Full wwPDB EM Validation Report ⓘ

Jun 23, 2024 – 07:44 am BST

PDB ID	:	8RDU
EMDB ID	:	EMD-19075
Title	:	Conformational Landscape of the Type V-K CRISPR-associated TransposonIntegration Assembly CAST V-K composite map
Authors	:	Tenjo-Castano, F.; Mesa, P.; Montoya, G.
Deposited on	:	2023-12-08
Resolution	:	2.30 Å(reported)
Based on initial model	:	.

This is a Full wwPDB EM Validation 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:

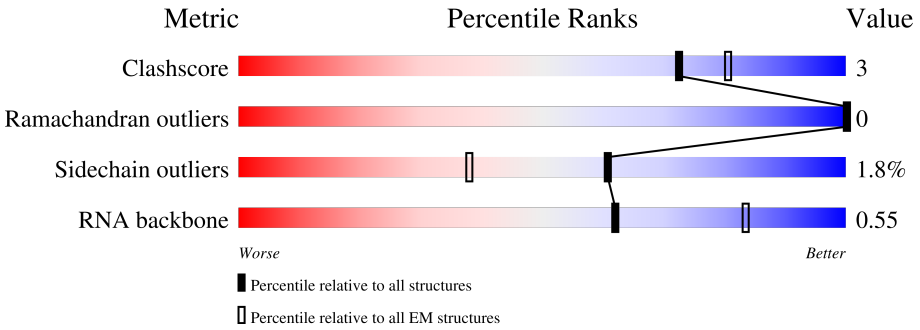
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	1	261	16% 62% 25% 7% 6%
2	2	68	24% 57% 37%
3	3	133	14% 39% 31% 26%
4	4	75	16% 17% 65%
5	5	74	16% 18% 65%
6	6	79	30% 29% 39%
7	7	15	7% 53% 40% 7%

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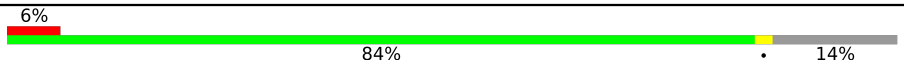
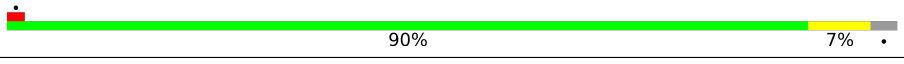
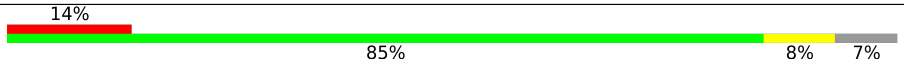
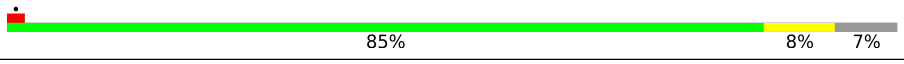
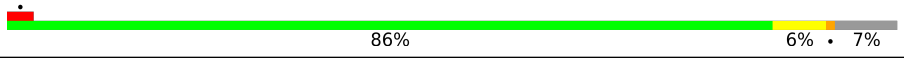
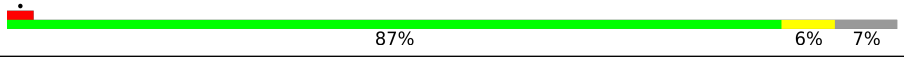
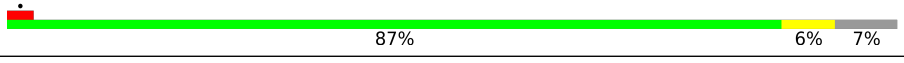
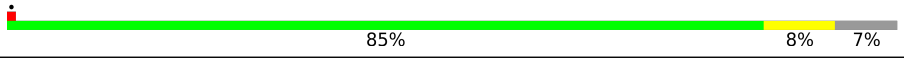
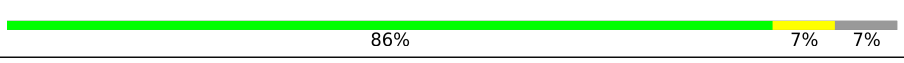
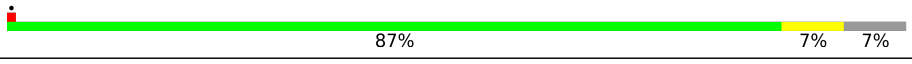
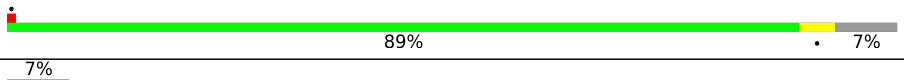
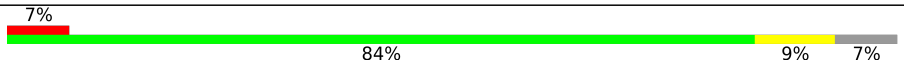
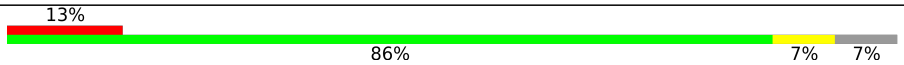
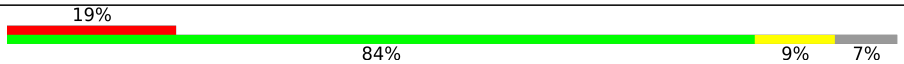
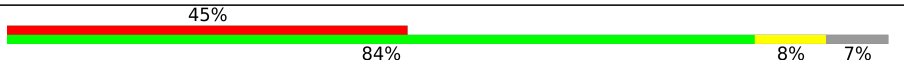
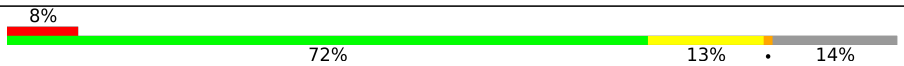
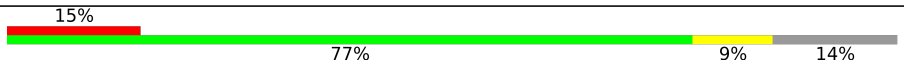
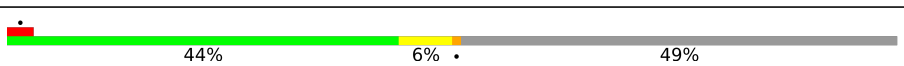
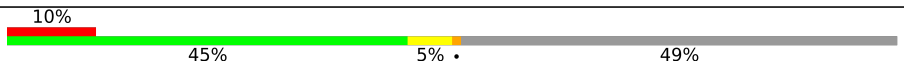
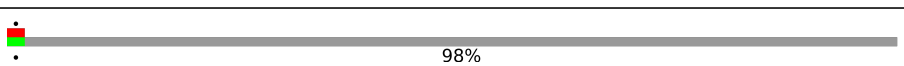
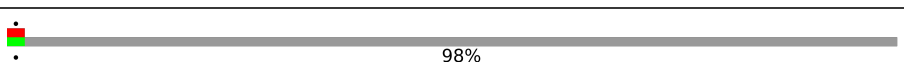
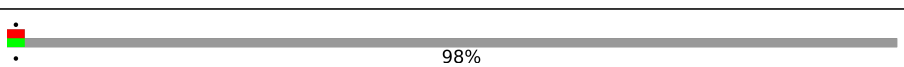
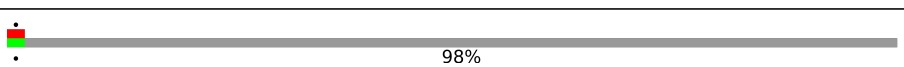
Mol	Chain	Length	Quality of chain
8	A	698	
9	B	90	
10	C	179	
11	D	276	
11	E	276	
11	F	276	
11	G	276	
11	H	276	
11	I	276	
11	J	276	
11	K	276	
11	L	276	
11	M	276	
11	N	276	
11	O	276	
11	P	276	
11	Q	276	
12	R	584	
12	S	584	
12	T	584	
12	U	584	
12	r	584	
12	s	584	
12	t	584	
12	u	584	

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 61430 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 RNA chain called sgRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	246	5239	2342	930	1722	245	0	0

- Molecule 2 is a DNA chain called Non-target strand - LE.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	2	67	1370	657	252	395	66	0	0

- Molecule 3 is a DNA chain called Target strand -LE.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	3	98	1995	958	344	595	98	0	0

- Molecule 4 is a DNA chain called LE.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	4	26	529	255	93	156	25	0	0

- Molecule 5 is a DNA chain called RE.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	5	26	535	257	94	158	26	0	0

- Molecule 6 is a DNA chain called Non-target strand - RE.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	6	48	986	470	187	281	48	0	0

- Molecule 7 is a DNA chain called Target strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	15	Total	C	N	O	P	0	0
			302	146	52	90	14		

- Molecule 8 is a protein called ShCas12k.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	602	Total	C	N	O	S	0	0
			4872	3072	882	903	15		

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-58	MET	-	initiating methionine	UNP A0A8X6EH11
A	-57	GLY	-	expression tag	UNP A0A8X6EH11
A	-56	SER	-	expression tag	UNP A0A8X6EH11
A	-55	SER	-	expression tag	UNP A0A8X6EH11
A	-54	HIS	-	expression tag	UNP A0A8X6EH11
A	-53	HIS	-	expression tag	UNP A0A8X6EH11
A	-52	HIS	-	expression tag	UNP A0A8X6EH11
A	-51	HIS	-	expression tag	UNP A0A8X6EH11
A	-50	HIS	-	expression tag	UNP A0A8X6EH11
A	-49	HIS	-	expression tag	UNP A0A8X6EH11
A	-48	SER	-	expression tag	UNP A0A8X6EH11
A	-47	SER	-	expression tag	UNP A0A8X6EH11
A	-46	GLY	-	expression tag	UNP A0A8X6EH11
A	-45	LEU	-	expression tag	UNP A0A8X6EH11
A	-44	VAL	-	expression tag	UNP A0A8X6EH11
A	-43	PRO	-	expression tag	UNP A0A8X6EH11
A	-42	ARG	-	expression tag	UNP A0A8X6EH11
A	-41	GLY	-	expression tag	UNP A0A8X6EH11
A	-40	SER	-	expression tag	UNP A0A8X6EH11
A	-39	HIS	-	expression tag	UNP A0A8X6EH11
A	-38	MET	-	expression tag	UNP A0A8X6EH11
A	-37	ALA	-	expression tag	UNP A0A8X6EH11
A	-36	SER	-	expression tag	UNP A0A8X6EH11
A	-35	TRP	-	expression tag	UNP A0A8X6EH11
A	-34	SER	-	expression tag	UNP A0A8X6EH11
A	-33	HIS	-	expression tag	UNP A0A8X6EH11
A	-32	PRO	-	expression tag	UNP A0A8X6EH11
A	-31	GLN	-	expression tag	UNP A0A8X6EH11
A	-30	PHE	-	expression tag	UNP A0A8X6EH11

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-29	GLU	-	expression tag	UNP A0A8X6EH11
A	-28	LYS	-	expression tag	UNP A0A8X6EH11
A	-27	GLY	-	expression tag	UNP A0A8X6EH11
A	-26	GLY	-	expression tag	UNP A0A8X6EH11
A	-25	GLY	-	expression tag	UNP A0A8X6EH11
A	-24	SER	-	expression tag	UNP A0A8X6EH11
A	-23	GLY	-	expression tag	UNP A0A8X6EH11
A	-22	GLY	-	expression tag	UNP A0A8X6EH11
A	-21	GLY	-	expression tag	UNP A0A8X6EH11
A	-20	SER	-	expression tag	UNP A0A8X6EH11
A	-19	GLY	-	expression tag	UNP A0A8X6EH11
A	-18	GLY	-	expression tag	UNP A0A8X6EH11
A	-17	SER	-	expression tag	UNP A0A8X6EH11
A	-16	ALA	-	expression tag	UNP A0A8X6EH11
A	-15	TRP	-	expression tag	UNP A0A8X6EH11
A	-14	SER	-	expression tag	UNP A0A8X6EH11
A	-13	HIS	-	expression tag	UNP A0A8X6EH11
A	-12	PRO	-	expression tag	UNP A0A8X6EH11
A	-11	GLN	-	expression tag	UNP A0A8X6EH11
A	-10	PHE	-	expression tag	UNP A0A8X6EH11
A	-9	GLU	-	expression tag	UNP A0A8X6EH11
A	-8	LYS	-	expression tag	UNP A0A8X6EH11
A	-7	GLU	-	expression tag	UNP A0A8X6EH11
A	-6	ASN	-	expression tag	UNP A0A8X6EH11
A	-5	LEU	-	expression tag	UNP A0A8X6EH11
A	-4	TYR	-	expression tag	UNP A0A8X6EH11
A	-3	PHE	-	expression tag	UNP A0A8X6EH11
A	-2	GLN	-	expression tag	UNP A0A8X6EH11
A	-1	GLY	-	expression tag	UNP A0A8X6EH11
A	0	GLY	-	expression tag	UNP A0A8X6EH11
A	1	SER	-	expression tag	UNP A0A8X6EH11

- Molecule 9 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	87	Total	C	N	O	S	0	0
			708	438	141	128	1		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	SER	-	expression tag	UNP A0A139X9A4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	3	ALA	THR	variant	UNP A0A139X9A4
B	7	GLU	GLN	variant	UNP A0A139X9A4
B	14	VAL	SER	variant	UNP A0A139X9A4
B	30	VAL	ILE	variant	UNP A0A139X9A4
B	42	LEU	GLU	variant	UNP A0A139X9A4
B	46	ALA	SER	variant	UNP A0A139X9A4
B	71	ILE	VAL	variant	UNP A0A139X9A4
B	73	LYS	GLN	variant	UNP A0A139X9A4
B	74	ASP	GLY	variant	UNP A0A139X9A4
B	78	LYS	HIS	variant	UNP A0A139X9A4

- Molecule 10 is a protein called TniQ.

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

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	168	GLY	-	expression tag	UNP A0A8J0PCL5
C	169	SER	-	expression tag	UNP A0A8J0PCL5
C	170	GLU	-	expression tag	UNP A0A8J0PCL5
C	171	PHE	-	expression tag	UNP A0A8J0PCL5
C	172	GLU	-	expression tag	UNP A0A8J0PCL5
C	173	LEU	-	expression tag	UNP A0A8J0PCL5
C	174	GLU	-	expression tag	UNP A0A8J0PCL5
C	175	ASN	-	expression tag	UNP A0A8J0PCL5
C	176	LEU	-	expression tag	UNP A0A8J0PCL5
C	177	TYR	-	expression tag	UNP A0A8J0PCL5
C	178	PHE	-	expression tag	UNP A0A8J0PCL5
C	179	GLN	-	expression tag	UNP A0A8J0PCL5

- Molecule 11 is a protein called ShTnsC.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		
11	E	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		
11	F	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		
11	H	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		
11	I	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		
11	J	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		
11	K	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		
11	L	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		
11	M	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		
11	N	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		
11	O	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		
11	P	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		
11	Q	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	SER	-	expression tag	UNP A0A8J0PCL3
E	1	SER	-	expression tag	UNP A0A8J0PCL3
F	1	SER	-	expression tag	UNP A0A8J0PCL3
G	1	SER	-	expression tag	UNP A0A8J0PCL3
H	1	SER	-	expression tag	UNP A0A8J0PCL3
I	1	SER	-	expression tag	UNP A0A8J0PCL3
J	1	SER	-	expression tag	UNP A0A8J0PCL3
K	1	SER	-	expression tag	UNP A0A8J0PCL3
L	1	SER	-	expression tag	UNP A0A8J0PCL3
M	1	SER	-	expression tag	UNP A0A8J0PCL3
N	1	SER	-	expression tag	UNP A0A8J0PCL3
O	1	SER	-	expression tag	UNP A0A8J0PCL3
P	1	SER	-	expression tag	UNP A0A8J0PCL3
Q	1	SER	-	expression tag	UNP A0A8J0PCL3

- Molecule 12 is a protein called TnsB.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	R	504	Total	C	N	O	S	0	0
			4043	2520	745	766	12		
12	S	500	Total	C	N	O	S	0	0
			4010	2501	737	760	12		
12	T	297	Total	C	N	O	S	0	0
			2393	1502	433	448	10		
12	U	299	Total	C	N	O	S	0	0
			2419	1518	442	449	10		
12	r	13	Total	C	N	O		0	0
			121	77	18	26			
12	s	13	Total	C	N	O		0	0
			121	77	18	26			
12	t	13	Total	C	N	O		0	0
			121	77	18	26			
12	u	13	Total	C	N	O		0	0
			121	77	18	26			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	1	SER	-	expression tag	UNP A0A979HMQ2
S	1	SER	-	expression tag	UNP A0A979HMQ2
T	1	SER	-	expression tag	UNP A0A979HMQ2
U	1	SER	-	expression tag	UNP A0A979HMQ2
r	1	SER	-	expression tag	UNP A0A979HMQ2
s	1	SER	-	expression tag	UNP A0A979HMQ2
t	1	SER	-	expression tag	UNP A0A979HMQ2
u	1	SER	-	expression tag	UNP A0A979HMQ2

- Molecule 13 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
13	1	1	Total	Mg	0
			1	1	
13	D	1	Total	Mg	0
			1	1	
13	E	1	Total	Mg	0
			1	1	
13	F	1	Total	Mg	0
			1	1	
13	G	1	Total	Mg	0
			1	1	

Continued on next page...

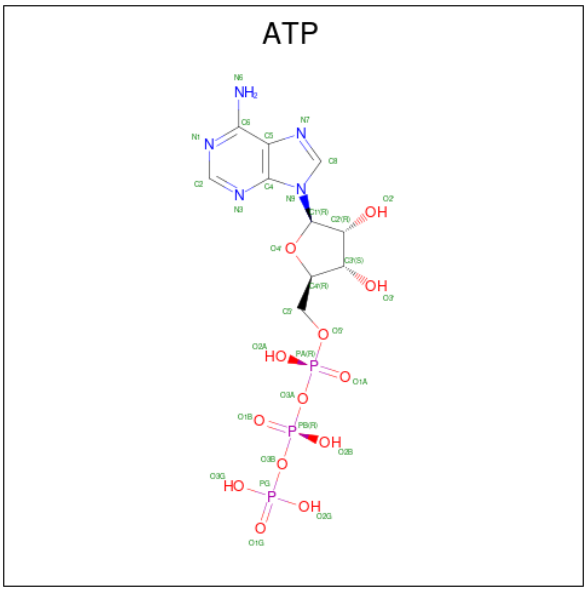
Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
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	N	1	Total Mg 1 1	0
13	O	1	Total Mg 1 1	0
13	P	1	Total Mg 1 1	0
13	Q	1	Total Mg 1 1	0
13	R	1	Total Mg 1 1	0
13	S	1	Total Mg 1 1	0

- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
14	C	2	Total Zn 2 2	0

- Molecule 15 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

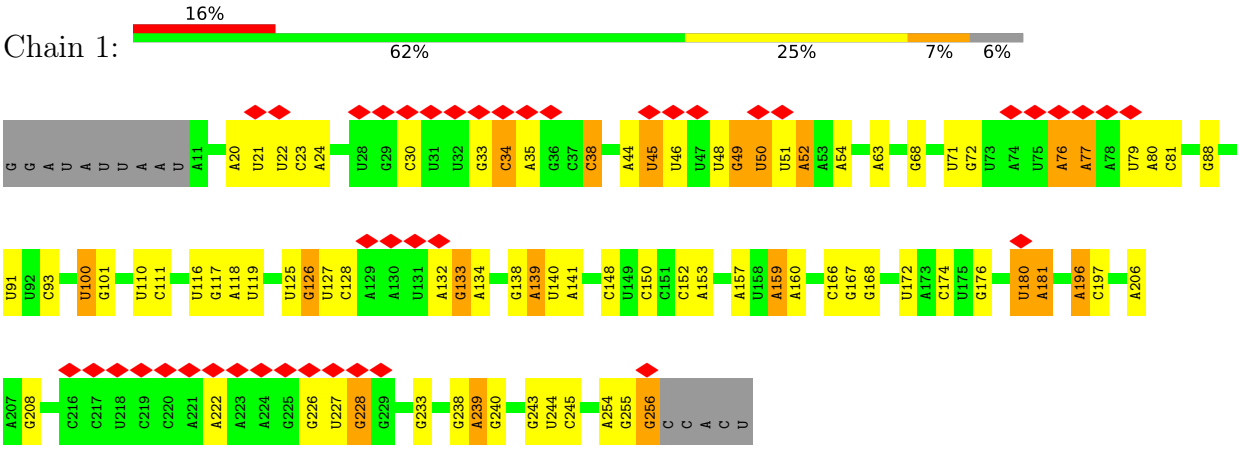
- Molecule 16 is water.

Mol	Chain	Residues	Atoms	AltConf
16	1	160	Total O 160 160	0
16	2	11	Total O 11 11	0
16	3	34	Total O 34 34	0
16	A	93	Total O 93 93	0
16	B	13	Total O 13 13	0
16	C	17	Total O 17 17	0
16	D	13	Total O 13 13	0
16	E	34	Total O 34 34	0
16	F	48	Total O 48 48	0
16	G	46	Total O 46 46	0
16	H	44	Total O 44 44	0
16	I	45	Total O 45 45	0
16	J	55	Total O 55 55	0
16	K	53	Total O 53 53	0
16	L	55	Total O 55 55	0
16	M	49	Total O 49 49	0
16	N	44	Total O 44 44	0
16	O	29	Total O 29 29	0
16	P	14	Total O 14 14	0
16	Q	4	Total O 4 4	0
16	r	1	Total O 1 1	0

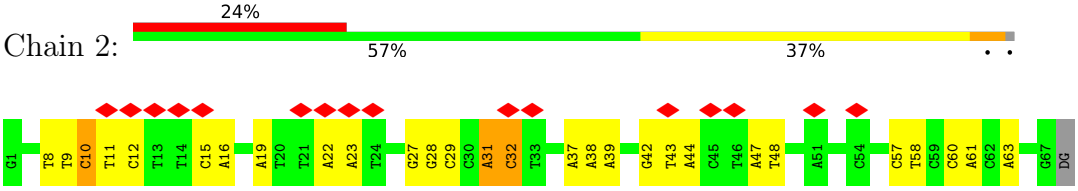
3 Residue-property plots (i)

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.

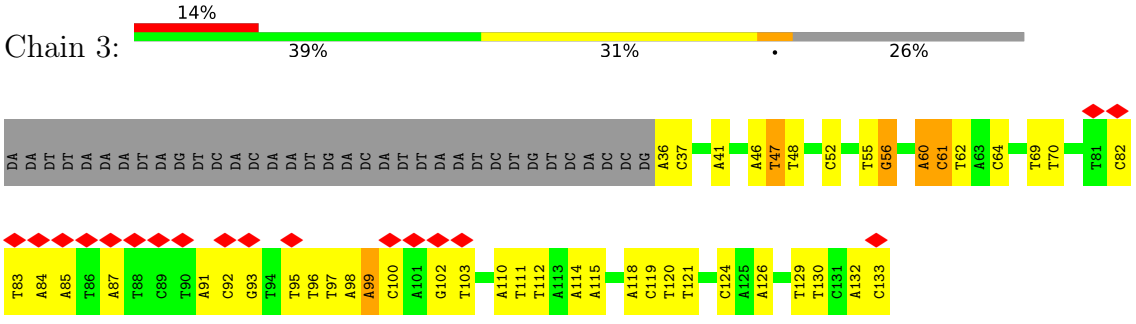
• Molecule 1: sgRNA



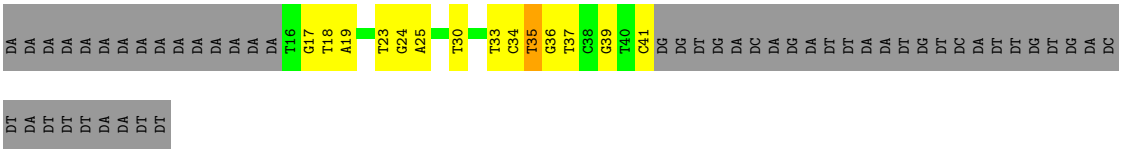
• Molecule 2: Non-target strand - LE



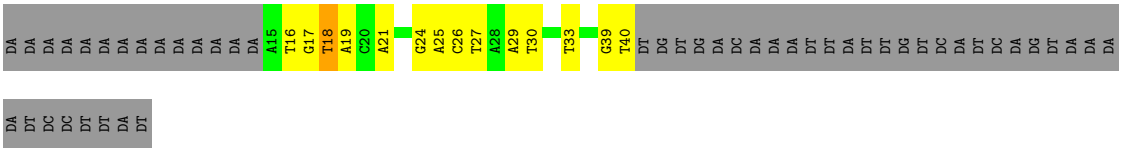
• Molecule 3: Target strand -LE



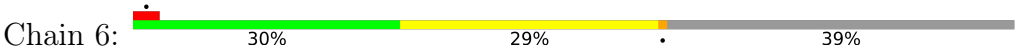
• Molecule 4: LE

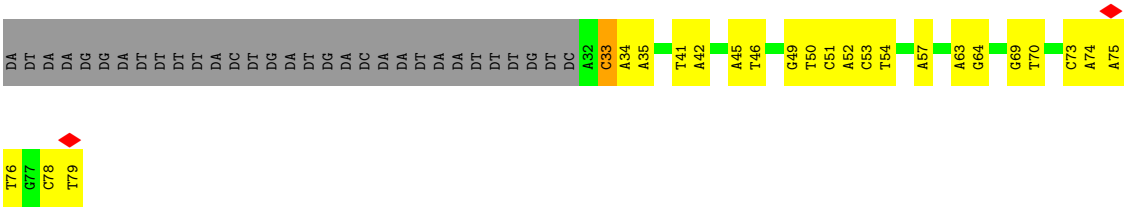


• Molecule 5: RE



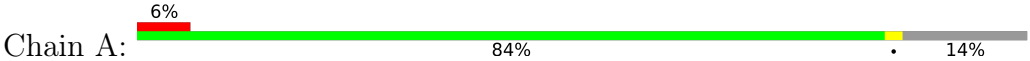
• Molecule 6: Non-target strand - RE

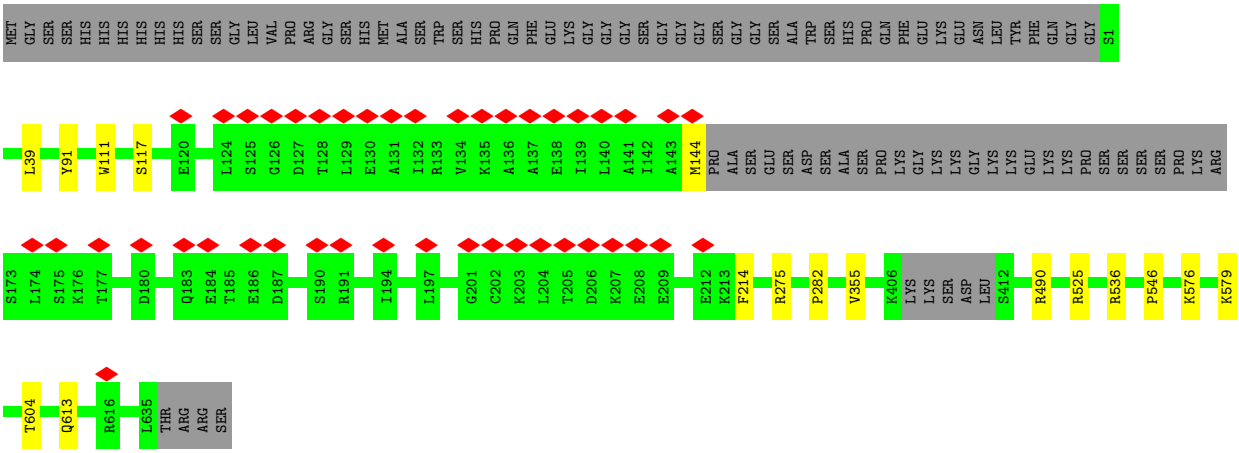




• Molecule 7: Target strand

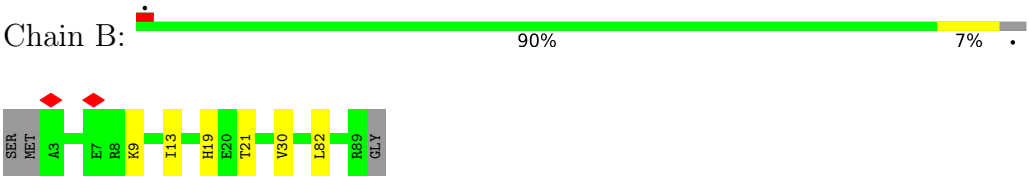
• Molecule 8: ShCas12k





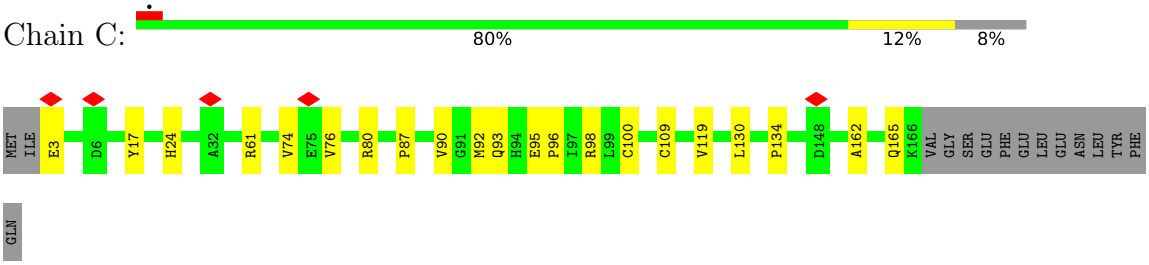
• Molecule 9: Small ribosomal subunit protein uS15

Chain B:



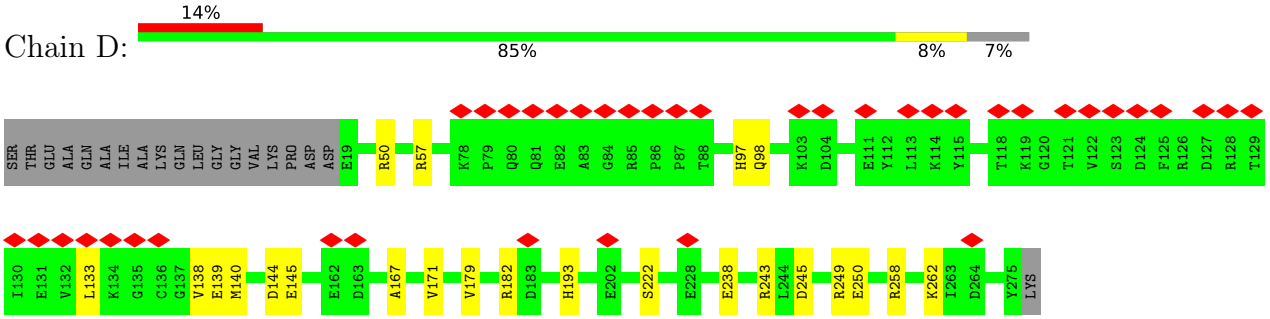
• Molecule 10: TniQ

Chain C:



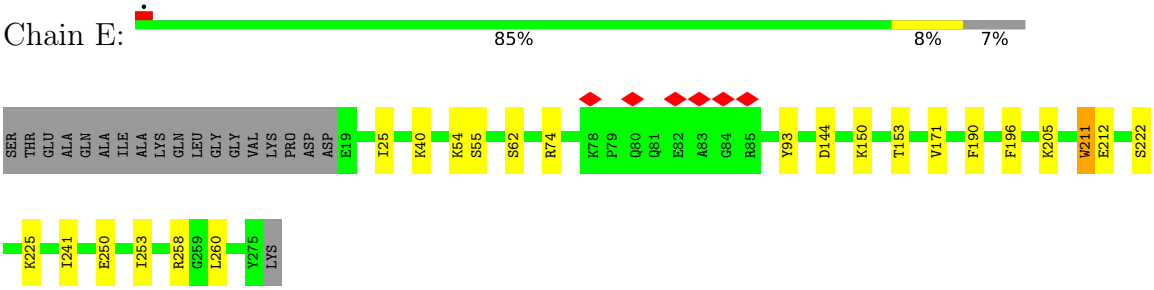
• Molecule 11: ShTnsC

Chain D:



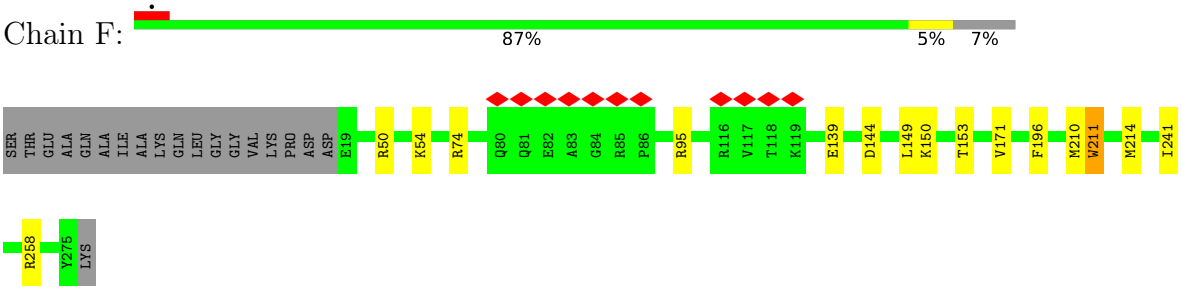
• Molecule 11: ShTnsC

Chain E:



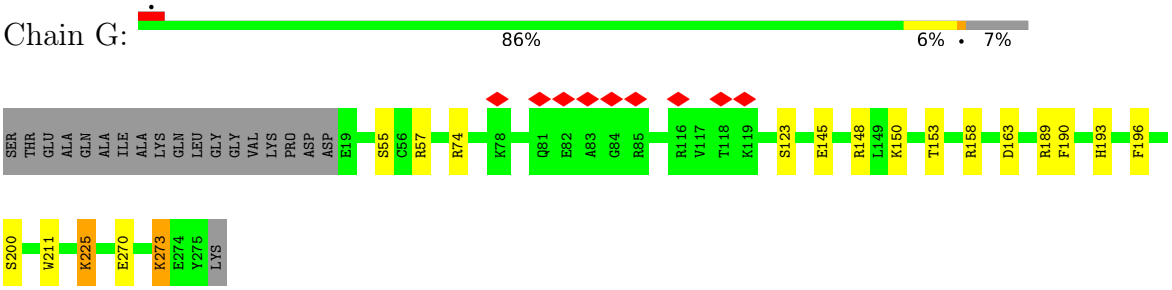
• Molecule 11: ShTnsC

Chain F:



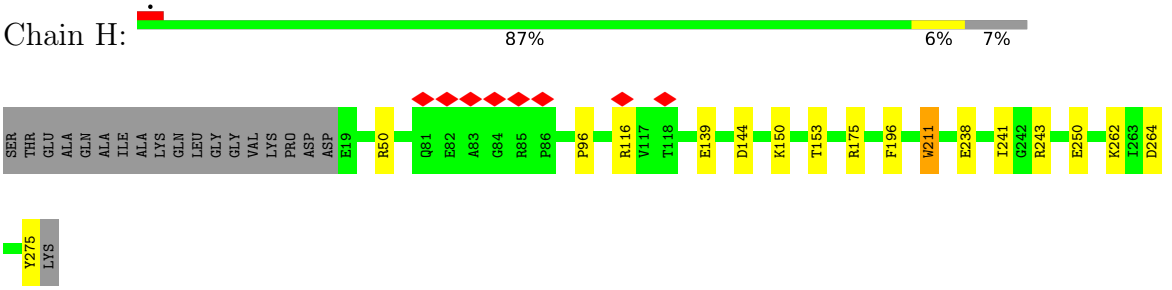
• Molecule 11: ShTnsC

Chain G:



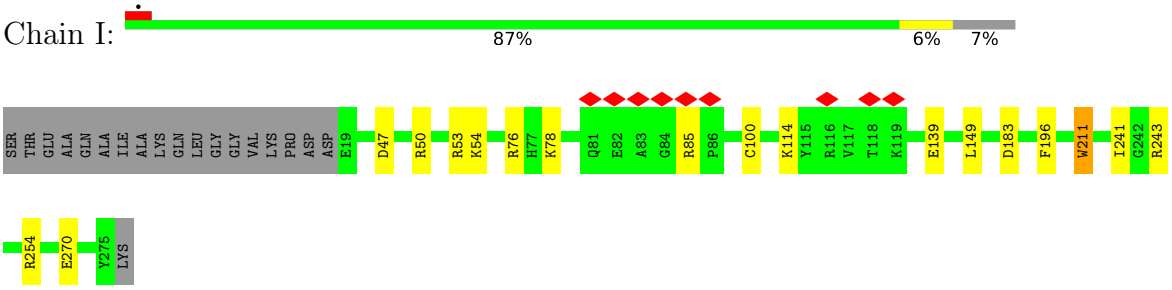
• Molecule 11: ShTnsC

Chain H:



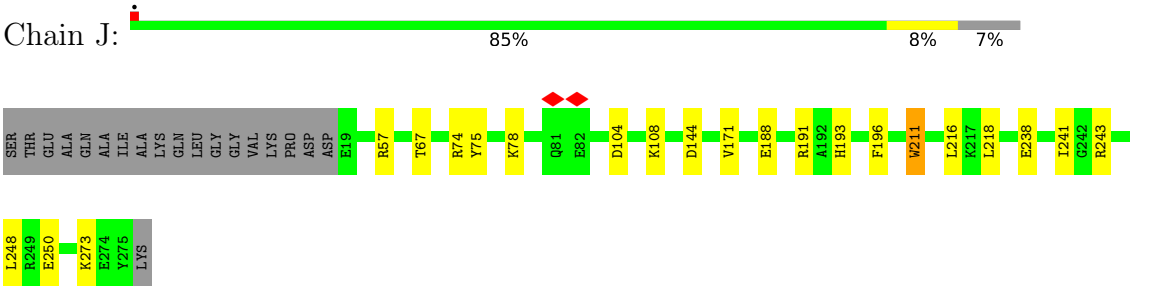
• Molecule 11: ShTnsC

Chain I:



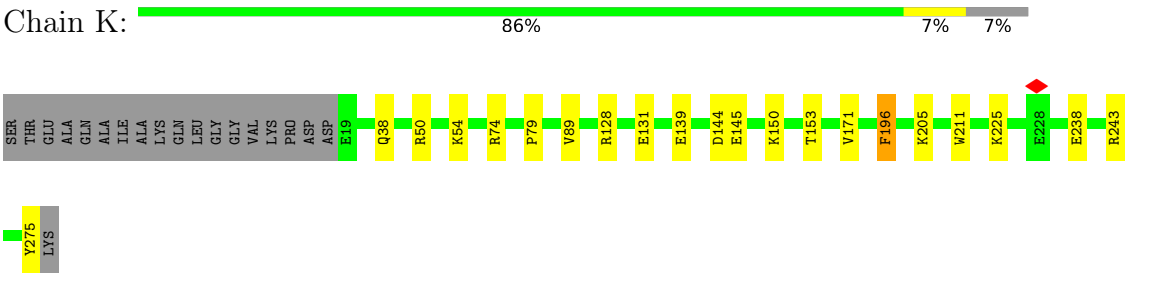
• Molecule 11: ShTnsC

Chain J:



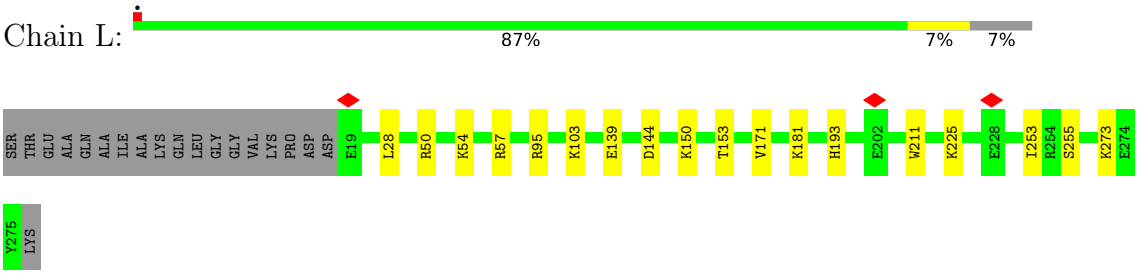
• Molecule 11: ShTnsC

Chain K:



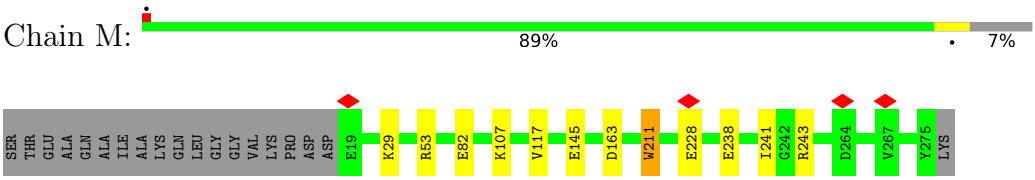
• Molecule 11: ShTnsC

Chain L:



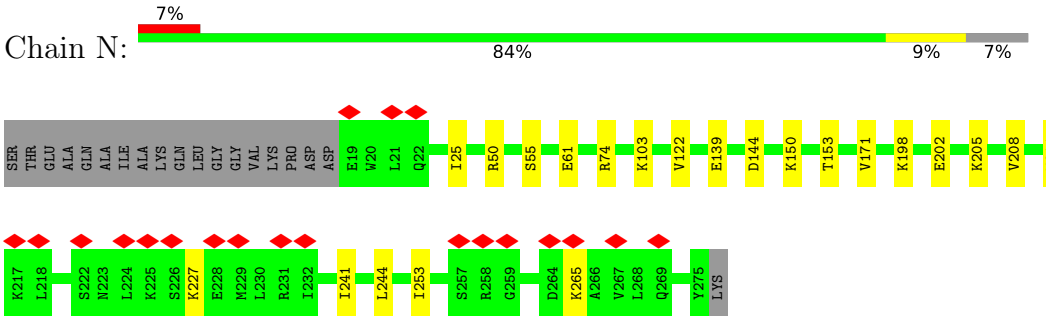
• Molecule 11: ShTnsC

Chain M:



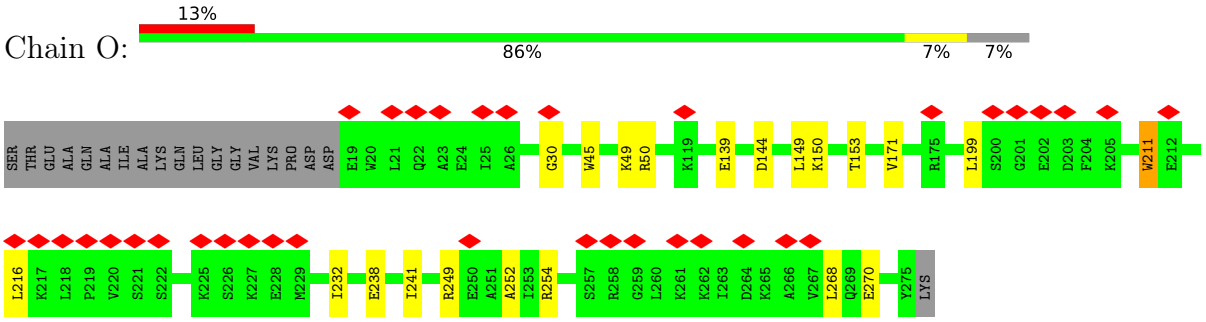
• Molecule 11: ShTnsC

Chain N:



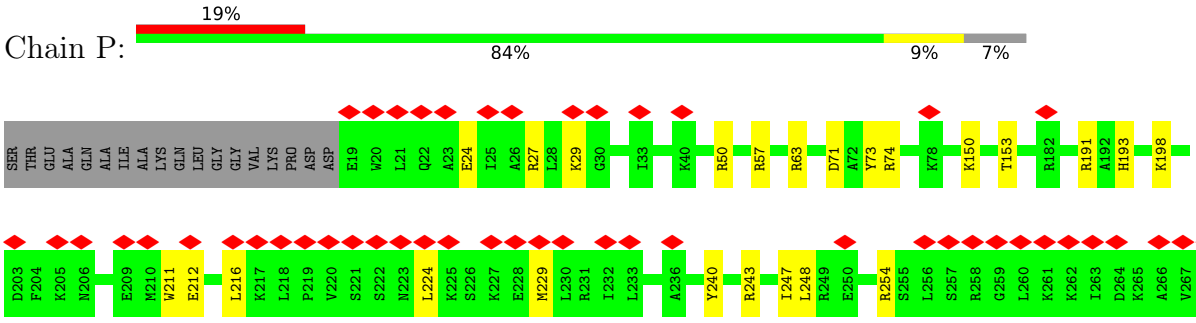
• Molecule 11: ShTnsC

Chain O:



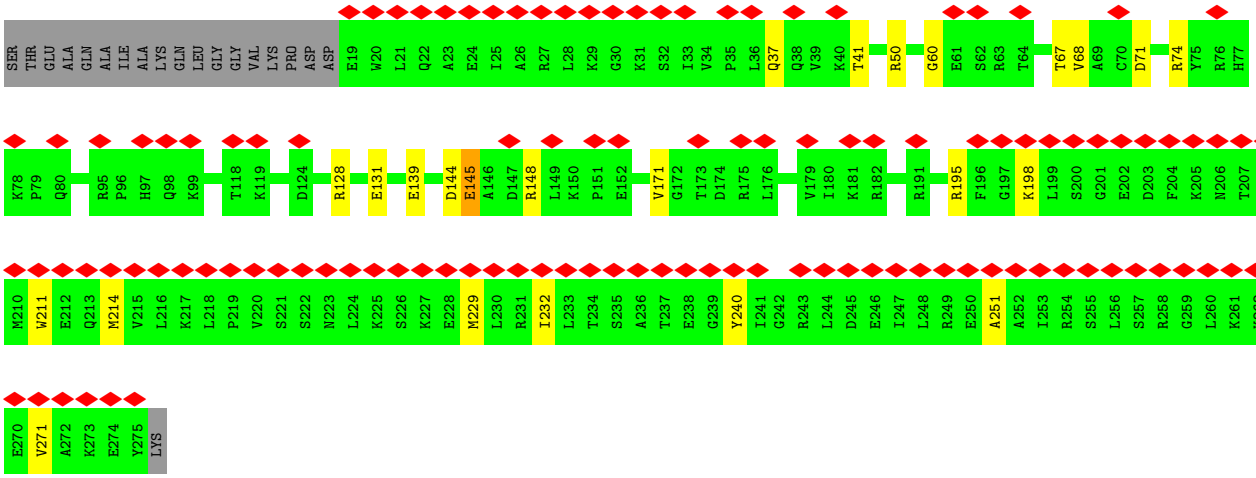
• Molecule 11: ShTnsC

Chain P:



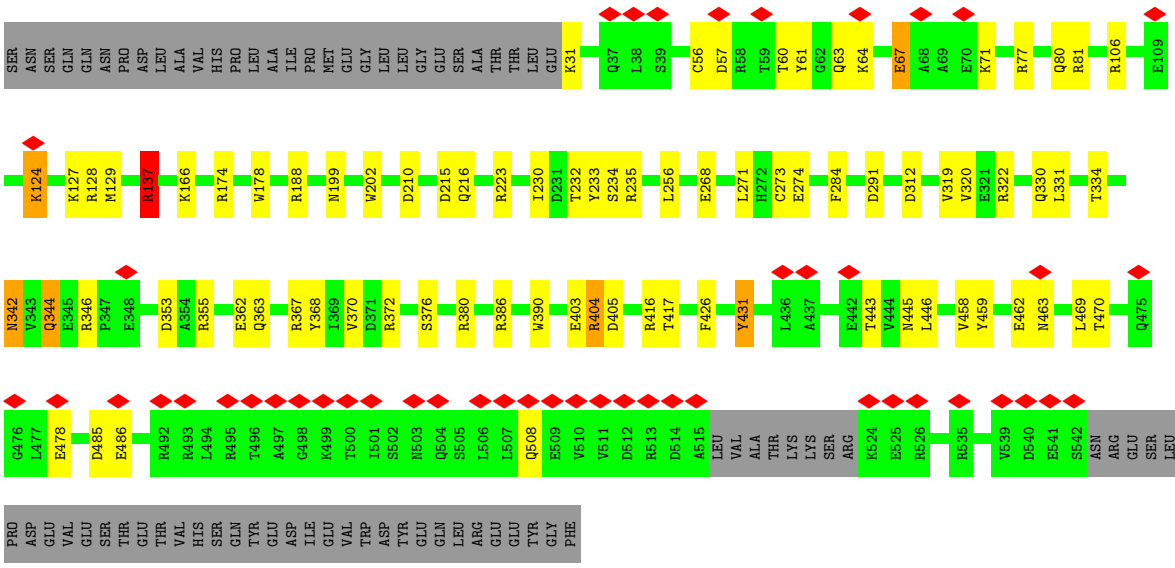
• Molecule 11: ShTnsC

Chain Q:



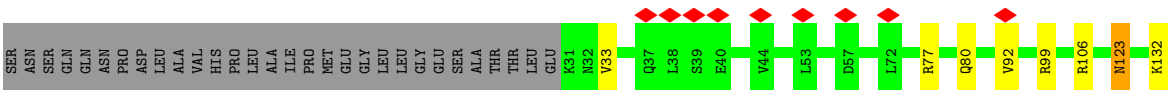
• Molecule 12: TnsB

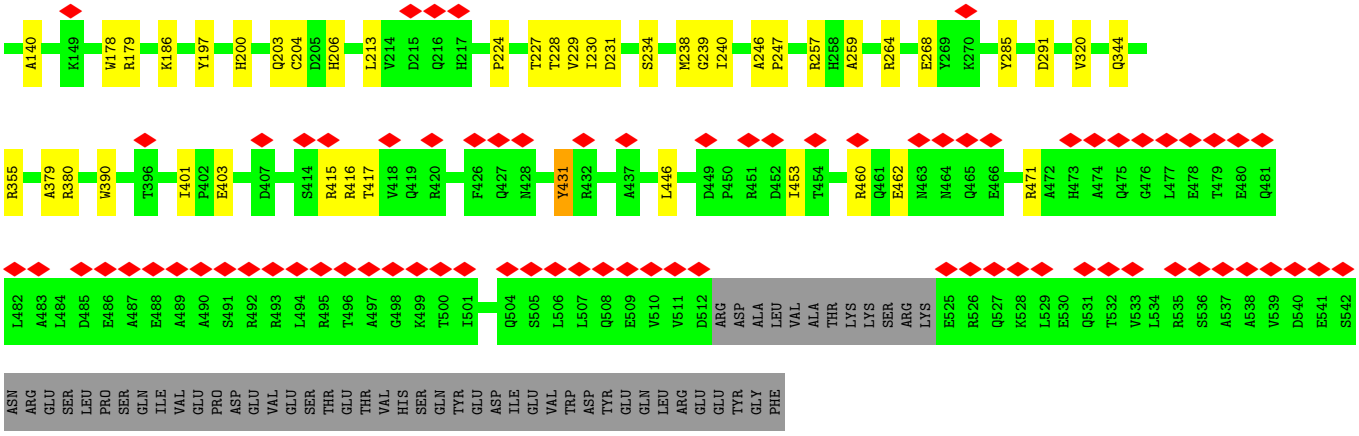
Chain R:



• Molecule 12: TnsB

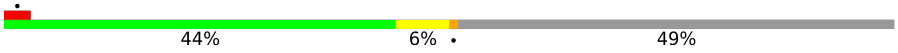
Chain S:

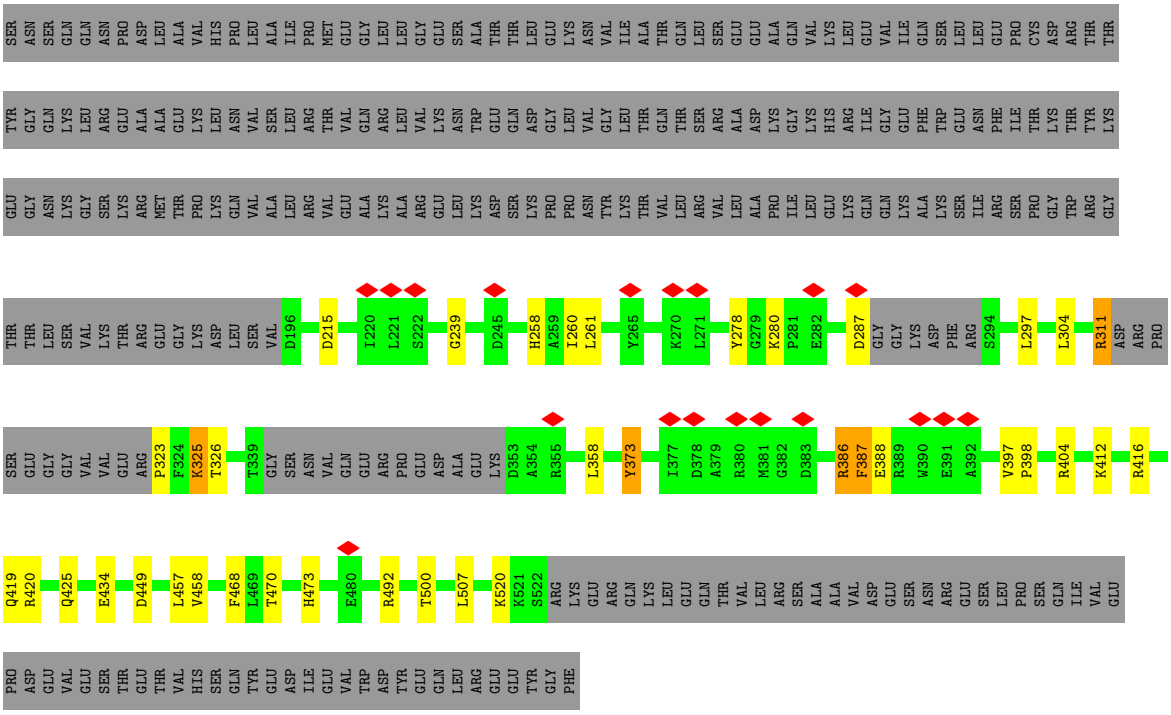




• Molecule 12: TnsB

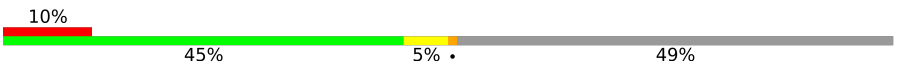
Chain T:

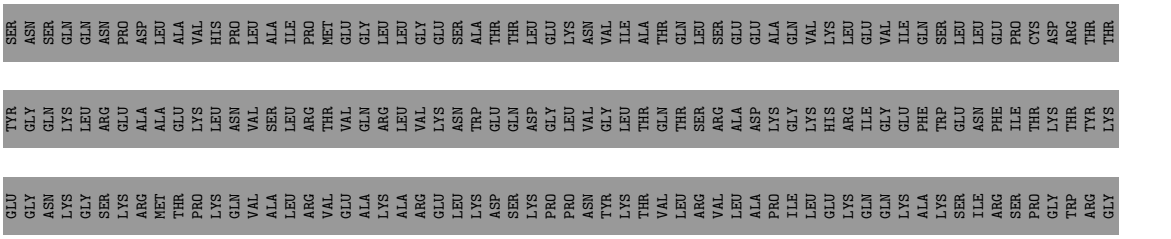


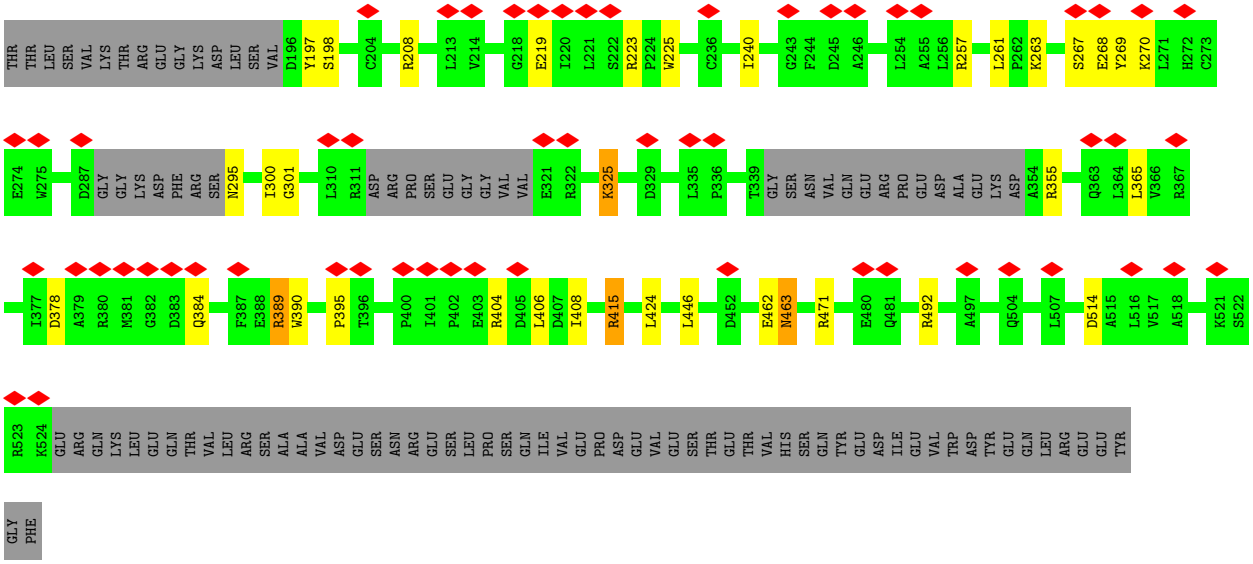


• Molecule 12: TnsB

Chain U:

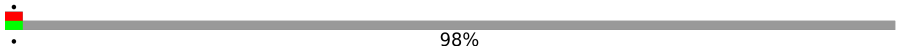


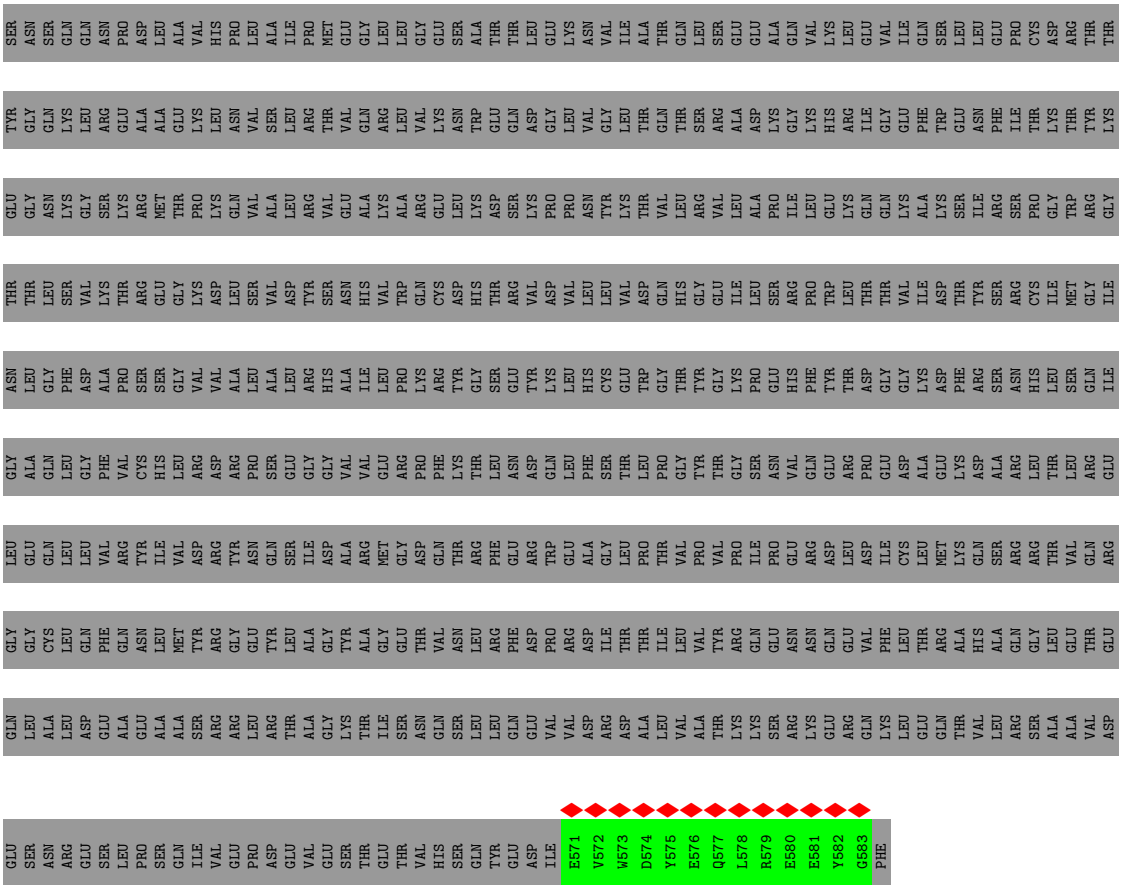




• Molecule 12: TnsB

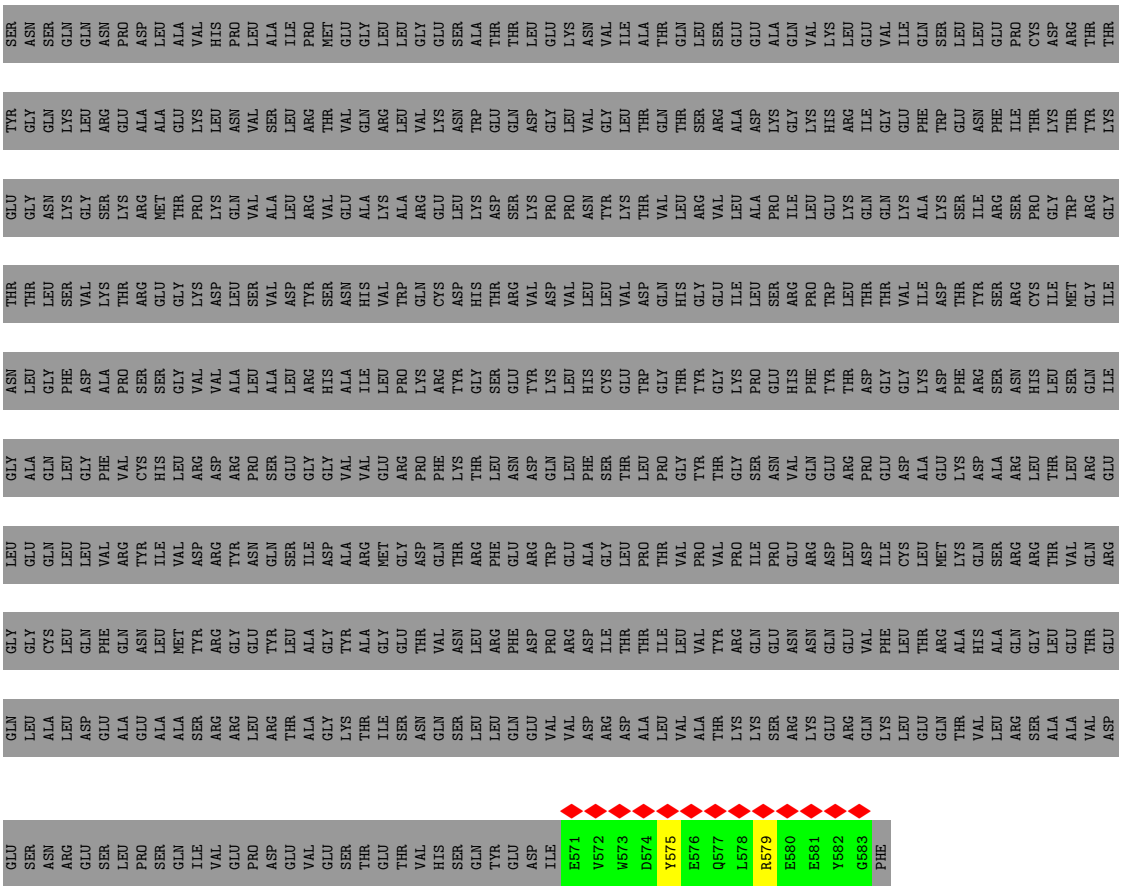
Chain r:





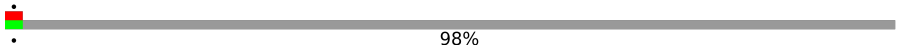
• Molecule 12: TnsB

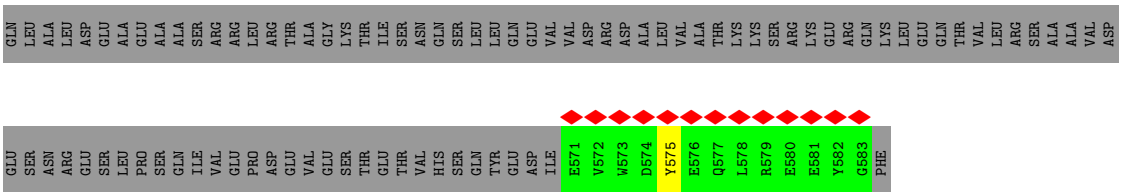
Chain s:



• Molecule 12: TnsB

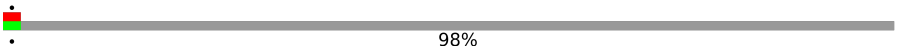
Chain t:

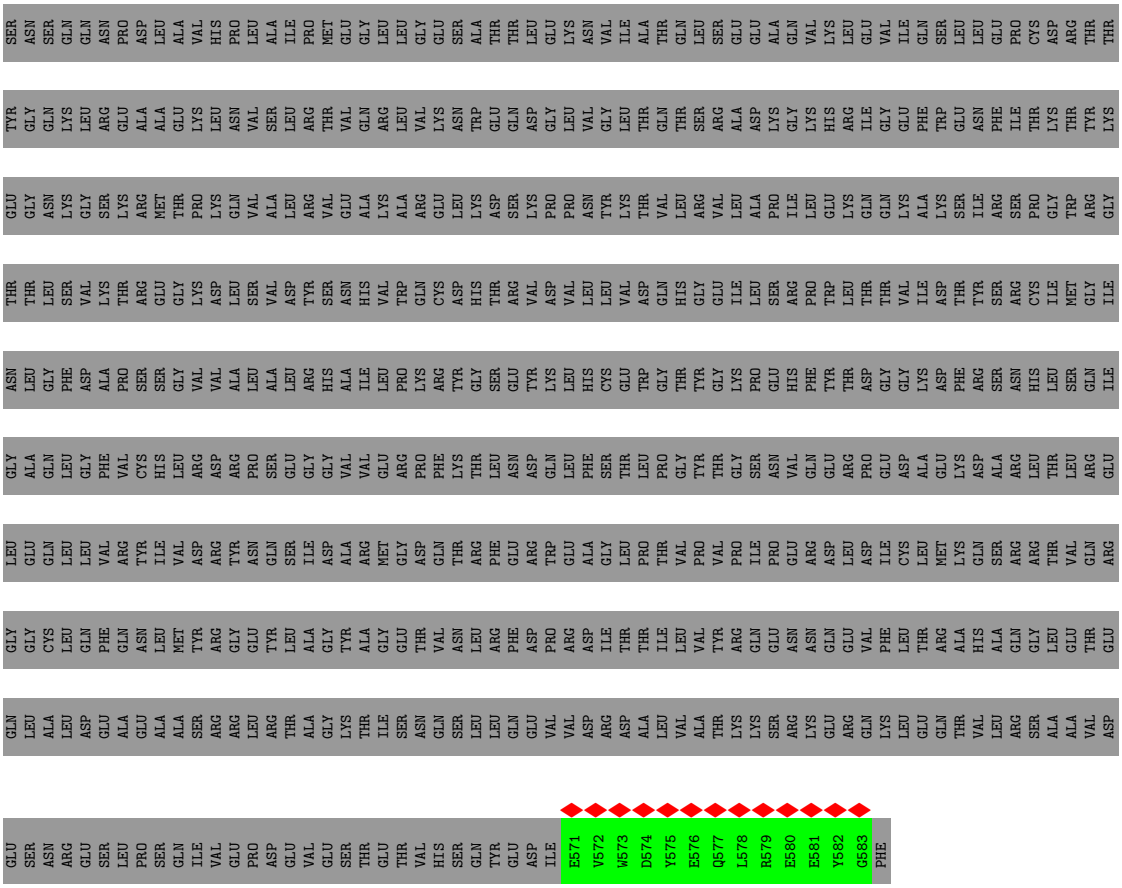




• Molecule 12: TnsB

Chain u:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	258000	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.284	Depositor
Minimum map value	-1.299	Depositor
Average map value	-0.006	Depositor
Map value standard deviation	0.087	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	173.99199, 175.448, 351.624	wwPDB
Map dimensions	239, 241, 483	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.7279999, 0.728, 0.728	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, ZN, 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	1	0.56	0/5858	1.07	3/9128 (0.0%)
2	2	0.72	0/1538	1.15	5/2371 (0.2%)
3	3	0.81	0/2232	1.21	12/3440 (0.3%)
4	4	0.86	0/592	1.18	4/912 (0.4%)
5	5	0.94	0/599	1.23	5/923 (0.5%)
6	6	0.85	0/1108	1.20	6/1707 (0.4%)
7	7	0.70	0/337	1.16	1/518 (0.2%)
8	A	0.30	0/4959	0.53	0/6686
9	B	0.29	0/713	0.55	0/952
10	C	0.32	0/1345	0.56	0/1819
11	D	0.28	0/2097	0.56	0/2817
11	E	0.31	0/2097	0.57	0/2817
11	F	0.33	0/2097	0.58	0/2817
11	G	0.33	0/2097	0.56	0/2817
11	H	0.34	0/2097	0.57	0/2817
11	I	0.33	0/2097	0.56	0/2817
11	J	0.33	0/2097	0.58	0/2817
11	K	0.34	0/2097	0.59	0/2817
11	L	0.34	0/2097	0.57	0/2817
11	M	0.33	0/2097	0.58	0/2817
11	N	0.33	0/2097	0.58	0/2817
11	O	0.31	0/2097	0.56	0/2817
11	P	0.29	0/2097	0.56	0/2817
11	Q	0.26	0/2097	0.56	0/2817
12	R	0.37	0/4112	0.61	0/5551
12	S	0.33	0/4079	0.60	0/5508
12	T	0.31	0/2439	0.60	0/3302
12	U	0.27	0/2465	0.58	0/3335
12	r	0.29	0/124	0.60	0/167
12	s	0.31	0/124	0.58	0/167
12	t	0.27	0/124	0.47	0/167
12	u	0.28	0/124	0.59	0/167

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
All	All	0.42	0/62230	0.73	36/86258 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
12	R	0	1
12	S	0	2
All	All	0	3

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	6	64	DG	O4'-C1'-N9	10.01	115.00	108.00
3	3	130	DT	P-O3'-C3'	-8.94	108.97	119.70
5	5	18	DT	O4'-C1'-N1	-7.25	102.92	108.00
2	2	10	DC	O4'-C4'-C3'	-6.86	101.76	104.50
3	3	126	DA	O4'-C1'-N9	6.40	112.48	108.00
2	2	31	DA	O4'-C1'-N9	6.31	112.41	108.00
3	3	100	DC	O4'-C1'-N1	6.21	112.35	108.00
3	3	124	DC	O4'-C1'-N1	6.20	112.34	108.00
3	3	61	DC	P-O3'-C3'	6.02	126.93	119.70
4	4	18	DT	O4'-C1'-N1	-6.01	103.79	108.00
4	4	35	DT	O4'-C4'-C3'	-5.96	102.12	104.50
1	1	196	A	P-O3'-C3'	5.90	126.78	119.70
3	3	56	DG	O4'-C1'-N9	-5.89	103.88	108.00
3	3	129	DT	P-O3'-C3'	-5.85	112.68	119.70
2	2	63	DA	O4'-C1'-N9	-5.84	103.91	108.00
3	3	52	DC	O4'-C1'-N1	5.80	112.06	108.00
5	5	40	DT	O4'-C1'-N1	5.68	111.98	108.00
5	5	39	DG	O4'-C1'-N9	5.48	111.84	108.00
2	2	32	DC	C1'-O4'-C4'	-5.48	104.62	110.10
3	3	64	DC	C3'-C2'-C1'	-5.41	96.01	102.50
6	6	57	DA	P-O3'-C3'	5.39	126.17	119.70
6	6	64	DG	C1'-O4'-C4'	-5.38	104.72	110.10
1	1	254	A	O4'-C1'-N9	5.36	112.49	108.20
3	3	60	DA	C1'-O4'-C4'	-5.34	104.76	110.10
4	4	33	DT	O4'-C1'-N1	5.33	111.73	108.00
3	3	47	DT	O4'-C1'-N1	5.30	111.71	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	5	33	DT	O4'-C1'-N1	5.29	111.70	108.00
2	2	29	DC	O4'-C1'-C2'	5.26	110.11	105.90
7	7	5	DT	P-O3'-C3'	5.23	125.98	119.70
6	6	33	DC	O4'-C1'-N1	5.22	111.66	108.00
1	1	30	C	O4'-C1'-N1	5.19	112.35	108.20
6	6	57	DA	O4'-C1'-C2'	5.17	110.04	105.90
5	5	40	DT	C1'-O4'-C4'	-5.16	104.94	110.10
4	4	35	DT	O4'-C1'-N1	5.11	111.58	108.00
3	3	99	DA	O4'-C1'-N9	-5.11	104.43	108.00
6	6	45	DA	O4'-C1'-N9	5.10	111.57	108.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	R	137	ARG	Sidechain
12	S	355	ARG	Sidechain
12	S	99	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	5239	0	2644	34	0
2	2	1370	0	758	20	0
3	3	1995	0	1113	32	0
4	4	529	0	297	11	0
5	5	535	0	297	9	0
6	6	986	0	540	16	0
7	7	302	0	171	7	0
8	A	4872	0	4938	10	0
9	B	708	0	748	3	0
10	C	1306	0	1285	12	0
11	D	2066	0	2157	13	0
11	E	2066	0	2157	13	0
11	F	2066	0	2157	11	0
11	G	2066	0	2157	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	H	2066	0	2157	10	0
11	I	2066	0	2157	11	0
11	J	2066	0	2157	12	0
11	K	2066	0	2157	11	0
11	L	2066	0	2157	7	0
11	M	2066	0	2157	6	0
11	N	2066	0	2157	11	0
11	O	2066	0	2157	10	0
11	P	2066	0	2157	12	0
11	Q	2066	0	2157	14	0
12	R	4043	0	4055	53	0
12	S	4010	0	4020	34	0
12	T	2393	0	2355	22	0
12	U	2419	0	2390	20	0
12	r	121	0	99	0	0
12	s	121	0	99	0	0
12	t	121	0	99	0	0
12	u	121	0	99	0	0
13	1	1	0	0	0	0
13	D	1	0	0	0	0
13	E	1	0	0	0	0
13	F	1	0	0	0	0
13	G	1	0	0	0	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	N	1	0	0	0	0
13	O	1	0	0	0	0
13	P	1	0	0	0	0
13	Q	1	0	0	0	0
13	R	1	0	0	0	0
13	S	1	0	0	0	0
14	C	2	0	0	0	0
15	D	31	0	12	0	0
15	E	31	0	12	1	0
15	F	31	0	12	0	0
15	G	31	0	12	0	0
15	H	31	0	12	0	0
15	I	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	J	31	0	12	1	0
15	K	31	0	12	0	0
15	L	31	0	12	0	0
15	M	31	0	12	0	0
15	N	31	0	12	0	0
15	O	31	0	12	0	0
15	P	31	0	12	1	0
15	Q	31	0	12	3	0
16	1	160	0	0	2	0
16	2	11	0	0	0	0
16	3	34	0	0	0	0
16	A	93	0	0	0	0
16	B	13	0	0	0	0
16	C	17	0	0	0	0
16	D	13	0	0	1	0
16	E	34	0	0	0	0
16	F	48	0	0	0	0
16	G	46	0	0	1	0
16	H	44	0	0	0	0
16	I	45	0	0	0	0
16	J	55	0	0	0	0
16	K	53	0	0	1	0
16	L	55	0	0	0	0
16	M	49	0	0	1	0
16	N	44	0	0	1	0
16	O	29	0	0	0	0
16	P	14	0	0	0	0
16	Q	4	0	0	0	0
16	r	1	0	0	0	0
All	All	61430	0	56373	387	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 3.

All (387) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:51:DC:H2'	6:6:52:DA:C8	2.15	0.82
12:R:268:GLU:O	12:R:363:GLN:NE2	2.19	0.74
1:1:256:G:OP2	10:C:61:ARG:NH1	2.19	0.74
11:N:50:ARG:NH1	11:N:139:GLU:OE2	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:100:U:H3	1:1:139:A:H2	1.37	0.72
5:5:19:DA:N3	12:R:322:ARG:NH1	2.41	0.69
8:A:282:PRO:HB3	8:A:355:VAL:HG22	1.75	0.68
12:R:376:SER:OG	12:R:386:ARG:NH1	2.27	0.68
10:C:100:CYS:O	10:C:165:GLN:NE2	2.27	0.67
10:C:95:GLU:HB3	10:C:96:PRO:HD3	1.77	0.67
12:R:403:GLU:OE1	12:R:404:ARG:NH1	2.28	0.66
11:J:188:GLU:OE1	11:J:191:ARG:NH1	2.29	0.66
11:H:50:ARG:NH1	11:H:139:GLU:OE2	2.23	0.65
1:1:239:A:OP2	8:A:525:ARG:NH2	2.29	0.65
6:6:73:DC:H2'	6:6:74:DA:C8	2.32	0.64
11:K:128:ARG:NH1	11:K:131:GLU:OE2	2.30	0.63
9:B:30:VAL:HG21	9:B:82:LEU:HD21	1.79	0.62
11:F:50:ARG:NH1	11:F:139:GLU:OE2	2.31	0.61
12:S:228:THR:HG22	12:S:240:ILE:HG22	1.83	0.61
5:5:18:DT:OP1	12:R:380:ARG:NH2	2.31	0.61
12:R:67:GLU:OE1	12:R:71:LYS:NZ	2.33	0.61
1:1:239:A:H2'	1:1:240:G:C8	2.35	0.60
11:O:50:ARG:NH1	11:O:139:GLU:OE2	2.30	0.60
1:1:239:A:H2'	1:1:240:G:H8	1.67	0.60
12:R:330:GLN:OE1	12:R:372:ARG:NH2	2.35	0.60
12:R:31:LYS:HE3	12:T:404:ARG:HG2	1.84	0.60
11:Q:251:ALA:HA	11:Q:271:VAL:HG21	1.84	0.59
11:J:67:THR:OG1	15:J:300:ATP:O2B	2.20	0.59
12:S:229:VAL:HG21	12:S:259:ALA:HB2	1.84	0.59
11:F:258:ARG:HH11	11:F:258:ARG:HG3	1.67	0.59
12:U:408:ILE:HD12	12:U:408:ILE:H	1.67	0.59
1:1:176:G:N7	16:1:406:HOH:O	2.32	0.59
11:N:55:SER:O	16:N:401:HOH:O	2.16	0.58
12:R:353:ASP:OD1	12:T:520:LYS:NZ	2.28	0.58
12:R:417:THR:HA	12:R:443:THR:HA	1.85	0.58
11:P:254:ARG:NH2	11:P:274:GLU:OE2	2.33	0.58
12:R:174:ARG:NH1	12:T:419:GLN:OE1	2.33	0.58
11:F:95:ARG:NH2	11:G:163:ASP:OD1	2.36	0.58
11:O:254:ARG:NH1	11:O:270:GLU:OE2	2.37	0.58
11:N:103:LYS:HG3	11:N:122:VAL:HG22	1.86	0.57
12:S:206:HIS:ND1	12:S:227:THR:OG1	2.26	0.57
2:2:10:DC:H2"	2:2:11:DT:H72	1.85	0.57
3:3:114:DA:H2'	3:3:115:DA:C8	2.39	0.57
11:P:212:GLU:HB2	11:P:224:LEU:HD12	1.87	0.57
2:2:44:DA:H5'	2:2:44:DA:C8	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:36:DA:H1'	3:3:37:DC:O5'	2.04	0.56
11:N:241:ILE:HD12	11:N:241:ILE:H	1.70	0.56
5:5:24:DG:H2"	5:5:25:DA:C8	2.40	0.56
11:D:222:SER:HA	11:D:262:LYS:HE3	1.87	0.56
12:S:178:TRP:O	12:S:380:ARG:NH1	2.38	0.56
12:R:56:CYS:SG	12:R:64:LYS:HD3	2.46	0.56
3:3:111:DT:H2'	3:3:112:DT:C6	2.41	0.56
3:3:91:DA:H2'	3:3:92:DC:C6	2.40	0.55
12:S:230:ILE:HD12	12:S:320:VAL:HA	1.87	0.55
11:Q:60:GLY:HA2	11:Q:195:ARG:NH2	2.22	0.55
11:K:205:LYS:HE3	11:K:225:LYS:HD2	1.89	0.55
11:E:150:LYS:O	11:E:153:THR:HG22	2.06	0.55
11:N:150:LYS:O	11:N:153:THR:HG22	2.06	0.55
2:2:57:DC:H2'	2:2:58:DT:H71	1.88	0.55
12:S:257:ARG:NH2	12:S:403:GLU:OE2	2.40	0.54
12:T:323:PRO:N	12:T:325:LYS:HZ2	2.06	0.54
12:U:325:LYS:H	12:U:325:LYS:HD3	1.73	0.54
6:6:69:DG:H3'	6:6:70:DT:H72	1.88	0.54
2:2:31:DA:H2"	2:2:32:DC:H6	1.72	0.54
11:D:245:ASP:OD1	11:D:249:ARG:NH1	2.34	0.54
10:C:92:MET:HG2	10:C:93:GLN:N	2.22	0.54
11:K:150:LYS:O	11:K:153:THR:HG22	2.07	0.54
12:T:373:TYR:O	12:T:386:ARG:NH1	2.41	0.54
1:1:23:C:H2'	1:1:24:A:C8	2.43	0.53
7:7:8:DC:H2'	7:7:9:DT:H72	1.91	0.53
11:E:258:ARG:HG3	11:E:260:LEU:HD23	1.90	0.53
12:T:386:ARG:H	12:T:386:ARG:HD2	1.74	0.53
11:Q:50:ARG:NH1	11:Q:139:GLU:OE1	2.40	0.53
11:N:25:ILE:HD12	11:N:253:ILE:HG23	1.91	0.53
11:O:150:LYS:O	11:O:153:THR:HG22	2.08	0.53
12:R:127:LYS:O	12:R:128:ARG:NH1	2.38	0.53
1:1:80:A:H2'	1:1:81:C:C6	2.44	0.53
12:R:273:CYS:HB3	12:R:370:VAL:HG12	1.90	0.53
12:U:267:SER:HA	12:U:270:LYS:HE3	1.90	0.53
12:T:434:GLU:OE2	12:T:473:HIS:NE2	2.31	0.52
1:1:180:U:O2'	1:1:181:A:OP1	2.26	0.52
6:6:49:DG:H2'	6:6:50:DT:H71	1.91	0.52
1:1:91:U:OP2	16:1:401:HOH:O	2.19	0.52
3:3:47:DT:H2'	3:3:48:DT:C6	2.45	0.52
1:1:244:U:H2'	1:1:245:C:C6	2.44	0.52
11:M:238:GLU:OE2	11:M:243:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:202:GLU:HA	11:N:205:LYS:HE2	1.91	0.52
7:7:10:DA:H2'	7:7:11:DC:C6	2.44	0.52
11:G:225:LYS:H	11:G:225:LYS:HD2	1.75	0.52
12:R:129:MET:HE1	12:R:137:ARG:HH12	1.74	0.52
3:3:61:DC:H1'	3:3:62:DT:O5'	2.10	0.52
11:I:50:ARG:NH1	11:I:139:GLU:OE2	2.36	0.52
12:R:342:ASN:HD21	12:S:344:GLN:NE2	2.08	0.52
1:1:133:G:H2'	1:1:134:A:C8	2.46	0.51
3:3:102:DG:H2'	3:3:103:DT:H71	1.91	0.51
11:D:250:GLU:OE1	11:E:54:LYS:NZ	2.33	0.51
11:Q:145:GLU:HG2	11:Q:148:ARG:NH2	2.25	0.51
11:F:150:LYS:O	11:F:153:THR:HG22	2.10	0.51
2:2:60:DC:H4'	2:2:61:DA:OP1	2.11	0.51
4:4:23:DT:H2"	4:4:24:DG:C8	2.46	0.51
11:H:275:TYR:OH	11:I:54:LYS:NZ	2.38	0.51
1:1:34:C:H2'	1:1:35:A:C8	2.45	0.51
1:1:126:G:H2'	1:1:127:U:C6	2.46	0.51
5:5:17:DG:OP2	12:T:420:ARG:NH2	2.39	0.51
12:S:231:ASP:HB2	12:S:238:MET:SD	2.50	0.51
11:H:262:LYS:NZ	11:H:264:ASP:OD1	2.37	0.51
1:1:125:U:H2'	1:1:126:G:C8	2.46	0.51
12:U:300:ILE:HD12	12:U:301:GLY:N	2.25	0.50
12:S:204:CYS:SG	12:S:229:VAL:HG12	2.52	0.50
11:Q:128:ARG:NH2	11:Q:131:GLU:OE2	2.40	0.50
12:S:77:ARG:NH1	12:S:80:GLN:OE1	2.44	0.50
12:T:287:ASP:OD1	12:T:311:ARG:NH2	2.40	0.50
7:7:5:DT:H5"	12:S:417:THR:HG21	1.94	0.50
11:P:150:LYS:O	11:P:153:THR:HG22	2.11	0.50
12:R:230:ILE:HD12	12:R:320:VAL:HA	1.93	0.50
12:R:331:LEU:O	12:R:334:THR:HG22	2.12	0.50
12:T:215:ASP:OD2	12:T:492:ARG:NH2	2.38	0.50
11:J:216:LEU:HD11	11:J:248:LEU:HB3	1.94	0.50
3:3:82:DC:H2"	3:3:83:DT:H71	1.94	0.50
11:E:250:GLU:OE1	11:F:54:LYS:NZ	2.40	0.50
11:P:24:GLU:OE1	11:P:27:ARG:NH1	2.41	0.50
12:R:291:ASP:OD1	12:R:291:ASP:N	2.44	0.49
11:F:144:ASP:HA	11:F:171:VAL:HB	1.95	0.49
11:M:211:TRP:CH2	11:M:241:ILE:HD11	2.46	0.49
12:U:257:ARG:HG3	12:U:261:LEU:HD23	1.94	0.49
11:K:238:GLU:OE2	11:K:243:ARG:NH1	2.35	0.49
11:O:30:GLY:O	11:O:249:ARG:NH2	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:R:462:GLU:O	12:R:463:ASN:ND2	2.45	0.49
5:5:16:DT:H2"	12:R:178:TRP:HA	1.95	0.49
11:D:238:GLU:OE2	11:D:243:ARG:NH1	2.39	0.49
11:E:25:ILE:HD12	11:E:253:ILE:HG23	1.94	0.49
11:Q:71:ASP:OD1	11:Q:74:ARG:NH2	2.38	0.49
11:P:63:ARG:NH1	15:P:300:ATP:H5'2	2.28	0.49
12:S:460:ARG:NH1	12:S:462:GLU:OE2	2.39	0.49
5:5:26:DC:H2'	5:5:27:DT:C7	2.42	0.49
11:G:150:LYS:O	11:G:153:THR:HG22	2.12	0.49
12:S:33:VAL:HG13	12:S:92:VAL:HG21	1.94	0.49
12:U:424:LEU:HD21	12:U:446:LEU:HD11	1.94	0.49
12:U:219:GLU:OE2	12:U:492:ARG:NH2	2.46	0.49
10:C:98:ARG:NH2	10:C:119:VAL:O	2.44	0.49
6:6:53:DC:OP1	12:T:416:ARG:NH1	2.43	0.48
3:3:69:DT:H2'	3:3:70:DT:H71	1.94	0.48
11:G:158:ARG:HD2	11:G:189:ARG:HD2	1.95	0.48
12:R:57:ASP:O	12:R:61:TYR:N	2.33	0.48
1:1:48:U:H2'	1:1:49:G:C8	2.48	0.48
1:1:93:C:OP1	8:A:490:ARG:NH1	2.46	0.48
1:1:227:U:H2'	1:1:228:G:C8	2.48	0.48
2:2:47:DA:H61	3:3:87:DA:H61	1.60	0.48
2:2:47:DA:H1'	2:2:48:DT:O4'	2.14	0.48
11:D:258:ARG:HG3	11:D:258:ARG:HH11	1.79	0.48
11:I:211:TRP:CH2	11:I:241:ILE:HD11	2.49	0.48
12:R:445:ASN:O	12:R:459:TYR:N	2.34	0.48
11:D:57:ARG:NH1	11:D:193:HIS:HB3	2.29	0.48
12:U:404:ARG:HA	12:U:404:ARG:CZ	2.43	0.48
2:2:31:DA:H2"	2:2:32:DC:C6	2.48	0.48
11:J:238:GLU:OE1	11:J:243:ARG:NH1	2.44	0.48
12:R:235:ARG:HH12	12:R:380:ARG:NH2	2.11	0.48
7:7:10:DA:H2'	7:7:11:DC:C5	2.49	0.47
11:I:254:ARG:NH1	11:I:270:GLU:OE2	2.47	0.47
12:R:235:ARG:HD2	12:R:319:VAL:HG13	1.95	0.47
12:R:485:ASP:OD1	12:R:486:GLU:N	2.46	0.47
11:D:179:VAL:HG12	11:D:182:ARG:NH2	2.29	0.47
1:1:76:A:H2'	1:1:77:A:C8	2.50	0.47
2:2:42:DG:H2"	2:2:43:DT:H5'	1.97	0.47
3:3:120:DT:H2'	3:3:121:DT:C6	2.50	0.47
11:E:205:LYS:HE3	11:E:225:LYS:HE2	1.95	0.47
11:F:210:MET:O	11:F:214:MET:HG2	2.15	0.47
11:P:216:LEU:HD11	11:P:248:LEU:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:U:240:ILE:HD13	12:U:365:LEU:HD21	1.96	0.47
10:C:162:ALA:HA	10:C:165:GLN:NE2	2.30	0.47
11:D:144:ASP:HA	11:D:171:VAL:HB	1.95	0.47
12:R:271:LEU:HD23	12:R:367:ARG:HD2	1.96	0.47
11:D:50:ARG:NH1	11:D:139:GLU:OE2	2.38	0.47
11:J:75:TYR:HA	11:J:78:LYS:HG2	1.97	0.47
3:3:36:DA:N6	4:4:41:DC:O4'	2.48	0.47
11:H:238:GLU:OE1	11:H:243:ARG:NH1	2.40	0.47
11:L:150:LYS:O	11:L:153:THR:HG22	2.15	0.47
11:O:211:TRP:CH2	11:O:241:ILE:HD11	2.50	0.47
12:R:344:GLN:HE21	12:R:344:GLN:HA	1.80	0.47
12:S:229:VAL:HG22	12:S:239:GLY:O	2.14	0.47
1:1:44:A:H5"	1:1:45:U:OP2	2.15	0.47
3:3:110:DA:H2'	3:3:111:DT:C6	2.49	0.47
12:R:215:ASP:OD1	12:R:216:GLN:N	2.47	0.47
1:1:21:U:H2'	1:1:22:U:C6	2.51	0.46
11:L:28:LEU:HB2	11:L:253:ILE:HD11	1.97	0.46
1:1:138:G:H21	1:1:141:A:H62	1.61	0.46
7:7:8:DC:H2"	7:7:9:DT:H5'	1.97	0.46
11:K:144:ASP:HA	11:K:171:VAL:HB	1.96	0.46
3:3:55:DT:H2"	3:3:56:DG:N7	2.30	0.46
3:3:114:DA:H5"	8:A:275:ARG:HB2	1.98	0.46
10:C:130:LEU:HD13	10:C:134:PRO:HD3	1.97	0.46
11:H:96:PRO:HD2	11:H:144:ASP:O	2.15	0.46
11:Q:37:GLN:O	11:Q:41:THR:HG23	2.16	0.46
3:3:41:DA:N6	4:4:36:DG:O6	2.49	0.46
11:H:150:LYS:O	11:H:153:THR:HG22	2.16	0.46
11:I:85:ARG:HA	11:I:85:ARG:NE	2.30	0.46
11:O:45:TRP:CZ2	11:O:49:LYS:HE2	2.51	0.46
12:R:137:ARG:NH1	12:U:514:ASP:OD2	2.49	0.46
12:S:431:TYR:OH	12:S:453:ILE:O	2.34	0.46
7:7:6:DT:H3'	12:S:416:ARG:NH1	2.30	0.46
11:Q:68:VAL:N	15:Q:302:ATP:O1A	2.37	0.46
12:R:458:VAL:HG13	12:R:469:LEU:HB2	1.96	0.46
12:S:123:ASN:O	12:S:123:ASN:ND2	2.45	0.46
12:R:368:TYR:O	12:R:372:ARG:HB3	2.15	0.46
3:3:60:DA:N6	4:4:17:DG:O6	2.49	0.46
3:3:132:DA:C2'	3:3:133:DC:H5"	2.46	0.46
5:5:30:DT:O4'	12:S:106:ARG:NH1	2.49	0.46
12:T:239:GLY:HA2	12:T:258:HIS:CD2	2.51	0.45
5:5:21:DA:H3'	12:S:132:LYS:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:110:U:H2'	1:1:111:C:C6	2.52	0.45
11:L:50:ARG:NH1	11:L:139:GLU:OE1	2.45	0.45
11:O:232:ILE:HD11	11:O:268:LEU:HD23	1.99	0.45
12:S:140:ALA:HA	12:T:507:LEU:HD11	1.97	0.45
1:1:100:U:N3	1:1:139:A:H2	2.10	0.45
2:2:38:DA:H1'	2:2:39:DA:C8	2.52	0.45
8:A:576:LYS:HA	8:A:579:LYS:HE3	1.98	0.45
3:3:55:DT:H2"	3:3:56:DG:C8	2.51	0.45
3:3:83:DT:H2"	3:3:84:DA:C5	2.51	0.45
10:C:3:GLU:O	11:E:74:ARG:NH2	2.49	0.45
11:G:55:SER:HB3	11:G:190:PHE:CE1	2.52	0.45
12:T:280:LYS:NZ	12:T:304:LEU:O	2.36	0.45
6:6:63:DA:OP2	12:R:346:ARG:NH1	2.50	0.45
11:P:57:ARG:NH1	11:P:193:HIS:HB3	2.32	0.45
12:R:188:ARG:NH2	12:R:312:ASP:O	2.49	0.45
6:6:41:DT:H2"	6:6:42:DA:C8	2.52	0.45
11:E:144:ASP:HA	11:E:171:VAL:HB	1.99	0.45
11:K:79:PRO:HB3	11:K:89:VAL:HG22	1.98	0.45
12:R:232:THR:O	12:R:235:ARG:NH2	2.49	0.45
12:R:199:ASN:HA	12:R:202:TRP:NE1	2.32	0.44
1:1:116:U:H3	1:1:160:A:H61	1.65	0.44
3:3:84:DA:H2"	3:3:85:DA:H5'	1.99	0.44
2:2:19:DA:H4'	8:A:111:TRP:CZ2	2.52	0.44
2:2:42:DG:C6	3:3:93:DG:N2	2.86	0.44
11:F:211:TRP:CH2	11:F:241:ILE:HD11	2.52	0.44
12:R:77:ARG:NH1	12:R:81:ARG:HH22	2.16	0.44
2:2:15:DC:H2"	2:2:16:DA:C8	2.52	0.44
4:4:39:DG:C8	4:4:39:DG:H5'	2.53	0.44
8:A:536:ARG:NH1	8:A:604:THR:OG1	2.46	0.44
11:Q:229:MET:HA	11:Q:232:ILE:HG12	2.00	0.44
11:D:140:MET:HG3	11:D:167:ALA:O	2.17	0.44
12:R:232:THR:O	12:R:235:ARG:NE	2.50	0.44
1:1:118:A:C2	1:1:159:A:H5"	2.53	0.44
11:M:107:LYS:HD3	11:M:117:VAL:HG21	1.99	0.44
11:N:213:GLN:HG3	11:N:214:MET:HG3	1.99	0.44
12:U:197:TYR:HB3	12:U:395:PRO:HD3	2.00	0.44
3:3:46:DA:H2'	3:3:47:DT:C7	2.48	0.44
11:K:50:ARG:NH1	11:K:139:GLU:OE1	2.50	0.44
12:R:273:CYS:SG	12:R:274:GLU:N	2.91	0.44
2:2:37:DA:H2"	2:2:38:DA:H5'	1.99	0.44
11:G:145:GLU:OE1	11:G:148:ARG:NE	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:200:SER:N	16:G:407:HOH:O	2.45	0.44
11:K:145:GLU:OE2	16:K:401:HOH:O	2.21	0.44
12:T:326:THR:O	12:T:373:TYR:OH	2.24	0.44
3:3:95:DT:H2'	3:3:96:DT:H72	1.99	0.43
10:C:24:HIS:NE2	10:C:109:CYS:HA	2.33	0.43
11:D:133:LEU:HD22	11:D:138:VAL:HG11	2.00	0.43
11:K:275:TYR:OH	11:L:54:LYS:NZ	2.41	0.43
12:R:458:VAL:HG12	12:R:470:THR:O	2.17	0.43
12:T:297:LEU:HD12	12:T:297:LEU:H	1.83	0.43
4:4:19:DA:H3'	12:S:379:ALA:HB2	1.99	0.43
11:J:144:ASP:HA	11:J:171:VAL:HB	2.01	0.43
11:Q:67:THR:HB	15:Q:302:ATP:O2A	2.18	0.43
1:1:20:A:H2'	1:1:21:U:C6	2.54	0.43
4:4:25:DA:OP1	12:U:415:ARG:NH2	2.38	0.43
11:I:47:ASP:OD2	11:I:76:ARG:NH2	2.51	0.43
12:R:355:ARG:HD3	12:R:355:ARG:C	2.38	0.43
12:U:263:LYS:HE2	12:U:263:LYS:HA	2.00	0.43
12:R:256:LEU:HD11	12:R:284:PHE:CZ	2.52	0.43
8:A:117:SER:HB3	8:A:214:PHE:CE2	2.53	0.43
9:B:9:LYS:O	9:B:13:ILE:HG12	2.18	0.43
11:Q:144:ASP:HA	11:Q:171:VAL:HB	1.99	0.43
12:R:199:ASN:HA	12:R:202:TRP:HE1	1.83	0.43
6:6:74:DA:H2'	6:6:75:DA:C8	2.54	0.43
6:6:75:DA:H3'	6:6:76:DT:H72	2.00	0.43
11:E:74:ARG:HD2	11:E:93:TYR:HB3	2.01	0.43
11:O:144:ASP:HA	11:O:171:VAL:HB	2.01	0.43
12:S:291:ASP:OD1	12:S:291:ASP:N	2.49	0.43
4:4:34:DC:H2"	4:4:35:DT:C6	2.54	0.43
11:D:145:GLU:OE2	16:D:401:HOH:O	2.21	0.43
11:F:95:ARG:HH22	11:G:163:ASP:CG	2.20	0.43
11:H:211:TRP:CH2	11:H:241:ILE:HD11	2.53	0.43
12:S:229:VAL:HG21	12:S:259:ALA:CB	2.47	0.43
1:1:117:G:H21	1:1:159:A:H2	1.65	0.43
9:B:19:HIS:CE1	9:B:21:THR:HG22	2.54	0.43
12:S:197:TYR:CD1	12:S:200:HIS:HB2	2.54	0.43
11:J:216:LEU:HB3	11:J:218:LEU:CD2	2.49	0.43
11:P:198:LYS:HE2	11:P:240:TYR:CZ	2.54	0.43
12:U:208:ARG:HD2	12:U:225:TRP:CZ3	2.53	0.43
6:6:46:DT:O2	12:S:106:ARG:NH2	2.52	0.42
11:I:243:ARG:NE	11:J:188:GLU:OE2	2.49	0.42
11:L:144:ASP:HA	11:L:171:VAL:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:145:GLU:OE2	16:M:401:HOH:O	2.21	0.42
11:J:57:ARG:NH1	11:J:193:HIS:HB3	2.34	0.42
12:S:203:GLN:HA	12:S:285:TYR:O	2.19	0.42
12:U:384:GLN:O	12:U:389:ARG:NH1	2.49	0.42
6:6:53:DC:H2"	6:6:54:DT:H5'	2.00	0.42
1:1:50:U:H2'	1:1:52:A:C8	2.54	0.42
1:1:125:U:H2'	1:1:126:G:O4'	2.20	0.42
11:K:38:GLN:HG2	11:K:196:PHE:CZ	2.54	0.42
4:4:30:DT:O2	12:R:106:ARG:NH1	2.51	0.42
11:D:97:HIS:ND1	11:D:98:GLN:O	2.50	0.42
12:R:234:SER:OG	12:R:390:TRP:HA	2.20	0.42
11:E:55:SER:HB3	11:E:190:PHE:CE1	2.54	0.42
11:I:100:CYS:HB3	11:I:149:LEU:HD23	2.01	0.42
11:J:104:ASP:O	11:J:108:LYS:HG2	2.20	0.42
11:L:95:ARG:NH2	11:M:163:ASP:OD2	2.42	0.42
11:Q:67:THR:HB	15:Q:302:ATP:PA	2.59	0.42
12:R:210:ASP:OD1	12:R:223:ARG:NH2	2.53	0.42
12:S:186:LYS:O	12:S:285:TYR:OH	2.28	0.42
12:U:268:GLU:HG2	12:U:269:TYR:CD1	2.54	0.42
10:C:87:PRO:HG2	10:C:90:VAL:HG21	2.02	0.42
11:G:57:ARG:NH1	11:G:193:HIS:HB3	2.35	0.42
11:G:270:GLU:HA	11:G:273:LYS:HD2	2.02	0.42
11:N:61:GLU:OE1	11:N:198:LYS:NZ	2.48	0.42
12:R:57:ASP:H	12:R:60:THR:HG1	1.60	0.42
1:1:152:C:H2'	1:1:153:A:C8	2.55	0.42
2:2:42:DG:H2'	2:2:43:DT:H72	2.01	0.42
11:J:211:TRP:CH2	11:J:241:ILE:HD11	2.54	0.42
12:R:235:ARG:HA	12:R:235:ARG:HD3	1.72	0.42
8:A:39:LEU:HD23	8:A:91:TYR:CD1	2.56	0.41
11:E:212:GLU:OE2	11:E:222:SER:N	2.51	0.41
11:I:53:ARG:HD3	11:I:53:ARG:HA	1.82	0.41
12:T:397:VAL:HG13	12:T:398:PRO:HD2	2.02	0.41
3:3:36:DA:C2	4:4:41:DC:C4	3.08	0.41
11:N:208:VAL:HG22	11:N:244:LEU:HD11	2.01	0.41
11:P:50:ARG:NH1	11:P:73:TYR:OH	2.53	0.41
11:Q:198:LYS:HE2	11:Q:240:TYR:CZ	2.55	0.41
12:S:401:ILE:HD12	12:S:401:ILE:O	2.20	0.41
1:1:38:C:OP2	1:1:38:C:H6	2.03	0.41
3:3:118:DA:H2'	3:3:119:DC:C6	2.54	0.41
11:P:71:ASP:OD1	11:P:74:ARG:NH2	2.36	0.41
12:T:260:ILE:HG23	12:T:261:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:97:DT:H2”	3:3:98:DA:C8	2.56	0.41
5:5:29:DA:H1’	5:5:30:DT:H5”	2.02	0.41
11:P:243:ARG:O	11:P:247:ILE:HG12	2.20	0.41
12:S:246:ALA:HB1	12:S:247:PRO:HD2	2.02	0.41
12:T:457:LEU:HD12	12:T:468:PHE:CE1	2.55	0.41
12:U:198:SER:HB3	12:U:390:TRP:CD1	2.56	0.41
2:2:23:DA:H5”	2:2:23:DA:C8	2.55	0.41
4:4:37:DT:O4	12:R:77:ARG:NH1	2.53	0.41
6:6:35:DA:H5”	12:S:80:GLN:NE2	2.35	0.41
10:C:17:TYR:O	10:C:80:ARG:NH2	2.53	0.41
11:E:211:TRP:CH2	11:E:241:ILE:HD11	2.56	0.41
11:H:175:ARG:NH2	11:I:183:ASP:OD1	2.54	0.41
12:T:458:VAL:HG12	12:T:470:THR:O	2.20	0.41
11:H:250:GLU:OE1	11:I:54:LYS:NZ	2.52	0.41
12:S:234:SER:OG	12:S:390:TRP:HA	2.21	0.41
1:1:71:U:H2’	1:1:72:G:C8	2.56	0.41
8:A:546:PRO:HB3	8:A:613:GLN:HB2	2.02	0.41
12:R:124:LYS:HD2	12:R:124:LYS:O	2.21	0.41
3:3:98:DA:H4’	3:3:99:DA:OP1	2.19	0.41
11:H:241:ILE:HD12	11:H:241:ILE:HA	1.91	0.41
11:P:57:ARG:NH1	11:P:191:ARG:O	2.53	0.41
12:S:203:GLN:O	12:S:229:VAL:HA	2.21	0.41
3:3:46:DA:H2’	3:3:47:DT:H72	2.03	0.41
3:3:82:DC:H2”	3:3:83:DT:C7	2.51	0.41
6:6:53:DC:OP2	12:T:425:GLN:NE2	2.53	0.41
11:N:144:ASP:HA	11:N:171:VAL:HB	2.02	0.41
3:3:61:DC:O2	3:3:61:DC:C2’	2.69	0.41
11:E:62:SER:OG	15:E:300:ATP:O3G	2.28	0.41
11:F:149:LEU:HB3	11:F:153:THR:CG2	2.51	0.41
11:L:57:ARG:O	11:L:193:HIS:HA	2.21	0.41
12:R:60:THR:HA	12:R:63:GLN:NE2	2.36	0.40
12:R:426:PHE:HB3	12:R:431:TYR:CE1	2.56	0.40
12:S:206:HIS:CD2	12:S:247:PRO:HB3	2.56	0.40
12:U:197:TYR:CG	12:U:395:PRO:HD3	2.55	0.40
1:1:148:C:H2’	1:1:150:C:C5	2.57	0.40
6:6:33:DC:H2”	6:6:34:DA:N7	2.36	0.40
10:C:74:VAL:HG12	10:C:76:VAL:H	1.86	0.40
11:F:258:ARG:HH11	11:F:258:ARG:CG	2.32	0.40
11:M:107:LYS:HE3	11:M:107:LYS:HB3	1.92	0.40
12:R:233:TYR:C	12:R:235:ARG:H	2.23	0.40
12:S:213:LEU:HD22	12:S:224:PRO:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:U:462:GLU:HG3	12:U:463:ASN:H	1.85	0.40
2:2:11:DT:H2'	2:2:12:DC:C5	2.56	0.40
11:J:250:GLU:OE1	11:K:54:LYS:NZ	2.49	0.40
11:O:149:LEU:HB3	11:O:153:THR:CG2	2.50	0.40
11:Q:60:GLY:HA2	11:Q:195:ARG:HH21	1.86	0.40
2:2:22:DA:H2"	2:2:23:DA:C5	2.57	0.40
2:2:27:DG:H1'	2:2:28:DG:C8	2.56	0.40
3:3:46:DA:H2'	3:3:47:DT:C6	2.56	0.40
6:6:78:DC:C2'	6:6:79:DT:H5"	2.51	0.40
6:6:79:DT:C5	7:7:1:DA:N6	2.89	0.40
11:O:216:LEU:HD22	11:O:252:ALA:HB2	2.03	0.40
12:U:270:LYS:HA	12:U:270:LYS:HE2	2.03	0.40
2:2:8:DT:H2'	2:2:9:DT:C5	2.56	0.40
12:T:387:PHE:CG	12:T:388:GLU:N	2.89	0.40

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	
8	A	596/698 (85%)	591 (99%)	5 (1%)	0	100	100
9	B	85/90 (94%)	82 (96%)	3 (4%)	0	100	100
10	C	162/179 (90%)	154 (95%)	8 (5%)	0	100	100
11	D	255/276 (92%)	252 (99%)	3 (1%)	0	100	100
11	E	255/276 (92%)	253 (99%)	2 (1%)	0	100	100
11	F	255/276 (92%)	253 (99%)	2 (1%)	0	100	100
11	G	255/276 (92%)	252 (99%)	3 (1%)	0	100	100
11	H	255/276 (92%)	251 (98%)	4 (2%)	0	100	100
11	I	255/276 (92%)	253 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	J	255/276 (92%)	253 (99%)	2 (1%)	0	100	100
11	K	255/276 (92%)	249 (98%)	6 (2%)	0	100	100
11	L	255/276 (92%)	253 (99%)	2 (1%)	0	100	100
11	M	255/276 (92%)	252 (99%)	3 (1%)	0	100	100
11	N	255/276 (92%)	253 (99%)	2 (1%)	0	100	100
11	O	255/276 (92%)	253 (99%)	2 (1%)	0	100	100
11	P	255/276 (92%)	250 (98%)	5 (2%)	0	100	100
11	Q	255/276 (92%)	244 (96%)	11 (4%)	0	100	100
12	R	500/584 (86%)	471 (94%)	29 (6%)	0	100	100
12	S	496/584 (85%)	470 (95%)	26 (5%)	0	100	100
12	T	289/584 (50%)	274 (95%)	15 (5%)	0	100	100
12	U	291/584 (50%)	266 (91%)	25 (9%)	0	100	100
12	r	11/584 (2%)	10 (91%)	1 (9%)	0	100	100
12	s	11/584 (2%)	10 (91%)	1 (9%)	0	100	100
12	t	11/584 (2%)	11 (100%)	0	0	100	100
12	u	11/584 (2%)	11 (100%)	0	0	100	100
All	All	6033/9503 (64%)	5871 (97%)	162 (3%)	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	
8	A	531/608 (87%)	530 (100%)	1 (0%)	93	97
9	B	76/78 (97%)	76 (100%)	0	100	100
10	C	136/150 (91%)	136 (100%)	0	100	100
11	D	224/238 (94%)	224 (100%)	0	100	100
11	E	224/238 (94%)	221 (99%)	3 (1%)	69	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
11	F	224/238 (94%)	221 (99%)	3 (1%)	69 82
11	G	224/238 (94%)	218 (97%)	6 (3%)	44 61
11	H	224/238 (94%)	221 (99%)	3 (1%)	69 82
11	I	224/238 (94%)	220 (98%)	4 (2%)	59 75
11	J	224/238 (94%)	220 (98%)	4 (2%)	59 75
11	K	224/238 (94%)	221 (99%)	3 (1%)	69 82
11	L	224/238 (94%)	218 (97%)	6 (3%)	44 61
11	M	224/238 (94%)	219 (98%)	5 (2%)	52 69
11	N	224/238 (94%)	220 (98%)	4 (2%)	59 75
11	O	224/238 (94%)	221 (99%)	3 (1%)	69 82
11	P	224/238 (94%)	221 (99%)	3 (1%)	69 82
11	Q	224/238 (94%)	221 (99%)	3 (1%)	69 82
12	R	439/512 (86%)	424 (97%)	15 (3%)	37 51
12	S	436/512 (85%)	428 (98%)	8 (2%)	59 75
12	T	259/512 (51%)	249 (96%)	10 (4%)	32 46
12	U	261/512 (51%)	251 (96%)	10 (4%)	33 47
12	r	12/512 (2%)	12 (100%)	0	100 100
12	s	12/512 (2%)	10 (83%)	2 (17%)	2 2
12	t	12/512 (2%)	11 (92%)	1 (8%)	11 14
12	u	12/512 (2%)	12 (100%)	0	100 100
All	All	5322/8264 (64%)	5225 (98%)	97 (2%)	61 75

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	A	144	MET
11	E	40	LYS
11	E	196	PHE
11	E	211	TRP
11	F	74	ARG
11	F	196	PHE
11	F	211	TRP
11	G	74	ARG
11	G	123	SER
11	G	196	PHE

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Mol	Chain	Res	Type
11	G	211	TRP
11	G	225	LYS
11	G	273	LYS
11	H	116	ARG
11	H	196	PHE
11	H	211	TRP
11	I	78	LYS
11	I	114	LYS
11	I	196	PHE
11	I	211	TRP
11	J	74	ARG
11	J	196	PHE
11	J	211	TRP
11	J	273	LYS
11	K	74	ARG
11	K	196	PHE
11	K	211	TRP
11	L	103	LYS
11	L	181	LYS
11	L	211	TRP
11	L	225	LYS
11	L	255	SER
11	L	273	LYS
11	M	29	LYS
11	M	53	ARG
11	M	82	GLU
11	M	211	TRP
11	M	228	GLU
11	N	74	ARG
11	N	211	TRP
11	N	227	LYS
11	N	265	LYS
11	O	199	LEU
11	O	211	TRP
11	O	238	GLU
11	P	29	LYS
11	P	211	TRP
11	P	229	MET
11	Q	145	GLU
11	Q	211	TRP
11	Q	214	MET
12	R	67	GLU

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Mol	Chain	Res	Type
12	R	80	GLN
12	R	124	LYS
12	R	137	ARG
12	R	166	LYS
12	R	342	ASN
12	R	344	GLN
12	R	362	GLU
12	R	404	ARG
12	R	405	ASP
12	R	416	ARG
12	R	431	TYR
12	R	446	LEU
12	R	478	GLU
12	R	508	GLN
12	S	123	ASN
12	S	179	ARG
12	S	264	ARG
12	S	268	GLU
12	S	415	ARG
12	S	431	TYR
12	S	446	LEU
12	S	471	ARG
12	T	278	TYR
12	T	311	ARG
12	T	325	LYS
12	T	358	LEU
12	T	373	TYR
12	T	386	ARG
12	T	387	PHE
12	T	412	LYS
12	T	449	ASP
12	T	500	THR
12	U	223	ARG
12	U	295	ASN
12	U	325	LYS
12	U	355	ARG
12	U	378	ASP
12	U	389	ARG
12	U	406	LEU
12	U	415	ARG
12	U	463	ASN
12	U	471	ARG

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Mol	Chain	Res	Type
12	s	575	TYR
12	s	579	ARG
12	t	575	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
8	A	521	GLN
10	C	94	HIS
10	C	135	ASN
10	C	152	HIS
11	D	206	ASN
11	H	213	GLN
11	N	213	GLN
11	Q	97	HIS
12	R	344	GLN
12	R	425	GLN
12	S	295	ASN
12	S	344	GLN
12	S	363	GLN
12	S	445	ASN
12	T	375	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	245/261 (93%)	45 (18%)	8 (3%)

All (45) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	33	G
1	1	34	C
1	1	38	C
1	1	45	U
1	1	46	U
1	1	50	U
1	1	51	U
1	1	52	A
1	1	54	A

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Mol	Chain	Res	Type
1	1	68	G
1	1	76	A
1	1	77	A
1	1	79	U
1	1	88	G
1	1	100	U
1	1	101	G
1	1	119	U
1	1	126	G
1	1	128	C
1	1	132	A
1	1	133	G
1	1	139	A
1	1	140	U
1	1	157	A
1	1	159	A
1	1	166	C
1	1	167	G
1	1	168	G
1	1	172	U
1	1	174	C
1	1	180	U
1	1	181	A
1	1	196	A
1	1	197	C
1	1	206	A
1	1	208	G
1	1	222	A
1	1	226	G
1	1	228	G
1	1	233	G
1	1	238	G
1	1	239	A
1	1	243	G
1	1	255	G
1	1	256	G

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	38	C
1	1	49	G

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Mol	Chain	Res	Type
1	1	63	A
1	1	76	A
1	1	167	G
1	1	196	A
1	1	238	G
1	1	239	A

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 33 ligands modelled in this entry, 19 are monoatomic - leaving 14 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	$\#\|Z\| > 2$
15	ATP	I	300	13	26,33,33	0.78	0	31,52,52	0.80	2 (6%)
15	ATP	D	300	13	26,33,33	0.79	0	31,52,52	0.83	1 (3%)
15	ATP	K	300	13	26,33,33	0.77	0	31,52,52	0.83	1 (3%)
15	ATP	J	300	13	26,33,33	0.80	0	31,52,52	0.84	2 (6%)
15	ATP	G	300	13	26,33,33	0.79	0	31,52,52	0.85	2 (6%)
15	ATP	O	300	13	26,33,33	0.71	0	31,52,52	0.82	2 (6%)
15	ATP	Q	302	13	26,33,33	0.64	0	31,52,52	0.76	2 (6%)
15	ATP	E	300	13	26,33,33	0.78	0	31,52,52	0.81	1 (3%)
15	ATP	L	300	13	26,33,33	0.74	0	31,52,52	0.77	1 (3%)
15	ATP	P	300	13	26,33,33	0.66	0	31,52,52	0.82	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	ATP	N	302	13	26,33,33	0.74	0	31,52,52	0.81	2 (6%)
15	ATP	F	300	13	26,33,33	0.78	0	31,52,52	0.84	1 (3%)
15	ATP	H	300	13	26,33,33	0.77	0	31,52,52	0.82	1 (3%)
15	ATP	M	300	13	26,33,33	0.75	0	31,52,52	0.89	2 (6%)

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
15	ATP	I	300	13	-	1/18/38/38	0/3/3/3
15	ATP	D	300	13	-	2/18/38/38	0/3/3/3
15	ATP	K	300	13	-	2/18/38/38	0/3/3/3
15	ATP	J	300	13	-	2/18/38/38	0/3/3/3
15	ATP	G	300	13	-	1/18/38/38	0/3/3/3
15	ATP	O	300	13	-	1/18/38/38	0/3/3/3
15	ATP	Q	302	13	-	4/18/38/38	0/3/3/3
15	ATP	E	300	13	-	1/18/38/38	0/3/3/3
15	ATP	L	300	13	-	1/18/38/38	0/3/3/3
15	ATP	P	300	13	-	1/18/38/38	0/3/3/3
15	ATP	N	302	13	-	2/18/38/38	0/3/3/3
15	ATP	F	300	13	-	1/18/38/38	0/3/3/3
15	ATP	H	300	13	-	1/18/38/38	0/3/3/3
15	ATP	M	300	13	-	1/18/38/38	0/3/3/3

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	F	300	ATP	C5-C6-N6	2.40	124.00	120.35
15	G	300	ATP	C5-C6-N6	2.38	123.97	120.35
15	K	300	ATP	C5-C6-N6	2.37	123.95	120.35
15	E	300	ATP	C5-C6-N6	2.35	123.92	120.35
15	P	300	ATP	C5-C6-N6	2.33	123.89	120.35
15	O	300	ATP	C5-C6-N6	2.32	123.88	120.35
15	N	302	ATP	C5-C6-N6	2.32	123.88	120.35
15	M	300	ATP	C5-C6-N6	2.31	123.87	120.35
15	H	300	ATP	C5-C6-N6	2.31	123.86	120.35
15	I	300	ATP	C5-C6-N6	2.31	123.86	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	J	300	ATP	C5-C6-N6	2.30	123.85	120.35
15	Q	302	ATP	C5-C6-N6	2.29	123.84	120.35
15	D	300	ATP	C5-C6-N6	2.26	123.79	120.35
15	L	300	ATP	C5-C6-N6	2.25	123.77	120.35
15	M	300	ATP	PB-O3B-PG	2.12	140.10	132.83
15	G	300	ATP	PB-O3B-PG	2.09	140.00	132.83
15	Q	302	ATP	PB-O3B-PG	2.07	139.93	132.83
15	O	300	ATP	PB-O3B-PG	2.06	139.90	132.83
15	J	300	ATP	PB-O3B-PG	2.05	139.85	132.83
15	P	300	ATP	PB-O3B-PG	2.03	139.80	132.83
15	N	302	ATP	PB-O3B-PG	2.02	139.76	132.83
15	I	300	ATP	PB-O3B-PG	2.01	139.72	132.83

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	Q	302	ATP	PA-O3A-PB-O1B
15	H	300	ATP	PA-O3A-PB-O2B
15	K	300	ATP	PA-O3A-PB-O2B
15	N	302	ATP	PA-O3A-PB-O2B
15	E	300	ATP	PA-O3A-PB-O2B
15	F	300	ATP	PA-O3A-PB-O2B
15	G	300	ATP	PA-O3A-PB-O2B
15	L	300	ATP	PA-O3A-PB-O2B
15	M	300	ATP	PA-O3A-PB-O2B
15	O	300	ATP	PA-O3A-PB-O2B
15	P	300	ATP	PA-O3A-PB-O1B
15	Q	302	ATP	PA-O3A-PB-O2B
15	D	300	ATP	PG-O3B-PB-O1B
15	D	300	ATP	PG-O3B-PB-O2B
15	I	300	ATP	PA-O3A-PB-O1B
15	J	300	ATP	PA-O3A-PB-O1B
15	J	300	ATP	PA-O3A-PB-O2B
15	K	300	ATP	PA-O3A-PB-O1B
15	N	302	ATP	PA-O3A-PB-O1B
15	Q	302	ATP	PG-O3B-PB-O1B
15	Q	302	ATP	PG-O3B-PB-O2B

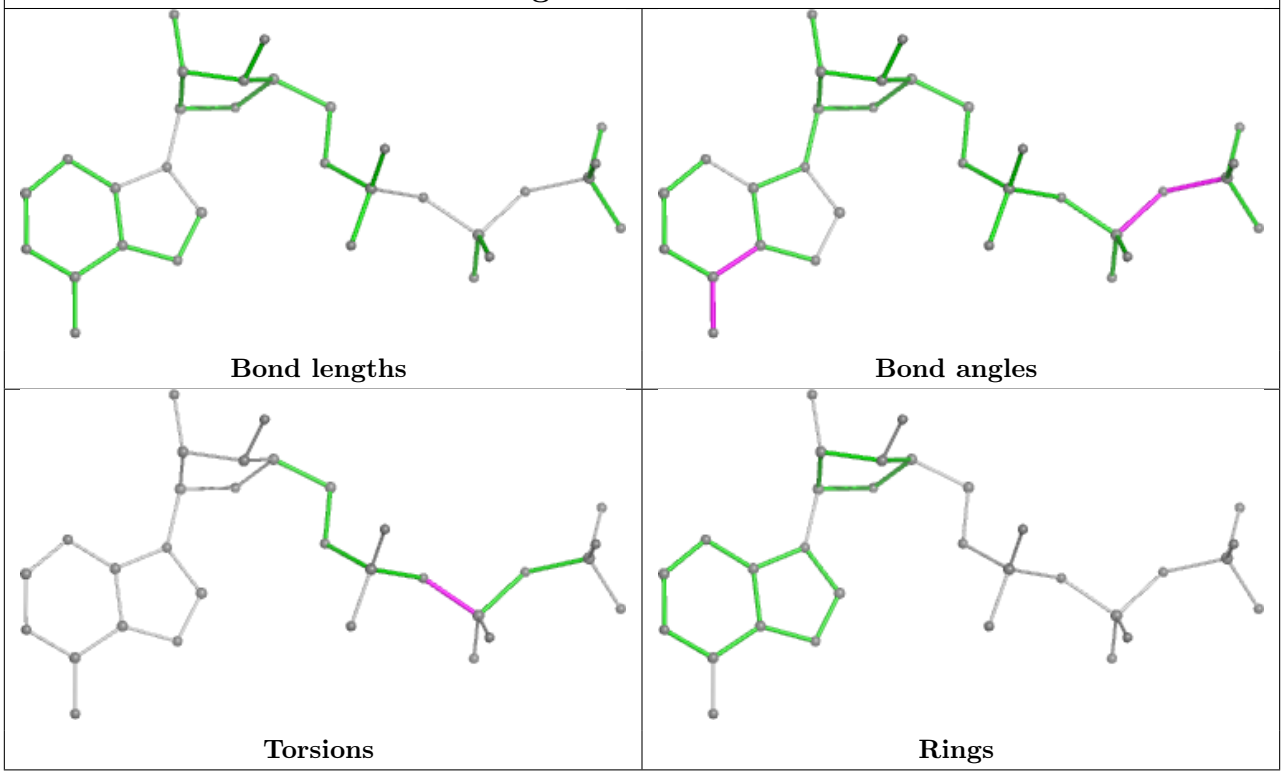
There are no ring outliers.

4 monomers are involved in 6 short contacts:

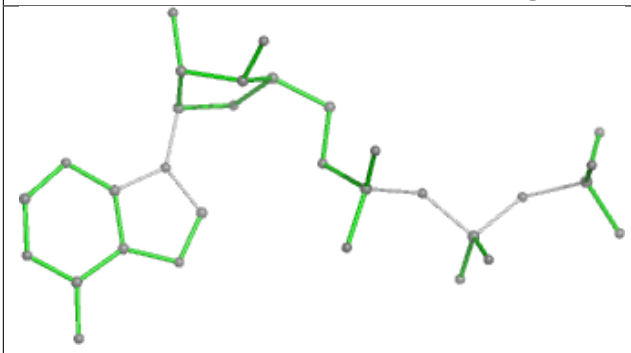
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	J	300	ATP	1	0
15	Q	302	ATP	3	0
15	E	300	ATP	1	0
15	P	300	ATP	1	0

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.

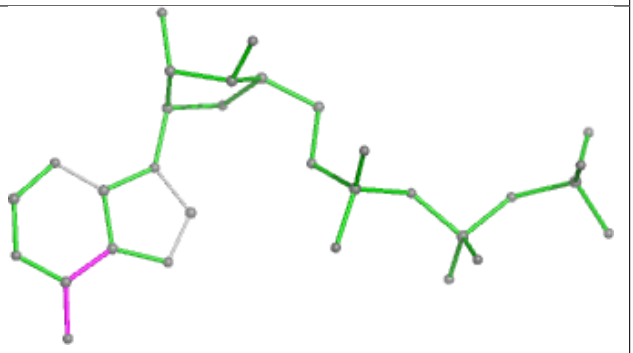
Ligand ATP I 300



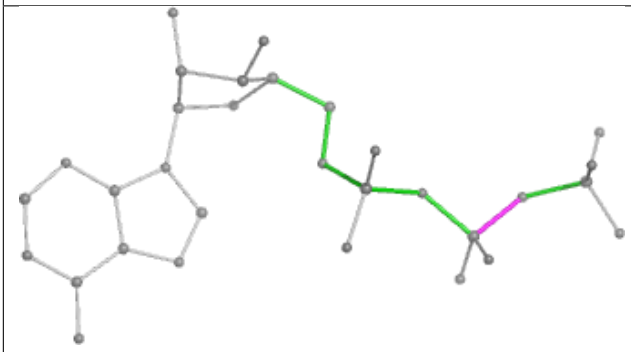
Ligand ATP D 300



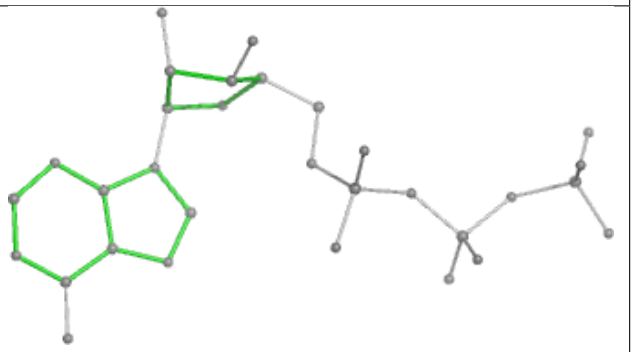
Bond lengths



Bond angles

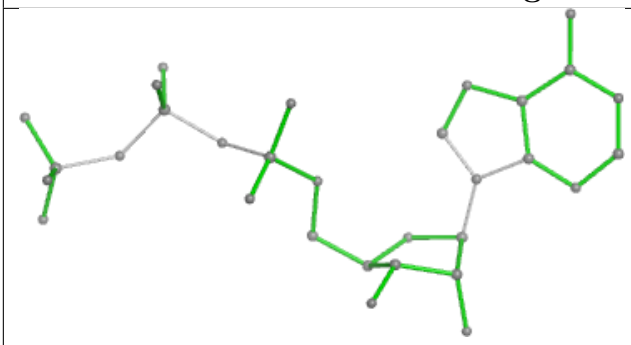


Torsions

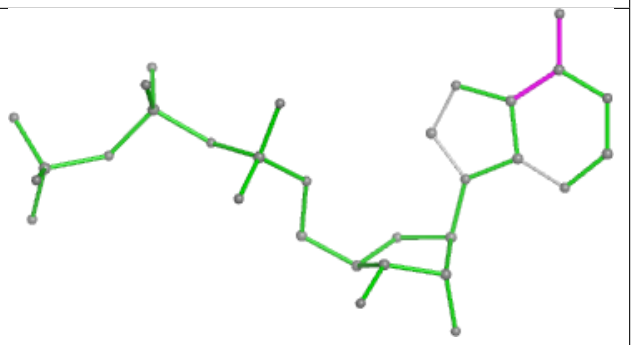


Rings

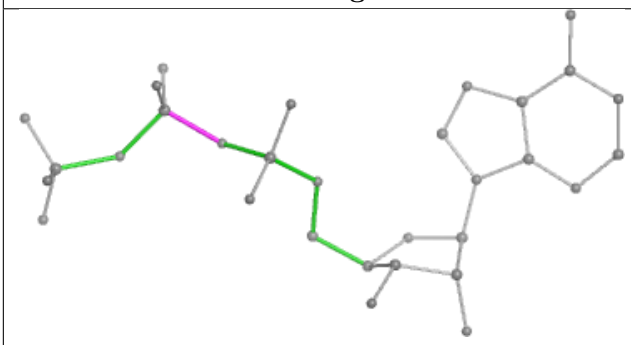
Ligand ATP K 300



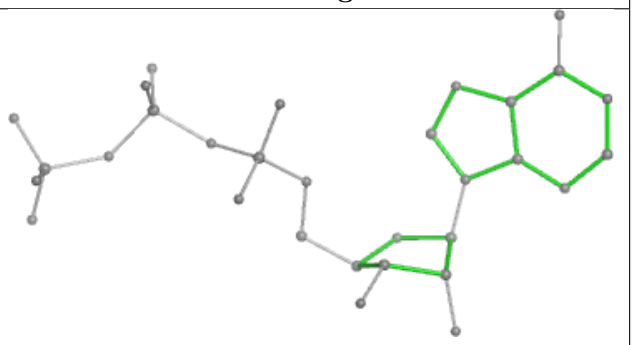
Bond lengths



Bond angles

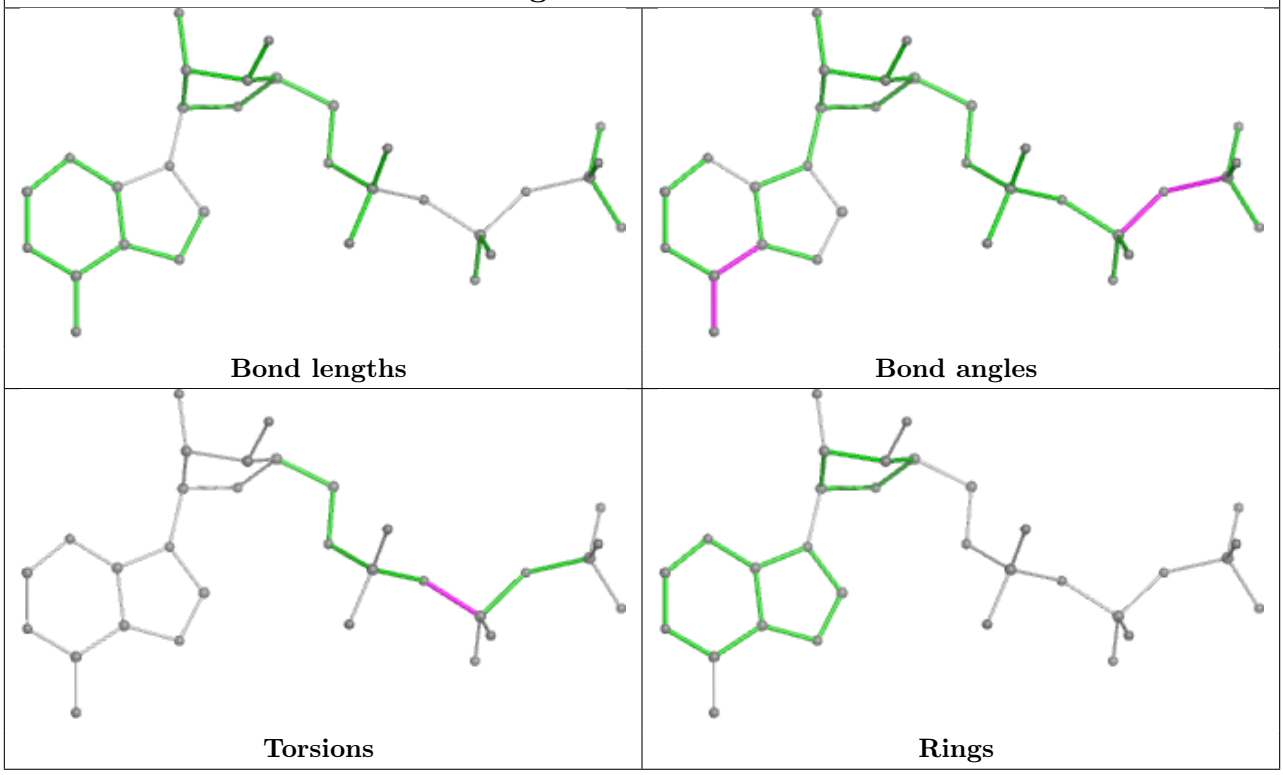


Torsions

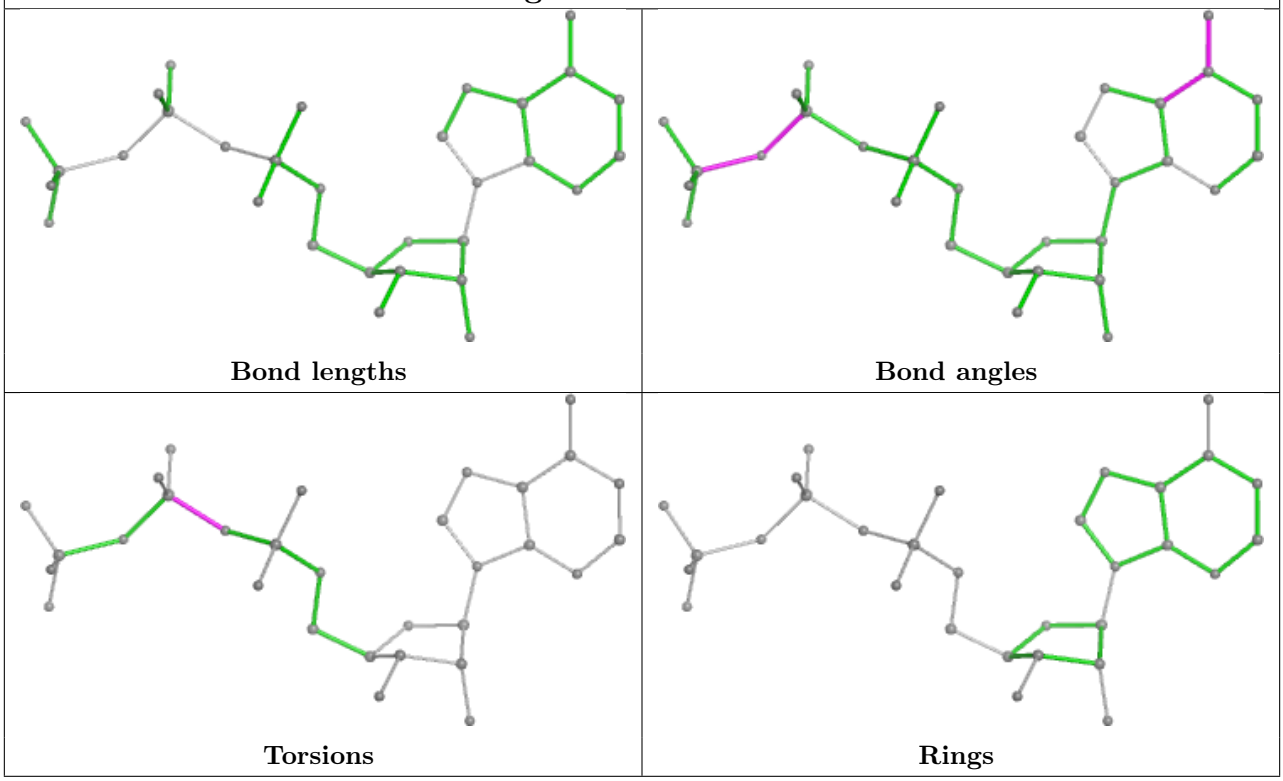


Rings

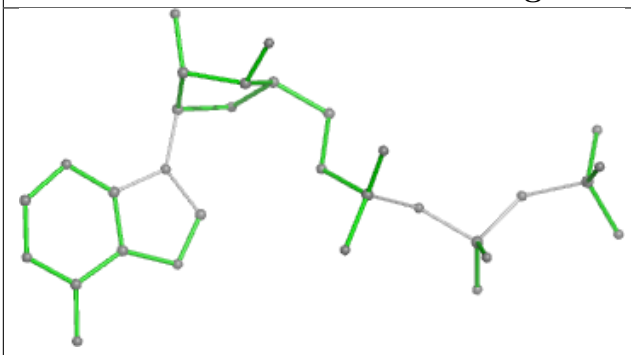
Ligand ATP J 300



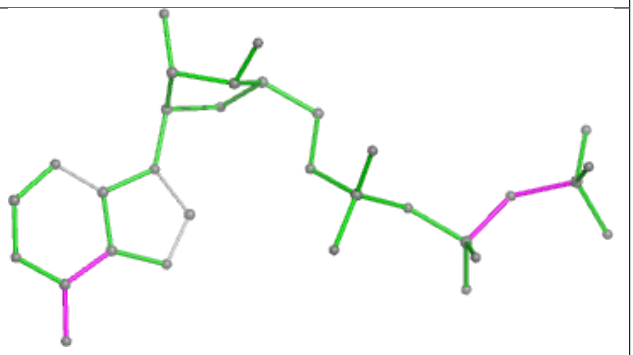
Ligand ATP G 300



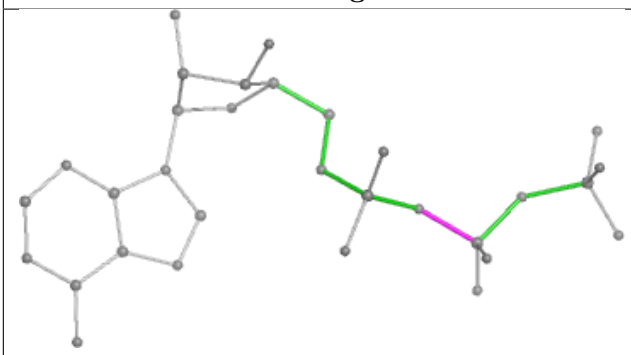
Ligand ATP O 300



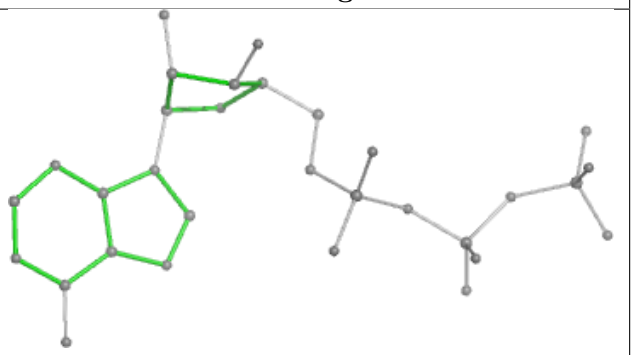
Bond lengths



Bond angles

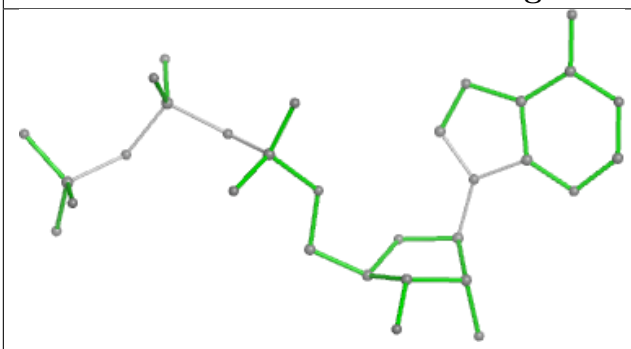


Torsions

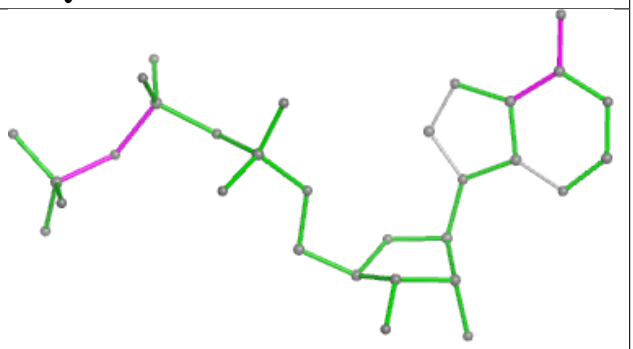


Rings

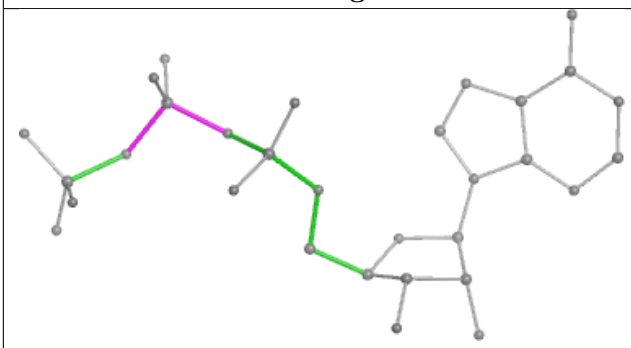
Ligand ATP Q 302



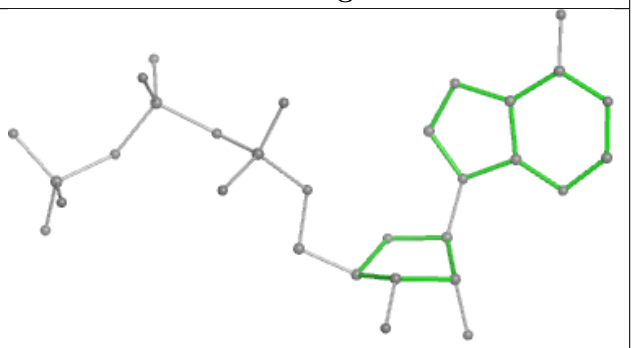
Bond lengths



Bond angles

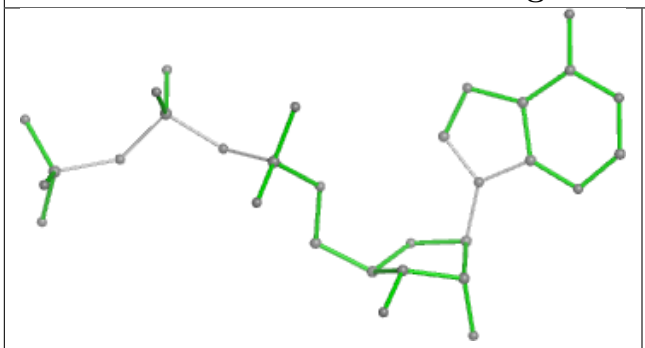


Torsions

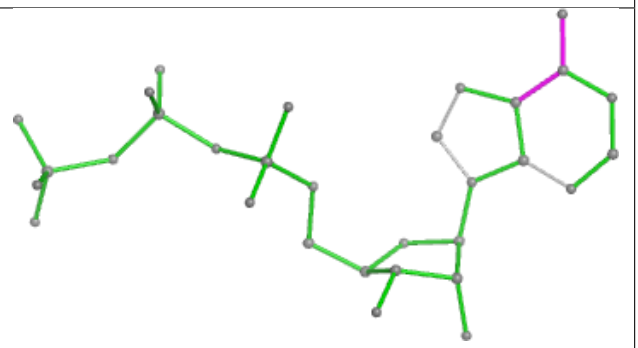


Rings

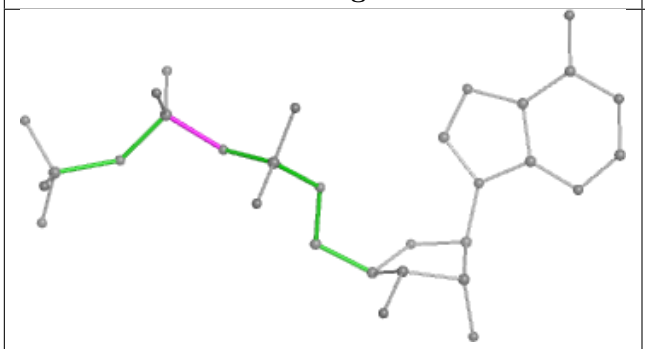
Ligand ATP E 300



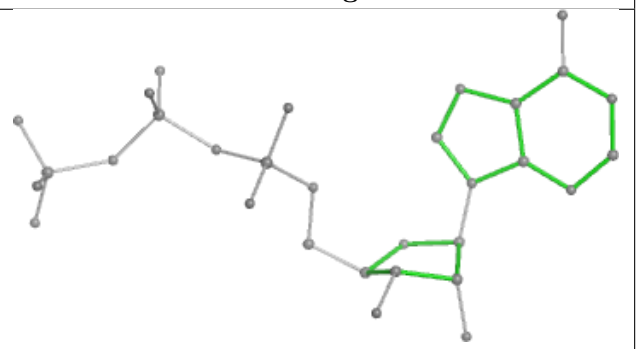
Bond lengths



Bond angles

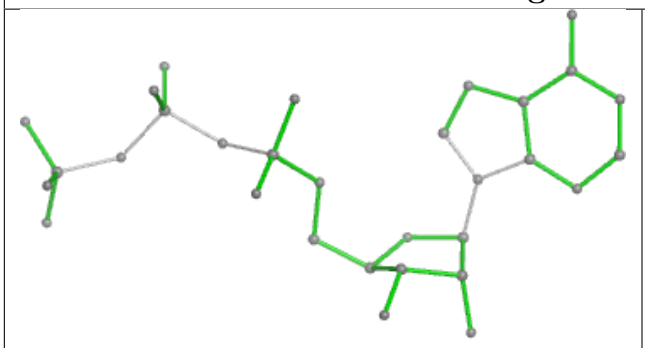


Torsions

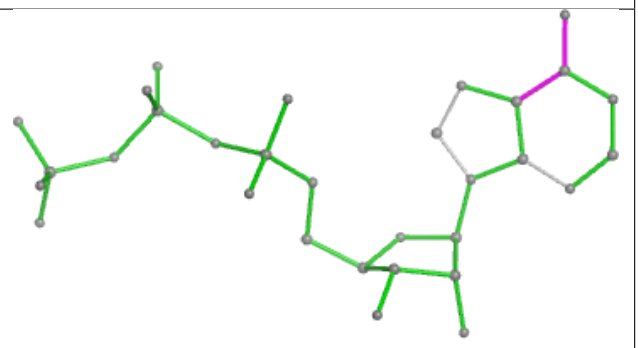


Rings

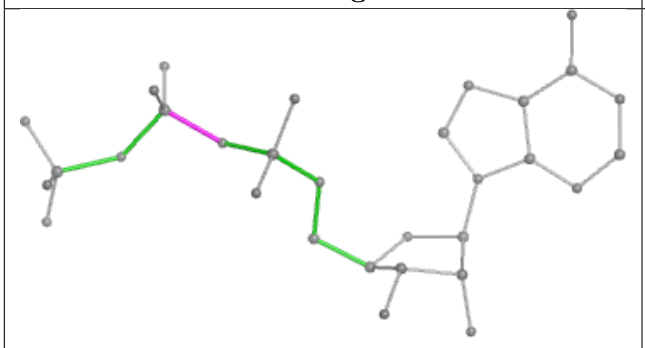
Ligand ATP L 300



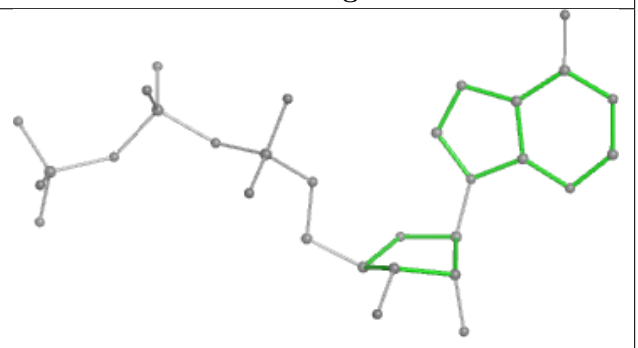
Bond lengths



Bond angles

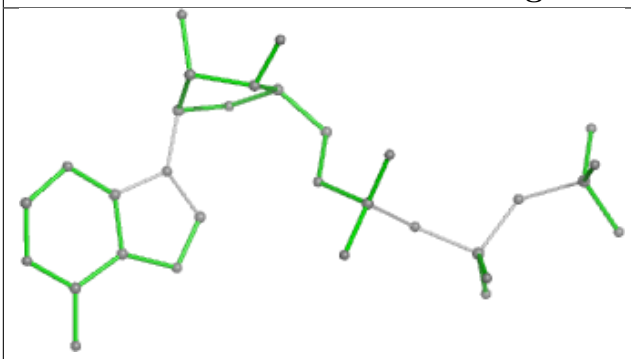


Torsions

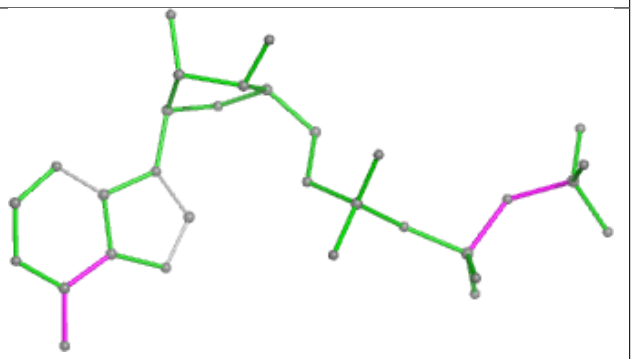


Rings

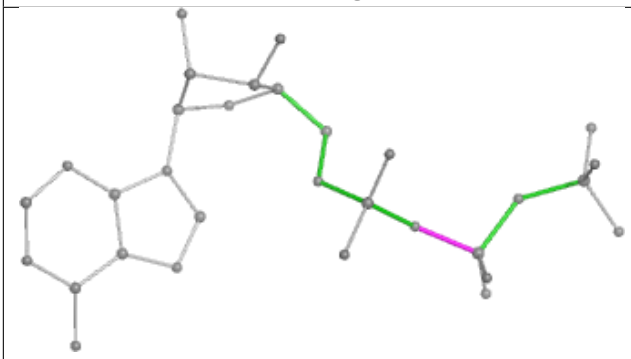
Ligand ATP P 300



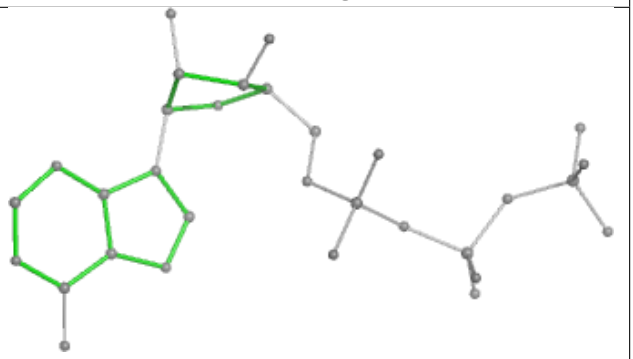
Bond lengths



Bond angles

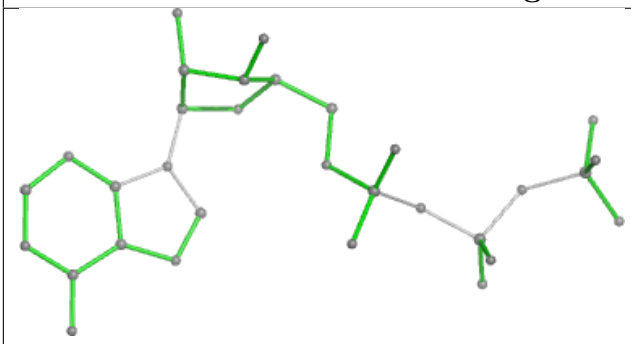


Torsions

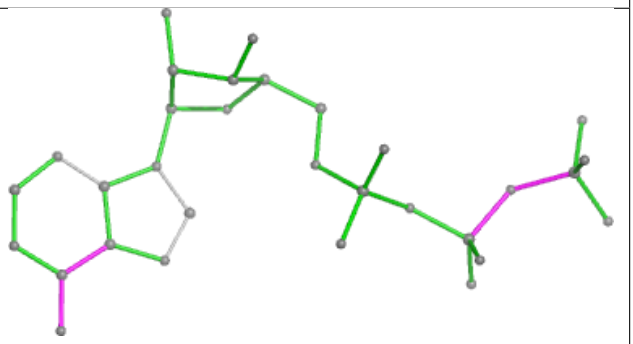


Rings

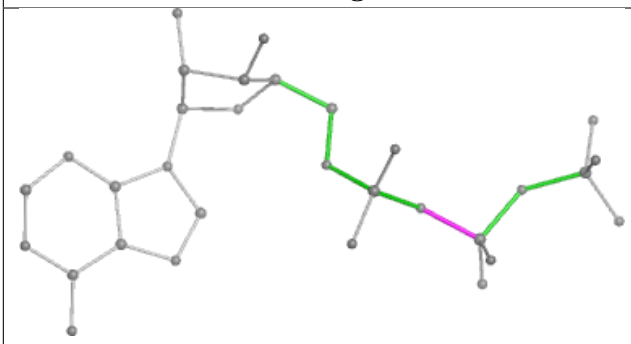
Ligand ATP N 302



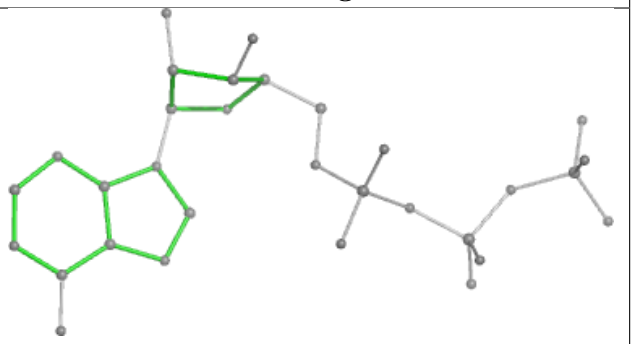
Bond lengths



Bond angles

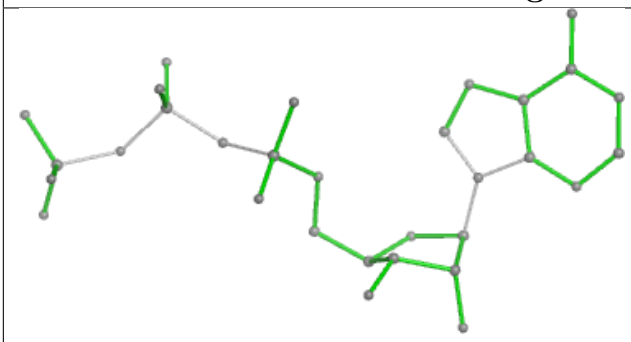


Torsions

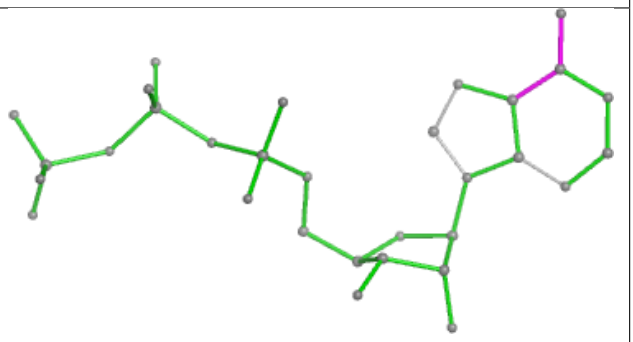


Rings

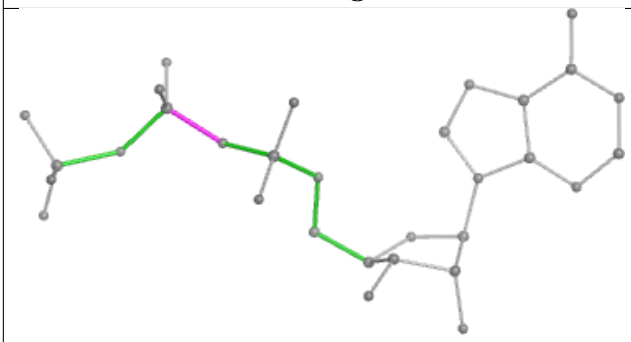
Ligand ATP F 300



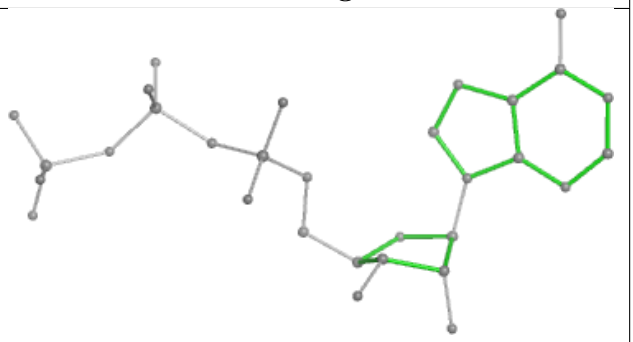
Bond lengths



Bond angles

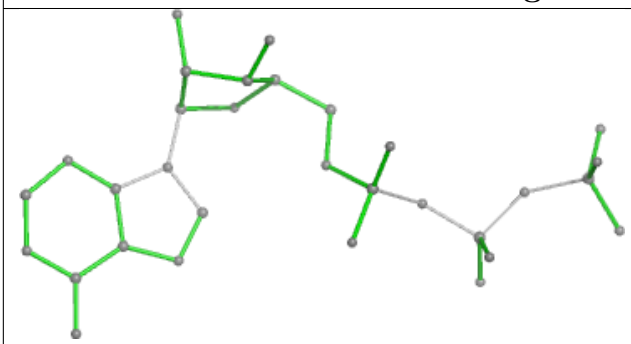


Torsions

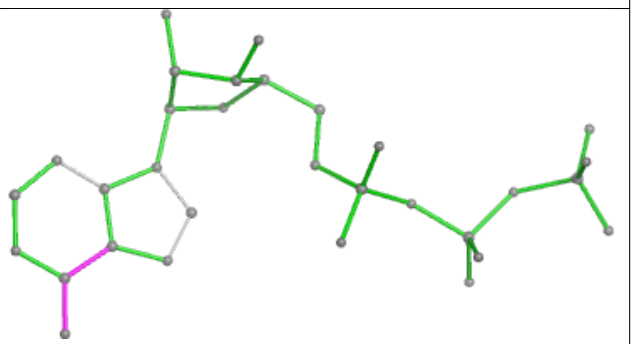


Rings

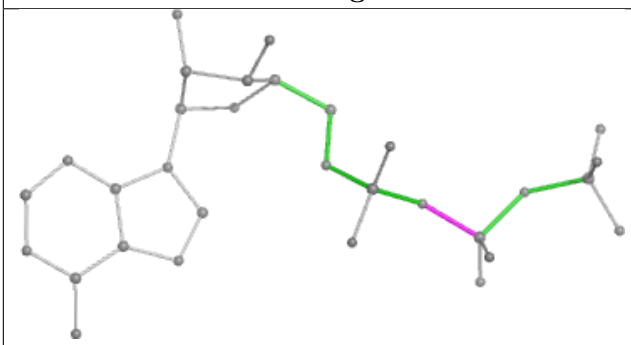
Ligand ATP H 300



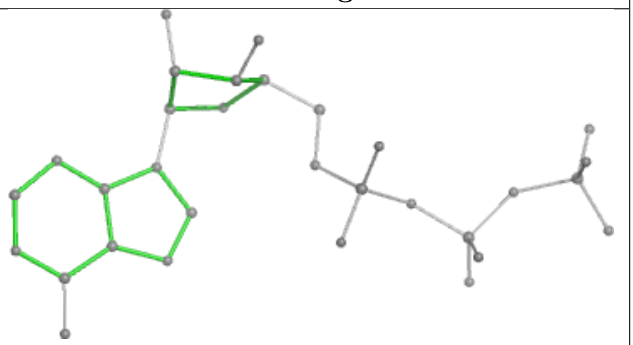
Bond lengths



Bond angles

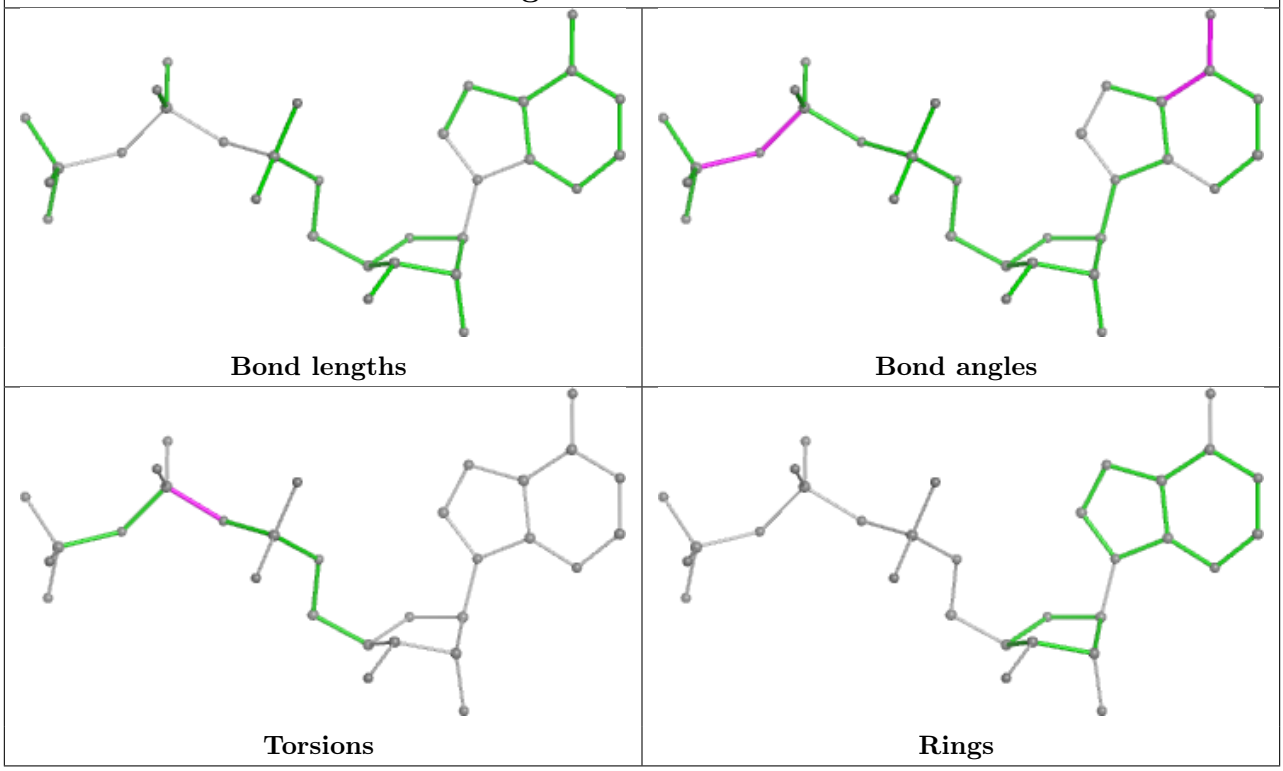


Torsions



Rings

Ligand ATP M 300



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.

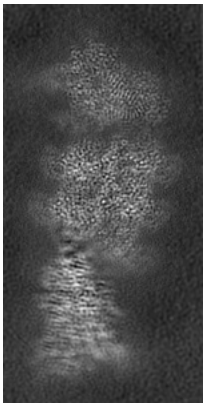
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-19075. These allow visual inspection of the internal detail of the map and identification of artifacts.

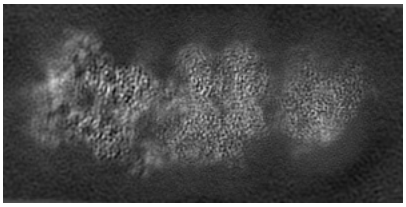
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

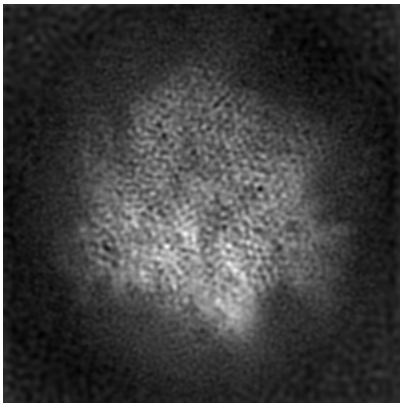
6.1.1 Primary map



X



Y

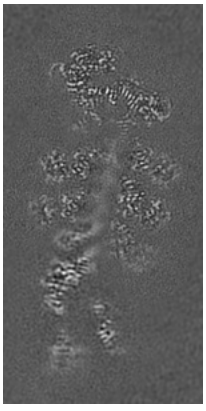


Z

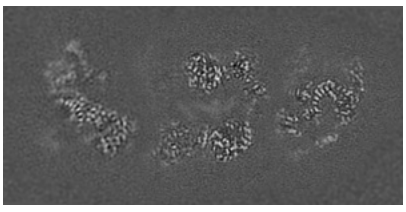
The images above show the map projected in three orthogonal directions.

6.2 Central slices

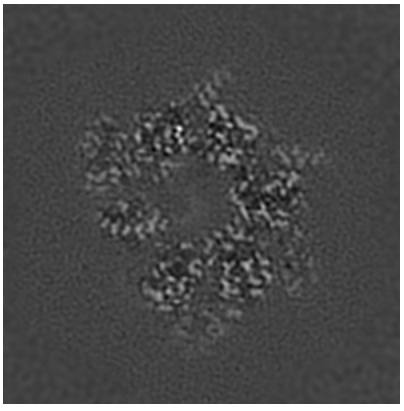
6.2.1 Primary map



X Index: 119



Y Index: 120

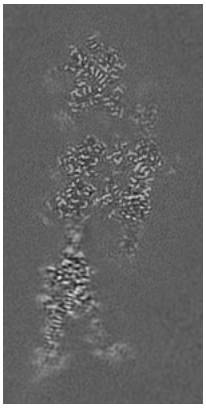


Z Index: 241

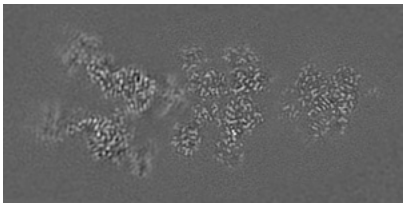
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

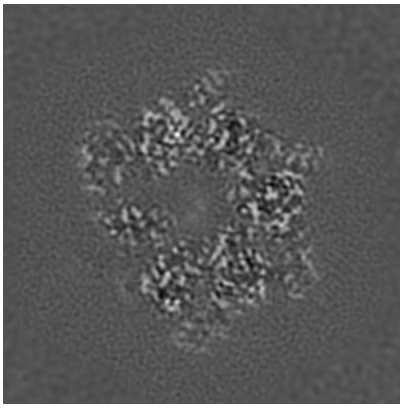
6.3.1 Primary map



X Index: 140



Y Index: 94

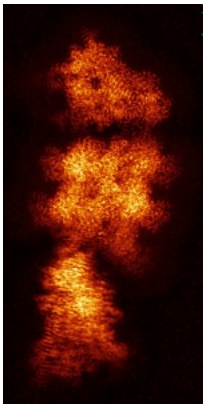


Z Index: 239

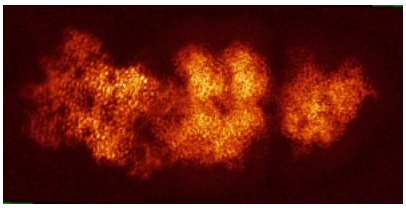
The images above show the largest variance slices of the map in three orthogonal directions.

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

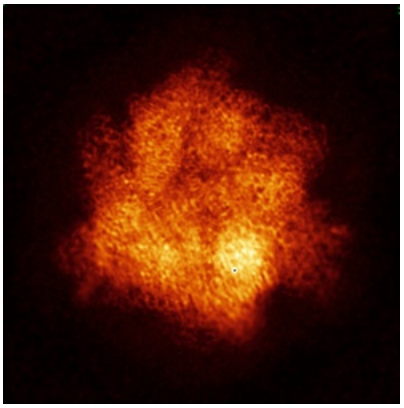
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.16. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

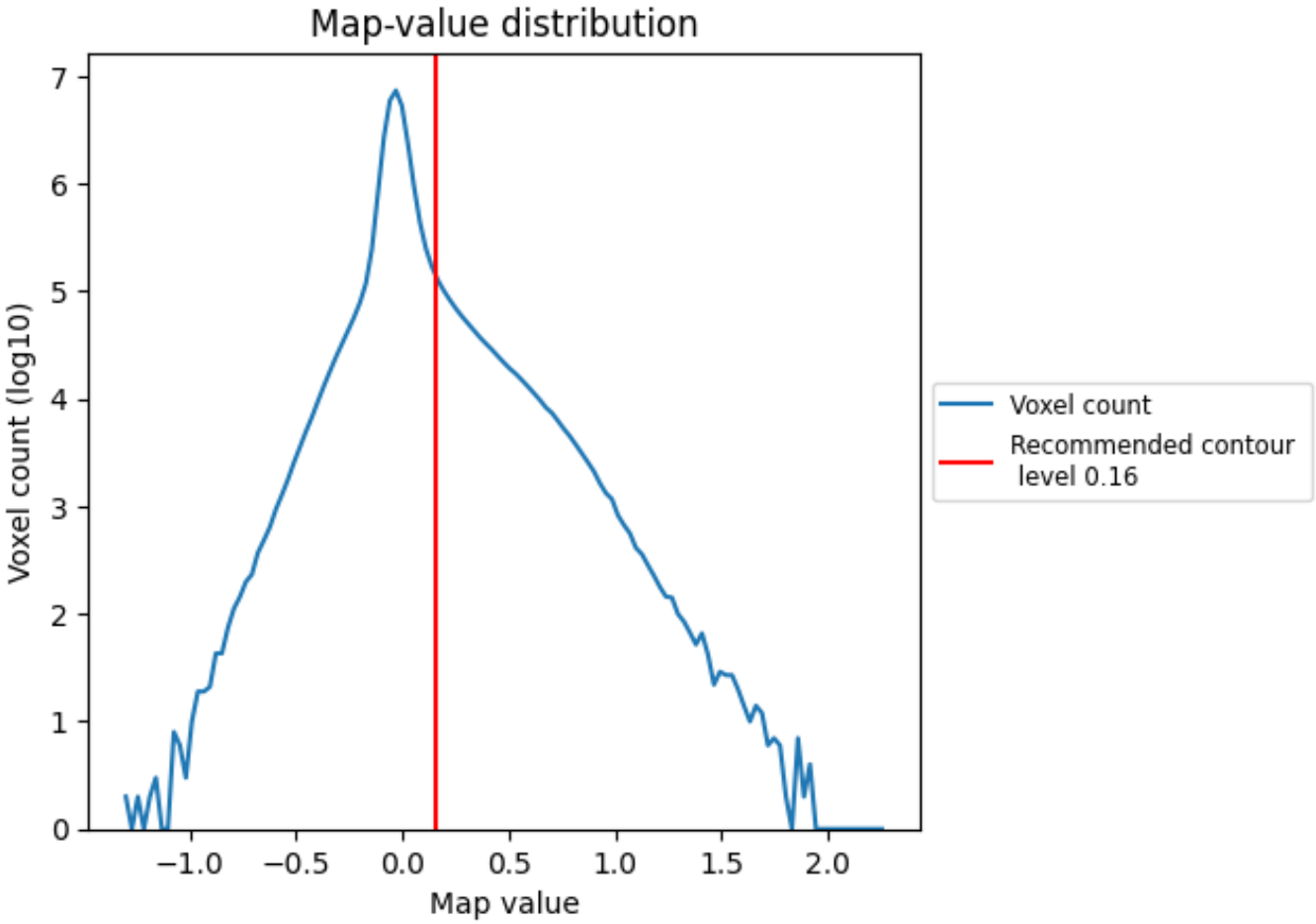
6.6 Mask visualisation (i)

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

7 Map analysis

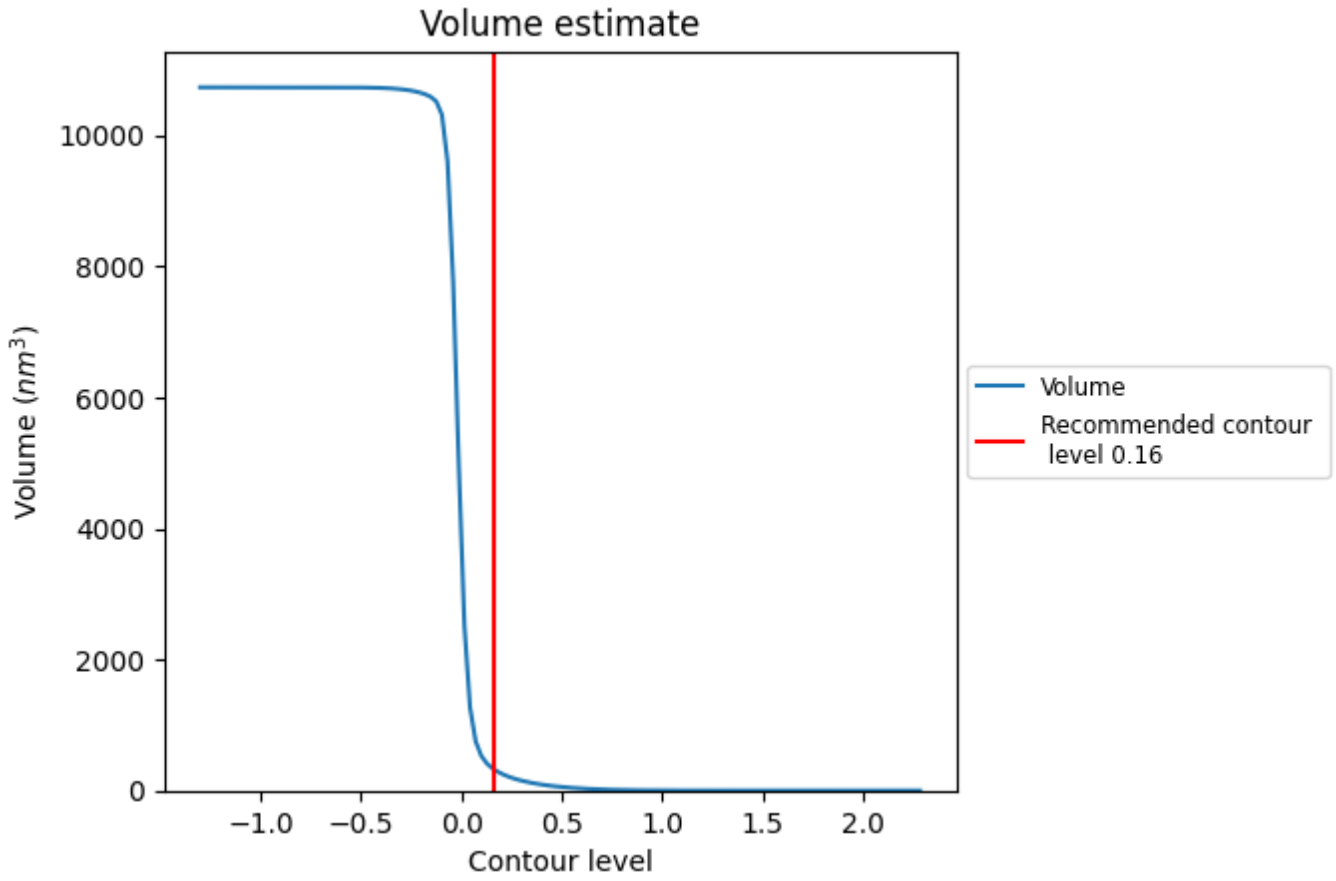
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

7.2 Volume estimate



The volume at the recommended contour level is 331 nm^3; this corresponds to an approximate mass of 299 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

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

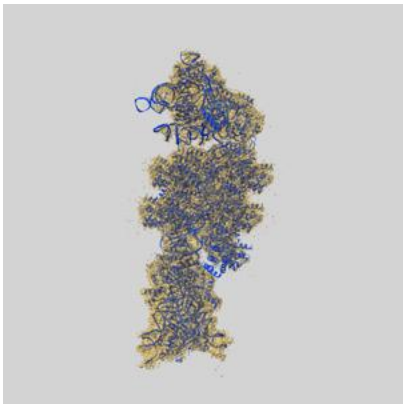
8 Fourier-Shell correlation (i)

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

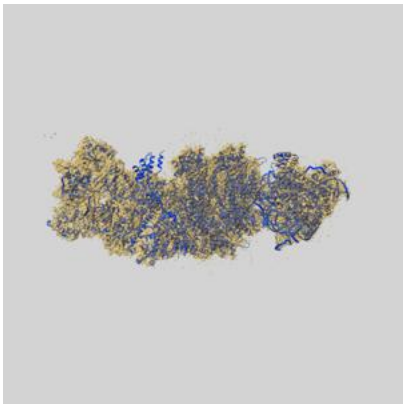
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-19075 and PDB model 8RDU. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay



X

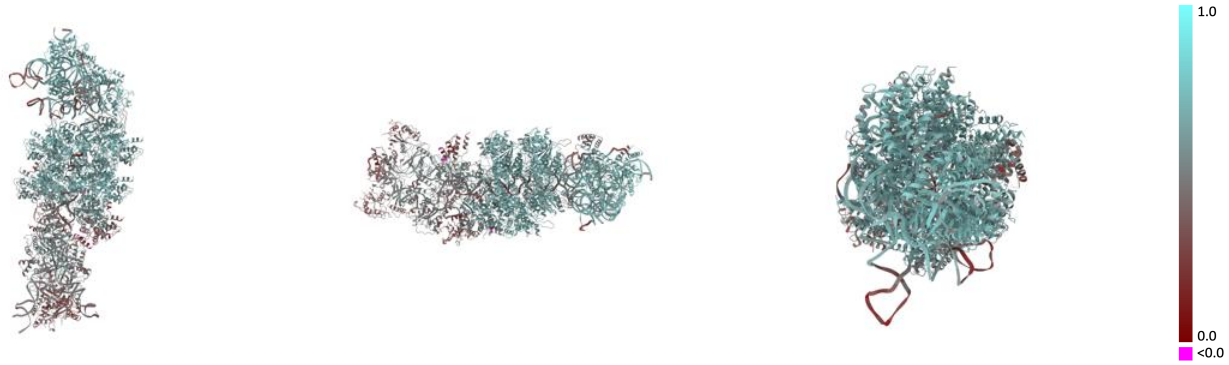


Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

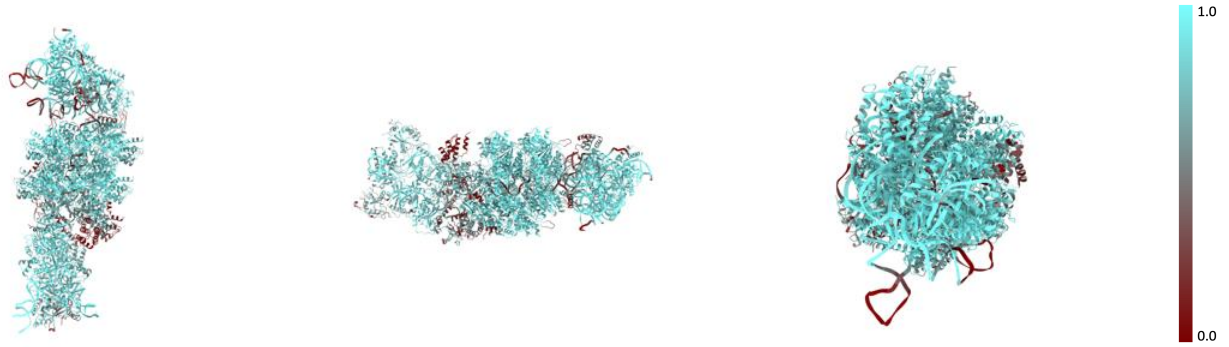
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

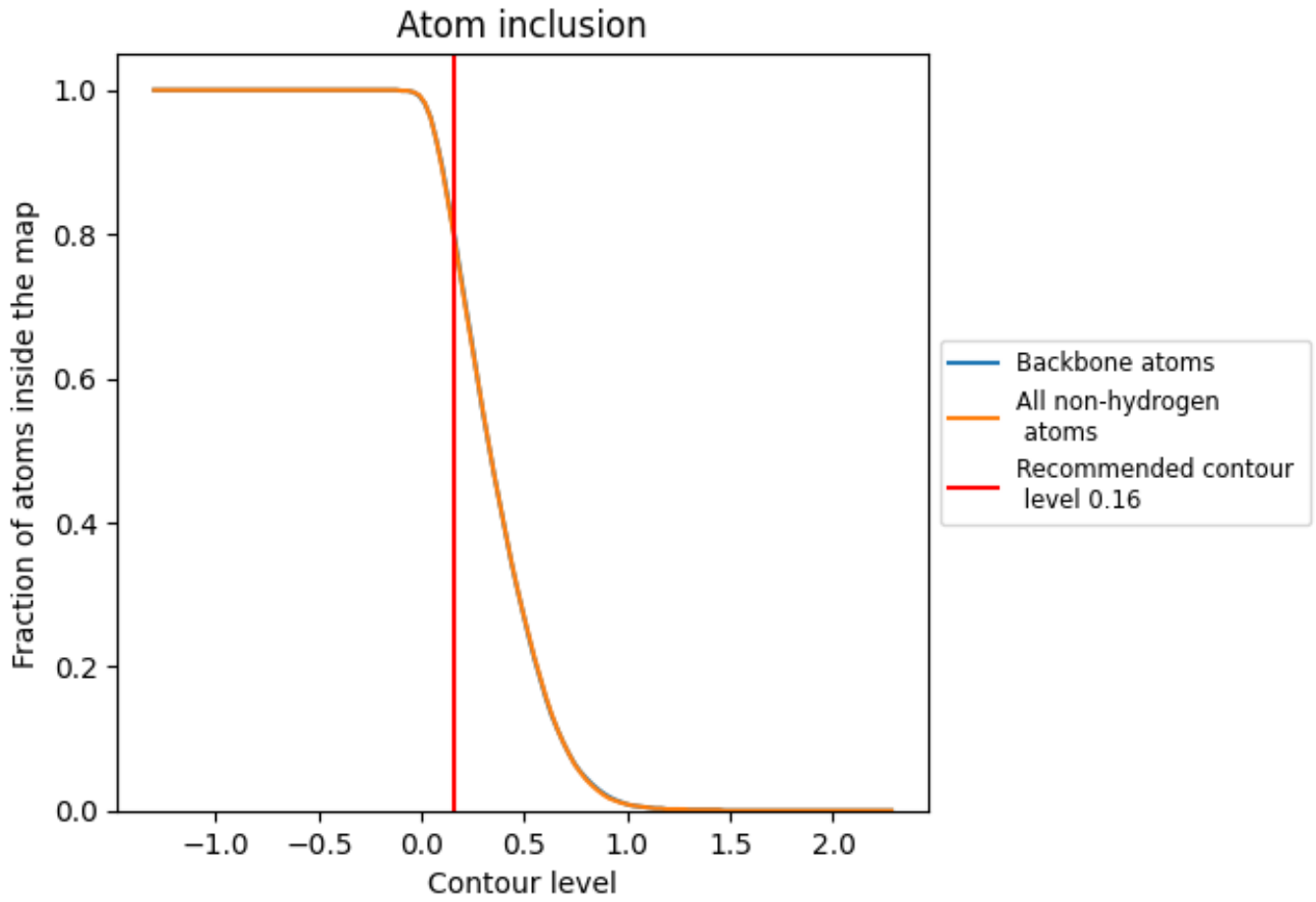
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.16).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 79% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7930	0.5590
1	0.7760	0.5750
2	0.6200	0.4700
3	0.7370	0.4960
4	0.8960	0.4850
5	0.9630	0.5080
6	0.8490	0.4590
7	0.7650	0.3970
A	0.8630	0.6470
B	0.8880	0.6530
C	0.8630	0.6490
D	0.7340	0.5870
E	0.8920	0.6480
F	0.8960	0.6500
G	0.8970	0.6370
H	0.9000	0.6460
I	0.9080	0.6540
J	0.9220	0.6560
K	0.9220	0.6530
L	0.9110	0.6470
M	0.8740	0.6220
N	0.8180	0.6040
O	0.7770	0.5930
P	0.7020	0.5510
Q	0.4220	0.4500
R	0.7940	0.4620
S	0.7140	0.4170
T	0.7810	0.4140
U	0.6430	0.3780
r	0.0600	0.2520
s	0.0430	0.2800
t	0.0600	0.3280
u	0.0260	0.3120