



# Full wwPDB NMR Structure Validation Report ⓘ

Jun 12, 2024 – 02:45 AM EDT

PDB ID : 2WWV  
Title : NMR structure of the IIAchitobiose-IIBchitobiose complex of the N,N'-diacetylchitobiose branch of the E. coli phosphotransferase system.  
Authors : Sang, Y.S.; Cai, M.; Clore, G.M.  
Deposited on : 2009-10-29

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

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>.

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

MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

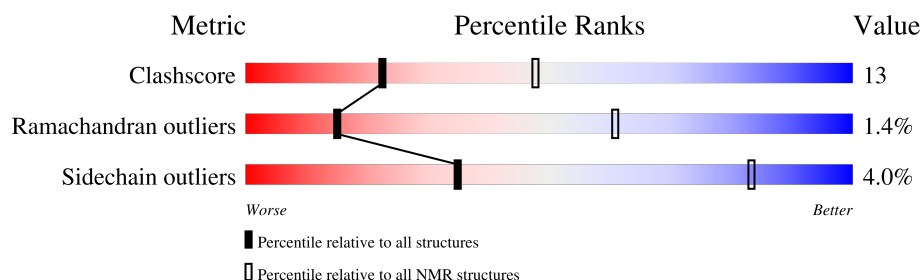
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	103	
1	B	103	
1	C	103	
2	D	103	

## 2 Ensemble composition and analysis

This entry contains 91 models. Model 91 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:1-A:62, A:70-A:103, B:1-B:62, B:70-B:103, C:1-C:62, C:70-C:103, D:10-D:19, D:38-D:40, D:57-D:60 (305)	0.11	91

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 10 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 3, 4, 11, 16, 18, 19, 22, 27, 28, 41, 45, 48, 49, 52, 68, 86
2	5, 6, 15, 21, 31, 43, 46, 58, 61, 64, 71, 75, 82, 85
3	10, 20, 26, 32, 38, 39, 47, 54, 60, 73, 79, 89
4	7, 12, 13, 24, 35, 40, 50, 53, 56, 70, 87
5	9, 23, 25, 34, 55, 57, 72, 77, 80, 90, 91
6	8, 29, 33, 36, 51, 63, 66, 69, 74, 76, 83
7	14, 30, 37, 42, 59, 67, 88
8	17, 78
9	65, 81
10	44, 84
Single-model clusters	62

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6423 atoms, of which 3301 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT.

Mol	Chain	Residues	Atoms						Trace
1	A	103	Total	C	H	N	O	S	0
			1605	490	823	134	151	7	
1	B	103	Total	C	H	N	O	S	0
			1605	490	823	134	151	7	
1	C	103	Total	C	H	N	O	S	0
			1605	490	823	134	151	7	

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	76	GLU	HIS	engineered mutation	UNP P69791
A	79	LEU	ASP	engineered mutation	UNP P69791
B	76	GLU	HIS	engineered mutation	UNP P69791
B	79	LEU	ASP	engineered mutation	UNP P69791
C	76	GLU	HIS	engineered mutation	UNP P69791
C	79	LEU	ASP	engineered mutation	UNP P69791

- Molecule 2 is a protein called N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT.

Mol	Chain	Residues	Atoms						Trace
2	D	103	Total	C	H	N	O	S	0
			1608	504	832	127	142	3	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	10	SER	CYS	engineered mutation	UNP P69795

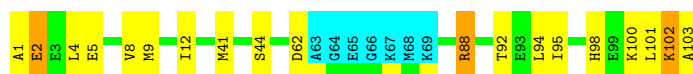
## 4 Residue-property plots

### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

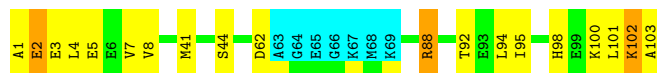
- Molecule 1: N<sub>1</sub>,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A:  75% 16% 7%



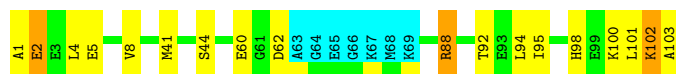
- Molecule 1: N<sub>1</sub>,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B:  75% 16% 7%



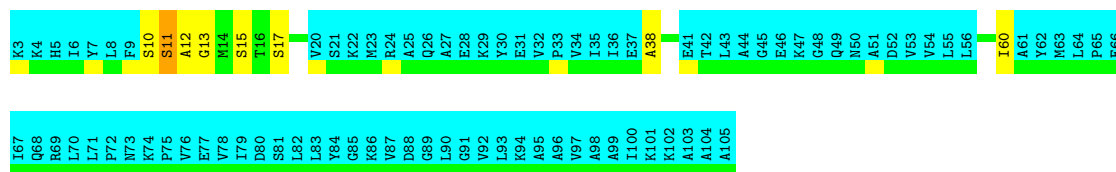
- Molecule 1: N<sub>1</sub>,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C:  76% 15% 7%



- Molecule 2: N<sub>1</sub>,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

Chain D:  9% 7% 83%



## 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

### 4.2.1 Score per residue for model 1

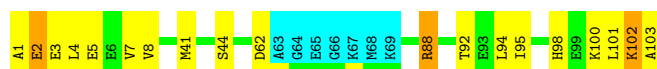
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A:  73% 17% 7%



- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B:  75% 16% 7%



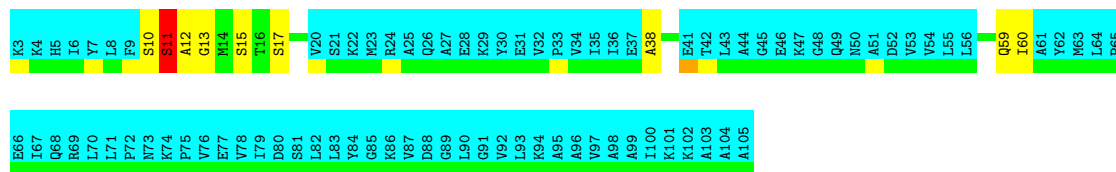
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C:  77% 14% 7%



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

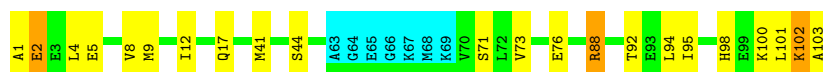
Chain D:  8% 8% 83%



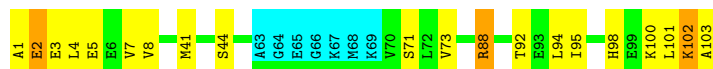
### 4.2.2 Score per residue for model 2

- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

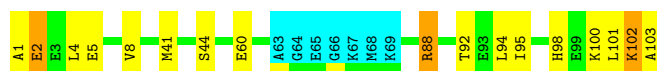
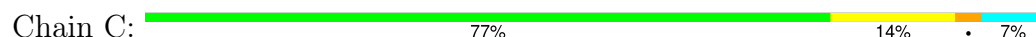
Chain A:  72% 18% 7%



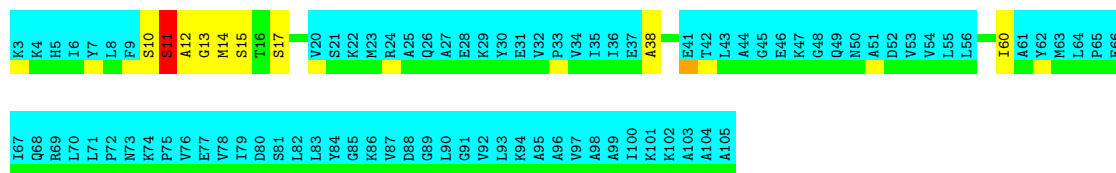
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

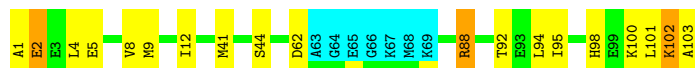


- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

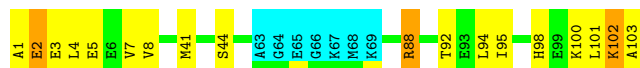


### 4.2.3 Score per residue for model 3


- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

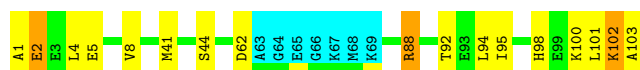


- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



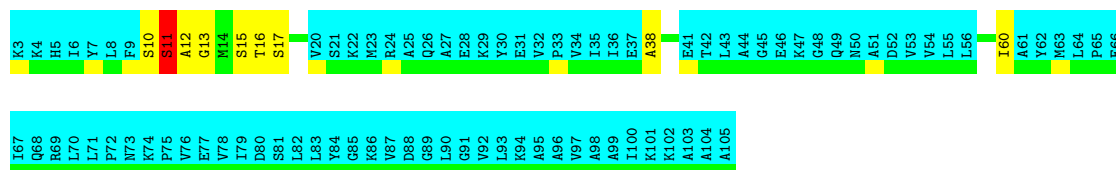
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C:  77% 14% 7%



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

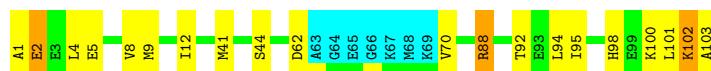
Chain D:  8% 8% 83%



#### 4.2.4 Score per residue for model 4

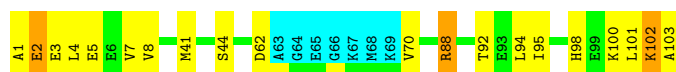
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A:  74% 17% 7%



- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B:  74% 17% 7%



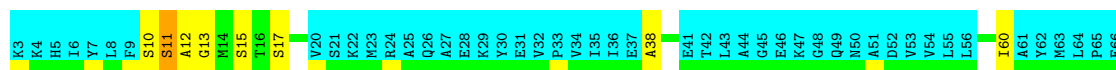
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C:  76% 15% 7%

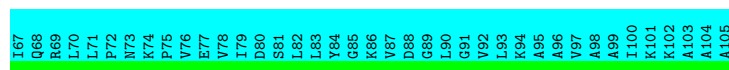


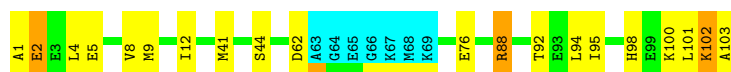
- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

Chain D:  9% 7% 83%

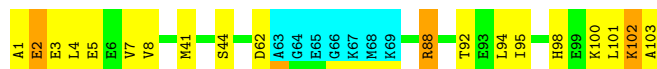




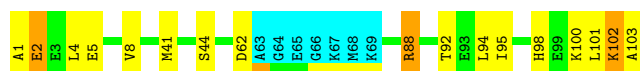
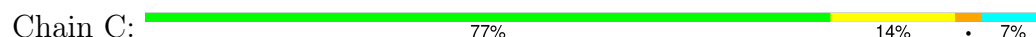




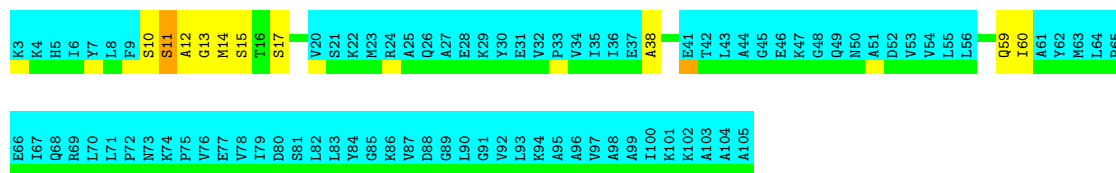
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT



#### 4.2.7 Score per residue for model 7


- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

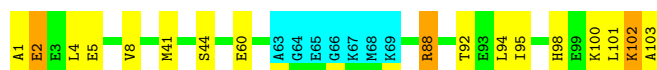


- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



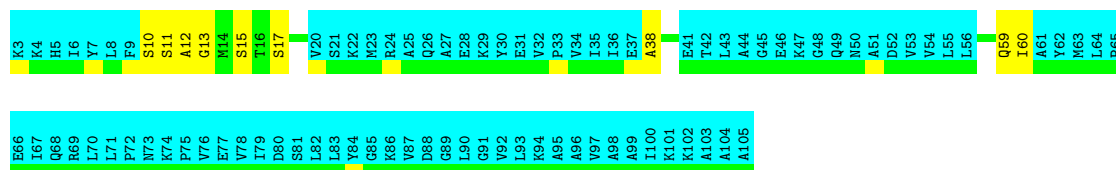
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C:  77% 14% 7%



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

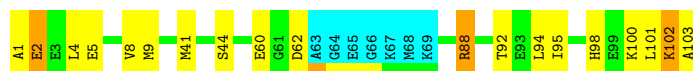
Chain D:  8% 9% 83%



#### 4.2.8 Score per residue for model 8

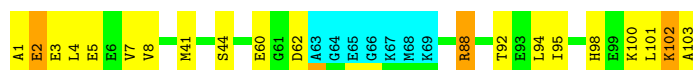
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A:  75% 16% 7%



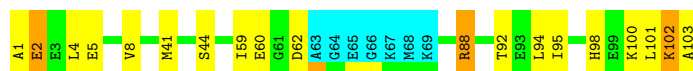
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B:  74% 17% 7%



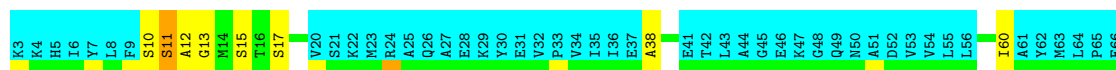
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

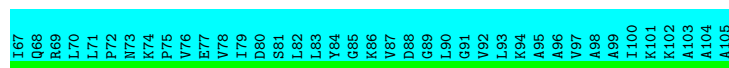
Chain C:  75% 16% 7%



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

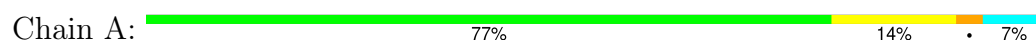
Chain D:  9% 7% 83%



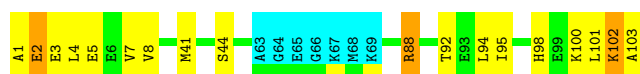


#### 4.2.9 Score per residue for model 9

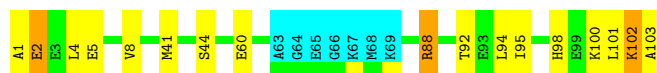
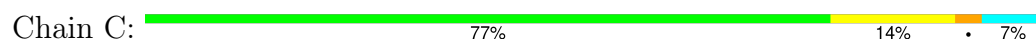
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



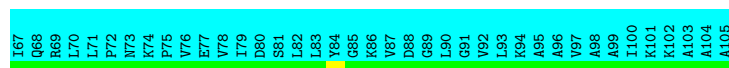
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



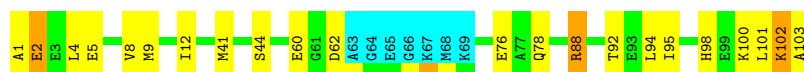
- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT



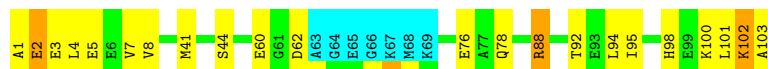
#### 4.2.10 Score per residue for model 10

- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

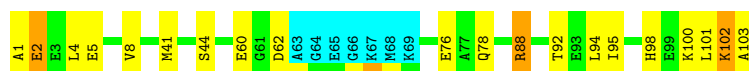




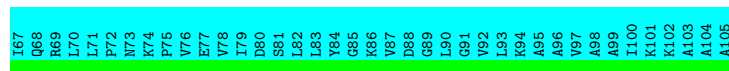
- Molecule 1: N<sub>1</sub>,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



- Molecule 1: N<sub>1</sub>,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

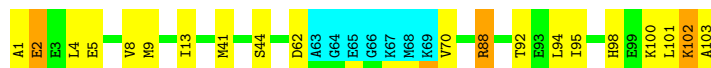


- Molecule 2: N<sub>1</sub>,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT



#### 4.2.11 Score per residue for model 11

- Molecule 1: N<sub>1</sub>,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



- Molecule 1: N<sub>1</sub>,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



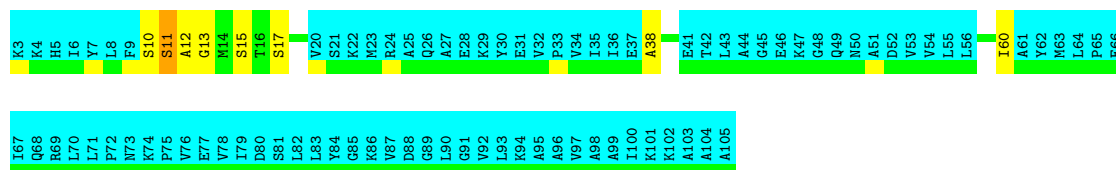
- Molecule 1: N<sub>1</sub>,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C:  75% 16% 7%



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

Chain D:  9% 7% 83%



#### 4.2.12 Score per residue for model 12

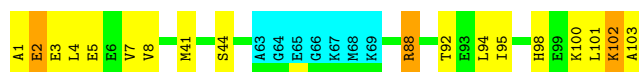
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A:  76% 15% 7%



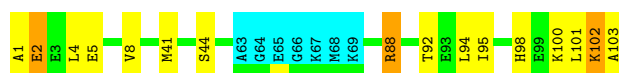
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B:  76% 15% 7%



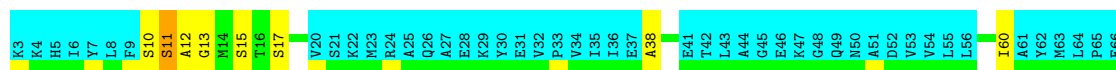
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

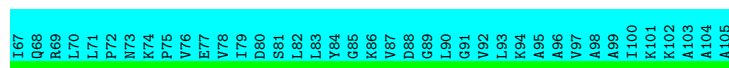
Chain C:  78% 13% 7%



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

Chain D:  9% 7% 83%

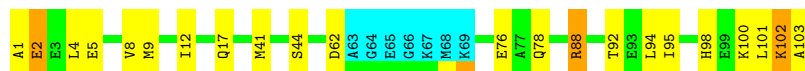




#### 4.2.13 Score per residue for model 13

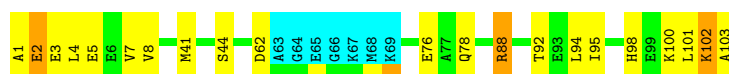
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A: 72% 18% 7%



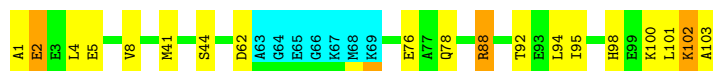
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B: 73% 17% 7%



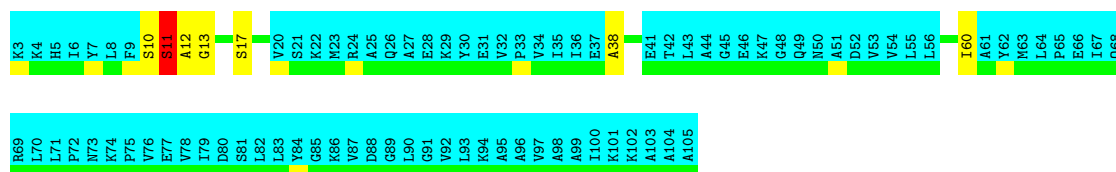
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C: 75% 16% 7%



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

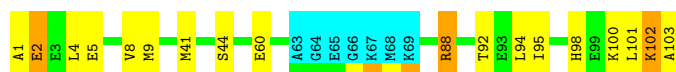
Chain D: 10% 6% 83%



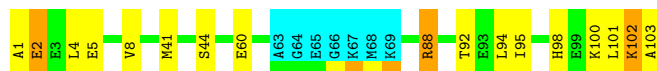
#### 4.2.14 Score per residue for model 14

- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

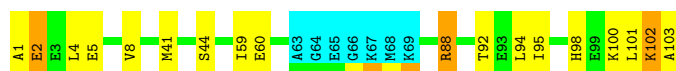
Chain A: 76% 15% 7%



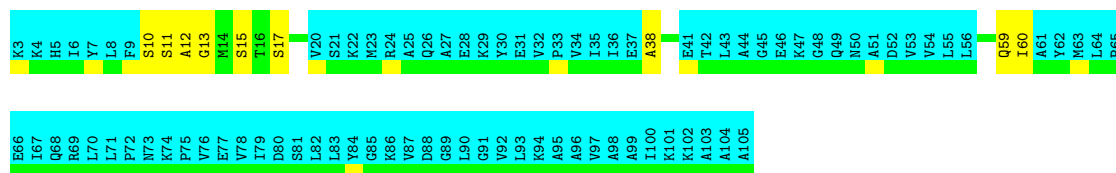
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

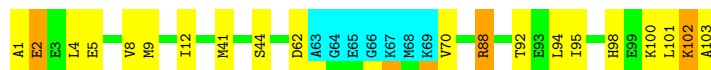


- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT



#### 4.2.15 Score per residue for model 15

- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT




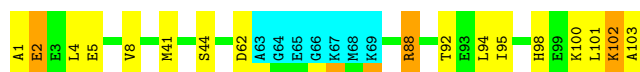
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

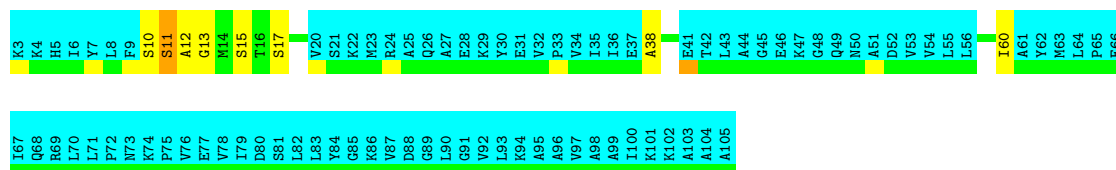


Chain C:  77% 14% 7%



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

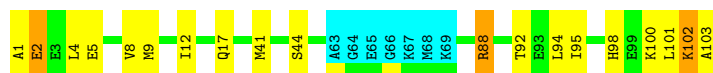
Chain D:  9% 7% 83%



#### 4.2.16 Score per residue for model 16

- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A:  75% 16% 7%



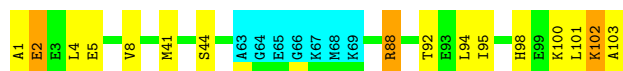
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B:  76% 15% 7%



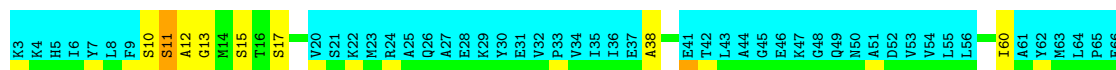
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

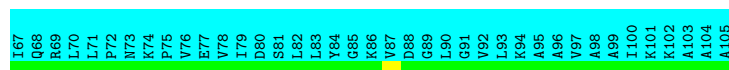
Chain C:  78% 13% 7%



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

Chain D:  9% 7% 83%

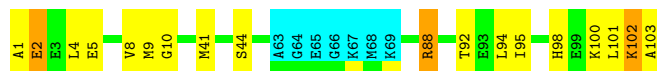




#### 4.2.17 Score per residue for model 17

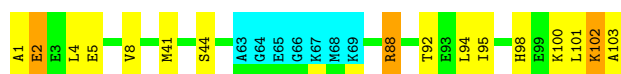
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A: 76% 15% 7%



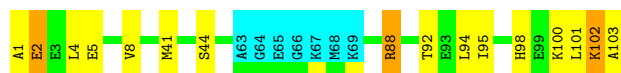
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B: 78% 13% 7%



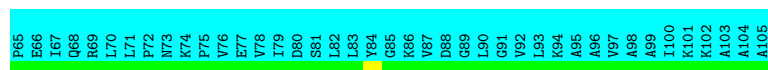
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C: 78% 13% 7%



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

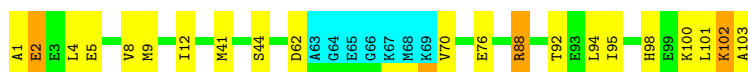
Chain D: 7% 9% 83%



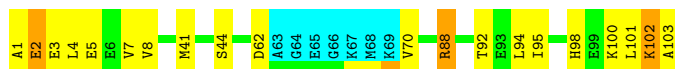
#### 4.2.18 Score per residue for model 18

- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

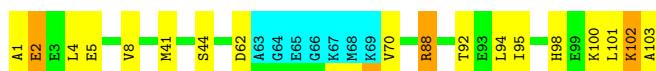
Chain A: 73% 17% 7%



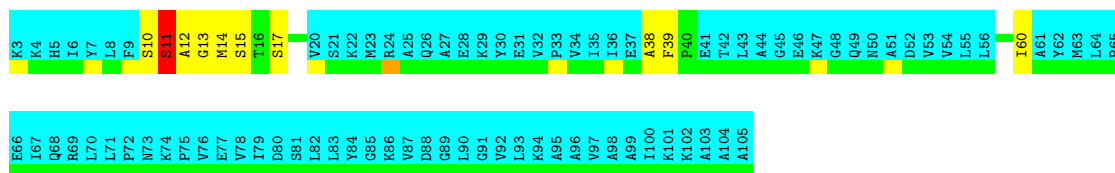
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

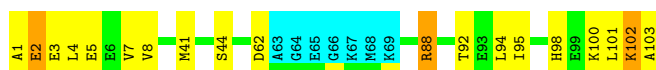


#### 4.2.19 Score per residue for model 19

- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

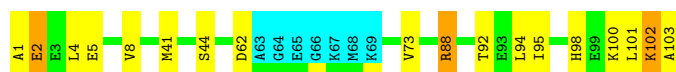


- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



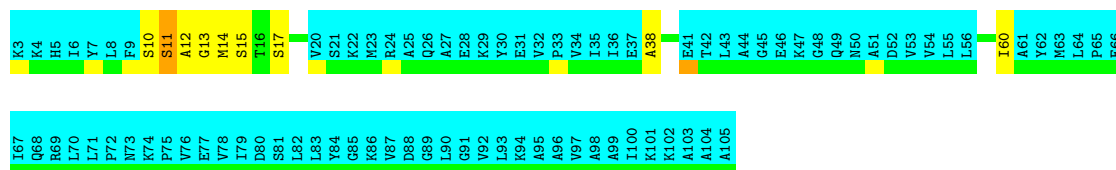
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C: 



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

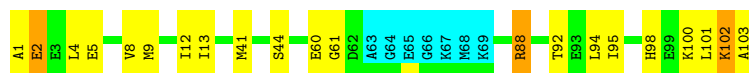
Chain D: 



#### 4.2.20 Score per residue for model 20

- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A: 



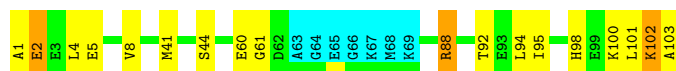
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B: 



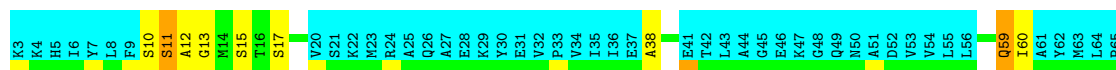
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

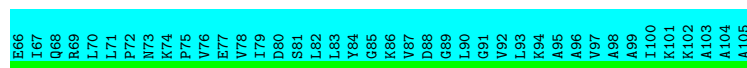
Chain C: 



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

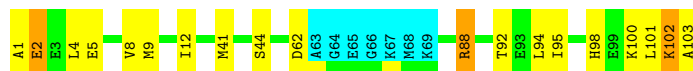
Chain D: 



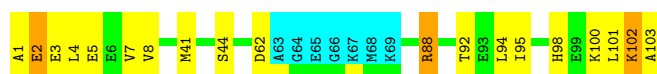


#### 4.2.21 Score per residue for model 21

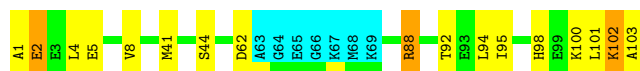
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



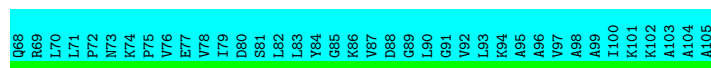
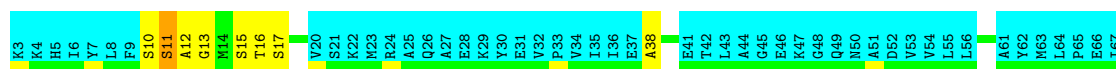
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

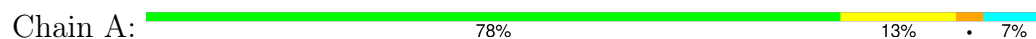


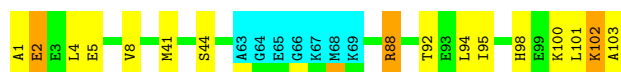
- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT



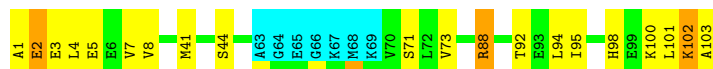
#### 4.2.22 Score per residue for model 22

- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

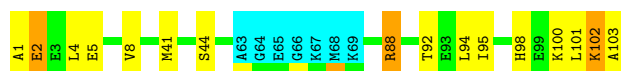




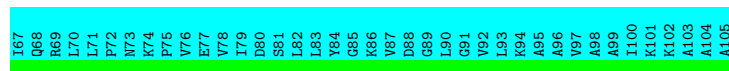
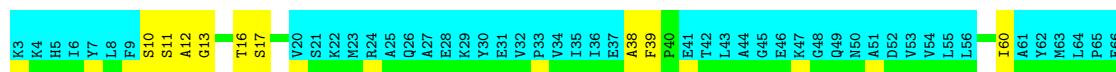
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

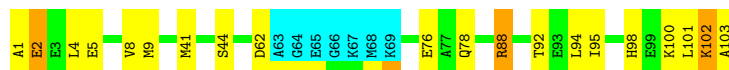


- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

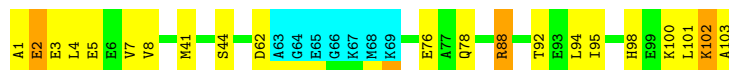


#### 4.2.23 Score per residue for model 23

- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

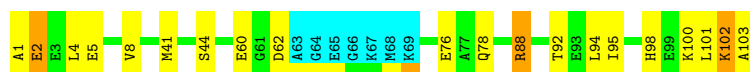


- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



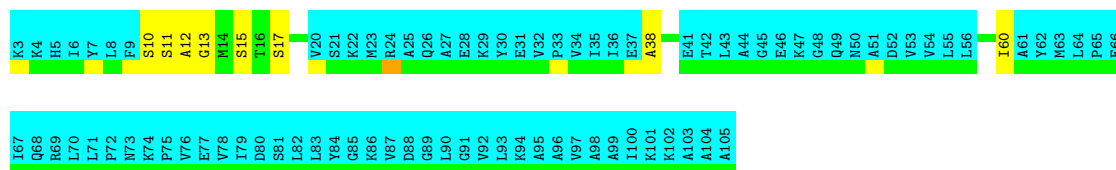
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C: 



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

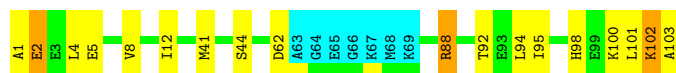
Chain D: 



#### 4.2.24 Score per residue for model 24

- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A: 



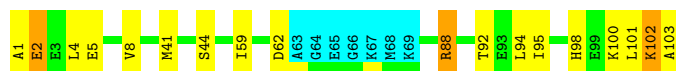
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B: 



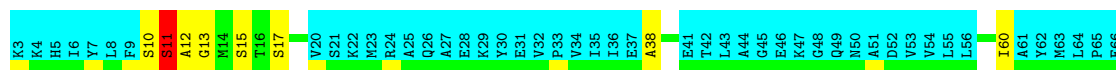
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

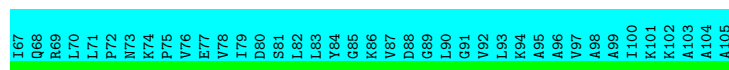
Chain C: 



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

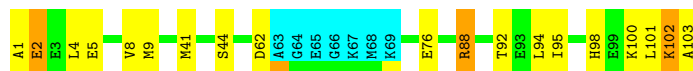
Chain D: 



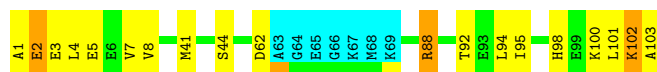


#### 4.2.25 Score per residue for model 25

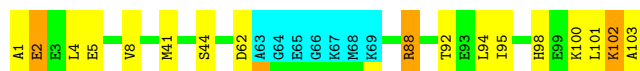
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



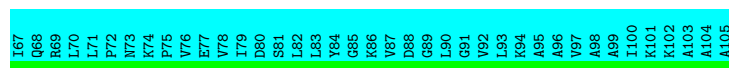
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT



#### 4.2.26 Score per residue for model 26

- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

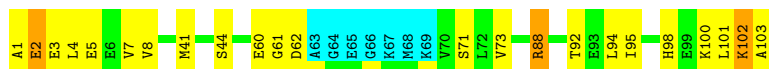






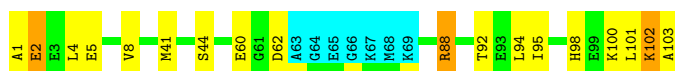
• Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B: 



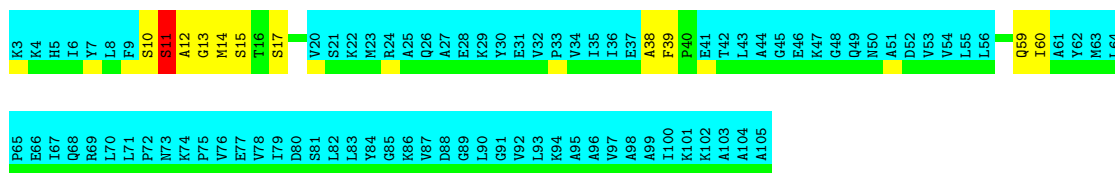
• Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C: 



• Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

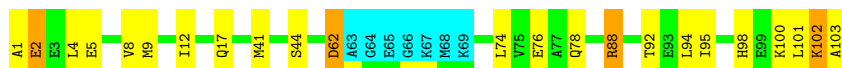
Chain D: 



#### 4.2.27 Score per residue for model 27

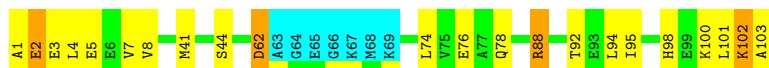
• Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A: 



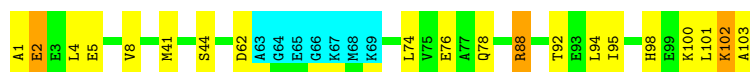
• Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B: 



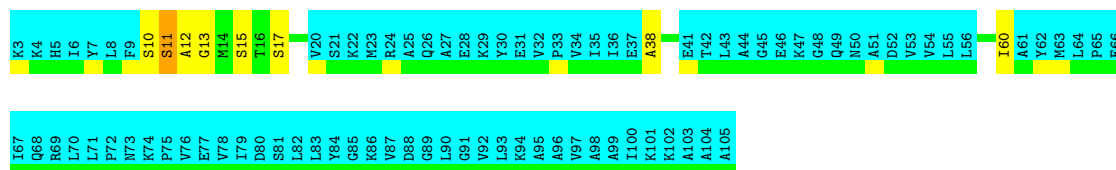
• Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C:  74% 17% 7%



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

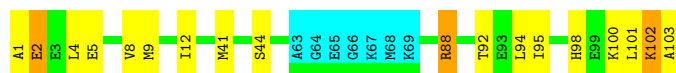
Chain D:  9% 7% 83%



#### 4.2.28 Score per residue for model 28

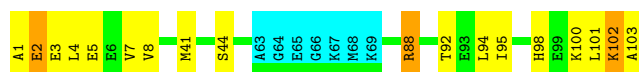
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A:  76% 15% 7%



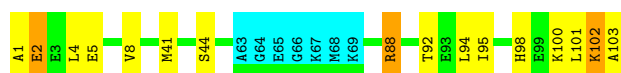
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B:  76% 15% 7%



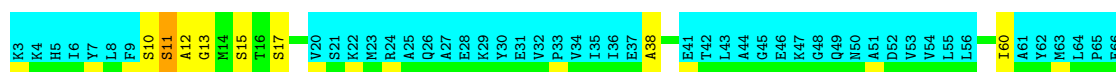
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

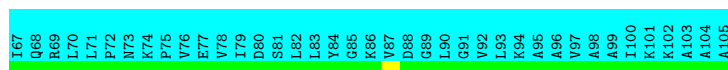
Chain C:  78% 13% 7%



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

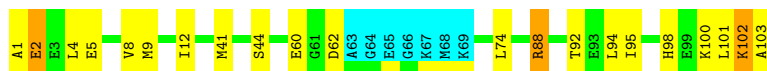
Chain D:  9% 7% 83%



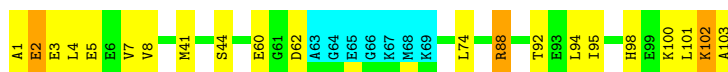


#### 4.2.29 Score per residue for model 29

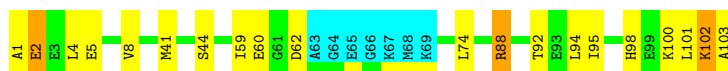
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



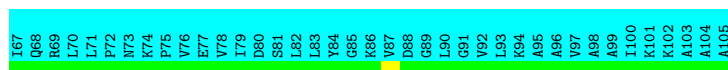
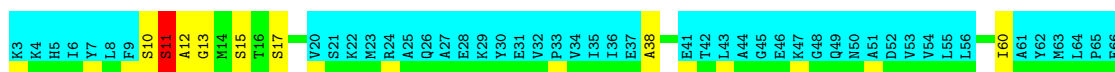
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



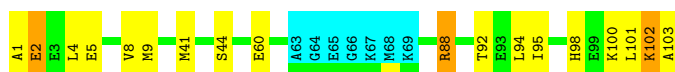
- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT



#### 4.2.30 Score per residue for model 30

- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

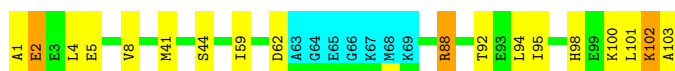




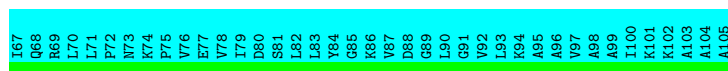
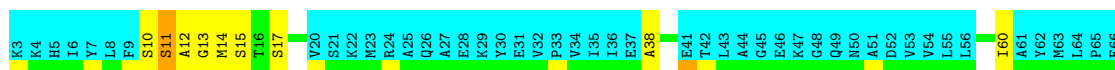
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

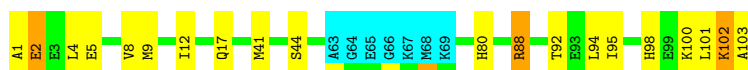


- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

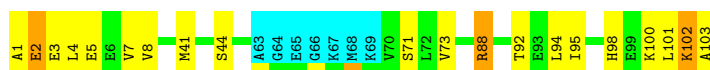


#### 4.2.31 Score per residue for model 31


- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

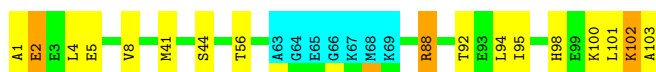


- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



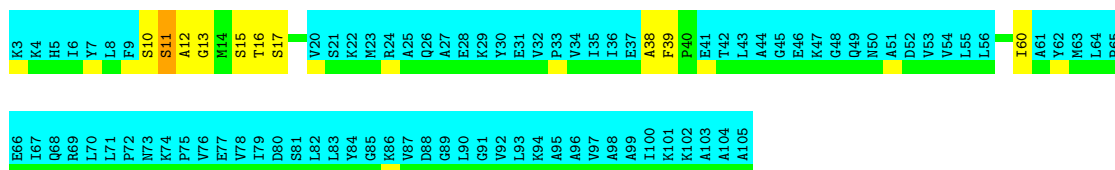
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C:  77% 14% 7%



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

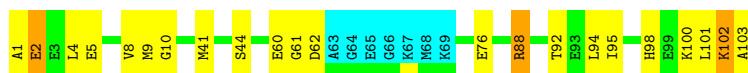
Chain D:  7% 9% 83%



#### 4.2.32 Score per residue for model 32

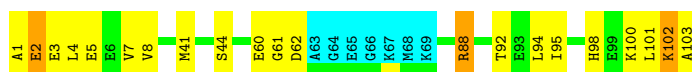
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A:  72% 18% 7%



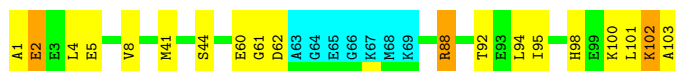
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B:  73% 17% 7%



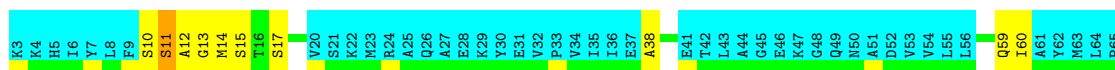
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

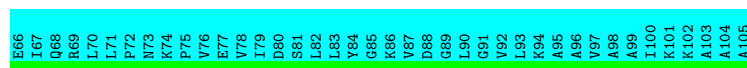
Chain C:  75% 16% 7%



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

Chain D:  7% 9% 83%





#### 4.2.33 Score per residue for model 33

- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A: 76% 15% 7%



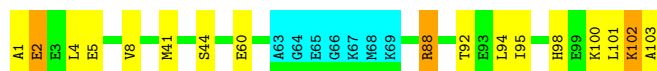
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B: 75% 16% 7%



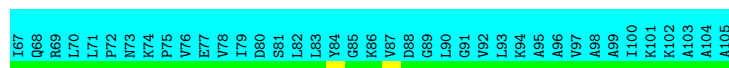
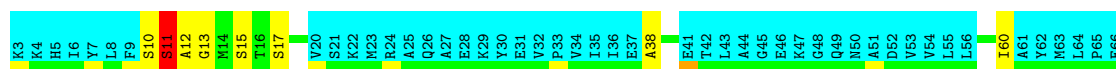
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C: 77% 14% 7%



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

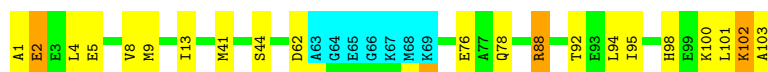
Chain D: 9% 7% 83%



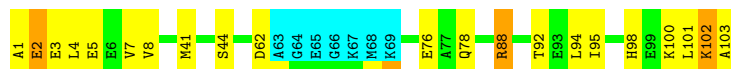
#### 4.2.34 Score per residue for model 34

- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

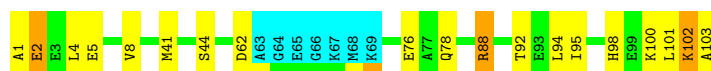
Chain A: 73% 17% 7%



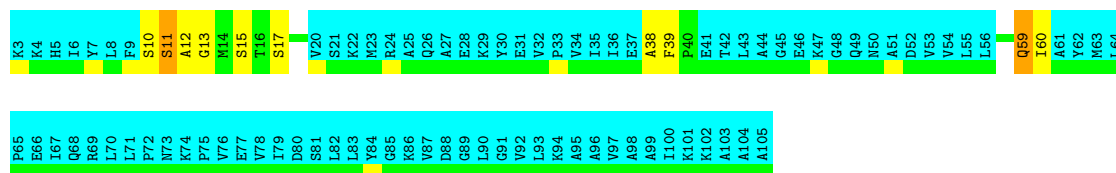
- Molecule 1: N<sub>1</sub>,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



- Molecule 1: N<sub>1</sub>,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

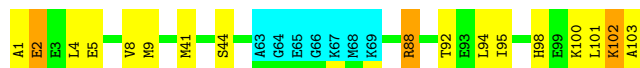


- Molecule 2: N<sub>1</sub>,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT



#### 4.2.35 Score per residue for model 35


- Molecule 1: N<sub>1</sub>,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

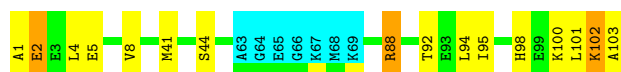


- Molecule 1: N<sub>1</sub>,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



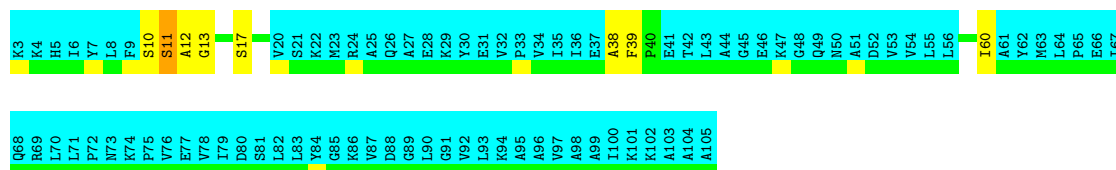
- Molecule 1: N<sub>1</sub>,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C:  78% 13% 7%



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

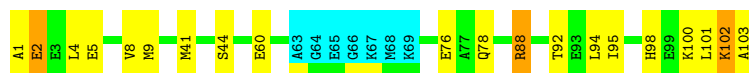
Chain D:  9% 7% 83%



#### 4.2.36 Score per residue for model 36

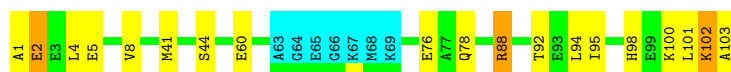
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A:  74% 17% 7%



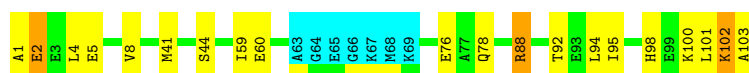
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B:  75% 16% 7%



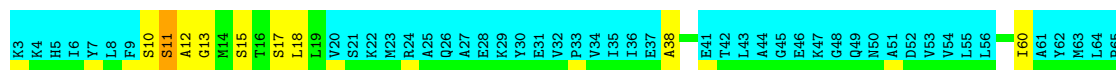
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C:  74% 17% 7%

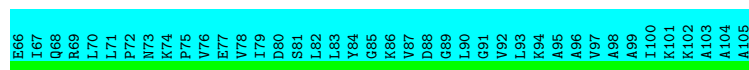


- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

Chain D:  8% 8% 83%







#### 4.2.37 Score per residue for model 37

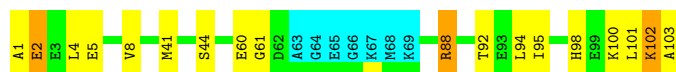
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A: 73% 17% 7%



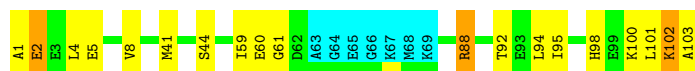
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B: 76% 15% 7%



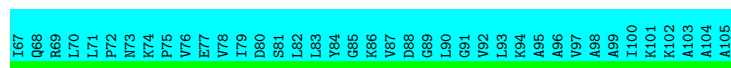
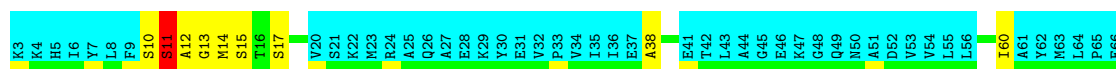
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C: 75% 16% 7%



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

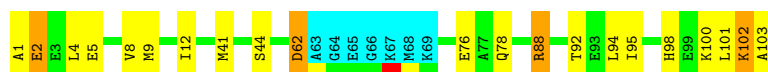
Chain D: 8% 8% 83%



#### 4.2.38 Score per residue for model 38

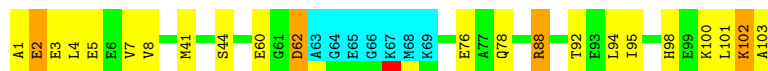
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A: 73% 17% 7%



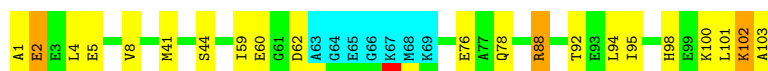
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B: 72% 17% 7%



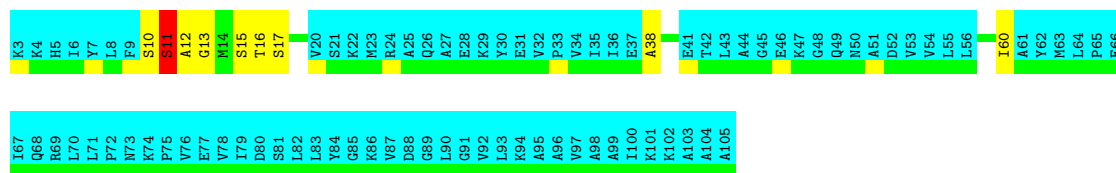
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C: 73% 17% 7%



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

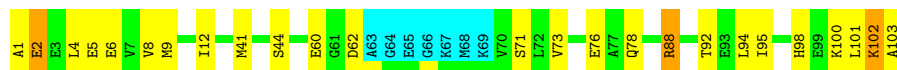
Chain D: 83% 8% 8%



#### 4.2.39 Score per residue for model 39

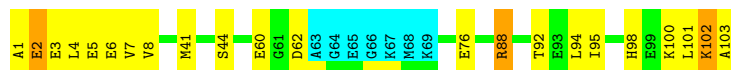
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A: 69% 21% 7%



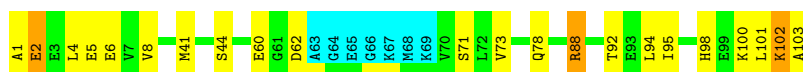
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B: 72% 18% 7%



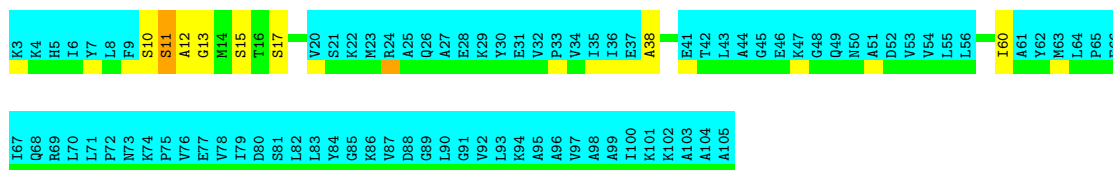
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C:  72% 18% 7%



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

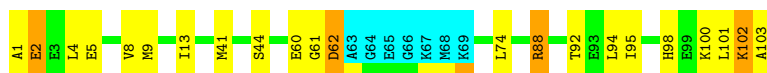
Chain D:  9% 7% 83%



#### 4.2.40 Score per residue for model 40

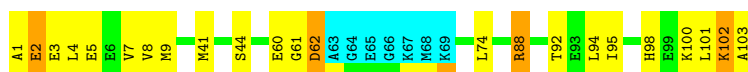
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A:  72% 17% 7%



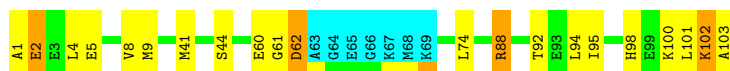
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B:  71% 18% 7%



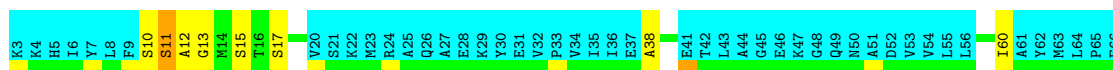
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

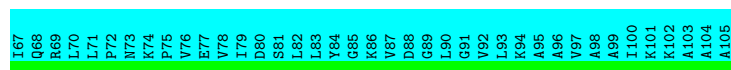
Chain C:  73% 17% 7%



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

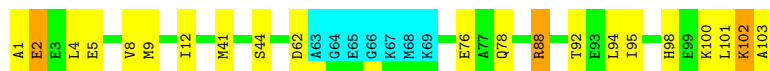
Chain D:  9% 7% 83%



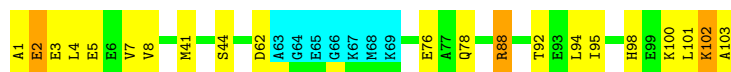


#### 4.2.41 Score per residue for model 41

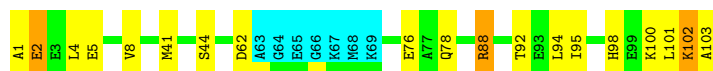
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



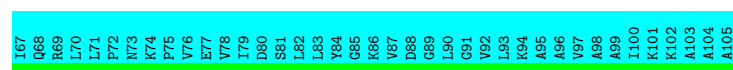
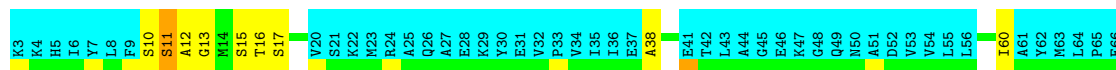
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



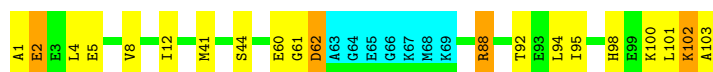
- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT



#### 4.2.42 Score per residue for model 42

- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT





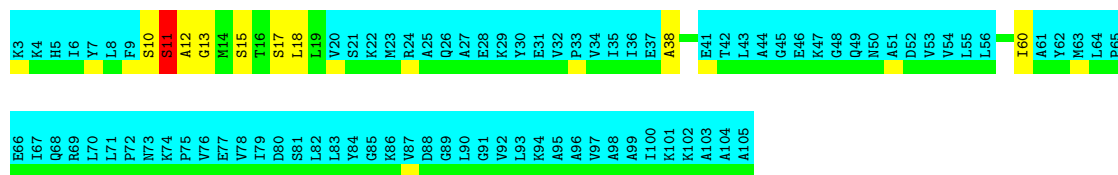
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

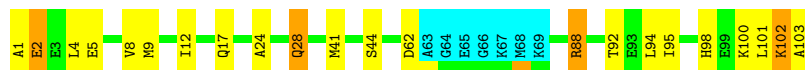


- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT



#### 4.2.43 Score per residue for model 43

- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



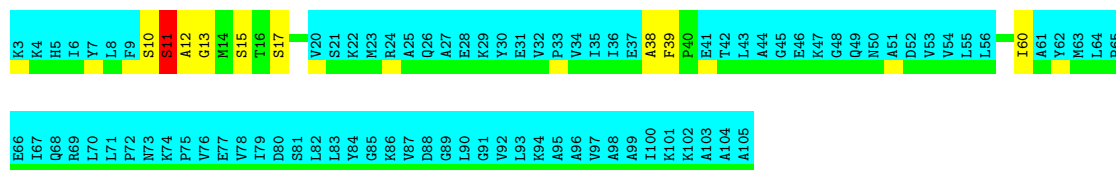
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C: 



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

Chain D: 



#### 4.2.44 Score per residue for model 44

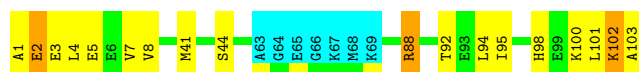
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A: 




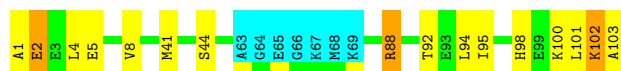
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B: 



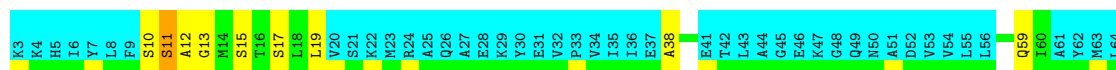
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

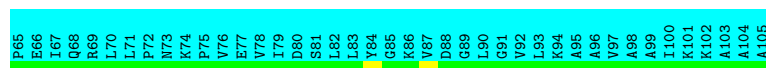
Chain C: 



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

Chain D: 

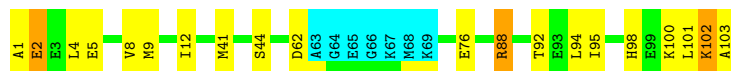




#### 4.2.45 Score per residue for model 45

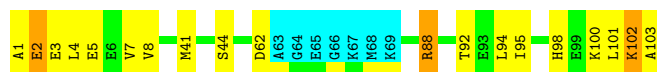
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A: 74% 17% 7%



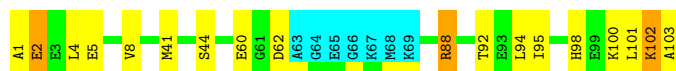
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B: 75% 16% 7%



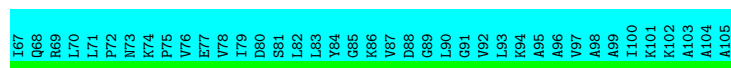
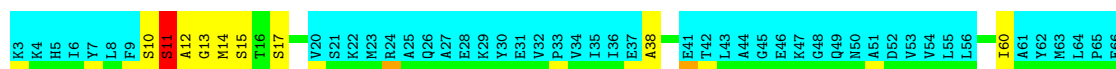
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C: 76% 15% 7%



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

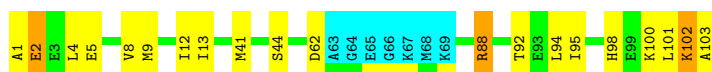
Chain D: 8% 8% 83%



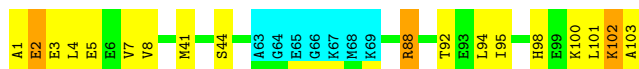
#### 4.2.46 Score per residue for model 46

- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

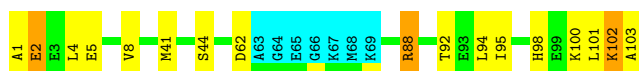
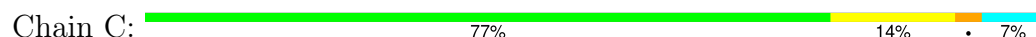
Chain A: 74% 17% 7%



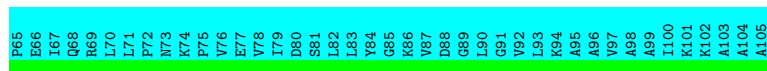
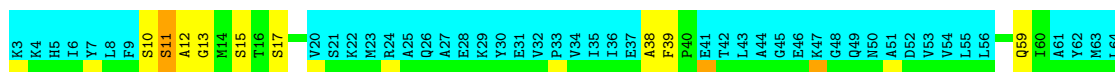
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

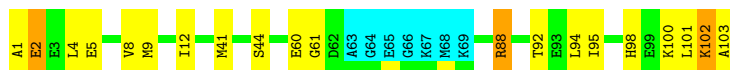


- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT



#### 4.2.47 Score per residue for model 47

- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



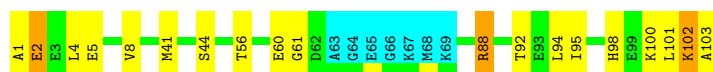
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

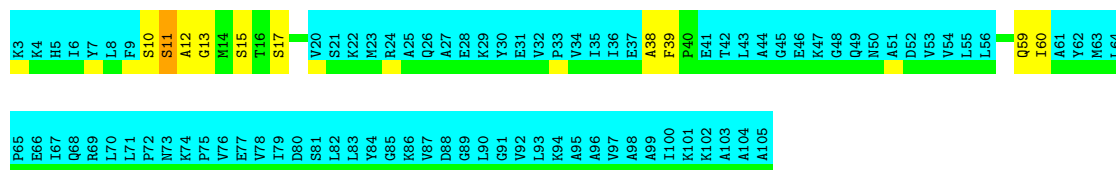


Chain C: 



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

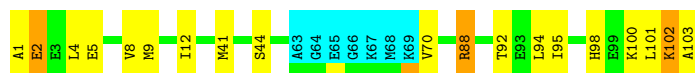
Chain D: 



#### 4.2.48 Score per residue for model 48

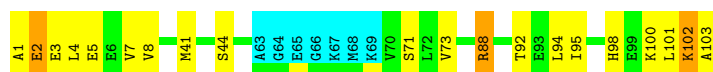
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A: 



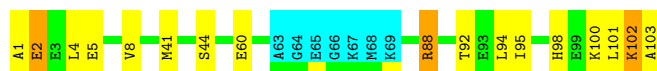
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B: 



- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

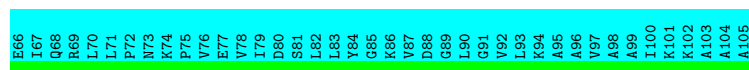
Chain C: 



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

Chain D: 

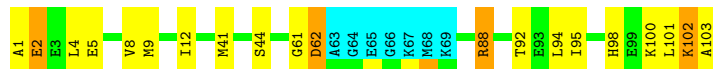




#### 4.2.49 Score per residue for model 49

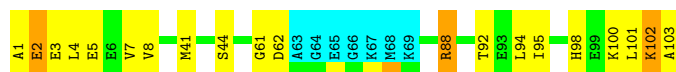
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A: 74% 16% 7%



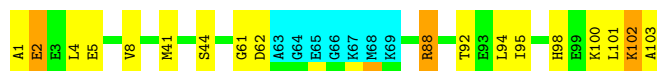
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B: 74% 17% 7%



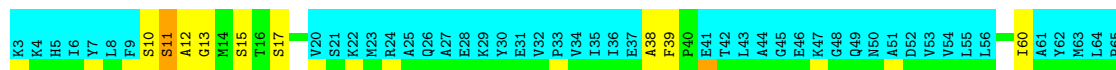
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C: 76% 15% 7%



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

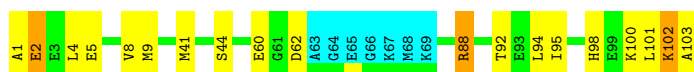
Chain D: 8% 8% 83%



#### 4.2.50 Score per residue for model 50

- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

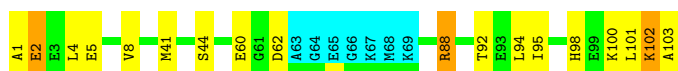
Chain A: 75% 16% 7%



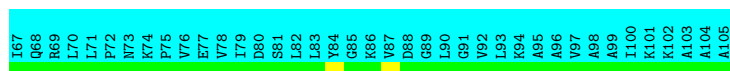
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

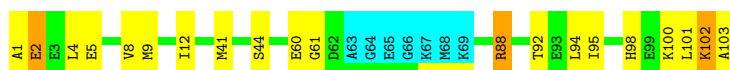


- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT



#### 4.2.51 Score per residue for model 51

- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

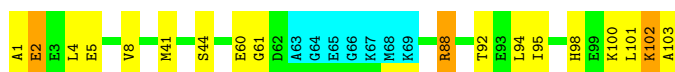


- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



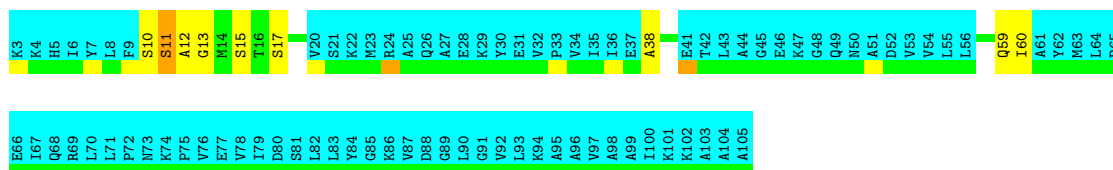
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C:  76% 15% 7%




- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

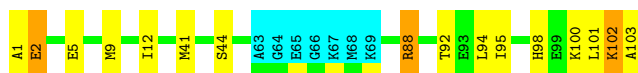
Chain D:  8% 8% 83%



#### 4.2.52 Score per residue for model 52

- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A:  78% 13% 7%



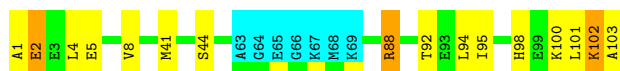
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B:  76% 15% 7%



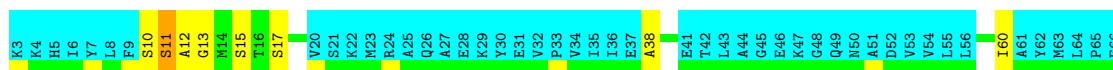
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

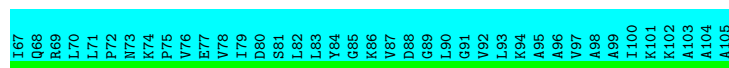
Chain C:  78% 13% 7%



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

Chain D:  9% 7% 83%

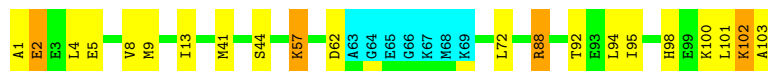




#### 4.2.53 Score per residue for model 53

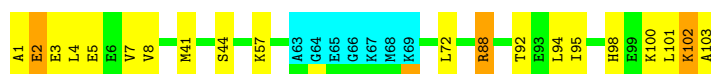
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A: 73% 17% 7%



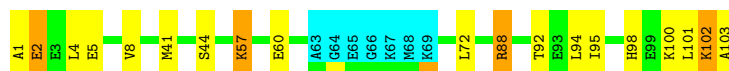
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B: 74% 17% 7%



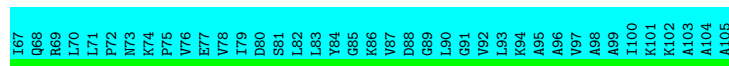
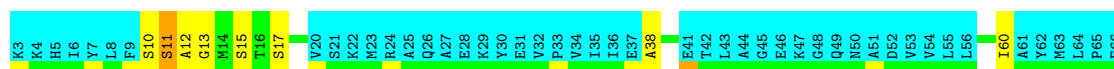
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C: 75% 15% 7%



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

Chain D: 9% 7% 83%



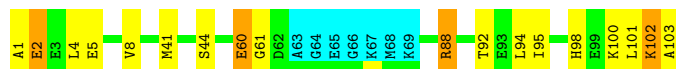
#### 4.2.54 Score per residue for model 54

- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

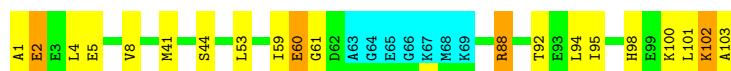
Chain A: 75% 15% 7%



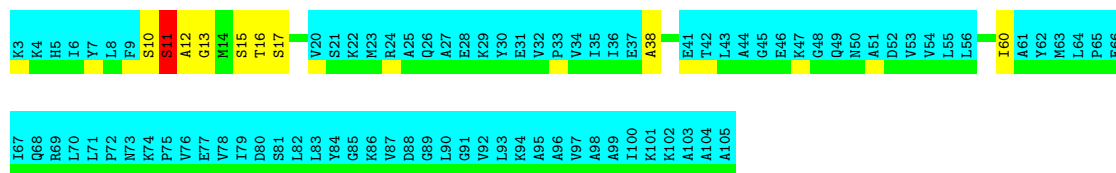
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

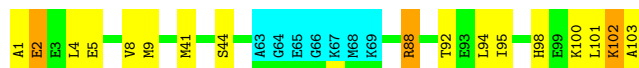


- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

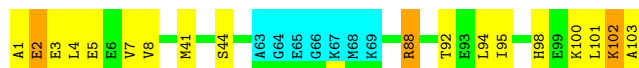


#### 4.2.55 Score per residue for model 55


- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



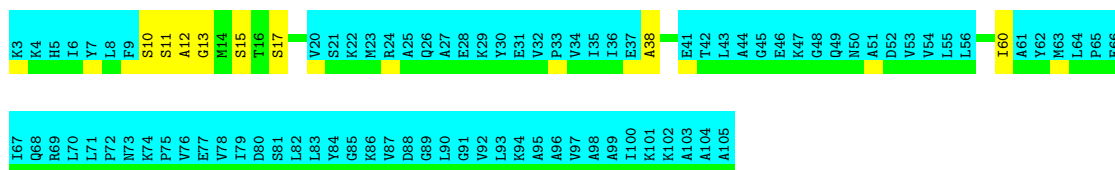
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C:  78% 13% 7%



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

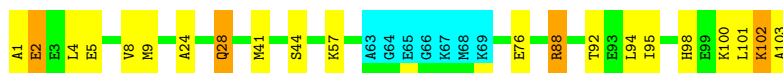
Chain D:  9% 8% 83%



#### 4.2.56 Score per residue for model 56

- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A:  73% 17% 7%



- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B:  73% 17% 7%



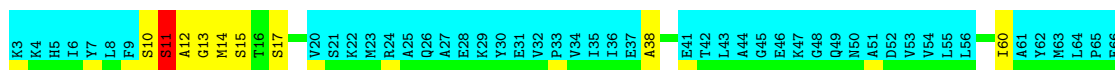
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

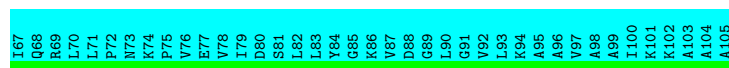
Chain C:  75% 15% 7%



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

Chain D:  8% 8% 83%

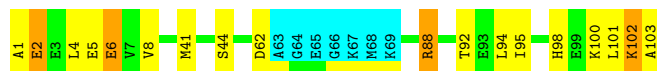




#### 4.2.57 Score per residue for model 57

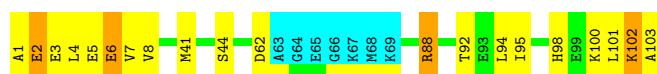
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A: 76% 14% 7%



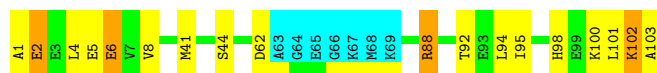
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B: 74% 16% 7%



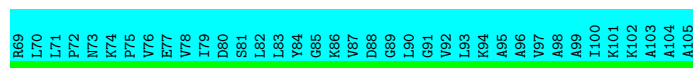
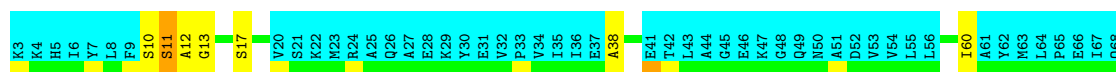
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C: 76% 14% 7%



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

Chain D: 10% 6% 83%

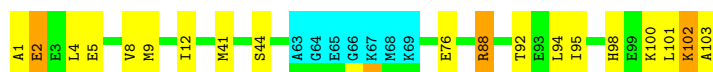


#### 4.2.58 Score per residue for model 58

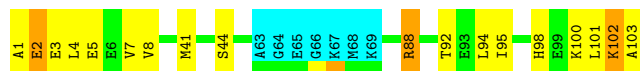
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A: 75% 16% 7%

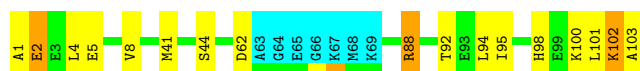
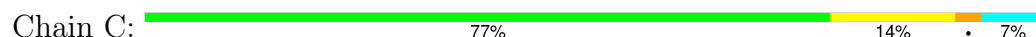




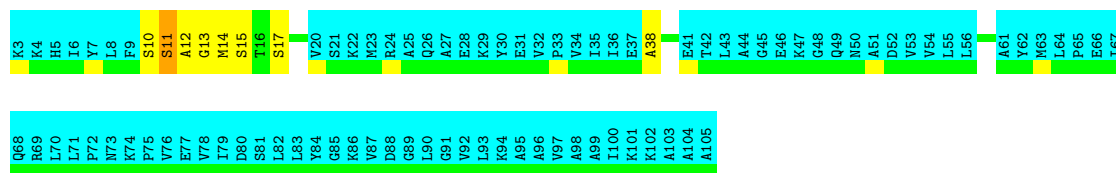
- Molecule 1: N<sub>1</sub>,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



- Molecule 1: N<sub>1</sub>,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

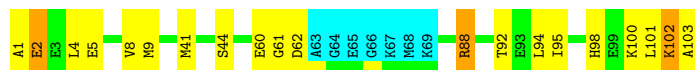


- Molecule 2: N<sub>1</sub>,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

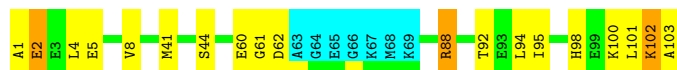


#### 4.2.59 Score per residue for model 59

- Molecule 1: N<sub>1</sub>,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

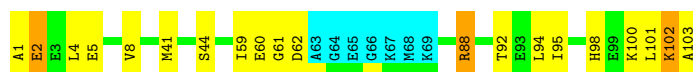


- Molecule 1: N<sub>1</sub>,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



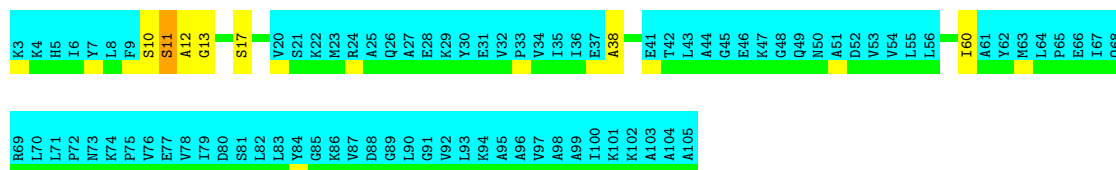
- Molecule 1: N<sub>1</sub>,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C:  74% 17% 7%



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

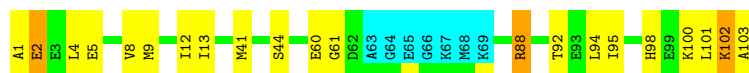
Chain D:  10% 6% 83%



#### 4.2.60 Score per residue for model 60

- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A:  73% 17% 7%



- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B:  74% 17% 7%



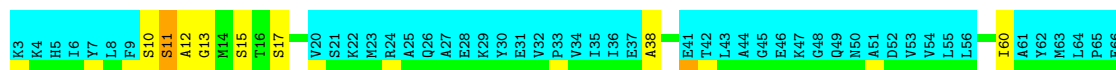
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

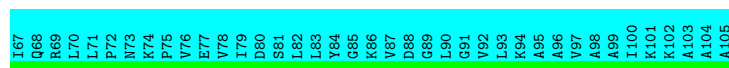
Chain C:  74% 17% 7%



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

Chain D:  9% 7% 83%

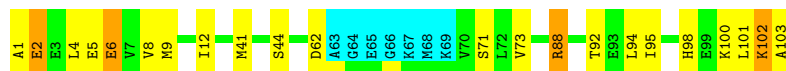




#### 4.2.61 Score per residue for model 61

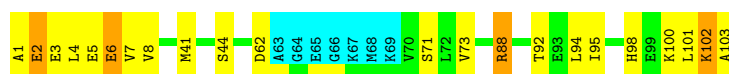
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A: 72% 17% 7%



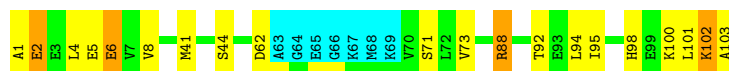
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B: 72% 17% 7%



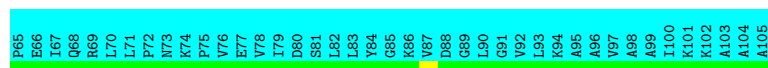
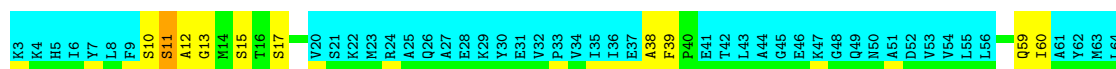
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C: 74% 16% 7%



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

Chain D: 7% 9% 83%



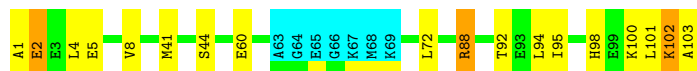
#### 4.2.62 Score per residue for model 62

- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

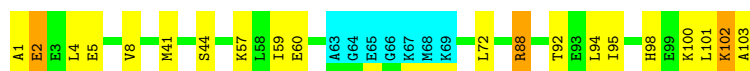
Chain A: 71% 19% 7%



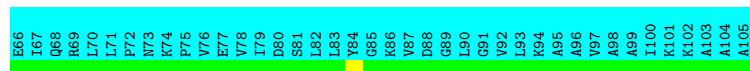
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

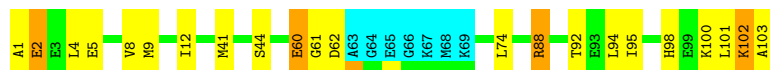


- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

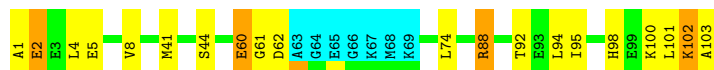


#### 4.2.63 Score per residue for model 63

- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



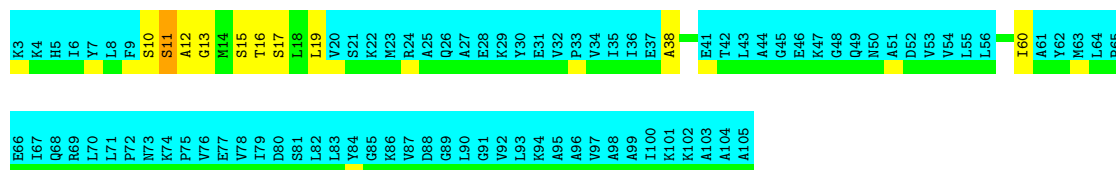
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C: 



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

Chain D: 




#### 4.2.64 Score per residue for model 64

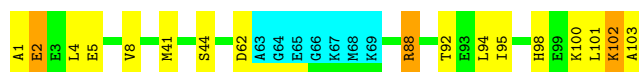
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A: 



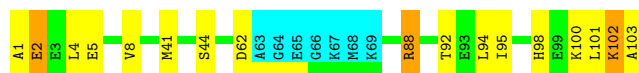
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B: 



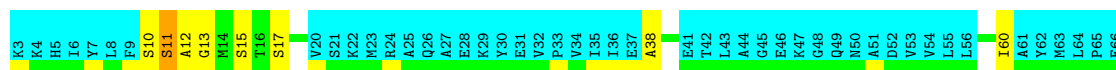
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C: 



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

Chain D: 



I67 Q68 R69 L70 L71 P72 P73 W74 K75 W76 E77 W78 W79 D80 S81 L82 L83 Y84 G85 K86 W87 D88 G89 L90 G91 G92 L93 K94 A95 A96 V97 V98 A99 I100 K101 K102 A103 A104 A105

#### 4.2.65 Score per residue for model 65

- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A:  73% 17% 7%

A1 E2 E3 L4 E5 E6 V7 V8 M9 I12 M41 S44 E60 G61 D62 A63 G64 E65 E66 K67 K68 K69 R88 T92 E93 L94 I95 H98 E99 K100 L101 K102 A103

- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B:  75% 15% 7%

A1 E2 E3 E5 V8 M41 S44 E60 G61 D62 A63 G64 E65 E66 K67 K68 K69 L74 R88 T92 E93 L94 I95 H98 E99 K100 L101 K102 A103

- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C:  76% 14% 7%

A1 E2 E3 E5 V8 M41 S44 E60 G61 D62 A63 G64 E65 E66 K67 K68 K69 R88 T92 E93 L94 I95 H98 E99 K100 L101 K102 A103

- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

Chain D:  8% 8% 83%

K3 K4 H5 I6 Y7 L8 F9 S10 S11 A12 Q13 S17 V20 S21 K22 K23 R24 A25 Q26 A27 E28 E29 Y30 Y31 P32 P33 V34 I35 I36 E37 A38 F39 P40 E41 T42 L43 A44 G45 E46 K47 G48 Q49 N50 A51 D52 V53 V54 L55 L56 Q59 I60 A61 Y62 M63 L64 P65 E66

I67 Q68 R69 L70 L71 P72 P73 W74 K75 W76 E77 W78 W79 D80 S81 L82 L83 Y84 G85 K86 W87 D88 G89 L90 G91 G92 L93 K94 A95 A96 V97 V98 A99 I100 K101 K102 A103 A104 A105

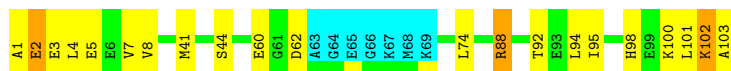
#### 4.2.66 Score per residue for model 66

- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

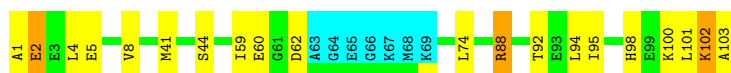
Chain A:  72% 18% 7%



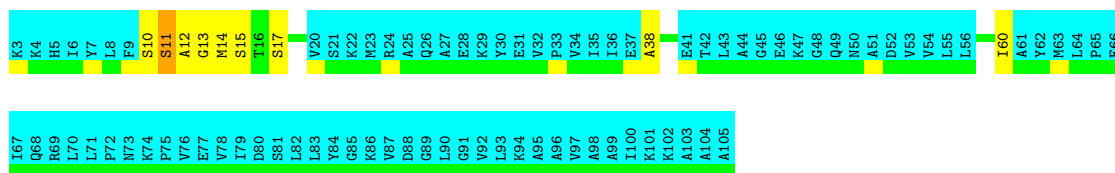
• Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



• Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

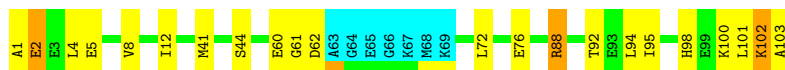


• Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT



#### 4.2.67 Score per residue for model 67

• Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

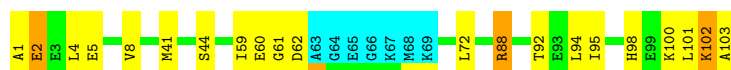


• Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



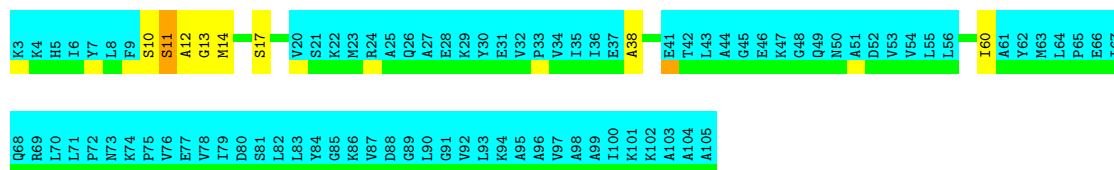
• Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C: 



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

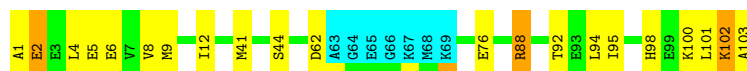
Chain D: 



#### 4.2.68 Score per residue for model 68

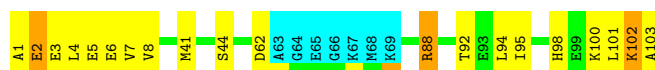
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A: 



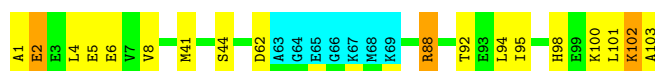
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B: 



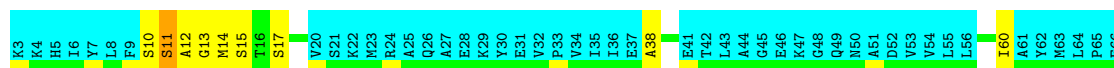
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C: 

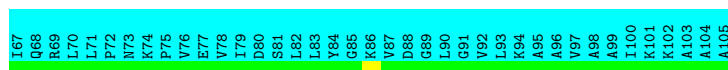


- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

Chain D: 



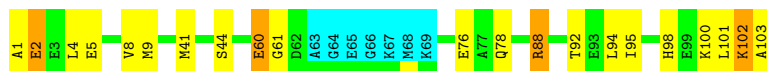




#### 4.2.69 Score per residue for model 69

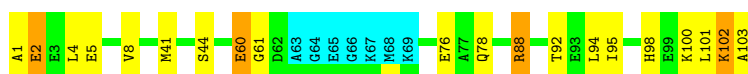
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A: 73% 17% 7%



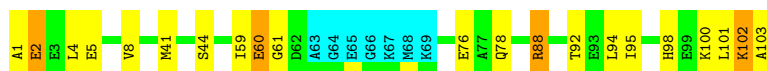
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B: 74% 16% 7%



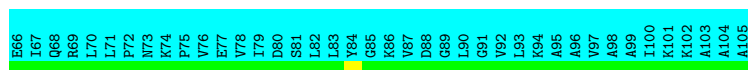
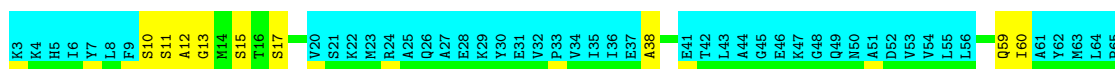
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C: 73% 17% 7%



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

Chain D: 8% 9% 83%



#### 4.2.70 Score per residue for model 70

- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A: 73% 17% 7%



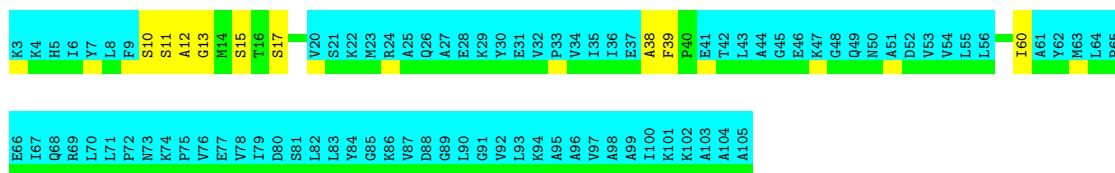
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

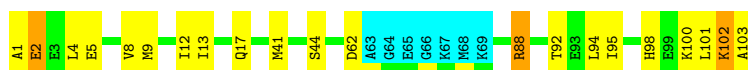


- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

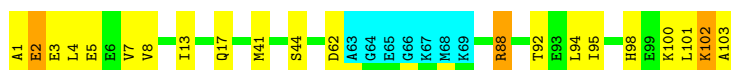


#### 4.2.71 Score per residue for model 71

- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



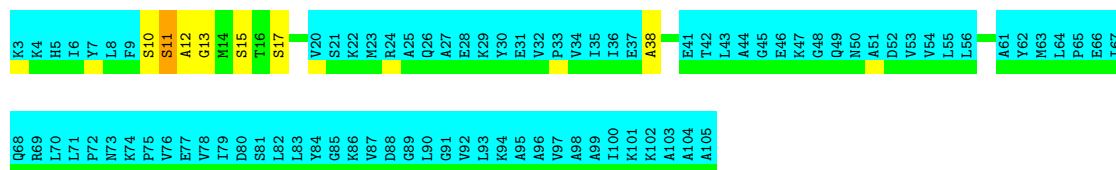
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C: 



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

Chain D: 



#### 4.2.72 Score per residue for model 72

- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A: 



- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B: 



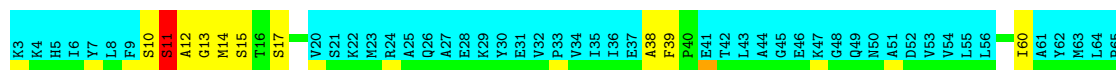
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

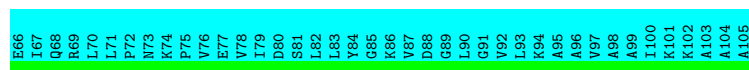
Chain C: 



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

Chain D: 

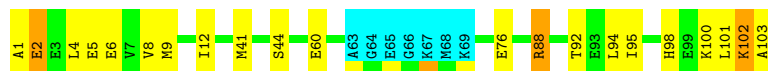




#### 4.2.73 Score per residue for model 73

- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A: 73% 17% 7%



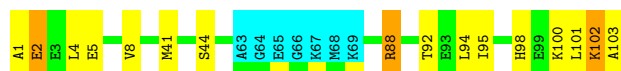
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B: 75% 16% 7%



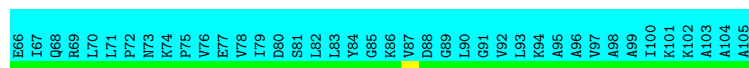
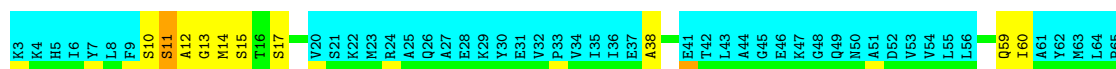
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C: 78% 13% 7%



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

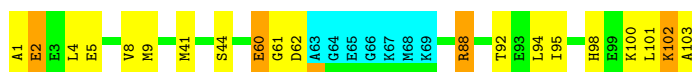
Chain D: 7% 9% 83%



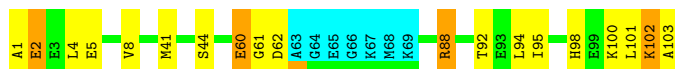
#### 4.2.74 Score per residue for model 74

- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

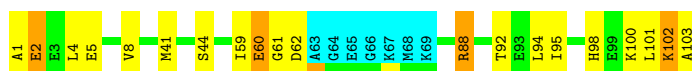
Chain A: 74% 16% 7%



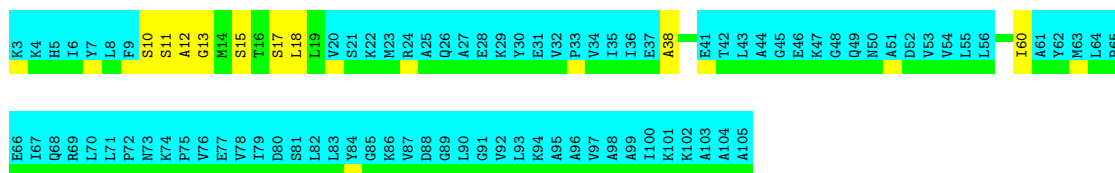
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

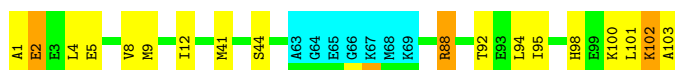


- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

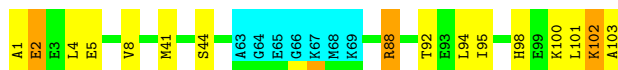


#### 4.2.75 Score per residue for model 75

- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

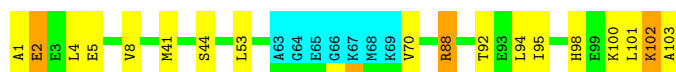


- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



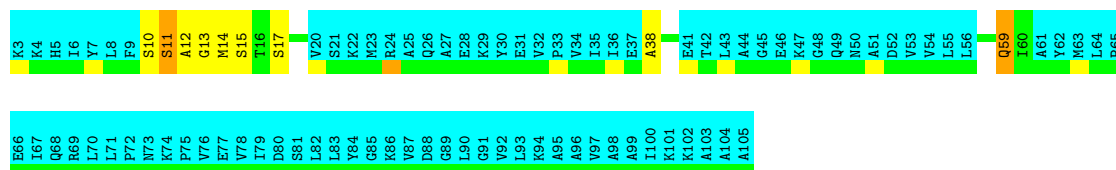
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C:  76% 15% 7%



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

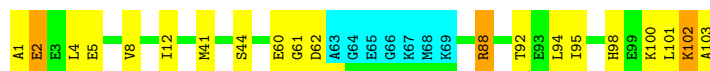
Chain D:  8% 7% 83%



#### 4.2.76 Score per residue for model 76

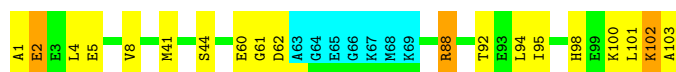
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A:  74% 17% 7%



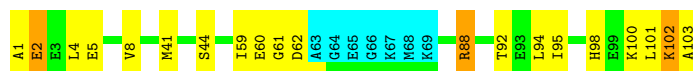
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B:  75% 16% 7%



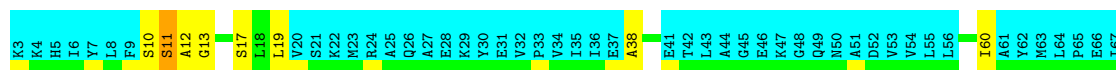
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

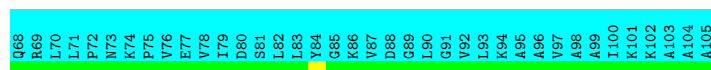
Chain C:  74% 17% 7%



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

Chain D:  9% 7% 83%





#### 4.2.77 Score per residue for model 77

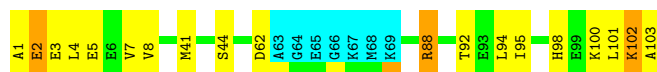
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A: 73% 17% 7%



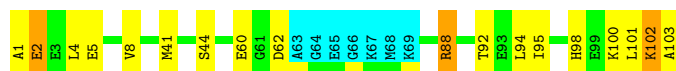
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B: 75% 16% 7%



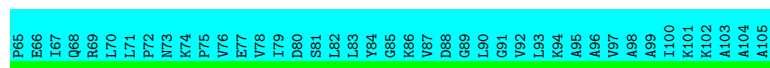
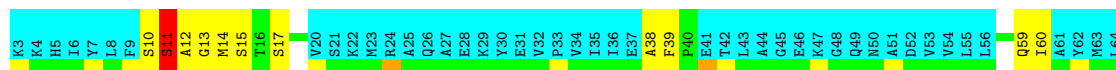
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C: 76% 15% 7%



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

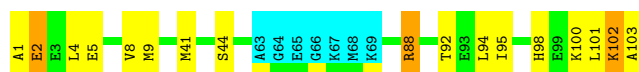
Chain D: 6% 10% 83%



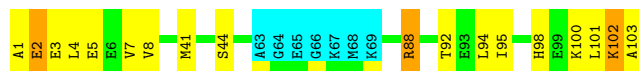
#### 4.2.78 Score per residue for model 78

- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

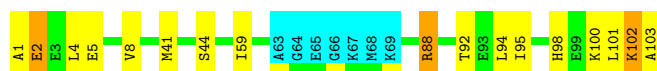
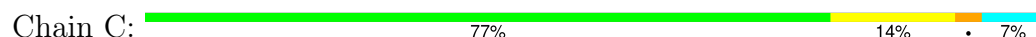
Chain A: 77% 14% 7%



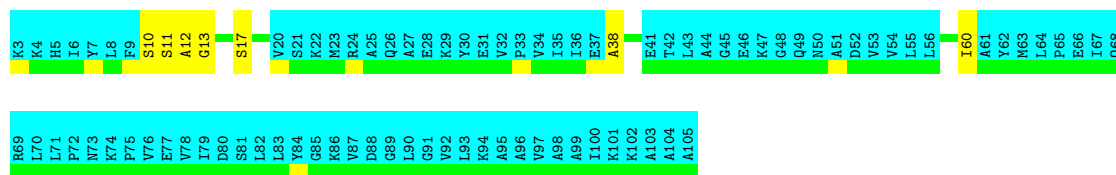
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

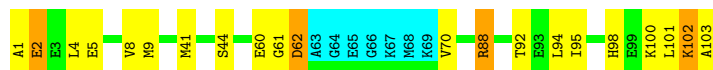


- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

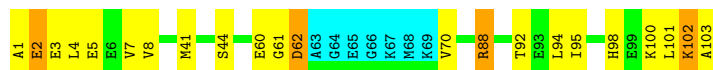


#### 4.2.79 Score per residue for model 79

- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



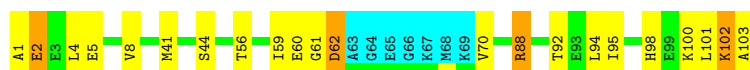
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

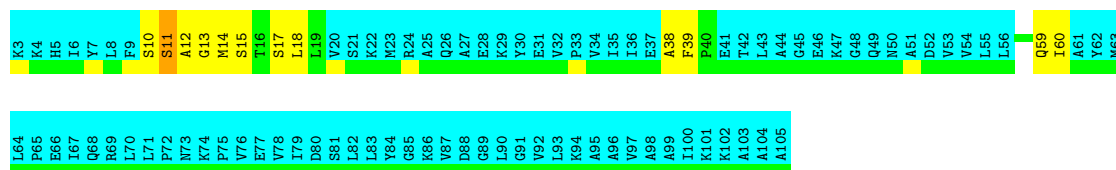


Chain C: 



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

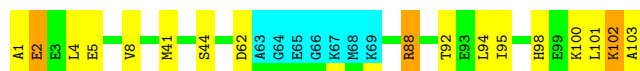
Chain D: 



#### 4.2.80 Score per residue for model 80

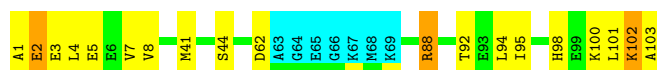
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A: 



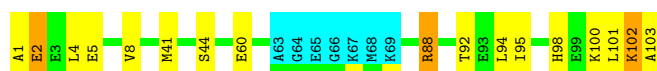
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B: 



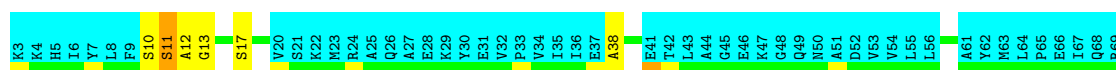
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

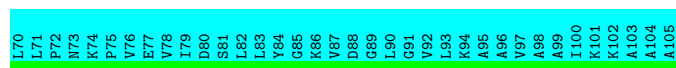
Chain C: 



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

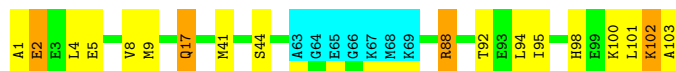
Chain D: 





#### 4.2.81 Score per residue for model 81

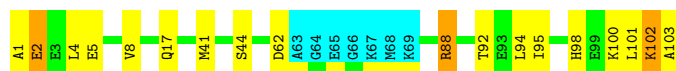
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



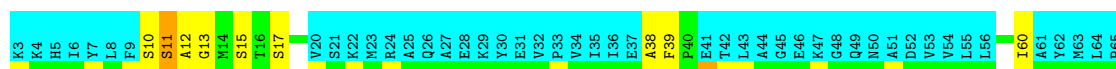
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

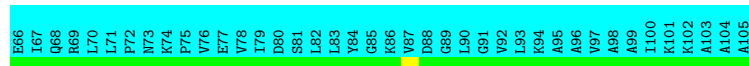


- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT



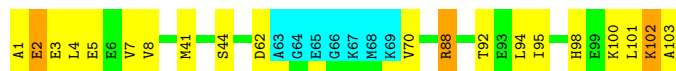
#### 4.2.82 Score per residue for model 82

- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

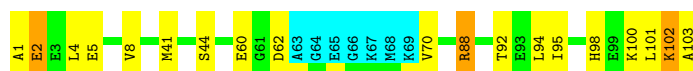




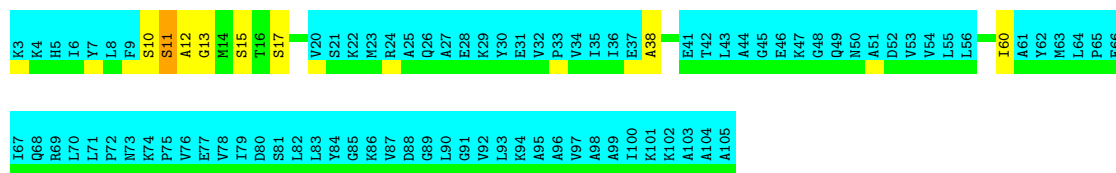
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT



#### 4.2.83 Score per residue for model 83

- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



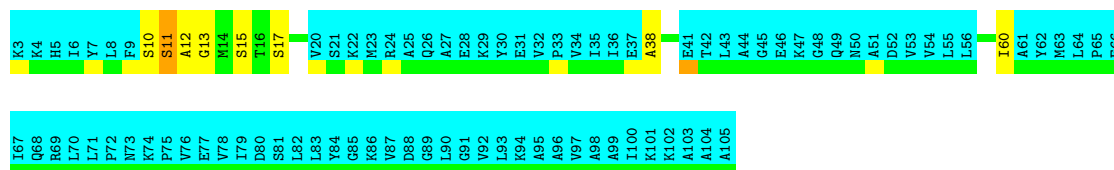
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C: 



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

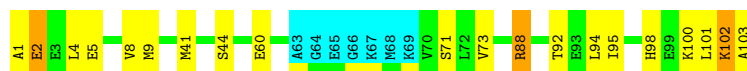
Chain D: 



#### 4.2.84 Score per residue for model 84

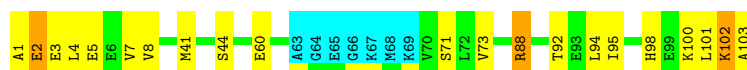
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A: 



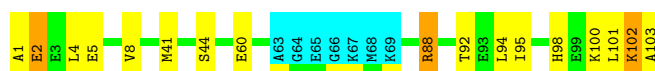
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B: 



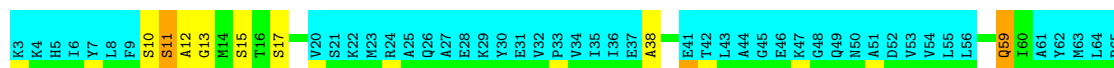
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

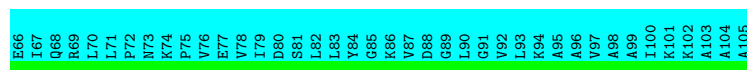
Chain C: 



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

Chain D: 





#### 4.2.85 Score per residue for model 85

- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

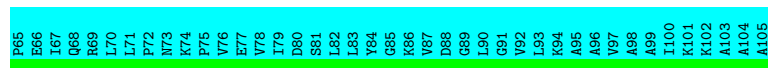


- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT



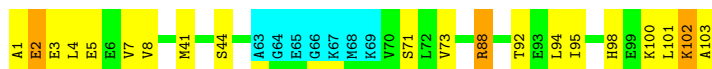
#### 4.2.86 Score per residue for model 86

- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

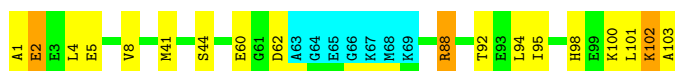




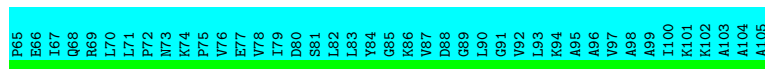
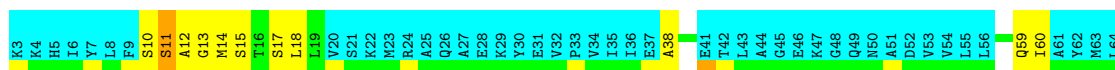
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

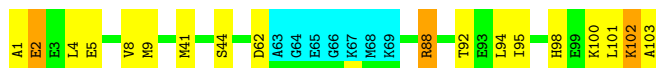


- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

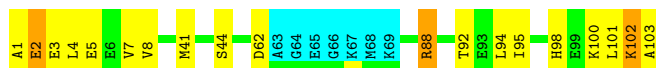


#### 4.2.87 Score per residue for model 87


- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



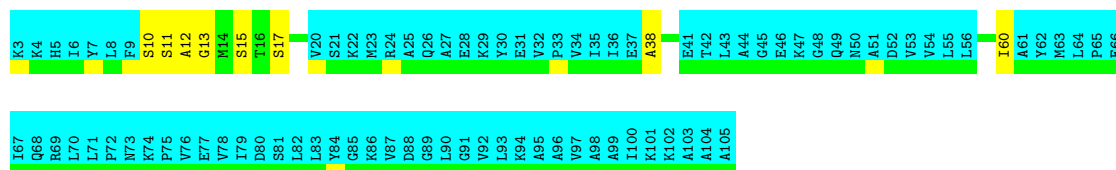
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C:  78% 13% 7%



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

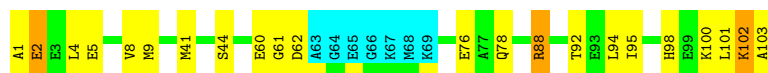
Chain D:  9% 8% 83%



#### 4.2.88 Score per residue for model 88

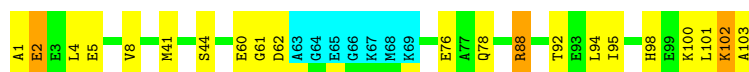
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A:  72% 18% 7%



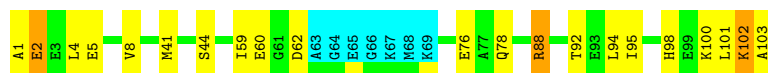
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B:  73% 17% 7%



- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

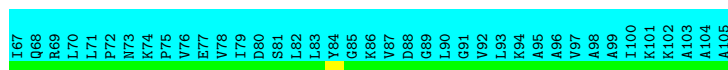
Chain C:  73% 17% 7%



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

Chain D:  9% 7% 83%

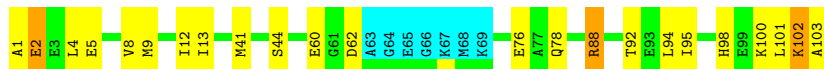




#### 4.2.89 Score per residue for model 89

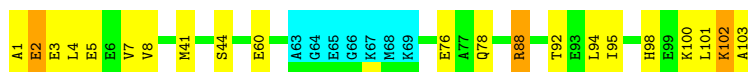
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A: 71% 19% 7%



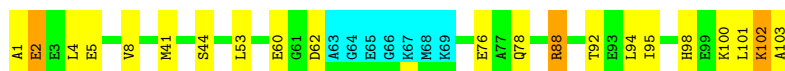
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B: 73% 17% 7%



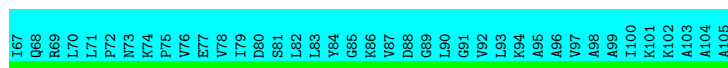
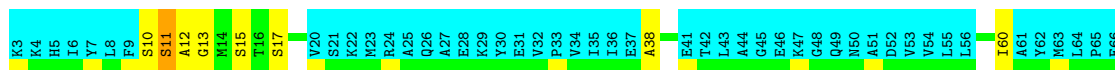
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C: 73% 17% 7%



- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

Chain D: 9% 7% 83%

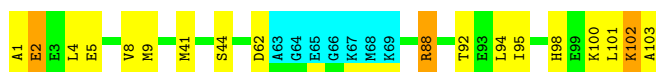


#### 4.2.90 Score per residue for model 90

- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

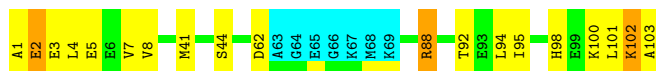
Chain A: 76% 15% 7%





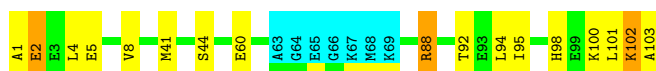
• Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B: 75% 16% 7%



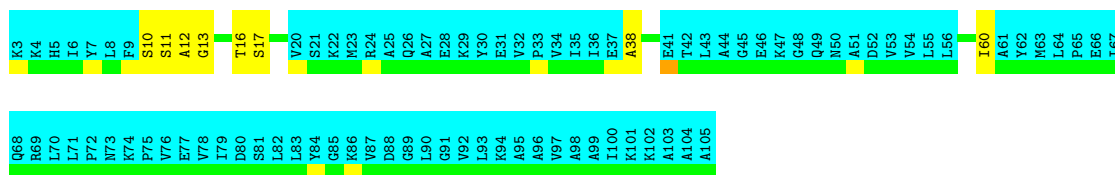
• Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C: 77% 14% 7%



• Molecule 2: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

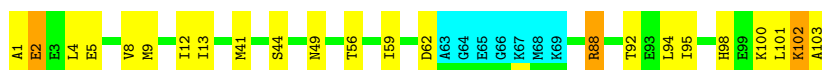
Chain D: 9% 8% 83%



#### 4.2.91 Score per residue for model 91 (medoid)

• Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A: 71% 19% 7%



• Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B: 72% 18% 7%



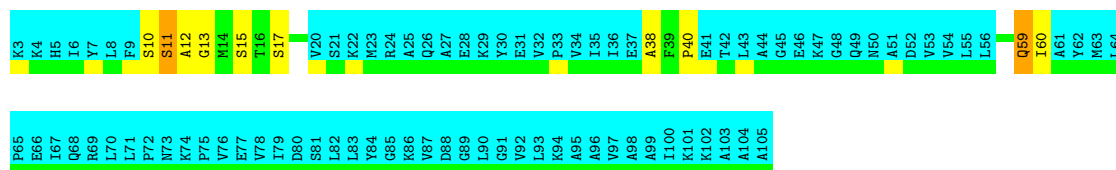
• Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C:  74% 17% 7%



• Molecule 2: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

Chain D:  7% 8% 83%



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *CONJOINED RIGID BODY AND TORSION ANGLE SIMULATED ANNEALING*.

Of the 91 calculated structures, 91 were deposited, based on the following criterion: *RESTRAINED REGULARIZED MEAN*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
Xplor-NIH	refinement	2.23
Xplor-NIH	structure solution	

No chemical shift data was provided.

## 6 Model quality

### 6.1 Standard geometry

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	734	771	768	18±2
1	B	734	771	768	18±2
1	C	734	771	768	17±2
2	D	115	116	116	9±2
All	All	210847	221039	220220	5425

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:17:GLN:N	1:B:17:GLN:OE1	0.72	2.22	81	1
1:A:17:GLN:N	1:A:17:GLN:OE1	0.71	2.22	81	1
1:A:4:LEU:O	1:A:8:VAL:HG23	0.70	1.86	41	90
1:B:4:LEU:O	1:B:8:VAL:HG23	0.69	1.87	24	91
1:B:1:ALA:O	1:B:5:GLU:HB2	0.69	1.88	86	4
1:A:1:ALA:O	1:A:5:GLU:HB2	0.68	1.88	90	4
1:C:4:LEU:O	1:C:8:VAL:HG23	0.68	1.87	16	91
1:C:1:ALA:O	1:C:5:GLU:HB2	0.68	1.89	86	4
1:A:9:MET:SD	2:D:59:GLN:NE2	0.65	2.69	7	2
2:D:59:GLN:N	2:D:59:GLN:OE1	0.65	2.30	91	6
2:D:13:GLY:O	2:D:17:SER:N	0.64	2.30	91	91

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:ILE:HD13	2:D:11:SER:OG	0.64	1.93	34	12
1:A:9:MET:SD	2:D:15:SER:OG	0.62	2.57	46	35
2:D:59:GLN:OE1	2:D:59:GLN:CA	0.61	2.48	91	2
1:A:6:GLU:N	1:A:6:GLU:OE1	0.60	2.34	68	4
1:A:6:GLU:OE2	2:D:59:GLN:NE2	0.60	2.34	65	3
1:A:76:GLU:OE1	2:D:14:MET:SD	0.60	2.60	37	20
1:C:102:LYS:HZ3	1:C:103:ALA:N	0.60	1.94	62	91
1:B:6:GLU:N	1:B:6:GLU:OE1	0.60	2.34	68	4
1:A:102:LYS:HZ3	1:A:103:ALA:N	0.60	1.95	36	91
1:A:17:GLN:OE1	1:A:17:GLN:CA	0.59	2.48	81	1
1:A:6:GLU:CD	2:D:59:GLN:HE22	0.59	2.00	62	1
1:A:9:MET:SD	2:D:15:SER:CB	0.59	2.90	41	76
1:C:59:ILE:O	2:D:17:SER:OG	0.59	2.21	76	19
1:B:17:GLN:OE1	1:B:17:GLN:CA	0.59	2.49	81	1
1:C:60:GLU:OE1	2:D:38:ALA:N	0.59	2.36	70	1
1:A:88:ARG:NH2	1:A:92:THR:OG1	0.58	2.37	5	91
2:D:13:GLY:O	2:D:17:SER:OG	0.58	2.22	45	91
1:C:6:GLU:OE1	1:C:6:GLU:N	0.58	2.36	68	4
1:C:60:GLU:O	1:C:60:GLU:CD	0.58	2.42	40	4
1:A:9:MET:C	2:D:59:GLN:HE22	0.58	2.02	32	1
1:C:24:ALA:O	1:C:28:GLN:OE1	0.58	2.22	43	3
1:C:17:GLN:HA	1:C:17:GLN:OE1	0.57	1.99	81	1
1:B:102:LYS:HZ3	1:B:103:ALA:N	0.57	1.98	65	91
2:D:10:SER:O	2:D:12:ALA:N	0.57	2.38	37	90
2:D:59:GLN:N	2:D:59:GLN:CD	0.56	2.59	20	6
1:A:24:ALA:O	1:A:28:GLN:OE1	0.56	2.24	43	3
2:D:13:GLY:O	2:D:17:SER:CB	0.56	2.54	43	88
1:B:24:ALA:O	1:B:28:GLN:OE1	0.56	2.23	43	3
1:B:6:GLU:OE1	1:B:6:GLU:O	0.55	2.24	83	1
2:D:59:GLN:H	2:D:59:GLN:CD	0.55	2.06	6	8
1:C:62:ASP:OD1	1:C:70:VAL:HG12	0.55	2.02	82	2
1:B:60:GLU:OE2	1:B:61:GLY:N	0.55	2.40	51	4
1:C:88:ARG:NH2	1:C:92:THR:OG1	0.54	2.41	11	91
1:A:6:GLU:O	1:A:6:GLU:CD	0.54	2.46	83	1
1:C:56:THR:HG21	2:D:39:PHE:CD1	0.54	2.38	79	4
1:A:60:GLU:OE2	1:A:61:GLY:N	0.54	2.41	51	4
1:A:6:GLU:OE1	1:A:9:MET:CE	0.53	2.56	70	1
1:C:6:GLU:O	1:C:6:GLU:OE1	0.53	2.26	83	1
1:A:62:ASP:OD1	1:A:70:VAL:HG12	0.53	2.03	82	2
1:A:1:ALA:N	1:A:5:GLU:CG	0.53	2.71	86	4
2:D:10:SER:C	2:D:12:ALA:H	0.53	2.06	91	91

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:2:GLU:O	1:B:6:GLU:OE1	0.53	2.26	68	1
1:A:10:GLY:N	2:D:59:GLN:HE22	0.53	2.02	32	1
1:C:62:ASP:OD2	2:D:14:MET:SD	0.53	2.67	50	2
1:B:1:ALA:N	1:B:5:GLU:CG	0.53	2.72	87	4
1:A:12:ILE:CG2	2:D:11:SER:O	0.53	2.57	64	54
1:C:88:ARG:NH1	1:C:88:ARG:C	0.52	2.63	5	91
1:A:60:GLU:OE1	1:A:61:GLY:N	0.52	2.42	67	2
1:C:1:ALA:N	1:C:5:GLU:CG	0.52	2.72	87	4
1:A:62:ASP:O	1:A:62:ASP:OD2	0.52	2.28	49	7
1:B:62:ASP:OD1	1:B:70:VAL:HG12	0.52	2.04	82	2
1:A:12:ILE:HG21	2:D:11:SER:O	0.52	2.04	91	7
1:A:2:GLU:O	1:A:6:GLU:OE1	0.52	2.27	68	1
1:C:2:GLU:O	1:C:6:GLU:OE1	0.52	2.28	68	1
1:B:62:ASP:O	1:B:62:ASP:OD1	0.52	2.28	76	6
1:B:62:ASP:O	1:B:62:ASP:OD2	0.52	2.28	49	7
1:B:88:ARG:NH2	1:B:92:THR:OG1	0.52	2.44	2	91
1:C:62:ASP:OD2	1:C:62:ASP:O	0.52	2.28	29	7
1:B:62:ASP:OD1	1:B:74:LEU:HD22	0.52	2.05	40	3
1:A:62:ASP:OD1	1:A:62:ASP:O	0.51	2.29	76	6
1:A:6:GLU:O	1:A:6:GLU:OE2	0.51	2.29	83	1
1:A:62:ASP:OD2	1:A:74:LEU:HD22	0.51	2.06	27	2
1:A:62:ASP:OD1	1:A:74:LEU:HD22	0.51	2.06	66	3
1:C:62:ASP:OD1	1:C:74:LEU:HD22	0.51	2.05	66	3
1:B:62:ASP:OD2	1:B:74:LEU:HD22	0.51	2.06	27	3
1:C:62:ASP:O	1:C:62:ASP:OD1	0.51	2.29	4	6
1:A:13:ILE:CD1	2:D:11:SER:OG	0.50	2.59	40	4
1:C:60:GLU:CD	1:C:60:GLU:C	0.50	2.70	54	19
1:C:62:ASP:OD2	1:C:74:LEU:HD22	0.50	2.06	27	2
1:B:60:GLU:HG3	1:B:61:GLY:N	0.50	2.22	69	4
1:B:6:GLU:OE1	1:B:9:MET:CE	0.49	2.59	70	1
1:C:6:GLU:OE1	1:C:9:MET:CE	0.49	2.60	70	1
1:C:13:ILE:HG22	1:C:17:GLN:HE21	0.49	1.66	71	1
1:B:2:GLU:O	1:B:6:GLU:OE2	0.49	2.31	39	2
1:B:57:LYS:HB2	1:B:57:LYS:NZ	0.49	2.21	53	1
1:A:5:GLU:OE2	2:D:15:SER:OG	0.49	2.30	55	6
1:A:13:ILE:HG22	1:A:17:GLN:HE21	0.49	1.67	71	1
1:B:13:ILE:HG22	1:B:17:GLN:HE21	0.49	1.68	71	1
1:C:94:LEU:O	1:C:98:HIS:ND1	0.49	2.46	27	91
1:A:94:LEU:O	1:A:98:HIS:ND1	0.48	2.45	14	91
1:C:88:ARG:C	1:C:88:ARG:HH11	0.48	2.11	35	91
1:C:60:GLU:OE2	1:C:61:GLY:N	0.48	2.45	32	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:60:GLU:O	1:C:60:GLU:OE2	0.48	2.31	84	1
1:B:62:ASP:OD1	1:B:62:ASP:C	0.48	2.52	11	1
1:C:60:GLU:HG3	1:C:61:GLY:N	0.48	2.23	63	4
1:A:28:GLN:OE1	1:A:36:ALA:C	0.48	2.51	85	2
1:A:56:THR:O	1:A:59:ILE:HG22	0.48	2.09	91	1
1:A:61:GLY:O	1:A:62:ASP:C	0.48	2.52	49	4
1:A:60:GLU:CD	1:A:60:GLU:C	0.48	2.72	63	17
1:C:28:GLN:OE1	1:C:36:ALA:C	0.48	2.52	85	2
1:A:5:GLU:O	1:A:5:GLU:OE1	0.48	2.31	40	1
1:B:57:LYS:NZ	1:B:57:LYS:CB	0.48	2.77	56	1
1:C:102:LYS:HZ3	1:C:102:LYS:HB3	0.48	1.69	75	2
1:B:60:GLU:CG	1:B:61:GLY:N	0.48	2.76	59	9
1:A:1:ALA:H2	1:A:5:GLU:CG	0.47	2.22	87	4
1:C:88:ARG:NH1	1:C:88:ARG:O	0.47	2.47	62	91
1:B:60:GLU:CD	1:B:60:GLU:C	0.47	2.72	63	18
1:C:2:GLU:O	1:C:6:GLU:OE2	0.47	2.32	39	1
1:C:56:THR:O	1:C:59:ILE:HG22	0.47	2.09	91	1
1:A:60:GLU:CG	1:A:61:GLY:N	0.47	2.77	60	9
1:A:13:ILE:CD1	2:D:60:ILE:HG23	0.47	2.40	64	1
1:B:61:GLY:O	1:B:62:ASP:C	0.47	2.53	49	3
1:B:28:GLN:OE1	1:B:36:ALA:C	0.47	2.52	72	2
1:C:101:LEU:O	1:C:102:LYS:CB	0.47	2.63	85	91
1:A:2:GLU:O	1:A:6:GLU:OE2	0.47	2.32	39	1
1:B:60:GLU:O	1:B:60:GLU:OE2	0.47	2.32	84	1
1:B:56:THR:O	1:B:59:ILE:HG22	0.47	2.09	91	1
1:B:60:GLU:OE1	1:B:61:GLY:N	0.47	2.48	79	3
1:C:1:ALA:O	1:C:5:GLU:N	0.47	2.40	62	91
1:A:62:ASP:OD1	1:A:62:ASP:C	0.47	2.53	11	1
1:B:60:GLU:O	1:B:60:GLU:CD	0.46	2.53	65	3
1:A:60:GLU:HG3	1:A:61:GLY:N	0.46	2.23	69	4
1:C:60:GLU:OE1	1:C:61:GLY:N	0.46	2.47	67	2
1:A:88:ARG:CZ	1:A:92:THR:OG1	0.46	2.64	8	91
1:A:102:LYS:HZ3	1:A:102:LYS:HB3	0.46	1.69	81	42
1:B:78:GLN:OE1	1:C:76:GLU:OE2	0.46	2.33	38	4
1:A:60:GLU:CD	1:A:60:GLU:O	0.46	2.53	65	3
2:D:59:GLN:OE1	2:D:59:GLN:HA	0.46	2.08	91	1
1:C:60:GLU:CG	1:C:61:GLY:N	0.46	2.78	54	9
1:B:1:ALA:N	1:B:5:GLU:HG2	0.46	2.26	90	4
1:A:102:LYS:HZ3	1:A:102:LYS:CB	0.46	2.24	17	42
1:B:60:GLU:OE2	1:B:60:GLU:C	0.46	2.54	47	3
1:C:62:ASP:OD1	1:C:62:ASP:C	0.46	2.53	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:94:LEU:O	1:B:98:HIS:ND1	0.46	2.46	45	91
1:C:59:ILE:O	2:D:17:SER:CB	0.46	2.64	63	19
1:A:76:GLU:OE2	1:C:78:GLN:OE1	0.46	2.34	10	4
1:B:88:ARG:NH1	1:B:88:ARG:C	0.46	2.70	8	90
1:C:102:LYS:HZ3	1:C:102:LYS:CB	0.46	2.23	75	2
2:D:59:GLN:CD	2:D:59:GLN:H	0.46	2.14	85	1
1:B:88:ARG:C	1:B:88:ARG:HH11	0.45	2.14	14	91
1:B:78:GLN:OE1	1:C:76:GLU:OE1	0.45	2.34	27	6
1:B:88:ARG:C	1:B:88:ARG:NH1	0.45	2.70	14	1
1:A:78:GLN:NE2	1:B:76:GLU:OE2	0.45	2.48	39	1
1:C:1:ALA:N	1:C:5:GLU:HG2	0.45	2.26	87	4
1:A:101:LEU:O	1:A:102:LYS:CB	0.45	2.64	76	91
1:C:60:GLU:C	1:C:60:GLU:OE2	0.45	2.55	20	4
1:C:57:LYS:CB	1:C:57:LYS:NZ	0.45	2.79	56	1
1:A:6:GLU:OE2	2:D:59:GLN:OE1	0.45	2.33	62	1
1:A:78:GLN:OE1	1:B:76:GLU:OE2	0.45	2.33	10	4
1:C:60:GLU:OE1	1:C:60:GLU:C	0.45	2.55	79	3
1:A:2:GLU:O	1:A:6:GLU:CD	0.45	2.55	57	3
1:A:102:LYS:HZ3	1:A:102:LYS:C	0.45	2.15	74	91
1:A:1:ALA:N	1:A:5:GLU:HG2	0.45	2.26	86	4
1:C:61:GLY:O	1:C:62:ASP:C	0.45	2.54	49	2
1:A:1:ALA:O	1:A:5:GLU:CB	0.45	2.65	10	88
2:D:10:SER:OG	2:D:16:THR:OG1	0.45	2.31	90	10
1:B:1:ALA:O	1:B:5:GLU:CB	0.45	2.65	43	91
1:A:60:GLU:OE1	1:A:60:GLU:C	0.45	2.55	67	2
1:A:57:LYS:CB	1:A:57:LYS:NZ	0.45	2.79	56	1
1:B:2:GLU:O	1:B:6:GLU:CD	0.45	2.55	57	3
1:C:62:ASP:OD2	1:C:70:VAL:HG12	0.45	2.12	79	1
1:C:1:ALA:O	1:C:5:GLU:CB	0.45	2.65	10	91
1:A:60:GLU:OE2	1:A:60:GLU:C	0.45	2.55	51	3
1:B:60:GLU:C	1:B:60:GLU:OE1	0.45	2.55	26	1
1:C:2:GLU:O	1:C:6:GLU:CD	0.44	2.55	57	3
1:C:62:ASP:OD2	1:C:62:ASP:N	0.44	2.50	86	6
1:A:5:GLU:OE1	2:D:15:SER:OG	0.44	2.31	47	3
1:C:70:VAL:HG11	2:D:14:MET:SD	0.44	2.53	75	2
1:B:78:GLN:HE22	1:C:76:GLU:CD	0.44	2.14	88	1
1:B:1:ALA:O	1:B:5:GLU:N	0.44	2.39	54	91
1:C:102:LYS:HZ3	1:C:102:LYS:C	0.44	2.16	64	91
1:A:78:GLN:OE1	1:B:76:GLU:OE1	0.44	2.36	36	6
1:B:101:LEU:O	1:B:102:LYS:CB	0.44	2.65	10	91
1:A:57:LYS:NZ	1:A:57:LYS:HB2	0.44	2.28	53	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:41:MET:SD	1:B:95:ILE:HD12	0.44	2.53	26	91
1:A:1:ALA:H2	1:A:5:GLU:HG2	0.44	1.72	86	4
1:B:1:ALA:O	1:B:2:GLU:C	0.44	2.56	60	91
1:A:60:GLU:O	1:A:60:GLU:OE2	0.44	2.35	84	1
1:A:1:ALA:O	1:A:5:GLU:N	0.44	2.41	75	91
1:C:100:LYS:C	1:C:102:LYS:H	0.44	2.17	4	91
1:C:1:ALA:H2	1:C:5:GLU:CG	0.44	2.25	86	4
1:C:49:ASN:OD1	1:C:49:ASN:C	0.43	2.57	91	1
1:C:62:ASP:CG	1:C:70:VAL:HG12	0.43	2.33	18	2
1:A:76:GLU:CD	1:C:78:GLN:HE22	0.43	2.16	88	1
1:A:41:MET:SD	1:A:95:ILE:HD12	0.43	2.54	62	91
1:A:61:GLY:O	1:A:62:ASP:O	0.43	2.36	79	1
1:C:1:ALA:O	1:C:2:GLU:C	0.43	2.56	76	91
1:A:62:ASP:OD2	1:A:62:ASP:N	0.43	2.51	32	5
1:C:41:MET:SD	1:C:95:ILE:HD12	0.43	2.54	76	91
1:A:76:GLU:OE1	1:C:78:GLN:OE1	0.43	2.36	27	6
1:C:62:ASP:N	1:C:62:ASP:OD1	0.43	2.51	39	4
1:A:60:GLU:C	1:A:60:GLU:OE2	0.43	2.57	63	1
1:C:13:ILE:HG22	1:C:17:GLN:NE2	0.43	2.29	71	1
1:B:60:GLU:OE1	1:B:60:GLU:C	0.43	2.57	79	1
1:B:100:LYS:C	1:B:102:LYS:H	0.43	2.16	24	91
1:C:1:ALA:H2	1:C:5:GLU:HG2	0.43	1.73	87	4
1:A:102:LYS:O	1:A:103:ALA:OXT	0.43	2.37	81	91
1:B:5:GLU:OE1	1:B:9:MET:SD	0.43	2.77	40	1
1:A:78:GLN:HE22	1:B:76:GLU:CD	0.43	2.17	88	1
1:A:9:MET:SD	2:D:15:SER:HB3	0.43	2.54	71	2
1:A:1:ALA:O	1:A:2:GLU:C	0.42	2.56	14	91
1:B:102:LYS:HZ3	1:B:102:LYS:C	0.42	2.18	62	91
2:D:10:SER:C	2:D:12:ALA:N	0.42	2.71	91	49
1:B:60:GLU:HG2	1:B:61:GLY:N	0.42	2.29	59	5
1:C:62:ASP:OD1	1:C:74:LEU:CD2	0.42	2.67	40	1
1:A:100:LYS:C	1:A:102:LYS:H	0.42	2.16	76	91
1:A:76:GLU:OE2	1:C:78:GLN:NE2	0.42	2.48	39	1
1:C:71:SER:OG	1:C:73:VAL:HG22	0.42	2.14	61	3
1:B:62:ASP:OD1	1:B:74:LEU:CD2	0.42	2.67	40	1
1:B:62:ASP:CG	1:B:70:VAL:HG12	0.42	2.35	4	2
1:C:60:GLU:OE2	1:C:60:GLU:C	0.42	2.58	51	2
1:C:62:ASP:N	1:C:62:ASP:OD2	0.42	2.52	64	2
1:B:102:LYS:HZ3	1:B:102:LYS:HB3	0.42	1.74	41	48
1:C:5:GLU:OE1	1:C:9:MET:SD	0.42	2.77	40	1
1:B:1:ALA:H2	1:B:5:GLU:HG2	0.42	1.75	90	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:3:GLU:O	1:B:7:VAL:N	0.42	2.40	81	73
1:B:62:ASP:N	1:B:62:ASP:OD2	0.42	2.53	32	2
1:C:57:LYS:HB2	1:C:57:LYS:NZ	0.42	2.29	53	1
1:A:62:ASP:OD2	1:A:70:VAL:HG12	0.42	2.15	79	1
1:B:1:ALA:H2	1:B:5:GLU:CG	0.42	2.27	88	3
1:A:49:ASN:OD1	1:A:49:ASN:C	0.42	2.57	91	1
1:C:102:LYS:O	1:C:103:ALA:OXT	0.42	2.38	7	91
1:A:9:MET:CE	2:D:59:GLN:NE2	0.42	2.82	7	1
1:C:60:GLU:HG2	1:C:61:GLY:N	0.42	2.29	59	5
1:A:62:ASP:N	1:A:62:ASP:OD1	0.42	2.53	89	5
1:A:62:ASP:OD1	1:A:74:LEU:CD2	0.42	2.68	40	1
1:B:13:ILE:HG22	1:B:17:GLN:NE2	0.42	2.30	71	1
1:B:49:ASN:OD1	1:B:49:ASN:C	0.42	2.57	91	1
1:B:71:SER:OG	1:B:73:VAL:HG22	0.42	2.14	84	8
1:A:62:ASP:CG	1:A:70:VAL:HG12	0.42	2.35	4	2
1:A:9:MET:SD	2:D:15:SER:HB2	0.42	2.54	75	2
1:B:28:GLN:NE2	1:B:28:GLN:CA	0.42	2.83	56	3
1:A:13:ILE:HG22	1:A:17:GLN:NE2	0.42	2.30	71	1
1:A:62:ASP:OD1	1:A:62:ASP:N	0.41	2.52	39	1
1:C:60:GLU:OE2	1:C:60:GLU:O	0.41	2.38	63	1
1:B:62:ASP:N	1:B:62:ASP:OD1	0.41	2.54	91	2
1:A:71:SER:OG	1:A:73:VAL:HG22	0.41	2.16	61	6
1:C:60:GLU:C	1:C:60:GLU:CD	0.41	2.79	32	1
1:B:60:GLU:C	1:B:60:GLU:OE2	0.41	2.59	69	2
1:A:6:GLU:CD	1:A:6:GLU:C	0.41	2.79	83	1
1:C:60:GLU:OE2	1:C:60:GLU:CA	0.41	2.69	70	1
1:B:88:ARG:NH1	1:B:88:ARG:O	0.41	2.54	2	91
1:B:88:ARG:HH11	1:B:88:ARG:CG	0.41	2.29	24	91
1:B:62:ASP:OD2	1:B:70:VAL:HG12	0.41	2.16	79	1
2:D:39:PHE:CD2	2:D:39:PHE:N	0.41	2.89	26	1
1:A:5:GLU:CG	2:D:15:SER:OG	0.41	2.69	42	1
1:B:62:ASP:OD1	1:B:62:ASP:N	0.41	2.53	50	1
1:C:62:ASP:C	1:C:62:ASP:OD2	0.41	2.59	81	1
1:A:6:GLU:OE1	2:D:59:GLN:NE2	0.41	2.54	1	1
1:B:62:ASP:C	1:B:62:ASP:OD2	0.41	2.59	66	1
1:A:12:ILE:HD13	1:A:80:HIS:CG	0.40	2.51	64	3
1:C:28:GLN:NE2	1:C:28:GLN:CA	0.40	2.83	56	2
1:B:60:GLU:C	1:B:60:GLU:CD	0.40	2.80	14	1
1:A:10:GLY:CA	2:D:59:GLN:HE21	0.40	2.29	17	1
1:C:8:VAL:HG21	1:C:73:VAL:HB	0.40	1.93	19	2
1:B:102:LYS:HZ3	1:B:102:LYS:CB	0.40	2.29	64	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:5:GLU:OE1	1:B:5:GLU:O	0.40	2.39	40	1
1:A:28:GLN:NE2	1:A:28:GLN:CA	0.40	2.83	56	1
1:B:61:GLY:O	1:B:62:ASP:O	0.40	2.38	79	1
1:B:1:ALA:H1	1:B:5:GLU:HG3	0.40	1.75	86	1
1:B:100:LYS:C	1:B:102:LYS:N	0.40	2.75	4	4
1:B:102:LYS:O	1:B:103:ALA:OXT	0.40	2.39	62	1
1:B:62:ASP:OD2	1:B:62:ASP:C	0.40	2.58	81	1
1:C:88:ARG:HH11	1:C:88:ARG:CG	0.40	2.30	87	1

## 6.3 Torsion angles

### 6.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	94/103 (91%)	90±0 (96±1%)	2±0 (3±1%)	1±0 (1±0%)	17	64
1	B	94/103 (91%)	91±0 (96±1%)	2±0 (3±1%)	1±0 (1±0%)	17	64
1	C	94/103 (91%)	91±0 (96±1%)	2±0 (2±0%)	1±0 (1±0%)	18	66
2	D	17/103 (17%)	14±0 (82±1%)	2±0 (12±1%)	1±0 (6±0%)	3	21
All	All	27209/37492 (73%)	25991 (96%)	824 (3%)	394 (1%)	15	61

All 7 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	2	GLU	91
1	B	2	GLU	91
1	C	2	GLU	91
2	D	11	SER	91
1	A	62	ASP	13
1	B	62	ASP	11
1	C	62	ASP	6

### 6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	77/81 (95%)	74±0 (96±0%)	3±0 (4±0%)	34	82
1	B	77/81 (95%)	74±0 (96±0%)	3±0 (4±0%)	34	82
1	C	77/81 (95%)	74±0 (96±0%)	3±0 (4±0%)	34	82
2	D	13/82 (16%)	13±1 (96±4%)	0±1 (4±4%)	38	86
All	All	22204/29575 (75%)	21307 (96%)	897 (4%)	35	83

All 24 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	44	SER	91
1	A	88	ARG	91
1	A	102	LYS	91
1	B	44	SER	91
1	B	88	ARG	91
1	B	102	LYS	91
1	C	44	SER	91
1	C	88	ARG	91
1	C	102	LYS	91
2	D	11	SER	33
2	D	59	GLN	9
1	A	60	GLU	4
1	B	60	GLU	4
1	C	60	GLU	4
1	A	6	GLU	4
1	A	28	GLN	3
1	B	28	GLN	3
1	C	28	GLN	3
1	B	6	GLU	3
1	C	6	GLU	3
1	C	57	LYS	2
1	A	57	LYS	1
1	A	17	GLN	1
1	B	17	GLN	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 6.7 Other polymers [i](#)

There are no such molecules in this entry.

### 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided