



Full wwPDB NMR Structure Validation Report ⓘ

Mar 20, 2026 – 03:04 AM UTC

PDB ID : 2KNY / pdb_00002kny
BMRB ID : 16483
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 ⓘ 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

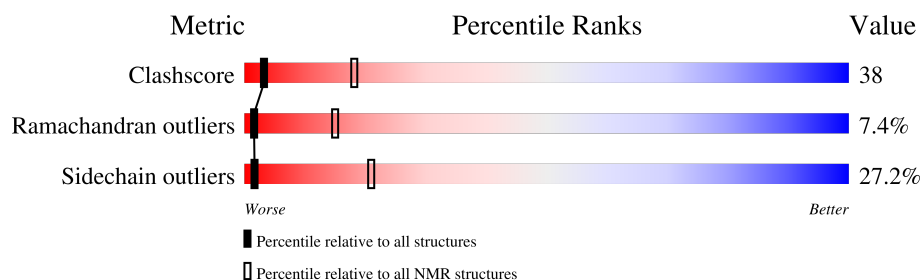
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment 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	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	80	24% 55% 5% 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)	0.84	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 (CCD ID: CA) (formula: Ca).

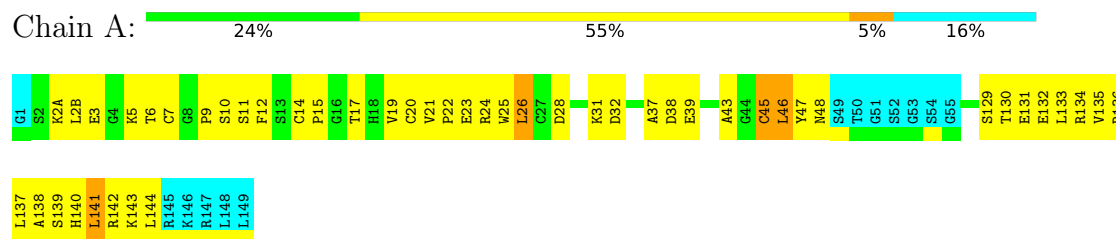
Mol	Chain	Residues	Atoms	
2	A	1	Total	Ca
			1	1

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, 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: LRP-1, linker, Apo-E

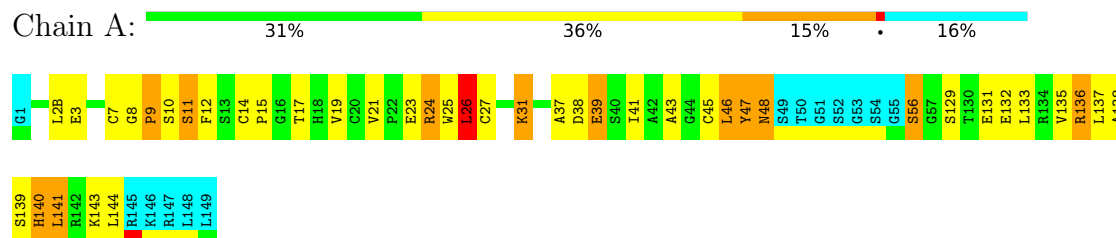


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

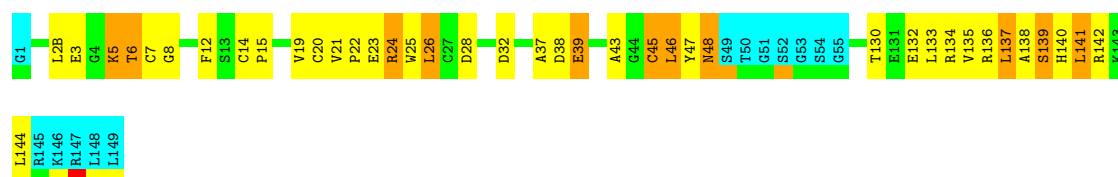
- Molecule 1: LRP-1, linker, Apo-E



4.2.2 Score per residue for model 2

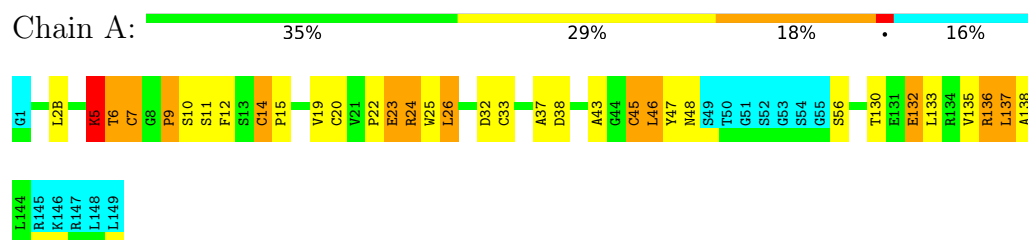
- Molecule 1: LRP-1, linker, Apo-E





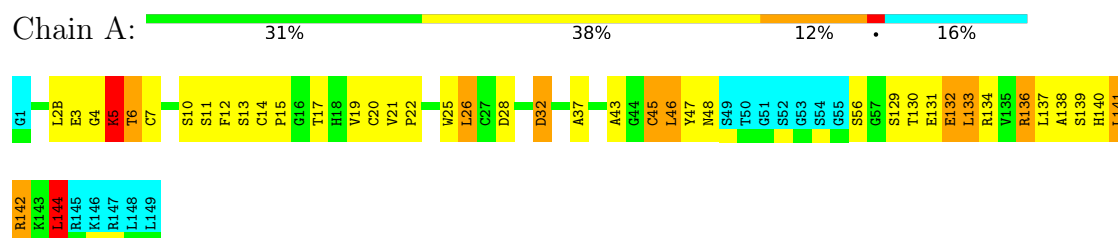
4.2.3 Score per residue for model 3

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



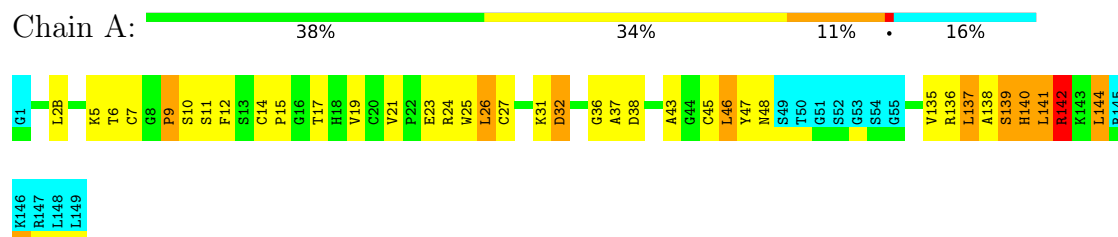
4.2.4 Score per residue for model 4

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



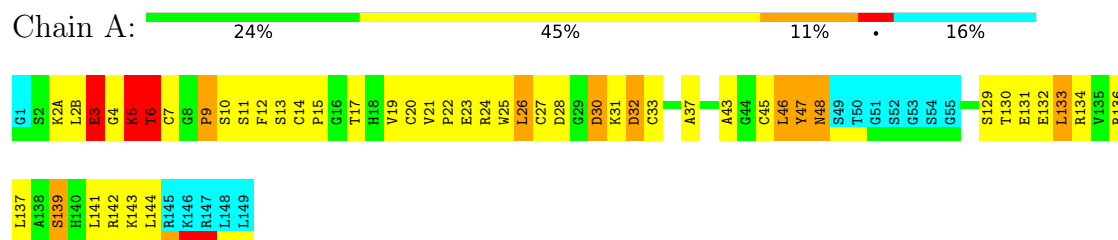
4.2.5 Score per residue for model 5

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



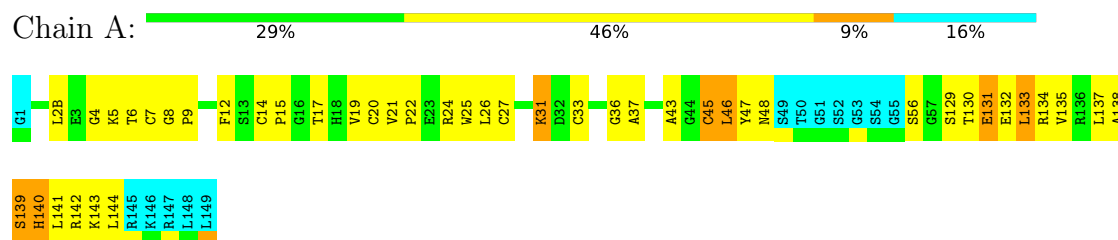
4.2.6 Score per residue for model 6

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



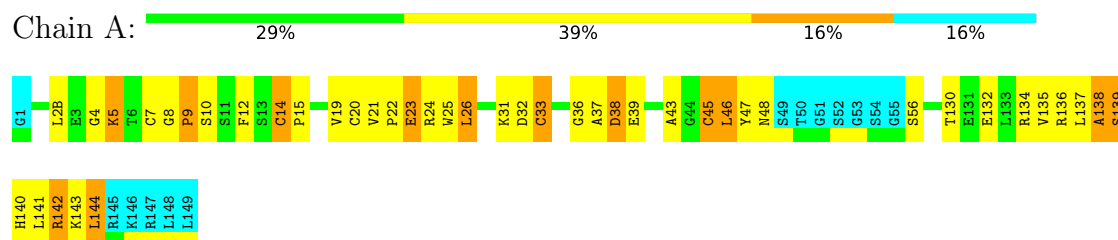
4.2.7 Score per residue for model 7 (medoid)

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



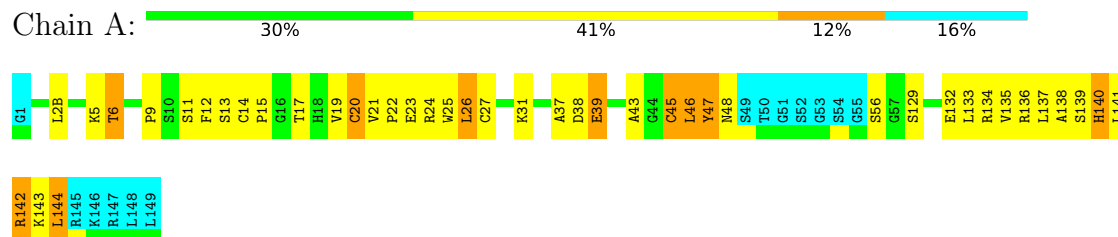
4.2.8 Score per residue for model 8

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



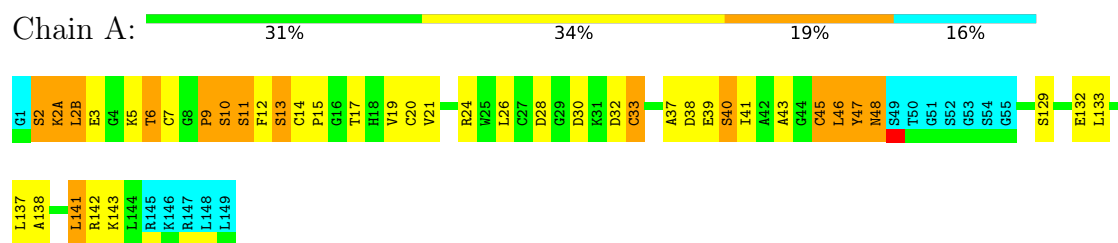
4.2.9 Score per residue for model 9

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



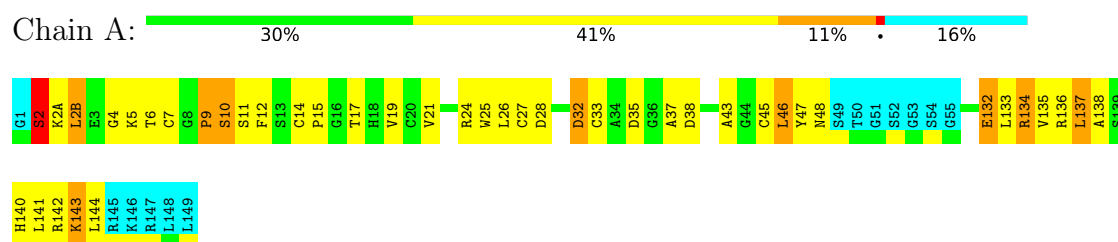
4.2.10 Score per residue for model 10

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



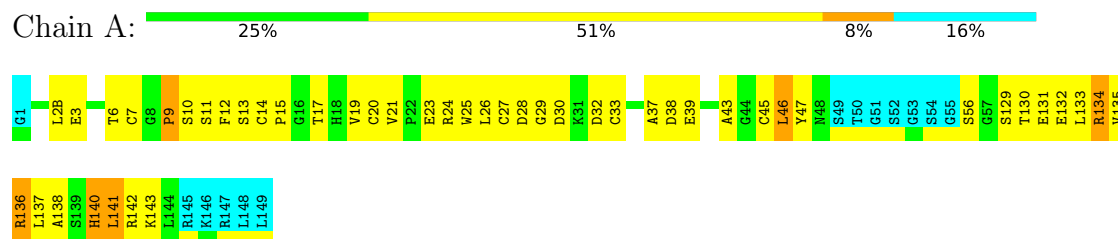
4.2.11 Score per residue for model 11

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



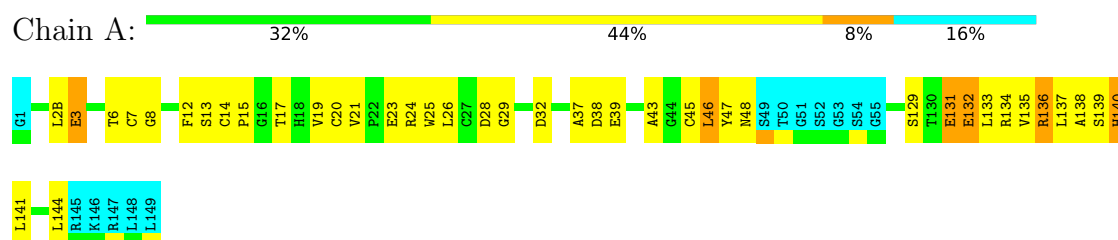
4.2.12 Score per residue for model 12

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



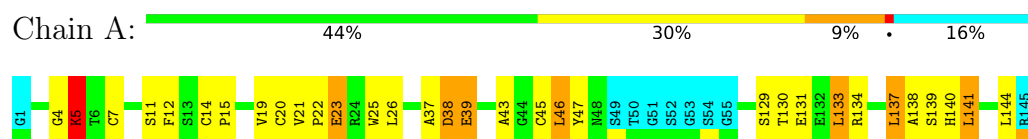
4.2.13 Score per residue for model 13

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



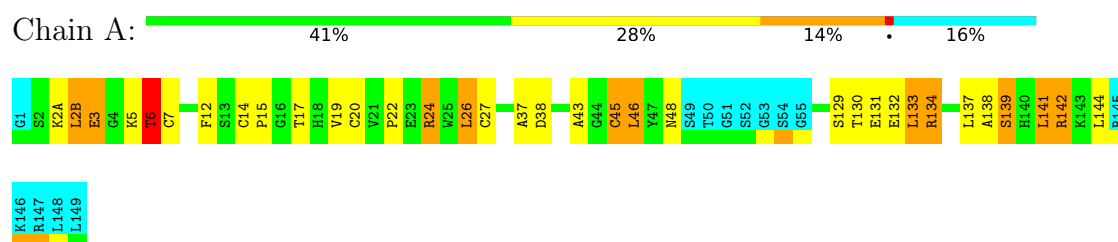
4.2.14 Score per residue for model 14

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



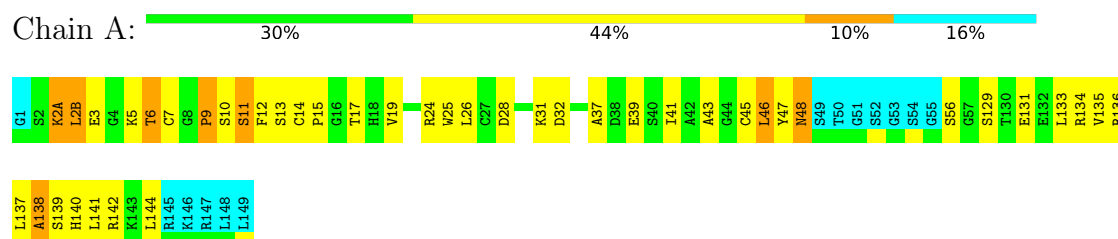
4.2.15 Score per residue for model 15

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



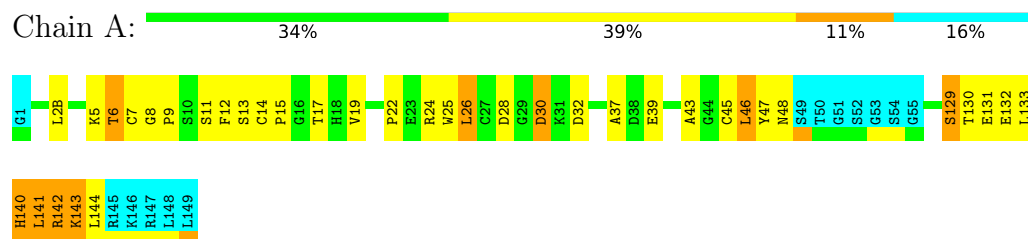
4.2.16 Score per residue for model 16

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



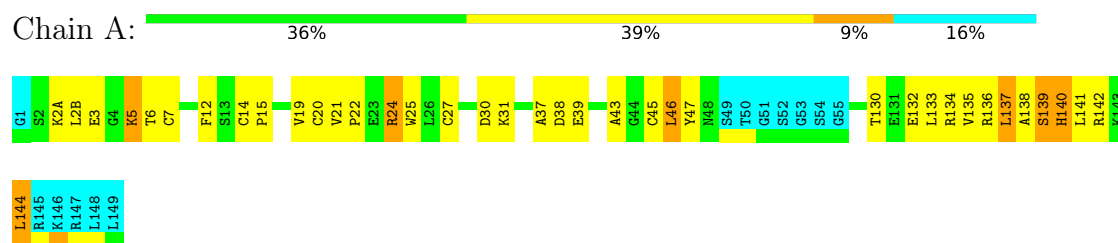
4.2.17 Score per residue for model 17

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



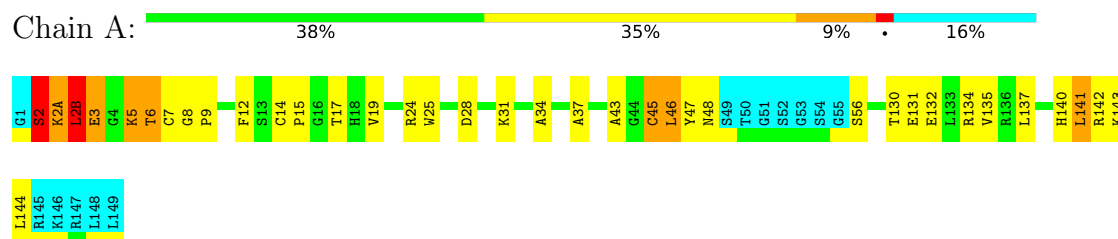
4.2.18 Score per residue for model 18

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



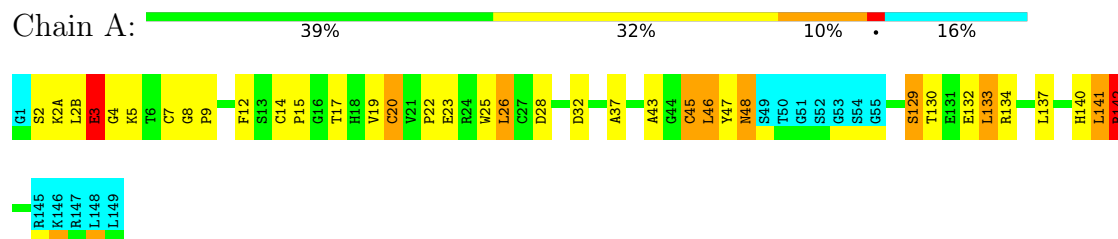
4.2.19 Score per residue for model 19

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



4.2.20 Score per residue for model 20

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



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)	working_cs.cif
Number of chemical shift lists	2
Total number of shifts	1122
Number of shifts mapped to atoms	999
Number of unparsed shifts	0
Number of shifts with mapping errors	123
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	84%

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	36±6
All	All	9900	9380	9380	724

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 38.

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	6
1:A:2(B):LEU:HD23	1:A:19:VAL:CG2	0.75	2.12	3	9
1:A:21:VAL:HG21	1:A:32:ASP:CG	0.74	2.07	12	1
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	6
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:39:GLU:N	1:A:39:GLU:CD	0.70	2.49	2	3
1:A:14:CYS:CB	1:A:19:VAL:HG13	0.70	2.17	3	20
1:A:45:CYS:C	1:A:46:LEU:HD22	0.70	2.11	3	20
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:2(B):LEU:HB2	1:A:19:VAL:HG21	0.65	1.67	10	2
1:A:26:LEU:HA	1:A:38:ASP:CG	0.65	2.17	8	4
1:A:2(A):LYS:C	1:A:2(B):LEU:HD12	0.65	2.17	20	2
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: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:2(B):LEU:HD21	1:A:21:VAL:HB	0.61	1.71	5	4
1:A:21:VAL:HG21	1:A:38:ASP:CG	0.61	2.20	9	4
1:A:47:TYR:O	1:A:48:ASN:CB	0.60	2.48	2	4
1:A:31:LYS:HA	1:A:39:GLU:CD	0.60	2.20	8	2
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:21:VAL:HG21	1:A:32:ASP:OD2	0.60	1.96	12	1
1:A:2(B):LEU:HD11	1:A:32:ASP:HB3	0.60	1.73	17	3
1:A:26:LEU:HD12	1:A:38:ASP:OD2	0.60	1.96	8	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:39:GLU:CD	1:A:39:GLU:N	0.57	2.62	8	1
1:A:46:LEU:HD13	1:A:46:LEU:N	0.57	2.15	7	16
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:137:LEU:HD13	1:A:137:LEU:C	0.57	2.25	16	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:PRO:O	1:A:26:LEU:HD13	0.56	2.00	6	7
1:A:2(B):LEU:HD11	1:A:32:ASP:OD2	0.56	2.01	8	1
1:A:23:GLU:HA	1:A:26:LEU:HD22	0.56	1.78	6	1
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:5:LYS:C	1:A:6:THR:HG23	0.54	2.27	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:HD22	1:A:137:LEU:C	0.52	2.28	5	3
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:2(B):LEU:O	1:A:3:GLU:C	0.51	2.54	20	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	12
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: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:46:LEU:N	1:A:46:LEU:HD13	0.50	2.21	1	2
1:A:9:PRO:O	1:A:11:SER:N	0.49	2.46	16	8
1:A:47:TYR:CD1	1:A:48:ASN:N	0.49	2.81	1	1

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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: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:39:GLU:N	1:A:39:GLU:OE1	0.48	2.47	8	2
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: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:21:VAL:HG11	1:A:33:CYS:SG	0.46	2.50	10	2
1:A:47:TYR:O	1:A:48:ASN:HB2	0.46	2.10	16	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:ND1	1:A:140:HIS:N	0.46	2.63	17	4
1:A:2(A):LYS:O	1:A:2(B):LEU:C	0.46	2.58	15	1
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
1:A:24:ARG:CG	1:A:138:ALA:C	0.45	2.89	1	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2(B):LEU:C	1:A:3:GLU:CG	0.45	2.90	6	1
1:A:129:SER:C	1:A:133:LEU:HD13	0.45	2.35	7	1
1:A:26:LEU:HD12	1:A:38:ASP:CG	0.45	2.36	8	3
1:A:12:PHE:O	1:A:21:VAL:CG1	0.45	2.65	10	3
1:A:22:PRO:CD	1:A:25:TRP:CD2	0.45	2.99	4	1
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:141:LEU:O	1:A:142:ARG:C	0.45	2.59	3	6
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:22:PRO:HD2	1:A:25:TRP:CE3	0.45	2.47	17	2
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:5:LYS:C	1:A:6:THR:CG2	0.44	2.90	15	2
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:137:LEU:C	1:A:137:LEU:HD22	0.44	2.38	3	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:LEU:HD12	1:A:38:ASP:HB2	0.43	1.89	15	1
1:A:135:VAL:O	1:A:135:VAL:HG12	0.43	2.12	3	3
1:A:24:ARG:HG2	1:A:135:VAL:O	0.43	2.13	1	1
1:A:47:TYR:C	1:A:47:TYR:CD1	0.43	2.97	3	2
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:5:LYS:C	1:A:6:THR:HG22	0.43	2.39	19	1
1:A:25:TRP:CD1	1:A:25:TRP:N	0.42	2.86	8	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:41:ILE:CD1	1:A:46:LEU:C	0.42	2.93	16	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:4:GLY:C	1:A:5:LYS:HG2	0.42	2.39	14	1
1:A:5:LYS:O	1:A:6:THR:HG23	0.42	2.15	15	1
1:A:135:VAL:HG12	1:A:135:VAL:O	0.42	2.14	5	1
1:A:21:VAL:HG21	1:A:32:ASP:OD1	0.42	2.14	12	1
1:A:21:VAL:CG2	1:A:25:TRP:CB	0.42	2.98	13	1
1:A:2(B):LEU:CD2	1:A:32:ASP:O	0.41	2.66	4	1
1:A:47:TYR:CD1	1:A:47:TYR:C	0.41	2.97	5	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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
1:A:46:LEU:HD23	1:A:131:GLU:CD	0.41	2.40	15	1
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: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:56:SER:CB	1:A:131:GLU:CD	0.41	2.94	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: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:24:ARG:HG3	1:A:138:ALA:C	0.40	2.42	1	1
1:A:6:THR:C	1:A:7:CYS:SG	0.40	3.04	4	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: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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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 [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	67/80 (84%)	50±2 (74±4%)	12±3 (19±4%)	5±2 (7±3%)	1	15
All	All	1340/1600 (84%)	992 (74%)	249 (19%)	99 (7%)	1	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	8	GLY	8
1	A	10	SER	8
1	A	3	GLU	7
1	A	5	LYS	7
1	A	31	LYS	6
1	A	142	ARG	6
1	A	47	TYR	4
1	A	6	THR	4
1	A	138	ALA	3
1	A	4	GLY	3
1	A	33	CYS	3
1	A	2	SER	3
1	A	2(B)	LEU	3
1	A	133	LEU	2
1	A	26	LEU	1
1	A	144	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%)	801 (73%)	299 (27%)	2	21

All 43 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	141	LEU	20
1	A	7	CYS	15
1	A	5	LYS	13
1	A	132	GLU	13
1	A	140	HIS	12
1	A	130	THR	12
1	A	26	LEU	11
1	A	6	THR	11
1	A	45	CYS	10
1	A	139	SER	10
1	A	20	CYS	9
1	A	28	ASP	9
1	A	56	SER	8
1	A	136	ARG	8
1	A	143	LYS	8
1	A	133	LEU	8
1	A	142	ARG	8
1	A	13	SER	8
1	A	144	LEU	8
1	A	3	GLU	7
1	A	24	ARG	7
1	A	39	GLU	6
1	A	137	LEU	6
1	A	32	ASP	6
1	A	131	GLU	5
1	A	134	ARG	4
1	A	11	SER	3
1	A	23	GLU	3

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Mol	Chain	Res	Type	Models (Total)
1	A	33	CYS	3
1	A	38	ASP	3
1	A	10	SER	3
1	A	30	ASP	3
1	A	2	SER	3
1	A	2(A)	LYS	3
1	A	2(B)	LEU	3
1	A	14	CYS	2
1	A	27	CYS	2
1	A	129	SER	2
1	A	40	SER	1
1	A	41	ILE	1
1	A	48	ASN	1
1	A	35	ASP	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 oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

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

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 [i](#)

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: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping [i](#)

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 [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	76	0.38 ± 0.25	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	68	-0.08 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}'$	56	-0.03 ± 0.31	None needed (< 0.5 ppm)
^{15}N	64	0.27 ± 0.32	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 81%, i.e. 670 atoms were assigned a chemical shift out of a possible 823. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	273/336 (81%)	112/138 (81%)	109/134 (81%)	52/64 (81%)
Sidechain	363/442 (82%)	247/286 (86%)	115/139 (83%)	1/17 (6%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	34/45 (76%)	19/23 (83%)	14/19 (74%)	1/3 (33%)
Overall	670/823 (81%)	378/447 (85%)	238/292 (82%)	54/84 (64%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 80%, i.e. 790 atoms were assigned a chemical shift out of a possible 982. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	324/405 (80%)	134/168 (80%)	128/160 (80%)	62/77 (81%)
Sidechain	432/532 (81%)	293/344 (85%)	138/164 (84%)	1/24 (4%)
Aromatic	34/45 (76%)	19/23 (83%)	14/19 (74%)	1/3 (33%)
Overall	790/982 (80%)	446/535 (83%)	280/343 (82%)	64/104 (62%)

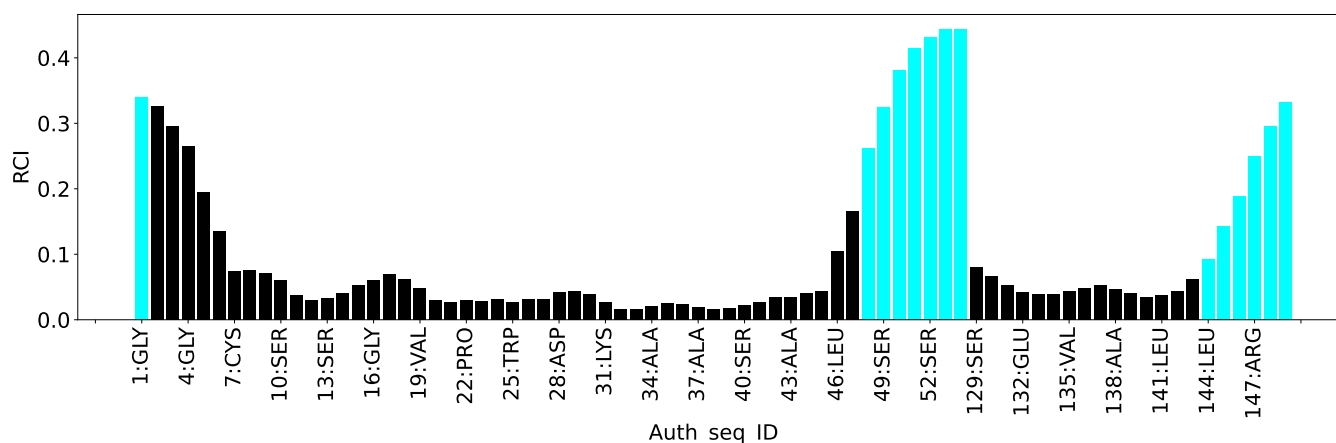
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

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. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



7.2 Chemical shift list 2

File name: working_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	297
Number of shifts mapped to atoms	174
Number of unparsed shifts	0
Number of shifts with mapping errors	123
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	29

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

- No matching atom found in the structure. All 123 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2	A	3	GLU	HD1	7.128	0.005	3
2	A	3	GLU	HD2	7.128	0.005	3
2	A	3	GLU	HE1	6.819	0.005	3
2	A	3	GLU	HE2	6.819	0.005	1
2	A	3	GLU	CD1	133.261	0.020	3
2	A	3	GLU	CE1	118.266	0.020	3
2	A	4	GLY	HB	4.199	0.001	1
2	A	4	GLY	HG21	1.2	0.005	1
2	A	4	GLY	HG22	1.2	0.005	1
2	A	4	GLY	HG23	1.2	0.005	1
2	A	4	GLY	CB	69.604	0.034	1
2	A	4	GLY	CG2	21.807	0.023	1
2	A	6	THR	HB2	2.004	0.005	4
2	A	6	THR	HB3	2.004	0.005	2
2	A	6	THR	HG3	2.238	0.005	2
2	A	7	CYS	HD11	0.843	0.005	2
2	A	7	CYS	HD12	0.843	0.005	2
2	A	7	CYS	HD13	0.843	0.005	2
2	A	7	CYS	HD21	0.884	0.005	2
2	A	7	CYS	HD22	0.884	0.005	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2	A	7	CYS	HD23	0.884	0.005	2
2	A	7	CYS	CD1	23.869	0.025	2
2	A	7	CYS	CD2	24.615	0.013	2
2	A	7	CYS	CG	26.96	0.020	1
2	A	8	GLY	HB2	1.875	0.005	2
2	A	8	GLY	HB3	1.875	0.005	2
2	A	8	GLY	HD2	3.184	0.005	2
2	A	8	GLY	HD3	3.184	0.005	2
2	A	8	GLY	CB	30.316	0.041	1
2	A	8	GLY	CD	43.331	0.011	1
2	A	8	GLY	CG	27.376	0.020	1
2	A	9	PRO	H	7.888	0.005	1
2	A	9	PRO	HG11	0.989	0.005	2
2	A	9	PRO	HG12	0.989	0.005	2
2	A	9	PRO	HG13	0.989	0.005	2
2	A	9	PRO	HG21	0.931	0.005	2
2	A	9	PRO	HG22	0.931	0.005	2
2	A	9	PRO	HG23	0.931	0.005	2
2	A	9	PRO	CG1	21.441	0.020	2
2	A	9	PRO	CG2	21.153	0.020	2
2	A	10	SER	HD2	3.172	0.005	2
2	A	10	SER	HD3	3.172	0.005	2
2	A	10	SER	CD	43.555	0.023	1
2	A	10	SER	CG	27.392	0.020	1
2	A	11	SER	HD11	0.851	0.005	2
2	A	11	SER	HD12	0.851	0.005	2
2	A	11	SER	HD13	0.851	0.005	2
2	A	11	SER	HD21	0.893	0.005	2
2	A	11	SER	HD22	0.893	0.005	2
2	A	11	SER	HD23	0.893	0.005	2
2	A	11	SER	CD1	23.458	0.028	2
2	A	11	SER	CD2	24.889	0.023	2
2	A	11	SER	CG	26.84	0.020	1
2	A	14	CYS	HD2	6.946	0.005	1
2	A	14	CYS	HE1	7.732	0.005	1
2	A	14	CYS	CD2	119.23	0.040	1
2	A	14	CYS	CE1	138.932	0.040	1
2	A	15	PRO	H	7.836	0.005	1
2	A	15	PRO	HD11	0.84	0.005	2
2	A	15	PRO	HD12	0.84	0.005	2
2	A	15	PRO	HD13	0.84	0.005	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2	A	15	PRO	HD21	0.901	0.005	2
2	A	15	PRO	HD22	0.901	0.005	2
2	A	15	PRO	HD23	0.901	0.005	2
2	A	15	PRO	CD1	23.117	0.018	2
2	A	15	PRO	CD2	25.16	0.032	2
2	A	16	GLY	HB2	1.852	0.005	2
2	A	16	GLY	HB3	1.852	0.005	2
2	A	16	GLY	CB	30.504	0.043	1
2	A	16	GLY	CD	43.542	0.020	1
2	A	16	GLY	CG	27.486	0.020	1
2	A	17	THR	HB2	1.838	0.005	4
2	A	17	THR	HB3	1.816	0.005	4
2	A	17	THR	HD2	1.688	0.005	4
2	A	17	THR	HD3	1.688	0.005	4
2	A	17	THR	HE2	2.995	0.005	2
2	A	17	THR	HE3	2.995	0.005	2
2	A	17	THR	HG3	1.404	0.005	2
2	A	17	THR	CD	29.284	0.005	1
2	A	17	THR	CE	42.203	0.031	1
2	A	18	HIS	HD11	0.851	0.005	2
2	A	18	HIS	HD12	0.851	0.005	2
2	A	18	HIS	HD13	0.851	0.005	2
2	A	18	HIS	HD21	0.891	0.005	2
2	A	18	HIS	HD22	0.891	0.005	2
2	A	18	HIS	HD23	0.891	0.005	2
2	A	18	HIS	CD1	23.468	0.023	2
2	A	19	VAL	HB2	1.799	0.005	2
2	A	19	VAL	HB3	1.799	0.005	2
2	A	19	VAL	HD2	3.212	0.005	2
2	A	19	VAL	HD3	3.212	0.005	2
2	A	19	VAL	CD	43.516	0.014	1
2	A	20	CYS	HD2	1.687	0.005	2
2	A	20	CYS	HD3	1.687	0.005	2
2	A	20	CYS	HE2	2.992	0.005	2
2	A	20	CYS	HE3	2.992	0.005	2
2	A	20	CYS	HG2	1.459	0.005	2
2	A	20	CYS	HG3	1.414	0.005	2
2	A	20	CYS	CD	29.118	0.008	1
2	A	20	CYS	CE	42.195	0.025	1
2	A	20	CYS	CG	24.845	0.006	1
2	A	21	VAL	HB2	1.845	0.005	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2	A	21	VAL	HB3	1.782	0.005	2
2	A	21	VAL	HD2	3.207	0.005	2
2	A	21	VAL	HD3	3.207	0.005	2
2	A	21	VAL	CD	43.517	0.014	1
2	A	22	PRO	H	8.267	0.002	1
2	A	22	PRO	HD11	0.861	0.005	2
2	A	22	PRO	HD12	0.861	0.005	2
2	A	22	PRO	HD13	0.861	0.005	2
2	A	22	PRO	HD21	0.928	0.005	2
2	A	22	PRO	HD22	0.928	0.005	2
2	A	22	PRO	HD23	0.928	0.005	2
2	A	22	PRO	CD1	23.431	0.015	2
2	A	22	PRO	CD2	25.081	0.014	2
2	A	23	GLU	HD11	0.856	0.005	2
2	A	23	GLU	HD12	0.856	0.005	2
2	A	23	GLU	HD13	0.856	0.005	2
2	A	23	GLU	HD21	0.9	0.005	2
2	A	23	GLU	HD22	0.9	0.005	2
2	A	23	GLU	HD23	0.9	0.005	2
2	A	23	GLU	CD1	23.746	0.020	2
2	A	23	GLU	CD2	25.234	0.020	2

7.2.2 Chemical shift referencing [i](#)

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

7.2.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 20%, i.e. 167 atoms were assigned a chemical shift out of a possible 823. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	97/336 (29%)	41/138 (30%)	40/134 (30%)	16/64 (25%)
Sidechain	69/442 (16%)	40/286 (14%)	29/139 (21%)	0/17 (0%)
Aromatic	1/45 (2%)	0/23 (0%)	1/19 (5%)	0/3 (0%)
Overall	167/823 (20%)	81/447 (18%)	70/292 (24%)	16/84 (19%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 17%, i.e. 170 atoms were assigned a chemical shift out of a possible

982. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	100/405 (25%)	43/168 (26%)	41/160 (26%)	16/77 (21%)
Sidechain	69/532 (13%)	40/344 (12%)	29/164 (18%)	0/24 (0%)
Aromatic	1/45 (2%)	0/23 (0%)	1/19 (5%)	0/3 (0%)
Overall	170/982 (17%)	83/535 (16%)	71/343 (21%)	16/104 (15%)

7.2.4 Statistically unusual chemical shifts ⓘ

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

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	A	18	HIS	CG	26.96	116.99 – 147.60	-34.4
2	A	18	HIS	CD2	24.95	103.95 – 136.66	-29.1
2	A	6	THR	CB	29.73	61.12 – 78.27	-23.3
2	A	10	SER	CB	30.55	56.28 – 71.32	-22.1
2	A	17	THR	CB	32.74	61.12 – 78.27	-21.6
2	A	11	SER	CB	42.20	56.28 – 71.32	-14.4
2	A	4	GLY	CA	62.97	38.93 – 51.79	13.7
2	A	6	THR	CG2	36.39	16.06 – 27.03	13.5
2	A	12	PHE	CB	18.77	29.72 – 50.07	-10.4
2	A	5	LYS	CG	36.24	19.35 – 30.45	10.2
2	A	8	GLY	CA	57.94	38.93 – 51.79	9.8
2	A	16	GLY	CA	57.38	38.93 – 51.79	9.3
2	A	22	PRO	CB	42.23	26.06 – 37.61	9.0
2	A	11	SER	HB2	1.63	2.61 – 5.13	-8.9
2	A	15	PRO	CB	41.92	26.06 – 37.61	8.7
2	A	11	SER	HB3	1.63	2.49 – 5.20	-8.2
2	A	23	GLU	CB	43.51	21.56 – 38.37	8.1
2	A	10	SER	HB2	1.86	2.61 – 5.13	-8.0
2	A	23	GLU	CG	27.28	30.20 – 42.01	-7.5
2	A	10	SER	HB3	1.86	2.49 – 5.20	-7.3
2	A	18	HIS	CB	42.34	19.76 – 40.75	5.8
2	A	6	THR	HG21	2.31	0.08 – 2.19	5.5
2	A	6	THR	HG22	2.31	0.08 – 2.19	5.5
2	A	6	THR	HG23	2.31	0.08 – 2.19	5.5
2	A	22	PRO	CA	55.22	55.85 – 70.84	-5.4
2	A	6	THR	HG3	2.24	0.08 – 2.19	5.2
2	A	3	GLU	CB	38.68	21.56 – 38.37	5.2
2	A	3	GLU	HB2	3.07	1.00 – 3.05	5.1
2	A	3	GLU	HB3	3.07	0.95 – 3.05	5.1

7.2.5 Random Coil Index (RCI) plots [i](#)

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. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

