



Full wwPDB NMR Structure Validation Report ⓘ

May 29, 2020 – 05:29 am BST

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

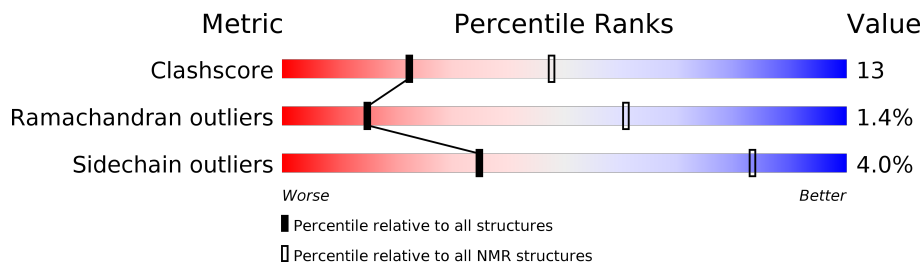
1 Overall quality at a glance

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 ≥ 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	75% 16% • 7%
1	B	103	75% 16% • 7%
1	C	103	76% 15% • 7%
2	D	103	9% 7% • 83%

2 Ensemble composition and analysis i

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)	0.06	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 6 clusters and 2 single-model clusters were found.

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

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 PHOSPHO-TRANSFERASE ENZYME IIA COMPONENT.

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

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 PHOSPHO-TRANSFERASE ENZYME IIB COMPONENT.

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

There is a discrepancy between the modelled and reference sequences:

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

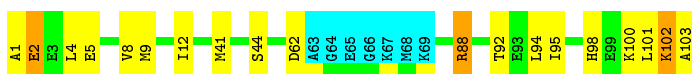
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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.

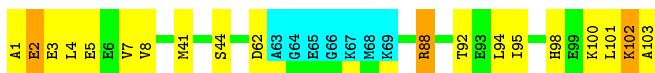
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A: 



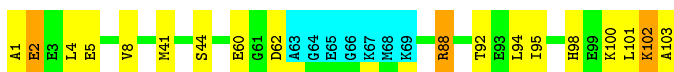
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B: 



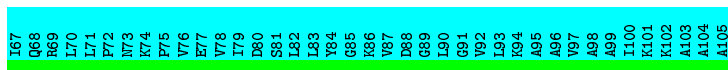
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C: 



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

Chain D: 



4.2 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

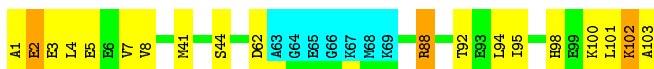
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A:  73% 17% 7%



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

Chain B:  75% 16% 7%



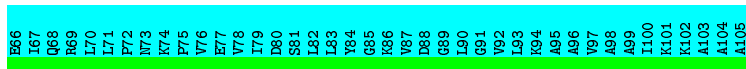
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C:  77% 14% 7%



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

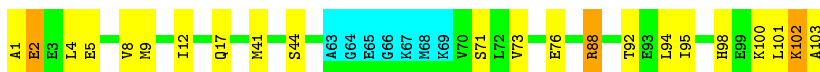
Chain D:  8% 8% 83%



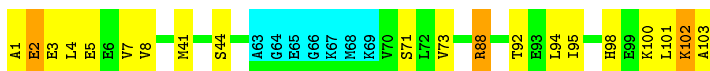
4.2.2 Score per residue for model 2

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

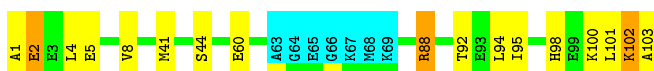
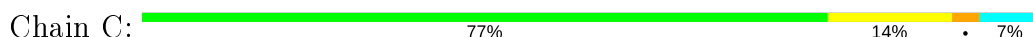
Chain A:  72% 18% 7%



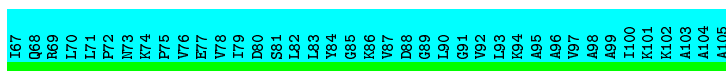
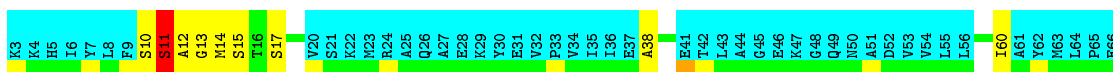
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



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

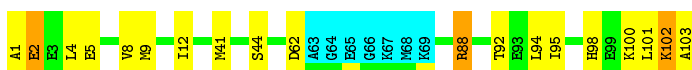


- Molecule 2: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

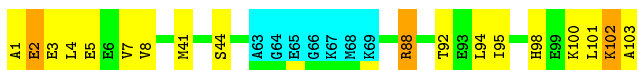


4.2.3 Score per residue for model 3

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

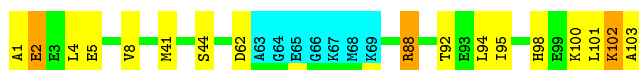


- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



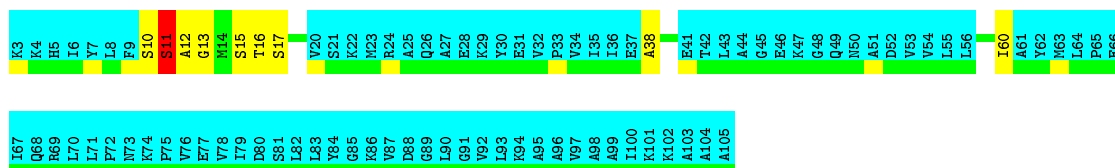
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C:  77% 14% 7%



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

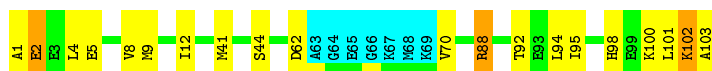
Chain D:  8% 8% 83%



4.2.4 Score per residue for model 4

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

Chain A:  74% 17% 7%



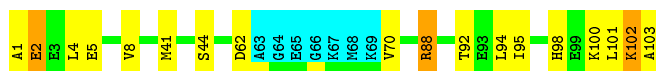
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B:  74% 17% 7%



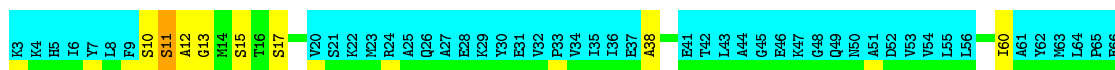
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

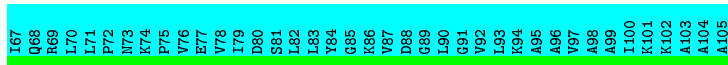
Chain C:  76% 15% 7%



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

Chain D:  9% 7% 83%



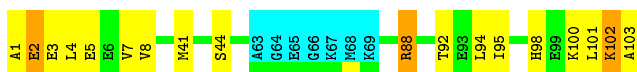


4.2.5 Score per residue for model 5

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



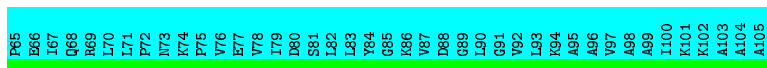
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



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



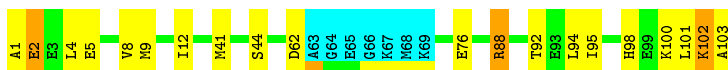
- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT



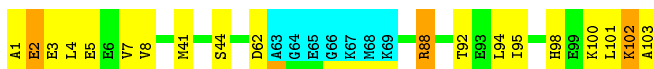
4.2.6 Score per residue for model 6

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

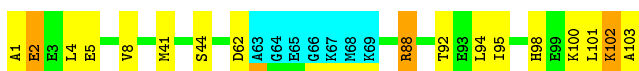
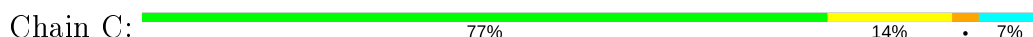




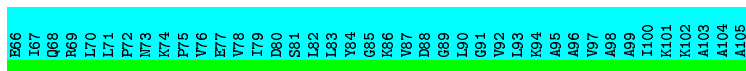
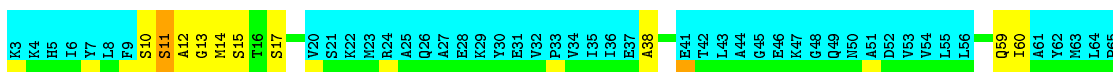
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



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

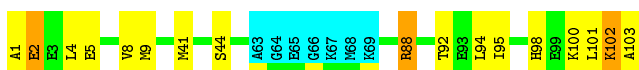


- Molecule 2: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

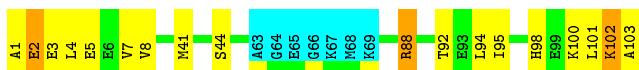


4.2.7 Score per residue for model 7


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



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



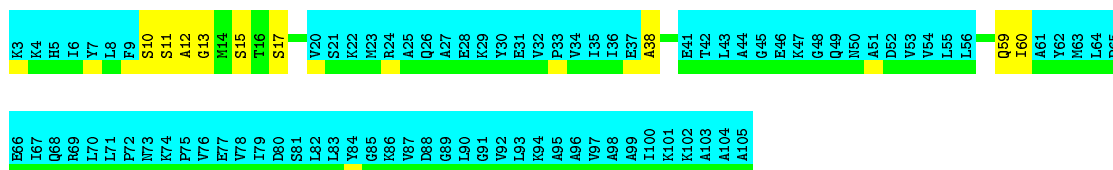
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C: 



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

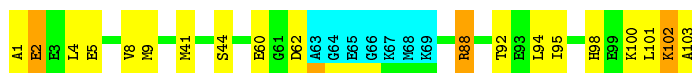
Chain D: 



4.2.8 Score per residue for model 8

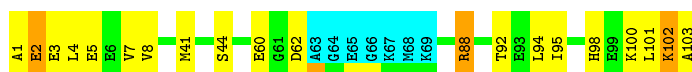
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A: 



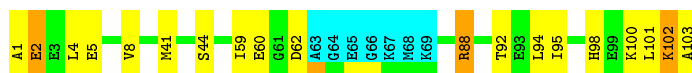
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B: 



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

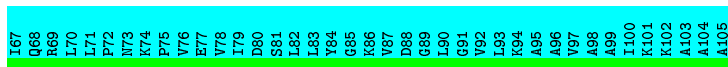
Chain C: 



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

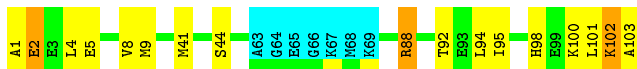
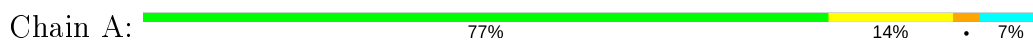
Chain D: 



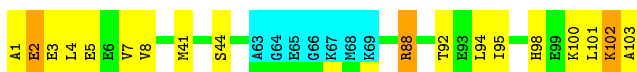


4.2.9 Score per residue for model 9

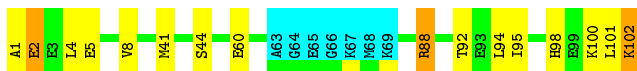
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



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



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



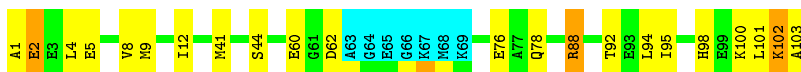
- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT



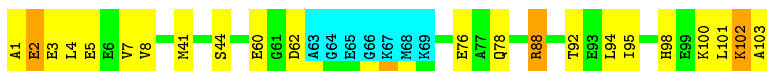
4.2.10 Score per residue for model 10

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

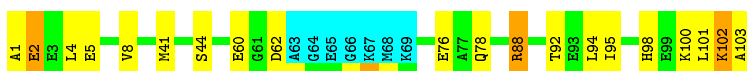




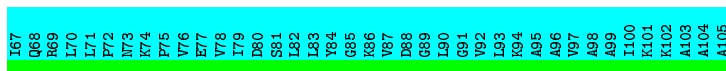
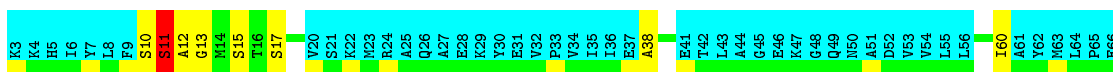
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



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



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

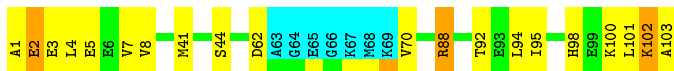


4.2.11 Score per residue for model 11

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



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



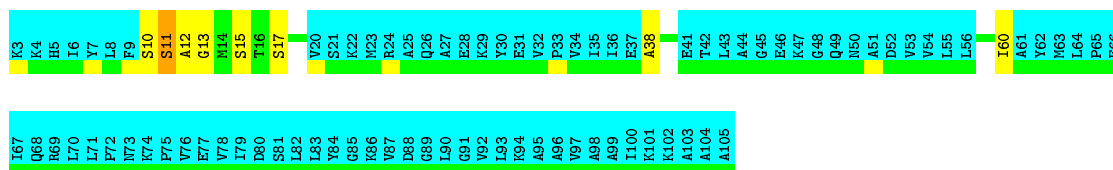
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C: 



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

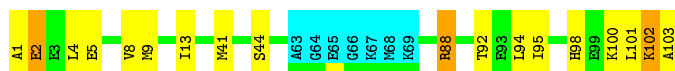
Chain D: 



4.2.12 Score per residue for model 12

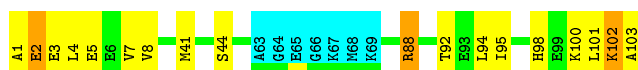
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A: 




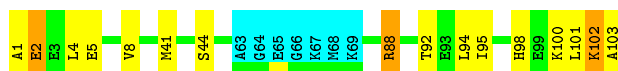
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B: 



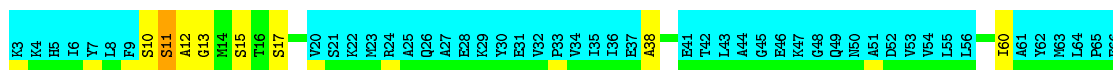
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

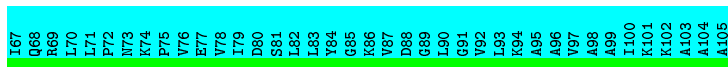
Chain C: 



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

Chain D: 



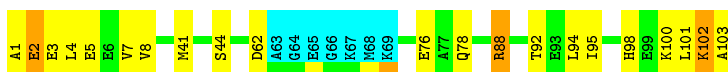


4.2.13 Score per residue for model 13

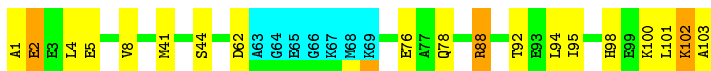
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



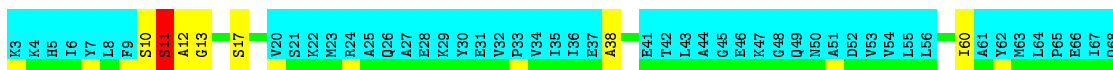
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



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



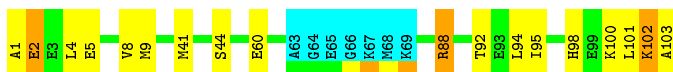
- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT



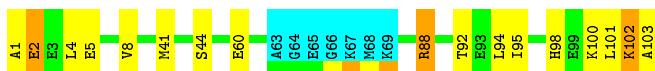
4.2.14 Score per residue for model 14

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

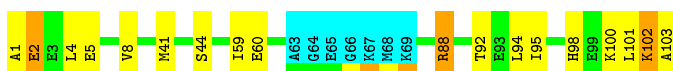




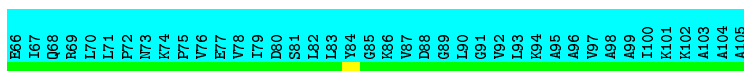
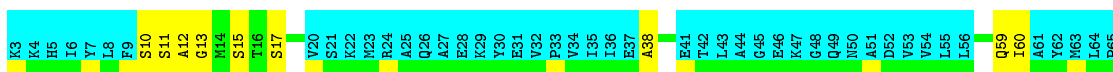
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



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

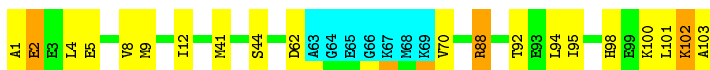


- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

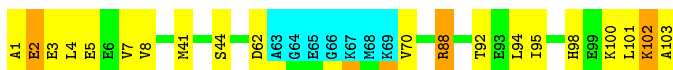


4.2.15 Score per residue for model 15

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

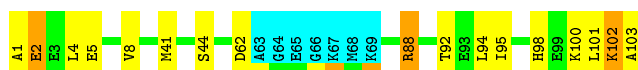


- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



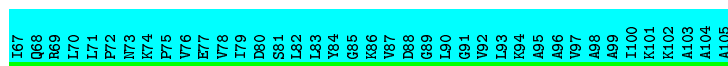
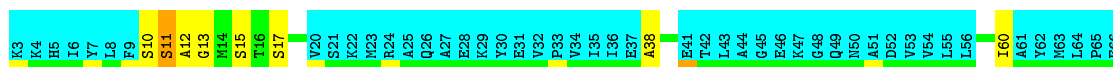
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C:  77% 14% 7%



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

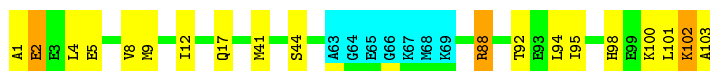
Chain D:  9% 7% 83%



4.2.16 Score per residue for model 16

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

Chain A:  75% 16% 7%




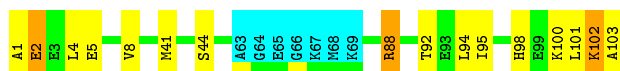
• Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B:  76% 15% 7%



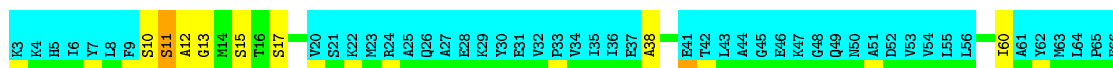
• Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C:  78% 13% 7%



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

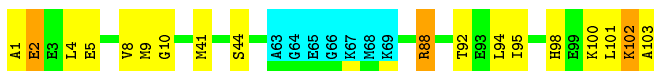
Chain D:  9% 7% 83%



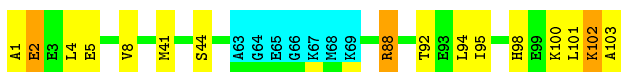


4.2.17 Score per residue for model 17

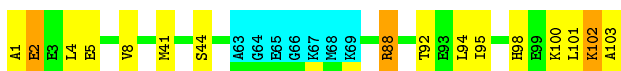
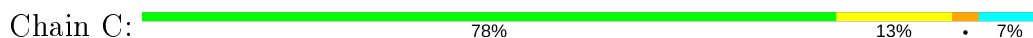
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



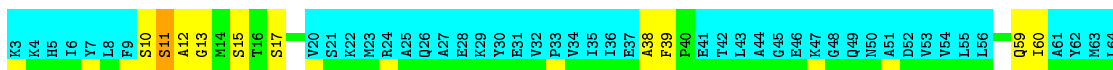
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



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



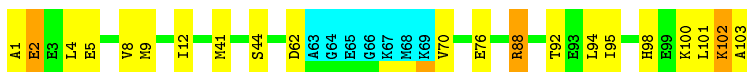
- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT



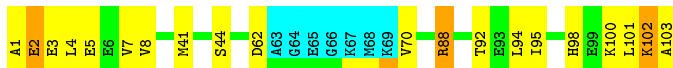
4.2.18 Score per residue for model 18

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

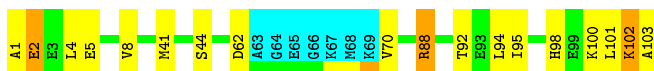




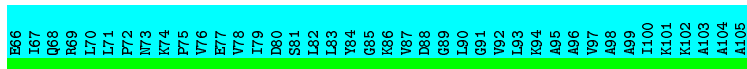
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



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



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



4.2.19 Score per residue for model 19

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

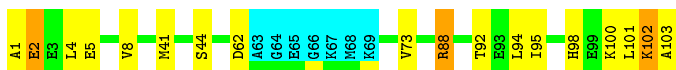


- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



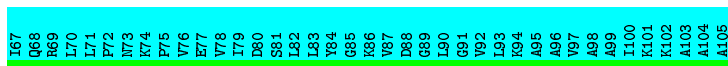
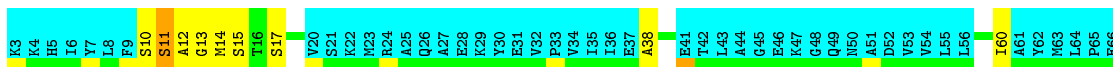
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C:  76% 15% 7%



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

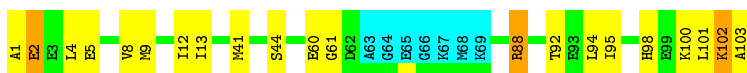
Chain D:  8% 8% 83%



4.2.20 Score per residue for model 20

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

Chain A:  73% 17% 7%




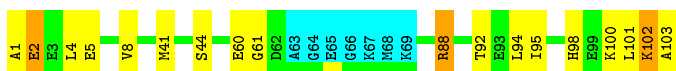
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B:  74% 17% 7%



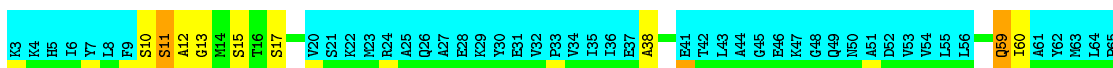
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

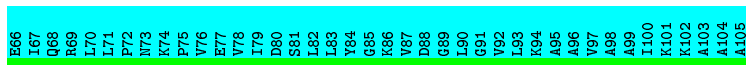
Chain C:  76% 15% 7%



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

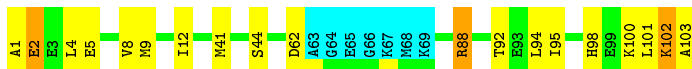
Chain D:  8% 7% 83%



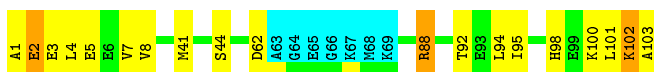


4.2.21 Score per residue for model 21

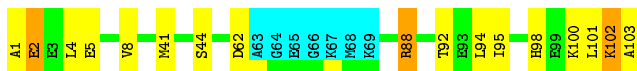
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



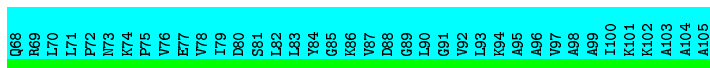
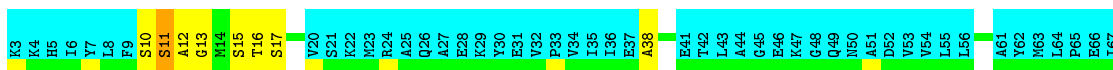
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



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

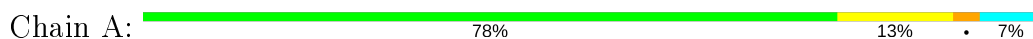


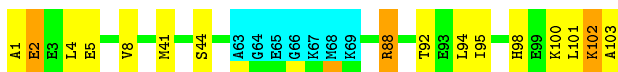
- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT



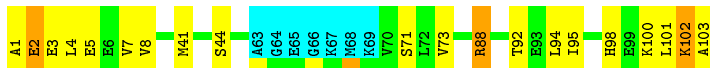
4.2.22 Score per residue for model 22

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

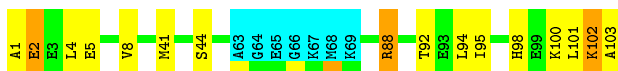
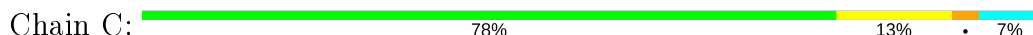




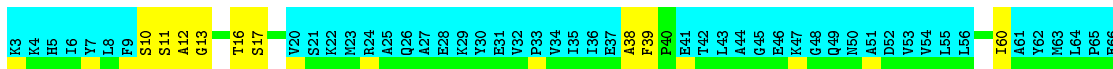
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



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

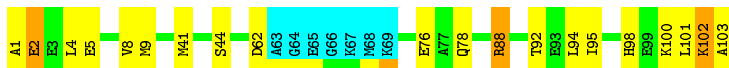


- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

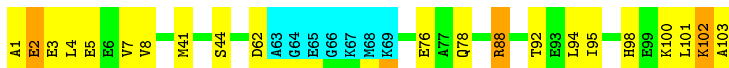


4.2.23 Score per residue for model 23

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

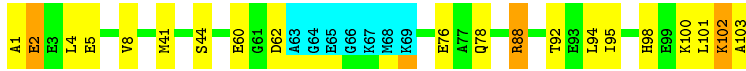


- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



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

Chain C: 



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

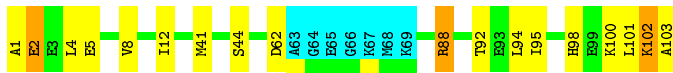
Chain D: 



4.2.24 Score per residue for model 24

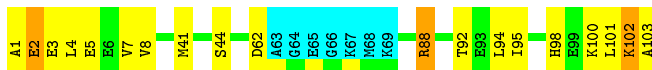
• Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A: 



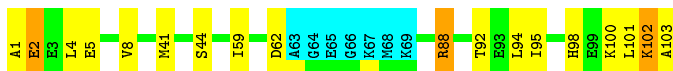
• Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B: 



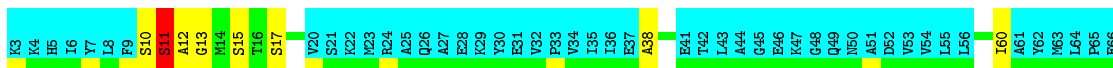
• Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C: 



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

Chain D: 



167
Q68
R69
L70
L71
P72
V73
K74
F75
V76
E77
V78
V79
D80
S81
L82
L83
Y84
G85
K86
R87
D88
G89
L90
G91
Y92
L93
K94
A95
A96
Y97
A98
A99
I100
K101
K102
A103
A104
A105

4.2.25 Score per residue for model 25

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

Chain A:  75% 16% 7%

A1
E2
E3
L4
E5
V8
M9
M41
S44
D62
A63
G64
E65
G66
K67
K68
K69
E76
R88
T92
E93
L94
I95
H98
E99
K100
L101
K102
A103

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

Chain B:  75% 16% 7%

A1
E2
E3
L4
E5
E6
V7
V8
M41
S44
D62
A63
G64
E65
G66
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 C:  77% 14% 7%

A1
E2
E3
L4
E5
V8
M41
S44
D62
A63
G64
E65
G66
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%

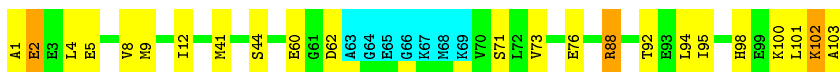
K3
K4
H5
I6
Y7
L8
F9
S10
S11
A12
G13
M14
S15
T16
S17
V20
K21
K22
M23
K24
A25
Q26
A27
E28
K29
Y30
E31
V32
P33
V34
I35
I36
E37
A38
E41
T42
L43
A44
G45
E46
K47
C48
Q49
M50
A51
D52
V53
V54
L55
L56
I60
A61
Y62
M63
L64
P65
E66

167
Q68
R69
L70
L71
P72
V73
K74
F75
V76
E77
V78
V79
D80
S81
L82
L83
Y84
G85
K86
R87
D88
G89
L90
G91
Y92
L93
K94
A95
A96
Y97
A98
A99
I100
K101
K102
A103
A104
A105

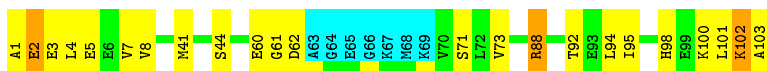
4.2.26 Score per residue for model 26

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

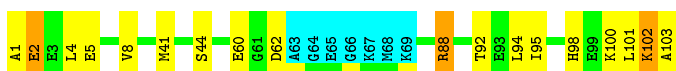
Chain A:  71% 19% 7%



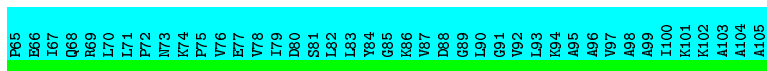
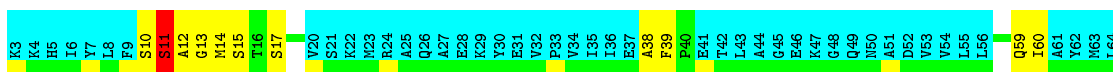
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



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

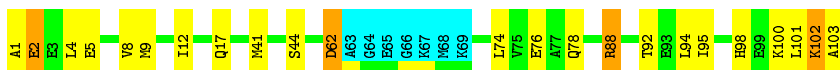


- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

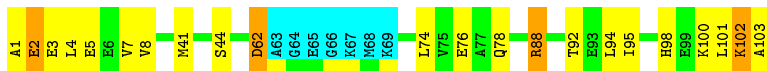


4.2.27 Score per residue for model 27

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

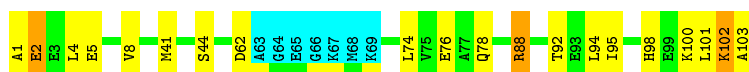


- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



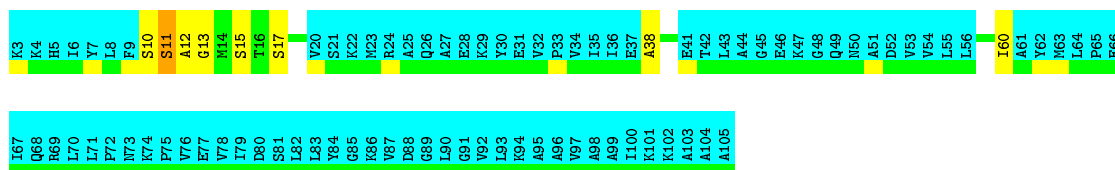
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C: 



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

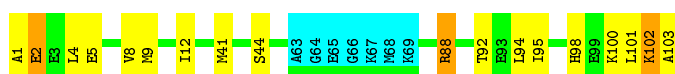
Chain D: 



4.2.28 Score per residue for model 28

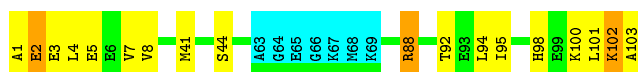
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A: 




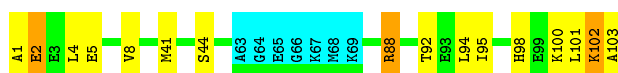
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B: 



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

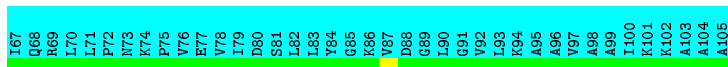
Chain C: 



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

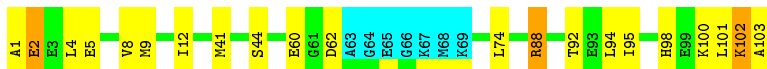
Chain D: 



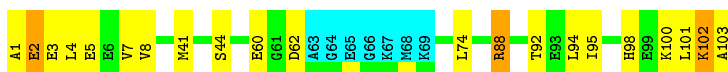


4.2.29 Score per residue for model 29

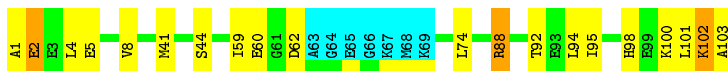
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



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



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



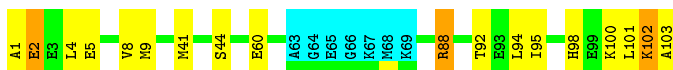
- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT



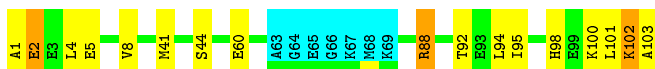
4.2.30 Score per residue for model 30

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

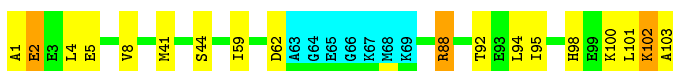




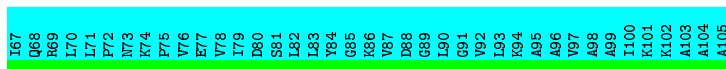
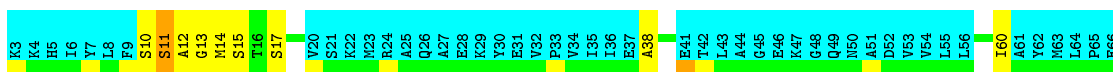
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



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

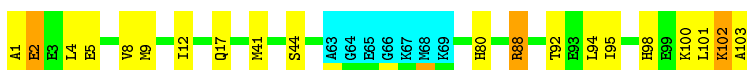


- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

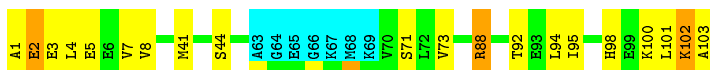


4.2.31 Score per residue for model 31


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

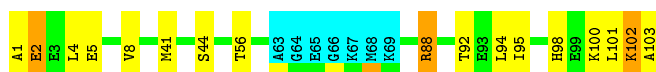


- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



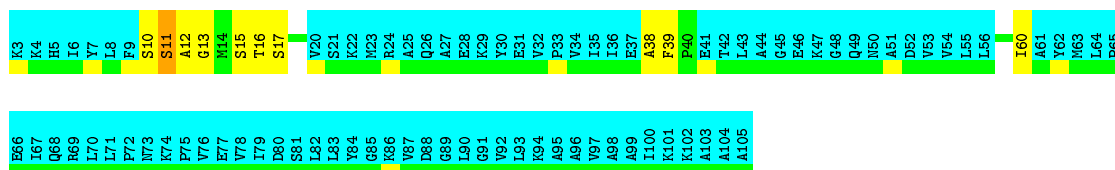
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C:  77% 14% 7%



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

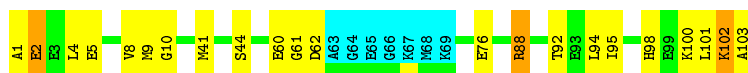
Chain D:  7% 9% 83%



4.2.32 Score per residue for model 32

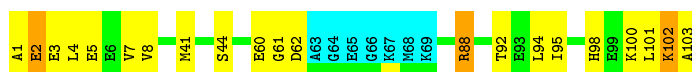
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A:  72% 18% 7%



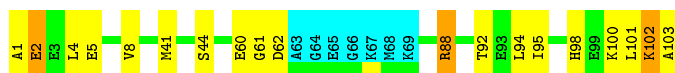
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

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%



E66
L67
Q68
R69
L70
L71
P72
M73
K74
P75
V76
E77
V78
I79
D80
S81
L82
L83
Y84
G85
K86
R87
D88
G89
L90
G91
Y92
L93
K94
A95
A96
Y97
A98
A99
I100
K101
K102
A103
A104
A105

4.2.33 Score per residue for model 33

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

Chain A:  76% 15% 7%

A1 E2 E3 L4 E5 V8 V9 I12 M41 S44 A63 G64 E65 G66 K67 M68 K69 R88 T92 E93 L94 I95 I98 E99 K100 L101 K102 A103

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

Chain B:  75% 16% 7%

A1 E2 E3 L4 E5 E6 V7 V8 M41 S44 E60 A63 G64 E65 G66 K67 M68 K69 R88 T92 E93 L94 I95 I98 E99 K100 L101 K102 A103

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

Chain C:  77% 14% 7%

A1 E2 E3 E5 V8 M41 S44 E60 A63 G64 E65 G66 K67 M68 K69 R88 T92 E93 L94 I95 I98 E99 K100 L101 K102 A103

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

Chain D:  9% 7% 83%

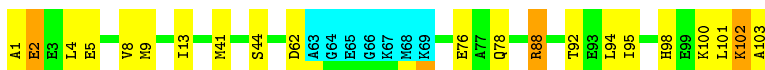
K3 K4 H5 I6 Y7 L8 V9 S10 S11 A12 G13 H14 S15 T16 S17 V20 S21 K22 M23 A24 A25 A26 Q26 A27 E28 K29 Y30 E31 E32 V32 P33 V34 I35 I36 E37 A38 E41 T42 L43 A44 G45 E46 K47 C48 Q49 N50 A51 D52 V53 V54 L55 L56 I60 A61 Y62 M63 L64 P65 E66

L67 Q68 R69 L70 L71 P72 M73 K74 P75 V76 E77 V78 I79 D80 S81 L82 L83 Y84 G85 K86 R87 D88 G89 L90 G91 Y92 L93 K94 A95 A96 Y97 A98 A99 I100 K101 K102 A103 A104 A105

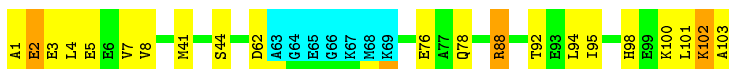
4.2.34 Score per residue for model 34

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

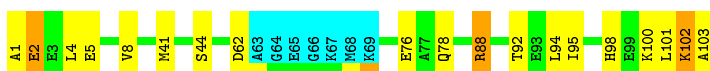
Chain A:  73% 17% 7%



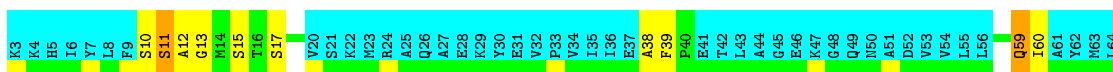
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



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

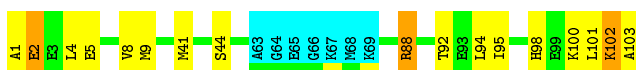


- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

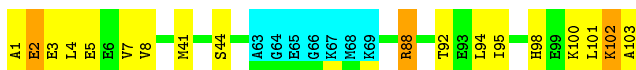


4.2.35 Score per residue for model 35


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

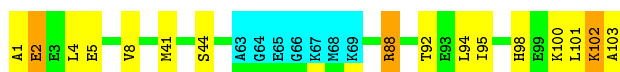


- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



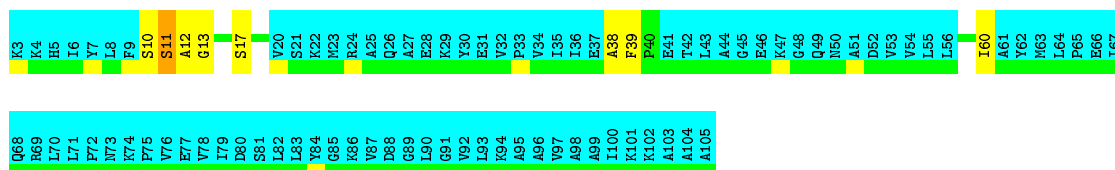
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C:  78% 13% 7%



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

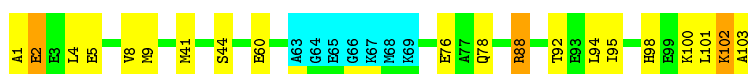
Chain D:  9% 7% 83%



4.2.36 Score per residue for model 36

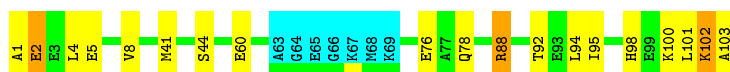
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A:  74% 17% 7%



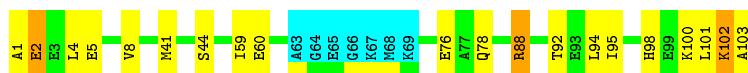
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B:  75% 16% 7%



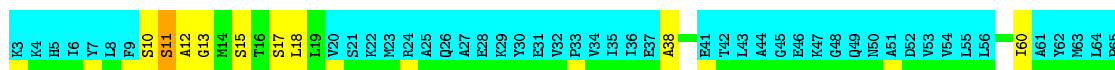
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C:  74% 17% 7%



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

Chain D:  8% 8% 83%



E66
L67
Q68
R69
L70
L71
P72
M73
K74
P75
V76
V77
V78
L79
D80
S81
L82
L83
Y84
G85
G86
R87
D88
G89
L90
G91
Y92
L93
K94
A95
A96
Y97
A98
A99
I100
K101
K102
A103
A104
A105


4.2.37 Score per residue for model 37

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

Chain A:  73% 17% 7%

A1
E2
E3
L4
E5
V8
M9
I12
M41
S44
E60
G61
D62
A63
G64
E65
G66
K67
M68
K69
E76
R88
T92
E93
L94
I95
H98
E99
K100
L101
K102
A103

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

Chain B:  76% 15% 7%

A1
E2
E3
L4
E5
V8
M41
S44
E60
G61
D62
A63
G64
E65
G66
K67
M68
K69
R88
T92
E93
L94
I95
H98
E99
K100
L101
K102
A103

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

Chain C:  75% 16% 7%

A1
E2
E3
L4
E5
V8
M41
S44
E59
E60
G61
D62
A63
G64
E65
G66
K67
M68
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%

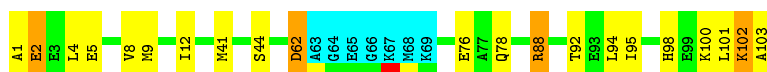
K3
K4
H5
I6
Y7
L8
F9
S10
S11
A12
G13
M14
S15
T16
S17
V20
S21
K22
M23
A24
A25
Q26
A27
E28
K29
Y30
E31
V32
P33
V34
I35
L36
E37
A38
E41
T42
L43
A44
G45
E46
K47
C48
Q49
M50
A51
D52
V53
V54
L55
L56
I60
A61
Y62
M63
L64
P65
E66

L67
Q68
R69
L70
L71
P72
M73
K74
P75
V76
V77
V78
L79
D80
S81
L82
L83
Y84
G85
G86
R87
D88
G89
L90
G91
Y92
L93
K94
A95
A96
Y97
A98
A99
I100
K101
K102
A103
A104
A105

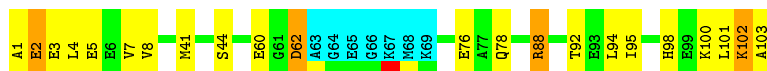
4.2.38 Score per residue for model 38

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

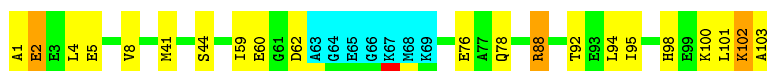
Chain A:  73% 17% 7%



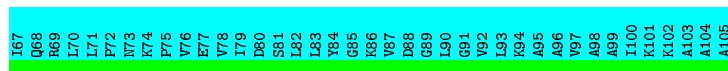
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



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

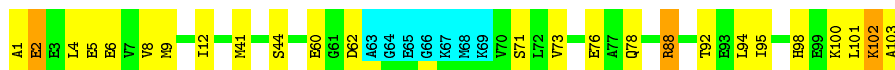


- Molecule 2: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT



4.2.39 Score per residue for model 39

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

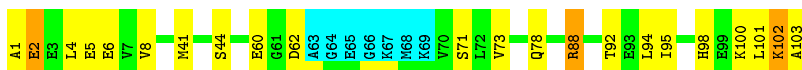


- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



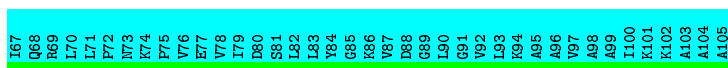
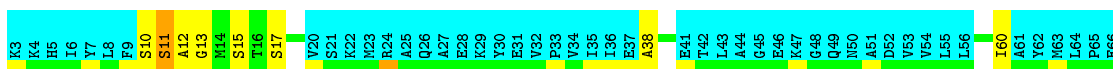
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C:  72% 18% 7%



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

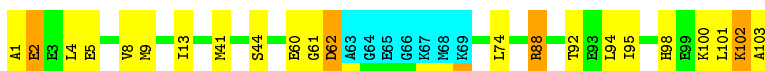
Chain D:  9% 7% 83%



4.2.40 Score per residue for model 40

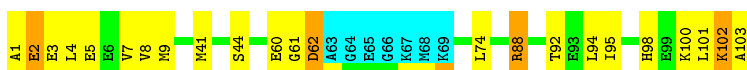
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A:  72% 17% 7%



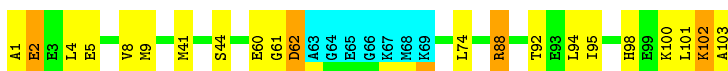
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B:  71% 18% 7%



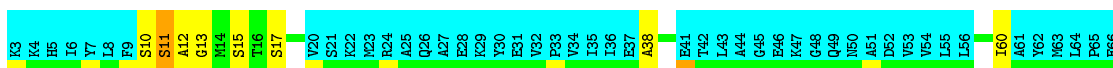
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

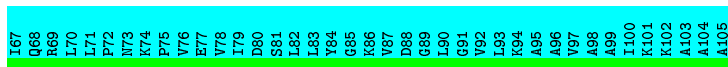
Chain C:  73% 17% 7%



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

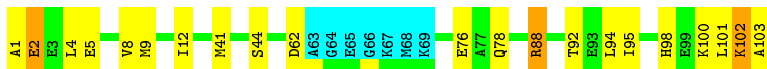
Chain D:  9% 7% 83%



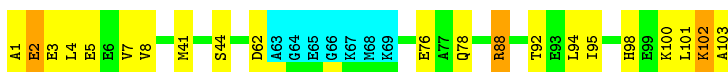


4.2.41 Score per residue for model 41

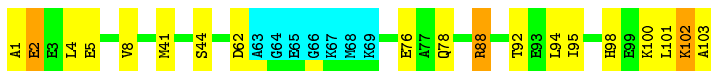
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



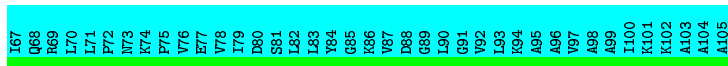
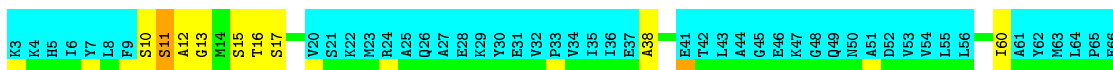
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



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



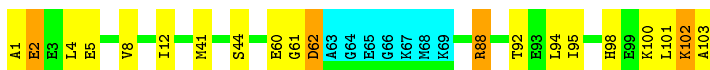
- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT



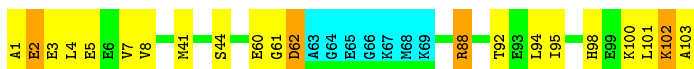
4.2.42 Score per residue for model 42

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

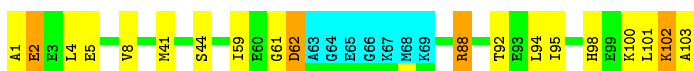




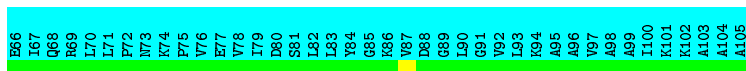
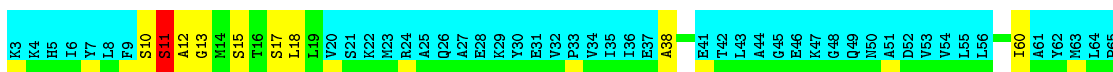
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



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

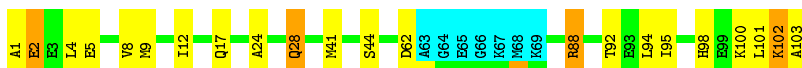


- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT



4.2.43 Score per residue for model 43

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

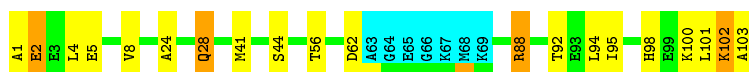


- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



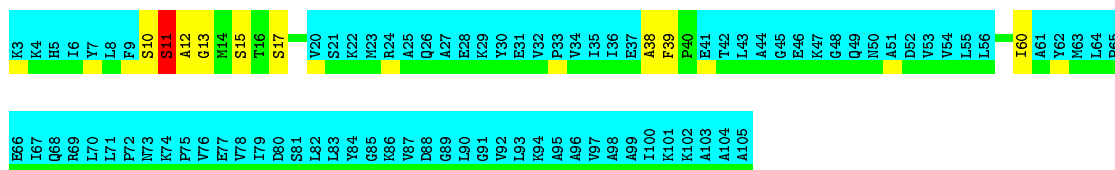
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C:  74% 16% 7%



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

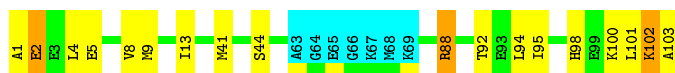
Chain D:  8% 8% 83%



4.2.44 Score per residue for model 44

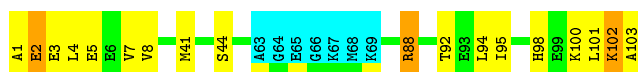
• Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A:  76% 15% 7%




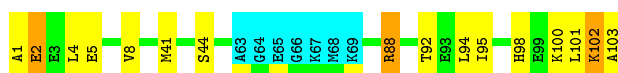
• Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B:  76% 15% 7%



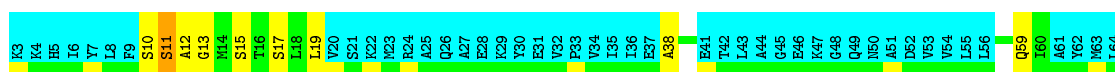
• Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C:  78% 13% 7%



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

Chain D:  8% 8% 83%



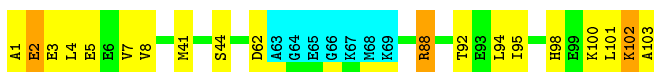


4.2.45 Score per residue for model 45

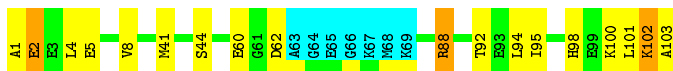
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



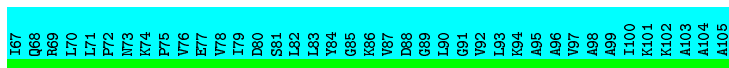
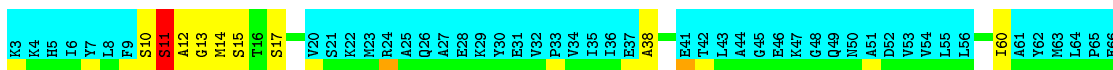
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



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



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



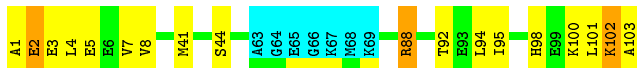
4.2.46 Score per residue for model 46

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





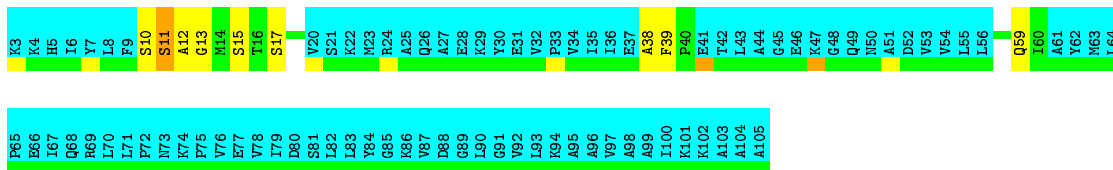
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



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

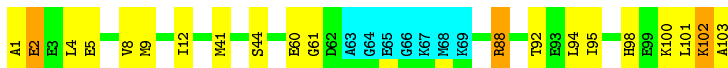


- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

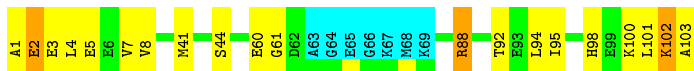


4.2.47 Score per residue for model 47

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



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



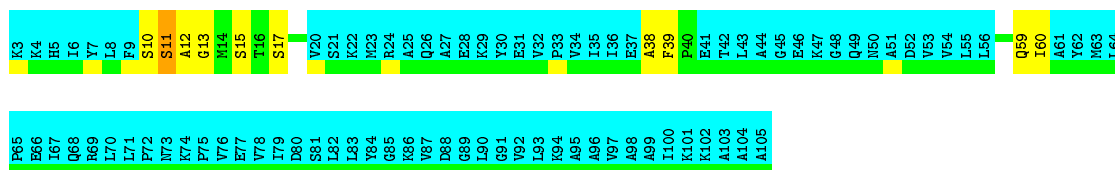
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C:  75% 16% 7%



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

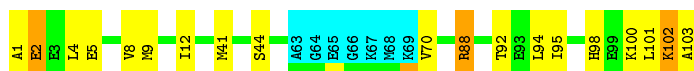
Chain D:  7% 9% 83%



4.2.48 Score per residue for model 48

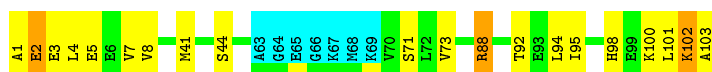
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A:  75% 16% 7%



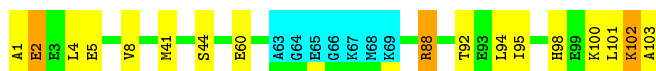
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B:  74% 17% 7%



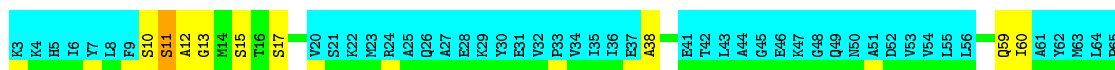
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C:  77% 14% 7%



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

Chain D:  8% 8% 83%



E66
I67
Q68
R69
L70
L71
P72
N73
K74
P75
V76
E77
W78
I79
D80
S81
L82
L83
Y84
G85
R86
W87
D88
G89
L90
G91
Y92
L93
K94
A95
A96
Y97
A98
A99
I100
K101
K102
A103
A104
A105

4.2.49 Score per residue for model 49

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

Chain A:  74% 16% 7%

A1 E2 E3 L4 E5 V8 N9 I12 M41 S44 G61 D62 A63 G64 G65 G66 K67 M68 K69 R88 T92 E93 L94 I95 H98 E99 K100 L101 K102 A103

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

Chain B:  74% 17% 7%

A1 E2 E3 L4 E5 V8 N9 M41 S44 G61 D62 A63 G64 G65 G66 K67 M68 K69 R88 T92 E93 L94 I95 H98 E99 K100 L101 K102 A103

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

Chain C:  76% 15% 7%

A1 E2 E3 L4 E5 V8 N9 M41 S44 G61 D62 A63 G64 G65 G66 K67 M68 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%

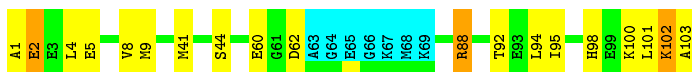
K3 K4 H5 L6 Y7 L8 F9 S10 S11 A12 G13 H14 S15 T16 S17 V20 K21 K22 M23 A24 A25 Q26 A27 E28 K29 Y30 E31 E32 V33 P34 I35 L36 E37 A38 F39 E40 E41 T42 L43 A44 G45 E46 K47 G48 Q49 N50 A51 D52 V53 V54 L55 L56 I60 A61 Y62 M63 L64 P65

E66
I67
Q68
R69
L70
L71
P72
N73
K74
P75
V76
E77
W78
I79
D80
S81
L82
L83
Y84
G85
R86
W87
D88
G89
L90
G91
Y92
L93
K94
A95
A96
Y97
A98
A99
I100
K101
K102
A103
A104
A105

4.2.50 Score per residue for model 50

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

Chain A:  75% 16% 7%



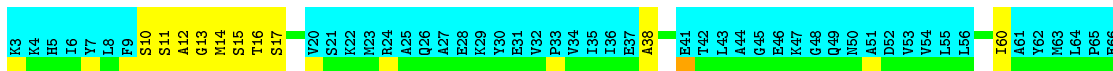
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



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

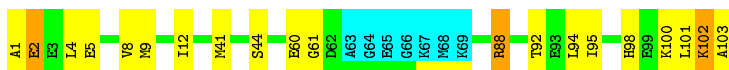


- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

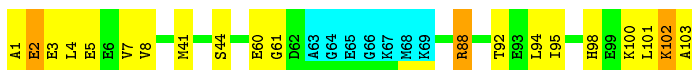


4.2.51 Score per residue for model 51

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

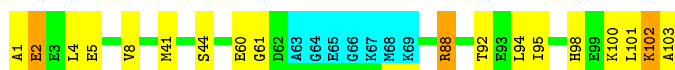


- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



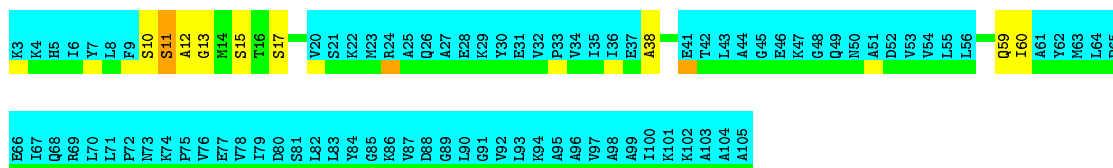
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C: 



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

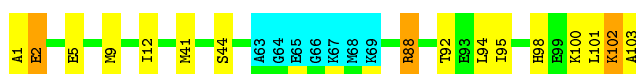
Chain D: 



4.2.52 Score per residue for model 52

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

Chain A: 




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

Chain B: 



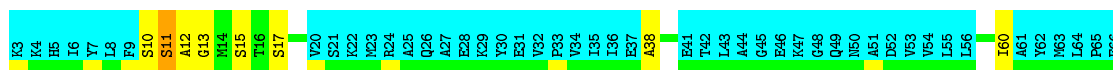
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C: 



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

Chain D: 



Q68 Q69 Q70 Q71 Q72 Q73 Q74 Q75 Q76 Q77 Q78 Q79 Q80 Q81 Q82 Q83 Q84 Q85 Q86 Q87 Q88 Q89 Q90 Q91 Q92 Q93 Q94 Q95 Q96 Q97 Q98 Q99 Q100 Q101 Q102 Q103 Q104 Q105

4.2.53 Score per residue for model 53

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

Chain A:  73% 17% 7%

A1 A2 A3 A4 A5 A6 A7 A8 A9 A10 A11 A12 A13 A14 A15 A16 A17 A18 A19 A20 A21 A22 A23 A24 A25 A26 A27 A28 A29 A30 A31 A32 A33 A34 A35 A36 A37 A38 A39 A40 A41 A42 A43 A44 A45 A46 A47 A48 A49 A50 A51 A52 A53 A54 A55 A56 A57 A58 A59 A60 A61 A62 A63 A64 A65 A66 A67 A68 A69 A70 A71 A72 A73 A74 A75 A76 A77 A78 A79 A80 A81 A82 A83 A84 A85 A86 A87 A88 A89 A90 A91 A92 A93 A94 A95 A96 A97 A98 A99 A100 A101 A102 A103 A104 A105

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

Chain B:  74% 17% 7%

A1 A2 A3 A4 A5 A6 A7 A8 A9 A10 A11 A12 A13 A14 A15 A16 A17 A18 A19 A20 A21 A22 A23 A24 A25 A26 A27 A28 A29 A30 A31 A32 A33 A34 A35 A36 A37 A38 A39 A40 A41 A42 A43 A44 A45 A46 A47 A48 A49 A50 A51 A52 A53 A54 A55 A56 A57 A58 A59 A60 A61 A62 A63 A64 A65 A66 A67 A68 A69 A70 A71 A72 A73 A74 A75 A76 A77 A78 A79 A80 A81 A82 A83 A84 A85 A86 A87 A88 A89 A90 A91 A92 A93 A94 A95 A96 A97 A98 A99 A100 A101 A102 A103 A104 A105

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

Chain C:  75% 15% 7%

A1 A2 A3 A4 A5 A6 A7 A8 A9 A10 A11 A12 A13 A14 A15 A16 A17 A18 A19 A20 A21 A22 A23 A24 A25 A26 A27 A28 A29 A30 A31 A32 A33 A34 A35 A36 A37 A38 A39 A40 A41 A42 A43 A44 A45 A46 A47 A48 A49 A50 A51 A52 A53 A54 A55 A56 A57 A58 A59 A60 A61 A62 A63 A64 A65 A66 A67 A68 A69 A70 A71 A72 A73 A74 A75 A76 A77 A78 A79 A80 A81 A82 A83 A84 A85 A86 A87 A88 A89 A90 A91 A92 A93 A94 A95 A96 A97 A98 A99 A100 A101 A102 A103 A104 A105

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

Chain D:  9% 7% 83%

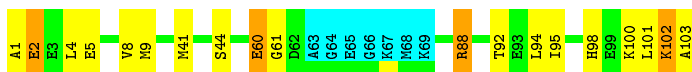
K3 K4 K5 K6 K7 K8 K9 K10 K11 K12 K13 K14 K15 K16 K17 K18 K19 K20 K21 K22 K23 K24 K25 K26 K27 K28 K29 K30 K31 K32 K33 K34 K35 K36 K37 K38 K39 K40 K41 K42 K43 K44 K45 K46 K47 K48 K49 K50 K51 K52 K53 K54 K55 K56 K57 K58 K59 K60 K61 K62 K63 K64 K65 K66 K67 K68 K69 K70 K71 K72 K73 K74 K75 K76 K77 K78 K79 K80 K81 K82 K83 K84 K85 K86 K87 K88 K89 K90 K91 K92 K93 K94 K95 K96 K97 K98 K99 K100 K101 K102 K103 K104 K105

Q68 Q69 Q70 Q71 Q72 Q73 Q74 Q75 Q76 Q77 Q78 Q79 Q80 Q81 Q82 Q83 Q84 Q85 Q86 Q87 Q88 Q89 Q90 Q91 Q92 Q93 Q94 Q95 Q96 Q97 Q98 Q99 Q100 Q101 Q102 Q103 Q104 Q105

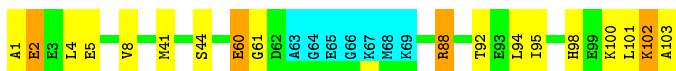
4.2.54 Score per residue for model 54

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

Chain A:  75% 15% 7%



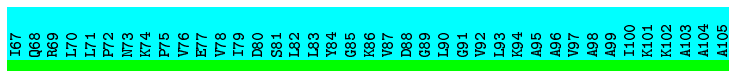
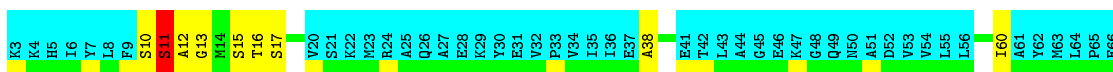
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



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

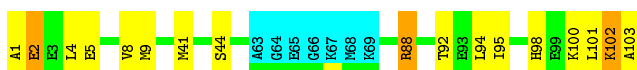


- Molecule 2: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

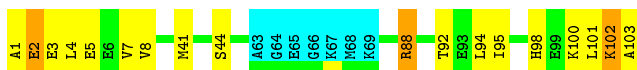


4.2.55 Score per residue for model 55

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



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



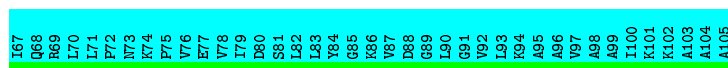
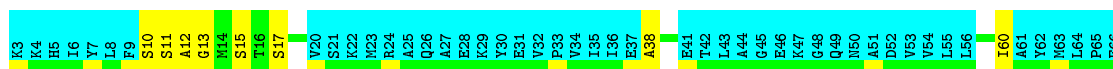
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

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%



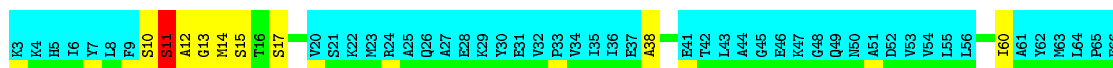
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

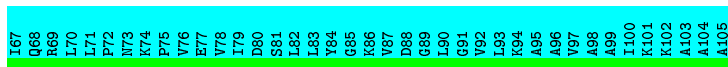
Chain C:  75% 15% 7%



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

Chain D:  8% 8% 83%



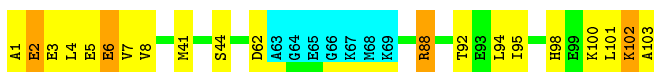


4.2.57 Score per residue for model 57

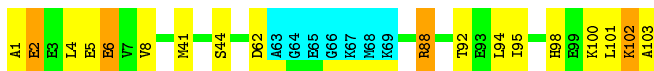
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



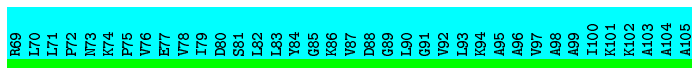
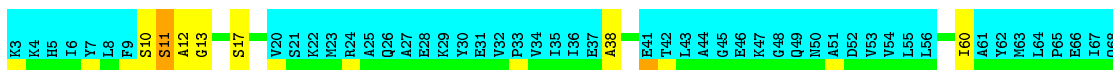
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



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



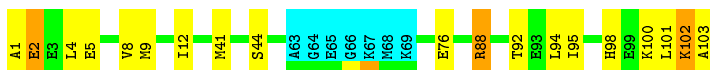
- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT



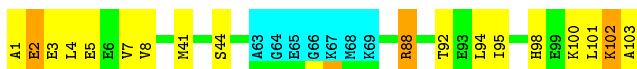
4.2.58 Score per residue for model 58

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

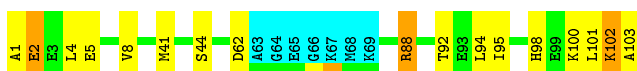




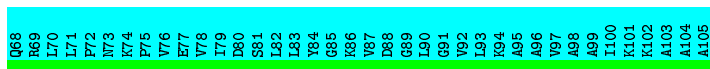
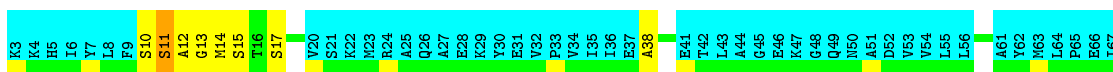
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



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

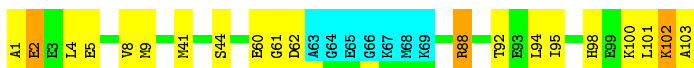


- Molecule 2: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

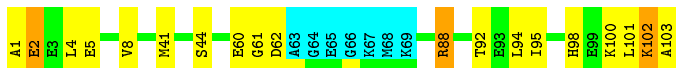


4.2.59 Score per residue for model 59

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

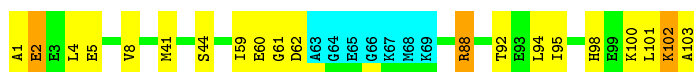


- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



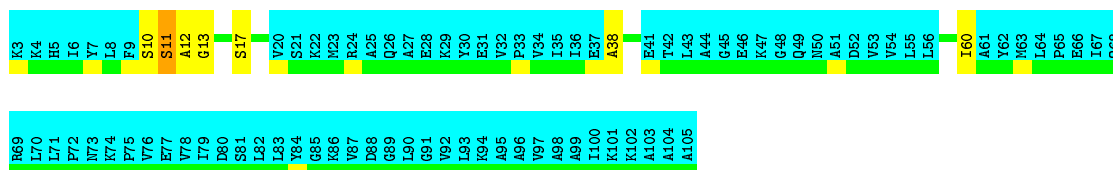
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C: 



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

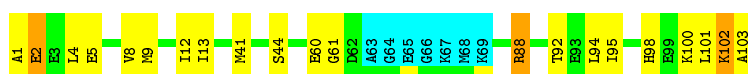
Chain D: 



4.2.60 Score per residue for model 60

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

Chain A: 




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

Chain B: 



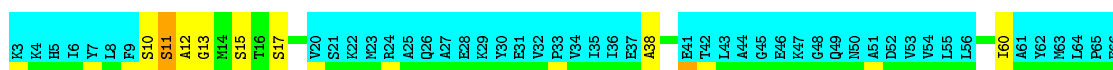
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

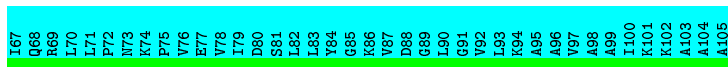
Chain C: 



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

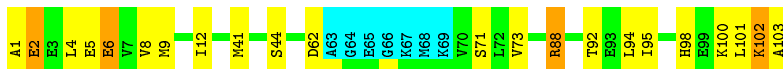
Chain D: 



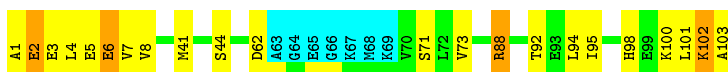


4.2.61 Score per residue for model 61

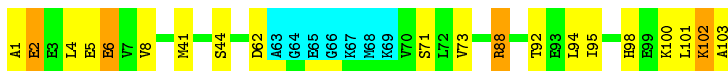
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



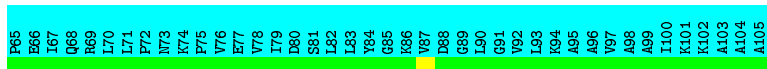
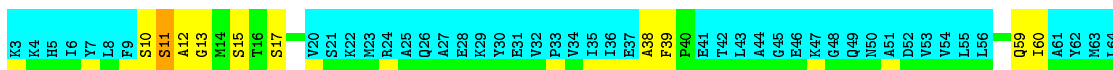
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



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



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



4.2.62 Score per residue for model 62

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

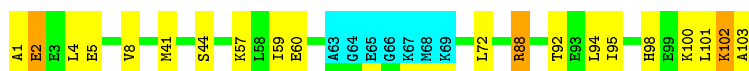




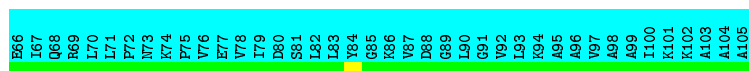
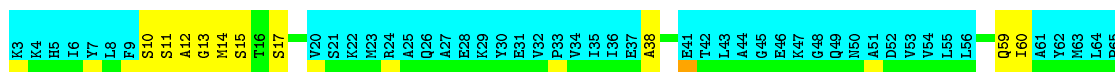
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



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

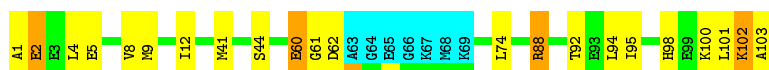


- Molecule 2: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

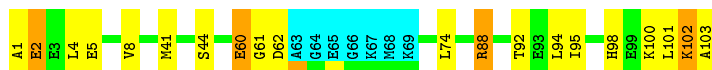


4.2.63 Score per residue for model 63

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



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



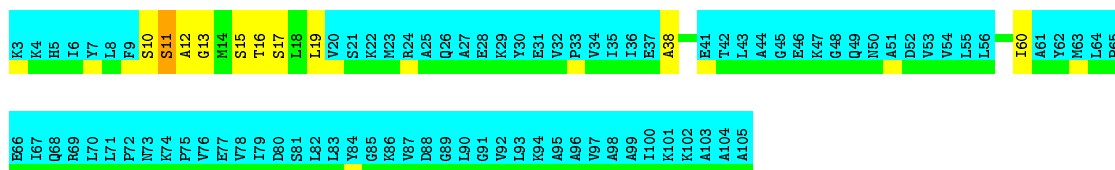
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C: 



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

Chain D: 



4.2.64 Score per residue for model 64

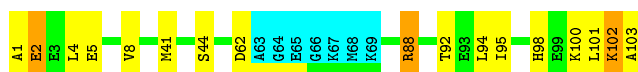
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A: 



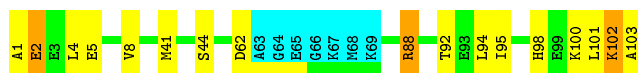
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B: 



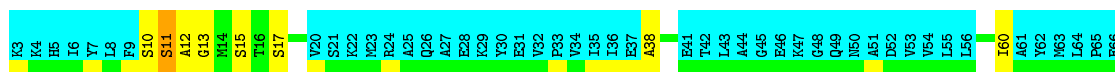
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

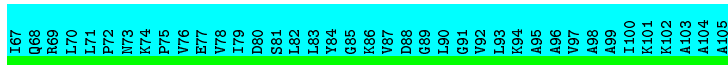
Chain C: 



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

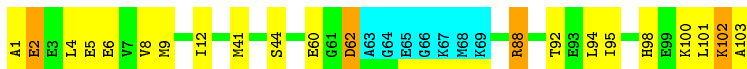
Chain D: 



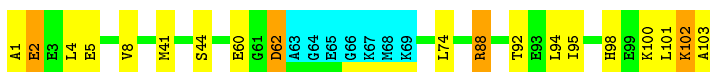


4.2.65 Score per residue for model 65

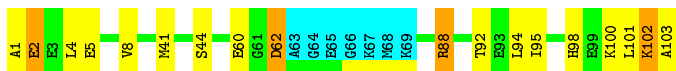
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



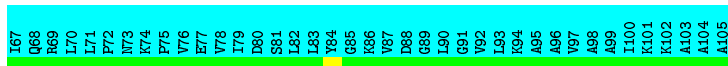
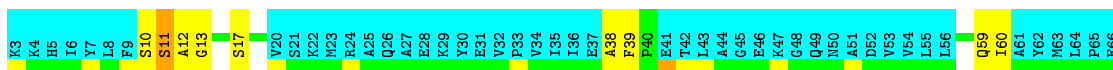
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



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



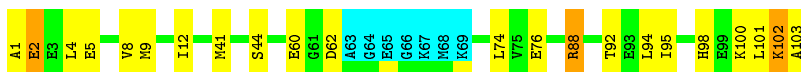
- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT



4.2.66 Score per residue for model 66

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

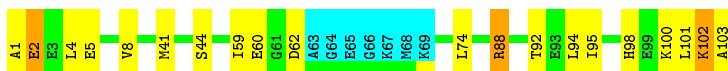




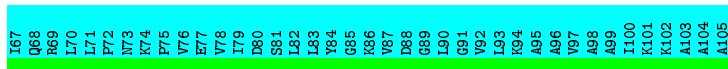
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



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



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



4.2.67 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



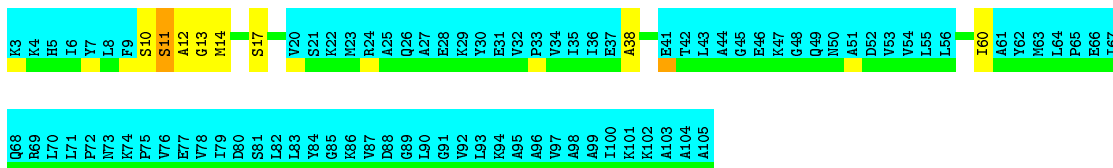
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C: 



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

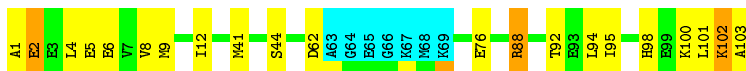
Chain D: 



4.2.68 Score per residue for model 68

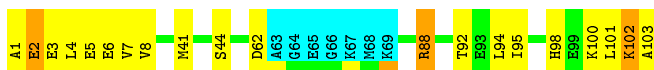
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A: 




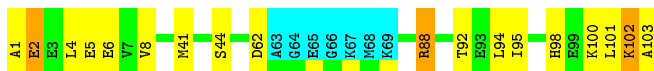
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B: 



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

Chain C: 



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

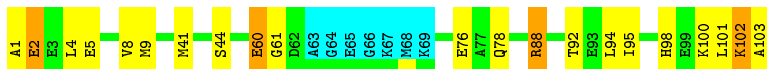
Chain D: 



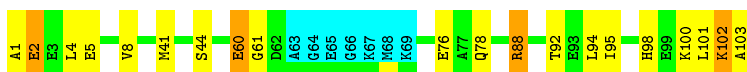


4.2.69 Score per residue for model 69

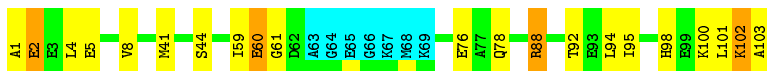
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



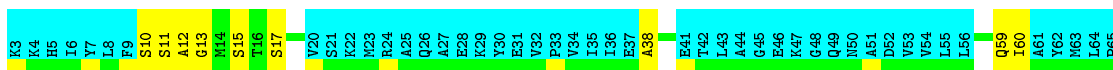
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



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



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



4.2.70 Score per residue for model 70

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

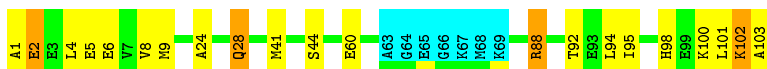




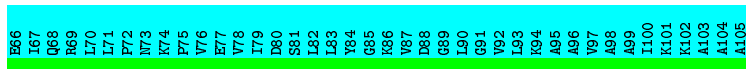
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



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



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



4.2.71 Score per residue for model 71

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

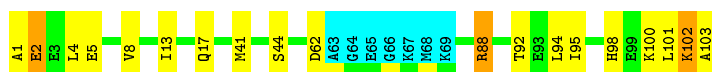


- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



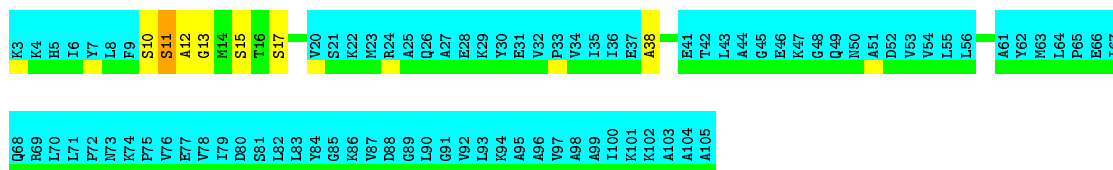
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C: 



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

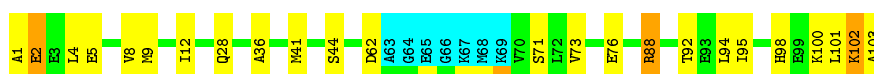
Chain D: 



4.2.72 Score per residue for model 72

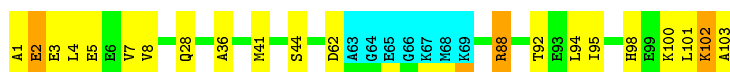
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A: 



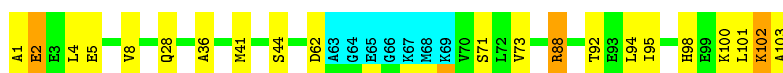
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B: 



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

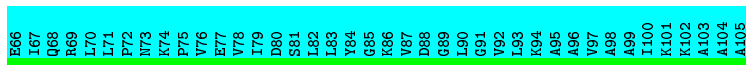
Chain C: 



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

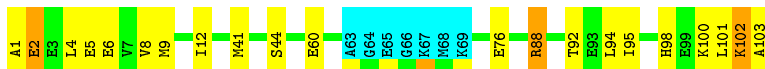
Chain D: 



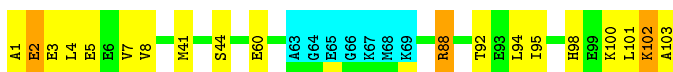


4.2.73 Score per residue for model 73

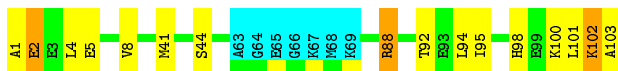
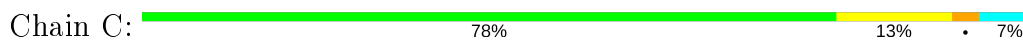
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



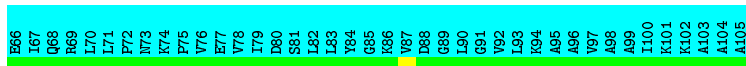
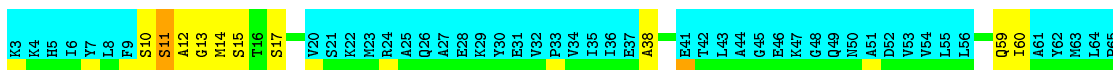
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



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



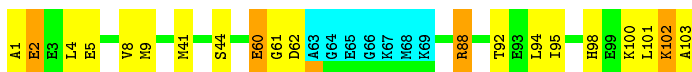
- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT



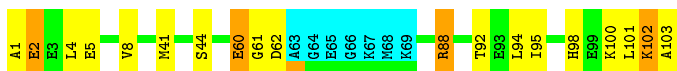
4.2.74 Score per residue for model 74

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

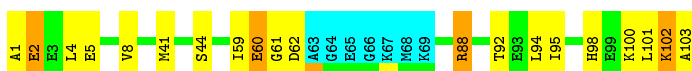




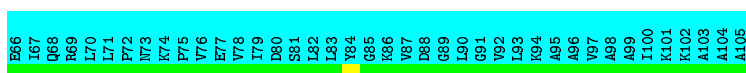
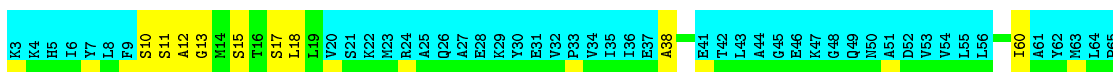
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



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

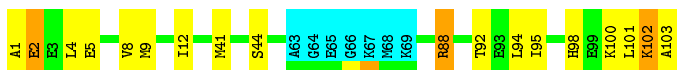


- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

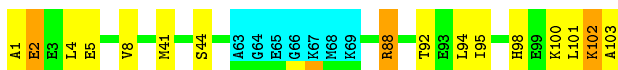
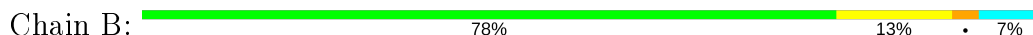


4.2.75 Score per residue for model 75

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

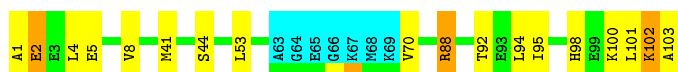


- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



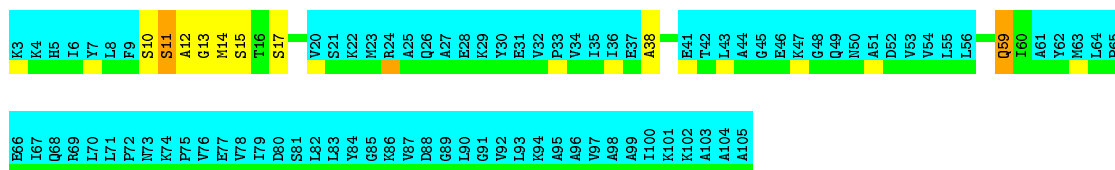
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C:  76% 15% 7%



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

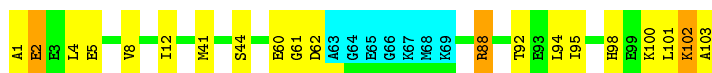
Chain D:  8% 7% 83%



4.2.76 Score per residue for model 76

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

Chain A:  74% 17% 7%



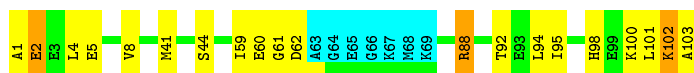
• Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B:  75% 16% 7%



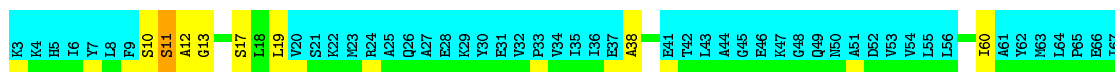
• Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

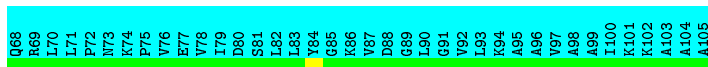
Chain C:  74% 17% 7%



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

Chain D:  9% 7% 83%

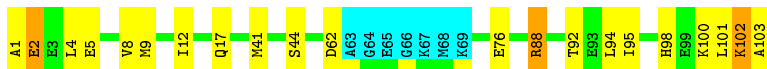




4.2.77 Score per residue for model 77

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

Chain A: 73% 17% 7%



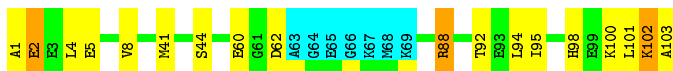
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B: 75% 16% 7%



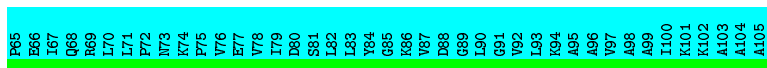
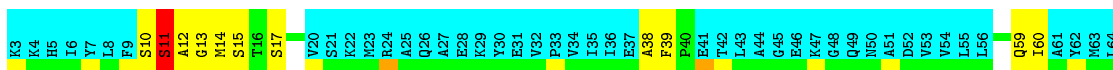
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C: 76% 15% 7%



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

Chain D: 6% 10% 83%



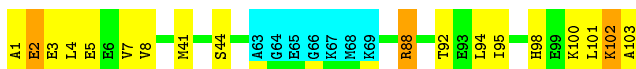
4.2.78 Score per residue for model 78

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

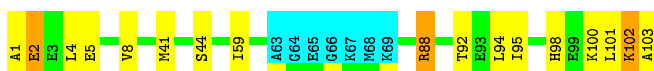
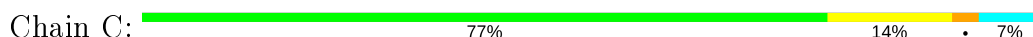
Chain A: 77% 14% 7%



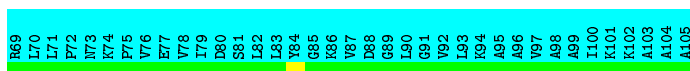
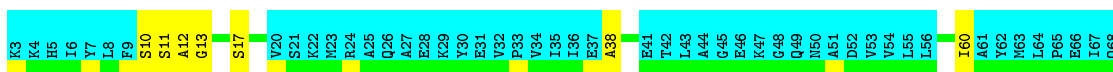
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



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

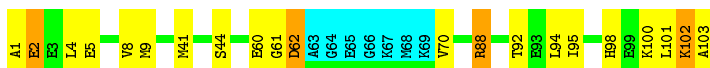


- Molecule 2: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

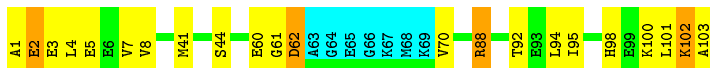


4.2.79 Score per residue for model 79

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

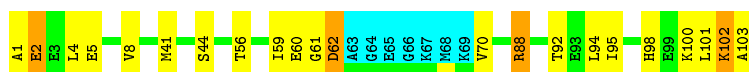


- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



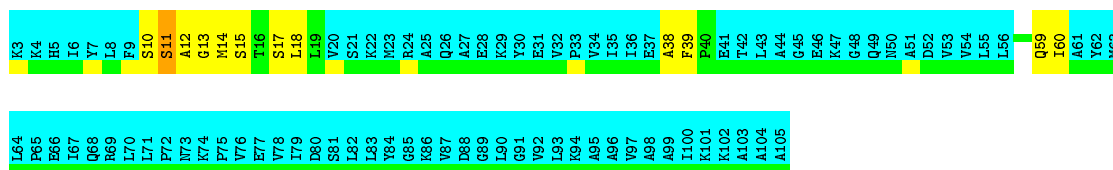
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C:  72% 17% 7%



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

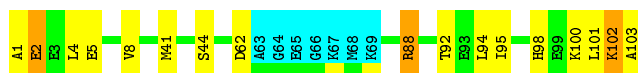
Chain D:  5% 11% 83%



4.2.80 Score per residue for model 80

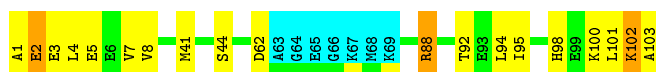
• Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A:  77% 14% 7%




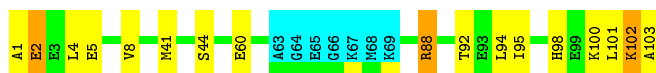
• Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

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:  11% 5% 83%



L70
L71
P72
M73
K74
P75
V76
E77
W78
I79
D80
S81
L82
L83
Y84
G85
K86
W87
D88
G89
L90
G91
Y92
L93
K94
A95
A96
Y97
A98
A99
I100
K101
K102
A103
A104
A105

4.2.81 Score per residue for model 81

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

Chain A:  76% 14% 7%

A1
E2
E3
L4
E5
V8
N9
Q17
M41
S44
A63
G64
E65
G66
K67
M68
K69
R88
T92
E93
L94
I95
H98
E99
K100
L101
K102
A103

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

Chain B:  74% 16% 7%

A1
E2
E3
L4
E5
E6
V7
V8
Q17
M41
S44
D62
A63
G64
E65
G66
K67
M68
K69
R88
T92
E93
L94
I95
H98
E99
K100
L101
K102
A103

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

Chain C:  76% 15% 7%

A1
E2
E3
L4
E5
V8
Q17
M41
S44
D62
A63
G64
E65
G66
K67
M68
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%

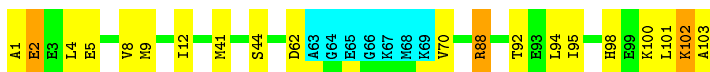
K3
K4
H5
I6
Y7
L8
F9
S10
S11
A12
G13
H14
S15
T16
S17
V20
S21
K22
M23
A24
A25
Q26
A27
E28
K29
Y30
E31
V32
P33
V34
I35
L36
E37
A38
F39
E40
E41
T42
L43
A44
G45
E46
K47
G48
Q49
N50
A51
D52
V53
V54
L55
L56
I60
A61
Y62
M63
L64
P65

E66
I67
Q68
R69
L70
L71
P72
M73
K74
P75
V76
E77
W78
I79
D80
S81
L82
L83
Y84
G85
K86
W87
D88
G89
L90
G91
Y92
L93
K94
A95
A96
Y97
A98
A99
I100
K101
K102
A103
A104
A105

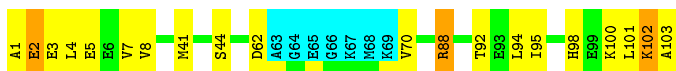
4.2.82 Score per residue for model 82

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

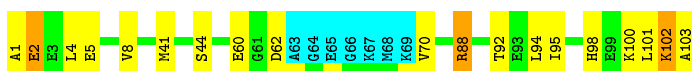
Chain A:  74% 17% 7%



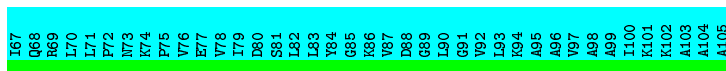
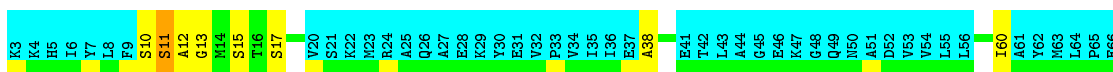
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



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



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

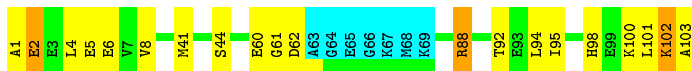


4.2.83 Score per residue for model 83

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



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



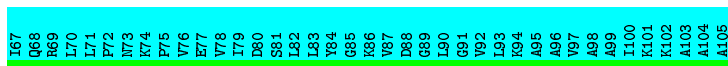
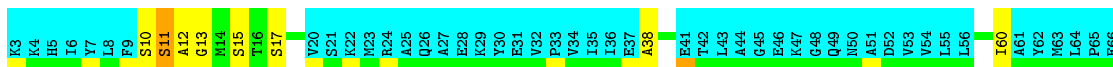
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C:  73% 17% 7%



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

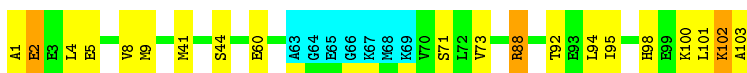
Chain D:  9% 7% 83%



4.2.84 Score per residue for model 84

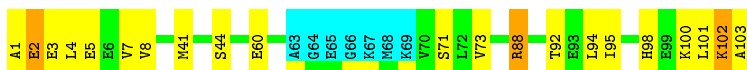
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain A:  74% 17% 7%



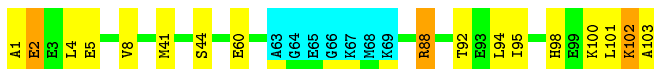
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B:  73% 17% 7%



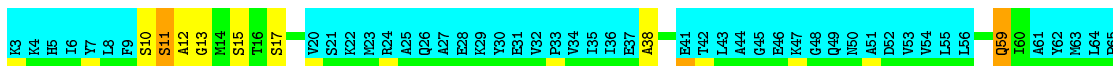
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C:  77% 14% 7%



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

Chain D:  9% 6% 83%



E66
L67
Q68
R69
L70
L71
P72
M73
K74
P75
V76
E77
V78
L79
D80
S81
L82
L83
Y84
G85
R86
D87
D88
G89
L90
G91
Y92
L93
K94
A95
A96
Y97
A98
A99
I100
K101
K102
A103
A104
A105

4.2.85 Score per residue for model 85

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

Chain A: 71% 18% 7%

A1
E2
E3
L4
E5
E6
V7
V8
N9
I12
Q28
A36
M41
S44
D62
A63
G64
E65
G66
K67
M68
K69
V70
R88
T92
E93
L94
I95
H98
E99
K100
L101
K102
A103

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

Chain B: 72% 17% 7%

A1
E2
E3
L4
E5
E6
V7
V8
Q28
A36
M41
S44
A63
G64
E65
G66
K67
M68
K69
V70
R88
T92
E93
L94
I95
H98
E99
K100
L101
K102
A103

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

Chain C: 73% 17% 7%

A1
E2
E3
L4
E5
E6
V7
V8
Q28
A36
M41
S44
E60
A63
G64
E65
G66
K67
M68
K69
V70
R88
T92
E93
L94
I95
H98
E99
K100
L101
K102
A103

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

Chain D: 7% 9% 83%

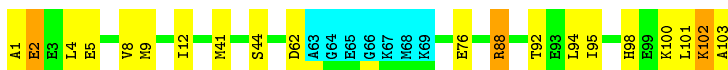
K3
K4
H5
L6
Y7
L8
F9
S10
S11
A12
G13
H14
S15
T16
S17
V20
S21
K22
M23
A24
A25
Q26
A27
E28
K29
Y30
E31
V32
P33
V34
I35
L36
E37
A38
F39
E40
E41
T42
L43
A44
G45
E46
K47
G48
Q49
N50
A51
D52
V53
V54
L55
L56
Q59
L60
A61
V62
M63
L64

P85
E86
Q88
R89
L90
L91
P92
M93
K94
P95
V96
E97
V98
L99
D80
S81
L82
L83
Y84
G85
R86
D87
D88
G89
L90
G91
Y92
L93
K94
A95
A96
Y97
A98
A99
I100
K101
K102
A103
A104
A105

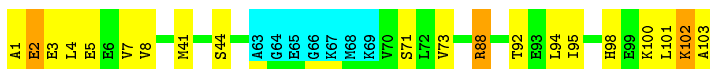
4.2.86 Score per residue for model 86

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

Chain A: 74% 17% 7%



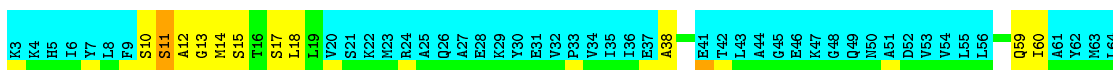
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



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

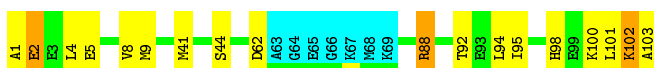


- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT

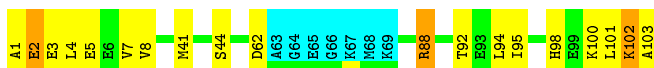


4.2.87 Score per residue for model 87


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



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



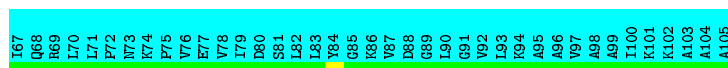
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C:  78% 13% 7%



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

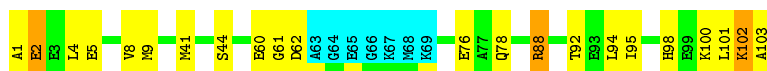
Chain D:  9% 8% 83%



4.2.88 Score per residue for model 88

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

Chain A:  72% 18% 7%



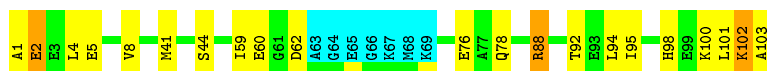
- Molecule 1: N,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain B:  73% 17% 7%



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

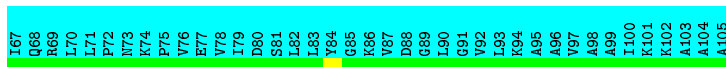
Chain C:  73% 17% 7%



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

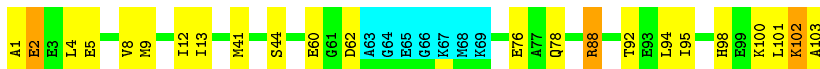
Chain D:  9% 7% 83%



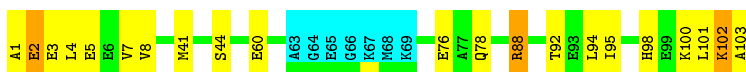


4.2.89 Score per residue for model 89

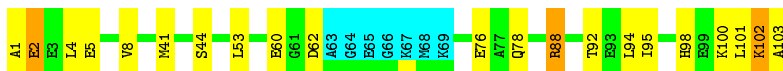
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



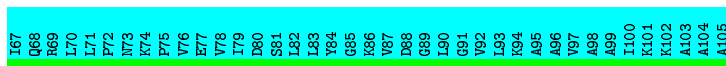
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



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

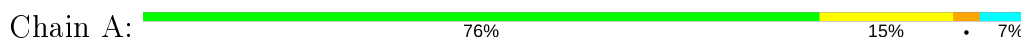


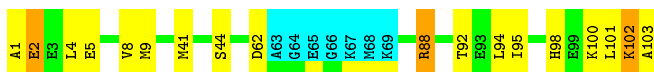
- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT



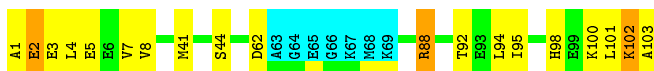
4.2.90 Score per residue for model 90

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

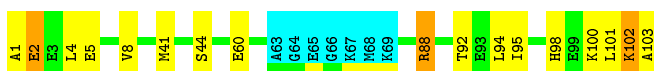




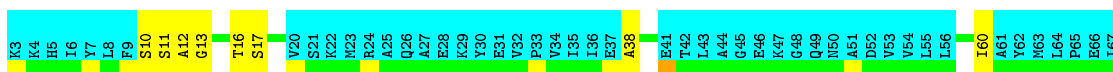
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



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

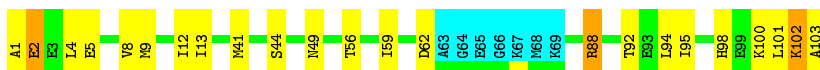


- Molecule 2: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIB COMPONENT



4.2.91 Score per residue for model 91 (medoid)

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

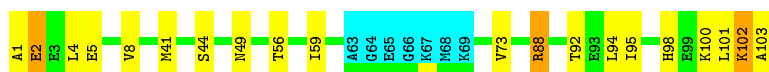


- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT



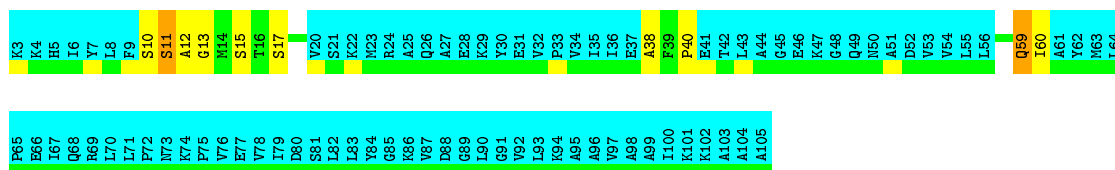
- Molecule 1: N\,N'-DIACETYLCHITOBIOSE-SPECIFIC PHOSPHOTRANSFERASE ENZYME IIA COMPONENT

Chain C:  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. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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 [i](#)

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:OE1	1:B:17:GLN:N	0.72	2.22	81	1
1:A:17:GLN:OE1	1:A:17:GLN:N	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	4
2:D:13:GLY:O	2:D:17:SER:N	0.64	2.30	91	91

Continued on next page...

Continued from previous page...

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:CA	2:D:59:GLN:OE1	0.61	2.48	91	1
1:A:6:GLU:OE1	1:A:6:GLU:N	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:OE1	1:B:6:GLU:N	0.60	2.34	68	2
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	3
1:C:60:GLU:O	1:C:60:GLU:CD	0.58	2.42	40	3
1:C:24:ALA:O	1:C:28:GLN:OE1	0.58	2.22	43	3
1:A:9:MET:C	2:D:59:GLN:HE22	0.58	2.02	32	1
2:D:59:GLN:OE1	2:D:59:GLN:N	0.57	2.37	84	2
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:CD	2:D:59:GLN:N	0.56	2.59	20	3
1:A:24:ALA:O	1:A:28:GLN:OE1	0.56	2.24	43	3
1:B:6:GLU:N	1:B:6:GLU:OE1	0.56	2.38	57	2
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
2:D:59:GLN:N	2:D:59:GLN:CD	0.55	2.59	34	3
1:C:60:GLU:CD	1:C:60:GLU:O	0.55	2.44	65	1
1:B:6:GLU:OE1	1:B:6:GLU:O	0.55	2.24	83	1
2:D:59:GLN:CD	2:D:59:GLN:H	0.55	2.06	6	4
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:CD	1:A:6:GLU:O	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:C:6:GLU:N	1:C:6:GLU:OE1	0.53	2.42	61	1
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
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	46	45
1:C:88:ARG:C	1:C:88:ARG:NH1	0.52	2.63	5	46
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:OD2	1:A:62:ASP:O	0.52	2.28	49	4
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	5
1:B:62:ASP:O	1:B:62:ASP:OD2	0.52	2.28	49	5
1:B:88:ARG:NH2	1:B:92:THR:OG1	0.52	2.44	2	91
1:C:62:ASP:O	1:C:62:ASP:OD2	0.52	2.28	29	2
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	4
1:A:6:GLU:OE2	1:A:6:GLU:O	0.51	2.29	83	1
1:A:62:ASP:OD2	1:A:74:LEU:HD22	0.51	2.06	27	2
1:C:62:ASP:OD1	1:C:74:LEU:HD22	0.51	2.05	66	3
1:A:62:ASP:OD1	1:A:74:LEU:HD22	0.51	2.06	66	3
1:B:62:ASP:OD2	1:B:74:LEU:HD22	0.51	2.06	27	3
1:C:62:ASP:OD1	1:C:62:ASP:O	0.51	2.29	4	4
1:B:62:ASP:OD2	1:B:62:ASP:O	0.50	2.29	1	2
1:A:13:ILE:CD1	2:D:11:SER:OG	0.50	2.59	40	4
1:C:62:ASP:OD2	1:C:62:ASP:O	0.50	2.30	49	5
1:C:60:GLU:C	1:C:60:GLU:CD	0.50	2.70	54	9
1:C:62:ASP:OD2	1:C:74:LEU:HD22	0.50	2.06	27	2
1:A:62:ASP:O	1:A:62:ASP:OD1	0.50	2.30	34	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:2:GLU:O	1:B:6:GLU:OE2	0.49	2.31	39	2
1:A:62:ASP:O	1:A:62:ASP:OD2	0.49	2.30	29	3
1:B:62:ASP:OD1	1:B:62:ASP:O	0.49	2.30	4	1
1:C:60:GLU:CD	1:C:60:GLU:C	0.49	2.71	69	11
1:B:57:LYS:NZ	1:B:57:LYS:HB2	0.49	2.21	53	1
1:A:5:GLU:OE2	2:D:15:SER:OG	0.49	2.30	55	6
1:C:62:ASP:O	1:C:62:ASP:OD1	0.49	2.30	65	2
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
2:D:59:GLN:H	2:D:59:GLN:CD	0.48	2.12	48	5
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	52
1:C:60:GLU:OE2	1:C:61:GLY:N	0.48	2.45	32	4
1:C:60:GLU:O	1:C:60:GLU:OE2	0.48	2.31	84	2
1:C:88:ARG:HH11	1:C:88:ARG:C	0.48	2.12	7	39
1:B:62:ASP:C	1:B:62:ASP:OD1	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	12
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	48
1:B:60:GLU:CD	1:B:60:GLU:C	0.47	2.72	63	11
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:C:88:ARG:O	1:C:88:ARG:NH1	0.47	2.47	14	43
1:B:60:GLU:C	1:B:60:GLU:CD	0.47	2.72	54	8
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:OE2	1:B:60:GLU:O	0.47	2.32	84	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:59:GLN:OE1	2:D:59:GLN:CA	0.47	2.61	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	21
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:HA	2:D:59:GLN:OE1	0.46	2.08	91	1
1:A:102:LYS:HB3	1:A:102:LYS:HZ3	0.46	1.69	17	21
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:CB	1:A:102:LYS:HZ3	0.46	2.24	17	19
1:A:102:LYS:HZ3	1:A:102:LYS:CB	0.46	2.24	81	23
1:B:60:GLU:C	1:B:60:GLU:OE2	0.46	2.54	47	2
1:C:62:ASP:OD1	1:C:62:ASP:C	0.46	2.53	11	1
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:C	1:B:88:ARG:NH1	0.46	2.70	8	51
1:B:88:ARG:NH1	1:B:88:ARG:C	0.46	2.70	36	40
1:C:102:LYS:HZ3	1:C:102:LYS:CB	0.46	2.23	75	2
1:B:88:ARG:C	1:B:88:ARG:HH11	0.45	2.14	14	54
1:B:88:ARG:HH11	1:B:88:ARG:C	0.45	2.14	37	37
1:B:78:GLN:OE1	1:C:76:GLU:OE1	0.45	2.34	27	6
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:NZ	1:C:57:LYS:CB	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:C	1:C:60:GLU:OE1	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:C	1:A:102:LYS:HZ3	0.45	2.15	74	40
1:A:1:ALA:N	1:A:5:GLU:HG2	0.45	2.26	86	4
1:A:102:LYS:HZ3	1:A:102:LYS:C	0.45	2.15	83	51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:60:GLU:OE2	1:B:60:GLU:C	0.45	2.55	20	3
1:B:1:ALA:O	1:B:5:GLU:CB	0.45	2.65	43	91
1:A:60:GLU:C	1:A:60:GLU:OE1	0.45	2.55	67	1
1:A:57:LYS:NZ	1:A:57:LYS:CB	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:C	1:A:60:GLU:OE2	0.45	2.55	51	3
1:B:60:GLU:OE1	1:B:60:GLU:C	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	5
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:C	1:C:102:LYS:HZ3	0.44	2.16	64	45
1:C:102:LYS:HZ3	1:C:102:LYS:C	0.44	2.16	72	46
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:HB2	1:A:57:LYS:NZ	0.44	2.28	53	1
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	63	91
1:A:60:GLU:O	1:A:60:GLU:OE2	0.44	2.35	84	1
1:C:100:LYS:C	1:C:102:LYS:H	0.44	2.17	4	91
1:A:1:ALA:O	1:A:5:GLU:N	0.44	2.41	75	91
1:C:1:ALA:H2	1:C:5:GLU:CG	0.44	2.25	86	4
1:C:49:ASN:C	1:C:49:ASN:OD1	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:C:60:GLU:OE2	1:C:60:GLU:C	0.43	2.57	63	2
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:N	1:A:62:ASP:OD2	0.43	2.51	32	2
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:OD2	0.43	2.51	19	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:62:ASP:OD1	1:C:62:ASP:N	0.43	2.51	39	1
1:A:60:GLU:OE2	1:A:60:GLU:C	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:C	1:B:60:GLU:OE1	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:C	1:B:102:LYS:HZ3	0.42	2.18	62	47
2:D:10:SER:C	2:D:12:ALA:N	0.42	2.71	91	49
1:B:102:LYS:HZ3	1:B:102:LYS:C	0.42	2.18	65	44
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:C:62:ASP:N	1:C:62:ASP:OD1	0.42	2.52	60	3
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:B:102:LYS:HB3	1:B:102:LYS:HZ3	0.42	1.74	41	27
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
1:B:3:GLU:O	1:B:7:VAL:N	0.42	2.40	81	73
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:C	1:A:49:ASN:OD1	0.42	2.57	91	1
1:B:62:ASP:OD2	1:B:62:ASP:N	0.42	2.53	32	1
1:C:102:LYS:O	1:C:103:ALA:OXT	0.42	2.38	7	91
1:A:62:ASP:OD2	1:A:62:ASP:N	0.42	2.52	3	3
1:B:102:LYS:HZ3	1:B:102:LYS:HB3	0.42	1.74	45	21
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	3
1:B:62:ASP:N	1:B:62:ASP:OD2	0.42	2.52	19	1
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:CA	1:B:28:GLN:NE2	0.42	2.83	56	3
1:A:13:ILE:HG22	1:A:17:GLN:NE2	0.42	2.30	71	1
1:A:60:GLU:C	1:A:60:GLU:CD	0.41	2.79	36	5
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:A:60:GLU:OE1	1:A:60:GLU:C	0.41	2.59	26	1
1:A:6:GLU:C	1:A:6:GLU:CD	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	11	46
1:B:88:ARG:HH11	1:B:88:ARG:CG	0.41	2.29	24	39
1:B:88:ARG:O	1:B:88:ARG:NH1	0.41	2.54	2	45
1:B:88:ARG:CG	1:B:88:ARG:HH11	0.41	2.29	35	52
1:A:62:ASP:OD1	1:A:62:ASP:N	0.41	2.53	70	3
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:OD2	1:C:62:ASP:C	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: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:5:GLU:O	1:B:5:GLU:OE1	0.40	2.39	40	1
1:B:102:LYS:HZ3	1:B:102:LYS:CB	0.40	2.29	64	3
1:A:28:GLN:CA	1:A:28:GLN:NE2	0.40	2.83	56	1
1:B:102:LYS:CB	1:B:102:LYS:HZ3	0.40	2.29	43	2
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 [i](#)

6.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all 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	C	2	GLU	91
1	A	2	GLU	91
1	B	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 [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all 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	B	88	ARG	91
1	B	102	LYS	91
1	C	44	SER	91
1	A	102	LYS	91
1	A	88	ARG	91
1	B	44	SER	91
1	C	88	ARG	91
1	A	44	SER	91
1	C	102	LYS	91
2	D	11	SER	33
2	D	59	GLN	9
1	A	6	GLU	4
1	C	60	GLU	4
1	B	60	GLU	4
1	A	60	GLU	4
1	C	28	GLN	3
1	C	6	GLU	3
1	A	28	GLN	3
1	B	28	GLN	3
1	B	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 carbohydrates 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