4	0.28	0/1648	0.62	2/2218 (0.1%)
4	G1	0.25	0/565	0.47	0/765
4	G2	0.26	0/565	0.47	0/765
4	G3	0.26	0/565	0.47	0/765
4	G4	0.25	0/565	0.46	0/765
4	H1	0.26	0/565	0.43	0/765
4	H2	0.25	0/565	0.44	0/765
4	H3	0.25	0/565	0.44	0/765
4	H4	0.25	0/565	0.43	0/765
5	I1	0.26	0/1160	0.54	0/1560
5	I2	0.26	0/1160	0.54	0/1560
5	I3	0.26	0/1160	0.54	0/1560
5	I4	0.26	0/1160	0.54	0/1560

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	J1	0.26	0/1169	0.53	0/1572
5	J2	0.26	0/1169	0.53	0/1572
5	J3	0.26	0/1169	0.53	0/1572
5	J4	0.26	0/1169	0.53	0/1572
6	K1	0.53	0/1765	0.98	0/2723
6	K2	0.55	0/1765	1.05	2/2723 (0.1%)
6	N1	0.51	0/1765	0.96	0/2723
6	N2	0.56	0/1740	0.98	0/2684
7	L1	0.54	0/1775	0.91	0/2736
7	L2	0.56	0/1775	0.98	0/2736
7	M1	0.53	0/1775	0.90	0/2736
7	M2	0.54	0/1754	0.91	0/2704
All	All	0.30	2/151622 (0.0%)	0.59	13/207105 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D1	119	GLU	C-N	12.91	1.63	1.34
2	D2	19	ASP	C-N	6.40	1.48	1.34

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F1	106	PRO	CA-N-CD	-7.84	100.53	111.50
3	F3	106	PRO	CA-N-CD	-7.83	100.54	111.50
3	F2	106	PRO	CA-N-CD	-7.82	100.56	111.50
3	F4	106	PRO	CA-N-CD	-7.82	100.56	111.50
3	F3	104	LEU	CA-CB-CG	7.56	132.69	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A1	11840	11708	11708	264	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A2	11840	11708	11708	266	0
1	A3	11840	11708	11708	266	0
1	A4	11840	11708	11708	254	0
1	B1	11840	11709	11707	266	0
1	B2	11840	11709	11707	265	0
1	B3	11840	11709	11707	266	0
1	B4	11840	11709	11707	260	0
2	C1	3460	3384	3376	245	0
2	C2	3460	3384	3371	374	0
2	D1	3460	3384	3378	241	0
2	D2	3460	3384	3374	376	0
3	E1	1722	1719	1718	63	0
3	E2	1722	1719	1718	61	0
3	E3	1722	1719	1718	62	0
3	E4	1722	1719	1718	63	0
3	F1	1619	1627	1626	38	0
3	F2	1619	1627	1626	36	0
3	F3	1619	1627	1626	36	0
3	F4	1619	1627	1626	37	0
4	G1	562	543	542	20	0
4	G2	562	543	542	21	0
4	G3	562	543	542	21	0
4	G4	562	543	542	20	0
4	H1	562	543	542	13	0
4	H2	562	543	542	14	0
4	H3	562	543	542	12	0
4	H4	562	543	542	13	0
5	I1	1135	1136	1136	30	0
5	I2	1135	1136	1136	31	0
5	I3	1135	1136	1136	33	0
5	I4	1135	1136	1136	34	0
5	J1	1144	1144	1144	66	0
5	J2	1144	1144	1144	38	0
5	J3	1144	1144	1144	36	0
5	J4	1144	1144	1144	68	0
6	K1	1577	872	872	74	0
6	K2	1577	872	872	49	0
6	N1	1577	872	872	33	0
6	N2	1555	861	861	72	0
7	L1	1580	862	863	30	0
7	L2	1580	862	863	27	0
7	M1	1580	862	863	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	M2	1561	851	852	37	0
8	A1	1	0	0	0	0
8	A2	1	0	0	0	0
8	A3	1	0	0	0	0
8	A4	1	0	0	0	0
8	B1	1	0	0	0	0
8	B2	1	0	0	0	0
8	B3	1	0	0	0	0
8	B4	1	0	0	0	0
9	A1	31	12	12	3	0
9	A2	31	12	12	2	0
9	A3	31	12	12	3	0
9	A4	31	12	12	2	0
9	B1	31	12	12	0	0
9	B2	31	12	12	0	0
9	B3	31	12	12	0	0
9	B4	31	12	12	0	0
10	G1	21	21	21	1	0
10	G2	21	21	21	1	0
10	G3	21	21	21	0	0
10	G4	21	21	21	1	0
10	H1	21	21	21	0	0
10	H2	21	21	21	0	0
10	H3	21	21	21	0	0
10	H4	21	21	21	0	0
All	All	148547	141230	141173	3628	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 13.

The worst 5 of 3628 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)
2:C2:113:TYR:CZ	2:D2:104:THR:HG23	1.17	1.70
2:C2:131:ILE:CD1	2:D2:163:SER:HB3	1.26	1.61
2:C2:159:PRO:CA	2:D2:127:MET:HB2	1.12	1.58
2:C1:113:TYR:CD1	2:D1:106:LEU:HA	1.04	1.56
2:C2:127:MET:CE	2:D2:158:ALA:HA	1.34	1.55

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A1	1465/1482 (99%)	1416 (97%)	49 (3%)	0	100	100
1	A2	1465/1482 (99%)	1417 (97%)	48 (3%)	0	100	100
1	A3	1465/1482 (99%)	1417 (97%)	48 (3%)	0	100	100
1	A4	1465/1482 (99%)	1416 (97%)	49 (3%)	0	100	100
1	B1	1465/1482 (99%)	1413 (96%)	52 (4%)	0	100	100
1	B2	1465/1482 (99%)	1413 (96%)	52 (4%)	0	100	100
1	B3	1465/1482 (99%)	1414 (96%)	51 (4%)	0	100	100
1	B4	1465/1482 (99%)	1413 (96%)	52 (4%)	0	100	100
2	C1	429/440 (98%)	410 (96%)	19 (4%)	0	100	100
2	C2	429/440 (98%)	408 (95%)	21 (5%)	0	100	100
2	D1	429/440 (98%)	410 (96%)	19 (4%)	0	100	100
2	D2	429/440 (98%)	408 (95%)	21 (5%)	0	100	100
3	E1	210/240 (88%)	207 (99%)	3 (1%)	0	100	100
3	E2	210/240 (88%)	207 (99%)	3 (1%)	0	100	100
3	E3	210/240 (88%)	207 (99%)	3 (1%)	0	100	100
3	E4	210/240 (88%)	207 (99%)	3 (1%)	0	100	100
3	F1	196/240 (82%)	186 (95%)	10 (5%)	0	100	100
3	F2	196/240 (82%)	186 (95%)	10 (5%)	0	100	100
3	F3	196/240 (82%)	186 (95%)	10 (5%)	0	100	100
3	F4	196/240 (82%)	186 (95%)	10 (5%)	0	100	100
4	G1	70/78 (90%)	69 (99%)	1 (1%)	0	100	100
4	G2	70/78 (90%)	69 (99%)	1 (1%)	0	100	100
4	G3	70/78 (90%)	69 (99%)	1 (1%)	0	100	100
4	G4	70/78 (90%)	69 (99%)	1 (1%)	0	100	100
4	H1	70/78 (90%)	66 (94%)	4 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	H2	70/78 (90%)	66 (94%)	4 (6%)	0	100	100
4	H3	70/78 (90%)	66 (94%)	4 (6%)	0	100	100
4	H4	70/78 (90%)	66 (94%)	4 (6%)	0	100	100
5	I1	132/151 (87%)	129 (98%)	3 (2%)	0	100	100
5	I2	132/151 (87%)	129 (98%)	3 (2%)	0	100	100
5	I3	132/151 (87%)	129 (98%)	3 (2%)	0	100	100
5	I4	132/151 (87%)	129 (98%)	3 (2%)	0	100	100
5	J1	133/151 (88%)	131 (98%)	2 (2%)	0	100	100
5	J2	133/151 (88%)	130 (98%)	3 (2%)	0	100	100
5	J3	133/151 (88%)	130 (98%)	3 (2%)	0	100	100
5	J4	133/151 (88%)	130 (98%)	3 (2%)	0	100	100
All	All	16680/17368 (96%)	16104 (96%)	576 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	A1	1269/1281 (99%)	1266 (100%)	3 (0%)	92	94
1	A2	1269/1281 (99%)	1266 (100%)	3 (0%)	92	94
1	A3	1269/1281 (99%)	1266 (100%)	3 (0%)	92	94
1	A4	1269/1281 (99%)	1266 (100%)	3 (0%)	92	94
1	B1	1269/1281 (99%)	1264 (100%)	5 (0%)	89	91
1	B2	1269/1281 (99%)	1264 (100%)	5 (0%)	89	91
1	B3	1269/1281 (99%)	1264 (100%)	5 (0%)	89	91
1	B4	1269/1281 (99%)	1264 (100%)	5 (0%)	89	91
2	C1	367/376 (98%)	363 (99%)	4 (1%)	70	80
2	C2	367/376 (98%)	363 (99%)	4 (1%)	70	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D1	367/376 (98%)	365 (100%)	2 (0%)	86	89
2	D2	367/376 (98%)	365 (100%)	2 (0%)	86	89
3	E1	189/212 (89%)	188 (100%)	1 (0%)	86	89
3	E2	189/212 (89%)	188 (100%)	1 (0%)	86	89
3	E3	189/212 (89%)	188 (100%)	1 (0%)	86	89
3	E4	189/212 (89%)	188 (100%)	1 (0%)	86	89
3	F1	177/212 (84%)	177 (100%)	0	100	100
3	F2	177/212 (84%)	177 (100%)	0	100	100
3	F3	177/212 (84%)	177 (100%)	0	100	100
3	F4	177/212 (84%)	177 (100%)	0	100	100
4	G1	63/67 (94%)	63 (100%)	0	100	100
4	G2	63/67 (94%)	63 (100%)	0	100	100
4	G3	63/67 (94%)	63 (100%)	0	100	100
4	G4	63/67 (94%)	63 (100%)	0	100	100
4	H1	63/67 (94%)	63 (100%)	0	100	100
4	H2	63/67 (94%)	63 (100%)	0	100	100
4	H3	63/67 (94%)	63 (100%)	0	100	100
4	H4	63/67 (94%)	63 (100%)	0	100	100
5	I1	121/136 (89%)	121 (100%)	0	100	100
5	I2	121/136 (89%)	121 (100%)	0	100	100
5	I3	121/136 (89%)	121 (100%)	0	100	100
5	I4	121/136 (89%)	121 (100%)	0	100	100
5	J1	122/136 (90%)	122 (100%)	0	100	100
5	J2	122/136 (90%)	122 (100%)	0	100	100
5	J3	122/136 (90%)	122 (100%)	0	100	100
5	J4	122/136 (90%)	122 (100%)	0	100	100
All	All	14560/15072 (97%)	14512 (100%)	48 (0%)	90	92

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B4	345	ARG
2	C1	228	LYS

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Mol	Chain	Res	Type
1	B4	658	LYS
2	C1	17	LYS
2	C2	116	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
2	C2	206	GLN
5	J1	60	GLN
2	D1	84	GLN
2	D2	206	GLN
1	A4	319	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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	$\# Z > 2$
10	PNS	H1	101	4	14,20,21	0.22	0	18,26,29	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	ATP	B3	2101	8	28,33,33	0.71	0	34,52,52	0.91	2 (5%)
9	ATP	B1	1502	8	28,33,33	0.71	0	34,52,52	0.91	2 (5%)
10	PNS	G4	101	4	14,20,21	0.23	0	18,26,29	0.34	0
10	PNS	G3	101	4	14,20,21	0.23	0	18,26,29	0.35	0
10	PNS	H4	101	4	14,20,21	0.23	0	18,26,29	0.45	0
10	PNS	H3	101	4	14,20,21	0.22	0	18,26,29	0.45	0
9	ATP	A2	2101	8	28,33,33	0.72	0	34,52,52	0.89	2 (5%)
9	ATP	B4	2101	8	28,33,33	0.70	0	34,52,52	0.91	2 (5%)
10	PNS	H2	101	4	14,20,21	0.21	0	18,26,29	0.45	0
9	ATP	A1	1502	8	28,33,33	0.72	0	34,52,52	0.89	1 (2%)
10	PNS	G1	101	4	14,20,21	0.23	0	18,26,29	0.34	0
9	ATP	A3	2101	8	28,33,33	0.73	0	34,52,52	0.88	2 (5%)
9	ATP	A4	1502	8	28,33,33	0.72	0	34,52,52	0.89	2 (5%)
9	ATP	B2	1502	8	28,33,33	0.72	0	34,52,52	0.91	2 (5%)
10	PNS	G2	101	4	14,20,21	0.23	0	18,26,29	0.35	0

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
10	PNS	H1	101	4	-	4/24/26/27	-
9	ATP	B3	2101	8	-	2/18/38/38	0/3/3/3
9	ATP	B1	1502	8	-	2/18/38/38	0/3/3/3
10	PNS	G4	101	4	-	3/24/26/27	-
10	PNS	G3	101	4	-	3/24/26/27	-
10	PNS	H4	101	4	-	4/24/26/27	-
10	PNS	H3	101	4	-	4/24/26/27	-
9	ATP	A2	2101	8	-	1/18/38/38	0/3/3/3
9	ATP	B4	2101	8	-	2/18/38/38	0/3/3/3
10	PNS	H2	101	4	-	4/24/26/27	-
9	ATP	A1	1502	8	-	1/18/38/38	0/3/3/3
10	PNS	G1	101	4	-	3/24/26/27	-
9	ATP	A3	2101	8	-	1/18/38/38	0/3/3/3
9	ATP	A4	1502	8	-	1/18/38/38	0/3/3/3
9	ATP	B2	1502	8	-	2/18/38/38	0/3/3/3
10	PNS	G2	101	4	-	3/24/26/27	-

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B2	1502	ATP	C5-C6-N6	2.34	123.88	120.31
9	B3	2101	ATP	C5-C6-N6	2.32	123.85	120.31
9	B1	1502	ATP	C5-C6-N6	2.32	123.84	120.31
9	B4	2101	ATP	C5-C6-N6	2.31	123.83	120.31
9	A2	2101	ATP	C5-C6-N6	2.30	123.81	120.31

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

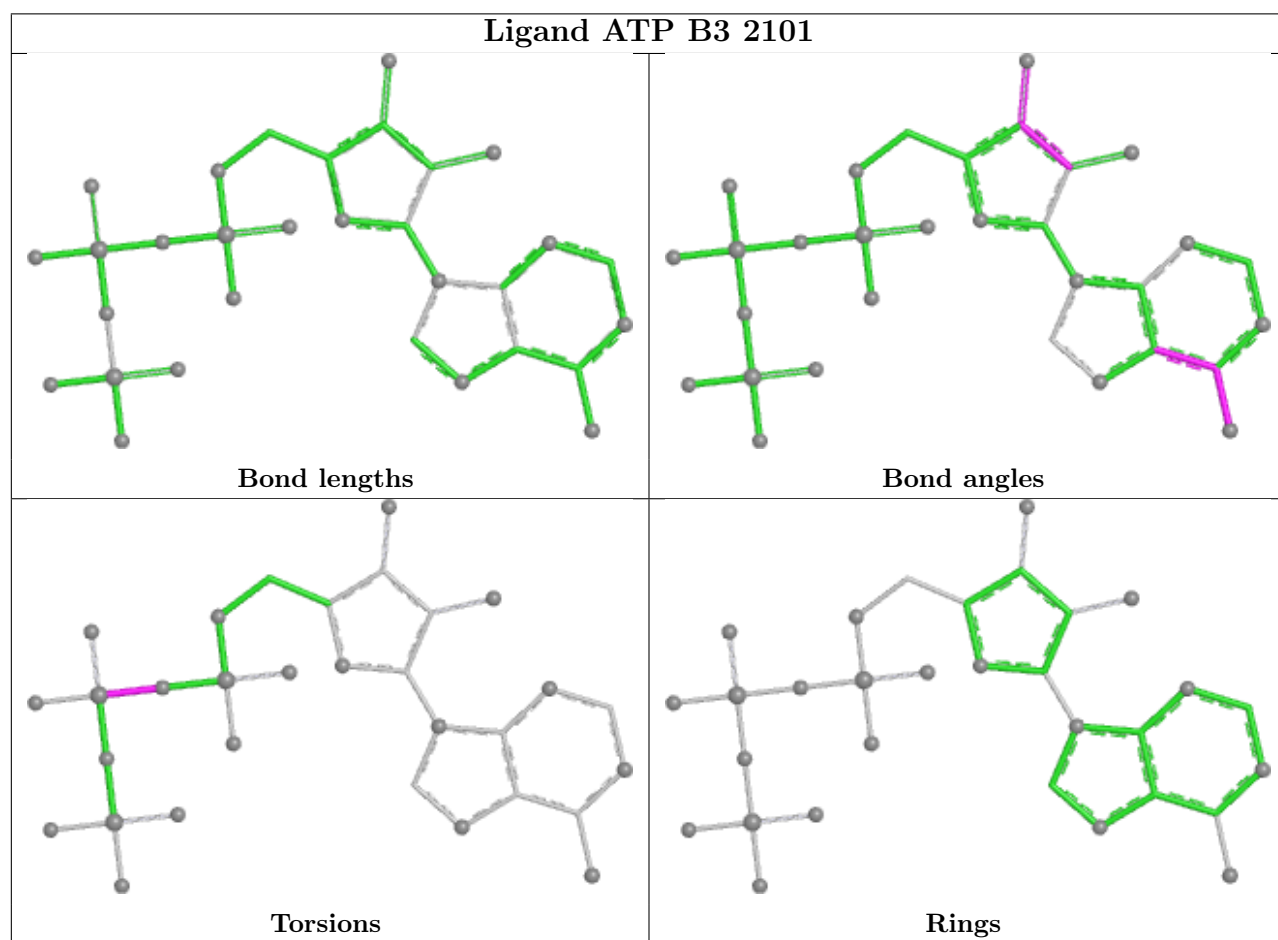
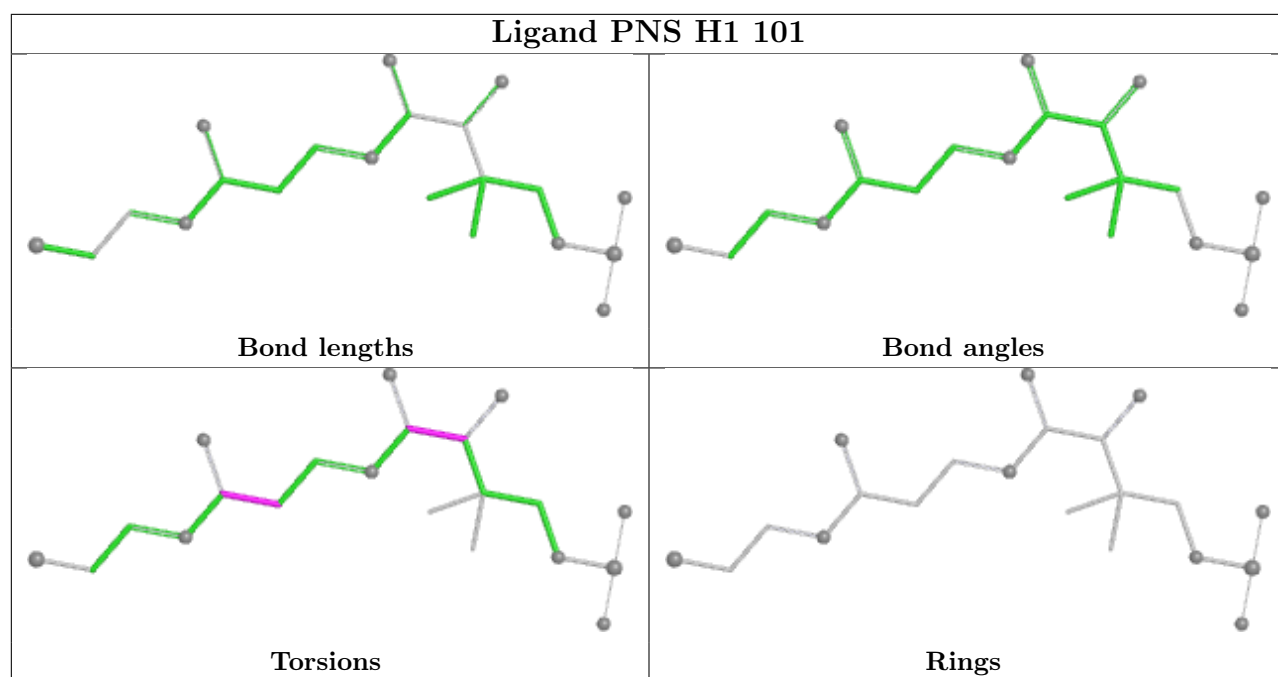
Mol	Chain	Res	Type	Atoms
9	A1	1502	ATP	PB-O3B-PG-O1G
9	A2	2101	ATP	PB-O3B-PG-O1G
9	A3	2101	ATP	PB-O3B-PG-O1G
9	A4	1502	ATP	PB-O3B-PG-O1G
10	H1	101	PNS	C37-C38-C39-N41

There are no ring outliers.

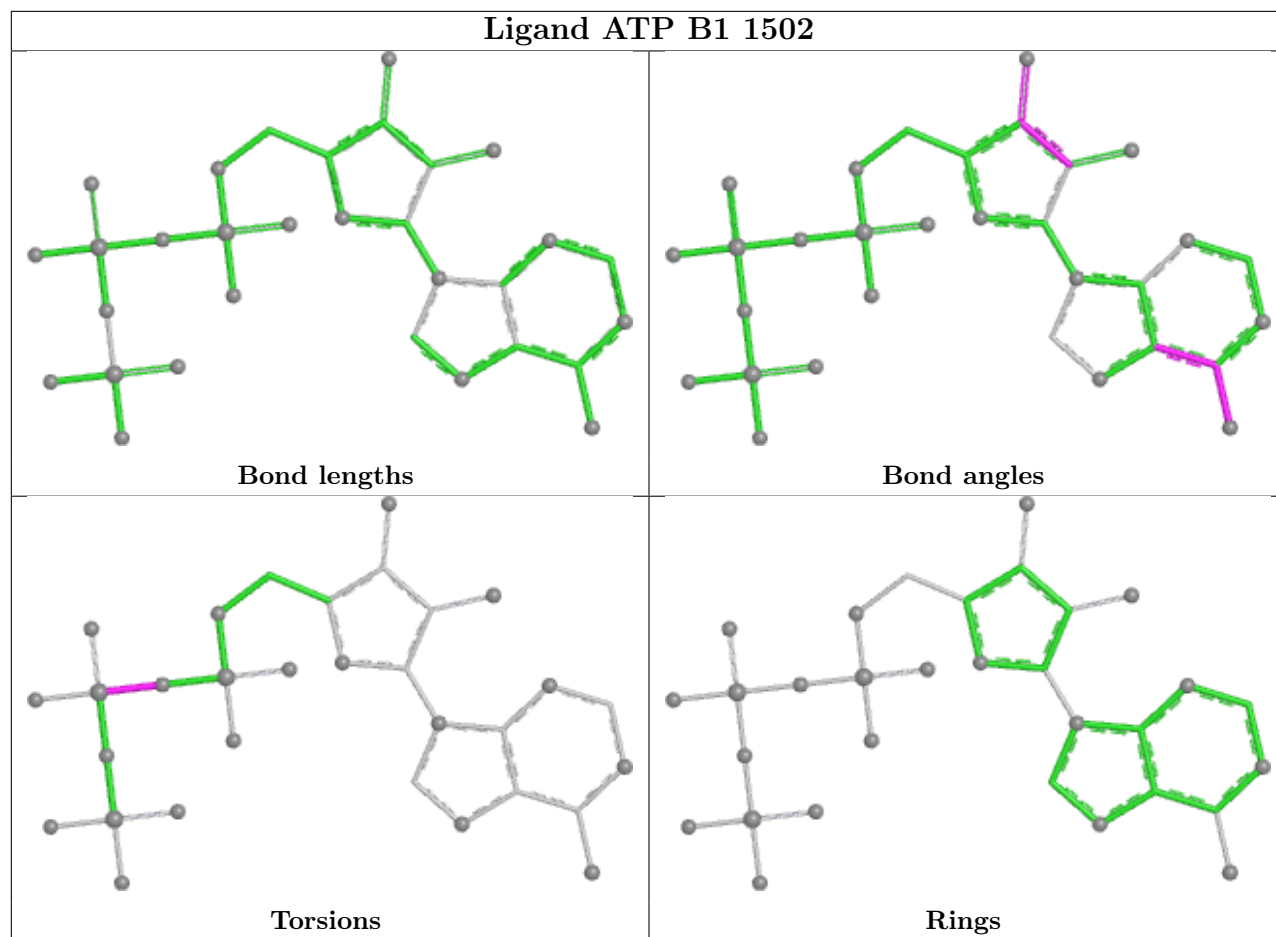
7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	G4	101	PNS	1	0
9	A2	2101	ATP	2	0
9	A1	1502	ATP	3	0
10	G1	101	PNS	1	0
9	A3	2101	ATP	3	0
9	A4	1502	ATP	2	0
10	G2	101	PNS	1	0

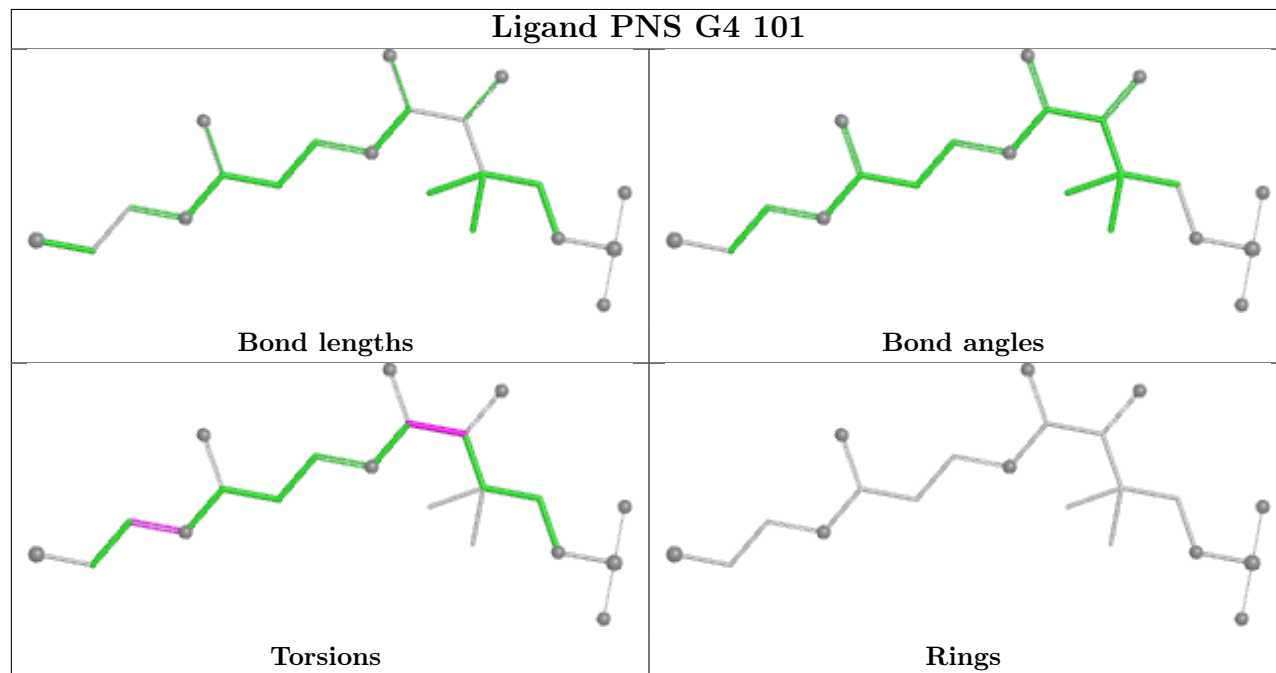
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

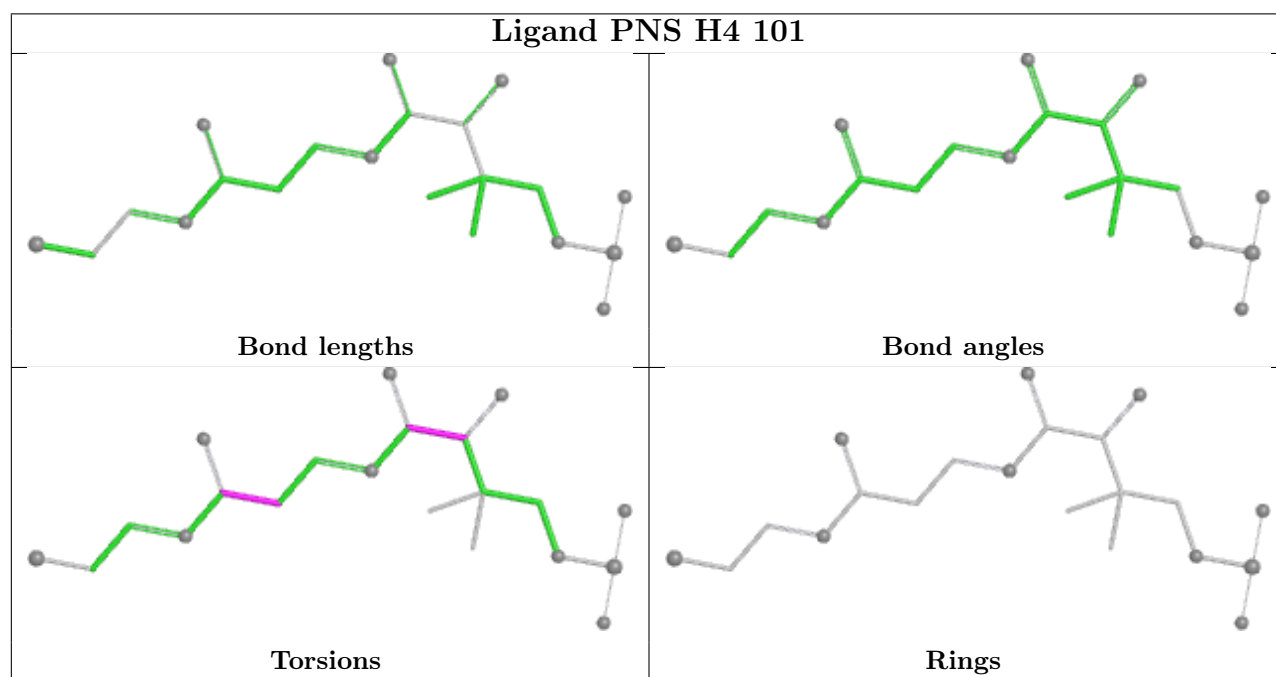
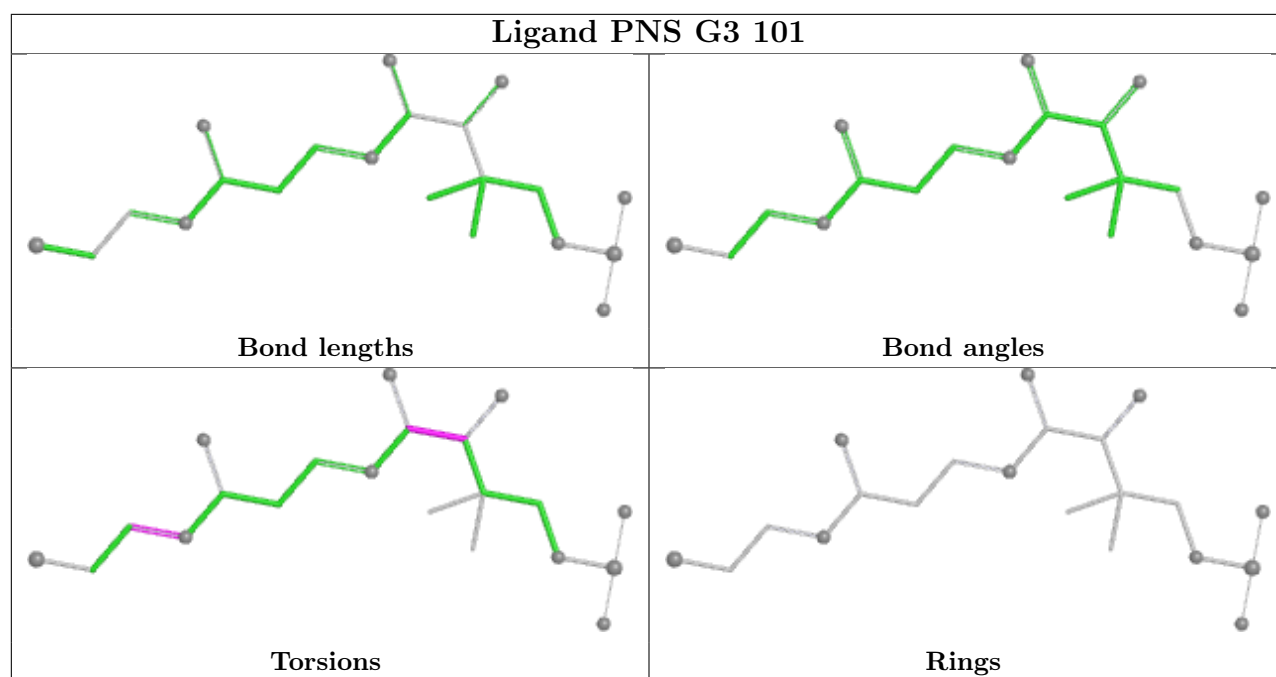


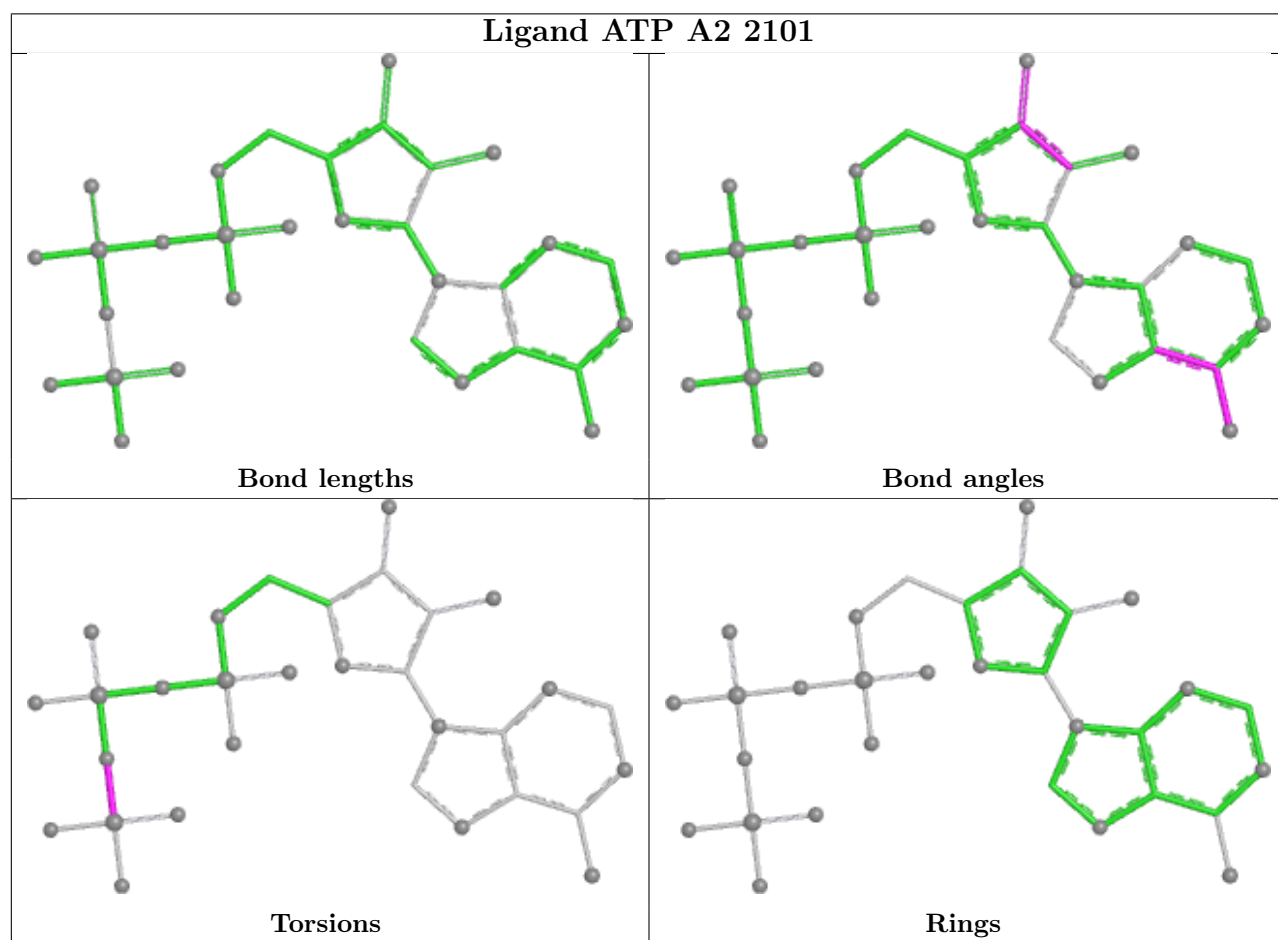
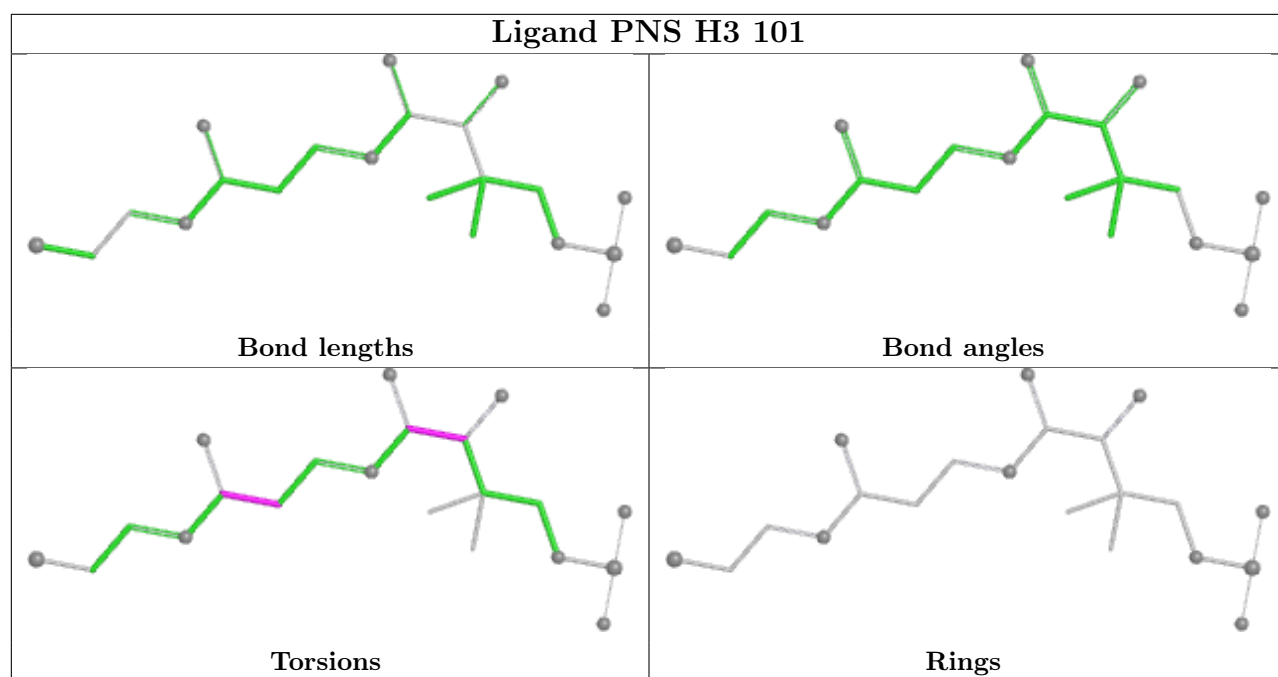
Ligand ATP B1 1502



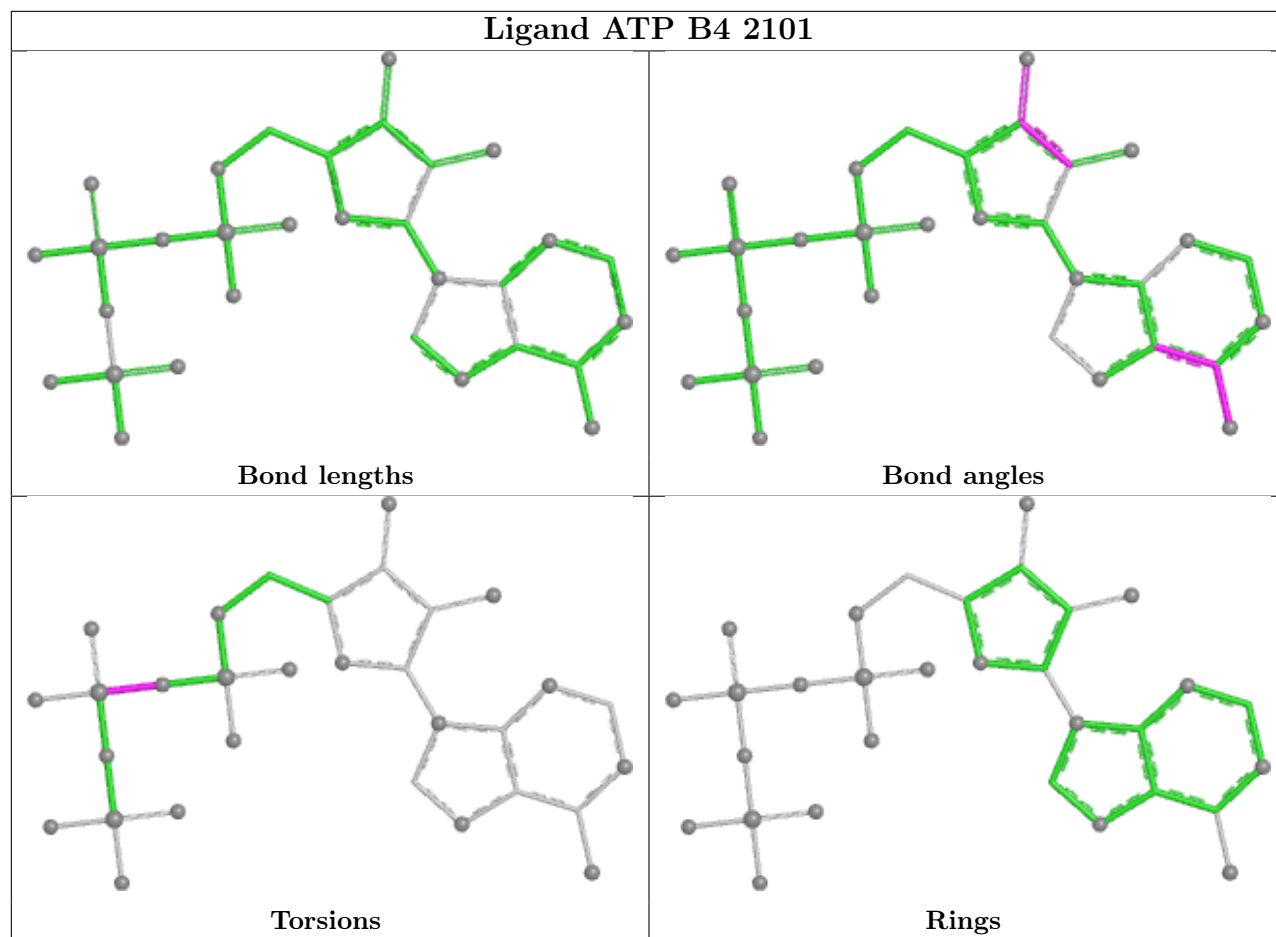
Ligand PNS G4 101



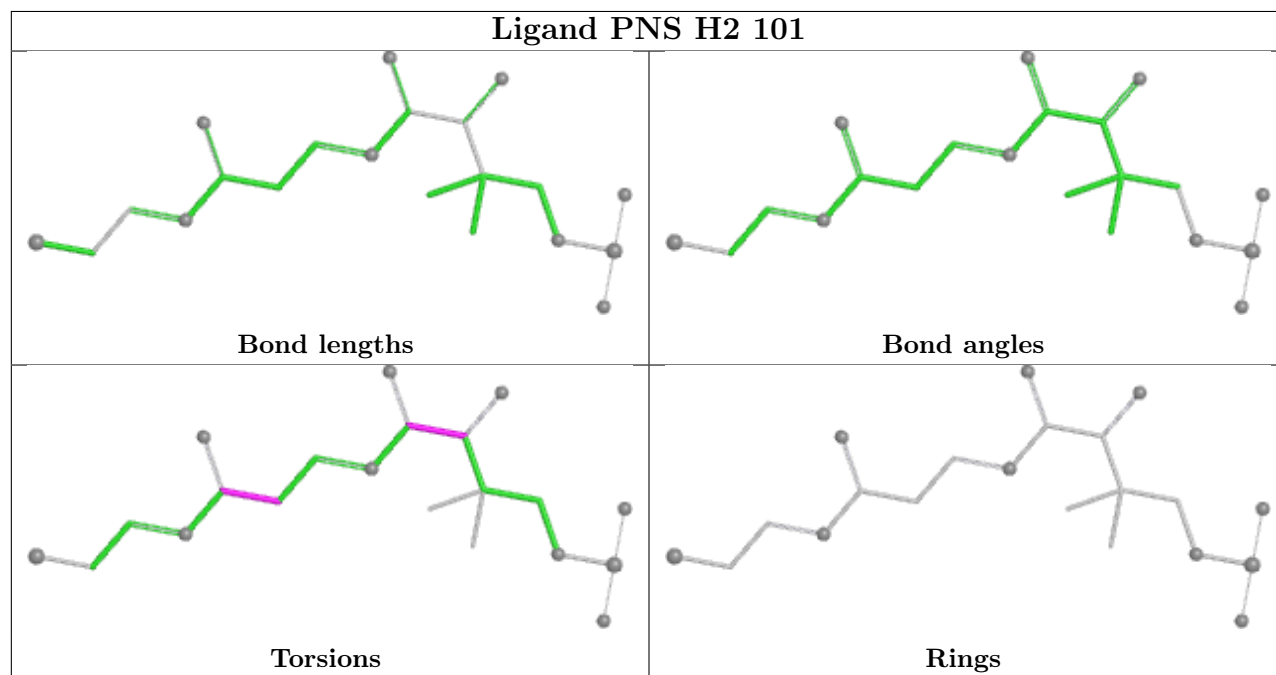




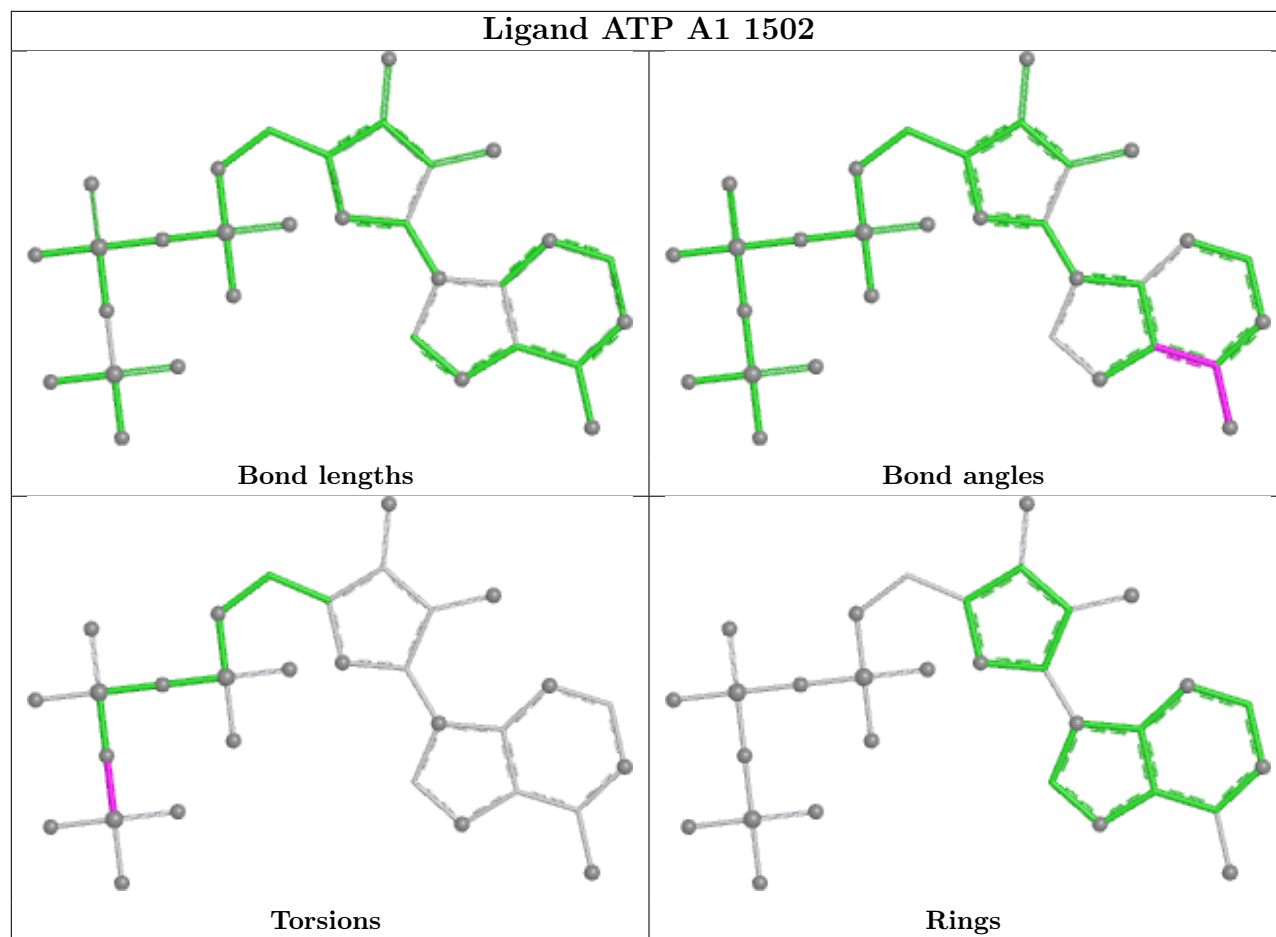
Ligand ATP B4 2101



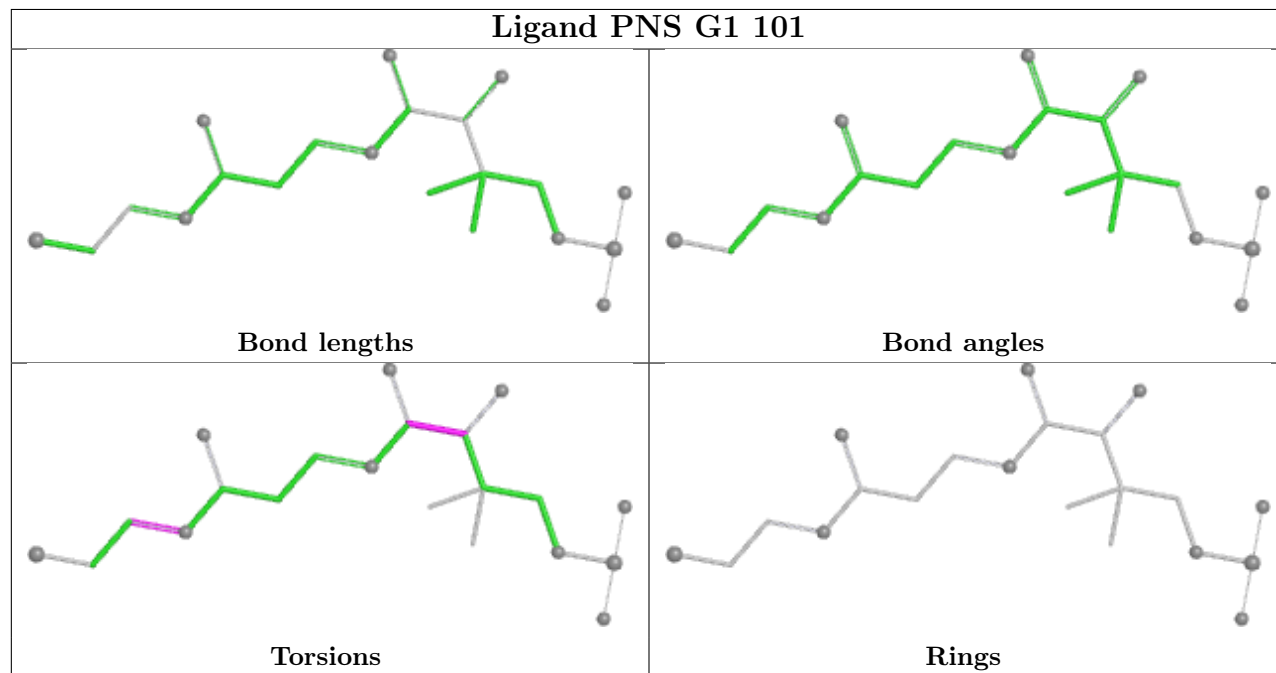
Ligand PNS H2 101

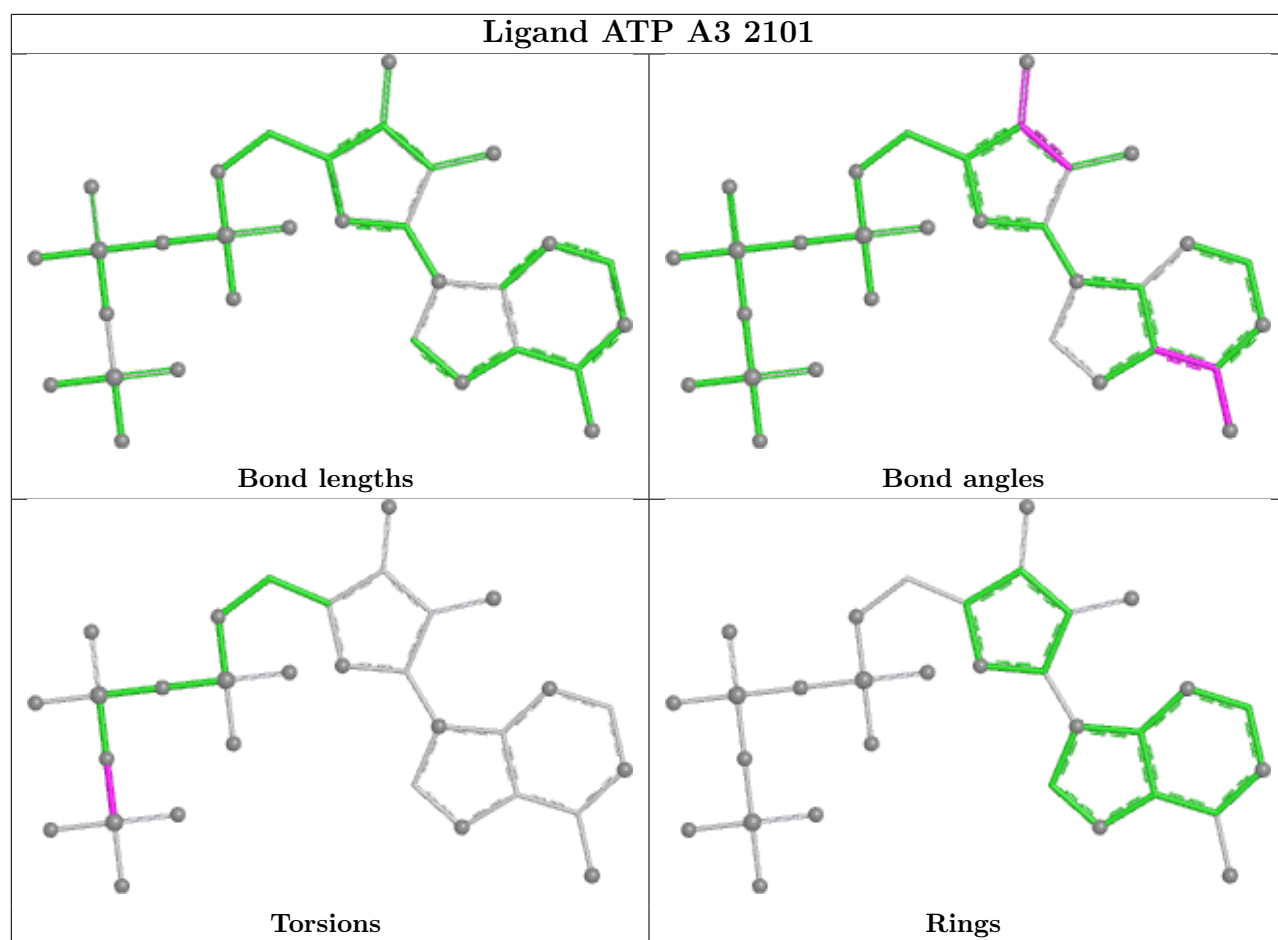


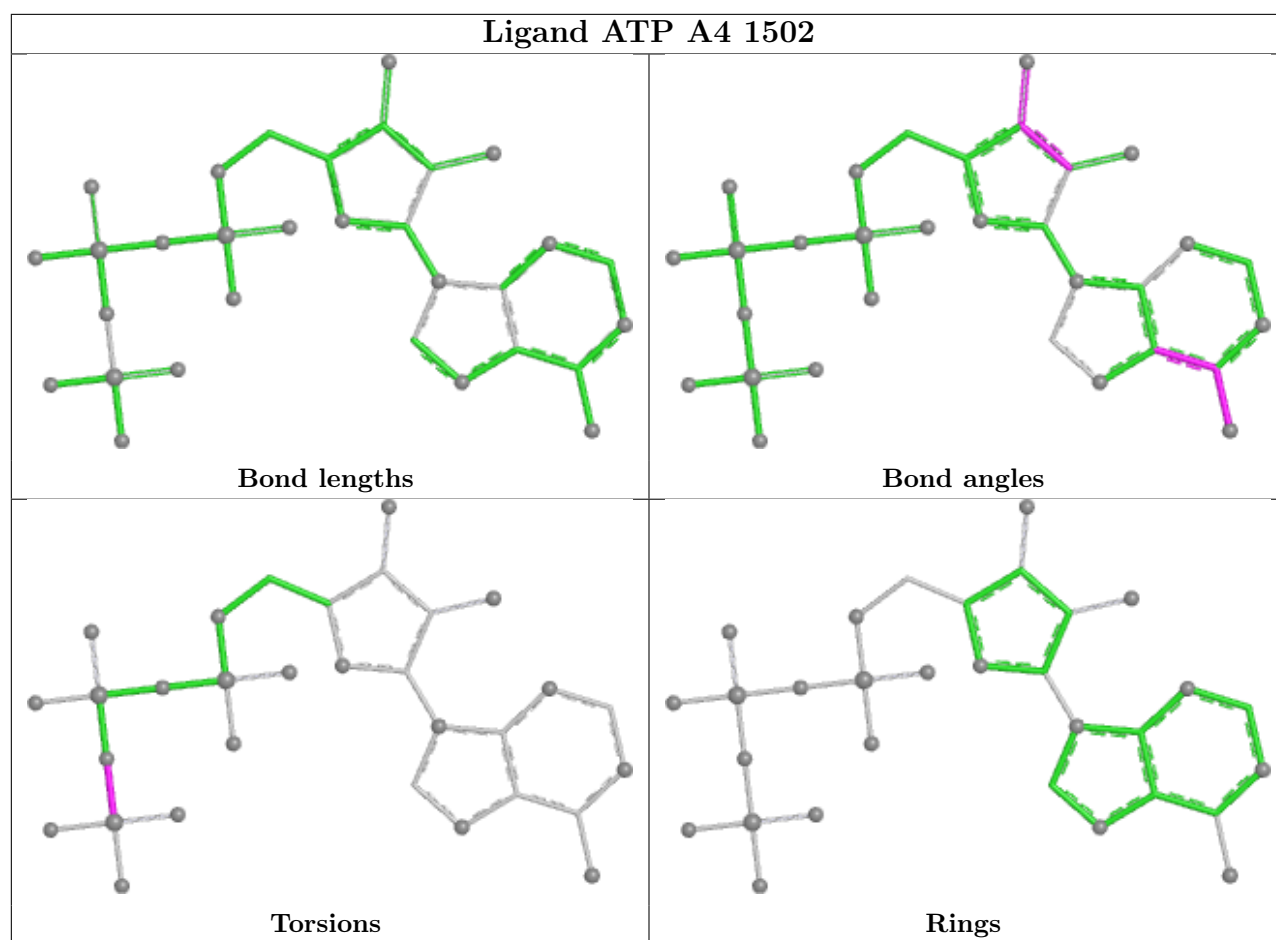
Ligand ATP A1 1502

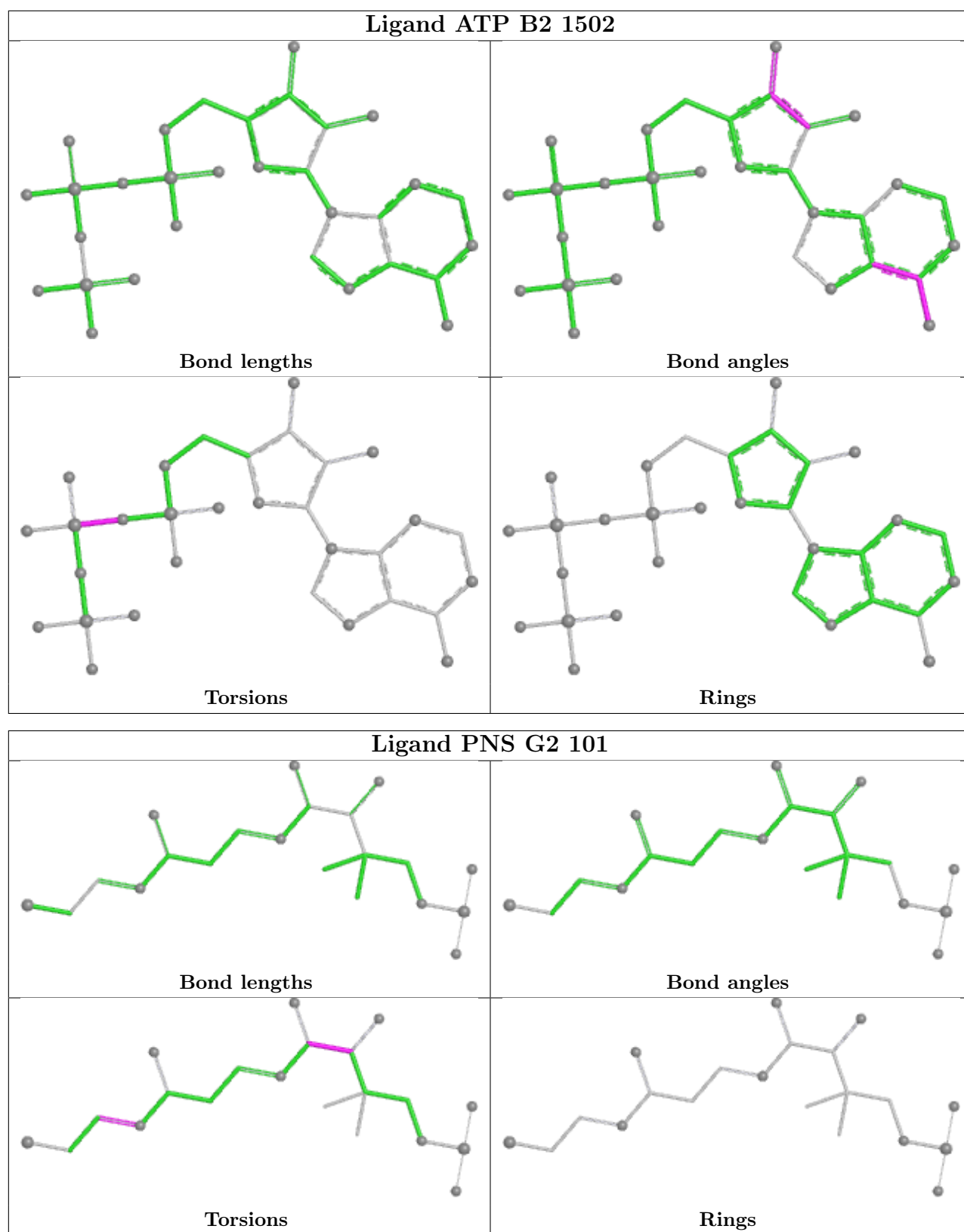


Ligand PNS G1 101









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	D1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D1	119:GLU	C	120:PHE	N	1.63

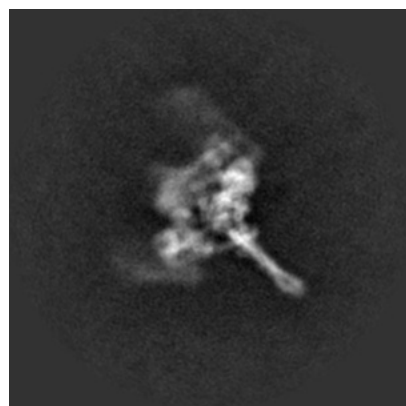
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12662. These allow visual inspection of the internal detail of the map and identification of artifacts.

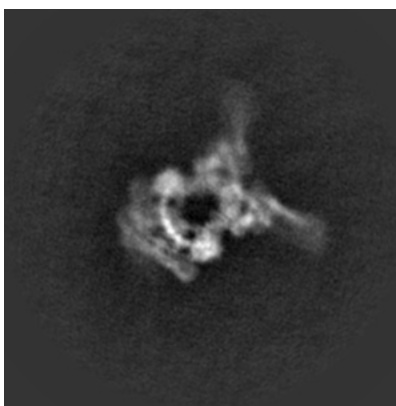
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

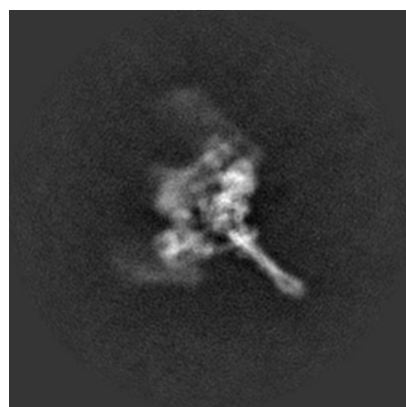


Y

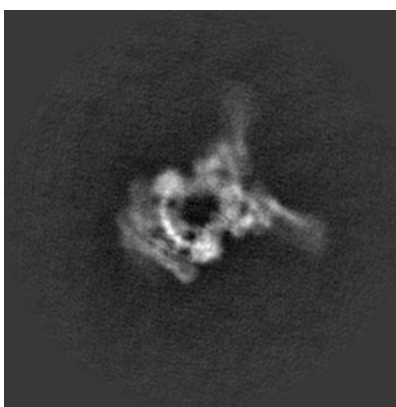


Z

6.1.2 Raw map



X



Y

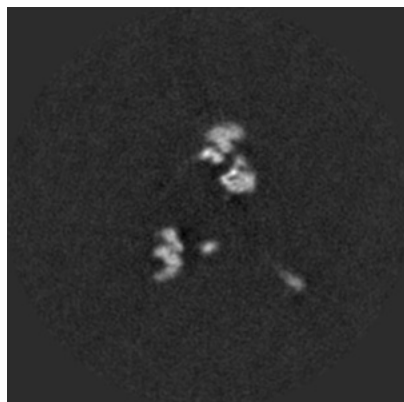


Z

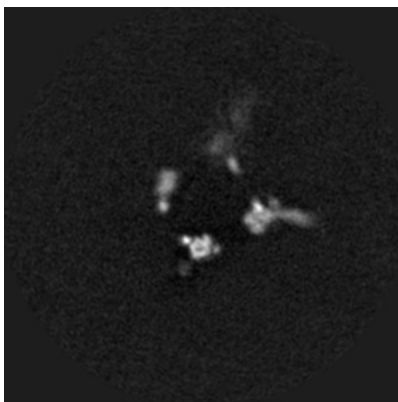
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

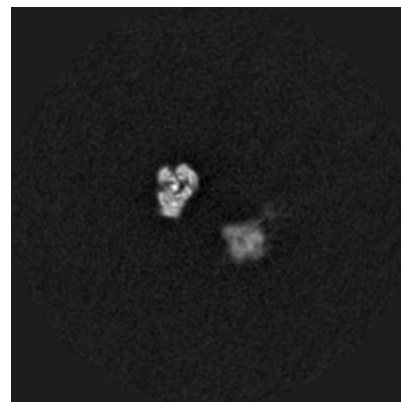
6.2.1 Primary map



X Index: 108

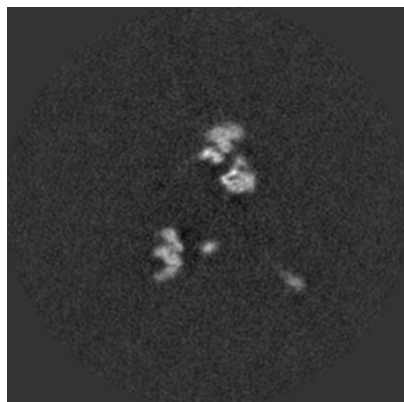


Y Index: 108

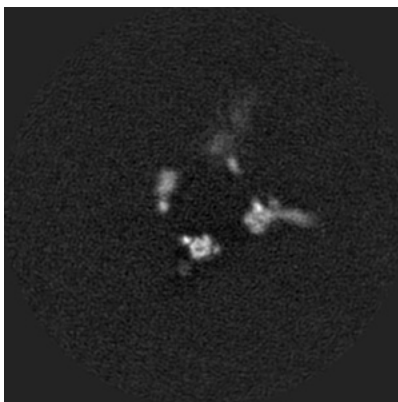


Z Index: 108

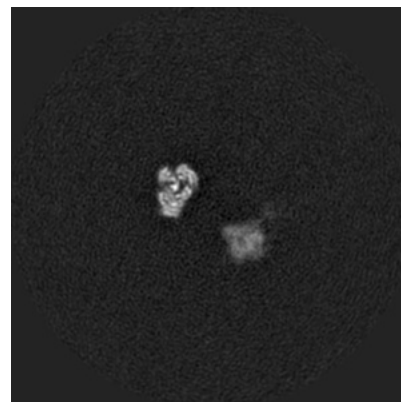
6.2.2 Raw map



X Index: 108



Y Index: 108

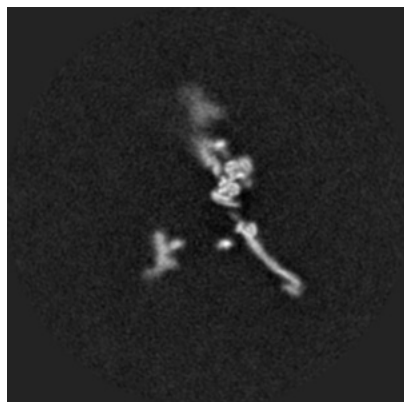


Z Index: 108

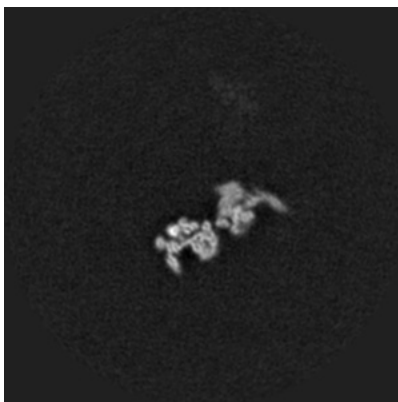
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 100



Y Index: 124

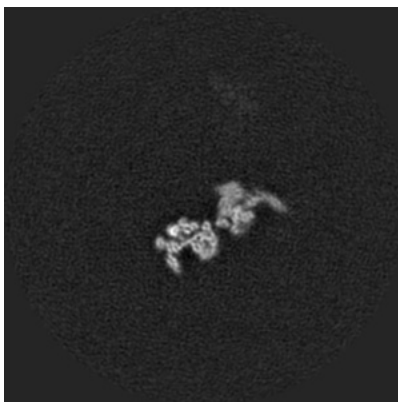


Z Index: 89

6.3.2 Raw map



X Index: 100



Y Index: 124



Z Index: 89

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

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

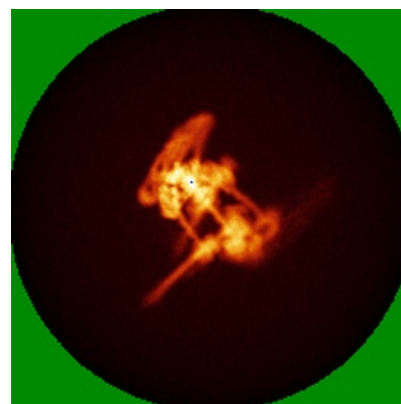
6.4.1 Primary map



X



Y

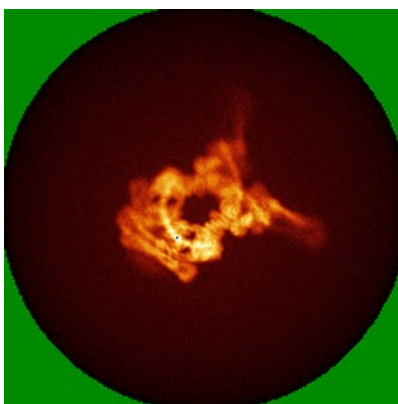


Z

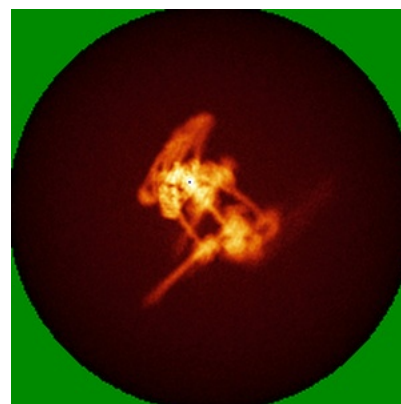
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.017. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

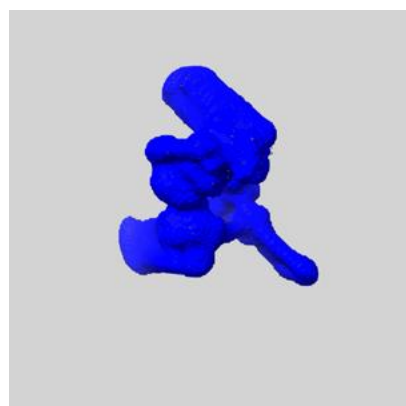
6.6 Mask visualisation [i](#)

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

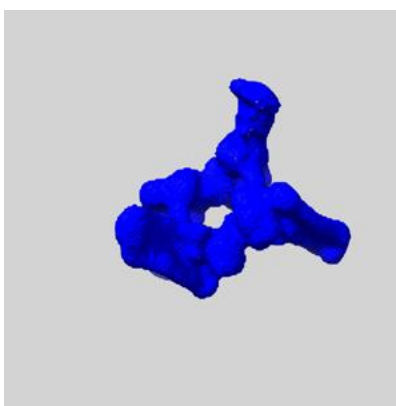
A mask typically either:

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

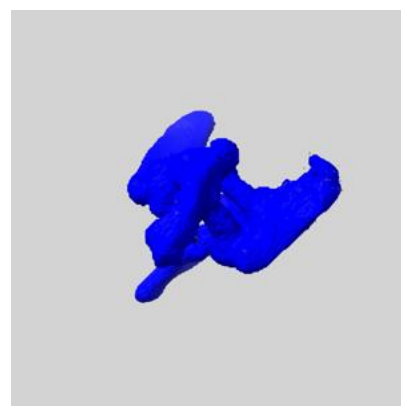
6.6.1 emd_12662_msk_1.map [i](#)



X



Y

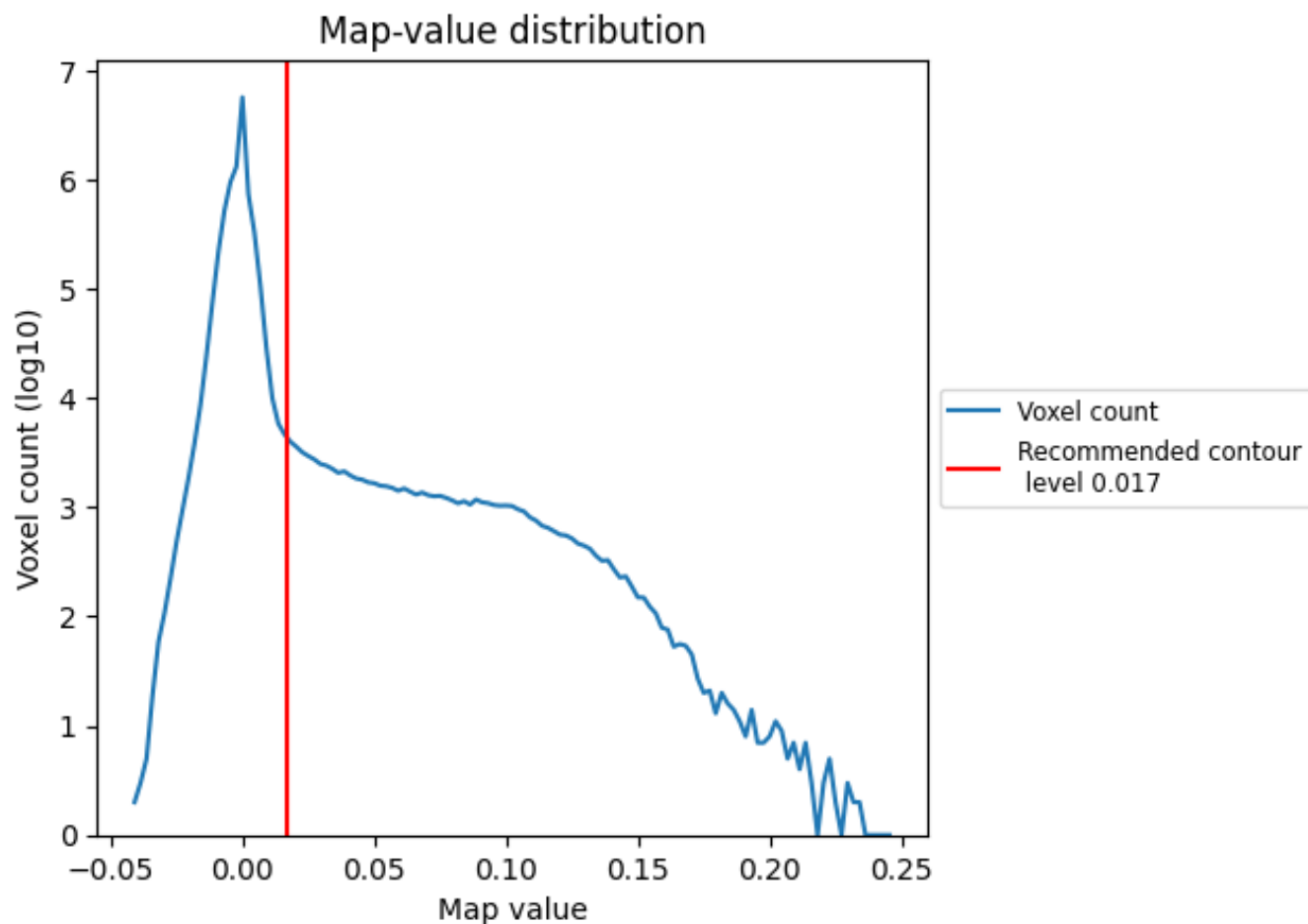


Z

7 Map analysis [i](#)

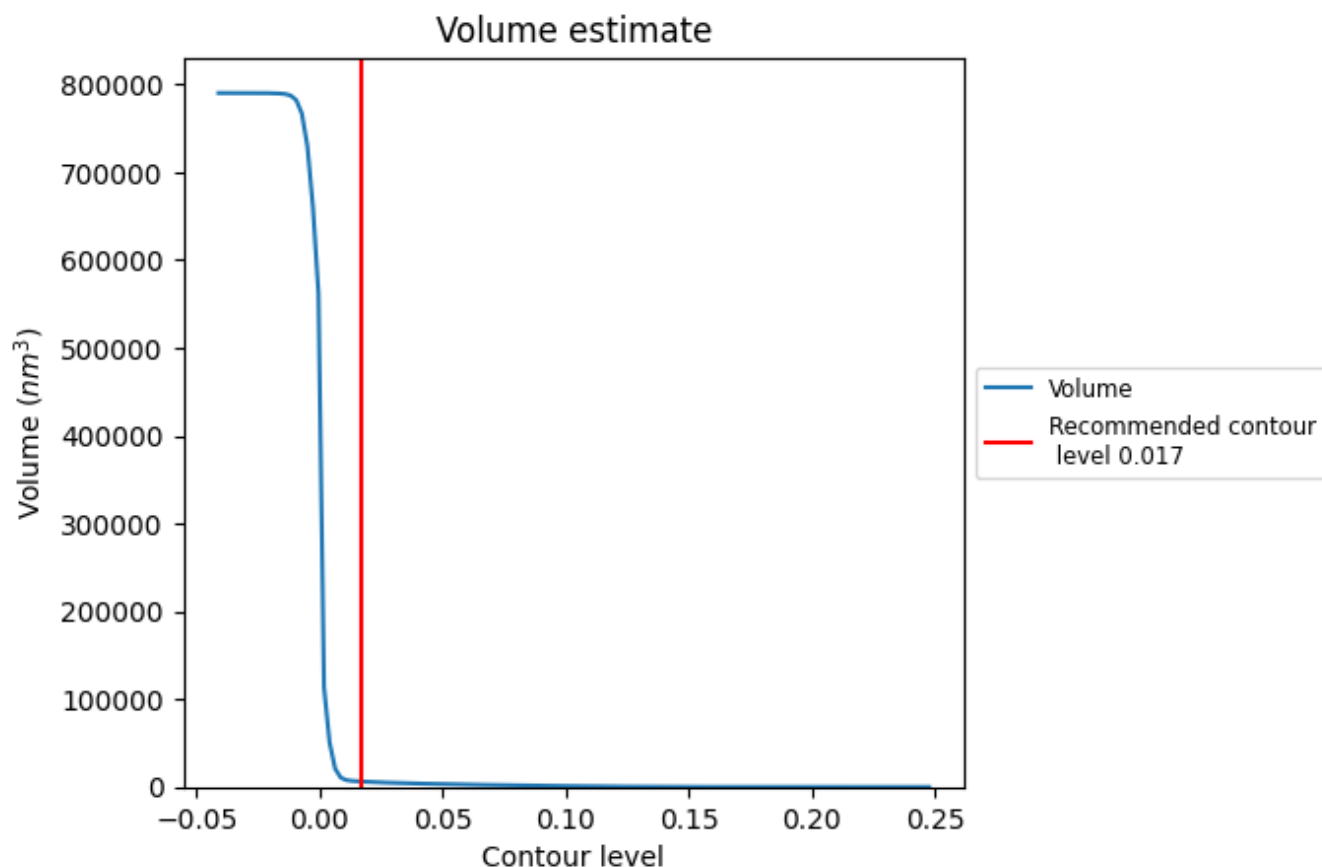
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

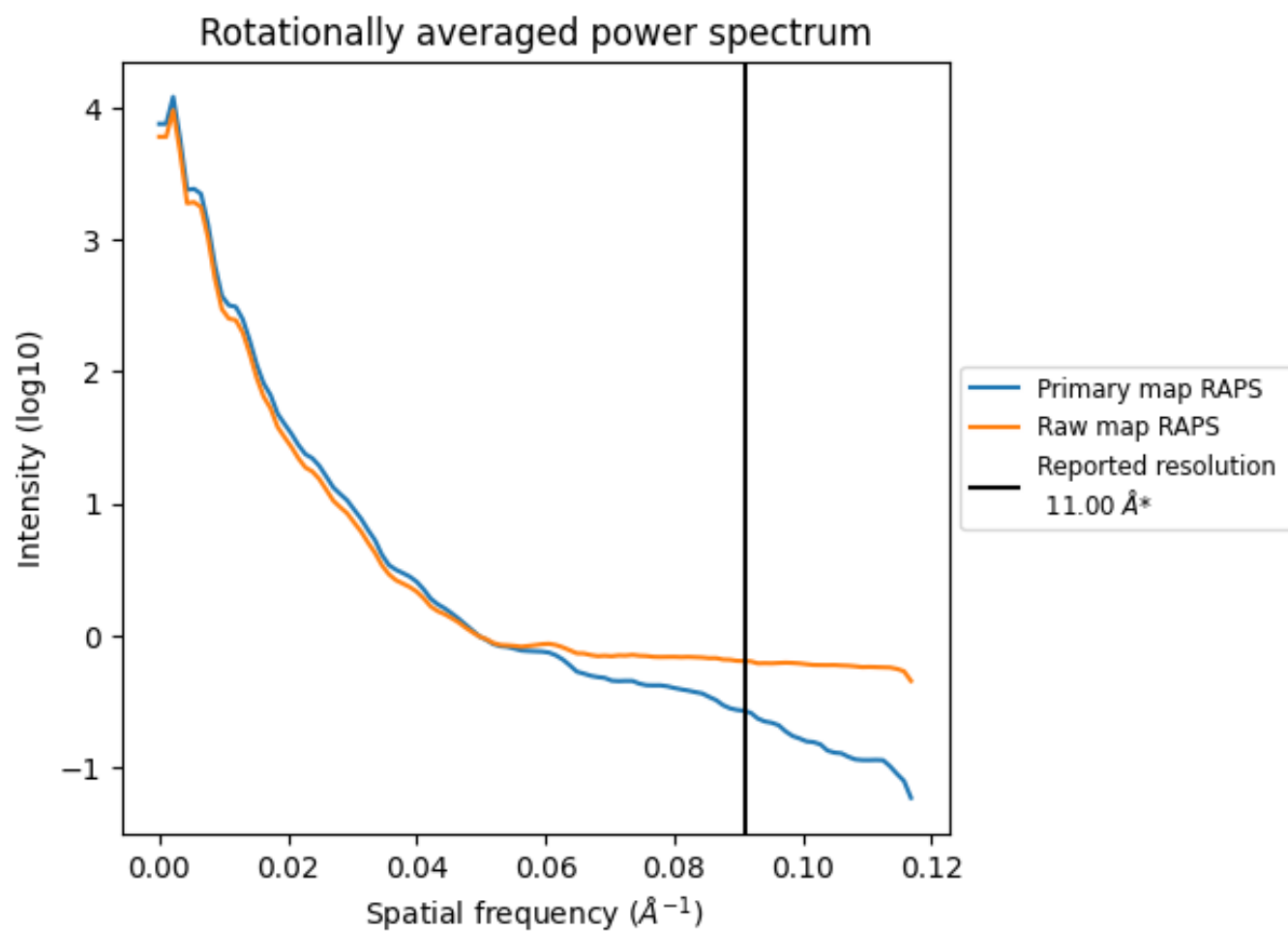
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 6204 nm^3 ; this corresponds to an approximate mass of 5605 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 ⓘ

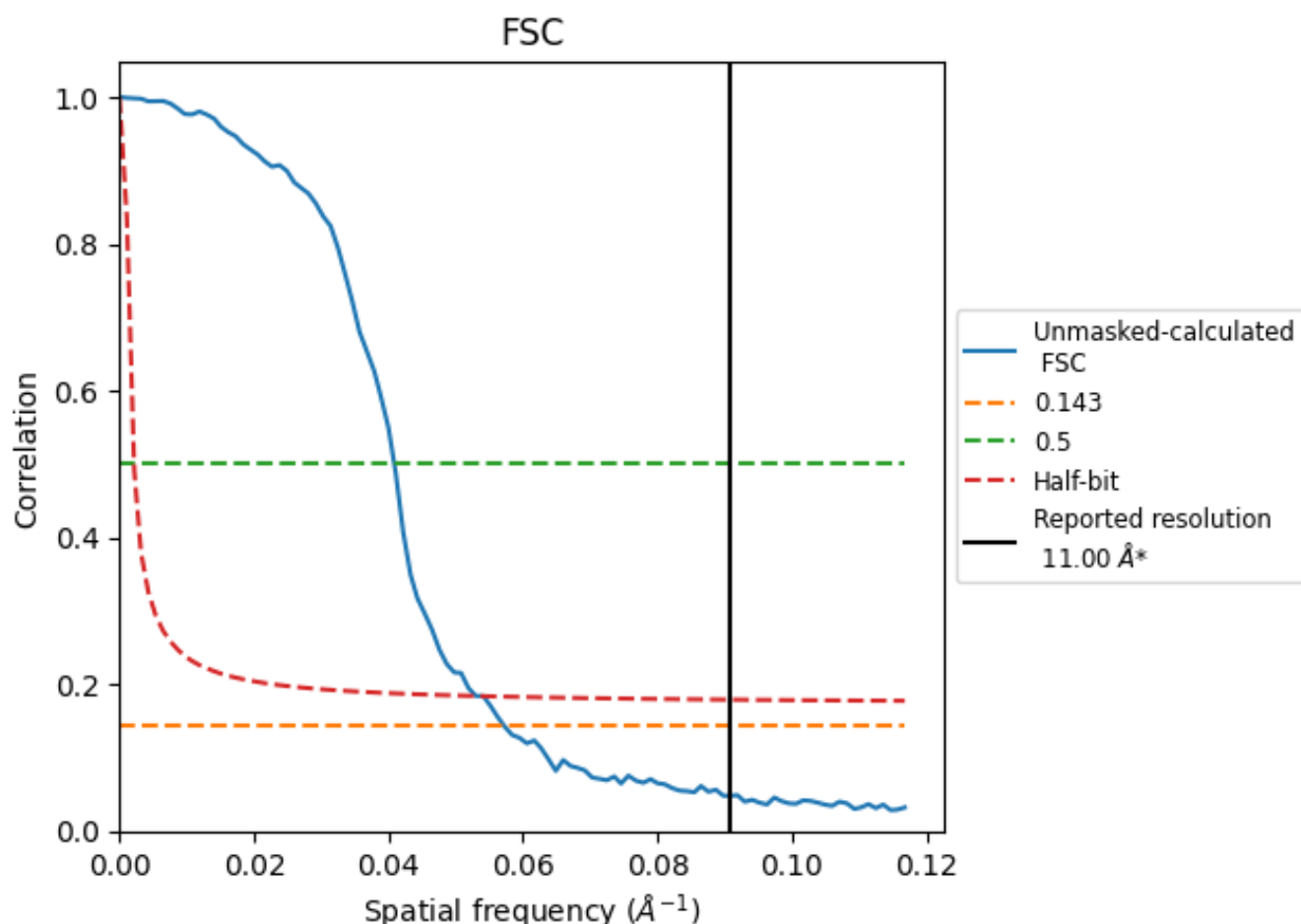


*Reported resolution corresponds to spatial frequency of 0.091 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.091 Å⁻¹

8.2 Resolution estimates [i](#)

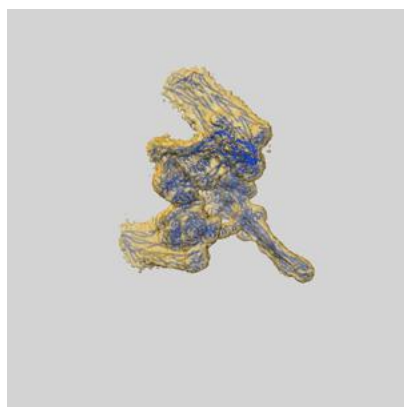
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	11.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	17.48	24.45	18.48

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 17.48 differs from the reported value 11.0 by more than 10 %

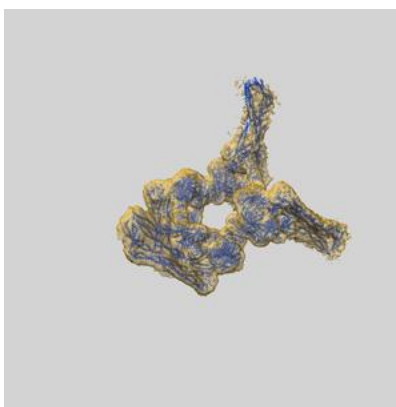
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12662 and PDB model 7NZ2. Per-residue inclusion information can be found in section [3](#) on page [11](#).

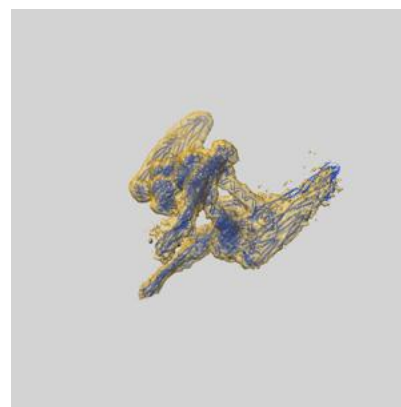
9.1 Map-model overlay [i](#)



X



Y



Z

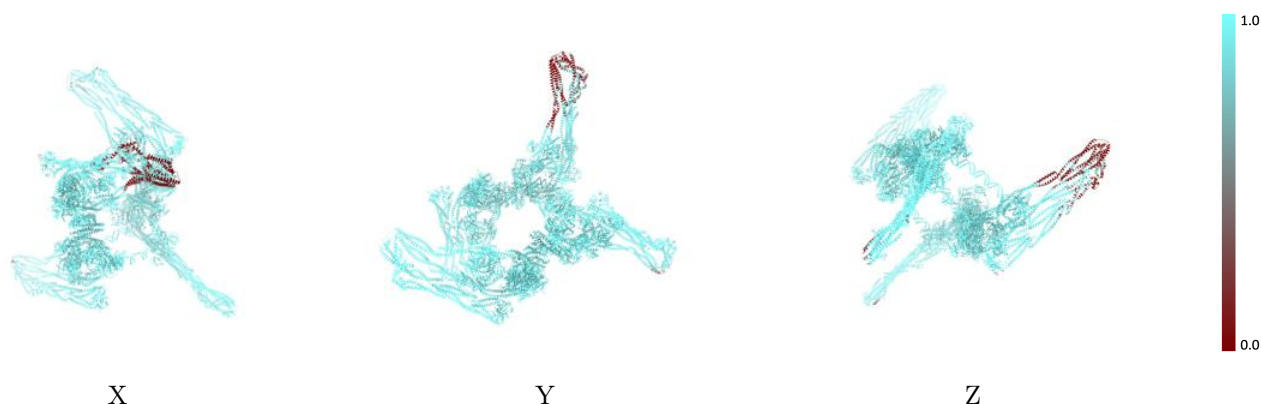
The images above show the 3D surface view of the map at the recommended contour level 0.017 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



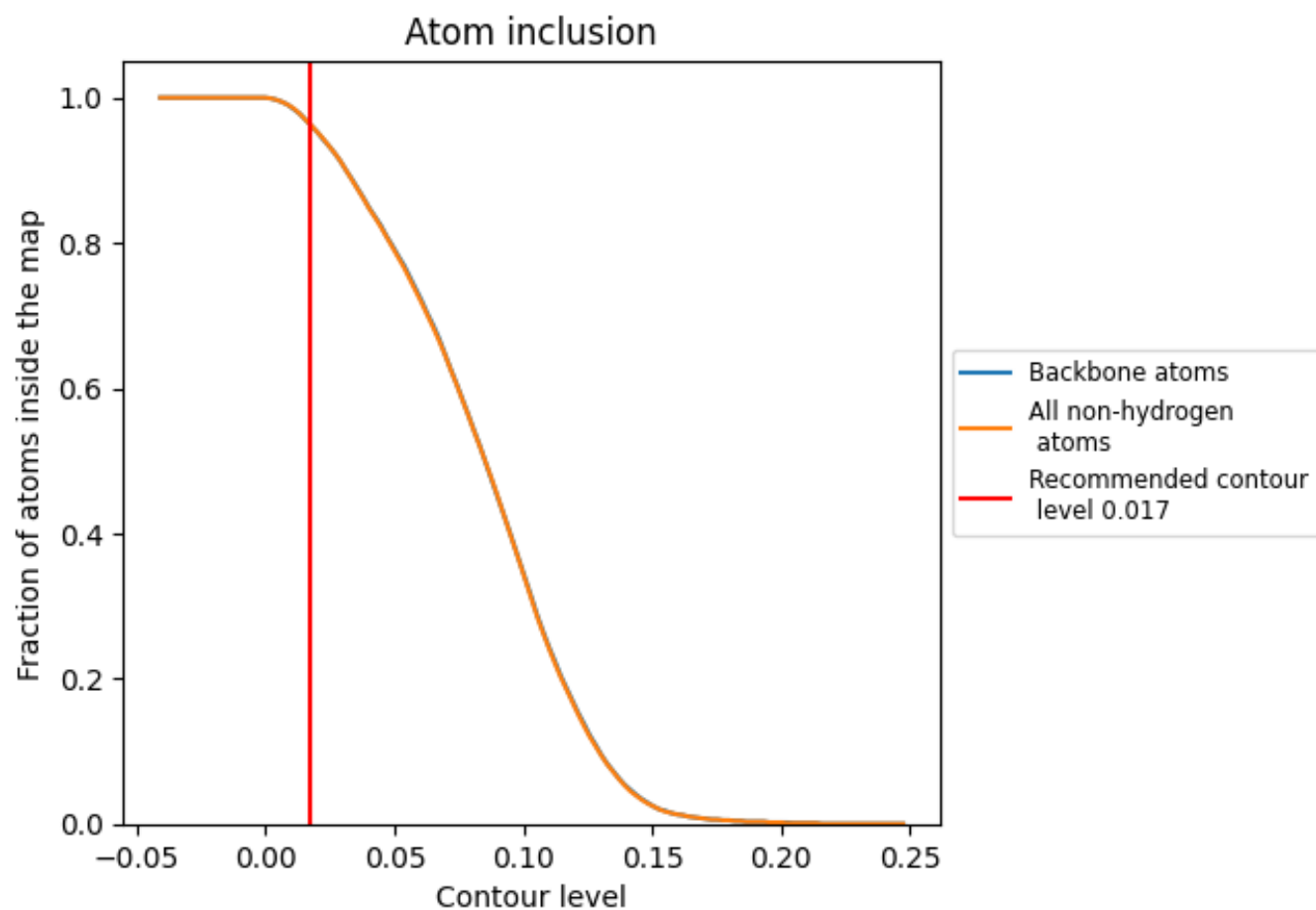
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.017).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ





















The table lists the average atom inclusion at the recommended contour level (0.017) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9640	 0.0870
A1	 1.0000	 0.1200
A2	 0.8050	 0.0360
A3	 0.9870	 0.0740
A4	 0.9840	 0.0800
B1	 1.0000	 0.1160
B2	 0.7990	 0.0440
B3	 0.9930	 0.0760
B4	 0.9880	 0.0840
C1	 1.0000	 0.1250
C2	 1.0000	 0.0670
D1	 1.0000	 0.1110
D2	 1.0000	 0.0880
E1	 1.0000	 0.1250
E2	 0.9990	 0.0580
E3	 1.0000	 0.0890
E4	 1.0000	 0.1120
F1	 0.9990	 0.1220
F2	 0.9990	 0.0640
F3	 0.9970	 0.0820
F4	 0.9990	 0.1010
G1	 1.0000	 0.1280
G2	 0.9780	 0.0670
G3	 0.9900	 0.0550
G4	 0.9930	 0.0840
H1	 1.0000	 0.1100
H2	 1.0000	 0.0500
H3	 1.0000	 0.0770
H4	 1.0000	 0.1000
I1	 1.0000	 0.1260
I2	 1.0000	 0.0400
I3	 1.0000	 0.0900
I4	 1.0000	 0.0850
J1	 1.0000	 0.1240
J2	 1.0000	 0.0590



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Chain	Atom inclusion	Q-score
J3	 1.0000	 0.0880
J4	 1.0000	 0.0870
K1	 1.0000	 0.1370
K2	 1.0000	 0.1200
L1	 1.0000	 0.1360
L2	 1.0000	 0.1240
M1	 1.0000	 0.1340
M2	 1.0000	 0.1100
N1	 1.0000	 0.1420
N2	 1.0000	 0.1060