



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 07:20 AM UTC

PDB ID : 2D21 / pdb_00002d21
Title : NMR Structure of stereo-array isotope labelled (SAIL) maltodextrin-binding protein (MBP)
Authors : Kainosho, M.; Torizawa, T.; Iwashita, Y.; Terauchi, T.; Ono, A.M.; Guntert, P.
Deposited on : 2005-09-02

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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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

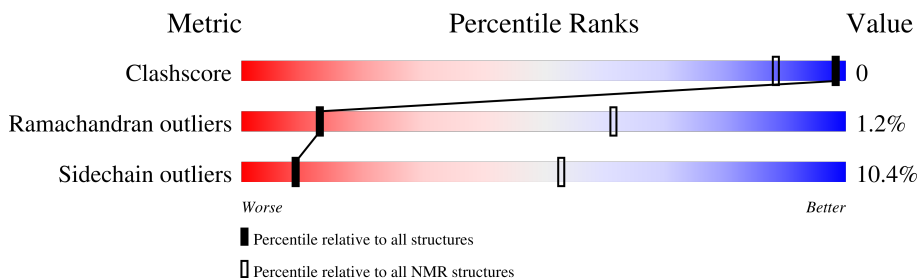
1 Overall quality at a glance

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	370	

2 Ensemble composition and analysis i

This entry contains 20 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:3-A:111, A:260-A:324 (174)	0.83	3
2	A:116-A:117, A:126-A:226, A:247-A:258, A:331-A:370 (155)	0.94	4

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 5 clusters and 3 single-model clusters were found.

Cluster number	Models
1	2, 8, 12, 15, 19
2	1, 3, 4, 14, 20
3	10, 13, 16
4	17, 18
5	6, 7
Single-model clusters	5; 9; 11

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5734 atoms, of which 2857 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Maltose-binding periplasmic protein.

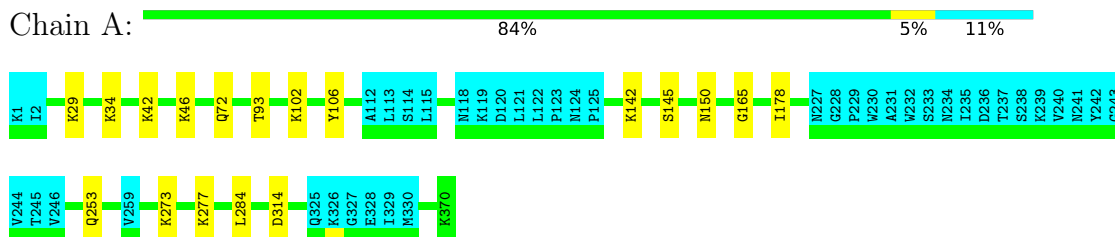
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	370	5734	1853	2857	469	549	6	0

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Maltose-binding periplasmic protein

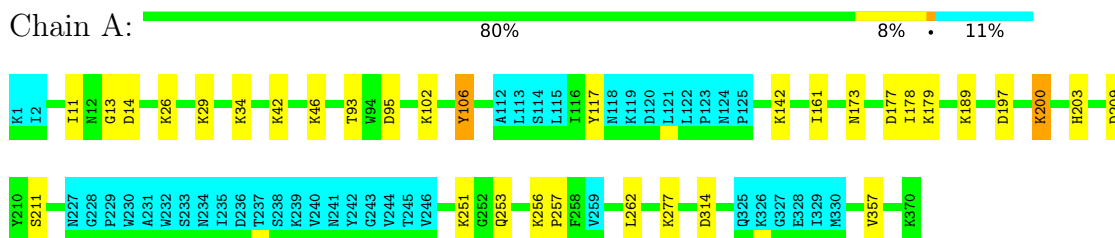


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

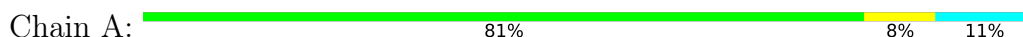
4.2.1 Score per residue for model 1

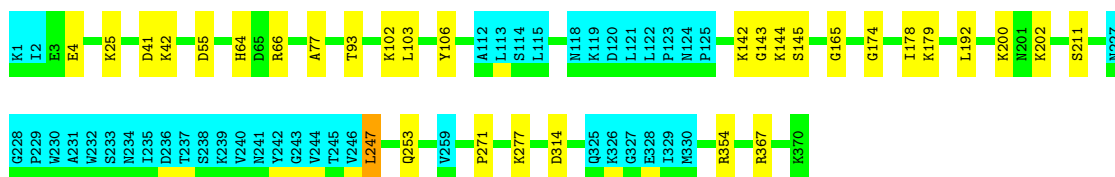
- Molecule 1: Maltose-binding periplasmic protein



4.2.2 Score per residue for model 2

- Molecule 1: Maltose-binding periplasmic protein

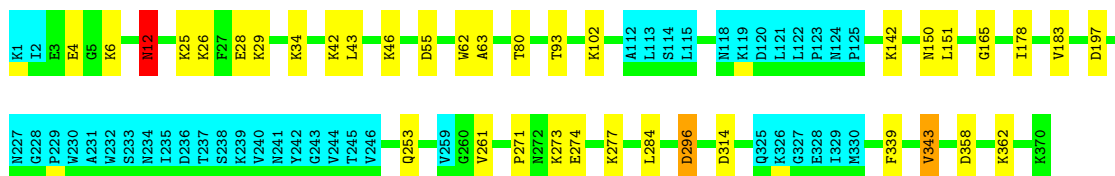




4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Maltose-binding periplasmic protein

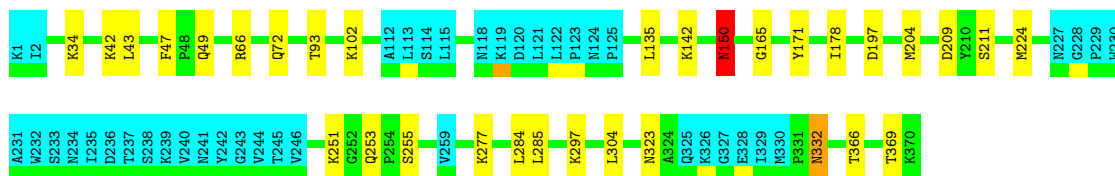
Chain A: 79% 9% 11%



4.2.4 Score per residue for model 4

- Molecule 1: Maltose-binding periplasmic protein

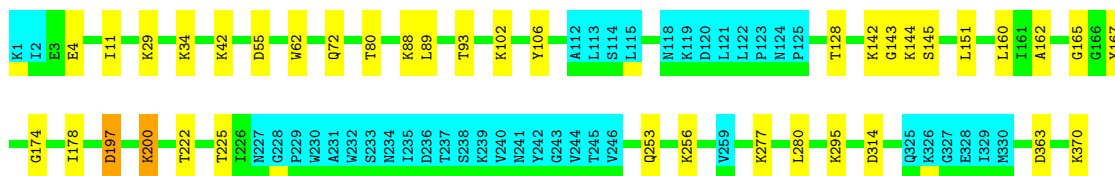
Chain A: 80% 8% 11%



4.2.5 Score per residue for model 5

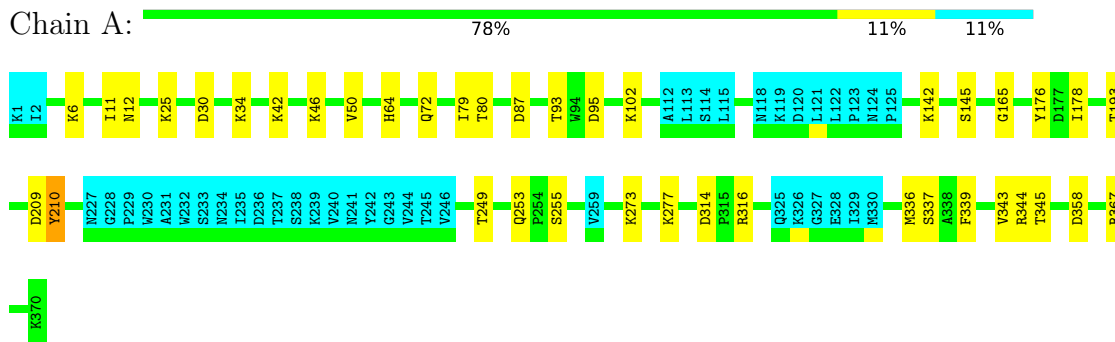
- Molecule 1: Maltose-binding periplasmic protein

Chain A: 79% 10% 11%



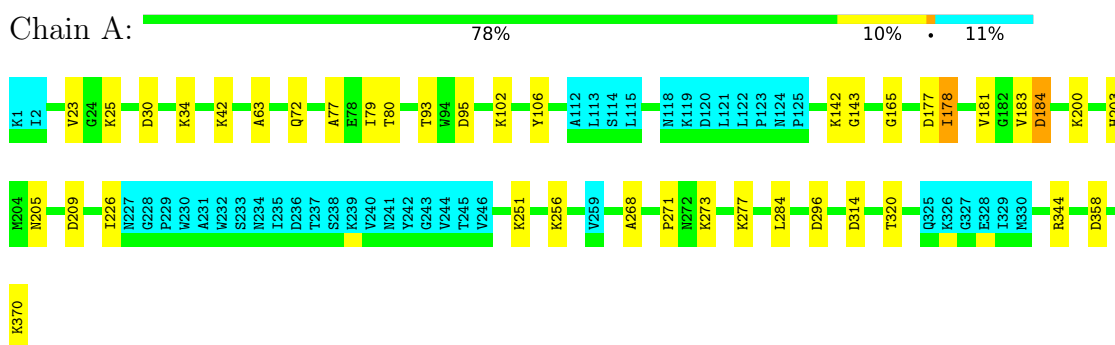
4.2.6 Score per residue for model 6

- Molecule 1: Maltose-binding periplasmic protein



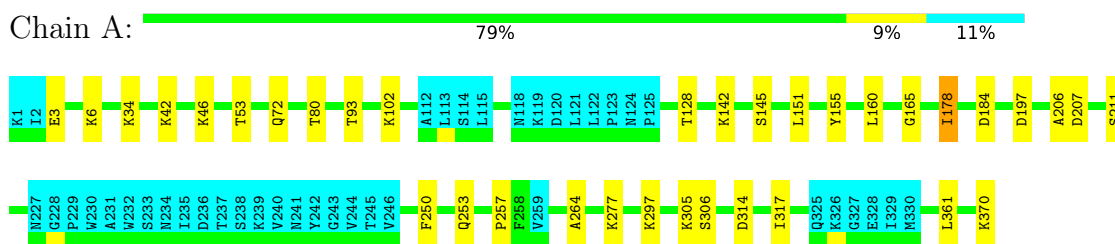
4.2.7 Score per residue for model 7

- Molecule 1: Maltose-binding periplasmic protein



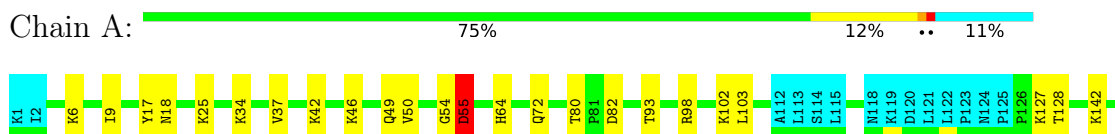
4.2.8 Score per residue for model 8

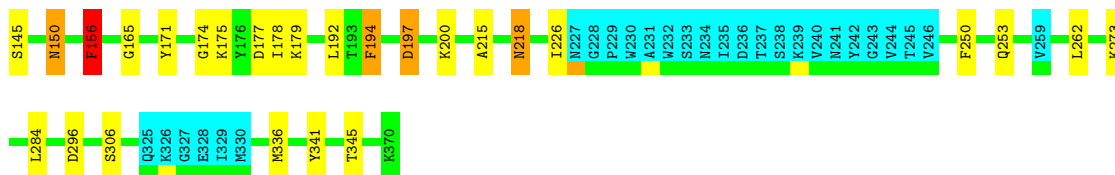
- Molecule 1: Maltose-binding periplasmic protein



4.2.9 Score per residue for model 9

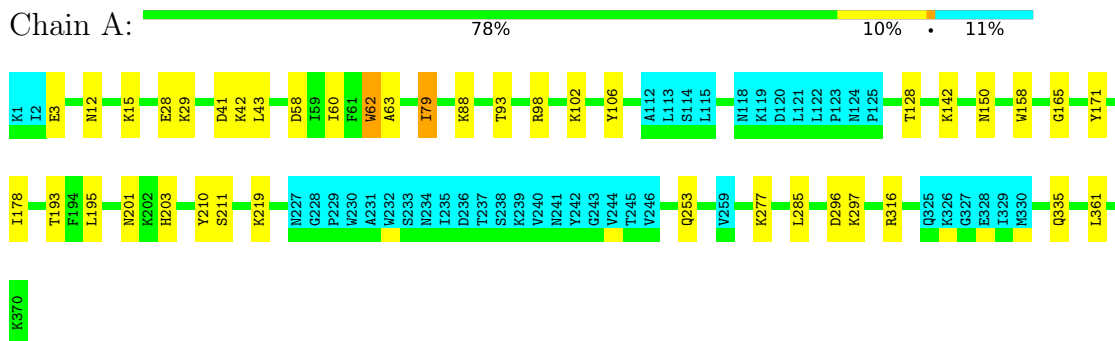
- Molecule 1: Maltose-binding periplasmic protein





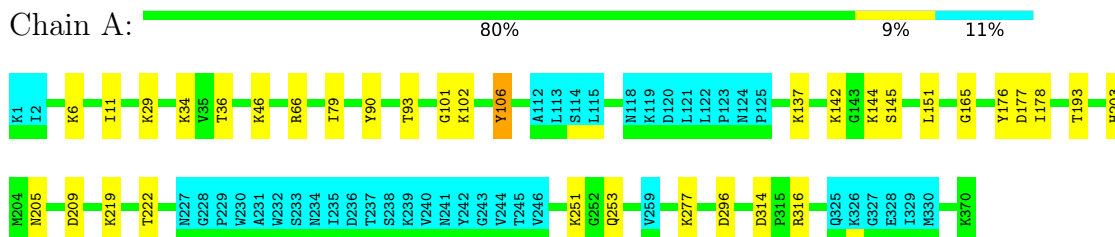
4.2.10 Score per residue for model 10

- Molecule 1: Maltose-binding periplasmic protein



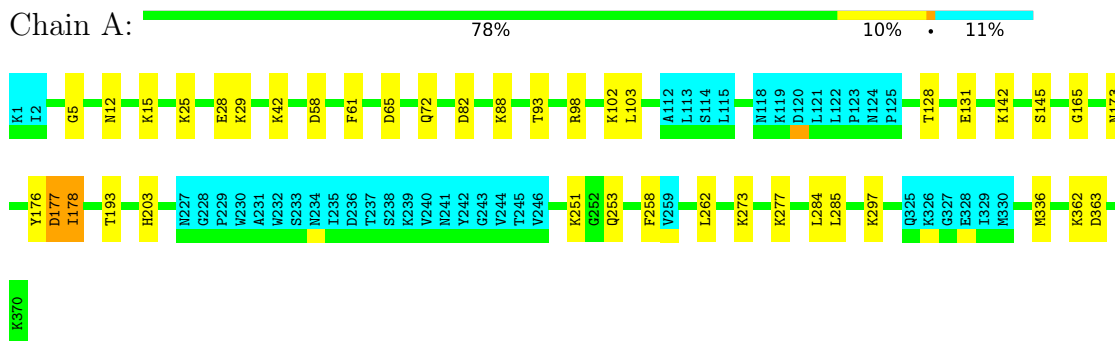
4.2.11 Score per residue for model 11

- Molecule 1: Maltose-binding periplasmic protein



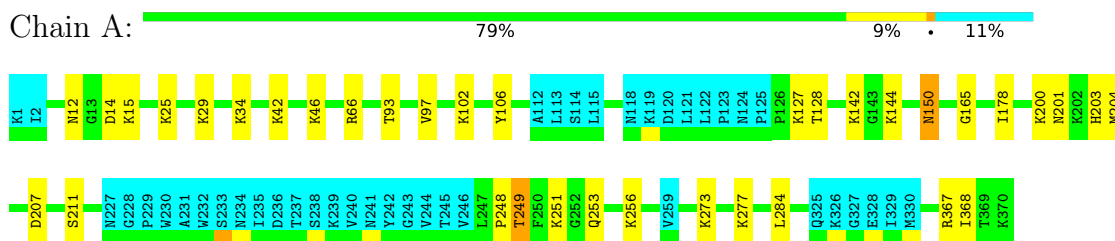
4.2.12 Score per residue for model 12

- Molecule 1: Maltose-binding periplasmic protein



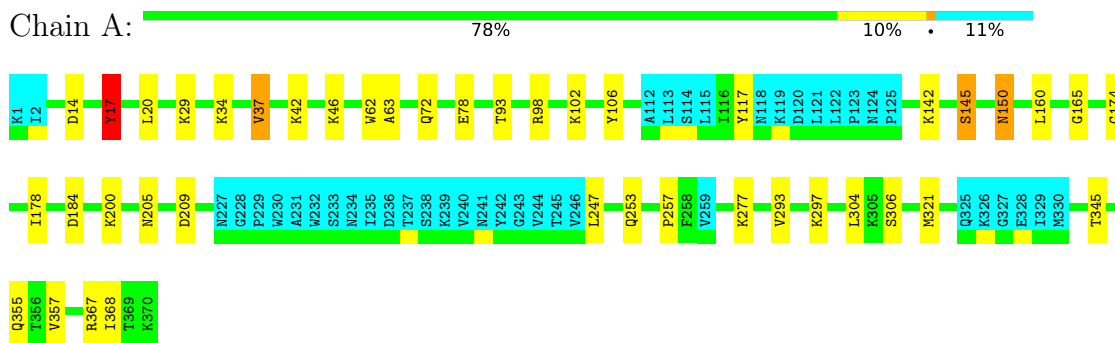
4.2.13 Score per residue for model 13

- Molecule 1: Maltose-binding periplasmic protein



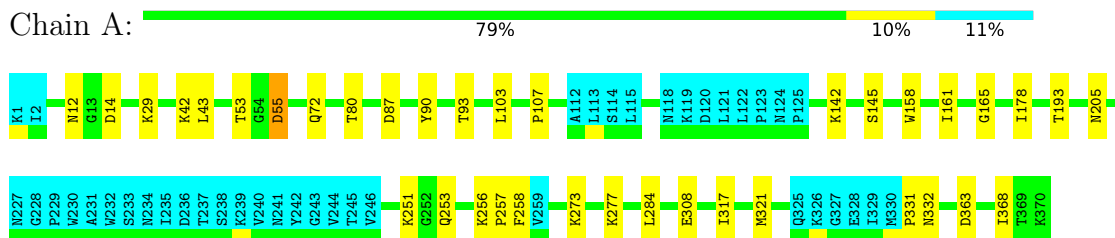
4.2.14 Score per residue for model 14

- Molecule 1: Maltose-binding periplasmic protein



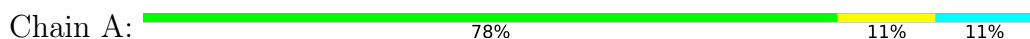
4.2.15 Score per residue for model 15

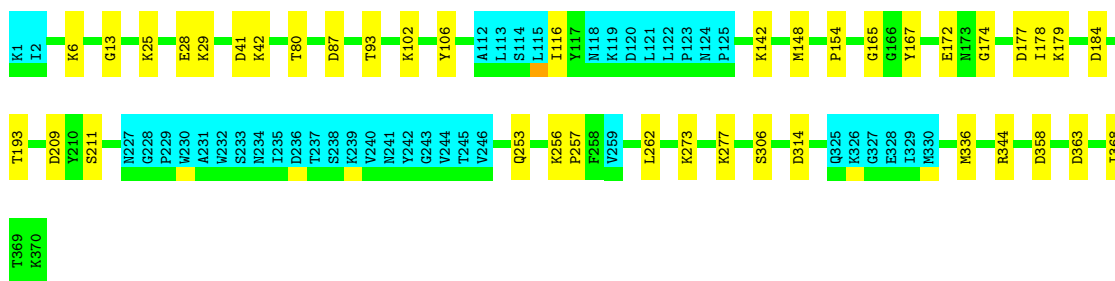
- Molecule 1: Maltose-binding periplasmic protein



4.2.16 Score per residue for model 16

- Molecule 1: Maltose-binding periplasmic protein

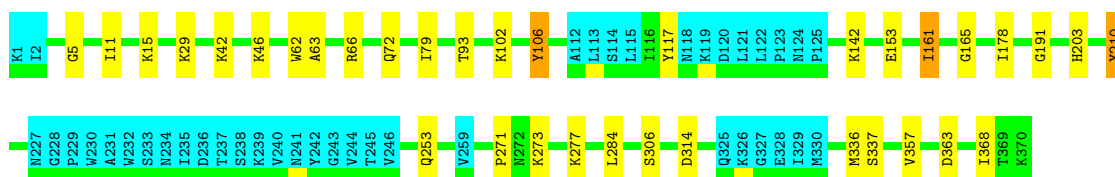




4.2.17 Score per residue for model 17

- Molecule 1: Maltose-binding periplasmic protein

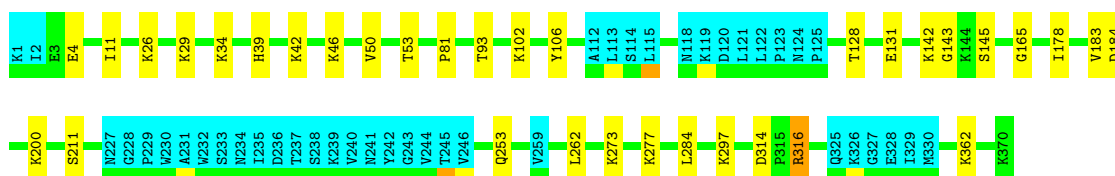
Chain A: 79% 9% 11%



4.2.18 Score per residue for model 18

- Molecule 1: Maltose-binding periplasmic protein

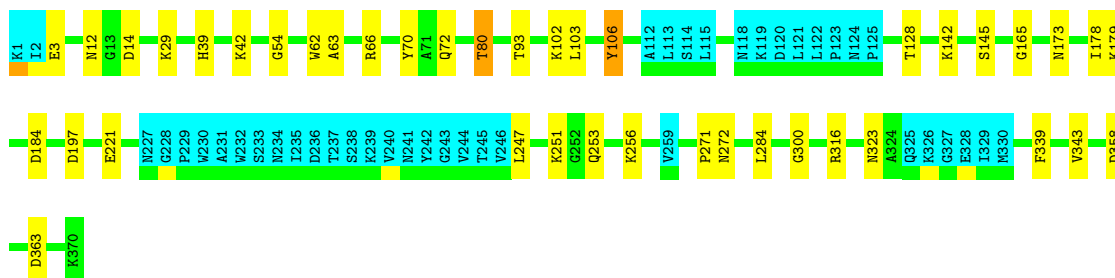
Chain A: 80% 9% 11%



4.2.19 Score per residue for model 19

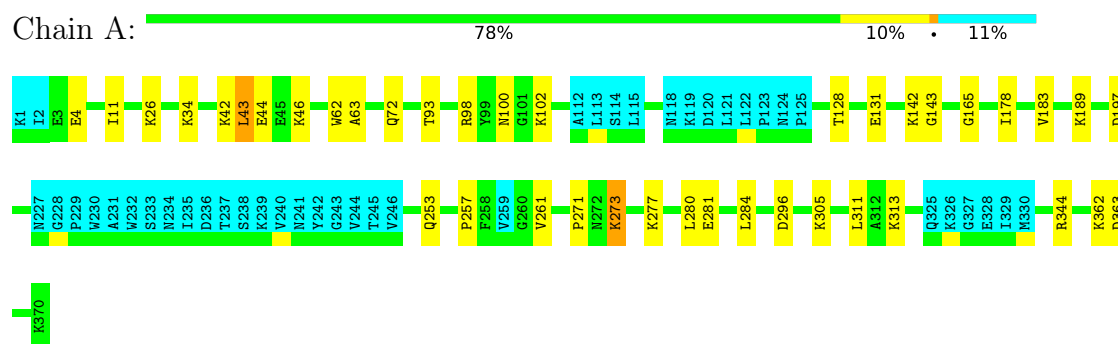
- Molecule 1: Maltose-binding periplasmic protein

Chain A: 78% 11% 11%



4.2.20 Score per residue for model 20

- Molecule 1: Maltose-binding periplasmic protein



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
OPALp	refinement	1.4
CYANA	structure solution	2.1

No chemical shift data was provided.

6 Model quality i

6.1 Standard geometry i

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	0.63±0.01	0±0/2621 (0.0± 0.0%)	1.35±0.02	5±3/3551 (0.1± 0.1%)
All	All	0.63	0/52420 (0.0%)	1.35	106/71020 (0.1%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	2.1±1.5
All	All	0	42

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	12	ASN	CA-CB-CG	8.01	120.61	112.60	3	2
1	A	150	ASN	CA-CB-CG	7.46	120.06	112.60	13	5
1	A	184	ASP	CA-CB-CG	7.12	119.72	112.60	7	1
1	A	3	GLU	CA-C-N	6.87	131.18	121.02	10	1
1	A	3	GLU	C-N-CA	6.87	131.18	121.02	10	1
1	A	13	GLY	N-CA-C	-6.65	104.85	112.29	1	1
1	A	368	ILE	N-CA-C	-6.59	106.14	111.81	15	3
1	A	357	VAL	CA-C-N	6.57	129.41	120.54	1	3
1	A	357	VAL	C-N-CA	6.57	129.41	120.54	1	3
1	A	194	PHE	CA-CB-CG	6.56	120.36	113.80	9	1
1	A	12	ASN	CA-C-N	6.42	127.22	120.03	6	1
1	A	12	ASN	C-N-CA	6.42	127.22	120.03	6	1
1	A	3	GLU	N-CA-C	-6.37	97.89	108.34	19	1
1	A	55	ASP	CA-CB-CG	6.31	118.91	112.60	15	3
1	A	30	ASP	CA-CB-CG	6.29	118.89	112.60	7	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	64	HIS	CB-CG-CD2	-6.17	123.18	131.20	2	3
1	A	296	ASP	CA-CB-CG	-6.11	106.49	112.60	3	1
1	A	218	ASN	CA-CB-CG	6.02	118.62	112.60	9	1
1	A	205	ASN	CA-C-N	5.92	128.49	120.38	11	1
1	A	205	ASN	C-N-CA	5.92	128.49	120.38	11	1
1	A	300	GLY	CA-C-N	5.92	131.58	121.87	19	1
1	A	300	GLY	C-N-CA	5.92	131.58	121.87	19	1
1	A	63	ALA	CA-C-N	5.91	129.01	120.38	7	1
1	A	63	ALA	C-N-CA	5.91	129.01	120.38	7	1
1	A	80	THR	CA-CB-CG2	5.81	120.38	110.50	19	1
1	A	369	THR	CB-CA-C	5.79	120.59	110.64	4	1
1	A	264	ALA	CA-C-N	5.75	126.03	121.61	8	1
1	A	264	ALA	C-N-CA	5.75	126.03	121.61	8	1
1	A	215	ALA	CA-C-N	5.71	127.94	120.28	9	1
1	A	215	ALA	C-N-CA	5.71	127.94	120.28	9	1
1	A	258	PHE	CA-CB-CG	5.71	119.51	113.80	12	1
1	A	339	PHE	CA-CB-CG	5.69	119.49	113.80	6	1
1	A	332	ASN	CA-CB-CG	5.69	118.29	112.60	4	1
1	A	201	ASN	CA-CB-CG	5.69	118.29	112.60	13	1
1	A	177	ASP	CA-CB-CG	5.67	118.27	112.60	12	4
1	A	311	LEU	N-CA-C	-5.67	104.57	112.45	20	1
1	A	317	ILE	N-CA-C	-5.67	105.58	110.74	15	1
1	A	14	ASP	CA-CB-CG	5.64	118.24	112.60	13	1
1	A	323	ASN	CA-CB-CG	-5.62	106.98	112.60	4	1
1	A	82	ASP	CA-C-N	5.61	128.07	120.38	9	2
1	A	82	ASP	C-N-CA	5.61	128.07	120.38	9	2
1	A	203	HIS	CB-CG-CD2	-5.55	123.99	131.20	11	3
1	A	362	LYS	CA-C-N	5.52	127.99	120.54	3	3
1	A	362	LYS	C-N-CA	5.52	127.99	120.54	3	3
1	A	80	THR	CB-CA-C	5.50	121.00	110.17	19	1
1	A	61	PHE	CA-CB-CG	5.43	119.23	113.80	12	1
1	A	26	LYS	N-CA-C	-5.43	105.26	111.07	3	1
1	A	160	LEU	N-CA-C	-5.43	104.24	111.24	14	1
1	A	54	GLY	CA-C-N	5.36	130.99	122.10	19	1
1	A	54	GLY	C-N-CA	5.36	130.99	122.10	19	1
1	A	273	LYS	CA-C-N	5.36	127.46	120.28	20	1
1	A	273	LYS	C-N-CA	5.36	127.46	120.28	20	1
1	A	197	ASP	CA-CB-CG	-5.35	107.25	112.60	9	1
1	A	320	THR	N-CA-C	-5.34	106.44	113.12	7	1
1	A	131	GLU	CA-C-N	5.34	124.60	120.33	20	1
1	A	131	GLU	C-N-CA	5.34	124.60	120.33	20	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	250	PHE	CA-CB-CG	5.24	119.04	113.80	9	2
1	A	154	PRO	CA-C-N	5.23	127.54	120.38	16	1
1	A	154	PRO	C-N-CA	5.23	127.54	120.38	16	1
1	A	210	TYR	CA-C-N	5.21	127.79	120.28	6	1
1	A	210	TYR	C-N-CA	5.21	127.79	120.28	6	1
1	A	41	ASP	N-CA-C	-5.19	107.50	113.88	16	1
1	A	39	HIS	CA-CB-CG	5.18	118.98	113.80	18	1
1	A	226	ILE	CB-CA-C	5.15	117.38	110.42	7	1
1	A	135	LEU	N-CA-C	-5.10	107.22	113.50	4	1
1	A	23	VAL	N-CA-C	-5.10	105.57	110.72	7	1
1	A	53	THR	N-CA-C	-5.09	106.41	113.18	15	1
1	A	363	ASP	CA-C-N	5.08	127.05	120.44	20	1
1	A	363	ASP	C-N-CA	5.08	127.05	120.44	20	1
1	A	203	HIS	CA-CB-CG	5.08	118.88	113.80	13	1
1	A	156	PHE	CA-CB-CG	-5.06	108.74	113.80	9	1
1	A	39	HIS	CA-C-N	5.05	125.05	120.21	19	1
1	A	39	HIS	C-N-CA	5.05	125.05	120.21	19	1
1	A	206	ALA	CA-C-N	5.03	130.52	121.66	8	1
1	A	206	ALA	C-N-CA	5.03	130.52	121.66	8	1
1	A	205	ASN	CA-CB-CG	5.03	117.63	112.60	14	1
1	A	368	ILE	CB-CA-C	5.03	115.48	111.06	14	1
1	A	179	LYS	N-CA-C	-5.00	105.54	111.69	16	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	66	ARG	Sidechain	5
1	A	106	TYR	Sidechain	4
1	A	98	ARG	Sidechain	4
1	A	367	ARG	Sidechain	3
1	A	171	TYR	Sidechain	3
1	A	176	TYR	Sidechain	3
1	A	316	ARG	Sidechain	3
1	A	117	TYR	Sidechain	2
1	A	167	TYR	Sidechain	2
1	A	210	TYR	Sidechain	2
1	A	17	TYR	Sidechain	2
1	A	90	TYR	Sidechain	2
1	A	354	ARG	Sidechain	1

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	47	PHE	Sidechain	1
1	A	344	ARG	Sidechain	1
1	A	155	TYR	Sidechain	1
1	A	156	PHE	Sidechain	1
1	A	341	TYR	Sidechain	1
1	A	70	TYR	Sidechain	1

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	2560	2533	2533	1±1
All	All	51200	50660	50660	29

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
1:A:43:LEU:HD22	1:A:44:GLU:N	0.54	2.16	20	1
1:A:62:TRP:CG	1:A:63:ALA:H	0.54	2.21	3	3
1:A:197:ASP:HA	1:A:200:LYS:HE3	0.50	1.83	1	2
1:A:339:PHE:O	1:A:343:VAL:HG23	0.49	2.07	3	1
1:A:161:ILE:H	1:A:161:ILE:HD13	0.49	1.67	17	1
1:A:77:ALA:HB2	1:A:268:ALA:HA	0.48	1.85	7	1
1:A:62:TRP:CD1	1:A:63:ALA:H	0.47	2.27	17	3
1:A:150:ASN:HD22	1:A:210:TYR:HB2	0.47	1.69	10	1
1:A:161:ILE:HG22	1:A:191:GLY:HA3	0.46	1.87	17	1
1:A:17:TYR:CE1	1:A:37:VAL:HG22	0.46	2.46	14	1
1:A:20:LEU:HA	1:A:293:VAL:HG22	0.46	1.88	14	1
1:A:12:ASN:HB3	1:A:43:LEU:HD21	0.46	1.88	3	1
1:A:339:PHE:O	1:A:343:VAL:HG22	0.45	2.11	19	1
1:A:249:THR:HG22	1:A:255:SER:H	0.45	1.71	6	1
1:A:79:ILE:HD12	1:A:106:TYR:CD2	0.42	2.49	10	2
1:A:317:ILE:HD12	1:A:317:ILE:H	0.42	1.75	8	1
1:A:345:THR:HG21	1:A:367:ARG:HH22	0.41	1.75	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:285:LEU:HD22	1:A:304:LEU:HD21	0.41	1.92	4	1
1:A:50:VAL:HG12	1:A:55:ASP:C	0.40	2.41	9	1
1:A:156:PHE:CZ	1:A:226:ILE:HG21	0.40	2.51	9	1
1:A:62:TRP:CG	1:A:63:ALA:N	0.40	2.88	3	1
1:A:93:THR:HG22	1:A:107:PRO:CB	0.40	2.46	15	1
1:A:9:ILE:HD12	1:A:37:VAL:HG22	0.40	1.92	9	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	328/370 (89%)	301±4 (92±1%)	23±5 (7±1%)	4±1 (1±0%)	13	61
All	All	6560/7400 (89%)	6022 (92%)	461 (7%)	77 (1%)	13	61

All 28 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	165	GLY	19
1	A	80	THR	7
1	A	257	PRO	6
1	A	271	PRO	6
1	A	143	GLY	5
1	A	174	GLY	5
1	A	173	ASN	3
1	A	178	ILE	3
1	A	14	ASP	3
1	A	5	GLY	2
1	A	251	LYS	1
1	A	77	ALA	1
1	A	202	LYS	1
1	A	150	ASN	1
1	A	162	ALA	1
1	A	3	GLU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	54	GLY	1
1	A	285	LEU	1
1	A	101	GLY	1
1	A	248	PRO	1
1	A	249	THR	1
1	A	145	SER	1
1	A	331	PRO	1
1	A	332	ASN	1
1	A	13	GLY	1
1	A	81	PRO	1
1	A	221	GLU	1
1	A	100	ASN	1

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	261/297 (88%)	234±3 (90±1%)	27±3 (10±1%)	9	53
All	All	5220/5940 (88%)	4676 (90%)	544 (10%)	9	53

All 129 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	142	LYS	20
1	A	178	ILE	20
1	A	42	LYS	19
1	A	93	THR	19
1	A	102	LYS	19
1	A	253	GLN	19
1	A	277	LYS	18
1	A	29	LYS	13
1	A	34	LYS	13
1	A	72	GLN	12
1	A	46	LYS	11
1	A	314	ASP	11
1	A	145	SER	11

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Mol	Chain	Res	Type	Models (Total)
1	A	273	LYS	11
1	A	284	LEU	11
1	A	106	TYR	10
1	A	128	THR	9
1	A	200	LYS	8
1	A	211	SER	8
1	A	25	LYS	8
1	A	11	ILE	7
1	A	209	ASP	7
1	A	256	LYS	7
1	A	197	ASP	7
1	A	251	LYS	7
1	A	6	LYS	6
1	A	296	ASP	6
1	A	297	LYS	6
1	A	363	ASP	6
1	A	193	THR	6
1	A	184	ASP	6
1	A	262	LEU	5
1	A	4	GLU	5
1	A	103	LEU	5
1	A	12	ASN	5
1	A	358	ASP	5
1	A	336	MET	5
1	A	306	SER	5
1	A	179	LYS	4
1	A	55	ASP	4
1	A	144	LYS	4
1	A	28	GLU	4
1	A	151	LEU	4
1	A	183	VAL	4
1	A	43	LEU	4
1	A	150	ASN	4
1	A	79	ILE	4
1	A	15	LYS	4
1	A	26	LYS	3
1	A	95	ASP	3
1	A	161	ILE	3
1	A	177	ASP	3
1	A	203	HIS	3
1	A	247	LEU	3
1	A	88	LYS	3

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Mol	Chain	Res	Type	Models (Total)
1	A	370	LYS	3
1	A	87	ASP	3
1	A	344	ARG	3
1	A	189	LYS	2
1	A	41	ASP	2
1	A	192	LEU	2
1	A	261	VAL	2
1	A	343	VAL	2
1	A	49	GLN	2
1	A	204	MET	2
1	A	62	TRP	2
1	A	160	LEU	2
1	A	222	THR	2
1	A	280	LEU	2
1	A	50	VAL	2
1	A	337	SER	2
1	A	345	THR	2
1	A	80	THR	2
1	A	205	ASN	2
1	A	53	THR	2
1	A	207	ASP	2
1	A	305	LYS	2
1	A	361	LEU	2
1	A	127	LYS	2
1	A	58	ASP	2
1	A	158	TRP	2
1	A	219	LYS	2
1	A	131	GLU	2
1	A	321	MET	2
1	A	316	ARG	2
1	A	14	ASP	1
1	A	274	GLU	1
1	A	224	MET	1
1	A	255	SER	1
1	A	332	ASN	1
1	A	366	THR	1
1	A	89	LEU	1
1	A	225	THR	1
1	A	295	LYS	1
1	A	181	VAL	1
1	A	18	ASN	1
1	A	175	LYS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	194	PHE	1
1	A	218	ASN	1
1	A	60	ILE	1
1	A	98	ARG	1
1	A	195	LEU	1
1	A	201	ASN	1
1	A	335	GLN	1
1	A	36	THR	1
1	A	137	LYS	1
1	A	65	ASP	1
1	A	285	LEU	1
1	A	97	VAL	1
1	A	249	THR	1
1	A	368	ILE	1
1	A	17	TYR	1
1	A	37	VAL	1
1	A	78	GLU	1
1	A	117	TYR	1
1	A	304	LEU	1
1	A	355	GLN	1
1	A	258	PHE	1
1	A	308	GLU	1
1	A	148	MET	1
1	A	172	GLU	1
1	A	153	GLU	1
1	A	210	TYR	1
1	A	362	LYS	1
1	A	66	ARG	1
1	A	272	ASN	1
1	A	323	ASN	1
1	A	281	GLU	1
1	A	313	LYS	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 oligosaccharides 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