



Full wwPDB NMR Structure Validation Report ⓘ

May 29, 2020 – 01:59 am BST

PDB ID : 2WCY
Title : NMR solution structure of factor I-like modules of complement C7.
Authors : Phelan, M.M.; Thai, C.T.; Soares, D.C.; Ogata, R.T.; Barlow, P.N.; Bramham, J.
Deposited on : 2009-03-17

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:

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

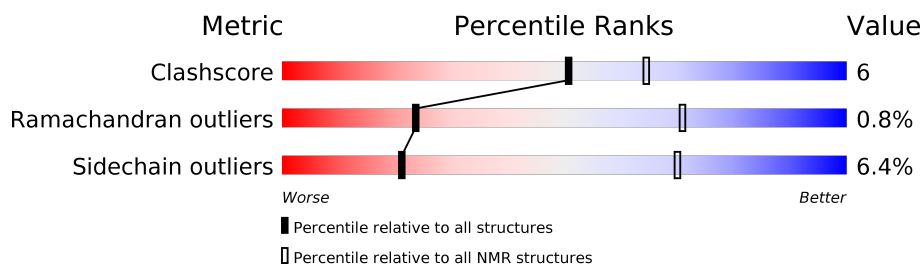
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 87%.

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	155	<div> <div style="width: 65%; background-color: green;"></div> <div style="width: 12%; background-color: yellow;"></div> <div style="width: 23%; background-color: cyan;"></div> </div> <div>65% 12% 23%</div>

2 Ensemble composition and analysis

This entry contains 48 models. Model 44 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:701-A:766, A:778-A:780, A:790-A:840 (120)	0.58	44

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 8 clusters and 2 single-model clusters were found.

Cluster number	Models
1	4, 6, 8, 16, 17, 18, 20, 22, 23, 24, 33, 34, 37, 39, 44, 46
2	1, 3, 5, 7, 9, 10, 11, 13, 15, 19, 21, 28, 41
3	12, 38, 42, 43
4	14, 36, 40, 45
5	2, 32, 48
6	27, 29
7	35, 47
8	25, 26
Single-model clusters	30; 31

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2296 atoms, of which 1129 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called COMPLEMENT COMPONENT C7.

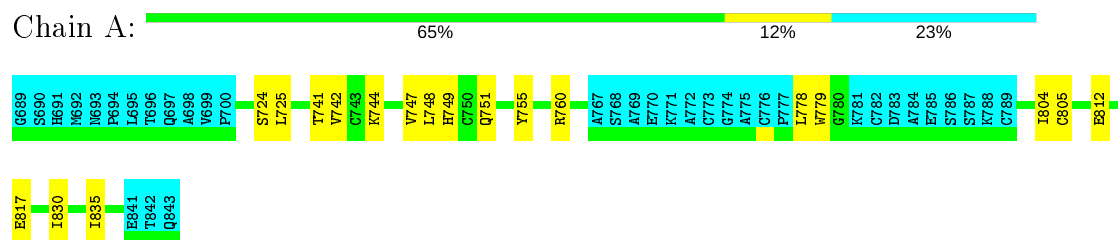
Mol	Chain	Residues	Atoms						Trace
1	A	155	Total	C	H	N	O	S	0
			2296	701	1129	214	230	22	

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: COMPLEMENT COMPONENT C7

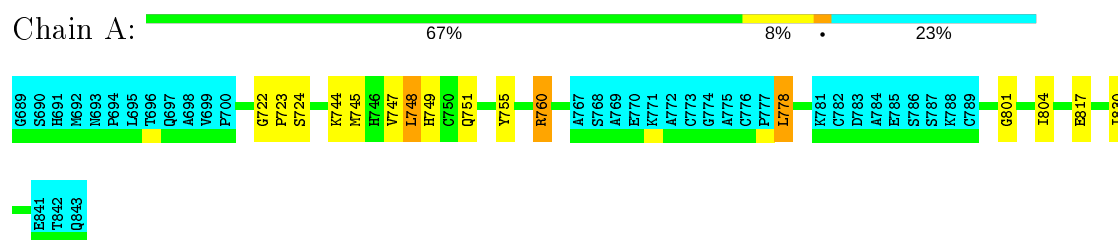


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

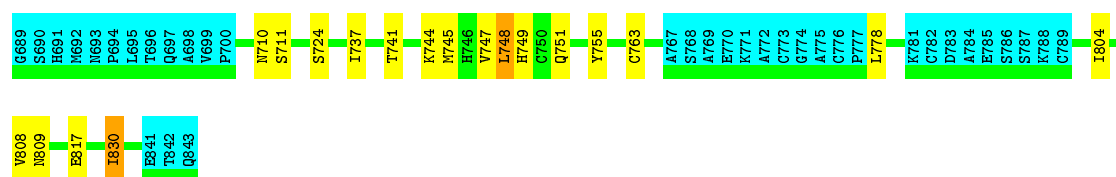
- Molecule 1: COMPLEMENT COMPONENT C7

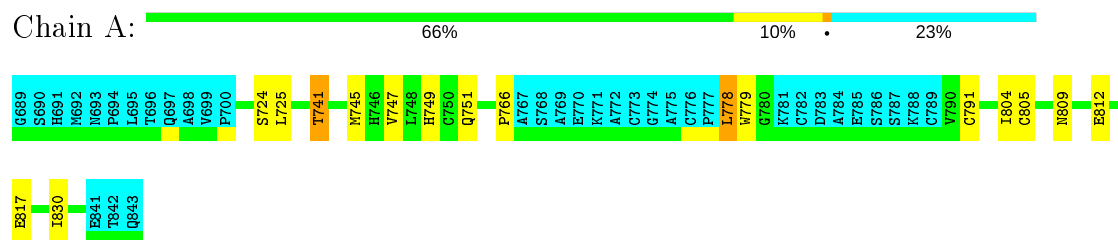


4.2.2 Score per residue for model 2

- Molecule 1: COMPLEMENT COMPONENT C7

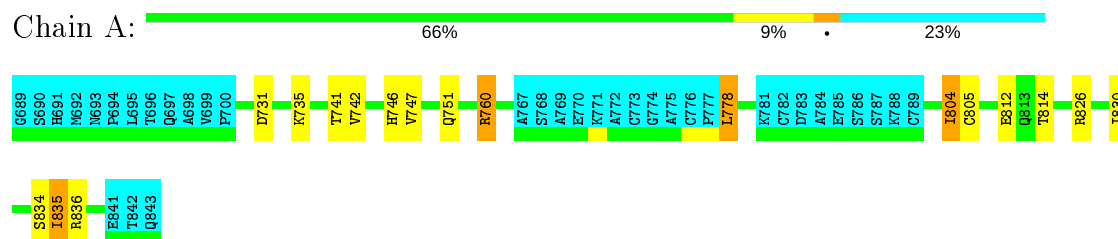






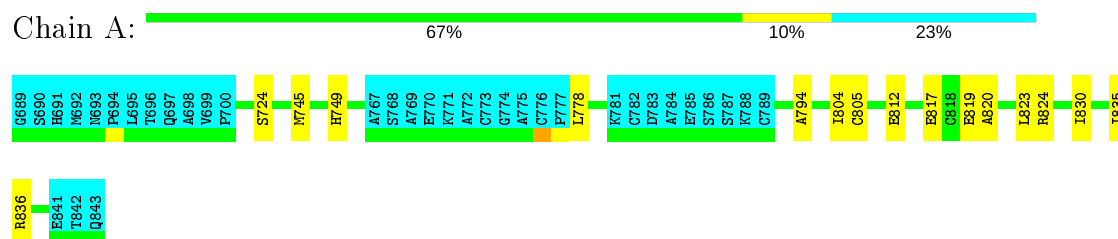
4.2.7 Score per residue for model 7

- Molecule 1: COMPLEMENT COMPONENT C7



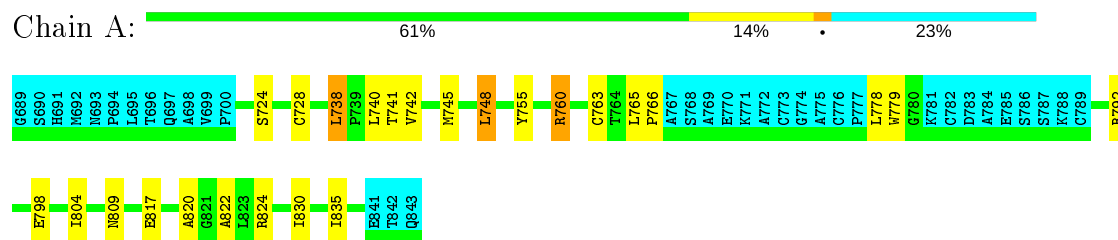
4.2.8 Score per residue for model 8

- Molecule 1: COMPLEMENT COMPONENT C7



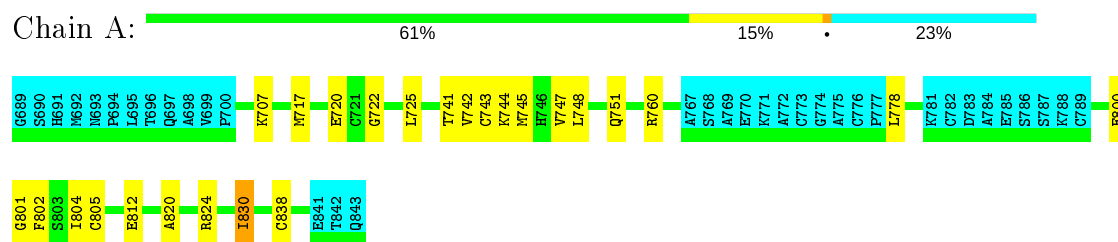
4.2.9 Score per residue for model 9

- Molecule 1: COMPLEMENT COMPONENT C7



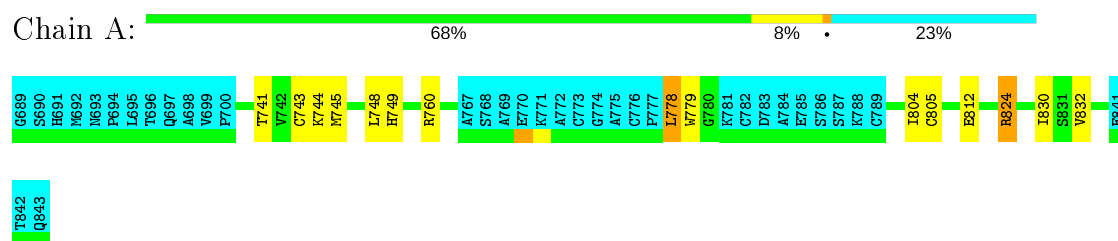
4.2.10 Score per residue for model 10

- Molecule 1: COMPLEMENT COMPONENT C7



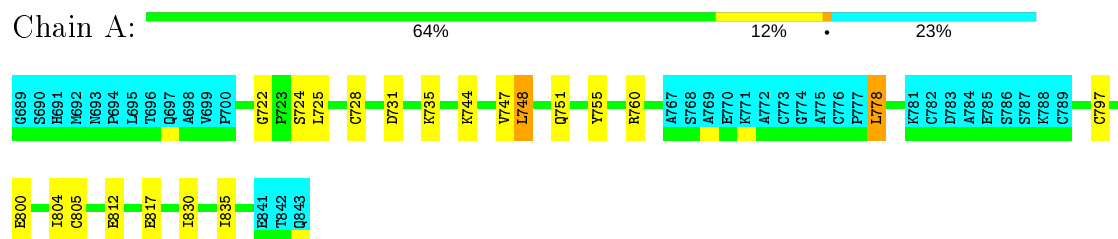
4.2.11 Score per residue for model 11

- Molecule 1: COMPLEMENT COMPONENT C7



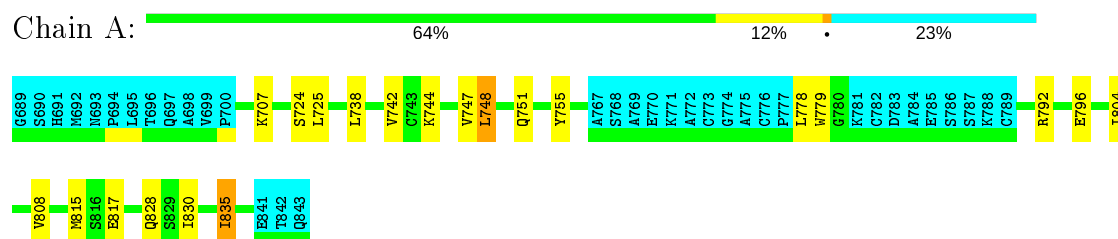
4.2.12 Score per residue for model 12

- Molecule 1: COMPLEMENT COMPONENT C7



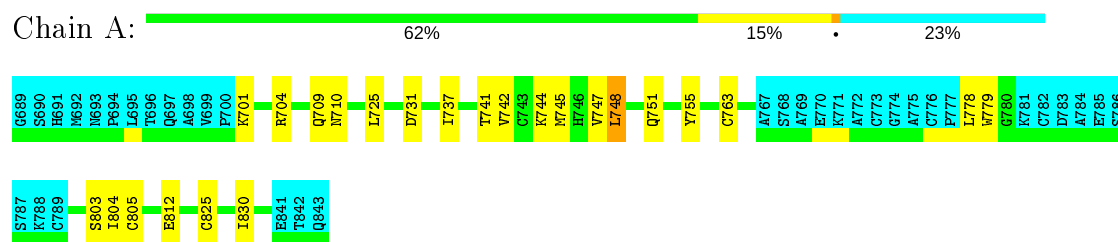
4.2.13 Score per residue for model 13

- Molecule 1: COMPLEMENT COMPONENT C7



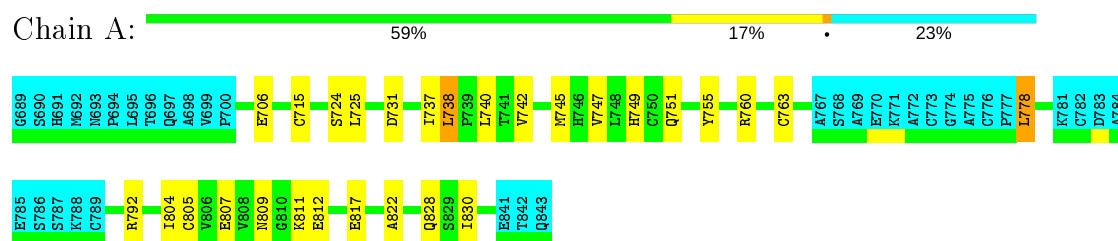
4.2.14 Score per residue for model 14

- Molecule 1: COMPLEMENT COMPONENT C7



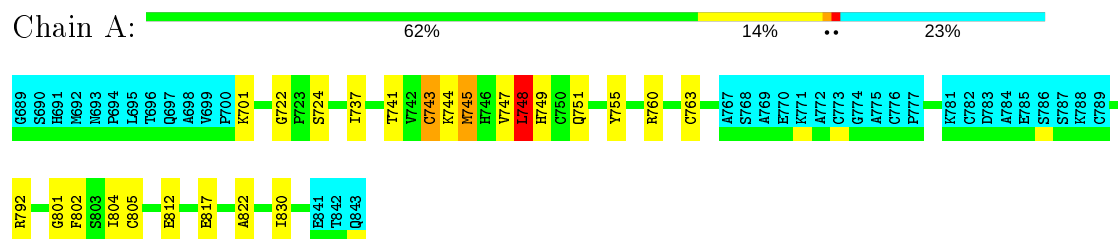
4.2.15 Score per residue for model 15

- Molecule 1: COMPLEMENT COMPONENT C7



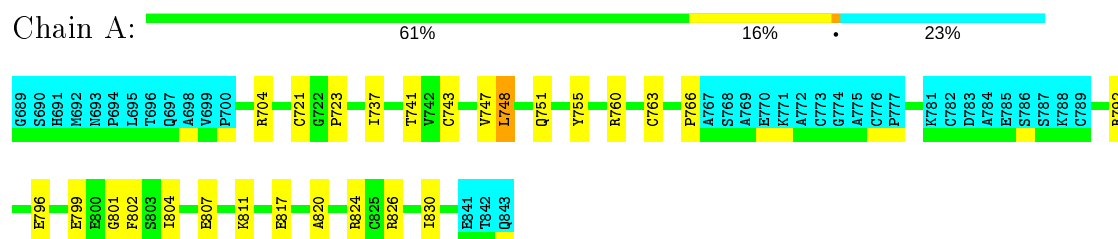
4.2.16 Score per residue for model 16

- Molecule 1: COMPLEMENT COMPONENT C7



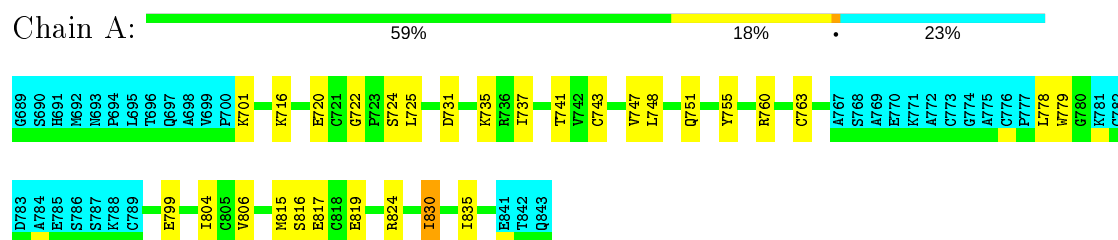
4.2.17 Score per residue for model 17

- Molecule 1: COMPLEMENT COMPONENT C7



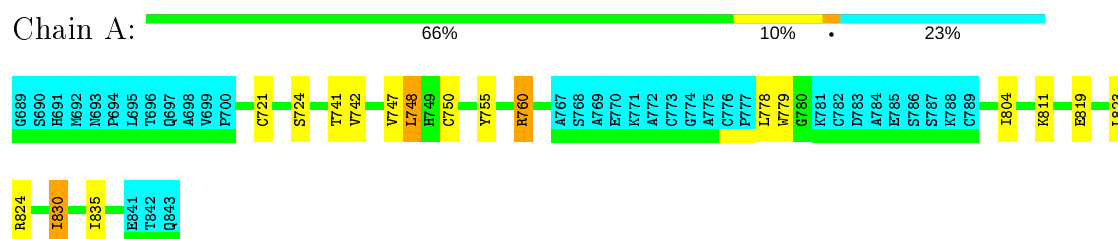
4.2.18 Score per residue for model 18

- Molecule 1: COMPLEMENT COMPONENT C7



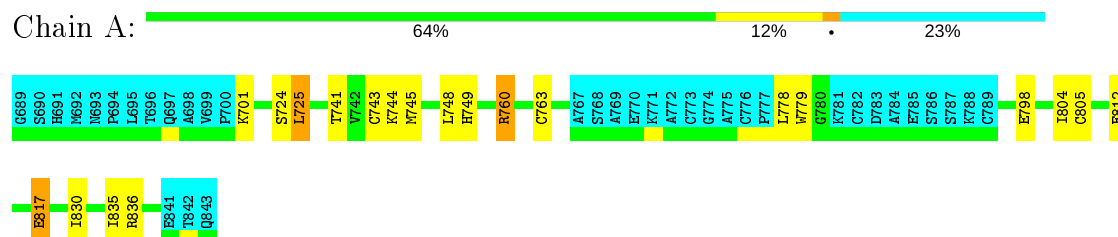
4.2.19 Score per residue for model 19

- Molecule 1: COMPLEMENT COMPONENT C7



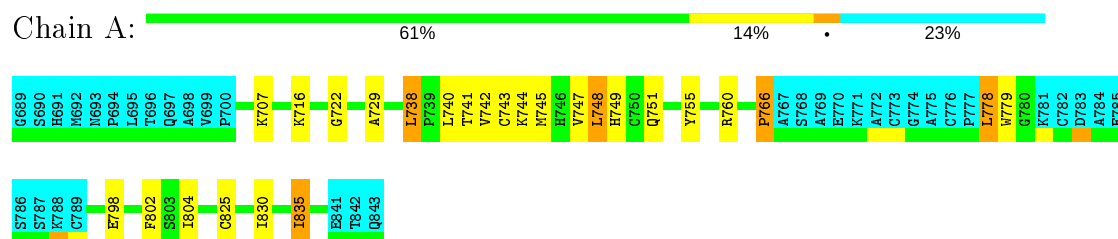
4.2.20 Score per residue for model 20

- Molecule 1: COMPLEMENT COMPONENT C7



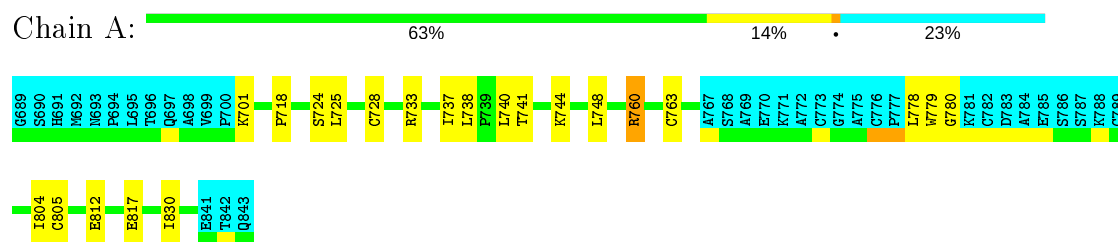
4.2.21 Score per residue for model 21

- Molecule 1: COMPLEMENT COMPONENT C7



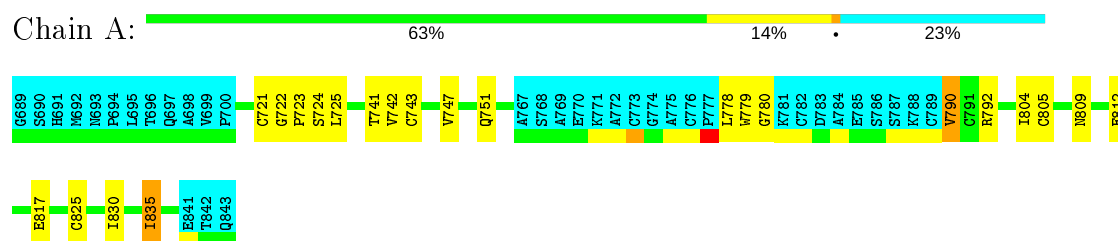
4.2.22 Score per residue for model 22

- Molecule 1: COMPLEMENT COMPONENT C7



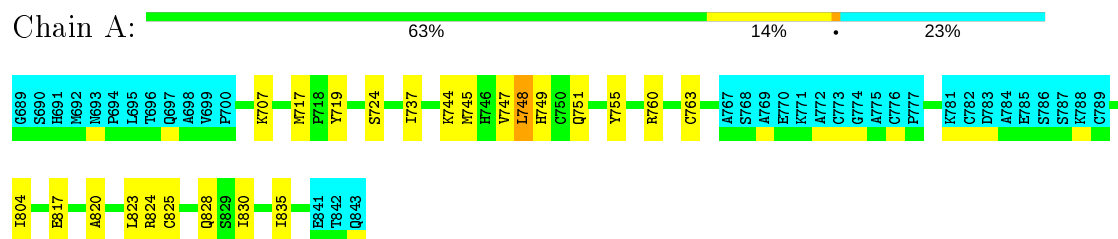
4.2.23 Score per residue for model 23

- Molecule 1: COMPLEMENT COMPONENT C7



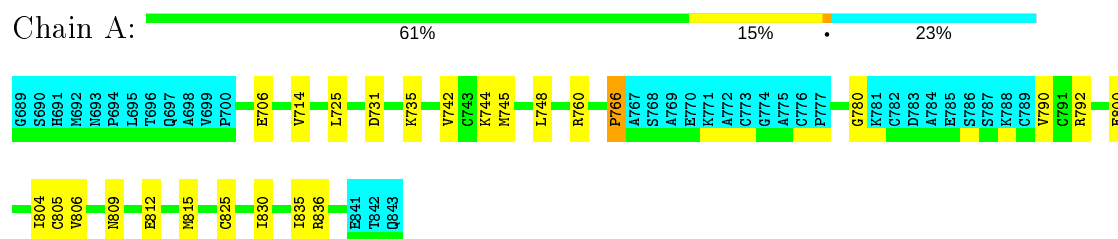
4.2.24 Score per residue for model 24

- Molecule 1: COMPLEMENT COMPONENT C7



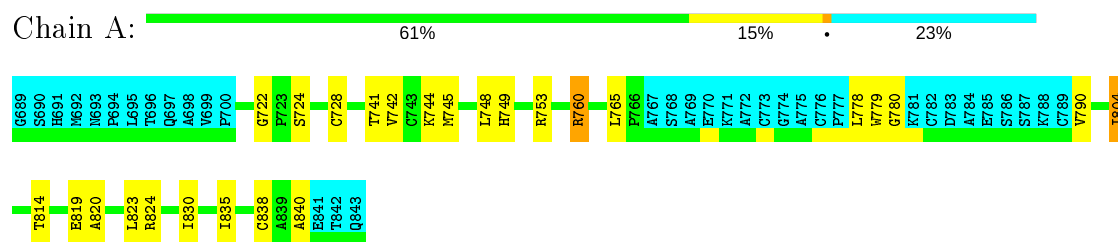
4.2.25 Score per residue for model 25

- Molecule 1: COMPLEMENT COMPONENT C7



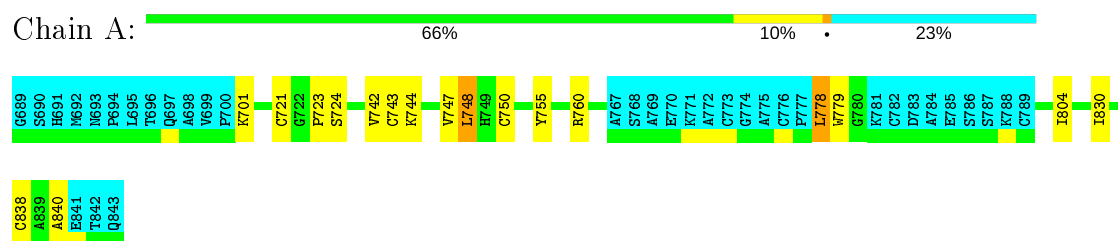
4.2.26 Score per residue for model 26

- Molecule 1: COMPLEMENT COMPONENT C7



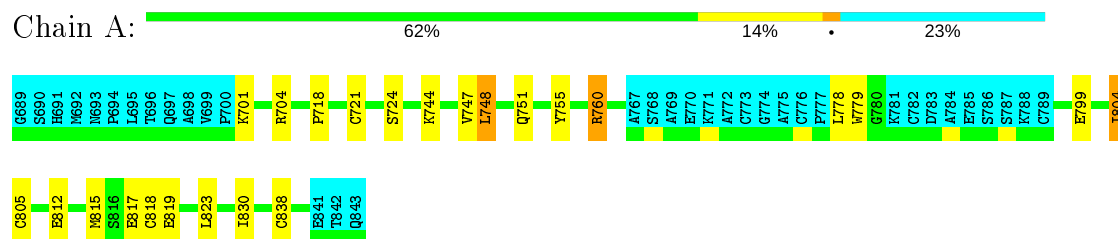
4.2.27 Score per residue for model 27

- Molecule 1: COMPLEMENT COMPONENT C7



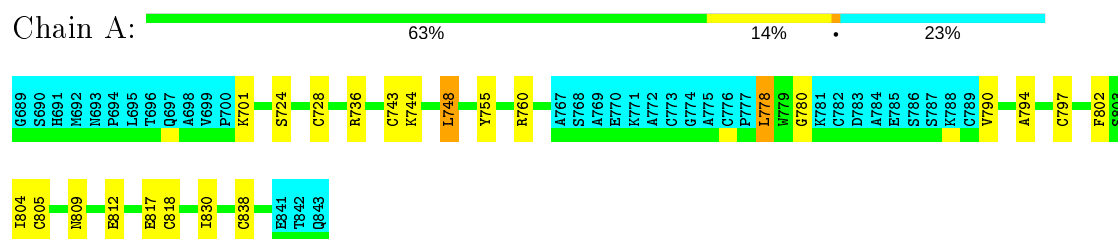
4.2.28 Score per residue for model 28

- Molecule 1: COMPLEMENT COMPONENT C7



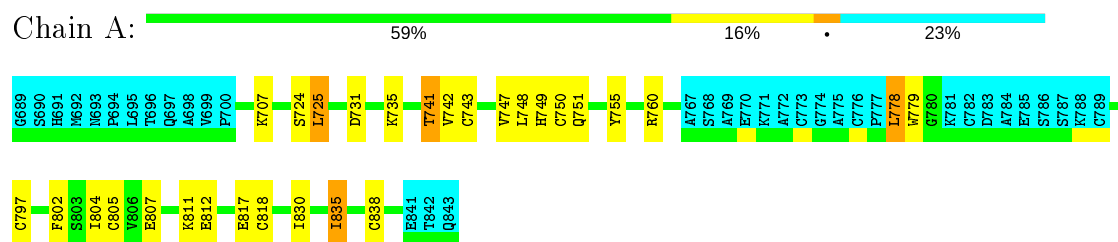
4.2.29 Score per residue for model 29

- Molecule 1: COMPLEMENT COMPONENT C7



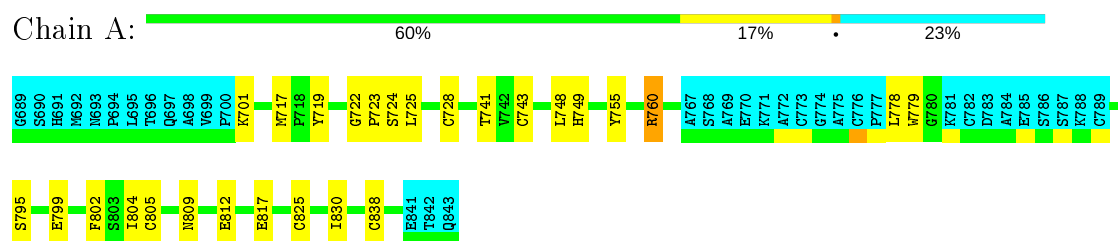
4.2.30 Score per residue for model 30

- Molecule 1: COMPLEMENT COMPONENT C7



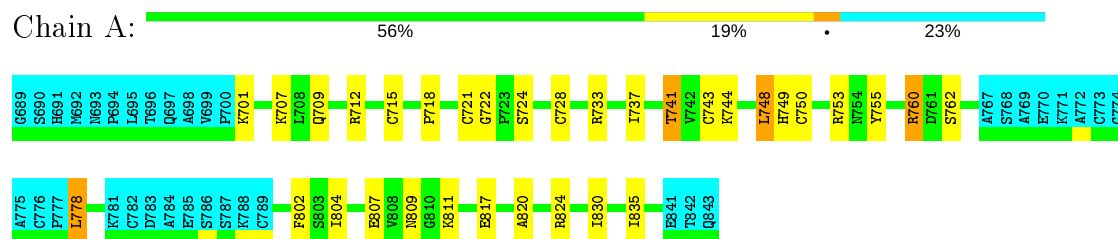
4.2.31 Score per residue for model 31

- Molecule 1: COMPLEMENT COMPONENT C7



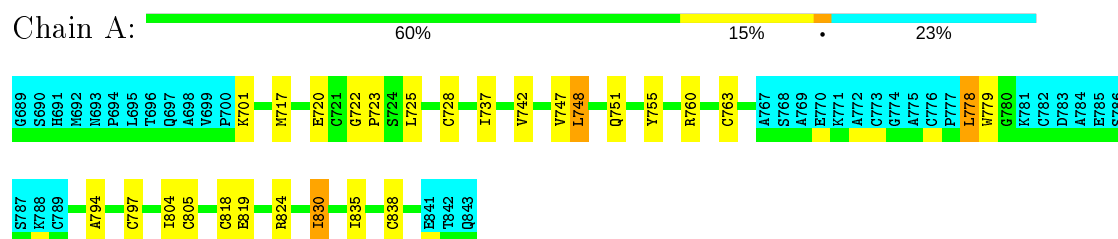
4.2.32 Score per residue for model 32

- Molecule 1: COMPLEMENT COMPONENT C7



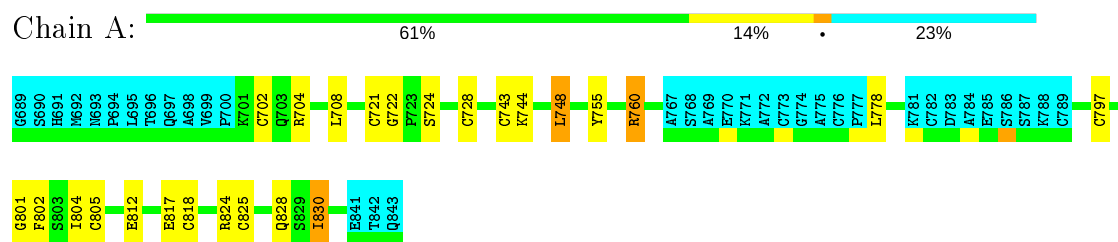
4.2.33 Score per residue for model 33

- Molecule 1: COMPLEMENT COMPONENT C7



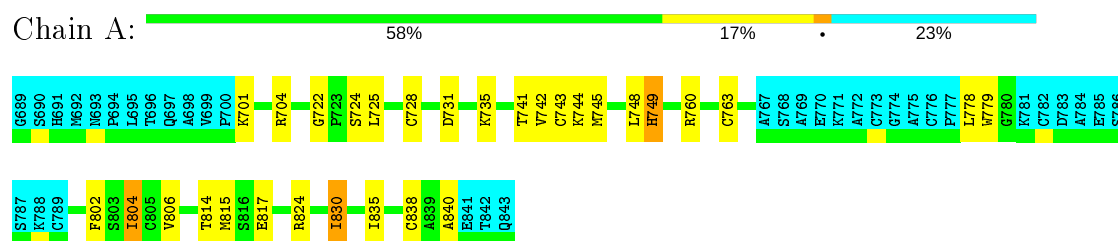
4.2.34 Score per residue for model 34

- Molecule 1: COMPLEMENT COMPONENT C7



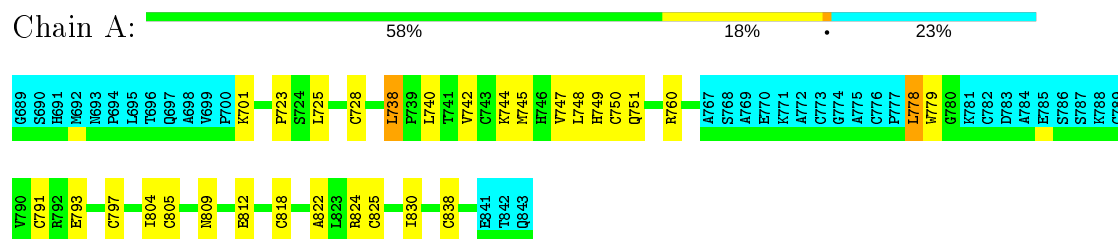
4.2.35 Score per residue for model 35

- Molecule 1: COMPLEMENT COMPONENT C7



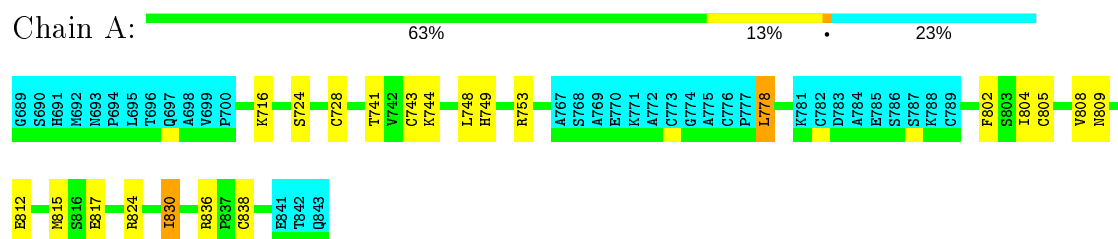
4.2.36 Score per residue for model 36

- Molecule 1: COMPLEMENT COMPONENT C7



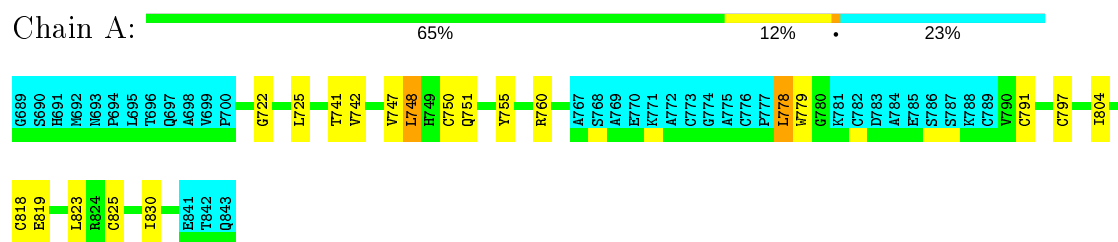
4.2.37 Score per residue for model 37

- Molecule 1: COMPLEMENT COMPONENT C7



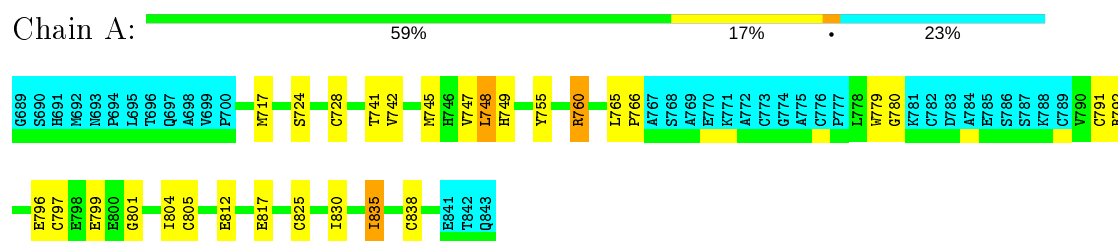
4.2.38 Score per residue for model 38

- Molecule 1: COMPLEMENT COMPONENT C7



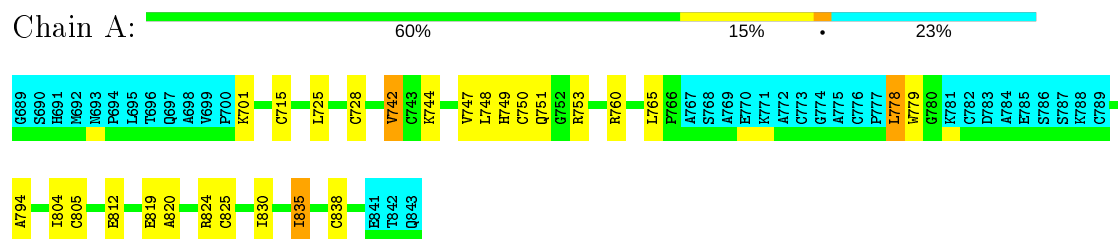
4.2.39 Score per residue for model 39

- Molecule 1: COMPLEMENT COMPONENT C7



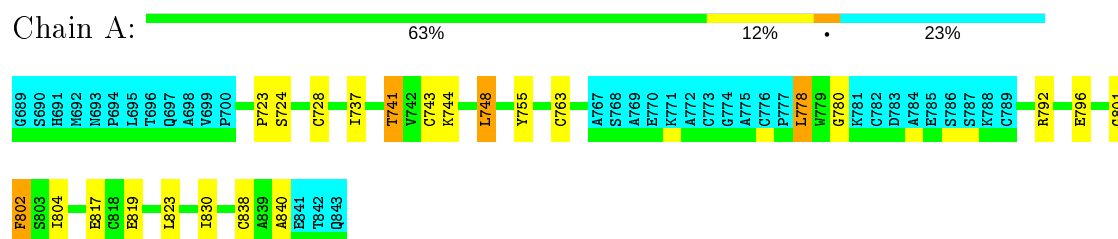
4.2.40 Score per residue for model 40

- Molecule 1: COMPLEMENT COMPONENT C7



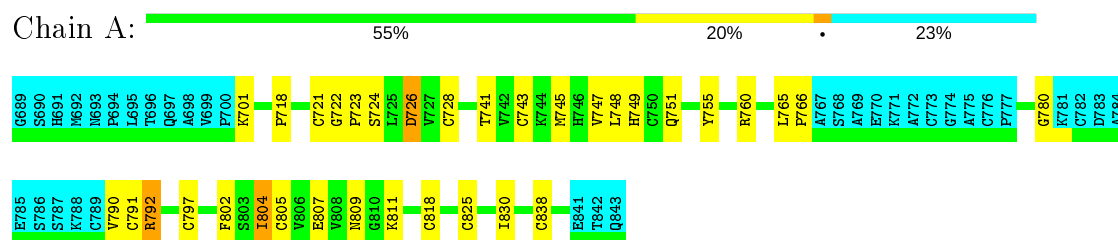
4.2.41 Score per residue for model 41

- Molecule 1: COMPLEMENT COMPONENT C7



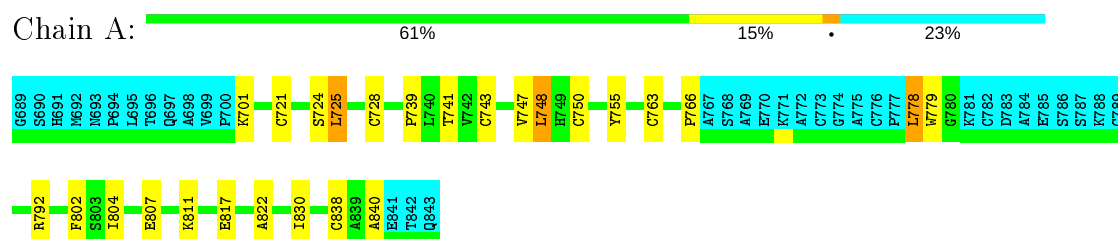
4.2.42 Score per residue for model 42

- Molecule 1: COMPLEMENT COMPONENT C7



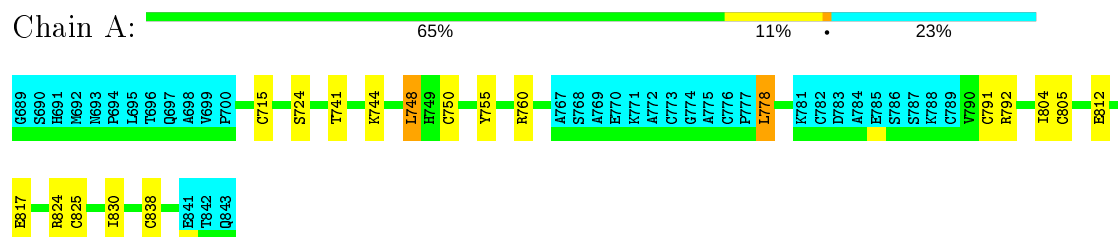
4.2.43 Score per residue for model 43

- Molecule 1: COMPLEMENT COMPONENT C7



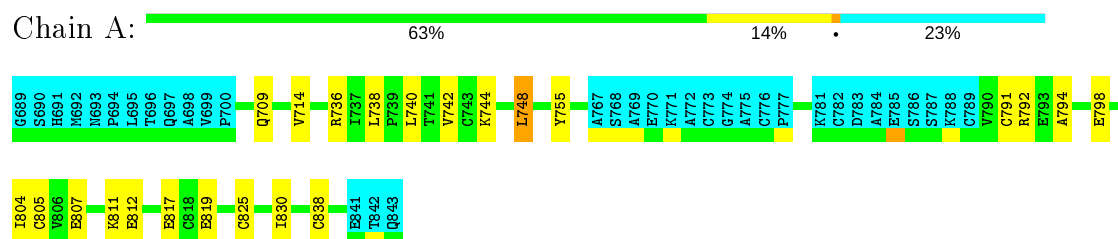
4.2.44 Score per residue for model 44 (medoid)

- Molecule 1: COMPLEMENT COMPONENT C7



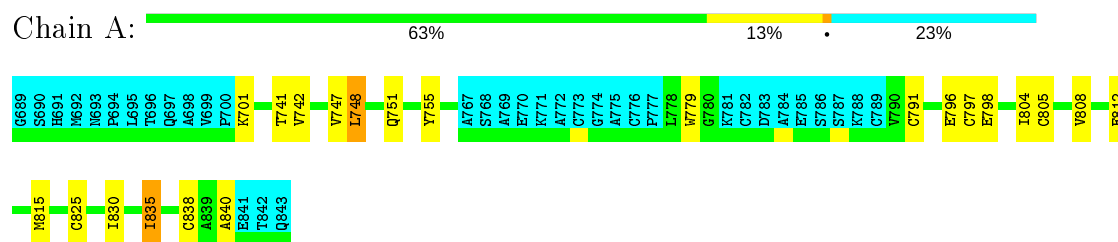
4.2.45 Score per residue for model 45

- Molecule 1: COMPLEMENT COMPONENT C7



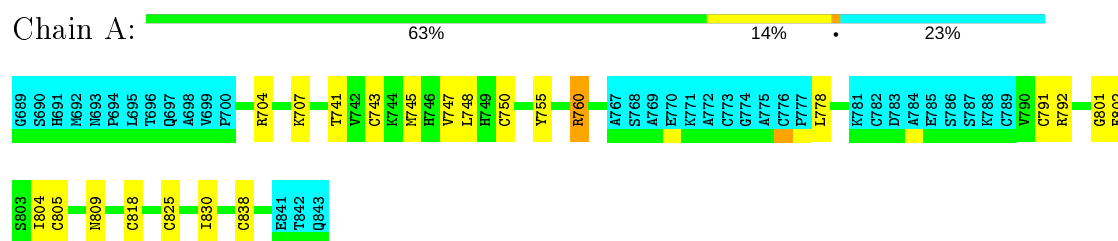
4.2.46 Score per residue for model 46

- Molecule 1: COMPLEMENT COMPONENT C7



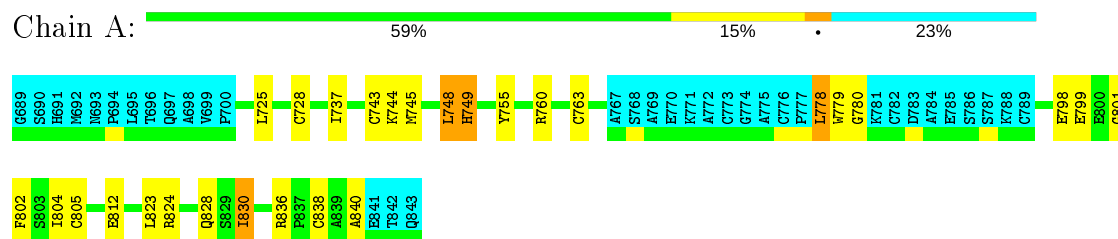
4.2.47 Score per residue for model 47

- Molecule 1: COMPLEMENT COMPONENT C7



4.2.48 Score per residue for model 48

- Molecule 1: COMPLEMENT COMPONENT C7



5 Refinement protocol and experimental data overview

The models were refined using the following method: *SIMULATED ANNEALING, RESTRAINED MOLECULAR DYNAMICS*.

Of the 200 calculated structures, 48 were deposited, based on the following criterion: *CONVERGED DATASETS OF 100 STRUCTURES EACH (1-25 AND 26-48)*.

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

Software name	Classification	Version
CNS	refinement	1.2
TopSpin	structure solution	1.3
CcpNmr Analysis	structure solution	1.0.15
CYANA	structure solution	2.1
CNS	structure solution	1.2

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 6 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	1676
Number of shifts mapped to atoms	1676
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	87%

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

COVALENT-GEOMETRY INFOmissingINFO

5.1 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	924	900	912	11±3
All	All	44352	43200	43426	519

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 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:728:CYS:SG	1:A:760:ARG:HA	0.75	2.21	26	10
1:A:794:ALA:HB1	1:A:819:GLU:HG2	0.75	1.58	33	1
1:A:725:LEU:HD13	1:A:779:TRP:CH2	0.69	2.22	3	5
1:A:738:LEU:HD13	1:A:740:LEU:HG	0.68	1.63	15	3
1:A:797:CYS:SG	1:A:818:CYS:HB2	0.68	2.28	42	5
1:A:797:CYS:SG	1:A:800:GLU:HA	0.68	2.29	12	1
1:A:724:SER:OG	1:A:742:VAL:HB	0.67	1.89	27	2
1:A:748:LEU:HD11	1:A:755:TYR:CD1	0.65	2.25	16	6
1:A:808:VAL:HG21	1:A:815:MET:HE1	0.65	1.69	37	3
1:A:748:LEU:HD11	1:A:755:TYR:CD2	0.65	2.25	14	4
1:A:721:CYS:SG	1:A:743:CYS:HB2	0.63	2.33	43	1
1:A:778:LEU:H	1:A:778:LEU:HD23	0.62	1.54	36	5
1:A:805:CYS:SG	1:A:812:GLU:HB3	0.62	2.35	40	28
1:A:724:SER:HA	1:A:817:GLU:CD	0.61	2.16	4	17
1:A:748:LEU:HD21	1:A:755:TYR:CD1	0.60	2.32	30	11
1:A:743:CYS:HA	1:A:802:PHE:CZ	0.59	2.32	42	10
1:A:824:ARG:HG2	1:A:830:ILE:HD11	0.59	1.74	34	6
1:A:838:CYS:SG	1:A:840:ALA:HB3	0.59	2.37	48	6
1:A:728:CYS:SG	1:A:739:PRO:HA	0.59	2.37	43	1
1:A:748:LEU:HD21	1:A:755:TYR:CD2	0.59	2.32	12	11
1:A:743:CYS:HA	1:A:802:PHE:CE1	0.59	2.32	17	3
1:A:724:SER:HA	1:A:817:GLU:OE1	0.58	1.98	18	7
1:A:724:SER:HA	1:A:817:GLU:OE2	0.58	1.99	9	6
1:A:805:CYS:SG	1:A:838:CYS:HB2	0.57	2.39	42	11
1:A:724:SER:OG	1:A:741:THR:HB	0.57	2.00	42	2
1:A:742:VAL:HG23	1:A:835:ILE:HB	0.57	1.77	35	10
1:A:778:LEU:HD23	1:A:778:LEU:H	0.56	1.60	43	7
1:A:824:ARG:HD2	1:A:830:ILE:HD11	0.56	1.75	37	1
1:A:744:LYS:O	1:A:748:LEU:HB3	0.56	2.00	2	19
1:A:728:CYS:SG	1:A:737:ILE:HG22	0.56	2.40	48	2
1:A:724:SER:HB2	1:A:741:THR:HG22	0.56	1.78	31	6
1:A:743:CYS:HA	1:A:802:PHE:CE2	0.56	2.34	31	4
1:A:728:CYS:SG	1:A:763:CYS:HB3	0.56	2.41	41	4
1:A:791:CYS:SG	1:A:825:CYS:HB3	0.56	2.41	44	6
1:A:791:CYS:HB3	1:A:825:CYS:SG	0.55	2.42	38	2
1:A:838:CYS:SG	1:A:840:ALA:HB2	0.54	2.42	46	1
1:A:728:CYS:SG	1:A:765:LEU:HD13	0.54	2.42	42	5
1:A:738:LEU:CD1	1:A:740:LEU:HG	0.54	2.32	15	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:725:LEU:HD13	1:A:817:GLU:HG3	0.54	1.80	4	1
1:A:778:LEU:HB2	1:A:779:TRP:CE3	0.53	2.38	18	6
1:A:745:MET:O	1:A:749:HIS:HB2	0.53	2.03	21	16
1:A:820:ALA:O	1:A:824:ARG:HG3	0.53	2.04	9	8
1:A:778:LEU:HG	1:A:779:TRP:CE3	0.53	2.38	40	11
1:A:737:ILE:HG22	1:A:763:CYS:HB3	0.53	1.80	14	8
1:A:724:SER:OG	1:A:743:CYS:HB3	0.53	2.04	41	1
1:A:780:GLY:HA2	1:A:790:VAL:O	0.53	2.04	23	3
1:A:747:VAL:O	1:A:751:GLN:HG3	0.52	2.04	4	9
1:A:824:ARG:HB3	1:A:830:ILE:HD11	0.52	1.81	3	1
1:A:819:GLU:O	1:A:823:LEU:HG	0.51	2.05	41	7
1:A:731:ASP:O	1:A:735:LYS:HA	0.51	2.06	35	6
1:A:738:LEU:HD23	1:A:740:LEU:HG	0.51	1.82	21	2
1:A:747:VAL:HA	1:A:750:CYS:SG	0.51	2.45	43	7
1:A:742:VAL:HG13	1:A:817:GLU:OE2	0.51	2.05	9	1
1:A:792:ARG:HD2	1:A:796:GLU:OE2	0.51	2.06	39	1
1:A:779:TRP:HA	1:A:797:CYS:SG	0.51	2.44	46	2
1:A:805:CYS:HB2	1:A:836:ARG:O	0.50	2.07	25	1
1:A:794:ALA:HA	1:A:797:CYS:SG	0.50	2.46	29	1
1:A:717:MET:O	1:A:720:GLU:HG3	0.50	2.06	33	1
1:A:718:PRO:HA	1:A:721:CYS:SG	0.50	2.45	28	3
1:A:807:GLU:HA	1:A:811:LYS:O	0.50	2.06	42	7
1:A:747:VAL:O	1:A:751:GLN:HG2	0.50	2.07	46	16
1:A:749:HIS:HA	1:A:753:ARG:O	0.49	2.08	40	4
1:A:823:LEU:HD23	1:A:828:GLN:HG2	0.49	1.84	24	2
1:A:741:THR:OG1	1:A:744:LYS:HD3	0.49	2.06	41	1
1:A:728:CYS:HB2	1:A:759:GLY:O	0.49	2.07	3	1
1:A:744:LYS:O	1:A:748:LEU:HG	0.49	2.06	35	10
1:A:725:LEU:CD2	1:A:817:GLU:HG3	0.49	2.37	23	1
1:A:792:ARG:HA	1:A:792:ARG:NE	0.49	2.23	44	1
1:A:717:MET:HB2	1:A:720:GLU:CG	0.49	2.38	33	1
1:A:743:CYS:SG	1:A:744:LYS:N	0.49	2.86	20	1
1:A:702:CYS:SG	1:A:708:LEU:HB2	0.49	2.48	34	2
1:A:778:LEU:HD13	1:A:778:LEU:H	0.48	1.67	3	6
1:A:792:ARG:O	1:A:822:ALA:HB1	0.48	2.08	9	4
1:A:709:GLN:CD	1:A:710:ASN:HB2	0.48	2.29	14	1
1:A:778:LEU:H	1:A:778:LEU:HD13	0.48	1.69	32	5
1:A:731:ASP:HA	1:A:755:TYR:CE1	0.48	2.44	14	1
1:A:725:LEU:HD22	1:A:779:TRP:CH2	0.48	2.43	20	1
1:A:806:VAL:HG11	1:A:815:MET:SD	0.47	2.48	25	3
1:A:721:CYS:HB2	1:A:743:CYS:SG	0.47	2.49	27	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:742:VAL:HG13	1:A:817:GLU:OE1	0.47	2.10	35	1
1:A:715:CYS:HB3	1:A:750:CYS:SG	0.47	2.49	40	2
1:A:709:GLN:OE1	1:A:714:VAL:HG22	0.47	2.10	45	1
1:A:792:ARG:HE	1:A:796:GLU:HG3	0.47	1.70	13	1
1:A:725:LEU:HD23	1:A:779:TRP:CH2	0.47	2.45	48	2
1:A:824:ARG:HA	1:A:830:ILE:HD11	0.47	1.86	18	1
1:A:778:LEU:HD12	1:A:778:LEU:H	0.47	1.69	22	2
1:A:748:LEU:HD11	1:A:755:TYR:CG	0.47	2.45	42	3
1:A:717:MET:HB3	1:A:719:TYR:CE1	0.46	2.45	31	1
1:A:725:LEU:O	1:A:742:VAL:HG23	0.46	2.11	10	7
1:A:731:ASP:HA	1:A:755:TYR:CE2	0.46	2.46	15	1
1:A:716:LYS:NZ	1:A:720:GLU:HB3	0.46	2.25	18	1
1:A:725:LEU:HD23	1:A:817:GLU:HG3	0.46	1.88	20	1
1:A:701:LYS:HD2	1:A:701:LYS:N	0.46	2.25	27	1
1:A:704:ARG:HA	1:A:704:ARG:CZ	0.46	2.39	47	1
1:A:794:ALA:HB1	1:A:819:GLU:HG3	0.46	1.85	45	3
1:A:721:CYS:SG	1:A:744:LYS:HA	0.46	2.50	34	1
1:A:709:GLN:HE22	1:A:714:VAL:HG11	0.46	1.71	45	1
1:A:726:ASP:O	1:A:765:LEU:HD21	0.45	2.11	3	1
1:A:723:PRO:CB	1:A:778:LEU:HG	0.45	2.42	41	1
1:A:834:SER:OG	1:A:836:ARG:HG2	0.45	2.11	7	1
1:A:760:ARG:HA	1:A:763:CYS:SG	0.45	2.51	20	2
1:A:748:LEU:HD11	1:A:755:TYR:CZ	0.45	2.46	30	1
1:A:748:LEU:HD12	1:A:749:HIS:N	0.45	2.26	37	1
1:A:709:GLN:O	1:A:712:ARG:HG2	0.45	2.12	32	1
1:A:742:VAL:HG13	1:A:835:ILE:HB	0.45	1.89	21	2
1:A:706:GLU:HA	1:A:714:VAL:O	0.45	2.11	25	1
1:A:724:SER:HG	1:A:743:CYS:HB3	0.45	1.70	41	1
1:A:742:VAL:HG22	1:A:835:ILE:HB	0.45	1.88	30	1
1:A:717:MET:O	1:A:720:GLU:HB3	0.44	2.11	10	1
1:A:824:ARG:CG	1:A:830:ILE:HD11	0.44	2.43	34	1
1:A:725:LEU:HD12	1:A:779:TRP:CZ3	0.44	2.48	38	1
1:A:724:SER:CB	1:A:741:THR:HG22	0.44	2.42	44	1
1:A:715:CYS:SG	1:A:750:CYS:HB3	0.44	2.53	32	1
1:A:742:VAL:CG2	1:A:835:ILE:HB	0.44	2.42	7	1
1:A:745:MET:HG3	1:A:835:ILE:HD13	0.43	1.90	20	1
1:A:726:ASP:OD2	1:A:765:LEU:HG	0.43	2.12	42	1
1:A:745:MET:HG2	1:A:835:ILE:CD1	0.43	2.43	26	2
1:A:741:THR:HB	1:A:743:CYS:SG	0.43	2.54	20	1
1:A:704:ARG:HD2	1:A:801:GLY:O	0.43	2.14	34	1
1:A:742:VAL:HB	1:A:817:GLU:OE2	0.43	2.13	45	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:745:MET:CG	1:A:835:ILE:HD13	0.43	2.43	20	1
1:A:804:ILE:O	1:A:814:THR:HA	0.43	2.13	35	3
1:A:721:CYS:O	1:A:723:PRO:HD2	0.43	2.14	17	1
1:A:704:ARG:HD3	1:A:801:GLY:O	0.43	2.14	17	1
1:A:778:LEU:HG	1:A:779:TRP:CZ3	0.43	2.48	33	2
1:A:725:LEU:HD12	1:A:779:TRP:CH2	0.43	2.49	31	1
1:A:728:CYS:HB2	1:A:763:CYS:SG	0.43	2.54	35	2
1:A:801:GLY:HA3	1:A:817:GLU:OE1	0.43	2.14	39	1
1:A:725:LEU:HD22	1:A:817:GLU:HG3	0.43	1.91	23	1
1:A:792:ARG:NE	1:A:792:ARG:HA	0.42	2.29	42	1
1:A:716:LYS:O	1:A:747:VAL:HG13	0.42	2.14	21	1
1:A:792:ARG:HB3	1:A:796:GLU:HB2	0.42	1.91	41	1
1:A:805:CYS:SG	1:A:838:CYS:HB3	0.42	2.55	31	3
1:A:778:LEU:HB2	1:A:818:CYS:SG	0.42	2.55	47	1
1:A:808:VAL:HG22	1:A:830:ILE:HG22	0.42	1.90	2	1
1:A:801:GLY:HA3	1:A:817:GLU:HB3	0.42	1.92	17	1
1:A:745:MET:HA	1:A:748:LEU:HB3	0.42	1.91	9	1
1:A:792:ARG:HD2	1:A:796:GLU:CD	0.42	2.35	17	1
1:A:804:ILE:HD13	1:A:804:ILE:H	0.42	1.73	28	2
1:A:793:GLU:HA	1:A:822:ALA:CB	0.42	2.44	36	1
1:A:706:GLU:HG2	1:A:715:CYS:SG	0.42	2.54	15	1
1:A:704:ARG:HA	1:A:704:ARG:NE	0.42	2.30	47	1
1:A:725:LEU:HD23	1:A:817:GLU:HG2	0.42	1.92	18	1
1:A:778:LEU:HD12	1:A:818:CYS:SG	0.42	2.54	28	2
1:A:728:CYS:SG	1:A:737:ILE:CG2	0.41	3.07	33	2
1:A:717:MET:C	1:A:747:VAL:HG11	0.41	2.36	39	1
1:A:725:LEU:O	1:A:742:VAL:HG12	0.41	2.14	40	1
1:A:725:LEU:HD22	1:A:817:GLU:CG	0.41	2.45	30	1
1:A:778:LEU:HD21	1:A:779:TRP:CZ3	0.41	2.50	35	1
1:A:746:HIS:NE2	1:A:835:ILE:HG12	0.41	2.31	7	1
1:A:717:MET:HB3	1:A:719:TYR:CE2	0.41	2.51	24	1
1:A:778:LEU:CD1	1:A:778:LEU:H	0.41	2.29	9	1
1:A:778:LEU:HA	1:A:799:GLU:HB3	0.41	1.93	18	1
1:A:815:MET:HB3	1:A:819:GLU:HG3	0.41	1.91	28	1
1:A:728:CYS:CB	1:A:763:CYS:SG	0.41	3.08	43	1
1:A:725:LEU:HB2	1:A:817:GLU:HG3	0.41	1.93	6	1
1:A:729:ALA:O	1:A:738:LEU:HD22	0.41	2.15	21	1
1:A:718:PRO:O	1:A:744:LYS:HG2	0.41	2.16	22	1
1:A:797:CYS:HB3	1:A:818:CYS:SG	0.41	2.56	33	1
1:A:824:ARG:NH2	1:A:832:VAL:HG21	0.41	2.31	11	1
1:A:723:PRO:HB2	1:A:778:LEU:CD2	0.41	2.46	27	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:737:ILE:HG21	1:A:762:SER:CB	0.41	2.45	32	1
1:A:724:SER:HB3	1:A:741:THR:CG2	0.40	2.46	4	1
1:A:724:SER:OG	1:A:743:CYS:HB2	0.40	2.16	30	1
1:A:805:CYS:HB3	1:A:834:SER:OG	0.40	2.16	3	1
1:A:816:SER:O	1:A:819:GLU:HB3	0.40	2.16	18	1
1:A:760:ARG:HD2	1:A:760:ARG:C	0.40	2.36	30	1
1:A:724:SER:HB2	1:A:741:THR:HB	0.40	1.94	6	1
1:A:748:LEU:HD21	1:A:755:TYR:CE2	0.40	2.52	33	1
1:A:797:CYS:CB	1:A:818:CYS:HB2	0.40	2.46	38	1

5.2 Torsion angles [i](#)

5.2.1 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	120/155 (77%)	112±2 (93±2%)	7±2 (6±2%)	1±1 (1±1%)	24	71
All	All	5760/7440 (77%)	5373 (93%)	340 (6%)	47 (1%)	24	71

All 10 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	722	GLY	17
1	A	766	PRO	9
1	A	801	GLY	8
1	A	723	PRO	6
1	A	800	GLU	2
1	A	701	LYS	1
1	A	711	SER	1
1	A	798	GLU	1
1	A	799	GLU	1
1	A	710	ASN	1

5.2.2 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	106/133 (80%)	99±1 (94±1%)	7±1 (6±1%)	21 70
All	All	5088/6384 (80%)	4763 (94%)	325 (6%)	21 70

All 40 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	804	ILE	48
1	A	830	ILE	48
1	A	760	ARG	31
1	A	778	LEU	29
1	A	748	LEU	27
1	A	741	THR	24
1	A	701	LYS	15
1	A	835	ILE	14
1	A	809	ASN	14
1	A	707	LYS	7
1	A	738	LEU	6
1	A	798	GLU	5
1	A	743	CYS	5
1	A	799	GLU	5
1	A	725	LEU	5
1	A	828	GLN	4
1	A	745	MET	4
1	A	749	HIS	4
1	A	704	ARG	3
1	A	742	VAL	2
1	A	766	PRO	2
1	A	836	ARG	2
1	A	733	ARG	2
1	A	736	ARG	2
1	A	721	CYS	2
1	A	802	PHE	1
1	A	716	LYS	1
1	A	811	LYS	1
1	A	796	GLU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	818	CYS	1
1	A	803	SER	1
1	A	817	GLU	1
1	A	795	SER	1
1	A	728	CYS	1
1	A	753	ARG	1
1	A	791	CYS	1
1	A	826	ARG	1
1	A	790	VAL	1
1	A	726	ASP	1
1	A	838	CYS	1

5.2.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.4 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.5 Ligand geometry [i](#)

There are no ligands in this entry.

5.6 Other polymers [i](#)

There are no such molecules in this entry.

5.7 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 87% for the well-defined parts and 83% for the entire structure.

6.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

6.1.1 Bookkeeping

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	1676
Number of shifts mapped to atoms	1676
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

6.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	147	-0.10 ± 0.20	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	136	0.33 ± 0.17	None needed (< 0.5 ppm)
$^{13}\text{C}'$	136	-0.95 ± 0.31	Should be applied
^{15}N	137	0.17 ± 0.47	None needed (< 0.5 ppm)

6.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 87%, i.e. 1270 atoms were assigned a chemical shift out of a possible 1453. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	582/590 (99%)	233/235 (99%)	235/240 (98%)	114/115 (99%)
Sidechain	636/798 (80%)	398/474 (84%)	220/279 (79%)	18/45 (40%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	52/65 (80%)	26/33 (79%)	24/26 (92%)	2/6 (33%)
Overall	1270/1453 (87%)	657/742 (89%)	479/545 (88%)	134/166 (81%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 83%, i.e. 1516 atoms were assigned a chemical shift out of a possible 1818. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	703/759 (93%)	283/302 (94%)	283/310 (91%)	137/147 (93%)
Sidechain	759/986 (77%)	477/587 (81%)	262/348 (75%)	20/51 (39%)
Aromatic	54/73 (74%)	27/37 (73%)	25/28 (89%)	2/8 (25%)
Overall	1516/1818 (83%)	787/926 (85%)	570/686 (83%)	159/206 (77%)

6.1.4 Statistically unusual chemical shifts ⓘ

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	703	GLN	HB2	-0.16	3.30 – 0.80	-8.9
1	A	792	ARG	HG2	-0.34	2.92 – 0.22	-7.1
1	A	744	LYS	CE	36.15	46.00 – 37.80	-7.0
1	A	703	GLN	HB3	0.27	3.37 – 0.67	-6.5

6.1.5 Random Coil Index (RCI) plots ⓘ

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:

