



Full wwPDB EM Validation Report ⓘ

Nov 3, 2022 – 07:27 AM EDT

PDB ID : 5URW
EMDB ID : EMD-8601
Title : Structure of the extended type VI secretion system sheath in *Myxococcus xanthus*
Authors : Chang, Y.-W.; Rettberg, L.A.; Jensen, G.J.
Deposited on : 2017-02-13
Resolution : 24.00 Å(reported)

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.dev43
MolProbity : 4.02b-467
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

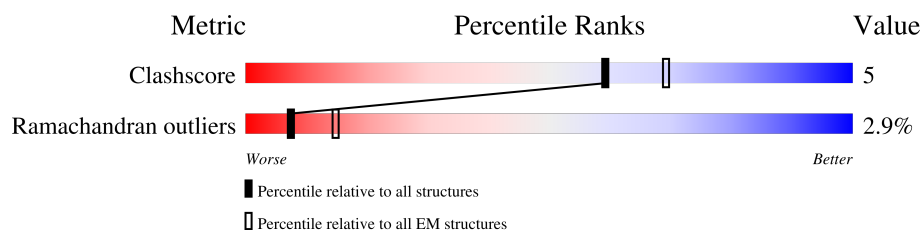
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 24.00 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

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

Mol	Chain	Length	Quality of chain
1	1A	164	<p>48% 82% 18%</p>
1	1C	164	<p>49% 82% 18%</p>
1	1E	164	<p>48% 82% 18%</p>
1	1G	164	<p>50% 82% 18%</p>
1	1I	164	<p>50% 82% 18%</p>
1	1K	164	<p>52% 82% 18%</p>
1	2A	164	<p>51% 81% 18%</p>
1	2C	164	<p>53% 81% 18%</p>
1	2E	164	<p>51% 82% 18%</p>

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Mol	Chain	Length	Quality of chain
1	2G	164	<div> <div>56%</div> <div>81%</div> <div>18%</div> </div>
1	2I	164	<div> <div>52%</div> <div>82%</div> <div>18%</div> </div>
1	2K	164	<div> <div>54%</div> <div>81%</div> <div>18%</div> </div>
1	3A	164	<div> <div>49%</div> <div>81%</div> <div>18%</div> </div>
1	3C	164	<div> <div>53%</div> <div>81%</div> <div>18%</div> </div>
1	3E	164	<div> <div>51%</div> <div>81%</div> <div>18%</div> </div>
1	3G	164	<div> <div>54%</div> <div>81%</div> <div>18%</div> </div>
1	3I	164	<div> <div>52%</div> <div>81%</div> <div>18%</div> </div>
1	3K	164	<div> <div>52%</div> <div>80%</div> <div>18%</div> </div>
2	1B	494	<div> <div>22%</div> <div>81%</div> <div>16%</div> </div>
2	1D	494	<div> <div>22%</div> <div>82%</div> <div>16%</div> </div>
2	1F	494	<div> <div>22%</div> <div>82%</div> <div>16%</div> </div>
2	1H	494	<div> <div>22%</div> <div>82%</div> <div>16%</div> </div>
2	1J	494	<div> <div>22%</div> <div>82%</div> <div>16%</div> </div>
2	1L	494	<div> <div>22%</div> <div>82%</div> <div>16%</div> </div>
2	2B	494	<div> <div>23%</div> <div>81%</div> <div>16%</div> </div>
2	2D	494	<div> <div>23%</div> <div>81%</div> <div>16%</div> </div>
2	2F	494	<div> <div>23%</div> <div>81%</div> <div>16%</div> </div>
2	2H	494	<div> <div>23%</div> <div>81%</div> <div>16%</div> </div>
2	2J	494	<div> <div>22%</div> <div>81%</div> <div>16%</div> </div>
2	2L	494	<div> <div>23%</div> <div>81%</div> <div>16%</div> </div>
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2	3F	494	<div> <div>23%</div> <div>82%</div> <div>16%</div> </div>
2	3H	494	<div> <div>23%</div> <div>82%</div> <div>16%</div> </div>

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Mol	Chain	Length	Quality of chain
2	3J	494	
2	3L	494	
3	11	163	
3	12	163	
3	13	163	
3	14	163	
3	15	163	
3	16	163	
3	21	163	
3	22	163	
3	23	163	
3	24	163	
3	25	163	
3	26	163	
3	31	163	
3	32	163	
3	33	163	
3	34	163	
3	35	163	
3	36	163	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 51048 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 TssB.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	1A	135	Total 540	C 270	N 135	O 135	0	0
1	1C	135	Total 540	C 270	N 135	O 135	0	0
1	1E	135	Total 540	C 270	N 135	O 135	0	0
1	1G	135	Total 540	C 270	N 135	O 135	0	0
1	1I	135	Total 540	C 270	N 135	O 135	0	0
1	1K	135	Total 540	C 270	N 135	O 135	0	0
1	2A	135	Total 540	C 270	N 135	O 135	0	0
1	2C	135	Total 540	C 270	N 135	O 135	0	0
1	2E	135	Total 540	C 270	N 135	O 135	0	0
1	2G	135	Total 540	C 270	N 135	O 135	0	0
1	2I	135	Total 540	C 270	N 135	O 135	0	0
1	2K	135	Total 540	C 270	N 135	O 135	0	0
1	3A	135	Total 540	C 270	N 135	O 135	0	0
1	3C	135	Total 540	C 270	N 135	O 135	0	0
1	3E	135	Total 540	C 270	N 135	O 135	0	0
1	3G	135	Total 540	C 270	N 135	O 135	0	0
1	3I	135	Total 540	C 270	N 135	O 135	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	3K	135	Total	C	N	O	0	0
			540	270	135	135		

- Molecule 2 is a protein called TssC.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	1B	414	Total	C	N	O	0	0
			1656	828	414	414		
2	1D	414	Total	C	N	O	0	0
			1656	828	414	414		
2	1F	414	Total	C	N	O	0	0
			1656	828	414	414		
2	1H	414	Total	C	N	O	0	0
			1656	828	414	414		
2	1J	414	Total	C	N	O	0	0
			1656	828	414	414		
2	1L	414	Total	C	N	O	0	0
			1656	828	414	414		
2	2B	414	Total	C	N	O	0	0
			1656	828	414	414		
2	2D	414	Total	C	N	O	0	0
			1656	828	414	414		
2	2F	414	Total	C	N	O	0	0
			1656	828	414	414		
2	2H	414	Total	C	N	O	0	0
			1656	828	414	414		
2	2J	414	Total	C	N	O	0	0
			1656	828	414	414		
2	2L	414	Total	C	N	O	0	0
			1656	828	414	414		
2	3B	414	Total	C	N	O	0	0
			1656	828	414	414		
2	3D	414	Total	C	N	O	0	0
			1656	828	414	414		
2	3F	414	Total	C	N	O	0	0
			1656	828	414	414		
2	3H	414	Total	C	N	O	0	0
			1656	828	414	414		
2	3J	414	Total	C	N	O	0	0
			1656	828	414	414		
2	3L	414	Total	C	N	O	0	0
			1656	828	414	414		

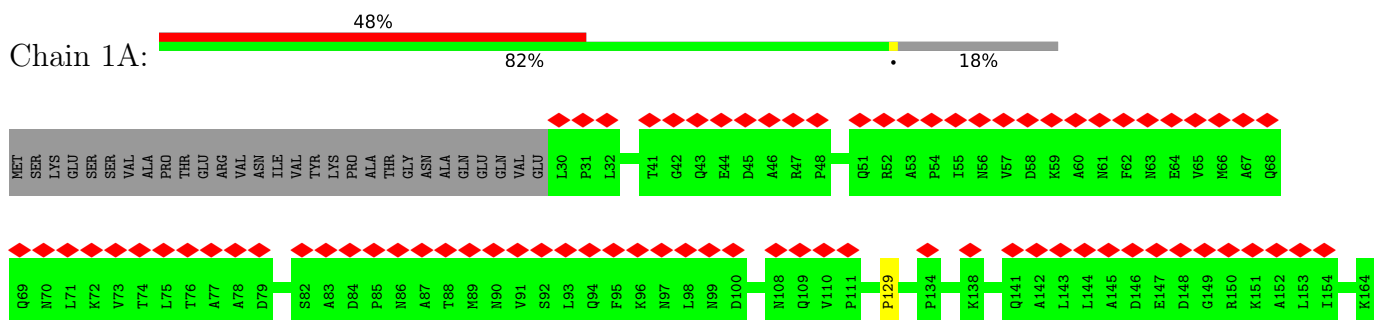
- Molecule 3 is a protein called Hcp.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	11	160	Total 640	C 320	N 160	O 160	0	0
3	12	160	Total 640	C 320	N 160	O 160	0	0
3	13	160	Total 640	C 320	N 160	O 160	0	0
3	14	160	Total 640	C 320	N 160	O 160	0	0
3	15	160	Total 640	C 320	N 160	O 160	0	0
3	16	160	Total 640	C 320	N 160	O 160	0	0
3	21	160	Total 640	C 320	N 160	O 160	0	0
3	22	160	Total 640	C 320	N 160	O 160	0	0
3	23	160	Total 640	C 320	N 160	O 160	0	0
3	24	160	Total 640	C 320	N 160	O 160	0	0
3	25	160	Total 640	C 320	N 160	O 160	0	0
3	26	160	Total 640	C 320	N 160	O 160	0	0
3	31	160	Total 640	C 320	N 160	O 160	0	0
3	32	160	Total 640	C 320	N 160	O 160	0	0
3	33	160	Total 640	C 320	N 160	O 160	0	0
3	34	160	Total 640	C 320	N 160	O 160	0	0
3	35	160	Total 640	C 320	N 160	O 160	0	0
3	36	160	Total 640	C 320	N 160	O 160	0	0

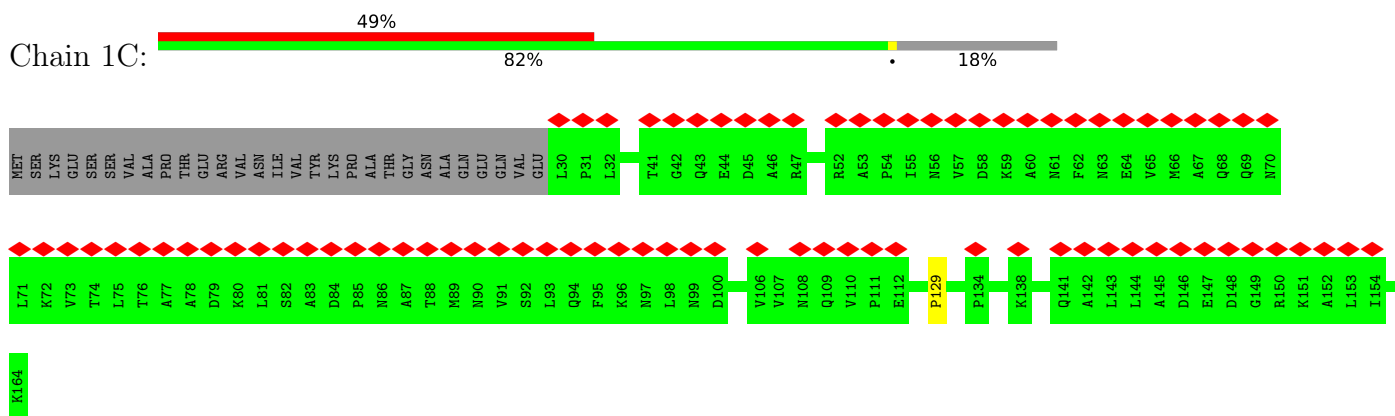
3 Residue-property plots

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

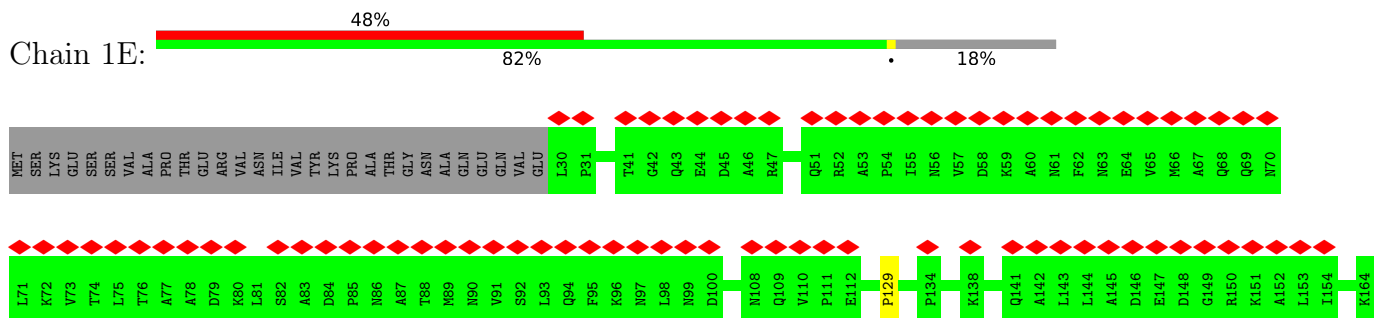
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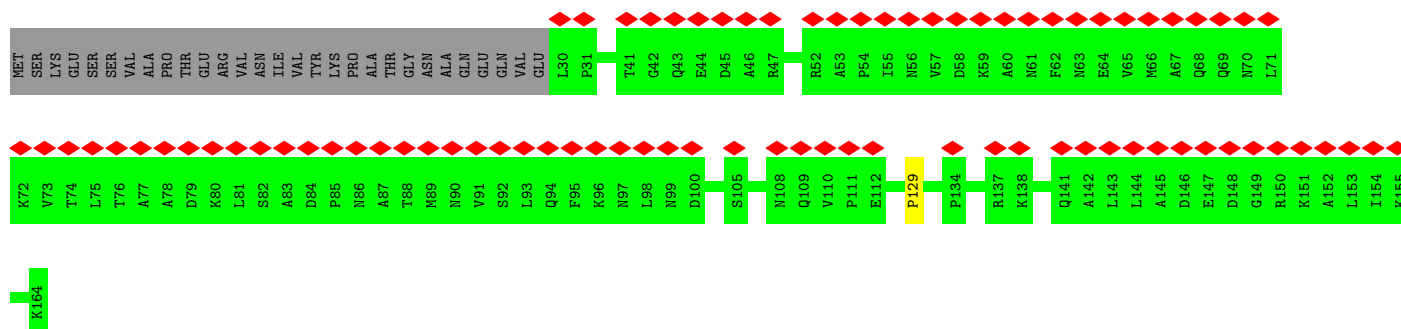
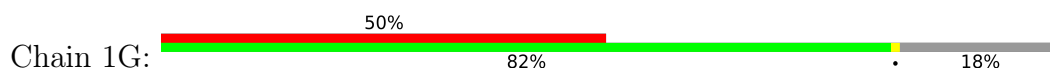
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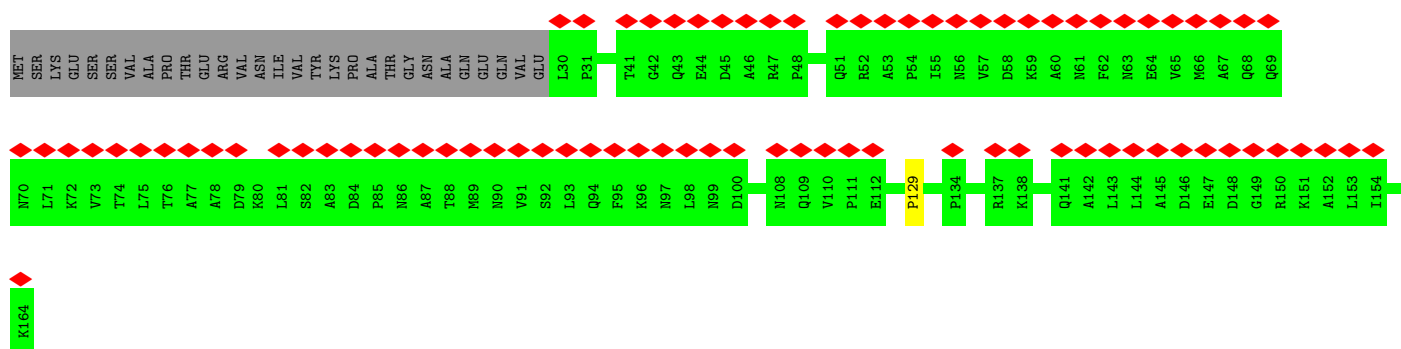
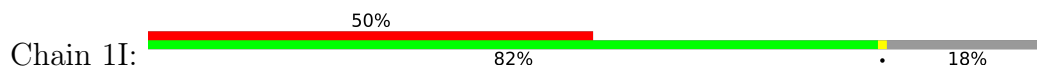
• Molecule 1: TssB



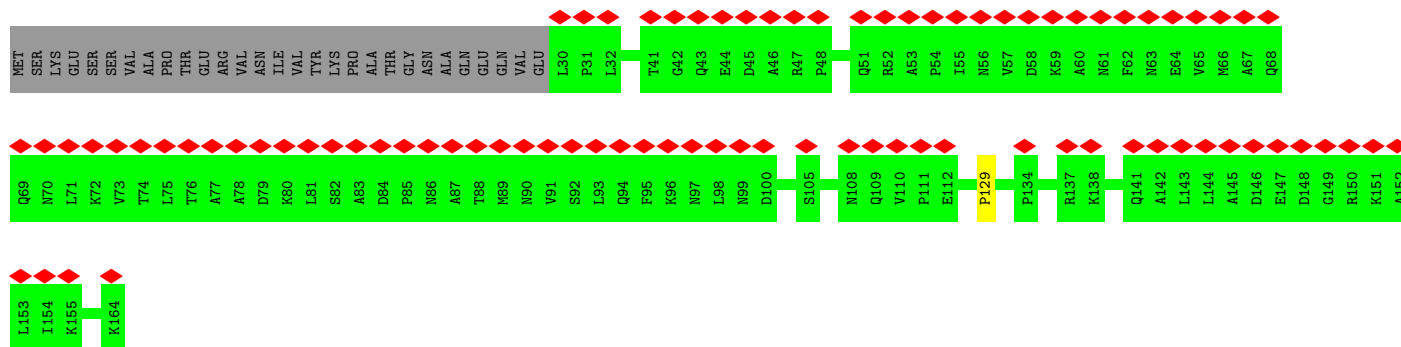
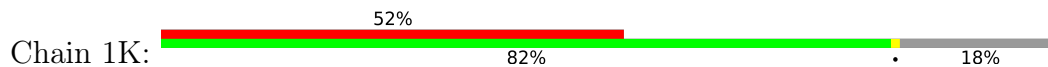
• Molecule 1: TssB



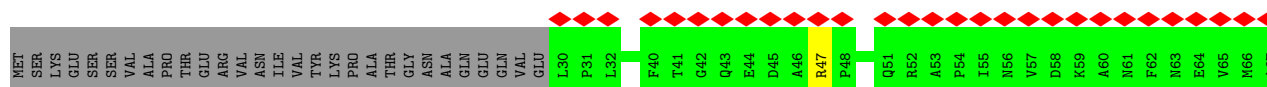
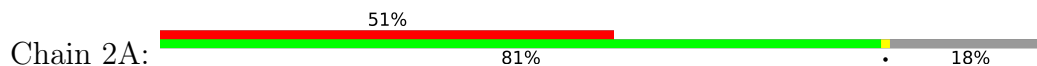
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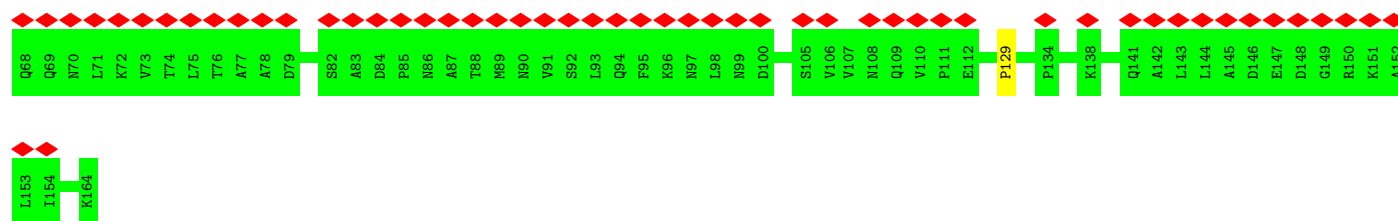


- Molecule 1: TssB

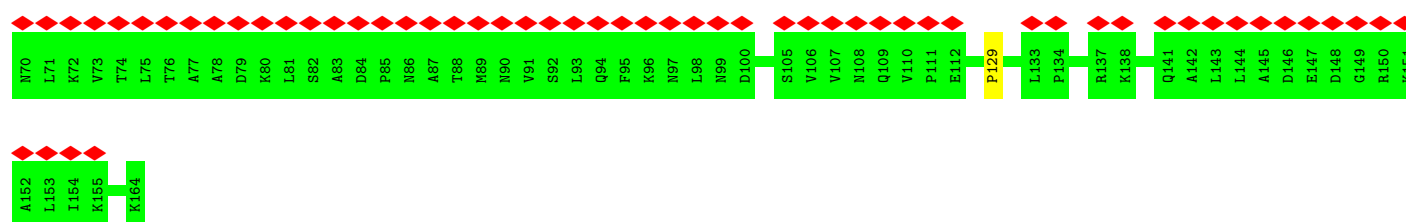
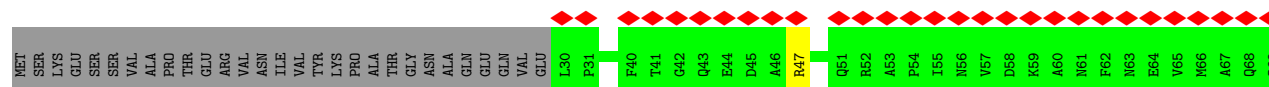
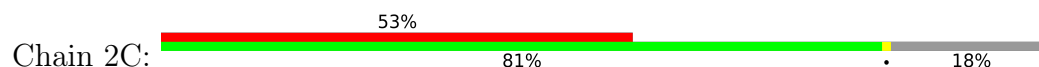


- Molecule 1: TssB

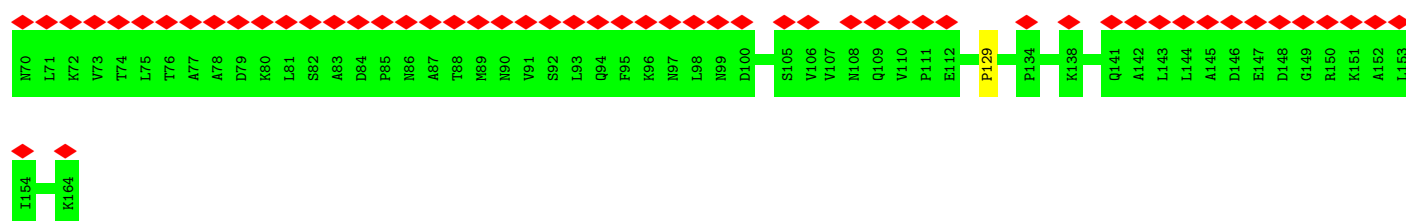
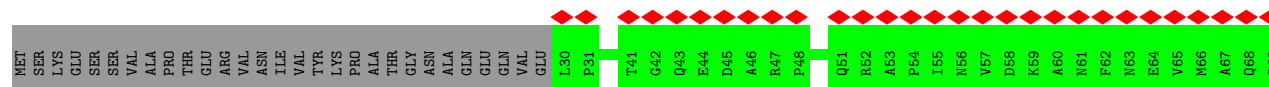
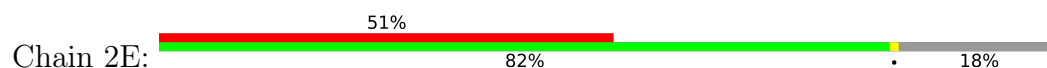




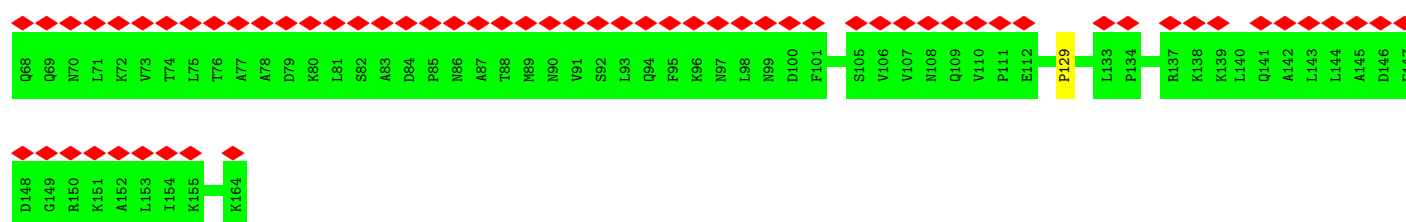
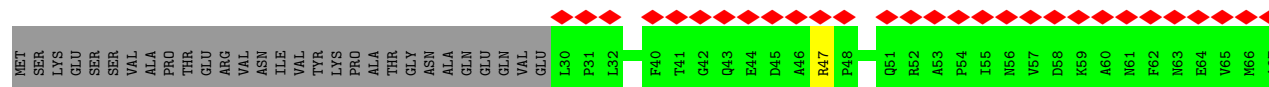
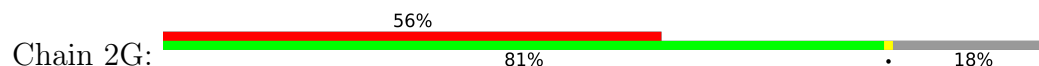
• Molecule 1: TssB



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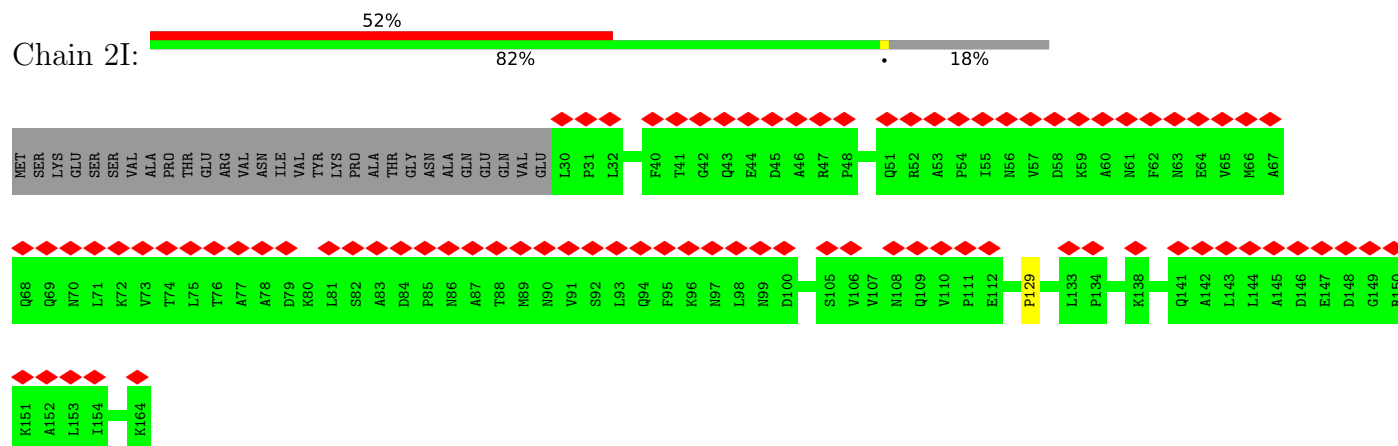


• Molecule 1: TssB



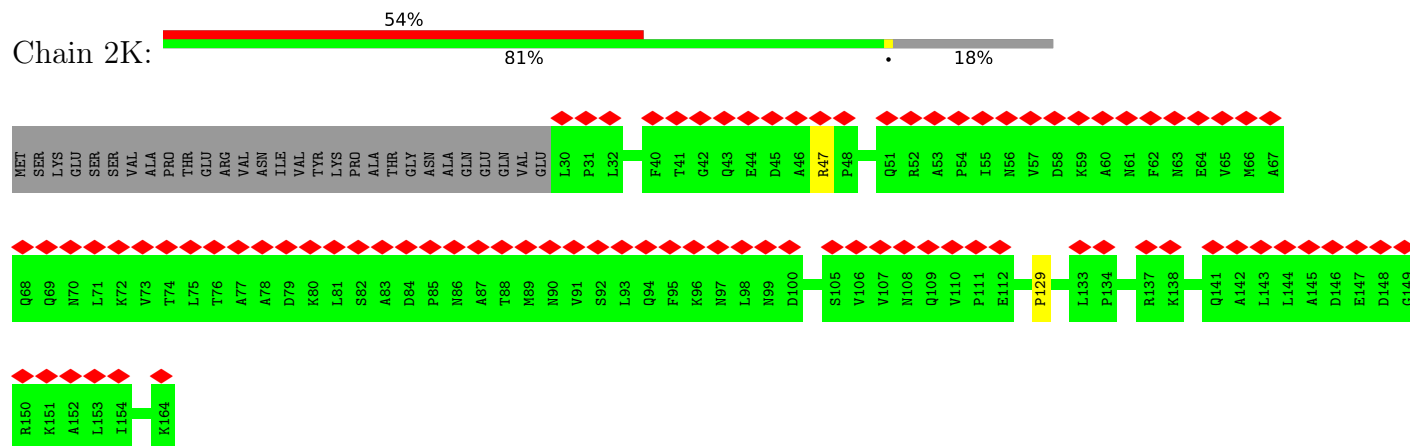
• Molecule 1: TssB

Chain 2I:



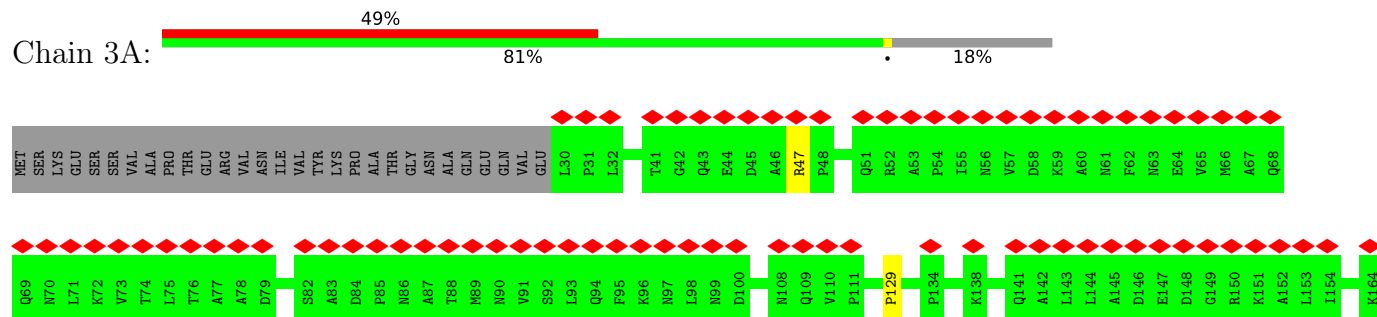
• Molecule 1: TssB

Chain 2K:



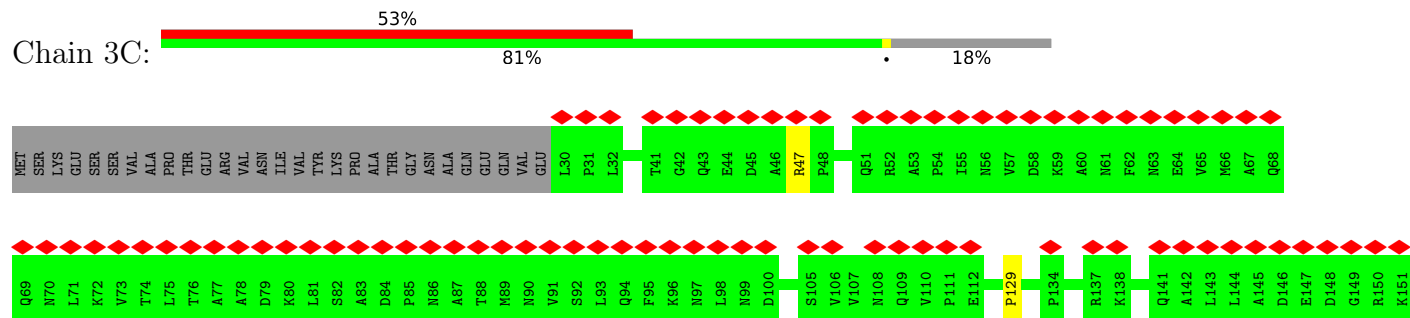
• Molecule 1: TssB

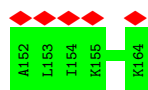
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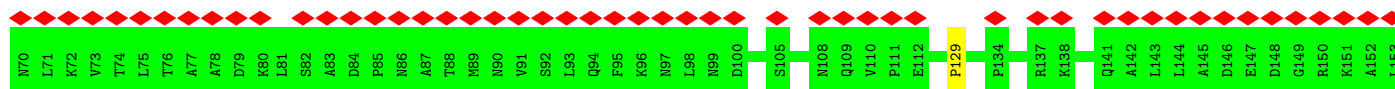
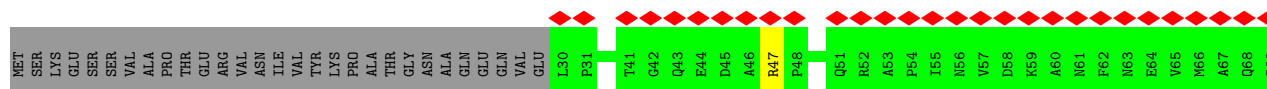
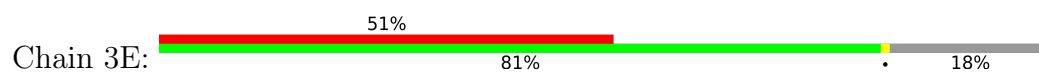
• Molecule 1: TssB

Chain 3C:

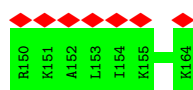
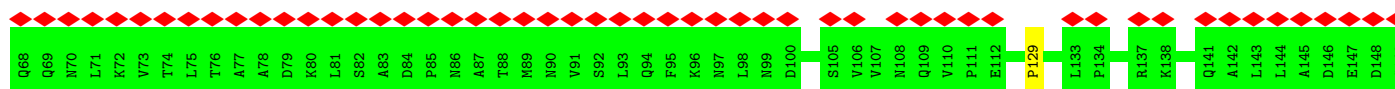
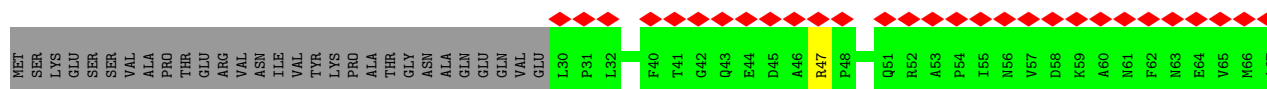
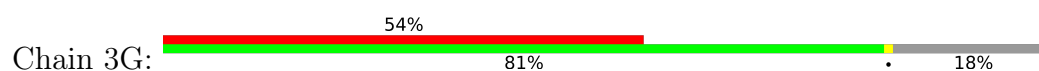




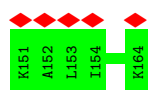
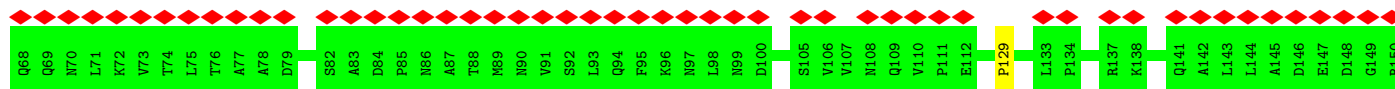
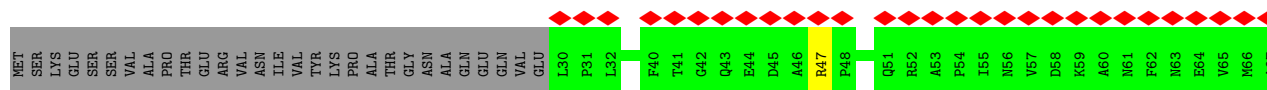
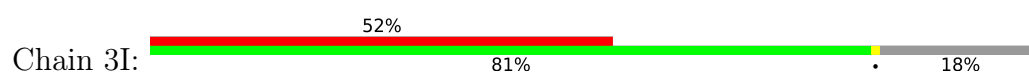
- Molecule 1: TssB




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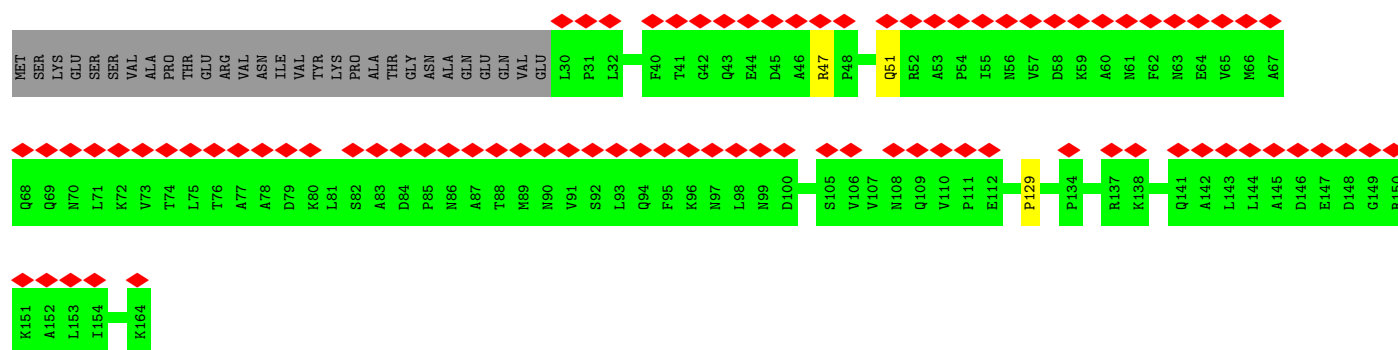


- Molecule 1: TssB




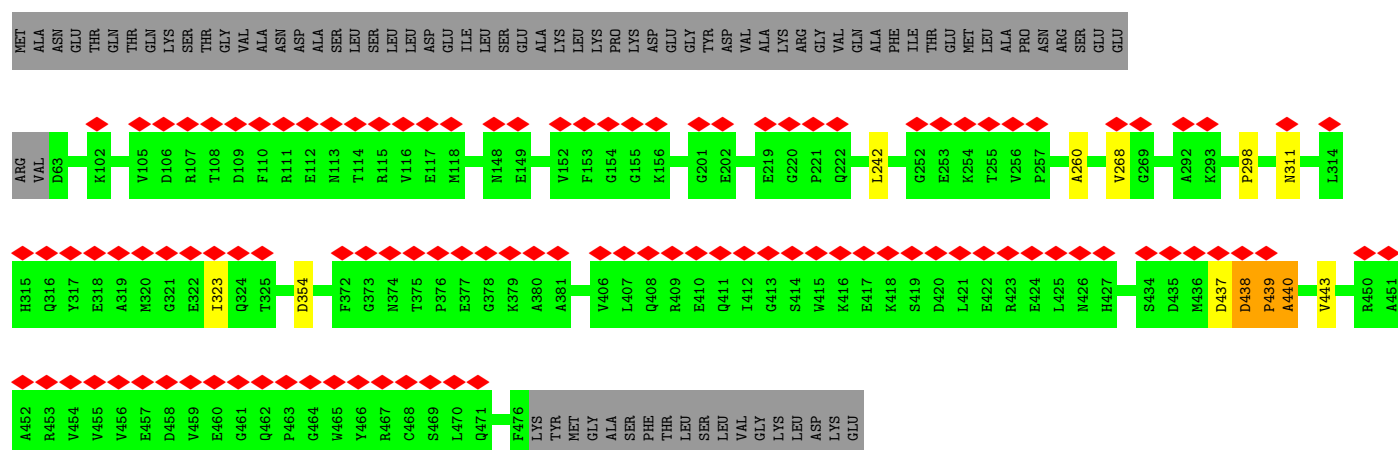
- Molecule 1: TssB

Chain 3K: 




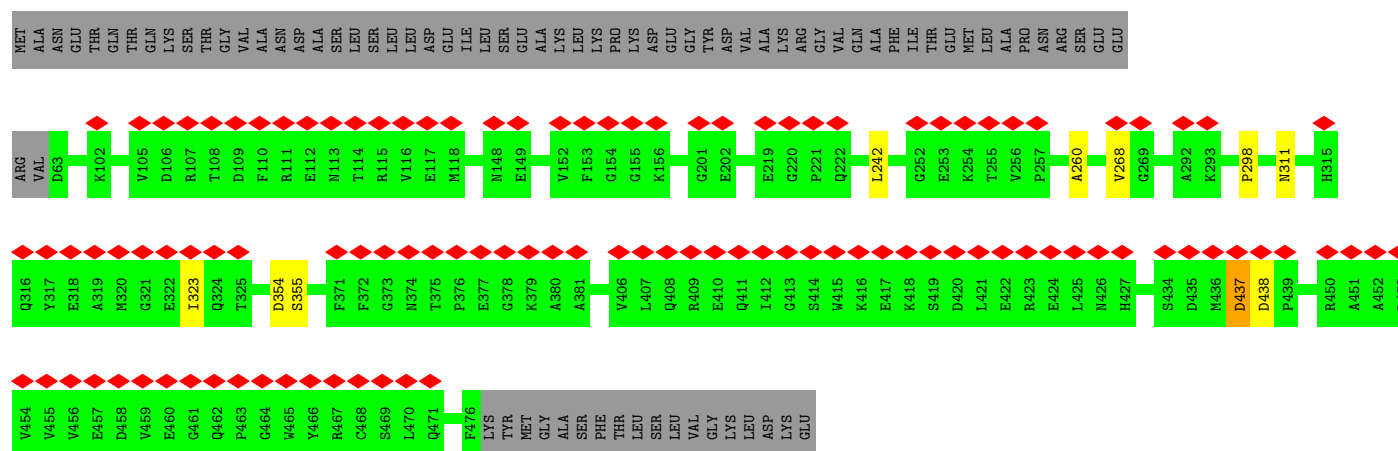
• Molecule 2: TssC

Chain 1B: 




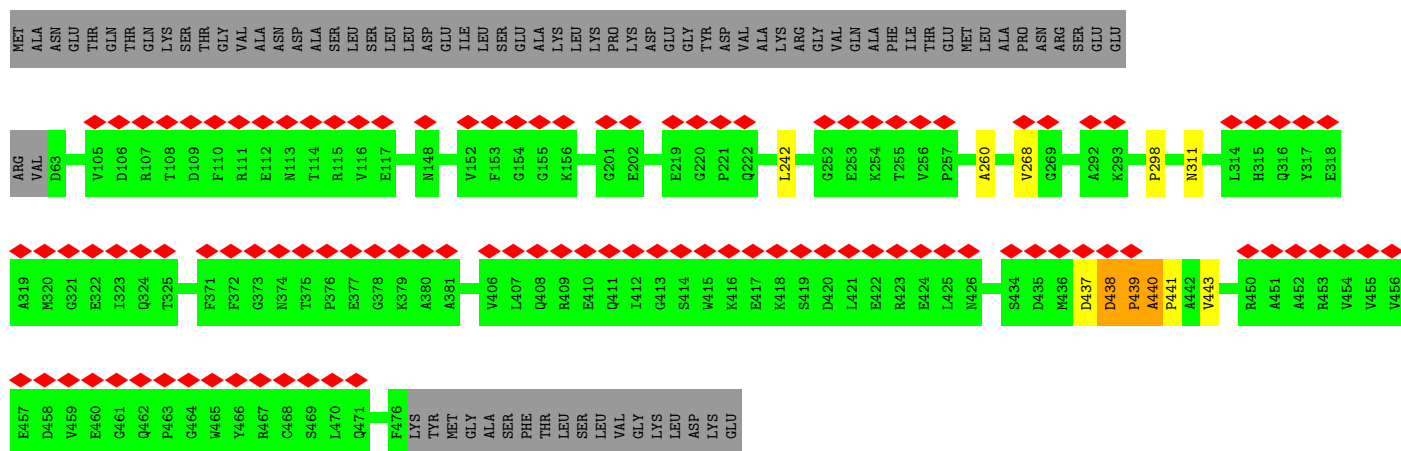
• Molecule 2: TssC

Chain 1D: 

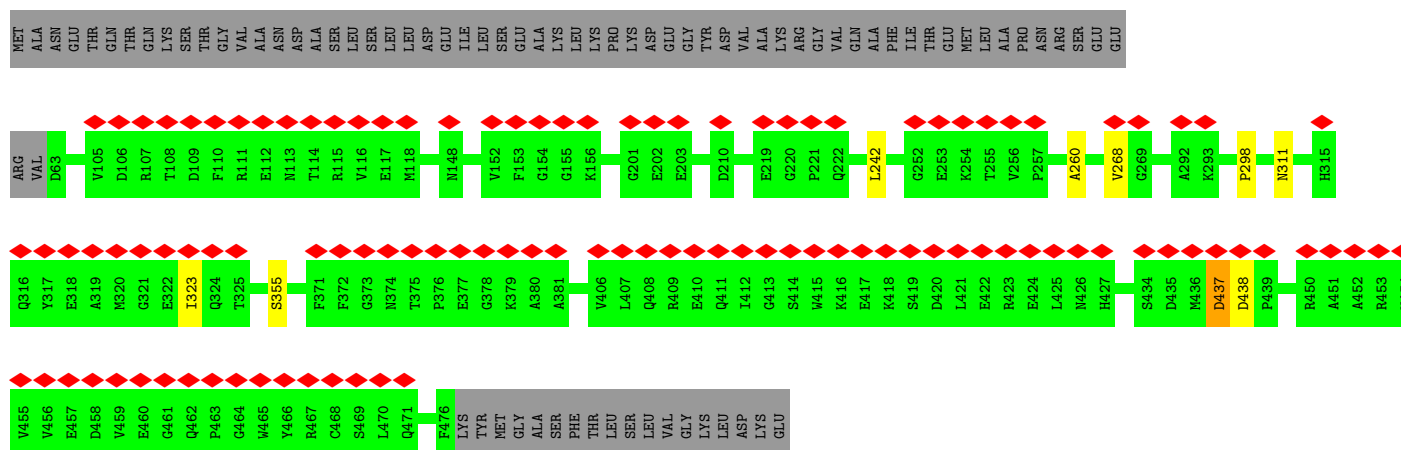
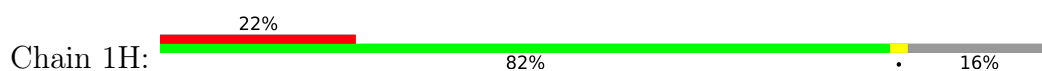


• Molecule 2: TssC

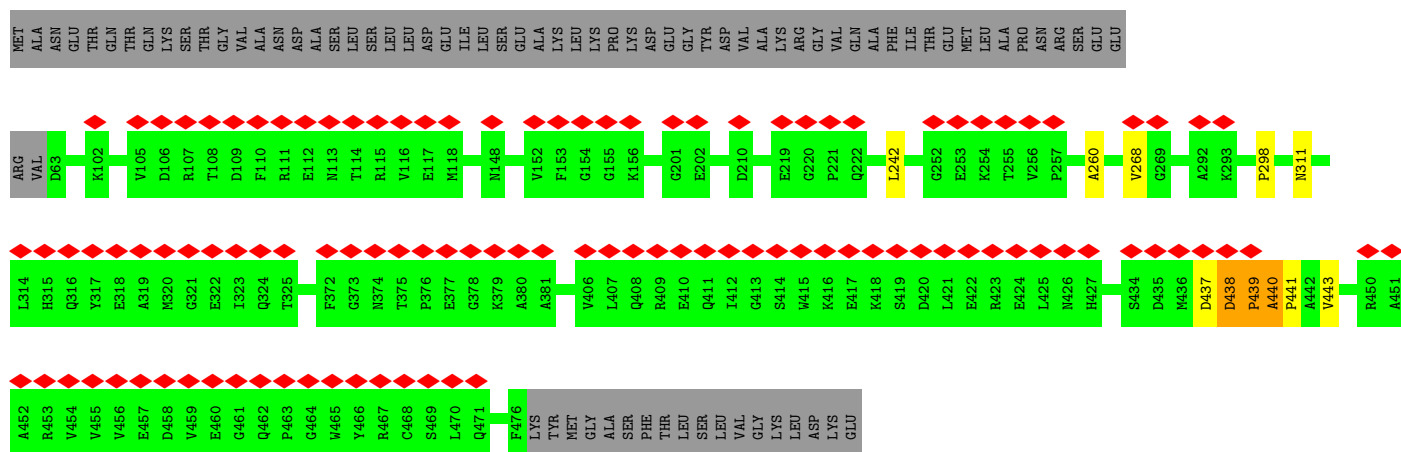
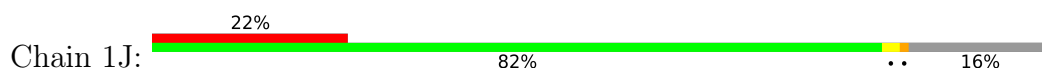
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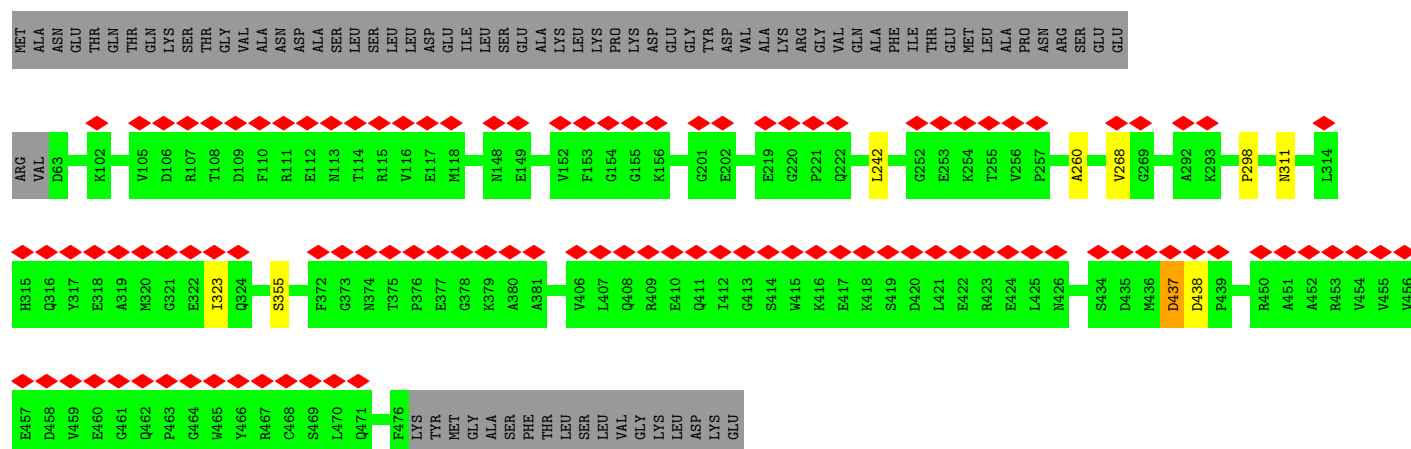
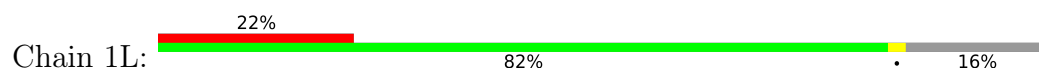
• Molecule 2: TssC



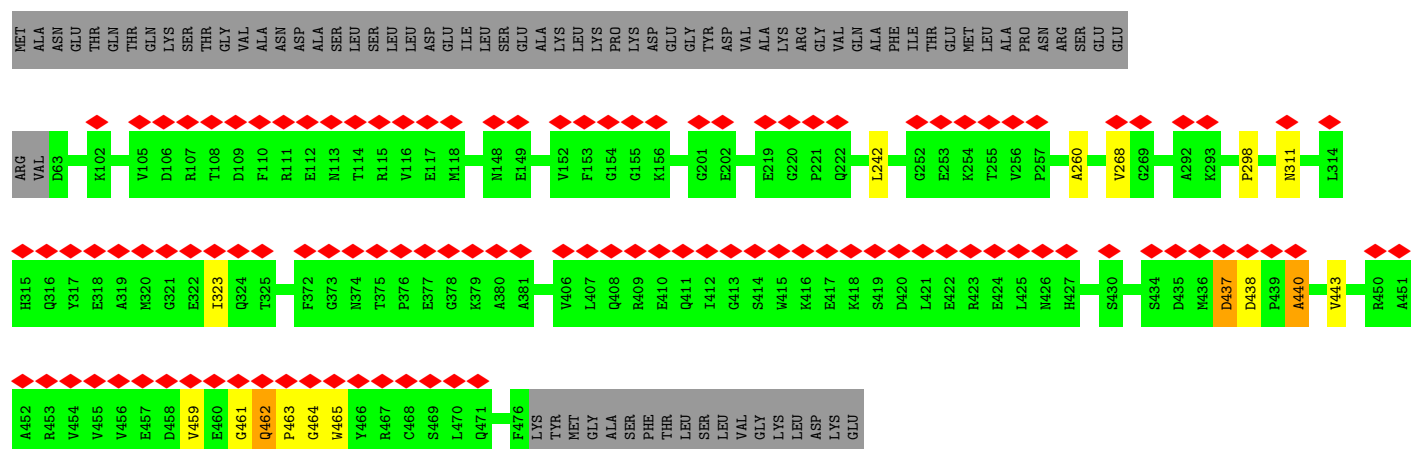
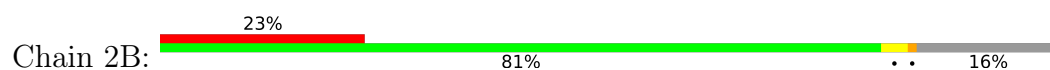
• Molecule 2: TssC



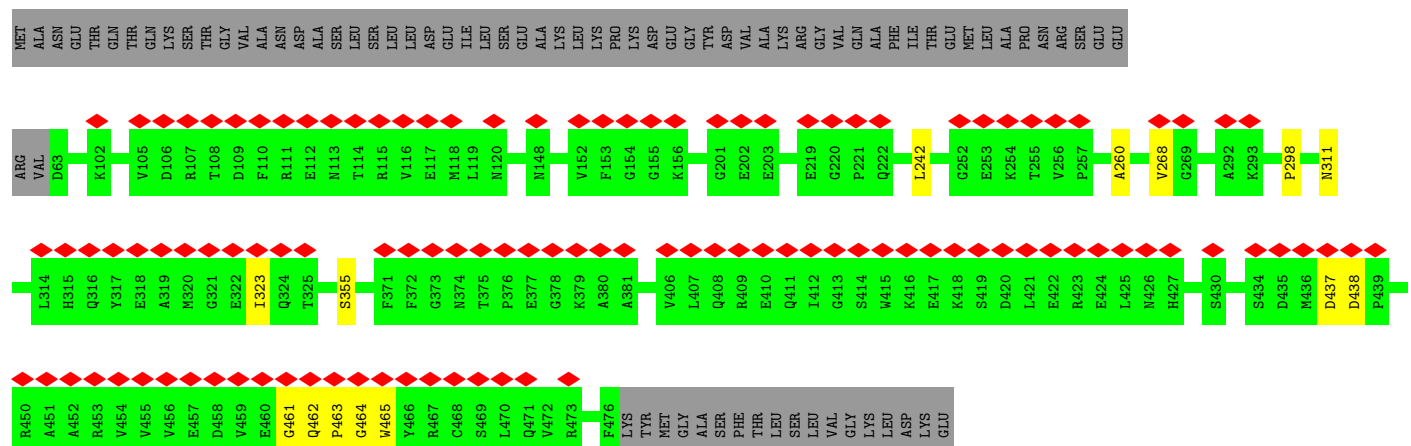
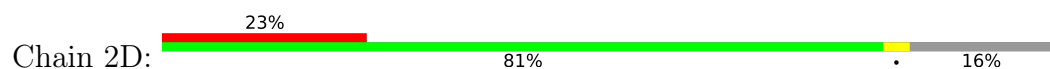
• Molecule 2: TssC




• Molecule 2: TssC

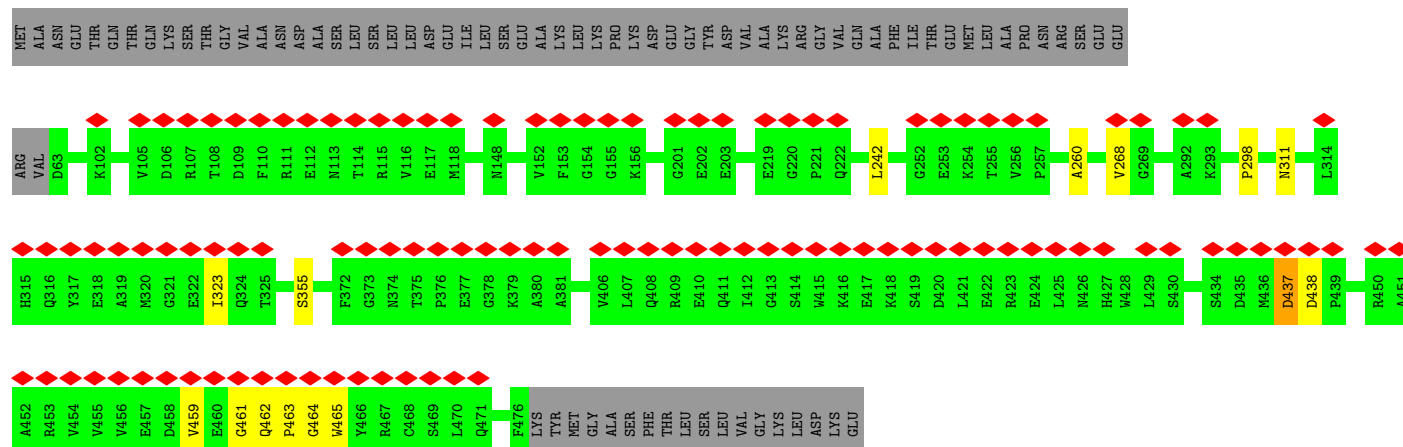


• Molecule 2: TssC




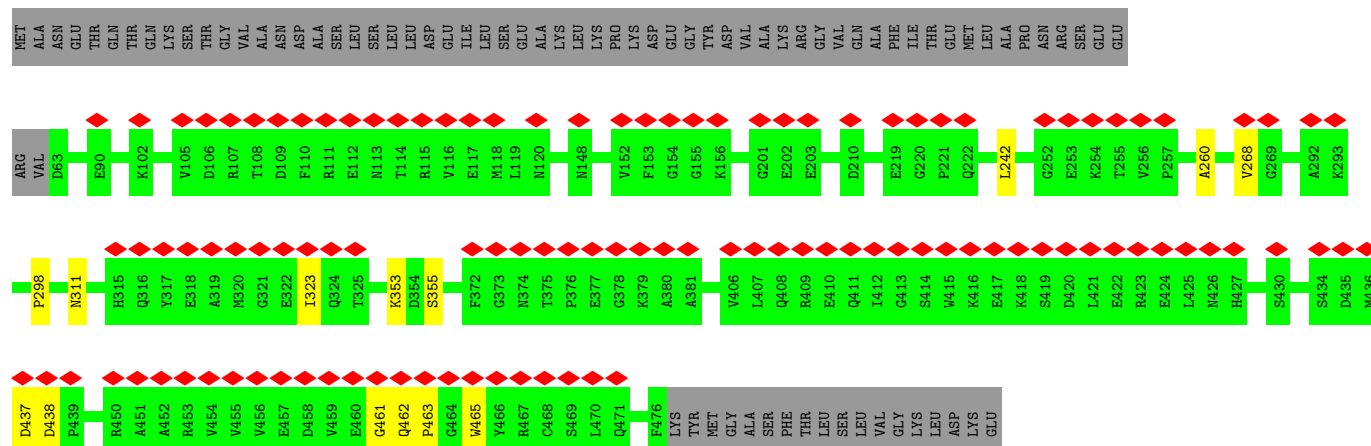
• Molecule 2: TssC

Chain 2F: 




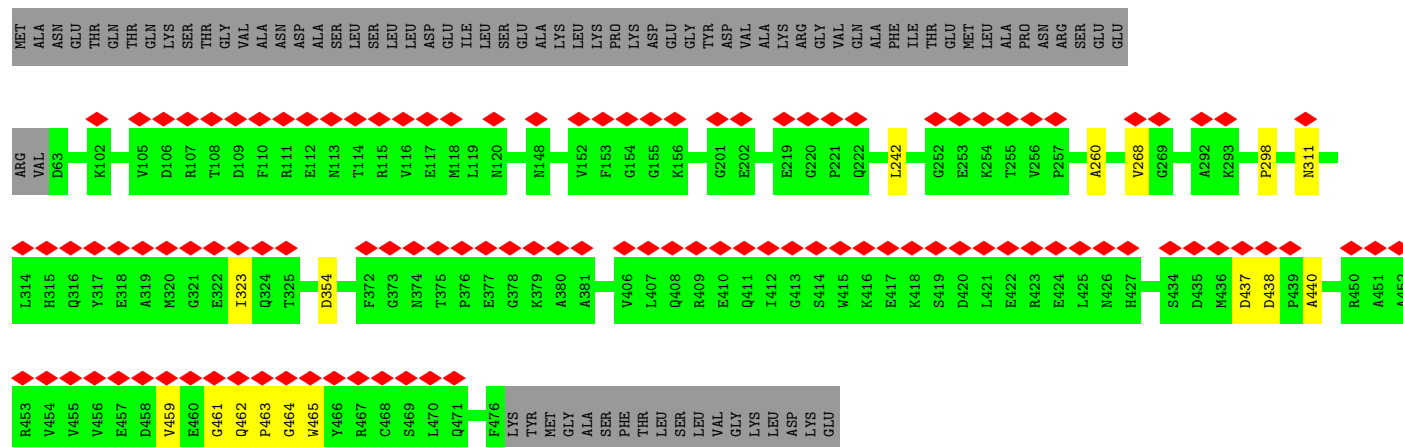
• Molecule 2: TssC

Chain 2H: 



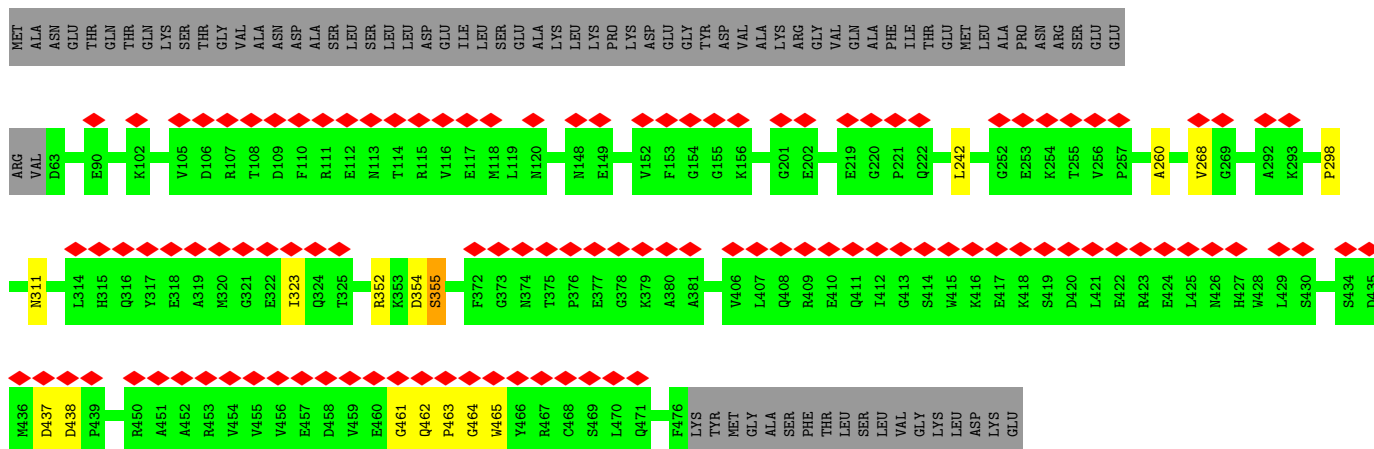
• Molecule 2: TssC

Chain 2J: 



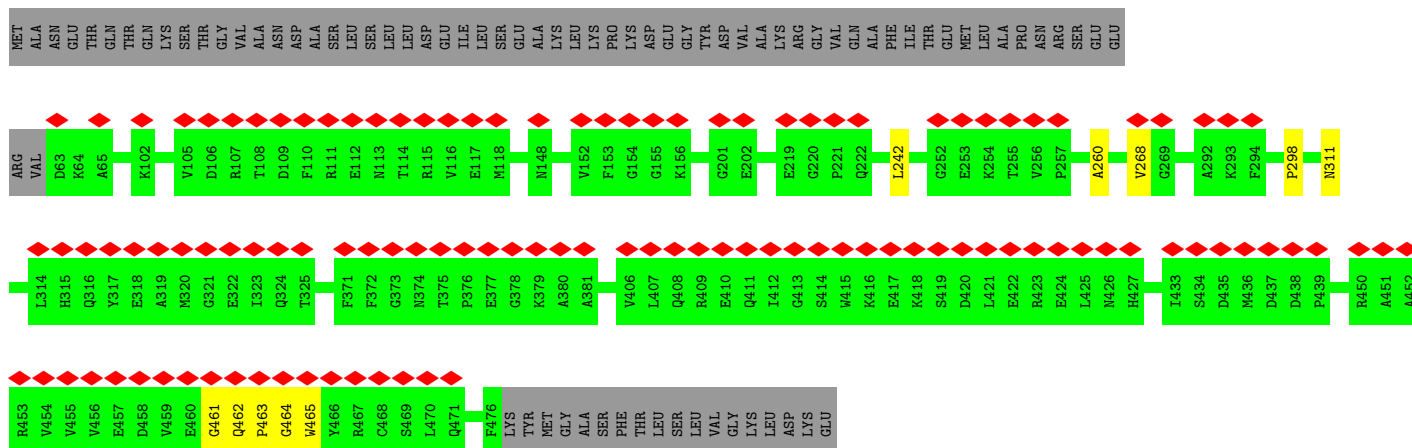
- Molecule 2: TssC

Chain 2L: 23% 81% 16%



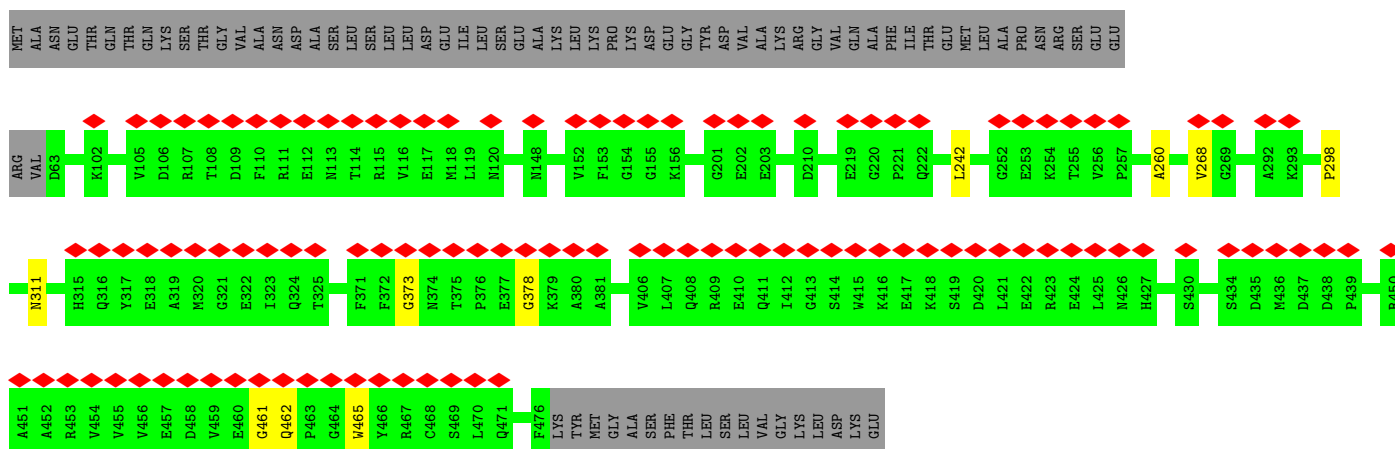
- Molecule 2: TssC

Chain 3B: 23% 82% 16%

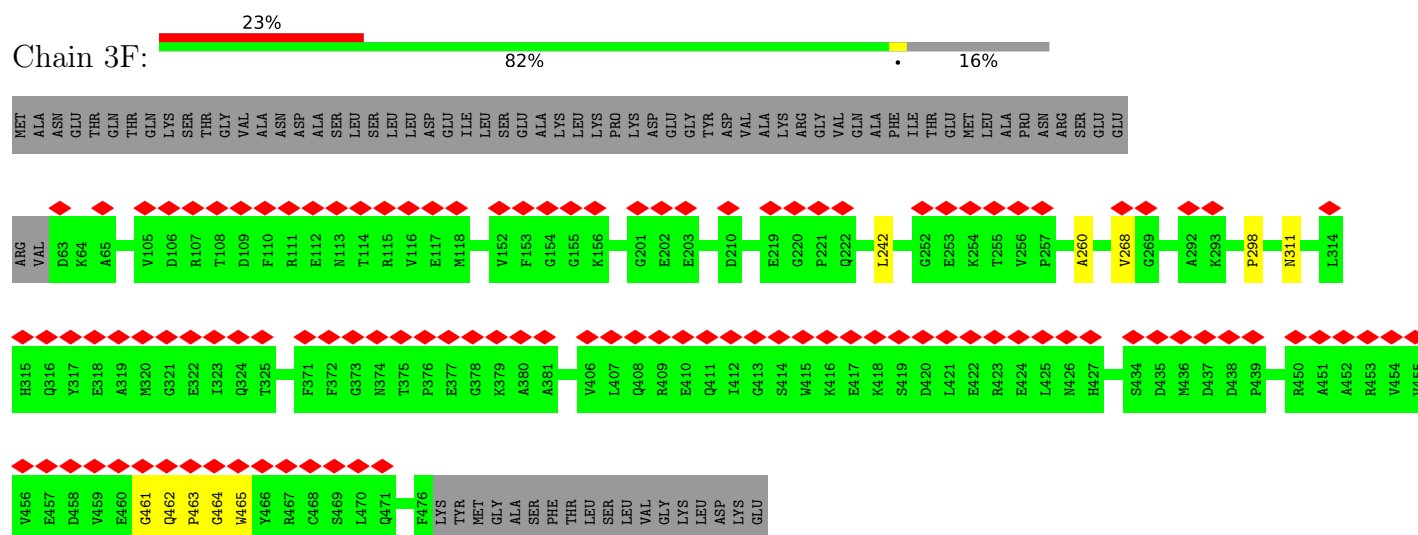


- Molecule 2: TssC

Chain 3D: 23% 82% 16%



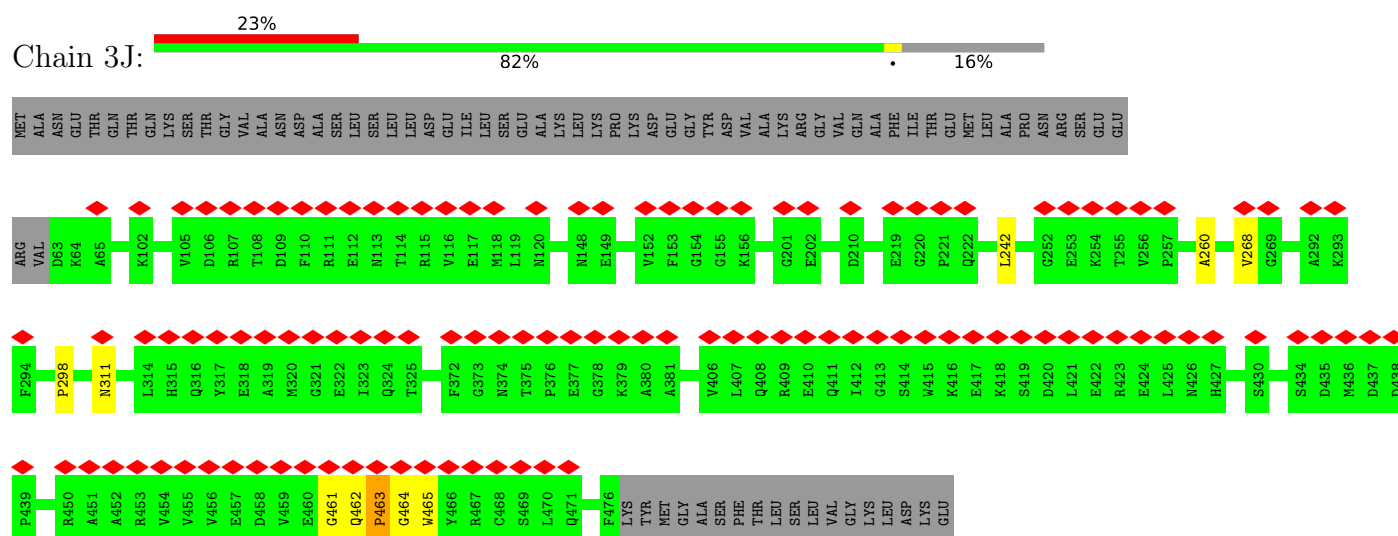
● Molecule 2: TssC



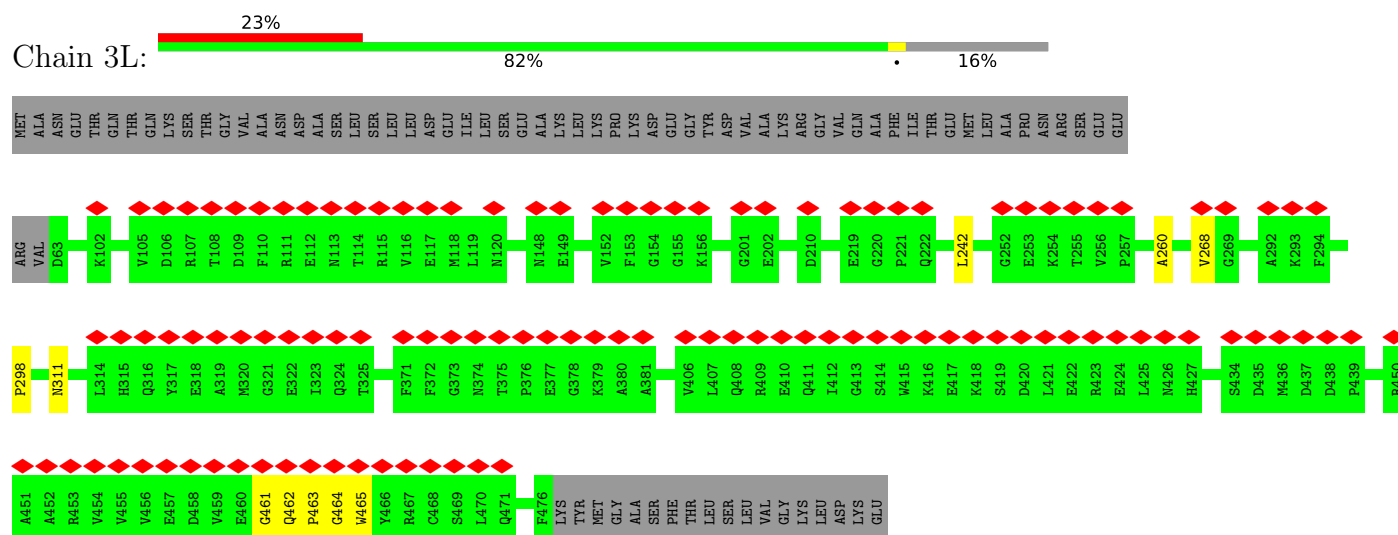
● Molecule 2: TssC



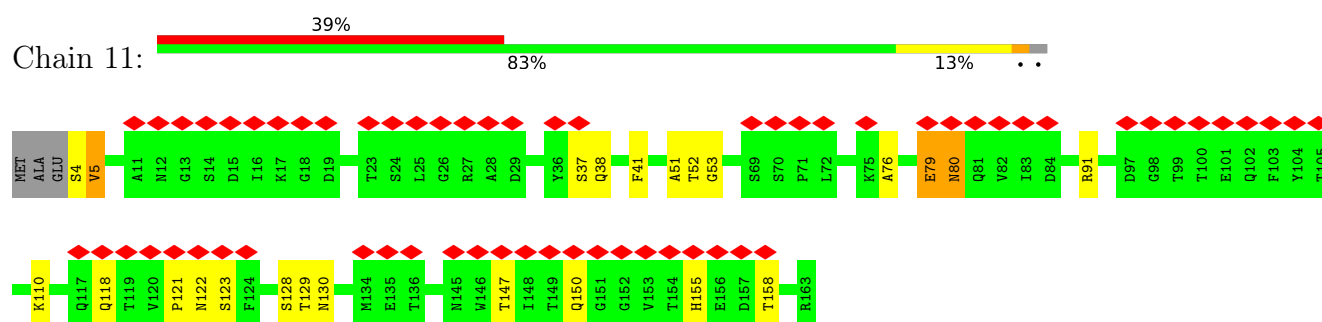
● Molecule 2: TssC



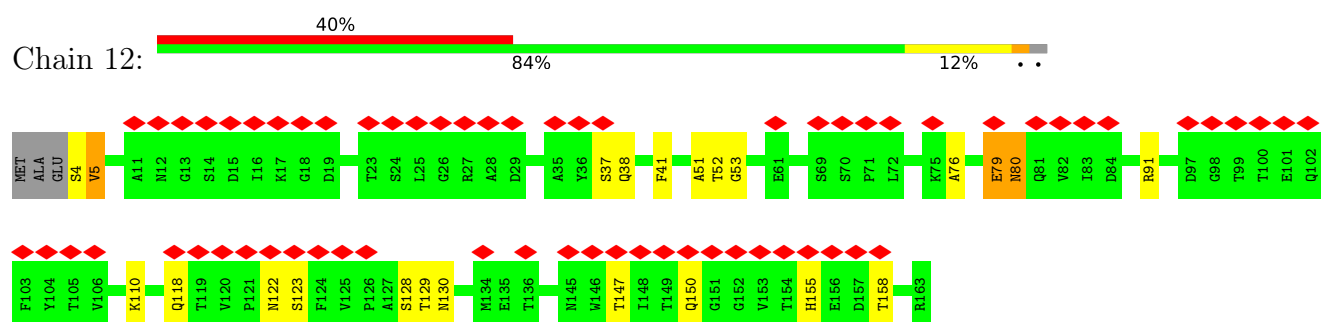
- Molecule 2: TssC



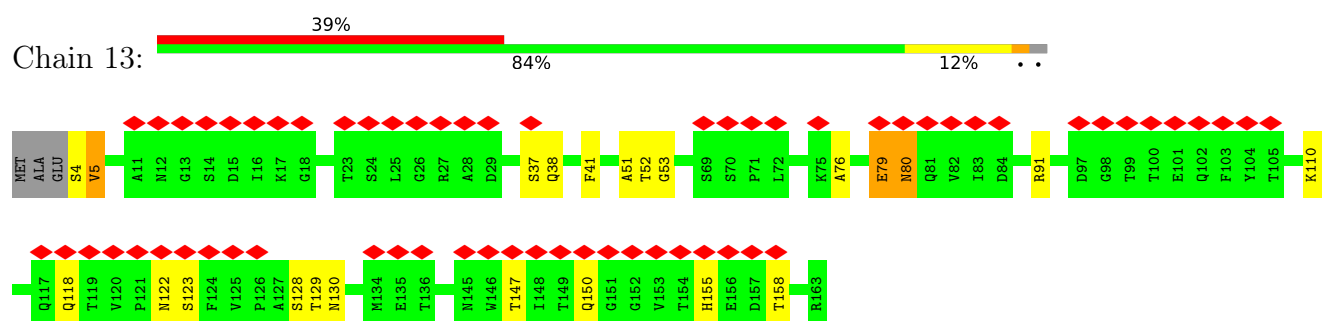
- Molecule 3: Hcp



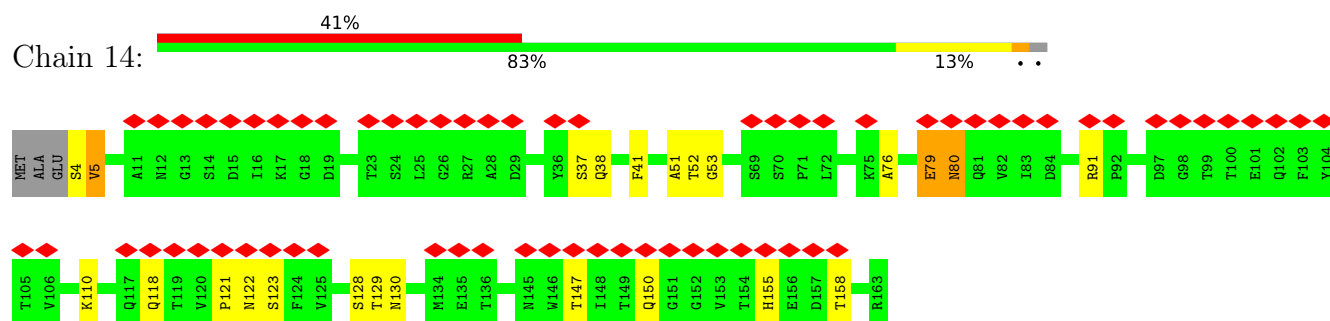
- Molecule 3: Hcp



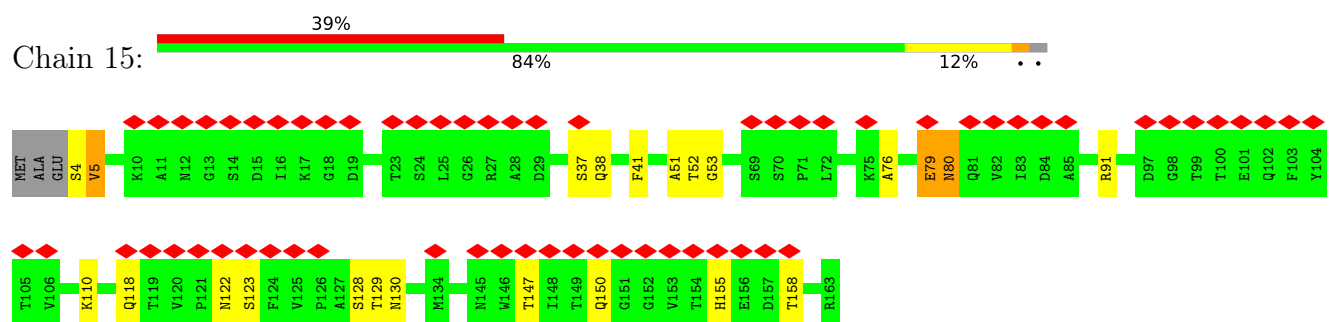
- Molecule 3: Hcp



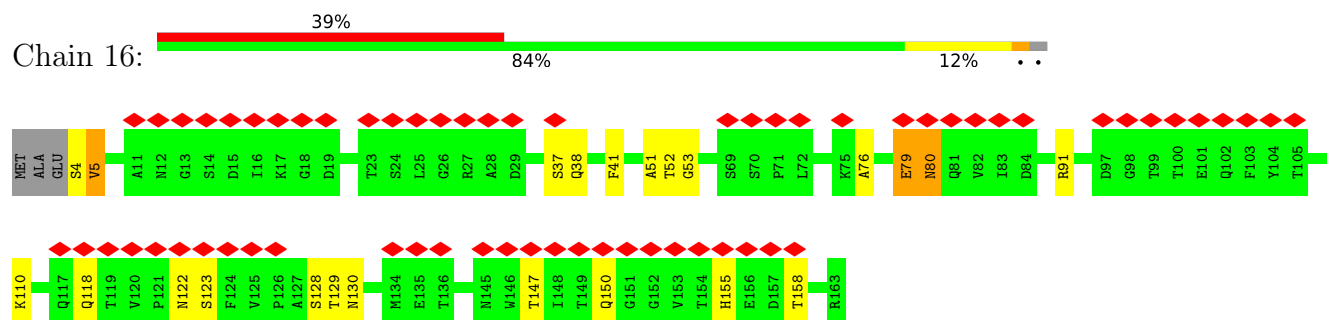
- Molecule 3: Hcp



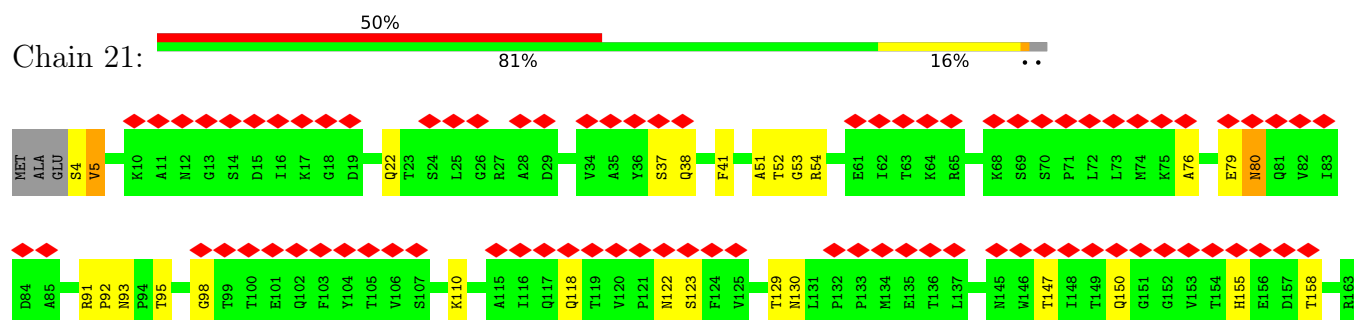
- Molecule 3: Hcp



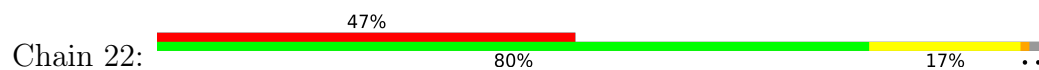
- Molecule 3: Hcp

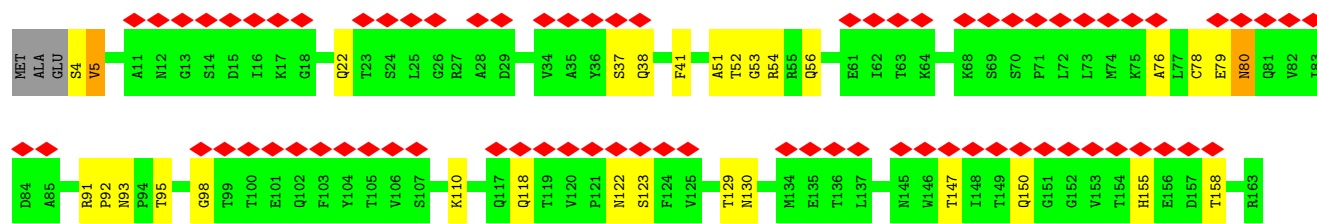


- Molecule 3: Hcp

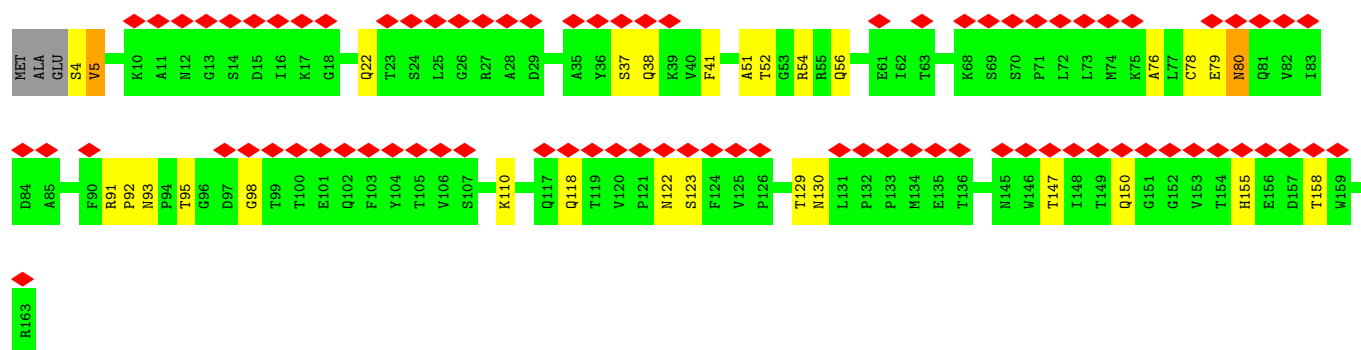
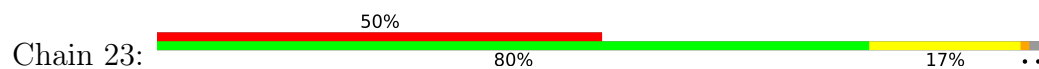


- Molecule 3: Hcp

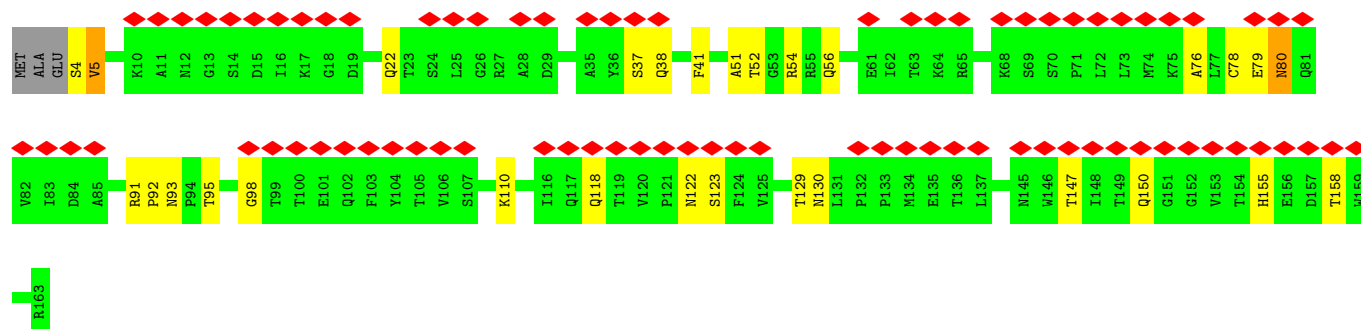
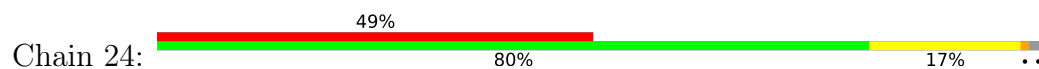




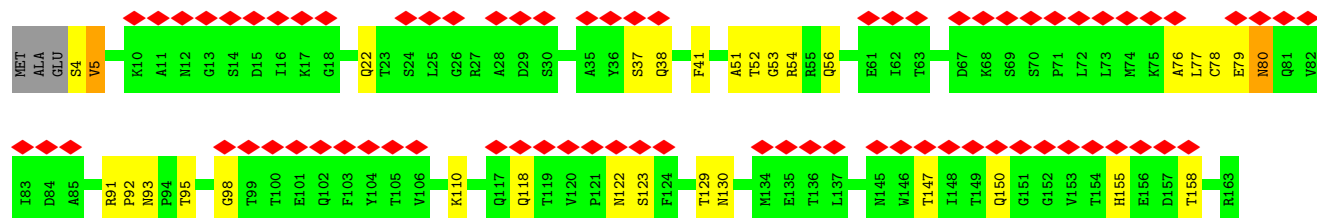
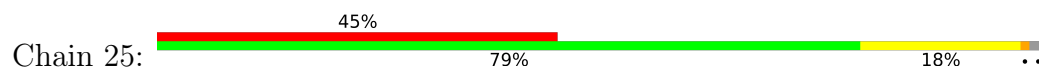
• Molecule 3: Hcp



• Molecule 3: Hcp

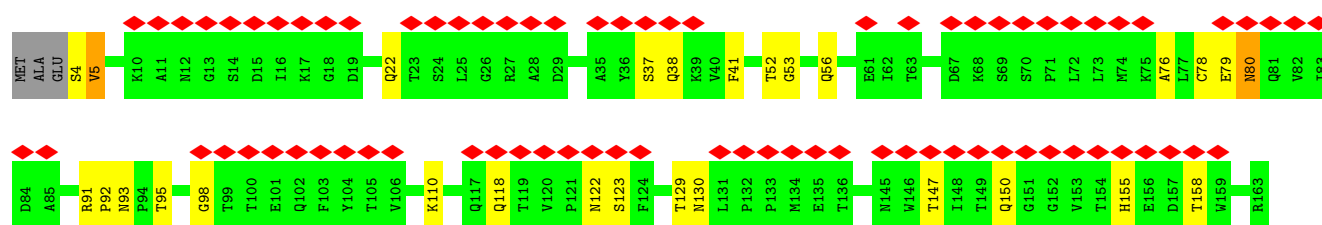


• Molecule 3: Hcp



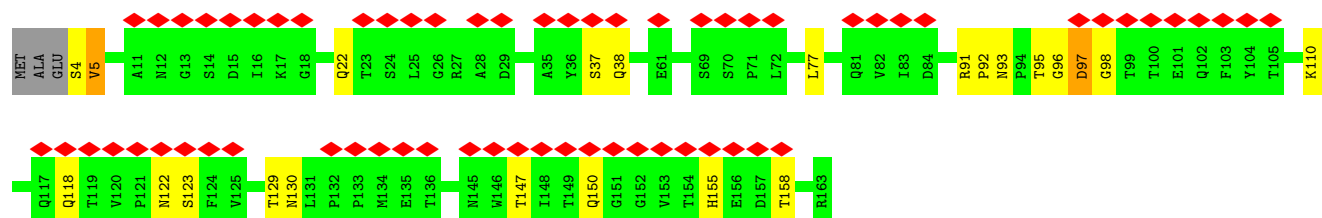
• Molecule 3: Hcp

Chain 26: 48% 81% 16% ..



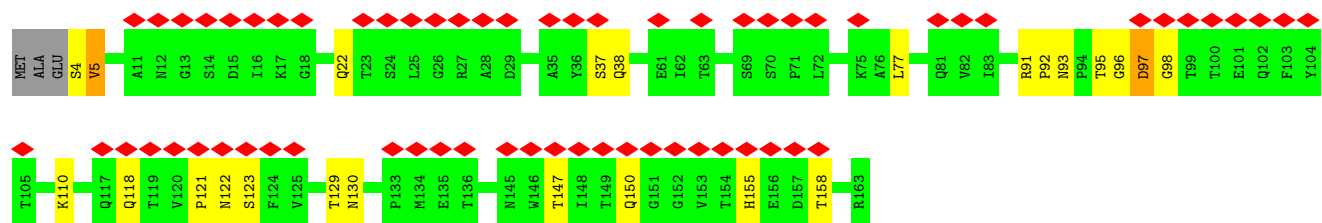
• Molecule 3: Hcp

Chain 31: 39% 84% 13% ..



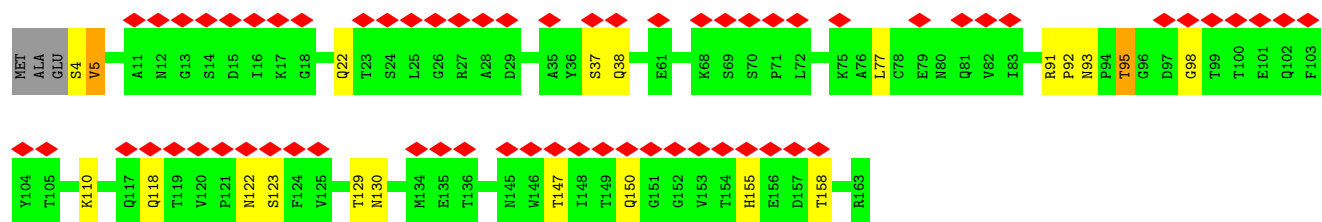
• Molecule 3: Hcp

Chain 32: 39% 83% 13% ..



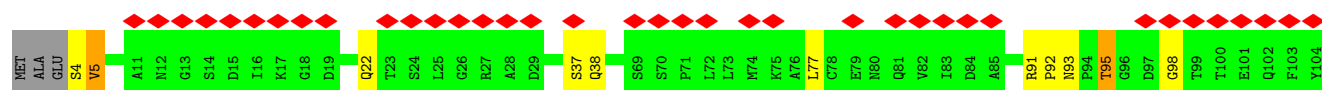
• Molecule 3: Hcp

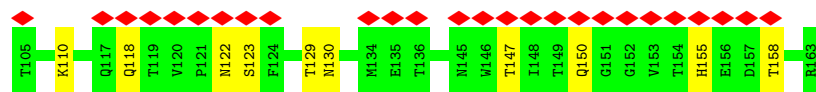
Chain 33: 39% 85% 12% ..



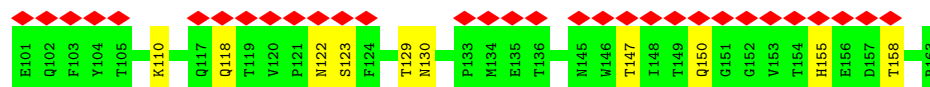
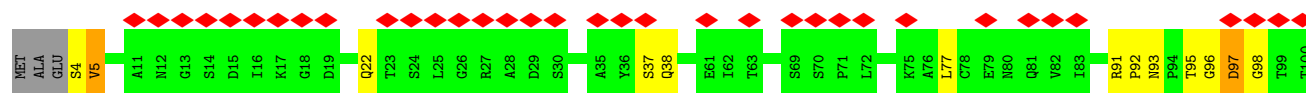
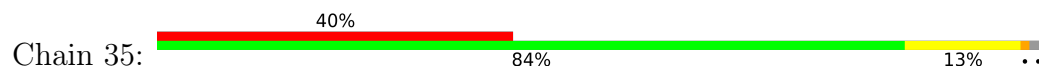
• Molecule 3: Hcp

Chain 34: 39% 85% 12% ..

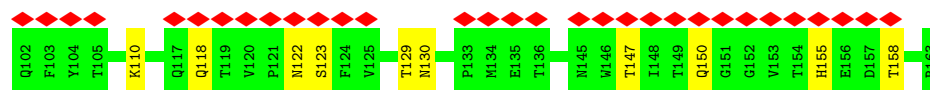
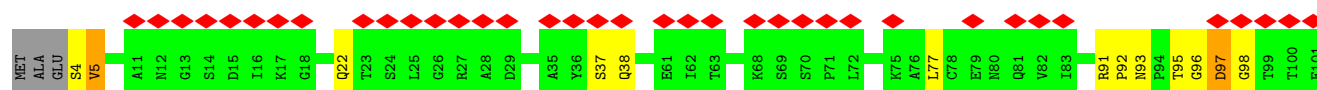
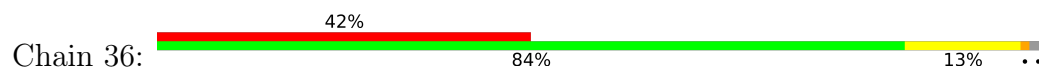




• Molecule 3: Hcp



• Molecule 3: Hcp



4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, Not provided	
Number of subtomograms used	687	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	248.659	Depositor
Minimum map value	-61.087	Depositor
Average map value	59.905	Depositor
Map value standard deviation	47.052	Depositor
Recommended contour level	130.0	Depositor
Map size (\AA)	390.00003, 390.00003, 468.00003	wwPDB
Map dimensions	50, 50, 60	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	7.8000007, 7.8000007, 7.8000007	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	1A	0.23	0/539	0.46	0/672
1	1C	0.23	0/539	0.46	0/672
1	1E	0.23	0/539	0.46	0/672
1	1G	0.23	0/539	0.46	0/672
1	1I	0.23	0/539	0.46	0/672
1	1K	0.23	0/539	0.46	0/672
1	2A	0.25	0/539	0.46	0/672
1	2C	0.23	0/539	0.46	0/672
1	2E	0.24	0/539	0.46	0/672
1	2G	0.23	0/539	0.46	0/672
1	2I	0.24	0/539	0.46	0/672
1	2K	0.24	0/539	0.47	0/672
1	3A	0.24	0/539	0.46	0/672
1	3C	0.24	0/539	0.47	0/672
1	3E	0.24	0/539	0.47	0/672
1	3G	0.24	0/539	0.48	0/672
1	3I	0.24	0/539	0.46	0/672
1	3K	0.23	0/539	0.47	0/672
2	1B	0.28	0/1655	0.47	0/2067
2	1D	0.27	0/1655	0.47	1/2067 (0.0%)
2	1F	0.27	0/1655	0.47	0/2067
2	1H	0.28	0/1655	0.48	1/2067 (0.0%)
2	1J	0.27	0/1655	0.47	0/2067
2	1L	0.27	0/1655	0.47	1/2067 (0.0%)
2	2B	0.32	0/1655	0.51	1/2067 (0.0%)
2	2D	0.28	0/1655	0.48	0/2067
2	2F	0.32	0/1655	0.50	1/2067 (0.0%)
2	2H	0.28	0/1655	0.48	0/2067
2	2J	0.31	0/1655	0.50	0/2067
2	2L	0.28	0/1655	0.48	0/2067
2	3B	0.27	0/1655	0.47	0/2067
2	3D	0.27	0/1655	0.47	0/2067
2	3F	0.26	0/1655	0.47	0/2067
2	3H	0.27	0/1655	0.47	0/2067

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	3J	0.28	0/1655	0.49	1/2067 (0.0%)
2	3L	0.27	0/1655	0.47	0/2067
3	11	0.38	0/639	0.64	0/797
3	12	0.38	0/639	0.65	0/797
3	13	0.38	0/639	0.65	0/797
3	14	0.38	0/639	0.64	0/797
3	15	0.38	0/639	0.65	0/797
3	16	0.38	0/639	0.65	0/797
3	21	0.45	1/639 (0.2%)	0.70	0/797
3	22	0.46	1/639 (0.2%)	0.70	0/797
3	23	0.45	1/639 (0.2%)	0.70	0/797
3	24	0.44	1/639 (0.2%)	0.69	0/797
3	25	0.44	1/639 (0.2%)	0.70	0/797
3	26	0.44	1/639 (0.2%)	0.71	0/797
3	31	0.44	1/639 (0.2%)	0.67	0/797
3	32	0.44	1/639 (0.2%)	0.67	0/797
3	33	0.45	1/639 (0.2%)	0.68	0/797
3	34	0.45	1/639 (0.2%)	0.66	0/797
3	35	0.45	1/639 (0.2%)	0.68	0/797
3	36	0.45	1/639 (0.2%)	0.67	0/797
All	All	0.31	12/50994 (0.0%)	0.53	6/63648 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	1B	0	1
2	1D	0	1
2	1F	0	1
2	1H	0	1
2	1J	0	1
2	1L	0	1
2	2D	0	1
2	2F	0	1
2	2H	0	1
2	2L	0	1
3	11	0	2
3	12	0	1
3	13	0	1
3	14	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	15	0	1
3	16	0	1
3	21	0	1
3	22	0	1
3	23	0	1
3	24	0	1
3	25	0	1
3	26	0	1
3	31	0	2
3	32	0	3
3	35	0	2
3	36	0	2
All	All	0	33

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	36	92	PRO	C-N	6.62	1.49	1.34
3	35	92	PRO	C-N	6.48	1.49	1.34
3	24	92	PRO	C-N	6.40	1.48	1.34
3	23	92	PRO	C-N	6.38	1.48	1.34
3	31	92	PRO	C-N	6.35	1.48	1.34
3	25	92	PRO	C-N	6.30	1.48	1.34
3	22	92	PRO	C-N	6.22	1.48	1.34
3	26	92	PRO	C-N	6.19	1.48	1.34
3	21	92	PRO	C-N	6.15	1.48	1.34
3	34	92	PRO	C-N	6.14	1.48	1.34
3	32	92	PRO	C-N	6.11	1.48	1.34
3	33	92	PRO	C-N	6.00	1.47	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1H	437	ASP	C-N-CA	-5.96	106.79	121.70
2	2B	437	ASP	C-N-CA	-5.78	107.24	121.70
2	2F	437	ASP	C-N-CA	-5.68	107.49	121.70
2	1D	437	ASP	C-N-CA	-5.27	108.52	121.70
2	1L	437	ASP	C-N-CA	-5.13	108.87	121.70
2	3J	463	PRO	N-CA-C	5.12	125.42	112.10

There are no chirality outliers.

All (33) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	11	121	PRO	Peptide
3	11	79	GLU	Peptide
3	12	79	GLU	Peptide
3	13	79	GLU	Peptide
3	14	121	PRO	Peptide
3	14	79	GLU	Peptide
3	15	79	GLU	Peptide
3	16	79	GLU	Peptide
2	1B	438	ASP	Peptide
2	1D	355	SER	Peptide
2	1F	438	ASP	Peptide
2	1H	355	SER	Peptide
2	1J	438	ASP	Peptide
2	1L	355	SER	Peptide
3	21	79	GLU	Peptide
3	22	79	GLU	Peptide
3	23	79	GLU	Peptide
3	24	79	GLU	Peptide
3	25	79	GLU	Peptide
3	26	79	GLU	Peptide
2	2D	355	SER	Peptide
2	2F	355	SER	Peptide
2	2H	355	SER	Peptide
2	2L	355	SER	Peptide
3	31	96	GLY	Peptide
3	31	97	ASP	Peptide
3	32	121	PRO	Peptide
3	32	96	GLY	Peptide
3	32	97	ASP	Peptide
3	35	96	GLY	Peptide
3	35	97	ASP	Peptide
3	36	96	GLY	Peptide
3	36	97	ASP	Peptide

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	1A	540	0	138	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1C	540	0	138	0	0
1	1E	540	0	138	0	0
1	1G	540	0	138	0	0
1	1I	540	0	138	0	0
1	1K	540	0	138	0	0
1	2A	540	0	138	1	0
1	2C	540	0	138	1	0
1	2E	540	0	138	0	0
1	2G	540	0	138	1	0
1	2I	540	0	138	0	0
1	2K	540	0	138	1	0
1	3A	540	0	138	1	0
1	3C	540	0	138	1	0
1	3E	540	0	138	1	0
1	3G	540	0	138	1	0
1	3I	540	0	138	1	0
1	3K	540	0	138	2	0
2	1B	1656	0	441	8	0
2	1D	1656	0	441	11	0
2	1F	1656	0	441	11	0
2	1H	1656	0	441	12	0
2	1J	1656	0	441	11	0
2	1L	1656	0	441	11	0
2	2B	1656	0	441	16	0
2	2D	1656	0	441	22	0
2	2F	1656	0	441	19	0
2	2H	1656	0	441	24	0
2	2J	1656	0	441	17	0
2	2L	1656	0	441	23	0
2	3B	1656	0	441	8	0
2	3D	1656	0	441	12	0
2	3F	1656	0	441	9	0
2	3H	1656	0	441	13	0
2	3J	1656	0	441	7	0
2	3L	1656	0	441	10	0
3	11	640	0	174	17	0
3	12	640	0	174	17	0
3	13	640	0	174	16	0
3	14	640	0	174	16	0
3	15	640	0	174	16	0
3	16	640	0	174	16	0
3	21	640	0	174	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	22	640	0	174	22	0
3	23	640	0	174	23	0
3	24	640	0	174	24	0
3	25	640	0	174	23	0
3	26	640	0	174	22	0
3	31	640	0	174	15	0
3	32	640	0	174	16	0
3	33	640	0	174	17	0
3	34	640	0	174	16	0
3	35	640	0	174	16	0
3	36	640	0	174	15	0
All	All	51048	0	13554	312	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 5.

All (312) 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)
3:14:76:ALA:O	3:14:80:ASN:CA	2.12	0.97
2:1B:438:ASP:O	2:2B:464:GLY:N	1.97	0.97
3:15:76:ALA:O	3:15:80:ASN:CA	2.13	0.95
2:2J:437:ASP:O	2:3J:461:GLY:N	1.99	0.94
2:2D:438:ASP:N	2:3D:462:GLN:O	2.01	0.93
2:1B:438:ASP:O	2:2B:465:TRP:N	2.02	0.93
2:2F:437:ASP:O	2:3F:461:GLY:N	2.02	0.92
2:1F:438:ASP:O	2:2F:464:GLY:N	2.04	0.91
2:2L:438:ASP:N	2:3L:462:GLN:O	2.02	0.91
2:2L:438:ASP:O	2:3L:465:TRP:N	2.04	0.91
2:1J:438:ASP:O	2:2J:464:GLY:N	2.02	0.91
3:16:76:ALA:O	3:16:80:ASN:CA	2.19	0.90
2:2H:438:ASP:N	2:3H:462:GLN:O	2.04	0.90
2:2D:438:ASP:O	2:3D:465:TRP:N	2.03	0.90
2:2B:437:ASP:O	2:3B:461:GLY:N	2.05	0.89
2:1L:438:ASP:O	2:2L:465:TRP:N	2.05	0.89
2:1D:437:ASP:O	2:2D:461:GLY:N	2.06	0.89
2:2H:438:ASP:O	2:3H:465:TRP:N	2.04	0.89
2:1D:438:ASP:N	2:2D:462:GLN:O	2.06	0.89
3:13:76:ALA:O	3:13:80:ASN:CA	2.20	0.88
2:1H:438:ASP:O	2:2H:465:TRP:N	2.05	0.88
2:1L:438:ASP:N	2:2L:462:GLN:O	2.06	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:24:76:ALA:O	3:24:80:ASN:CA	2.22	0.88
2:1H:437:ASP:O	2:2H:461:GLY:N	2.07	0.88
2:1D:438:ASP:O	2:2D:465:TRP:N	2.05	0.88
2:1L:437:ASP:O	2:2L:461:GLY:N	2.06	0.88
2:2J:438:ASP:O	2:3J:464:GLY:N	2.06	0.88
2:2L:437:ASP:O	2:3L:461:GLY:N	2.07	0.87
3:26:76:ALA:O	3:26:80:ASN:CA	2.23	0.87
2:1H:438:ASP:N	2:2H:462:GLN:O	2.07	0.87
3:23:76:ALA:O	3:23:80:ASN:CA	2.23	0.86
2:2F:438:ASP:N	2:3F:462:GLN:O	2.08	0.86
2:2D:437:ASP:O	2:3D:461:GLY:N	2.09	0.85
2:1J:438:ASP:O	2:2J:465:TRP:N	2.09	0.85
2:2B:438:ASP:O	2:3B:465:TRP:N	2.08	0.85
2:2F:438:ASP:O	2:3F:465:TRP:N	2.08	0.85
2:1F:438:ASP:O	2:2F:465:TRP:N	2.10	0.85
3:25:76:ALA:O	3:25:80:ASN:CA	2.25	0.84
3:22:76:ALA:O	3:22:80:ASN:CA	2.25	0.84
3:24:52:THR:N	3:34:93:ASN:O	2.10	0.84
3:23:52:THR:N	3:33:93:ASN:O	2.11	0.84
2:2H:437:ASP:O	2:3H:461:GLY:N	2.10	0.83
3:21:76:ALA:O	3:21:80:ASN:CA	2.27	0.83
3:11:76:ALA:O	3:11:80:ASN:CA	2.28	0.82
2:2J:438:ASP:O	2:3J:465:TRP:N	2.13	0.80
3:13:52:THR:N	3:23:93:ASN:O	2.15	0.80
3:14:52:THR:N	3:24:93:ASN:O	2.15	0.80
3:12:52:THR:N	3:22:93:ASN:O	2.15	0.80
3:16:52:THR:N	3:26:93:ASN:O	2.16	0.79
3:15:52:THR:N	3:25:93:ASN:O	2.15	0.79
3:11:52:THR:N	3:21:93:ASN:O	2.16	0.79
3:12:76:ALA:O	3:12:80:ASN:CA	2.30	0.79
3:22:52:THR:N	3:32:93:ASN:O	2.16	0.78
2:1H:437:ASP:N	2:2H:462:GLN:O	2.16	0.77
3:21:52:THR:N	3:31:93:ASN:O	2.17	0.77
2:2D:437:ASP:C	2:3D:462:GLN:H	1.89	0.76
3:25:52:THR:N	3:35:93:ASN:O	2.18	0.76
2:2B:437:ASP:N	2:3B:462:GLN:O	2.19	0.75
3:25:80:ASN:O	3:34:98:GLY:N	2.16	0.75
2:2H:437:ASP:C	2:3H:462:GLN:H	1.90	0.73
2:2L:437:ASP:C	2:3L:462:GLN:H	1.92	0.72
3:33:5:VAL:N	3:34:130:ASN:H	1.88	0.72
3:35:5:VAL:N	3:36:130:ASN:H	1.88	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:32:5:VAL:N	3:33:130:ASN:H	1.88	0.71
3:21:5:VAL:N	3:22:130:ASN:H	1.89	0.71
3:24:80:ASN:O	3:33:98:GLY:N	2.21	0.71
3:22:5:VAL:N	3:23:130:ASN:H	1.89	0.70
3:31:130:ASN:H	3:36:5:VAL:N	1.88	0.70
2:2J:437:ASP:C	2:3J:462:GLN:O	2.29	0.70
3:34:5:VAL:N	3:35:130:ASN:H	1.88	0.70
3:24:5:VAL:N	3:25:130:ASN:H	1.89	0.70
3:25:5:VAL:N	3:26:130:ASN:H	1.90	0.70
3:26:52:THR:N	3:36:93:ASN:O	2.24	0.70
3:31:5:VAL:N	3:32:130:ASN:H	1.89	0.70
2:1F:438:ASP:C	2:2F:465:TRP:H	1.94	0.70
2:1D:437:ASP:C	2:2D:462:GLN:H	1.95	0.69
3:23:5:VAL:N	3:24:130:ASN:H	1.89	0.69
2:1H:437:ASP:C	2:2H:462:GLN:H	1.95	0.69
3:14:5:VAL:N	3:15:130:ASN:H	1.91	0.69
3:21:130:ASN:H	3:26:5:VAL:N	1.89	0.69
2:1L:437:ASP:N	2:2L:462:GLN:O	2.26	0.69
3:11:130:ASN:H	3:16:5:VAL:N	1.91	0.69
2:2B:438:ASP:O	2:3B:464:GLY:N	2.25	0.69
2:1D:437:ASP:N	2:2D:462:GLN:O	2.26	0.68
3:15:5:VAL:N	3:16:130:ASN:H	1.91	0.68
3:13:5:VAL:N	3:14:130:ASN:H	1.91	0.68
2:1J:438:ASP:C	2:2J:465:TRP:H	1.95	0.68
2:1L:437:ASP:C	2:2L:462:GLN:H	1.96	0.68
3:11:5:VAL:N	3:12:130:ASN:H	1.91	0.68
3:12:5:VAL:N	3:13:130:ASN:H	1.91	0.67
3:25:52:THR:CA	3:35:98:GLY:HA2	2.24	0.67
2:2B:438:ASP:N	2:3B:462:GLN:O	2.28	0.67
2:2F:437:ASP:N	2:3F:462:GLN:O	2.29	0.65
2:2F:437:ASP:C	2:3F:462:GLN:H	1.99	0.65
2:2F:438:ASP:O	2:3F:464:GLY:N	2.31	0.63
2:1J:438:ASP:CA	2:2J:459:VAL:O	2.47	0.63
2:1F:438:ASP:CA	2:2F:459:VAL:O	2.47	0.63
2:2J:438:ASP:N	2:3J:462:GLN:O	2.32	0.63
3:26:80:ASN:O	3:35:98:GLY:N	2.33	0.61
2:2B:437:ASP:O	2:3B:462:GLN:N	2.32	0.60
3:12:79:GLU:C	3:21:98:GLY:HA3	2.22	0.60
2:2L:437:ASP:N	2:3L:462:GLN:O	2.35	0.60
2:1H:437:ASP:CA	2:2H:461:GLY:H	2.16	0.59
2:2F:437:ASP:C	2:3F:462:GLN:O	2.41	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2H:323:ILE:O	1:3G:47:ARG:N	2.36	0.59
3:13:79:GLU:C	3:22:98:GLY:HA3	2.22	0.59
2:1F:440:ALA:H	2:2F:464:GLY:HA3	1.68	0.59
2:1B:438:ASP:C	2:2B:465:TRP:H	2.02	0.58
2:2B:437:ASP:C	2:3B:462:GLN:H	2.07	0.58
2:2B:437:ASP:C	2:3B:462:GLN:O	2.41	0.58
3:23:80:ASN:O	3:32:98:GLY:N	2.37	0.58
3:11:79:GLU:C	3:26:98:GLY:HA3	2.23	0.58
2:2F:437:ASP:O	2:3F:462:GLN:N	2.36	0.58
2:2D:437:ASP:CA	2:3D:461:GLY:H	2.16	0.58
3:14:79:GLU:C	3:23:98:GLY:HA3	2.25	0.57
3:16:79:GLU:C	3:25:98:GLY:HA3	2.25	0.57
2:2L:437:ASP:CA	2:3L:461:GLY:H	2.17	0.57
3:15:79:GLU:C	3:24:98:GLY:HA3	2.25	0.57
2:1D:437:ASP:CA	2:2D:461:GLY:H	2.18	0.56
2:1L:437:ASP:CA	2:2L:461:GLY:H	2.18	0.56
2:2D:323:ILE:O	1:3C:47:ARG:N	2.38	0.56
2:1B:438:ASP:CA	2:2B:459:VAL:O	2.53	0.56
2:2F:323:ILE:O	1:3E:47:ARG:N	2.39	0.55
2:1D:437:ASP:C	2:2D:462:GLN:O	2.44	0.55
2:2L:437:ASP:C	2:3L:462:GLN:O	2.45	0.55
2:1L:437:ASP:C	2:2L:462:GLN:O	2.44	0.55
3:24:51:ALA:C	3:34:93:ASN:O	2.44	0.55
3:26:52:THR:CA	3:36:98:GLY:HA2	2.37	0.55
2:2J:437:ASP:N	2:3J:462:GLN:O	2.40	0.55
2:2H:437:ASP:CA	2:3H:461:GLY:H	2.19	0.55
2:2H:437:ASP:N	2:3H:462:GLN:O	2.40	0.55
2:2L:323:ILE:O	1:3K:47:ARG:N	2.40	0.55
3:21:53:GLY:N	3:31:98:GLY:HA2	2.22	0.54
3:26:53:GLY:N	3:36:98:GLY:HA2	2.22	0.54
3:22:52:THR:CA	3:32:98:GLY:HA2	2.38	0.54
2:1H:437:ASP:C	2:2H:462:GLN:O	2.45	0.54
2:2D:437:ASP:N	2:3D:462:GLN:O	2.40	0.54
3:34:4:SER:C	3:35:130:ASN:H	2.10	0.54
2:1B:439:PRO:N	2:2B:462:GLN:O	2.41	0.54
2:2D:437:ASP:C	2:3D:462:GLN:O	2.46	0.54
2:2J:323:ILE:O	1:3I:47:ARG:N	2.41	0.54
2:2D:437:ASP:CA	2:3D:462:GLN:H	2.20	0.54
3:33:4:SER:C	3:34:130:ASN:H	2.10	0.54
2:1B:437:ASP:O	2:2B:461:GLY:N	2.41	0.53
3:23:51:ALA:C	3:33:93:ASN:O	2.45	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:31:4:SER:C	3:32:130:ASN:H	2.12	0.53
3:31:130:ASN:H	3:36:4:SER:C	2.12	0.53
3:11:4:SER:O	3:12:130:ASN:O	2.27	0.53
3:12:4:SER:O	3:13:130:ASN:O	2.27	0.53
3:13:4:SER:O	3:14:130:ASN:O	2.27	0.53
3:32:4:SER:C	3:33:130:ASN:H	2.11	0.52
3:11:130:ASN:O	3:16:4:SER:O	2.27	0.52
3:35:4:SER:C	3:36:130:ASN:H	2.11	0.52
3:14:4:SER:O	3:15:130:ASN:O	2.27	0.52
2:1J:440:ALA:H	2:2J:464:GLY:HA3	1.74	0.52
3:15:4:SER:O	3:16:130:ASN:O	2.27	0.52
2:2H:437:ASP:C	2:3H:462:GLN:O	2.46	0.52
3:21:130:ASN:H	3:26:4:SER:C	2.13	0.52
3:16:53:GLY:N	3:26:98:GLY:HA2	2.25	0.51
3:22:4:SER:C	3:23:130:ASN:H	2.13	0.51
3:25:4:SER:C	3:26:130:ASN:H	2.14	0.51
2:2H:437:ASP:O	2:3H:462:GLN:N	2.43	0.51
3:23:4:SER:C	3:24:130:ASN:H	2.14	0.51
3:23:52:THR:CA	3:33:98:GLY:HA2	2.40	0.51
3:24:38:GLN:O	3:25:118:GLN:CA	2.59	0.51
2:2L:437:ASP:CA	2:3L:462:GLN:H	2.24	0.51
3:31:38:GLN:O	3:32:118:GLN:CA	2.59	0.51
2:1D:437:ASP:O	2:2D:462:GLN:N	2.44	0.51
3:13:38:GLN:O	3:14:118:GLN:CA	2.59	0.51
3:21:118:GLN:CA	3:26:38:GLN:O	2.59	0.51
3:25:5:VAL:CA	3:25:91:ARG:O	2.59	0.51
3:25:38:GLN:O	3:26:118:GLN:CA	2.59	0.51
3:11:38:GLN:O	3:12:118:GLN:CA	2.59	0.50
3:21:4:SER:C	3:22:130:ASN:H	2.13	0.50
3:21:38:GLN:O	3:22:118:GLN:CA	2.59	0.50
3:32:5:VAL:CA	3:32:91:ARG:O	2.59	0.50
3:33:5:VAL:CA	3:33:91:ARG:O	2.59	0.50
3:23:38:GLN:O	3:24:118:GLN:CA	2.59	0.50
3:35:5:VAL:CA	3:35:91:ARG:O	2.59	0.50
3:22:5:VAL:CA	3:22:91:ARG:O	2.59	0.50
3:22:38:GLN:O	3:23:118:GLN:CA	2.59	0.50
3:23:5:VAL:CA	3:23:91:ARG:O	2.59	0.50
3:34:38:GLN:O	3:35:118:GLN:CA	2.59	0.50
3:11:118:GLN:CA	3:16:38:GLN:O	2.59	0.50
3:12:38:GLN:O	3:13:118:GLN:CA	2.59	0.50
3:24:5:VAL:CA	3:24:91:ARG:O	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:33:38:GLN:O	3:34:118:GLN:CA	2.59	0.50
3:35:38:GLN:O	3:36:118:GLN:CA	2.59	0.50
2:1D:323:ILE:O	1:2C:47:ARG:N	2.45	0.50
2:1J:438:ASP:C	2:2J:464:GLY:H	2.08	0.50
3:11:5:VAL:H	3:12:129:THR:CA	2.25	0.50
3:15:5:VAL:H	3:16:129:THR:CA	2.25	0.50
2:1L:437:ASP:O	2:2L:462:GLN:N	2.44	0.50
2:2L:437:ASP:O	2:3L:462:GLN:N	2.44	0.50
3:32:38:GLN:O	3:33:118:GLN:CA	2.59	0.50
3:12:5:VAL:H	3:13:129:THR:CA	2.25	0.50
3:34:5:VAL:CA	3:34:91:ARG:O	2.59	0.50
3:15:38:GLN:O	3:16:118:GLN:CA	2.59	0.50
3:24:52:THR:CA	3:34:98:GLY:HA2	2.41	0.50
3:31:5:VAL:CA	3:31:91:ARG:O	2.60	0.50
3:15:5:VAL:CA	3:15:91:ARG:O	2.60	0.50
3:24:4:SER:C	3:25:130:ASN:H	2.14	0.50
3:31:118:GLN:CA	3:36:38:GLN:O	2.59	0.50
3:14:5:VAL:H	3:15:129:THR:CA	2.25	0.49
3:14:38:GLN:O	3:15:118:GLN:CA	2.59	0.49
3:26:5:VAL:CA	3:26:91:ARG:O	2.59	0.49
3:14:5:VAL:CA	3:14:91:ARG:O	2.60	0.49
2:2D:437:ASP:O	2:3D:462:GLN:N	2.45	0.49
3:21:5:VAL:CA	3:21:91:ARG:O	2.59	0.49
3:36:5:VAL:CA	3:36:91:ARG:O	2.59	0.49
2:1L:323:ILE:O	1:2K:47:ARG:N	2.45	0.49
3:12:5:VAL:CA	3:12:91:ARG:O	2.60	0.49
3:11:53:GLY:N	3:21:98:GLY:HA2	2.27	0.49
3:11:129:THR:CA	3:16:5:VAL:H	2.25	0.49
3:13:5:VAL:CA	3:13:91:ARG:O	2.60	0.49
2:1H:437:ASP:CA	2:2H:462:GLN:H	2.25	0.49
3:15:53:GLY:N	3:25:98:GLY:HA2	2.27	0.49
2:2H:437:ASP:CA	2:3H:462:GLN:H	2.24	0.49
3:25:4:SER:O	3:26:130:ASN:O	2.31	0.49
3:16:5:VAL:CA	3:16:91:ARG:O	2.60	0.49
3:21:130:ASN:O	3:26:4:SER:O	2.31	0.49
3:11:5:VAL:CA	3:11:91:ARG:O	2.60	0.49
3:21:4:SER:O	3:22:130:ASN:O	2.31	0.49
3:22:53:GLY:N	3:32:98:GLY:HA2	2.27	0.48
3:13:5:VAL:H	3:14:129:THR:CA	2.25	0.48
2:2H:438:ASP:O	2:3H:464:GLY:N	2.46	0.48
3:25:51:ALA:C	3:35:93:ASN:O	2.52	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1F:440:ALA:H	2:2F:464:GLY:CA	2.26	0.48
2:1H:437:ASP:O	2:2H:462:GLN:N	2.47	0.48
3:31:4:SER:O	3:32:130:ASN:O	2.32	0.48
2:1F:438:ASP:C	2:2F:464:GLY:H	2.07	0.48
3:22:51:ALA:C	3:32:93:ASN:O	2.51	0.48
3:31:130:ASN:O	3:36:4:SER:O	2.32	0.48
3:24:4:SER:O	3:25:130:ASN:O	2.31	0.48
3:35:4:SER:O	3:36:130:ASN:O	2.32	0.48
3:22:4:SER:O	3:23:130:ASN:O	2.31	0.48
3:33:4:SER:O	3:34:130:ASN:O	2.32	0.48
3:23:4:SER:O	3:24:130:ASN:O	2.31	0.47
3:32:4:SER:O	3:33:130:ASN:O	2.32	0.47
3:24:51:ALA:O	3:34:95:THR:N	2.48	0.47
3:34:4:SER:O	3:35:130:ASN:O	2.32	0.47
3:11:130:ASN:H	3:16:4:SER:C	2.18	0.47
2:2L:354:ASP:O	1:3K:51:GLN:N	2.48	0.47
2:1F:437:ASP:O	2:2F:461:GLY:N	2.48	0.46
3:11:4:SER:C	3:12:130:ASN:H	2.18	0.46
2:2B:323:ILE:O	1:3A:47:ARG:N	2.47	0.46
2:1D:437:ASP:CA	2:2D:462:GLN:H	2.28	0.46
2:1D:438:ASP:O	2:2D:464:GLY:N	2.48	0.46
2:1J:440:ALA:H	2:2J:464:GLY:CA	2.29	0.46
2:1L:437:ASP:CA	2:2L:462:GLN:H	2.28	0.46
3:23:5:VAL:H	3:24:129:THR:CA	2.29	0.46
3:21:129:THR:CA	3:26:5:VAL:H	2.29	0.46
3:12:53:GLY:N	3:22:98:GLY:HA2	2.31	0.46
3:13:4:SER:C	3:14:130:ASN:H	2.19	0.46
3:21:5:VAL:H	3:22:129:THR:CA	2.29	0.46
3:12:4:SER:C	3:13:130:ASN:H	2.18	0.45
3:24:5:VAL:H	3:25:129:THR:CA	2.29	0.45
2:1B:323:ILE:O	1:2A:47:ARG:N	2.50	0.45
2:1J:437:ASP:O	2:2J:462:GLN:O	2.34	0.45
3:14:53:GLY:N	3:24:98:GLY:HA2	2.31	0.45
2:2L:352:ARG:O	2:2L:355:SER:N	2.42	0.45
3:23:51:ALA:O	3:33:95:THR:N	2.50	0.45
2:3H:373:GLY:O	2:3H:378:GLY:HA3	2.17	0.45
3:14:4:SER:C	3:15:130:ASN:H	2.18	0.45
3:31:5:VAL:H	3:32:129:THR:CA	2.30	0.45
3:32:5:VAL:H	3:33:129:THR:CA	2.30	0.45
3:15:4:SER:C	3:16:130:ASN:H	2.18	0.45
3:22:5:VAL:H	3:23:129:THR:CA	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:25:5:VAL:H	3:26:129:THR:CA	2.29	0.45
2:1F:437:ASP:O	2:2F:462:GLN:O	2.34	0.45
2:2H:438:ASP:C	2:3H:462:GLN:O	2.56	0.44
2:1F:440:ALA:O	2:1F:443:VAL:N	2.46	0.44
2:1H:323:ILE:O	1:2G:47:ARG:N	2.50	0.44
2:2F:437:ASP:CA	2:3F:461:GLY:H	2.30	0.44
3:23:54:ARG:CA	3:24:78:CYS:O	2.66	0.44
3:31:129:THR:CA	3:36:5:VAL:H	2.30	0.44
3:21:51:ALA:C	3:31:93:ASN:O	2.55	0.44
3:35:5:VAL:H	3:36:129:THR:CA	2.31	0.44
3:34:5:VAL:H	3:35:129:THR:CA	2.31	0.43
2:1L:438:ASP:O	2:2L:464:GLY:N	2.51	0.43
2:2L:438:ASP:O	2:3L:464:GLY:N	2.51	0.43
3:13:53:GLY:N	3:23:98:GLY:HA2	2.33	0.43
3:24:54:ARG:CA	3:25:78:CYS:O	2.66	0.43
2:1J:437:ASP:O	2:2J:461:GLY:N	2.51	0.43
2:2D:437:ASP:C	2:3D:462:GLN:N	2.67	0.43
3:33:5:VAL:H	3:34:129:THR:CA	2.31	0.43
2:2H:437:ASP:C	2:3H:462:GLN:N	2.68	0.42
3:22:54:ARG:CA	3:23:78:CYS:O	2.67	0.42
3:12:51:ALA:CA	3:22:93:ASN:O	2.67	0.42
2:2B:440:ALA:O	2:2B:443:VAL:N	2.49	0.42
3:14:51:ALA:CA	3:24:93:ASN:O	2.68	0.42
2:1F:439:PRO:O	2:1F:441:PRO:N	2.53	0.42
3:21:52:THR:CA	3:31:98:GLY:HA2	2.49	0.42
2:1J:439:PRO:O	2:1J:441:PRO:N	2.53	0.42
3:24:80:ASN:C	3:33:98:GLY:H	2.19	0.42
3:25:54:ARG:CA	3:26:78:CYS:O	2.67	0.42
3:13:51:ALA:CA	3:23:93:ASN:O	2.67	0.42
3:21:54:ARG:CA	3:22:78:CYS:O	2.68	0.42
3:25:53:GLY:N	3:35:98:GLY:HA2	2.35	0.42
2:2D:438:ASP:C	2:3D:462:GLN:O	2.58	0.41
3:11:79:GLU:O	3:11:80:ASN:C	2.59	0.41
3:15:51:ALA:CA	3:25:93:ASN:O	2.68	0.41
2:3D:373:GLY:O	2:3D:378:GLY:HA3	2.19	0.41
2:1J:440:ALA:O	2:1J:443:VAL:N	2.45	0.41
3:16:51:ALA:CA	3:26:93:ASN:O	2.69	0.41
3:26:52:THR:C	3:36:98:GLY:HA2	2.41	0.41
3:11:51:ALA:CA	3:21:93:ASN:O	2.69	0.41
2:1H:437:ASP:C	2:2H:462:GLN:N	2.70	0.41
2:2J:438:ASP:CA	2:3J:462:GLN:O	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:12:79:GLU:O	3:12:80:ASN:C	2.59	0.40
2:1B:440:ALA:O	2:1B:443:VAL:N	2.46	0.40
2:1H:437:ASP:C	2:2H:461:GLY:H	2.25	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	
1	1A	133/164 (81%)	129 (97%)	3 (2%)	1 (1%)	19	60
1	1C	133/164 (81%)	129 (97%)	3 (2%)	1 (1%)	19	60
1	1E	133/164 (81%)	128 (96%)	4 (3%)	1 (1%)	19	60
1	1G	133/164 (81%)	129 (97%)	3 (2%)	1 (1%)	19	60
1	1I	133/164 (81%)	128 (96%)	4 (3%)	1 (1%)	19	60
1	1K	133/164 (81%)	129 (97%)	3 (2%)	1 (1%)	19	60
1	2A	133/164 (81%)	129 (97%)	3 (2%)	1 (1%)	19	60
1	2C	133/164 (81%)	128 (96%)	4 (3%)	1 (1%)	19	60
1	2E	133/164 (81%)	127 (96%)	5 (4%)	1 (1%)	19	60
1	2G	133/164 (81%)	128 (96%)	4 (3%)	1 (1%)	19	60
1	2I	133/164 (81%)	128 (96%)	4 (3%)	1 (1%)	19	60
1	2K	133/164 (81%)	128 (96%)	4 (3%)	1 (1%)	19	60
1	3A	133/164 (81%)	128 (96%)	4 (3%)	1 (1%)	19	60
1	3C	133/164 (81%)	128 (96%)	4 (3%)	1 (1%)	19	60
1	3E	133/164 (81%)	129 (97%)	3 (2%)	1 (1%)	19	60
1	3G	133/164 (81%)	129 (97%)	3 (2%)	1 (1%)	19	60
1	3I	133/164 (81%)	128 (96%)	4 (3%)	1 (1%)	19	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3K	133/164 (81%)	128 (96%)	4 (3%)	1 (1%)	19	60
2	1B	412/494 (83%)	390 (95%)	14 (3%)	8 (2%)	8	38
2	1D	412/494 (83%)	391 (95%)	15 (4%)	6 (2%)	10	46
2	1F	412/494 (83%)	391 (95%)	14 (3%)	7 (2%)	9	42
2	1H	412/494 (83%)	390 (95%)	17 (4%)	5 (1%)	13	50
2	1J	412/494 (83%)	391 (95%)	14 (3%)	7 (2%)	9	42
2	1L	412/494 (83%)	391 (95%)	16 (4%)	5 (1%)	13	50
2	2B	412/494 (83%)	386 (94%)	18 (4%)	8 (2%)	8	38
2	2D	412/494 (83%)	387 (94%)	19 (5%)	6 (2%)	10	46
2	2F	412/494 (83%)	387 (94%)	19 (5%)	6 (2%)	10	46
2	2H	412/494 (83%)	386 (94%)	19 (5%)	7 (2%)	9	42
2	2J	412/494 (83%)	387 (94%)	17 (4%)	8 (2%)	8	38
2	2L	412/494 (83%)	387 (94%)	19 (5%)	6 (2%)	10	46
2	3B	412/494 (83%)	390 (95%)	16 (4%)	6 (2%)	10	46
2	3D	412/494 (83%)	391 (95%)	16 (4%)	5 (1%)	13	50
2	3F	412/494 (83%)	390 (95%)	16 (4%)	6 (2%)	10	46
2	3H	412/494 (83%)	390 (95%)	17 (4%)	5 (1%)	13	50
2	3J	412/494 (83%)	390 (95%)	16 (4%)	6 (2%)	10	46
2	3L	412/494 (83%)	391 (95%)	15 (4%)	6 (2%)	10	46
3	11	158/163 (97%)	125 (79%)	21 (13%)	12 (8%)	1	13
3	12	158/163 (97%)	125 (79%)	21 (13%)	12 (8%)	1	13
3	13	158/163 (97%)	125 (79%)	21 (13%)	12 (8%)	1	13
3	14	158/163 (97%)	125 (79%)	21 (13%)	12 (8%)	1	13
3	15	158/163 (97%)	125 (79%)	21 (13%)	12 (8%)	1	13
3	16	158/163 (97%)	125 (79%)	21 (13%)	12 (8%)	1	13
3	21	158/163 (97%)	125 (79%)	20 (13%)	13 (8%)	1	12
3	22	158/163 (97%)	125 (79%)	19 (12%)	14 (9%)	1	11
3	23	158/163 (97%)	125 (79%)	19 (12%)	14 (9%)	1	11
3	24	158/163 (97%)	126 (80%)	18 (11%)	14 (9%)	1	11
3	25	158/163 (97%)	126 (80%)	17 (11%)	15 (10%)	0	10
3	26	158/163 (97%)	125 (79%)	19 (12%)	14 (9%)	1	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	31	158/163 (97%)	126 (80%)	19 (12%)	13 (8%)	1	12
3	32	158/163 (97%)	126 (80%)	19 (12%)	13 (8%)	1	12
3	33	158/163 (97%)	125 (79%)	21 (13%)	12 (8%)	1	13
3	34	158/163 (97%)	125 (79%)	21 (13%)	12 (8%)	1	13
3	35	158/163 (97%)	125 (79%)	20 (13%)	13 (8%)	1	12
3	36	158/163 (97%)	125 (79%)	20 (13%)	13 (8%)	1	12
All	All	12654/14778 (86%)	11570 (91%)	721 (6%)	363 (3%)	7	29

All (363) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1A	129	PRO
2	1B	242	LEU
1	1C	129	PRO
2	1D	242	LEU
1	1E	129	PRO
2	1F	242	LEU
1	1G	129	PRO
2	1H	242	LEU
1	1I	129	PRO
2	1J	242	LEU
1	1K	129	PRO
2	1L	242	LEU
3	11	5	VAL
3	11	122	ASN
3	11	123	SER
3	12	5	VAL
3	12	122	ASN
3	12	123	SER
3	13	5	VAL
3	13	80	ASN
3	13	122	ASN
3	13	123	SER
3	14	5	VAL
3	14	80	ASN
3	14	122	ASN
3	14	123	SER
3	15	5	VAL
3	15	80	ASN
3	15	122	ASN

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Mol	Chain	Res	Type
3	15	123	SER
3	16	5	VAL
3	16	122	ASN
3	16	123	SER
1	2A	129	PRO
2	2B	242	LEU
2	2B	462	GLN
1	2C	129	PRO
2	2D	242	LEU
1	2E	129	PRO
2	2F	242	LEU
2	2F	463	PRO
1	2G	129	PRO
2	2H	242	LEU
1	2I	129	PRO
2	2J	242	LEU
2	2J	463	PRO
1	2K	129	PRO
2	2L	242	LEU
3	21	5	VAL
3	21	95	THR
3	21	122	ASN
3	21	123	SER
3	22	5	VAL
3	22	95	THR
3	22	122	ASN
3	22	123	SER
3	23	5	VAL
3	23	95	THR
3	23	122	ASN
3	23	123	SER
3	24	5	VAL
3	24	95	THR
3	24	122	ASN
3	24	123	SER
3	25	5	VAL
3	25	80	ASN
3	25	95	THR
3	25	122	ASN
3	25	123	SER
3	26	5	VAL
3	26	95	THR

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Mol	Chain	Res	Type
3	26	122	ASN
3	26	123	SER
1	3A	129	PRO
2	3B	242	LEU
1	3C	129	PRO
2	3D	242	LEU
1	3E	129	PRO
2	3F	242	LEU
1	3G	129	PRO
2	3H	242	LEU
1	3I	129	PRO
2	3J	242	LEU
2	3J	463	PRO
1	3K	129	PRO
2	3L	242	LEU
3	31	5	VAL
3	31	95	THR
3	31	97	ASP
3	31	122	ASN
3	31	123	SER
3	32	5	VAL
3	32	95	THR
3	32	97	ASP
3	32	122	ASN
3	32	123	SER
3	33	5	VAL
3	33	95	THR
3	33	122	ASN
3	33	123	SER
3	34	5	VAL
3	34	95	THR
3	34	122	ASN
3	34	123	SER
3	35	5	VAL
3	35	95	THR
3	35	97	ASP
3	35	122	ASN
3	35	123	SER
3	36	5	VAL
3	36	95	THR
3	36	97	ASP
3	36	122	ASN

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Mol	Chain	Res	Type
3	36	123	SER
2	1B	298	PRO
2	1D	298	PRO
2	1F	298	PRO
2	1H	298	PRO
2	1J	298	PRO
2	1L	298	PRO
3	11	80	ASN
3	11	150	GLN
3	11	155	HIS
3	12	80	ASN
3	12	150	GLN
3	12	155	HIS
3	13	150	GLN
3	13	155	HIS
3	14	150	GLN
3	14	155	HIS
3	15	150	GLN
3	15	155	HIS
3	16	80	ASN
3	16	150	GLN
3	16	155	HIS
2	2B	298	PRO
2	2B	463	PRO
2	2D	298	PRO
2	2F	298	PRO
2	2H	298	PRO
2	2J	298	PRO
2	2L	298	PRO
3	21	22	GLN
3	21	150	GLN
3	21	155	HIS
3	22	150	GLN
3	22	155	HIS
3	23	150	GLN
3	23	155	HIS
3	24	80	ASN
3	24	150	GLN
3	24	155	HIS
3	25	150	GLN
3	25	155	HIS
3	26	150	GLN

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Mol	Chain	Res	Type
3	26	155	HIS
2	3B	298	PRO
2	3B	463	PRO
2	3D	298	PRO
2	3F	298	PRO
2	3H	298	PRO
2	3J	298	PRO
2	3L	298	PRO
3	31	150	GLN
3	31	155	HIS
3	32	150	GLN
3	32	155	HIS
3	33	22	GLN
3	33	150	GLN
3	33	155	HIS
3	34	22	GLN
3	34	150	GLN
3	34	155	HIS
3	35	22	GLN
3	35	150	GLN
3	35	155	HIS
3	36	22	GLN
3	36	150	GLN
3	36	155	HIS
2	1B	260	ALA
2	1B	354	ASP
2	1D	260	ALA
2	1F	260	ALA
2	1F	439	PRO
2	1H	260	ALA
2	1J	260	ALA
2	1J	439	PRO
2	1L	260	ALA
3	11	37	SER
3	11	41	PHE
3	11	158	THR
3	12	37	SER
3	12	41	PHE
3	12	158	THR
3	13	37	SER
3	13	41	PHE
3	13	158	THR

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Mol	Chain	Res	Type
3	14	37	SER
3	14	41	PHE
3	14	158	THR
3	15	37	SER
3	15	41	PHE
3	15	158	THR
3	16	37	SER
3	16	41	PHE
3	16	158	THR
2	2B	260	ALA
2	2D	260	ALA
2	2F	260	ALA
2	2H	260	ALA
2	2H	463	PRO
2	2J	260	ALA
2	2L	260	ALA
3	21	37	SER
3	21	41	PHE
3	21	80	ASN
3	21	158	THR
3	22	22	GLN
3	22	37	SER
3	22	41	PHE
3	22	80	ASN
3	22	158	THR
3	23	22	GLN
3	23	37	SER
3	23	41	PHE
3	23	80	ASN
3	23	158	THR
3	24	22	GLN
3	24	37	SER
3	24	41	PHE
3	24	158	THR
3	25	22	GLN
3	25	37	SER
3	25	41	PHE
3	25	158	THR
3	26	22	GLN
3	26	37	SER
3	26	41	PHE
3	26	80	ASN

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Mol	Chain	Res	Type
3	26	158	THR
2	3B	260	ALA
2	3D	260	ALA
2	3F	260	ALA
2	3F	463	PRO
2	3H	260	ALA
2	3J	260	ALA
2	3L	260	ALA
3	31	22	GLN
3	31	37	SER
3	31	158	THR
3	32	22	GLN
3	32	37	SER
3	32	158	THR
3	33	37	SER
3	33	158	THR
3	34	37	SER
3	34	158	THR
3	35	37	SER
3	35	158	THR
3	36	37	SER
3	36	158	THR
2	1B	311	ASN
2	1D	311	ASN
2	1F	311	ASN
2	1H	311	ASN
2	1J	311	ASN
2	1L	311	ASN
3	11	110	LYS
3	11	128	SER
3	11	147	THR
3	12	110	LYS
3	12	128	SER
3	12	147	THR
3	13	110	LYS
3	13	128	SER
3	13	147	THR
3	14	110	LYS
3	14	128	SER
3	14	147	THR
3	15	110	LYS
3	15	128	SER

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Mol	Chain	Res	Type
3	15	147	THR
3	16	110	LYS
3	16	128	SER
3	16	147	THR
2	2B	311	ASN
2	2D	311	ASN
2	2D	463	PRO
2	2F	311	ASN
2	2H	311	ASN
2	2J	311	ASN
2	2L	311	ASN
2	2L	463	PRO
3	21	110	LYS
3	21	147	THR
3	22	110	LYS
3	22	147	THR
3	23	56	GLN
3	23	110	LYS
3	23	147	THR
3	24	56	GLN
3	24	110	LYS
3	24	147	THR
3	25	110	LYS
3	25	147	THR
3	26	110	LYS
3	26	147	THR
2	3B	311	ASN
2	3D	311	ASN
2	3F	311	ASN
2	3H	311	ASN
2	3J	311	ASN
2	3L	311	ASN
3	31	110	LYS
3	31	147	THR
3	32	110	LYS
3	32	147	THR
3	33	110	LYS
3	33	147	THR
3	34	110	LYS
3	34	147	THR
3	35	110	LYS
3	35	147	THR

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Mol	Chain	Res	Type
3	36	110	LYS
3	36	147	THR
2	1B	440	ALA
2	1D	354	ASP
2	1F	440	ALA
2	1J	440	ALA
2	2J	354	ASP
3	22	56	GLN
3	25	56	GLN
3	25	77	LEU
2	1D	268	VAL
2	1F	268	VAL
2	1H	268	VAL
2	1J	268	VAL
2	2B	268	VAL
2	2D	268	VAL
2	2F	268	VAL
2	2H	268	VAL
2	2H	353	LYS
2	2J	268	VAL
3	26	56	GLN
2	3B	268	VAL
2	3D	268	VAL
2	3F	268	VAL
2	3H	268	VAL
2	3J	268	VAL
3	31	77	LEU
3	32	77	LEU
3	33	77	LEU
3	34	77	LEU
3	35	77	LEU
3	36	77	LEU
2	1B	268	VAL
2	1L	268	VAL
2	2L	268	VAL
2	3L	268	VAL
2	3L	463	PRO
2	1B	439	PRO
2	2J	440	ALA
2	2B	440	ALA

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8601. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

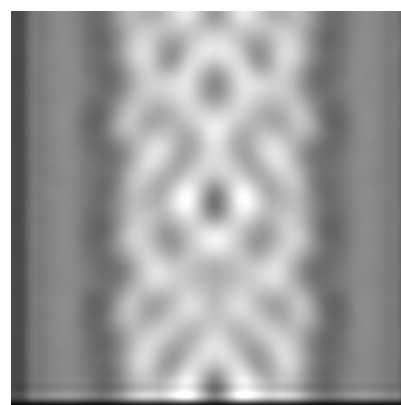
6.1.1 Primary map



X



Y

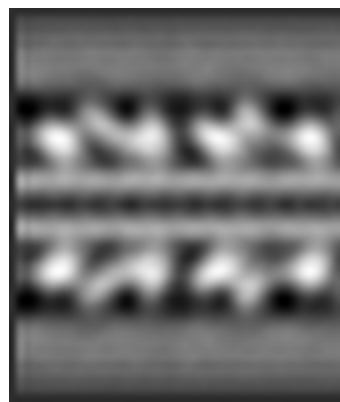


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 25



Y Index: 25

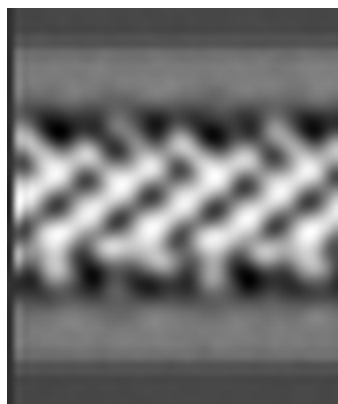


Z Index: 30

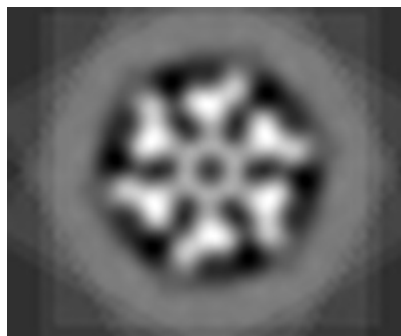
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 16



Y Index: 26

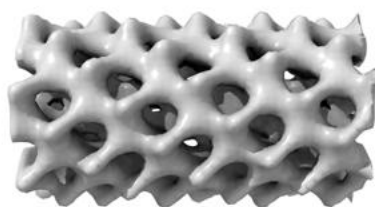


Z Index: 21

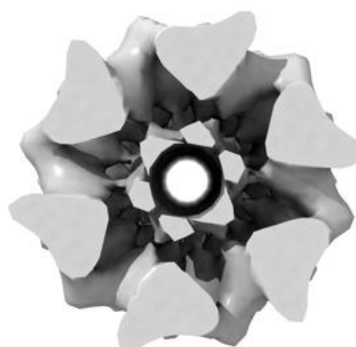
The images above show the largest variance slices of the map in three orthogonal directions.

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

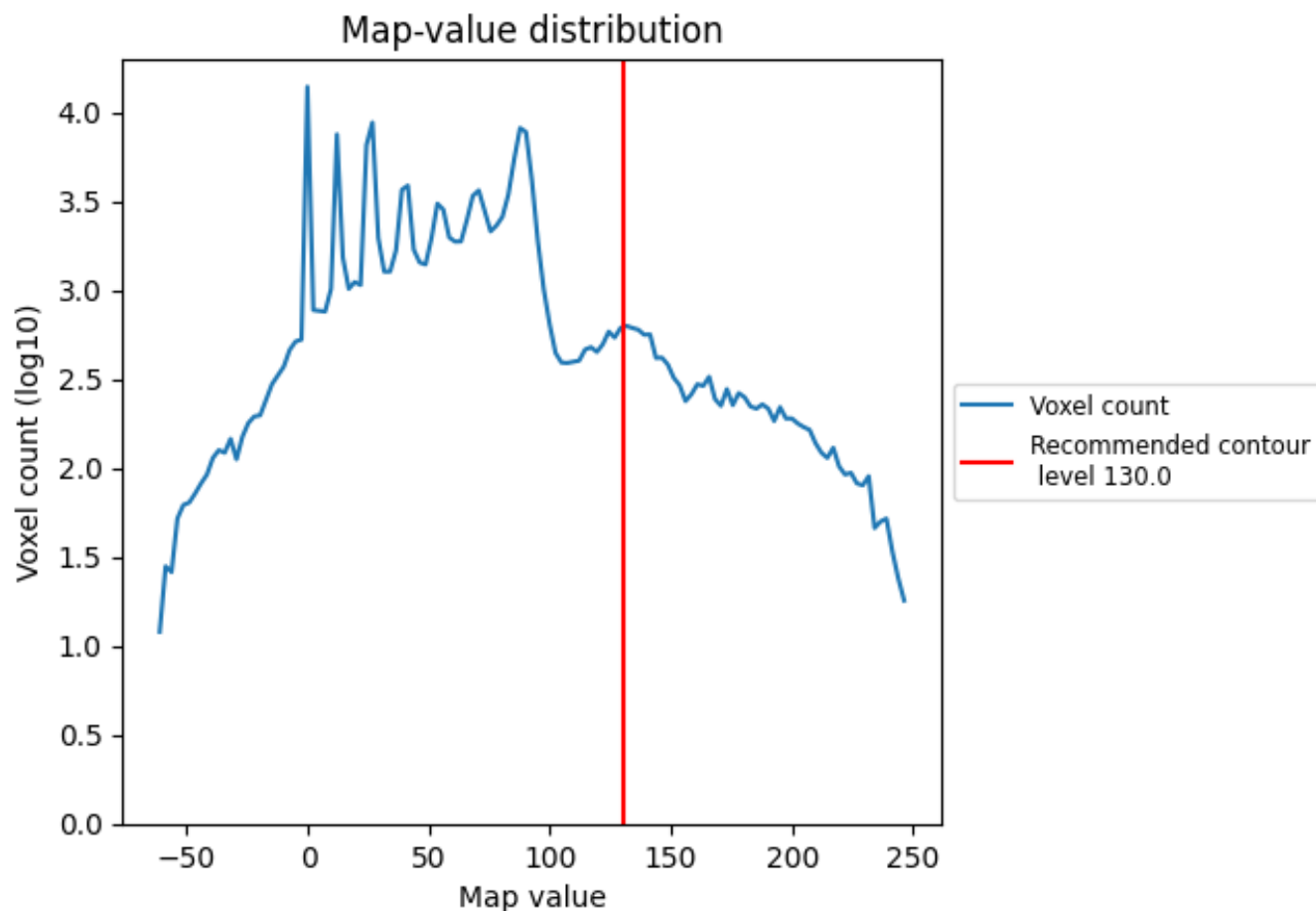
6.5 Mask visualisation

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

7 Map analysis [i](#)

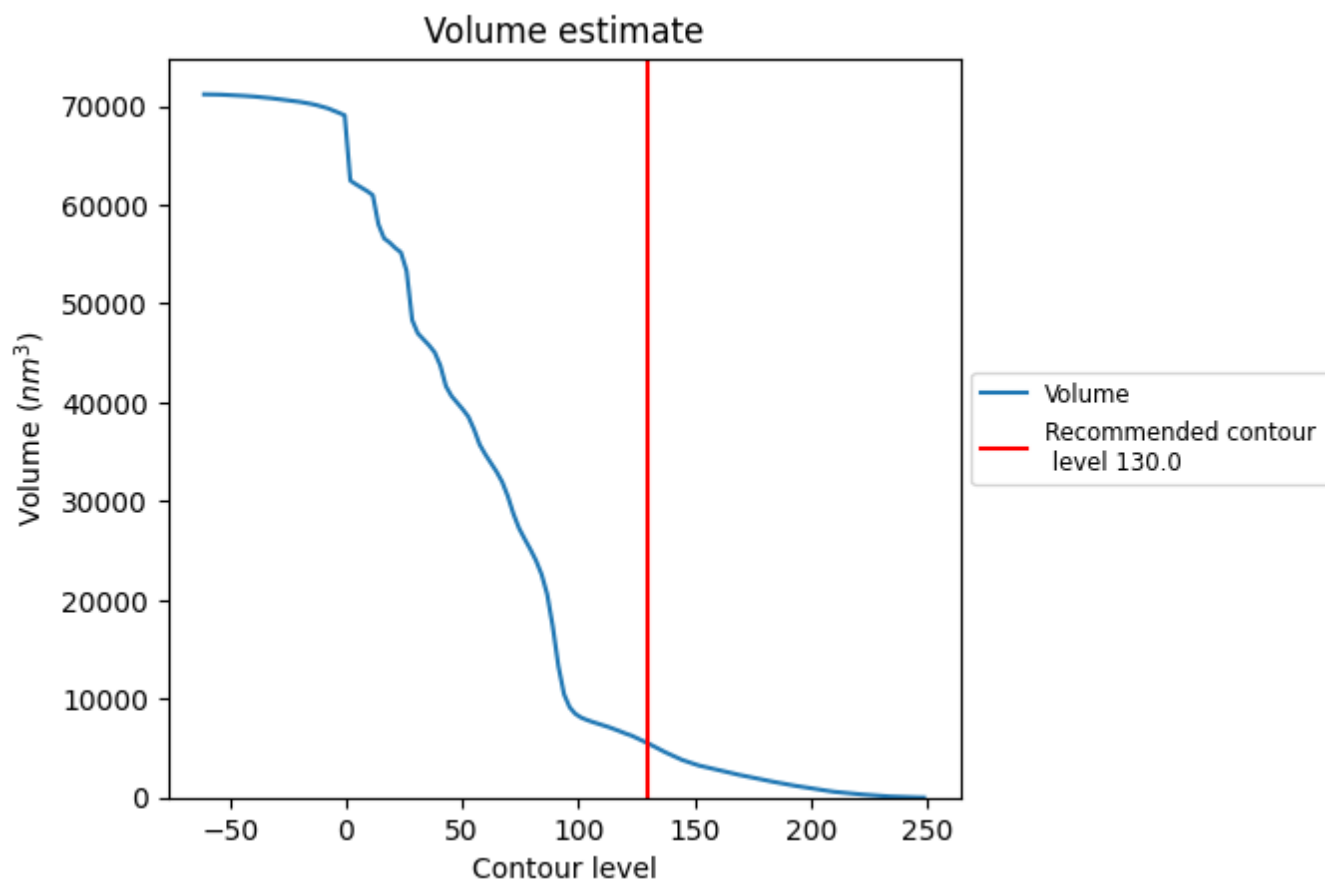
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5480 nm³; this corresponds to an approximate mass of 4950 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](#)

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

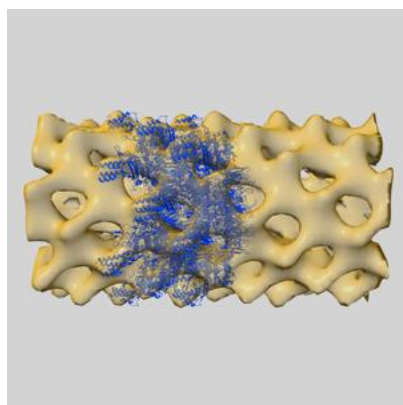
8 Fourier-Shell correlation ⓘ

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

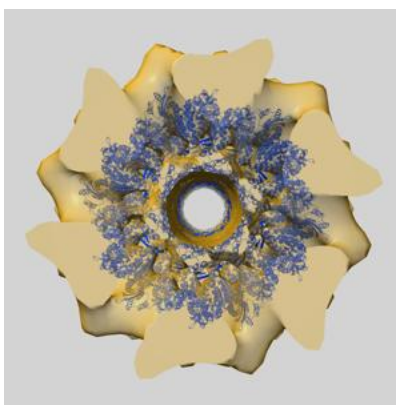
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8601 and PDB model 5URW. Per-residue inclusion information can be found in section [3](#) on page [8](#).

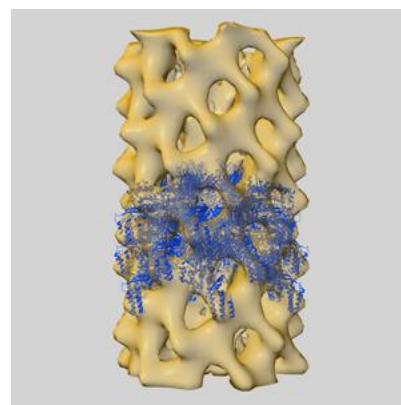
9.1 Map-model overlay [i](#)



X



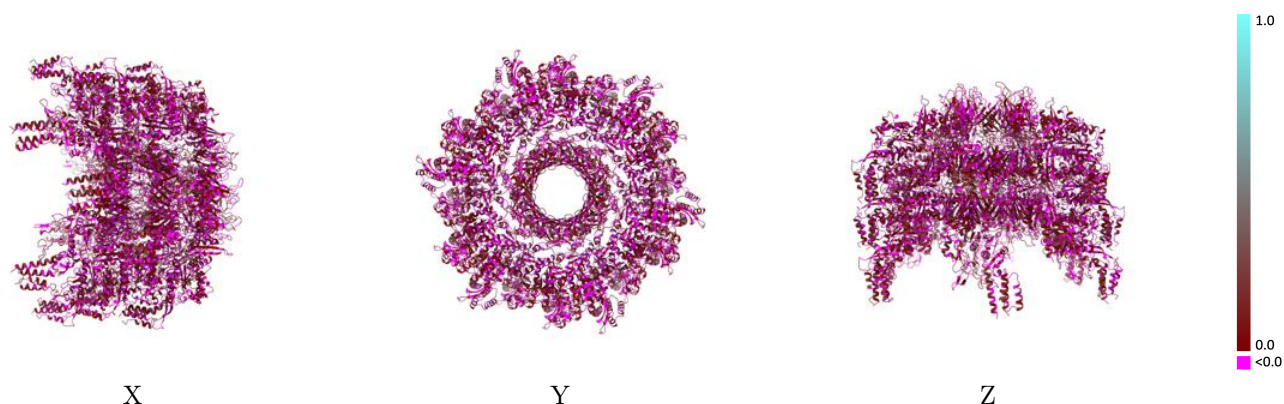
Y



Z

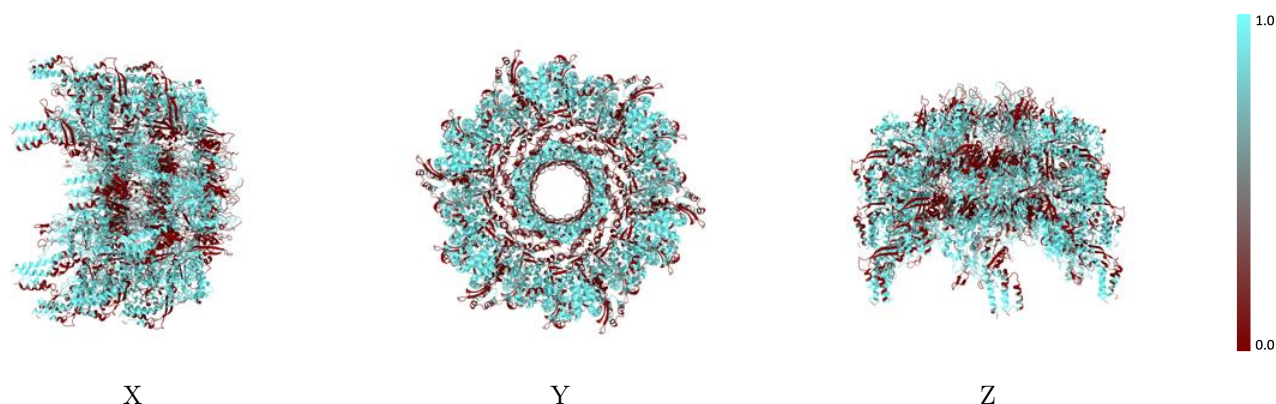
The images above show the 3D surface view of the map at the recommended contour level 130.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



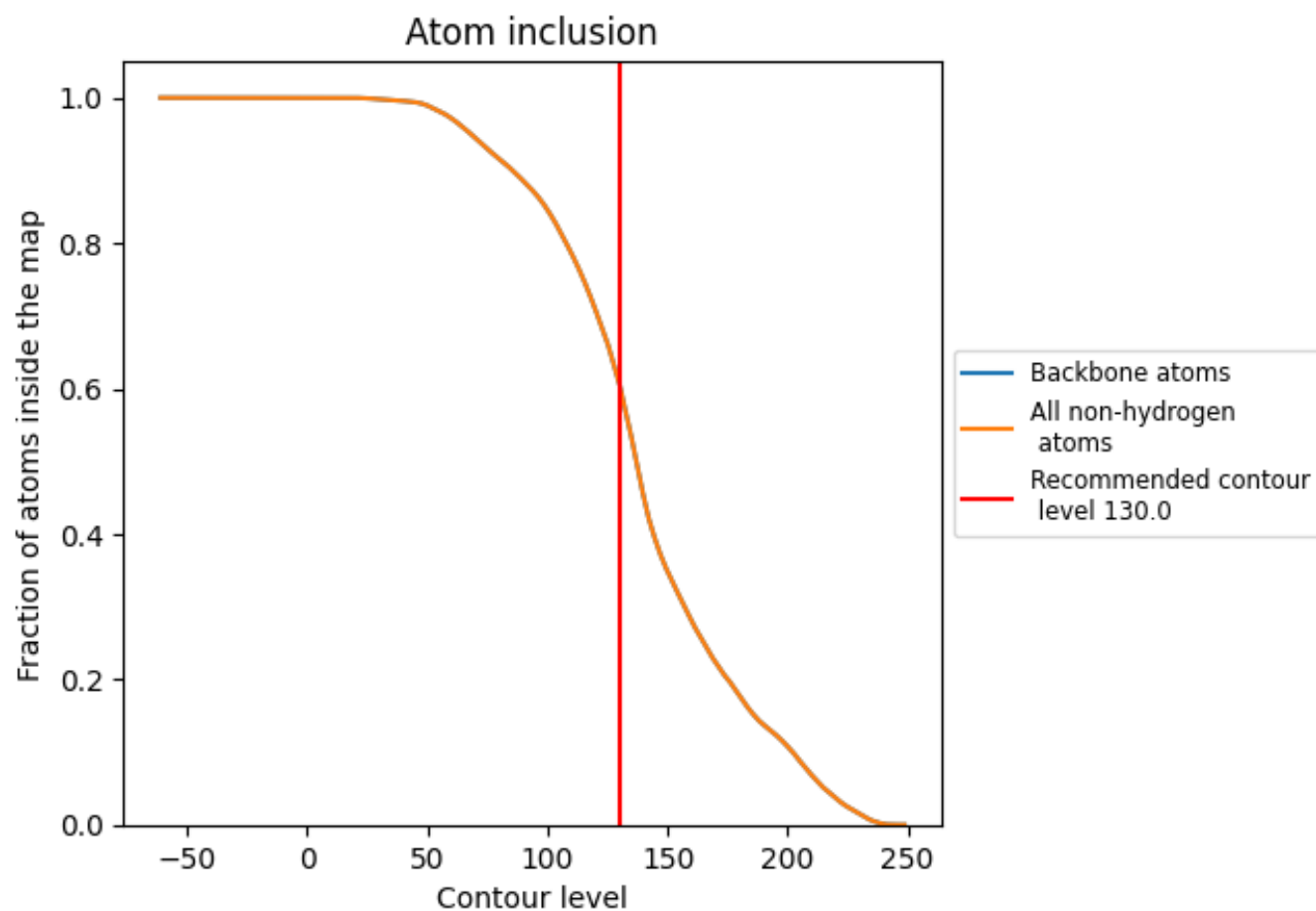
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (130.0).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 61% 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 (130.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6058	 0.0420
11	 0.5641	 0.0580
12	 0.5719	 0.0580
13	 0.5734	 0.0520
14	 0.5437	 0.0470
15	 0.5719	 0.0490
16	 0.5687	 0.0450
1A	 0.3963	 0.0170
1B	 0.7186	 0.0430
1C	 0.3611	 0.0290
1D	 0.7228	 0.0460
1E	 0.3963	 0.0480
1F	 0.7252	 0.0440
1G	 0.3519	 0.0370
1H	 0.7234	 0.0450
1I	 0.3722	 0.0270
1J	 0.7228	 0.0450
1K	 0.3463	 0.0190
1L	 0.7271	 0.0430
21	 0.4641	 0.0530
22	 0.4719	 0.0500
23	 0.4688	 0.0540
24	 0.4656	 0.0460
25	 0.4828	 0.0390
26	 0.4797	 0.0580
2A	 0.3593	 0.0200
2B	 0.7114	 0.0460
2C	 0.3278	 0.0250
2D	 0.7132	 0.0440
2E	 0.3519	 0.0350
2F	 0.7162	 0.0430
2G	 0.3056	 0.0270
2H	 0.7132	 0.0490
2I	 0.3407	 0.0170
2J	 0.7132	 0.0480



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Chain	Atom inclusion	Q-score
2K	 0.3167	 0.0080
2L	 0.7126	 0.0410
3I	 0.5563	 0.0600
32	 0.5547	 0.0490
33	 0.5578	 0.0660
34	 0.5578	 0.0470
35	 0.5437	 0.0440
36	 0.5547	 0.0730
3A	 0.3796	 0.0190
3B	 0.7107	 0.0450
3C	 0.3537	 0.0250
3D	 0.7198	 0.0400
3E	 0.3667	 0.0370
3F	 0.7210	 0.0490
3G	 0.3167	 0.0150
3H	 0.7162	 0.0440
3I	 0.3556	 0.0120
3J	 0.7126	 0.0400
3K	 0.3407	 0.0020
3L	 0.7162	 0.0470