Full wwPDB NMR Structure Validation Report (i)

May 28, 2020 – 10:38 pm BST

PDB ID	:	2KNY
Title	:	Fusion construct of CR17 from LRP-1 and ApoE residues 130-149
Authors	:	Guttman, M.; Komives, E.A.
Deposited on	:	2009-09-08

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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

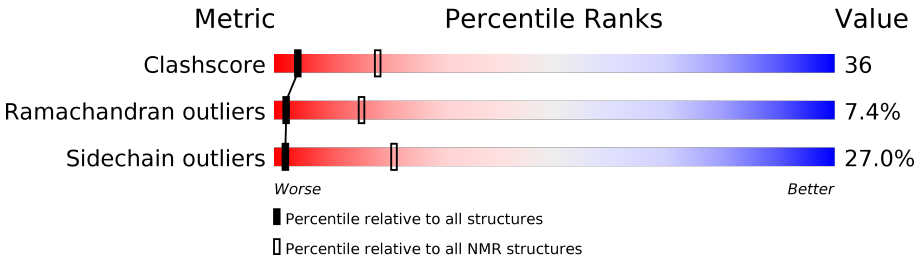
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.11
Ideal geometry (proteins)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 84%.

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	80	24% 56% • 16%

2 Ensemble composition and analysis

This entry contains 20 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 9 as representative, based on the following criterion: *closest to the average*.

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:2-A:48, A:56-A:57, A:129-A:144 (65)	0.48	7

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 4 clusters and 1 single-model cluster was found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1150 atoms, of which 566 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called LRP-1, linker, Apo-E.

Mol	Chain	Residues	Atoms						Trace
1	A	80	Total	C	H	N	O	S	0
			1149	350	566	109	118	6	

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	linker	UNP Q07954
A	2	SER	-	linker	UNP Q07954
A	2A	LYS	-	linker	UNP Q07954
A	2B	LEU	-	linker	UNP Q07954
A	51	GLY	-	linker	UNP Q07954
A	52	SER	-	linker	UNP Q07954
A	53	GLY	-	linker	UNP Q07954
A	54	SER	-	linker	UNP Q07954
A	55	GLY	-	linker	UNP Q07954
A	56	SER	-	linker	UNP Q07954
A	57	GLY	-	linker	UNP Q07954

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	
2	A	1	Total	Ca
			1	1

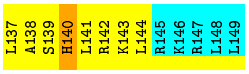
4 Residue-property plots

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: LRP-1, linker, Apo-E

Chain A:



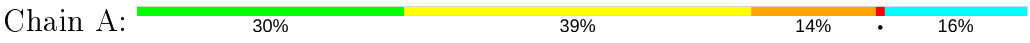
4.2 Scores per residue for each member of the ensemble

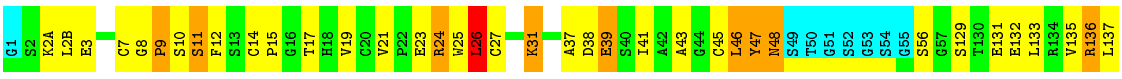
Colouring as in section 4.1 above.

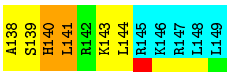
4.2.1 Score per residue for model 1

- Molecule 1: LRP-1, linker, Apo-E

Chain A:



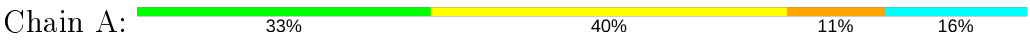


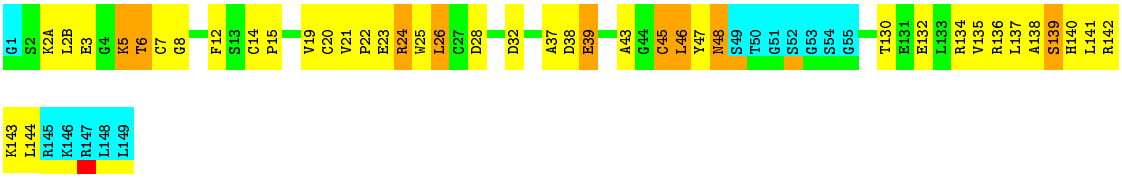


4.2.2 Score per residue for model 2

- Molecule 1: LRP-1, linker, Apo-E

Chain A:

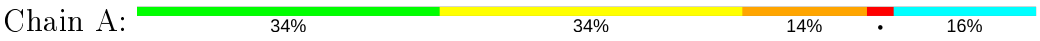


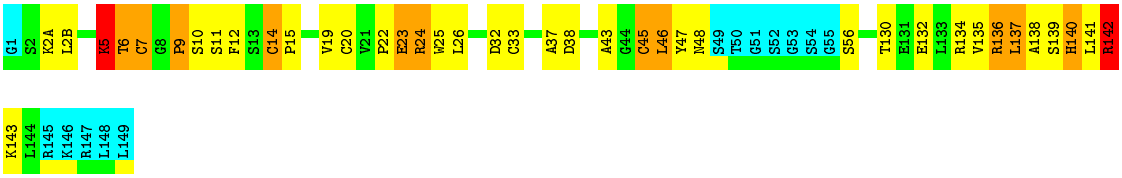


4.2.3 Score per residue for model 3

- Molecule 1: LRP-1, linker, Apo-E

Chain A:

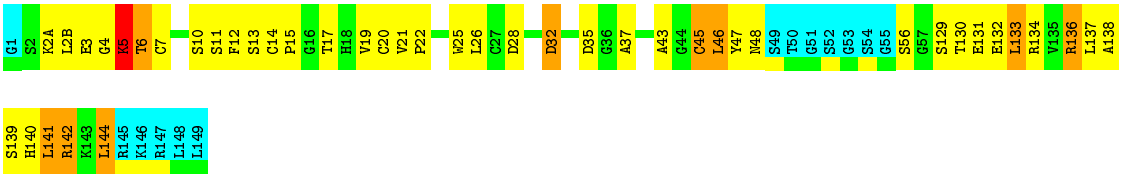




4.2.4 Score per residue for model 4

- Molecule 1: LRP-1, linker, Apo-E

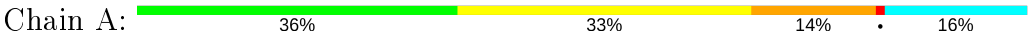
Chain A:

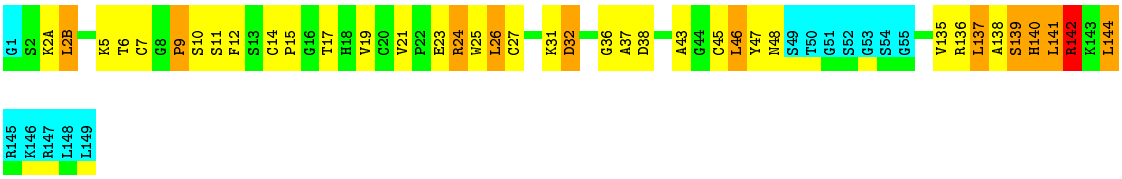


4.2.5 Score per residue for model 5

- Molecule 1: LRP-1, linker, Apo-E

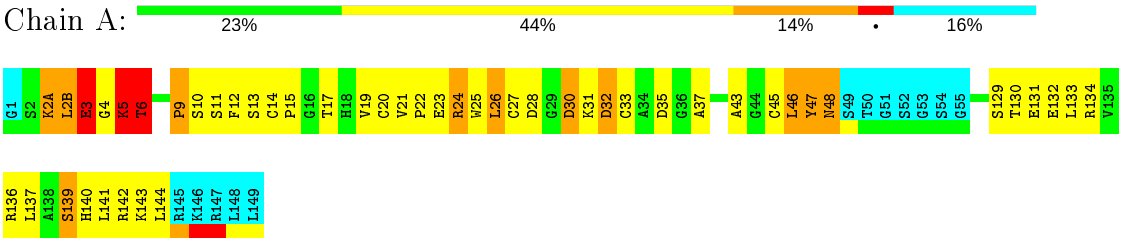
Chain A:





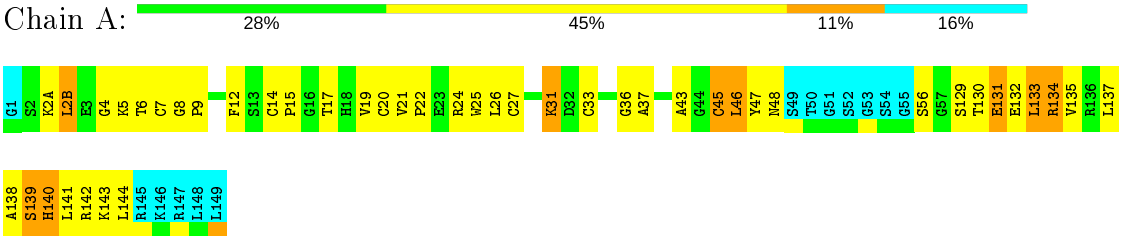
4.2.6 Score per residue for model 6

- Molecule 1: LRP-1, linker, Apo-E



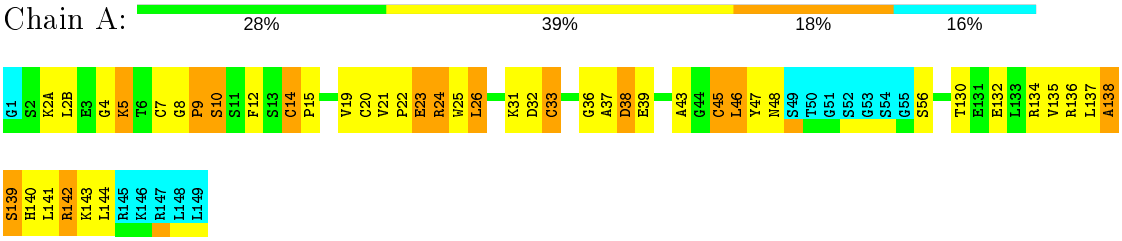
4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: LRP-1, linker, Apo-E



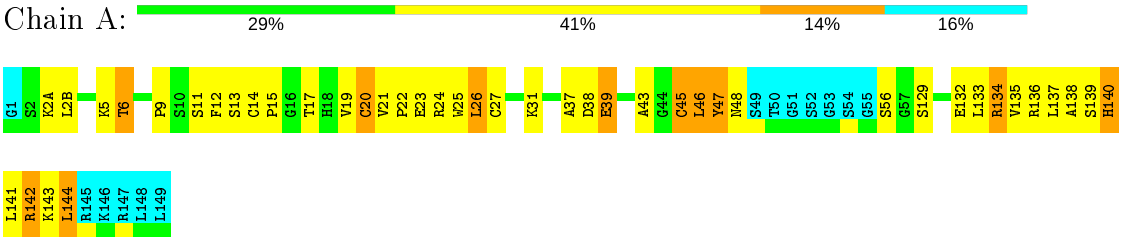
4.2.8 Score per residue for model 8

- Molecule 1: LRP-1, linker, Apo-E



4.2.9 Score per residue for model 9

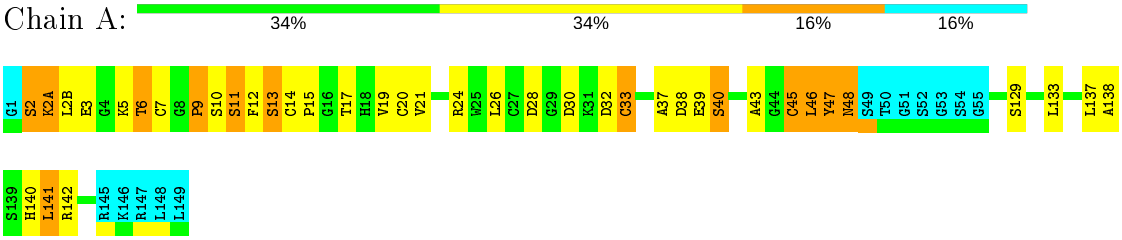
- Molecule 1: LRP-1, linker, Apo-E



4.2.10 Score per residue for model 10

• Molecule 1: LRP-1, linker, Apo-E

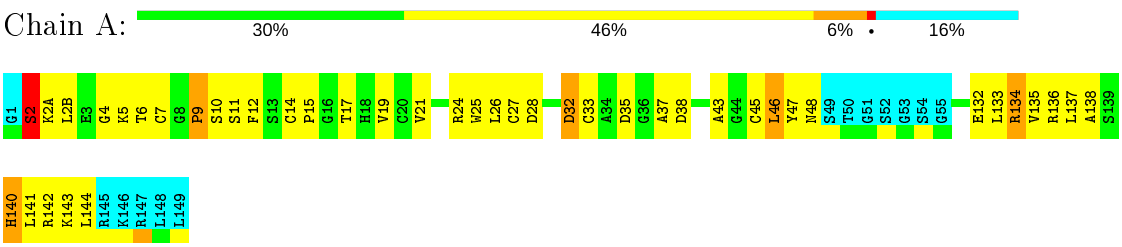
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: LRP-1, linker, Apo-E

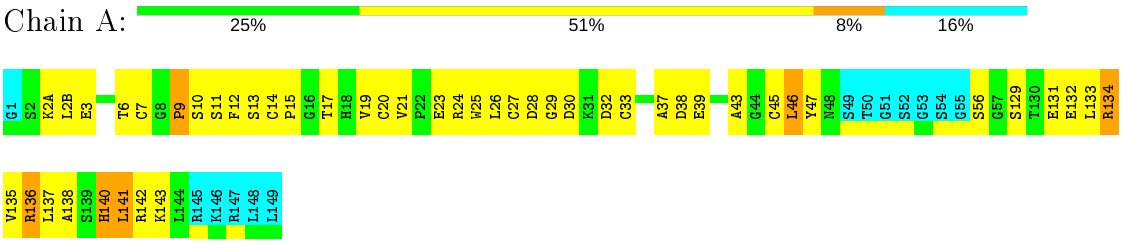
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: LRP-1, linker, Apo-E

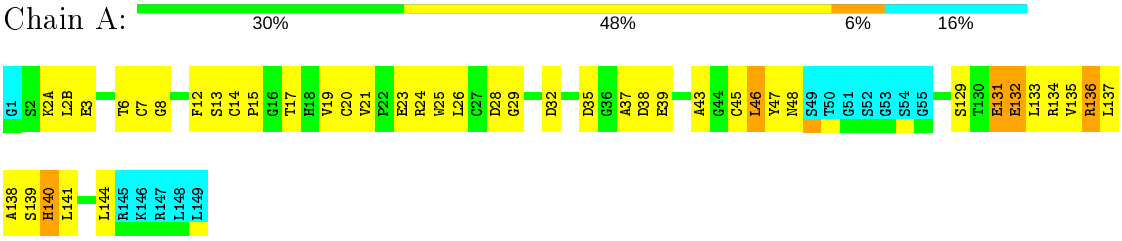
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: LRP-1, linker, Apo-E

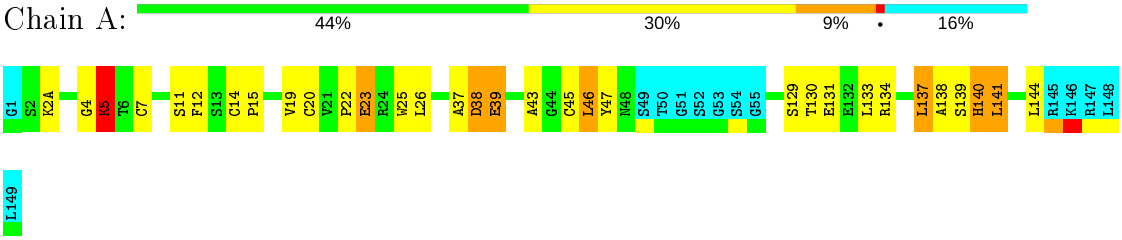
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: LRP-1, linker, Apo-E

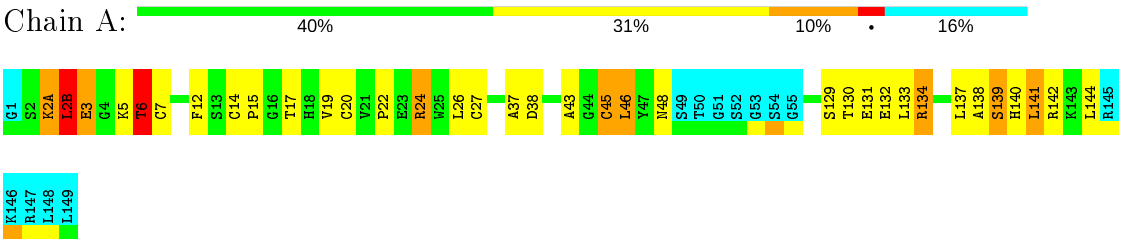
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: LRP-1, linker, Apo-E

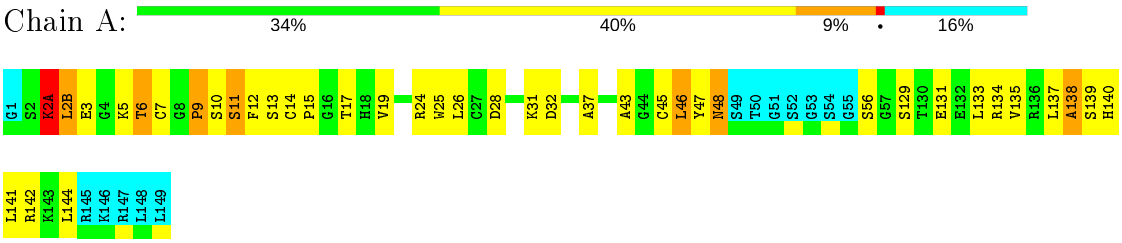
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: LRP-1, linker, Apo-E

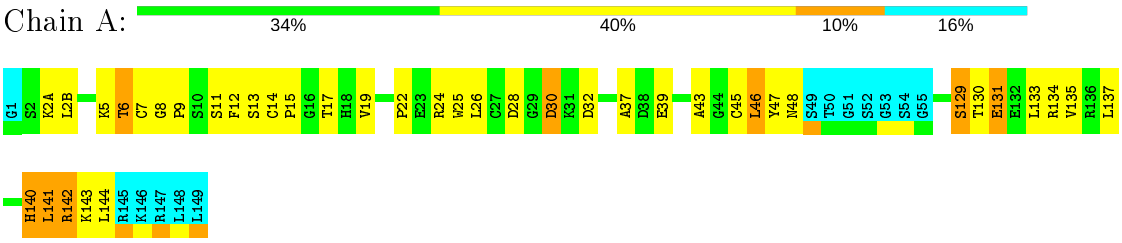
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: LRP-1, linker, Apo-E

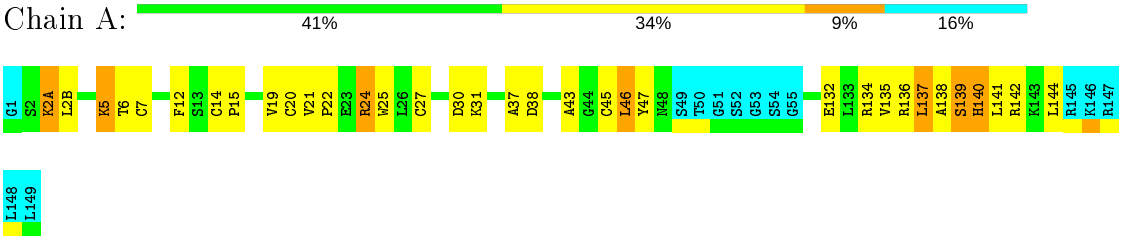
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: LRP-1, linker, Apo-E

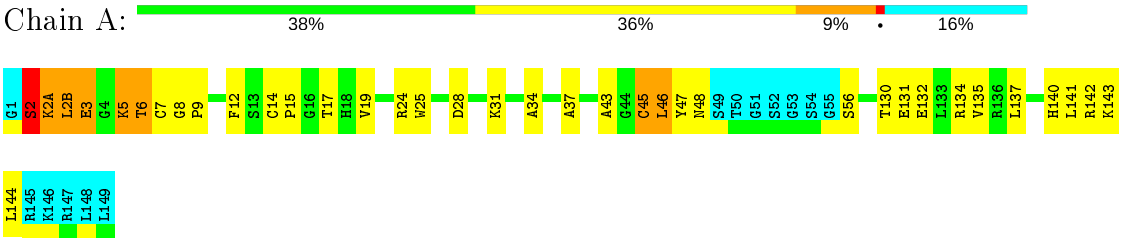
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: LRP-1, linker, Apo-E

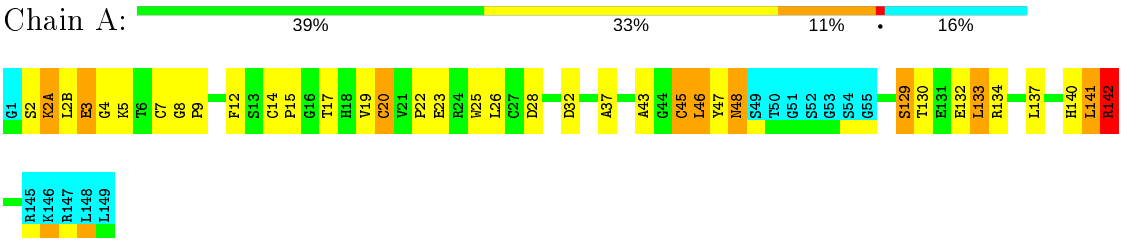
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: LRP-1, linker, Apo-E

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DGSA-distance geometry simulated annealing.*

Of the 328 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations.*

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

Software name	Classification	Version
ARIA	refinement	2.2
CNS	refinement	1.2
CNS	structure solution	1.2
TALOS	refinement	

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

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	2
Total number of shifts	1112
Number of shifts mapped to atoms	825
Number of unparsed shifts	0
Number of shifts with mapping errors	287
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	84%

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

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	494	469	469	35±5
All	All	9900	9380	9380	694

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 36.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2(B):LEU:HD23	1:A:19:VAL:HG21	0.85	1.48	17	10
1:A:14:CYS:HB2	1:A:19:VAL:HG13	0.78	1.55	9	17
1:A:137:LEU:O	1:A:137:LEU:HD13	0.78	1.78	1	3
1:A:137:LEU:HD13	1:A:137:LEU:O	0.75	1.81	9	3
1:A:2(B):LEU:HD23	1:A:19:VAL:CG2	0.75	2.12	3	9
1:A:26:LEU:HD12	1:A:38:ASP:OD1	0.74	1.80	9	3
1:A:137:LEU:HD22	1:A:137:LEU:O	0.73	1.83	18	3
1:A:6:THR:HG21	1:A:142:ARG:NE	0.73	1.97	2	1
1:A:129:SER:O	1:A:133:LEU:HD13	0.72	1.84	10	13
1:A:139:SER:O	1:A:144:LEU:HD13	0.72	1.85	5	5
1:A:21:VAL:HG11	1:A:38:ASP:HB3	0.72	1.60	13	3
1:A:21:VAL:HG22	1:A:25:TRP:HB2	0.72	1.60	12	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:VAL:HG11	1:A:38:ASP:HB2	0.71	1.62	1	2
1:A:131:GLU:O	1:A:135:VAL:HG23	0.71	1.86	12	5
1:A:14:CYS:CB	1:A:19:VAL:HG13	0.70	2.17	3	20
1:A:21:VAL:HG21	1:A:32:ASP:CG	0.70	2.07	12	1
1:A:2:SER:OG	1:A:19:VAL:HG11	0.69	1.87	19	1
1:A:5:LYS:HG2	1:A:6:THR:HG22	0.68	1.63	18	1
1:A:2(B):LEU:HD21	1:A:32:ASP:O	0.67	1.90	4	2
1:A:24:ARG:HB2	1:A:138:ALA:HB3	0.67	1.65	15	10
1:A:2(B):LEU:HD23	1:A:19:VAL:HG22	0.67	1.66	5	4
1:A:12:PHE:CE2	1:A:43:ALA:HB2	0.67	2.25	9	19
1:A:46:LEU:HD21	1:A:134:ARG:HD2	0.66	1.67	20	14
1:A:39:GLU:CD	1:A:39:GLU:N	0.66	2.49	2	2
1:A:2(B):LEU:HB2	1:A:19:VAL:HG21	0.65	1.67	10	2
1:A:45:CYS:C	1:A:46:LEU:HD22	0.65	2.11	3	19
1:A:12:PHE:CD2	1:A:43:ALA:HB2	0.64	2.26	17	11
1:A:2(B):LEU:HD21	1:A:32:ASP:OD1	0.64	1.92	10	1
1:A:2(B):LEU:HD13	1:A:32:ASP:O	0.63	1.93	11	1
1:A:24:ARG:HA	1:A:135:VAL:HG13	0.63	1.69	16	4
1:A:39:GLU:N	1:A:39:GLU:CD	0.62	2.52	9	2
1:A:2(B):LEU:CB	1:A:19:VAL:HG21	0.62	2.24	10	2
1:A:27:CYS:HB2	1:A:135:VAL:HG21	0.62	1.71	11	5
1:A:137:LEU:O	1:A:137:LEU:HD22	0.62	1.95	5	3
1:A:2(B):LEU:HD21	1:A:21:VAL:HB	0.61	1.71	5	4
1:A:47:TYR:O	1:A:48:ASN:CB	0.60	2.48	2	4
1:A:5:LYS:O	1:A:7:CYS:N	0.60	2.35	15	1
1:A:2(B):LEU:HD13	1:A:25:TRP:CZ3	0.60	2.31	19	1
1:A:2(B):LEU:HD11	1:A:32:ASP:HB3	0.60	1.73	17	3
1:A:21:VAL:HG21	1:A:32:ASP:OD2	0.60	1.96	12	1
1:A:26:LEU:HD12	1:A:38:ASP:OD2	0.60	1.96	8	2
1:A:26:LEU:HA	1:A:38:ASP:CG	0.60	2.17	8	2
1:A:2(A):LYS:C	1:A:2(B):LEU:HD12	0.60	2.17	20	2
1:A:141:LEU:HD23	1:A:142:ARG:HD3	0.60	1.72	12	1
1:A:24:ARG:CB	1:A:138:ALA:HB3	0.59	2.27	13	7
1:A:137:LEU:HD13	1:A:138:ALA:N	0.59	2.13	5	4
1:A:140:HIS:HA	1:A:144:LEU:HD12	0.58	1.73	7	3
1:A:2(A):LYS:O	1:A:2(B):LEU:HD12	0.58	1.99	18	3
1:A:46:LEU:HD13	1:A:46:LEU:N	0.57	2.15	7	9
1:A:2(B):LEU:HD12	1:A:25:TRP:CZ3	0.57	2.35	2	2
1:A:17:THR:HB	1:A:19:VAL:HG12	0.57	1.76	15	8
1:A:6:THR:HG23	1:A:142:ARG:NE	0.57	2.14	10	1
1:A:22:PRO:O	1:A:26:LEU:HD13	0.56	2.00	6	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2(B):LEU:HD11	1:A:32:ASP:OD2	0.56	2.01	8	1
1:A:46:LEU:N	1:A:46:LEU:HD13	0.56	2.14	20	9
1:A:23:GLU:HA	1:A:26:LEU:HD22	0.56	1.78	6	1
1:A:21:VAL:HG21	1:A:38:ASP:CG	0.56	2.20	9	1
1:A:31:LYS:HA	1:A:39:GLU:CD	0.56	2.20	8	2
1:A:139:SER:O	1:A:144:LEU:HD12	0.56	2.00	6	5
1:A:140:HIS:O	1:A:144:LEU:HD12	0.55	2.00	11	2
1:A:24:ARG:O	1:A:135:VAL:HG13	0.55	2.02	3	1
1:A:21:VAL:HG22	1:A:25:TRP:CB	0.55	2.32	13	3
1:A:6:THR:HG23	1:A:142:ARG:NH1	0.55	2.16	16	2
1:A:23:GLU:O	1:A:26:LEU:HB2	0.55	2.02	5	9
1:A:26:LEU:CD1	1:A:38:ASP:OD1	0.55	2.54	9	3
1:A:2(B):LEU:HD11	1:A:21:VAL:CB	0.54	2.32	2	1
1:A:46:LEU:HD21	1:A:134:ARG:CD	0.54	2.32	20	6
1:A:5:LYS:CE	1:A:6:THR:O	0.54	2.56	4	2
1:A:26:LEU:HD11	1:A:43:ALA:HB1	0.53	1.79	9	2
1:A:26:LEU:HA	1:A:38:ASP:HB2	0.53	1.80	14	1
1:A:24:ARG:HD2	1:A:135:VAL:HG12	0.53	1.79	8	2
1:A:17:THR:CB	1:A:19:VAL:HG12	0.53	2.33	15	12
1:A:137:LEU:C	1:A:137:LEU:HD13	0.52	2.25	16	8
1:A:12:PHE:CD2	1:A:26:LEU:HD11	0.52	2.40	5	1
1:A:15:PRO:HG2	1:A:37:ALA:HB1	0.52	1.80	2	12
1:A:6:THR:HG22	1:A:142:ARG:CZ	0.52	2.35	17	2
1:A:12:PHE:HB3	1:A:26:LEU:HD11	0.52	1.81	16	7
1:A:15:PRO:HD2	1:A:37:ALA:CB	0.52	2.35	13	13
1:A:26:LEU:HA	1:A:38:ASP:O	0.51	2.04	8	3
1:A:2(B):LEU:HD11	1:A:21:VAL:HB	0.51	1.82	2	1
1:A:45:CYS:O	1:A:46:LEU:HD22	0.51	2.06	10	3
1:A:12:PHE:O	1:A:21:VAL:HG12	0.51	2.04	10	4
1:A:25:TRP:N	1:A:25:TRP:CD1	0.51	2.79	20	8
1:A:23:GLU:HG3	1:A:26:LEU:HD22	0.51	1.83	14	1
1:A:137:LEU:HA	1:A:140:HIS:CE1	0.51	2.40	9	4
1:A:41:ILE:HD12	1:A:46:LEU:H	0.50	1.64	1	1
1:A:22:PRO:HD2	1:A:25:TRP:CD2	0.50	2.41	4	6
1:A:10:SER:OG	1:A:138:ALA:HB2	0.50	2.05	8	1
1:A:2(B):LEU:O	1:A:3:GLU:CB	0.50	2.60	19	1
1:A:137:LEU:HD13	1:A:137:LEU:C	0.50	2.27	15	8
1:A:45:CYS:O	1:A:47:TYR:CD2	0.50	2.65	2	13
1:A:41:ILE:HD12	1:A:46:LEU:N	0.50	2.22	1	1
1:A:47:TYR:CD1	1:A:48:ASN:N	0.49	2.81	1	1
1:A:9:PRO:O	1:A:11:SER:N	0.49	2.46	16	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:ARG:HB3	1:A:138:ALA:HB3	0.49	1.83	3	1
1:A:24:ARG:HG2	1:A:138:ALA:HB3	0.49	1.83	1	1
1:A:5:LYS:C	1:A:6:THR:HG23	0.49	2.27	2	1
1:A:15:PRO:HD2	1:A:37:ALA:HB3	0.49	1.84	1	3
1:A:141:LEU:HD23	1:A:142:ARG:NH1	0.49	2.23	5	2
1:A:5:LYS:HE3	1:A:22:PRO:HG3	0.49	1.84	3	1
1:A:2(A):LYS:O	1:A:3:GLU:N	0.49	2.45	15	3
1:A:21:VAL:CG1	1:A:38:ASP:OD1	0.49	2.60	2	3
1:A:5:LYS:CE	1:A:25:TRP:CZ2	0.49	2.96	18	1
1:A:140:HIS:CA	1:A:144:LEU:HD12	0.48	2.38	7	2
1:A:17:THR:OG1	1:A:19:VAL:HG12	0.48	2.08	4	9
1:A:132:GLU:O	1:A:136:ARG:N	0.48	2.45	18	7
1:A:130:THR:HA	1:A:133:LEU:HD22	0.48	1.85	15	1
1:A:46:LEU:HD21	1:A:134:ARG:NE	0.48	2.24	6	1
1:A:7:CYS:HA	1:A:11:SER:CB	0.48	2.38	10	1
1:A:4:GLY:O	1:A:5:LYS:HB2	0.48	2.09	4	1
1:A:25:TRP:CD1	1:A:25:TRP:N	0.48	2.81	14	5
1:A:39:GLU:N	1:A:39:GLU:OE1	0.48	2.47	8	1
1:A:141:LEU:HD23	1:A:142:ARG:CZ	0.48	2.39	20	1
1:A:38:ASP:OD1	1:A:39:GLU:OE2	0.47	2.32	8	1
1:A:2(B):LEU:O	1:A:5:LYS:CE	0.47	2.62	19	1
1:A:46:LEU:HD21	1:A:134:ARG:HE	0.47	1.68	6	1
1:A:132:GLU:O	1:A:136:ARG:CB	0.47	2.63	11	4
1:A:24:ARG:HB2	1:A:138:ALA:CB	0.47	2.39	5	2
1:A:137:LEU:C	1:A:137:LEU:HD22	0.47	2.28	5	1
1:A:25:TRP:O	1:A:38:ASP:OD1	0.47	2.33	8	2
1:A:138:ALA:HB1	1:A:142:ARG:HG3	0.47	1.87	9	1
1:A:5:LYS:CE	1:A:25:TRP:CH2	0.47	2.98	19	1
1:A:2(B):LEU:O	1:A:3:GLU:C	0.47	2.54	20	1
1:A:47:TYR:O	1:A:48:ASN:HB2	0.46	2.10	16	2
1:A:21:VAL:HG11	1:A:33:CYS:SG	0.46	2.50	10	2
1:A:15:PRO:CD	1:A:37:ALA:CB	0.46	2.93	12	4
1:A:140:HIS:CD2	1:A:140:HIS:N	0.46	2.83	5	3
1:A:2(B):LEU:HD23	1:A:20:CYS:O	0.46	2.10	9	1
1:A:26:LEU:O	1:A:38:ASP:OD1	0.46	2.34	10	1
1:A:140:HIS:N	1:A:140:HIS:ND1	0.46	2.63	17	3
1:A:137:LEU:O	1:A:140:HIS:NE2	0.46	2.48	17	4
1:A:5:LYS:O	1:A:6:THR:HB	0.46	2.11	3	1
1:A:140:HIS:CE1	1:A:142:ARG:NH2	0.46	2.84	8	1
1:A:137:LEU:O	1:A:140:HIS:CD2	0.46	2.68	14	3
1:A:24:ARG:HG3	1:A:139:SER:HA	0.45	1.87	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:LYS:HD2	1:A:25:TRP:CZ3	0.45	2.46	14	1
1:A:19:VAL:HG22	1:A:20:CYS:N	0.45	2.27	8	5
1:A:22:PRO:CD	1:A:25:TRP:CD2	0.45	2.99	4	1
1:A:12:PHE:O	1:A:21:VAL:CG1	0.45	2.65	10	3
1:A:28:ASP:OD1	1:A:29:GLY:N	0.45	2.50	12	2
1:A:2(B):LEU:O	1:A:3:GLU:HB2	0.45	2.12	19	1
1:A:2(B):LEU:HD11	1:A:21:VAL:CG2	0.45	2.41	2	1
1:A:22:PRO:HB3	1:A:142:ARG:HG3	0.45	1.88	3	1
1:A:12:PHE:N	1:A:21:VAL:O	0.45	2.46	4	2
1:A:21:VAL:CG2	1:A:38:ASP:OD2	0.45	2.65	8	1
1:A:24:ARG:CA	1:A:135:VAL:HG13	0.45	2.41	16	1
1:A:134:ARG:O	1:A:138:ALA:HB3	0.45	2.11	18	1
1:A:46:LEU:HD23	1:A:131:GLU:HG3	0.45	1.89	1	1
1:A:6:THR:OG1	1:A:7:CYS:N	0.45	2.50	3	3
1:A:22:PRO:HG2	1:A:25:TRP:CE2	0.45	2.47	4	1
1:A:22:PRO:HB3	1:A:142:ARG:CG	0.45	2.42	17	1
1:A:24:ARG:HG3	1:A:139:SER:CA	0.45	2.42	18	1
1:A:135:VAL:O	1:A:135:VAL:HG12	0.45	2.12	3	2
1:A:22:PRO:HD2	1:A:25:TRP:CE3	0.45	2.47	17	2
1:A:137:LEU:HD22	1:A:137:LEU:C	0.45	2.32	18	1
1:A:22:PRO:HG2	1:A:25:TRP:CD2	0.44	2.47	4	1
1:A:26:LEU:CD1	1:A:38:ASP:OD2	0.44	2.65	8	1
1:A:12:PHE:CE2	1:A:43:ALA:CB	0.44	3.01	15	1
1:A:2(B):LEU:HD13	1:A:32:ASP:HB3	0.44	1.87	2	1
1:A:24:ARG:HD3	1:A:139:SER:CB	0.44	2.42	8	1
1:A:140:HIS:ND1	1:A:140:HIS:N	0.44	2.65	1	1
1:A:5:LYS:HE2	1:A:6:THR:O	0.44	2.13	3	1
1:A:138:ALA:HB1	1:A:142:ARG:CG	0.44	2.42	9	1
1:A:5:LYS:HG2	1:A:6:THR:N	0.44	2.28	6	1
1:A:12:PHE:CD2	1:A:43:ALA:CB	0.44	2.99	17	3
1:A:6:THR:HG21	1:A:142:ARG:CZ	0.44	2.43	2	1
1:A:2:SER:HB2	1:A:2(B):LEU:HD13	0.44	1.89	20	1
1:A:30:ASP:O	1:A:39:GLU:CG	0.44	2.66	10	2
1:A:45:CYS:SG	1:A:47:TYR:CE1	0.44	3.11	16	2
1:A:6:THR:CG2	1:A:142:ARG:NH1	0.44	2.80	9	2
1:A:2(B):LEU:HD13	1:A:25:TRP:CE3	0.44	2.48	19	1
1:A:25:TRP:O	1:A:38:ASP:OD2	0.43	2.36	9	1
1:A:136:ARG:O	1:A:140:HIS:CE1	0.43	2.71	12	3
1:A:40:SER:CB	1:A:48:ASN:OD1	0.43	2.66	10	1
1:A:21:VAL:HG21	1:A:38:ASP:HB3	0.43	1.90	11	1
1:A:26:LEU:HD12	1:A:38:ASP:HB2	0.43	1.89	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:ARG:HG2	1:A:135:VAL:O	0.43	2.13	1	1
1:A:2(B):LEU:HD13	1:A:32:ASP:OD1	0.43	2.14	5	1
1:A:6:THR:HG22	1:A:142:ARG:NE	0.43	2.29	5	1
1:A:24:ARG:O	1:A:24:ARG:CD	0.43	2.66	6	1
1:A:45:CYS:SG	1:A:47:TYR:CZ	0.43	3.12	11	7
1:A:13:SER:HA	1:A:20:CYS:HA	0.43	1.90	10	1
1:A:47:TYR:CD2	1:A:56:SER:OG	0.43	2.72	19	1
1:A:31:LYS:HD2	1:A:36:GLY:HA3	0.43	1.90	7	1
1:A:137:LEU:O	1:A:140:HIS:CG	0.43	2.72	14	2
1:A:5:LYS:CD	1:A:22:PRO:CG	0.43	2.97	18	1
1:A:21:VAL:CG2	1:A:25:TRP:HB2	0.43	2.44	4	1
1:A:26:LEU:O	1:A:39:GLU:HA	0.43	2.14	13	2
1:A:47:TYR:O	1:A:48:ASN:HB3	0.43	2.14	20	2
1:A:2(A):LYS:O	1:A:25:TRP:CZ3	0.43	2.72	6	1
1:A:25:TRP:NE1	1:A:143:LYS:CD	0.42	2.82	12	3
1:A:11:SER:HA	1:A:22:PRO:HA	0.42	1.90	4	3
1:A:27:CYS:CB	1:A:131:GLU:OE2	0.42	2.67	6	1
1:A:30:ASP:O	1:A:32:ASP:N	0.42	2.52	6	1
1:A:32:ASP:OD1	1:A:33:CYS:N	0.42	2.53	12	1
1:A:12:PHE:CE2	1:A:15:PRO:HD3	0.42	2.49	10	6
1:A:24:ARG:N	1:A:138:ALA:HB3	0.42	2.30	11	1
1:A:2(B):LEU:HD11	1:A:21:VAL:HG23	0.42	1.90	2	1
1:A:30:ASP:O	1:A:39:GLU:OE2	0.42	2.38	12	1
1:A:39:GLU:OE1	1:A:39:GLU:N	0.42	2.52	9	1
1:A:5:LYS:O	1:A:6:THR:HG23	0.42	2.15	15	1
1:A:21:VAL:CG2	1:A:25:TRP:CB	0.42	2.98	13	1
1:A:21:VAL:HG21	1:A:32:ASP:OD1	0.42	2.14	12	1
1:A:2(B):LEU:CD2	1:A:32:ASP:O	0.41	2.66	4	1
1:A:21:VAL:HG11	1:A:38:ASP:CB	0.41	2.41	13	1
1:A:2(B):LEU:CB	1:A:19:VAL:CG2	0.41	2.97	4	2
1:A:46:LEU:HD23	1:A:131:GLU:OE1	0.41	2.15	15	1
1:A:31:LYS:HA	1:A:39:GLU:CG	0.41	2.46	1	1
1:A:36:GLY:HA2	1:A:39:GLU:OE1	0.41	2.14	8	1
1:A:27:CYS:SG	1:A:47:TYR:CZ	0.41	3.13	9	1
1:A:2:SER:CA	1:A:32:ASP:O	0.41	2.68	11	1
1:A:12:PHE:O	1:A:21:VAL:N	0.41	2.53	13	2
1:A:2(A):LYS:O	1:A:2(B):LEU:C	0.41	2.58	15	1
1:A:5:LYS:HD2	1:A:22:PRO:HG3	0.41	1.93	3	1
1:A:45:CYS:O	1:A:47:TYR:CD1	0.41	2.73	12	2
1:A:6:THR:CG2	1:A:142:ARG:CZ	0.41	2.99	11	1
1:A:2(B):LEU:O	1:A:3:GLU:CG	0.41	2.69	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:PRO:CB	1:A:142:ARG:HG3	0.41	2.45	20	1
1:A:31:LYS:HB3	1:A:36:GLY:HA2	0.41	1.91	7	2
1:A:45:CYS:O	1:A:47:TYR:CE2	0.41	2.74	6	1
1:A:26:LEU:HG	1:A:43:ALA:HB1	0.41	1.91	15	1
1:A:45:CYS:SG	1:A:47:TYR:CE2	0.41	3.14	18	1
1:A:26:LEU:HA	1:A:38:ASP:OD1	0.41	2.14	1	1
1:A:22:PRO:CD	1:A:25:TRP:CE3	0.41	3.03	4	1
1:A:22:PRO:HG2	1:A:25:TRP:CG	0.41	2.51	4	1
1:A:2(B):LEU:O	1:A:4:GLY:N	0.41	2.53	6	2
1:A:24:ARG:CG	1:A:138:ALA:C	0.41	2.89	1	1
1:A:135:VAL:HG12	1:A:135:VAL:O	0.41	2.16	2	2
1:A:25:TRP:NE1	1:A:143:LYS:CE	0.41	2.83	3	1
1:A:5:LYS:HE3	1:A:25:TRP:CZ2	0.41	2.50	18	1
1:A:2(B):LEU:CD2	1:A:19:VAL:CG2	0.41	2.99	1	1
1:A:22:PRO:HG2	1:A:25:TRP:CD1	0.41	2.51	4	1
1:A:9:PRO:CG	1:A:142:ARG:NH2	0.41	2.83	8	1
1:A:5:LYS:CD	1:A:22:PRO:HG3	0.41	2.46	3	1
1:A:2(B):LEU:C	1:A:3:GLU:CG	0.41	2.90	6	1
1:A:129:SER:C	1:A:133:LEU:HD13	0.41	2.35	7	1
1:A:2(B):LEU:HD11	1:A:32:ASP:HB2	0.41	1.93	10	1
1:A:5:LYS:HE2	1:A:25:TRP:CZ2	0.41	2.51	18	1
1:A:21:VAL:CG2	1:A:38:ASP:OD1	0.40	2.70	5	2
1:A:5:LYS:O	1:A:6:THR:CB	0.40	2.69	3	1
1:A:26:LEU:HD12	1:A:38:ASP:CG	0.40	2.36	8	1
1:A:5:LYS:N	1:A:5:LYS:HD2	0.40	2.31	6	1
1:A:5:LYS:HD3	1:A:25:TRP:CH2	0.40	2.50	19	1
1:A:24:ARG:CG	1:A:139:SER:N	0.40	2.85	1	1
1:A:24:ARG:HA	1:A:135:VAL:CG1	0.40	2.44	13	1
1:A:141:LEU:O	1:A:142:ARG:C	0.40	2.59	3	1
1:A:141:LEU:HD23	1:A:142:ARG:HE	0.40	1.77	4	1
1:A:5:LYS:HD2	1:A:22:PRO:CG	0.40	2.46	8	1
1:A:24:ARG:CB	1:A:138:ALA:CB	0.40	2.99	9	1
1:A:40:SER:HA	1:A:48:ASN:HA	0.40	1.93	10	1
1:A:5:LYS:C	1:A:6:THR:CG2	0.40	2.90	15	1
1:A:137:LEU:O	1:A:140:HIS:CE1	0.40	2.74	1	1
1:A:25:TRP:CD1	1:A:143:LYS:HE3	0.40	2.51	7	1
1:A:11:SER:CB	1:A:142:ARG:NH2	0.40	2.84	9	1
1:A:24:ARG:HD2	1:A:24:ARG:O	0.40	2.16	9	1
1:A:6:THR:CG2	1:A:142:ARG:NE	0.40	2.84	19	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	67/80 (84%)	50±2 (74±4%)	12±3 (19±4%)	5±2 (7±3%)	2	15
All	All	1340/1600 (84%)	992 (74%)	249 (19%)	99 (7%)	2	15

All 19 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	48	ASN	15
1	A	9	PRO	14
1	A	10	SER	8
1	A	8	GLY	8
1	A	3	GLU	7
1	A	5	LYS	7
1	A	142	ARG	6
1	A	31	LYS	6
1	A	6	THR	4
1	A	47	TYR	4
1	A	33	CYS	3
1	A	4	GLY	3
1	A	138	ALA	3
1	A	2(B)	LEU	3
1	A	2	SER	3
1	A	133	LEU	2
1	A	144	LEU	1
1	A	26	LEU	1
1	A	2(A)	LYS	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	55/64 (86%)	40±3 (73±5%)	15±3 (27±5%)	2 21
All	All	1100/1280 (86%)	803 (73%)	297 (27%)	2 21

All 42 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	46	LEU	20
1	A	2(A)	LYS	20
1	A	141	LEU	19
1	A	140	HIS	17
1	A	7	CYS	14
1	A	5	LYS	13
1	A	6	THR	11
1	A	139	SER	10
1	A	24	ARG	10
1	A	130	THR	10
1	A	45	CYS	10
1	A	20	CYS	9
1	A	28	ASP	9
1	A	142	ARG	8
1	A	132	GLU	8
1	A	13	SER	8
1	A	56	SER	8
1	A	134	ARG	7
1	A	136	ARG	7
1	A	143	LYS	6
1	A	26	LEU	6
1	A	131	GLU	6
1	A	32	ASP	6
1	A	144	LEU	5
1	A	3	GLU	4
1	A	39	GLU	4
1	A	2(B)	LEU	4
1	A	137	LEU	4
1	A	35	ASP	4
1	A	23	GLU	3
1	A	11	SER	3
1	A	30	ASP	3
1	A	33	CYS	3
1	A	38	ASP	3
1	A	2	SER	3
1	A	133	LEU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	10	SER	2
1	A	14	CYS	2
1	A	27	CYS	2
1	A	129	SER	2
1	A	40	SER	1
1	A	48	ASN	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 carbohydrates in this entry.

6.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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

The completeness of assignment taking into account all chemical shift lists is 84% for the well-defined parts and 83% for the entire structure.

7.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 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	825
Number of shifts mapped to atoms	825
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	76	0.44 ± 0.31	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	68	-0.11 ± 0.12	None needed (< 0.5 ppm)
$^{13}C'$	56	-0.01 ± 0.27	None needed (< 0.5 ppm)
^{15}N	64	0.29 ± 0.59	None needed (< 0.5 ppm)

7.1.3 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 84%, i.e. 636 atoms were assigned a chemical shift out of a possible 754. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	277/329 (84%)	110/131 (84%)	113/134 (84%)	54/64 (84%)
Sidechain	322/382 (84%)	201/226 (89%)	120/139 (86%)	1/17 (6%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	37/43 (86%)	19/23 (83%)	17/17 (100%)	1/3 (33%)
Overall	636/754 (84%)	330/380 (87%)	250/290 (86%)	56/84 (67%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 83%, i.e. 742 atoms were assigned a chemical shift out of a possible 899. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	326/394 (83%)	130/157 (83%)	132/160 (82%)	64/77 (83%)
Sidechain	379/462 (82%)	236/274 (86%)	142/164 (87%)	1/24 (4%)
Aromatic	37/43 (86%)	19/23 (83%)	17/17 (100%)	1/3 (33%)
Overall	742/899 (83%)	385/454 (85%)	291/341 (85%)	66/104 (63%)

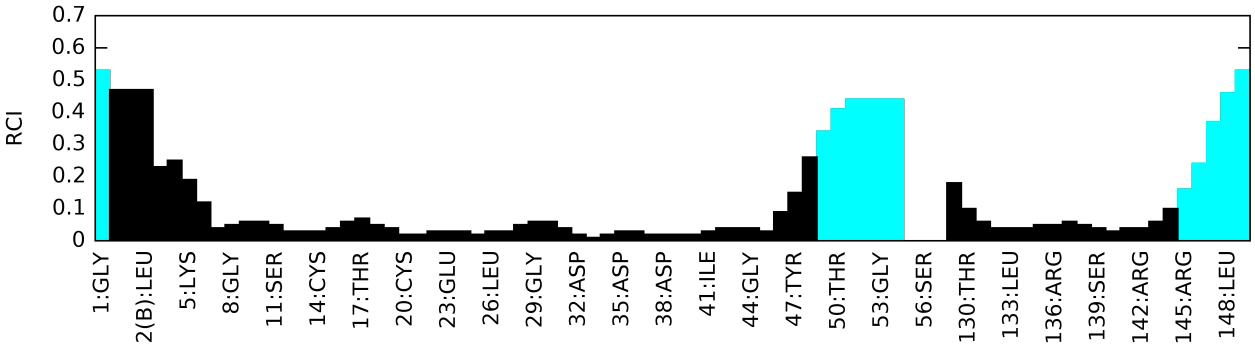
7.1.4 Statistically unusual chemical shifts

There are no statistically unusual chemical shifts.

7.1.5 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:



7.2 Chemical shift list 2

File name: input_cs.cif

Chemical shift list name: *assigned_chem_shift_list_2*

7.2.1 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	287
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	287
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- Chain not found in structure. All 287 occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	11	LEU	C	177.886	0.021	1
UNMAPPED	19	ARG	H	8.104	0.003	1
UNMAPPED	22	LEU	HB2	1.631	0.005	2
UNMAPPED	14	HIS	HA	4.519	0.005	1
UNMAPPED	15	LEU	CB	41.916	0.031	1
UNMAPPED	23	LEU	HD21	0.9	0.005	2
UNMAPPED	20	LYS	H	8.131	0.003	1
UNMAPPED	23	LEU	HD11	0.856	0.005	2
UNMAPPED	3	TYR	C	176.445	0.014	1
UNMAPPED	17	LYS	HE3	2.995	0.005	2
UNMAPPED	20	LYS	CD	29.118	0.008	1
UNMAPPED	14	HIS	HE1	7.732	0.005	1
UNMAPPED	12	ALA	H	8.101	0.005	1
UNMAPPED	3	TYR	HE1	6.819	0.005	3
UNMAPPED	19	ARG	CD	43.516	0.014	1
UNMAPPED	5	GLU	C	177.254	0.002	1
UNMAPPED	8	ARG	N	119.541	0.01	1
UNMAPPED	3	TYR	CB	38.682	0.085	1
UNMAPPED	15	LEU	HD21	0.901	0.005	2
UNMAPPED	21	ARG	CA	56.203	0.027	1
UNMAPPED	14	HIS	CB	30.749	0.103	1
UNMAPPED	13	SER	CA	60.163	0.032	1
UNMAPPED	8	ARG	C	177.749	0.022	1
UNMAPPED	23	LEU	HD22	0.9	0.005	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	20	LYS	HB2	1.825	0.005	2
UNMAPPED	10	ARG	HA	4.239	0.005	1
UNMAPPED	15	LEU	HB3	1.532	0.005	2
UNMAPPED	3	TYR	HD1	7.128	0.005	3
UNMAPPED	11	LEU	H	8.22	0.005	1
UNMAPPED	18	LEU	HD11	0.851	0.005	2
UNMAPPED	18	LEU	HD21	0.891	0.005	2
UNMAPPED	18	LEU	HB3	1.573	0.005	2
UNMAPPED	16	ARG	CG	27.486	0.02	1
UNMAPPED	20	LYS	HB3	1.765	0.005	2
UNMAPPED	18	LEU	N	121.33	0.004	1
UNMAPPED	18	LEU	CA	55.577	0.01	1
UNMAPPED	7	LEU	HD11	0.843	0.005	2
UNMAPPED	15	LEU	HD12	0.84	0.005	2
UNMAPPED	10	ARG	HD2	3.172	0.005	2
UNMAPPED	15	LEU	HD11	0.84	0.005	2
UNMAPPED	23	LEU	N	127.626	0.007	1
UNMAPPED	5	GLU	H	8.191	0.005	1
UNMAPPED	12	ALA	N	122.649	0.01	1
UNMAPPED	6	GLU	HG3	2.238	0.005	2
UNMAPPED	12	ALA	CA	53.698	0.02	1
UNMAPPED	22	LEU	HD11	0.861	0.005	2
UNMAPPED	15	LEU	H	7.836	0.005	1
UNMAPPED	16	ARG	CD	43.542	0.02	1
UNMAPPED	8	ARG	CD	43.331	0.011	1
UNMAPPED	6	GLU	C	177.662	0.023	1
UNMAPPED	20	LYS	HE3	2.992	0.005	2
UNMAPPED	8	ARG	CA	57.94	0.007	1
UNMAPPED	21	ARG	CB	30.917	0.01	1
UNMAPPED	21	ARG	HA	4.315	0.005	1
UNMAPPED	17	LYS	N	120.082	0.007	1
UNMAPPED	8	ARG	CB	30.316	0.041	1
UNMAPPED	21	ARG	CG	27.175	0.02	1
UNMAPPED	20	LYS	HG3	1.414	0.005	2
UNMAPPED	4	THR	HG23	1.2	0.005	1
UNMAPPED	21	ARG	HD2	3.207	0.005	2
UNMAPPED	23	LEU	HD13	0.856	0.005	2
UNMAPPED	21	ARG	HD3	3.207	0.005	2
UNMAPPED	18	LEU	HD22	0.891	0.005	2
UNMAPPED	22	LEU	CA	55.224	0.025	1
UNMAPPED	14	HIS	HB2	3.172	0.005	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	11	LEU	HD13	0.851	0.005	2
UNMAPPED	18	LEU	CB	42.343	0.014	1
UNMAPPED	12	ALA	HA	4.25	0.005	1
UNMAPPED	18	LEU	C	177.558	0.019	1
UNMAPPED	17	LYS	HB3	1.816	0.005	2
UNMAPPED	17	LYS	HG2	1.493	0.005	2
UNMAPPED	7	LEU	N	121.231	0.022	1
UNMAPPED	8	ARG	HA	4.129	0.005	1
UNMAPPED	23	LEU	HB3	1.577	0.005	2
UNMAPPED	7	LEU	CG	26.96	0.02	1
UNMAPPED	3	TYR	HB3	3.067	0.005	2
UNMAPPED	7	LEU	HB3	1.599	0.005	2
UNMAPPED	7	LEU	HD21	0.884	0.005	2
UNMAPPED	1	GLY	CA	44.166	0.005	1
UNMAPPED	7	LEU	CB	42.011	0.01	1
UNMAPPED	7	LEU	HD22	0.884	0.005	2
UNMAPPED	11	LEU	HA	4.267	0.005	1
UNMAPPED	6	GLU	CA	57.922	0.023	1
UNMAPPED	15	LEU	C	178.142	0.023	1
UNMAPPED	9	VAL	CG2	21.153	0.02	2
UNMAPPED	11	LEU	HD23	0.893	0.005	2
UNMAPPED	6	GLU	CB	29.726	0.023	1
UNMAPPED	8	ARG	HD3	3.184	0.005	2
UNMAPPED	10	ARG	HB3	1.863	0.005	2
UNMAPPED	19	ARG	HD3	3.212	0.005	2
UNMAPPED	6	GLU	CG	36.393	0.023	1
UNMAPPED	21	ARG	HB2	1.845	0.005	2
UNMAPPED	9	VAL	HG23	0.931	0.005	2
UNMAPPED	23	LEU	H	7.697	0.002	1
UNMAPPED	5	GLU	N	122.429	0.007	1
UNMAPPED	14	HIS	CD2	119.23	0.04	1
UNMAPPED	3	TYR	HE2	6.819	0.005	3
UNMAPPED	15	LEU	N	119.936	0.005	1
UNMAPPED	13	SER	HB2	3.96	0.005	2
UNMAPPED	9	VAL	HG11	0.989	0.005	2
UNMAPPED	9	VAL	HB	2.107	0.005	1
UNMAPPED	22	LEU	N	123.638	0.006	1
UNMAPPED	20	LYS	HG2	1.459	0.005	2
UNMAPPED	13	SER	HB3	3.915	0.005	2
UNMAPPED	22	LEU	CG	26.923	0.02	1
UNMAPPED	22	LEU	HD21	0.928	0.005	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	9	VAL	N	119.007	0.007	1
UNMAPPED	10	ARG	C	177.527	0.013	1
UNMAPPED	22	LEU	HD22	0.928	0.005	2
UNMAPPED	20	LYS	N	121.499	0.009	1
UNMAPPED	2	SER	CA	58.148	0.019	1
UNMAPPED	7	LEU	CD1	23.869	0.025	2
UNMAPPED	15	LEU	HD22	0.901	0.005	2
UNMAPPED	2	SER	CB	64.047	0.009	1
UNMAPPED	23	LEU	HA	4.18	0.005	1
UNMAPPED	17	LYS	HD2	1.688	0.005	2
UNMAPPED	9	VAL	H	7.888	0.005	1
UNMAPPED	6	GLU	HB2	2.004	0.005	2
UNMAPPED	17	LYS	CD	29.284	0.005	1
UNMAPPED	10	ARG	CG	27.392	0.02	1
UNMAPPED	3	TYR	HD2	7.128	0.005	3
UNMAPPED	4	THR	HB	4.199	0.001	1
UNMAPPED	17	LYS	HD3	1.688	0.005	2
UNMAPPED	18	LEU	HD12	0.851	0.005	2
UNMAPPED	4	THR	HA	4.129	0.002	1
UNMAPPED	16	ARG	N	119.352	0.004	1
UNMAPPED	4	THR	H	7.933	0.002	1
UNMAPPED	17	LYS	C	177.022	0.026	1
UNMAPPED	5	GLU	HG2	2.282	0.005	2
UNMAPPED	17	LYS	H	7.968	0.005	1
UNMAPPED	20	LYS	CE	42.195	0.025	1
UNMAPPED	2	SER	HA	4.502	0.002	1
UNMAPPED	22	LEU	CD2	25.081	0.014	2
UNMAPPED	10	ARG	HD3	3.172	0.005	2
UNMAPPED	7	LEU	HD13	0.843	0.005	2
UNMAPPED	12	ALA	HB1	1.446	0.005	1
UNMAPPED	22	LEU	HB3	1.631	0.005	2
UNMAPPED	6	GLU	HG2	2.305	0.005	2
UNMAPPED	12	ALA	CB	18.765	0.02	1
UNMAPPED	12	ALA	HB2	1.446	0.005	1
UNMAPPED	19	ARG	CB	30.666	0.018	1
UNMAPPED	17	LYS	HG3	1.404	0.005	2
UNMAPPED	14	HIS	CA	57.918	0.012	1
UNMAPPED	22	LEU	HD13	0.861	0.005	2
UNMAPPED	11	LEU	CD1	23.458	0.028	2
UNMAPPED	20	LYS	CG	24.845	0.006	1
UNMAPPED	8	ARG	HB2	1.875	0.005	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	11	LEU	CD2	24.889	0.023	2
UNMAPPED	10	ARG	N	122.489	0.005	1
UNMAPPED	21	ARG	CD	43.517	0.014	1
UNMAPPED	20	LYS	HD2	1.687	0.005	2
UNMAPPED	22	LEU	H	8.267	0.002	1
UNMAPPED	19	ARG	HA	4.275	0.005	1
UNMAPPED	16	ARG	HB2	1.852	0.005	2
UNMAPPED	14	HIS	C	176.407	0.023	1
UNMAPPED	11	LEU	CB	42.197	0.031	1
UNMAPPED	4	THR	CG2	21.807	0.023	1
UNMAPPED	17	LYS	CG	25.009	0.014	1
UNMAPPED	11	LEU	HD12	0.851	0.005	2
UNMAPPED	19	ARG	N	120.507	0.014	1
UNMAPPED	17	LYS	CB	32.739	0.008	1
UNMAPPED	11	LEU	HD11	0.851	0.005	2
UNMAPPED	17	LYS	HB2	1.838	0.005	2
UNMAPPED	16	ARG	CA	57.384	0.02	1
UNMAPPED	17	LYS	CA	57.108	0.018	1
UNMAPPED	5	GLU	HA	4.173	0.005	1
UNMAPPED	22	LEU	C	176.086	0.011	1
UNMAPPED	20	LYS	HA	4.268	0.005	1
UNMAPPED	2	SER	HB2	3.883	0.005	2
UNMAPPED	7	LEU	HB2	1.599	0.005	2
UNMAPPED	7	LEU	CA	56.6	0.019	1
UNMAPPED	13	SER	CB	63.225	0.027	1
UNMAPPED	11	LEU	CA	56.045	0.028	1
UNMAPPED	7	LEU	HD23	0.884	0.005	2
UNMAPPED	1	GLY	HA2	3.756	0.005	2
UNMAPPED	11	LEU	N	121.382	0.021	1
UNMAPPED	19	ARG	HB2	1.799	0.005	2
UNMAPPED	14	HIS	HB3	3.172	0.005	2
UNMAPPED	20	LYS	CB	33.102	0.035	1
UNMAPPED	11	LEU	HD21	0.893	0.005	2
UNMAPPED	6	GLU	N	120.275	0.004	1
UNMAPPED	21	ARG	HB3	1.782	0.005	2
UNMAPPED	5	GLU	HB3	2.025	0.005	2
UNMAPPED	10	ARG	H	8.135	0.005	1
UNMAPPED	5	GLU	CG	36.236	0.028	1
UNMAPPED	13	SER	N	113.685	0.028	1
UNMAPPED	9	VAL	HG21	0.931	0.005	2
UNMAPPED	5	GLU	CB	29.937	0.023	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	11	LEU	HB2	1.634	0.005	2
UNMAPPED	18	LEU	CD2	24.952	0.026	2
UNMAPPED	15	LEU	CG	26.736	0.058	1
UNMAPPED	15	LEU	CD1	23.117	0.018	2
UNMAPPED	5	GLU	CA	57.78	0.017	1
UNMAPPED	9	VAL	HA	3.925	0.005	1
UNMAPPED	4	THR	CA	62.967	0.018	1
UNMAPPED	14	HIS	HD2	6.946	0.005	1
UNMAPPED	16	ARG	H	7.927	0.005	1
UNMAPPED	15	LEU	CA	56.064	0.023	1
UNMAPPED	19	ARG	C	176.326	0.02	1
UNMAPPED	23	LEU	CD2	25.234	0.02	2
UNMAPPED	21	ARG	H	8.22	0.003	1
UNMAPPED	23	LEU	HD12	0.856	0.005	2
UNMAPPED	18	LEU	CG	26.957	0.02	1
UNMAPPED	8	ARG	H	8.066	0.005	1
UNMAPPED	18	LEU	HA	4.265	0.005	1
UNMAPPED	22	LEU	CB	42.226	0.031	1
UNMAPPED	17	LYS	HE2	2.995	0.005	2
UNMAPPED	22	LEU	HD23	0.928	0.005	2
UNMAPPED	4	THR	C	175.127	0.004	1
UNMAPPED	7	LEU	CD2	24.615	0.013	2
UNMAPPED	15	LEU	HD23	0.901	0.005	2
UNMAPPED	16	ARG	CB	30.504	0.043	1
UNMAPPED	3	TYR	CA	58.921	0.016	1
UNMAPPED	16	ARG	C	177.026	0.012	1
UNMAPPED	20	LYS	C	176.28	0.015	1
UNMAPPED	6	GLU	HB3	2.004	0.005	2
UNMAPPED	10	ARG	CD	43.555	0.023	1
UNMAPPED	18	LEU	HD13	0.851	0.005	2
UNMAPPED	19	ARG	HB3	1.799	0.005	2
UNMAPPED	10	ARG	CA	57.52	0.053	1
UNMAPPED	13	SER	H	8.205	0.006	1
UNMAPPED	18	LEU	HD23	0.891	0.005	2
UNMAPPED	13	SER	HA	4.239	0.005	1
UNMAPPED	10	ARG	CB	30.548	0.039	1
UNMAPPED	7	LEU	H	8.034	0.005	1
UNMAPPED	18	LEU	HB2	1.66	0.005	2
UNMAPPED	23	LEU	CD1	23.746	0.02	2
UNMAPPED	5	GLU	HG3	2.282	0.005	2
UNMAPPED	21	ARG	C	175.855	0.013	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	18	LEU	H	7.953	0.002	1
UNMAPPED	9	VAL	C	177.245	0.023	1
UNMAPPED	6	GLU	H	8.305	0.005	1
UNMAPPED	6	GLU	HA	4.123	0.005	1
UNMAPPED	23	LEU	CA	56.685	0.012	1
UNMAPPED	3	TYR	HA	4.595	0.005	1
UNMAPPED	7	LEU	HD12	0.843	0.005	2
UNMAPPED	15	LEU	HD13	0.84	0.005	2
UNMAPPED	19	ARG	HD2	3.212	0.005	2
UNMAPPED	23	LEU	CB	43.512	0.024	1
UNMAPPED	20	LYS	HD3	1.687	0.005	2
UNMAPPED	17	LYS	HA	4.217	0.005	1
UNMAPPED	12	ALA	HB3	1.446	0.005	1
UNMAPPED	19	ARG	CA	56.388	0.013	1
UNMAPPED	15	LEU	HG	1.42	0.005	1
UNMAPPED	22	LEU	HD12	0.861	0.005	2
UNMAPPED	7	LEU	HA	4.145	0.005	1
UNMAPPED	8	ARG	CG	27.376	0.02	1
UNMAPPED	21	ARG	N	121.496	0.038	1
UNMAPPED	8	ARG	HB3	1.875	0.005	2
UNMAPPED	19	ARG	CG	27.247	0.02	1
UNMAPPED	15	LEU	HA	4.169	0.005	1
UNMAPPED	20	LYS	CA	56.435	0.047	1
UNMAPPED	23	LEU	HD23	0.9	0.005	2
UNMAPPED	4	THR	HG21	1.2	0.005	1
UNMAPPED	16	ARG	HB3	1.852	0.005	2
UNMAPPED	22	LEU	HA	4.364	0.005	1
UNMAPPED	4	THR	HG22	1.2	0.005	1
UNMAPPED	23	LEU	CG	27.282	0.02	1
UNMAPPED	3	TYR	CD1	133.261	0.02	3
UNMAPPED	9	VAL	CA	64.025	0.029	1
UNMAPPED	17	LYS	CE	42.203	0.031	1
UNMAPPED	9	VAL	CB	32.339	0.038	1
UNMAPPED	16	ARG	HA	4.178	0.005	1
UNMAPPED	22	LEU	CD1	23.431	0.015	2
UNMAPPED	2	SER	HB3	3.836	0.002	2
UNMAPPED	23	LEU	HB2	1.577	0.005	2
UNMAPPED	20	LYS	HE2	2.992	0.005	2
UNMAPPED	3	TYR	HB2	3.067	0.005	2
UNMAPPED	3	TYR	CE1	118.266	0.02	3
UNMAPPED	4	THR	CB	69.604	0.034	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	14	HIS	CE1	138.932	0.04	1
UNMAPPED	11	LEU	HB3	1.634	0.005	2
UNMAPPED	1	GLY	HA3	3.756	0.005	2
UNMAPPED	11	LEU	CG	26.84	0.02	1
UNMAPPED	15	LEU	CD2	25.16	0.032	2
UNMAPPED	9	VAL	HG12	0.989	0.005	2
UNMAPPED	4	THR	N	114.36	0.005	1
UNMAPPED	9	VAL	CG1	21.441	0.02	2
UNMAPPED	11	LEU	HD22	0.893	0.005	2
UNMAPPED	8	ARG	HD2	3.184	0.005	2
UNMAPPED	5	GLU	HB2	2.025	0.005	2
UNMAPPED	10	ARG	HB2	1.863	0.005	2
UNMAPPED	9	VAL	HG13	0.989	0.005	2
UNMAPPED	9	VAL	HG22	0.931	0.005	2
UNMAPPED	15	LEU	HB2	1.691	0.005	2
UNMAPPED	18	LEU	CD1	23.468	0.023	2
UNMAPPED	7	LEU	C	178.026	0.026	1

7.2.2 Chemical shift referencing

No chemical shift referencing corrections were calculated (not enough data).

7.2.3 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 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 754. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/329 (0%)	0/131 (0%)	0/134 (0%)	0/64 (0%)
Sidechain	0/382 (0%)	0/226 (0%)	0/139 (0%)	0/17 (0%)
Aromatic	0/43 (0%)	0/23 (0%)	0/17 (0%)	0/3 (0%)
Overall	0/754 (0%)	0/380 (0%)	0/290 (0%)	0/84 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 899. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/394 (0%)	0/157 (0%)	0/160 (0%)	0/77 (0%)
Sidechain	0/462 (0%)	0/274 (0%)	0/164 (0%)	0/24 (0%)
Aromatic	0/43 (0%)	0/23 (0%)	0/17 (0%)	0/3 (0%)
Overall	0/899 (0%)	0/454 (0%)	0/341 (0%)	0/104 (0%)

7.2.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.2.5 Random Coil Index (RCI) plots (i)

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned_chem_shift_list_2). RCI is only applicable to proteins.