Full wwPDB NMR Structure Validation Report (i)

Apr 27, 2016 – 08:53 AM BST

PDB ID	:	2V93
Title	:	EQUILLIBRIUM MIXTURE OF OPEN AND PARTIALLY-CLOSED SPECIES IN THE APO STATE OF MALTODEXTRIN-BINDING PROTEIN BY PARAMAGNETIC RELAXATION ENHANCEMENT NMR
Authors	:	Clore, G.M.; Tang, C.
Deposited on	:	2007-08-21

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
http://wwpdb.org/validation/2016/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

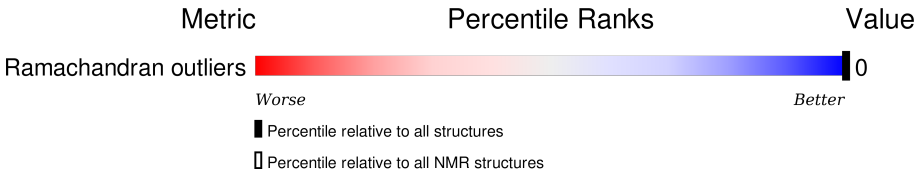
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

1 Overall quality at a glance (i)

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)
Ramachandran outliers	111179	9975

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	370	95%

2 Ensemble composition and analysis

This entry contains 50 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 39 is the overall representative, medoid model (most similar to other models).

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:81-A:87, A:103-A:105, A:266-A:268, A:311-A:313 (16)	-0.00	39

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

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

NmrClust was unable to cluster the ensemble.

Error message: No clusters in NmrClust output

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3792 atoms, of which 1003 are hydrogens and 0 are deuteriums.

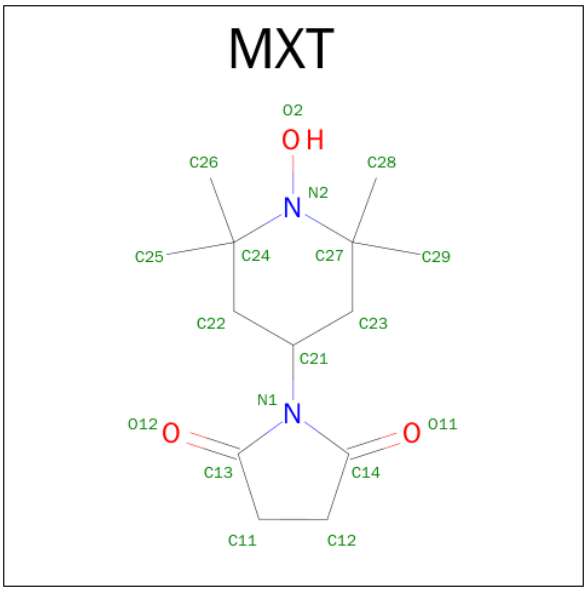
- Molecule 1 is a protein called MALTOSE-BINDING PERIPLASMIC PROTEIN.

Mol	Chain	Residues	Atoms						Trace
1	A	366	Total	C	H	N	O	S	0
			2904	1169	547	583	581	24	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	CYS	ASP	ENGINEERED MUTATION	UNP P0AEY0
A	211	CYS	SER	ENGINEERED MUTATION	UNP P0AEY0

- Molecule 2 is 1-(1-HYDROXY-2,2,6,6-TETRAMETHYLPIPERIDIN-4-YL)PYRROLIDIN E-2,5-DIONE (three-letter code: MXT) (formula: $C_{13}H_{22}N_2O_3$).



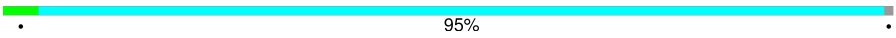
Mol	Chain	Residues	Atoms				
2	A	1	Total	C	H	N	O
			444	156	228	24	36
2	A	1	Total	C	H	N	O
			444	156	228	24	36

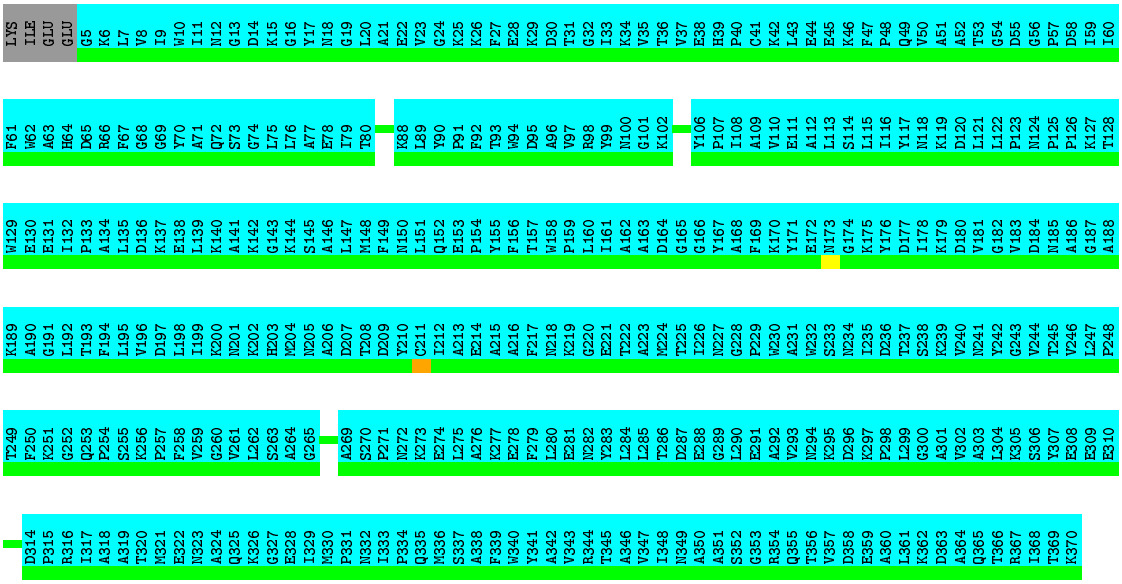
4 Residue-property plots

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: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: 

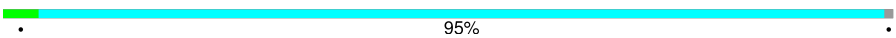


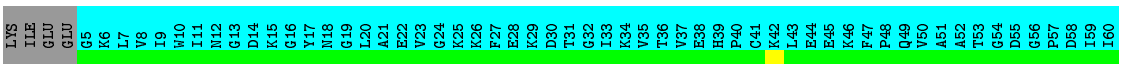
4.2 Scores per residue for each member of the ensemble

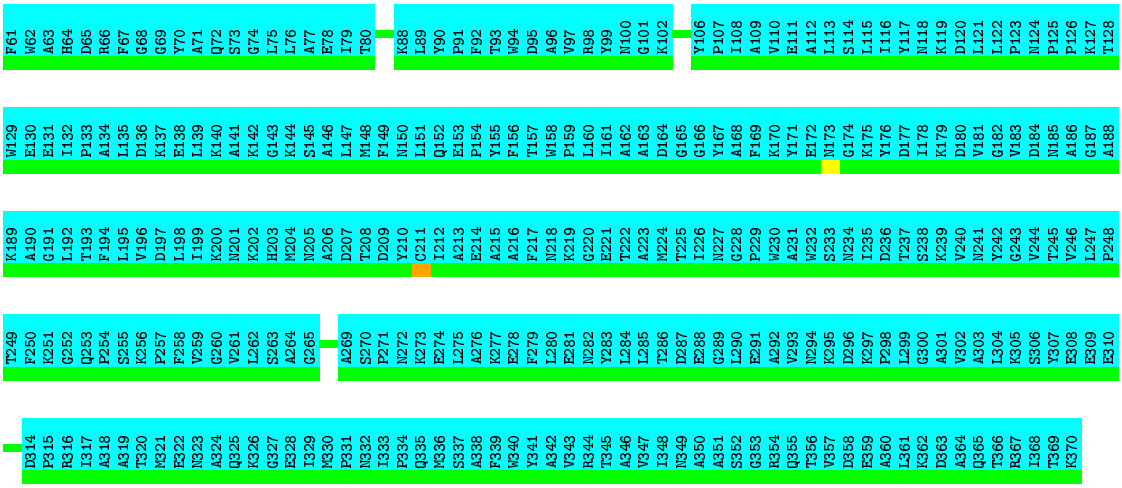
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: 

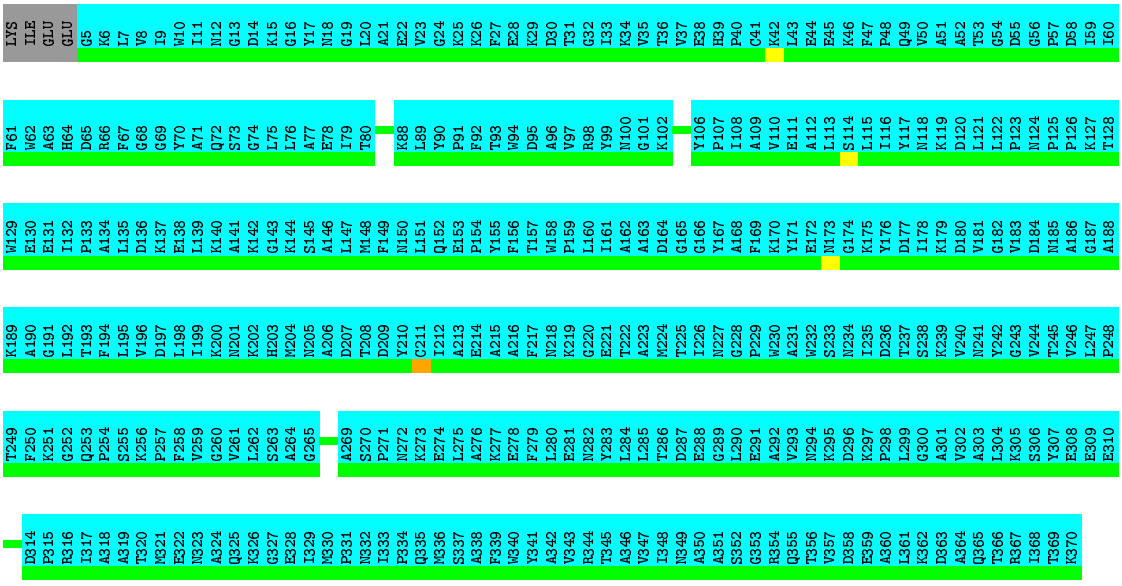




4.2.2 Score per residue for model 2

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

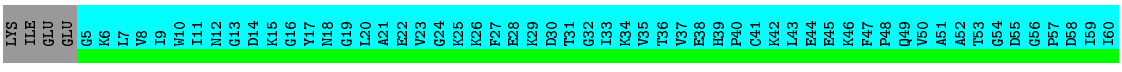
Chain A: 95%

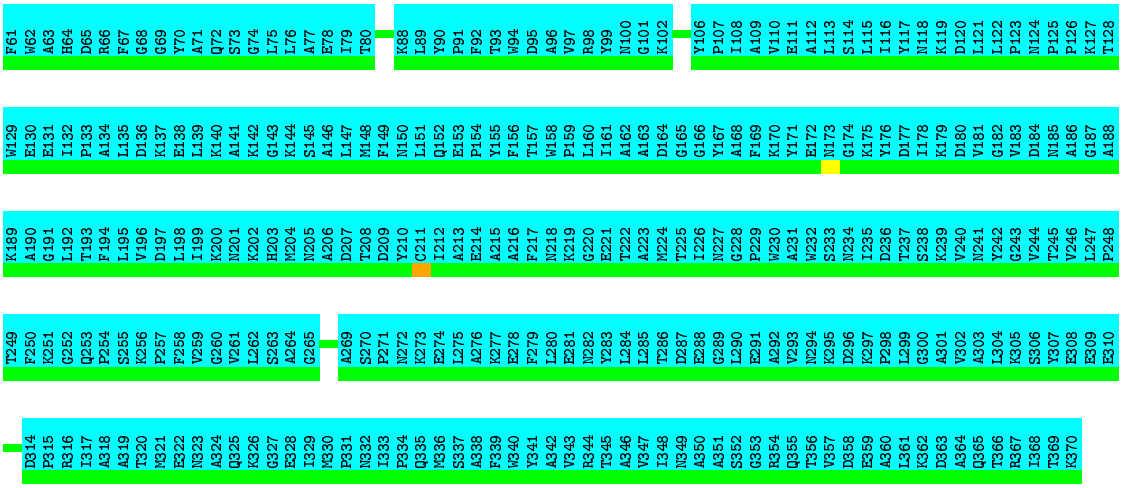


4.2.3 Score per residue for model 3

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: 95%

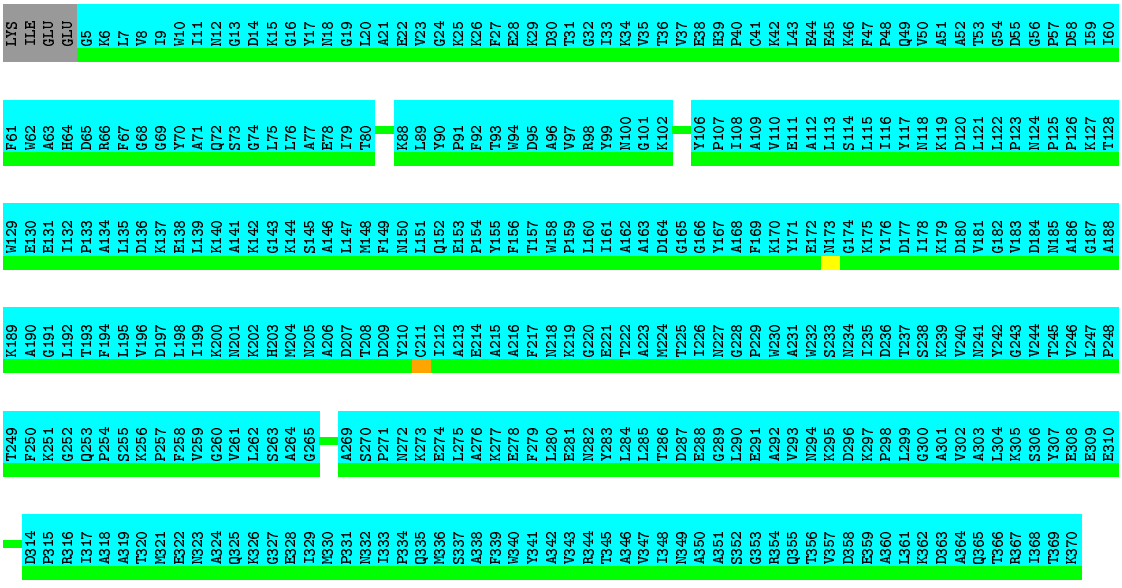




4.2.4 Score per residue for model 4

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

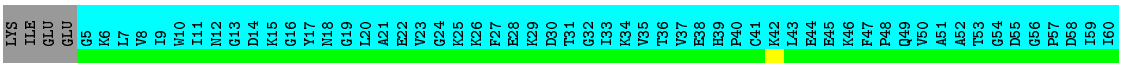
Chain A: 95%

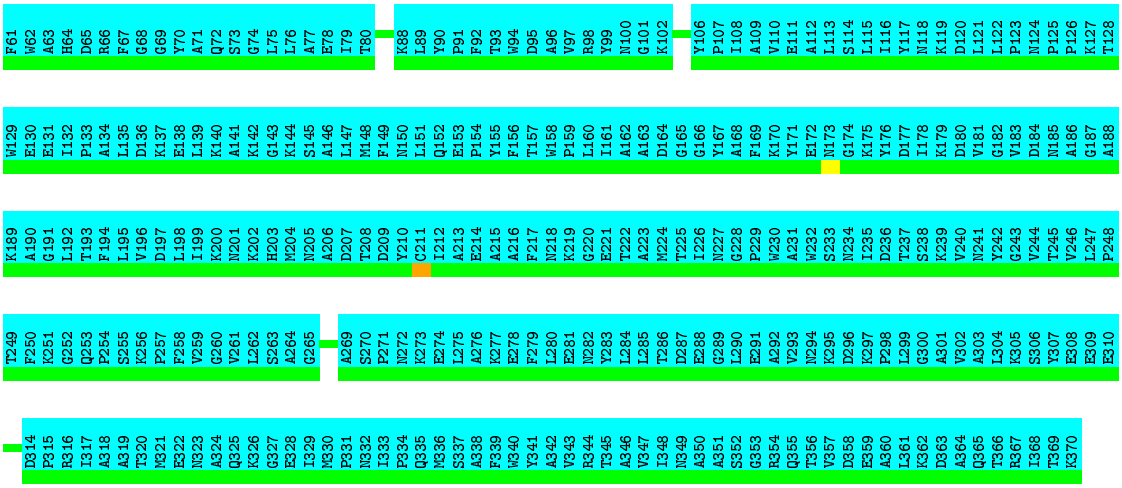


4.2.5 Score per residue for model 5

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: 95%

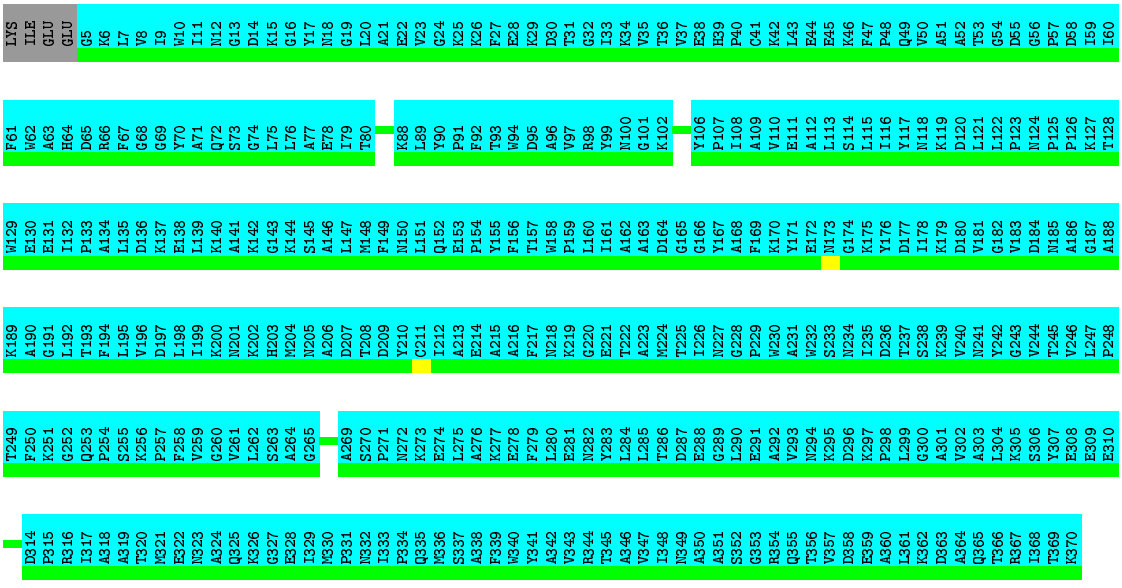




4.2.6 Score per residue for model 6

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

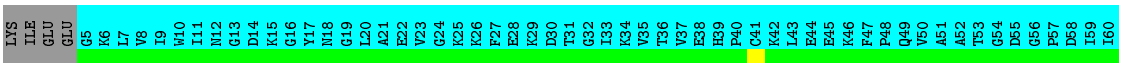
Chain A: 95%

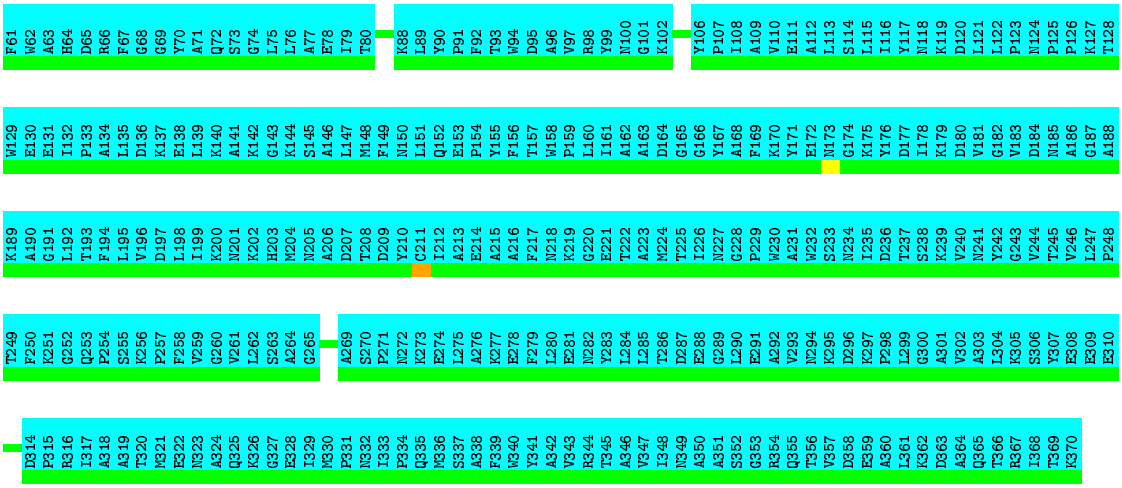


4.2.7 Score per residue for model 7

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: 95%

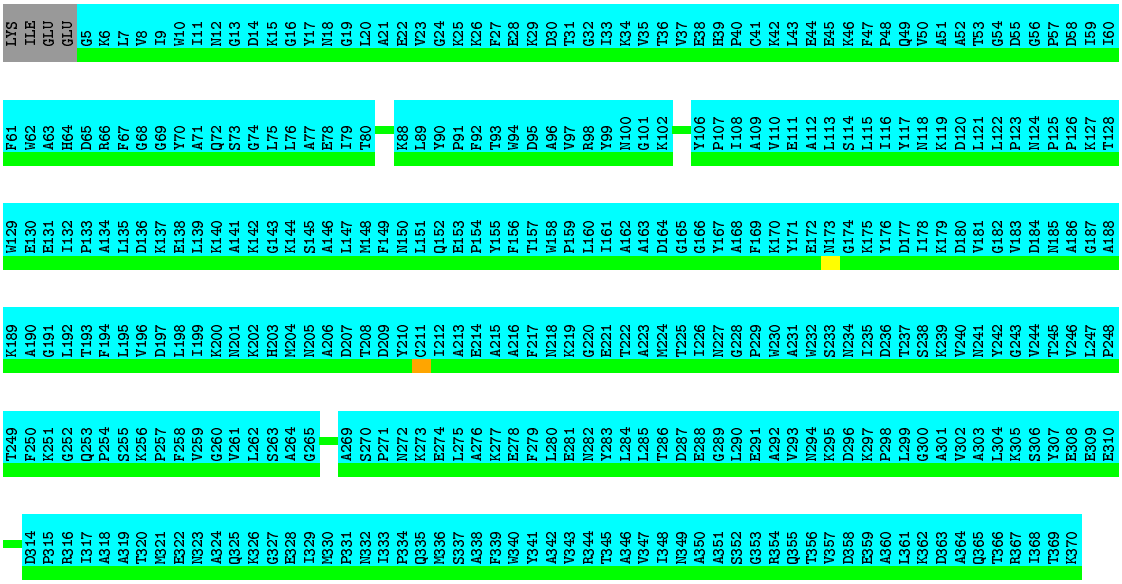




4.2.8 Score per residue for model 8

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

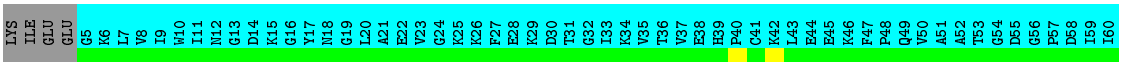
Chain A: 95%

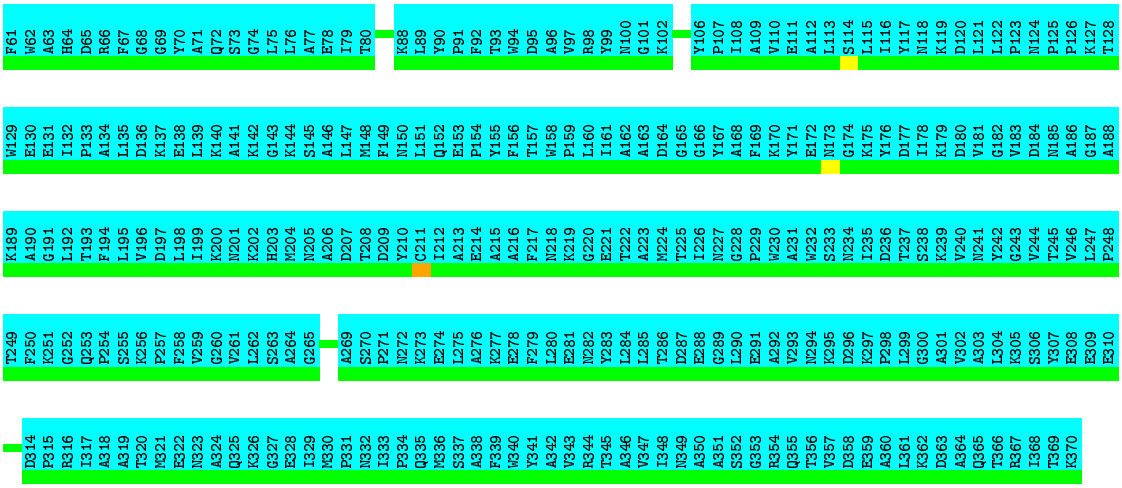


4.2.9 Score per residue for model 9

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

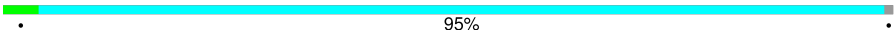
Chain A: 95%

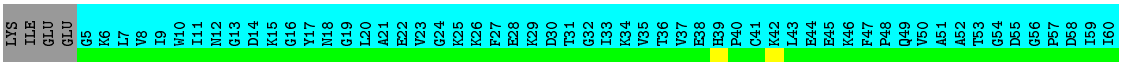




4.2.10 Score per residue for model 10

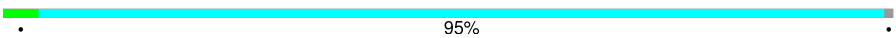
- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

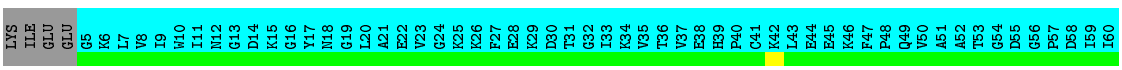
Chain A: 

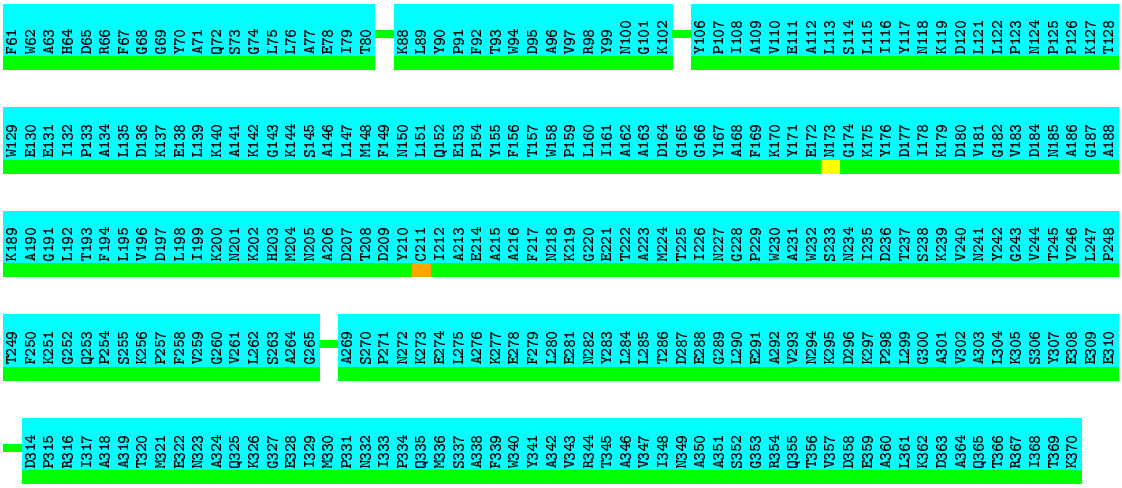


4.2.11 Score per residue for model 11

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: 

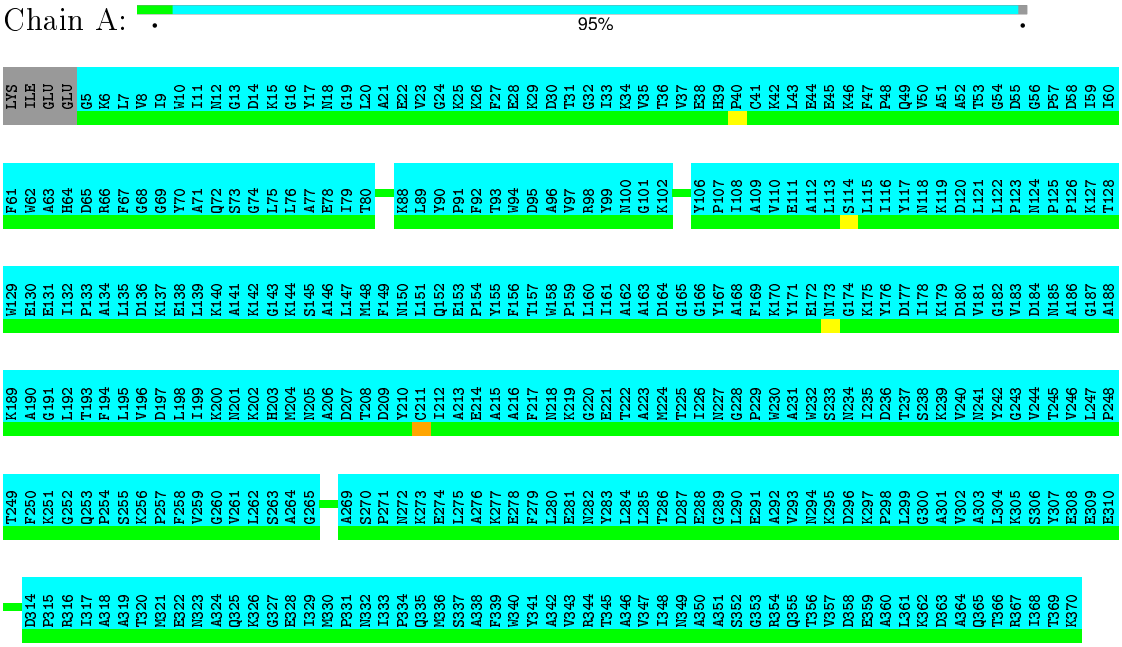




4.2.12 Score per residue for model 12

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

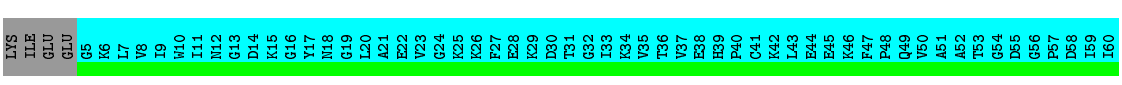
Chain A:

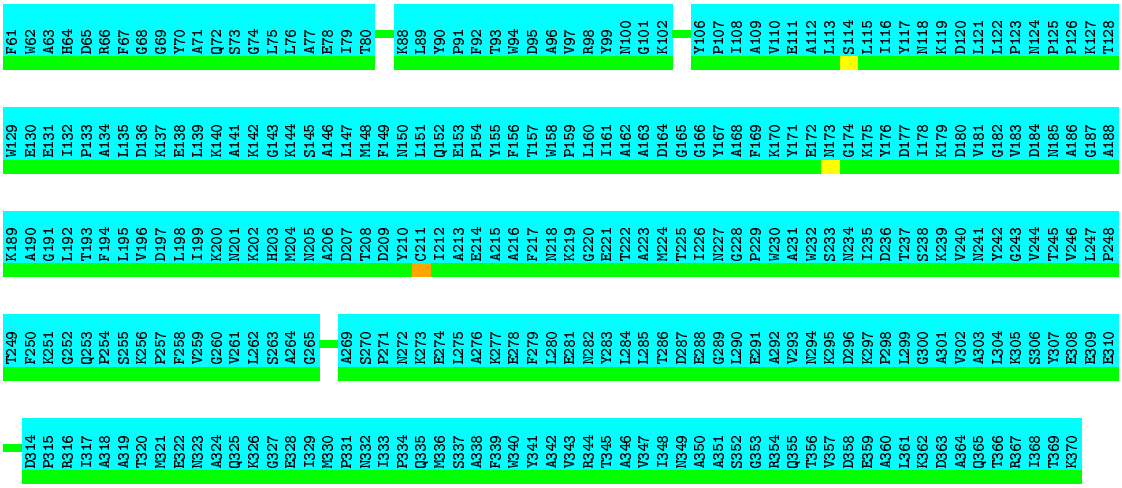


4.2.13 Score per residue for model 13

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A:

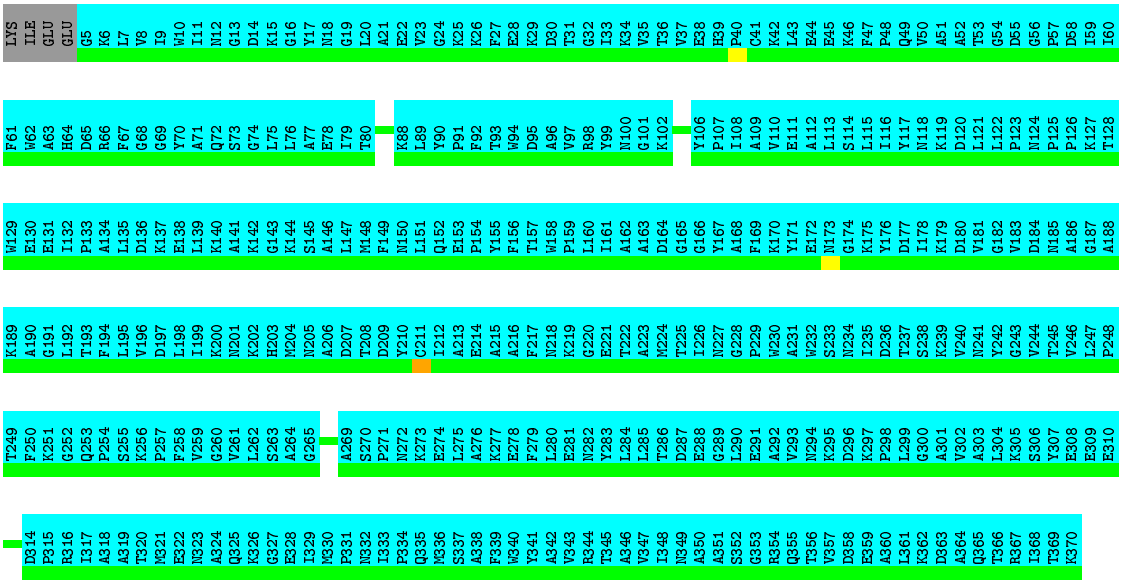




4.2.14 Score per residue for model 14

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

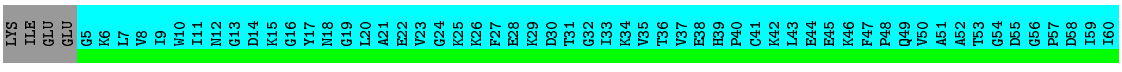
Chain A: 95%

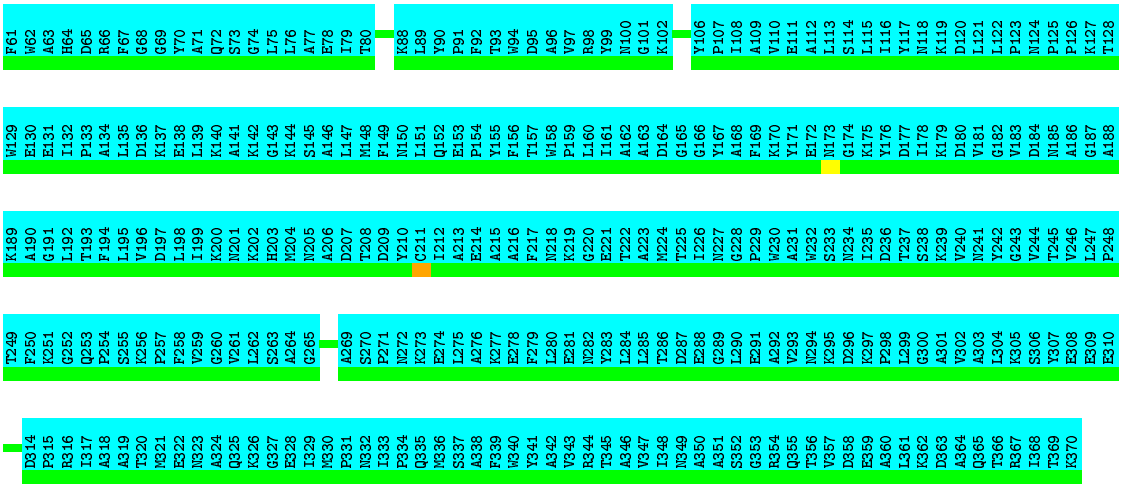


4.2.15 Score per residue for model 15

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: 95%

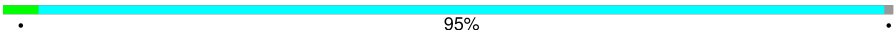


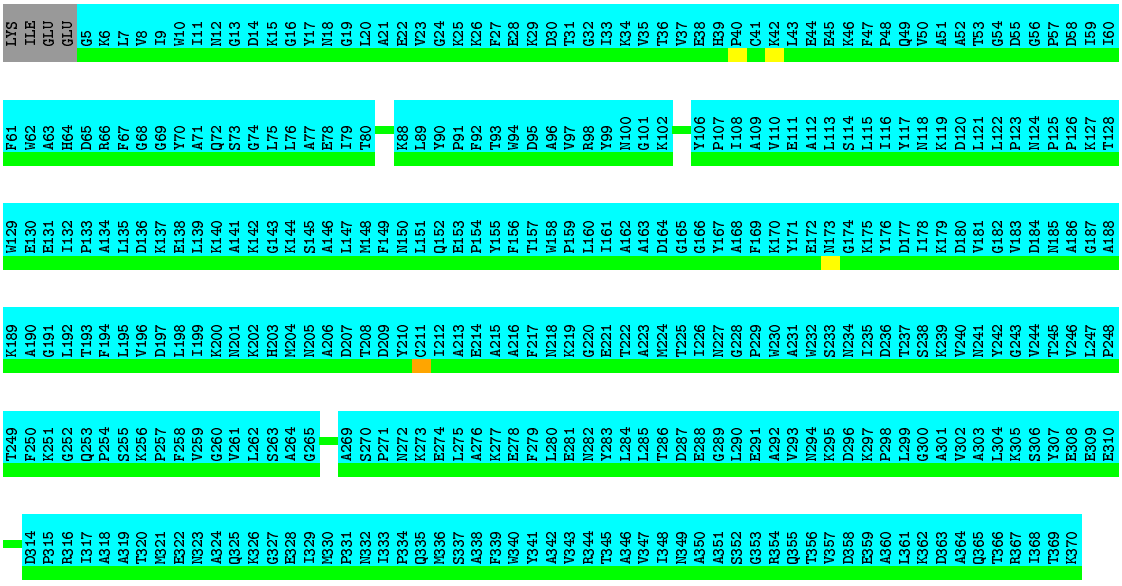


4.2.16 Score per residue for model 16

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A:

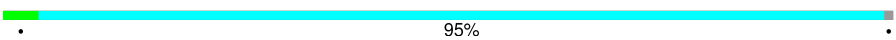


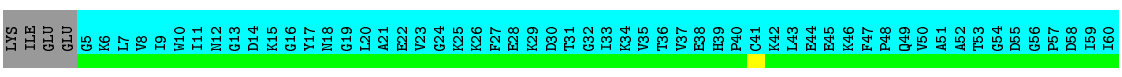


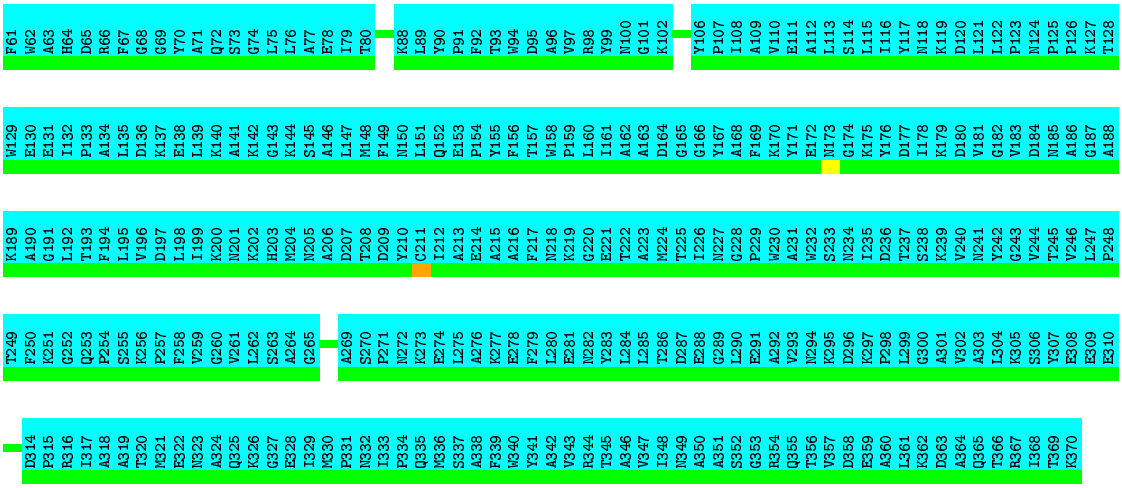
4.2.17 Score per residue for model 17

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A:



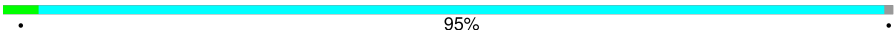


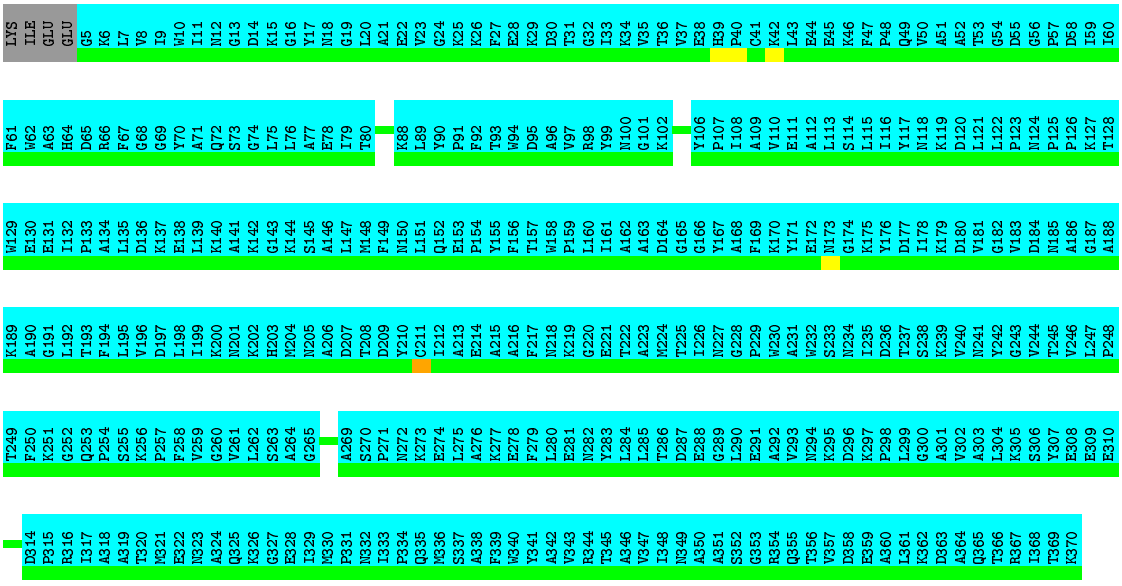


4.2.18 Score per residue for model 18

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A:

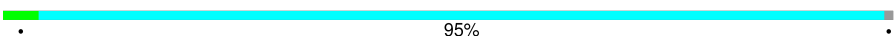


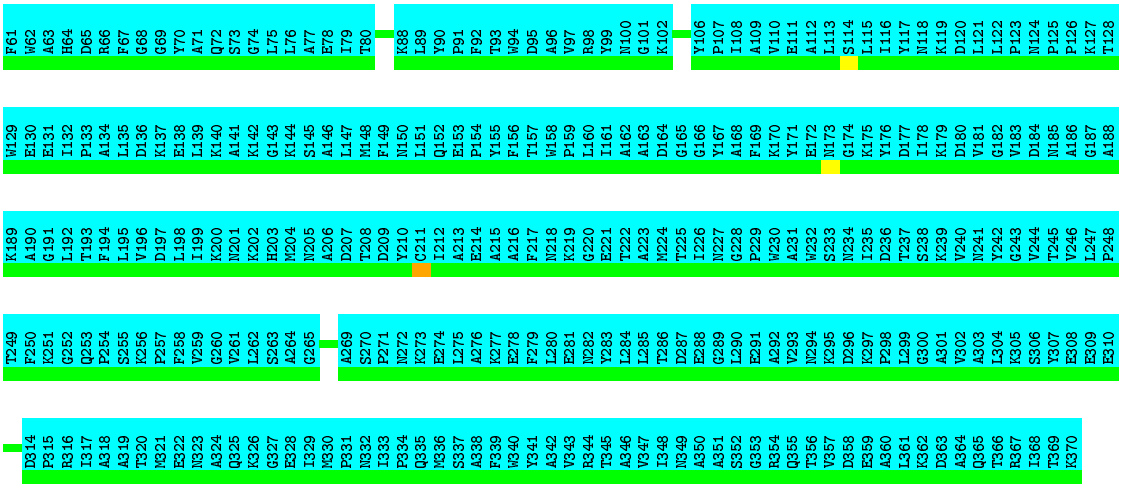


4.2.19 Score per residue for model 19

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A:

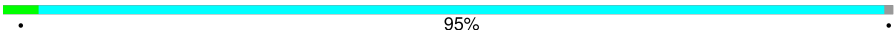


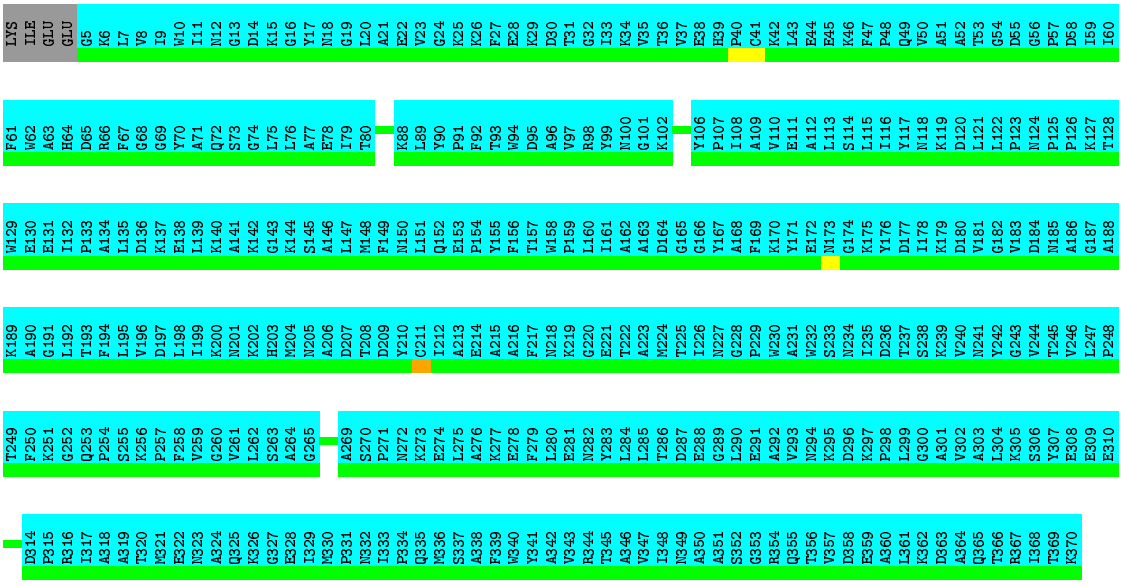


4.2.20 Score per residue for model 20

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A:

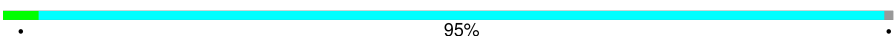


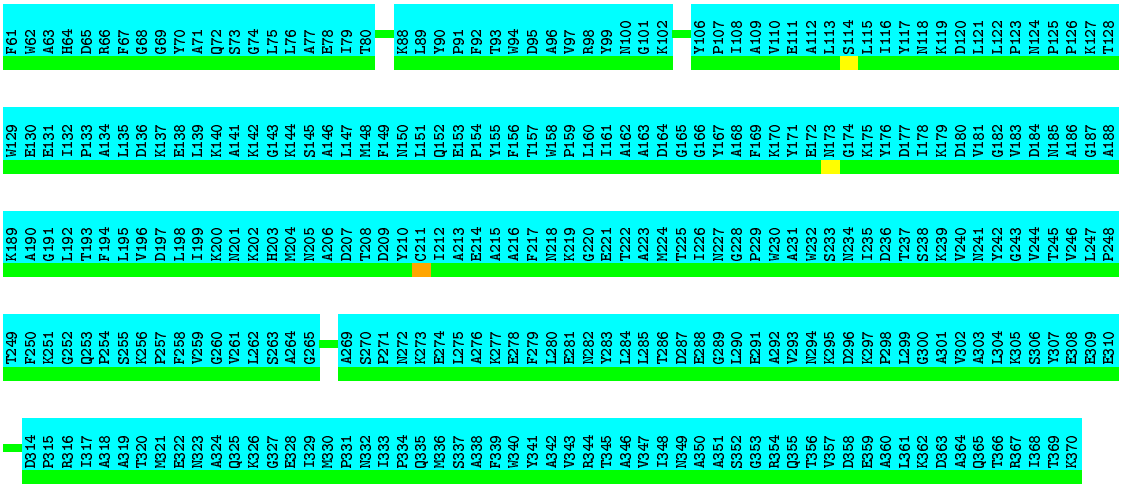


4.2.21 Score per residue for model 21

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A:

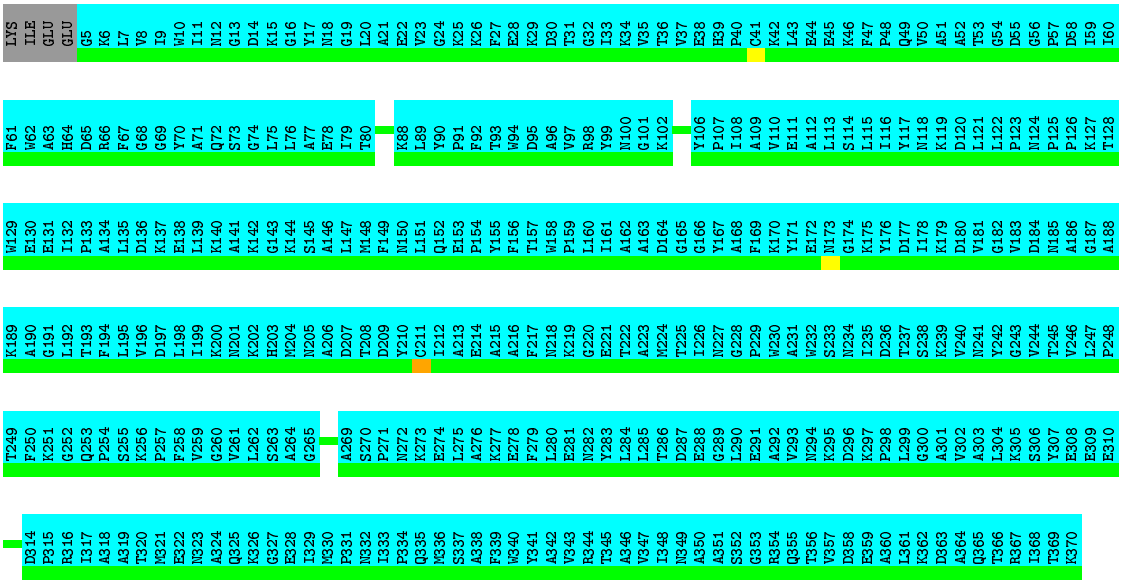




4.2.22 Score per residue for model 22

• Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

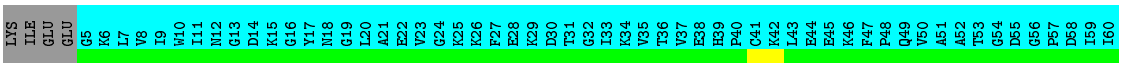
Chain A: 95%

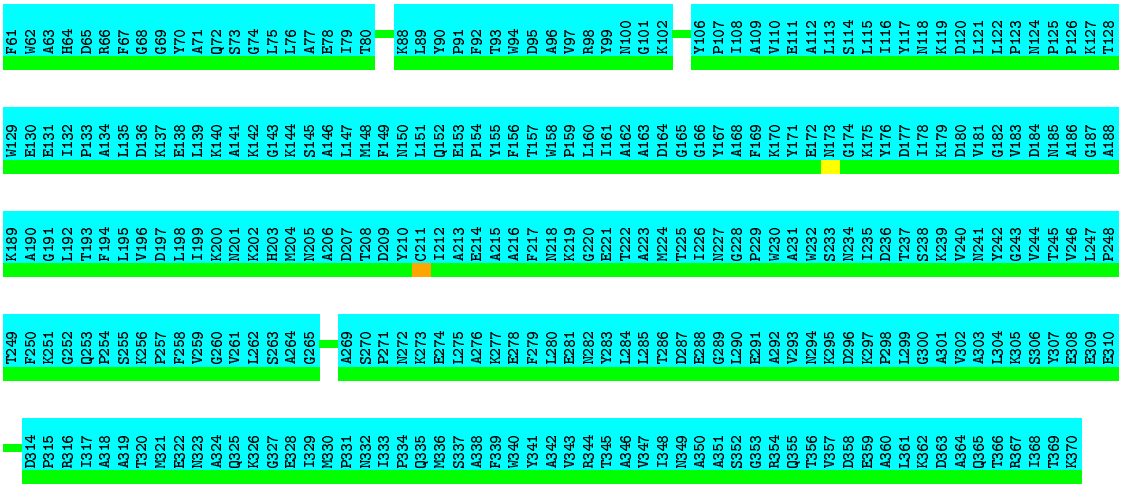


4.2.23 Score per residue for model 23

• Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: 95%

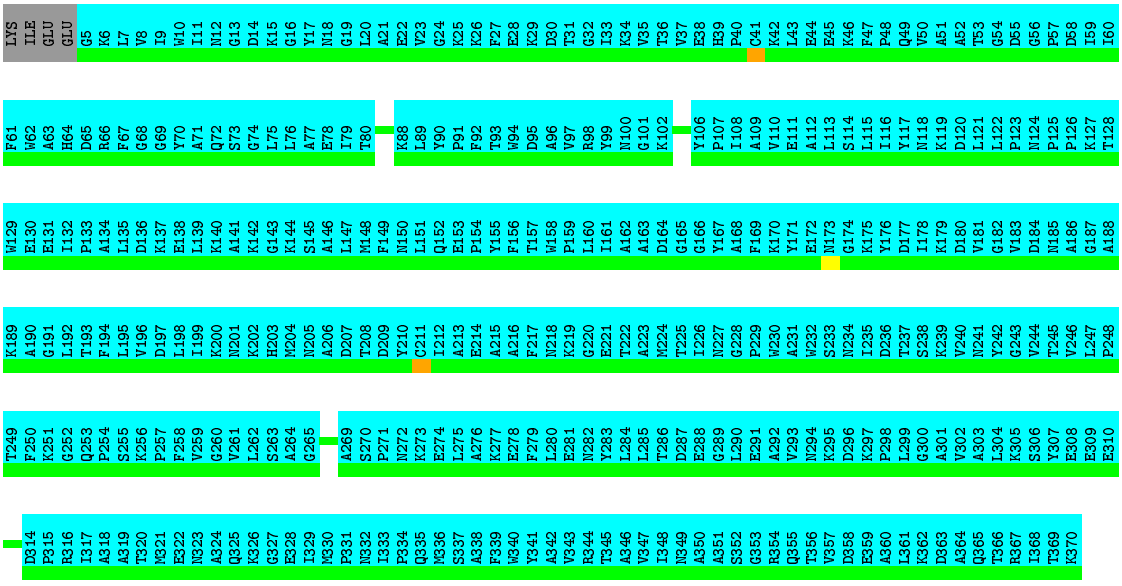




4.2.24 Score per residue for model 24

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

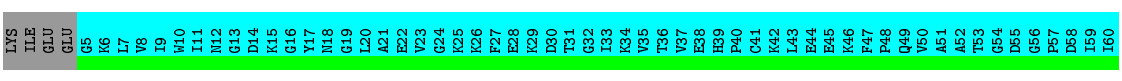
Chain A: 95%

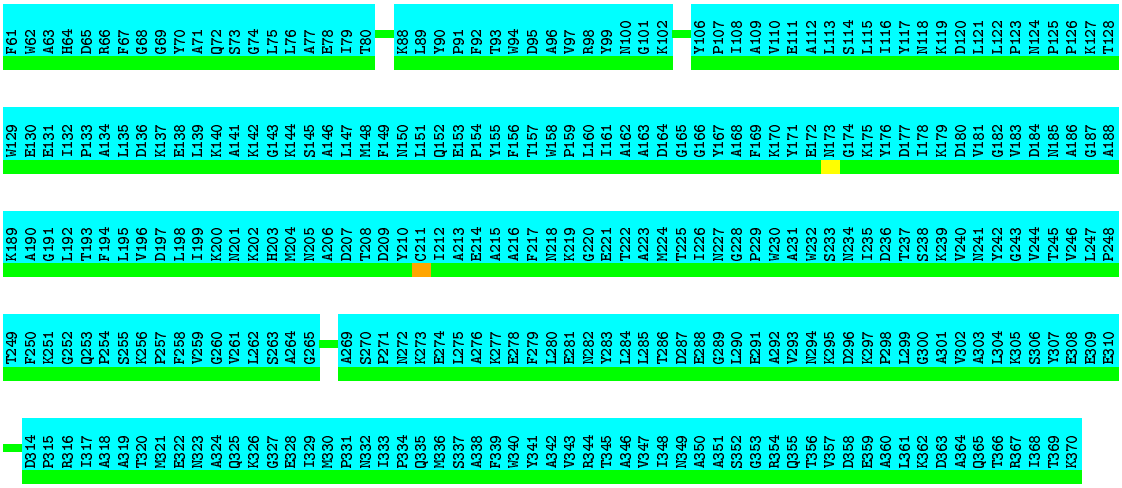


4.2.25 Score per residue for model 25

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: 95%

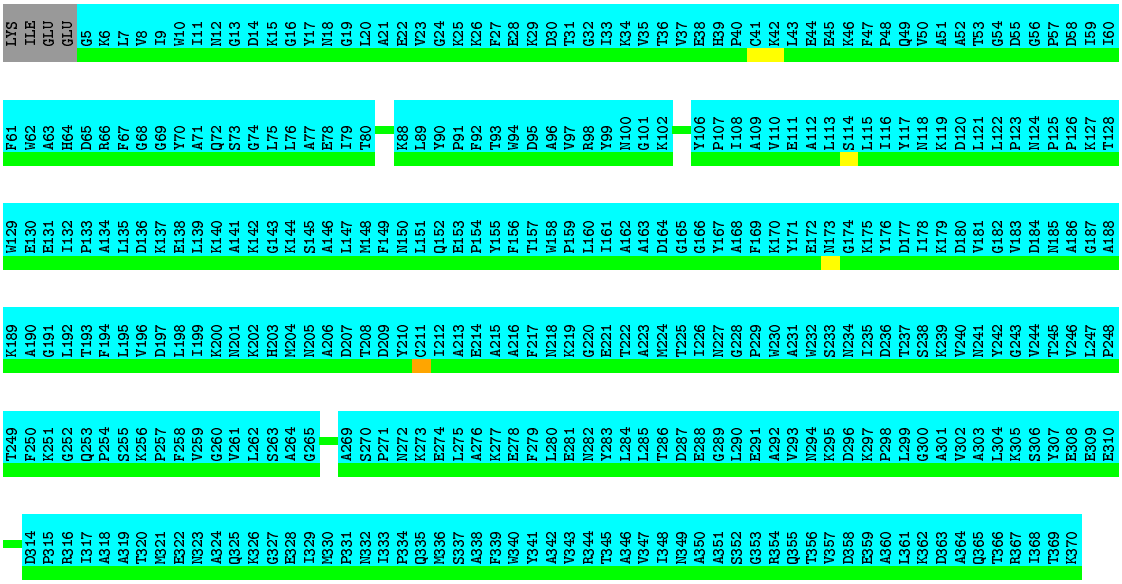




4.2.26 Score per residue for model 26

• Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

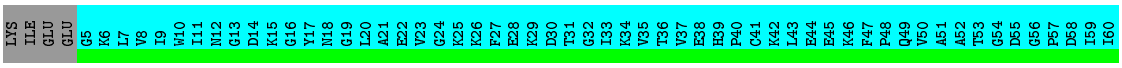
Chain A: 95%

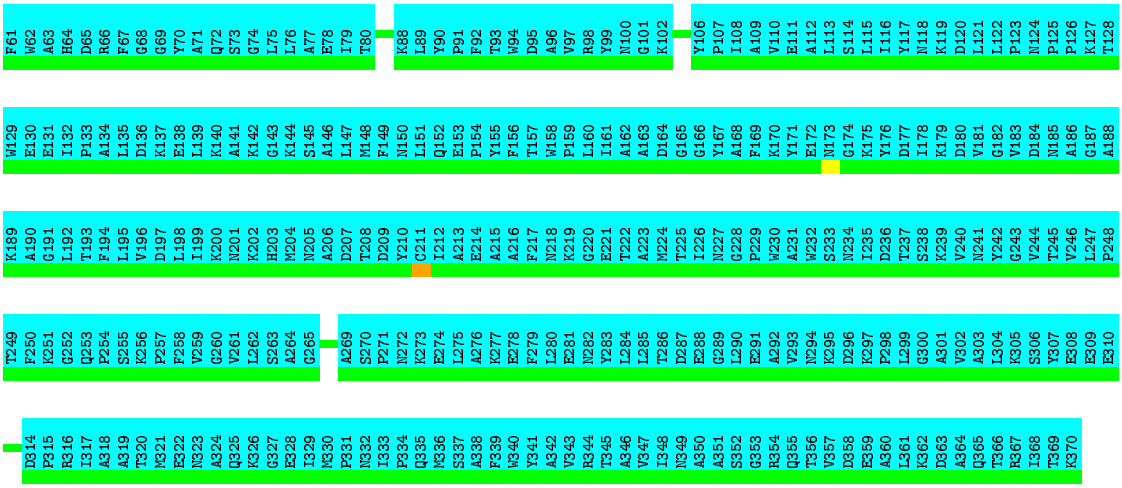


4.2.27 Score per residue for model 27

• Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: 95%

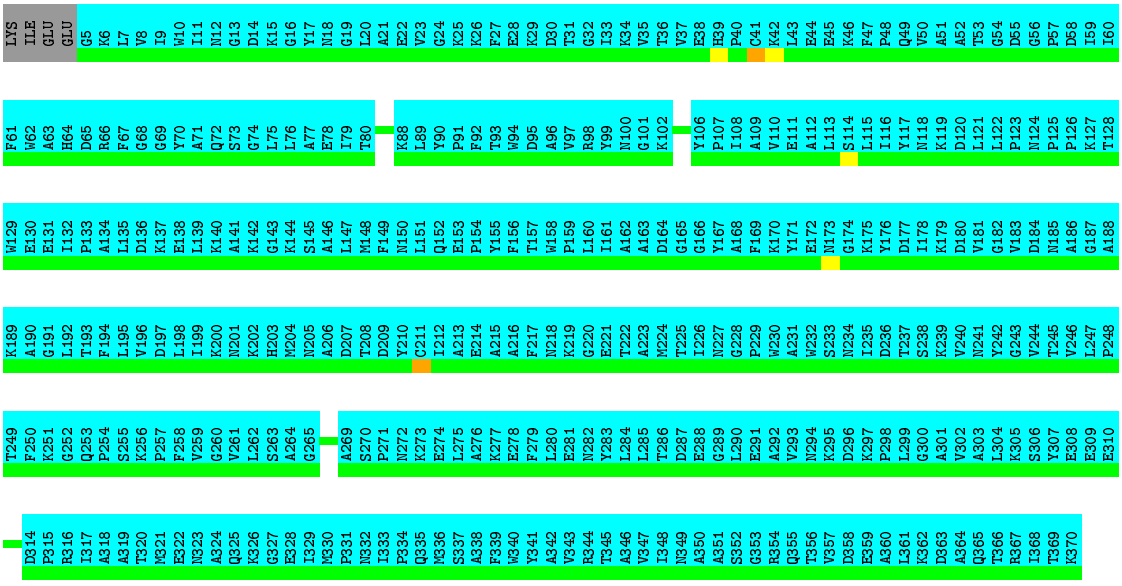




4.2.28 Score per residue for model 28

• Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

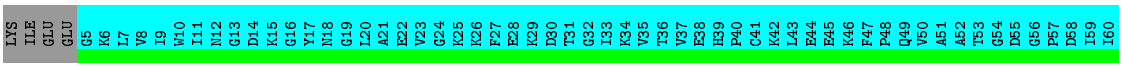
Chain A: 95%

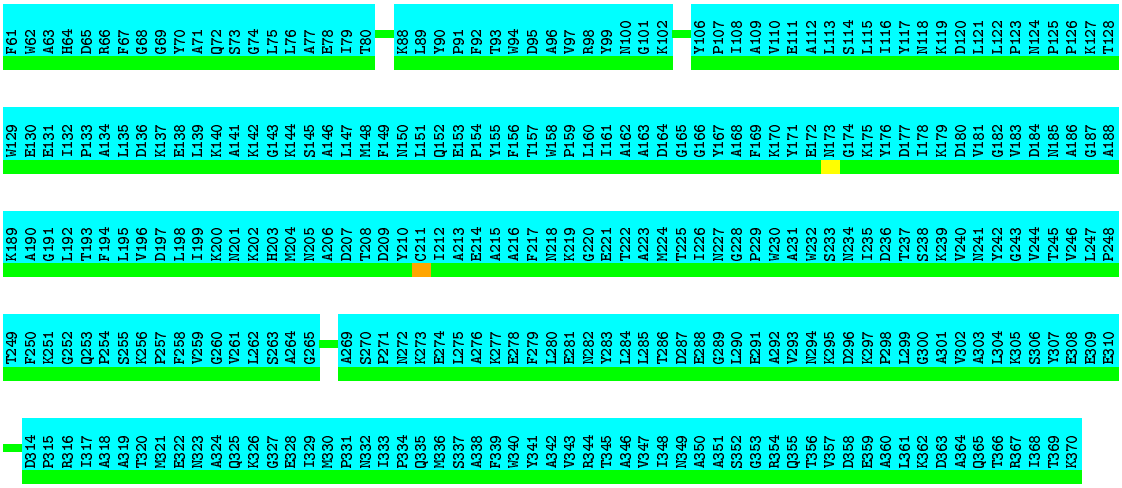


4.2.29 Score per residue for model 29

• Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: 95%

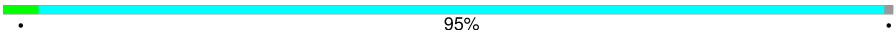


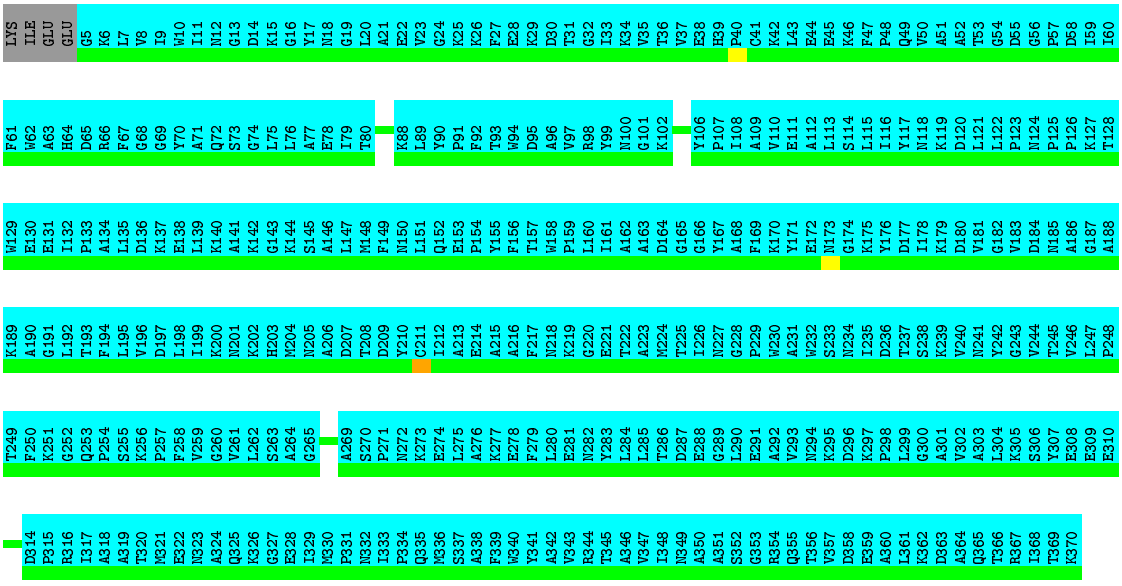


4.2.30 Score per residue for model 30

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A:

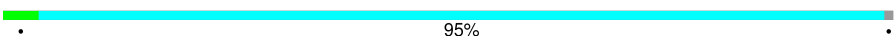


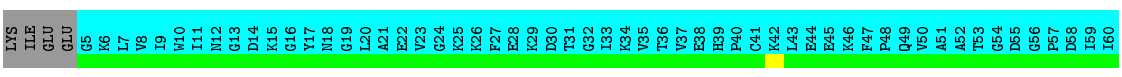


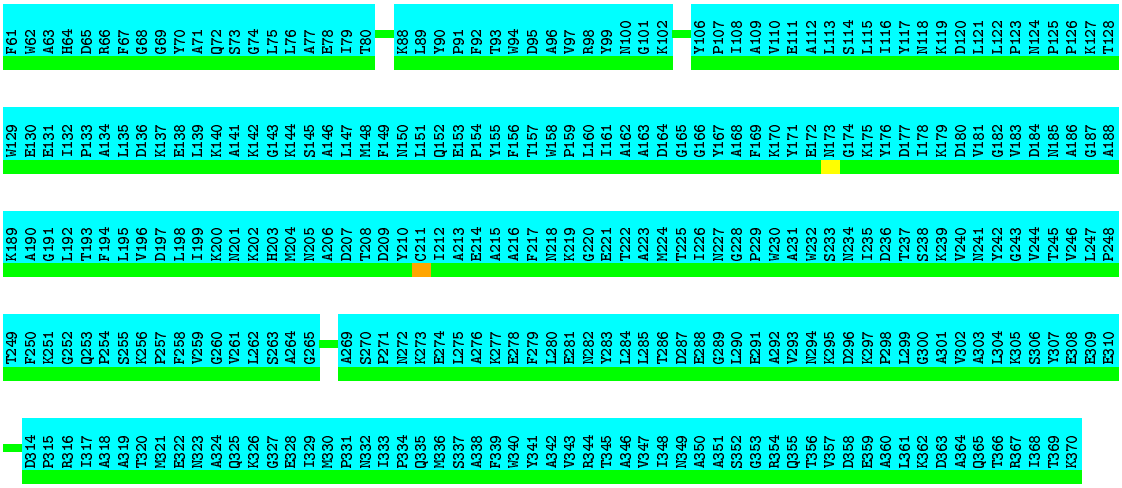
4.2.31 Score per residue for model 31

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A:



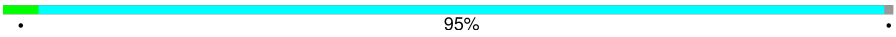


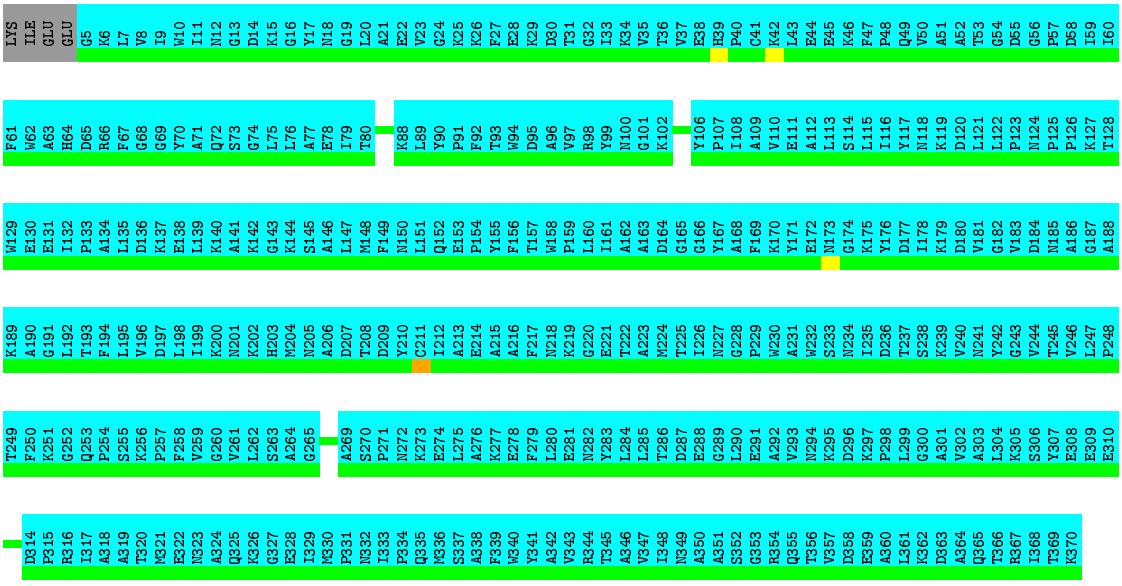


4.2.32 Score per residue for model 32

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A:

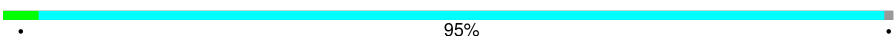


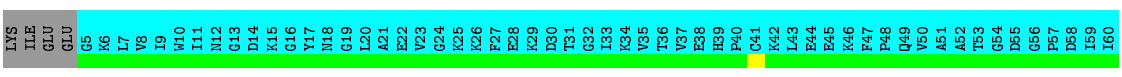


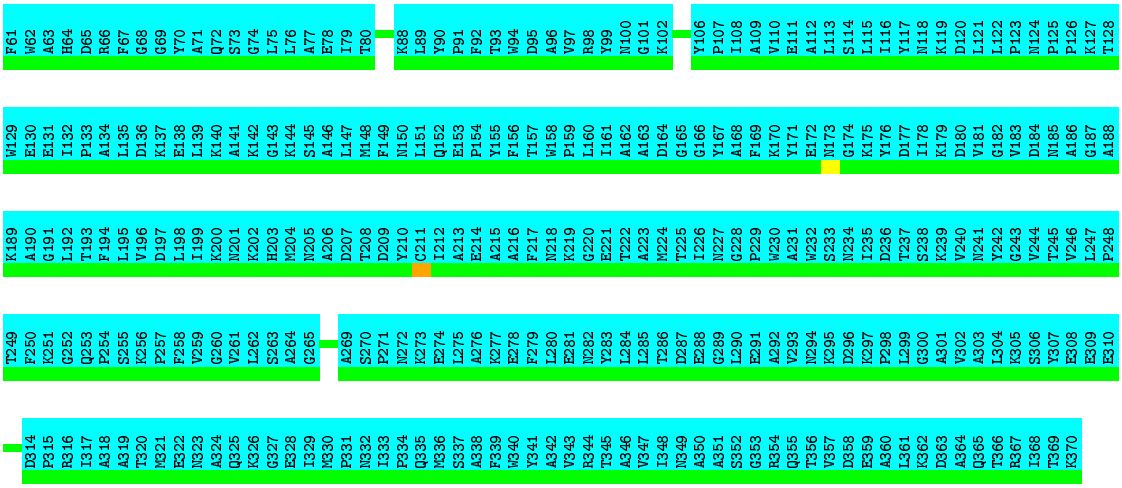
4.2.33 Score per residue for model 33

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A:



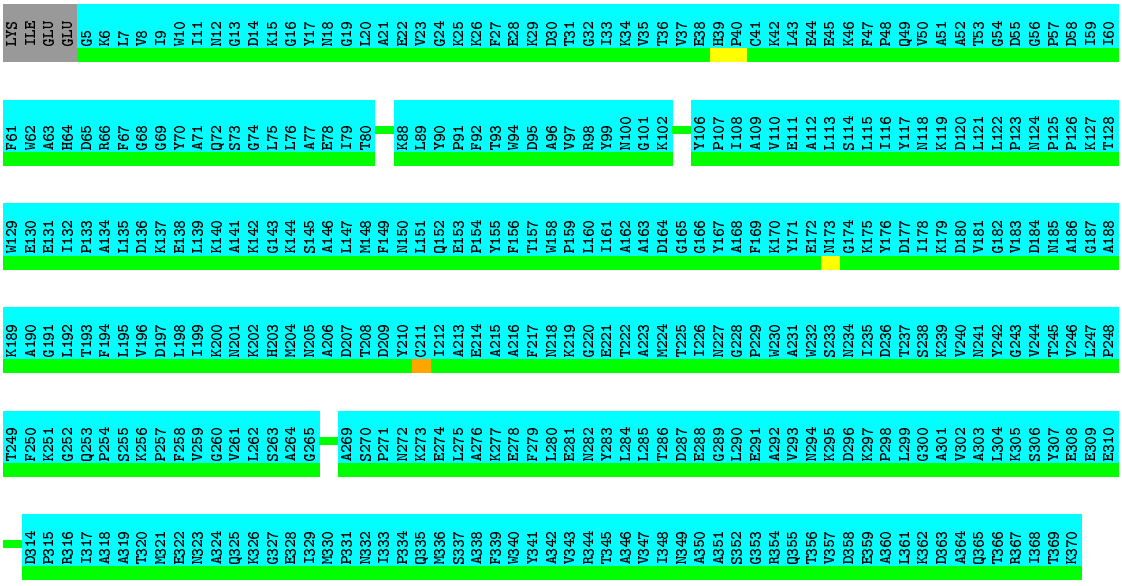




4.2.34 Score per residue for model 34

• Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

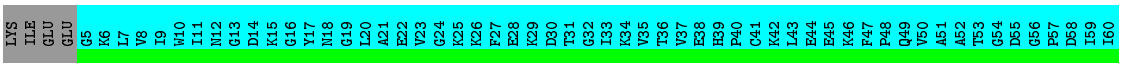
Chain A: 95%

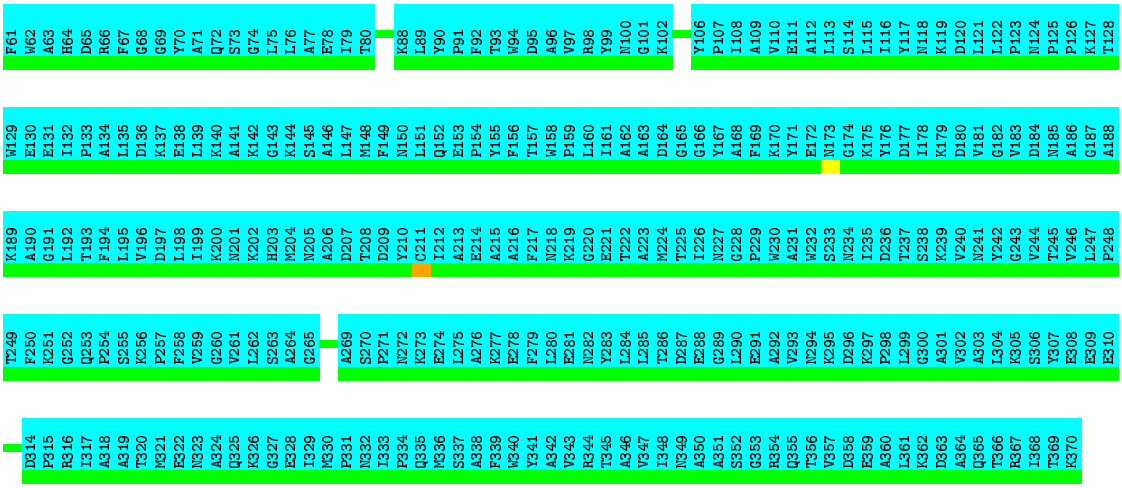


4.2.35 Score per residue for model 35

• Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: 95%

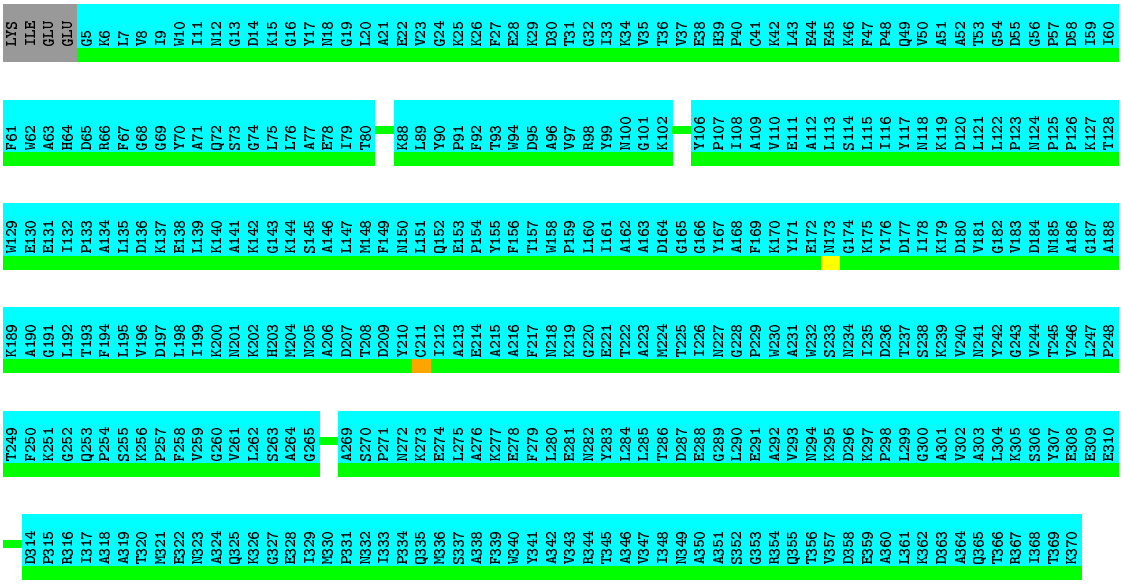




4.2.36 Score per residue for model 36

• Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

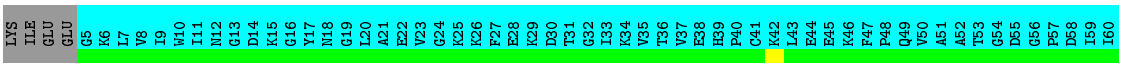
Chain A: 95%

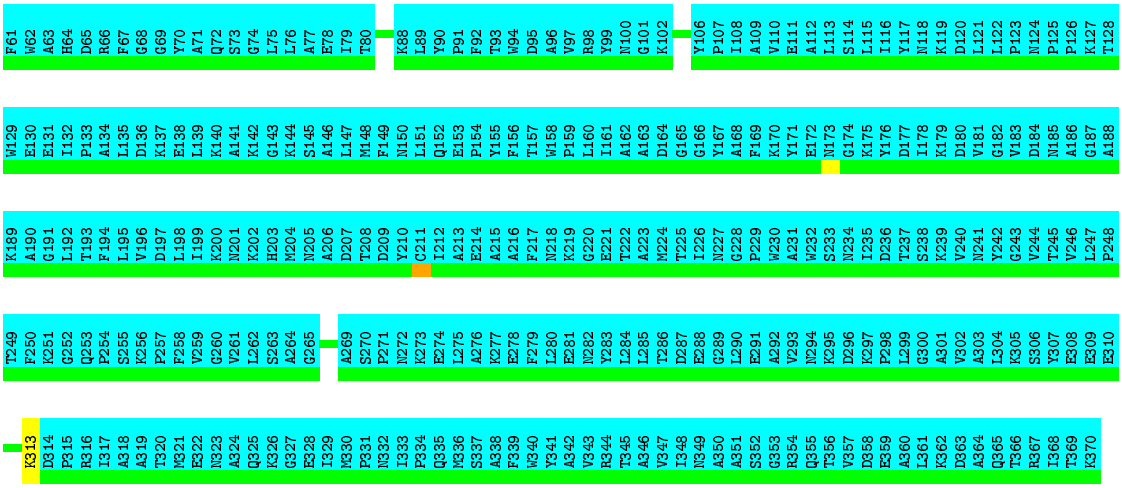


4.2.37 Score per residue for model 37

• Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: 95%

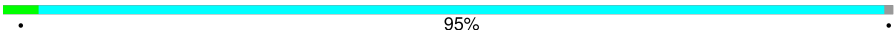


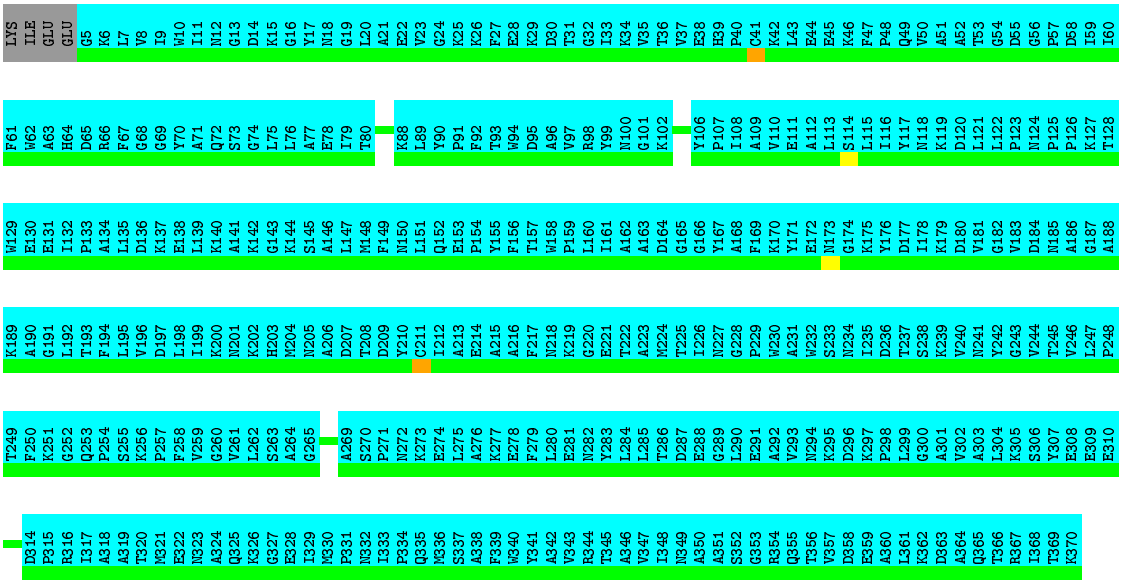


4.2.38 Score per residue for model 38

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A:

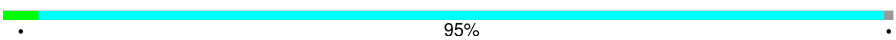


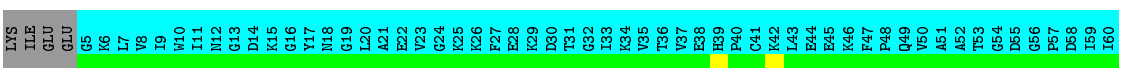


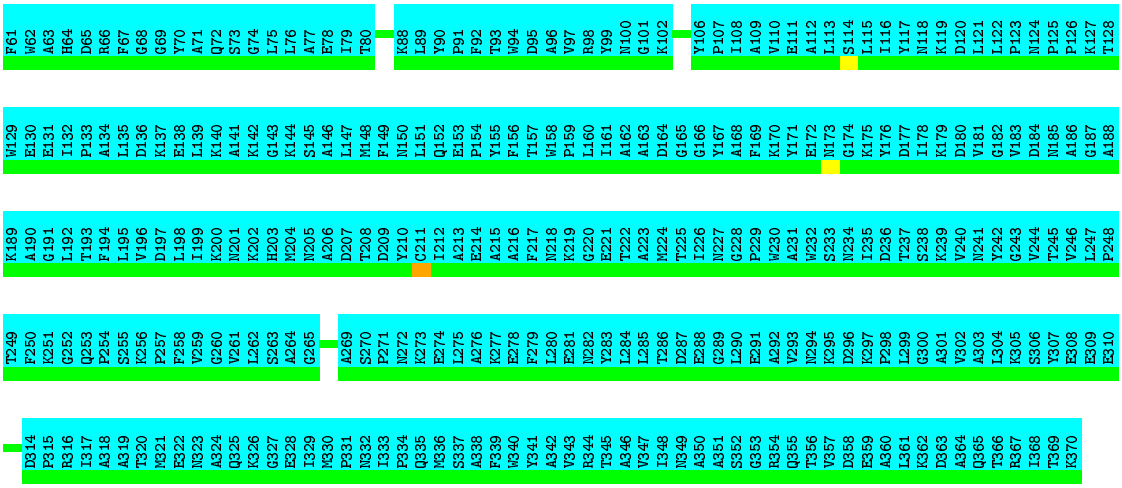
4.2.39 Score per residue for model 39 (medoid)

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A:



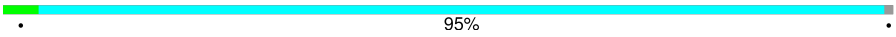


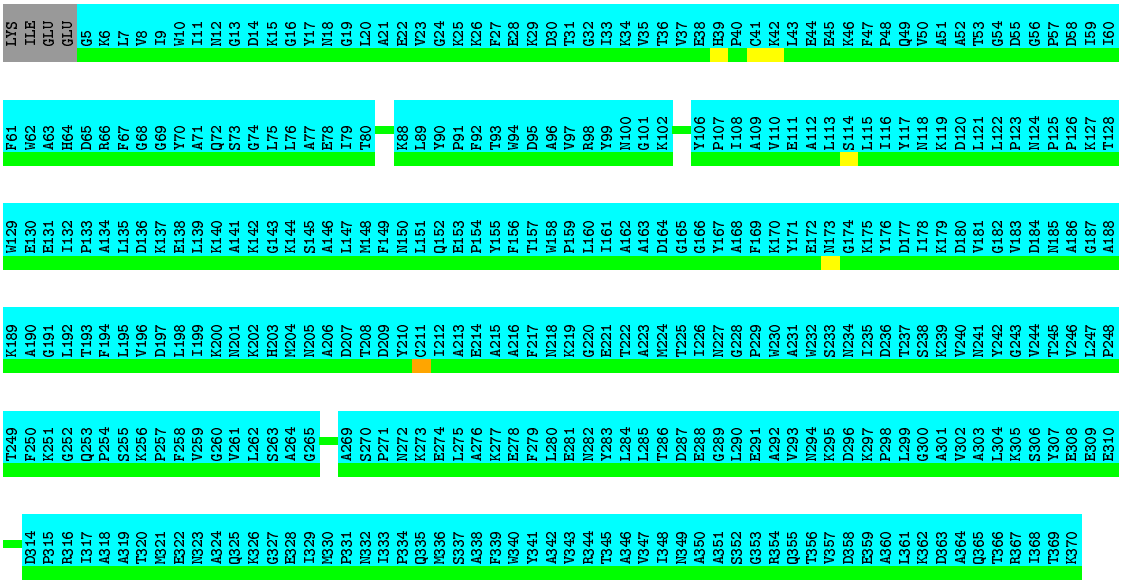


4.2.40 Score per residue for model 40

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A:

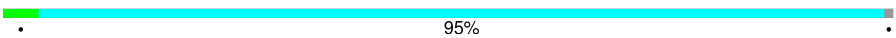


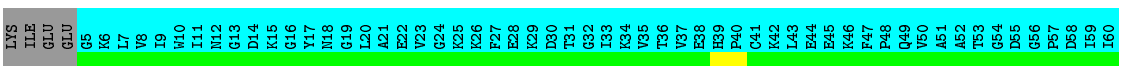


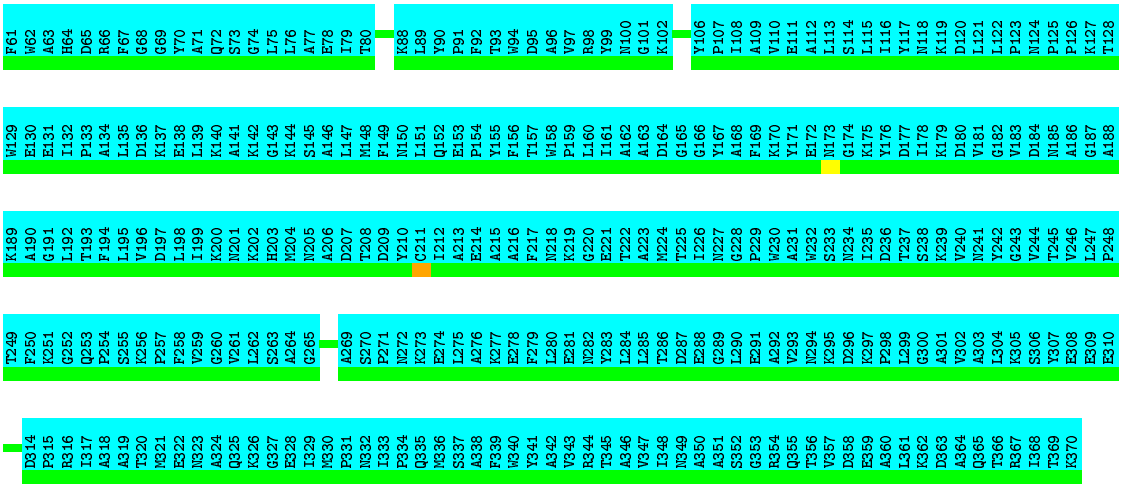
4.2.41 Score per residue for model 41

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A:

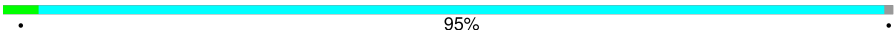


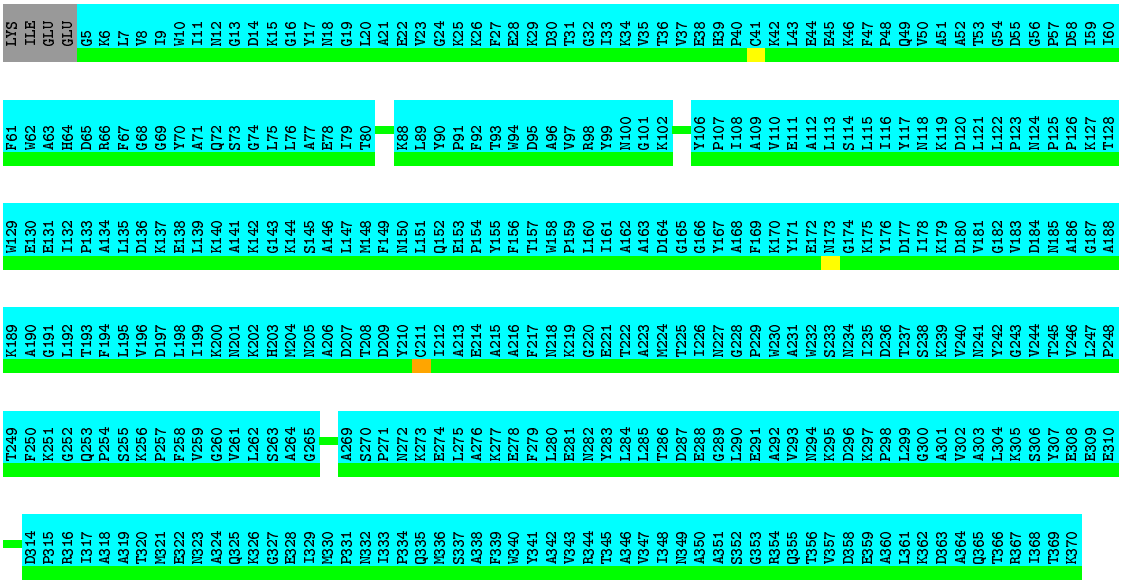




4.2.42 Score per residue for model 42

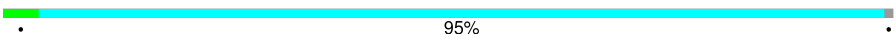
- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

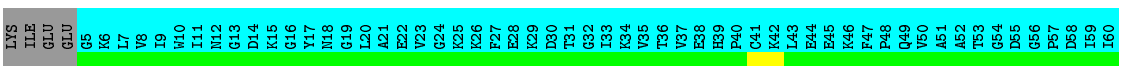
Chain A: 

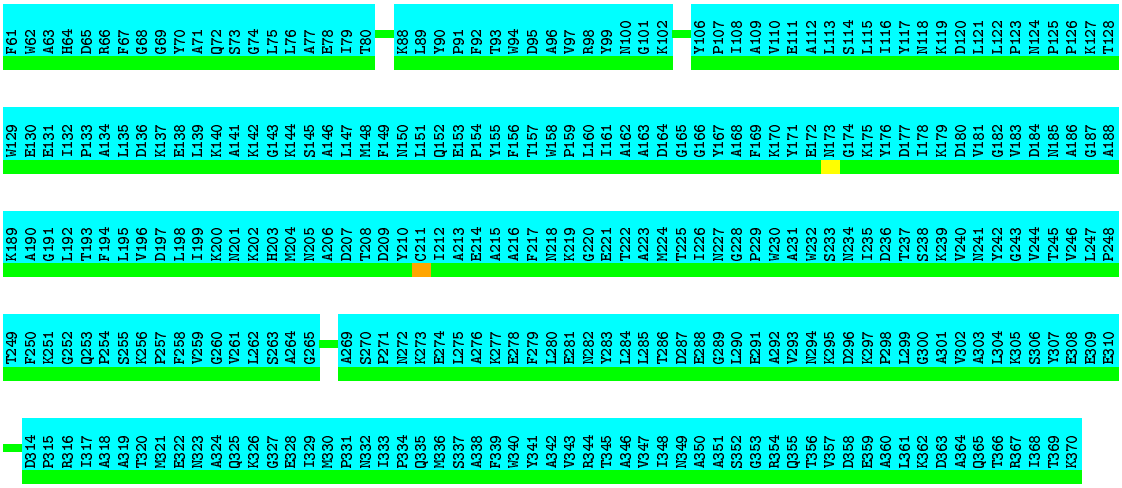


4.2.43 Score per residue for model 43

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: 

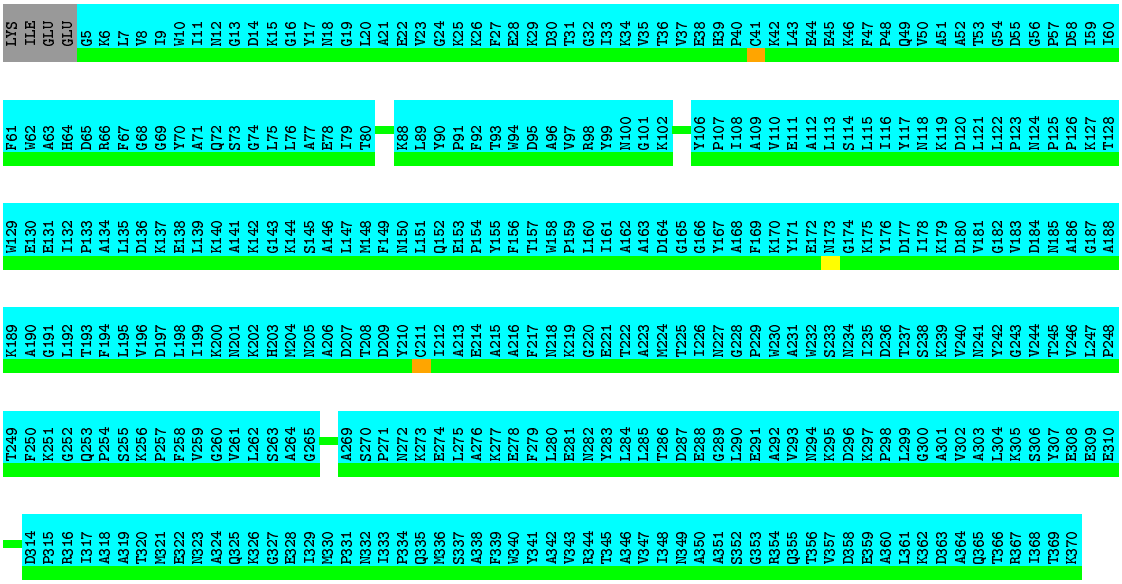




4.2.44 Score per residue for model 44

• Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

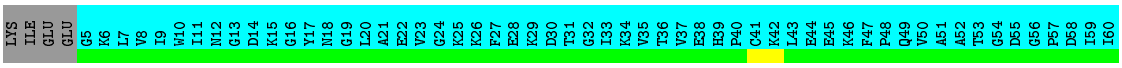
Chain A: 95%

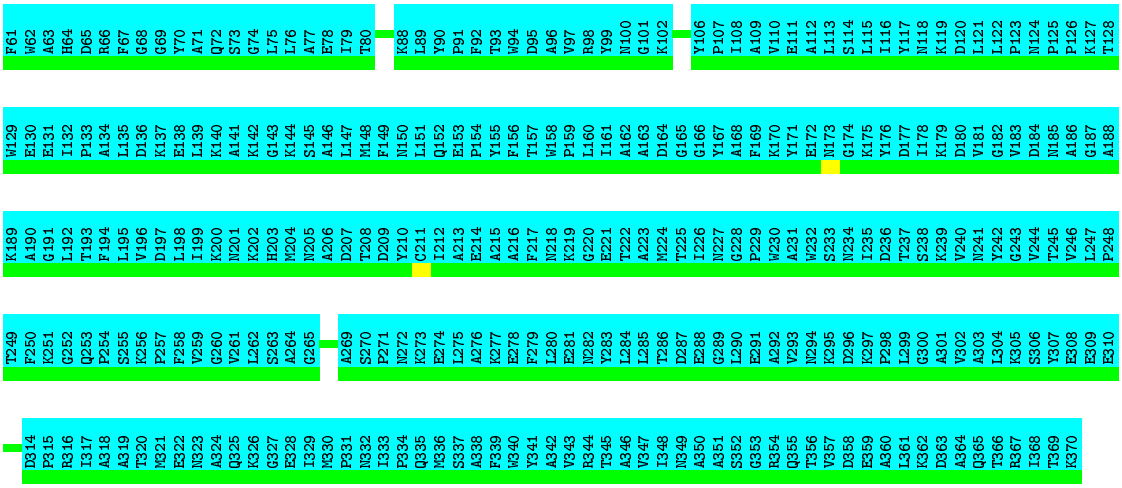


4.2.45 Score per residue for model 45

• Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: 95%

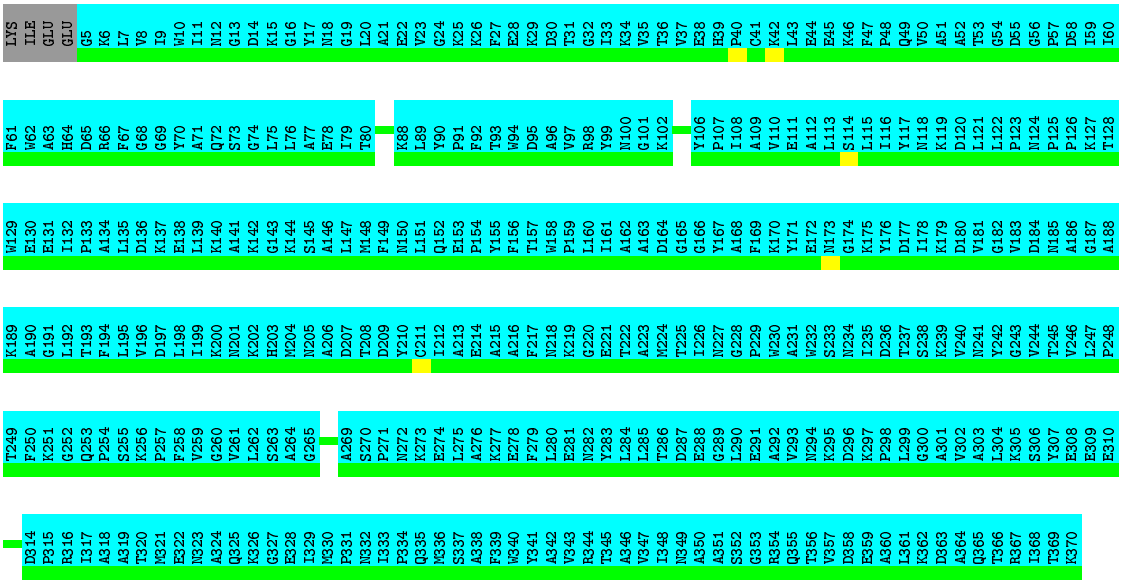




4.2.46 Score per residue for model 46

• Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

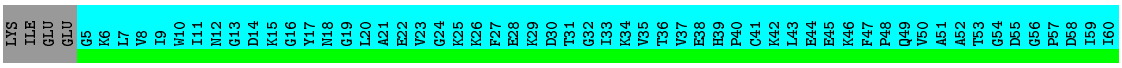
Chain A: 95%

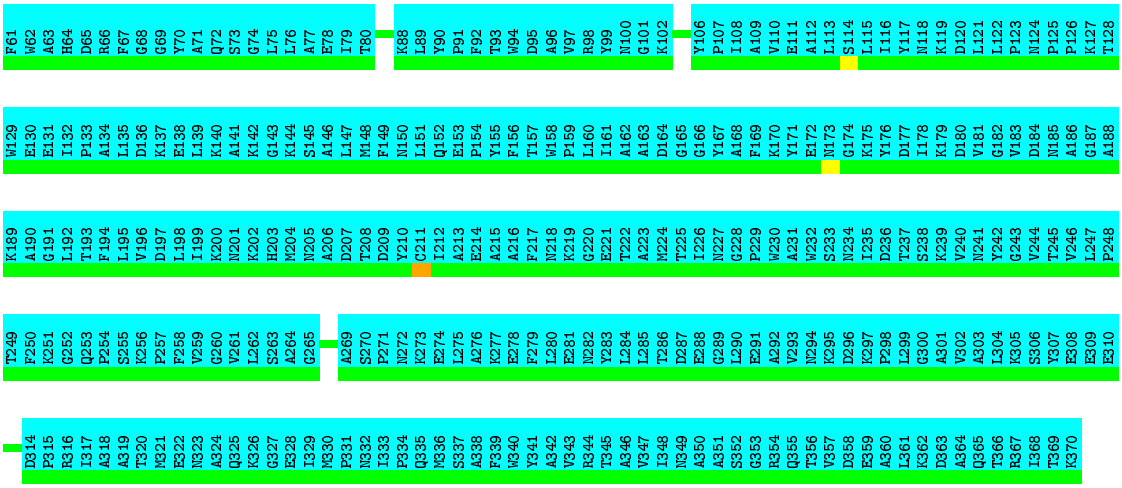


4.2.47 Score per residue for model 47

• Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: 95%

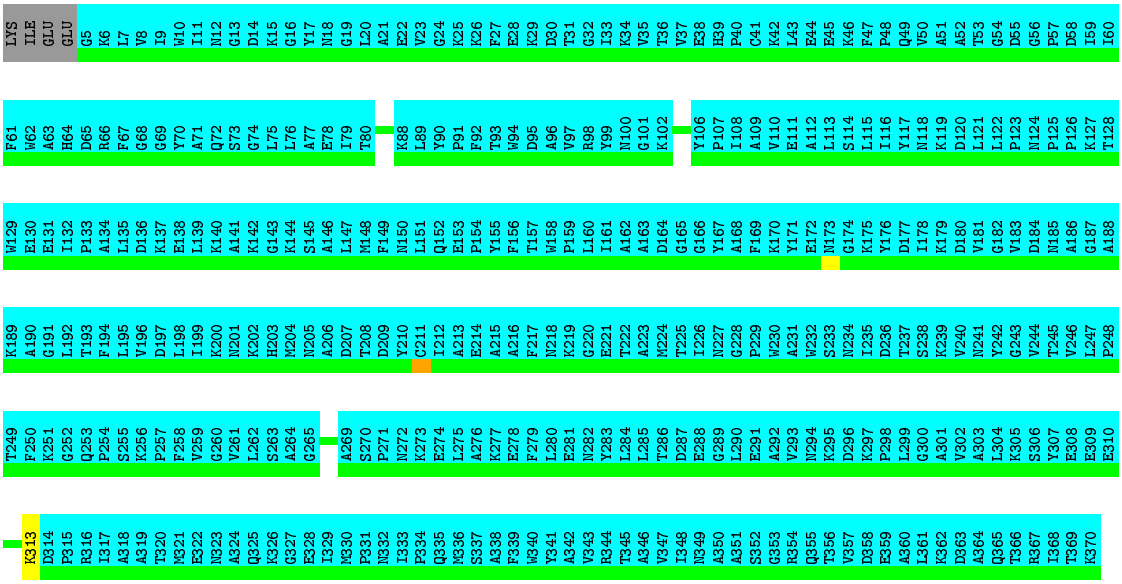




4.2.48 Score per residue for model 48

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

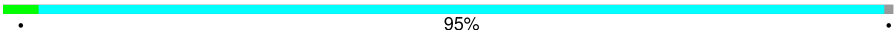
Chain A:

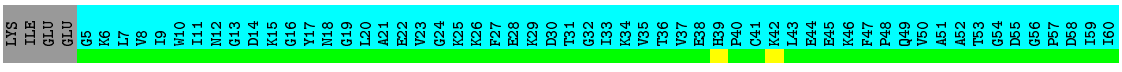


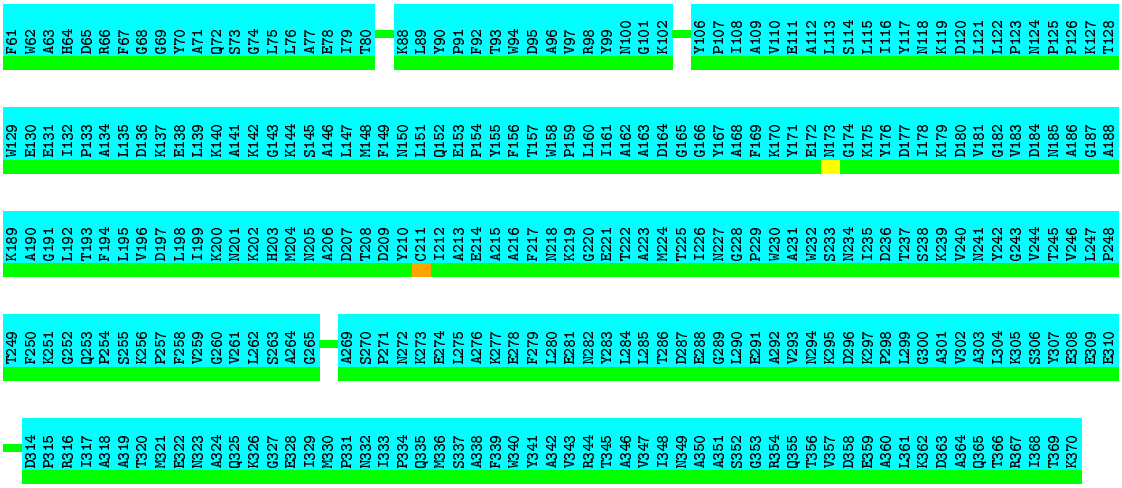
4.2.49 Score per residue for model 49

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A:



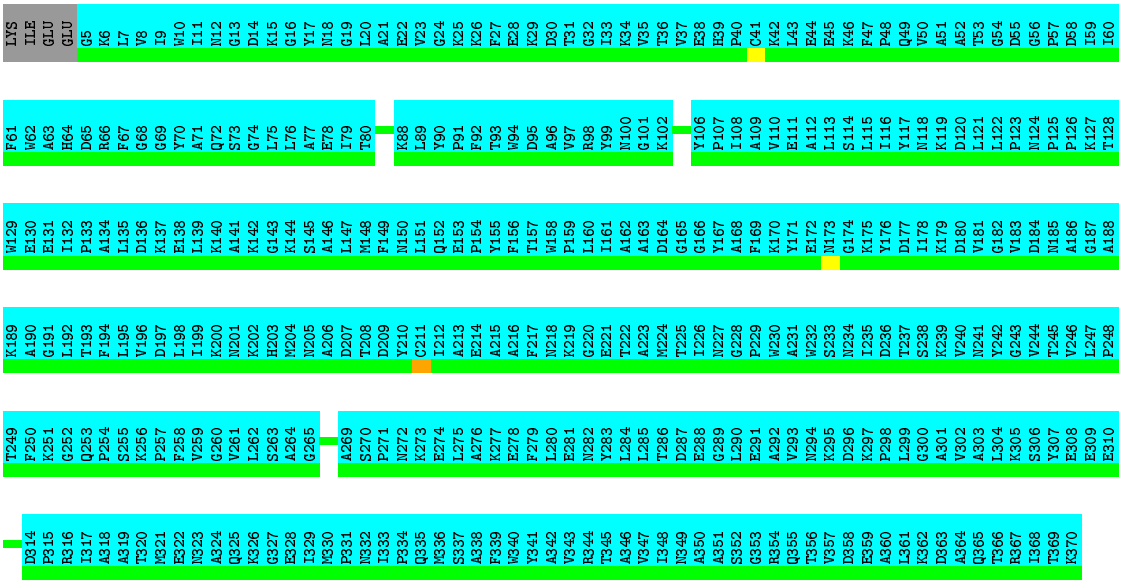




4.2.50 Score per residue for model 50

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: 95%



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 50 were deposited, based on the following criterion: *PRE AND VDW ENERGIES*.

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

Software name
A PRE PEUDOPOTENTIAL, A QUARTIC VAN DER WAALS REPULSION TERM TO PREVENT AT
XPLOR-NIH

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

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MXT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.00±0.01	0±0/64 (0.0±0.0%)	1.17±0.04	0±0/80 (0.1±0.2%)
All	All	1.00	0/3200 (0.0%)	1.17	2/4000 (0.1%)

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	313	LYS	O-C-N	-5.74	113.51	122.70	48	2

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	-2113	-424	14	0±0
2	A	432	456	500	14±4
All	All	-84050	1600	25660	695

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:600[A]:MXT:O11	2:A:600[A]:MXT:H231	0.83	1.73	29	3
2:A:600[B]:MXT:O11	2:A:600[B]:MXT:H231	0.83	1.73	46	4
2:A:500[F]:MXT:H231	2:A:500[F]:MXT:O11	0.83	1.73	24	10
2:A:500[D]:MXT:H231	2:A:500[D]:MXT:O11	0.83	1.73	10	4
2:A:500[A]:MXT:H231	2:A:500[A]:MXT:O11	0.82	1.75	24	3
2:A:600[B]:MXT:H231	2:A:600[B]:MXT:O11	0.82	1.74	14	8
2:A:500[D]:MXT:O11	2:A:500[D]:MXT:H231	0.82	1.74	29	10
2:A:500[C]:MXT:H231	2:A:500[C]:MXT:O11	0.81	1.75	2	9
2:A:600[A]:MXT:H231	2:A:600[A]:MXT:O11	0.81	1.75	40	8
2:A:500[B]:MXT:O11	2:A:500[B]:MXT:H231	0.81	1.73	13	3
2:A:600[D]:MXT:O11	2:A:600[D]:MXT:H231	0.81	1.75	43	8
2:A:500[C]:MXT:O11	2:A:500[C]:MXT:H231	0.81	1.73	21	7
2:A:500[E]:MXT:H231	2:A:500[E]:MXT:O11	0.80	1.73	50	15
2:A:500[E]:MXT:O11	2:A:500[E]:MXT:H231	0.79	1.75	35	9
2:A:500[B]:MXT:H231	2:A:500[B]:MXT:O11	0.78	1.77	34	4
2:A:600[D]:MXT:H231	2:A:600[D]:MXT:O11	0.77	1.76	44	2
2:A:500[F]:MXT:O11	2:A:500[F]:MXT:H231	0.71	1.86	7	6
2:A:500[A]:MXT:O11	2:A:500[A]:MXT:H231	0.71	1.84	19	3
2:A:600[F]:MXT:O11	2:A:600[F]:MXT:H231	0.69	1.86	17	2
2:A:600[D]:MXT:H231	2:A:600[D]:MXT:O12	0.68	1.89	14	8
2:A:500[B]:MXT:O12	2:A:500[B]:MXT:H231	0.68	1.88	45	7
2:A:600[A]:MXT:H231	2:A:600[A]:MXT:O12	0.68	1.89	3	5
2:A:600[E]:MXT:H231	2:A:600[E]:MXT:O12	0.67	1.89	45	13
2:A:600[F]:MXT:O12	2:A:600[F]:MXT:H231	0.67	1.88	32	9
2:A:600[E]:MXT:O12	2:A:600[E]:MXT:H231	0.67	1.89	4	11
2:A:500[A]:MXT:O12	2:A:500[A]:MXT:H231	0.66	1.89	40	4
2:A:600[C]:MXT:H231	2:A:600[C]:MXT:O11	0.66	1.90	37	1
2:A:600[C]:MXT:H231	2:A:600[C]:MXT:O12	0.66	1.89	3	6
2:A:600[F]:MXT:H231	2:A:600[F]:MXT:O12	0.66	1.89	24	9
2:A:600[C]:MXT:O12	2:A:600[C]:MXT:H231	0.65	1.90	14	4
2:A:500[B]:MXT:H231	2:A:500[B]:MXT:O12	0.65	1.91	20	3
2:A:600[A]:MXT:O12	2:A:600[A]:MXT:H231	0.65	1.91	7	2
2:A:500[A]:MXT:H231	2:A:500[A]:MXT:O12	0.65	1.91	32	7
2:A:600[E]:MXT:H231	2:A:600[E]:MXT:O11	0.64	1.91	31	1
2:A:600[D]:MXT:O12	2:A:600[D]:MXT:H231	0.63	1.91	12	5
2:A:600[B]:MXT:O12	2:A:600[B]:MXT:H231	0.63	1.92	44	3
2:A:600[B]:MXT:H231	2:A:600[B]:MXT:O12	0.62	1.95	47	3
2:A:500[D]:MXT:O12	2:A:500[D]:MXT:H231	0.61	1.94	16	3
2:A:500[D]:MXT:H231	2:A:500[D]:MXT:O12	0.60	1.96	17	3
2:A:500[C]:MXT:C23	2:A:500[C]:MXT:O11	0.58	2.52	49	2
2:A:500[E]:MXT:C23	2:A:500[E]:MXT:O11	0.57	2.52	19	3
2:A:600[D]:MXT:C23	2:A:600[D]:MXT:O11	0.57	2.53	33	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:500[B]:MXT:C22	2:A:500[B]:MXT:O11	0.57	2.52	37	5
2:A:500[A]:MXT:O11	2:A:500[A]:MXT:C22	0.57	2.53	16	8
2:A:600[A]:MXT:O11	2:A:600[A]:MXT:C23	0.57	2.52	33	4
2:A:500[B]:MXT:C23	2:A:500[B]:MXT:O11	0.57	2.52	34	5
2:A:500[C]:MXT:O11	2:A:500[C]:MXT:C22	0.57	2.53	32	3
2:A:500[D]:MXT:O11	2:A:500[D]:MXT:C23	0.57	2.52	4	6
2:A:500[D]:MXT:O11	2:A:500[D]:MXT:C22	0.57	2.52	13	3
2:A:500[A]:MXT:C22	2:A:500[A]:MXT:O11	0.57	2.53	4	7
2:A:600[C]:MXT:O11	2:A:600[C]:MXT:C22	0.57	2.53	24	2
2:A:600[B]:MXT:H221	2:A:600[B]:MXT:O11	0.56	2.00	36	2
2:A:500[E]:MXT:O12	2:A:500[E]:MXT:H231	0.56	2.00	27	2
2:A:500[A]:MXT:O11	2:A:500[A]:MXT:H221	0.56	2.00	26	7
2:A:600[D]:MXT:H221	2:A:600[D]:MXT:O11	0.56	2.00	49	3
2:A:500[F]:MXT:O11	2:A:500[F]:MXT:H221	0.56	2.00	41	1
2:A:500[D]:MXT:C22	2:A:500[D]:MXT:O11	0.56	2.52	32	3
2:A:500[B]:MXT:O11	2:A:500[B]:MXT:C23	0.56	2.53	24	3
2:A:500[A]:MXT:H221	2:A:500[A]:MXT:O11	0.56	2.00	12	8
2:A:500[F]:MXT:O12	2:A:500[F]:MXT:H231	0.56	1.98	22	2
2:A:500[E]:MXT:O11	2:A:500[E]:MXT:H221	0.56	2.00	42	2
2:A:600[D]:MXT:O11	2:A:600[D]:MXT:C23	0.56	2.53	43	2
2:A:500[F]:MXT:O11	2:A:500[F]:MXT:C23	0.55	2.53	7	7
2:A:500[C]:MXT:C22	2:A:500[C]:MXT:O11	0.55	2.54	19	5
2:A:600[E]:MXT:O11	2:A:600[E]:MXT:H221	0.55	2.01	18	3
2:A:600[B]:MXT:C23	2:A:600[B]:MXT:O11	0.55	2.52	17	2
2:A:500[C]:MXT:O11	2:A:500[C]:MXT:C23	0.55	2.52	14	3
2:A:500[D]:MXT:C23	2:A:500[D]:MXT:O11	0.55	2.54	21	5
2:A:600[B]:MXT:O11	2:A:600[B]:MXT:C23	0.55	2.53	26	5
2:A:600[D]:MXT:C22	2:A:600[D]:MXT:O11	0.54	2.55	1	3
2:A:500[D]:MXT:O11	2:A:500[D]:MXT:H221	0.54	2.03	47	3
2:A:500[A]:MXT:O11	2:A:500[A]:MXT:C23	0.54	2.55	9	3
2:A:600[C]:MXT:C22	2:A:600[C]:MXT:O11	0.53	2.56	15	4
2:A:500[C]:MXT:H231	2:A:500[C]:MXT:O12	0.52	2.02	31	1
2:A:500[F]:MXT:C22	2:A:500[F]:MXT:O11	0.52	2.57	41	2
2:A:600[F]:MXT:O11	2:A:600[F]:MXT:C22	0.52	2.57	47	4
2:A:500[E]:MXT:O11	2:A:500[E]:MXT:C23	0.52	2.58	9	4
2:A:600[B]:MXT:O11	2:A:600[B]:MXT:H221	0.52	2.04	41	1
2:A:600[E]:MXT:C22	2:A:600[E]:MXT:O11	0.52	2.58	48	2
2:A:600[D]:MXT:O11	2:A:600[D]:MXT:C22	0.51	2.58	22	2
2:A:500[D]:MXT:H221	2:A:500[D]:MXT:O11	0.51	2.05	50	2
2:A:600[B]:MXT:C22	2:A:600[B]:MXT:O11	0.51	2.59	4	3
2:A:600[C]:MXT:O11	2:A:600[C]:MXT:H221	0.51	2.05	28	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:500[F]:MXT:C23	2:A:500[F]:MXT:O11	0.51	2.54	24	3
2:A:600[F]:MXT:C22	2:A:600[F]:MXT:O11	0.51	2.58	46	3
2:A:600[D]:MXT:O11	2:A:600[D]:MXT:H221	0.51	2.05	41	1
2:A:600[E]:MXT:O11	2:A:600[E]:MXT:C22	0.51	2.59	32	5
2:A:600[C]:MXT:H221	2:A:600[C]:MXT:O11	0.50	2.06	24	1
2:A:500[F]:MXT:O11	2:A:500[F]:MXT:C22	0.50	2.58	46	1
2:A:500[C]:MXT:O11	2:A:500[C]:MXT:H221	0.49	2.05	32	1
2:A:500[F]:MXT:H221	2:A:500[F]:MXT:O11	0.49	2.06	29	1
2:A:600[E]:MXT:H221	2:A:600[E]:MXT:O11	0.49	2.08	22	3
2:A:600[A]:MXT:O11	2:A:600[A]:MXT:C22	0.49	2.60	49	1
2:A:500[B]:MXT:O11	2:A:500[B]:MXT:H221	0.49	2.07	11	2
2:A:600[A]:MXT:H221	2:A:600[A]:MXT:O11	0.48	2.07	4	1
2:A:500[E]:MXT:C22	2:A:500[E]:MXT:O11	0.48	2.61	42	2
2:A:500[B]:MXT:O11	2:A:500[B]:MXT:C22	0.48	2.61	29	2
2:A:500[B]:MXT:H221	2:A:500[B]:MXT:O11	0.48	2.09	37	1
2:A:500[A]:MXT:C23	2:A:500[A]:MXT:O11	0.48	2.57	5	2
2:A:600[F]:MXT:C23	2:A:600[F]:MXT:O11	0.47	2.62	45	1
2:A:500[B]:MXT:O11	2:A:500[B]:MXT:H222	0.47	2.10	29	5
2:A:600[E]:MXT:H222	2:A:600[E]:MXT:O11	0.46	2.10	43	6
2:A:600[F]:MXT:H231	2:A:600[F]:MXT:O11	0.46	2.09	8	2
2:A:600[B]:MXT:H222	2:A:600[B]:MXT:O11	0.46	2.11	30	2
2:A:600[F]:MXT:H221	2:A:600[F]:MXT:O11	0.46	2.09	30	1
2:A:600[F]:MXT:H222	2:A:600[F]:MXT:O11	0.46	2.10	19	6
2:A:500[D]:MXT:H222	2:A:500[D]:MXT:O11	0.46	2.10	42	3
2:A:600[D]:MXT:H222	2:A:600[D]:MXT:O11	0.46	2.10	10	3
2:A:500[A]:MXT:H222	2:A:500[A]:MXT:O11	0.46	2.11	34	2
2:A:500[C]:MXT:H222	2:A:500[C]:MXT:O11	0.46	2.11	1	5
2:A:600[E]:MXT:O11	2:A:600[E]:MXT:H222	0.46	2.10	25	3
2:A:600[E]:MXT:C23	2:A:600[E]:MXT:O11	0.46	2.63	42	1
2:A:600[A]:MXT:H222	2:A:600[A]:MXT:O11	0.46	2.11	27	1
2:A:500[B]:MXT:H222	2:A:500[B]:MXT:O11	0.45	2.11	14	1
2:A:500[C]:MXT:O11	2:A:500[C]:MXT:H222	0.45	2.11	24	3
2:A:600[C]:MXT:H222	2:A:600[C]:MXT:O11	0.45	2.11	49	3
2:A:500[F]:MXT:O11	2:A:500[F]:MXT:H222	0.45	2.11	1	1
2:A:600[A]:MXT:C23	2:A:600[A]:MXT:O11	0.45	2.64	44	1
2:A:500[E]:MXT:H222	2:A:500[E]:MXT:O11	0.45	2.12	11	2
2:A:600[F]:MXT:O11	2:A:600[F]:MXT:H222	0.44	2.10	4	3
2:A:600[A]:MXT:O11	2:A:600[A]:MXT:H222	0.44	2.11	49	1
2:A:600[B]:MXT:O11	2:A:600[B]:MXT:C22	0.44	2.66	50	1
2:A:600[A]:MXT:O12	2:A:600[A]:MXT:C22	0.44	2.66	38	5
2:A:500[F]:MXT:H222	2:A:500[F]:MXT:O11	0.44	2.11	46	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:600[C]:MXT:C22	2:A:600[C]:MXT:O12	0.44	2.66	31	6
2:A:500[E]:MXT:C22	2:A:500[E]:MXT:O12	0.43	2.66	38	2
2:A:500[E]:MXT:O12	2:A:500[E]:MXT:C22	0.43	2.66	6	2
2:A:500[B]:MXT:C23	2:A:500[B]:MXT:O12	0.43	2.67	17	1
2:A:600[A]:MXT:C22	2:A:600[A]:MXT:O12	0.43	2.66	28	4
2:A:600[A]:MXT:O12	2:A:600[A]:MXT:C23	0.43	2.67	43	1
2:A:600[F]:MXT:C23	2:A:600[F]:MXT:O12	0.43	2.67	6	1
2:A:500[D]:MXT:O12	2:A:500[D]:MXT:C23	0.43	2.66	16	3
2:A:500[A]:MXT:O12	2:A:500[A]:MXT:C22	0.43	2.67	23	3
2:A:600[B]:MXT:O12	2:A:600[B]:MXT:C22	0.43	2.66	20	2
2:A:500[B]:MXT:O12	2:A:500[B]:MXT:C22	0.43	2.66	36	5
2:A:500[B]:MXT:O12	2:A:500[B]:MXT:C23	0.43	2.66	23	3
2:A:500[F]:MXT:O12	2:A:500[F]:MXT:C22	0.43	2.66	40	4
2:A:600[B]:MXT:O12	2:A:600[B]:MXT:C23	0.43	2.66	43	1
2:A:600[C]:MXT:O12	2:A:600[C]:MXT:C23	0.43	2.67	6	2
2:A:600[B]:MXT:C22	2:A:600[B]:MXT:O12	0.43	2.67	24	1
2:A:600[F]:MXT:C22	2:A:600[F]:MXT:O12	0.43	2.66	5	2
2:A:600[E]:MXT:C23	2:A:600[E]:MXT:O12	0.43	2.66	41	4
2:A:600[E]:MXT:C22	2:A:600[E]:MXT:O12	0.43	2.67	21	2
2:A:600[B]:MXT:C23	2:A:600[B]:MXT:O12	0.43	2.66	47	1
2:A:600[D]:MXT:O12	2:A:600[D]:MXT:C23	0.42	2.67	28	3
2:A:500[F]:MXT:C22	2:A:500[F]:MXT:O12	0.42	2.66	5	3
2:A:600[C]:MXT:O11	2:A:600[C]:MXT:H231	0.42	2.14	13	1
2:A:600[D]:MXT:C23	2:A:600[D]:MXT:O12	0.42	2.68	19	1
2:A:600[E]:MXT:O12	2:A:600[E]:MXT:C23	0.42	2.66	46	4
2:A:600[A]:MXT:C22	2:A:600[A]:MXT:O11	0.42	2.68	27	1
2:A:500[D]:MXT:C22	2:A:500[D]:MXT:O12	0.42	2.68	27	1
2:A:500[B]:MXT:C22	2:A:500[B]:MXT:O12	0.42	2.67	41	1
2:A:500[F]:MXT:H221	2:A:500[F]:MXT:O12	0.42	2.15	3	1
2:A:600[F]:MXT:O12	2:A:600[F]:MXT:C22	0.42	2.67	39	1
2:A:500[C]:MXT:O12	2:A:500[C]:MXT:C22	0.41	2.66	28	1
2:A:500[D]:MXT:H221	2:A:500[D]:MXT:O12	0.41	2.16	46	1
2:A:600[A]:MXT:O12	2:A:600[A]:MXT:H221	0.41	2.16	23	2
2:A:600[D]:MXT:O12	2:A:600[D]:MXT:C22	0.41	2.68	15	1
2:A:600[A]:MXT:H221	2:A:600[A]:MXT:O12	0.41	2.15	9	2
2:A:600[F]:MXT:O12	2:A:600[F]:MXT:C23	0.41	2.67	24	2
2:A:500[A]:MXT:O12	2:A:500[A]:MXT:C23	0.41	2.67	29	1
2:A:500[A]:MXT:C23	2:A:500[A]:MXT:O12	0.41	2.70	10	1
2:A:600[C]:MXT:C23	2:A:600[C]:MXT:O12	0.41	2.67	46	1
2:A:500[F]:MXT:O12	2:A:500[F]:MXT:H221	0.41	2.15	45	2
2:A:500[A]:MXT:O12	2:A:500[A]:MXT:H221	0.40	2.16	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:600[B]:MXT:H221	2:A:600[B]:MXT:O12	0.40	2.16	13	1
2:A:500[E]:MXT:O12	2:A:500[E]:MXT:H221	0.40	2.15	17	1
2:A:600[B]:MXT:O12	2:A:600[B]:MXT:H221	0.40	2.16	39	1

6.3 Torsion angles

6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	16/370 (4%)	15±0 (94±0%)	1±0 (6±0%)	0±0 (0±0%)	100	100
All	All	800/18500 (4%)	750 (94%)	50 (6%)	0 (0%)	100	100

There are no Ramachandran outliers.

6.3.2 Protein sidechains

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	0	-	-	-
All	All	0	-	-	-

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

6.3.3 RNA

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)

24 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	MXT	A	500[A]	1	19,19,19	1.90±0.00	0±0 (0±0%)
2	MXT	A	500[B]	1	19,19,19	1.90±0.00	0±0 (0±0%)
2	MXT	A	500[C]	1	19,19,19	1.89±0.00	0±0 (0±0%)
2	MXT	A	500[D]	1	19,19,19	1.88±0.00	0±0 (0±0%)
2	MXT	A	500[E]	1	19,19,19	1.89±0.00	0±0 (0±0%)
2	MXT	A	500[F]	1	19,19,19	1.91±0.00	0±0 (0±0%)
2	MXT	A	500[U]	1	19,19,19	1.90±0.00	0±0 (0±0%)
2	MXT	A	500[V]	1	19,19,19	1.90±0.00	0±0 (0±0%)
2	MXT	A	500[W]	1	19,19,19	1.89±0.00	0±0 (0±0%)
2	MXT	A	500[X]	1	19,19,19	1.88±0.00	0±0 (0±0%)
2	MXT	A	500[Y]	1	19,19,19	1.89±0.00	0±0 (0±0%)
2	MXT	A	500[Z]	1	19,19,19	1.91±0.00	0±0 (0±0%)
2	MXT	A	600[A]	1	19,19,19	1.89±0.00	0±0 (0±0%)
2	MXT	A	600[B]	1	19,19,19	1.89±0.00	0±0 (0±0%)
2	MXT	A	600[C]	1	19,19,19	1.90±0.00	0±0 (0±0%)
2	MXT	A	600[D]	1	19,19,19	1.89±0.00	0±0 (0±0%)
2	MXT	A	600[E]	1	19,19,19	1.90±0.00	0±0 (0±0%)
2	MXT	A	600[F]	1	19,19,19	1.89±0.00	0±0 (0±0%)
2	MXT	A	600[U]	1	19,19,19	1.89±0.00	0±0 (0±0%)
2	MXT	A	600[V]	1	19,19,19	1.89±0.00	0±0 (0±0%)
2	MXT	A	600[W]	1	19,19,19	1.90±0.00	0±0 (0±0%)
2	MXT	A	600[X]	1	19,19,19	1.89±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	MXT	A	600[Y]	1	19,19,19	1.90±0.00	0±0 (0±0%)
2	MXT	A	600[Z]	1	19,19,19	1.89±0.00	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	MXT	A	500[A]	1	21,31,31	1.38±0.01	0±0 (0±0%)
2	MXT	A	500[B]	1	21,31,31	1.38±0.01	0±0 (0±0%)
2	MXT	A	500[C]	1	21,31,31	1.38±0.01	0±0 (0±0%)
2	MXT	A	500[D]	1	21,31,31	1.37±0.01	0±0 (0±0%)
2	MXT	A	500[E]	1	21,31,31	1.37±0.01	0±0 (0±0%)
2	MXT	A	500[F]	1	21,31,31	1.40±0.01	0±0 (0±0%)
2	MXT	A	500[U]	1	21,31,31	1.38±0.01	0±0 (0±0%)
2	MXT	A	500[V]	1	21,31,31	1.38±0.01	0±0 (0±0%)
2	MXT	A	500[W]	1	21,31,31	1.38±0.01	0±0 (0±0%)
2	MXT	A	500[X]	1	21,31,31	1.37±0.01	0±0 (0±0%)
2	MXT	A	500[Y]	1	21,31,31	1.37±0.01	0±0 (0±0%)
2	MXT	A	500[Z]	1	21,31,31	1.40±0.01	0±0 (0±0%)
2	MXT	A	600[A]	1	21,31,31	1.38±0.01	0±0 (0±0%)
2	MXT	A	600[B]	1	21,31,31	1.36±0.01	0±0 (0±0%)
2	MXT	A	600[C]	1	21,31,31	1.39±0.01	0±0 (0±0%)
2	MXT	A	600[D]	1	21,31,31	1.40±0.01	0±0 (0±0%)
2	MXT	A	600[E]	1	21,31,31	1.40±0.01	0±0 (0±0%)
2	MXT	A	600[F]	1	21,31,31	1.35±0.01	0±0 (0±0%)
2	MXT	A	600[U]	1	21,31,31	1.38±0.01	0±0 (0±0%)
2	MXT	A	600[V]	1	21,31,31	1.36±0.01	0±0 (0±0%)
2	MXT	A	600[W]	1	21,31,31	1.39±0.01	0±0 (0±0%)
2	MXT	A	600[X]	1	21,31,31	1.40±0.01	0±0 (0±0%)
2	MXT	A	600[Y]	1	21,31,31	1.40±0.01	0±0 (0±0%)
2	MXT	A	600[Z]	1	21,31,31	1.35±0.01	0±0 (0±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MXT	A	500[A]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	500[B]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	500[C]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	500[D]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	500[E]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	500[F]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	500[U]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	500[V]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	500[W]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	500[X]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	500[Y]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	500[Z]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	600[A]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	600[B]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	600[C]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	600[D]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	600[E]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	600[F]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	600[U]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	600[V]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	600[W]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	600[X]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	600[Y]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	600[Z]	1	-	0±0,4,39,39	0±0,2,2,2

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided