wwPDB EM Validation Summary Report (i)

Dec 5, 2022 – 02:24 PM EST

PDB ID	:	8EA4
EMDB ID	:	EMD-27972
Title	:	V-K CAST Transpososome from Scytonema hofmanni, minor configuration
Authors	:	Rizo, A.R.; Park, J.-U.; Tsai, A.W.; Kellogg, E.K.
Deposited on	:	2022-08-27
Resolution	:	3.00 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 (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:

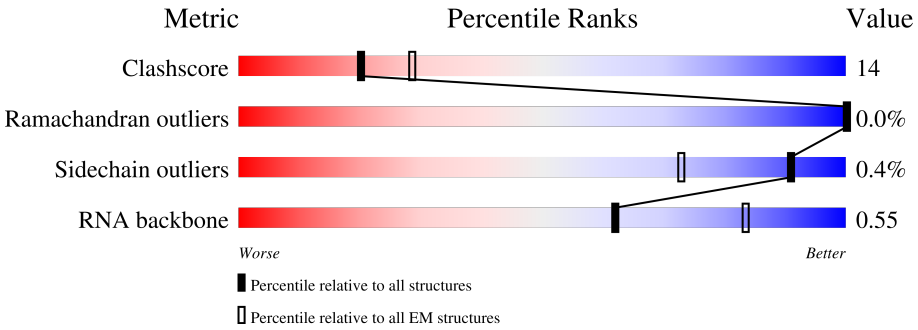
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	276	6%, 79%, 13%, 7%
1	B	276	82%, 10%, 7%
1	C	276	82%, 11%, 7%
1	D	276	81%, 12%, 7%
1	E	276	81%, 12%, 7%
1	F	276	81%, 12%, 7%
1	G	276	78%, 15%, 7%

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Mol	Chain	Length	Quality of chain
1	H	276	82% 11% 7%
1	I	276	80% 13% 7%
1	J	276	80% 13% 7%
1	K	276	80% 13% 7%
1	L	276	80% 12% 7%
1	M	276	11% 81% 12% 7%
2	O	639	11% 80% 14% 6%
3	Q	167	83% 14%
4	S	89	87% 10%
5	W	584	12% 72% 16% 12%
5	X	584	22% 72% 13% 13%
5	Y	584	17% 45% 7% 48%
5	Z	584	22% 45% 6% 48%
5	w	584	98%
5	x	584	98%
5	y	584	98%
5	z	584	98%
6	1	141	23% 44% 30%
7	2	51	24% 27% 45%
8	3	71	18% 46% 32%
9	4	75	24% 39% 36%
10	5	50	12% 44% 44%
11	6	20	45% 25% 5% 25%
12	7	265	5% 44% 30% 11% 13%

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	ATP	I	302	-	-	X	-
14	ATP	M	302	-	-	X	-

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 58049 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called TnsC.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		
1	B	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		
1	C	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		
1	D	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		
1	E	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		
1	F	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		
1	G	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		
1	H	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		
1	I	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		
1	J	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		
1	K	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		
1	L	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		
1	M	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		

- Molecule 2 is a protein called Cas12k.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	O	601	Total	C	N	O	S	0	0
			4865	3069	881	900	15		

- Molecule 3 is a protein called TniQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Q	164	Total	C	N	O	S	0	0
			1306	832	240	220	14		

- Molecule 4 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	S	87	Total	C	N	O	S	0	0
			702	433	140	128	1		

- Molecule 5 is a protein called TnsB.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	W	514	Total	C	N	O	S	0	0
			4122	2570	760	780	12		
5	X	507	Total	C	N	O	S	0	0
			4068	2537	748	771	12		
5	Y	304	Total	C	N	O	S	0	0
			2453	1537	449	457	10		
5	Z	301	Total	C	N	O	S	0	0
			2426	1522	442	452	10		
5	w	14	Total	C	N	O		0	0
			129	83	19	27			
5	x	14	Total	C	N	O		0	0
			129	83	19	27			
5	y	14	Total	C	N	O		0	0
			129	83	19	27			
5	z	14	Total	C	N	O		0	0
			129	83	19	27			

- Molecule 6 is a DNA chain called Target-LE.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1	98	Total	C	N	O	P	0	0
			2010	961	368	583	98		

- Molecule 7 is a DNA chain called LE_R.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	2	28	Total	C	N	O	P	0	0
			573	275	103	168	27		

- Molecule 8 is a DNA chain called Non-target_R.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	3	48	Total 980	C 470	N 169	O 293	P 48	0	0

- Molecule 9 is a DNA chain called RE_F.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	4	48	Total 982	C 468	N 183	O 283	P 48	0	0

- Molecule 10 is a DNA chain called RE_R1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	5	28	Total 573	C 277	N 98	O 171	P 27	0	0

- Molecule 11 is a DNA chain called RE_R2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	6	15	Total 301	C 144	N 54	O 89	P 14	0	0

- Molecule 12 is a RNA chain called sg_RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	7	230	Total 4896	C 2187	N 863	O 1616	P 230	0	0

- Molecule 13 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
13	A	1	Total 1	Mg 1	0
13	B	1	Total 1	Mg 1	0
13	C	1	Total 1	Mg 1	0
13	D	1	Total 1	Mg 1	0
13	E	1	Total 1	Mg 1	0
13	F	1	Total 1	Mg 1	0

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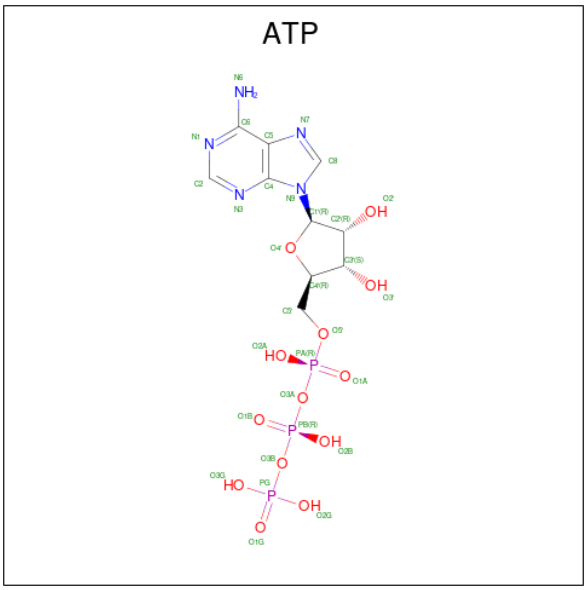
Mol	Chain	Residues	Atoms	AltConf
13	G	1	Total Mg 1 1	0
13	H	1	Total Mg 1 1	0
13	I	1	Total Mg 1 1	0
13	J	1	Total Mg 1 1	0
13	K	1	Total Mg 1 1	0
13	L	1	Total Mg 1 1	0
13	M	1	Total Mg 1 1	0
13	W	1	Total Mg 1 1	0
13	X	1	Total Mg 1 1	0

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



Mol	Chain	Residues	Atoms	AltConf
14	A	1	Total C N O P 31 10 5 13 3	0
14	B	1	Total C N O P 31 10 5 13 3	0

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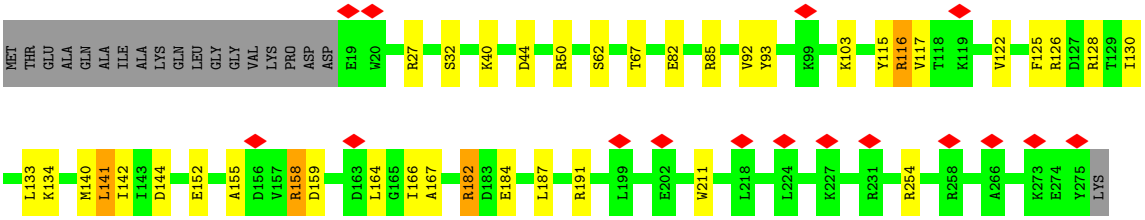
Mol	Chain	Residues	Atoms					AltConf
14	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
14	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
14	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
14	F	1	Total	C	N	O	P	0
			31	10	5	13	3	
14	G	1	Total	C	N	O	P	0
			31	10	5	13	3	
14	H	1	Total	C	N	O	P	0
			31	10	5	13	3	
14	I	1	Total	C	N	O	P	0
			31	10	5	13	3	
14	J	1	Total	C	N	O	P	0
			31	10	5	13	3	
14	K	1	Total	C	N	O	P	0
			31	10	5	13	3	
14	L	1	Total	C	N	O	P	0
			31	10	5	13	3	
14	M	1	Total	C	N	O	P	0
			31	10	5	13	3	

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.

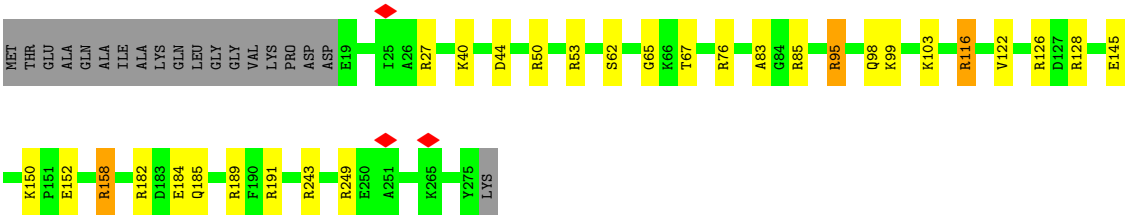
- Molecule 1: TnsC

Chain A:



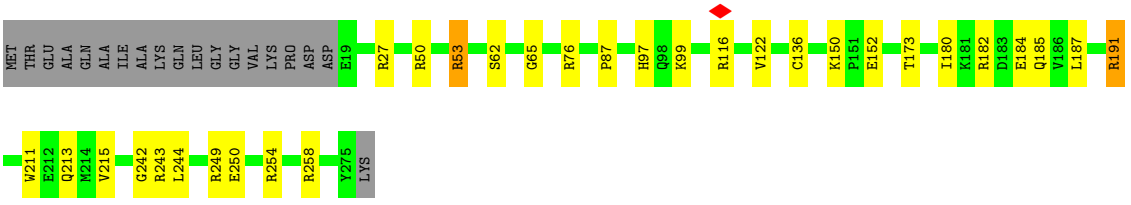
- Molecule 1: TnsC

Chain B:



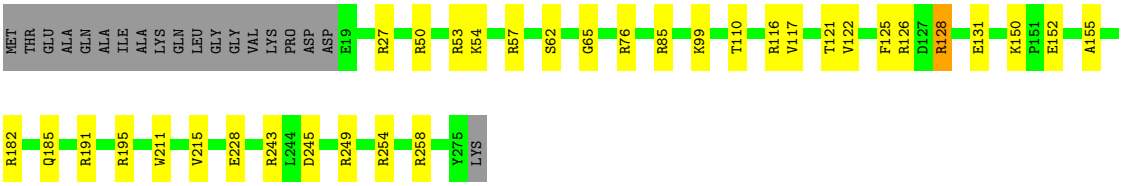
- Molecule 1: TnsC

Chain C:



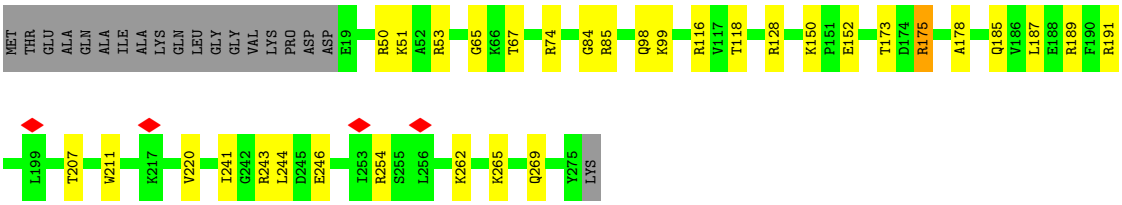
- Molecule 1: TnsC

Chain D:



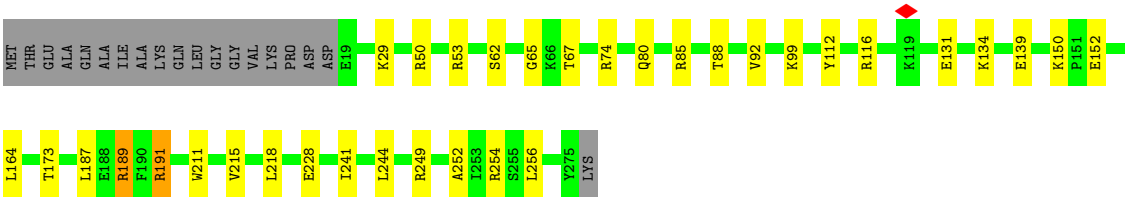
• Molecule 1: TnsC

Chain E:



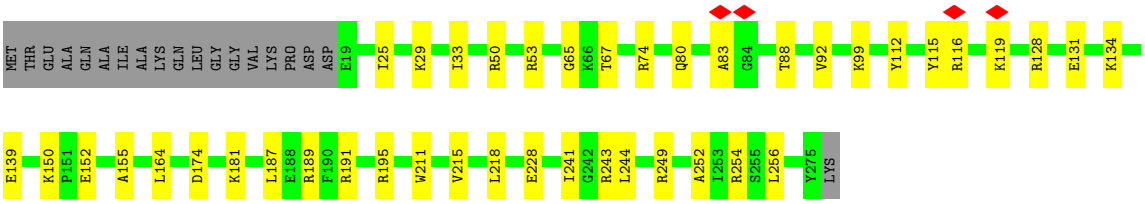
• Molecule 1: TnsC

Chain F:



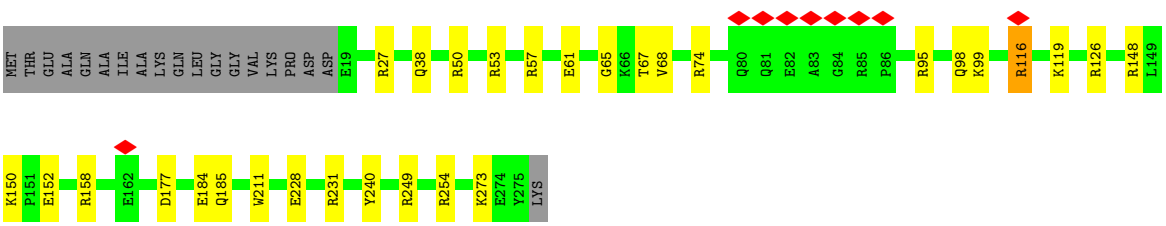
• Molecule 1: TnsC

Chain G:



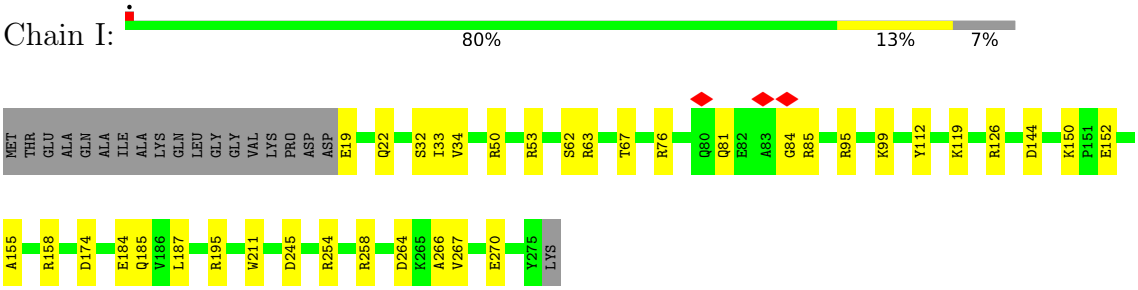
• Molecule 1: TnsC

Chain H:



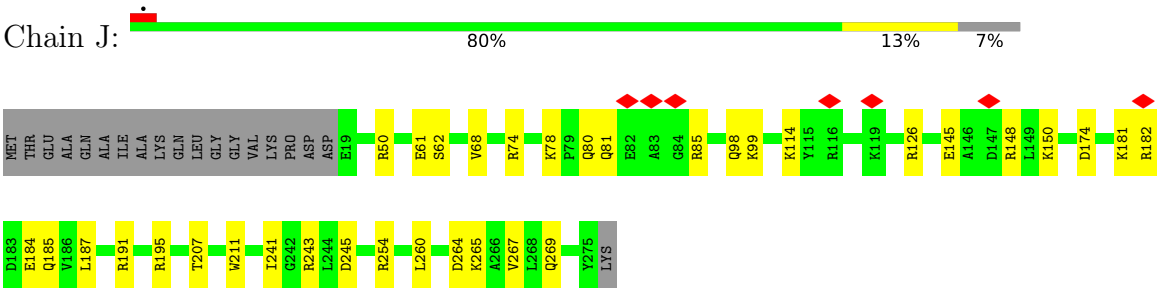
• Molecule 1: TnsC

Chain I:



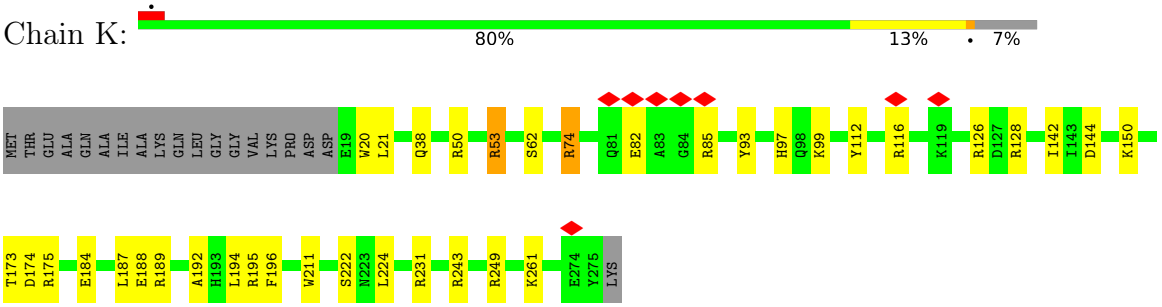
• Molecule 1: TnsC

Chain J:



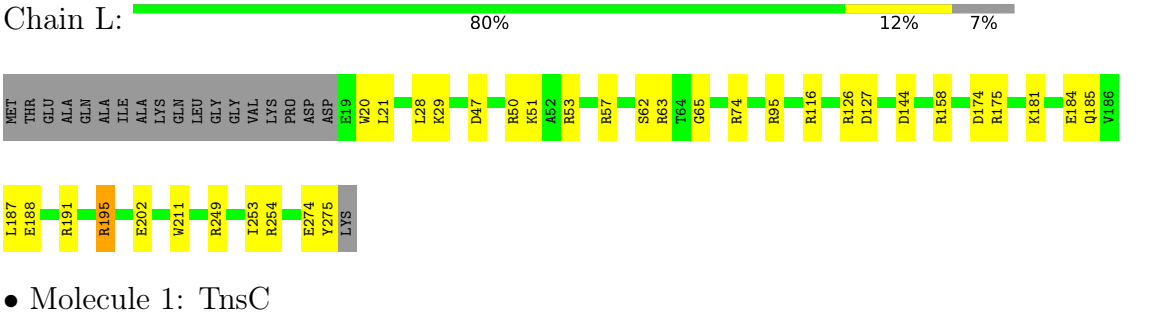
• Molecule 1: TnsC

Chain K:



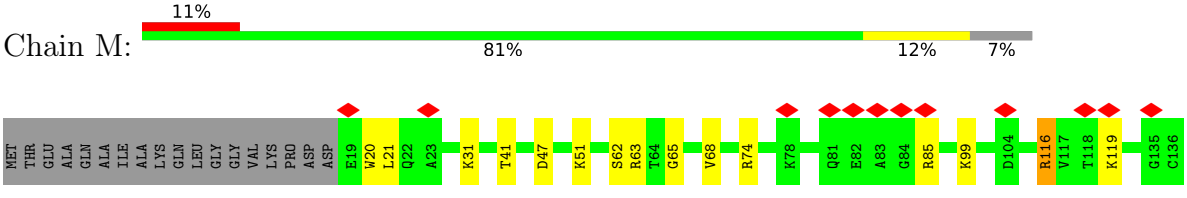
• Molecule 1: TnsC

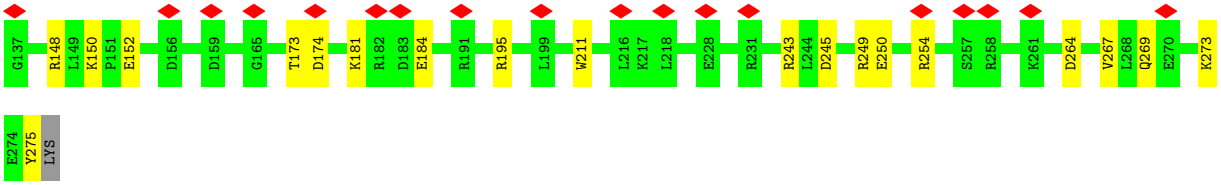
Chain L:



• Molecule 1: TnsC

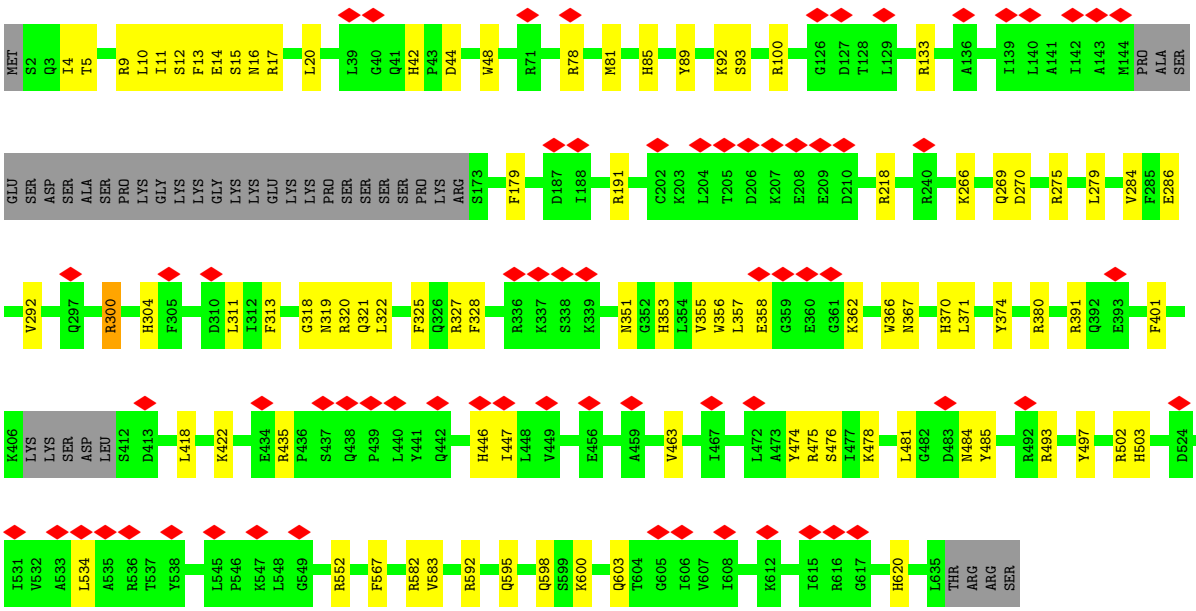
Chain M:





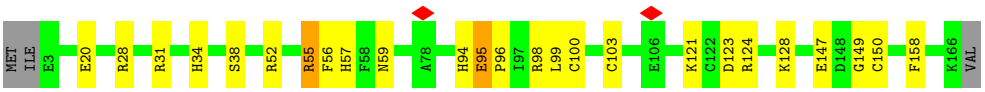
• Molecule 2: Cas12k

Chain O:



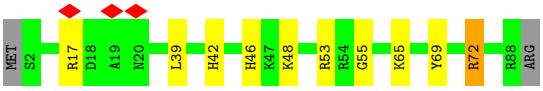
• Molecule 3: TniQ

Chain Q:



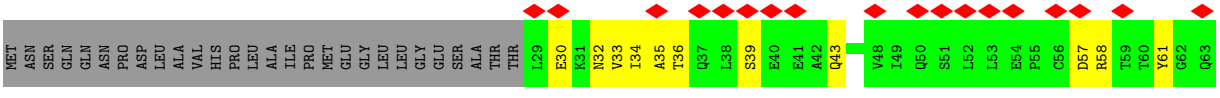
• Molecule 4: 30S ribosomal protein S15

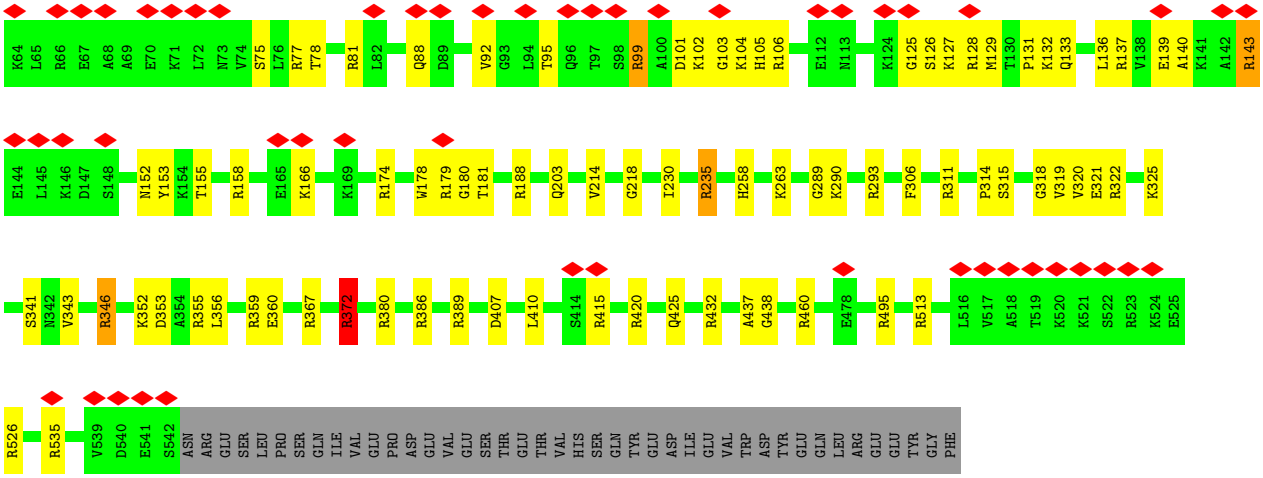
Chain S:



• Molecule 5: TnsB

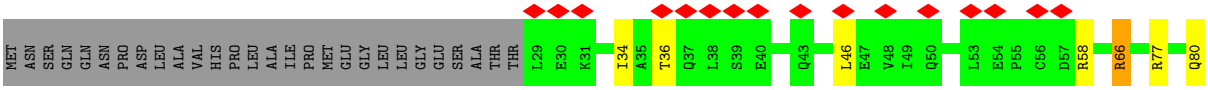
Chain W:

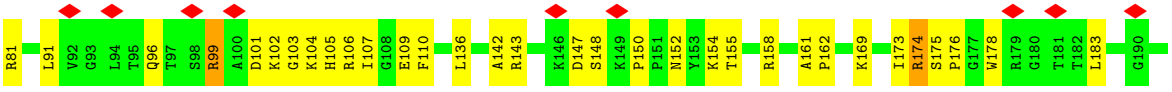


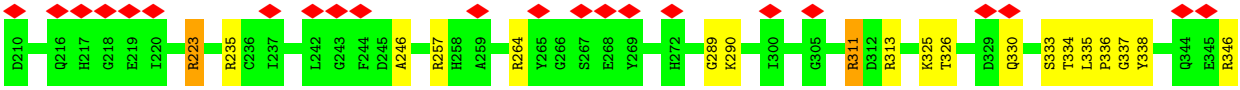


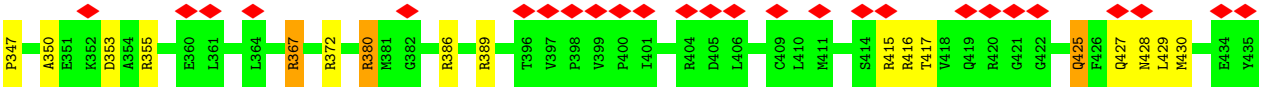
• Molecule 5: TnsB

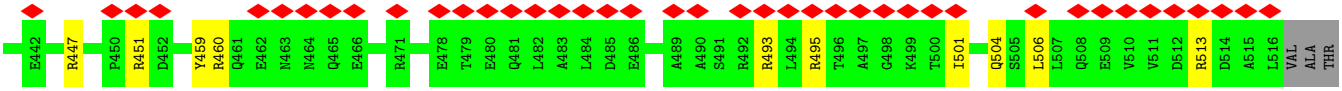
Chain X:

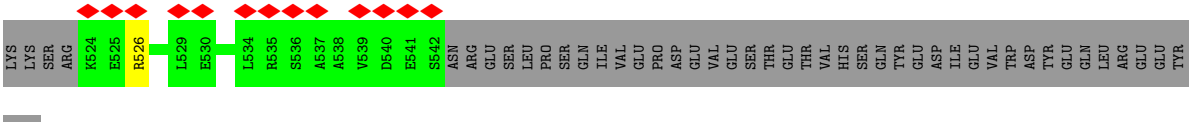






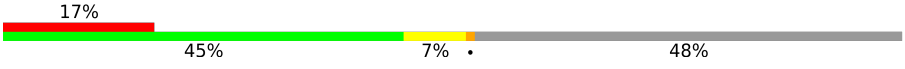


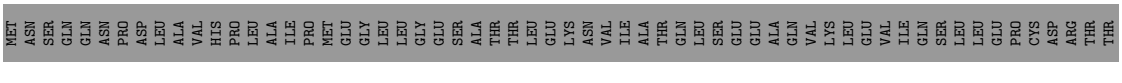


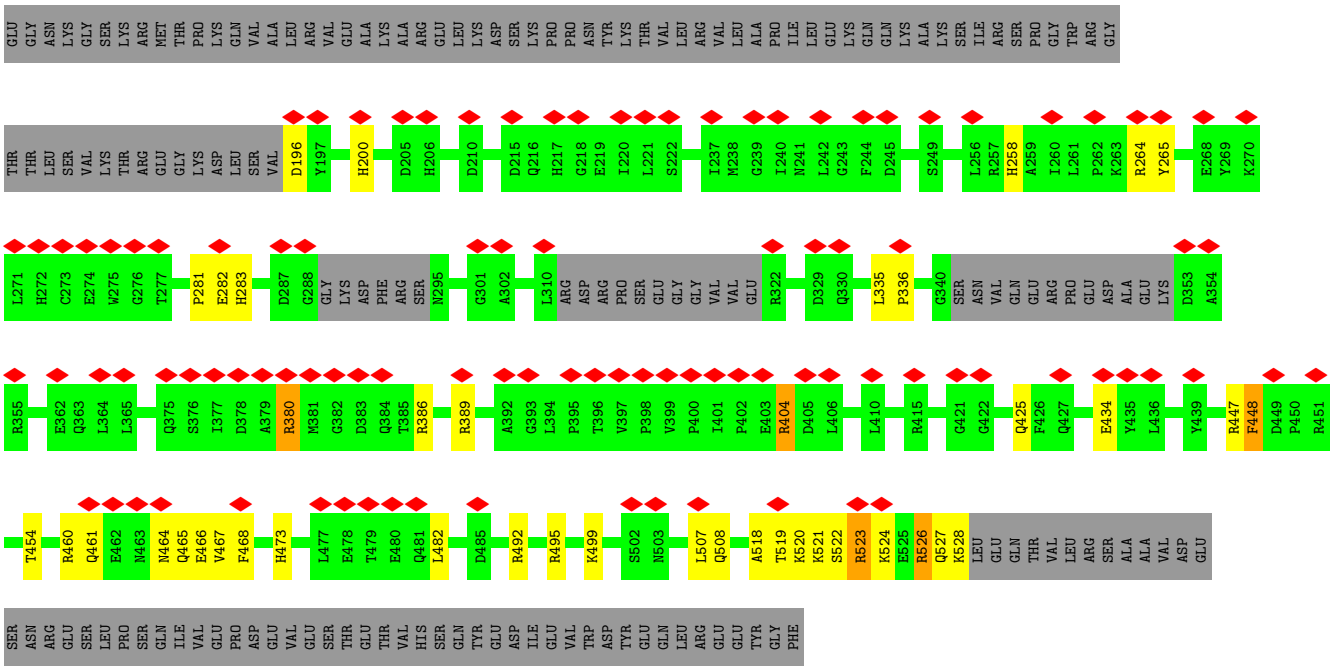


• Molecule 5: TnsB

Chain Y:

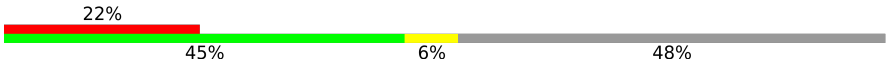


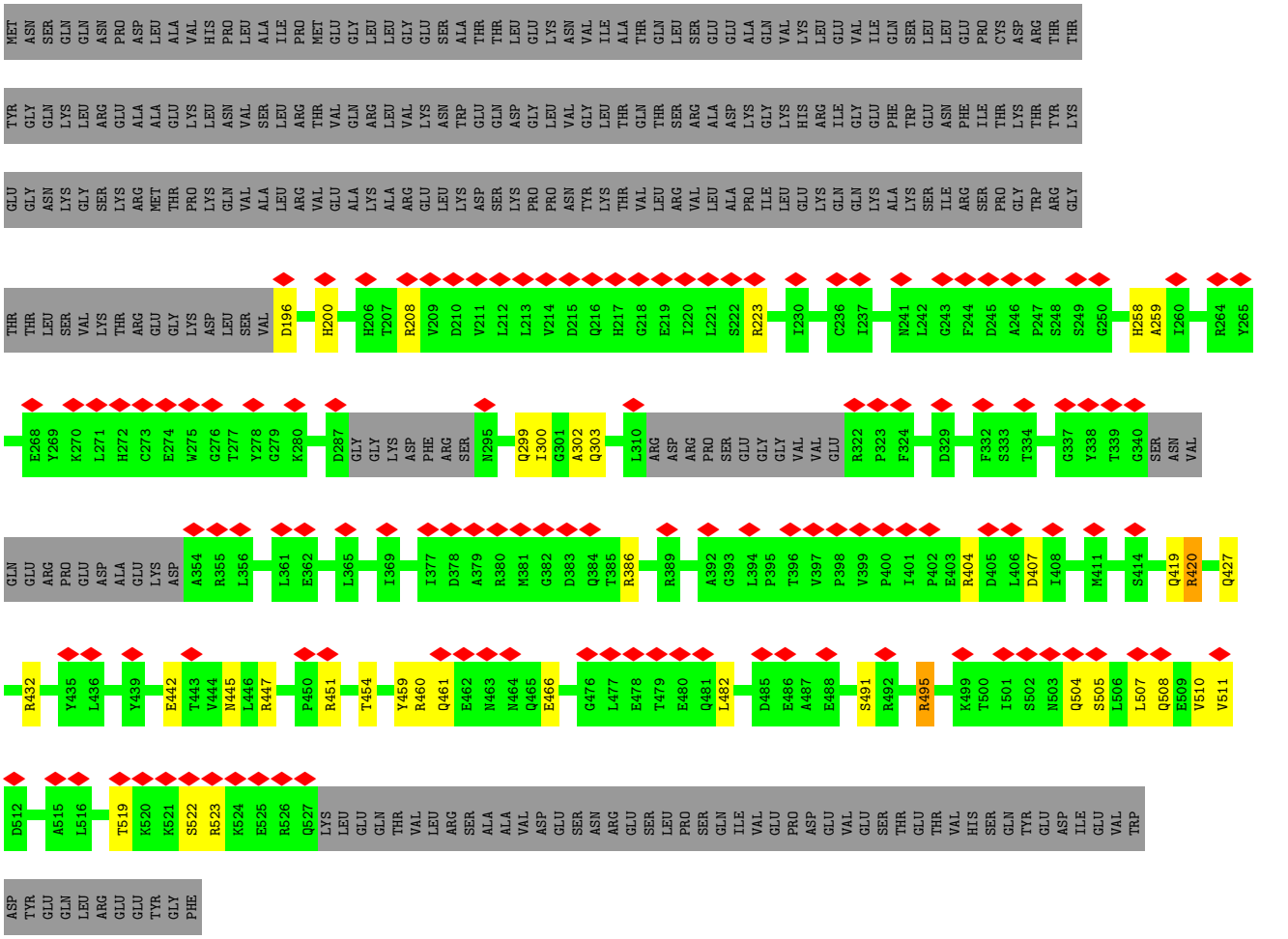




• Molecule 5: TnsB

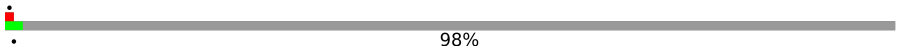
Chain Z:

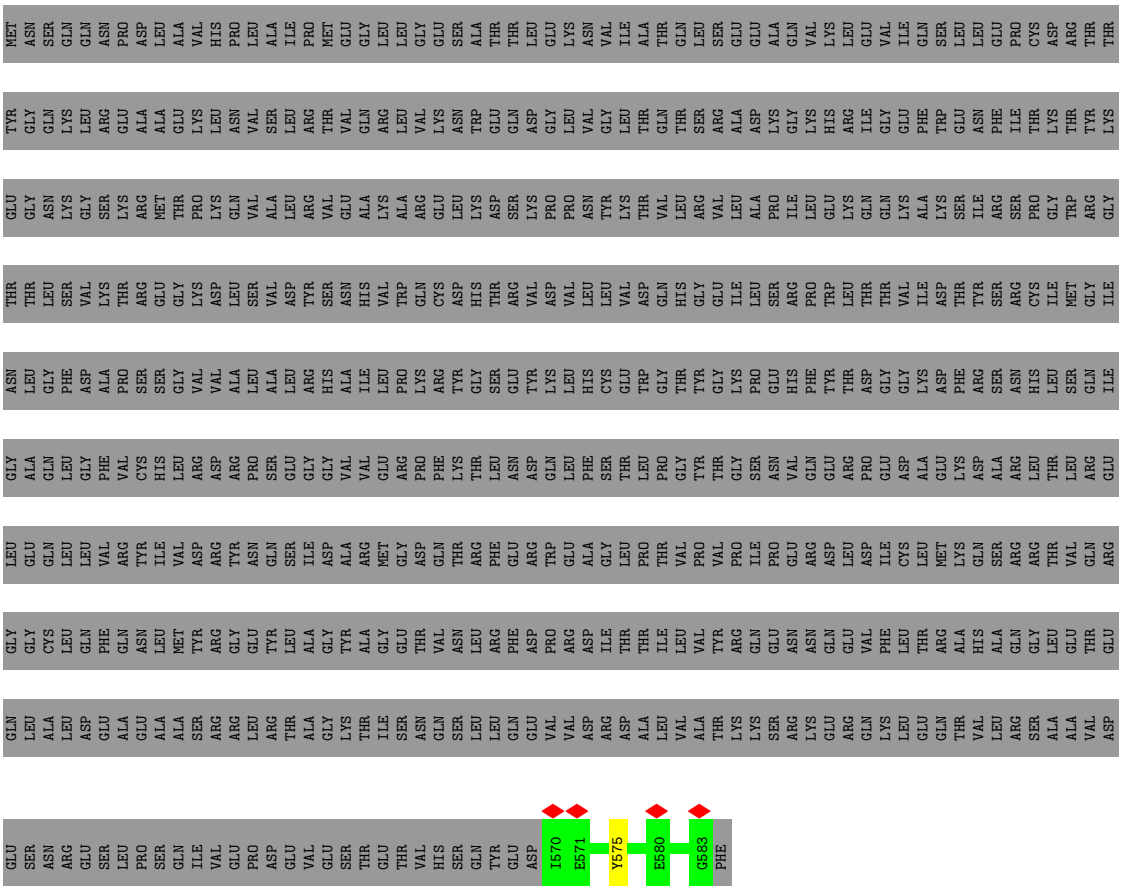




• Molecule 5: TnsB

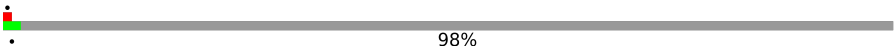
Chain w:

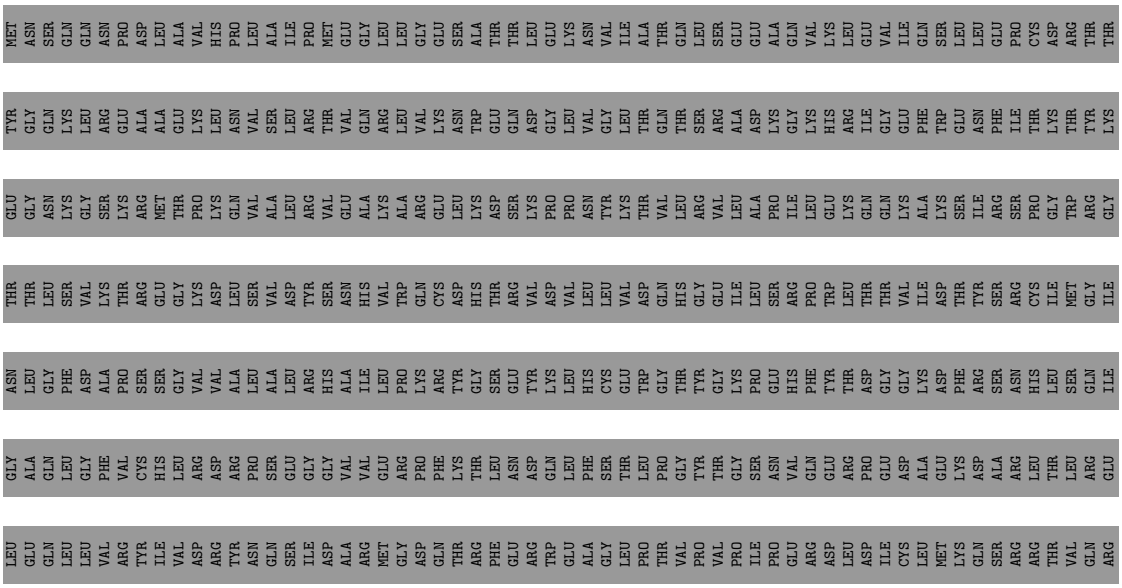


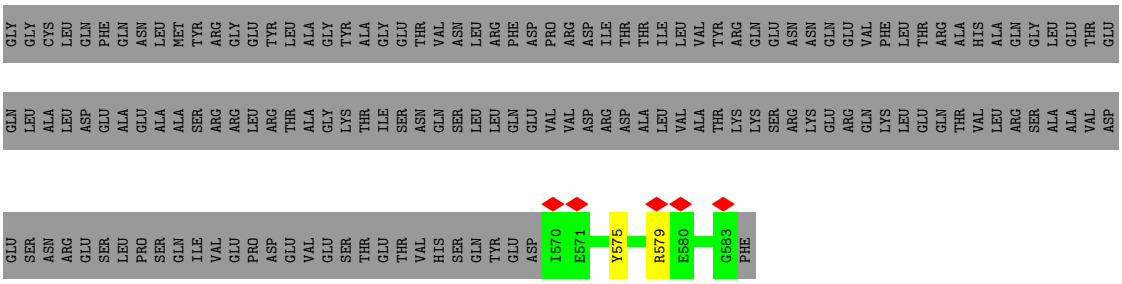


• Molecule 5: TnsB

Chain x:

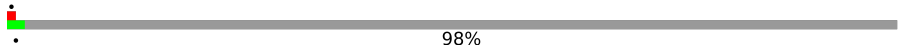


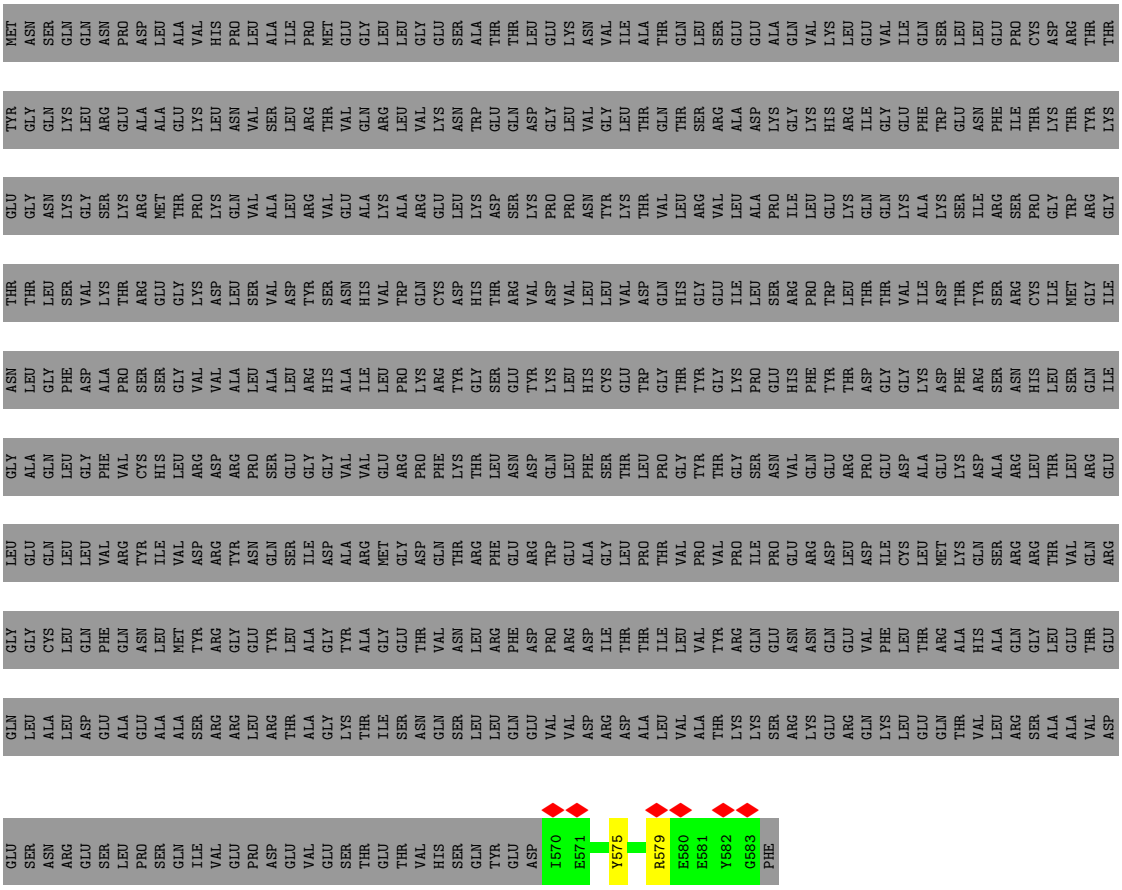




• Molecule 5: TnsB

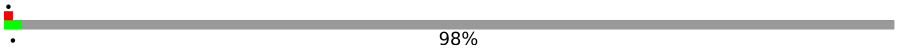
Chain y:

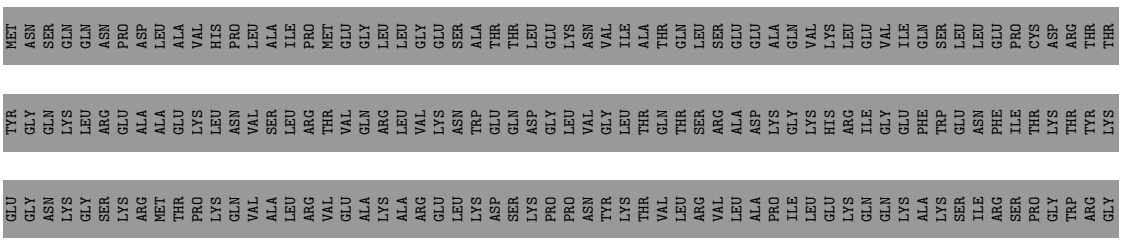


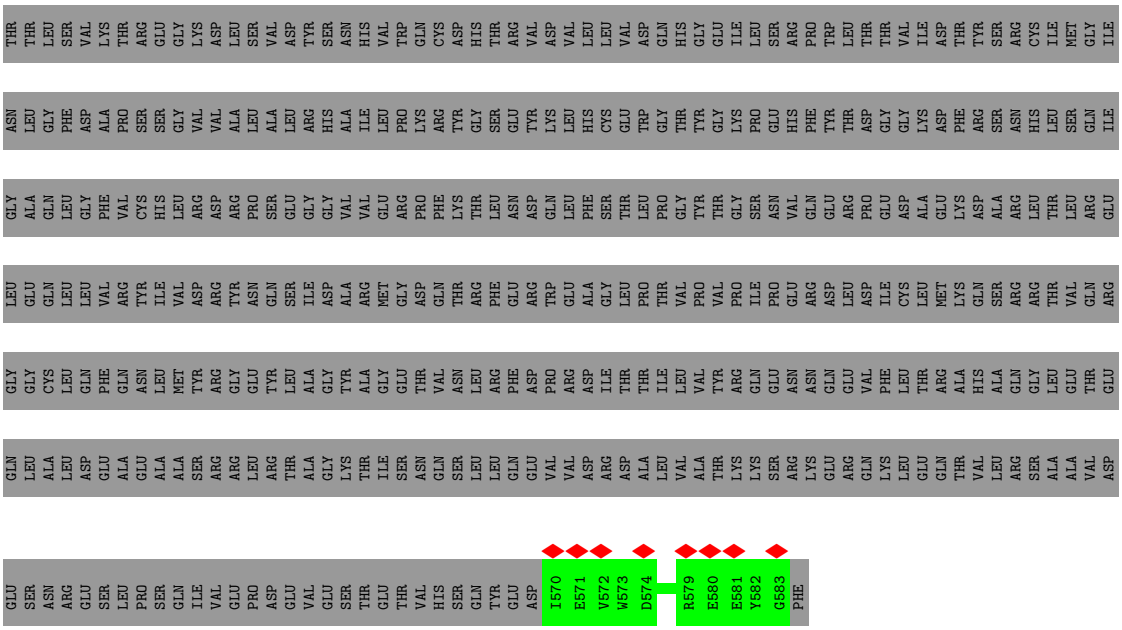


• Molecule 5: TnsB

Chain z:

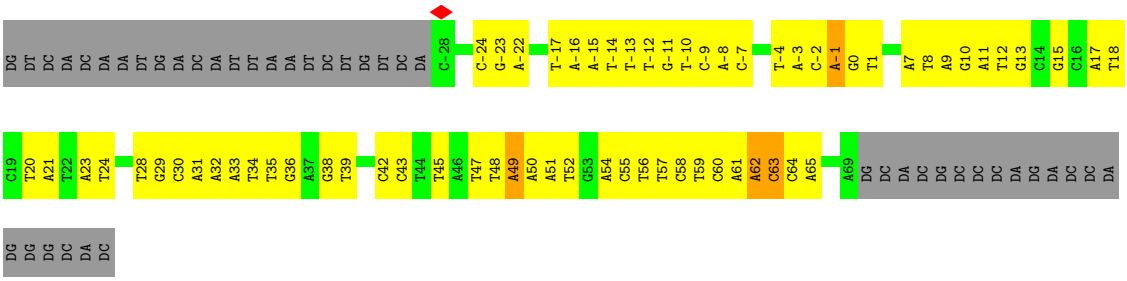






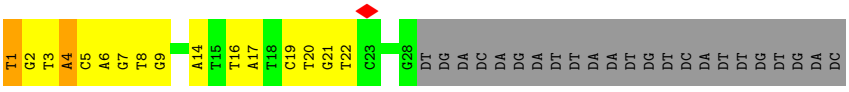
- Molecule 6: Target-LE

Chain 1:



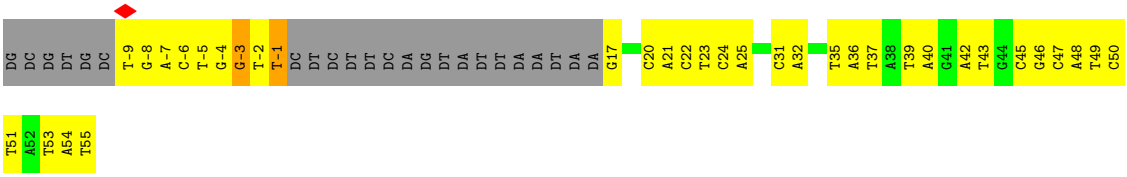
- Molecule 7: LE_R

Chain 2:



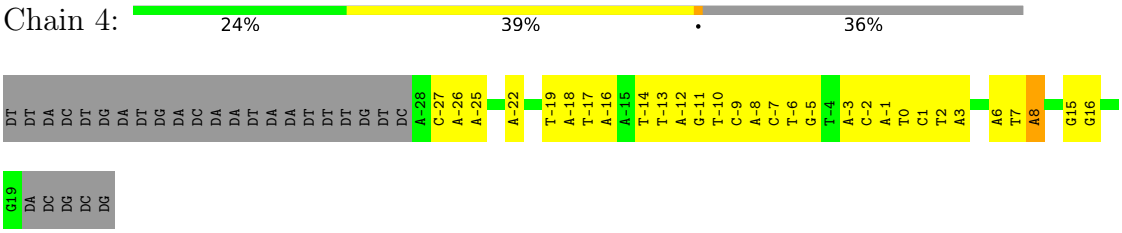
- Molecule 8: Non-target_R

Chain 3:



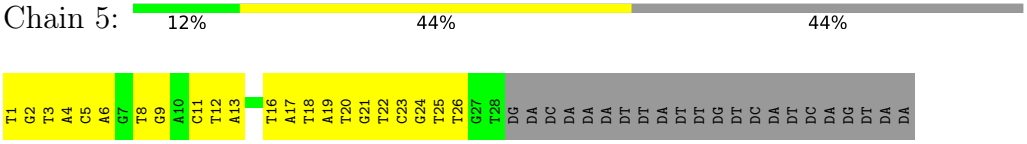
- Molecule 9: RE_F

Chain 4:



• Molecule 10: RE_R1

Chain 5:

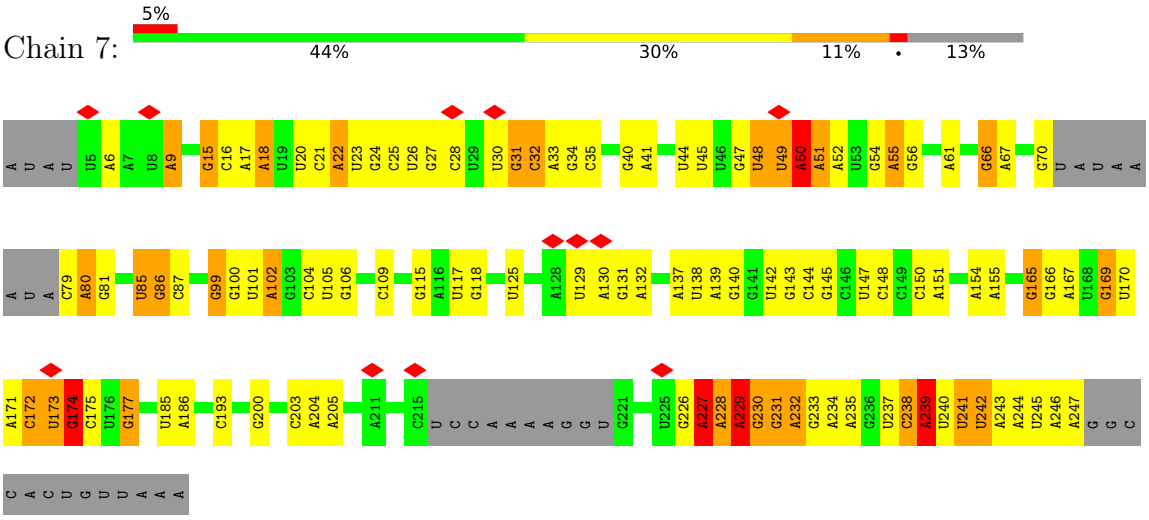


• Molecule 11: RE_R2

Chain 6:

• Molecule 12: sg_RNA

Chain 7:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	67096	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)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.885	Depositor
Minimum map value	-0.359	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	576.18, 576.18, 576.18	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.067, 1.067, 1.067	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	A	0.86	0/2097	0.95	7/2817 (0.2%)
1	B	0.85	0/2097	0.99	10/2817 (0.4%)
1	C	0.86	0/2097	0.96	9/2817 (0.3%)
1	D	0.76	0/2097	1.06	17/2817 (0.6%)
1	E	0.81	0/2097	1.00	9/2817 (0.3%)
1	F	0.87	0/2097	0.94	7/2817 (0.2%)
1	G	0.87	0/2097	0.94	7/2817 (0.2%)
1	H	0.77	0/2097	1.02	11/2817 (0.4%)
1	I	0.82	0/2097	1.01	10/2817 (0.4%)
1	J	0.80	0/2097	0.95	6/2817 (0.2%)
1	K	0.86	0/2097	1.01	9/2817 (0.3%)
1	L	0.86	0/2097	1.04	11/2817 (0.4%)
1	M	0.85	0/2097	0.95	5/2817 (0.2%)
2	O	0.66	0/4952	0.95	16/6677 (0.2%)
3	Q	0.69	0/1345	1.00	4/1819 (0.2%)
4	S	0.73	0/710	1.01	3/950 (0.3%)
5	W	0.72	0/4192	0.94	14/5659 (0.2%)
5	X	0.72	0/4137	1.06	26/5585 (0.5%)
5	Y	0.73	0/2499	0.90	7/3379 (0.2%)
5	Z	0.74	0/2472	0.98	10/3345 (0.3%)
5	w	0.80	0/132	1.29	2/178 (1.1%)
5	x	1.15	0/132	0.98	1/178 (0.6%)
5	y	0.92	0/132	1.10	1/178 (0.6%)
5	z	0.81	0/132	1.14	0/178
6	1	0.71	1/2256 (0.0%)	1.17	23/3479 (0.7%)
7	2	0.75	1/642 (0.2%)	1.34	10/990 (1.0%)
8	3	0.63	0/1095	1.14	7/1685 (0.4%)
9	4	0.56	0/1102	0.95	3/1697 (0.2%)
10	5	0.47	0/641	0.95	0/989
11	6	0.59	0/336	1.08	3/516 (0.6%)
12	7	0.48	0/5470	0.99	43/8517 (0.5%)
All	All	0.75	2/59638 (0.0%)	1.00	291/82620 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	2
1	D	0	1
1	H	0	1
1	I	0	2
1	L	0	1
4	S	0	1
5	W	0	3
5	X	0	4
5	Y	0	3
5	Z	0	1
6	1	0	3
7	2	0	1
8	3	0	2
9	4	0	1
12	7	0	4
All	All	0	31

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	2	4	DA	C5-C4	-5.41	1.34	1.38
6	1	-1	DA	C5-C4	-5.00	1.35	1.38

The worst 5 of 291 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	X	425	GLN	CB-CA-C	12.57	135.54	110.40
7	2	4	DA	N1-C6-N6	-11.22	111.86	118.60
12	7	230	G	P-O3'-C3'	-10.51	107.09	119.70
12	7	174	G	N3-C2-N2	-9.82	113.02	119.90
12	7	48	U	C3'-C2'-C1'	9.67	109.23	101.50

There are no chirality outliers.

5 of 31 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	182	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	191	ARG	Sidechain
1	C	53	ARG	Sidechain
1	D	128	ARG	Sidechain
1	H	240	TYR	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	2066	0	2157	58	0
1	B	2066	0	2157	53	0
1	C	2066	0	2157	48	0
1	D	2066	0	2157	30	0
1	E	2066	0	2156	46	0
1	F	2066	0	2156	48	0
1	G	2066	0	2158	71	0
1	H	2066	0	2157	35	0
1	I	2066	0	2157	37	0
1	J	2066	0	2157	54	0
1	K	2066	0	2156	69	0
1	L	2066	0	2152	53	0
1	M	2066	0	2155	75	0
2	O	4865	0	4924	219	0
3	Q	1306	0	1290	44	0
4	S	702	0	721	15	0
5	W	4122	0	4147	341	0
5	X	4068	0	4081	150	0
5	Y	2453	0	2421	108	0
5	Z	2426	0	2390	98	0
5	w	129	0	110	0	0
5	x	129	0	110	0	0
5	y	129	0	110	0	0
5	z	129	0	110	0	0
6	1	2010	0	1107	150	0
7	2	573	0	319	56	0
8	3	980	0	547	45	0
9	4	982	0	540	101	0
10	5	573	0	322	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	6	301	0	169	11	0
12	7	4896	0	2469	144	0
13	A	1	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	D	1	0	0	0	0
13	E	1	0	0	0	0
13	F	1	0	0	1	0
13	G	1	0	0	1	0
13	H	1	0	0	0	0
13	I	1	0	0	0	0
13	J	1	0	0	0	0
13	K	1	0	0	0	0
13	L	1	0	0	0	0
13	M	1	0	0	0	0
13	W	1	0	0	0	0
13	X	1	0	0	0	0
14	A	31	0	12	4	0
14	B	31	0	12	3	0
14	C	31	0	12	3	0
14	D	31	0	12	4	0
14	E	31	0	12	2	0
14	F	31	0	12	1	0
14	G	31	0	12	6	0
14	H	31	0	12	7	0
14	I	31	0	12	13	0
14	J	31	0	12	4	0
14	K	31	0	12	3	0
14	L	31	0	12	6	0
14	M	31	0	12	12	0
All	All	58049	0	54075	1425	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

The worst 5 of 1425 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:53:ARG:CG	1:L:29:LYS:NZ	1.71	1.51
1:G:218:LEU:CD2	1:G:256:LEU:HD11	1.43	1.49
5:X:155:THR:CG2	9:4:-12:DA:H2'	1.40	1.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:218:LEU:CD2	1:F:256:LEU:HD11	1.43	1.45
5:W:143:ARG:HH22	5:Z:504:GLN:CD	1.09	1.45

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	255/276 (92%)	250 (98%)	5 (2%)	0	100	100
1	B	255/276 (92%)	254 (100%)	1 (0%)	0	100	100
1	C	255/276 (92%)	250 (98%)	5 (2%)	0	100	100
1	D	255/276 (92%)	248 (97%)	7 (3%)	0	100	100
1	E	255/276 (92%)	252 (99%)	3 (1%)	0	100	100
1	F	255/276 (92%)	251 (98%)	4 (2%)	0	100	100
1	G	255/276 (92%)	251 (98%)	4 (2%)	0	100	100
1	H	255/276 (92%)	250 (98%)	5 (2%)	0	100	100
1	I	255/276 (92%)	252 (99%)	3 (1%)	0	100	100
1	J	255/276 (92%)	253 (99%)	2 (1%)	0	100	100
1	K	255/276 (92%)	251 (98%)	4 (2%)	0	100	100
1	L	255/276 (92%)	252 (99%)	3 (1%)	0	100	100
1	M	255/276 (92%)	250 (98%)	5 (2%)	0	100	100
2	O	595/639 (93%)	585 (98%)	10 (2%)	0	100	100
3	Q	162/167 (97%)	152 (94%)	9 (6%)	1 (1%)	25	64
4	S	85/89 (96%)	83 (98%)	2 (2%)	0	100	100
5	W	512/584 (88%)	492 (96%)	20 (4%)	0	100	100
5	X	503/584 (86%)	485 (96%)	17 (3%)	1 (0%)	47	82

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	Y	296/584 (51%)	284 (96%)	12 (4%)	0	100	100
5	Z	293/584 (50%)	280 (96%)	13 (4%)	0	100	100
5	w	12/584 (2%)	12 (100%)	0	0	100	100
5	x	12/584 (2%)	12 (100%)	0	0	100	100
5	y	12/584 (2%)	12 (100%)	0	0	100	100
5	z	12/584 (2%)	12 (100%)	0	0	100	100
All	All	5809/9155 (64%)	5673 (98%)	134 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	X	176	PRO
3	Q	95	GLU

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	224/238 (94%)	221 (99%)	3 (1%)	69	89
1	B	224/238 (94%)	224 (100%)	0	100	100
1	C	224/238 (94%)	224 (100%)	0	100	100
1	D	224/238 (94%)	224 (100%)	0	100	100
1	E	224/238 (94%)	224 (100%)	0	100	100
1	F	224/238 (94%)	224 (100%)	0	100	100
1	G	224/238 (94%)	224 (100%)	0	100	100
1	H	224/238 (94%)	223 (100%)	1 (0%)	91	97
1	I	224/238 (94%)	223 (100%)	1 (0%)	91	97
1	J	224/238 (94%)	221 (99%)	3 (1%)	69	89
1	K	224/238 (94%)	223 (100%)	1 (0%)	91	97
1	L	224/238 (94%)	223 (100%)	1 (0%)	91	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	M	224/238 (94%)	222 (99%)	2 (1%)	78 92
2	O	529/564 (94%)	527 (100%)	2 (0%)	91 97
3	Q	136/139 (98%)	136 (100%)	0	100 100
4	S	75/77 (97%)	75 (100%)	0	100 100
5	W	448/512 (88%)	446 (100%)	2 (0%)	91 97
5	X	442/512 (86%)	441 (100%)	1 (0%)	93 98
5	Y	264/512 (52%)	262 (99%)	2 (1%)	81 93
5	Z	261/512 (51%)	261 (100%)	0	100 100
5	w	13/512 (2%)	13 (100%)	0	100 100
5	x	13/512 (2%)	12 (92%)	1 (8%)	13 42
5	y	13/512 (2%)	12 (92%)	1 (8%)	13 42
5	z	13/512 (2%)	13 (100%)	0	100 100
All	All	5119/7970 (64%)	5098 (100%)	21 (0%)	91 97

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	W	235	ARG
5	Y	264	ARG
5	y	575	TYR
5	Y	380	ARG
5	X	380	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
5	W	217	HIS
5	X	96	GLN
5	Y	473	HIS
5	Y	419	GLN
5	Y	461	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	7	227/265 (85%)	54 (23%)	5 (2%)

5 of 54 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
12	7	9	A
12	7	15	G
12	7	18	A
12	7	22	A
12	7	24	G

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
12	7	48	U
12	7	49	U
12	7	50	A
12	7	130	A
12	7	173	U

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 28 ligands modelled in this entry, 15 are monoatomic - leaving 13 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	$\#\|Z\| > 2$
14	ATP	K	302	13	26,33,33	0.65	0	31,52,52	0.72	1 (3%)
14	ATP	B	302	13	26,33,33	0.67	0	31,52,52	0.72	1 (3%)
14	ATP	D	302	13	26,33,33	0.65	0	31,52,52	0.74	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	ATP	L	302	13	26,33,33	0.67	0	31,52,52	0.73	1 (3%)
14	ATP	M	302	13	26,33,33	0.66	0	31,52,52	0.74	1 (3%)
14	ATP	J	302	13	26,33,33	0.66	0	31,52,52	0.73	1 (3%)
14	ATP	E	302	13	26,33,33	0.66	0	31,52,52	0.72	1 (3%)
14	ATP	A	302	13	26,33,33	0.65	0	31,52,52	0.73	1 (3%)
14	ATP	H	302	13	26,33,33	0.67	0	31,52,52	0.73	1 (3%)
14	ATP	I	302	13	26,33,33	0.66	0	31,52,52	0.74	1 (3%)
14	ATP	C	302	13	26,33,33	0.66	0	31,52,52	0.73	1 (3%)
14	ATP	G	302	13	26,33,33	0.66	0	31,52,52	0.72	1 (3%)
14	ATP	F	302	13	26,33,33	0.66	0	31,52,52	0.72	1 (3%)

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
14	ATP	K	302	13	-	1/18/38/38	0/3/3/3
14	ATP	B	302	13	-	6/18/38/38	0/3/3/3
14	ATP	D	302	13	-	3/18/38/38	0/3/3/3
14	ATP	L	302	13	-	5/18/38/38	0/3/3/3
14	ATP	M	302	13	-	2/18/38/38	0/3/3/3
14	ATP	J	302	13	-	4/18/38/38	0/3/3/3
14	ATP	E	302	13	-	2/18/38/38	0/3/3/3
14	ATP	A	302	13	-	4/18/38/38	0/3/3/3
14	ATP	H	302	13	-	7/18/38/38	0/3/3/3
14	ATP	I	302	13	-	6/18/38/38	0/3/3/3
14	ATP	C	302	13	-	4/18/38/38	0/3/3/3
14	ATP	G	302	13	-	7/18/38/38	0/3/3/3
14	ATP	F	302	13	-	1/18/38/38	0/3/3/3

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	M	302	ATP	C5-C6-N6	2.36	123.93	120.35
14	D	302	ATP	C5-C6-N6	2.32	123.88	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	I	302	ATP	C5-C6-N6	2.32	123.88	120.35
14	H	302	ATP	C5-C6-N6	2.30	123.85	120.35
14	A	302	ATP	C5-C6-N6	2.30	123.85	120.35

There are no chirality outliers.

5 of 52 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	302	ATP	C5'-O5'-PA-O3A
14	B	302	ATP	PB-O3B-PG-O2G
14	B	302	ATP	O4'-C4'-C5'-O5'
14	G	302	ATP	PB-O3B-PG-O2G
14	G	302	ATP	C5'-O5'-PA-O3A

There are no ring outliers.

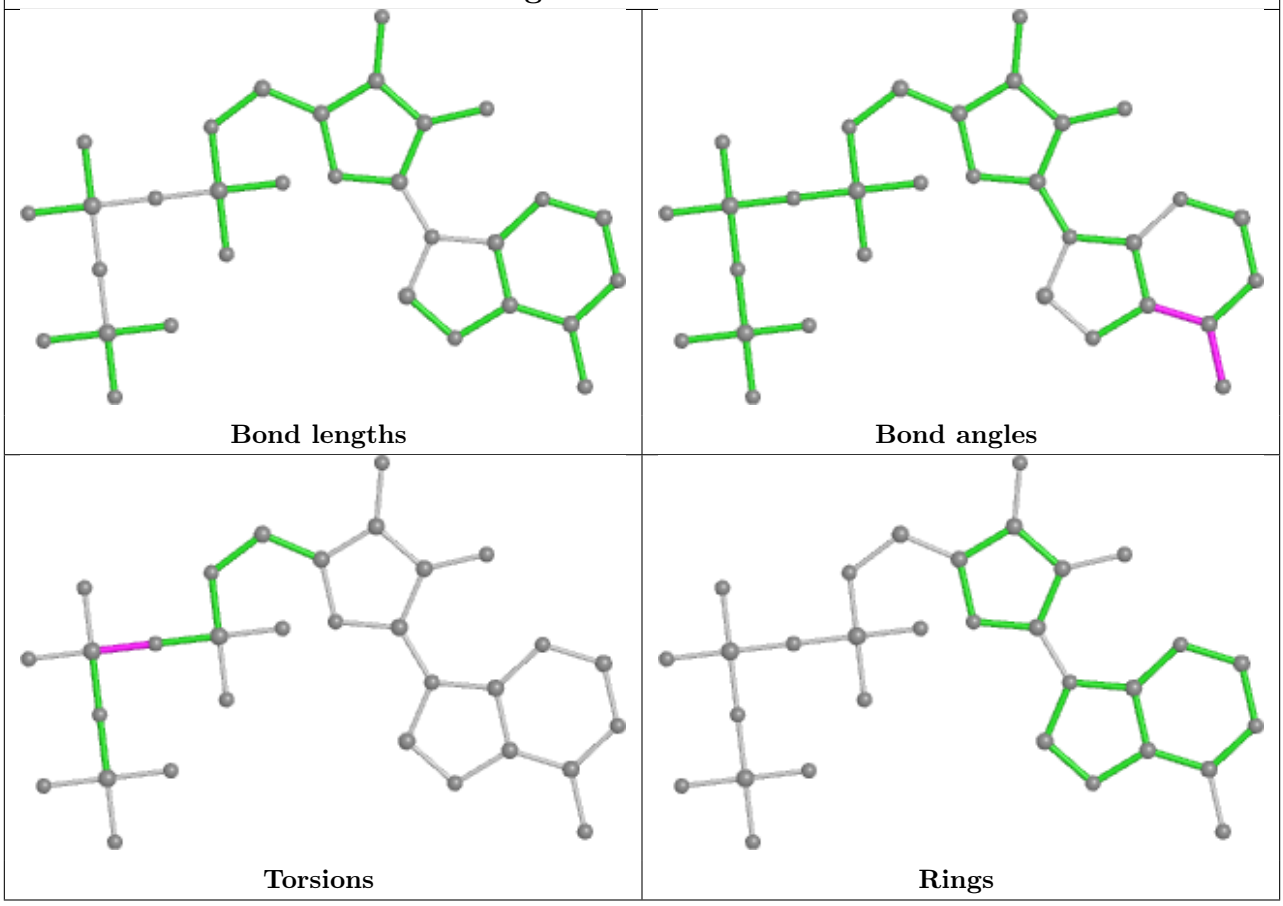
13 monomers are involved in 68 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	K	302	ATP	3	0
14	B	302	ATP	3	0
14	D	302	ATP	4	0
14	L	302	ATP	6	0
14	M	302	ATP	12	0
14	J	302	ATP	4	0
14	E	302	ATP	2	0
14	A	302	ATP	4	0
14	H	302	ATP	7	0
14	I	302	ATP	13	0
14	C	302	ATP	3	0
14	G	302	ATP	6	0
14	F	302	ATP	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 ATP K 302



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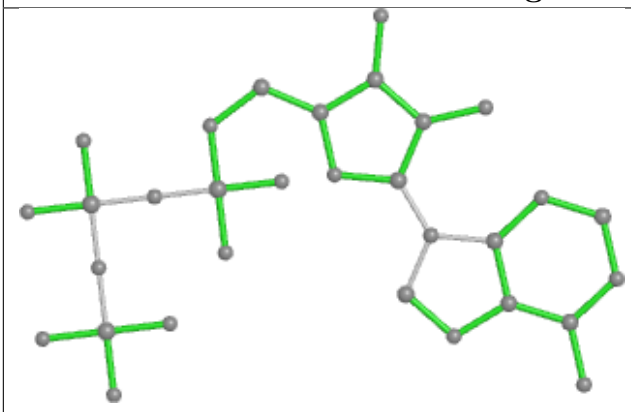

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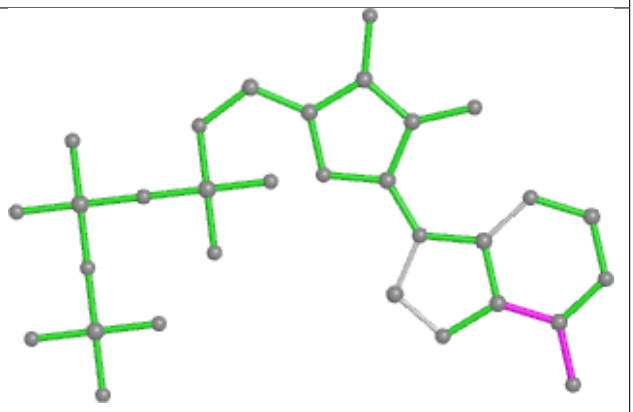
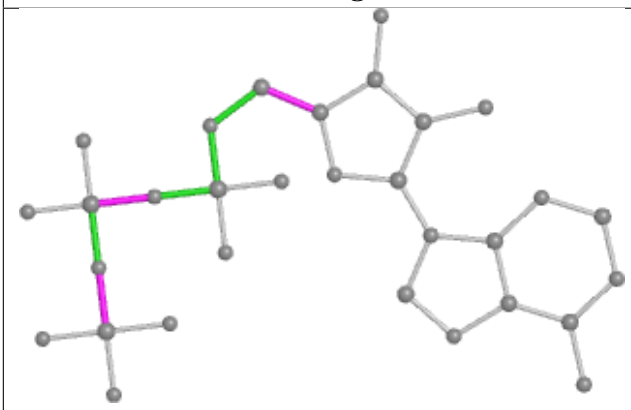
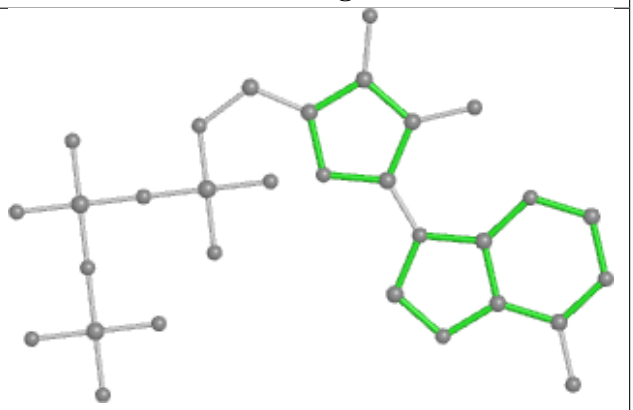


Bond angles

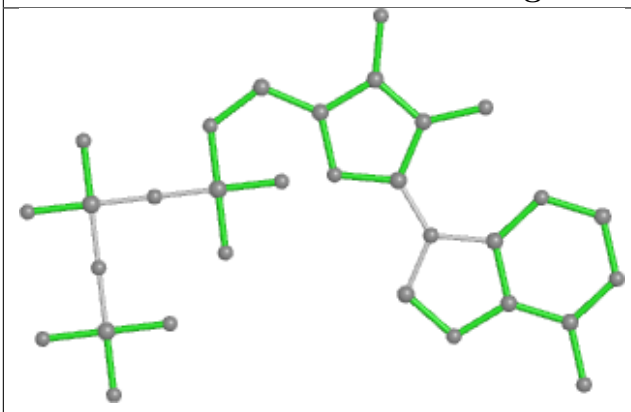


Torsions



Rings

Ligand ATP D 302



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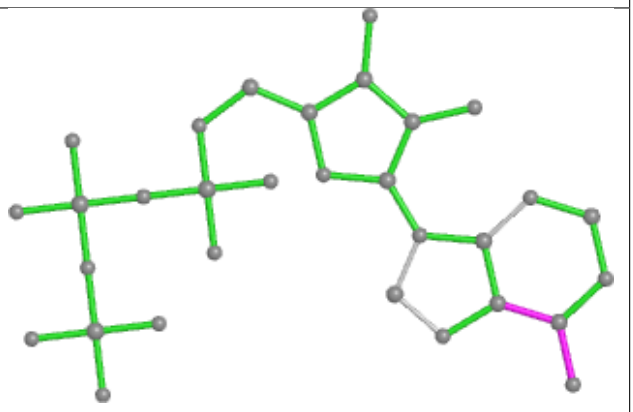

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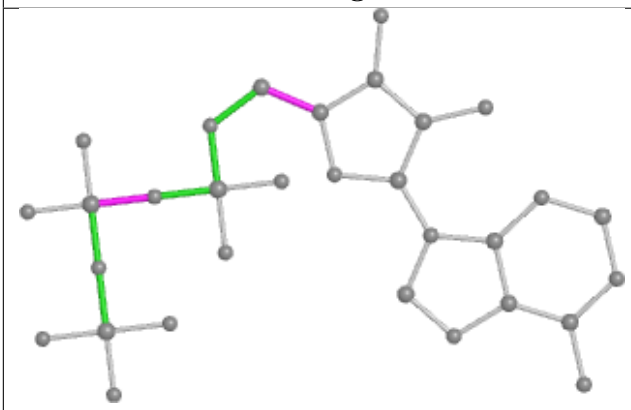

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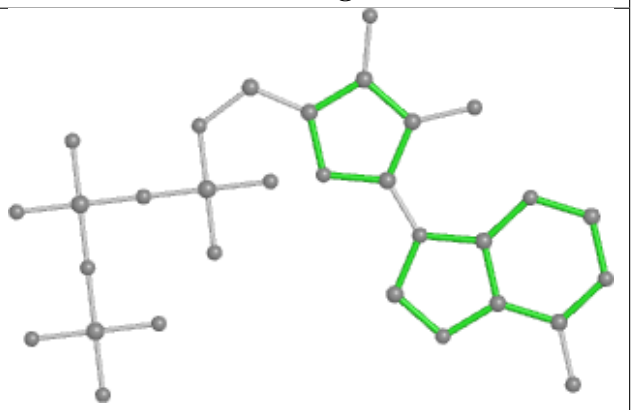

Rings

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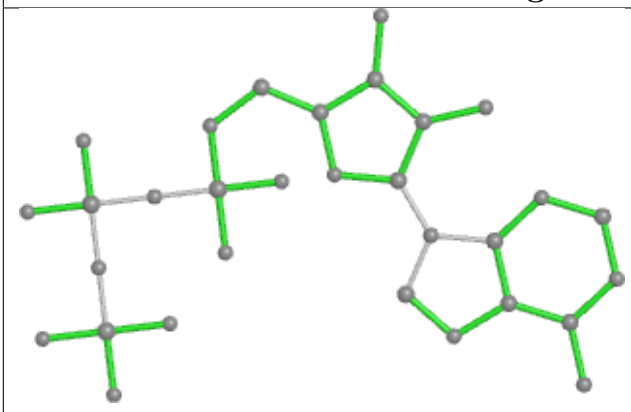

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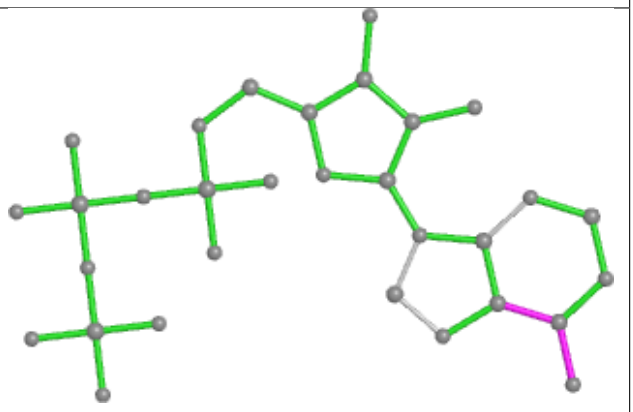

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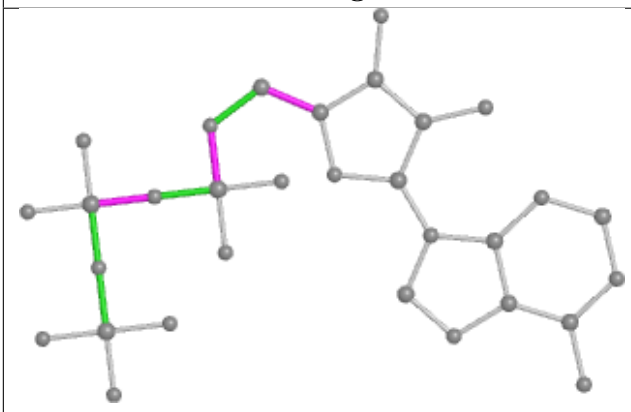

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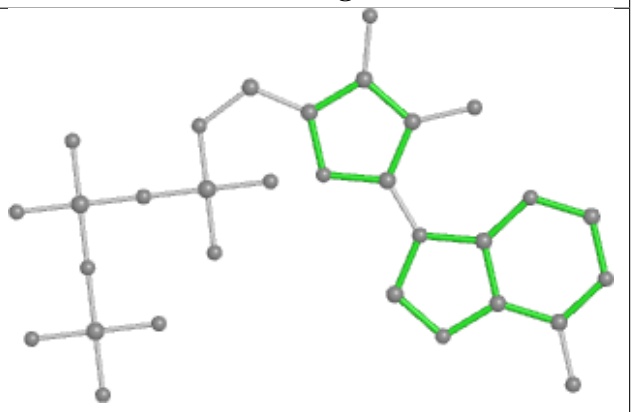
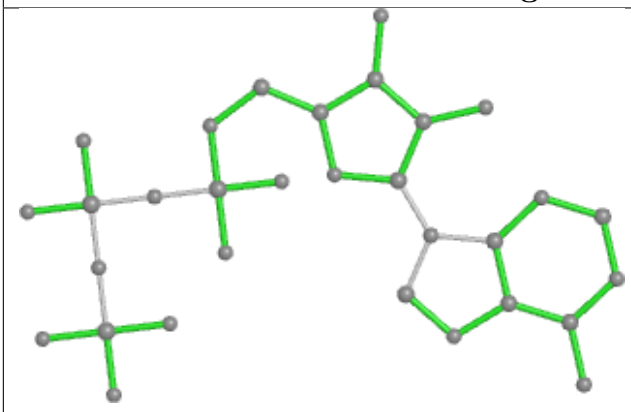


Rings

Ligand ATP M 302



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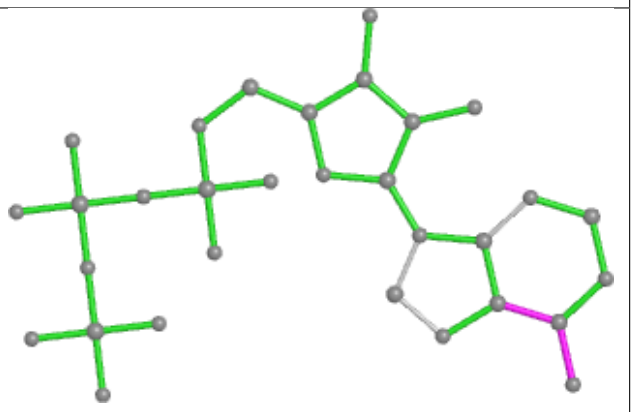

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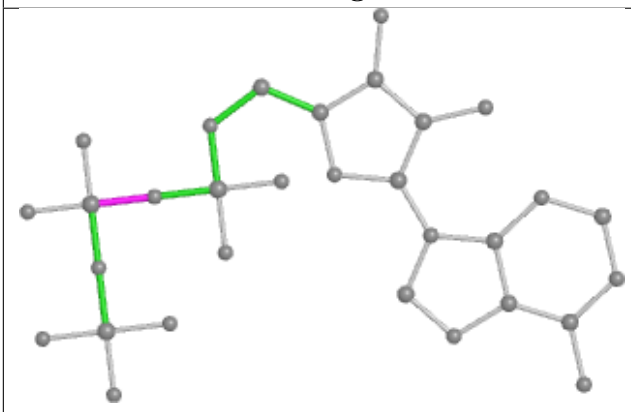

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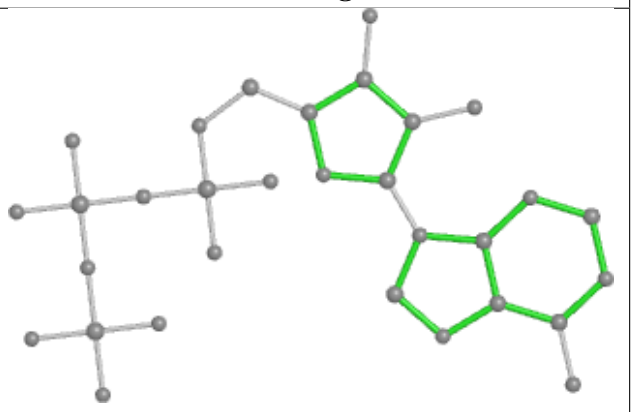

Rings

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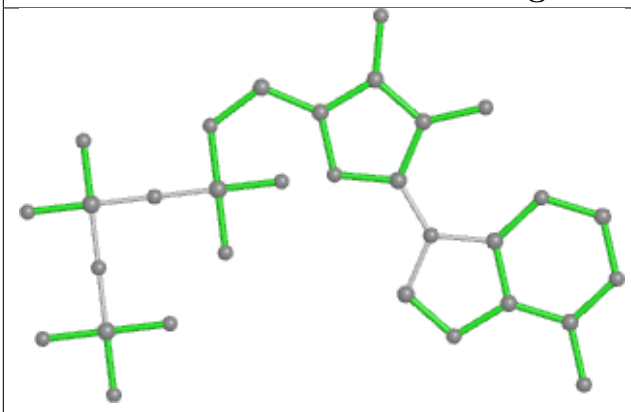

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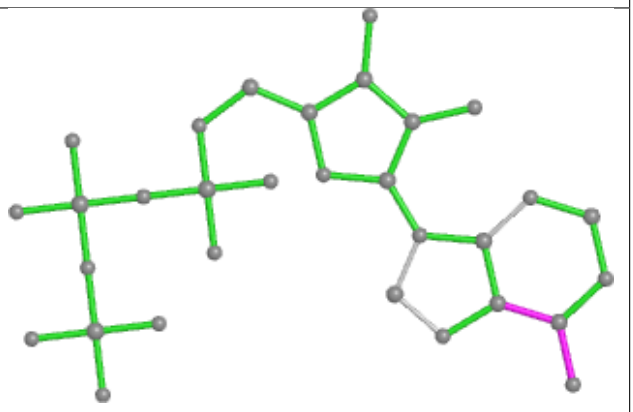

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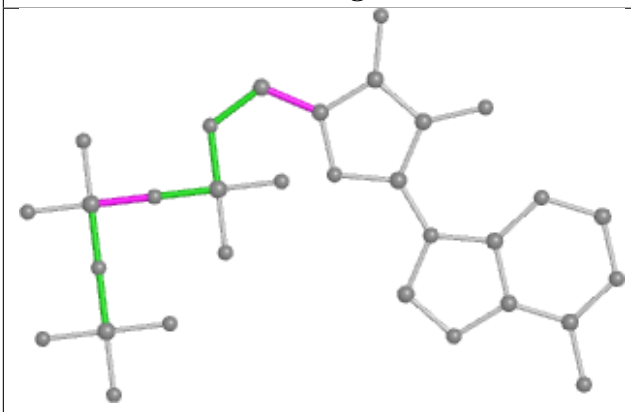

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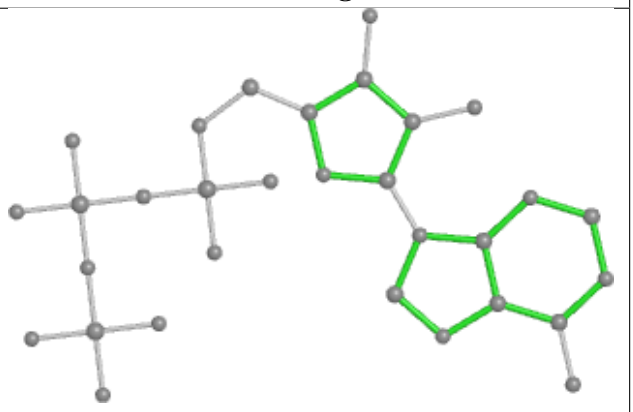

Rings

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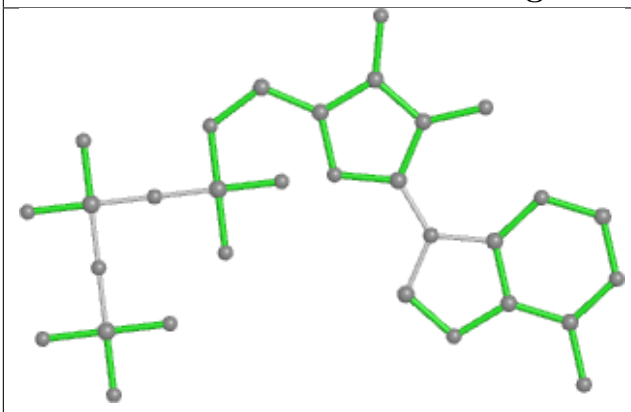

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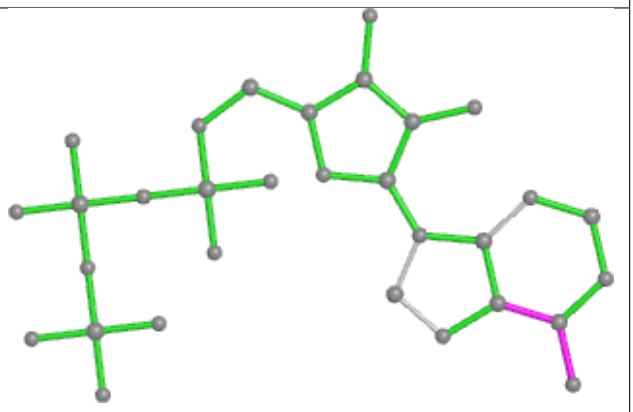

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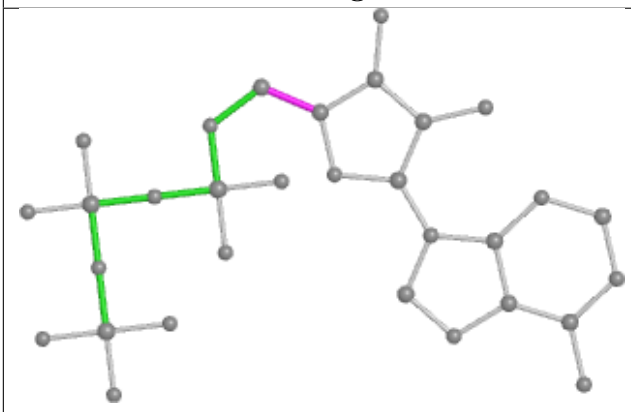

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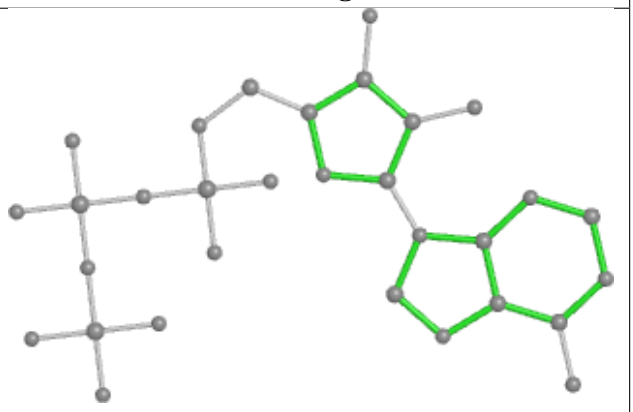

Rings

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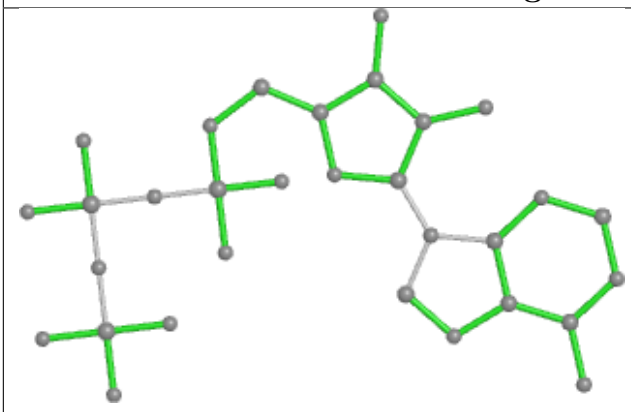

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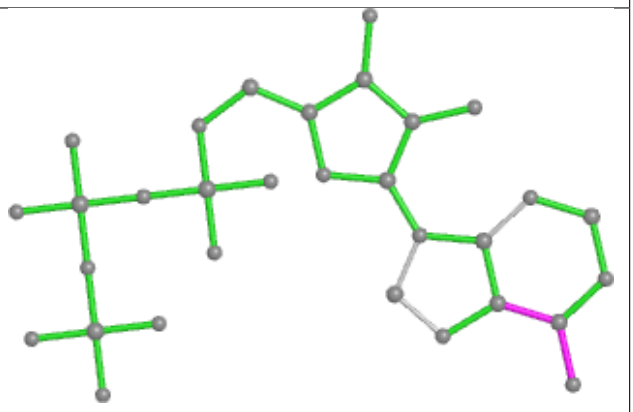

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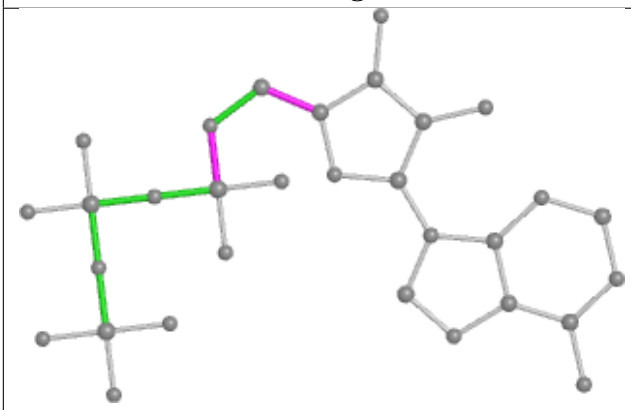

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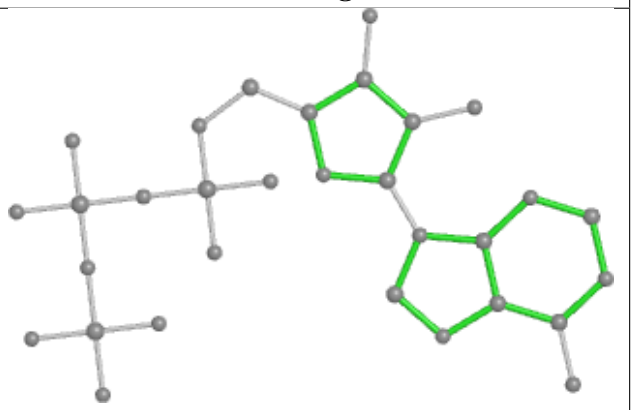

Rings

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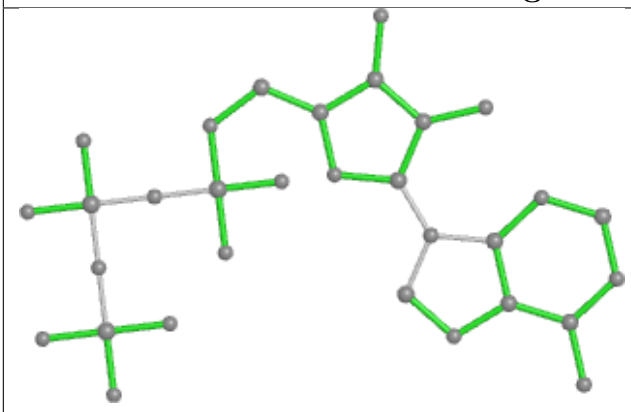

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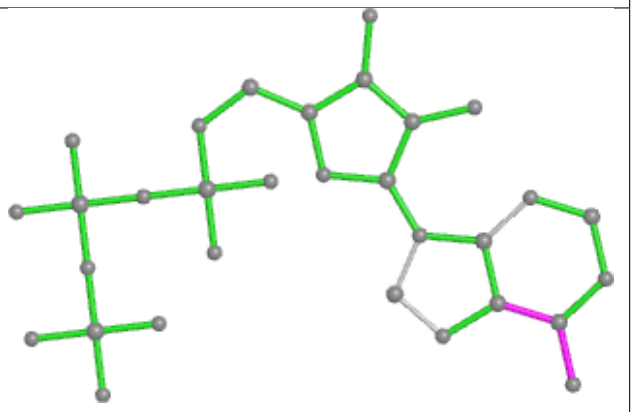
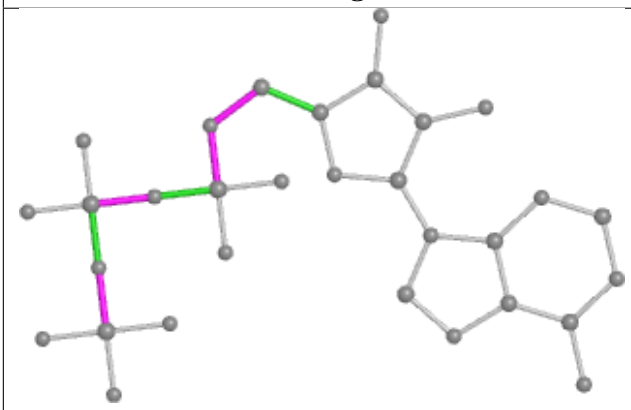


Bond angles



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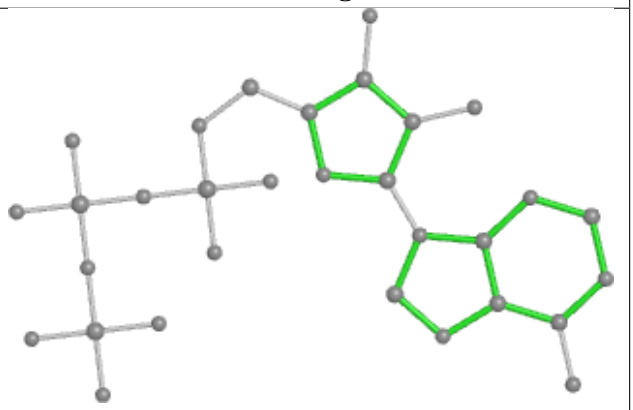
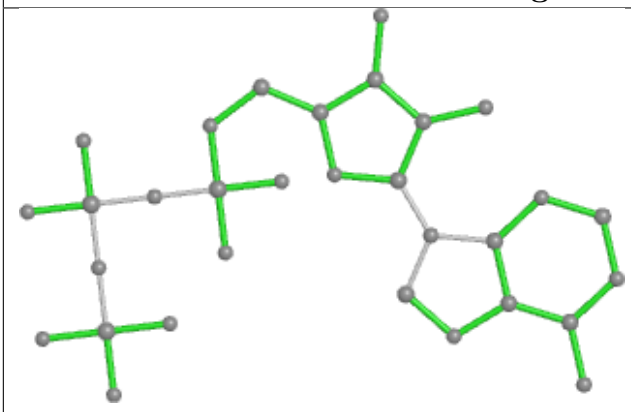


Rings

Ligand ATP I 302



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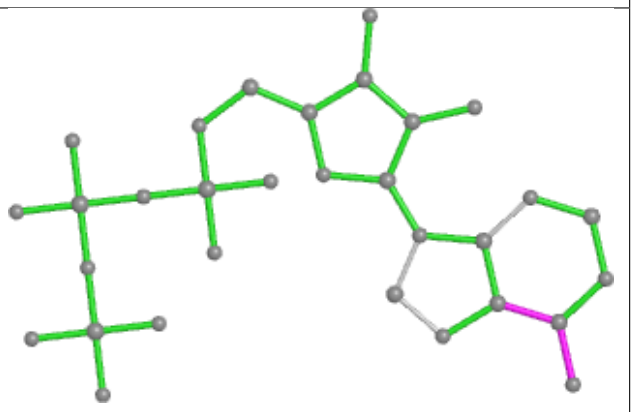
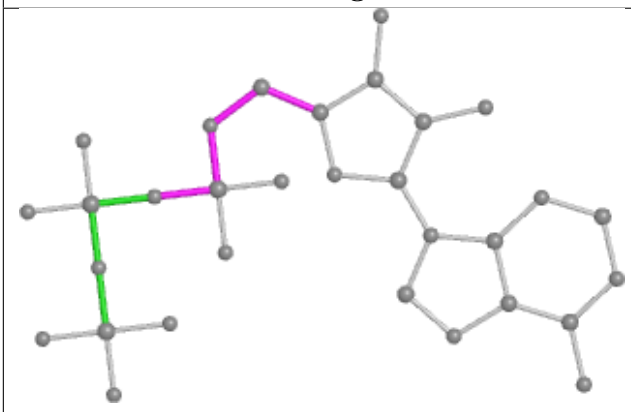
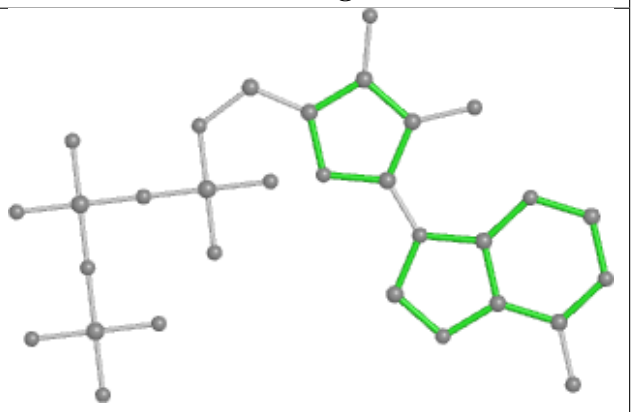


Bond angles

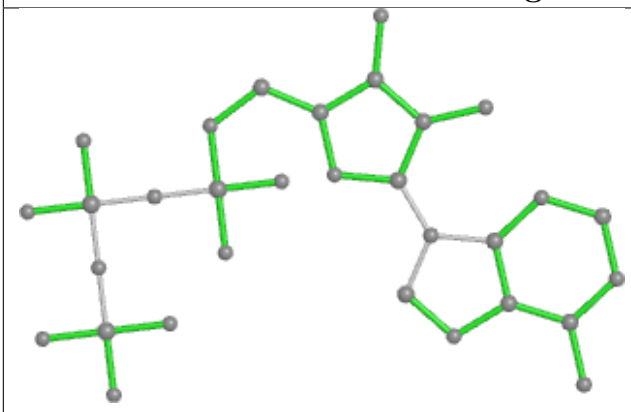


Torsions

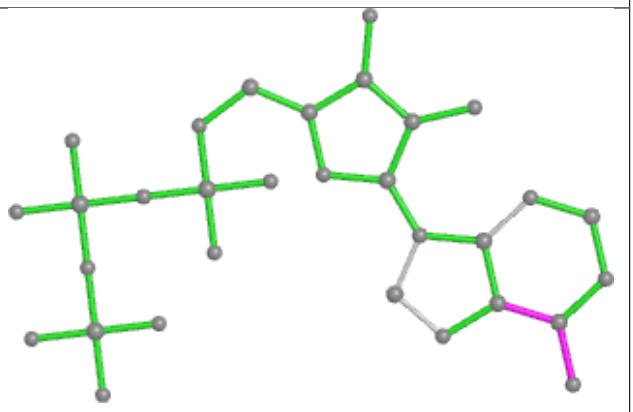


Rings

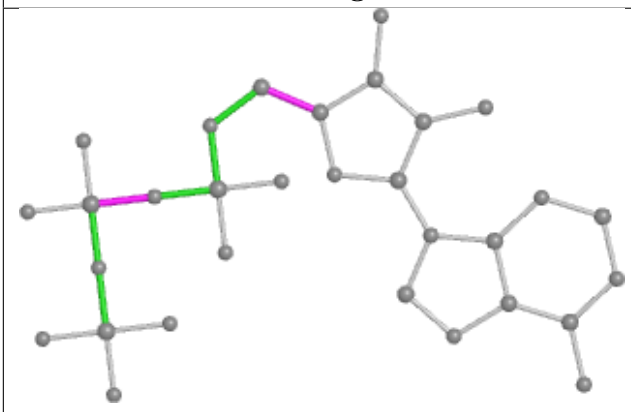
Ligand ATP C 302



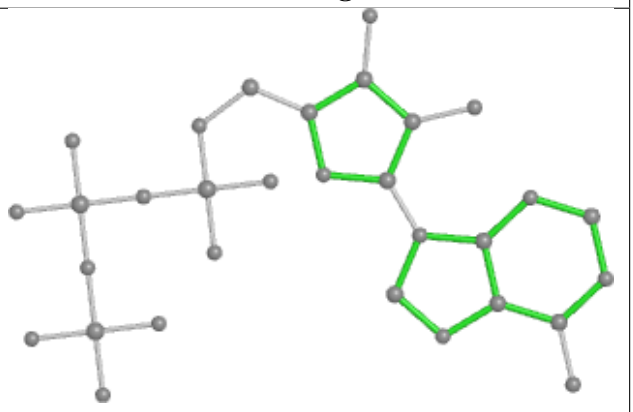
Bond lengths



Bond angles

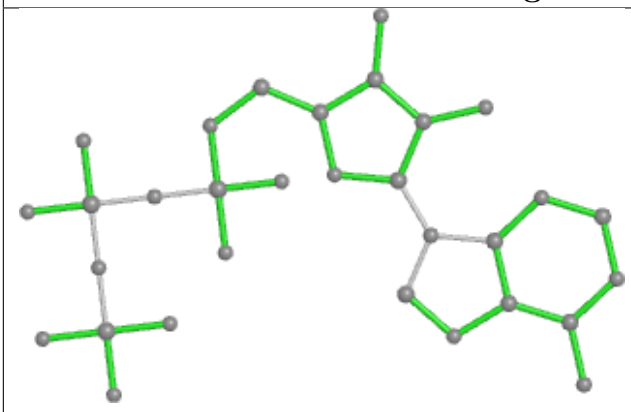


Torsions

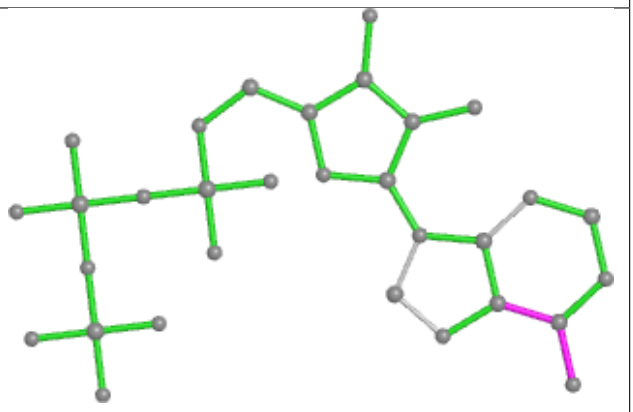


Rings

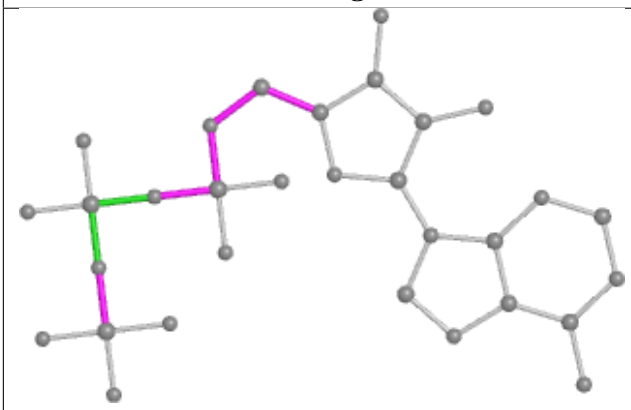
Ligand ATP G 302



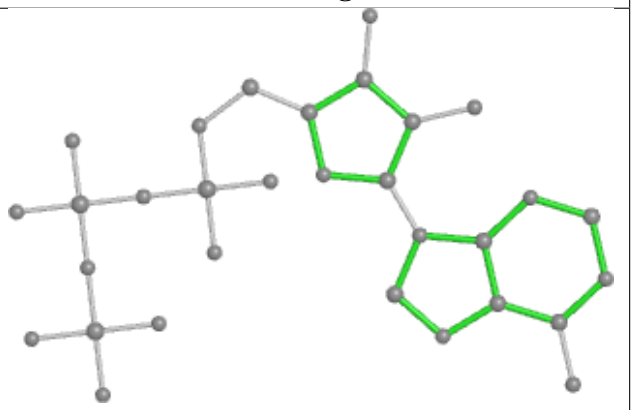
Bond lengths



Bond angles

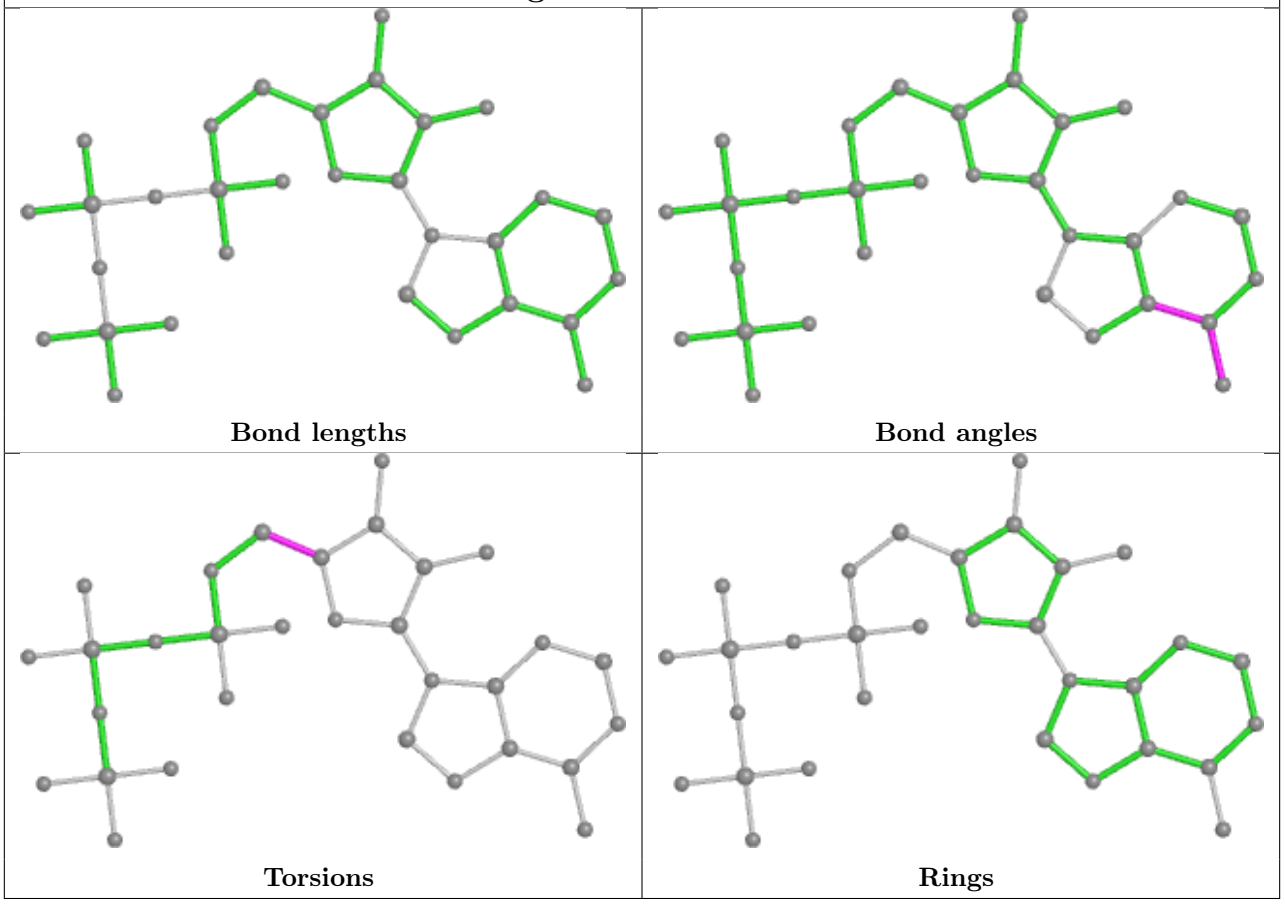


Torsions



Rings

Ligand ATP F 302



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.

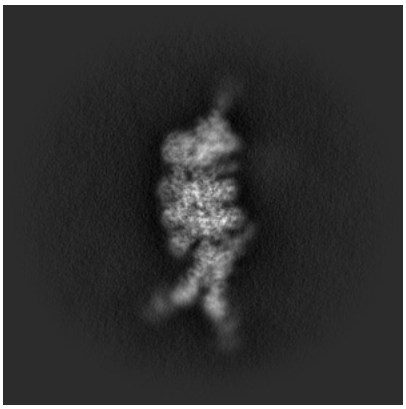
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-27972. These allow visual inspection of the internal detail of the map and identification of artifacts.

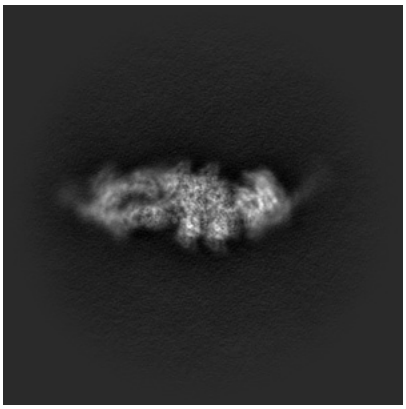
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

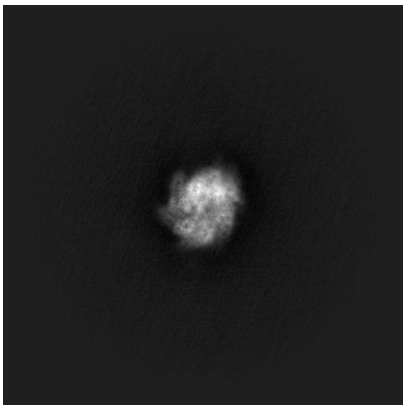
6.1.1 Primary map



X

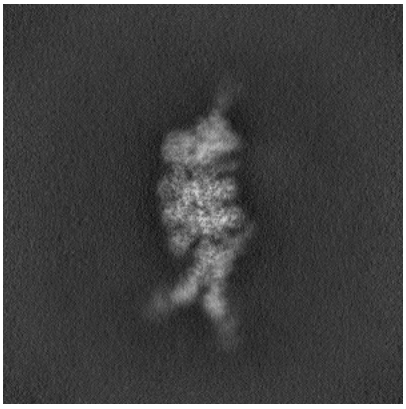


Y

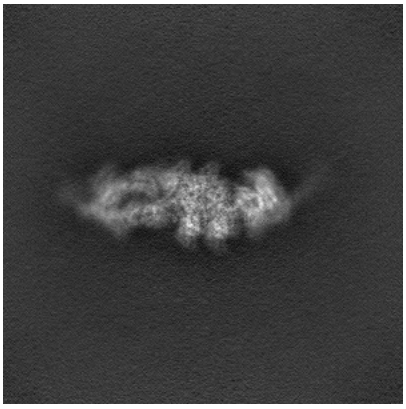


Z

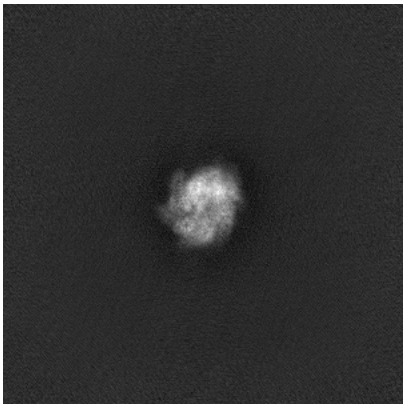
6.1.2 Raw map



X



Y

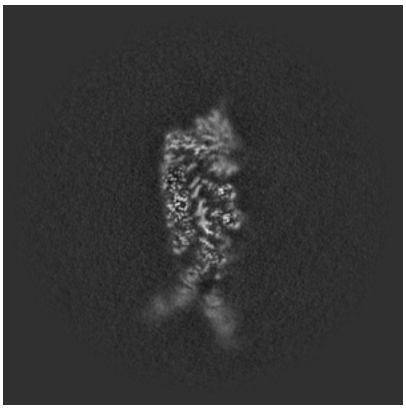


Z

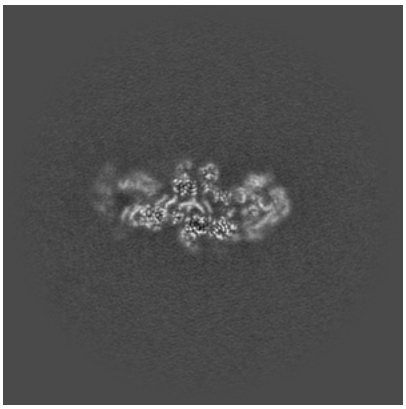
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

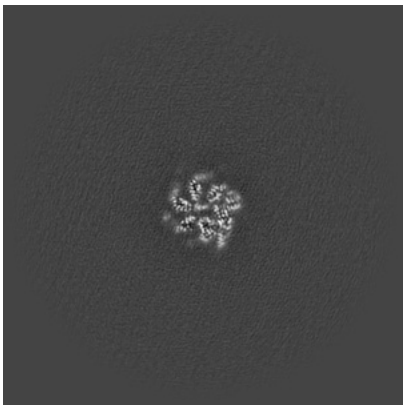
6.2.1 Primary map



X Index: 270

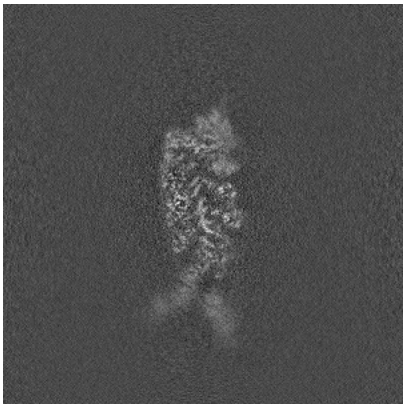


Y Index: 270

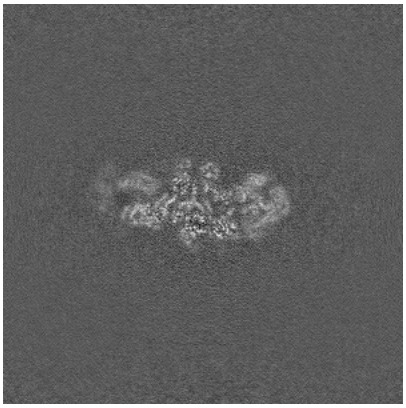


Z Index: 270

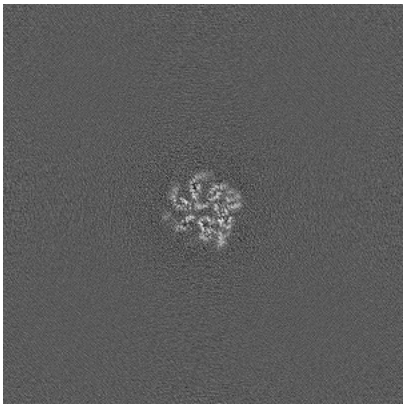
6.2.2 Raw map



X Index: 270



Y Index: 270

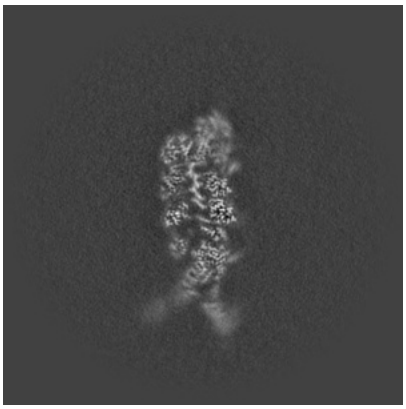


Z Index: 270

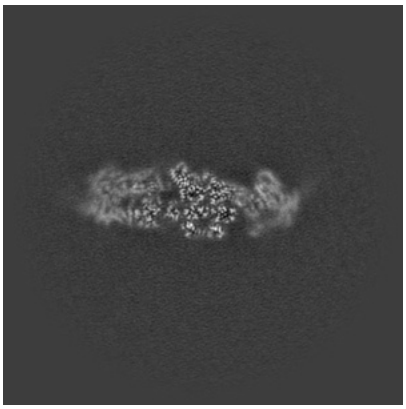
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

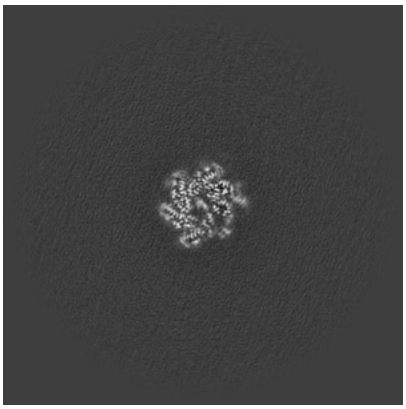
6.3.1 Primary map



X Index: 264

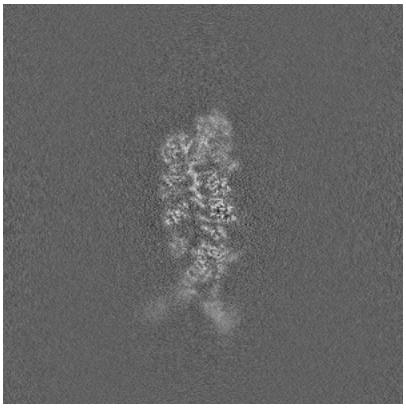


Y Index: 286

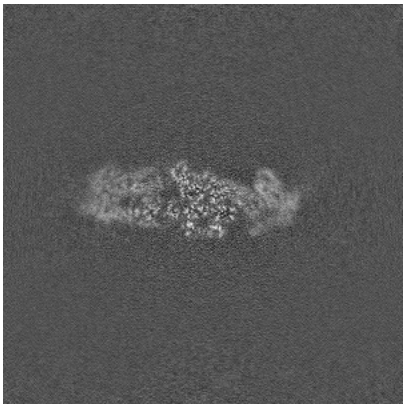


Z Index: 249

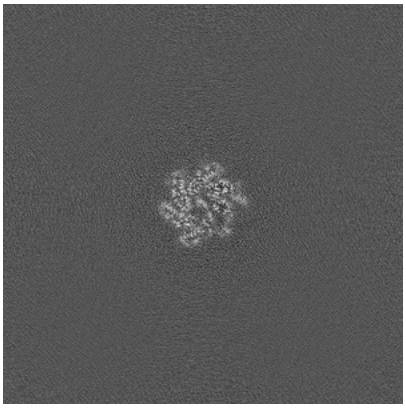
6.3.2 Raw map



X Index: 264



Y Index: 286



Z Index: 249

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

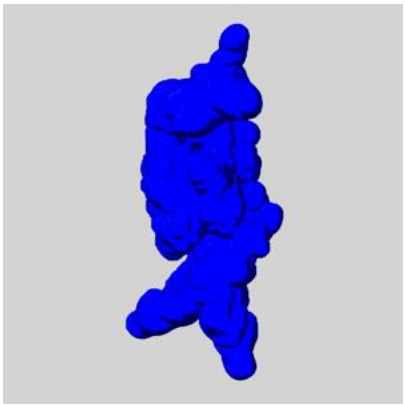
6.5 Mask visualisation (i)

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

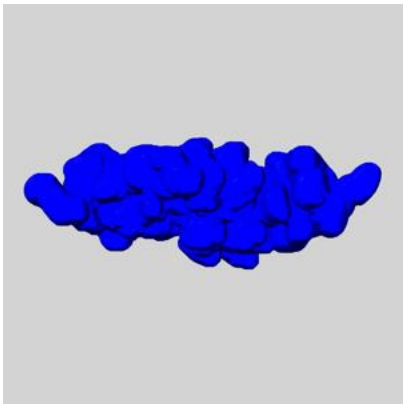
A mask typically either:

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

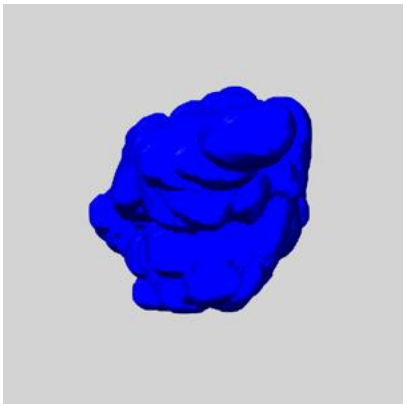
6.5.1 emd_27972_msk_1.map (i)



X



Y

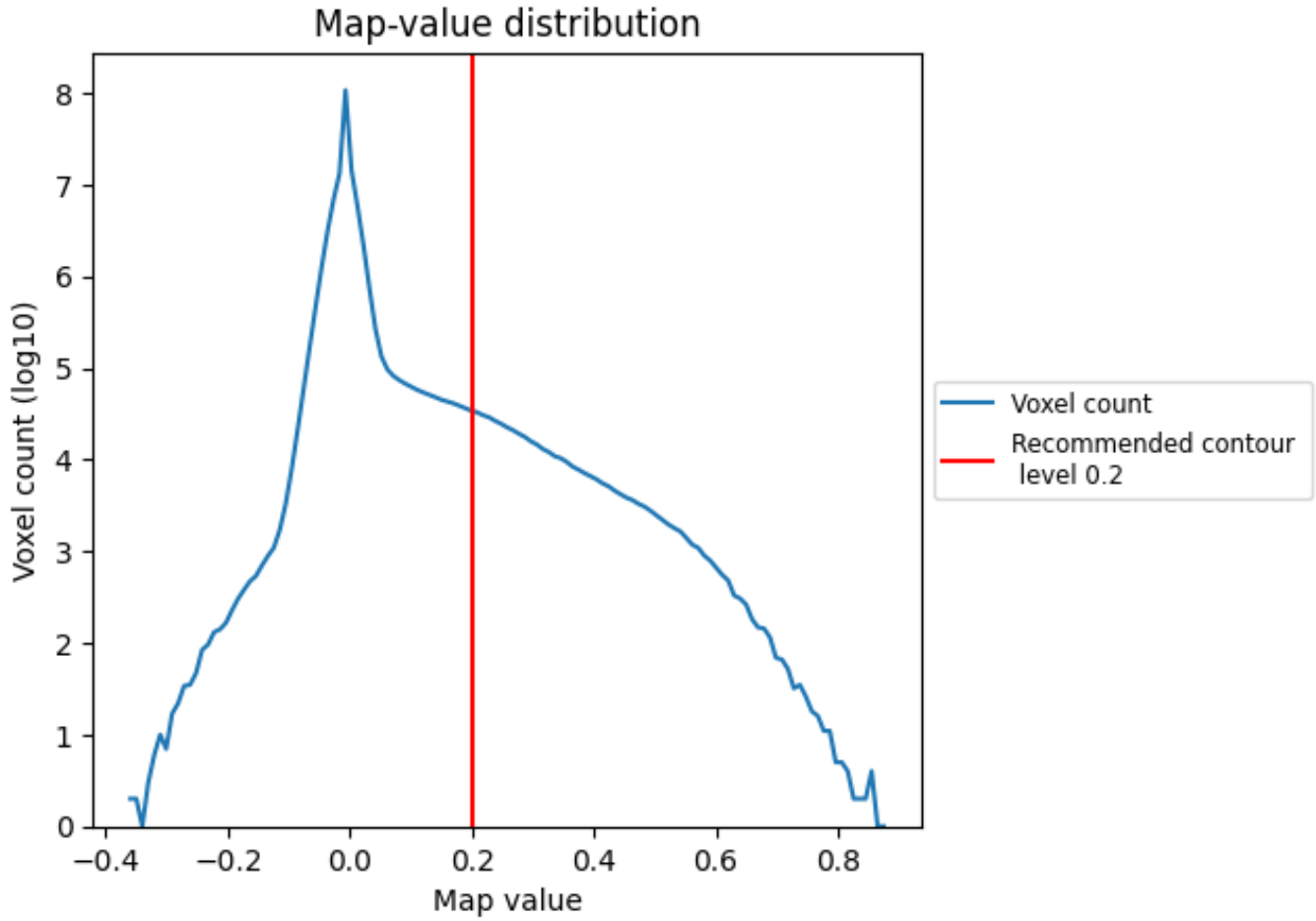


Z

7 Map analysis

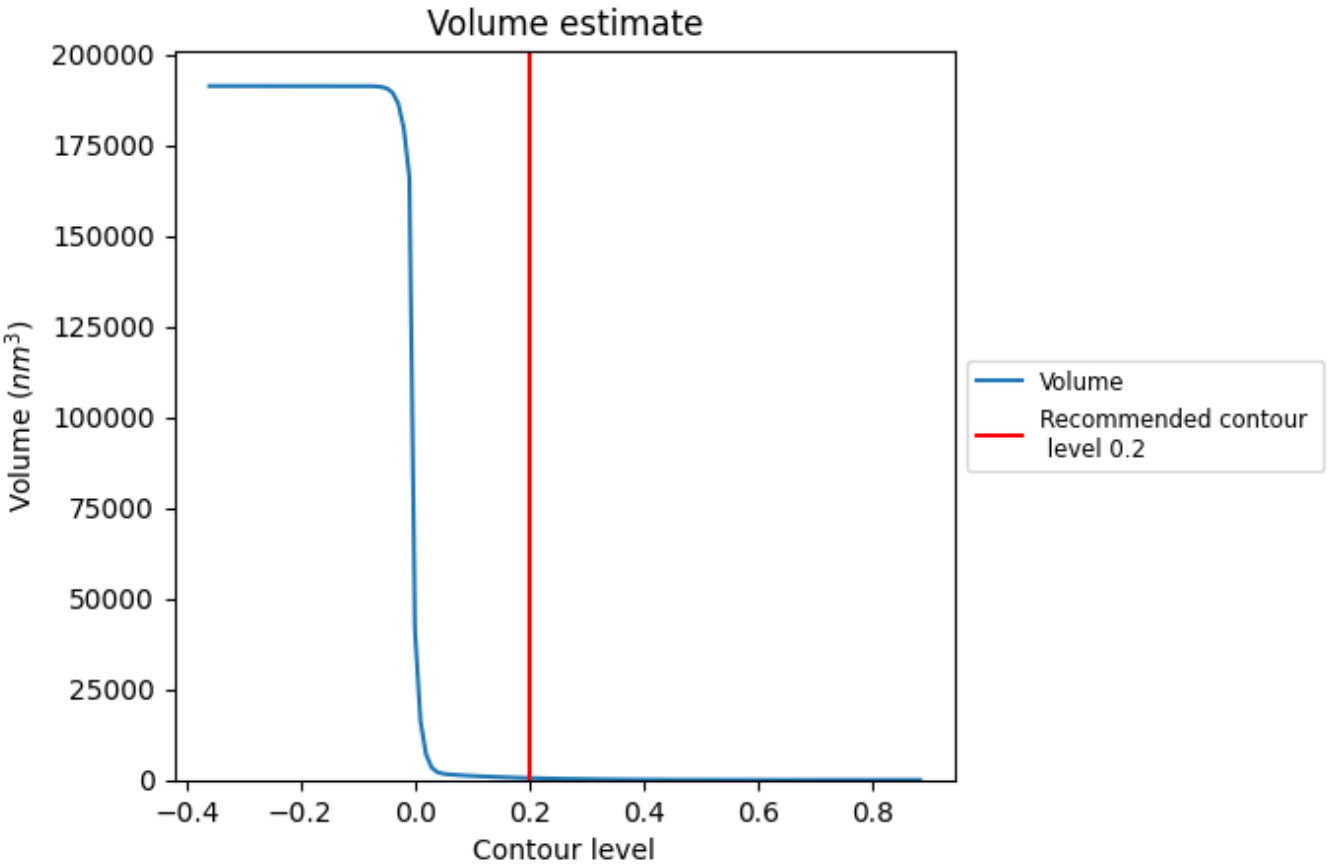
This section contains the results of statistical analysis of the map.

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.

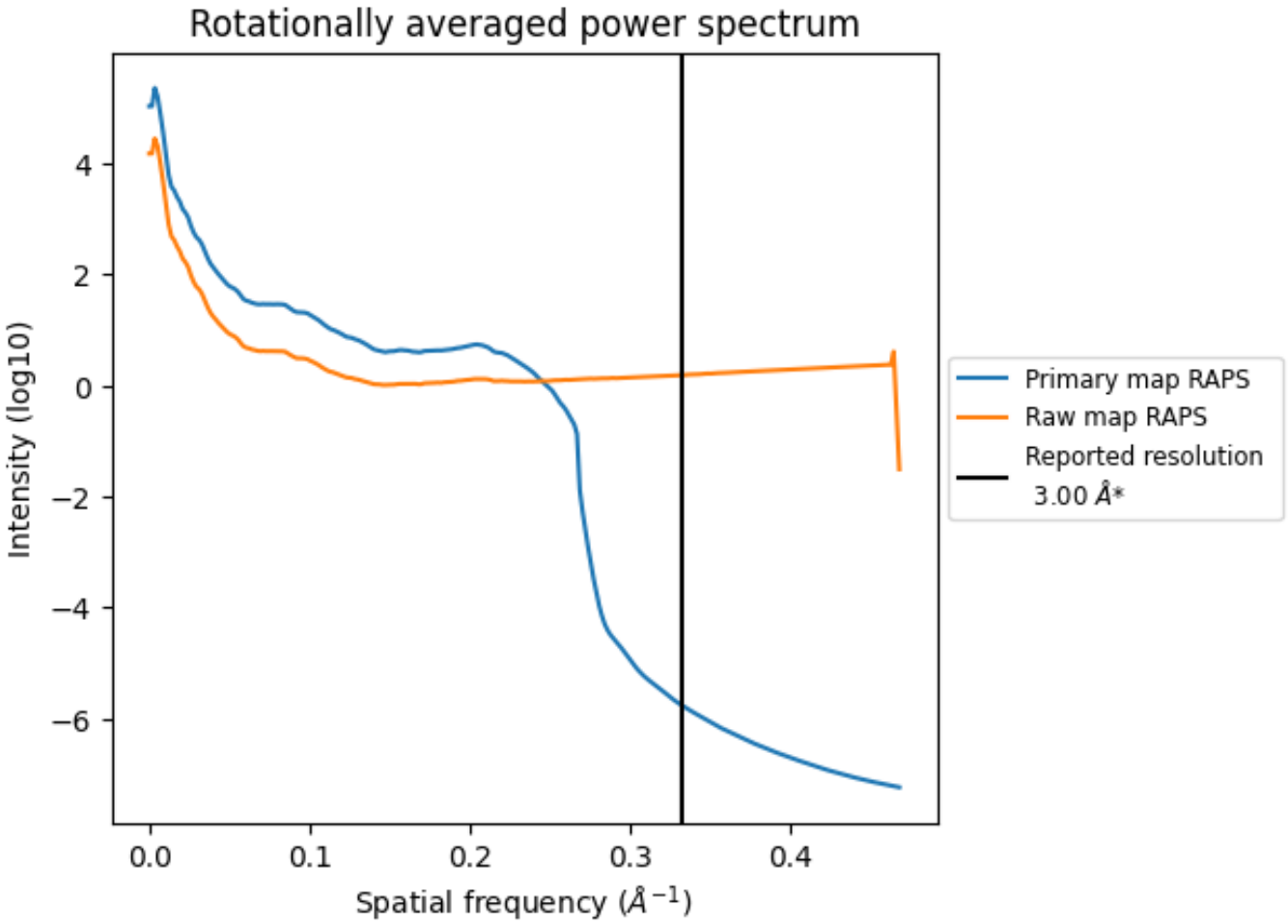
7.2 Volume estimate (i)



The volume at the recommended contour level is 525 nm^3; this corresponds to an approximate mass of 475 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)

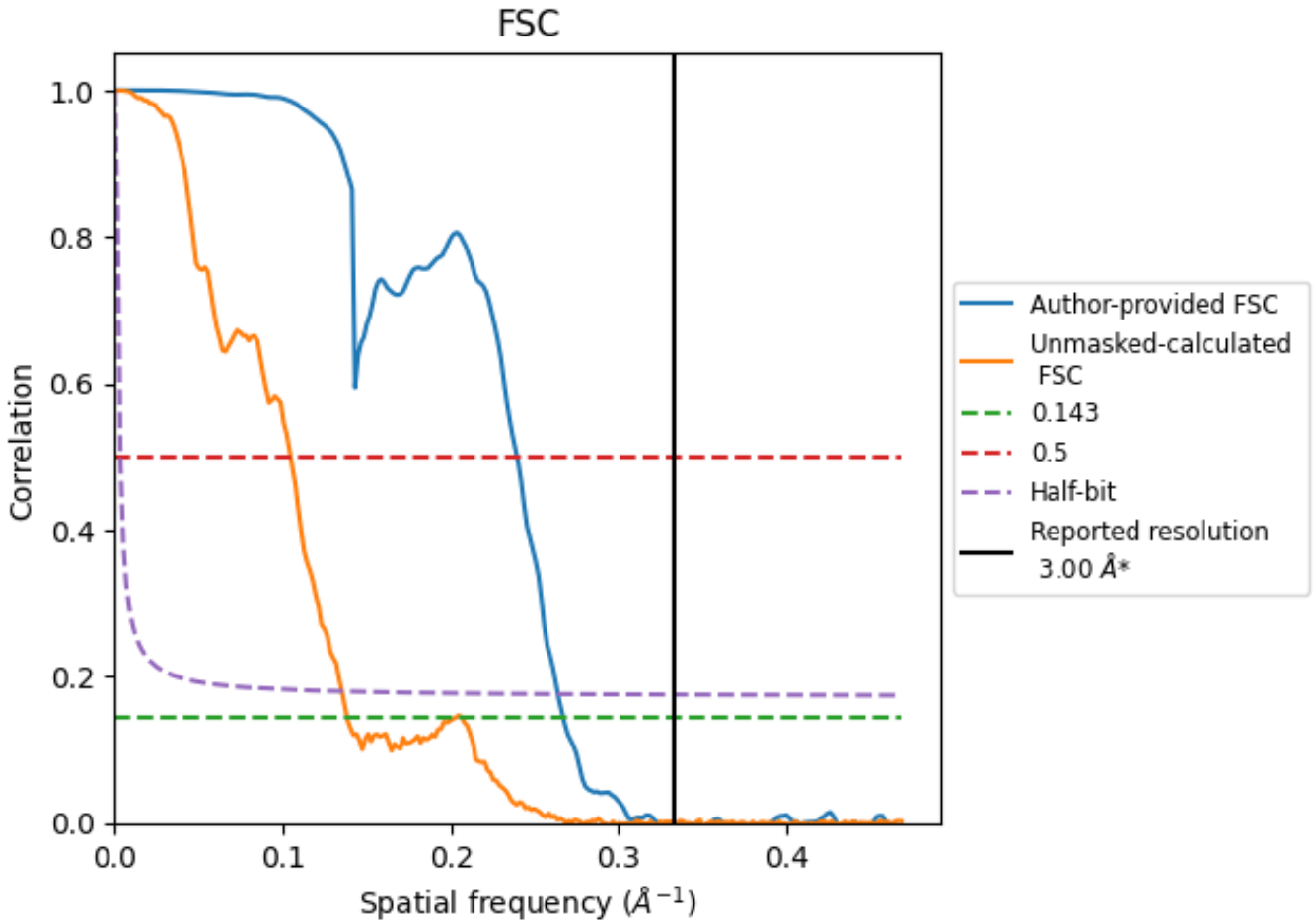


*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.74	4.17	3.79
Unmasked-calculated*	7.22	9.54	7.39

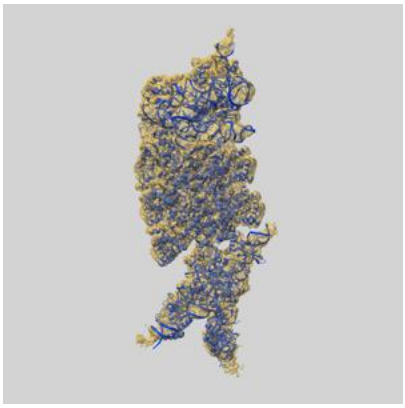
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.74 differs from the reported value 3.0 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.22 differs from the reported value 3.0 by more than 10 %

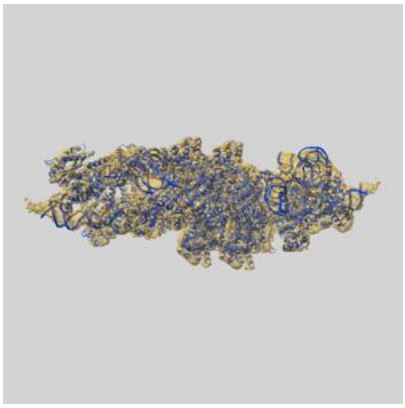
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-27972 and PDB model 8EA4. Per-residue inclusion information can be found in section 3 on page 10.

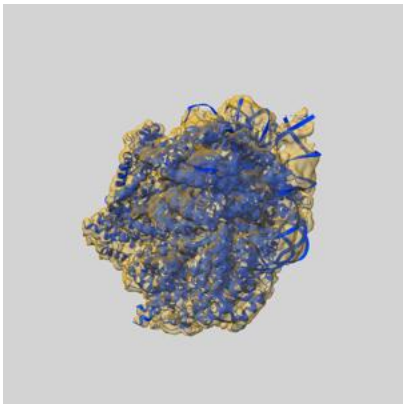
9.1 Map-model overlay



X



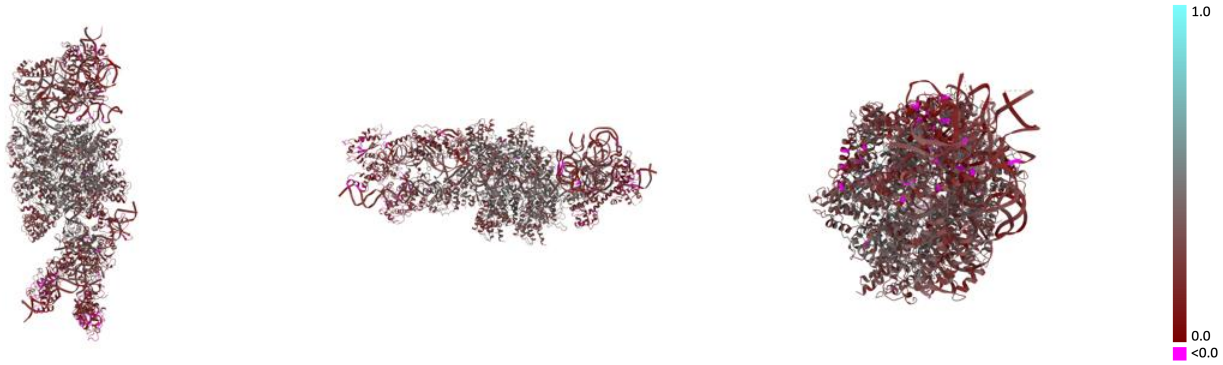
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 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.

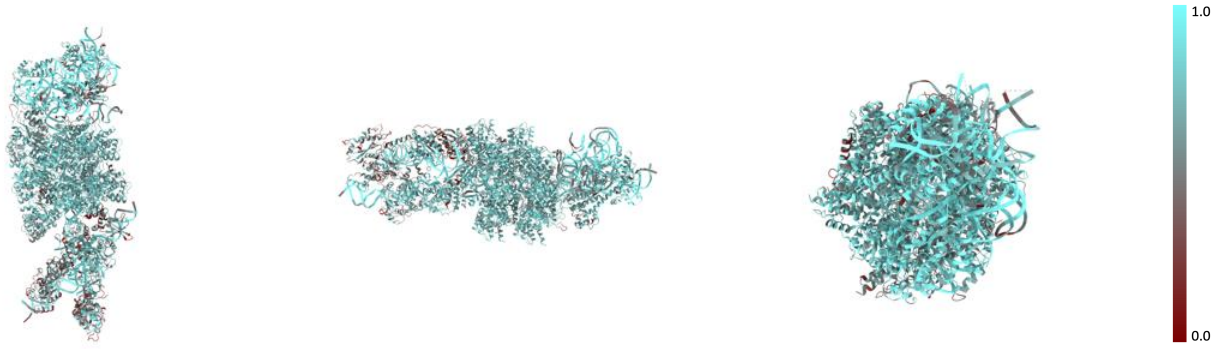
9.2 Q-score mapped to coordinate model



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.

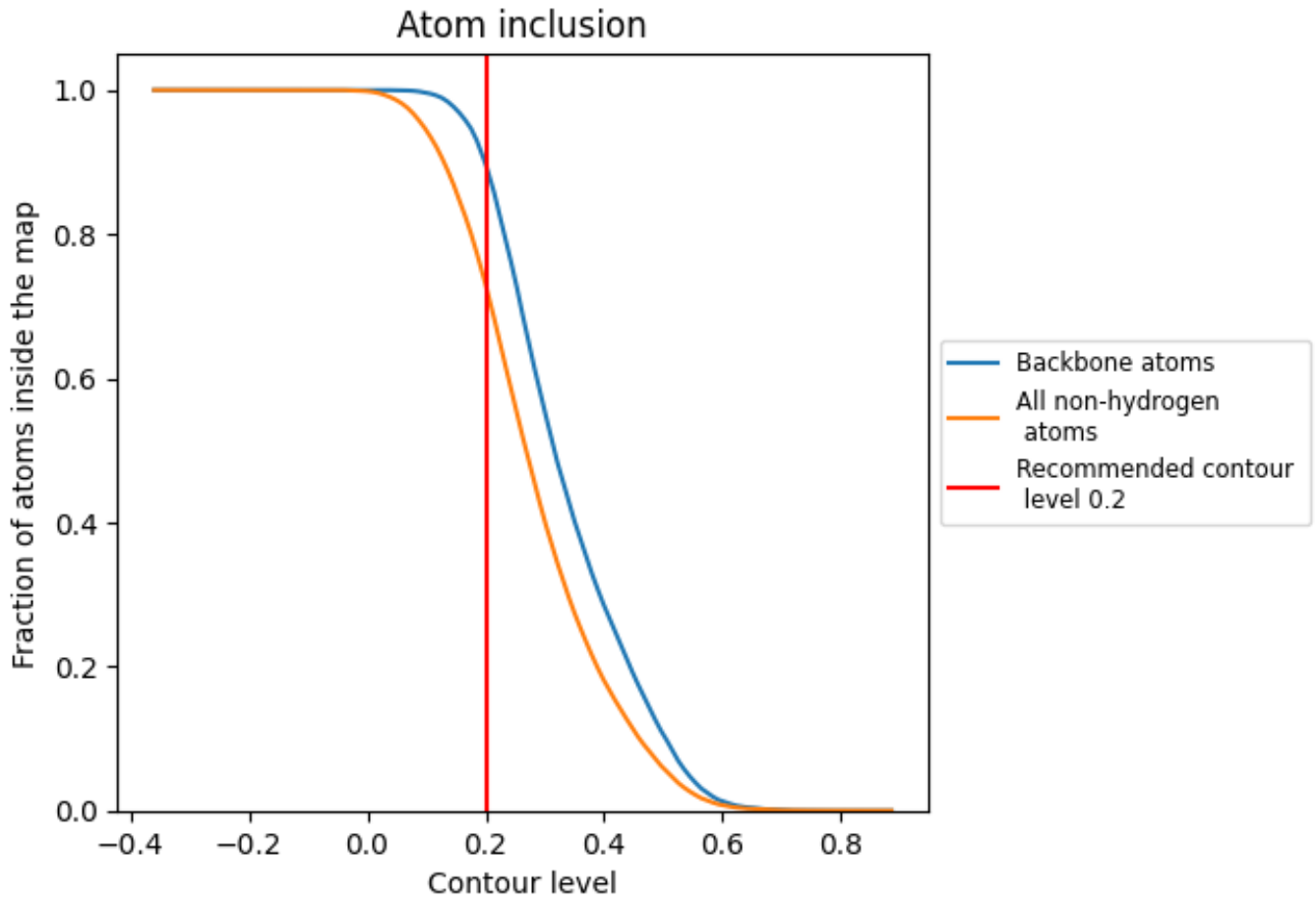
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 73% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7295	0.3020
1	0.9000	0.3110
2	0.7801	0.2550
3	0.9051	0.3400
4	0.8595	0.2740
5	0.8866	0.2830
6	0.8173	0.2510
7	0.8407	0.2300
A	0.6779	0.3330
B	0.7559	0.3630
C	0.7809	0.3660
D	0.7848	0.3790
E	0.7672	0.3550
F	0.7941	0.3800
G	0.7882	0.3810
H	0.7809	0.3770
I	0.7667	0.3690
J	0.7667	0.3770
K	0.7652	0.3740
L	0.7956	0.3810
M	0.6245	0.3470
O	0.6953	0.2160
Q	0.8085	0.3450
S	0.7706	0.2620
W	0.6811	0.3130
X	0.5816	0.2280
Y	0.5193	0.1420
Z	0.4667	0.1690
w	0.4919	0.2160
x	0.4677	0.2820
y	0.4435	0.1870
z	0.3710	0.2020