



Full wwPDB NMR Structure Validation Report ⓘ

Feb 20, 2018 – 05:25 am GMT

PDB ID : 1A6X
Title : STRUCTURE OF THE APO-BIOTIN CARBOXYL CARRIER PROTEIN (APO-BCCP87) OF ESCHERICHIA COLI ACETYL-COA CARBOXYLASE, NMR, 49 STRUCTURES
Authors : Yao, X.; Wei, D.; Soden Junior, C.; Summers, M.F.; Beckett, D.
Deposited on : 1998-03-04

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 : 20171227.v01 (using entries in the PDB archive December 27th 2017)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk30686
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

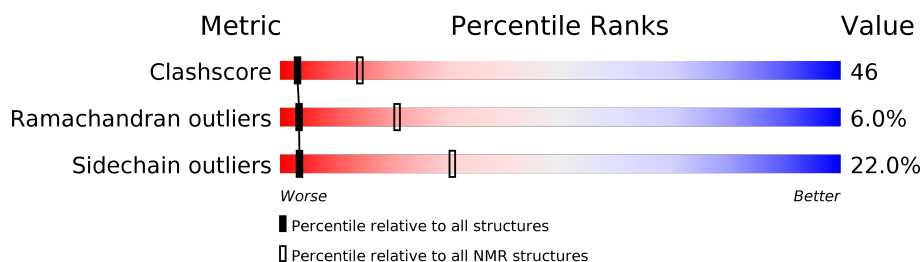
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	136279	12091
Ramachandran outliers	132675	10835
Sidechain outliers	132484	10811

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	87	

2 Ensemble composition and analysis

This entry contains 49 models. Model 12 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:81-A:156 (76)	0.27	12

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 9 clusters and 4 single-model clusters were found.

Cluster number	Models
1	2, 4, 7, 10, 12, 17, 20, 21, 24, 30, 31, 32, 39, 41, 44, 49
2	6, 14, 19, 29, 33, 38, 42
3	15, 18, 22, 27, 28, 34, 43
4	1, 11, 13, 23
5	8, 35, 40
6	46, 48
7	3, 9
8	5, 37
9	25, 45
Single-model clusters	16; 26; 36; 47

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1206 atoms, of which 556 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXYLASE.

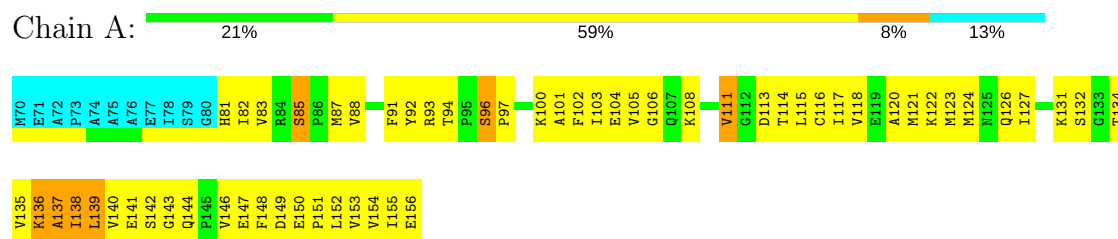
Mol	Chain	Residues	Atoms						Trace
1	A	87	Total	C	H	N	O	S	0
			1206	411	556	105	128	6	

4 Residue-property plots [i](#)

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: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE

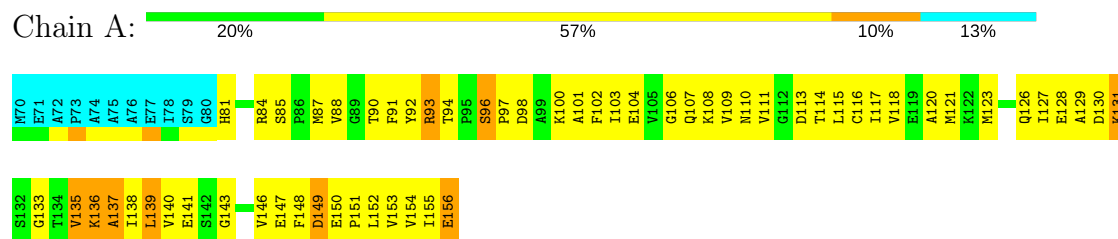


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

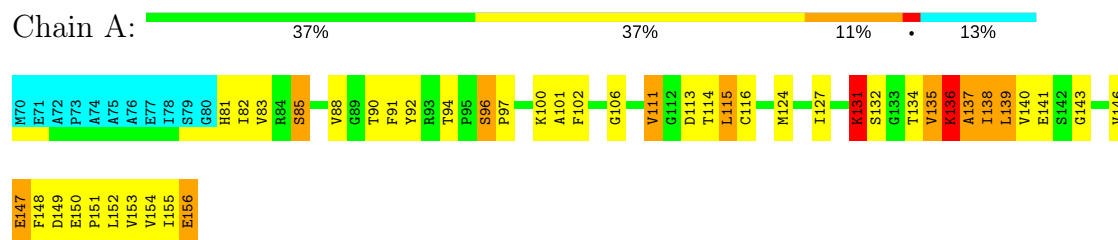
4.2.1 Score per residue for model 1

- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE



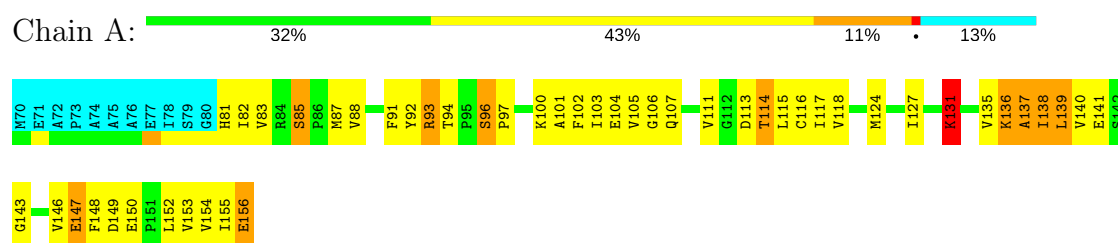
4.2.2 Score per residue for model 2

- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE



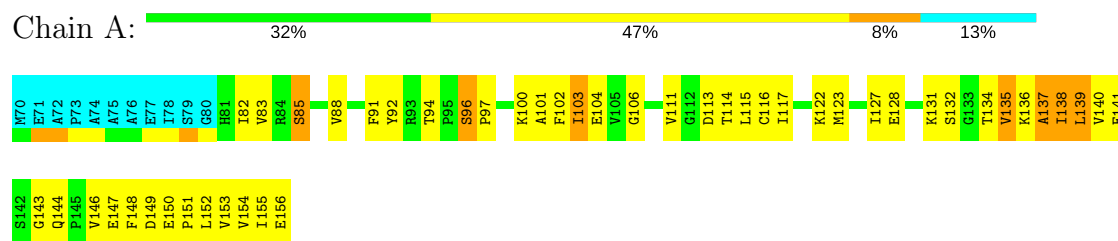
4.2.3 Score per residue for model 3

- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE



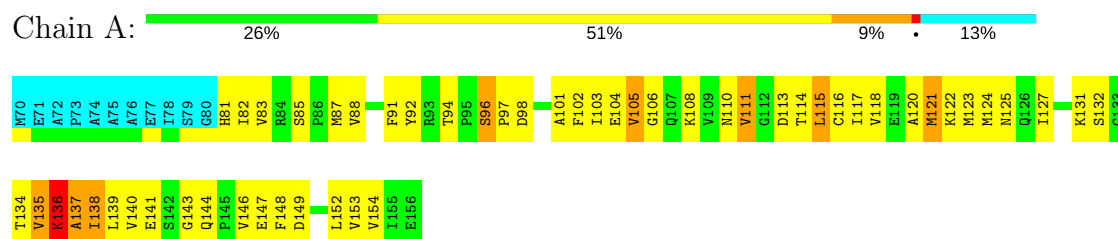
4.2.4 Score per residue for model 4

- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE



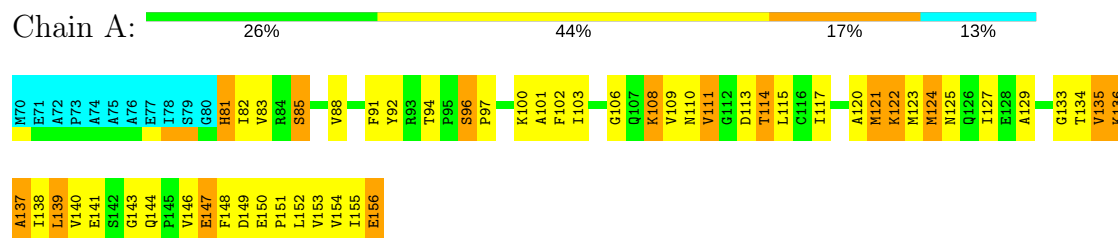
4.2.5 Score per residue for model 5

- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE



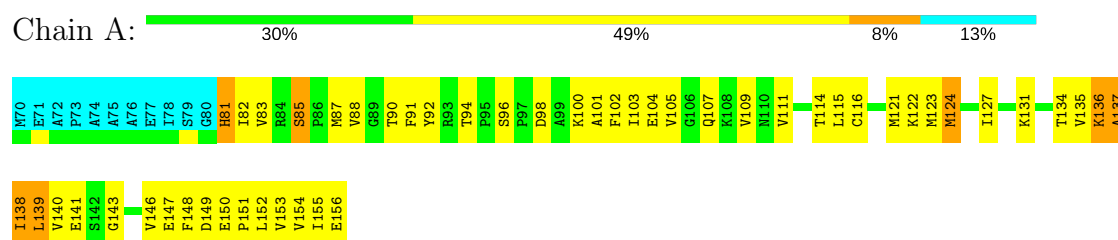
4.2.6 Score per residue for model 6

- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE



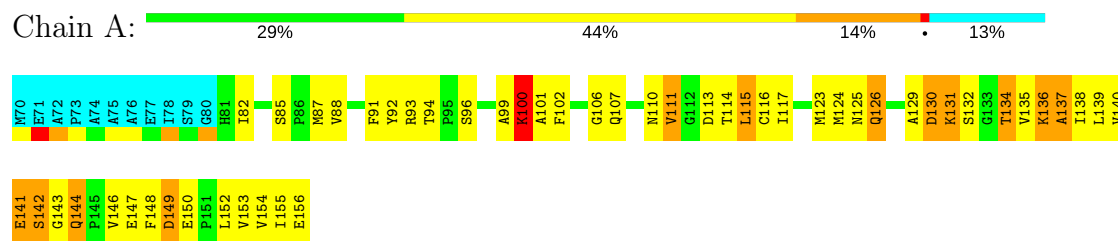
4.2.7 Score per residue for model 7

- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE



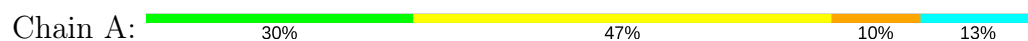
4.2.8 Score per residue for model 8

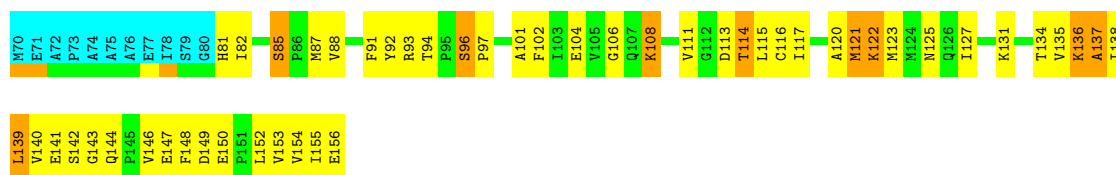
- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE



4.2.9 Score per residue for model 9

- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE

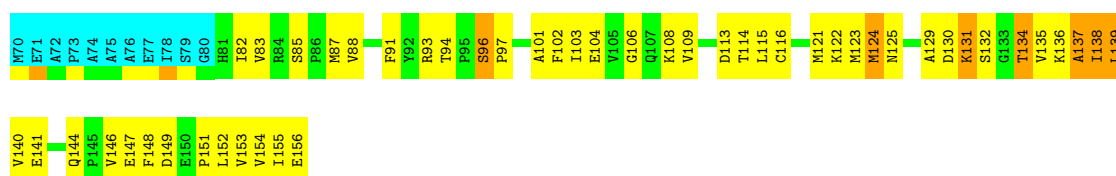




4.2.10 Score per residue for model 10

- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE

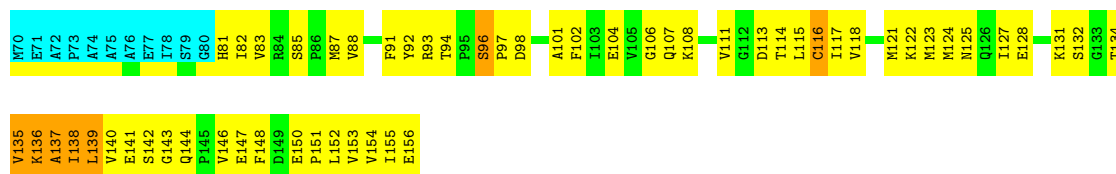
Chain A: 31% 48% 8% 13%



4.2.11 Score per residue for model 11

- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE

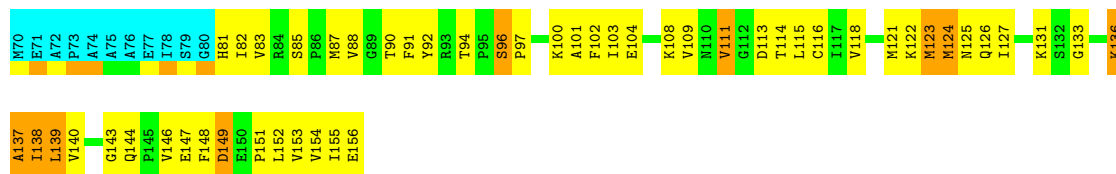
Chain A: 23% 56% 8% 13%



4.2.12 Score per residue for model 12 (medoid)

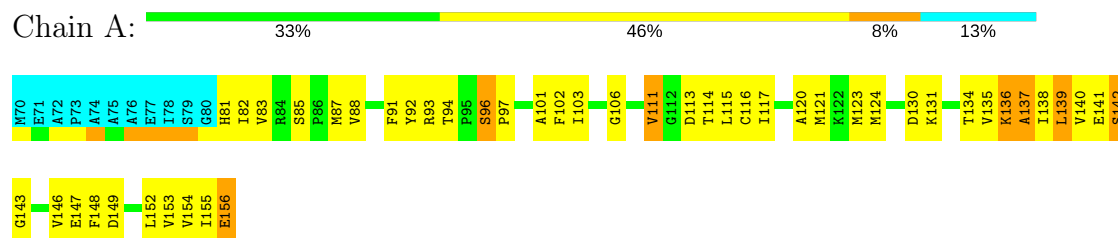
- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE

Chain A: 29% 48% 10% 13%



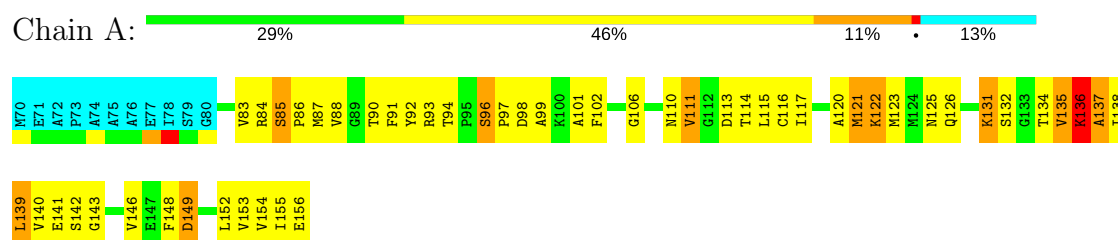
4.2.13 Score per residue for model 13

- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE



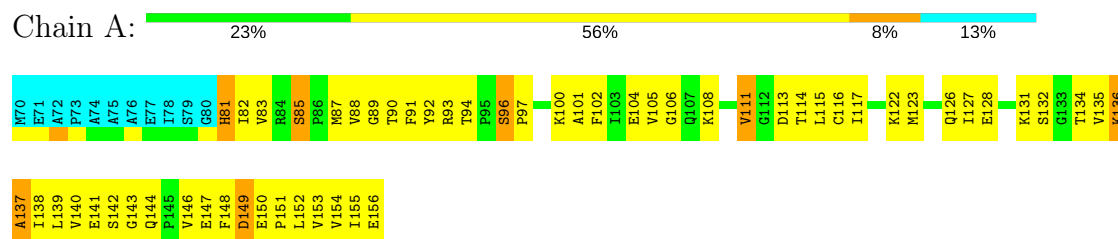
4.2.14 Score per residue for model 14

- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE



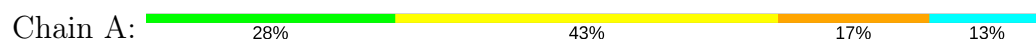
4.2.15 Score per residue for model 15

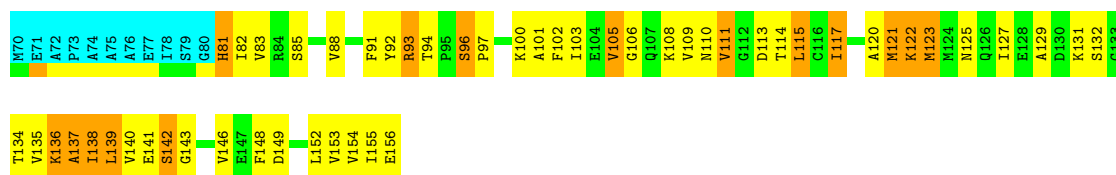
- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE



4.2.16 Score per residue for model 16

- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE

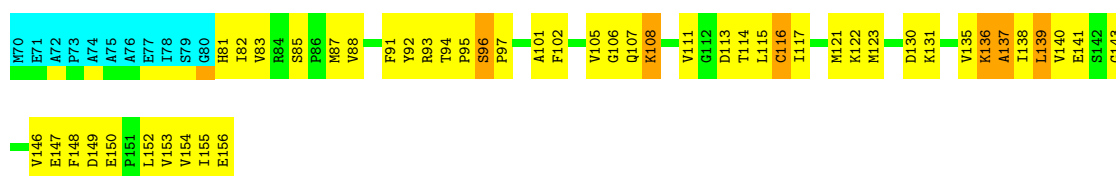




4.2.17 Score per residue for model 17

- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE

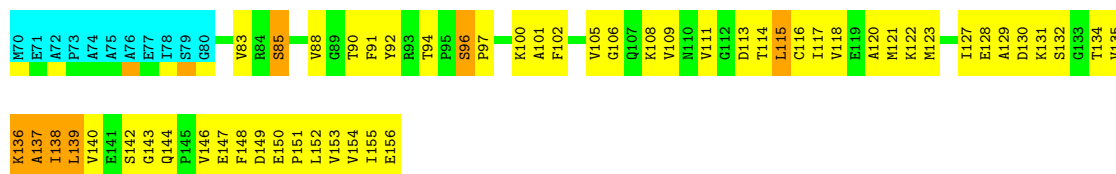
Chain A: 32% 48% 7% 13%



4.2.18 Score per residue for model 18

- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE

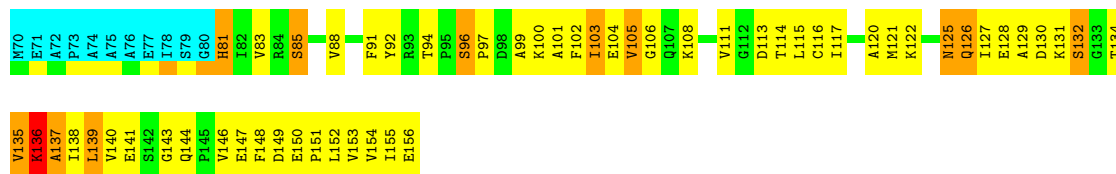
Chain A: 25% 54% 8% 13%



4.2.19 Score per residue for model 19

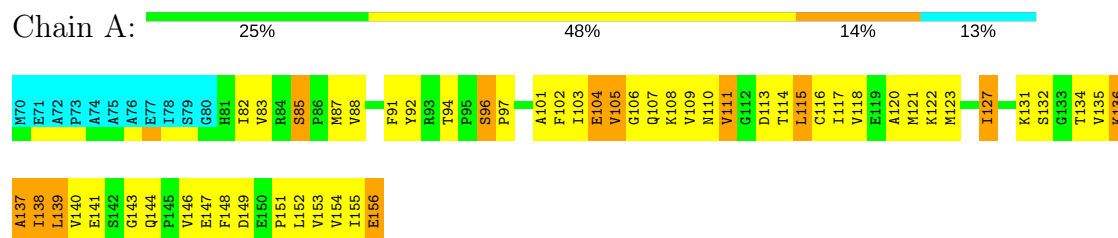
- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE

Chain A: 23% 51% 13% 13%



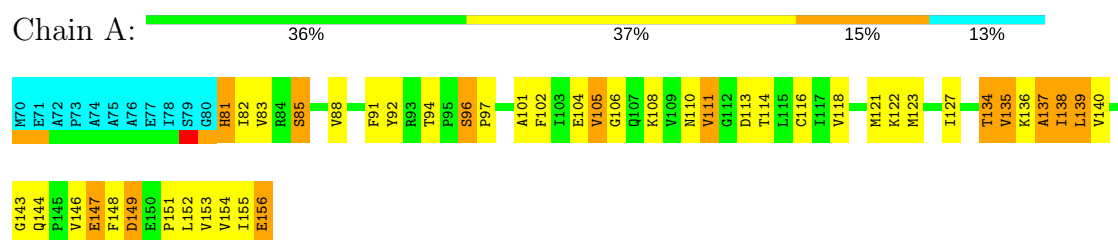
4.2.20 Score per residue for model 20

- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE



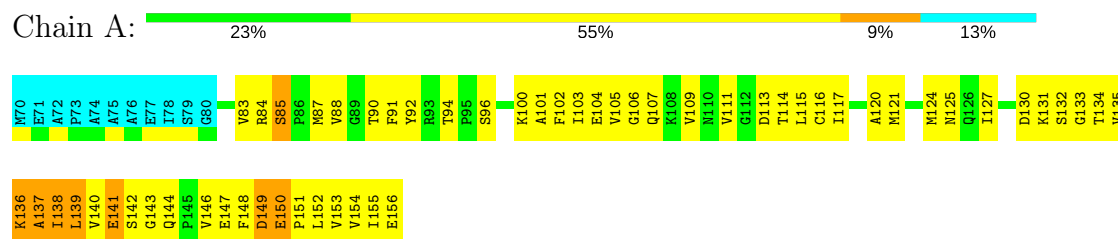
4.2.21 Score per residue for model 21

- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE



4.2.22 Score per residue for model 22

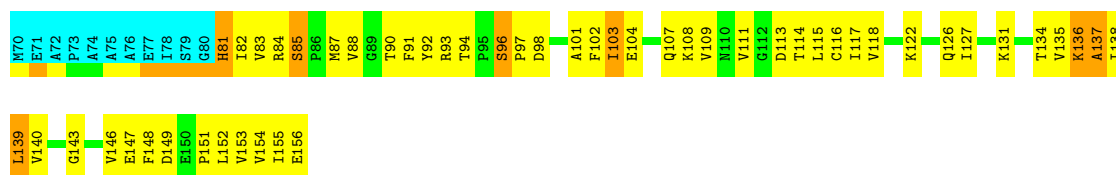
- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE



4.2.23 Score per residue for model 23

- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE

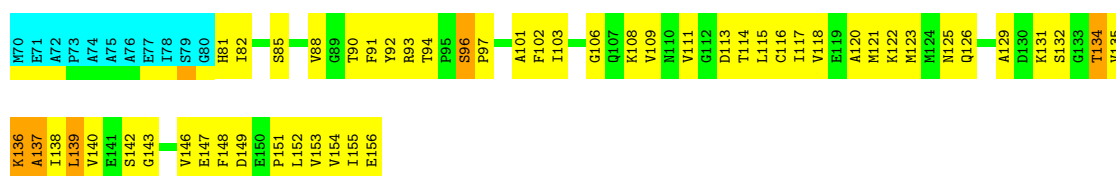




4.2.24 Score per residue for model 24

- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE

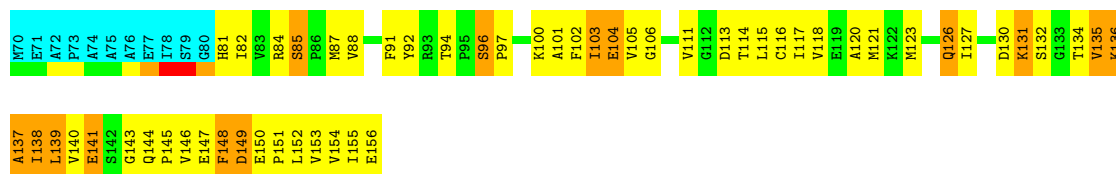
Chain A: 28% 54% 6% 13%



4.2.25 Score per residue for model 25

- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE

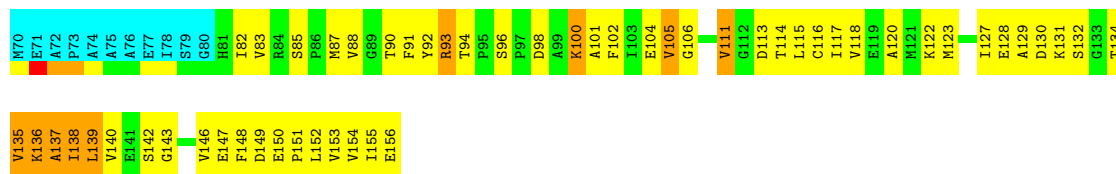
Chain A: 24% 47% 16% 13%



4.2.26 Score per residue for model 26

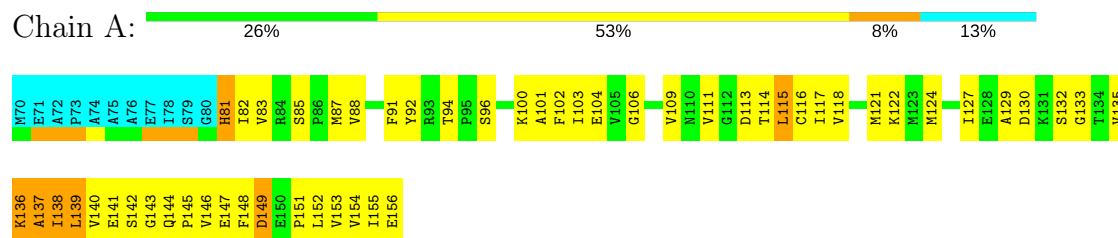
- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE

Chain A: 25% 52% 10% 13%



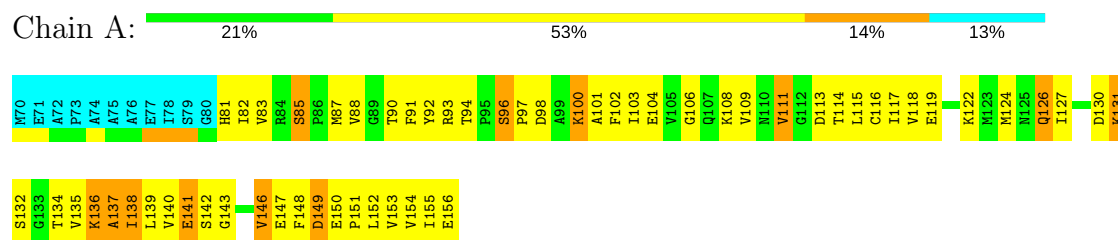
4.2.27 Score per residue for model 27

- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE



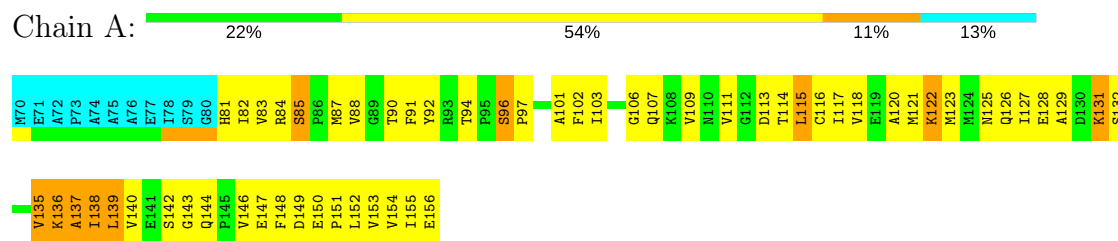
4.2.28 Score per residue for model 28

- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE



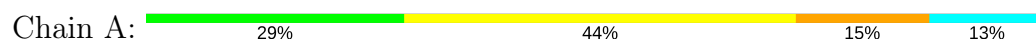
4.2.29 Score per residue for model 29

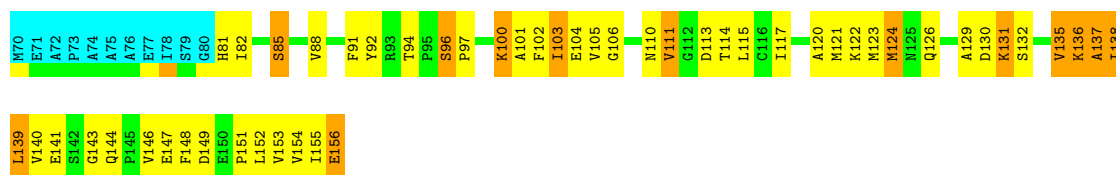
- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE



4.2.30 Score per residue for model 30

- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE

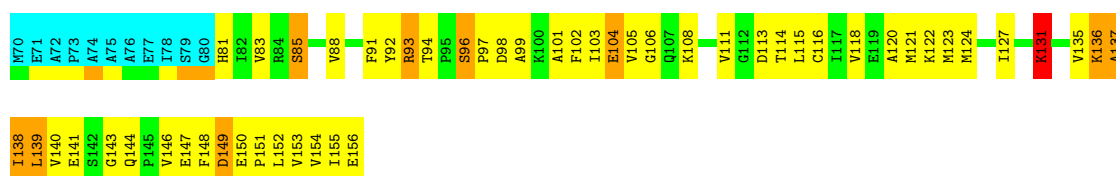




4.2.31 Score per residue for model 31

- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE

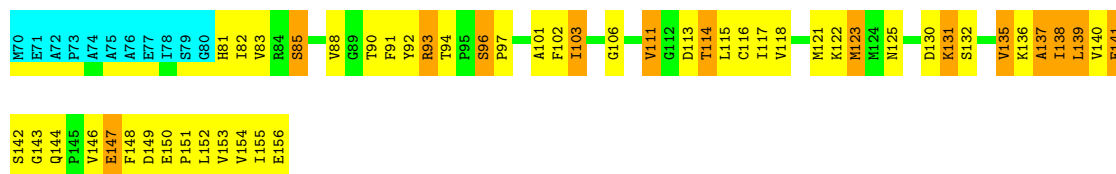
Chain A: 28% 48% 10% 13%



4.2.32 Score per residue for model 32

- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE

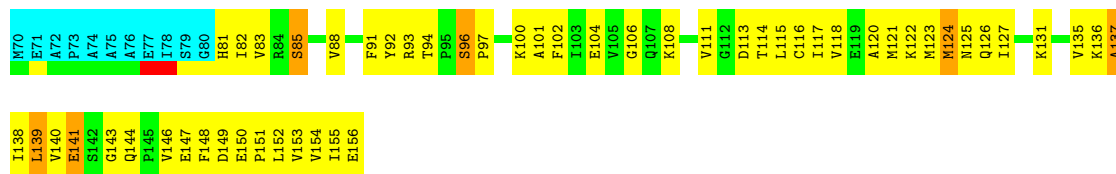
Chain A: 29% 43% 16% 13%



4.2.33 Score per residue for model 33

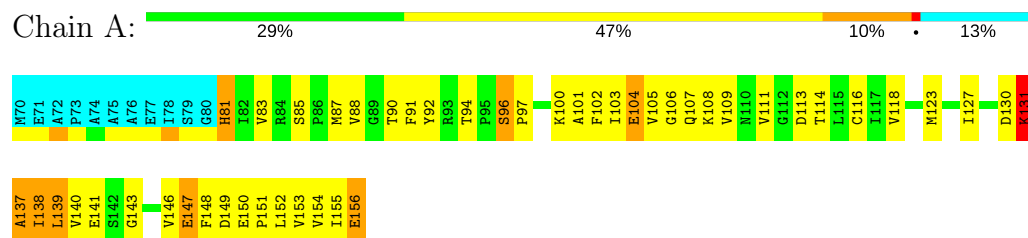
- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE

Chain A: 26% 54% 7% 13%



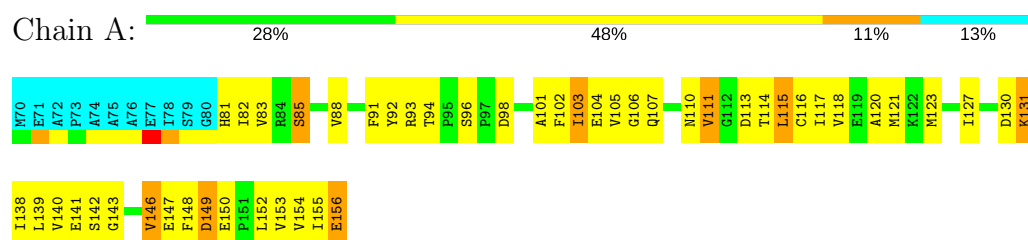
4.2.34 Score per residue for model 34

- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE



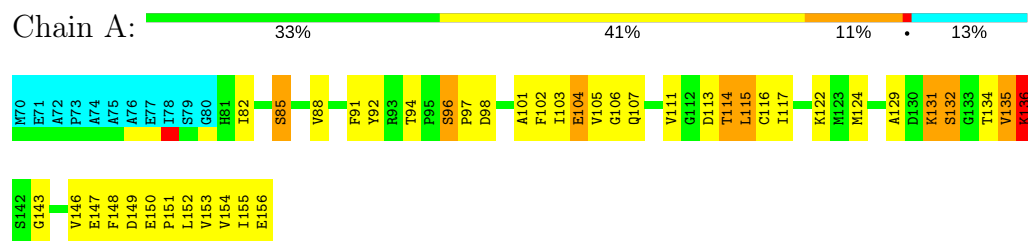
4.2.35 Score per residue for model 35

- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE



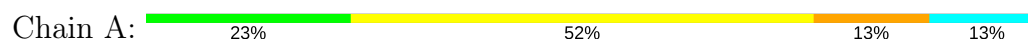
4.2.36 Score per residue for model 36

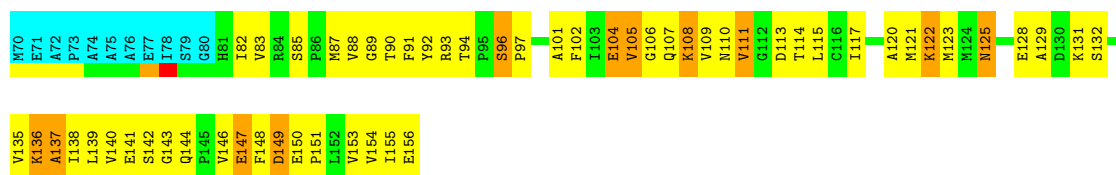
- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE



4.2.37 Score per residue for model 37

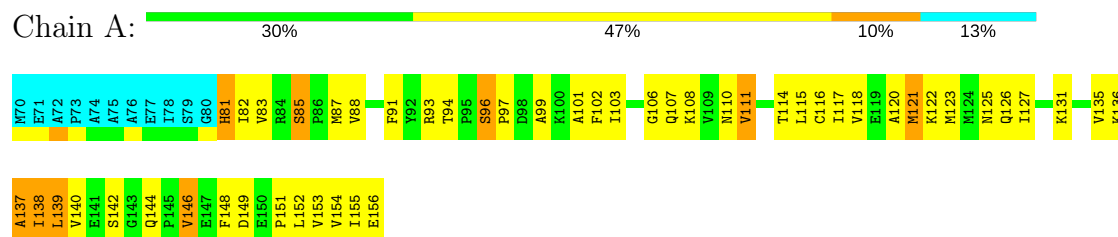
- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE





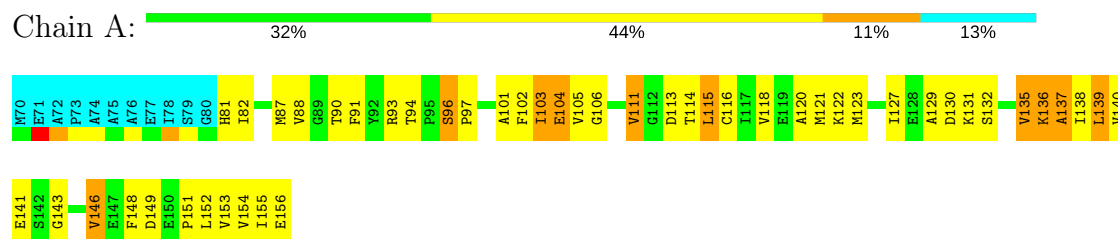
4.2.38 Score per residue for model 38

- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE



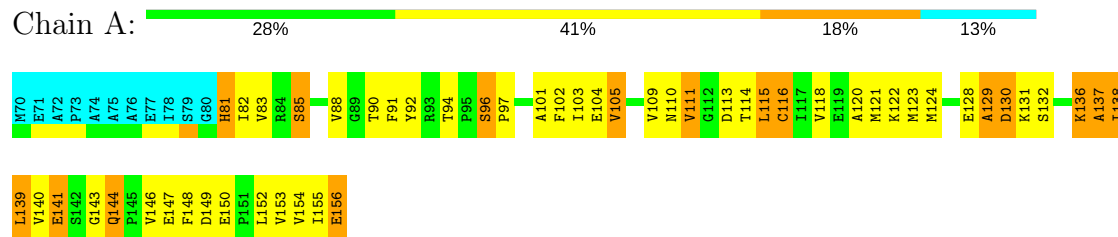
4.2.39 Score per residue for model 39

- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE



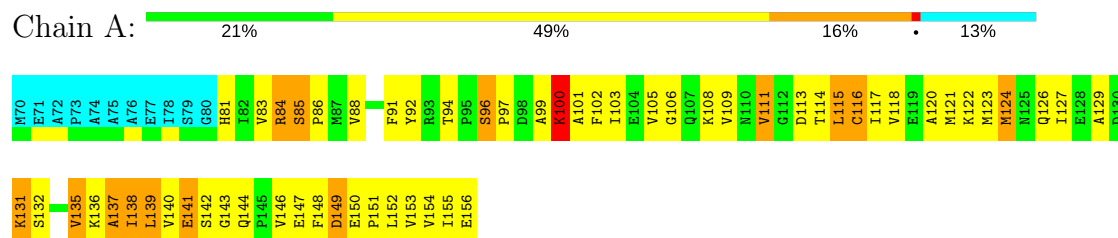
4.2.40 Score per residue for model 40

- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE



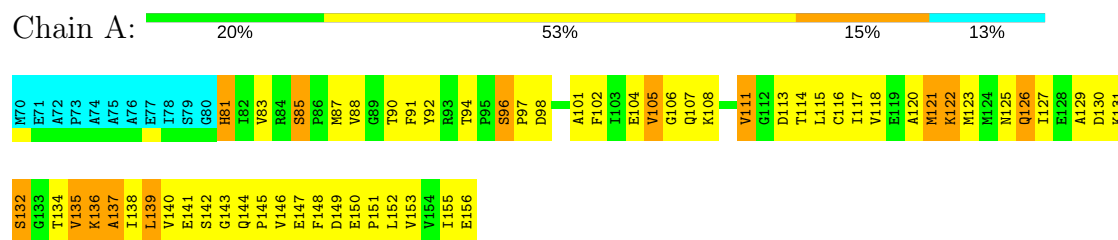
4.2.41 Score per residue for model 41

- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE



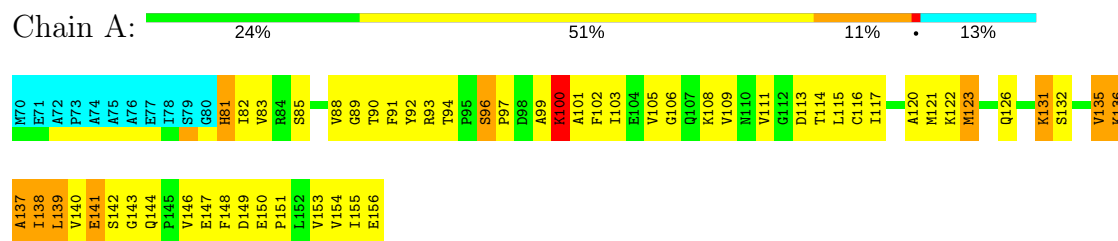
4.2.42 Score per residue for model 42

- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE



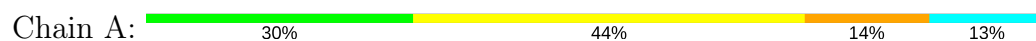
4.2.43 Score per residue for model 43

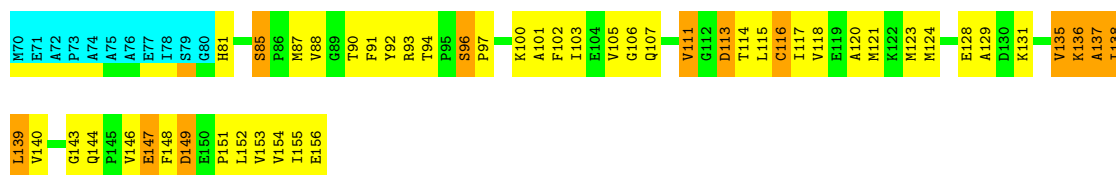
- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE



4.2.44 Score per residue for model 44

- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE

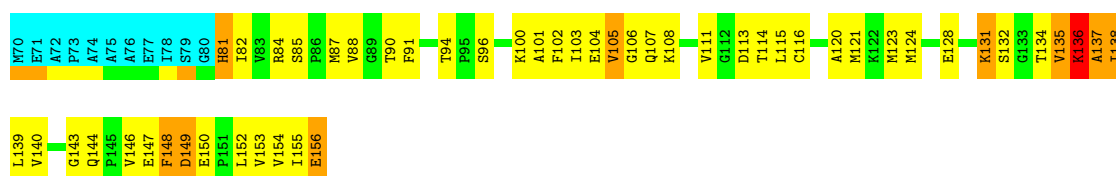




4.2.45 Score per residue for model 45

- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE

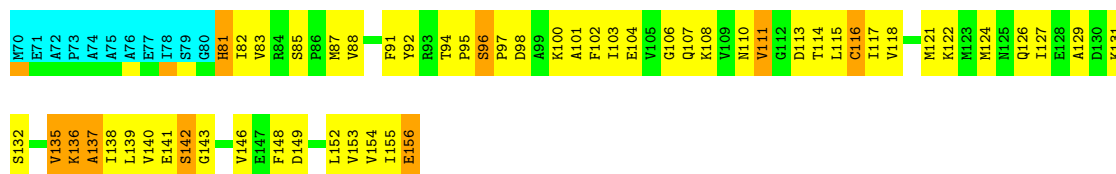
Chain A: 30% 46% 10% 13%



4.2.46 Score per residue for model 46

- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE

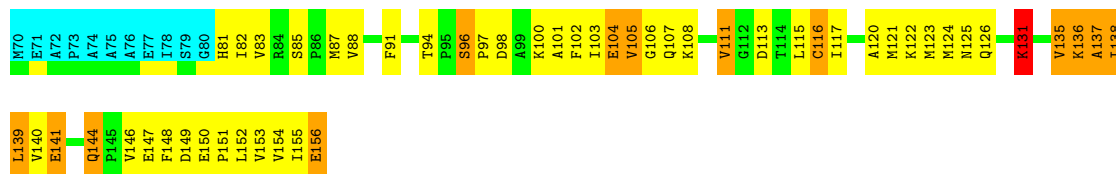
Chain A: 25% 52% 10% 13%



4.2.47 Score per residue for model 47

- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE

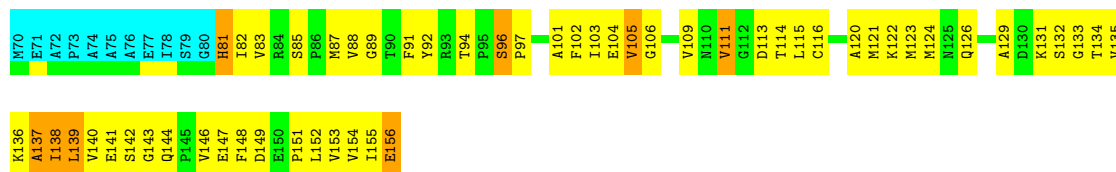
Chain A: 28% 44% 15% 13%



4.2.48 Score per residue for model 48

- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE

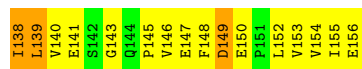
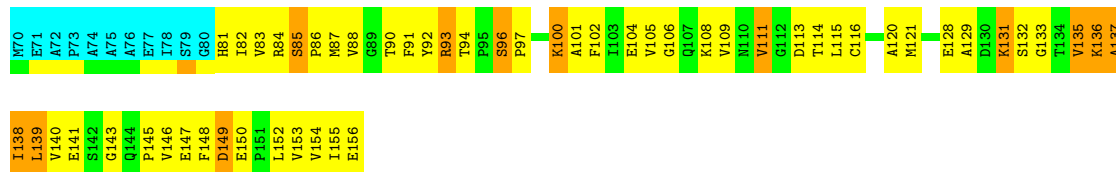
Chain A:  24% 54% 9% 13%



4.2.49 Score per residue for model 49

- Molecule 1: APO-BIOTIN CARBOXYL CARRIER PROTEIN OF ACETYL-COA CARBOXY-LASE

Chain A:  25% 48% 14% 13%



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *distance geometry*.

Of the 49 calculated structures, 49 were deposited, based on the following criterion: *LEAST RESTRAINT VIOLATION*.

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

Software name	Classification	Version
DIANA	refinement	
DIANA	structure solution	

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

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

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	579	498	590	54±7
All	All	28371	24402	28910	2624

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 46.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:138:ILE:HD12	1:A:153:VAL:HG13	1.05	1.26	25	7
1:A:138:ILE:HG23	1:A:153:VAL:HG22	1.02	1.32	6	46
1:A:115:LEU:HD21	1:A:127:ILE:HG22	1.00	1.24	38	10
1:A:82:ILE:CD1	1:A:154:VAL:HG13	0.99	1.86	27	14
1:A:81:HIS:CE1	1:A:155:ILE:HD13	0.94	1.97	6	2
1:A:102:PHE:CZ	1:A:117:ILE:HD11	0.91	2.01	47	16
1:A:115:LEU:HD21	1:A:155:ILE:CD1	0.90	1.97	43	4
1:A:116:CYS:O	1:A:117:ILE:HD13	0.90	1.67	8	8
1:A:102:PHE:CD2	1:A:117:ILE:HD11	0.89	2.02	16	1
1:A:115:LEU:HD13	1:A:129:ALA:HB2	0.89	1.44	42	10
1:A:115:LEU:HD21	1:A:155:ILE:HD11	0.89	1.40	19	4
1:A:139:LEU:HD21	1:A:154:VAL:HG23	0.87	1.45	43	36
1:A:102:PHE:CE1	1:A:114:THR:HG21	0.86	2.04	21	47
1:A:102:PHE:CD1	1:A:114:THR:HG21	0.86	2.06	32	42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:138:ILE:HD13	1:A:153:VAL:HG13	0.85	1.47	23	1
1:A:103:ILE:HD12	1:A:103:ILE:O	0.85	1.72	12	2
1:A:109:VAL:HG21	1:A:115:LEU:HD21	0.82	1.50	29	3
1:A:94:THR:HG22	1:A:101:ALA:HA	0.81	1.52	16	49
1:A:82:ILE:HD13	1:A:154:VAL:HG13	0.80	1.50	24	12
1:A:139:LEU:HD21	1:A:154:VAL:CG2	0.80	2.07	27	26
1:A:83:VAL:HG21	1:A:115:LEU:HD13	0.80	1.51	5	5
1:A:83:VAL:HG21	1:A:115:LEU:CD2	0.79	2.07	40	6
1:A:82:ILE:HG13	1:A:154:VAL:HG13	0.79	1.54	37	15
1:A:85:SER:OG	1:A:152:LEU:HD21	0.79	1.78	14	1
1:A:85:SER:HB2	1:A:152:LEU:HD21	0.79	1.54	49	8
1:A:138:ILE:HD12	1:A:153:VAL:CG1	0.78	2.09	27	4
1:A:82:ILE:HD12	1:A:154:VAL:HG22	0.78	1.51	48	4
1:A:102:PHE:CE2	1:A:117:ILE:HD11	0.78	2.14	16	21
1:A:114:THR:HG23	1:A:126:GLN:CD	0.78	1.99	19	4
1:A:88:VAL:HG13	1:A:147:GLU:HA	0.77	1.55	17	23
1:A:82:ILE:CG1	1:A:154:VAL:HG13	0.77	2.09	17	15
1:A:82:ILE:HD11	1:A:154:VAL:HG13	0.77	1.56	40	12
1:A:109:VAL:HG21	1:A:115:LEU:HD11	0.76	1.56	37	4
1:A:93:ARG:CZ	1:A:138:ILE:HD13	0.75	2.11	35	1
1:A:115:LEU:HD23	1:A:129:ALA:HB2	0.75	1.56	41	6
1:A:83:VAL:HG12	1:A:152:LEU:HD12	0.75	1.58	34	13
1:A:137:ALA:C	1:A:138:ILE:HD13	0.75	2.02	25	4
1:A:83:VAL:HG21	1:A:115:LEU:HD23	0.74	1.59	37	13
1:A:102:PHE:O	1:A:103:ILE:HD13	0.73	1.84	13	1
1:A:82:ILE:HG12	1:A:154:VAL:HG13	0.73	1.59	17	6
1:A:139:LEU:HD23	1:A:139:LEU:N	0.73	1.98	11	19
1:A:85:SER:HA	1:A:152:LEU:HD11	0.72	1.61	22	28
1:A:115:LEU:HD21	1:A:127:ILE:CG2	0.72	2.14	20	9
1:A:103:ILE:HD12	1:A:109:VAL:HG11	0.72	1.62	6	1
1:A:139:LEU:N	1:A:139:LEU:HD23	0.72	1.99	18	12
1:A:118:VAL:CG2	1:A:127:ILE:HD11	0.71	2.14	42	21
1:A:114:THR:HG23	1:A:126:GLN:CG	0.71	2.15	24	13
1:A:117:ILE:HG23	1:A:125:ASN:O	0.71	1.85	5	11
1:A:120:ALA:HB3	1:A:123:MET:CG	0.71	2.16	14	1
1:A:82:ILE:HD13	1:A:154:VAL:HG22	0.71	1.60	2	1
1:A:138:ILE:N	1:A:138:ILE:HD13	0.70	2.01	25	2
1:A:88:VAL:HG22	1:A:147:GLU:HA	0.70	1.64	22	9
1:A:93:ARG:NH1	1:A:138:ILE:HD12	0.70	2.02	24	1
1:A:102:PHE:CE2	1:A:117:ILE:CG1	0.70	2.75	47	13
1:A:82:ILE:CD1	1:A:154:VAL:HG22	0.70	2.17	2	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:SER:HB3	1:A:152:LEU:HD11	0.70	1.64	11	3
1:A:117:ILE:HD12	1:A:126:GLN:HG3	0.69	1.63	8	7
1:A:117:ILE:HD12	1:A:117:ILE:N	0.69	2.01	16	1
1:A:87:MET:CG	1:A:118:VAL:HG11	0.69	2.17	44	2
1:A:103:ILE:HD12	1:A:115:LEU:HD13	0.68	1.63	36	1
1:A:102:PHE:CD1	1:A:114:THR:CG2	0.68	2.76	46	39
1:A:138:ILE:C	1:A:139:LEU:HD23	0.68	2.08	25	5
1:A:83:VAL:HG11	1:A:115:LEU:HD11	0.68	1.64	15	3
1:A:103:ILE:CD1	1:A:109:VAL:HG11	0.68	2.18	48	6
1:A:103:ILE:HD11	1:A:109:VAL:HG11	0.68	1.65	48	4
1:A:88:VAL:HG13	1:A:146:VAL:O	0.68	1.87	15	10
1:A:139:LEU:HD12	1:A:151:PRO:HB2	0.68	1.64	19	32
1:A:91:PHE:HB2	1:A:146:VAL:HG11	0.68	1.65	16	38
1:A:85:SER:CB	1:A:152:LEU:HD21	0.68	2.19	49	1
1:A:136:LYS:HD3	1:A:154:VAL:HG12	0.67	1.65	13	6
1:A:134:THR:O	1:A:135:VAL:HG12	0.67	1.88	2	9
1:A:85:SER:CA	1:A:152:LEU:HD11	0.67	2.20	16	15
1:A:115:LEU:HD23	1:A:129:ALA:CB	0.67	2.20	36	4
1:A:116:CYS:SG	1:A:127:ILE:HD12	0.67	2.30	38	3
1:A:146:VAL:HG12	1:A:152:LEU:CD2	0.66	2.19	8	5
1:A:81:HIS:CE1	1:A:83:VAL:HG22	0.66	2.25	23	7
1:A:115:LEU:CD2	1:A:127:ILE:HG22	0.66	2.14	38	8
1:A:85:SER:HB3	1:A:152:LEU:HD21	0.66	1.66	21	1
1:A:134:THR:O	1:A:134:THR:HG23	0.66	1.89	14	1
1:A:93:ARG:HD2	1:A:138:ILE:HG21	0.66	1.68	9	8
1:A:138:ILE:CD1	1:A:153:VAL:HG13	0.66	2.18	11	9
1:A:88:VAL:HG22	1:A:148:PHE:H	0.66	1.51	5	43
1:A:81:HIS:CE1	1:A:155:ILE:CD1	0.66	2.78	6	1
1:A:82:ILE:HD12	1:A:154:VAL:HG13	0.65	1.67	40	1
1:A:91:PHE:CD2	1:A:152:LEU:HD13	0.64	2.27	11	8
1:A:88:VAL:HG22	1:A:148:PHE:N	0.64	2.07	35	34
1:A:136:LYS:O	1:A:137:ALA:HB2	0.64	1.93	28	49
1:A:138:ILE:HG23	1:A:153:VAL:CG2	0.64	2.23	33	33
1:A:138:ILE:HA	1:A:153:VAL:HG13	0.64	1.70	26	5
1:A:81:HIS:CE1	1:A:155:ILE:HD12	0.64	2.27	32	2
1:A:103:ILE:HD11	1:A:114:THR:O	0.63	1.92	45	2
1:A:114:THR:HG23	1:A:126:GLN:HG3	0.63	1.71	15	9
1:A:103:ILE:O	1:A:103:ILE:HG23	0.63	1.94	32	4
1:A:91:PHE:HD2	1:A:152:LEU:HD13	0.62	1.54	11	11
1:A:83:VAL:CG2	1:A:115:LEU:HD23	0.62	2.24	37	2
1:A:103:ILE:HD11	1:A:115:LEU:HD12	0.62	1.71	48	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:117:ILE:HD12	1:A:126:GLN:CG	0.62	2.25	8	7
1:A:115:LEU:CD2	1:A:129:ALA:HB2	0.62	2.24	29	4
1:A:81:HIS:CE1	1:A:131:LYS:CD	0.62	2.83	47	4
1:A:103:ILE:HG21	1:A:115:LEU:HD13	0.62	1.68	29	1
1:A:136:LYS:HB3	1:A:154:VAL:HG12	0.62	1.71	26	14
1:A:134:THR:O	1:A:134:THR:HG22	0.62	1.95	2	1
1:A:81:HIS:CE1	1:A:83:VAL:HG23	0.61	2.30	6	4
1:A:138:ILE:HG23	1:A:153:VAL:HG13	0.61	1.73	12	12
1:A:91:PHE:CE2	1:A:116:CYS:SG	0.61	2.94	26	37
1:A:91:PHE:CD2	1:A:152:LEU:HD22	0.61	2.31	16	3
1:A:120:ALA:HB3	1:A:123:MET:HG3	0.60	1.72	14	1
1:A:85:SER:OG	1:A:146:VAL:HG21	0.60	1.96	16	5
1:A:81:HIS:CE1	1:A:82:ILE:O	0.60	2.55	48	1
1:A:83:VAL:HG11	1:A:115:LEU:CD1	0.60	2.26	15	1
1:A:93:ARG:HH12	1:A:103:ILE:HD11	0.60	1.57	38	1
1:A:93:ARG:CZ	1:A:138:ILE:CD1	0.60	2.80	37	8
1:A:91:PHE:CE1	1:A:140:VAL:HG13	0.60	2.31	39	48
1:A:106:GLY:H	1:A:135:VAL:HG11	0.60	1.57	21	45
1:A:134:THR:HG22	1:A:156:GLU:HB3	0.60	1.74	11	2
1:A:81:HIS:CE1	1:A:130:ASP:OD2	0.60	2.55	40	1
1:A:81:HIS:NE2	1:A:155:ILE:HD13	0.60	2.12	6	1
1:A:117:ILE:HD13	1:A:126:GLN:HA	0.60	1.74	25	3
1:A:138:ILE:HD13	1:A:138:ILE:N	0.59	2.12	27	2
1:A:109:VAL:HG21	1:A:115:LEU:CD1	0.59	2.27	37	1
1:A:138:ILE:CG2	1:A:153:VAL:HG22	0.59	2.26	48	28
1:A:102:PHE:CZ	1:A:117:ILE:CD1	0.59	2.83	47	7
1:A:146:VAL:HG12	1:A:152:LEU:HD21	0.59	1.75	8	2
1:A:85:SER:OG	1:A:152:LEU:HD11	0.59	1.98	15	1
1:A:115:LEU:HD11	1:A:155:ILE:HD11	0.59	1.75	36	1
1:A:91:PHE:CD1	1:A:140:VAL:HG13	0.58	2.33	24	11
1:A:115:LEU:CD2	1:A:155:ILE:HD11	0.58	2.21	19	1
1:A:90:THR:HG23	1:A:143:GLY:O	0.58	1.98	28	13
1:A:118:VAL:HG23	1:A:127:ILE:HD11	0.58	1.75	42	4
1:A:139:LEU:HD21	1:A:154:VAL:HG21	0.58	1.74	27	4
1:A:103:ILE:HD13	1:A:109:VAL:HG11	0.58	1.76	41	2
1:A:148:PHE:O	1:A:149:ASP:CB	0.57	2.52	45	43
1:A:117:ILE:CG2	1:A:124:MET:HE2	0.57	2.30	41	1
1:A:102:PHE:CE2	1:A:117:ILE:CD1	0.57	2.86	46	4
1:A:82:ILE:HG12	1:A:154:VAL:HG22	0.57	1.76	8	1
1:A:146:VAL:CG1	1:A:152:LEU:HD22	0.56	2.30	35	3
1:A:103:ILE:HG21	1:A:115:LEU:HD23	0.56	1.77	19	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:109:VAL:HG21	1:A:115:LEU:CD2	0.56	2.28	29	1
1:A:108:LYS:HG2	1:A:134:THR:HG23	0.56	1.77	9	1
1:A:103:ILE:HG23	1:A:103:ILE:O	0.56	2.00	30	2
1:A:134:THR:HG22	1:A:134:THR:O	0.56	2.01	19	4
1:A:103:ILE:HD11	1:A:115:LEU:HD22	0.56	1.77	36	1
1:A:139:LEU:N	1:A:139:LEU:CD2	0.55	2.69	6	8
1:A:136:LYS:HD2	1:A:154:VAL:HG12	0.55	1.78	37	1
1:A:138:ILE:HD12	1:A:138:ILE:H	0.55	1.62	7	11
1:A:135:VAL:HG22	1:A:136:LYS:H	0.55	1.61	26	9
1:A:93:ARG:CZ	1:A:138:ILE:HD12	0.55	2.30	33	8
1:A:102:PHE:CE2	1:A:117:ILE:HG12	0.55	2.37	19	8
1:A:105:VAL:HG22	1:A:138:ILE:HD11	0.55	1.77	21	11
1:A:81:HIS:C	1:A:82:ILE:HD12	0.55	2.22	38	2
1:A:93:ARG:HH21	1:A:116:CYS:HB3	0.55	1.62	49	2
1:A:93:ARG:NH1	1:A:103:ILE:CG2	0.55	2.70	44	1
1:A:135:VAL:HA	1:A:155:ILE:HD13	0.55	1.78	21	1
1:A:91:PHE:CD2	1:A:140:VAL:HG11	0.55	2.36	43	31
1:A:85:SER:CB	1:A:152:LEU:HD11	0.55	2.32	16	2
1:A:139:LEU:CD2	1:A:139:LEU:N	0.54	2.69	11	13
1:A:138:ILE:H	1:A:138:ILE:HD12	0.54	1.62	38	6
1:A:83:VAL:HG21	1:A:115:LEU:CD1	0.54	2.31	5	2
1:A:105:VAL:CG2	1:A:138:ILE:HD11	0.54	2.32	21	4
1:A:146:VAL:CG1	1:A:152:LEU:CD2	0.54	2.86	11	5
1:A:115:LEU:HD13	1:A:129:ALA:CB	0.54	2.26	48	1
1:A:82:ILE:HG13	1:A:154:VAL:HG22	0.54	1.80	26	1
1:A:118:VAL:HG21	1:A:127:ILE:HD11	0.54	1.80	38	8
1:A:81:HIS:CE1	1:A:131:LYS:HD3	0.54	2.38	2	3
1:A:93:ARG:HH11	1:A:138:ILE:HG21	0.54	1.63	32	1
1:A:102:PHE:CE1	1:A:117:ILE:HD11	0.54	2.38	47	3
1:A:82:ILE:CD1	1:A:154:VAL:CG1	0.54	2.81	6	3
1:A:81:HIS:CE1	1:A:131:LYS:HD2	0.53	2.38	47	4
1:A:146:VAL:CG1	1:A:152:LEU:HD21	0.53	2.33	8	3
1:A:81:HIS:CD2	1:A:155:ILE:CG2	0.53	2.91	12	1
1:A:111:VAL:O	1:A:111:VAL:HG13	0.53	2.04	2	11
1:A:91:PHE:HB3	1:A:140:VAL:HG21	0.53	1.81	28	25
1:A:81:HIS:CD2	1:A:155:ILE:HG22	0.53	2.39	34	1
1:A:111:VAL:HG13	1:A:111:VAL:O	0.53	2.04	42	8
1:A:136:LYS:HE3	1:A:154:VAL:HG12	0.53	1.80	33	1
1:A:115:LEU:HD23	1:A:129:ALA:CA	0.52	2.34	36	1
1:A:111:VAL:HG23	1:A:130:ASP:HA	0.52	1.81	42	2
1:A:103:ILE:H	1:A:103:ILE:HD13	0.52	1.64	19	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:91:PHE:HE2	1:A:116:CYS:HG	0.52	1.48	19	10
1:A:138:ILE:HG12	1:A:153:VAL:HG13	0.52	1.81	33	6
1:A:117:ILE:CG2	1:A:124:MET:CE	0.52	2.88	41	1
1:A:96:SER:CB	1:A:97:PRO:CD	0.52	2.88	44	42
1:A:136:LYS:CE	1:A:154:VAL:CG1	0.52	2.87	41	1
1:A:82:ILE:CG1	1:A:154:VAL:HG22	0.52	2.34	26	2
1:A:134:THR:O	1:A:135:VAL:CG1	0.52	2.58	42	9
1:A:88:VAL:HG22	1:A:147:GLU:CA	0.52	2.34	22	2
1:A:138:ILE:HG22	1:A:140:VAL:O	0.52	2.04	1	2
1:A:115:LEU:HD12	1:A:116:CYS:SG	0.52	2.45	22	4
1:A:146:VAL:HG12	1:A:152:LEU:HD22	0.52	1.82	35	2
1:A:138:ILE:HD13	1:A:153:VAL:CG1	0.51	2.29	23	1
1:A:91:PHE:CG	1:A:140:VAL:HG11	0.51	2.41	43	7
1:A:129:ALA:O	1:A:130:ASP:CB	0.51	2.57	40	1
1:A:91:PHE:C	1:A:91:PHE:CD1	0.51	2.84	6	24
1:A:136:LYS:CB	1:A:154:VAL:O	0.51	2.59	16	32
1:A:134:THR:CG2	1:A:135:VAL:N	0.51	2.74	10	10
1:A:82:ILE:N	1:A:82:ILE:HD12	0.51	2.21	30	1
1:A:81:HIS:O	1:A:82:ILE:HD13	0.51	2.06	47	2
1:A:103:ILE:HD13	1:A:103:ILE:H	0.51	1.65	23	1
1:A:155:ILE:CG2	1:A:156:GLU:N	0.51	2.74	32	46
1:A:147:GLU:O	1:A:150:GLU:CB	0.51	2.59	8	9
1:A:91:PHE:CD1	1:A:91:PHE:C	0.51	2.85	40	23
1:A:102:PHE:CE2	1:A:117:ILE:HG13	0.51	2.41	19	9
1:A:111:VAL:HG22	1:A:130:ASP:C	0.51	2.27	30	1
1:A:136:LYS:CD	1:A:156:GLU:CB	0.51	2.89	17	1
1:A:120:ALA:O	1:A:121:MET:CG	0.50	2.60	48	16
1:A:100:LYS:CD	1:A:100:LYS:N	0.50	2.70	30	1
1:A:103:ILE:CG2	1:A:104:GLU:N	0.50	2.74	45	1
1:A:117:ILE:HG22	1:A:124:MET:CE	0.50	2.37	41	1
1:A:106:GLY:N	1:A:135:VAL:HG11	0.50	2.21	21	6
1:A:111:VAL:O	1:A:111:VAL:CG1	0.50	2.59	16	12
1:A:91:PHE:CE1	1:A:140:VAL:CG1	0.50	2.94	45	19
1:A:115:LEU:CD1	1:A:116:CYS:SG	0.50	3.00	2	5
1:A:96:SER:HB2	1:A:99:ALA:HB2	0.50	1.83	31	4
1:A:134:THR:HG22	1:A:135:VAL:H	0.50	1.66	9	3
1:A:120:ALA:HB3	1:A:123:MET:SD	0.50	2.46	14	1
1:A:90:THR:CG2	1:A:143:GLY:O	0.50	2.60	18	9
1:A:111:VAL:CG1	1:A:111:VAL:O	0.50	2.60	26	7
1:A:85:SER:OG	1:A:146:VAL:CG2	0.50	2.60	29	10
1:A:121:MET:O	1:A:122:LYS:CG	0.50	2.60	32	7

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:93:ARG:NH1	1:A:103:ILE:HD11	0.50	2.21	38	1
1:A:114:THR:CG2	1:A:126:GLN:CG	0.50	2.90	19	2
1:A:115:LEU:HD13	1:A:129:ALA:HA	0.49	1.84	40	1
1:A:151:PRO:O	1:A:152:LEU:HD23	0.49	2.07	7	3
1:A:81:HIS:HE1	1:A:83:VAL:HG22	0.49	1.62	23	1
1:A:141:GLU:CB	1:A:144:GLN:NE2	0.49	2.75	47	1
1:A:87:MET:HG3	1:A:118:VAL:HG11	0.49	1.84	44	2
1:A:145:PRO:O	1:A:146:VAL:HG13	0.49	2.08	49	1
1:A:136:LYS:O	1:A:137:ALA:CB	0.49	2.60	27	22
1:A:115:LEU:HD11	1:A:155:ILE:CD1	0.49	2.37	19	2
1:A:92:TYR:CE1	1:A:143:GLY:HA2	0.49	2.43	5	44
1:A:103:ILE:HD13	1:A:109:VAL:CG1	0.49	2.38	41	2
1:A:102:PHE:CZ	1:A:117:ILE:CG1	0.49	2.96	19	2
1:A:134:THR:O	1:A:134:THR:CG2	0.49	2.59	14	2
1:A:103:ILE:O	1:A:103:ILE:CG2	0.49	2.60	32	1
1:A:91:PHE:CE2	1:A:140:VAL:HG11	0.49	2.43	48	21
1:A:93:ARG:NH2	1:A:138:ILE:CD1	0.49	2.76	37	2
1:A:81:HIS:CG	1:A:82:ILE:N	0.48	2.81	11	3
1:A:108:LYS:C	1:A:108:LYS:CD	0.48	2.80	17	1
1:A:103:ILE:CG2	1:A:103:ILE:O	0.48	2.60	30	1
1:A:155:ILE:HG22	1:A:156:GLU:N	0.48	2.24	42	6
1:A:91:PHE:CB	1:A:140:VAL:HG21	0.48	2.38	46	7
1:A:81:HIS:CB	1:A:131:LYS:NZ	0.48	2.77	46	1
1:A:120:ALA:O	1:A:122:LYS:N	0.48	2.46	6	11
1:A:81:HIS:N	1:A:81:HIS:ND1	0.48	2.62	45	1
1:A:140:VAL:HG22	1:A:141:GLU:N	0.48	2.23	19	7
1:A:138:ILE:N	1:A:138:ILE:CD1	0.48	2.70	11	2
1:A:82:ILE:HD12	1:A:82:ILE:N	0.47	2.23	3	1
1:A:90:THR:O	1:A:118:VAL:HG13	0.47	2.09	24	5
1:A:89:GLY:N	1:A:146:VAL:HG22	0.47	2.25	43	4
1:A:115:LEU:HD21	1:A:155:ILE:HD13	0.47	1.86	48	3
1:A:96:SER:CB	1:A:99:ALA:HB2	0.47	2.39	38	1
1:A:125:ASN:N	1:A:125:ASN:ND2	0.47	2.63	19	2
1:A:115:LEU:HD12	1:A:129:ALA:HA	0.47	1.86	10	2
1:A:91:PHE:CZ	1:A:153:VAL:CG2	0.47	2.98	26	5
1:A:120:ALA:HB1	1:A:121:MET:SD	0.47	2.50	31	1
1:A:81:HIS:HE1	1:A:83:VAL:HG23	0.47	1.68	32	1
1:A:93:ARG:NH1	1:A:138:ILE:HD13	0.47	2.24	35	1
1:A:117:ILE:CG2	1:A:125:ASN:O	0.47	2.63	8	6
1:A:85:SER:HB2	1:A:152:LEU:HD11	0.47	1.85	35	1
1:A:126:GLN:CG	1:A:127:ILE:N	0.47	2.78	12	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:GLU:CG	1:A:128:GLU:O	0.47	2.62	37	1
1:A:116:CYS:C	1:A:117:ILE:HD13	0.47	2.30	47	2
1:A:124:MET:CG	1:A:124:MET:O	0.47	2.63	47	1
1:A:91:PHE:CE2	1:A:152:LEU:HB3	0.46	2.45	49	8
1:A:130:ASP:O	1:A:131:LYS:CD	0.46	2.63	22	1
1:A:81:HIS:NE2	1:A:155:ILE:HD12	0.46	2.26	32	2
1:A:100:LYS:N	1:A:100:LYS:CD	0.46	2.77	3	1
1:A:115:LEU:HD22	1:A:129:ALA:HA	0.46	1.87	37	2
1:A:91:PHE:CB	1:A:146:VAL:HG11	0.46	2.36	13	7
1:A:108:LYS:HG3	1:A:134:THR:HG22	0.46	1.87	45	1
1:A:103:ILE:CG2	1:A:115:LEU:O	0.46	2.64	1	2
1:A:88:VAL:HG13	1:A:147:GLU:HG2	0.46	1.88	2	2
1:A:88:VAL:HG13	1:A:147:GLU:CD	0.46	2.31	44	1
1:A:103:ILE:HD12	1:A:109:VAL:CG1	0.46	2.40	40	1
1:A:103:ILE:C	1:A:103:ILE:HD13	0.46	2.30	32	1
1:A:120:ALA:O	1:A:123:MET:CG	0.46	2.64	43	2
1:A:103:ILE:HG21	1:A:115:LEU:HA	0.46	1.88	19	2
1:A:134:THR:HG22	1:A:135:VAL:N	0.46	2.26	23	7
1:A:88:VAL:HG13	1:A:147:GLU:HG3	0.46	1.88	10	1
1:A:81:HIS:CD2	1:A:131:LYS:HB3	0.46	2.45	40	1
1:A:149:ASP:OD1	1:A:150:GLU:N	0.46	2.49	45	1
1:A:138:ILE:HD12	1:A:138:ILE:N	0.46	2.26	7	6
1:A:103:ILE:HD13	1:A:103:ILE:N	0.46	2.26	19	1
1:A:81:HIS:O	1:A:81:HIS:ND1	0.45	2.49	29	2
1:A:109:VAL:HG22	1:A:133:GLY:O	0.45	2.10	1	7
1:A:83:VAL:O	1:A:152:LEU:N	0.45	2.50	6	24
1:A:124:MET:N	1:A:124:MET:SD	0.45	2.90	10	4
1:A:125:ASN:ND2	1:A:125:ASN:N	0.45	2.64	37	2
1:A:124:MET:SD	1:A:124:MET:N	0.45	2.90	2	3
1:A:81:HIS:CD2	1:A:155:ILE:HG21	0.45	2.47	12	1
1:A:103:ILE:CD1	1:A:115:LEU:O	0.45	2.65	43	1
1:A:115:LEU:N	1:A:127:ILE:O	0.45	2.50	6	3
1:A:141:GLU:O	1:A:143:GLY:N	0.45	2.49	43	6
1:A:117:ILE:HG22	1:A:124:MET:HE2	0.45	1.88	41	1
1:A:123:MET:O	1:A:125:ASN:ND2	0.45	2.50	32	5
1:A:136:LYS:CD	1:A:155:ILE:O	0.45	2.64	13	3
1:A:128:GLU:O	1:A:128:GLU:CG	0.45	2.64	29	1
1:A:93:ARG:NH2	1:A:103:ILE:O	0.45	2.50	43	2
1:A:138:ILE:CD1	1:A:138:ILE:N	0.45	2.70	25	1
1:A:85:SER:OG	1:A:146:VAL:HG23	0.45	2.11	34	1
1:A:81:HIS:C	1:A:81:HIS:ND1	0.45	2.70	16	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:124:MET:SD	1:A:126:GLN:NE2	0.45	2.90	46	1
1:A:108:LYS:CG	1:A:109:VAL:N	0.45	2.80	16	5
1:A:103:ILE:CD1	1:A:103:ILE:C	0.45	2.85	32	1
1:A:96:SER:CB	1:A:97:PRO:HD2	0.45	2.42	43	27
1:A:101:ALA:HB3	1:A:104:GLU:HG3	0.44	1.88	46	1
1:A:81:HIS:NE2	1:A:130:ASP:OD2	0.44	2.50	35	1
1:A:84:ARG:HH21	1:A:149:ASP:HA	0.44	1.72	14	1
1:A:138:ILE:CD1	1:A:153:VAL:CG1	0.44	2.93	12	2
1:A:91:PHE:CD1	1:A:140:VAL:CG1	0.44	3.00	18	6
1:A:141:GLU:OE2	1:A:144:GLN:NE2	0.44	2.50	40	1
1:A:93:ARG:NH2	1:A:115:LEU:O	0.44	2.50	31	1
1:A:114:THR:OG1	1:A:126:GLN:NE2	0.44	2.50	15	2
1:A:138:ILE:CA	1:A:153:VAL:HG13	0.44	2.41	26	1
1:A:148:PHE:O	1:A:149:ASP:CG	0.44	2.56	1	8
1:A:81:HIS:ND1	1:A:81:HIS:O	0.44	2.50	19	1
1:A:147:GLU:OE2	1:A:148:PHE:N	0.44	2.51	3	1
1:A:114:THR:HG22	1:A:115:LEU:H	0.44	1.72	14	6
1:A:139:LEU:CD2	1:A:154:VAL:HG23	0.44	2.36	21	3
1:A:115:LEU:HD11	1:A:155:ILE:HD12	0.44	1.88	19	1
1:A:85:SER:CB	1:A:146:VAL:CG2	0.44	2.96	28	1
1:A:134:THR:CG2	1:A:156:GLU:CD	0.44	2.86	10	1
1:A:136:LYS:CB	1:A:155:ILE:C	0.44	2.86	25	1
1:A:95:PRO:HD3	1:A:102:PHE:CE2	0.43	2.47	46	2
1:A:136:LYS:CD	1:A:154:VAL:HG12	0.43	2.43	48	1
1:A:91:PHE:CZ	1:A:140:VAL:CG1	0.43	3.01	2	6
1:A:141:GLU:O	1:A:142:SER:C	0.43	2.56	13	4
1:A:114:THR:HG22	1:A:115:LEU:N	0.43	2.28	36	15
1:A:90:THR:HG22	1:A:91:PHE:N	0.43	2.29	23	4
1:A:136:LYS:HE2	1:A:154:VAL:CG1	0.43	2.43	41	1
1:A:138:ILE:N	1:A:138:ILE:HD12	0.43	2.28	38	4
1:A:120:ALA:HB3	1:A:125:ASN:ND2	0.43	2.28	47	2
1:A:117:ILE:CD1	1:A:117:ILE:N	0.43	2.71	16	1
1:A:149:ASP:O	1:A:149:ASP:OD1	0.43	2.37	1	3
1:A:136:LYS:CD	1:A:156:GLU:HB2	0.43	2.43	17	2
1:A:149:ASP:C	1:A:149:ASP:OD1	0.43	2.57	14	5
1:A:147:GLU:O	1:A:148:PHE:C	0.43	2.55	25	1
1:A:136:LYS:CB	1:A:154:VAL:HG12	0.43	2.40	26	1
1:A:91:PHE:CZ	1:A:116:CYS:SG	0.43	3.11	29	1
1:A:141:GLU:OE1	1:A:142:SER:N	0.43	2.52	41	1
1:A:136:LYS:HD3	1:A:156:GLU:CB	0.43	2.43	17	1
1:A:136:LYS:CE	1:A:154:VAL:HG12	0.43	2.44	41	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:134:THR:O	1:A:135:VAL:O	0.43	2.37	19	9
1:A:114:THR:CG2	1:A:126:GLN:HG3	0.43	2.44	43	3
1:A:130:ASP:O	1:A:131:LYS:CG	0.43	2.67	35	2
1:A:90:THR:C	1:A:146:VAL:HG13	0.43	2.34	37	1
1:A:111:VAL:HG23	1:A:132:SER:H	0.43	1.73	46	2
1:A:149:ASP:OD1	1:A:149:ASP:C	0.42	2.57	25	4
1:A:148:PHE:O	1:A:149:ASP:OD1	0.42	2.37	31	5
1:A:141:GLU:O	1:A:144:GLN:N	0.42	2.49	8	2
1:A:108:LYS:CD	1:A:133:GLY:O	0.42	2.67	6	1
1:A:134:THR:HB	1:A:156:GLU:CG	0.42	2.44	10	1
1:A:125:ASN:HD22	1:A:125:ASN:N	0.42	2.12	19	1
1:A:135:VAL:O	1:A:156:GLU:N	0.42	2.52	26	1
1:A:128:GLU:O	1:A:129:ALA:C	0.42	2.56	40	3
1:A:138:ILE:HG23	1:A:153:VAL:CG1	0.42	2.44	32	1
1:A:136:LYS:CE	1:A:136:LYS:HA	0.42	2.45	43	1
1:A:108:LYS:O	1:A:109:VAL:CG1	0.42	2.68	37	2
1:A:114:THR:CG2	1:A:126:GLN:CD	0.42	2.86	33	2
1:A:148:PHE:O	1:A:149:ASP:OD2	0.42	2.38	49	11
1:A:115:LEU:HD23	1:A:129:ALA:HA	0.42	1.90	36	1
1:A:147:GLU:O	1:A:149:ASP:N	0.42	2.53	45	1
1:A:149:ASP:OD1	1:A:149:ASP:O	0.42	2.38	28	2
1:A:134:THR:N	1:A:156:GLU:O	0.42	2.50	4	1
1:A:87:MET:HG3	1:A:118:VAL:CG1	0.42	2.44	44	1
1:A:115:LEU:HD23	1:A:129:ALA:N	0.42	2.29	46	1
1:A:103:ILE:CD1	1:A:114:THR:O	0.42	2.63	45	1
1:A:145:PRO:C	1:A:146:VAL:CG1	0.42	2.88	25	2
1:A:81:HIS:CG	1:A:131:LYS:HD2	0.42	2.50	42	1
1:A:87:MET:CG	1:A:118:VAL:CG1	0.42	2.95	44	1
1:A:117:ILE:HG22	1:A:118:VAL:N	0.42	2.29	1	1
1:A:113:ASP:O	1:A:129:ALA:CB	0.42	2.68	44	1
1:A:99:ALA:O	1:A:100:LYS:O	0.41	2.38	43	3
1:A:121:MET:SD	1:A:121:MET:N	0.41	2.93	31	1
1:A:147:GLU:CB	1:A:150:GLU:HG3	0.41	2.45	3	10
1:A:82:ILE:CD1	1:A:154:VAL:CG2	0.41	2.97	46	1
1:A:149:ASP:O	1:A:149:ASP:OD2	0.41	2.38	31	2
1:A:91:PHE:CG	1:A:140:VAL:HG21	0.41	2.49	37	1
1:A:117:ILE:CD1	1:A:126:GLN:HB2	0.41	2.45	25	2
1:A:81:HIS:CG	1:A:131:LYS:HB2	0.41	2.50	5	1
1:A:131:LYS:O	1:A:132:SER:C	0.41	2.58	40	28
1:A:110:ASN:O	1:A:111:VAL:C	0.41	2.59	40	12
1:A:103:ILE:N	1:A:103:ILE:CD1	0.41	2.83	19	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:134:THR:HG22	1:A:156:GLU:OE1	0.41	2.16	24	1
1:A:137:ALA:O	1:A:154:VAL:HG23	0.41	2.16	17	1
1:A:135:VAL:O	1:A:156:GLU:CB	0.41	2.69	45	1
1:A:84:ARG:O	1:A:85:SER:C	0.41	2.59	25	2
1:A:104:GLU:O	1:A:105:VAL:C	0.41	2.59	48	22
1:A:149:ASP:OD2	1:A:149:ASP:C	0.41	2.59	31	1
1:A:130:ASP:O	1:A:131:LYS:CB	0.41	2.67	25	1
1:A:148:PHE:C	1:A:148:PHE:CD1	0.41	2.94	13	2
1:A:136:LYS:HD2	1:A:156:GLU:CB	0.41	2.46	48	1
1:A:135:VAL:HG22	1:A:136:LYS:N	0.41	2.31	25	4
1:A:140:VAL:CG2	1:A:141:GLU:N	0.41	2.84	19	1
1:A:103:ILE:HD13	1:A:103:ILE:C	0.41	2.35	39	1
1:A:103:ILE:CD1	1:A:109:VAL:CG1	0.41	2.98	16	3
1:A:148:PHE:CD1	1:A:148:PHE:C	0.41	2.94	5	2
1:A:144:GLN:N	1:A:144:GLN:NE2	0.41	2.68	8	1
1:A:88:VAL:HG13	1:A:147:GLU:CG	0.41	2.45	44	1
1:A:103:ILE:CG1	1:A:103:ILE:O	0.41	2.69	29	1
1:A:117:ILE:CG2	1:A:124:MET:HG2	0.41	2.46	27	1
1:A:95:PRO:CD	1:A:102:PHE:CE2	0.41	3.04	17	1
1:A:88:VAL:HG11	1:A:147:GLU:OE1	0.41	2.16	28	1
1:A:136:LYS:NZ	1:A:156:GLU:OE1	0.41	2.50	31	1
1:A:134:THR:O	1:A:135:VAL:C	0.41	2.60	21	1
1:A:147:GLU:CG	1:A:148:PHE:N	0.41	2.84	12	1
1:A:81:HIS:ND1	1:A:81:HIS:N	0.41	2.66	46	1
1:A:91:PHE:HB2	1:A:146:VAL:CG1	0.41	2.46	28	3
1:A:150:GLU:OE2	1:A:151:PRO:O	0.41	2.39	22	1
1:A:149:ASP:C	1:A:149:ASP:OD2	0.41	2.59	27	1
1:A:130:ASP:N	1:A:130:ASP:OD1	0.41	2.54	8	1
1:A:145:PRO:O	1:A:146:VAL:CG1	0.40	2.69	49	1
1:A:84:ARG:O	1:A:86:PRO:N	0.40	2.54	14	3
1:A:83:VAL:HG23	1:A:155:ILE:CD1	0.40	2.46	20	1
1:A:81:HIS:CE1	1:A:82:ILE:C	0.40	2.95	48	1
1:A:150:GLU:CG	1:A:151:PRO:HD2	0.40	2.46	26	1
1:A:90:THR:CA	1:A:146:VAL:HG22	0.40	2.46	39	1
1:A:149:ASP:OD1	1:A:150:GLU:OE2	0.40	2.40	25	1
1:A:120:ALA:O	1:A:121:MET:C	0.40	2.59	5	1
1:A:121:MET:O	1:A:122:LYS:C	0.40	2.59	6	2
1:A:150:GLU:OE1	1:A:151:PRO:O	0.40	2.40	37	2
1:A:85:SER:OG	1:A:147:GLU:C	0.40	2.60	45	1
1:A:81:HIS:CE1	1:A:83:VAL:CG2	0.40	3.02	15	1
1:A:85:SER:HB3	1:A:146:VAL:CG2	0.40	2.47	18	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:102:PHE:CE1	1:A:114:THR:CG2	0.40	2.95	27	1
1:A:144:GLN:CG	1:A:145:PRO:HD2	0.40	2.47	42	1
1:A:85:SER:OG	1:A:150:GLU:O	0.40	2.40	33	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	75/87 (86%)	58±2 (78±2%)	12±2 (16±3%)	5±2 (6±2%)	3	21
All	All	3675/4263 (86%)	2865 (78%)	589 (16%)	221 (6%)	3	21

All 16 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	137	ALA	49
1	A	111	VAL	48
1	A	135	VAL	24
1	A	131	LYS	17
1	A	142	SER	15
1	A	105	VAL	13
1	A	121	MET	11
1	A	136	LYS	9
1	A	100	LYS	9
1	A	132	SER	8
1	A	116	CYS	8
1	A	114	THR	5
1	A	148	PHE	2
1	A	130	ASP	1
1	A	149	ASP	1
1	A	129	ALA	1

6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	66/72 (92%)	51±2 (78±3%)	15±2 (22±3%)	3 31
All	All	3234/3528 (92%)	2523 (78%)	711 (22%)	3 31

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	139	LEU	49
1	A	96	SER	49
1	A	113	ASP	47
1	A	136	LYS	38
1	A	85	SER	38
1	A	123	MET	35
1	A	141	GLU	31
1	A	138	ILE	31
1	A	87	MET	30
1	A	144	GLN	29
1	A	122	LYS	26
1	A	81	HIS	25
1	A	100	LYS	23
1	A	108	LYS	22
1	A	124	MET	20
1	A	107	GLN	20
1	A	104	GLU	18
1	A	131	LYS	17
1	A	149	ASP	16
1	A	156	GLU	15
1	A	115	LEU	14
1	A	98	ASP	14
1	A	103	ILE	14
1	A	130	ASP	12
1	A	147	GLU	10
1	A	150	GLU	9
1	A	121	MET	8
1	A	128	GLU	8
1	A	93	ARG	7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	142	SER	7
1	A	134	THR	6
1	A	126	GLN	5
1	A	84	ARG	5
1	A	146	VAL	4
1	A	110	ASN	2
1	A	127	ILE	2
1	A	125	ASN	2
1	A	119	GLU	1
1	A	116	CYS	1
1	A	117	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 carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided