Full wwPDB NMR Structure Validation Report (i)

Jun 5, 2023 – 06:22 AM EDT

PDB ID	:	2LV3
BMRB ID	:	17636
Title	:	Structure-functional characterization of Grx domain of Mus musculus TGR
Authors	:	Dobrovolska, O.; Shumilina, E.; Gladyshev, V.; Dikiy, A.
Deposited on	:	2012-06-28

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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

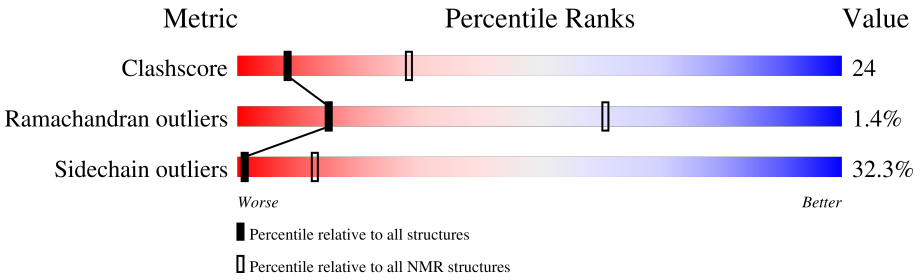
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 87%.

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	118	39% 34% 8% 6% 14%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 11 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:27-A:121 (95)	0.43	11

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. No single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1638 atoms, of which 821 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Thioredoxin reductase 3.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	102	1638	508	821	150	156	3	0

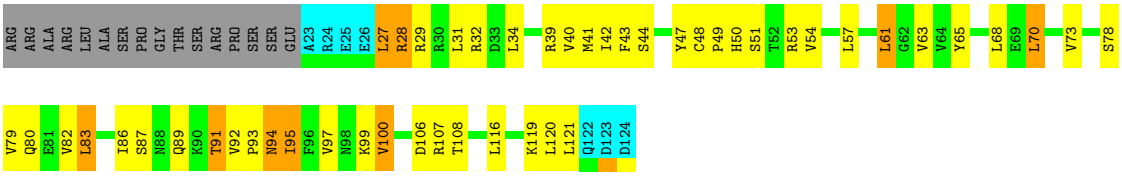
4 Residue-property plots (i)

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: Thioredoxin reductase 3

Chain A: 39% 34% 8% 6% 14%



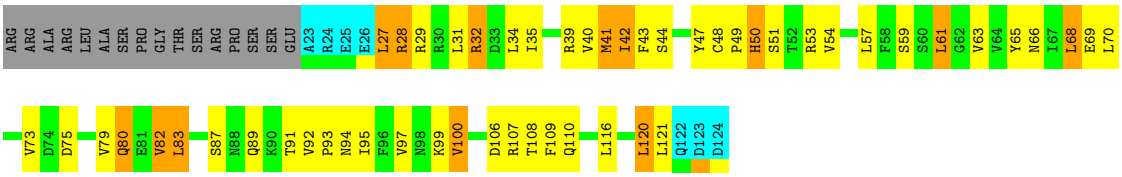
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Thioredoxin reductase 3

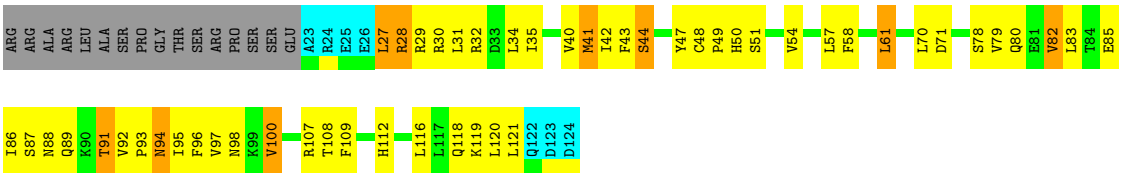
Chain A: 36% 34% 11% 6% 14%



4.2.2 Score per residue for model 2

• Molecule 1: Thioredoxin reductase 3

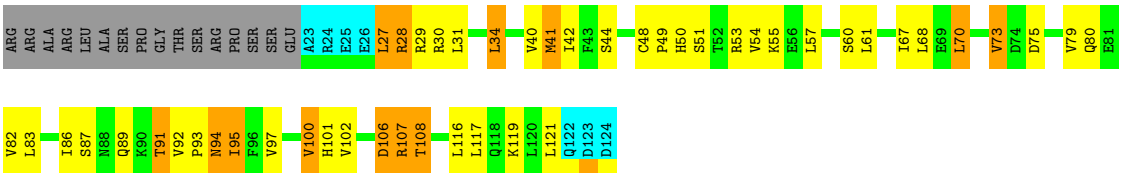
Chain A: 36% 36% 8% 6% 14%



4.2.3 Score per residue for model 3

- Molecule 1: Thioredoxin reductase 3

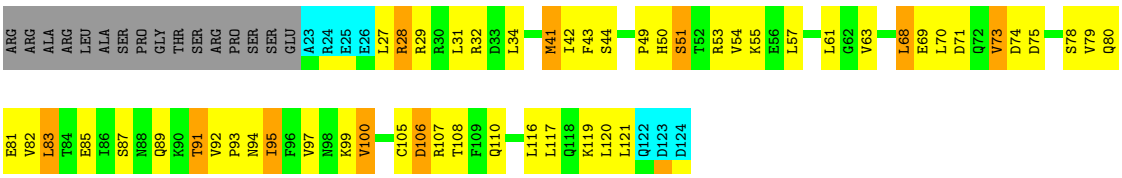
Chain A: 40% 30% 11% 6% 14%



4.2.4 Score per residue for model 4

- Molecule 1: Thioredoxin reductase 3

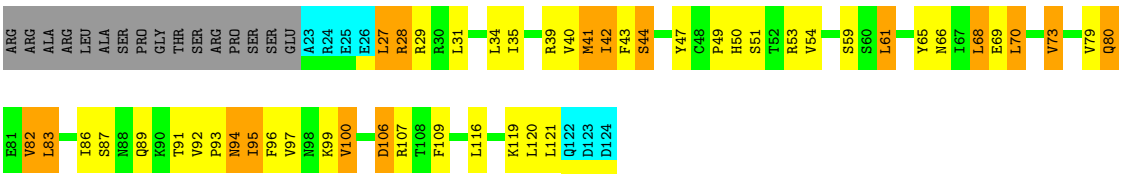
Chain A: 36% 36% 8% 6% 14%



4.2.5 Score per residue for model 5

- Molecule 1: Thioredoxin reductase 3

Chain A: 39% 28% 14% 6% 14%



4.2.6 Score per residue for model 6

- Molecule 1: Thioredoxin reductase 3

Chain A: 39% 32% 9% 6% 14%

ARG ARG ALA ARG LEU ALA SER PRO GLY THR SER ARG PRO SER SER GLU A23 R24 E25 E26 L27 R28 R29 L34 R39 V40 M41 I42 F43 S44 K45 S46 Y47 C48 P49 H50 S51 T52 R53 V54 L57 I61 G62 V63 L68 E69 L70 D71 Q72 V73 S78 V79 V82

L83 T84 E85 I86 S87 N88 Q89 K90 T91 V92 P93 N94 I95 F96 V97 N98 K99 V100 D106 R107 T108 F109 Q110 L116 K119 L120 L121 Q122 D123 D124

4.2.7 Score per residue for model 7

- Molecule 1: Thioredoxin reductase 3

Chain A: 34% 35% 12% 6% 14%

ARG ARG ALA ARG LEU ALA SER PRO GLY THR SER ARG PRO SER SER GLU A23 R24 E25 E26 L27 R28 R29 R30 L31 R32 D33 L34 I35 E36 R39 V40 M41 I42 F43 S44 K45 S46 Y47 C48 P49 H50 S51 T52 R53 V54 L57 S60 L61 G62 V63 V64 Y65 L68 E69 L70

V73 D74 D75 G76 A77 S78 V79 Q80 E81 V82 L83 T84 E85 I86 S87 N88 Q89 K90 T91 V92 P93 N94 I95 F96 V97 N98 K99 V100 R107 T108 L116 L117 Q118 K119 L120 L121 Q122 D123 D124

4.2.8 Score per residue for model 8

- Molecule 1: Thioredoxin reductase 3

Chain A: 42% 29% 9% 6% 14%

ARG ARG ALA ARG LEU ALA SER PRO GLY THR SER ARG PRO SER SER GLU A23 R24 E25 E26 L27 R28 R29 L34 R39 V40 M41 I42 F43 S44 C48 P49 H50 S51 T52 R53 V54 L57 L61 G62 V63 I67 L68 E69 L70 V73 D74 D75 S78 V79 Q80 E81

V82 L83 S87 N88 Q89 K90 T91 V92 P93 N94 I95 F96 V97 N98 K99 V100 D106 R107 T108 H112 L116 L120 L121 Q122 D123 D124

4.2.9 Score per residue for model 9

- Molecule 1: Thioredoxin reductase 3

Chain A: 34% 36% 10% 6% 14%

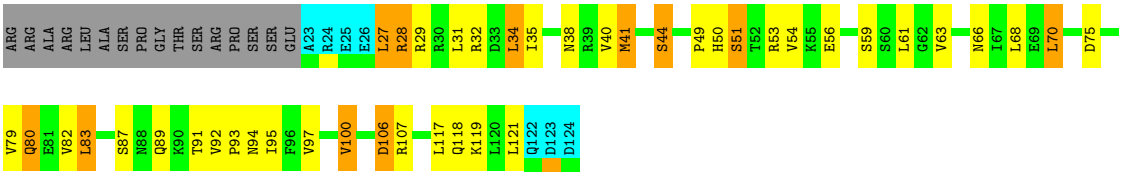
ARG ARG ALA ARG LEU ALA SER PRO GLY THR SER ARG PRO SER SER GLU A23 R24 E25 E26 L27 R28 R29 R30 L34 V40 M41 I42 F43 S44 K45 S46 Y47 C48 P49 H50 S51 T52 R53 V54 K55 E56 L57 L61 Y65 N66 I67 L68 E69 L70 V73 G76 A77 S78

V79 Q80 E81 V82 L83 T84 E85 I86 S87 N88 Q89 K90 T91 V92 P93 N94 I95 F96 V97 N98 K99 V100 H101 V102 D106 R107 T108 H112 L116 K119 L120 L121 Q122 D123 D124

4.2.10 Score per residue for model 10

- Molecule 1: Thioredoxin reductase 3

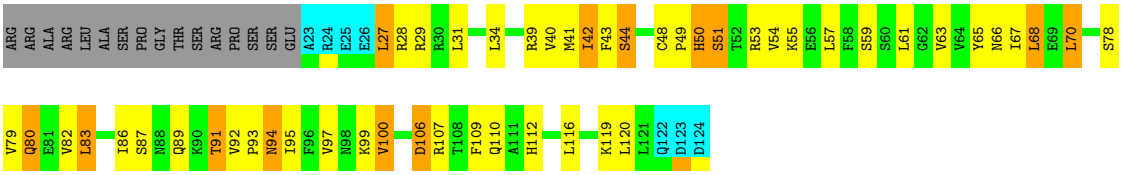
Chain A: 44% 27% 9% 6% 14%



4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: Thioredoxin reductase 3

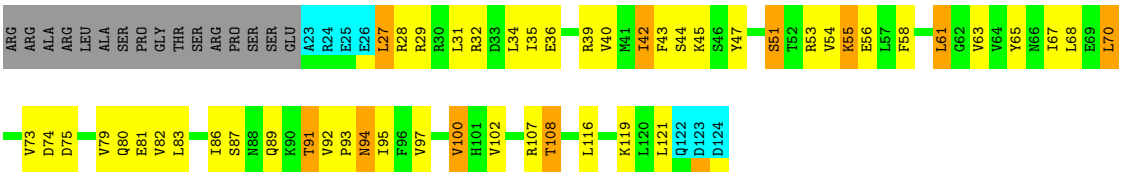
Chain A: 37% 32% 11% 6% 14%



4.2.12 Score per residue for model 12

- Molecule 1: Thioredoxin reductase 3

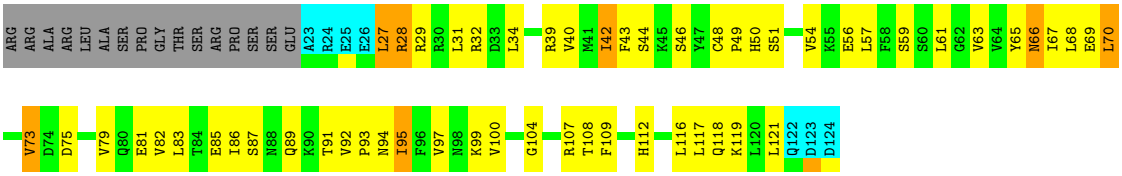
Chain A: 37% 35% 8% 6% 14%



4.2.13 Score per residue for model 13

- Molecule 1: Thioredoxin reductase 3

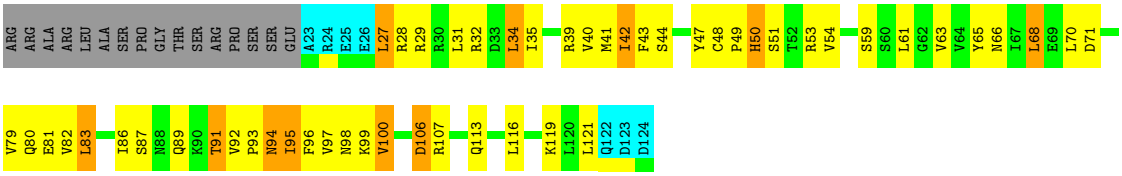
Chain A: 33% 42% 6% 6% 14%



4.2.14 Score per residue for model 14

- Molecule 1: Thioredoxin reductase 3

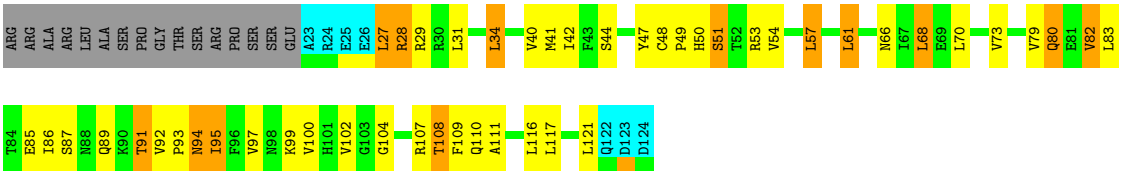
Chain A: 36% 35% 9% 6% 14%



4.2.15 Score per residue for model 15

- Molecule 1: Thioredoxin reductase 3

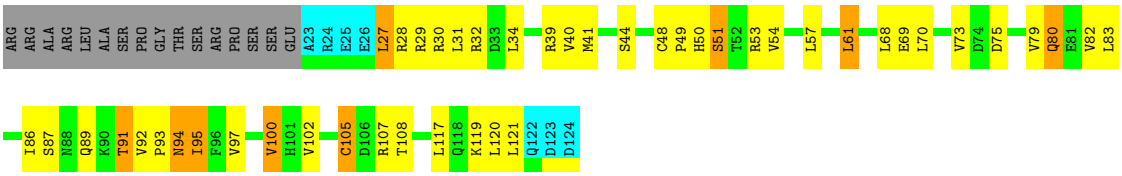
Chain A: 40% 30% 11% 6% 14%



4.2.16 Score per residue for model 16

- Molecule 1: Thioredoxin reductase 3

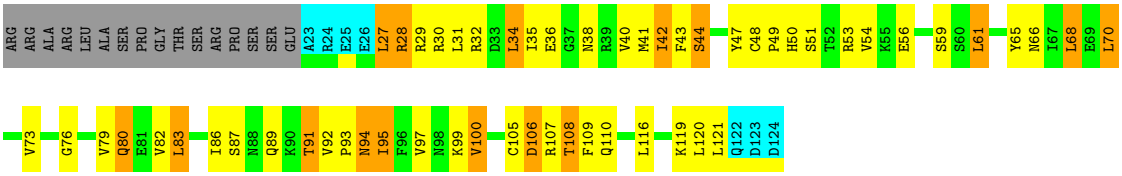
Chain A: 42% 31% 8% 6% 14%



4.2.17 Score per residue for model 17

- Molecule 1: Thioredoxin reductase 3

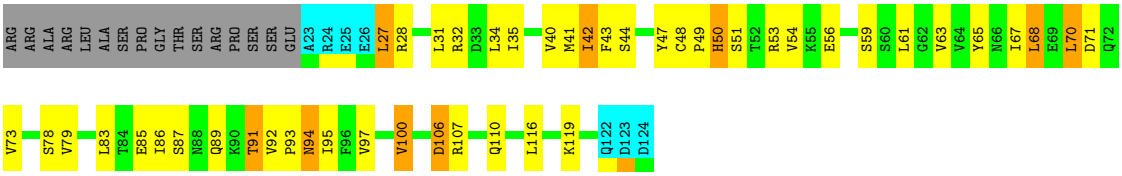
Chain A: 33% 34% 14% 6% 14%



4.2.18 Score per residue for model 18

- Molecule 1: Thioredoxin reductase 3

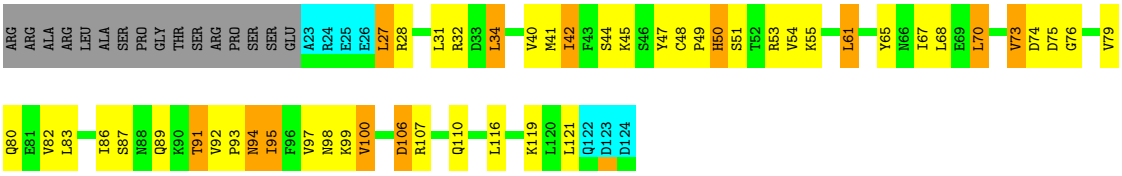
Chain A: 41% 32% 8% 6% 14%



4.2.19 Score per residue for model 19

- Molecule 1: Thioredoxin reductase 3

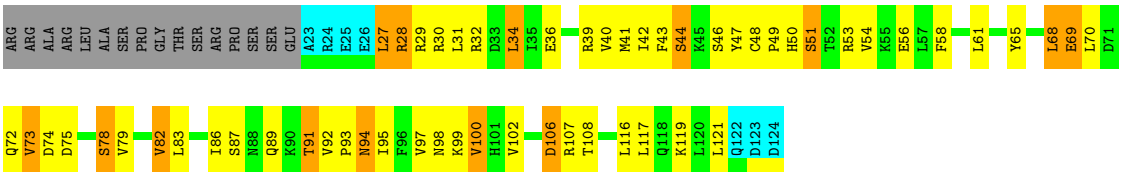
Chain A: 39% 31% 10% 6% 14%



4.2.20 Score per residue for model 20

- Molecule 1: Thioredoxin reductase 3

Chain A: 32% 36% 12% 6% 14%



5 Refinement protocol and experimental data overview (i)

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

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
CYANA 2.1	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	1
Total number of shifts	1400
Number of shifts mapped to atoms	1248
Number of unparsed shifts	0
Number of shifts with mapping errors	152
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	87%

6 Model quality (i)

6.1 Standard geometry (i)

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 (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	758	775	775	37±4
All	All	15160	15500	15500	747

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 24.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:102:VAL:HG11	1:A:108:THR:HG23	0.99	1.35	15	4
1:A:31:LEU:HD13	1:A:83:LEU:HD23	0.92	1.41	10	1
1:A:83:LEU:HD22	1:A:86:ILE:HD12	0.87	1.44	16	9
1:A:70:LEU:HD12	1:A:92:VAL:HG11	0.87	1.47	16	1
1:A:83:LEU:HD12	1:A:86:ILE:HD12	0.85	1.48	19	2
1:A:83:LEU:HD23	1:A:86:ILE:HD12	0.82	1.52	13	3
1:A:40:VAL:HG22	1:A:97:VAL:HG23	0.82	1.52	12	13
1:A:70:LEU:HD11	1:A:92:VAL:HG21	0.82	1.49	12	8
1:A:27:LEU:HD21	1:A:79:VAL:HA	0.78	1.55	6	20
1:A:61:LEU:HD23	1:A:121:LEU:HD11	0.77	1.55	3	2
1:A:97:VAL:HG13	1:A:120:LEU:HD22	0.75	1.56	1	2
1:A:100:VAL:HG11	1:A:120:LEU:HD11	0.74	1.57	8	4
1:A:42:ILE:HD11	1:A:65:TYR:CD1	0.73	2.19	17	3
1:A:70:LEU:HD13	1:A:92:VAL:HG11	0.73	1.61	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:83:LEU:HD22	1:A:92:VAL:HG12	0.71	1.61	6	3
1:A:27:LEU:CD1	1:A:79:VAL:HG22	0.69	2.17	4	1
1:A:27:LEU:HD11	1:A:79:VAL:CG2	0.69	2.17	6	4
1:A:27:LEU:HD11	1:A:79:VAL:HG23	0.69	1.64	7	4
1:A:28:ARG:CG	1:A:82:VAL:HG21	0.68	2.18	3	3
1:A:57:LEU:HD23	1:A:108:THR:HG22	0.68	1.64	9	4
1:A:67:ILE:O	1:A:68:LEU:HD23	0.66	1.91	12	5
1:A:67:ILE:O	1:A:68:LEU:HD13	0.66	1.90	18	2
1:A:34:LEU:HD23	1:A:43:PHE:CZ	0.65	2.26	12	6
1:A:41:MET:C	1:A:42:ILE:HD13	0.65	2.11	11	7
1:A:97:VAL:HG11	1:A:121:LEU:CD2	0.65	2.21	8	14
1:A:49:PRO:O	1:A:91:THR:HG21	0.65	1.92	15	16
1:A:97:VAL:HG13	1:A:98:ASN:ND2	0.65	2.06	2	2
1:A:31:LEU:HD21	1:A:79:VAL:HG23	0.64	1.68	13	13
1:A:69:GLU:O	1:A:73:VAL:HG13	0.64	1.91	20	3
1:A:27:LEU:HD13	1:A:79:VAL:HG22	0.64	1.69	4	1
1:A:41:MET:CE	1:A:68:LEU:HD11	0.64	2.23	20	4
1:A:31:LEU:HD21	1:A:79:VAL:HG13	0.64	1.70	4	1
1:A:42:ILE:HD11	1:A:65:TYR:HB2	0.64	1.70	19	7
1:A:69:GLU:O	1:A:73:VAL:HG23	0.63	1.92	16	2
1:A:116:LEU:O	1:A:116:LEU:HD13	0.63	1.94	8	5
1:A:57:LEU:HD21	1:A:117:LEU:HD23	0.63	1.70	15	1
1:A:43:PHE:CD2	1:A:83:LEU:HD11	0.63	2.28	8	2
1:A:70:LEU:O	1:A:73:VAL:HG22	0.62	1.95	9	6
1:A:83:LEU:CD1	1:A:86:ILE:HD12	0.62	2.25	3	2
1:A:28:ARG:CD	1:A:82:VAL:HG21	0.62	2.25	3	2
1:A:43:PHE:HB3	1:A:70:LEU:HD11	0.61	1.72	20	2
1:A:83:LEU:HD23	1:A:86:ILE:CD1	0.61	2.24	13	1
1:A:57:LEU:HD21	1:A:108:THR:O	0.61	1.96	3	1
1:A:42:ILE:HG22	1:A:94:ASN:O	0.61	1.96	12	4
1:A:40:VAL:HG12	1:A:42:ILE:CD1	0.61	2.26	7	5
1:A:102:VAL:CG1	1:A:117:LEU:HD11	0.60	2.26	3	1
1:A:31:LEU:HD13	1:A:83:LEU:HG	0.60	1.72	13	2
1:A:83:LEU:HD22	1:A:86:ILE:CD1	0.60	2.25	14	7
1:A:57:LEU:HG	1:A:108:THR:HG22	0.60	1.72	8	1
1:A:83:LEU:HD12	1:A:92:VAL:HG12	0.60	1.72	2	4
1:A:83:LEU:HD12	1:A:92:VAL:CG1	0.60	2.27	16	6
1:A:97:VAL:HG11	1:A:121:LEU:HD23	0.60	1.74	13	11
1:A:61:LEU:O	1:A:61:LEU:HD13	0.60	1.97	8	1
1:A:34:LEU:HD22	1:A:41:MET:CE	0.59	2.28	10	4
1:A:97:VAL:HG22	1:A:98:ASN:OD1	0.59	1.97	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:VAL:HG13	1:A:98:ASN:OD1	0.59	1.97	8	1
1:A:83:LEU:HD11	1:A:94:ASN:OD1	0.59	1.97	19	1
1:A:40:VAL:HG22	1:A:97:VAL:CG2	0.58	2.27	12	7
1:A:43:PHE:CD2	1:A:83:LEU:HD21	0.58	2.33	6	2
1:A:44:SER:O	1:A:70:LEU:HD12	0.58	1.98	20	6
1:A:27:LEU:HD11	1:A:79:VAL:CA	0.58	2.27	17	14
1:A:41:MET:HE3	1:A:68:LEU:HD11	0.58	1.75	7	4
1:A:75:ASP:O	1:A:79:VAL:HG23	0.58	1.99	4	1
1:A:34:LEU:HD21	1:A:68:LEU:HD13	0.57	1.76	4	1
1:A:39:ARG:HG3	1:A:40:VAL:HG23	0.57	1.75	16	2
1:A:48:CYS:HB3	1:A:91:THR:HG22	0.57	1.75	14	15
1:A:34:LEU:HD22	1:A:41:MET:SD	0.57	2.38	2	4
1:A:70:LEU:HD11	1:A:92:VAL:HG11	0.57	1.75	17	4
1:A:61:LEU:HD22	1:A:117:LEU:HD23	0.57	1.77	4	2
1:A:35:ILE:HD12	1:A:96:PHE:HB2	0.57	1.77	2	3
1:A:34:LEU:HD21	1:A:68:LEU:CD1	0.57	2.29	12	2
1:A:70:LEU:CD1	1:A:92:VAL:HG11	0.56	2.29	17	5
1:A:97:VAL:HG22	1:A:98:ASN:CG	0.56	2.21	8	1
1:A:31:LEU:O	1:A:35:ILE:HD12	0.56	2.00	12	3
1:A:78:SER:O	1:A:82:VAL:HG23	0.56	2.01	6	5
1:A:57:LEU:HD12	1:A:57:LEU:O	0.55	2.01	1	4
1:A:95:ILE:HG21	1:A:108:THR:HG21	0.55	1.76	17	3
1:A:67:ILE:C	1:A:68:LEU:HD13	0.55	2.21	18	1
1:A:44:SER:O	1:A:70:LEU:HD22	0.55	2.01	6	1
1:A:83:LEU:CD2	1:A:86:ILE:HD12	0.55	2.26	16	2
1:A:83:LEU:HD11	1:A:94:ASN:ND2	0.55	2.17	14	11
1:A:28:ARG:HG3	1:A:82:VAL:HG21	0.55	1.79	17	2
1:A:34:LEU:HD21	1:A:68:LEU:HD22	0.55	1.79	7	1
1:A:83:LEU:HD21	1:A:94:ASN:OD1	0.54	2.02	2	3
1:A:97:VAL:O	1:A:100:VAL:HG12	0.54	2.03	8	17
1:A:57:LEU:HD21	1:A:112:HIS:HB2	0.54	1.79	2	1
1:A:27:LEU:HD11	1:A:79:VAL:HG22	0.54	1.78	6	1
1:A:70:LEU:HD12	1:A:79:VAL:HG11	0.54	1.79	6	1
1:A:34:LEU:HD21	1:A:68:LEU:HD12	0.54	1.78	13	2
1:A:41:MET:HE3	1:A:68:LEU:HD21	0.54	1.80	16	1
1:A:34:LEU:O	1:A:34:LEU:HD23	0.54	2.02	18	1
1:A:97:VAL:CG1	1:A:120:LEU:HD22	0.53	2.33	6	2
1:A:68:LEU:N	1:A:68:LEU:HD22	0.53	2.18	18	2
1:A:34:LEU:HD21	1:A:68:LEU:CD2	0.53	2.34	7	1
1:A:42:ILE:O	1:A:68:LEU:HD12	0.53	2.02	1	4
1:A:51:SER:O	1:A:54:VAL:HG12	0.53	2.04	4	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:55:LYS:HE3	1:A:67:ILE:HG23	0.53	1.81	11	1
1:A:43:PHE:HB3	1:A:70:LEU:HD21	0.53	1.80	6	4
1:A:83:LEU:HD22	1:A:92:VAL:CG1	0.53	2.34	6	3
1:A:41:MET:HG3	1:A:68:LEU:HD11	0.53	1.81	16	2
1:A:28:ARG:HG2	1:A:82:VAL:HG21	0.53	1.80	10	1
1:A:28:ARG:CG	1:A:82:VAL:HG11	0.53	2.34	4	7
1:A:27:LEU:HD11	1:A:79:VAL:CB	0.53	2.34	8	10
1:A:34:LEU:HD22	1:A:41:MET:HE2	0.53	1.81	10	1
1:A:97:VAL:HG22	1:A:98:ASN:ND2	0.52	2.18	8	1
1:A:42:ILE:HD11	1:A:65:TYR:CE1	0.52	2.38	12	1
1:A:102:VAL:CG1	1:A:108:THR:HG23	0.52	2.34	12	2
1:A:42:ILE:HD13	1:A:42:ILE:N	0.52	2.20	19	8
1:A:70:LEU:CD2	1:A:92:VAL:HG11	0.52	2.35	9	6
1:A:67:ILE:C	1:A:68:LEU:HD23	0.51	2.24	8	1
1:A:27:LEU:HD11	1:A:79:VAL:HA	0.51	1.82	10	9
1:A:70:LEU:HD22	1:A:79:VAL:CG1	0.51	2.35	16	1
1:A:34:LEU:HD13	1:A:41:MET:HE2	0.51	1.81	20	1
1:A:116:LEU:HD23	1:A:116:LEU:O	0.51	2.06	4	8
1:A:27:LEU:HD23	1:A:28:ARG:N	0.51	2.20	8	1
1:A:34:LEU:HD12	1:A:34:LEU:O	0.51	2.06	9	4
1:A:108:THR:HG23	1:A:117:LEU:HD21	0.51	1.82	20	1
1:A:41:MET:SD	1:A:68:LEU:HD11	0.51	2.46	15	1
1:A:92:VAL:N	1:A:93:PRO:CD	0.51	2.73	5	20
1:A:79:VAL:O	1:A:83:LEU:HD12	0.51	2.05	12	2
1:A:31:LEU:HD13	1:A:83:LEU:CD2	0.51	2.28	10	1
1:A:34:LEU:HD13	1:A:43:PHE:CE1	0.51	2.41	18	1
1:A:31:LEU:HD13	1:A:83:LEU:HD12	0.51	1.82	1	2
1:A:97:VAL:HG13	1:A:120:LEU:CD2	0.51	2.33	1	2
1:A:57:LEU:HD11	1:A:112:HIS:CG	0.51	2.41	9	2
1:A:28:ARG:HD2	1:A:82:VAL:HG21	0.51	1.82	17	1
1:A:54:VAL:HA	1:A:57:LEU:HD23	0.50	1.83	8	3
1:A:27:LEU:HD21	1:A:79:VAL:CA	0.50	2.36	4	1
1:A:108:THR:HG22	1:A:117:LEU:HD21	0.50	1.83	15	1
1:A:61:LEU:HG	1:A:121:LEU:HD12	0.50	1.83	5	9
1:A:31:LEU:HD21	1:A:79:VAL:HG22	0.50	1.81	19	2
1:A:57:LEU:HD11	1:A:61:LEU:HD23	0.50	1.83	16	1
1:A:97:VAL:HG21	1:A:121:LEU:HD22	0.50	1.82	14	1
1:A:35:ILE:HD13	1:A:41:MET:HB3	0.50	1.82	2	1
1:A:57:LEU:HD12	1:A:112:HIS:CB	0.50	2.35	8	2
1:A:70:LEU:HD12	1:A:79:VAL:CG1	0.50	2.36	6	1
1:A:108:THR:O	1:A:117:LEU:HD22	0.50	2.07	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:83:LEU:HD13	1:A:83:LEU:O	0.50	2.07	2	6
1:A:49:PRO:O	1:A:50:HIS:CB	0.49	2.60	18	19
1:A:43:PHE:CE2	1:A:83:LEU:HD21	0.49	2.42	11	2
1:A:55:LYS:CE	1:A:67:ILE:HG23	0.49	2.38	19	1
1:A:34:LEU:HD22	1:A:41:MET:CG	0.49	2.37	18	1
1:A:28:ARG:HB3	1:A:82:VAL:HG21	0.49	1.83	8	2
1:A:35:ILE:HD11	1:A:41:MET:HE3	0.49	1.84	18	1
1:A:57:LEU:CD2	1:A:108:THR:HG22	0.48	2.38	9	1
1:A:28:ARG:HG3	1:A:82:VAL:HG11	0.48	1.85	1	5
1:A:73:VAL:HG12	1:A:75:ASP:H	0.48	1.69	12	3
1:A:61:LEU:CD2	1:A:117:LEU:HD23	0.48	2.39	10	1
1:A:54:VAL:HG21	1:A:95:ILE:HD12	0.48	1.84	9	9
1:A:108:THR:CG2	1:A:117:LEU:HD21	0.48	2.39	20	1
1:A:70:LEU:HD23	1:A:79:VAL:HG13	0.47	1.85	2	2
1:A:95:ILE:HD11	1:A:104:GLY:CA	0.47	2.39	15	1
1:A:40:VAL:HG11	1:A:58:PHE:CD2	0.47	2.44	2	2
1:A:31:LEU:CD2	1:A:79:VAL:HG13	0.47	2.39	4	1
1:A:63:VAL:HG11	1:A:121:LEU:HD13	0.47	1.87	6	3
1:A:55:LYS:HE2	1:A:67:ILE:HG23	0.47	1.86	19	1
1:A:83:LEU:HD12	1:A:86:ILE:CD1	0.47	2.33	19	1
1:A:91:THR:C	1:A:93:PRO:CD	0.47	2.83	20	20
1:A:70:LEU:HD21	1:A:92:VAL:HG11	0.47	1.86	9	4
1:A:70:LEU:HB3	1:A:79:VAL:HG11	0.47	1.84	9	3
1:A:102:VAL:HG22	1:A:120:LEU:CD2	0.47	2.40	9	1
1:A:63:VAL:HG11	1:A:121:LEU:CD1	0.47	2.39	10	1
1:A:102:VAL:HG11	1:A:117:LEU:HD11	0.47	1.87	3	2
1:A:40:VAL:CG2	1:A:97:VAL:HG23	0.46	2.39	15	3
1:A:107:ARG:CZ	1:A:116:LEU:HD21	0.46	2.40	3	1
1:A:57:LEU:HD21	1:A:109:PHE:CD2	0.46	2.45	13	1
1:A:43:PHE:CD2	1:A:68:LEU:HD12	0.46	2.45	17	1
1:A:61:LEU:HD13	1:A:61:LEU:C	0.46	2.29	8	1
1:A:41:MET:HE2	1:A:68:LEU:HD11	0.46	1.87	14	1
1:A:32:ARG:O	1:A:35:ILE:HD12	0.46	2.11	18	2
1:A:73:VAL:HG21	1:A:79:VAL:HG11	0.46	1.87	20	1
1:A:28:ARG:HD3	1:A:82:VAL:HG21	0.46	1.88	3	1
1:A:97:VAL:HG11	1:A:121:LEU:HD22	0.46	1.88	16	2
1:A:43:PHE:HD2	1:A:83:LEU:HD21	0.45	1.68	6	1
1:A:34:LEU:HD13	1:A:43:PHE:CZ	0.45	2.46	18	1
1:A:34:LEU:HD13	1:A:41:MET:SD	0.45	2.52	6	1
1:A:79:VAL:O	1:A:83:LEU:HB2	0.45	2.11	8	1
1:A:91:THR:C	1:A:93:PRO:HD3	0.45	2.32	3	19

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:ILE:HD11	1:A:65:TYR:CD2	0.45	2.46	5	1
1:A:42:ILE:HD11	1:A:65:TYR:CB	0.45	2.42	19	2
1:A:41:MET:SD	1:A:68:LEU:HD21	0.45	2.51	17	1
1:A:57:LEU:HD21	1:A:117:LEU:CD2	0.45	2.39	15	2
1:A:57:LEU:HD22	1:A:108:THR:HG22	0.45	1.89	15	1
1:A:58:PHE:CD1	1:A:121:LEU:HD13	0.45	2.46	20	1
1:A:42:ILE:HD12	1:A:55:LYS:HG2	0.45	1.88	3	1
1:A:31:LEU:HD12	1:A:82:VAL:HG13	0.45	1.88	12	1
1:A:83:LEU:HD23	1:A:92:VAL:CG1	0.45	2.42	19	1
1:A:111:ALA:HB3	1:A:117:LEU:HD13	0.44	1.88	15	1
1:A:57:LEU:CD2	1:A:117:LEU:HD23	0.44	2.41	15	1
1:A:42:ILE:HD13	1:A:66:ASN:O	0.44	2.12	13	1
1:A:83:LEU:HD13	1:A:83:LEU:C	0.44	2.32	2	4
1:A:42:ILE:CD1	1:A:42:ILE:N	0.43	2.81	19	3
1:A:83:LEU:HD12	1:A:92:VAL:HG13	0.43	1.89	15	1
1:A:79:VAL:CG1	1:A:80:GLN:N	0.43	2.81	17	10
1:A:31:LEU:HD12	1:A:82:VAL:CG2	0.43	2.43	14	1
1:A:34:LEU:HD11	1:A:41:MET:CE	0.43	2.43	4	1
1:A:31:LEU:HD12	1:A:82:VAL:CG1	0.43	2.44	17	2
1:A:55:LYS:NZ	1:A:67:ILE:HG23	0.43	2.28	3	1
1:A:43:PHE:CE1	1:A:68:LEU:HD13	0.43	2.48	11	2
1:A:40:VAL:HG13	1:A:97:VAL:HB	0.43	1.91	8	1
1:A:40:VAL:HG21	1:A:63:VAL:CG1	0.43	2.43	12	1
1:A:57:LEU:HD23	1:A:108:THR:O	0.43	2.14	4	1
1:A:42:ILE:HD12	1:A:65:TYR:CD2	0.43	2.48	13	1
1:A:42:ILE:N	1:A:42:ILE:CD1	0.43	2.82	5	1
1:A:58:PHE:CD2	1:A:121:LEU:HD13	0.43	2.48	12	1
1:A:43:PHE:CG	1:A:83:LEU:HD11	0.42	2.48	6	1
1:A:41:MET:HE1	1:A:43:PHE:CD2	0.42	2.50	8	1
1:A:75:ASP:O	1:A:79:VAL:HG12	0.42	2.14	20	1
1:A:73:VAL:HG23	1:A:76:GLY:N	0.42	2.30	19	4
1:A:120:LEU:O	1:A:120:LEU:HD13	0.42	2.15	11	1
1:A:70:LEU:HD23	1:A:92:VAL:HG11	0.42	1.91	14	1
1:A:70:LEU:HD12	1:A:92:VAL:CG1	0.42	2.34	16	1
1:A:54:VAL:CG2	1:A:108:THR:HG21	0.42	2.44	1	1
1:A:42:ILE:HD13	1:A:55:LYS:HG2	0.42	1.90	12	1
1:A:40:VAL:HG22	1:A:97:VAL:HB	0.42	1.92	16	1
1:A:42:ILE:HD11	1:A:65:TYR:CE2	0.41	2.50	20	1
1:A:100:VAL:HG11	1:A:120:LEU:HD21	0.41	1.92	16	1
1:A:34:LEU:HD11	1:A:68:LEU:CD1	0.41	2.44	19	1
1:A:55:LYS:HZ3	1:A:67:ILE:HD12	0.41	1.76	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:120:LEU:C	1:A:120:LEU:HD13	0.41	2.36	5	1
1:A:57:LEU:HD12	1:A:112:HIS:HB2	0.41	1.92	11	1
1:A:97:VAL:O	1:A:98:ASN:CG	0.41	2.59	2	2
1:A:95:ILE:HD11	1:A:104:GLY:HA3	0.41	1.91	13	1
1:A:61:LEU:HD12	1:A:121:LEU:HD12	0.41	1.93	8	1
1:A:70:LEU:HD22	1:A:79:VAL:HG13	0.41	1.91	16	1
1:A:27:LEU:HD21	1:A:79:VAL:N	0.40	2.31	4	1
1:A:28:ARG:HG2	1:A:82:VAL:HG11	0.40	1.93	10	1
1:A:54:VAL:HG22	1:A:108:THR:HG21	0.40	1.91	8	1
1:A:61:LEU:CD1	1:A:121:LEU:HD12	0.40	2.46	8	1
1:A:27:LEU:HD11	1:A:79:VAL:HB	0.40	1.94	2	1
1:A:83:LEU:CD1	1:A:92:VAL:HG12	0.40	2.46	2	1
1:A:34:LEU:HD23	1:A:43:PHE:HZ	0.40	1.71	9	1
1:A:120:LEU:HD13	1:A:120:LEU:C	0.40	2.37	11	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	95/118 (81%)	88±1 (92±1%)	6±1 (6±2%)	1±1 (1±1%)	15	61
All	All	1900/2360 (81%)	1753 (92%)	121 (6%)	26 (1%)	15	61

All 3 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	106	ASP	14
1	A	73	VAL	11
1	A	105	CYS	1

6.3.2 Protein sidechains (i)

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	87/106 (82%)	59±4 (68±4%)	28±4 (32±4%)	1 13
All	All	1740/2120 (82%)	1178 (68%)	562 (32%)	1 13

All 62 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	44	SER	20
1	A	87	SER	20
1	A	89	GLN	20
1	A	94	ASN	20
1	A	95	ILE	20
1	A	100	VAL	20
1	A	107	ARG	20
1	A	27	LEU	19
1	A	28	ARG	19
1	A	29	ARG	18
1	A	53	ARG	18
1	A	119	LYS	17
1	A	61	LEU	16
1	A	91	THR	15
1	A	42	ILE	14
1	A	70	LEU	14
1	A	47	TYR	13
1	A	80	GLN	13
1	A	99	LYS	13
1	A	32	ARG	12
1	A	68	LEU	12
1	A	106	ASP	12
1	A	34	LEU	11
1	A	83	LEU	11
1	A	82	VAL	10
1	A	39	ARG	9
1	A	63	VAL	9
1	A	66	ASN	9
1	A	51	SER	9
1	A	41	MET	8
1	A	59	SER	8
1	A	110	GLN	8
1	A	85	GLU	8

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Mol	Chain	Res	Type	Models (Total)
1	A	109	PHE	7
1	A	78	SER	7
1	A	56	GLU	7
1	A	30	ARG	6
1	A	81	GLU	6
1	A	50	HIS	5
1	A	71	ASP	5
1	A	75	ASP	5
1	A	74	ASP	5
1	A	108	THR	4
1	A	45	LYS	4
1	A	36	GLU	4
1	A	116	LEU	4
1	A	120	LEU	3
1	A	118	GLN	3
1	A	105	CYS	3
1	A	46	SER	3
1	A	60	SER	2
1	A	55	LYS	2
1	A	38	ASN	2
1	A	69	GLU	2
1	A	88	ASN	1
1	A	101	HIS	1
1	A	90	LYS	1
1	A	40	VAL	1
1	A	98	ASN	1
1	A	113	GLN	1
1	A	57	LEU	1
1	A	72	GLN	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 monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 87% for the well-defined parts and 87% 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	1400
Number of shifts mapped to atoms	1248
Number of unparsed shifts	0
Number of shifts with mapping errors	152
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.

- No matching atom found in the structure. All 152 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	7	ARG	H	8.165	0.020	1
1	A	7	ARG	HA	4.224	0.020	1
1	A	7	ARG	HB2	1.79	0.020	2
1	A	7	ARG	HB3	1.697	0.020	2
1	A	7	ARG	HG2	1.54	0.020	1
1	A	7	ARG	HG3	1.54	0.020	1
1	A	7	ARG	CA	56.136	0.3	1
1	A	7	ARG	CB	30.583	0.3	1
1	A	7	ARG	CG	27.289	0.3	1
1	A	7	ARG	N	121.462	0.3	1
1	A	8	ARG	H	8.412	0.020	1
1	A	8	ARG	HA	4.232	0.020	1
1	A	8	ARG	HB2	1.72	0.020	1
1	A	8	ARG	HB3	1.72	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	8	ARG	CA	56.208	0.3	1
1	A	8	ARG	CB	30.583	0.3	1
1	A	8	ARG	N	123.153	0.3	1
1	A	9	ALA	H	8.284	0.020	1
1	A	9	ALA	HA	4.202	0.020	1
1	A	9	ALA	HB1	1.286	0.020	1
1	A	9	ALA	HB2	1.286	0.020	1
1	A	9	ALA	HB3	1.286	0.020	1
1	A	9	ALA	CA	52.403	0.3	1
1	A	9	ALA	CB	18.943	0.3	1
1	A	9	ALA	N	126.117	0.3	1
1	A	10	ARG	H	8.285	0.020	1
1	A	10	ARG	HA	4.216	0.020	1
1	A	10	ARG	HB2	1.699	0.020	1
1	A	10	ARG	HB3	1.699	0.020	1
1	A	10	ARG	HD2	3.105	0.020	1
1	A	10	ARG	HD3	3.105	0.020	1
1	A	10	ARG	CA	55.998	0.3	1
1	A	10	ARG	CB	30.681	0.3	1
1	A	10	ARG	CD	43.227	0.3	1
1	A	10	ARG	N	121.268	0.3	1
1	A	11	LEU	H	8.305	0.020	1
1	A	11	LEU	HA	4.265	0.020	1
1	A	11	LEU	HB2	1.516	0.020	1
1	A	11	LEU	HB3	1.516	0.020	1
1	A	11	LEU	HG	1.556	0.020	1
1	A	11	LEU	HD11	0.843	0.020	2
1	A	11	LEU	HD12	0.843	0.020	2
1	A	11	LEU	HD13	0.843	0.020	2
1	A	11	LEU	HD21	0.778	0.020	2
1	A	11	LEU	HD22	0.778	0.020	2
1	A	11	LEU	HD23	0.778	0.020	2
1	A	11	LEU	CA	54.96	0.3	1
1	A	11	LEU	CB	42.448	0.3	1
1	A	11	LEU	CG	27.16	0.3	1
1	A	11	LEU	CD1	24.649	0.3	1
1	A	11	LEU	CD2	23.484	0.3	1
1	A	11	LEU	N	124.359	0.3	1
1	A	12	ALA	H	8.274	0.020	1
1	A	12	ALA	HA	4.241	0.020	1
1	A	12	ALA	HB1	1.282	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	12	ALA	HB2	1.282	0.020	1
1	A	12	ALA	HB3	1.282	0.020	1
1	A	12	ALA	CA	52.248	0.3	1
1	A	12	ALA	CB	19.312	0.3	1
1	A	12	ALA	N	125.64	0.3	1
1	A	13	SER	H	8.278	0.020	1
1	A	13	SER	HA	4.635	0.020	1
1	A	13	SER	HB2	3.66	0.020	1
1	A	13	SER	HB3	3.66	0.020	1
1	A	13	SER	CA	56.34	0.3	1
1	A	13	SER	CB	63.214	0.3	1
1	A	13	SER	N	117.457	0.3	1
1	A	14	PRO	HA	4.367	0.020	1
1	A	14	PRO	HB2	2.231	0.020	2
1	A	14	PRO	HB3	1.89	0.020	2
1	A	14	PRO	HG2	1.94	0.020	1
1	A	14	PRO	HG3	1.94	0.020	1
1	A	14	PRO	HD2	3.74	0.020	2
1	A	14	PRO	HD3	3.662	0.020	2
1	A	14	PRO	C	177.125	0.3	1
1	A	14	PRO	CA	63.544	0.3	1
1	A	14	PRO	CB	32.131	0.3	1
1	A	14	PRO	CG	27.439	0.3	1
1	A	14	PRO	CD	50.794	0.3	1
1	A	15	GLY	H	8.455	0.020	1
1	A	15	GLY	HA2	3.915	0.020	1
1	A	15	GLY	HA3	3.915	0.020	1
1	A	15	GLY	C	174.413	0.3	1
1	A	15	GLY	CA	45.276	0.3	1
1	A	15	GLY	N	109.946	0.3	1
1	A	16	THR	H	7.98	0.020	1
1	A	16	THR	HA	4.313	0.020	1
1	A	16	THR	HB	4.177	0.020	1
1	A	16	THR	HG21	1.106	0.020	1
1	A	16	THR	HG22	1.106	0.020	1
1	A	16	THR	HG23	1.106	0.020	1
1	A	16	THR	CA	61.621	0.3	1
1	A	16	THR	CB	69.819	0.3	1
1	A	16	THR	CG2	21.482	0.3	1
1	A	16	THR	N	113.735	0.3	1
1	A	17	SER	H	8.349	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	17	SER	HA	4.388	0.020	1
1	A	17	SER	HB2	3.766	0.020	1
1	A	17	SER	HB3	3.766	0.020	1
1	A	17	SER	CA	58.272	0.3	1
1	A	17	SER	CB	63.741	0.3	1
1	A	17	SER	N	119.262	0.3	1
1	A	18	ARG	H	8.342	0.020	1
1	A	18	ARG	HA	4.561	0.020	1
1	A	18	ARG	HB2	1.748	0.020	2
1	A	18	ARG	HB3	1.638	0.020	2
1	A	18	ARG	HG2	1.586	0.020	1
1	A	18	ARG	HG3	1.586	0.020	1
1	A	18	ARG	HD2	3.11	0.020	1
1	A	18	ARG	HD3	3.11	0.020	1
1	A	18	ARG	C	174.009	0.3	1
1	A	18	ARG	CA	53.878	0.3	1
1	A	18	ARG	CB	30.005	0.3	1
1	A	18	ARG	CG	26.539	0.3	1
1	A	18	ARG	CD	43.209	0.3	1
1	A	18	ARG	N	124.559	0.3	1
1	A	19	PRO	HA	4.366	0.020	1
1	A	19	PRO	HB2	2.225	0.020	2
1	A	19	PRO	HB3	1.831	0.020	2
1	A	19	PRO	HG2	1.953	0.020	1
1	A	19	PRO	HG3	1.953	0.020	1
1	A	19	PRO	HD2	3.74	0.020	1
1	A	19	PRO	HD3	3.74	0.020	1
1	A	19	PRO	CA	63.306	0.3	1
1	A	19	PRO	CB	31.782	0.3	1
1	A	19	PRO	CG	27.143	0.3	1
1	A	19	PRO	CD	50.809	0.3	1
1	A	20	SER	H	8.564	0.020	1
1	A	20	SER	HA	4.344	0.020	1
1	A	20	SER	HB2	3.961	0.020	2
1	A	20	SER	HB3	3.851	0.020	2
1	A	20	SER	CA	58.503	0.3	1
1	A	20	SER	CB	63.538	0.3	1
1	A	20	SER	N	118.012	0.3	1
1	A	21	SER	H	8.41	0.020	1
1	A	21	SER	HA	4.259	0.020	1
1	A	21	SER	HB2	3.872	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	21	SER	HB3	3.872	0.020	1
1	A	21	SER	CA	59.909	0.3	1
1	A	21	SER	CB	63.144	0.3	1
1	A	21	SER	N	123.738	0.3	1
1	A	22	GLU	H	8.447	0.020	1
1	A	22	GLU	HA	4.078	0.020	1
1	A	22	GLU	HB2	1.956	0.020	1
1	A	22	GLU	HB3	1.956	0.020	1
1	A	22	GLU	HG2	2.232	0.020	1
1	A	22	GLU	HG3	2.232	0.020	1
1	A	22	GLU	C	178.352	0.3	1
1	A	22	GLU	CA	58.731	0.3	1
1	A	22	GLU	CB	29.267	0.3	1
1	A	22	GLU	CG	36.644	0.3	1
1	A	22	GLU	N	123.738	0.3	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	116	-0.43 ± 0.20	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	109	0.32 ± 0.15	None needed (< 0.5 ppm)
$^{13}C'$	83	-0.31 ± 0.14	None needed (< 0.5 ppm)
^{15}N	112	-0.73 ± 0.53	None needed (imprecise)

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 87%, i.e. 1174 atoms were assigned a chemical shift out of a possible 1349. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	448/477 (94%)	191/194 (98%)	166/190 (87%)	91/93 (98%)
Sidechain	666/793 (84%)	451/514 (88%)	203/241 (84%)	12/38 (32%)
Aromatic	60/79 (76%)	30/40 (75%)	30/36 (83%)	0/3 (0%)
Overall	1174/1349 (87%)	672/748 (90%)	399/467 (85%)	103/134 (77%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 87%, i.e. 1248 atoms were assigned a chemical shift out of a possible

1438. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	482/512 (94%)	205/208 (99%)	179/204 (88%)	98/100 (98%)
Sidechain	706/847 (83%)	478/546 (88%)	215/259 (83%)	13/42 (31%)
Aromatic	60/79 (76%)	30/40 (75%)	30/36 (83%)	0/3 (0%)
Overall	1248/1438 (87%)	713/794 (90%)	424/499 (85%)	111/145 (77%)

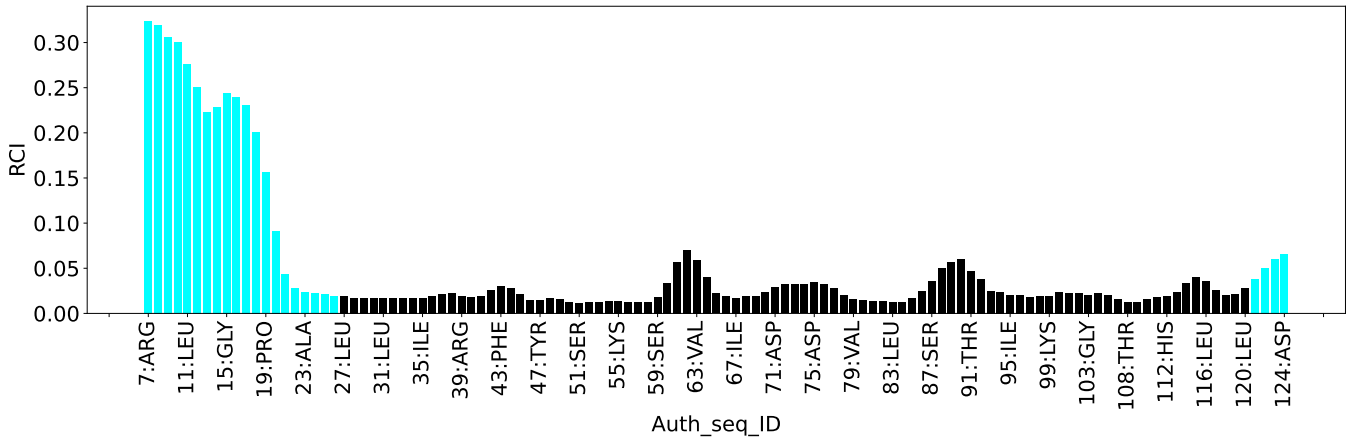
7.1.4 Statistically unusual chemical shifts (i)

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:



8 NMR restraints analysis (i)

No restraints data found

9 Distance violation analysis (i)

No distance restraints data found

10 Dihedral-angle violation analysis (i)

Dihedral angle analysis failed due to data error in the dihedral angle restraints, possibly missing target value