



Full wwPDB NMR Structure Validation Report ⓘ

Mar 19, 2026 – 12:04 PM UTC

PDB ID : 2C34 / pdb_00002c34
BMRB ID : 6794
Title : Leishmania mexicana ICP
Authors : Smith, B.O.; Picken, N.C.; Bromek, K.; Westrop, G.D.; Mottram, J.C.;
Coombs, G.H.
Deposited on : 2005-10-04

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

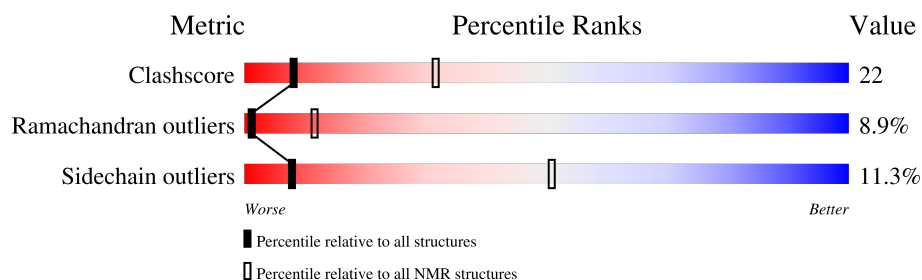
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 91%.

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	116	34% 34% . 27%

2 Ensemble composition and analysis

This entry contains 38 models. Model 1 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:10-A:29, A:34-A:43, A:47-A:60, A:73-A:113 (85)	0.50	1

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 5 clusters and 9 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1855 atoms, of which 938 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called INHIBITOR OF CYSTEINE PEPTIDASES.

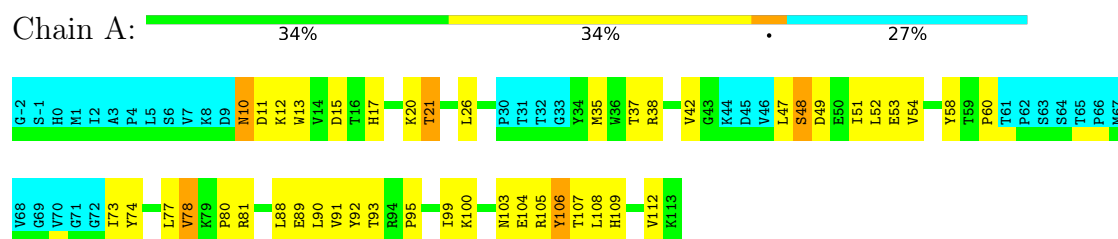
Mol	Chain	Residues	Atoms						Trace
1	A	116	Total	C	H	N	O	S	0
			1855	587	938	159	167	4	

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: INHIBITOR OF CYSTEINE PEPTIDASES

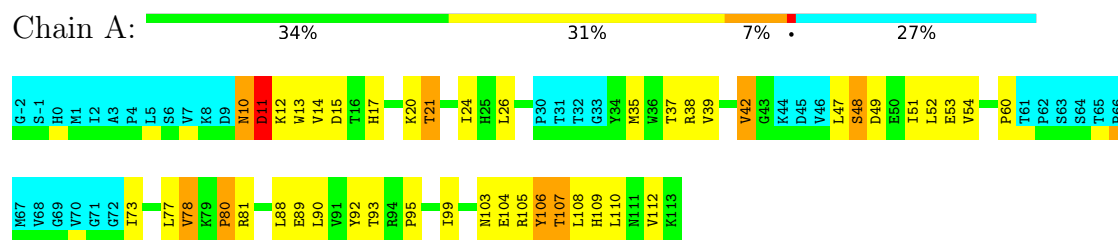


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: INHIBITOR OF CYSTEINE PEPTIDASES



4.2.2 Score per residue for model 2

• Molecule 1: INHIBITOR OF CYSTEINE PEPTIDASES

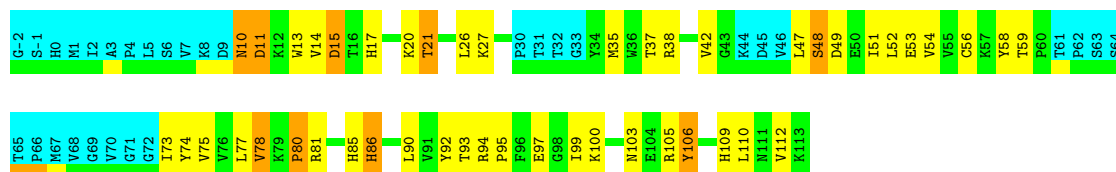




4.2.3 Score per residue for model 3

- Molecule 1: INHIBITOR OF CYSTEINE PEPTIDASES

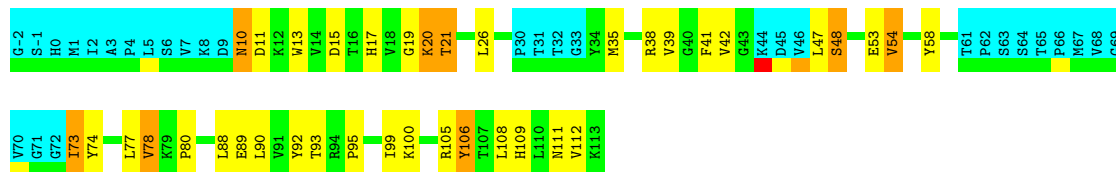
Chain A: 33% 33% 8% 27%



4.2.4 Score per residue for model 4

- Molecule 1: INHIBITOR OF CYSTEINE PEPTIDASES

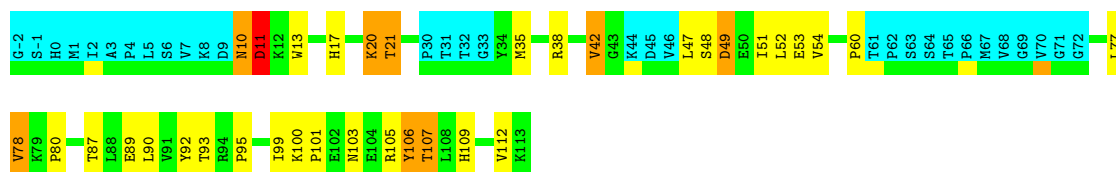
Chain A: 41% 26% 7% 27%



4.2.5 Score per residue for model 5

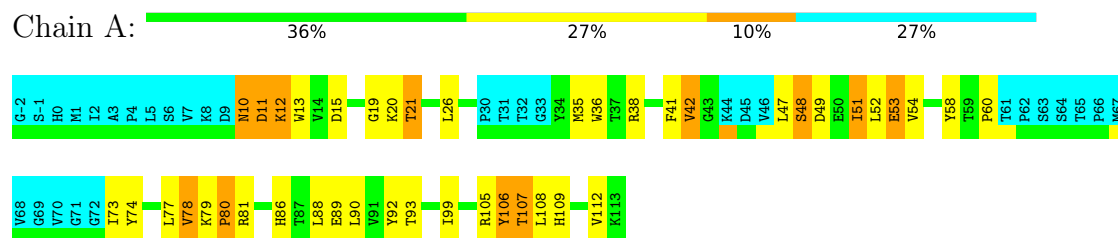
- Molecule 1: INHIBITOR OF CYSTEINE PEPTIDASES

Chain A: 43% 22% 7% 27%



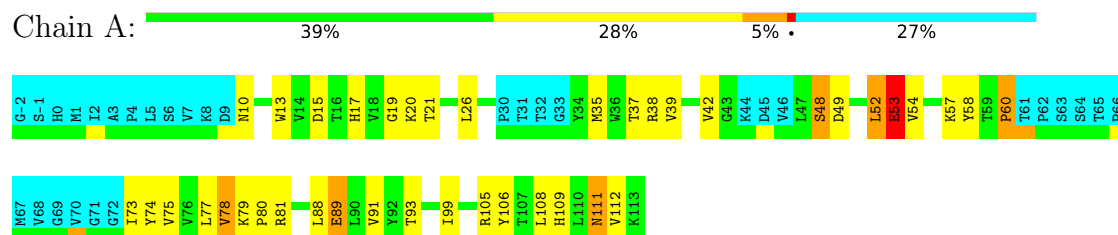
4.2.6 Score per residue for model 6

- Molecule 1: INHIBITOR OF CYSTEINE PEPTIDASES



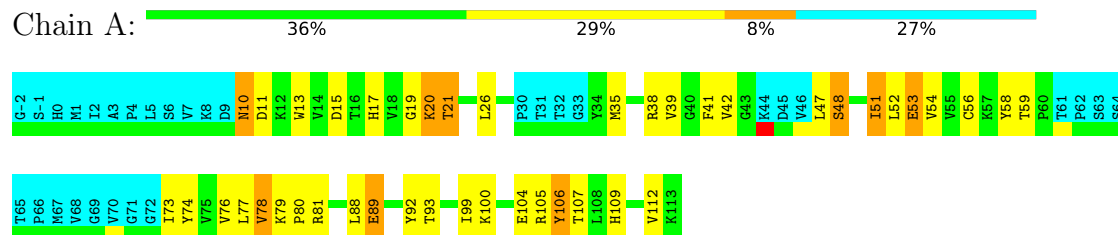
4.2.7 Score per residue for model 7

- Molecule 1: INHIBITOR OF CYSTEINE PEPTIDASES



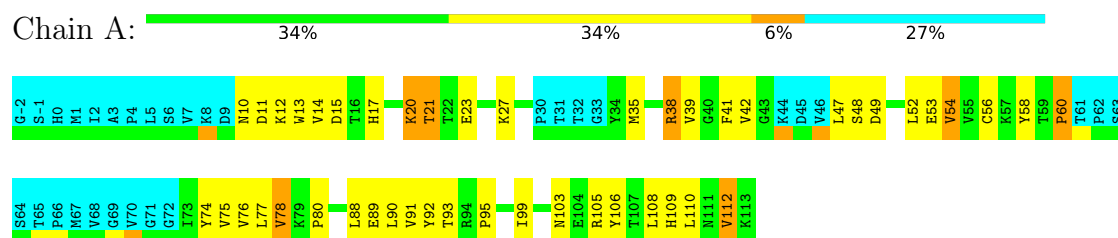
4.2.8 Score per residue for model 8

- Molecule 1: INHIBITOR OF CYSTEINE PEPTIDASES



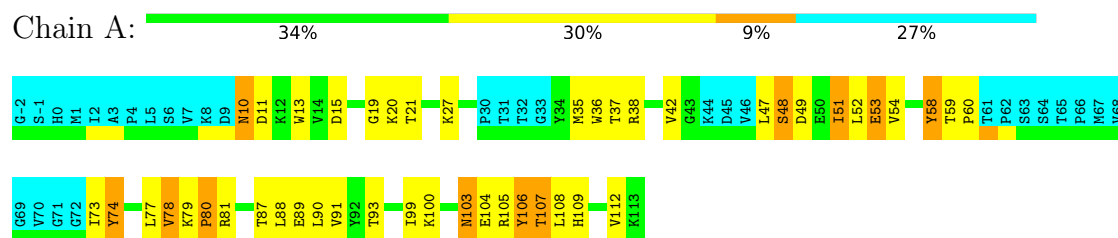
4.2.9 Score per residue for model 9

- Molecule 1: INHIBITOR OF CYSTEINE PEPTIDASES



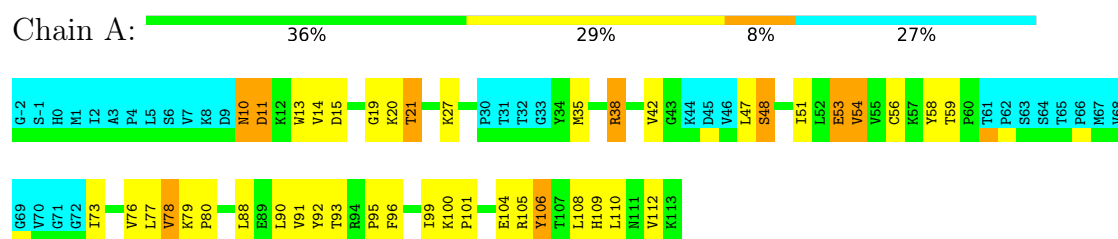
4.2.10 Score per residue for model 10

- Molecule 1: INHIBITOR OF CYSTEINE PEPTIDASES



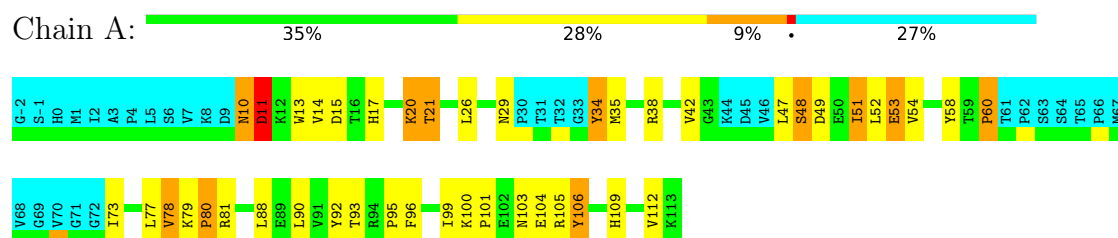
4.2.11 Score per residue for model 11

- Molecule 1: INHIBITOR OF CYSTEINE PEPTIDASES



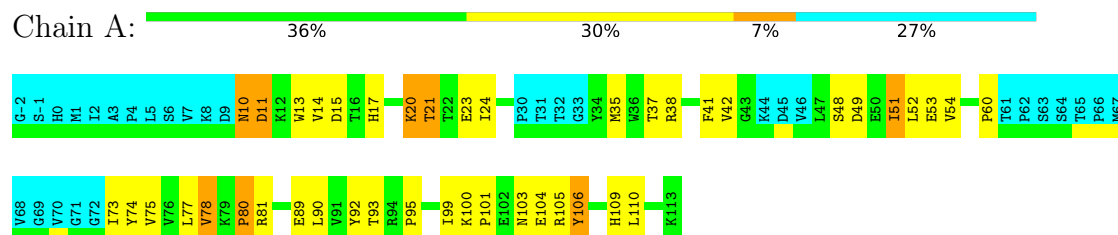
4.2.12 Score per residue for model 12

- Molecule 1: INHIBITOR OF CYSTEINE PEPTIDASES



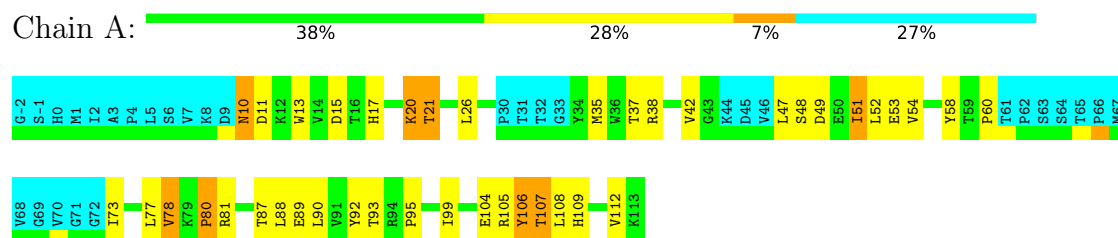
4.2.13 Score per residue for model 13

- Molecule 1: INHIBITOR OF CYSTEINE PEPTIDASES



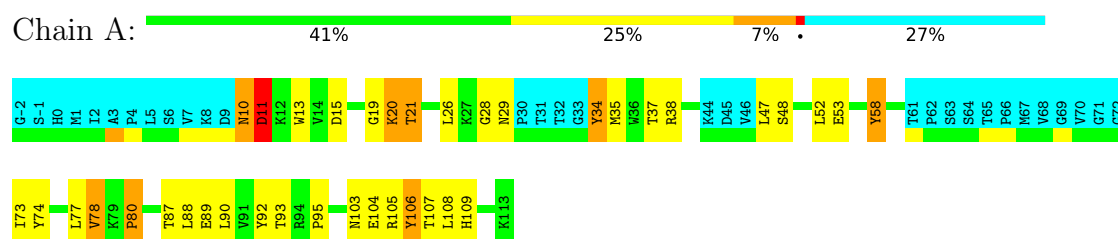
4.2.14 Score per residue for model 14

- Molecule 1: INHIBITOR OF CYSTEINE PEPTIDASES



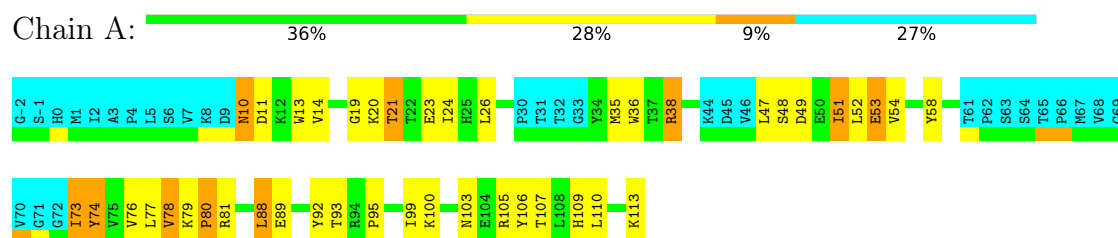
4.2.15 Score per residue for model 15

- Molecule 1: INHIBITOR OF CYSTEINE PEPTIDASES



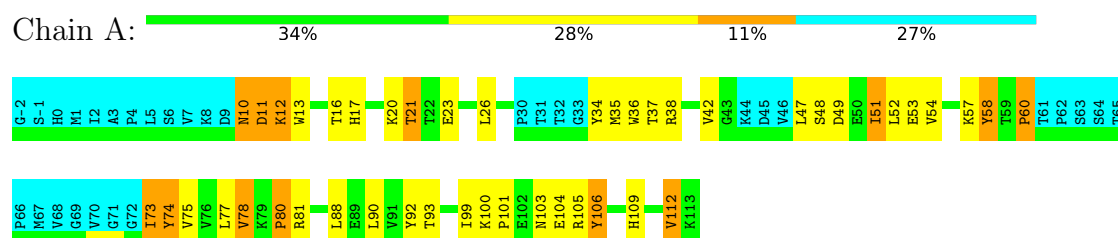
4.2.16 Score per residue for model 16

- Molecule 1: INHIBITOR OF CYSTEINE PEPTIDASES



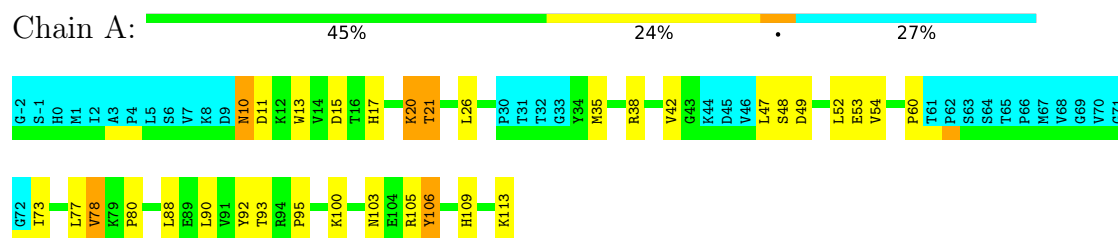
4.2.17 Score per residue for model 17

- Molecule 1: INHIBITOR OF CYSTEINE PEPTIDASES



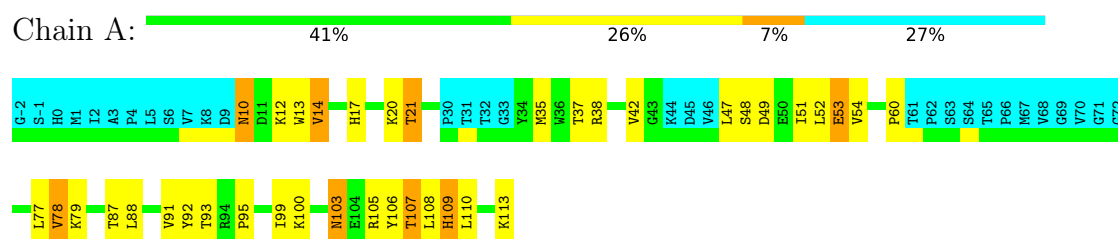
4.2.18 Score per residue for model 18

- Molecule 1: INHIBITOR OF CYSTEINE PEPTIDASES



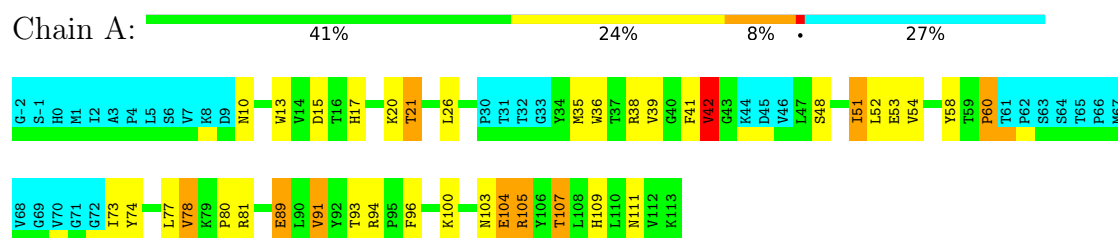
4.2.19 Score per residue for model 19

- Molecule 1: INHIBITOR OF CYSTEINE PEPTIDASES



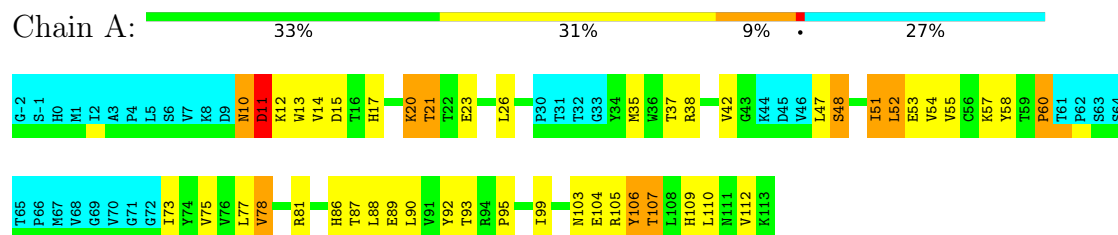
4.2.20 Score per residue for model 20

- Molecule 1: INHIBITOR OF CYSTEINE PEPTIDASES



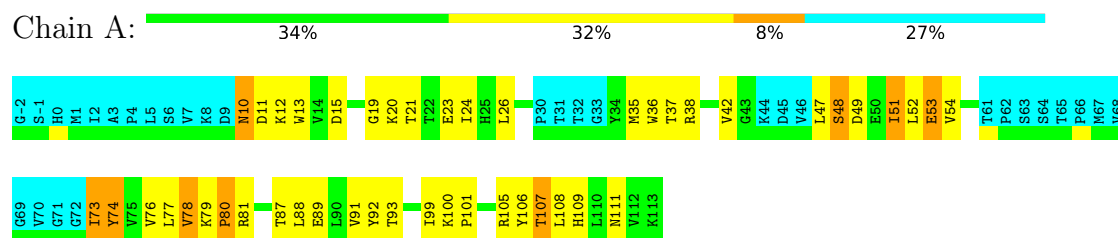
4.2.21 Score per residue for model 21

- Molecule 1: INHIBITOR OF CYSTEINE PEPTIDASES



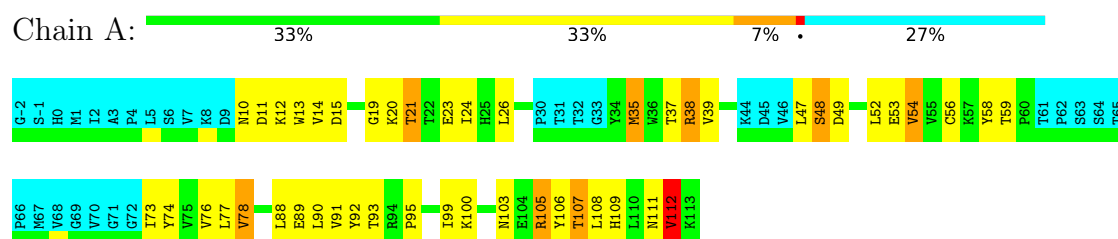
4.2.22 Score per residue for model 22

- Molecule 1: INHIBITOR OF CYSTEINE PEPTIDASES



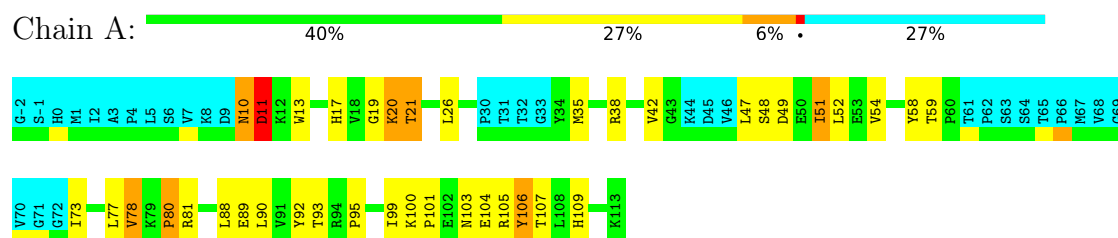
4.2.23 Score per residue for model 23

- Molecule 1: INHIBITOR OF CYSTEINE PEPTIDASES



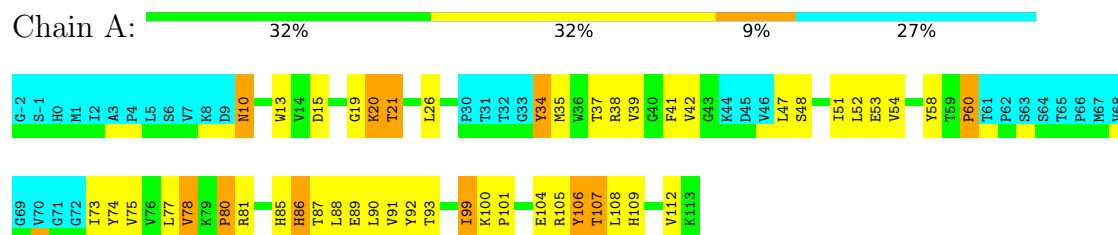
4.2.24 Score per residue for model 24

- Molecule 1: INHIBITOR OF CYSTEINE PEPTIDASES



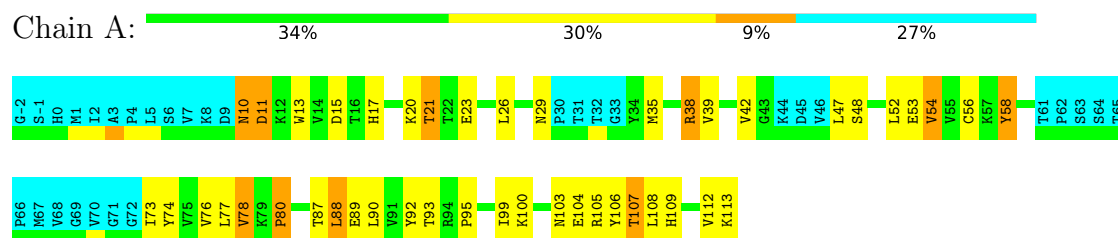
4.2.25 Score per residue for model 25

- Molecule 1: INHIBITOR OF CYSTEINE PEPTIDASES



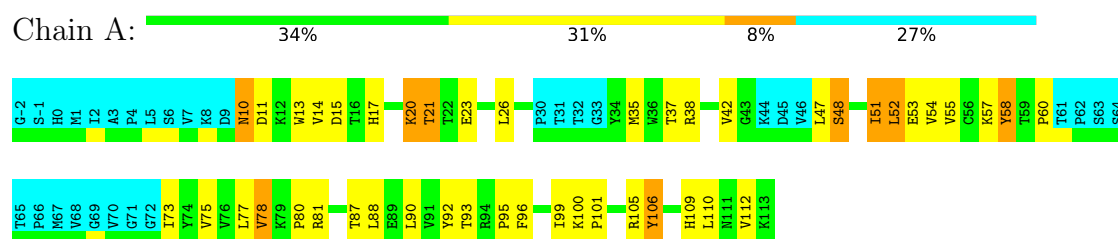
4.2.26 Score per residue for model 26

- Molecule 1: INHIBITOR OF CYSTEINE PEPTIDASES



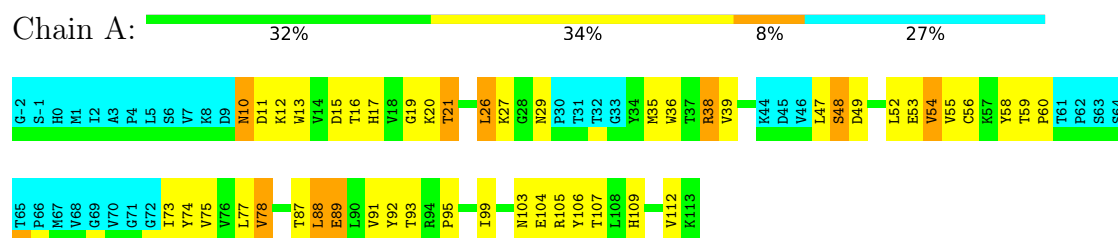
4.2.27 Score per residue for model 27

- Molecule 1: INHIBITOR OF CYSTEINE PEPTIDASES



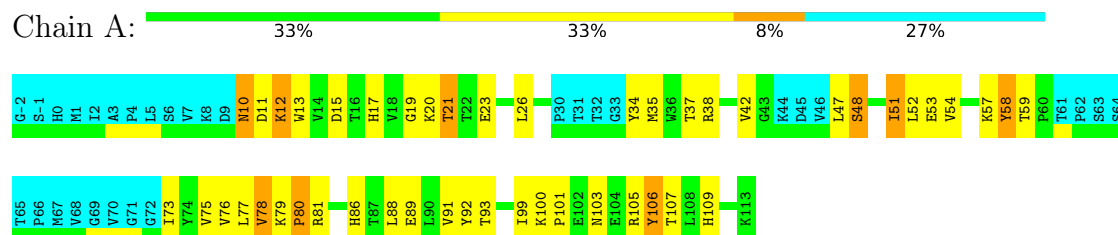
4.2.28 Score per residue for model 28

- Molecule 1: INHIBITOR OF CYSTEINE PEPTIDASES



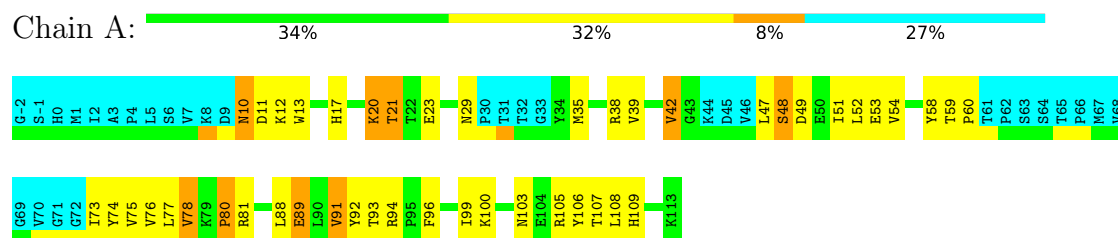
4.2.29 Score per residue for model 29

- Molecule 1: INHIBITOR OF CYSTEINE PEPTIDASES



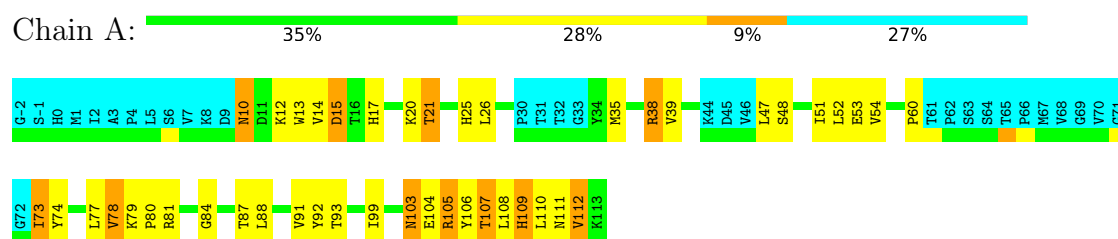
4.2.30 Score per residue for model 30

- Molecule 1: INHIBITOR OF CYSTEINE PEPTIDASES



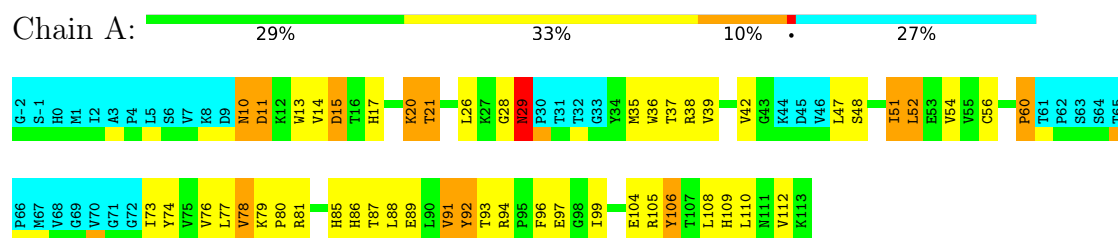
4.2.31 Score per residue for model 31

- Molecule 1: INHIBITOR OF CYSTEINE PEPTIDASES



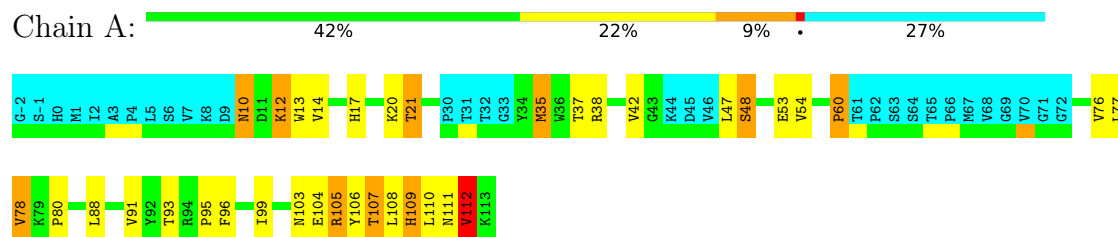
4.2.32 Score per residue for model 32

- Molecule 1: INHIBITOR OF CYSTEINE PEPTIDASES



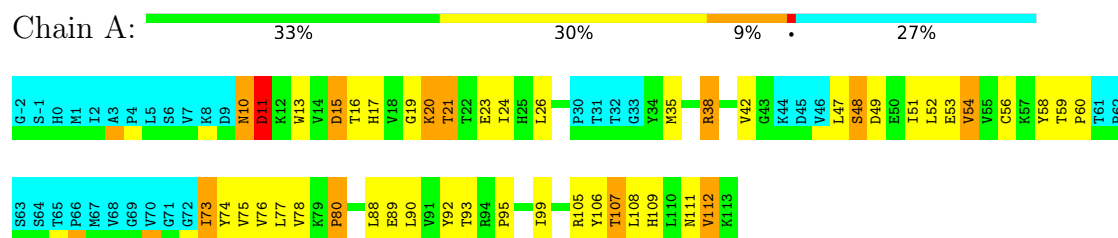
4.2.33 Score per residue for model 33

- Molecule 1: INHIBITOR OF CYSTEINE PEPTIDASES



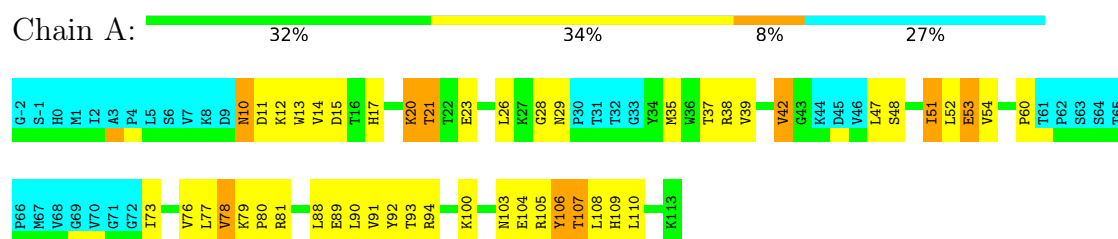
4.2.34 Score per residue for model 34

- Molecule 1: INHIBITOR OF CYSTEINE PEPTIDASES



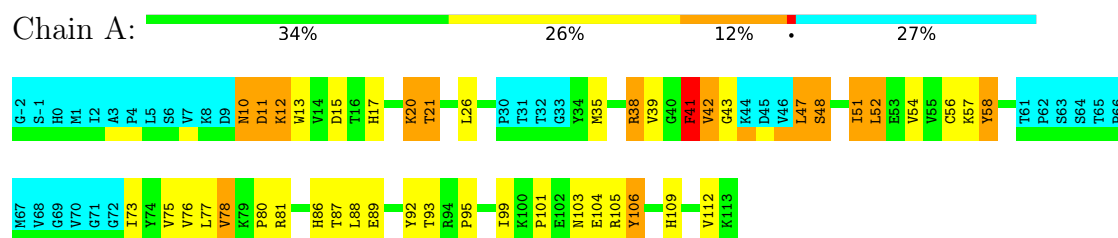
4.2.35 Score per residue for model 35

- Molecule 1: INHIBITOR OF CYSTEINE PEPTIDASES



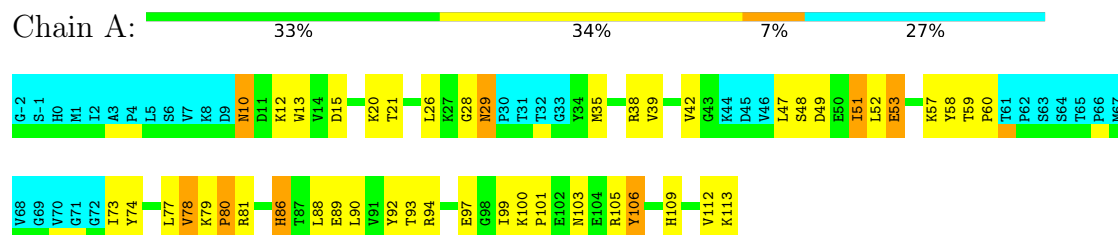
4.2.36 Score per residue for model 36

- Molecule 1: INHIBITOR OF CYSTEINE PEPTIDASES



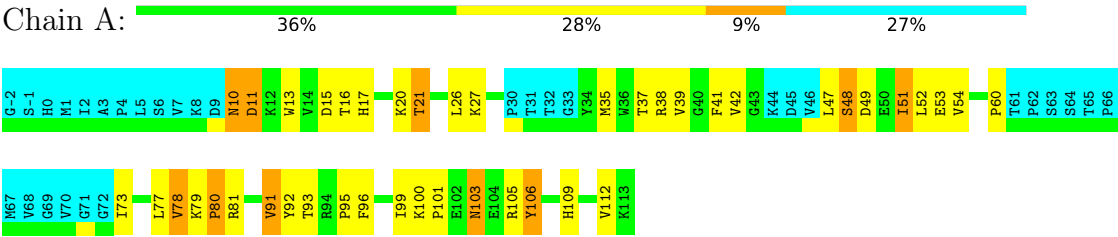
4.2.37 Score per residue for model 37

- Molecule 1: INHIBITOR OF CYSTEINE PEPTIDASES



4.2.38 Score per residue for model 38

● Molecule 1: INHIBITOR OF CYSTEINE PEPTIDASES



5 Refinement protocol and experimental data overview

The models were refined using the following method: *ARIA-ALIKE*.

Of the 50 calculated structures, 38 were deposited, based on the following criterion: *LOWEST RESTRAINT ENERGY*.

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

Software name	Classification	Version
CNS	refinement	1.1
CcpNmr Analysis	structure solution	ANALYSIS

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	1440
Number of shifts mapped to atoms	1422
Number of unparsed shifts	0
Number of shifts with mapping errors	18
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	91%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.33±0.01	0±0/727 (0.0± 0.0%)	0.69±0.02	0±0/986 (0.0± 0.0%)
All	All	0.33	0/27626 (0.0%)	0.69	1/37468 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	41	PHE	CA-CB-CG	5.55	119.35	113.80	36	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	708	722	717	31±5
All	All	26904	27436	27246	1190

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:VAL:HG21	1:A:93:THR:HG21	0.80	1.53	4	22

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:ARG:NH2	1:A:47:LEU:HD12	0.76	1.95	28	1
1:A:10:ASN:HB2	1:A:106:TYR:HA	0.69	1.62	7	23
1:A:35:MET:HE2	1:A:37:THR:HB	0.68	1.64	2	8
1:A:93:THR:HB	1:A:99:ILE:HG23	0.66	1.66	36	32
1:A:42:VAL:HG11	1:A:93:THR:HG23	0.65	1.68	32	13
1:A:41:PHE:CG	1:A:47:LEU:HD22	0.65	2.26	36	1
1:A:21:THR:HG22	1:A:77:LEU:HD22	0.64	1.70	34	36
1:A:41:PHE:C	1:A:41:PHE:CD1	0.64	2.76	36	1
1:A:38:ARG:NH1	1:A:90:LEU:HD21	0.64	2.08	2	5
1:A:41:PHE:CD2	1:A:47:LEU:HD22	0.63	2.28	36	1
1:A:54:VAL:HG22	1:A:78:VAL:HG13	0.63	1.70	33	21
1:A:105:ARG:HG3	1:A:106:TYR:N	0.63	2.08	23	35
1:A:38:ARG:NH1	1:A:90:LEU:HD11	0.62	2.09	9	2
1:A:14:VAL:HG22	1:A:15:ASP:H	0.62	1.54	2	8
1:A:38:ARG:NH2	1:A:47:LEU:HD13	0.62	2.10	11	2
1:A:38:ARG:HE	1:A:47:LEU:HB2	0.62	1.55	28	1
1:A:38:ARG:HE	1:A:47:LEU:HB3	0.60	1.57	11	4
1:A:10:ASN:HB3	1:A:105:ARG:O	0.59	1.97	9	33
1:A:13:TRP:CD1	1:A:13:TRP:N	0.59	2.70	22	10
1:A:13:TRP:HA	1:A:109:HIS:HB2	0.58	1.73	20	34
1:A:58:TYR:C	1:A:58:TYR:CD1	0.58	2.82	27	23
1:A:38:ARG:NE	1:A:47:LEU:HB2	0.58	2.14	28	1
1:A:13:TRP:CD1	1:A:87:THR:HG1	0.58	2.16	31	1
1:A:76:VAL:HG11	1:A:88:LEU:HD21	0.57	1.76	2	6
1:A:89:GLU:HA	1:A:107:THR:HG23	0.57	1.77	14	10
1:A:38:ARG:NH1	1:A:54:VAL:HG11	0.57	2.15	26	2
1:A:41:PHE:O	1:A:42:VAL:C	0.57	2.48	36	3
1:A:78:VAL:HG11	1:A:88:LEU:HB2	0.56	1.75	16	7
1:A:14:VAL:N	1:A:109:HIS:HB2	0.56	2.14	23	4
1:A:52:LEU:HD22	1:A:78:VAL:HG12	0.56	1.78	21	9
1:A:39:VAL:HG12	1:A:89:GLU:O	0.56	2.01	4	1
1:A:17:HIS:O	1:A:112:VAL:HG13	0.55	2.02	7	2
1:A:36:TRP:HB2	1:A:74:TYR:CD1	0.55	2.37	22	4
1:A:38:ARG:HH21	1:A:47:LEU:HD13	0.55	1.62	11	3
1:A:38:ARG:HB2	1:A:47:LEU:HB3	0.55	1.77	5	25
1:A:38:ARG:NE	1:A:54:VAL:HG11	0.55	2.17	34	2
1:A:52:LEU:HD23	1:A:80:PRO:HA	0.55	1.79	34	22
1:A:38:ARG:NH1	1:A:88:LEU:HD11	0.54	2.17	34	2
1:A:13:TRP:H	1:A:13:TRP:CD1	0.54	2.20	30	5
1:A:12:LYS:HG3	1:A:13:TRP:N	0.54	2.18	19	2
1:A:37:THR:HG23	1:A:42:VAL:HG22	0.54	1.79	22	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:VAL:HG22	1:A:109:HIS:HB2	0.54	1.78	33	3
1:A:89:GLU:HA	1:A:107:THR:HA	0.54	1.79	2	7
1:A:35:MET:HB3	1:A:95:PRO:HD3	0.54	1.80	18	1
1:A:77:LEU:N	1:A:77:LEU:HD22	0.54	2.18	20	2
1:A:93:THR:CB	1:A:99:ILE:HG23	0.54	2.33	8	4
1:A:14:VAL:HG22	1:A:15:ASP:N	0.53	2.18	35	7
1:A:52:LEU:O	1:A:54:VAL:HG23	0.53	2.02	7	8
1:A:14:VAL:HG12	1:A:109:HIS:HB2	0.53	1.80	31	1
1:A:13:TRP:HA	1:A:109:HIS:HA	0.53	1.80	19	4
1:A:38:ARG:HH11	1:A:90:LEU:HD11	0.53	1.62	4	2
1:A:91:VAL:HG23	1:A:104:GLU:O	0.53	2.04	33	2
1:A:54:VAL:HG13	1:A:78:VAL:HG13	0.53	1.78	28	4
1:A:41:PHE:O	1:A:43:GLY:N	0.52	2.43	36	1
1:A:21:THR:HG22	1:A:77:LEU:HD12	0.52	1.81	20	2
1:A:10:ASN:N	1:A:10:ASN:OD1	0.52	2.43	11	16
1:A:13:TRP:CD1	1:A:13:TRP:H	0.52	2.21	15	9
1:A:93:THR:O	1:A:95:PRO:HD3	0.52	2.05	15	22
1:A:35:MET:O	1:A:92:TYR:HA	0.51	2.05	3	31
1:A:89:GLU:C	1:A:90:LEU:HD12	0.51	2.30	9	1
1:A:103:ASN:HD22	1:A:103:ASN:N	0.51	2.03	10	17
1:A:48:SER:HB2	1:A:54:VAL:N	0.51	2.21	4	2
1:A:38:ARG:CZ	1:A:54:VAL:HG11	0.51	2.35	34	3
1:A:88:LEU:O	1:A:88:LEU:HD13	0.51	2.05	16	2
1:A:35:MET:HE3	1:A:95:PRO:HG3	0.51	1.83	18	1
1:A:10:ASN:HD22	1:A:105:ARG:HB3	0.51	1.66	8	9
1:A:10:ASN:HD22	1:A:105:ARG:HG2	0.50	1.67	23	2
1:A:57:LYS:HB2	1:A:75:VAL:HB	0.50	1.81	17	5
1:A:42:VAL:HG21	1:A:93:THR:CG2	0.50	2.35	8	3
1:A:53:GLU:HB3	1:A:79:LYS:HB2	0.50	1.84	31	3
1:A:73:ILE:CG2	1:A:74:TYR:N	0.49	2.75	31	3
1:A:23:GLU:HA	1:A:77:LEU:HD23	0.49	1.84	16	7
1:A:52:LEU:HB3	1:A:78:VAL:HG12	0.49	1.85	26	3
1:A:24:ILE:HB	1:A:76:VAL:HB	0.49	1.85	16	2
1:A:38:ARG:NH1	1:A:54:VAL:HG21	0.49	2.22	25	11
1:A:38:ARG:HD3	1:A:54:VAL:HG11	0.49	1.84	11	4
1:A:37:THR:CG2	1:A:42:VAL:HG22	0.49	2.38	32	4
1:A:58:TYR:C	1:A:58:TYR:HD1	0.49	2.16	36	6
1:A:78:VAL:HG21	1:A:88:LEU:HD22	0.49	1.84	15	5
1:A:10:ASN:O	1:A:11:ASP:C	0.49	2.55	3	11
1:A:35:MET:N	1:A:93:THR:O	0.49	2.45	1	24
1:A:37:THR:HG21	1:A:42:VAL:HA	0.49	1.84	22	13

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:ARG:HD3	1:A:88:LEU:HD21	0.49	1.84	4	1
1:A:35:MET:HE3	1:A:95:PRO:HG2	0.49	1.83	36	1
1:A:13:TRP:HE1	1:A:107:THR:HB	0.49	1.68	19	5
1:A:39:VAL:HG23	1:A:89:GLU:HB2	0.49	1.85	36	2
1:A:53:GLU:HB2	1:A:81:ARG:HG3	0.49	1.82	31	3
1:A:91:VAL:HG12	1:A:104:GLU:O	0.48	2.08	20	1
1:A:11:ASP:HB2	1:A:13:TRP:NE1	0.48	2.23	22	2
1:A:51:ILE:O	1:A:81:ARG:HB2	0.48	2.08	20	23
1:A:90:LEU:HB2	1:A:106:TYR:O	0.48	2.09	34	17
1:A:38:ARG:HD2	1:A:54:VAL:HG21	0.48	1.84	19	9
1:A:15:ASP:HA	1:A:111:ASN:N	0.48	2.24	7	1
1:A:39:VAL:HG22	1:A:91:VAL:HB	0.48	1.86	9	4
1:A:38:ARG:HA	1:A:89:GLU:O	0.48	2.08	6	12
1:A:42:VAL:HB	1:A:93:THR:HG21	0.48	1.86	30	4
1:A:78:VAL:HG11	1:A:88:LEU:HD22	0.48	1.85	9	1
1:A:10:ASN:ND2	1:A:105:ARG:HB3	0.48	2.24	10	9
1:A:17:HIS:HB2	1:A:20:LYS:HD3	0.48	1.85	3	25
1:A:26:LEU:O	1:A:73:ILE:HB	0.48	2.09	12	24
1:A:88:LEU:HB3	1:A:108:LEU:HB3	0.48	1.85	34	16
1:A:39:VAL:HG23	1:A:89:GLU:O	0.48	2.08	2	4
1:A:21:THR:CG2	1:A:77:LEU:HD12	0.47	2.40	20	2
1:A:56:CYS:SG	1:A:76:VAL:HG22	0.47	2.49	36	7
1:A:38:ARG:NH1	1:A:90:LEU:CD2	0.47	2.77	26	2
1:A:73:ILE:HG23	1:A:74:TYR:N	0.47	2.25	31	1
1:A:19:GLY:O	1:A:21:THR:N	0.47	2.47	24	16
1:A:87:THR:CG2	1:A:107:THR:HG22	0.47	2.40	14	4
1:A:38:ARG:HH11	1:A:54:VAL:HG21	0.47	1.70	13	3
1:A:93:THR:HA	1:A:103:ASN:HD22	0.47	1.68	18	1
1:A:15:ASP:HA	1:A:111:ASN:HB3	0.47	1.86	23	1
1:A:12:LYS:C	1:A:109:HIS:HB3	0.47	2.34	31	1
1:A:29:ASN:O	1:A:29:ASN:CG	0.47	2.57	32	1
1:A:38:ARG:HH12	1:A:90:LEU:HD21	0.47	1.69	34	1
1:A:108:LEU:O	1:A:110:LEU:N	0.47	2.48	33	1
1:A:73:ILE:C	1:A:74:TYR:CG	0.47	2.93	3	1
1:A:21:THR:CG2	1:A:77:LEU:HD22	0.47	2.40	32	7
1:A:38:ARG:NH1	1:A:38:ARG:HG3	0.47	2.25	9	2
1:A:14:VAL:CG2	1:A:15:ASP:N	0.47	2.78	31	2
1:A:78:VAL:HG21	1:A:108:LEU:CD1	0.46	2.40	23	1
1:A:48:SER:HB3	1:A:54:VAL:N	0.46	2.25	36	14
1:A:10:ASN:CB	1:A:106:TYR:HA	0.46	2.40	9	3
1:A:87:THR:HG22	1:A:88:LEU:N	0.46	2.24	15	7

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:78:VAL:CG2	1:A:88:LEU:HD22	0.46	2.40	2	3
1:A:26:LEU:N	1:A:73:ILE:O	0.46	2.48	16	4
1:A:77:LEU:N	1:A:77:LEU:CD2	0.46	2.79	7	2
1:A:105:ARG:NE	1:A:107:THR:HG23	0.46	2.26	33	2
1:A:23:GLU:HG3	1:A:75:VAL:HG23	0.46	1.88	13	2
1:A:38:ARG:NH2	1:A:48:SER:HA	0.45	2.25	7	1
1:A:34:TYR:N	1:A:34:TYR:CD1	0.45	2.84	12	3
1:A:12:LYS:CG	1:A:13:TRP:N	0.45	2.79	19	2
1:A:108:LEU:HD23	1:A:110:LEU:HD11	0.45	1.88	31	2
1:A:55:VAL:HB	1:A:77:LEU:HB2	0.45	1.88	27	3
1:A:10:ASN:HB2	1:A:105:ARG:O	0.45	2.11	33	2
1:A:78:VAL:HG21	1:A:108:LEU:HD23	0.45	1.87	4	3
1:A:12:LYS:O	1:A:109:HIS:HB3	0.45	2.12	23	4
1:A:78:VAL:HG11	1:A:88:LEU:HG	0.45	1.88	26	1
1:A:39:VAL:HG22	1:A:91:VAL:CG2	0.45	2.42	38	4
1:A:58:TYR:O	1:A:58:TYR:CD1	0.45	2.69	3	1
1:A:100:LYS:HB2	1:A:103:ASN:ND2	0.45	2.26	5	7
1:A:36:TRP:HB2	1:A:74:TYR:CZ	0.45	2.46	28	1
1:A:35:MET:HE2	1:A:58:TYR:CE2	0.45	2.46	36	1
1:A:100:LYS:HB3	1:A:101:PRO:HD2	0.45	1.89	24	12
1:A:38:ARG:NE	1:A:47:LEU:HB3	0.45	2.26	8	3
1:A:38:ARG:CZ	1:A:54:VAL:HB	0.45	2.42	28	1
1:A:88:LEU:HG	1:A:90:LEU:HG	0.45	1.89	21	8
1:A:38:ARG:HH11	1:A:88:LEU:HD11	0.45	1.71	2	2
1:A:93:THR:OG1	1:A:99:ILE:HA	0.45	2.12	8	4
1:A:14:VAL:HG23	1:A:110:LEU:HD23	0.45	1.90	11	3
1:A:38:ARG:HH11	1:A:38:ARG:HG3	0.45	1.71	28	1
1:A:38:ARG:HH22	1:A:56:CYS:H	0.45	1.53	28	1
1:A:20:LYS:N	1:A:80:PRO:HD2	0.44	2.27	24	5
1:A:27:LYS:N	1:A:27:LYS:HD2	0.44	2.28	28	1
1:A:57:LYS:O	1:A:75:VAL:HG12	0.44	2.13	7	1
1:A:52:LEU:HD22	1:A:80:PRO:HA	0.44	1.90	15	1
1:A:113:LYS:HA	1:A:113:LYS:HE2	0.44	1.89	26	2
1:A:93:THR:OG1	1:A:99:ILE:HG12	0.44	2.12	7	1
1:A:93:THR:HA	1:A:103:ASN:ND2	0.44	2.28	18	1
1:A:111:ASN:O	1:A:112:VAL:C	0.44	2.60	33	3
1:A:14:VAL:H	1:A:109:HIS:HB2	0.44	1.71	23	2
1:A:48:SER:HB3	1:A:54:VAL:HG23	0.44	1.89	36	1
1:A:92:TYR:O	1:A:103:ASN:HB3	0.44	2.13	36	2
1:A:93:THR:OG1	1:A:94:ARG:N	0.44	2.50	35	3
1:A:24:ILE:HD11	1:A:108:LEU:HD21	0.44	1.90	23	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:LYS:HE3	1:A:12:LYS:HA	0.44	1.90	29	4
1:A:38:ARG:NH2	1:A:41:PHE:CE2	0.44	2.86	38	3
1:A:38:ARG:NH1	1:A:88:LEU:HD21	0.44	2.27	23	1
1:A:53:GLU:HB2	1:A:79:LYS:O	0.44	2.13	22	10
1:A:23:GLU:HA	1:A:76:VAL:O	0.44	2.12	23	4
1:A:27:LYS:HD3	1:A:27:LYS:N	0.43	2.28	3	1
1:A:24:ILE:O	1:A:74:TYR:O	0.43	2.36	22	3
1:A:54:VAL:HG22	1:A:78:VAL:CG1	0.43	2.44	38	8
1:A:27:LYS:H	1:A:27:LYS:HD2	0.43	1.72	10	3
1:A:39:VAL:C	1:A:41:PHE:H	0.43	2.20	4	1
1:A:35:MET:HG3	1:A:58:TYR:CE2	0.43	2.48	30	3
1:A:36:TRP:HB2	1:A:74:TYR:CD2	0.43	2.48	20	2
1:A:34:TYR:CD1	1:A:34:TYR:N	0.43	2.87	25	2
1:A:14:VAL:O	1:A:110:LEU:HA	0.43	2.13	13	7
1:A:89:GLU:HB3	1:A:107:THR:HG23	0.43	1.89	16	1
1:A:17:HIS:O	1:A:80:PRO:HG2	0.43	2.14	29	3
1:A:52:LEU:HD23	1:A:80:PRO:CA	0.43	2.44	16	5
1:A:48:SER:OG	1:A:53:GLU:HA	0.43	2.14	8	1
1:A:38:ARG:HD3	1:A:88:LEU:HD11	0.43	1.89	9	1
1:A:80:PRO:CB	1:A:112:VAL:HG11	0.43	2.43	31	1
1:A:48:SER:CB	1:A:54:VAL:H	0.43	2.27	29	1
1:A:105:ARG:HE	1:A:107:THR:HG23	0.43	1.74	33	2
1:A:38:ARG:HA	1:A:90:LEU:HA	0.42	1.91	9	1
1:A:91:VAL:HA	1:A:105:ARG:HA	0.42	1.89	20	1
1:A:58:TYR:O	1:A:60:PRO:HD3	0.42	2.14	17	1
1:A:39:VAL:HG23	1:A:89:GLU:C	0.42	2.39	23	2
1:A:88:LEU:HB3	1:A:108:LEU:CB	0.42	2.44	33	1
1:A:75:VAL:O	1:A:75:VAL:HG13	0.42	2.15	25	3
1:A:11:ASP:HB3	1:A:107:THR:O	0.42	2.13	23	1
1:A:38:ARG:HH11	1:A:88:LEU:HD21	0.42	1.72	23	1
1:A:92:TYR:HB2	1:A:104:GLU:HB3	0.42	1.90	28	1
1:A:52:LEU:HG	1:A:86:HIS:HB3	0.42	1.90	37	2
1:A:94:ARG:HB2	1:A:97:GLU:HB2	0.42	1.91	3	3
1:A:38:ARG:HD2	1:A:88:LEU:HD12	0.42	1.90	27	1
1:A:28:GLY:O	1:A:29:ASN:O	0.42	2.38	32	1
1:A:35:MET:HE2	1:A:37:THR:CB	0.42	2.42	2	1
1:A:52:LEU:O	1:A:54:VAL:N	0.42	2.52	7	2
1:A:27:LYS:HD3	1:A:27:LYS:H	0.42	1.74	3	1
1:A:56:CYS:HA	1:A:75:VAL:O	0.42	2.15	28	2
1:A:11:ASP:HA	1:A:107:THR:O	0.41	2.15	24	1
1:A:38:ARG:HG3	1:A:38:ARG:HH11	0.41	1.75	34	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:VAL:HG11	1:A:88:LEU:HD21	0.41	1.92	4	1
1:A:87:THR:HG1	1:A:109:HIS:CE1	0.41	2.32	25	2
1:A:36:TRP:HB2	1:A:74:TYR:CE2	0.41	2.50	6	1
1:A:27:LYS:HD2	1:A:27:LYS:N	0.41	2.30	9	2
1:A:48:SER:HB2	1:A:52:LEU:O	0.41	2.15	28	2
1:A:16:THR:HG22	1:A:112:VAL:HG22	0.41	1.92	17	1
1:A:12:LYS:HD3	1:A:108:LEU:HD13	0.41	1.91	30	2
1:A:39:VAL:CG1	1:A:89:GLU:HB3	0.41	2.45	37	3
1:A:76:VAL:HG12	1:A:78:VAL:HG22	0.41	1.92	23	1
1:A:47:LEU:HD12	1:A:56:CYS:HB3	0.41	1.92	34	1
1:A:39:VAL:CG2	1:A:89:GLU:HB2	0.41	2.45	36	1
1:A:38:ARG:HD3	1:A:54:VAL:HG21	0.41	1.91	28	1
1:A:84:GLY:N	1:A:112:VAL:HG23	0.41	2.31	31	1
1:A:15:ASP:HA	1:A:111:ASN:H	0.41	1.75	22	1
1:A:21:THR:OG1	1:A:79:LYS:HE3	0.41	2.15	32	1
1:A:99:ILE:O	1:A:103:ASN:CG	0.41	2.64	33	1
1:A:47:LEU:HD23	1:A:47:LEU:N	0.41	2.31	36	1
1:A:85:HIS:C	1:A:86:HIS:HD1	0.41	2.24	32	3
1:A:53:GLU:HG2	1:A:81:ARG:CZ	0.41	2.46	7	1
1:A:42:VAL:CG2	1:A:93:THR:HG21	0.41	2.39	25	2
1:A:15:ASP:HA	1:A:111:ASN:O	0.41	2.15	31	1
1:A:91:VAL:HG22	1:A:92:TYR:N	0.41	2.31	25	3
1:A:88:LEU:C	1:A:88:LEU:HD22	0.41	2.41	26	1
1:A:14:VAL:O	1:A:109:HIS:O	0.41	2.39	31	1
1:A:58:TYR:O	1:A:59:THR:C	0.41	2.64	3	1
1:A:38:ARG:NE	1:A:54:VAL:HB	0.41	2.30	28	1
1:A:24:ILE:HG22	1:A:26:LEU:HG	0.40	1.94	1	1
1:A:35:MET:SD	1:A:95:PRO:HG3	0.40	2.56	15	1
1:A:87:THR:HG21	1:A:107:THR:HB	0.40	1.92	19	1
1:A:38:ARG:CD	1:A:47:LEU:HB3	0.40	2.47	8	1
1:A:53:GLU:HG2	1:A:81:ARG:NE	0.40	2.31	21	1
1:A:10:ASN:HD22	1:A:11:ASP:H	0.40	1.58	1	1
1:A:103:ASN:N	1:A:103:ASN:HD22	0.40	2.12	29	1
1:A:111:ASN:HD22	1:A:111:ASN:C	0.40	2.23	4	1
1:A:58:TYR:CD1	1:A:58:TYR:C	0.40	3.00	14	1
1:A:15:ASP:O	1:A:16:THR:HB	0.40	2.15	34	1
1:A:38:ARG:CZ	1:A:90:LEU:HD21	0.40	2.46	2	1
1:A:38:ARG:HE	1:A:47:LEU:CB	0.40	2.28	4	1
1:A:56:CYS:HB2	1:A:76:VAL:HA	0.40	1.93	9	1
1:A:26:LEU:N	1:A:26:LEU:HD22	0.40	2.31	31	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	84/116 (72%)	58±3 (70±3%)	18±3 (22±4%)	7±2 (9±2%)	1	11
All	All	3192/4408 (72%)	2220 (70%)	689 (22%)	283 (9%)	1	11

All 21 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	SER	37
1	A	21	THR	34
1	A	80	PRO	29
1	A	20	LYS	29
1	A	11	ASP	27
1	A	106	TYR	25
1	A	51	ILE	24
1	A	49	ASP	23
1	A	60	PRO	23
1	A	42	VAL	6
1	A	112	VAL	4
1	A	29	ASN	4
1	A	73	ILE	3
1	A	28	GLY	3
1	A	74	TYR	3
1	A	109	HIS	3
1	A	111	ASN	2
1	A	53	GLU	1
1	A	15	ASP	1
1	A	38	ARG	1
1	A	101	PRO	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	79/104 (76%)	70±2 (89±3%)	9±2 (11±3%)	8	51
All	All	3002/3952 (76%)	2664 (89%)	338 (11%)	8	51

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	78	VAL	38
1	A	10	ASN	35
1	A	53	GLU	31
1	A	112	VAL	24
1	A	15	ASP	20
1	A	104	GLU	17
1	A	107	THR	17
1	A	11	ASP	14
1	A	12	LYS	11
1	A	38	ARG	10
1	A	74	TYR	10
1	A	100	LYS	9
1	A	91	VAL	9
1	A	96	PHE	8
1	A	89	GLU	7
1	A	54	VAL	7
1	A	58	TYR	7
1	A	86	HIS	6
1	A	59	THR	6
1	A	73	ILE	6
1	A	52	LEU	5
1	A	105	ARG	5
1	A	103	ASN	4
1	A	34	TYR	3
1	A	88	LEU	3
1	A	113	LYS	3
1	A	99	ILE	3
1	A	42	VAL	2
1	A	35	MET	2
1	A	16	THR	2
1	A	26	LEU	2
1	A	92	TYR	2
1	A	49	ASP	1
1	A	27	LYS	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	14	VAL	1
1	A	25	HIS	1
1	A	39	VAL	1
1	A	29	ASN	1
1	A	41	PHE	1
1	A	47	LEU	1
1	A	57	LYS	1
1	A	79	LYS	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](#)

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

The completeness of assignment taking into account all chemical shift lists is 91% for the well-defined parts and 89% 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

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	1440
Number of shifts mapped to atoms	1422
Number of unparsed shifts	0
Number of shifts with mapping errors	18
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	19

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

- No matching atom found in the structure. All 18 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	MET	HA2	3.879	0.003	1
1	A	1	MET	HA3	3.879	0.003	1
1	A	2	ILE	HB2	3.829	0.003	1
1	A	2	ILE	HB3	3.829	0.003	1
1	A	4	PRO	H	8.452	0.003	1
1	A	5	LEU	HG12	1.461	0.008	2
1	A	5	LEU	HG13	1.161	0.006	2
1	A	5	LEU	HG21	0.886	0.017	1
1	A	5	LEU	HG22	0.886	0.017	1
1	A	5	LEU	HG23	0.886	0.017	1
1	A	5	LEU	CG1	27.281	0.042	1
1	A	5	LEU	CG2	17.42	0.022	1
1	A	7	VAL	HB2	1.918	0.008	2
1	A	7	VAL	HB3	2.275	0.013	2

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	7	VAL	HD2	3.665	0.012	2
1	A	7	VAL	HD3	3.806	0.001	2
1	A	7	VAL	HG3	2.025	0.001	2
1	A	7	VAL	CD	50.622	0.000	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	113	-0.09 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	102	0.20 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}'$	113	1.92 ± 0.28	Should be applied
^{15}N	105	-0.57 ± 0.53	None needed (imprecise)

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 91%, i.e. 1135 atoms were assigned a chemical shift out of a possible 1243. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	423/423 (100%)	172/172 (100%)	170/170 (100%)	81/81 (100%)
Sidechain	627/691 (91%)	424/449 (94%)	194/215 (90%)	9/27 (33%)
Aromatic	85/129 (66%)	45/62 (73%)	38/55 (69%)	2/12 (17%)
Overall	1135/1243 (91%)	641/683 (94%)	402/440 (91%)	92/120 (77%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 89%, i.e. 1421 atoms were assigned a chemical shift out of a possible 1602. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	556/575 (97%)	226/235 (96%)	226/232 (97%)	104/108 (96%)
Sidechain	780/890 (88%)	527/582 (91%)	244/279 (87%)	9/29 (31%)
Aromatic	85/137 (62%)	45/66 (68%)	38/57 (67%)	2/14 (14%)
Overall	1421/1602 (89%)	798/883 (90%)	508/568 (89%)	115/151 (76%)

7.1.4 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
1	A	6	SER	CB	18.34	56.28 – 71.32	-30.2
1	A	2	ILE	CB	64.04	28.63 – 48.45	12.9
1	A	6	SER	HB2	1.36	2.61 – 5.13	-10.0
1	A	6	SER	HB3	1.36	2.49 – 5.20	-9.2
1	A	92	TYR	HB3	-0.19	0.93 – 4.76	-7.9
1	A	3	ALA	HB2	3.27	0.14 – 2.58	7.8
1	A	5	LEU	CD1	12.86	16.71 – 32.55	-7.4
1	A	3	ALA	HB3	3.15	0.14 – 2.58	7.3
1	A	26	LEU	HD11	-1.03	-0.61 – 2.12	-6.6
1	A	26	LEU	HD12	-1.03	-0.61 – 2.12	-6.6
1	A	26	LEU	HD13	-1.03	-0.61 – 2.12	-6.6
1	A	8	LYS	CB	43.45	24.03 – 41.47	6.1
1	A	34	TYR	HB3	0.60	0.93 – 4.76	-5.9
1	A	1	MET	CA	43.39	45.26 – 67.07	-5.9
1	A	3	ALA	CB	29.16	10.19 – 27.75	5.8
1	A	30	PRO	C	168.43	169.47 – 184.06	-5.7
1	A	94	ARG	HG2	0.16	0.26 – 2.87	-5.4
1	A	4	PRO	CA	55.70	55.85 – 70.84	-5.1
1	A	113	LYS	C	167.21	167.28 – 186.22	-5.0

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. 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:

