



Full wwPDB NMR Structure Validation Report ⓘ

May 29, 2020 – 12:00 am BST

PDB ID : 2MF6
Title : Solution NMR structure of Chimeric Avidin, ChiAVD(I117Y), in the biotin bound form
Authors : Tossavainen, H.; Kukkurainen, S.; Maatta, J.A.E.; Pihlajamaa, T.; Hytonen, V.P.; Kulomaa, M.S.; Permi, P.
Deposited on : 2013-10-07

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

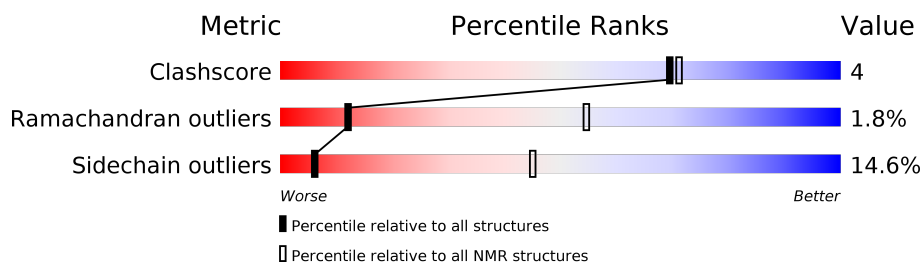
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 19%.

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	129	74% 18% • 8%
1	B	129	74% 17% • 8%
1	C	129	73% 19% • 8%
1	D	129	72% 19% • 8%

2 Ensemble composition and analysis

This entry contains 15 models. Model 10 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:3-A:54, A:57-A:123, D:3-D:54, D:57-D:123, B:3-B:54, B:57-B:123, C:3-C:54, C:57-C:123 (476)	0.23	10

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 3 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8072 atoms, of which 4020 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Avidin, Avidin-related protein 4/5.

Mol	Chain	Residues	Atoms						Trace
1	A	129	Total 2018	C 636	H 1005	N 181	O 192	S 4	0
1	D	129	Total 2018	C 636	H 1005	N 181	O 192	S 4	0
1	B	129	Total 2018	C 636	H 1005	N 181	O 192	S 4	0
1	C	129	Total 2018	C 636	H 1005	N 181	O 192	S 4	0

There are 16 discrepancies between the modelled and reference sequences:

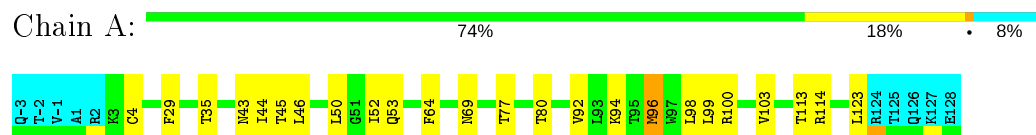
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLN	-	EXPRESSION TAG	UNP P02701
A	-2	THR	-	EXPRESSION TAG	UNP P02701
A	-1	VAL	-	EXPRESSION TAG	UNP P02701
A	117	TYR	ILE	ENGINEERED MUTATION	UNP P02701
D	-3	GLN	-	EXPRESSION TAG	UNP P02701
D	-2	THR	-	EXPRESSION TAG	UNP P02701
D	-1	VAL	-	EXPRESSION TAG	UNP P02701
D	117	TYR	ILE	ENGINEERED MUTATION	UNP P02701
B	-3	GLN	-	EXPRESSION TAG	UNP P02701
B	-2	THR	-	EXPRESSION TAG	UNP P02701
B	-1	VAL	-	EXPRESSION TAG	UNP P02701
B	117	TYR	ILE	ENGINEERED MUTATION	UNP P02701
C	-3	GLN	-	EXPRESSION TAG	UNP P02701
C	-2	THR	-	EXPRESSION TAG	UNP P02701
C	-1	VAL	-	EXPRESSION TAG	UNP P02701
C	117	TYR	ILE	ENGINEERED MUTATION	UNP P02701

4 Residue-property plots

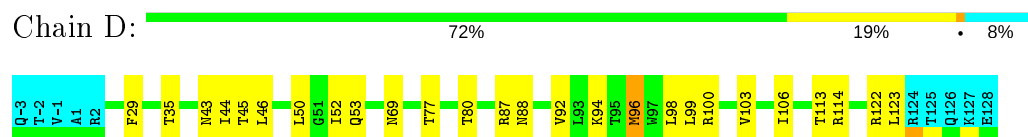
4.1 Average score per residue in the NMR ensemble

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.

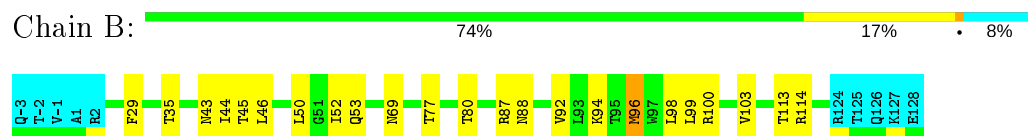
- Molecule 1: Avidin, Avidin-related protein 4/5



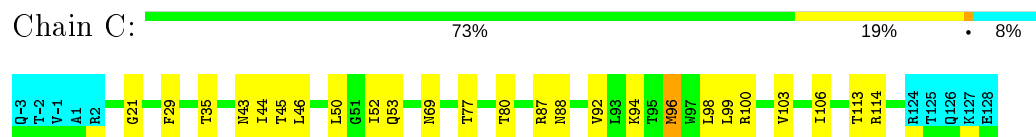
- Molecule 1: Avidin, Avidin-related protein 4/5



- Molecule 1: Avidin, Avidin-related protein 4/5



- Molecule 1: Avidin, Avidin-related protein 4/5

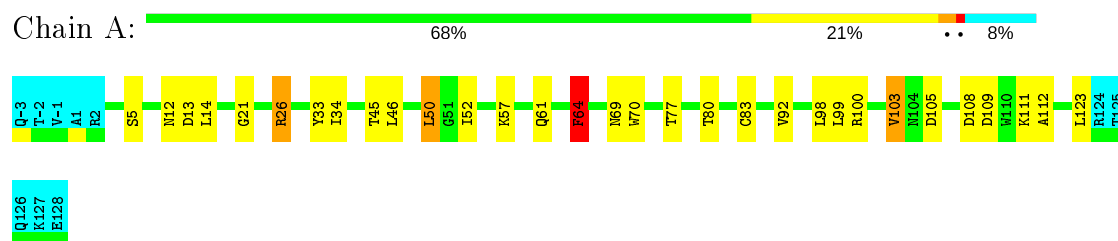


4.2 Scores per residue for each member of the ensemble

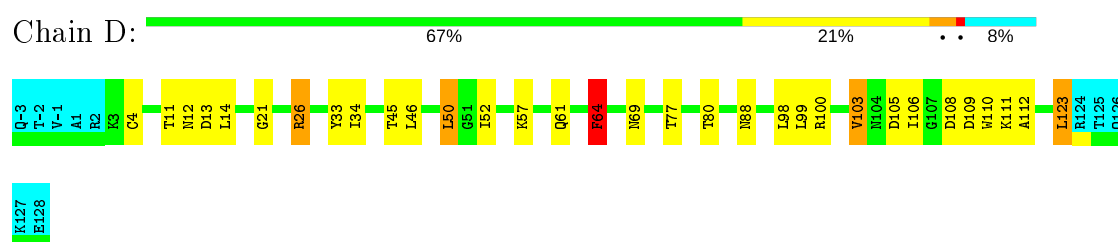
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

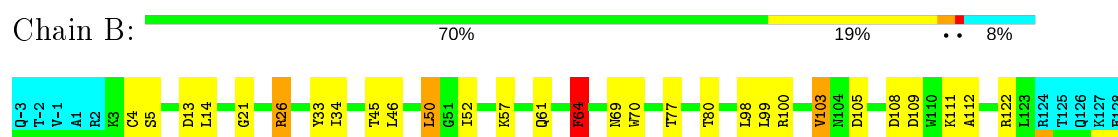
- Molecule 1: Avidin, Avidin-related protein 4/5



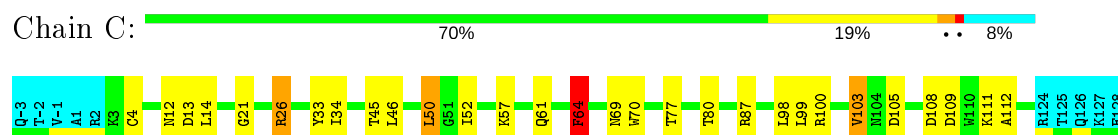
- Molecule 1: Avidin, Avidin-related protein 4/5



- Molecule 1: Avidin, Avidin-related protein 4/5

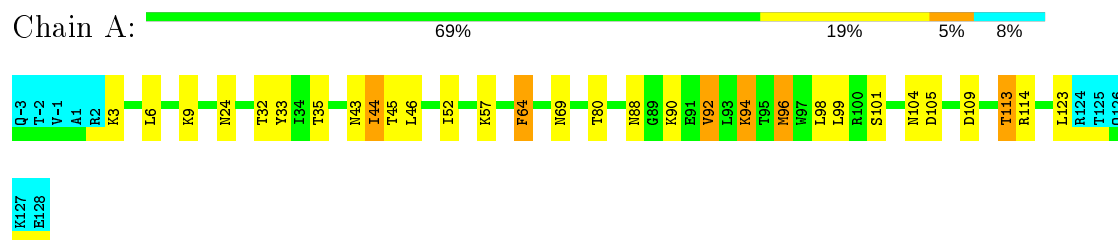


- Molecule 1: Avidin, Avidin-related protein 4/5

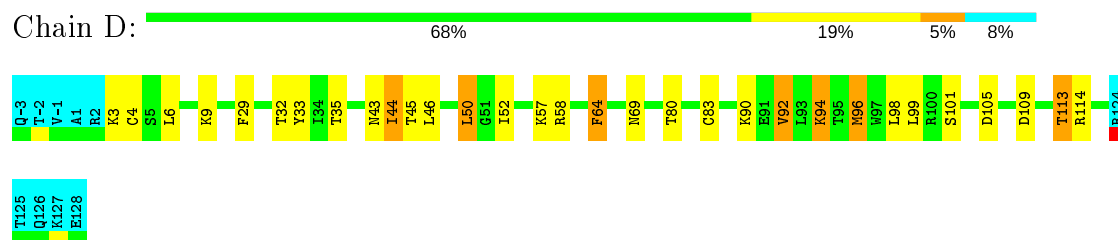


4.2.2 Score per residue for model 2

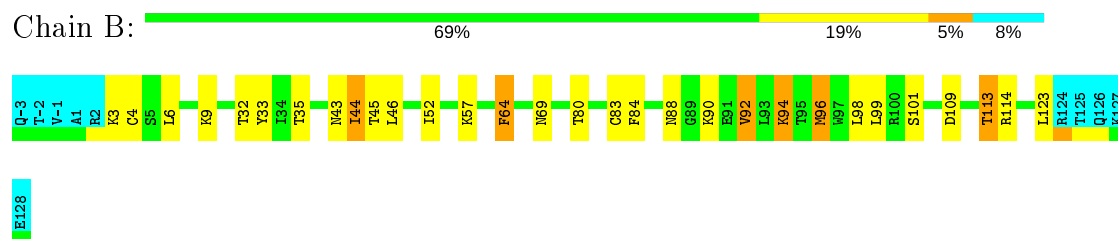
- Molecule 1: Avidin, Avidin-related protein 4/5



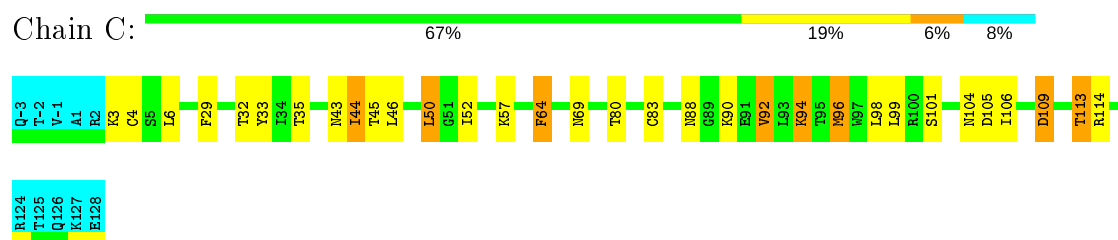
- Molecule 1: Avidin, Avidin-related protein 4/5



- Molecule 1: Avidin, Avidin-related protein 4/5

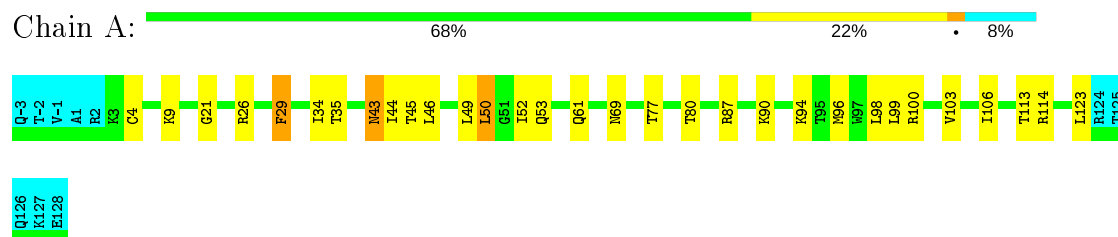


- Molecule 1: Avidin, Avidin-related protein 4/5

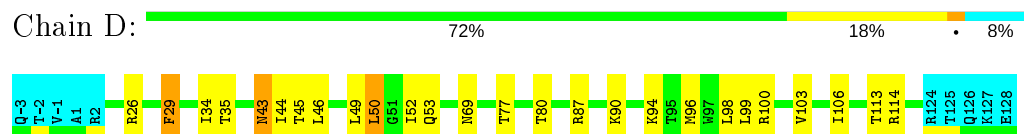


4.2.3 Score per residue for model 3

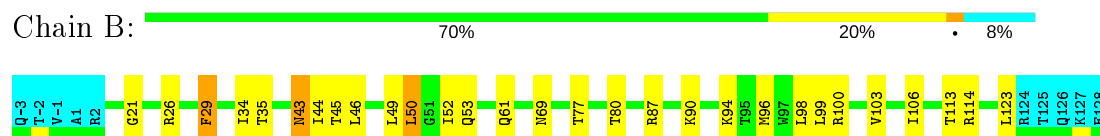
- Molecule 1: Avidin, Avidin-related protein 4/5



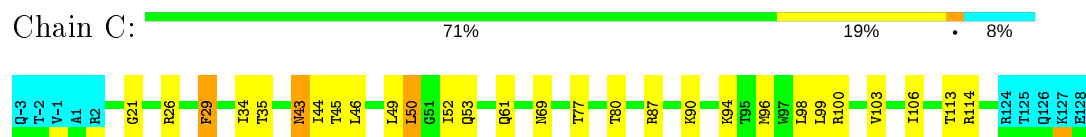
- Molecule 1: Avidin, Avidin-related protein 4/5



- Molecule 1: Avidin, Avidin-related protein 4/5

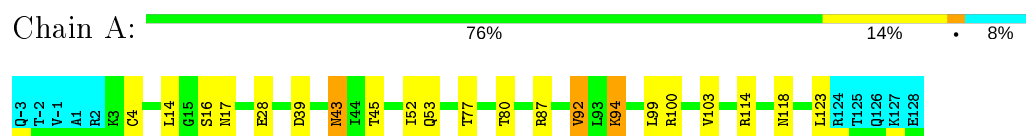


- Molecule 1: Avidin, Avidin-related protein 4/5

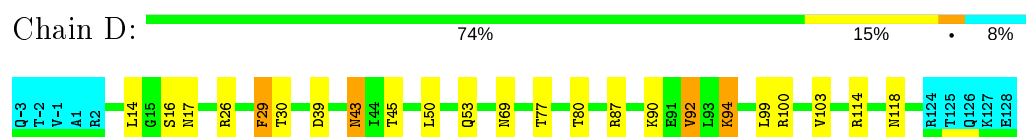


4.2.4 Score per residue for model 4

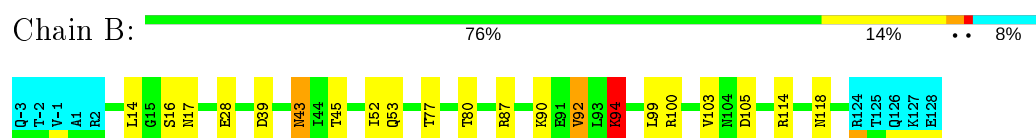
- Molecule 1: Avidin, Avidin-related protein 4/5



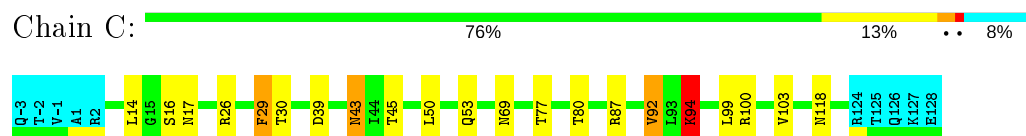
- Molecule 1: Avidin, Avidin-related protein 4/5



- Molecule 1: Avidin, Avidin-related protein 4/5



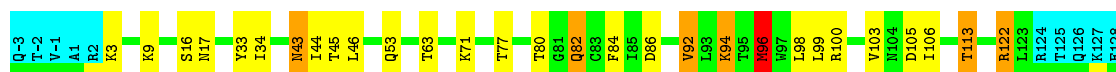
- Molecule 1: Avidin, Avidin-related protein 4/5



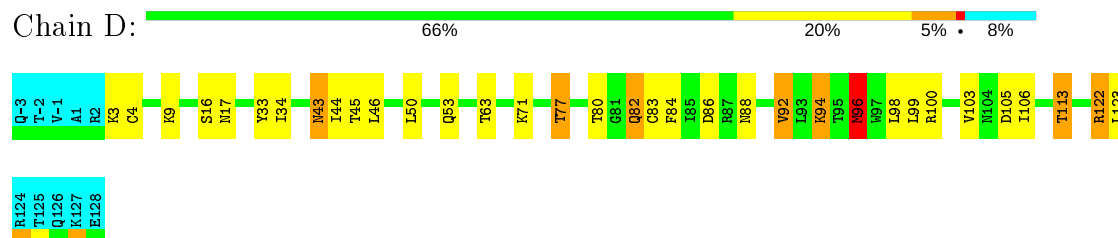
4.2.5 Score per residue for model 5

- Molecule 1: Avidin, Avidin-related protein 4/5

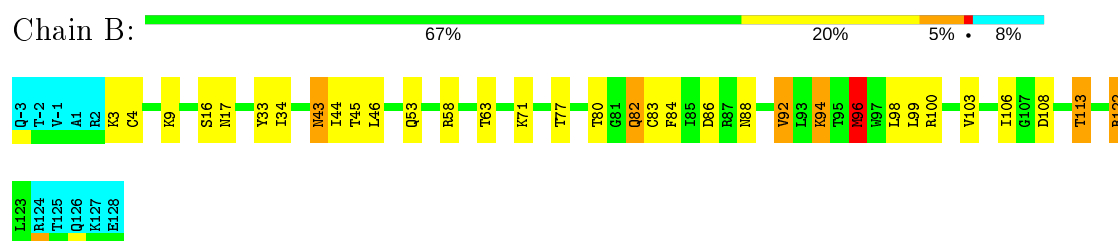




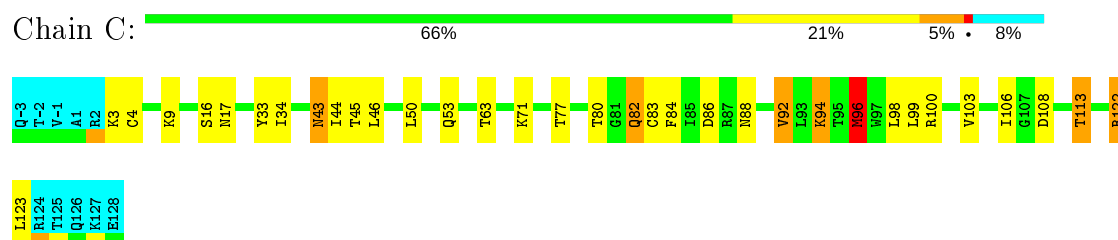
- Molecule 1: Avidin, Avidin-related protein 4/5



- Molecule 1: Avidin, Avidin-related protein 4/5

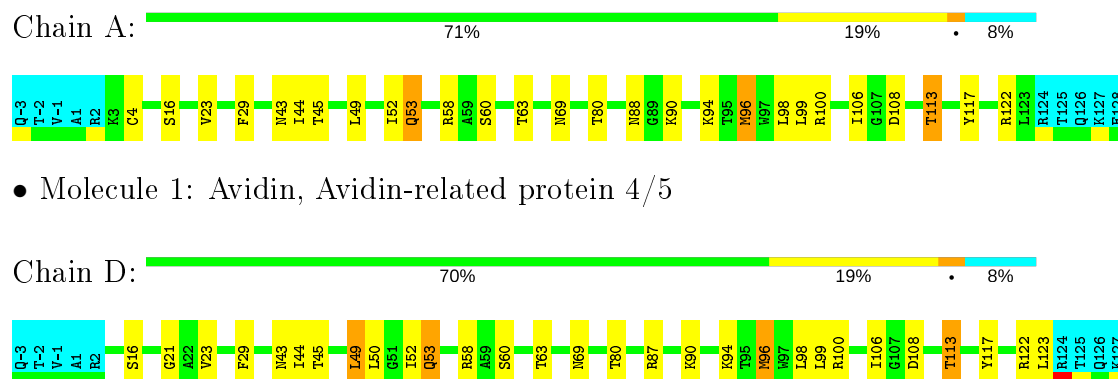


- Molecule 1: Avidin, Avidin-related protein 4/5



4.2.6 Score per residue for model 6

- Molecule 1: Avidin, Avidin-related protein 4/5

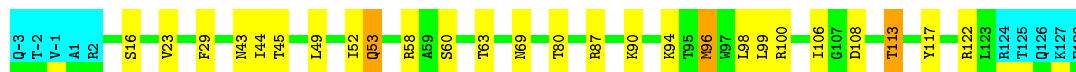


- Molecule 1: Avidin, Avidin-related protein 4/5

E128

- Molecule 1: Avidin, Avidin-related protein 4/5

Chain B: 



- Molecule 1: Avidin, Avidin-related protein 4/5

Chain C: 

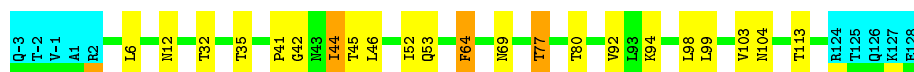


E128

4.2.7 Score per residue for model 7

- Molecule 1: Avidin, Avidin-related protein 4/5

Chain A: 



- Molecule 1: Avidin, Avidin-related protein 4/5

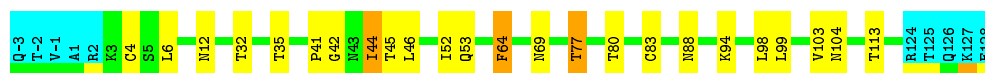
Chain D: 



E128

- Molecule 1: Avidin, Avidin-related protein 4/5

Chain B: 



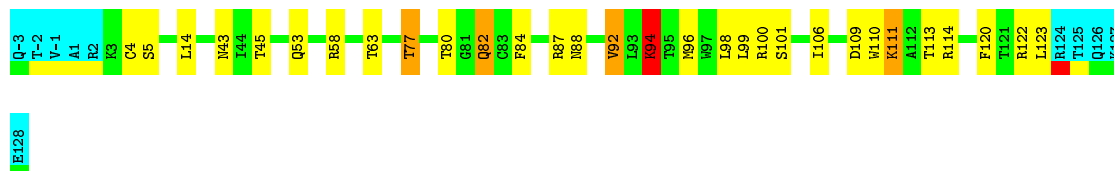
- Molecule 1: Avidin, Avidin-related protein 4/5

Chain C: 

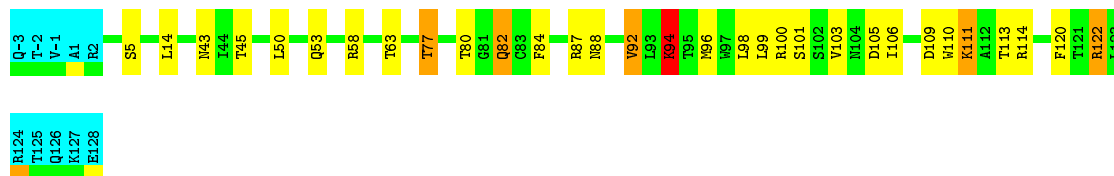


4.2.8 Score per residue for model 8

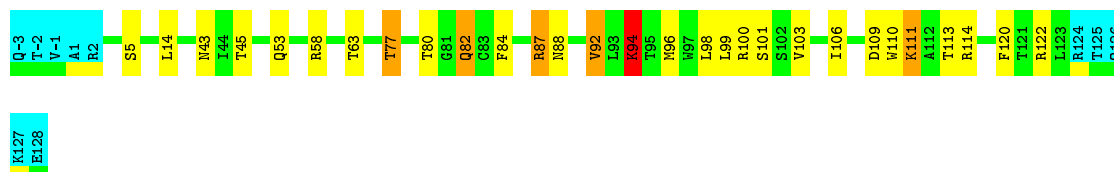
- Molecule 1: Avidin, Avidin-related protein 4/5



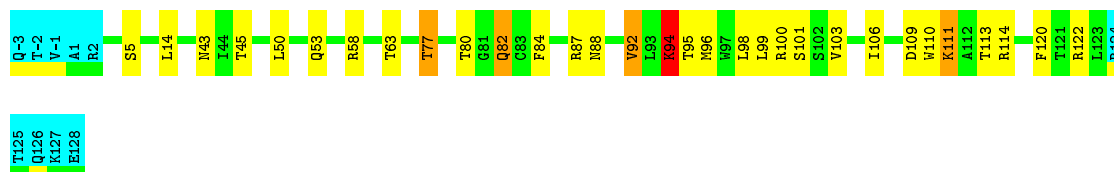
- Molecule 1: Avidin, Avidin-related protein 4/5



- Molecule 1: Avidin, Avidin-related protein 4/5



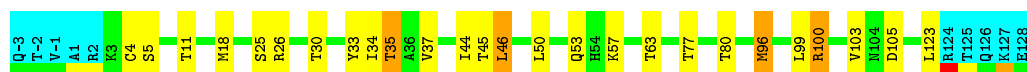
- Molecule 1: Avidin, Avidin-related protein 4/5



4.2.9 Score per residue for model 9

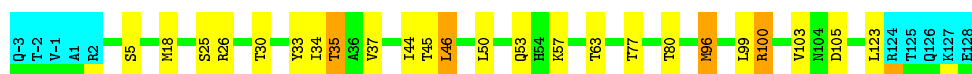
- Molecule 1: Avidin, Avidin-related protein 4/5

Chain A: 



- Molecule 1: Avidin, Avidin-related protein 4/5

Chain D: 



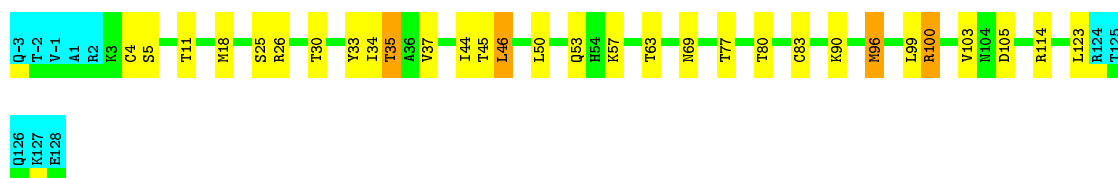
- Molecule 1: Avidin, Avidin-related protein 4/5

Chain B: 



- Molecule 1: Avidin, Avidin-related protein 4/5

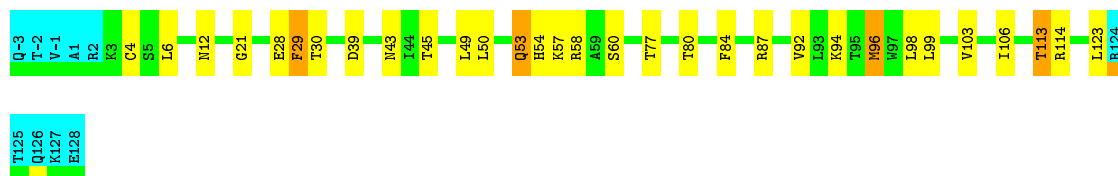
Chain C: 



4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: Avidin, Avidin-related protein 4/5

Chain A: 



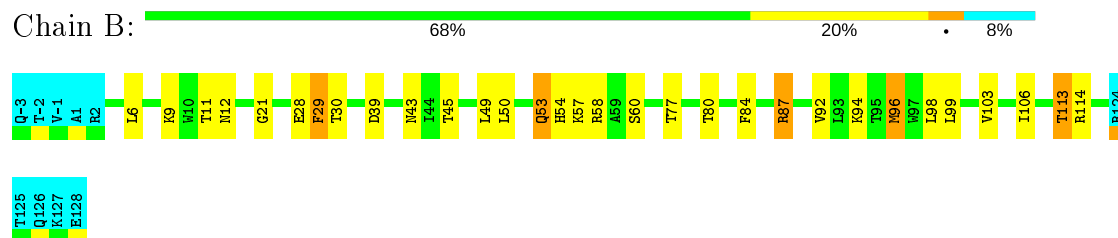
- Molecule 1: Avidin, Avidin-related protein 4/5

Chain D: 

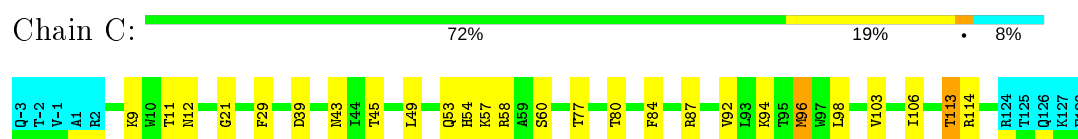


E128

- Molecule 1: Avidin, Avidin-related protein 4/5

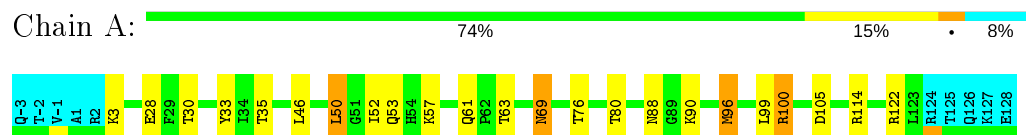


- Molecule 1: Avidin, Avidin-related protein 4/5

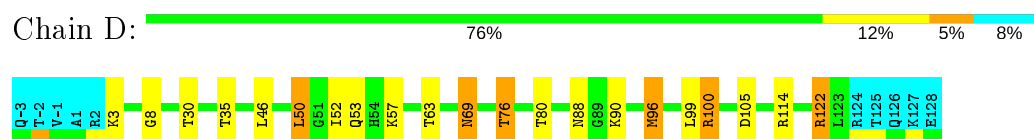


4.2.11 Score per residue for model 11

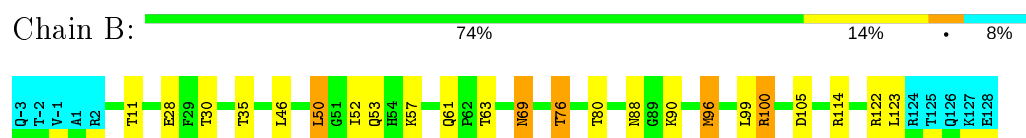
- Molecule 1: Avidin, Avidin-related protein 4/5



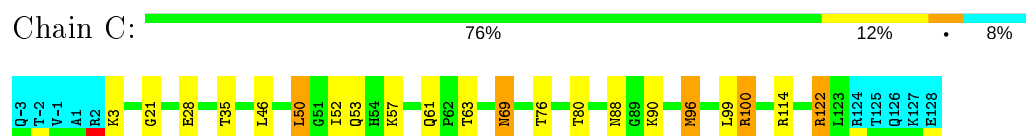
- Molecule 1: Avidin, Avidin-related protein 4/5



- Molecule 1: Avidin, Avidin-related protein 4/5

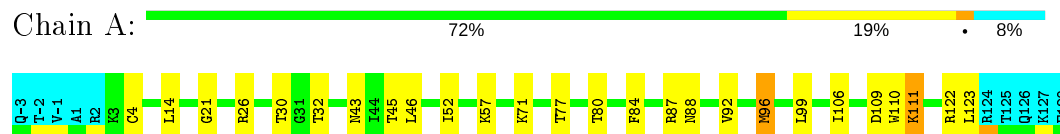


- Molecule 1: Avidin, Avidin-related protein 4/5

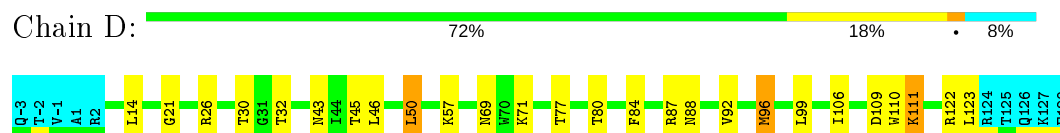


4.2.12 Score per residue for model 12

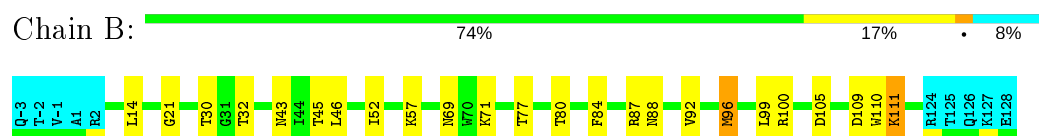
- Molecule 1: Avidin, Avidin-related protein 4/5



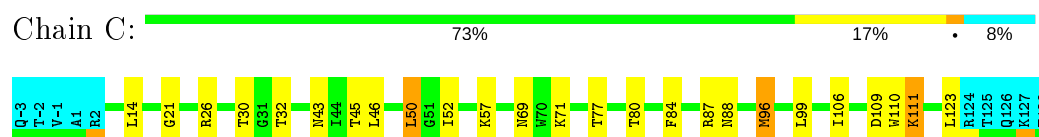
- Molecule 1: Avidin, Avidin-related protein 4/5



- Molecule 1: Avidin, Avidin-related protein 4/5

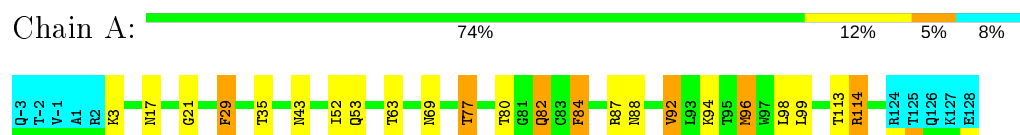


- Molecule 1: Avidin, Avidin-related protein 4/5

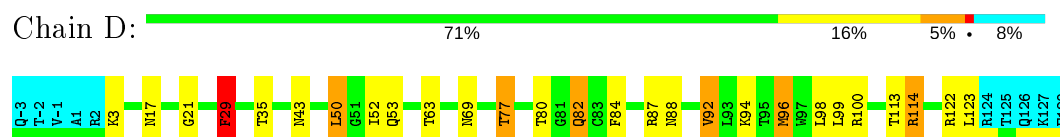


4.2.13 Score per residue for model 13

- Molecule 1: Avidin, Avidin-related protein 4/5

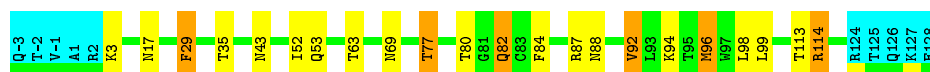


- Molecule 1: Avidin, Avidin-related protein 4/5



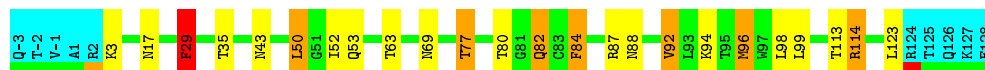
- Molecule 1: Avidin, Avidin-related protein 4/5





- Molecule 1: Avidin, Avidin-related protein 4/5

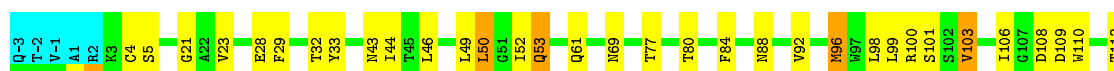
Chain C:



4.2.14 Score per residue for model 14

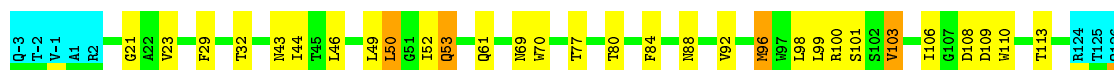
- Molecule 1: Avidin, Avidin-related protein 4/5

Chain A:



- Molecule 1: Avidin, Avidin-related protein 4/5

Chain D:



- Molecule 1: Avidin, Avidin-related protein 4/5

Chain B:



- Molecule 1: Avidin, Avidin-related protein 4/5

Chain C:





4.2.15 Score per residue for model 15

- Molecule 1: Avidin, Avidin-related protein 4/5

Chain A: 70% 19% 8%



- Molecule 1: Avidin, Avidin-related protein 4/5

Chain D: 68% 20% 8%



- Molecule 1: Avidin, Avidin-related protein 4/5

Chain B: 70% 19% 8%



- Molecule 1: Avidin, Avidin-related protein 4/5

Chain C: 68% 20% 8%



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 15 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
SPARKY	structure solution	
X-PLOR NIH	structure solution	
AMBER	refinement	
X-PLOR NIH	refinement	

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	1389
Number of shifts mapped to atoms	1389
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	19%

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	928	914	914	9±3
1	B	928	914	916	9±2
1	C	928	914	916	9±3
1	D	928	914	916	9±3
All	All	55680	54840	54930	410

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 4.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:LEU:HD12	1:D:50:LEU:HD12	0.72	1.62	3	4
1:B:50:LEU:HD12	1:C:50:LEU:HD12	0.72	1.61	3	4
1:D:77:THR:HG23	1:D:99:LEU:HD12	0.69	1.64	8	2
1:A:77:THR:HG23	1:A:99:LEU:HD12	0.69	1.64	8	2
1:B:77:THR:HG23	1:B:99:LEU:HD12	0.69	1.64	8	2
1:B:98:LEU:HD21	1:B:113:THR:CG2	0.68	2.18	14	8
1:A:98:LEU:HD21	1:A:113:THR:CG2	0.68	2.19	6	8
1:C:98:LEU:HD21	1:C:113:THR:CG2	0.68	2.18	2	8
1:D:98:LEU:HD21	1:D:113:THR:CG2	0.68	2.19	2	8
1:A:34:ILE:HD11	1:A:46:LEU:CD1	0.68	2.19	9	2
1:D:98:LEU:HD21	1:D:113:THR:HG23	0.67	1.66	13	6
1:D:34:ILE:HD11	1:D:46:LEU:CD1	0.67	2.19	9	1
1:C:77:THR:HG23	1:C:99:LEU:HD12	0.67	1.64	8	2
1:A:98:LEU:HD21	1:A:113:THR:HG23	0.67	1.66	13	6
1:B:98:LEU:HD21	1:B:113:THR:HG23	0.66	1.66	13	6
1:C:34:ILE:HD11	1:C:46:LEU:CD1	0.66	2.19	9	2
1:B:34:ILE:HD11	1:B:46:LEU:CD1	0.66	2.19	9	2
1:C:98:LEU:HD21	1:C:113:THR:HG23	0.65	1.67	13	6
1:B:94:LYS:HE2	1:C:106:ILE:HD11	0.64	1.70	6	3
1:B:106:ILE:HD11	1:C:94:LYS:HE2	0.63	1.69	6	3
1:A:94:LYS:HE2	1:D:106:ILE:HD11	0.62	1.71	6	3
1:A:106:ILE:HD11	1:D:94:LYS:HE2	0.62	1.69	6	3
1:B:103:VAL:HG11	1:B:108:ASP:HB3	0.62	1.72	14	1
1:A:103:VAL:HG11	1:A:108:ASP:HB3	0.60	1.73	14	1
1:B:35:THR:HG22	1:B:37:VAL:O	0.59	1.97	9	1
1:C:103:VAL:HG11	1:C:108:ASP:HB3	0.59	1.73	14	1
1:C:33:TYR:C	1:C:34:ILE:HD12	0.59	2.17	9	2
1:A:33:TYR:C	1:A:34:ILE:HD12	0.59	2.17	9	2
1:D:33:TYR:C	1:D:34:ILE:HD12	0.59	2.18	9	2
1:B:33:TYR:C	1:B:34:ILE:HD12	0.59	2.17	9	2
1:D:103:VAL:HG11	1:D:108:ASP:HB3	0.59	1.75	14	1
1:D:35:THR:HG22	1:D:37:VAL:O	0.59	1.97	9	1
1:A:35:THR:HG22	1:A:37:VAL:O	0.58	1.97	9	1
1:C:35:THR:HG22	1:C:37:VAL:O	0.58	1.99	9	1
1:A:110:TRP:CZ2	1:A:111:LYS:HE3	0.57	2.34	8	2
1:D:110:TRP:CZ2	1:D:111:LYS:HE3	0.57	2.34	8	2
1:B:110:TRP:CZ2	1:B:111:LYS:HE3	0.57	2.34	8	2
1:C:110:TRP:CZ2	1:C:111:LYS:HE3	0.57	2.34	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:69:ASN:HB2	1:C:52:ILE:HG21	0.56	1.77	6	9
1:D:34:ILE:HD11	1:D:46:LEU:HD12	0.56	1.77	5	2
1:A:34:ILE:HD11	1:A:46:LEU:HD12	0.55	1.77	5	2
1:C:92:VAL:HG11	1:C:94:LYS:HD3	0.55	1.79	13	1
1:A:69:ASN:HB2	1:D:52:ILE:HG21	0.55	1.78	6	8
1:B:11:THR:HB	1:B:123:LEU:HD13	0.55	1.77	11	1
1:B:34:ILE:HD11	1:B:46:LEU:HD12	0.55	1.77	5	2
1:B:52:ILE:HG21	1:C:69:ASN:HB2	0.55	1.79	6	10
1:A:52:ILE:HG21	1:D:69:ASN:HB2	0.54	1.79	6	10
1:B:32:THR:HB	1:B:46:LEU:HD11	0.54	1.80	14	5
1:C:34:ILE:HD11	1:C:46:LEU:HD12	0.54	1.77	5	2
1:D:92:VAL:HG11	1:D:94:LYS:HD3	0.54	1.78	13	1
1:A:123:LEU:HD23	1:A:123:LEU:C	0.54	2.23	8	3
1:B:6:LEU:HD21	1:B:64:PHE:CE2	0.53	2.38	7	2
1:B:92:VAL:HG11	1:B:94:LYS:HD3	0.53	1.79	13	1
1:A:32:THR:HB	1:A:46:LEU:HD11	0.53	1.81	14	5
1:A:92:VAL:HG11	1:A:94:LYS:HD3	0.53	1.79	13	1
1:D:98:LEU:HD21	1:D:113:THR:HG22	0.53	1.81	5	1
1:C:32:THR:HB	1:C:46:LEU:HD11	0.53	1.81	14	5
1:D:32:THR:HB	1:D:46:LEU:HD11	0.52	1.81	14	5
1:A:6:LEU:HD21	1:A:64:PHE:CE2	0.52	2.40	7	2
1:D:6:LEU:HD21	1:D:64:PHE:CE2	0.52	2.39	7	2
1:C:6:LEU:HD21	1:C:64:PHE:CE2	0.52	2.39	7	2
1:B:98:LEU:HD21	1:B:113:THR:HG22	0.52	1.81	5	2
1:D:103:VAL:CG2	1:D:112:ALA:HB2	0.51	2.36	1	1
1:B:103:VAL:CG2	1:B:112:ALA:HB2	0.51	2.35	1	1
1:A:103:VAL:CG2	1:A:112:ALA:HB2	0.51	2.36	1	1
1:C:4:CYS:HB2	1:C:83:CYS:HG	0.51	1.66	2	1
1:A:98:LEU:HD21	1:A:113:THR:HG22	0.50	1.82	5	1
1:D:123:LEU:HD23	1:D:123:LEU:C	0.50	2.26	15	2
1:C:103:VAL:CG2	1:C:112:ALA:HB2	0.50	2.35	1	1
1:D:34:ILE:HG13	1:D:46:LEU:HD12	0.49	1.84	1	1
1:D:110:TRP:CD1	1:B:14:LEU:HD11	0.49	2.42	12	4
1:B:4:CYS:HB2	1:B:83:CYS:HG	0.49	1.67	2	1
1:D:29:PHE:O	1:D:50:LEU:HD12	0.49	2.07	2	2
1:D:82:GLN:HB3	1:D:84:PHE:CE1	0.49	2.42	13	1
1:A:82:GLN:HB3	1:A:84:PHE:CE1	0.49	2.43	13	1
1:C:98:LEU:HD21	1:C:113:THR:HG22	0.49	1.81	5	1
1:B:106:ILE:HD11	1:C:94:LYS:CE	0.49	2.38	6	2
1:A:34:ILE:HG13	1:A:46:LEU:HD12	0.49	1.84	1	1
1:B:34:ILE:HG13	1:B:46:LEU:HD12	0.49	1.85	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:92:VAL:HG11	1:D:94:LYS:CD	0.49	2.38	15	5
1:C:82:GLN:HB3	1:C:84:PHE:CE1	0.49	2.42	13	1
1:C:29:PHE:O	1:C:50:LEU:HD12	0.48	2.08	2	2
1:C:34:ILE:HG13	1:C:46:LEU:HD12	0.48	1.84	1	1
1:A:69:ASN:CB	1:D:52:ILE:HG21	0.48	2.39	11	2
1:B:82:GLN:HB3	1:B:84:PHE:CE1	0.48	2.43	13	1
1:D:35:THR:O	1:D:44:ILE:HG21	0.48	2.09	2	3
1:A:92:VAL:HG11	1:A:94:LYS:CD	0.48	2.39	8	5
1:B:35:THR:O	1:B:44:ILE:HG21	0.47	2.08	2	3
1:B:113:THR:HG21	1:C:96:MET:HG3	0.47	1.86	3	2
1:C:23:VAL:HG21	1:C:53:GLN:HG3	0.47	1.85	6	2
1:B:96:MET:HG3	1:C:113:THR:HG21	0.47	1.86	3	2
1:A:23:VAL:HG21	1:A:53:GLN:HG3	0.47	1.87	14	2
1:B:69:ASN:CB	1:C:52:ILE:HG21	0.47	2.39	11	2
1:C:92:VAL:HG11	1:C:94:LYS:CD	0.47	2.39	15	5
1:B:92:VAL:HG11	1:B:94:LYS:CD	0.47	2.39	15	5
1:B:106:ILE:HD12	1:C:84:PHE:HB2	0.47	1.87	8	1
1:A:110:TRP:CD1	1:C:14:LEU:HD11	0.47	2.45	12	3
1:A:14:LEU:HD11	1:C:110:TRP:CD1	0.47	2.44	12	3
1:C:35:THR:O	1:C:44:ILE:HG21	0.47	2.10	2	3
1:B:52:ILE:HG21	1:C:69:ASN:CB	0.47	2.40	11	3
1:D:14:LEU:HD11	1:B:110:TRP:CD1	0.47	2.44	12	3
1:C:82:GLN:HB3	1:C:84:PHE:CZ	0.46	2.45	13	3
1:A:94:LYS:CE	1:D:106:ILE:HD11	0.46	2.39	6	2
1:A:52:ILE:HG21	1:D:69:ASN:CB	0.46	2.41	11	2
1:A:35:THR:O	1:A:44:ILE:HG21	0.46	2.11	2	3
1:B:84:PHE:HB2	1:C:106:ILE:HD12	0.46	1.87	8	2
1:B:94:LYS:CE	1:C:106:ILE:HD11	0.46	2.40	6	3
1:D:82:GLN:HB3	1:D:84:PHE:CZ	0.46	2.45	13	3
1:B:82:GLN:HB3	1:B:84:PHE:CZ	0.46	2.46	5	3
1:A:106:ILE:HD11	1:D:94:LYS:CE	0.46	2.38	6	2
1:A:106:ILE:HD12	1:D:84:PHE:HB2	0.46	1.87	8	1
1:A:113:THR:HG21	1:D:96:MET:HG3	0.46	1.86	3	2
1:A:82:GLN:HB3	1:A:84:PHE:CZ	0.46	2.46	5	2
1:B:23:VAL:HG21	1:B:53:GLN:HG3	0.46	1.87	14	2
1:A:96:MET:HG3	1:D:113:THR:HG21	0.46	1.86	3	2
1:A:34:ILE:HD11	1:A:46:LEU:HD11	0.45	1.86	9	1
1:A:84:PHE:HB2	1:D:106:ILE:HD12	0.45	1.88	8	1
1:B:96:MET:SD	1:C:113:THR:HG21	0.45	2.51	5	1
1:A:96:MET:SD	1:D:113:THR:HG21	0.45	2.51	5	1
1:D:123:LEU:C	1:D:123:LEU:HD23	0.45	2.32	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:34:ILE:HD11	1:D:46:LEU:HD11	0.45	1.86	9	1
1:C:14:LEU:HD22	1:C:118:ASN:HD21	0.45	1.72	4	1
1:B:4:CYS:CB	1:B:83:CYS:HG	0.45	2.25	9	3
1:B:113:THR:HG21	1:C:96:MET:SD	0.45	2.51	5	1
1:D:14:LEU:HD22	1:D:118:ASN:HD21	0.45	1.72	4	1
1:D:4:CYS:HB2	1:D:83:CYS:HG	0.45	1.71	2	1
1:B:106:ILE:CD1	1:C:92:VAL:HG21	0.44	2.43	10	3
1:B:34:ILE:HD11	1:B:46:LEU:HD11	0.44	1.87	9	1
1:C:34:ILE:HD11	1:C:46:LEU:HD11	0.44	1.87	9	1
1:B:92:VAL:HG21	1:C:106:ILE:CD1	0.44	2.43	10	4
1:D:23:VAL:HG21	1:D:53:GLN:HG3	0.44	1.87	6	2
1:C:4:CYS:SG	1:C:83:CYS:SG	0.44	3.16	15	1
1:C:30:THR:HG22	1:C:50:LEU:CD1	0.44	2.42	4	2
1:C:4:CYS:CB	1:C:83:CYS:HG	0.44	2.25	2	2
1:D:30:THR:HG22	1:D:50:LEU:CD1	0.44	2.42	4	2
1:C:108:ASP:HA	1:C:110:TRP:CD1	0.44	2.48	14	1
1:B:4:CYS:SG	1:B:83:CYS:SG	0.44	3.16	15	1
1:A:82:GLN:NE2	1:D:103:VAL:H	0.43	2.11	8	1
1:B:52:ILE:HG21	1:C:69:ASN:HB3	0.43	1.90	11	1
1:B:108:ASP:HA	1:B:110:TRP:CD1	0.43	2.49	14	1
1:A:52:ILE:CG2	1:D:69:ASN:HD22	0.43	2.27	6	1
1:B:69:ASN:HD22	1:C:52:ILE:CG2	0.43	2.26	6	1
1:D:49:LEU:C	1:D:49:LEU:HD12	0.43	2.34	6	1
1:D:11:THR:HB	1:D:123:LEU:HD12	0.43	1.90	1	1
1:A:113:THR:HG21	1:D:96:MET:SD	0.43	2.53	5	1
1:C:92:VAL:CG1	1:C:94:LYS:HD3	0.43	2.44	13	1
1:A:106:ILE:CD1	1:D:92:VAL:HG21	0.43	2.43	10	4
1:D:108:ASP:HA	1:D:110:TRP:CD1	0.43	2.48	14	1
1:A:92:VAL:CG1	1:A:94:LYS:HD3	0.43	2.44	13	1
1:D:12:ASN:HD22	1:D:14:LEU:H	0.43	1.57	1	1
1:A:108:ASP:HA	1:A:110:TRP:CD1	0.43	2.48	14	1
1:C:49:LEU:HD12	1:C:49:LEU:C	0.43	2.34	6	1
1:D:123:LEU:CD2	1:D:123:LEU:C	0.42	2.87	12	1
1:B:14:LEU:HD22	1:B:118:ASN:HD21	0.42	1.73	4	1
1:C:34:ILE:N	1:C:34:ILE:HD12	0.42	2.30	9	2
1:A:6:LEU:HD12	1:A:53:GLN:CD	0.42	2.34	10	1
1:D:123:LEU:C	1:D:123:LEU:CD2	0.42	2.87	5	1
1:B:52:ILE:CG2	1:C:69:ASN:HD22	0.42	2.27	6	1
1:B:82:GLN:NE2	1:C:103:VAL:H	0.42	2.12	8	1
1:A:52:ILE:HG21	1:D:69:ASN:HB3	0.42	1.91	11	1
1:B:92:VAL:CG1	1:B:94:LYS:HD3	0.42	2.44	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:34:ILE:HD12	1:B:34:ILE:N	0.42	2.30	9	1
1:A:92:VAL:HG21	1:D:106:ILE:CD1	0.42	2.45	5	6
1:D:34:ILE:HD12	1:D:34:ILE:N	0.42	2.29	9	1
1:A:123:LEU:C	1:A:123:LEU:HD23	0.42	2.35	15	2
1:A:69:ASN:HB3	1:D:52:ILE:HG21	0.42	1.92	11	1
1:C:82:GLN:CB	1:C:84:PHE:CZ	0.42	3.03	8	1
1:D:92:VAL:CG1	1:D:94:LYS:HD3	0.41	2.43	13	1
1:D:4:CYS:CB	1:D:83:CYS:HG	0.41	2.27	7	1
1:A:123:LEU:CD2	1:A:123:LEU:C	0.41	2.88	8	1
1:D:82:GLN:CB	1:D:84:PHE:CZ	0.41	3.03	8	1
1:B:82:GLN:CB	1:B:84:PHE:CZ	0.41	3.03	8	1
1:D:90:LYS:HB3	1:D:90:LYS:NZ	0.41	2.31	4	1
1:A:82:GLN:CB	1:A:84:PHE:CZ	0.41	3.04	8	1
1:B:6:LEU:HD12	1:B:53:GLN:CD	0.41	2.36	10	1
1:A:52:ILE:HG21	1:D:69:ASN:HD22	0.41	1.76	6	1
1:B:69:ASN:HB3	1:C:52:ILE:HG21	0.41	1.92	11	1
1:C:12:ASN:HD22	1:C:14:LEU:H	0.41	1.59	1	1
1:A:64:PHE:CZ	1:A:83:CYS:HB2	0.41	2.51	1	1
1:A:12:ASN:HD22	1:A:14:LEU:H	0.41	1.58	1	1
1:A:34:ILE:N	1:A:34:ILE:HD12	0.41	2.30	1	2
1:B:34:ILE:N	1:B:34:ILE:HD12	0.41	2.30	1	1
1:D:34:ILE:N	1:D:34:ILE:HD12	0.41	2.30	1	1
1:A:69:ASN:HD22	1:D:52:ILE:CG2	0.41	2.29	6	1
1:A:14:LEU:HD22	1:A:118:ASN:HD21	0.41	1.75	4	1
1:D:6:LEU:HD12	1:D:53:GLN:CD	0.41	2.36	10	1
1:A:52:ILE:HD11	1:D:50:LEU:HB2	0.40	1.93	1	1
1:B:103:VAL:H	1:C:82:GLN:NE2	0.40	2.13	8	1
1:A:77:THR:HG23	1:A:99:LEU:CD1	0.40	2.44	13	1
1:C:77:THR:HG23	1:C:99:LEU:CD1	0.40	2.44	13	1

5.2 Torsion angles ⓘ

5.2.1 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	119/129 (92%)	111±2 (93±2%)	6±2 (5±2%)	2±1 (2±1%)	13	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	119/129 (92%)	111±2 (94±2%)	6±2 (5±1%)	2±1 (2±1%)	13	56
1	C	119/129 (92%)	111±2 (93±2%)	6±2 (5±2%)	2±1 (2±1%)	11	53
1	D	119/129 (92%)	111±2 (93±2%)	6±2 (5±2%)	2±1 (2±1%)	11	52
All	All	7140/7740 (92%)	6665 (93%)	345 (5%)	130 (2%)	12	54

All 36 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	C	21	GLY	8
1	C	43	ASN	8
1	B	43	ASN	8
1	A	43	ASN	8
1	D	43	ASN	8
1	D	21	GLY	7
1	A	44	ILE	6
1	C	44	ILE	6
1	A	21	GLY	6
1	B	44	ILE	6
1	D	44	ILE	6
1	D	103	VAL	5
1	B	21	GLY	5
1	A	103	VAL	5
1	C	103	VAL	5
1	B	103	VAL	5
1	D	87	ARG	2
1	C	87	ARG	2
1	D	57	LYS	2
1	D	9	LYS	2
1	C	57	LYS	2
1	B	87	ARG	2
1	B	57	LYS	2
1	A	57	LYS	2
1	D	41	PRO	1
1	C	42	GLY	1
1	C	9	LYS	1
1	D	42	GLY	1
1	A	42	GLY	1
1	B	42	GLY	1
1	D	8	GLY	1
1	A	41	PRO	1

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Mol	Chain	Res	Type	Models (Total)
1	B	41	PRO	1
1	B	9	LYS	1
1	C	41	PRO	1
1	A	9	LYS	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	102/111 (92%)	87±3 (85±3%)	15±3 (15±3%)	6	44
1	B	102/111 (92%)	87±3 (85±3%)	15±3 (15±3%)	6	45
1	C	102/111 (92%)	87±3 (86±3%)	15±3 (14±3%)	6	45
1	D	102/111 (92%)	87±3 (86±3%)	15±3 (14±3%)	6	45
All	All	6120/6660 (92%)	5225 (85%)	895 (15%)	6	45

All 241 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	D	80	THR	15
1	B	80	THR	15
1	C	80	THR	15
1	A	80	THR	15
1	B	99	LEU	13
1	A	99	LEU	13
1	D	99	LEU	13
1	B	53	GLN	12
1	D	45	THR	12
1	D	53	GLN	12
1	C	53	GLN	12
1	A	45	THR	12
1	C	99	LEU	12
1	A	53	GLN	12
1	B	45	THR	12
1	C	45	THR	12
1	D	96	MET	10

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Mol	Chain	Res	Type	Models (Total)
1	C	96	MET	10
1	A	96	MET	10
1	B	96	MET	10
1	A	4	CYS	9
1	C	88	ASN	8
1	D	88	ASN	8
1	B	88	ASN	8
1	D	50	LEU	7
1	A	88	ASN	7
1	D	105	ASP	7
1	C	50	LEU	7
1	D	63	THR	6
1	B	50	LEU	6
1	D	29	PHE	6
1	B	63	THR	6
1	D	109	ASP	6
1	B	105	ASP	6
1	A	109	ASP	6
1	A	63	THR	6
1	A	50	LEU	6
1	C	63	THR	6
1	B	109	ASP	6
1	C	109	ASP	6
1	C	29	PHE	6
1	D	30	THR	5
1	B	30	THR	5
1	D	87	ARG	5
1	C	43	ASN	5
1	A	43	ASN	5
1	B	29	PHE	5
1	A	105	ASP	5
1	D	122	ARG	5
1	D	123	LEU	5
1	B	122	ARG	5
1	B	43	ASN	5
1	B	87	ARG	5
1	A	30	THR	5
1	D	77	THR	5
1	C	87	ARG	5
1	B	90	LYS	5
1	D	3	LYS	5
1	C	3	LYS	5

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Mol	Chain	Res	Type	Models (Total)
1	A	87	ARG	5
1	A	29	PHE	5
1	C	90	LYS	5
1	A	3	LYS	5
1	D	43	ASN	5
1	D	17	ASN	4
1	B	98	LEU	4
1	B	77	THR	4
1	B	57	LYS	4
1	B	49	LEU	4
1	C	98	LEU	4
1	D	98	LEU	4
1	D	90	LYS	4
1	A	5	SER	4
1	C	57	LYS	4
1	A	98	LEU	4
1	D	49	LEU	4
1	B	28	GLU	4
1	A	122	ARG	4
1	A	57	LYS	4
1	B	3	LYS	4
1	A	49	LEU	4
1	A	90	LYS	4
1	A	17	ASN	4
1	C	49	LEU	4
1	A	61	GLN	4
1	B	61	GLN	4
1	C	30	THR	4
1	C	77	THR	4
1	C	17	ASN	4
1	B	17	ASN	4
1	A	28	GLU	4
1	C	61	GLN	4
1	C	123	LEU	4
1	D	57	LYS	4
1	C	122	ARG	4
1	C	105	ASP	4
1	A	77	THR	4
1	D	103	VAL	3
1	A	82	GLN	3
1	A	16	SER	3
1	B	5	SER	3

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Mol	Chain	Res	Type	Models (Total)
1	D	84	PHE	3
1	A	111	LYS	3
1	C	46	LEU	3
1	A	104	ASN	3
1	C	16	SER	3
1	B	64	PHE	3
1	A	46	LEU	3
1	D	82	GLN	3
1	C	111	LYS	3
1	B	16	SER	3
1	C	84	PHE	3
1	A	101	SER	3
1	C	101	SER	3
1	D	64	PHE	3
1	C	94	LYS	3
1	B	111	LYS	3
1	D	46	LEU	3
1	D	16	SER	3
1	B	101	SER	3
1	A	84	PHE	3
1	C	64	PHE	3
1	D	111	LYS	3
1	D	101	SER	3
1	C	104	ASN	3
1	B	94	LYS	3
1	A	103	VAL	3
1	B	46	LEU	3
1	B	82	GLN	3
1	A	123	LEU	3
1	A	64	PHE	3
1	C	103	VAL	3
1	B	84	PHE	3
1	C	82	GLN	3
1	B	103	VAL	3
1	A	12	ASN	2
1	B	39	ASP	2
1	C	108	ASP	2
1	A	100	ARG	2
1	C	60	SER	2
1	D	60	SER	2
1	D	39	ASP	2
1	C	11	THR	2

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Mol	Chain	Res	Type	Models (Total)
1	B	9	LYS	2
1	C	71	LYS	2
1	D	5	SER	2
1	A	9	LYS	2
1	B	108	ASP	2
1	D	35	THR	2
1	B	11	THR	2
1	D	9	LYS	2
1	D	100	ARG	2
1	A	94	LYS	2
1	D	12	ASN	2
1	C	100	ARG	2
1	C	35	THR	2
1	C	12	ASN	2
1	B	12	ASN	2
1	B	4	CYS	2
1	D	94	LYS	2
1	B	71	LYS	2
1	A	39	ASP	2
1	C	5	SER	2
1	C	4	CYS	2
1	B	100	ARG	2
1	A	60	SER	2
1	D	4	CYS	2
1	C	39	ASP	2
1	B	35	THR	2
1	D	104	ASN	2
1	B	60	SER	2
1	D	61	GLN	2
1	A	35	THR	2
1	D	71	LYS	2
1	B	123	LEU	2
1	B	104	ASN	2
1	A	71	LYS	2
1	D	69	ASN	1
1	B	86	ASP	1
1	A	108	ASP	1
1	B	73	SER	1
1	C	18	MET	1
1	B	54	HIS	1
1	C	26	ARG	1
1	A	25	SER	1

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Mol	Chain	Res	Type	Models (Total)
1	C	120	PHE	1
1	C	83	CYS	1
1	B	83	CYS	1
1	A	11	THR	1
1	A	58	ARG	1
1	C	114	ARG	1
1	D	114	ARG	1
1	C	9	LYS	1
1	C	95	THR	1
1	B	25	SER	1
1	B	26	ARG	1
1	C	54	HIS	1
1	D	18	MET	1
1	B	13	ASP	1
1	A	114	ARG	1
1	C	118	ASN	1
1	B	18	MET	1
1	D	54	HIS	1
1	A	24	ASN	1
1	D	118	ASN	1
1	D	117	TYR	1
1	C	86	ASP	1
1	B	69	ASN	1
1	B	117	TYR	1
1	D	58	ARG	1
1	C	117	TYR	1
1	C	13	ASP	1
1	A	54	HIS	1
1	A	69	ASN	1
1	D	83	CYS	1
1	B	76	THR	1
1	A	13	ASP	1
1	A	86	ASP	1
1	D	108	ASP	1
1	C	76	THR	1
1	A	73	SER	1
1	A	120	PHE	1
1	C	58	ARG	1
1	C	69	ASN	1
1	B	114	ARG	1
1	D	25	SER	1
1	D	120	PHE	1

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Mol	Chain	Res	Type	Models (Total)
1	C	25	SER	1
1	D	76	THR	1
1	D	86	ASP	1
1	A	118	ASN	1
1	B	58	ARG	1
1	A	117	TYR	1
1	C	28	GLU	1
1	A	26	ARG	1
1	D	13	ASP	1
1	D	26	ARG	1
1	B	118	ASN	1
1	B	120	PHE	1
1	A	76	THR	1
1	A	18	MET	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 19% for the well-defined parts and 19% 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	1389
Number of shifts mapped to atoms	1389
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	12

6.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	127	-0.40 ± 0.05	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	111	-1.35 ± 0.18	Should be applied
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	116	1.07 ± 0.34	Should be applied

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 19%, i.e. 1114 atoms were assigned a chemical shift out of a possible 5736. 15 out of 64 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	456/2356 (19%)	228/940 (24%)	118/952 (12%)	110/464 (24%)
Sidechain	537/2844 (19%)	335/1656 (20%)	202/1040 (19%)	0/148 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	121/536 (23%)	66/284 (23%)	51/232 (22%)	4/20 (20%)
Overall	1114/5736 (19%)	629/2880 (22%)	371/2224 (17%)	114/632 (18%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 19%, i.e. 1193 atoms were assigned a chemical shift out of a possible 6304. 16 out of 68 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	486/2556 (19%)	243/1020 (24%)	127/1032 (12%)	116/504 (23%)
Sidechain	586/3212 (18%)	367/1872 (20%)	219/1156 (19%)	0/184 (0%)
Aromatic	121/536 (23%)	66/284 (23%)	51/232 (22%)	4/20 (20%)
Overall	1193/6304 (19%)	676/3176 (21%)	397/2420 (16%)	120/708 (17%)

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	111	LYS	HB3	-0.72	3.10 – 0.40	-9.1
1	A	93	LEU	HD21	-1.18	2.14 – -0.66	-6.9
1	A	93	LEU	HD22	-1.18	2.14 – -0.66	-6.9
1	A	93	LEU	HD23	-1.18	2.14 – -0.66	-6.9
1	A	68	VAL	HG21	-0.90	2.20 – -0.60	-6.1
1	A	68	VAL	HG22	-0.90	2.20 – -0.60	-6.1
1	A	68	VAL	HG23	-0.90	2.20 – -0.60	-6.1
1	A	118	ASN	CB	48.78	47.13 – 30.23	6.0
1	A	37	VAL	HG21	-0.78	2.20 – -0.60	-5.6
1	A	37	VAL	HG22	-0.78	2.20 – -0.60	-5.6
1	A	37	VAL	HG23	-0.78	2.20 – -0.60	-5.6
1	A	12	ASN	HB3	1.03	4.41 – 1.11	-5.2

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:

