



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 12:26 PM UTC

PDB ID : 1Z87 / pdb_00001z87
Title : solution structure of the split PH-PDZ Supramodule of alpha-Syntrophin
Authors : Yan, J.; Xu, W.; Wen, W.; Long, J.F.; Adams, M.E.; Froehner, S.C.; Zhang, M.
Deposited on : 2005-03-30

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

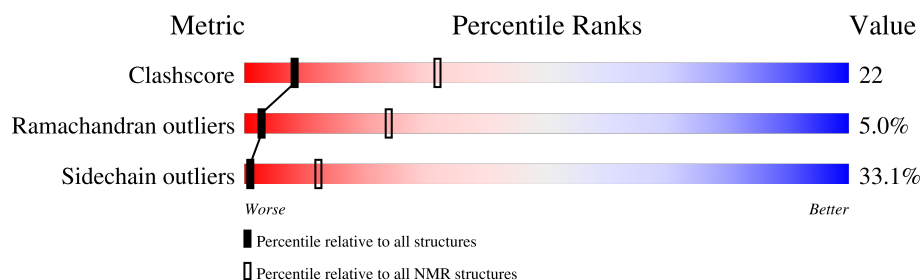
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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

Mol	Chain	Length	Quality of chain
1	A	263	

2 Ensemble composition and analysis

This entry contains 15 models. Model 3 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:8-A:17, A:27-A:45, A:206-A:221, A:228-A:264 (82)	0.78	1
2	A:79-A:163 (85)	0.80	3

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 1 single-model cluster was found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 3906 atoms, of which 1960 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Alpha-1-syntrophin.

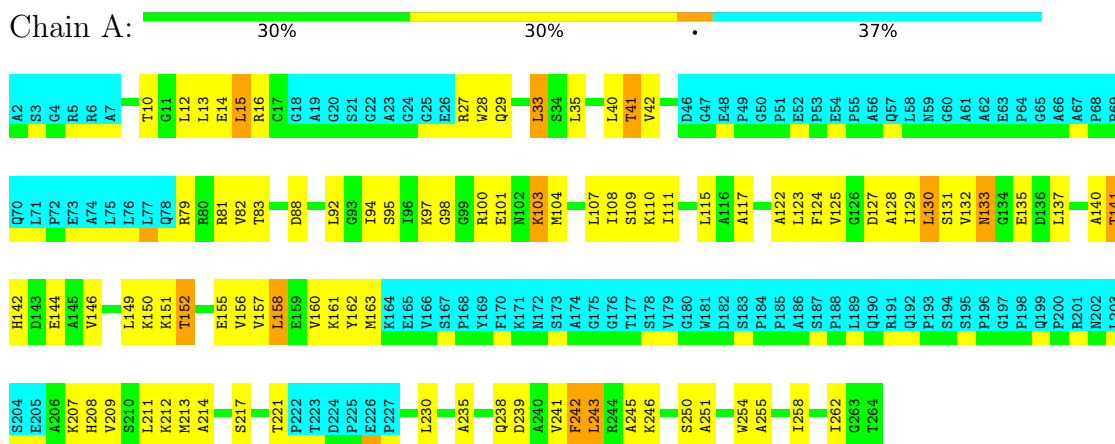
Mol	Chain	Residues	Atoms						Trace
1	A	263	Total	C	H	N	O	S	0
			3906	1207	1960	355	378	6	

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Alpha-1-syntrophin

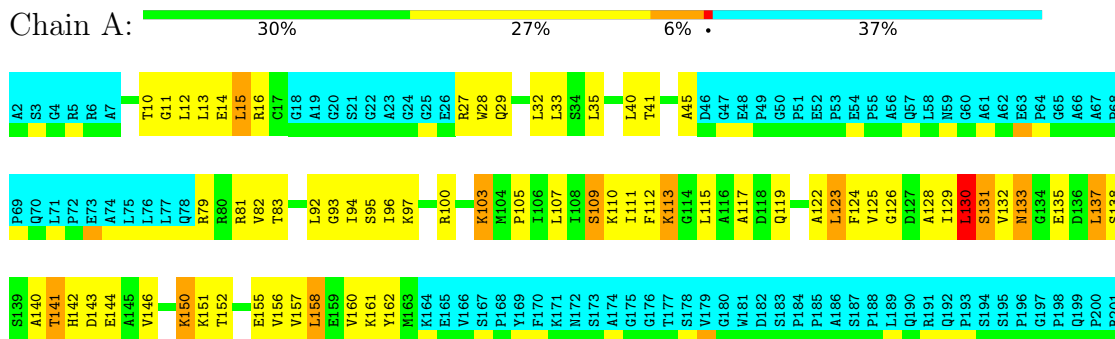


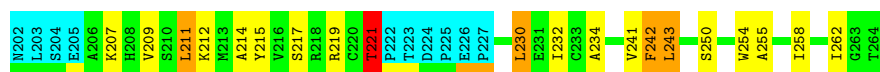
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

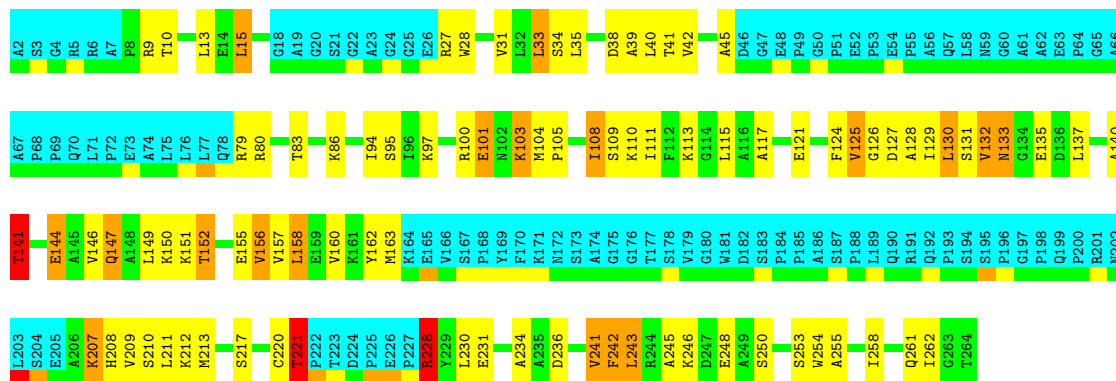
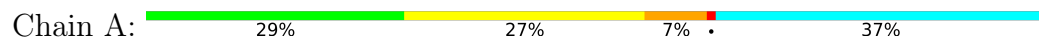
- Molecule 1: Alpha-1-syntrophin





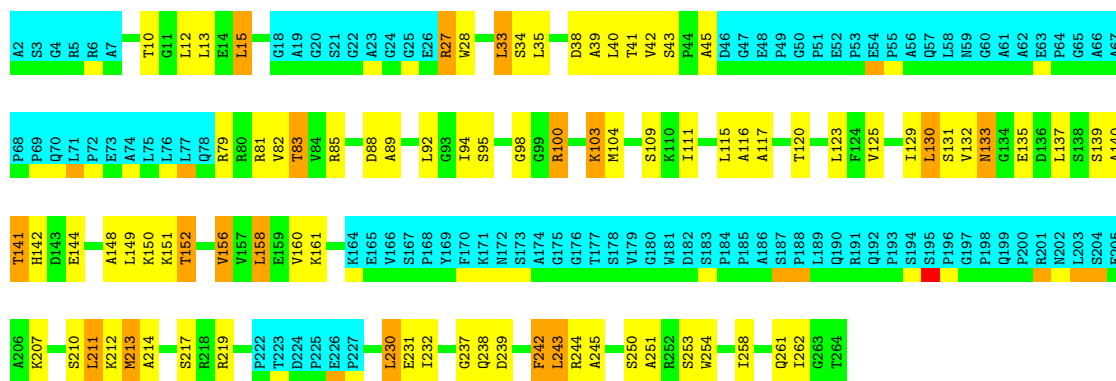
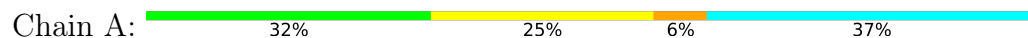
4.2.2 Score per residue for model 2

- Molecule 1: Alpha-1-syntrophin



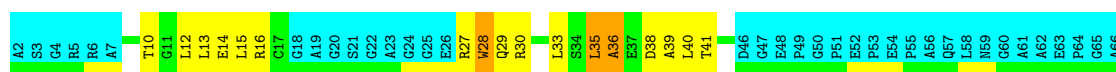
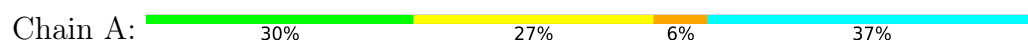
4.2.3 Score per residue for model 3 (medoid)

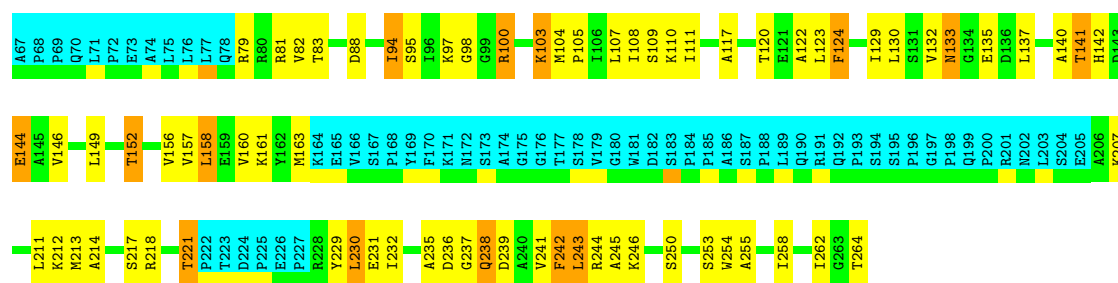
- Molecule 1: Alpha-1-syntrophin



4.2.4 Score per residue for model 4

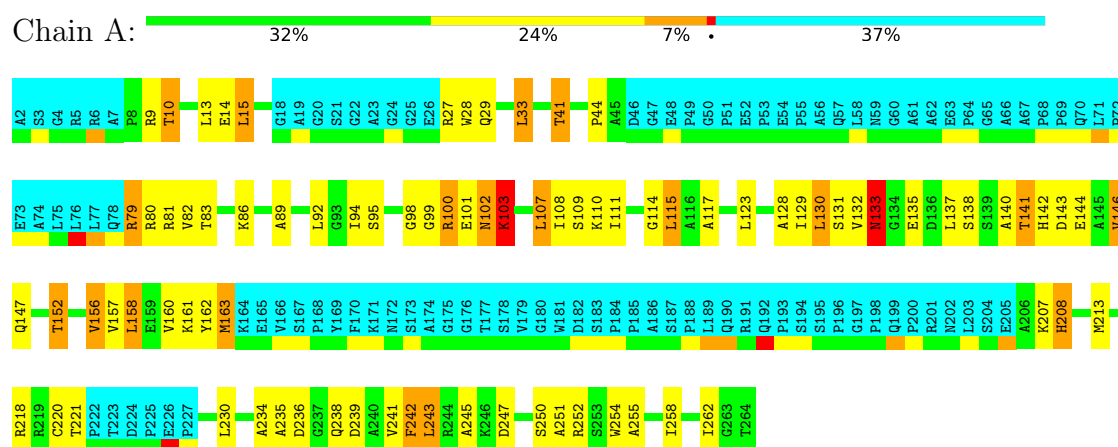
- Molecule 1: Alpha-1-syntrophin





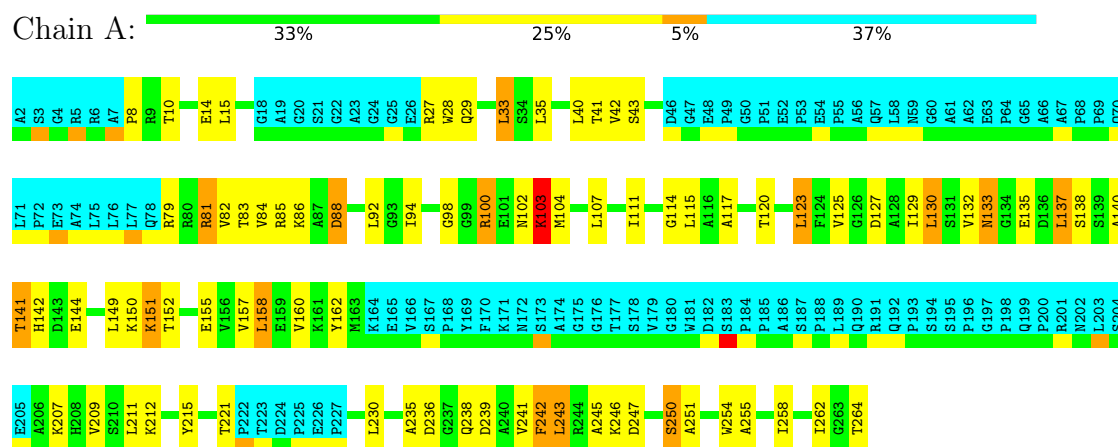
4.2.5 Score per residue for model 5

- Molecule 1: Alpha-1-syntrophin



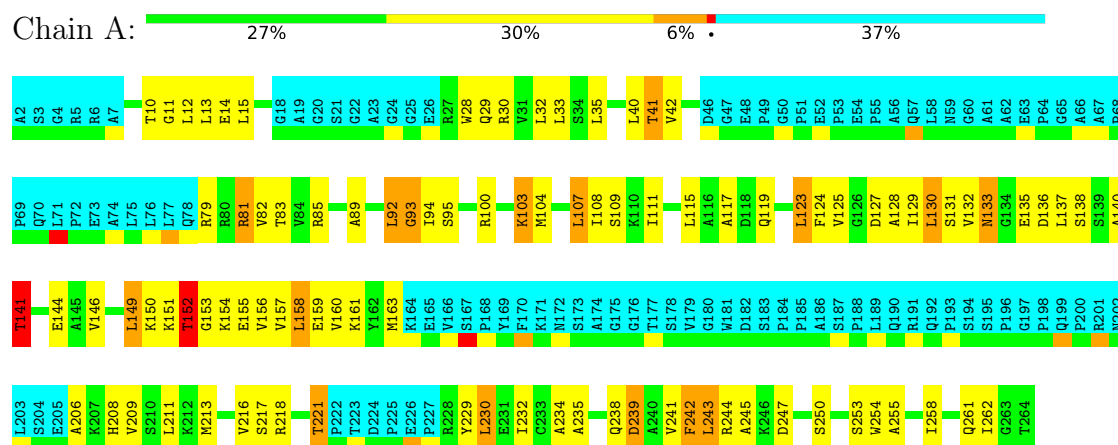
4.2.6 Score per residue for model 6

- Molecule 1: Alpha-1-syntrophin



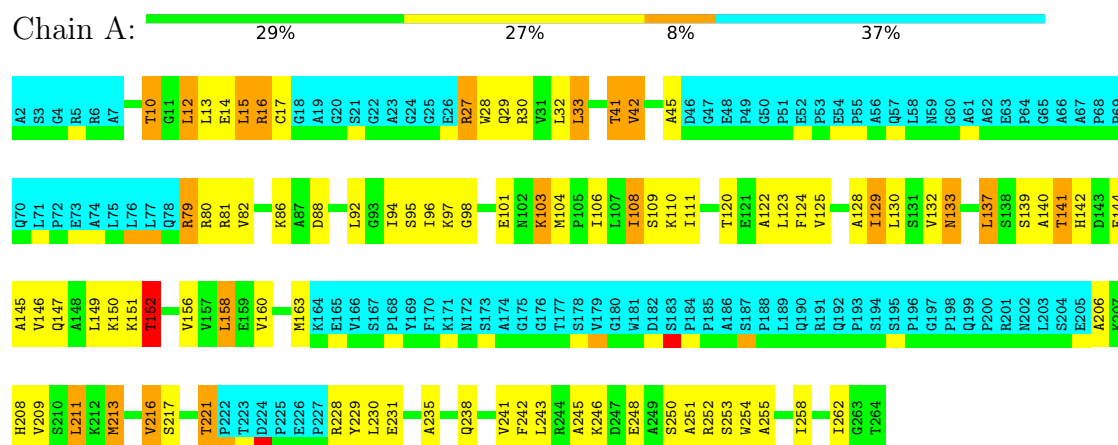
4.2.7 Score per residue for model 7

- Molecule 1: Alpha-1-syntrophin



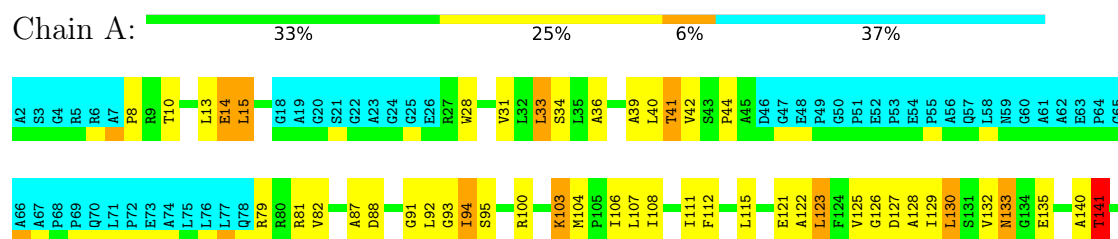
4.2.8 Score per residue for model 8

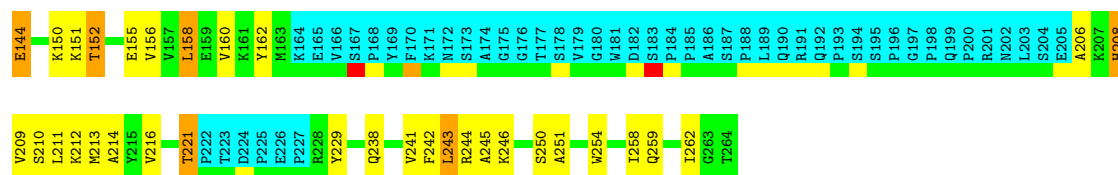
- Molecule 1: Alpha-1-syntrophin



4.2.9 Score per residue for model 9

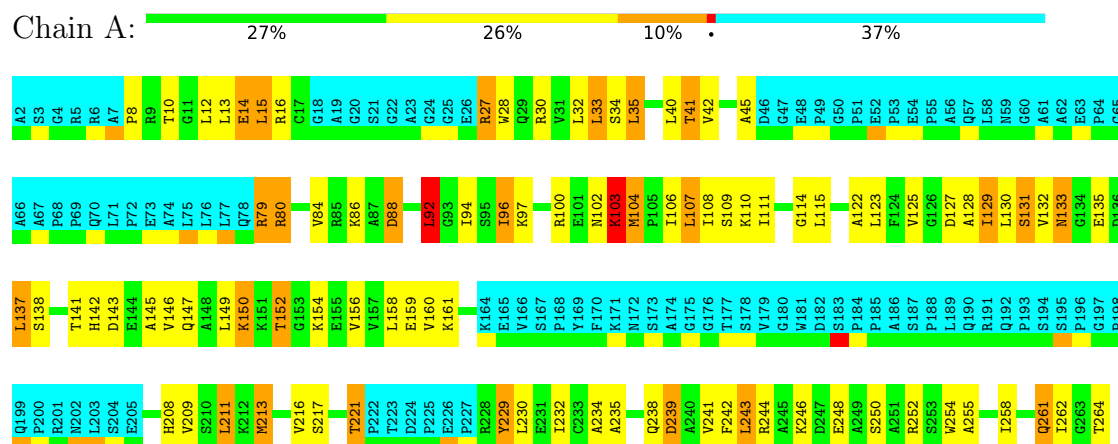
- Molecule 1: Alpha-1-syntrophin





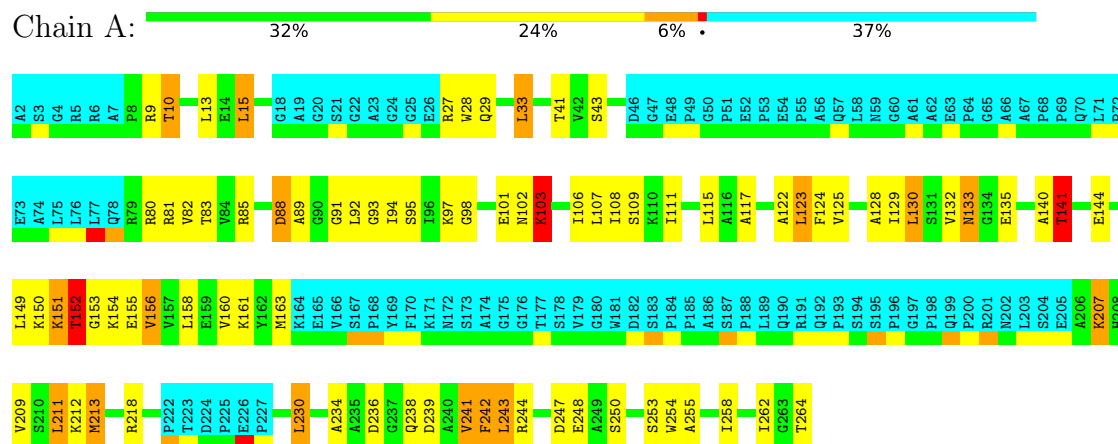
4.2.10 Score per residue for model 10

- Molecule 1: Alpha-1-syntrophin



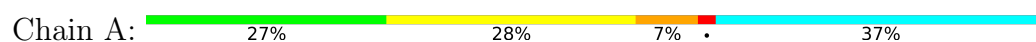
4.2.11 Score per residue for model 11

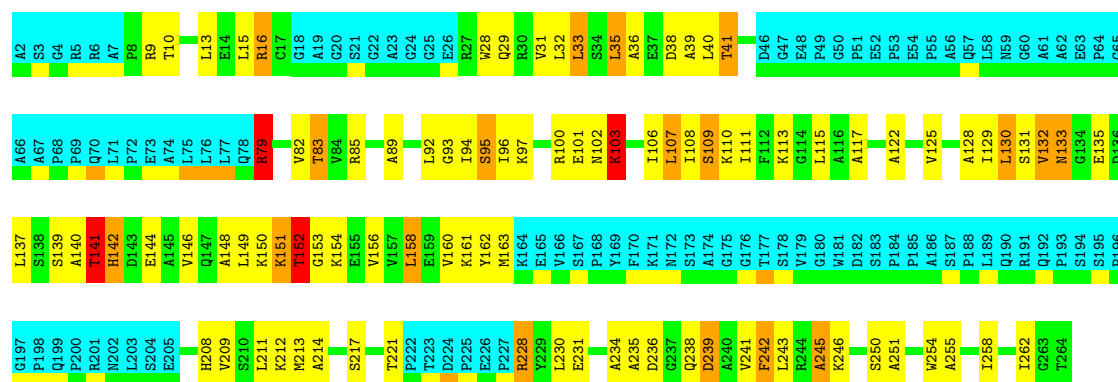
- Molecule 1: Alpha-1-syntrophin



4.2.12 Score per residue for model 12

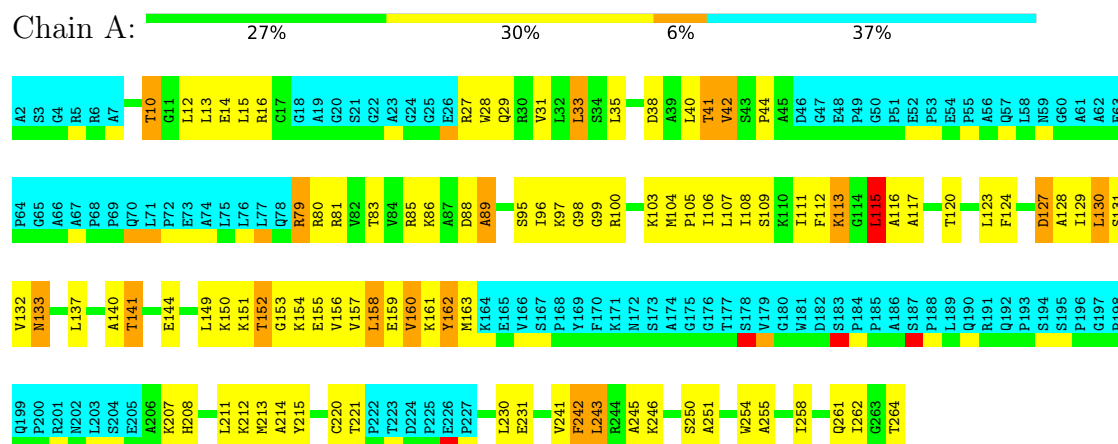
- Molecule 1: Alpha-1-syntrophin





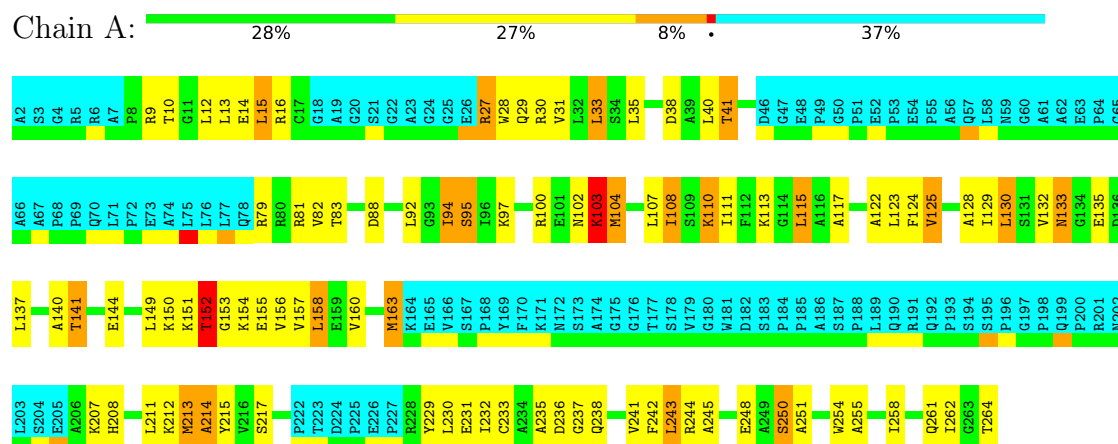
4.2.13 Score per residue for model 13

- Molecule 1: Alpha-1-syntrophin



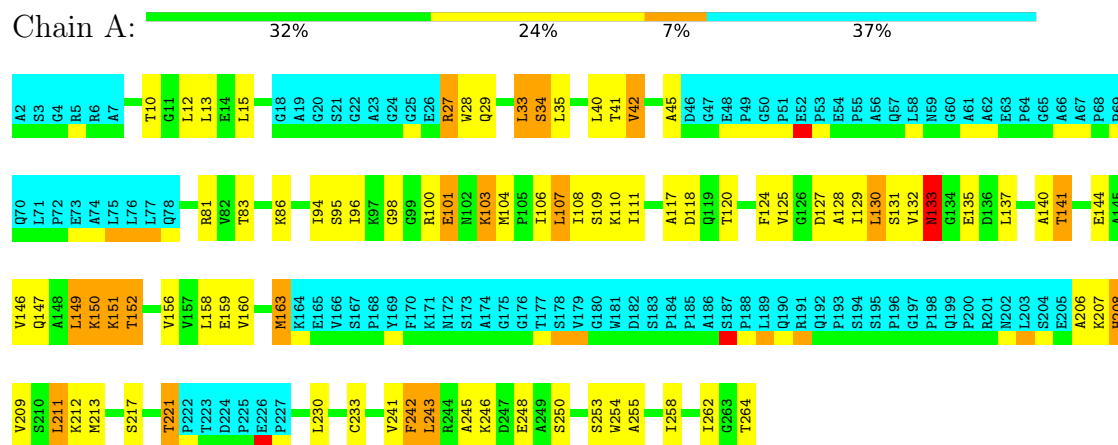
4.2.14 Score per residue for model 14

- Molecule 1: Alpha-1-syntrophin



4.2.15 Score per residue for model 15

• Molecule 1: Alpha-1-syntrophin



5 Refinement protocol and experimental data overview ⓘ

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

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
CNS	refinement	1.1

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.28±0.00	0±0/1285 (0.0± 0.0%)	0.61±0.02	0±0/1727 (0.0± 0.0%)
All	All	0.28	0/19275 (0.0%)	0.61	1/25905 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	156	VAL	N-CA-C	5.19	111.77	106.21	2	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1271	1326	1324	56±7
All	All	19065	19890	19860	846

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 22.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:230:LEU:HD21	1:A:255:ALA:HB2	1.04	1.27	15	7

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:96:ILE:HD11	1:A:146:VAL:HG22	0.98	1.26	8	1
1:A:258:ILE:HG22	1:A:262:ILE:HD11	0.98	1.34	6	4
1:A:83:THR:HG23	1:A:157:VAL:HG22	0.93	1.37	5	7
1:A:245:ALA:HB2	1:A:251:ALA:HB2	0.92	1.39	14	1
1:A:13:LEU:HD13	1:A:243:LEU:HD13	0.90	1.41	14	2
1:A:132:VAL:HG13	1:A:158:LEU:HD12	0.87	1.45	3	5
1:A:108:ILE:HG21	1:A:111:ILE:HD11	0.86	1.47	13	5
1:A:152:THR:HG21	1:A:156:VAL:HG13	0.85	1.46	9	8
1:A:230:LEU:HD22	1:A:255:ALA:HB2	0.84	1.49	1	4
1:A:140:ALA:HB1	1:A:144:GLU:CB	0.82	2.04	1	13
1:A:258:ILE:HG22	1:A:262:ILE:CD1	0.81	2.06	2	11
1:A:13:LEU:CD1	1:A:243:LEU:HD13	0.80	2.07	14	1
1:A:245:ALA:HB3	1:A:251:ALA:HB2	0.80	1.52	6	6
1:A:230:LEU:CD2	1:A:255:ALA:HB2	0.80	2.06	5	8
1:A:111:ILE:HG23	1:A:117:ALA:HB1	0.79	1.53	14	10
1:A:230:LEU:HD21	1:A:255:ALA:CB	0.79	2.06	15	1
1:A:40:LEU:HD23	1:A:211:LEU:HD12	0.78	1.56	7	2
1:A:40:LEU:HD23	1:A:211:LEU:HD21	0.77	1.53	10	3
1:A:82:VAL:HG13	1:A:122:ALA:HB3	0.77	1.56	14	7
1:A:149:LEU:HD12	1:A:150:LYS:N	0.77	1.93	2	9
1:A:140:ALA:HB1	1:A:144:GLU:HB3	0.77	1.55	13	13
1:A:130:LEU:HD12	1:A:131:SER:OG	0.76	1.81	1	1
1:A:232:ILE:CD1	1:A:243:LEU:HD21	0.75	2.11	14	1
1:A:242:PHE:C	1:A:243:LEU:HD13	0.74	2.07	13	9
1:A:242:PHE:C	1:A:243:LEU:HD22	0.74	2.07	8	4
1:A:258:ILE:CG2	1:A:262:ILE:HD11	0.74	2.12	6	7
1:A:129:ILE:HA	1:A:160:VAL:HG12	0.73	1.60	6	14
1:A:12:LEU:O	1:A:13:LEU:HD23	0.72	1.84	1	5
1:A:242:PHE:O	1:A:243:LEU:HD22	0.72	1.84	5	4
1:A:12:LEU:HD21	1:A:45:ALA:CB	0.72	2.15	1	2
1:A:137:LEU:HD23	1:A:140:ALA:HB3	0.72	1.62	8	2
1:A:132:VAL:HG23	1:A:158:LEU:HD12	0.72	1.60	9	3
1:A:235:ALA:HB3	1:A:238:GLN:HG3	0.71	1.61	14	2
1:A:211:LEU:HD12	1:A:262:ILE:HG12	0.70	1.61	15	2
1:A:100:ARG:CB	1:A:141:THR:HG22	0.70	2.16	3	4
1:A:14:GLU:C	1:A:15:LEU:HD23	0.70	2.12	10	2
1:A:152:THR:OG1	1:A:156:VAL:HG22	0.69	1.87	11	2
1:A:33:LEU:HD12	1:A:42:VAL:HG13	0.69	1.62	7	6
1:A:38:ASP:C	1:A:211:LEU:HD13	0.69	2.12	14	2
1:A:36:ALA:HB3	1:A:39:ALA:O	0.68	1.88	9	3
1:A:213:MET:HB3	1:A:235:ALA:HB2	0.68	1.63	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:245:ALA:CB	1:A:251:ALA:HB2	0.68	2.17	14	5
1:A:108:ILE:HG21	1:A:111:ILE:CD1	0.68	2.17	13	3
1:A:13:LEU:HD21	1:A:254:TRP:NE1	0.68	2.03	10	8
1:A:146:VAL:HG12	1:A:150:LYS:CE	0.67	2.19	15	1
1:A:209:VAL:CG1	1:A:234:ALA:HB2	0.67	2.20	11	4
1:A:82:VAL:HG21	1:A:123:LEU:HG	0.66	1.65	1	1
1:A:232:ILE:HD12	1:A:243:LEU:HD11	0.66	1.67	3	4
1:A:213:MET:HE2	1:A:213:MET:C	0.66	2.14	3	1
1:A:235:ALA:HB3	1:A:238:GLN:OE1	0.66	1.90	12	1
1:A:94:ILE:HG23	1:A:117:ALA:HB2	0.66	1.66	11	7
1:A:28:TRP:CD1	1:A:28:TRP:N	0.66	2.61	4	15
1:A:13:LEU:HD13	1:A:243:LEU:CD1	0.65	2.21	14	1
1:A:209:VAL:HG13	1:A:239:ASP:HB2	0.65	1.66	11	1
1:A:214:ALA:HB3	1:A:262:ILE:HD13	0.65	1.67	1	5
1:A:94:ILE:HG22	1:A:111:ILE:HA	0.65	1.69	2	12
1:A:15:LEU:HD23	1:A:16:ARG:O	0.65	1.91	8	2
1:A:98:GLY:HA3	1:A:106:ILE:HD13	0.65	1.66	11	3
1:A:146:VAL:HG12	1:A:150:LYS:HE3	0.65	1.69	15	1
1:A:115:LEU:HD22	1:A:115:LEU:N	0.65	2.07	13	1
1:A:107:LEU:CD2	1:A:128:ALA:HB2	0.65	2.22	10	7
1:A:40:LEU:CD2	1:A:211:LEU:HD21	0.65	2.21	10	1
1:A:123:LEU:HD13	1:A:123:LEU:N	0.64	2.07	6	2
1:A:96:ILE:HD12	1:A:142:HIS:CE1	0.64	2.26	8	1
1:A:207:LYS:HE2	1:A:241:VAL:HG13	0.64	1.68	2	1
1:A:221:THR:HG21	1:A:229:TYR:CE2	0.64	2.27	7	1
1:A:15:LEU:HD22	1:A:242:PHE:O	0.64	1.93	14	4
1:A:93:GLY:HA3	1:A:115:LEU:HD13	0.62	1.71	1	3
1:A:156:VAL:HG12	1:A:158:LEU:HD12	0.62	1.71	4	4
1:A:107:LEU:HD23	1:A:128:ALA:HB2	0.62	1.72	5	4
1:A:243:LEU:HD13	1:A:243:LEU:N	0.62	2.10	4	8
1:A:221:THR:HG21	1:A:229:TYR:CZ	0.62	2.29	7	1
1:A:137:LEU:HD22	1:A:140:ALA:CB	0.61	2.25	7	2
1:A:85:ARG:O	1:A:89:ALA:HB3	0.61	1.96	3	3
1:A:12:LEU:HD21	1:A:45:ALA:HB2	0.61	1.72	3	2
1:A:140:ALA:HB1	1:A:144:GLU:HB2	0.61	1.72	4	10
1:A:258:ILE:HG22	1:A:262:ILE:HD12	0.61	1.73	14	10
1:A:35:LEU:HD21	1:A:261:GLN:HG3	0.61	1.70	3	3
1:A:245:ALA:HB1	1:A:250:SER:CB	0.60	2.26	4	3
1:A:152:THR:OG1	1:A:153:GLY:N	0.60	2.31	11	4
1:A:211:LEU:HD12	1:A:262:ILE:CG1	0.60	2.26	15	2
1:A:101:GLU:N	1:A:141:THR:HG22	0.60	2.11	8	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:137:LEU:HB3	1:A:140:ALA:HB3	0.60	1.73	13	3
1:A:13:LEU:HD12	1:A:33:LEU:HB2	0.60	1.74	3	1
1:A:214:ALA:O	1:A:262:ILE:HD13	0.60	1.96	4	1
1:A:235:ALA:HB3	1:A:238:GLN:HG2	0.60	1.73	7	4
1:A:13:LEU:HD22	1:A:244:ARG:O	0.59	1.97	4	1
1:A:92:LEU:HD12	1:A:92:LEU:O	0.59	1.97	6	1
1:A:211:LEU:HD22	1:A:262:ILE:HG12	0.59	1.75	10	2
1:A:107:LEU:HD23	1:A:128:ALA:HA	0.59	1.73	11	1
1:A:82:VAL:HG11	1:A:123:LEU:HG	0.59	1.73	14	1
1:A:94:ILE:HD13	1:A:94:ILE:N	0.59	2.13	4	1
1:A:30:ARG:HD2	1:A:45:ALA:HB3	0.59	1.73	8	1
1:A:137:LEU:HD12	1:A:140:ALA:HB3	0.58	1.74	1	1
1:A:211:LEU:HD23	1:A:262:ILE:HG13	0.58	1.72	1	1
1:A:114:GLY:O	1:A:115:LEU:HD12	0.58	1.97	6	2
1:A:234:ALA:HB3	1:A:239:ASP:CB	0.58	2.28	7	3
1:A:42:VAL:O	1:A:206:ALA:HB1	0.58	1.99	7	4
1:A:40:LEU:HD23	1:A:211:LEU:HD11	0.58	1.75	12	2
1:A:94:ILE:HD12	1:A:96:ILE:CG2	0.58	2.28	8	2
1:A:94:ILE:HD12	1:A:96:ILE:HG23	0.57	1.75	8	3
1:A:116:ALA:O	1:A:120:THR:HG23	0.57	1.99	13	2
1:A:40:LEU:HD23	1:A:211:LEU:CD1	0.57	2.28	1	2
1:A:111:ILE:HG23	1:A:117:ALA:CB	0.57	2.26	14	3
1:A:108:ILE:O	1:A:125:VAL:HG23	0.57	2.00	7	1
1:A:213:MET:HE2	1:A:213:MET:O	0.56	2.00	11	1
1:A:245:ALA:HB2	1:A:251:ALA:CB	0.56	2.25	14	1
1:A:243:LEU:HD22	1:A:243:LEU:N	0.56	2.16	13	2
1:A:211:LEU:HD21	1:A:262:ILE:HA	0.56	1.76	7	1
1:A:82:VAL:HG13	1:A:122:ALA:CB	0.56	2.30	11	2
1:A:41:THR:HG23	1:A:208:HIS:CG	0.56	2.35	10	6
1:A:129:ILE:CA	1:A:160:VAL:HG12	0.56	2.30	1	12
1:A:83:THR:CG2	1:A:157:VAL:HG22	0.56	2.27	6	3
1:A:132:VAL:HG22	1:A:158:LEU:HG	0.56	1.78	14	4
1:A:39:ALA:N	1:A:211:LEU:HD13	0.56	2.16	3	1
1:A:123:LEU:HD12	1:A:123:LEU:O	0.56	2.01	5	1
1:A:39:ALA:N	1:A:211:LEU:HD12	0.56	2.16	2	1
1:A:35:LEU:HD12	1:A:40:LEU:HB3	0.56	1.78	3	2
1:A:245:ALA:HB1	1:A:250:SER:HB2	0.56	1.76	4	2
1:A:82:VAL:HG21	1:A:123:LEU:HD12	0.56	1.77	6	1
1:A:11:GLY:O	1:A:32:LEU:HD12	0.56	2.01	7	1
1:A:38:ASP:O	1:A:211:LEU:HD13	0.56	2.01	14	1
1:A:11:GLY:C	1:A:32:LEU:HD12	0.56	2.26	7	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:100:ARG:HB3	1:A:141:THR:HG22	0.56	1.78	3	2
1:A:13:LEU:HD13	1:A:243:LEU:CD2	0.55	2.31	11	3
1:A:108:ILE:HG13	1:A:123:LEU:HD21	0.55	1.78	10	1
1:A:143:ASP:O	1:A:146:VAL:HG12	0.55	2.01	10	2
1:A:114:GLY:C	1:A:115:LEU:HD22	0.55	2.27	10	1
1:A:10:THR:HG22	1:A:33:LEU:O	0.55	2.01	13	3
1:A:15:LEU:HD12	1:A:243:LEU:HD12	0.54	1.79	1	1
1:A:132:VAL:HG12	1:A:158:LEU:HD12	0.54	1.78	2	1
1:A:108:ILE:O	1:A:125:VAL:HG13	0.54	2.02	11	1
1:A:132:VAL:HG21	1:A:137:LEU:HD11	0.54	1.79	12	1
1:A:243:LEU:N	1:A:243:LEU:HD22	0.54	2.17	7	1
1:A:15:LEU:N	1:A:15:LEU:HD23	0.54	2.16	9	1
1:A:209:VAL:HG22	1:A:239:ASP:OD2	0.54	2.03	12	1
1:A:149:LEU:C	1:A:149:LEU:HD12	0.54	2.28	11	4
1:A:13:LEU:HD12	1:A:33:LEU:HD13	0.54	1.80	8	3
1:A:91:GLY:O	1:A:115:LEU:HD22	0.54	2.02	9	1
1:A:243:LEU:HD22	1:A:243:LEU:H	0.54	1.61	7	3
1:A:125:VAL:O	1:A:125:VAL:HG13	0.54	2.02	2	3
1:A:40:LEU:O	1:A:40:LEU:HD12	0.54	2.03	9	5
1:A:106:ILE:HG23	1:A:142:HIS:CE1	0.54	2.38	8	1
1:A:232:ILE:CD1	1:A:243:LEU:HD11	0.54	2.33	4	2
1:A:96:ILE:HD11	1:A:146:VAL:CG2	0.54	2.19	8	1
1:A:114:GLY:O	1:A:115:LEU:HD22	0.53	2.02	10	1
1:A:152:THR:CG2	1:A:156:VAL:HG22	0.53	2.33	13	1
1:A:230:LEU:HD11	1:A:251:ALA:HB1	0.53	1.79	14	1
1:A:152:THR:HG21	1:A:156:VAL:HA	0.53	1.79	5	1
1:A:132:VAL:HG13	1:A:158:LEU:CD1	0.53	2.34	7	2
1:A:38:ASP:HA	1:A:211:LEU:HD22	0.53	1.78	13	1
1:A:229:TYR:CZ	1:A:242:PHE:CD1	0.53	2.97	8	1
1:A:214:ALA:HB3	1:A:262:ILE:CD1	0.53	2.33	1	1
1:A:102:ASN:C	1:A:103:LYS:HG3	0.53	2.26	10	1
1:A:38:ASP:C	1:A:211:LEU:HD12	0.53	2.28	2	1
1:A:13:LEU:HD13	1:A:243:LEU:HD23	0.53	1.81	1	2
1:A:152:THR:HG21	1:A:156:VAL:CG1	0.53	2.33	15	3
1:A:125:VAL:O	1:A:125:VAL:HG22	0.53	2.04	3	2
1:A:96:ILE:HD12	1:A:106:ILE:CG2	0.53	2.34	15	3
1:A:137:LEU:HD23	1:A:140:ALA:CB	0.52	2.32	8	2
1:A:127:ASP:HB3	1:A:160:VAL:HG11	0.52	1.79	13	1
1:A:149:LEU:HD12	1:A:149:LEU:C	0.52	2.29	3	5
1:A:100:ARG:HB2	1:A:141:THR:HG22	0.52	1.79	5	3
1:A:209:VAL:HG12	1:A:211:LEU:H	0.52	1.63	15	5

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:156:VAL:HG12	1:A:158:LEU:CD1	0.52	2.34	14	2
1:A:82:VAL:HG11	1:A:123:LEU:CD1	0.52	2.34	11	1
1:A:137:LEU:HD13	1:A:140:ALA:HB3	0.52	1.81	14	2
1:A:113:LYS:HB3	1:A:115:LEU:HD13	0.52	1.81	13	1
1:A:82:VAL:CG1	1:A:122:ALA:HB3	0.52	2.35	11	1
1:A:108:ILE:CD1	1:A:108:ILE:N	0.51	2.74	2	3
1:A:33:LEU:HD13	1:A:243:LEU:HG	0.51	1.82	5	2
1:A:96:ILE:CD1	1:A:142:HIS:CE1	0.51	2.94	8	1
1:A:94:ILE:CG2	1:A:117:ALA:HB2	0.51	2.36	3	3
1:A:215:TYR:CE1	1:A:264:THR:HG21	0.51	2.40	6	1
1:A:94:ILE:HD13	1:A:94:ILE:H	0.50	1.65	4	1
1:A:215:TYR:CD1	1:A:264:THR:HG21	0.50	2.41	14	1
1:A:112:PHE:O	1:A:115:LEU:HD12	0.50	2.05	1	1
1:A:210:SER:O	1:A:211:LEU:HD23	0.50	2.06	2	1
1:A:82:VAL:HG11	1:A:123:LEU:HD23	0.50	1.82	7	1
1:A:213:MET:HE2	1:A:214:ALA:N	0.50	2.21	3	1
1:A:132:VAL:HG13	1:A:158:LEU:HG	0.50	1.82	4	1
1:A:15:LEU:HD23	1:A:15:LEU:N	0.50	2.22	10	1
1:A:96:ILE:HD12	1:A:142:HIS:CD2	0.50	2.42	10	2
1:A:81:ARG:O	1:A:81:ARG:HG2	0.50	2.06	7	1
1:A:137:LEU:HD11	1:A:148:ALA:CB	0.50	2.37	3	1
1:A:229:TYR:CZ	1:A:242:PHE:CE1	0.50	3.00	8	1
1:A:132:VAL:CG1	1:A:158:LEU:HD12	0.50	2.27	3	2
1:A:209:VAL:HG22	1:A:239:ASP:CB	0.50	2.37	11	1
1:A:207:LYS:CE	1:A:241:VAL:HG13	0.49	2.37	2	1
1:A:81:ARG:O	1:A:81:ARG:CG	0.49	2.60	7	1
1:A:146:VAL:HA	1:A:149:LEU:HD23	0.49	1.83	15	2
1:A:15:LEU:HD12	1:A:31:VAL:HG21	0.49	1.85	2	1
1:A:92:LEU:HD21	1:A:149:LEU:HD13	0.49	1.83	8	1
1:A:96:ILE:HD12	1:A:106:ILE:HG21	0.49	1.84	12	1
1:A:16:ARG:CG	1:A:28:TRP:CD1	0.49	2.95	4	1
1:A:115:LEU:HD23	1:A:117:ALA:HB3	0.49	1.83	13	1
1:A:132:VAL:CG2	1:A:137:LEU:HD12	0.49	2.38	7	1
1:A:129:ILE:HG21	1:A:132:VAL:CG2	0.49	2.38	4	1
1:A:30:ARG:O	1:A:31:VAL:HG13	0.49	2.07	14	1
1:A:88:ASP:O	1:A:89:ALA:HB2	0.49	2.08	13	1
1:A:132:VAL:O	1:A:133:ASN:C	0.49	2.56	4	15
1:A:245:ALA:HB2	1:A:254:TRP:HD1	0.49	1.67	2	1
1:A:82:VAL:HG22	1:A:122:ALA:HB1	0.49	1.84	12	1
1:A:213:MET:HA	1:A:264:THR:HG21	0.48	1.85	10	1
1:A:94:ILE:HG23	1:A:117:ALA:CB	0.48	2.39	7	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:229:TYR:CE1	1:A:242:PHE:CD1	0.48	3.01	8	1
1:A:229:TYR:CE2	1:A:242:PHE:CE1	0.48	3.02	8	1
1:A:229:TYR:CZ	1:A:242:PHE:CZ	0.48	3.01	10	1
1:A:209:VAL:HG22	1:A:239:ASP:HB3	0.48	1.85	11	1
1:A:97:LYS:N	1:A:142:HIS:CE1	0.48	2.81	8	1
1:A:132:VAL:HG12	1:A:158:LEU:CD1	0.48	2.37	2	1
1:A:92:LEU:HD22	1:A:149:LEU:HD13	0.48	1.84	7	1
1:A:128:ALA:HB3	1:A:163:MET:SD	0.48	2.49	5	1
1:A:242:PHE:CD1	1:A:243:LEU:N	0.48	2.82	14	2
1:A:130:LEU:HD23	1:A:130:LEU:N	0.48	2.23	13	1
1:A:150:LYS:HG2	1:A:151:LYS:N	0.48	2.24	14	1
1:A:100:ARG:HG3	1:A:141:THR:HG23	0.48	1.86	7	1
1:A:209:VAL:HG13	1:A:234:ALA:HB2	0.48	1.86	11	1
1:A:82:VAL:HG11	1:A:123:LEU:HD13	0.48	1.86	11	1
1:A:133:ASN:HD21	1:A:156:VAL:HG13	0.48	1.67	14	1
1:A:97:LYS:C	1:A:142:HIS:CE1	0.47	2.92	8	1
1:A:82:VAL:HG11	1:A:123:LEU:HD12	0.47	1.87	1	1
1:A:83:THR:O	1:A:120:THR:HG21	0.47	2.09	4	1
1:A:105:PRO:O	1:A:107:LEU:HD12	0.47	2.08	1	3
1:A:98:GLY:N	1:A:142:HIS:CD2	0.47	2.83	3	4
1:A:123:LEU:HD12	1:A:123:LEU:C	0.47	2.35	5	1
1:A:108:ILE:HD11	1:A:123:LEU:HD21	0.47	1.85	9	1
1:A:35:LEU:HD11	1:A:258:ILE:HG12	0.47	1.87	12	1
1:A:31:VAL:HG12	1:A:44:PRO:HA	0.47	1.87	13	2
1:A:150:LYS:CG	1:A:151:LYS:N	0.47	2.77	3	5
1:A:216:VAL:CG2	1:A:217:SER:N	0.47	2.77	8	1
1:A:137:LEU:HD21	1:A:145:ALA:HA	0.46	1.86	10	1
1:A:147:GLN:HA	1:A:150:LYS:HD2	0.46	1.87	15	1
1:A:80:ARG:HH11	1:A:122:ALA:HB1	0.46	1.70	10	1
1:A:211:LEU:HD22	1:A:262:ILE:HA	0.46	1.87	2	1
1:A:245:ALA:HB1	1:A:250:SER:OG	0.46	2.11	15	1
1:A:79:ARG:HD3	1:A:130:LEU:HD11	0.46	1.86	13	2
1:A:108:ILE:HD11	1:A:123:LEU:HD11	0.46	1.88	10	1
1:A:41:THR:HB	1:A:208:HIS:CD2	0.46	2.46	15	1
1:A:132:VAL:HG23	1:A:158:LEU:CD1	0.46	2.39	15	1
1:A:98:GLY:N	1:A:142:HIS:CE1	0.46	2.84	8	1
1:A:35:LEU:HD23	1:A:261:GLN:HB2	0.46	1.86	10	1
1:A:155:GLU:O	1:A:155:GLU:CG	0.46	2.64	13	3
1:A:242:PHE:C	1:A:242:PHE:CD1	0.46	2.94	5	7
1:A:102:ASN:C	1:A:103:LYS:CD	0.46	2.89	6	5
1:A:40:LEU:HD23	1:A:211:LEU:HD22	0.45	1.87	15	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:ALA:CB	1:A:163:MET:HE2	0.45	2.41	15	1
1:A:137:LEU:CD2	1:A:140:ALA:HB3	0.45	2.37	8	1
1:A:212:LYS:O	1:A:213:MET:CB	0.45	2.64	14	1
1:A:111:ILE:HG22	1:A:111:ILE:O	0.45	2.12	14	2
1:A:245:ALA:HB1	1:A:250:SER:HB3	0.45	1.88	2	2
1:A:83:THR:HG23	1:A:157:VAL:CG2	0.45	2.26	5	1
1:A:250:SER:O	1:A:254:TRP:CD1	0.45	2.70	2	15
1:A:137:LEU:HD11	1:A:148:ALA:HB1	0.45	1.88	3	1
1:A:13:LEU:HB2	1:A:243:LEU:HD12	0.45	1.88	5	1
1:A:216:VAL:HG21	1:A:259:GLN:CG	0.45	2.42	9	1
1:A:15:LEU:CD1	1:A:243:LEU:HD12	0.45	2.41	11	1
1:A:140:ALA:O	1:A:141:THR:O	0.45	2.35	1	7
1:A:147:GLN:HA	1:A:150:LYS:HG2	0.45	1.88	2	1
1:A:211:LEU:O	1:A:262:ILE:HG23	0.45	2.12	4	1
1:A:123:LEU:HD22	1:A:123:LEU:H	0.45	1.72	11	1
1:A:33:LEU:HD12	1:A:42:VAL:CG1	0.45	2.42	13	1
1:A:115:LEU:N	1:A:115:LEU:CD2	0.45	2.78	13	1
1:A:13:LEU:HD12	1:A:33:LEU:HD22	0.45	1.89	11	1
1:A:137:LEU:HD13	1:A:140:ALA:CB	0.45	2.42	14	1
1:A:148:ALA:O	1:A:152:THR:HG22	0.44	2.12	12	1
1:A:220:CYS:C	1:A:221:THR:HG22	0.44	2.36	2	1
1:A:12:LEU:CD2	1:A:45:ALA:HB2	0.44	2.40	3	1
1:A:96:ILE:CG1	1:A:142:HIS:CE1	0.44	3.00	8	1
1:A:15:LEU:HD22	1:A:243:LEU:HB3	0.44	1.90	9	1
1:A:129:ILE:C	1:A:130:LEU:HD23	0.44	2.38	13	1
1:A:129:ILE:HG22	1:A:130:LEU:N	0.44	2.28	1	12
1:A:108:ILE:HG22	1:A:125:VAL:HA	0.44	1.90	2	1
1:A:235:ALA:HB3	1:A:238:GLN:CG	0.44	2.43	7	1
1:A:97:LYS:CA	1:A:142:HIS:CE1	0.44	3.00	8	1
1:A:34:SER:HB2	1:A:41:THR:HG23	0.44	1.90	15	1
1:A:92:LEU:HD21	1:A:94:ILE:HG12	0.44	1.87	1	1
1:A:105:PRO:HG3	1:A:163:MET:HE3	0.44	1.90	2	1
1:A:229:TYR:CD1	1:A:229:TYR:C	0.44	2.96	14	1
1:A:106:ILE:HG22	1:A:129:ILE:HD12	0.44	1.90	11	1
1:A:35:LEU:HD11	1:A:211:LEU:HD21	0.43	1.90	1	1
1:A:146:VAL:O	1:A:149:LEU:HG	0.43	2.13	12	1
1:A:230:LEU:HD11	1:A:251:ALA:CB	0.43	2.42	14	1
1:A:221:THR:CG2	1:A:229:TYR:CE2	0.43	2.99	7	1
1:A:243:LEU:N	1:A:243:LEU:CD1	0.43	2.82	10	1
1:A:103:LYS:CD	1:A:103:LYS:N	0.43	2.82	5	5
1:A:41:THR:HG1	1:A:208:HIS:CE1	0.43	2.31	9	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:216:VAL:HG11	1:A:258:ILE:HB	0.43	1.89	7	2
1:A:79:ARG:CD	1:A:130:LEU:HD11	0.43	2.44	13	1
1:A:152:THR:CG2	1:A:156:VAL:HG13	0.43	2.41	4	1
1:A:129:ILE:HG12	1:A:158:LEU:HD23	0.43	1.90	7	1
1:A:209:VAL:HG12	1:A:210:SER:N	0.43	2.29	9	1
1:A:145:ALA:O	1:A:149:LEU:HD23	0.43	2.14	8	1
1:A:128:ALA:HB3	1:A:163:MET:HE3	0.43	1.91	8	1
1:A:216:VAL:CG1	1:A:258:ILE:HG21	0.43	2.44	7	1
1:A:13:LEU:HD12	1:A:243:LEU:HG	0.42	1.89	2	1
1:A:242:PHE:CD1	1:A:242:PHE:O	0.42	2.72	2	1
1:A:40:LEU:HD12	1:A:40:LEU:C	0.42	2.39	10	1
1:A:229:TYR:CD1	1:A:229:TYR:O	0.42	2.72	4	1
1:A:232:ILE:HD12	1:A:243:LEU:HD21	0.42	1.87	14	1
1:A:13:LEU:CD1	1:A:33:LEU:HD22	0.42	2.44	11	1
1:A:94:ILE:CG2	1:A:117:ALA:CB	0.42	2.98	4	6
1:A:95:SER:O	1:A:109:SER:CB	0.42	2.67	1	2
1:A:214:ALA:HB3	1:A:262:ILE:HG21	0.42	1.90	14	1
1:A:82:VAL:HG12	1:A:83:THR:N	0.42	2.29	1	5
1:A:96:ILE:HG13	1:A:142:HIS:NE2	0.42	2.29	8	1
1:A:115:LEU:CD2	1:A:117:ALA:HB3	0.42	2.45	13	1
1:A:93:GLY:CA	1:A:115:LEU:HD13	0.42	2.44	1	1
1:A:232:ILE:HB	1:A:241:VAL:HG23	0.42	1.92	1	1
1:A:27:ARG:C	1:A:28:TRP:CD1	0.42	2.98	4	1
1:A:41:THR:HG1	1:A:208:HIS:CD2	0.42	2.32	5	2
1:A:82:VAL:O	1:A:157:VAL:HA	0.42	2.14	7	1
1:A:10:THR:CG2	1:A:32:LEU:HD21	0.42	2.44	8	1
1:A:221:THR:CG2	1:A:229:TYR:CE1	0.42	3.03	10	1
1:A:82:VAL:HG21	1:A:123:LEU:HD23	0.42	1.91	5	1
1:A:108:ILE:HG21	1:A:111:ILE:CG1	0.42	2.45	5	2
1:A:142:HIS:O	1:A:146:VAL:HG23	0.42	2.14	8	2
1:A:84:VAL:HG11	1:A:92:LEU:CD1	0.42	2.44	10	1
1:A:42:VAL:HG12	1:A:43:SER:N	0.42	2.30	6	1
1:A:211:LEU:HD11	1:A:262:ILE:HG12	0.42	1.91	7	1
1:A:102:ASN:O	1:A:103:LYS:HG2	0.41	2.15	11	4
1:A:133:ASN:OD1	1:A:152:THR:HG23	0.41	2.14	5	1
1:A:42:VAL:HG23	1:A:207:LYS:O	0.41	2.15	15	1
1:A:216:VAL:CG1	1:A:258:ILE:CG2	0.41	2.98	7	2
1:A:107:LEU:HD21	1:A:128:ALA:HB2	0.41	1.92	9	1
1:A:211:LEU:HD23	1:A:262:ILE:CG1	0.41	2.45	3	3
1:A:101:GLU:N	1:A:141:THR:HG23	0.41	2.30	2	1
1:A:31:VAL:HG12	1:A:32:LEU:N	0.41	2.30	12	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:150:LYS:O	1:A:151:LYS:C	0.41	2.63	12	1
1:A:95:SER:O	1:A:110:LYS:N	0.41	2.54	14	1
1:A:16:ARG:HG3	1:A:28:TRP:CD1	0.41	2.49	4	1
1:A:262:ILE:HG22	1:A:264:THR:H	0.41	1.76	15	1
1:A:123:LEU:O	1:A:124:PHE:CG	0.41	2.73	1	1
1:A:213:MET:HE3	1:A:264:THR:HG23	0.41	1.91	11	1
1:A:40:LEU:HB3	1:A:211:LEU:HD11	0.41	1.92	4	1
1:A:100:ARG:HB2	1:A:141:THR:HG23	0.41	1.91	6	1
1:A:84:VAL:HG12	1:A:85:ARG:N	0.41	2.31	6	1
1:A:123:LEU:HD13	1:A:123:LEU:H	0.41	1.73	6	1
1:A:132:VAL:HG12	1:A:158:LEU:HG	0.41	1.92	12	1
1:A:111:ILE:O	1:A:111:ILE:HG22	0.41	2.15	15	1
1:A:128:ALA:O	1:A:130:LEU:HD23	0.41	2.16	2	1
1:A:82:VAL:O	1:A:158:LEU:N	0.41	2.53	1	1
1:A:128:ALA:HB2	1:A:163:MET:HG3	0.41	1.93	2	1
1:A:81:ARG:N	1:A:81:ARG:HD2	0.41	2.30	7	1
1:A:234:ALA:HB3	1:A:239:ASP:HB3	0.41	1.93	7	1
1:A:106:ILE:HG23	1:A:142:HIS:ND1	0.41	2.31	8	1
1:A:93:GLY:O	1:A:112:PHE:CD1	0.41	2.74	9	1
1:A:106:ILE:H	1:A:106:ILE:HD12	0.41	1.76	9	1
1:A:242:PHE:CD1	1:A:242:PHE:C	0.41	2.99	9	1
1:A:131:SER:O	1:A:159:GLU:CB	0.41	2.69	10	2
1:A:112:PHE:CD1	1:A:112:PHE:N	0.41	2.88	13	1
1:A:128:ALA:CB	1:A:163:MET:HE3	0.41	2.46	14	1
1:A:147:GLN:O	1:A:151:LYS:HG3	0.41	2.15	15	1
1:A:211:LEU:HD21	1:A:262:ILE:HG12	0.41	1.93	7	1
1:A:15:LEU:HD12	1:A:243:LEU:HD11	0.40	1.91	5	1
1:A:128:ALA:HB3	1:A:163:MET:CE	0.40	2.45	8	1
1:A:258:ILE:CG2	1:A:262:ILE:CD1	0.40	2.99	14	2
1:A:207:LYS:HD2	1:A:241:VAL:HG22	0.40	1.92	11	1
1:A:102:ASN:O	1:A:104:MET:N	0.40	2.55	14	1
1:A:141:THR:O	1:A:142:HIS:C	0.40	2.65	1	1
1:A:109:SER:C	1:A:125:VAL:HG23	0.40	2.42	3	1
1:A:230:LEU:HD21	1:A:251:ALA:HB1	0.40	1.93	3	1
1:A:102:ASN:C	1:A:104:MET:N	0.40	2.79	14	2
1:A:146:VAL:O	1:A:150:LYS:CB	0.40	2.69	1	1
1:A:16:ARG:HG2	1:A:28:TRP:CD1	0.40	2.51	4	1
1:A:12:LEU:HD21	1:A:30:ARG:HD3	0.40	1.93	8	1
1:A:115:LEU:N	1:A:115:LEU:HD12	0.40	2.32	2	1
1:A:150:LYS:HG3	1:A:151:LYS:N	0.40	2.32	2	1
1:A:35:LEU:HD13	1:A:254:TRP:CZ3	0.40	2.51	4	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:106:ILE:HD12	1:A:106:ILE:H	0.40	1.77	10	1
1:A:13:LEU:HD22	1:A:245:ALA:HA	0.40	1.92	13	1
1:A:133:ASN:ND2	1:A:156:VAL:HG13	0.40	2.32	14	1
1:A:132:VAL:CG1	1:A:158:LEU:CD1	0.40	2.99	2	1
1:A:39:ALA:CA	1:A:211:LEU:HD12	0.40	2.47	4	1
1:A:15:LEU:HD23	1:A:16:ARG:N	0.40	2.31	12	1
1:A:128:ALA:CB	1:A:163:MET:CE	0.40	2.99	14	1

6.3 Torsion angles

6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	166/263 (63%)	127±3 (77±2%)	31±3 (18±2%)	8±2 (5±1%)	3	24
All	All	2490/3945 (63%)	1905 (77%)	460 (18%)	125 (5%)	3	24

All 32 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	103	LYS	15
1	A	133	ASN	15
1	A	141	THR	15
1	A	27	ARG	10
1	A	79	ARG	9
1	A	125	VAL	7
1	A	124	PHE	5
1	A	152	THR	5
1	A	221	THR	4
1	A	88	ASP	4
1	A	126	GLY	3
1	A	45	ALA	3
1	A	237	GLY	3
1	A	89	ALA	3
1	A	113	LYS	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	228	ARG	2
1	A	99	GLY	2
1	A	93	GLY	2
1	A	151	LYS	2
1	A	115	LEU	2
1	A	130	LEU	1
1	A	36	ALA	1
1	A	44	PRO	1
1	A	87	ALA	1
1	A	92	LEU	1
1	A	91	GLY	1
1	A	211	LEU	1
1	A	245	ALA	1
1	A	153	GLY	1
1	A	213	MET	1
1	A	214	ALA	1
1	A	248	GLU	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	131/201 (65%)	88±5 (67±4%)	43±5 (33±4%)	1	12
All	All	1965/3015 (65%)	1315 (67%)	650 (33%)	1	12

All 111 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	10	THR	15
1	A	130	LEU	15
1	A	152	THR	15
1	A	15	LEU	14
1	A	33	LEU	14
1	A	41	THR	14
1	A	103	LYS	14
1	A	158	LEU	14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	135	GLU	13
1	A	243	LEU	13
1	A	241	VAL	13
1	A	81	ARG	12
1	A	95	SER	12
1	A	213	MET	12
1	A	29	GLN	11
1	A	109	SER	11
1	A	242	PHE	11
1	A	104	MET	11
1	A	14	GLU	10
1	A	212	LYS	10
1	A	221	THR	10
1	A	100	ARG	10
1	A	110	LYS	9
1	A	123	LEU	9
1	A	161	LYS	9
1	A	217	SER	9
1	A	246	LYS	9
1	A	97	LYS	8
1	A	131	SER	8
1	A	207	LYS	8
1	A	92	LEU	8
1	A	162	TYR	7
1	A	35	LEU	7
1	A	79	ARG	7
1	A	86	LYS	7
1	A	127	ASP	7
1	A	231	GLU	7
1	A	236	ASP	7
1	A	253	SER	7
1	A	88	ASP	7
1	A	163	MET	7
1	A	16	ARG	6
1	A	27	ARG	6
1	A	80	ARG	6
1	A	239	ASP	6
1	A	244	ARG	6
1	A	107	LEU	6
1	A	154	LYS	6
1	A	137	LEU	5
1	A	138	SER	5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	150	LYS	5
1	A	151	LYS	5
1	A	211	LEU	5
1	A	230	LEU	5
1	A	9	ARG	5
1	A	34	SER	5
1	A	101	GLU	5
1	A	141	THR	5
1	A	155	GLU	5
1	A	248	GLU	5
1	A	115	LEU	5
1	A	238	GLN	5
1	A	113	LYS	4
1	A	124	PHE	4
1	A	144	GLU	4
1	A	147	GLN	4
1	A	208	HIS	4
1	A	42	VAL	4
1	A	83	THR	4
1	A	156	VAL	4
1	A	218	ARG	4
1	A	247	ASP	4
1	A	108	ILE	3
1	A	146	VAL	3
1	A	228	ARG	3
1	A	261	GLN	3
1	A	38	ASP	3
1	A	139	SER	3
1	A	30	ARG	3
1	A	94	ILE	3
1	A	252	ARG	3
1	A	120	THR	3
1	A	12	LEU	3
1	A	119	GLN	2
1	A	215	TYR	2
1	A	219	ARG	2
1	A	121	GLU	2
1	A	132	VAL	2
1	A	43	SER	2
1	A	264	THR	2
1	A	133	ASN	2
1	A	220	CYS	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	250	SER	2
1	A	149	LEU	2
1	A	159	GLU	2
1	A	129	ILE	2
1	A	229	TYR	2
1	A	85	ARG	2
1	A	233	CYS	2
1	A	143	ASP	1
1	A	210	SER	1
1	A	28	TRP	1
1	A	102	ASN	1
1	A	136	ASP	1
1	A	17	CYS	1
1	A	216	VAL	1
1	A	32	LEU	1
1	A	96	ILE	1
1	A	142	HIS	1
1	A	160	VAL	1
1	A	118	ASP	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided