



Full wwPDB NMR Structure Validation Report ⓘ

Jan 13, 2021 – 06:07 AM GMT

PDB ID : 7A2D
Title : Structure-function analyses of dual-BON domain protein DolP identifies phospholipid binding as a new mechanism for protein localisation to the cell division site
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Deposited on : 2020-08-17

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.16
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.16

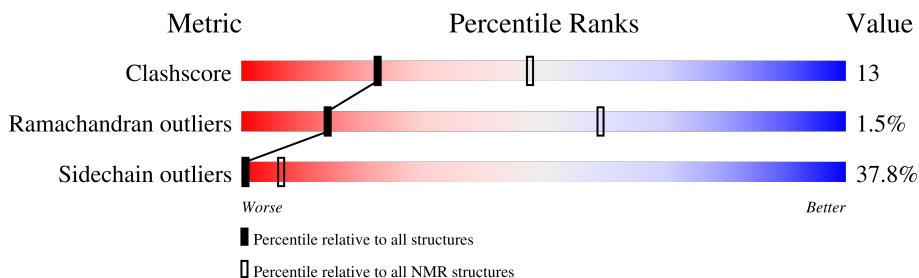
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 79%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	182	

2 Ensemble composition and analysis

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

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:46-A:113 (68)	0.32	7
2	A:118-A:191 (74)	0.41	20

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 3 clusters and 5 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2667 atoms, of which 1351 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Uncharacterized protein YraP.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	178	2667	812	1351	238	264	2	0

There are 11 discrepancies between the modelled and reference sequences:

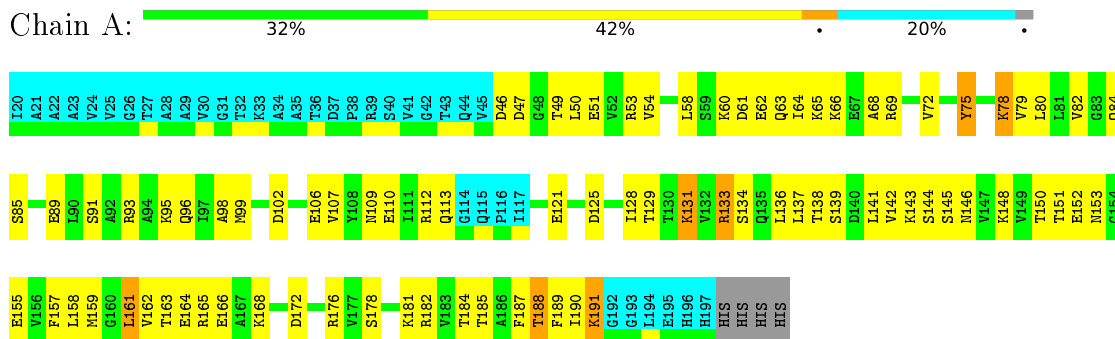
Chain	Residue	Modelled	Actual	Comment	Reference
A	20	ILE	VAL	conflict	UNP P64596
A	192	GLY	-	expression tag	UNP P64596
A	193	GLY	-	expression tag	UNP P64596
A	194	LEU	-	expression tag	UNP P64596
A	195	GLU	-	expression tag	UNP P64596
A	196	HIS	-	expression tag	UNP P64596
A	197	HIS	-	expression tag	UNP P64596
A	198	HIS	-	expression tag	UNP P64596
A	199	HIS	-	expression tag	UNP P64596
A	200	HIS	-	expression tag	UNP P64596
A	201	HIS	-	expression tag	UNP P64596

4 Residue-property plots [i](#)

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: Uncharacterized protein YraP

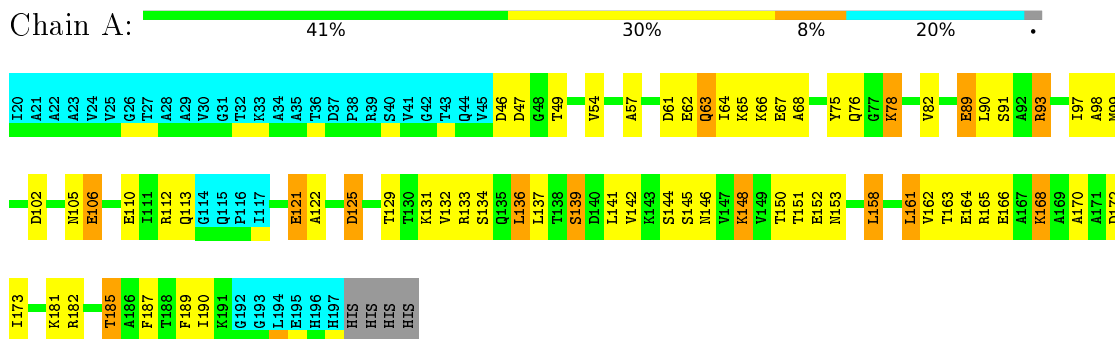


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

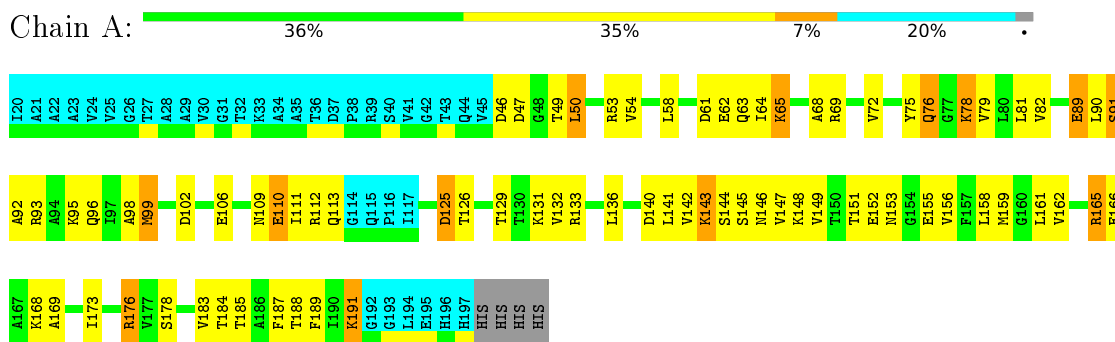
4.2.1 Score per residue for model 1

- Molecule 1: Uncharacterized protein YraP



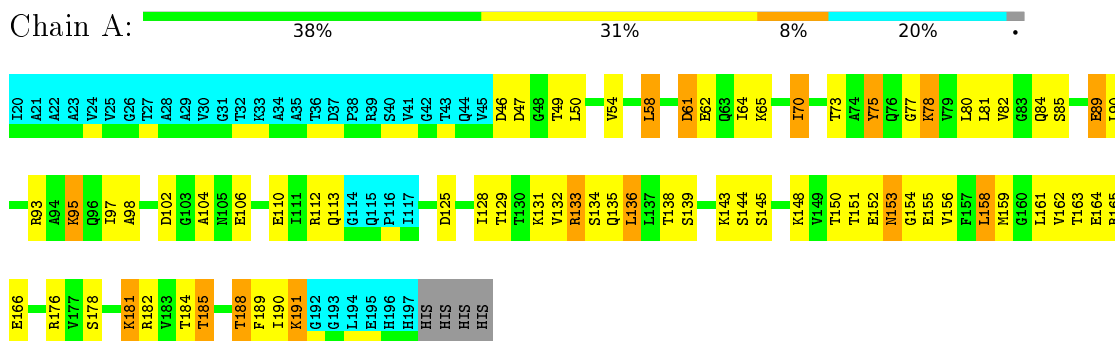
4.2.2 Score per residue for model 2

- Molecule 1: Uncharacterized protein YraP



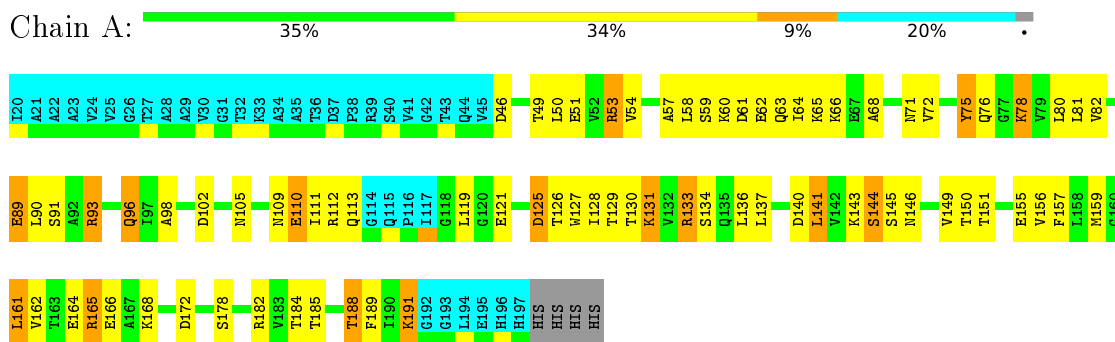
4.2.3 Score per residue for model 3

- Molecule 1: Uncharacterized protein YraP



4.2.4 Score per residue for model 4

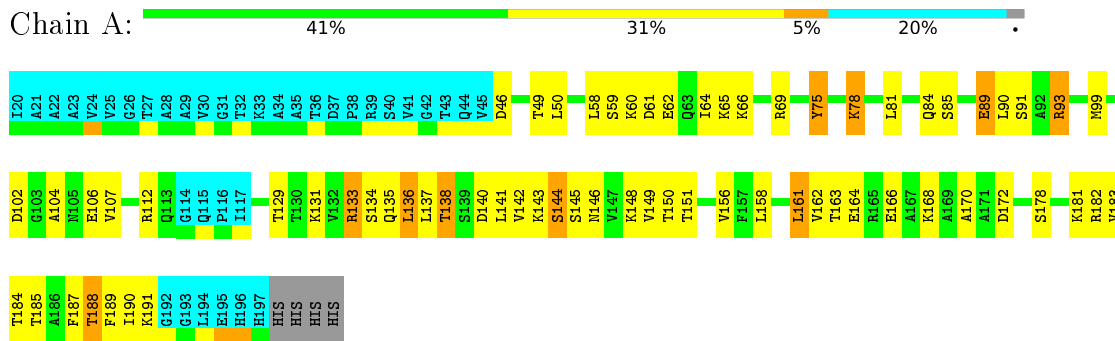
- Molecule 1: Uncharacterized protein YraP



4.2.5 Score per residue for model 5

• Molecule 1: Uncharacterized protein YraP

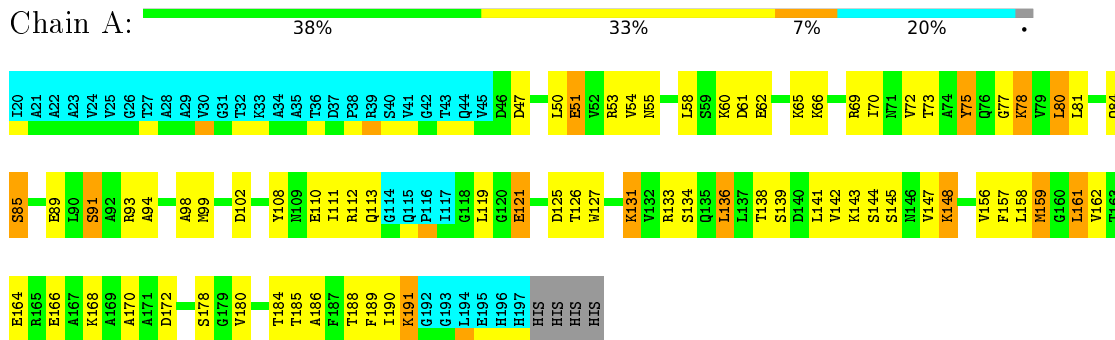
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: Uncharacterized protein YraP

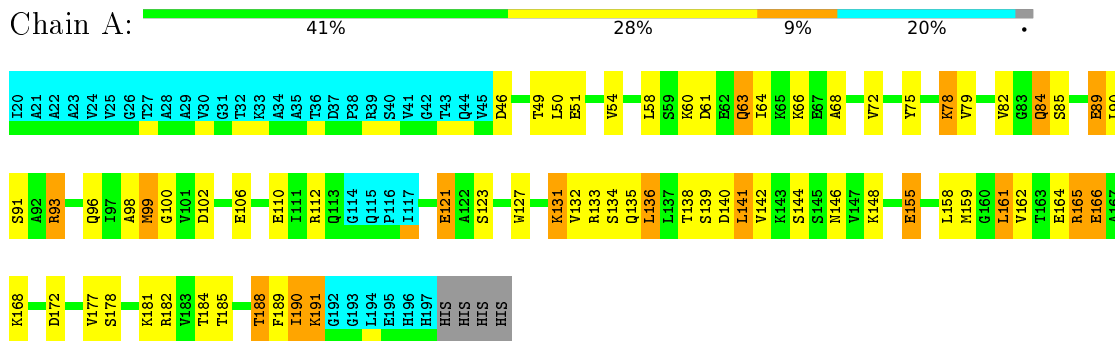
Chain A:



4.2.7 Score per residue for model 7

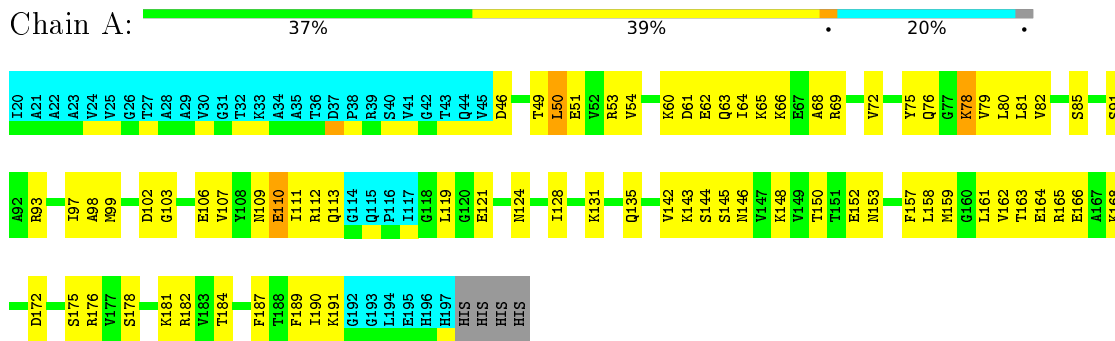
• Molecule 1: Uncharacterized protein YraP

Chain A:



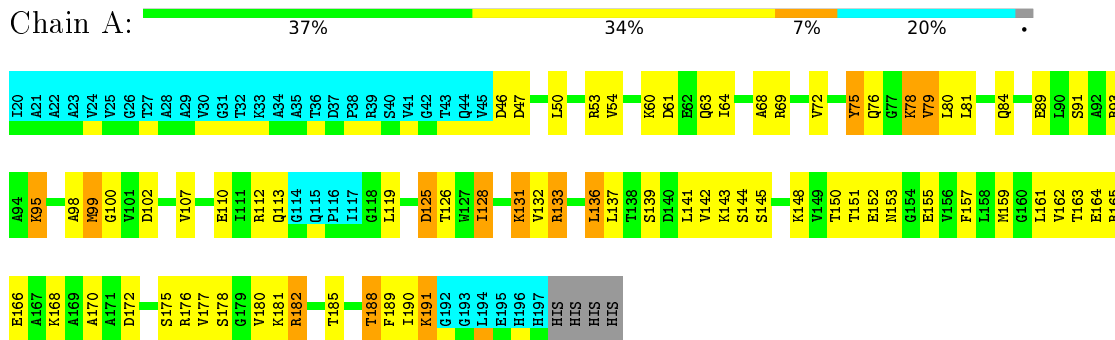
4.2.8 Score per residue for model 8

- Molecule 1: Uncharacterized protein YraP



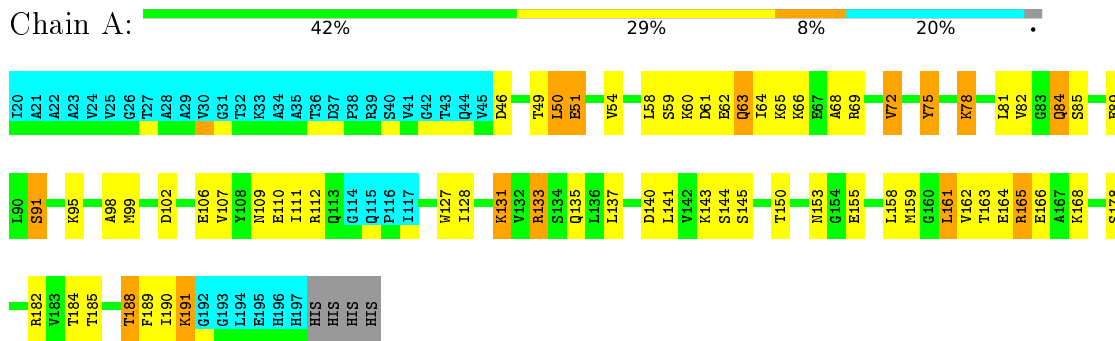
4.2.9 Score per residue for model 9

- Molecule 1: Uncharacterized protein YraP



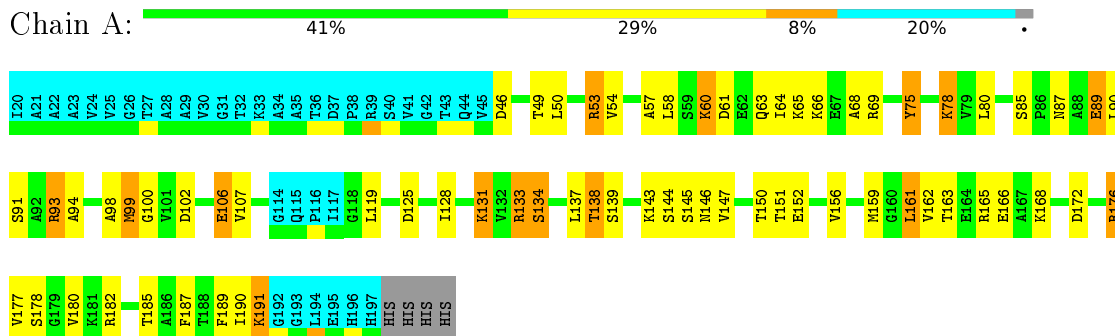
4.2.10 Score per residue for model 10

- Molecule 1: Uncharacterized protein YraP



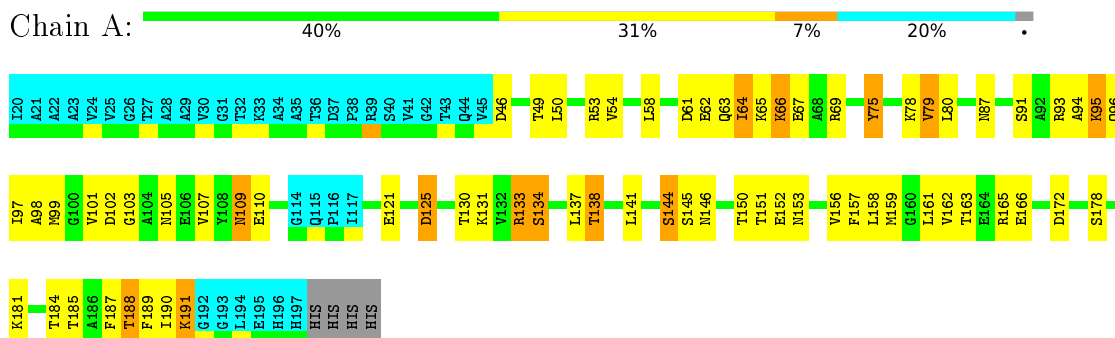
4.2.11 Score per residue for model 11

- Molecule 1: Uncharacterized protein YraP



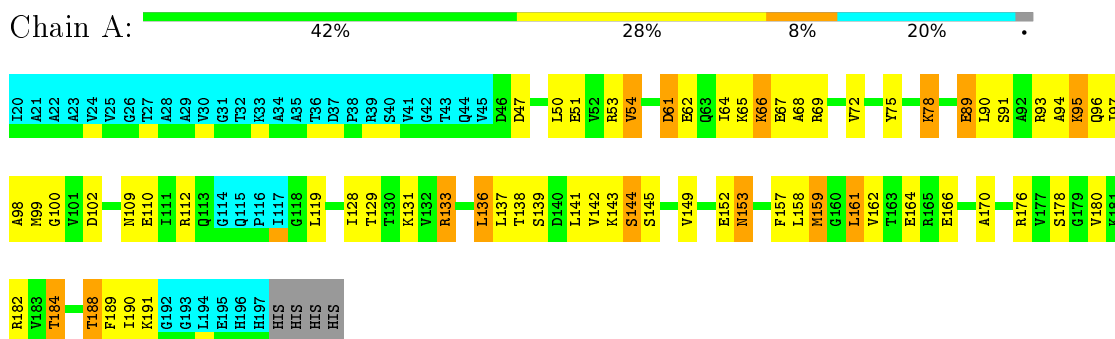
4.2.12 Score per residue for model 12

- Molecule 1: Uncharacterized protein YraP



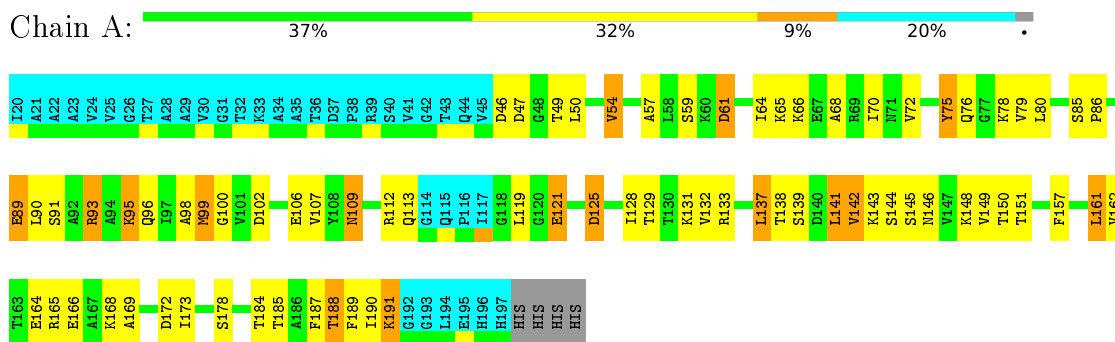
4.2.13 Score per residue for model 13

- Molecule 1: Uncharacterized protein YraP



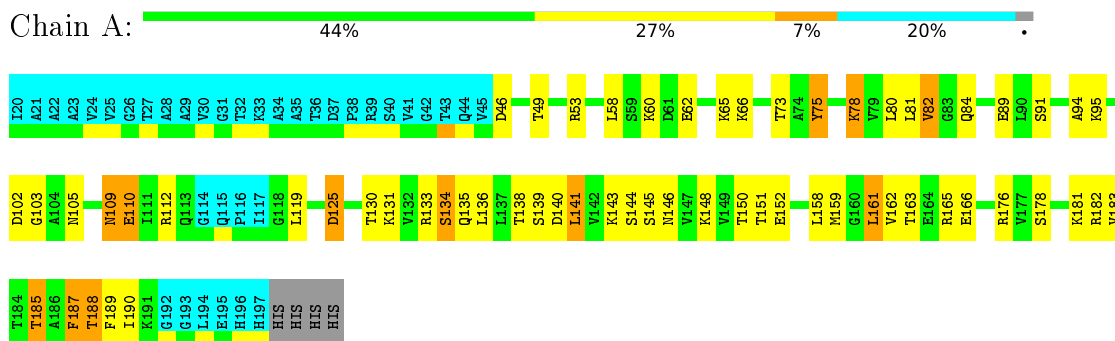
4.2.14 Score per residue for model 14

- Molecule 1: Uncharacterized protein YraP



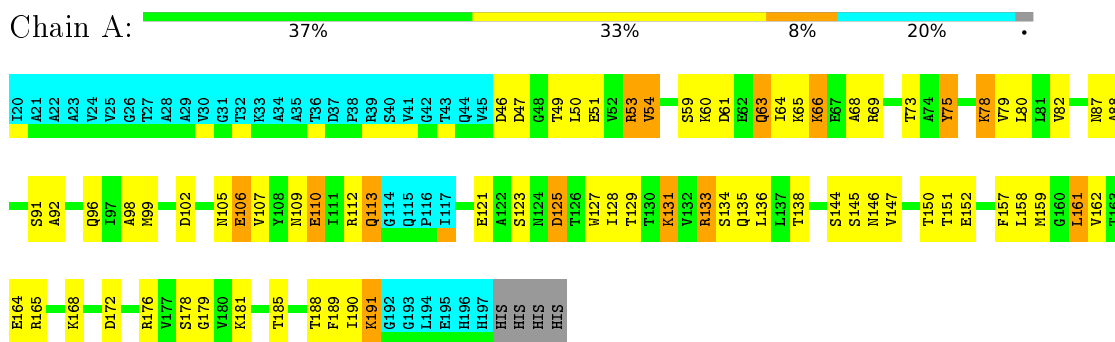
4.2.15 Score per residue for model 15

- Molecule 1: Uncharacterized protein YraP



4.2.16 Score per residue for model 16

- Molecule 1: Uncharacterized protein YraP



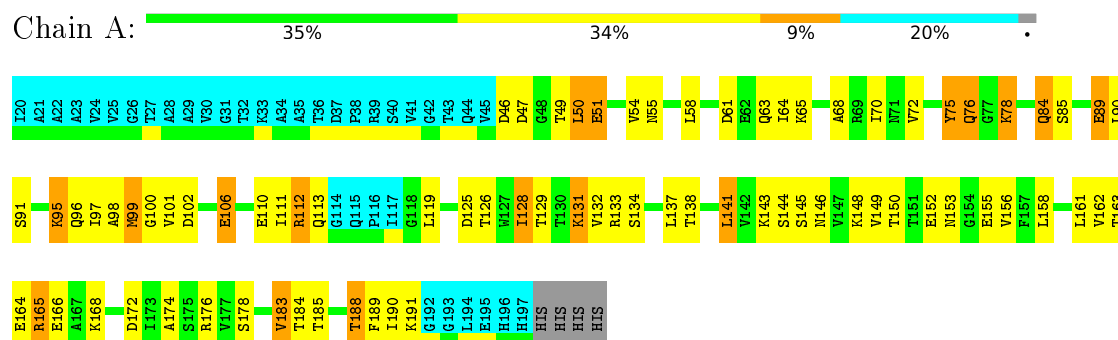
4.2.17 Score per residue for model 17

• Molecule 1: Uncharacterized protein YraP



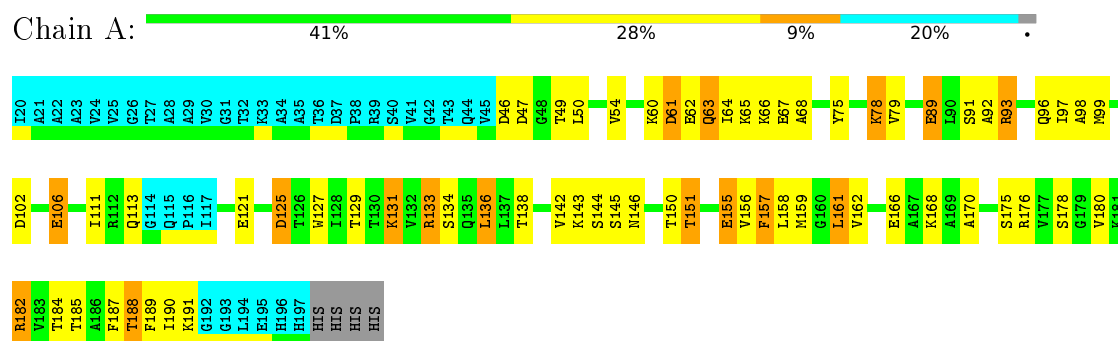
4.2.18 Score per residue for model 18

• Molecule 1: Uncharacterized protein YraP



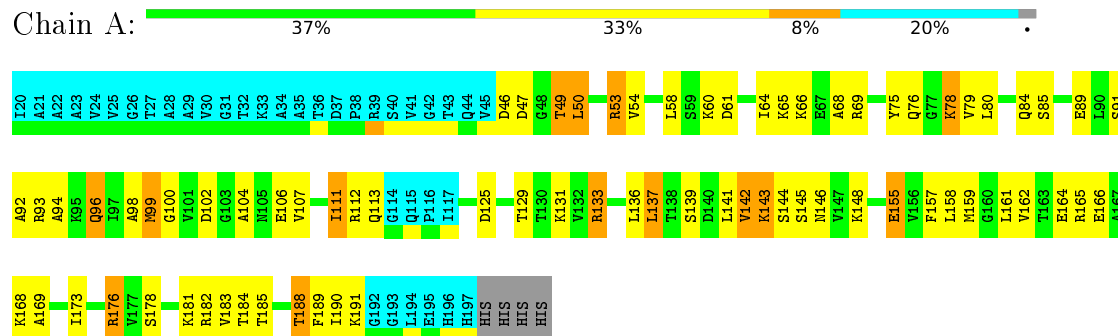
4.2.19 Score per residue for model 19

• Molecule 1: Uncharacterized protein YraP



4.2.20 Score per residue for model 20 (medoid)

• Molecule 1: Uncharacterized protein YraP



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 100 calculated structures, 20 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
ARIA	refinement	2.3
CYANA	structure calculation	
PROCHECK / PROCHECK-NMR	refinement	
CYANA	refinement	2.1

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1881
Number of shifts mapped to atoms	1881
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	79%

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	1075	1103	1103	28±4
All	All	21500	22060	22060	550

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

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:ASP:HB3	1:A:49:THR:HB	0.92	1.40	14	17
1:A:142:VAL:HB	1:A:166:GLU:HG2	0.91	1.37	7	1
1:A:54:VAL:HA	1:A:98:ALA:HB1	0.80	1.52	13	16
1:A:137:LEU:HD22	1:A:144:SER:HA	0.79	1.54	13	3
1:A:64:ILE:HD13	1:A:94:ALA:HB2	0.74	1.58	13	2
1:A:162:VAL:O	1:A:189:PHE:HA	0.74	1.83	15	20
1:A:75:TYR:CD1	1:A:161:LEU:HD22	0.73	2.18	15	3
1:A:136:LEU:HD11	1:A:170:ALA:HA	0.73	1.60	6	7
1:A:139:SER:HB2	1:A:142:VAL:HG12	0.73	1.60	1	2
1:A:142:VAL:HA	1:A:166:GLU:HG2	0.73	1.57	20	8
1:A:95:LYS:HE3	1:A:107:VAL:HG23	0.73	1.61	17	1
1:A:127:TRP:CZ2	1:A:131:LYS:HE2	0.71	2.19	4	3
1:A:75:TYR:CD1	1:A:161:LEU:HG	0.71	2.21	5	12
1:A:163:THR:HG22	1:A:190:ILE:O	0.70	1.86	17	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:133:ARG:O	1:A:137:LEU:HG	0.70	1.86	20	7
1:A:151:THR:HG23	1:A:156:VAL:HG22	0.70	1.62	17	6
1:A:75:TYR:CE2	1:A:78:LYS:HD2	0.70	2.21	10	16
1:A:75:TYR:HD1	1:A:161:LEU:HD22	0.69	1.47	15	3
1:A:161:LEU:HD13	1:A:188:THR:HB	0.68	1.64	15	2
1:A:142:VAL:HB	1:A:166:GLU:CG	0.66	2.17	7	1
1:A:78:LYS:HB3	1:A:106:GLU:HB2	0.65	1.67	17	3
1:A:79:VAL:HB	1:A:107:VAL:HG13	0.64	1.67	12	1
1:A:130:THR:HA	1:A:133:ARG:HE	0.64	1.53	12	3
1:A:66:LYS:HG2	1:A:67:GLU:HG2	0.64	1.69	13	2
1:A:125:ASP:HA	1:A:151:THR:HB	0.63	1.70	2	9
1:A:64:ILE:HD11	1:A:93:ARG:HD2	0.63	1.71	11	2
1:A:63:GLN:HA	1:A:66:LYS:HG2	0.63	1.70	19	1
1:A:158:LEU:HB2	1:A:185:THR:HG23	0.62	1.69	7	2
1:A:64:ILE:HD11	1:A:93:ARG:HD3	0.62	1.71	19	3
1:A:174:ALA:HB1	1:A:183:VAL:HG11	0.62	1.71	18	1
1:A:128:ILE:HA	1:A:131:LYS:HD3	0.62	1.72	11	2
1:A:161:LEU:HG	1:A:190:ILE:HG13	0.62	1.72	20	2
1:A:162:VAL:HB	1:A:166:GLU:HB2	0.61	1.72	19	12
1:A:161:LEU:HG	1:A:190:ILE:HG12	0.61	1.72	15	1
1:A:61:ASP:HB3	1:A:64:ILE:HB	0.61	1.73	1	10
1:A:75:TYR:O	1:A:78:LYS:HG3	0.61	1.96	10	1
1:A:161:LEU:HG	1:A:190:ILE:CG1	0.60	2.26	15	3
1:A:129:THR:HG23	1:A:149:VAL:HG23	0.60	1.73	13	1
1:A:63:GLN:HA	1:A:66:LYS:HB3	0.60	1.74	10	3
1:A:141:LEU:HD13	1:A:165:ARG:HG2	0.60	1.74	4	1
1:A:146:ASN:HB3	1:A:162:VAL:HG12	0.59	1.74	8	2
1:A:95:LYS:HD2	1:A:107:VAL:HB	0.59	1.73	12	1
1:A:156:VAL:HG12	1:A:180:VAL:HG21	0.59	1.73	6	2
1:A:128:ILE:HA	1:A:131:LYS:HG3	0.59	1.75	17	1
1:A:78:LYS:CB	1:A:106:GLU:HB2	0.59	2.28	7	3
1:A:64:ILE:O	1:A:68:ALA:HB3	0.58	1.98	20	14
1:A:151:THR:HG23	1:A:156:VAL:HB	0.58	1.73	19	2
1:A:75:TYR:HE1	1:A:188:THR:HG21	0.58	1.58	17	5
1:A:89:GLU:HG3	1:A:90:LEU:N	0.57	2.12	4	7
1:A:84:GLN:HB2	1:A:112:ARG:HB3	0.57	1.74	18	1
1:A:95:LYS:HD3	1:A:109:ASN:HB2	0.57	1.74	10	1
1:A:64:ILE:HG12	1:A:94:ALA:HB2	0.57	1.75	12	2
1:A:78:LYS:HB3	1:A:106:GLU:HG3	0.57	1.76	16	5
1:A:54:VAL:O	1:A:58:LEU:HG	0.57	1.99	6	3
1:A:81:LEU:HB2	1:A:109:ASN:HD22	0.56	1.60	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:LYS:HG3	1:A:67:GLU:HG3	0.56	1.77	19	1
1:A:72:VAL:HA	1:A:81:LEU:HD23	0.56	1.76	9	3
1:A:168:LYS:O	1:A:172:ASP:HB2	0.56	1.99	1	1
1:A:78:LYS:CB	1:A:106:GLU:HG3	0.56	2.30	16	3
1:A:51:GLU:HG2	1:A:72:VAL:HG22	0.56	1.77	10	3
1:A:143:LYS:HB2	1:A:146:ASN:HB2	0.56	1.78	20	5
1:A:75:TYR:CZ	1:A:78:LYS:HD2	0.56	2.36	7	8
1:A:132:VAL:HG21	1:A:149:VAL:HG21	0.56	1.77	14	3
1:A:161:LEU:HD23	1:A:188:THR:HB	0.55	1.79	10	10
1:A:95:LYS:HE3	1:A:107:VAL:HB	0.55	1.77	14	2
1:A:129:THR:HG23	1:A:149:VAL:HG13	0.55	1.79	5	4
1:A:161:LEU:HD22	1:A:190:ILE:HG13	0.55	1.79	6	5
1:A:148:LYS:O	1:A:158:LEU:HA	0.54	2.02	6	3
1:A:89:GLU:HG2	1:A:90:LEU:N	0.54	2.17	7	3
1:A:134:SER:O	1:A:138:THR:HB	0.54	2.02	12	3
1:A:109:ASN:HD21	1:A:111:ILE:HD11	0.54	1.62	8	2
1:A:158:LEU:HD11	1:A:185:THR:HG23	0.54	1.80	17	1
1:A:132:VAL:O	1:A:136:LEU:HG	0.54	2.03	3	1
1:A:139:SER:HB2	1:A:142:VAL:CG1	0.53	2.33	7	1
1:A:162:VAL:HB	1:A:166:GLU:HB3	0.53	1.81	7	1
1:A:95:LYS:HG3	1:A:96:GLN:N	0.53	2.18	14	3
1:A:139:SER:HB3	1:A:142:VAL:HG13	0.53	1.81	20	3
1:A:76:GLN:HG3	1:A:78:LYS:HG3	0.53	1.81	2	2
1:A:50:LEU:HG	1:A:53:ARG:HH12	0.53	1.64	16	1
1:A:93:ARG:HA	1:A:96:GLN:HG3	0.52	1.79	4	1
1:A:50:LEU:O	1:A:54:VAL:HG12	0.52	2.05	13	2
1:A:50:LEU:HD21	1:A:104:ALA:HB2	0.52	1.80	20	1
1:A:139:SER:HB2	1:A:142:VAL:HG22	0.52	1.81	17	1
1:A:129:THR:O	1:A:133:ARG:HB2	0.52	2.05	1	4
1:A:149:VAL:HG12	1:A:158:LEU:HG	0.52	1.82	13	1
1:A:85:SER:O	1:A:113:GLN:HB2	0.51	2.06	18	3
1:A:81:LEU:HD13	1:A:95:LYS:HE3	0.51	1.82	3	1
1:A:142:VAL:HG22	1:A:166:GLU:HA	0.51	1.81	9	2
1:A:159:MET:HG2	1:A:186:ALA:HB3	0.51	1.81	6	1
1:A:161:LEU:CD1	1:A:188:THR:HB	0.51	2.35	15	2
1:A:82:VAL:HA	1:A:110:GLU:O	0.51	2.05	4	8
1:A:54:VAL:HG13	1:A:98:ALA:HB1	0.50	1.82	9	1
1:A:157:PHE:HD1	1:A:184:THR:HB	0.50	1.65	13	1
1:A:141:LEU:HD22	1:A:165:ARG:HG2	0.50	1.83	7	1
1:A:155:GLU:HG3	1:A:182:ARG:HB2	0.50	1.82	7	1
1:A:58:LEU:HD21	1:A:70:ILE:HB	0.50	1.83	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:110:GLU:O	1:A:110:GLU:HG3	0.50	2.06	8	1
1:A:127:TRP:O	1:A:131:LYS:HG2	0.50	2.07	19	3
1:A:82:VAL:HG12	1:A:110:GLU:HG3	0.50	1.82	2	1
1:A:58:LEU:HD22	1:A:94:ALA:HB1	0.50	1.84	6	3
1:A:78:LYS:HB2	1:A:106:GLU:HB2	0.50	1.84	10	3
1:A:62:GLU:O	1:A:66:LYS:HB3	0.50	2.06	13	1
1:A:84:GLN:HB2	1:A:112:ARG:HB2	0.50	1.82	7	1
1:A:46:ASP:HB3	1:A:49:THR:CB	0.49	2.36	2	10
1:A:62:GLU:O	1:A:66:LYS:HB2	0.49	2.07	6	1
1:A:91:SER:HB2	1:A:111:ILE:HG13	0.49	1.84	10	1
1:A:76:GLN:HG3	1:A:188:THR:HG21	0.49	1.85	14	1
1:A:132:VAL:O	1:A:136:LEU:HB2	0.49	2.08	7	2
1:A:136:LEU:HG	1:A:142:VAL:HG11	0.49	1.85	5	1
1:A:143:LYS:HB3	1:A:146:ASN:HB2	0.49	1.85	4	1
1:A:129:THR:O	1:A:133:ARG:HB3	0.49	2.07	20	3
1:A:137:LEU:HG	1:A:144:SER:HB3	0.49	1.83	17	1
1:A:54:VAL:HG13	1:A:98:ALA:CB	0.49	2.38	9	1
1:A:63:GLN:HA	1:A:66:LYS:HB2	0.48	1.84	1	1
1:A:61:ASP:CB	1:A:64:ILE:HD12	0.48	2.38	13	5
1:A:130:THR:HA	1:A:133:ARG:NE	0.48	2.22	15	1
1:A:93:ARG:HA	1:A:96:GLN:HG2	0.48	1.85	7	1
1:A:57:ALA:CB	1:A:98:ALA:HA	0.48	2.39	14	3
1:A:156:VAL:HB	1:A:183:VAL:HG23	0.47	1.84	5	1
1:A:54:VAL:CA	1:A:98:ALA:HB1	0.47	2.37	11	1
1:A:141:LEU:HD13	1:A:165:ARG:HB3	0.47	1.86	15	2
1:A:50:LEU:HG	1:A:53:ARG:NH1	0.47	2.24	16	1
1:A:81:LEU:O	1:A:109:ASN:HA	0.47	2.10	2	1
1:A:185:THR:HB	1:A:187:PHE:CD1	0.47	2.44	1	1
1:A:132:VAL:HG12	1:A:177:VAL:HG11	0.47	1.86	7	1
1:A:50:LEU:HD12	1:A:53:ARG:HD3	0.47	1.87	2	1
1:A:84:GLN:HA	1:A:111:ILE:HG22	0.47	1.86	20	1
1:A:79:VAL:O	1:A:107:VAL:HA	0.47	2.09	14	2
1:A:161:LEU:HA	1:A:188:THR:OG1	0.47	2.08	6	1
1:A:99:MET:HG3	1:A:100:GLY:N	0.47	2.25	13	7
1:A:54:VAL:HG11	1:A:81:LEU:HD21	0.47	1.87	9	1
1:A:50:LEU:HG	1:A:53:ARG:HE	0.46	1.69	8	1
1:A:125:ASP:HB2	1:A:151:THR:O	0.46	2.11	4	1
1:A:169:ALA:O	1:A:173:ILE:HG12	0.46	2.11	14	4
1:A:125:ASP:HB2	1:A:151:THR:HB	0.46	1.88	19	2
1:A:121:GLU:HG3	1:A:122:ALA:N	0.46	2.26	1	1
1:A:161:LEU:HB3	1:A:190:ILE:HG13	0.46	1.88	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:172:ASP:O	1:A:176:ARG:HG3	0.46	2.10	11	1
1:A:132:VAL:HG12	1:A:177:VAL:HG21	0.46	1.88	9	1
1:A:134:SER:O	1:A:138:THR:HG23	0.46	2.11	7	2
1:A:91:SER:CB	1:A:111:ILE:HG13	0.45	2.40	10	3
1:A:132:VAL:HA	1:A:173:ILE:HG21	0.45	1.87	1	2
1:A:51:GLU:O	1:A:55:ASN:HB2	0.45	2.11	18	2
1:A:173:ILE:HA	1:A:176:ARG:HD2	0.45	1.87	20	2
1:A:50:LEU:HD21	1:A:104:ALA:HA	0.45	1.88	5	1
1:A:95:LYS:O	1:A:99:MET:HG3	0.45	2.11	2	1
1:A:46:ASP:O	1:A:50:LEU:HB2	0.45	2.12	18	3
1:A:185:THR:HB	1:A:187:PHE:CE1	0.45	2.46	15	1
1:A:82:VAL:HG12	1:A:110:GLU:HG2	0.45	1.87	8	1
1:A:93:ARG:O	1:A:97:ILE:HG12	0.45	2.12	13	1
1:A:47:ASP:OD2	1:A:75:TYR:HA	0.45	2.12	16	1
1:A:50:LEU:O	1:A:54:VAL:HG22	0.45	2.11	6	1
1:A:165:ARG:HG2	1:A:166:GLU:N	0.45	2.27	10	1
1:A:190:ILE:HG22	1:A:190:ILE:O	0.44	2.11	19	3
1:A:61:ASP:HB3	1:A:64:ILE:HD12	0.44	1.89	14	1
1:A:75:TYR:HD1	1:A:161:LEU:HG	0.44	1.70	4	1
1:A:78:LYS:HB3	1:A:106:GLU:CG	0.44	2.43	11	1
1:A:161:LEU:HD22	1:A:190:ILE:CG1	0.44	2.42	1	4
1:A:155:GLU:HA	1:A:182:ARG:O	0.44	2.12	9	1
1:A:78:LYS:NZ	1:A:159:MET:SD	0.44	2.90	13	3
1:A:137:LEU:HD11	1:A:144:SER:HA	0.44	1.89	4	1
1:A:155:GLU:HG3	1:A:182:ARG:HB3	0.44	1.88	20	1
1:A:75:TYR:CE1	1:A:188:THR:HG21	0.44	2.46	20	1
1:A:54:VAL:CG1	1:A:72:VAL:HG21	0.44	2.42	14	1
1:A:92:ALA:O	1:A:96:GLN:HG2	0.44	2.12	20	4
1:A:136:LEU:HB3	1:A:142:VAL:HG11	0.44	1.89	2	1
1:A:125:ASP:CA	1:A:151:THR:HB	0.44	2.42	2	2
1:A:61:ASP:O	1:A:65:LYS:HG2	0.44	2.13	2	1
1:A:53:ARG:HG3	1:A:54:VAL:N	0.43	2.28	20	3
1:A:95:LYS:HD3	1:A:109:ASN:OD1	0.43	2.14	14	2
1:A:61:ASP:OD1	1:A:63:GLN:HG2	0.43	2.13	1	1
1:A:156:VAL:HG13	1:A:183:VAL:HG13	0.43	1.91	18	1
1:A:139:SER:HB2	1:A:142:VAL:CG2	0.43	2.44	17	1
1:A:143:LYS:HG3	1:A:166:GLU:OE2	0.43	2.14	6	1
1:A:54:VAL:CG2	1:A:72:VAL:HG21	0.43	2.44	7	3
1:A:61:ASP:CG	1:A:64:ILE:HD12	0.43	2.34	2	1
1:A:80:LEU:HD12	1:A:108:TYR:HB2	0.43	1.91	6	1
1:A:57:ALA:HB3	1:A:98:ALA:HA	0.42	1.91	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:82:VAL:HG11	1:A:148:LYS:HE3	0.42	1.91	7	1
1:A:89:GLU:O	1:A:93:ARG:HB3	0.42	2.14	19	2
1:A:95:LYS:HD3	1:A:109:ASN:HB3	0.42	1.91	15	1
1:A:75:TYR:HB2	1:A:161:LEU:HD12	0.42	1.90	6	1
1:A:57:ALA:HA	1:A:60:LYS:HB2	0.42	1.90	11	1
1:A:128:ILE:O	1:A:131:LYS:HG2	0.42	2.14	18	2
1:A:151:THR:HG23	1:A:156:VAL:CB	0.42	2.44	19	1
1:A:84:GLN:HG3	1:A:112:ARG:HB2	0.42	1.91	10	1
1:A:63:GLN:HA	1:A:66:LYS:HE3	0.42	1.90	11	1
1:A:77:GLY:O	1:A:104:ALA:HA	0.42	2.13	3	1
1:A:165:ARG:HA	1:A:165:ARG:HD3	0.42	1.45	2	1
1:A:112:ARG:HD2	1:A:112:ARG:HA	0.42	1.59	10	1
1:A:50:LEU:HD12	1:A:50:LEU:HA	0.42	1.75	10	1
1:A:161:LEU:HD23	1:A:188:THR:O	0.42	2.15	18	1
1:A:141:LEU:HD13	1:A:165:ARG:HD2	0.42	1.90	17	1
1:A:141:LEU:HG	1:A:141:LEU:H	0.41	1.44	14	2
1:A:88:ALA:HB2	1:A:113:GLN:NE2	0.41	2.29	16	1
1:A:111:ILE:C	1:A:113:GLN:H	0.41	2.18	18	1
1:A:50:LEU:O	1:A:53:ARG:HG2	0.41	2.15	13	2
1:A:72:VAL:HG12	1:A:81:LEU:HD22	0.41	1.90	2	1
1:A:190:ILE:O	1:A:190:ILE:HG22	0.41	2.15	10	1
1:A:54:VAL:HG13	1:A:72:VAL:HG21	0.41	1.93	13	1
1:A:58:LEU:CD2	1:A:94:ALA:HB1	0.41	2.45	20	2
1:A:161:LEU:HD13	1:A:190:ILE:HG12	0.41	1.92	13	1
1:A:79:VAL:HG13	1:A:107:VAL:HG22	0.41	1.93	9	1
1:A:125:ASP:CB	1:A:151:THR:HB	0.41	2.45	12	1
1:A:82:VAL:HG12	1:A:110:GLU:HB3	0.41	1.90	7	1
1:A:71:ASN:HB3	1:A:82:VAL:HG23	0.41	1.93	4	1
1:A:155:GLU:CG	1:A:182:ARG:HB3	0.41	2.46	19	1
1:A:157:PHE:HA	1:A:184:THR:O	0.41	2.15	19	1
1:A:127:TRP:CH2	1:A:179:GLY:HA3	0.41	2.50	16	1
1:A:75:TYR:CE1	1:A:76:GLN:HG2	0.41	2.51	18	1
1:A:142:VAL:HG13	1:A:166:GLU:HG2	0.41	1.93	6	1
1:A:132:VAL:HG21	1:A:149:VAL:HG11	0.41	1.92	17	1
1:A:113:GLN:OE1	1:A:113:GLN:HA	0.40	2.16	3	1
1:A:75:TYR:O	1:A:76:GLN:HB2	0.40	2.15	9	1
1:A:79:VAL:HG13	1:A:107:VAL:HG13	0.40	1.93	8	1
1:A:131:LYS:H	1:A:131:LYS:HG2	0.40	1.57	10	1
1:A:133:ARG:HG2	1:A:137:LEU:HD11	0.40	1.93	10	1
1:A:155:GLU:CG	1:A:182:ARG:HB2	0.40	2.46	7	1
1:A:147:VAL:HG21	1:A:158:LEU:HD23	0.40	1.93	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:154:GLY:HA3	1:A:181:LYS:HD3	0.40	1.93	3	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	142/182 (78%)	137±2 (97±1%)	3±2 (2±1%)	2±1 (1±0%)	14	59
All	All	2840/3640 (78%)	2742 (97%)	56 (2%)	42 (1%)	14	59

All 4 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	102	ASP	20
1	A	191	LYS	16
1	A	153	ASN	5
1	A	77	GLY	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	117/144 (81%)	73±4 (62±3%)	44±4 (38±3%)	1	6
All	All	2340/2880 (81%)	1455 (62%)	885 (38%)	1	6

All 100 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	131	LYS	20
1	A	78	LYS	20
1	A	144	SER	20
1	A	145	SER	19
1	A	178	SER	19
1	A	91	SER	19
1	A	65	LYS	18
1	A	89	GLU	17
1	A	185	THR	17
1	A	188	THR	16
1	A	125	ASP	15
1	A	150	THR	15
1	A	161	LEU	15
1	A	112	ARG	15
1	A	168	LYS	15
1	A	99	MET	15
1	A	141	LEU	14
1	A	184	THR	14
1	A	165	ARG	14
1	A	191	LYS	14
1	A	133	ARG	14
1	A	164	GLU	14
1	A	93	ARG	14
1	A	136	LEU	13
1	A	158	LEU	13
1	A	159	MET	13
1	A	60	LYS	12
1	A	176	ARG	12
1	A	80	LEU	12
1	A	75	TYR	12
1	A	69	ARG	12
1	A	152	GLU	11
1	A	62	GLU	11
1	A	181	LYS	11
1	A	182	ARG	11
1	A	143	LYS	11
1	A	47	ASP	11
1	A	110	GLU	11
1	A	148	LYS	11
1	A	63	GLN	11
1	A	134	SER	10
1	A	66	LYS	10
1	A	119	LEU	10

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Mol	Chain	Res	Type	Models (Total)
1	A	138	THR	10
1	A	50	LEU	10
1	A	172	ASP	10
1	A	157	PHE	10
1	A	155	GLU	9
1	A	84	GLN	9
1	A	187	PHE	9
1	A	61	ASP	9
1	A	85	SER	9
1	A	113	GLN	9
1	A	135	GLN	8
1	A	106	GLU	8
1	A	146	ASN	8
1	A	128	ILE	8
1	A	97	ILE	7
1	A	53	ARG	7
1	A	58	LEU	7
1	A	139	SER	7
1	A	140	ASP	7
1	A	153	ASN	6
1	A	79	VAL	6
1	A	109	ASN	6
1	A	76	GLN	6
1	A	121	GLU	6
1	A	95	LYS	6
1	A	59	SER	6
1	A	51	GLU	6
1	A	126	THR	6
1	A	73	THR	5
1	A	105	ASN	5
1	A	107	VAL	5
1	A	137	LEU	4
1	A	183	VAL	4
1	A	54	VAL	3
1	A	87	ASN	3
1	A	70	ILE	3
1	A	142	VAL	3
1	A	123	SER	3
1	A	81	LEU	3
1	A	180	VAL	3
1	A	96	GLN	3
1	A	147	VAL	3

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Mol	Chain	Res	Type	Models (Total)
1	A	175	SER	3
1	A	111	ILE	2
1	A	72	VAL	2
1	A	82	VAL	1
1	A	151	THR	1
1	A	124	ASN	1
1	A	67	GLU	1
1	A	166	GLU	1
1	A	101	VAL	1
1	A	64	ILE	1
1	A	46	ASP	1
1	A	49	THR	1
1	A	177	VAL	1
1	A	86	PRO	1
1	A	190	ILE	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 79% for the well-defined parts and 79% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *YraP_assignments_nmrstarformat.txt*

7.1.1 Bookkeeping [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1881
Number of shifts mapped to atoms	1881
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	176	-1.20 \pm 0.09	Should be applied
$^{13}\text{C}_\beta$	160	-0.93 \pm 0.10	Should be applied
$^{13}\text{C}'$	171	-0.08 \pm 0.07	None needed (< 0.5 ppm)
^{15}N	172	-0.43 \pm 0.36	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 79%, i.e. 1328 atoms were assigned a chemical shift out of a possible 1683. 21 out of 27 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	685/708 (97%)	264/283 (93%)	281/284 (99%)	140/141 (99%)
Sidechain	608/920 (66%)	356/529 (67%)	252/342 (74%)	0/49 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	35/55 (64%)	18/29 (62%)	17/25 (68%)	0/1 (0%)
Overall	1328/1683 (79%)	638/841 (76%)	550/651 (84%)	140/191 (73%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 79%, i.e. 1620 atoms were assigned a chemical shift out of a possible 2051. 27 out of 33 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	847/884 (96%)	328/353 (93%)	347/356 (97%)	172/175 (98%)
Sidechain	738/1096 (67%)	431/629 (69%)	307/412 (75%)	0/55 (0%)
Aromatic	35/71 (49%)	18/37 (49%)	17/29 (59%)	0/5 (0%)
Overall	1620/2051 (79%)	777/1019 (76%)	671/797 (84%)	172/235 (73%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

