



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 06:23 PM UTC

PDB ID : 1SR2 / pdb_00001sr2
Title : Solution structure of the Escherichia coli YojN Histidine-Phosphotransferase (HPt) domain
Authors : Rogov, V.V.; Bernhard, F.; Loehr, F.; Doetsch, V.
Deposited on : 2004-03-22

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 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

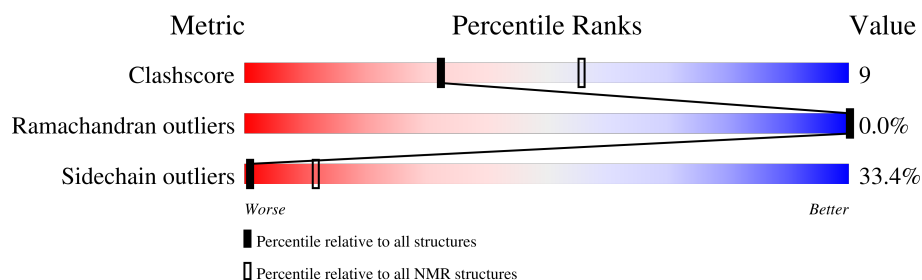
1 Overall quality at a glance

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	116	

2 Ensemble composition and analysis

This entry contains 25 models. Model 9 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:802-A:890 (89)	0.63	9

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 4 single-model clusters were found.

Cluster number	Models
1	5, 6, 12, 18, 20, 25
2	1, 4, 9, 13, 15
3	7, 16, 21, 24
4	10, 19
5	11, 17
6	3, 14
Single-model clusters	2; 8; 22; 23

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1806 atoms, of which 903 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Putative sensor-like histidine kinase yojN.

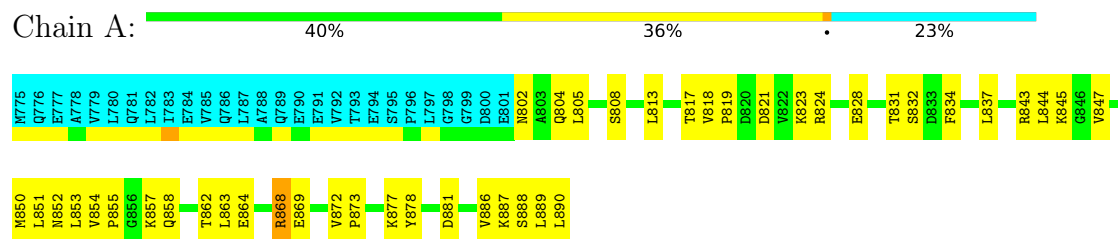
Mol	Chain	Residues	Atoms						Trace
1	A	116	Total	C	H	N	O	S	0
			1806	573	903	146	181	3	

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: Putative sensor-like histidine kinase yojN

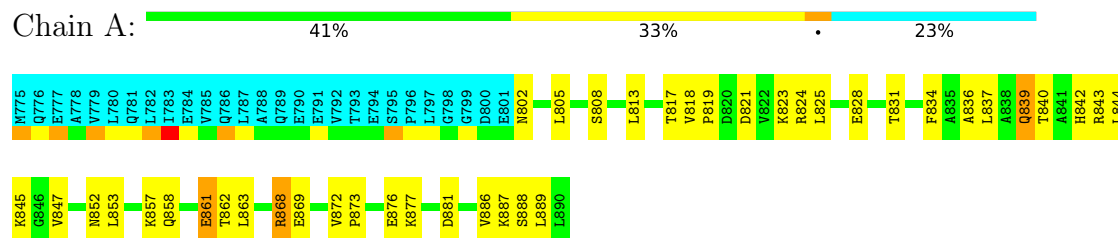


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

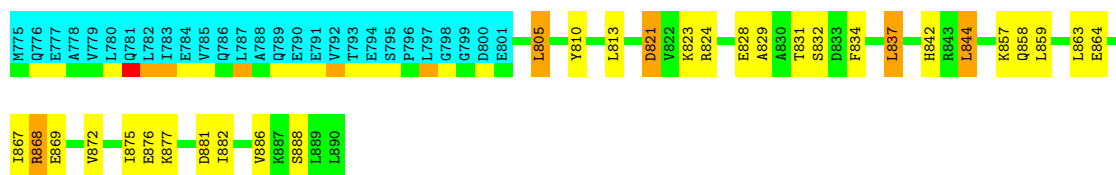
- Molecule 1: Putative sensor-like histidine kinase yojN



4.2.2 Score per residue for model 2

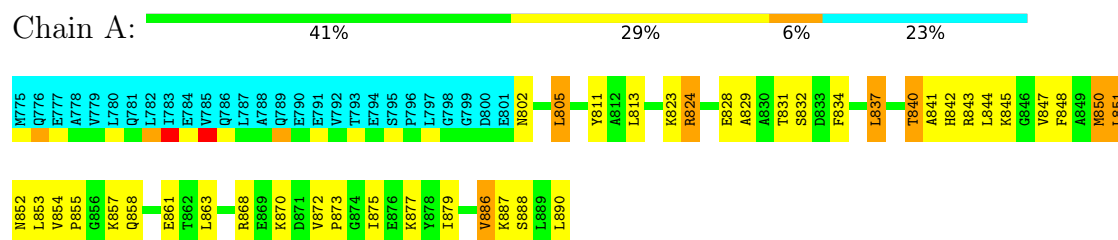
- Molecule 1: Putative sensor-like histidine kinase yojN





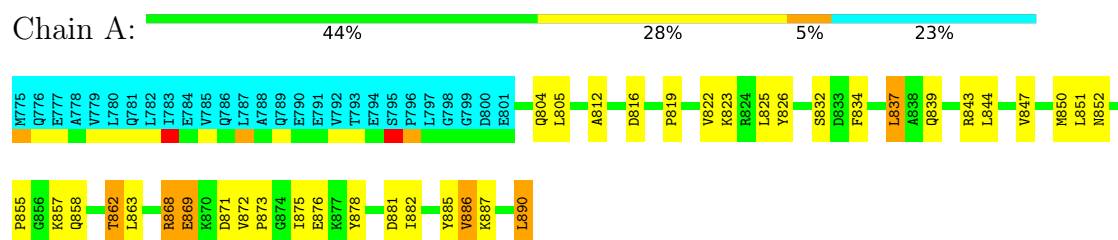
4.2.3 Score per residue for model 3

- Molecule 1: Putative sensor-like histidine kinase yojN



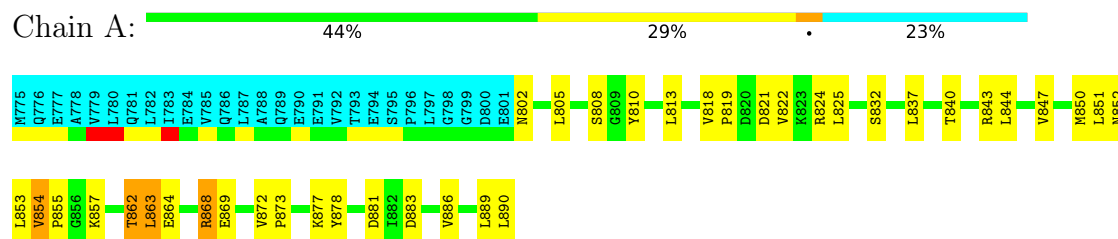
4.2.4 Score per residue for model 4

- Molecule 1: Putative sensor-like histidine kinase yojN



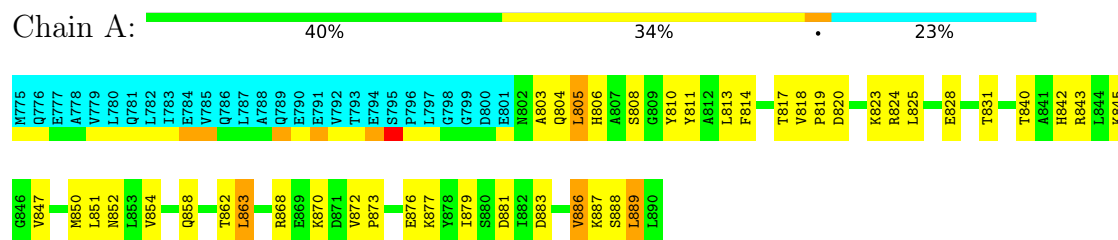
4.2.5 Score per residue for model 5

- Molecule 1: Putative sensor-like histidine kinase yojN



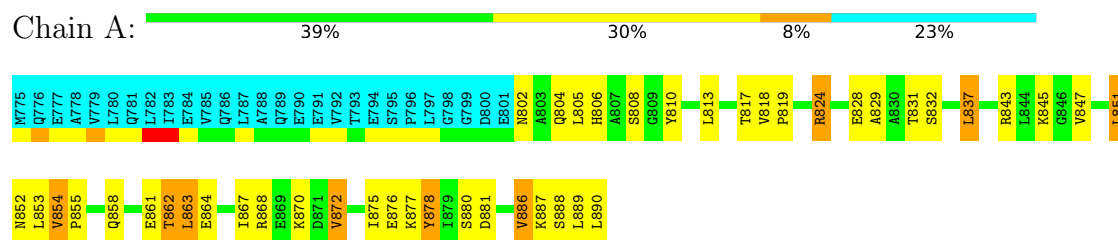
4.2.6 Score per residue for model 6

- Molecule 1: Putative sensor-like histidine kinase yojN



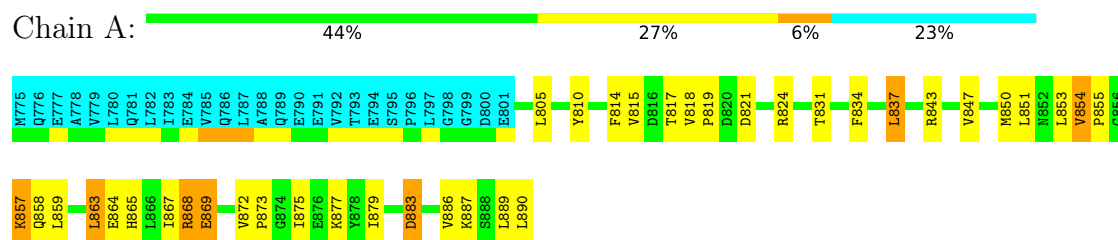
4.2.7 Score per residue for model 7

- Molecule 1: Putative sensor-like histidine kinase yojN



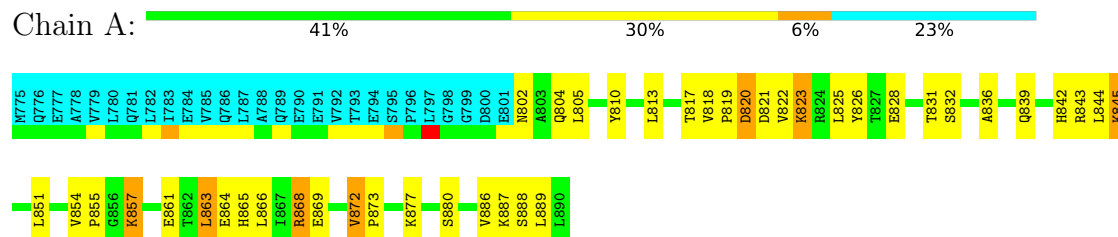
4.2.8 Score per residue for model 8

- Molecule 1: Putative sensor-like histidine kinase yojN



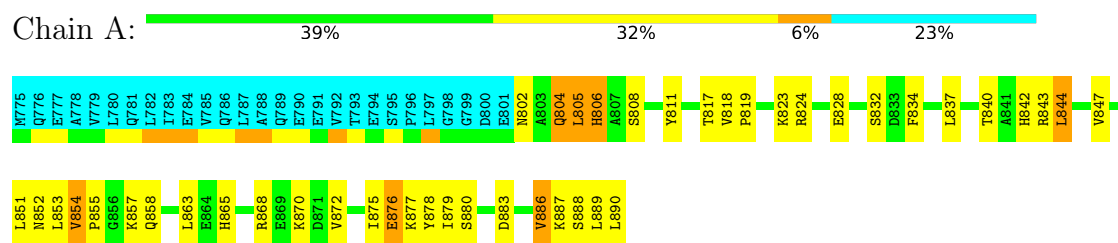
4.2.9 Score per residue for model 9 (medoid)

- Molecule 1: Putative sensor-like histidine kinase yojN



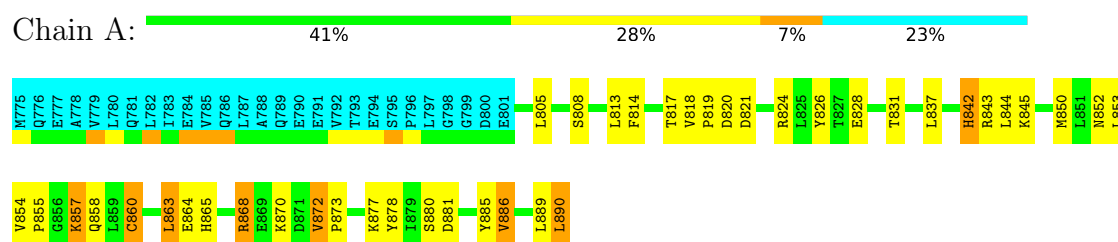
4.2.10 Score per residue for model 10

- Molecule 1: Putative sensor-like histidine kinase yojN



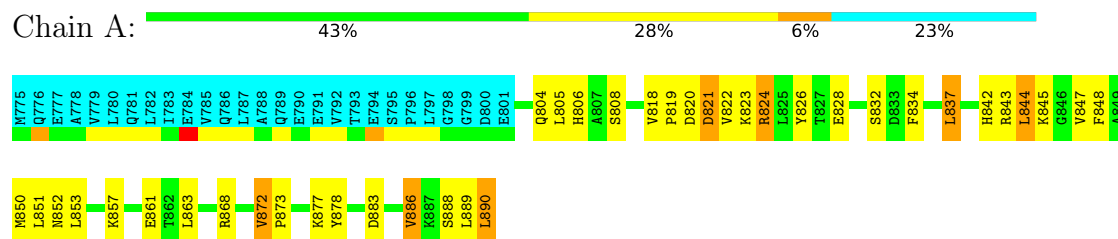
4.2.11 Score per residue for model 11

- Molecule 1: Putative sensor-like histidine kinase yojN



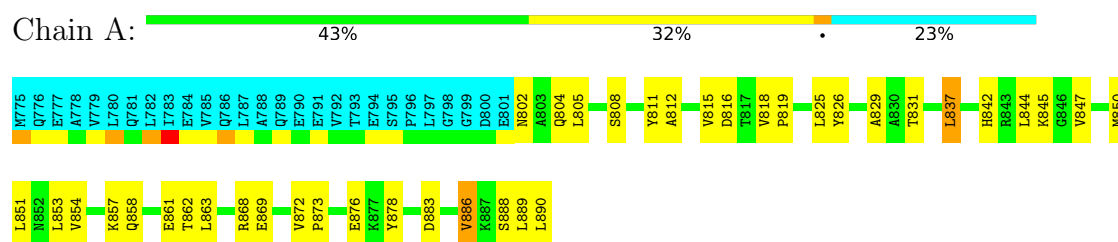
4.2.12 Score per residue for model 12

- Molecule 1: Putative sensor-like histidine kinase yojN



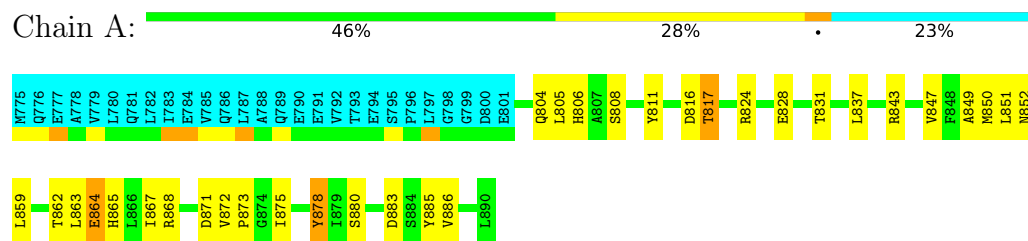
4.2.13 Score per residue for model 13

- Molecule 1: Putative sensor-like histidine kinase yojN



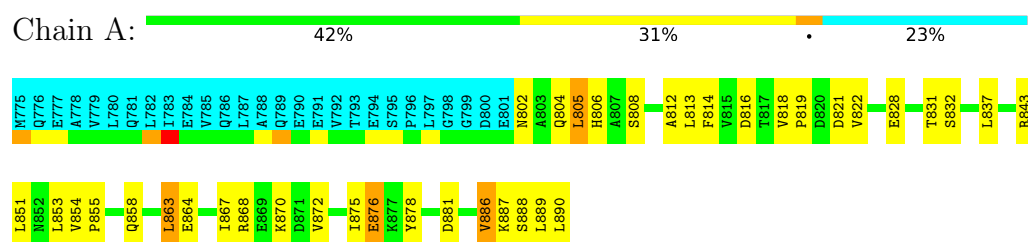
4.2.14 Score per residue for model 14

- Molecule 1: Putative sensor-like histidine kinase yojN



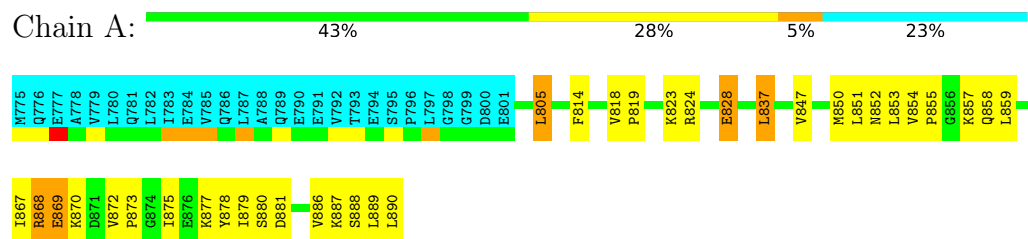
4.2.15 Score per residue for model 15

- Molecule 1: Putative sensor-like histidine kinase yojN



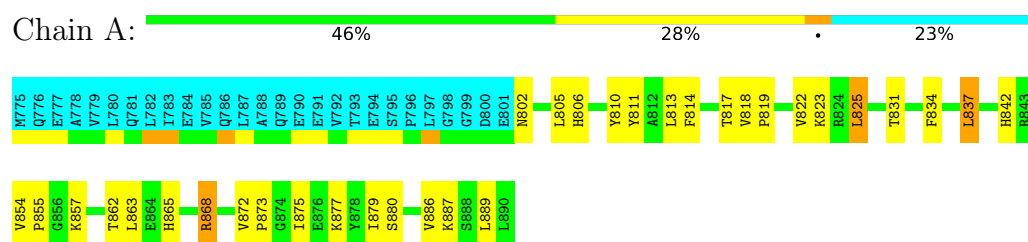
4.2.16 Score per residue for model 16

- Molecule 1: Putative sensor-like histidine kinase yojN



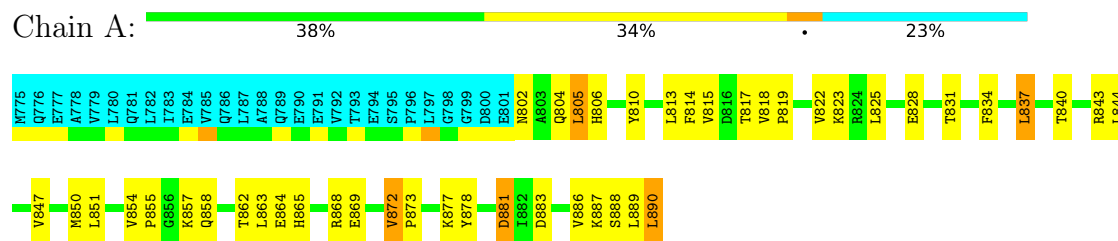
4.2.17 Score per residue for model 17

- Molecule 1: Putative sensor-like histidine kinase yojN



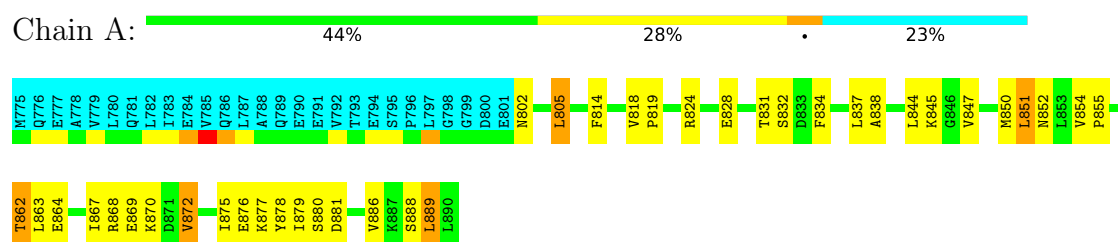
4.2.18 Score per residue for model 18

- Molecule 1: Putative sensor-like histidine kinase yojN



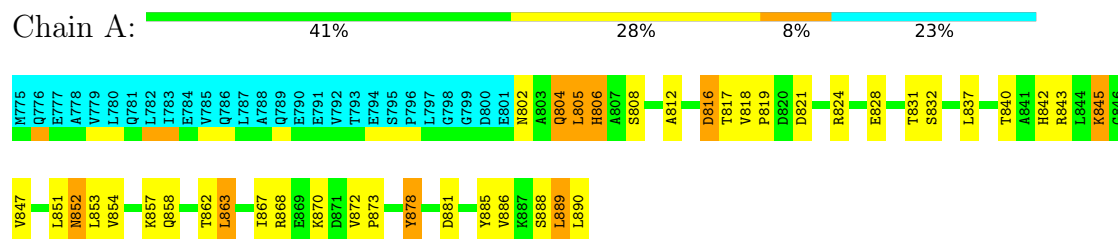
4.2.19 Score per residue for model 19

- Molecule 1: Putative sensor-like histidine kinase yojN



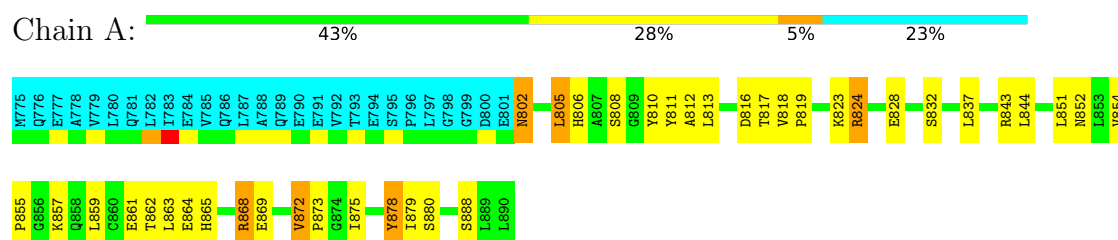
4.2.20 Score per residue for model 20

- Molecule 1: Putative sensor-like histidine kinase yojN



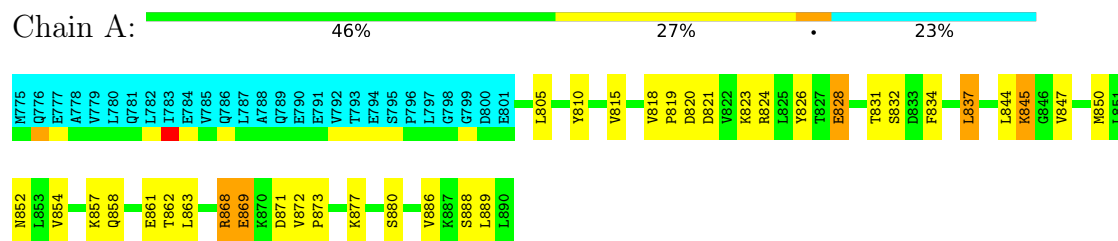
4.2.21 Score per residue for model 21

- Molecule 1: Putative sensor-like histidine kinase yojN



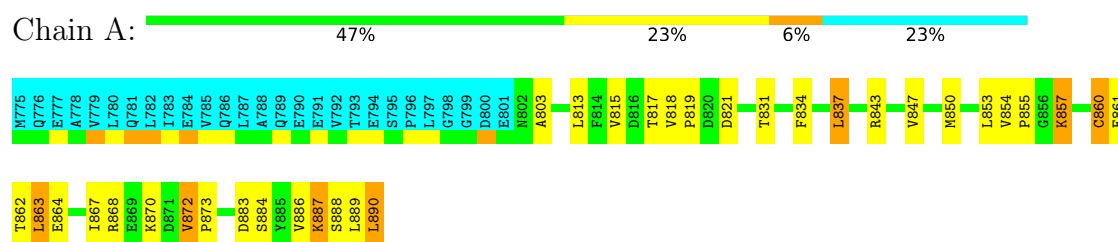
4.2.22 Score per residue for model 22

- Molecule 1: Putative sensor-like histidine kinase yojN



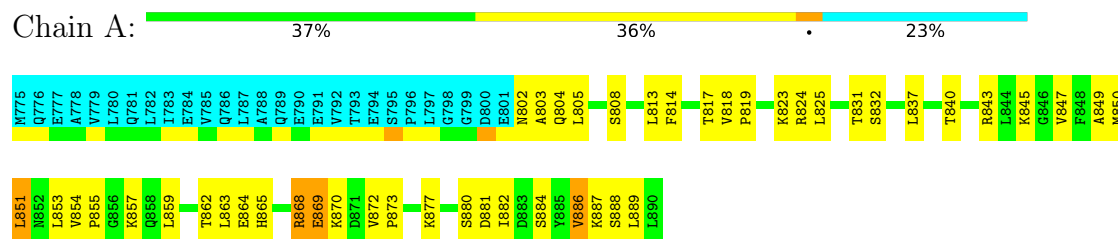
4.2.23 Score per residue for model 23

- Molecule 1: Putative sensor-like histidine kinase yojN



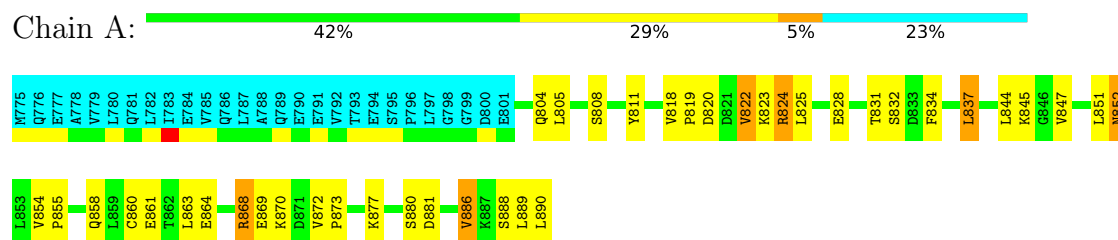
4.2.24 Score per residue for model 24

- Molecule 1: Putative sensor-like histidine kinase yojN



4.2.25 Score per residue for model 25

- Molecule 1: Putative sensor-like histidine kinase yojN



5 Refinement protocol and experimental data overview

The models were refined using the following method: *Energy minimization*.

Of the 50 calculated structures, 25 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
DYANA	structure solution	1.5
CNS	refinement	1.1

No chemical shift data was provided.

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	698	703	700	12±3
All	All	17450	17575	17500	298

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 9.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:802:ASN:HA	1:A:805:LEU:HD23	0.83	1.47	20	5
1:A:854:VAL:HG13	1:A:855:PRO:HD3	0.79	1.55	7	1
1:A:820:ASP:HA	1:A:823:LYS:HD3	0.73	1.59	9	1
1:A:863:LEU:HG	1:A:878:TYR:CD2	0.66	2.26	16	1
1:A:854:VAL:HB	1:A:855:PRO:HD3	0.65	1.68	19	11
1:A:818:VAL:HG11	1:A:886:VAL:HG21	0.64	1.69	7	3
1:A:847:VAL:O	1:A:851:LEU:HG	0.64	1.92	5	17
1:A:840:THR:HA	1:A:843:ARG:HD3	0.63	1.69	20	1
1:A:865:HIS:HA	1:A:868:ARG:HG2	0.62	1.69	24	3
1:A:857:LYS:HA	1:A:860:CYS:SG	0.62	2.34	11	2
1:A:818:VAL:HB	1:A:819:PRO:HD3	0.62	1.71	16	19
1:A:829:ALA:HA	1:A:837:LEU:HD11	0.62	1.72	3	4
1:A:886:VAL:O	1:A:890:LEU:HG	0.61	1.95	7	13
1:A:824:ARG:O	1:A:828:GLU:HG2	0.61	1.94	1	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:863:LEU:HG	1:A:878:TYR:HB3	0.60	1.71	15	5
1:A:872:VAL:HB	1:A:873:PRO:HD3	0.59	1.74	16	11
1:A:859:LEU:HB3	1:A:878:TYR:HE1	0.59	1.57	16	1
1:A:825:LEU:HD23	1:A:837:LEU:HG	0.59	1.74	17	1
1:A:822:VAL:HG11	1:A:883:ASP:HB2	0.59	1.75	12	1
1:A:842:HIS:HA	1:A:845:LYS:HD2	0.58	1.73	9	2
1:A:823:LYS:HA	1:A:826:TYR:HD2	0.58	1.58	9	1
1:A:834:PHE:HA	1:A:837:LEU:HB2	0.58	1.75	17	11
1:A:814:PHE:HE1	1:A:886:VAL:HG22	0.58	1.59	15	1
1:A:865:HIS:O	1:A:869:GLU:HG2	0.57	1.99	18	1
1:A:841:ALA:O	1:A:845:LYS:HG3	0.57	1.98	3	1
1:A:819:PRO:HA	1:A:822:VAL:HG22	0.57	1.76	4	1
1:A:805:LEU:HD11	1:A:814:PHE:HB2	0.56	1.76	16	3
1:A:838:ALA:HA	1:A:867:ILE:HD13	0.56	1.78	19	1
1:A:805:LEU:HB3	1:A:811:TYR:HD1	0.55	1.60	3	1
1:A:816:ASP:O	1:A:817:THR:HB	0.54	2.02	14	1
1:A:810:TYR:HB3	1:A:851:LEU:HD22	0.54	1.79	6	2
1:A:845:LYS:HE2	1:A:861:GLU:HG2	0.53	1.78	25	4
1:A:851:LEU:O	1:A:852:ASN:HB2	0.53	2.03	4	4
1:A:862:THR:HB	1:A:878:TYR:CE2	0.53	2.39	21	7
1:A:868:ARG:HG3	1:A:869:GLU:N	0.52	2.19	4	9
1:A:811:TYR:OH	1:A:890:LEU:HA	0.52	2.04	25	1
1:A:814:PHE:CZ	1:A:886:VAL:HG23	0.51	2.40	16	3
1:A:836:ALA:O	1:A:839:GLN:HG3	0.51	2.05	9	2
1:A:821:ASP:HB3	1:A:844:LEU:HD21	0.51	1.81	2	1
1:A:872:VAL:HA	1:A:875:ILE:HD12	0.51	1.82	14	2
1:A:814:PHE:CE1	1:A:886:VAL:HG22	0.50	2.41	6	2
1:A:864:GLU:HA	1:A:867:ILE:HD12	0.50	1.84	15	1
1:A:825:LEU:HG	1:A:840:THR:HG21	0.50	1.84	1	1
1:A:803:ALA:HA	1:A:806:HIS:CD2	0.50	2.42	6	1
1:A:863:LEU:O	1:A:867:ILE:HG12	0.49	2.07	20	3
1:A:863:LEU:HA	1:A:866:LEU:HD12	0.49	1.84	9	1
1:A:812:ALA:O	1:A:816:ASP:HB2	0.49	2.08	4	5
1:A:865:HIS:O	1:A:868:ARG:HG3	0.49	2.07	11	4
1:A:842:HIS:O	1:A:845:LYS:HG2	0.49	2.07	11	2
1:A:840:THR:O	1:A:843:ARG:HG2	0.49	2.07	10	1
1:A:859:LEU:HB3	1:A:878:TYR:CE1	0.49	2.41	16	1
1:A:824:ARG:HB3	1:A:840:THR:HG21	0.49	1.84	3	1
1:A:875:ILE:O	1:A:879:ILE:HG13	0.49	2.08	16	6
1:A:865:HIS:O	1:A:869:GLU:HB2	0.48	2.09	8	1
1:A:819:PRO:O	1:A:822:VAL:HG22	0.48	2.08	25	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:815:VAL:HG12	1:A:890:LEU:HD22	0.48	1.85	23	3
1:A:845:LYS:HA	1:A:860:CYS:SG	0.48	2.49	11	1
1:A:872:VAL:N	1:A:873:PRO:HD2	0.48	2.24	14	9
1:A:883:ASP:O	1:A:887:LYS:HG2	0.48	2.09	18	4
1:A:828:GLU:HB2	1:A:837:LEU:HD12	0.48	1.84	22	1
1:A:842:HIS:HA	1:A:845:LYS:HD3	0.47	1.85	3	1
1:A:851:LEU:HB2	1:A:853:LEU:HG	0.47	1.84	16	1
1:A:837:LEU:HB3	1:A:867:ILE:HD12	0.47	1.86	8	1
1:A:814:PHE:CZ	1:A:886:VAL:HG22	0.47	2.44	11	2
1:A:820:ASP:O	1:A:823:LYS:HG2	0.47	2.10	9	1
1:A:872:VAL:O	1:A:876:GLU:HG2	0.47	2.10	10	3
1:A:883:ASP:O	1:A:886:VAL:HG12	0.47	2.10	18	1
1:A:805:LEU:HG	1:A:806:HIS:N	0.46	2.24	20	2
1:A:805:LEU:HA	1:A:810:TYR:CE1	0.46	2.46	2	1
1:A:886:VAL:HG13	1:A:890:LEU:HD21	0.46	1.86	25	1
1:A:871:ASP:O	1:A:875:ILE:HG12	0.46	2.10	4	1
1:A:854:VAL:HA	1:A:857:LYS:HD3	0.45	1.88	8	1
1:A:849:ALA:HB2	1:A:857:LYS:HD2	0.45	1.87	24	2
1:A:867:ILE:HA	1:A:875:ILE:HD11	0.45	1.87	2	3
1:A:864:GLU:HG3	1:A:865:HIS:N	0.45	2.26	14	1
1:A:875:ILE:O	1:A:879:ILE:HG12	0.45	2.11	21	1
1:A:863:LEU:HG	1:A:878:TYR:CE2	0.45	2.46	16	1
1:A:804:GLN:HG3	1:A:805:LEU:N	0.45	2.27	20	1
1:A:834:PHE:HA	1:A:837:LEU:HB3	0.45	1.88	19	1
1:A:806:HIS:HA	1:A:811:TYR:HB2	0.44	1.87	21	2
1:A:828:GLU:HB2	1:A:837:LEU:HD13	0.44	1.89	12	2
1:A:847:VAL:O	1:A:850:MET:HB3	0.44	2.12	3	1
1:A:862:THR:HB	1:A:878:TYR:HE2	0.44	1.71	13	1
1:A:884:SER:HA	1:A:887:LYS:HB2	0.44	1.88	23	1
1:A:818:VAL:O	1:A:822:VAL:HG22	0.44	2.13	15	1
1:A:872:VAL:O	1:A:876:GLU:HG3	0.44	2.13	15	1
1:A:814:PHE:O	1:A:819:PRO:HD3	0.44	2.13	8	2
1:A:857:LYS:O	1:A:861:GLU:HG2	0.44	2.12	9	2
1:A:834:PHE:HA	1:A:837:LEU:HD12	0.43	1.90	1	1
1:A:854:VAL:HB	1:A:855:PRO:CD	0.43	2.43	24	2
1:A:819:PRO:HA	1:A:822:VAL:CG2	0.43	2.43	4	2
1:A:855:PRO:HG2	1:A:885:TYR:OH	0.43	2.13	11	2
1:A:878:TYR:HA	1:A:881:ASP:HB2	0.43	1.90	18	1
1:A:854:VAL:N	1:A:855:PRO:HD2	0.43	2.29	10	2
1:A:868:ARG:HG3	1:A:869:GLU:HG2	0.42	1.90	16	2
1:A:844:LEU:HA	1:A:847:VAL:HG22	0.42	1.89	1	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:802:ASN:HB2	1:A:889:LEU:HD23	0.42	1.91	20	1
1:A:818:VAL:O	1:A:822:VAL:HG13	0.42	2.15	25	1
1:A:886:VAL:HG22	1:A:890:LEU:HD21	0.42	1.91	18	1
1:A:844:LEU:HB3	1:A:860:CYS:SG	0.42	2.55	25	1
1:A:842:HIS:HA	1:A:845:LYS:CD	0.42	2.43	6	1
1:A:845:LYS:HE2	1:A:861:GLU:HA	0.42	1.90	7	1
1:A:802:ASN:HB3	1:A:889:LEU:HG	0.42	1.91	19	1
1:A:837:LEU:HD21	1:A:875:ILE:HG21	0.42	1.91	19	1
1:A:863:LEU:HD13	1:A:867:ILE:HD11	0.41	1.92	16	1
1:A:887:LYS:HA	1:A:890:LEU:HD12	0.41	1.91	16	1
1:A:814:PHE:CZ	1:A:889:LEU:HB3	0.41	2.50	6	1
1:A:868:ARG:HD2	1:A:869:GLU:OE2	0.41	2.15	5	1
1:A:821:ASP:OD1	1:A:843:ARG:HD2	0.41	2.16	12	1
1:A:818:VAL:N	1:A:819:PRO:HD2	0.41	2.30	23	1
1:A:822:VAL:HA	1:A:825:LEU:HD12	0.41	1.93	9	1
1:A:845:LYS:HD2	1:A:861:GLU:HG2	0.41	1.92	22	1
1:A:883:ASP:O	1:A:887:LYS:HB2	0.41	2.16	8	1
1:A:845:LYS:HE3	1:A:861:GLU:HG2	0.41	1.91	3	1
1:A:863:LEU:HD11	1:A:879:ILE:HG12	0.40	1.92	6	1
1:A:821:ASP:HB3	1:A:844:LEU:HD11	0.40	1.92	12	1
1:A:857:LYS:HG2	1:A:858:GLN:N	0.40	2.31	8	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	88/116 (76%)	86±1 (98±1%)	2±1 (2±1%)	0±0 (0±0%)	100	100
All	All	2200/2900 (76%)	2156 (98%)	43 (2%)	1 (0%)	100	100

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	817	THR	1

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	75/98 (77%)	50±3 (67±4%)	25±3 (33±4%)	1	12
All	All	1875/2450 (77%)	1249 (67%)	626 (33%)	1	12

All 63 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	863	LEU	25
1	A	868	ARG	25
1	A	805	LEU	24
1	A	889	LEU	20
1	A	837	LEU	20
1	A	831	THR	19
1	A	886	VAL	19
1	A	888	SER	19
1	A	877	LYS	18
1	A	857	LYS	17
1	A	823	LYS	15
1	A	843	ARG	15
1	A	858	GLN	15
1	A	832	SER	15
1	A	850	MET	15
1	A	808	SER	14
1	A	813	LEU	14
1	A	852	ASN	14
1	A	853	LEU	14
1	A	881	ASP	14
1	A	864	GLU	14
1	A	817	THR	13
1	A	844	LEU	13
1	A	862	THR	12
1	A	870	LYS	12
1	A	804	GLN	12
1	A	880	SER	12
1	A	821	ASP	11
1	A	802	ASN	9

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Mol	Chain	Res	Type	Models (Total)
1	A	887	LYS	9
1	A	872	VAL	9
1	A	824	ARG	9
1	A	854	VAL	9
1	A	825	LEU	8
1	A	842	HIS	7
1	A	876	GLU	7
1	A	851	LEU	7
1	A	869	GLU	7
1	A	806	HIS	7
1	A	810	TYR	7
1	A	845	LYS	7
1	A	890	LEU	6
1	A	820	ASP	6
1	A	828	GLU	6
1	A	878	TYR	6
1	A	859	LEU	5
1	A	840	THR	5
1	A	826	TYR	5
1	A	822	VAL	4
1	A	883	ASP	4
1	A	811	TYR	4
1	A	882	ILE	3
1	A	839	GLN	2
1	A	861	GLU	2
1	A	848	PHE	2
1	A	815	VAL	2
1	A	865	HIS	2
1	A	860	CYS	2
1	A	871	ASP	2
1	A	885	TYR	2
1	A	847	VAL	2
1	A	816	ASP	1
1	A	884	SER	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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