



Full wwPDB NMR Structure Validation Report ⓘ

Sep 29, 2024 – 06:38 AM EDT

PDB ID : 2N4I
BMRB ID : 17833
Title : The solution structure of Skint-1, a critical determinant of dendritic epidermal gamma-delta T cell selection
Authors : Salim, M.; Knowles, T.J.; Hart, R.; Mohammed, F.; Woodward, M.J.; Willcox, C.R.; Overduin, M.; Hayday, A.C.; Willcox, B.E.
Deposited on : 2015-06-18

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 : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.39

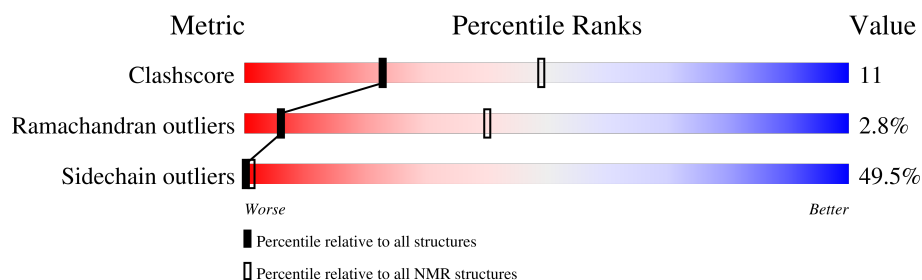
1 Overall quality at a glance

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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	119	

2 Ensemble composition and analysis

This entry contains 20 models. Model 13 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:27-A:66, A:74-A:141 (108)	1.13	13

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 6 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1880 atoms, of which 926 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Selection and upkeep of intraepithelial T-cells protein 1.

Mol	Chain	Residues	Atoms						Trace
1	A	119	Total	C	H	N	O	S	0
			1880	606	926	157	186	5	

There is a discrepancy between the modelled and reference sequences:

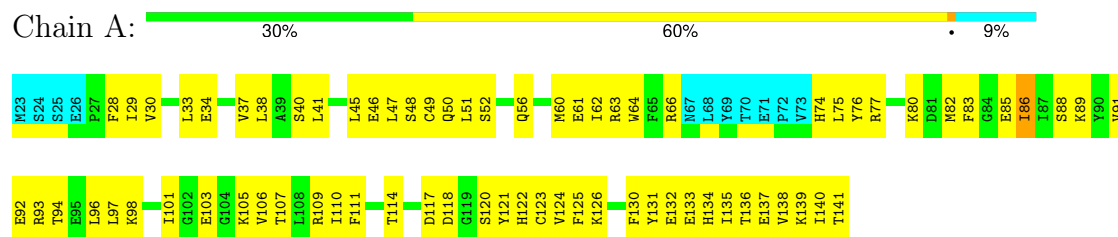
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	initiating methionine	UNP A7TZE6

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: Selection and upkeep of intraepithelial T-cells protein 1

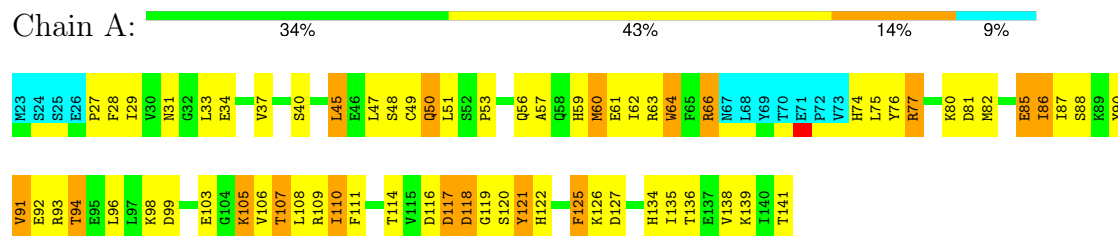


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

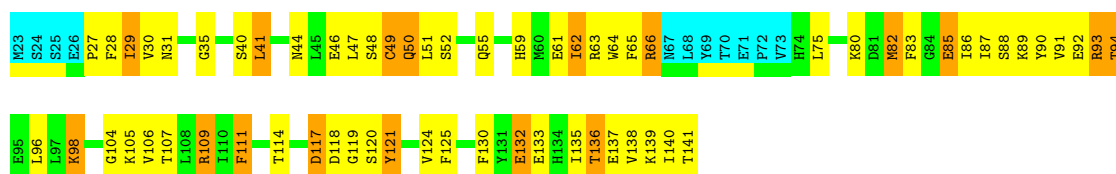
- Molecule 1: Selection and upkeep of intraepithelial T-cells protein 1



4.2.2 Score per residue for model 2

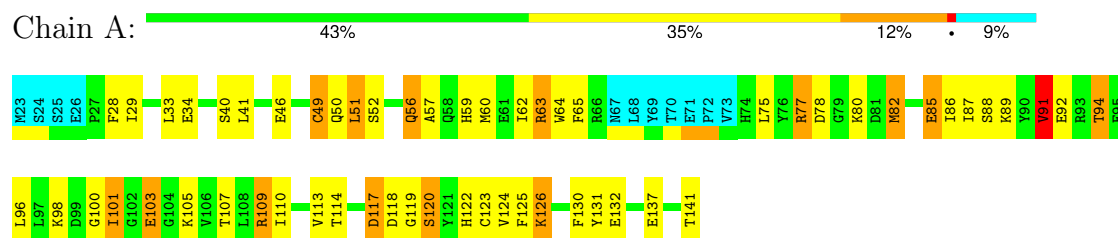
- Molecule 1: Selection and upkeep of intraepithelial T-cells protein 1





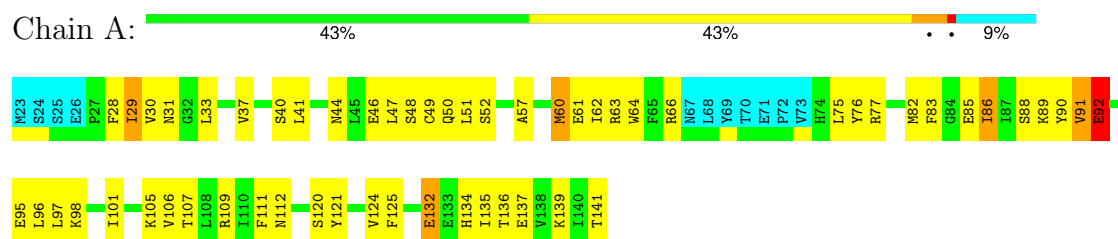
4.2.3 Score per residue for model 3

- Molecule 1: Selection and upkeep of intraepithelial T-cells protein 1



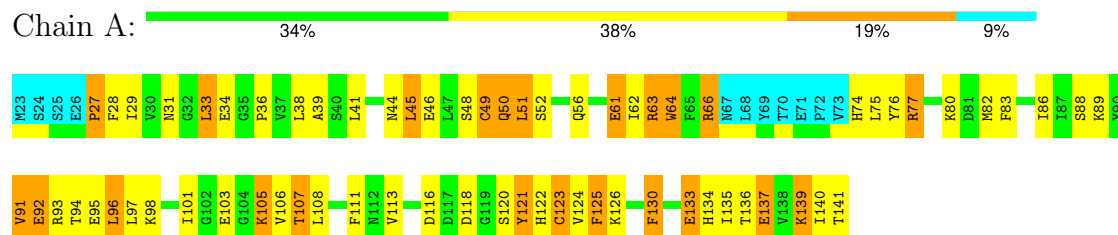
4.2.4 Score per residue for model 4

- Molecule 1: Selection and upkeep of intraepithelial T-cells protein 1



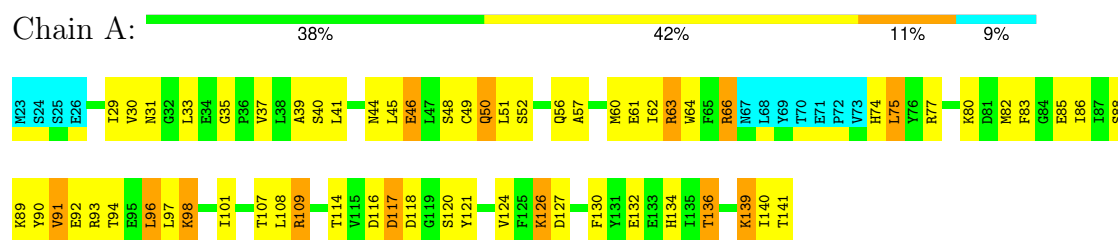
4.2.5 Score per residue for model 5

- Molecule 1: Selection and upkeep of intraepithelial T-cells protein 1



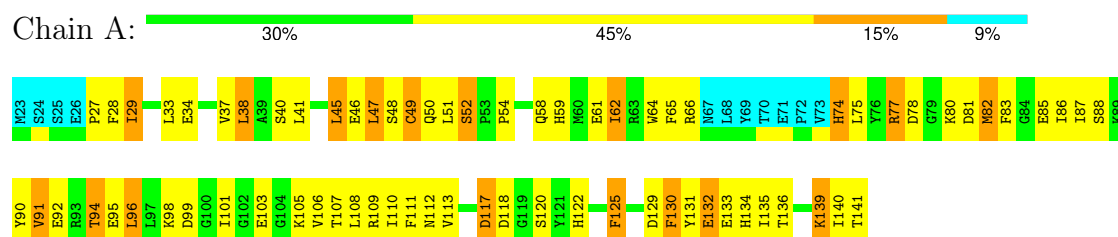
4.2.6 Score per residue for model 6

- Molecule 1: Selection and upkeep of intraepithelial T-cells protein 1



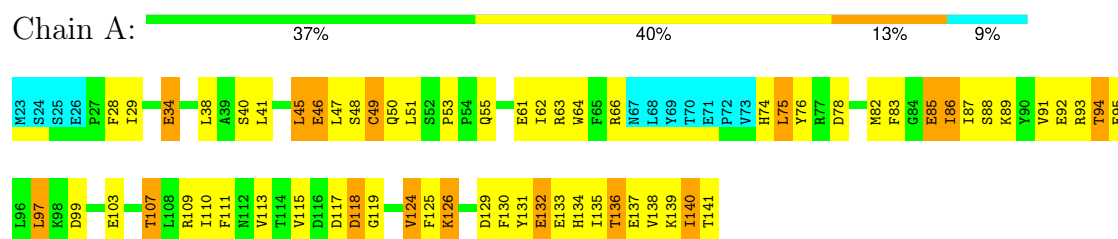
4.2.7 Score per residue for model 7

- Molecule 1: Selection and upkeep of intraepithelial T-cells protein 1



4.2.8 Score per residue for model 8

- Molecule 1: Selection and upkeep of intraepithelial T-cells protein 1



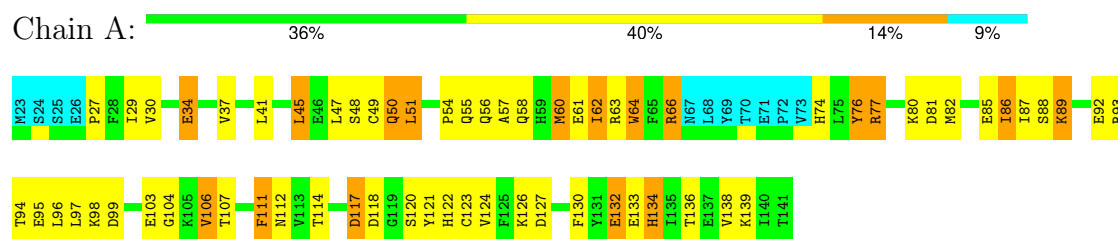
4.2.9 Score per residue for model 9

- Molecule 1: Selection and upkeep of intraepithelial T-cells protein 1



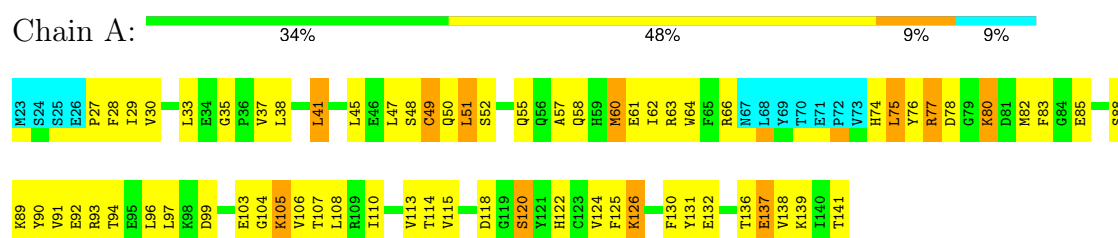
4.2.10 Score per residue for model 10

- Molecule 1: Selection and upkeep of intraepithelial T-cells protein 1



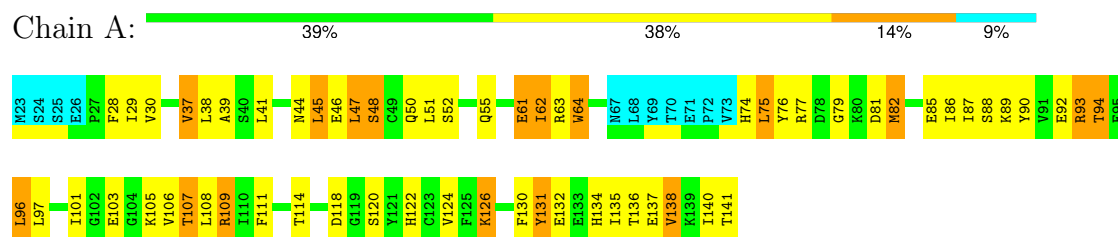
4.2.11 Score per residue for model 11

- Molecule 1: Selection and upkeep of intraepithelial T-cells protein 1



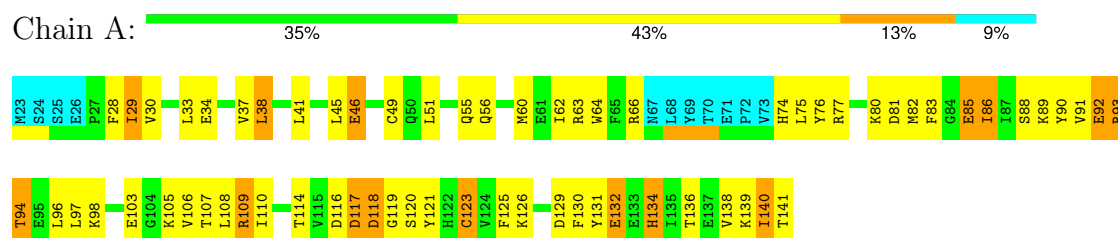
4.2.12 Score per residue for model 12

- Molecule 1: Selection and upkeep of intraepithelial T-cells protein 1



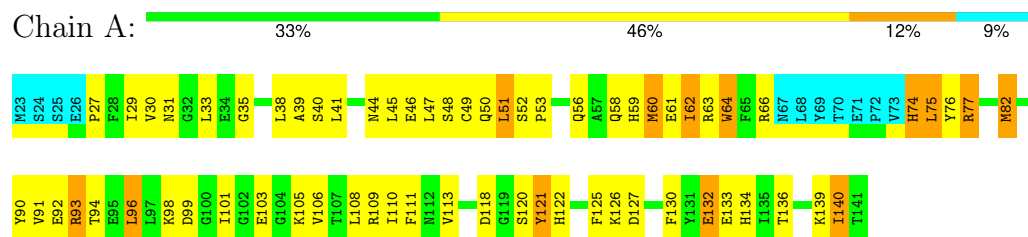
4.2.13 Score per residue for model 13 (medoid)

- Molecule 1: Selection and upkeep of intraepithelial T-cells protein 1



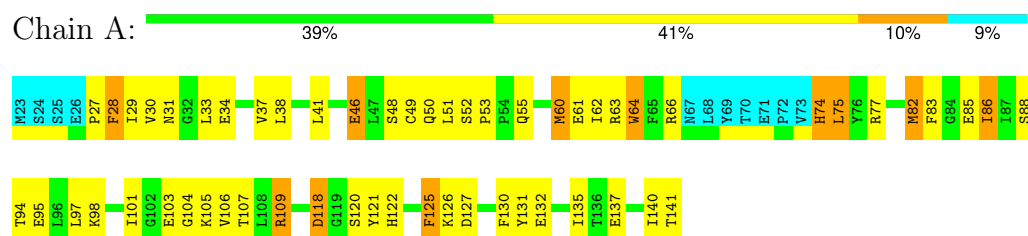
4.2.14 Score per residue for model 14

- Molecule 1: Selection and upkeep of intraepithelial T-cells protein 1



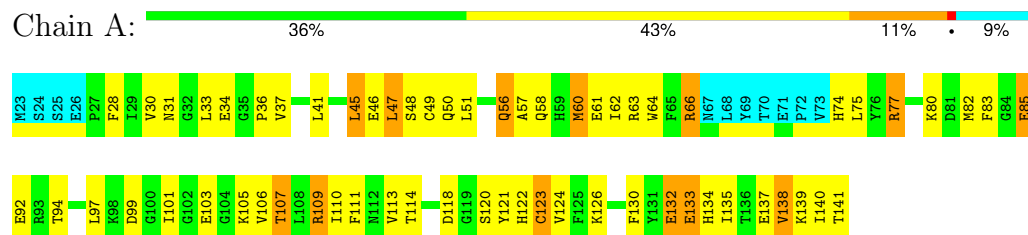
4.2.15 Score per residue for model 15

- Molecule 1: Selection and upkeep of intraepithelial T-cells protein 1



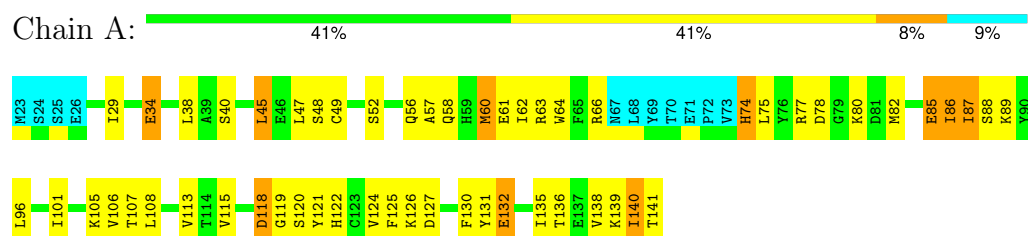
4.2.16 Score per residue for model 16

- Molecule 1: Selection and upkeep of intraepithelial T-cells protein 1



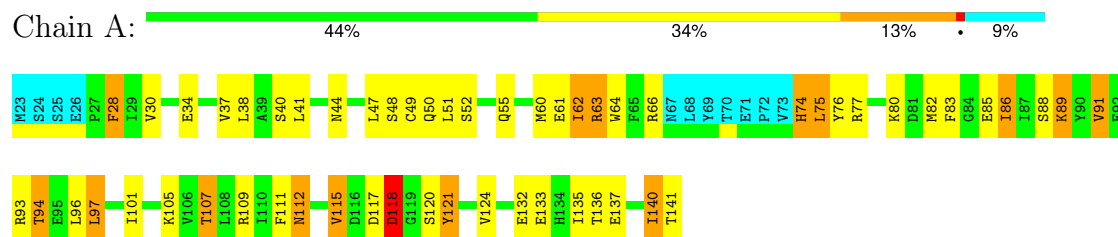
4.2.17 Score per residue for model 17

- Molecule 1: Selection and upkeep of intraepithelial T-cells protein 1



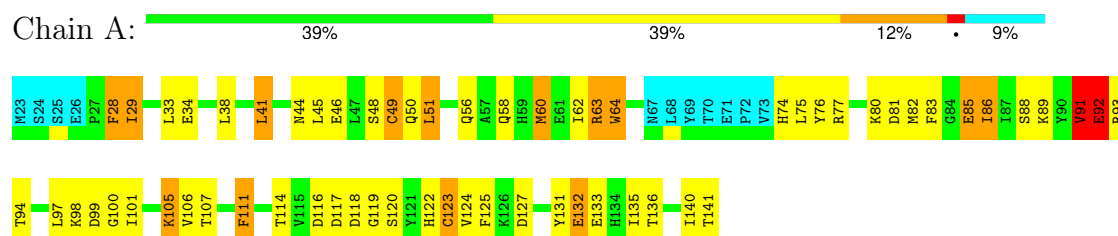
4.2.18 Score per residue for model 18

- Molecule 1: Selection and upkeep of intraepithelial T-cells protein 1



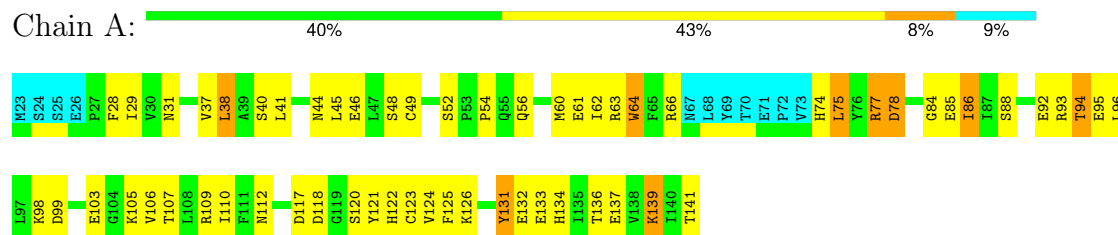
4.2.19 Score per residue for model 19

- Molecule 1: Selection and upkeep of intraepithelial T-cells protein 1



4.2.20 Score per residue for model 20

- Molecule 1: Selection and upkeep of intraepithelial T-cells protein 1



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing, torsion angle dynamics*.

Of the 100 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
CYANA	structure solution	
ARIA	refinement	
CYANA	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	1289
Number of shifts mapped to atoms	1289
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	84%

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	867	844	840	19±4
All	All	17340	16880	16800	374

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 11.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:GLU:HB3	1:A:75:LEU:HD11	0.92	1.42	14	4
1:A:61:GLU:HG2	1:A:75:LEU:HD13	0.84	1.48	20	1
1:A:74:HIS:HA	1:A:85:GLU:HB2	0.83	1.47	14	2
1:A:63:ARG:HB3	1:A:124:VAL:HB	0.82	1.52	20	4
1:A:74:HIS:HA	1:A:85:GLU:HB3	0.79	1.55	6	2
1:A:35:GLY:HA3	1:A:136:THR:HG23	0.78	1.52	9	3
1:A:29:ILE:HA	1:A:132:GLU:HG3	0.76	1.58	19	11
1:A:61:GLU:HB2	1:A:126:LYS:HB2	0.74	1.57	11	6
1:A:126:LYS:HG2	1:A:131:TYR:HB3	0.74	1.59	15	3
1:A:60:MET:HG3	1:A:127:ASP:HA	0.73	1.58	17	6
1:A:27:PRO:HB2	1:A:130:PHE:HB3	0.73	1.60	7	1
1:A:87:ILE:HG12	1:A:94:THR:HB	0.73	1.59	2	1
1:A:94:THR:HG23	1:A:110:ILE:HG12	0.73	1.60	7	5
1:A:45:LEU:HG	1:A:113:VAL:HB	0.72	1.60	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:ARG:HB3	1:A:124:VAL:HG12	0.72	1.60	5	1
1:A:45:LEU:HD23	1:A:110:ILE:HB	0.71	1.63	7	3
1:A:45:LEU:HD11	1:A:138:VAL:HG21	0.70	1.61	16	1
1:A:82:MET:HB3	1:A:85:GLU:HB3	0.70	1.63	1	1
1:A:74:HIS:HB2	1:A:85:GLU:HB2	0.69	1.63	10	2
1:A:45:LEU:HD22	1:A:113:VAL:HG21	0.67	1.65	17	1
1:A:91:VAL:HG12	1:A:94:THR:HG23	0.67	1.64	18	1
1:A:93:ARG:HB3	1:A:111:PHE:HB2	0.67	1.66	14	3
1:A:30:VAL:HG23	1:A:132:GLU:HB3	0.66	1.65	14	6
1:A:62:ILE:HD13	1:A:96:LEU:HD21	0.66	1.67	7	1
1:A:49:CYS:HB2	1:A:64:TRP:CZ3	0.66	2.26	11	2
1:A:46:GLU:HG3	1:A:109:ARG:HG3	0.65	1.68	6	8
1:A:61:GLU:HG2	1:A:75:LEU:HD12	0.65	1.67	6	2
1:A:39:ALA:O	1:A:140:ILE:HA	0.65	1.92	12	3
1:A:34:GLU:HB2	1:A:136:THR:HG23	0.65	1.66	8	2
1:A:124:VAL:HG23	1:A:133:GLU:HB3	0.65	1.68	5	1
1:A:66:ARG:HB3	1:A:121:TYR:HA	0.65	1.67	16	1
1:A:118:ASP:HB2	1:A:140:ILE:HG12	0.65	1.68	18	1
1:A:74:HIS:CE1	1:A:87:ILE:HA	0.64	2.28	7	1
1:A:50:GLN:HG3	1:A:105:LYS:HD2	0.64	1.70	11	1
1:A:47:LEU:HD23	1:A:108:LEU:HD23	0.62	1.70	1	1
1:A:63:ARG:HB2	1:A:75:LEU:HB2	0.62	1.72	8	1
1:A:74:HIS:HE1	1:A:87:ILE:HA	0.62	1.55	7	2
1:A:120:SER:HA	1:A:137:GLU:HA	0.61	1.70	3	2
1:A:63:ARG:NH1	1:A:124:VAL:HB	0.61	2.11	8	1
1:A:121:TYR:CE2	1:A:138:VAL:HB	0.61	2.30	2	1
1:A:66:ARG:HA	1:A:121:TYR:HA	0.60	1.72	9	2
1:A:30:VAL:HG11	1:A:134:HIS:HB2	0.60	1.73	16	1
1:A:57:ALA:HA	1:A:60:MET:HG2	0.60	1.72	10	1
1:A:57:ALA:HA	1:A:60:MET:SD	0.59	2.36	1	4
1:A:108:LEU:HD21	1:A:110:ILE:HD12	0.59	1.72	1	1
1:A:96:LEU:HD12	1:A:108:LEU:HD13	0.59	1.74	14	4
1:A:63:ARG:HH11	1:A:124:VAL:HB	0.59	1.58	8	1
1:A:93:ARG:HB3	1:A:111:PHE:HB3	0.58	1.75	18	2
1:A:75:LEU:HD22	1:A:82:MET:HB2	0.58	1.74	15	1
1:A:66:ARG:HB2	1:A:121:TYR:HA	0.57	1.76	10	2
1:A:28:PHE:HB2	1:A:53:PRO:HA	0.57	1.74	1	1
1:A:64:TRP:CZ3	1:A:121:TYR:HB3	0.57	2.35	15	2
1:A:79:GLY:HA2	1:A:96:LEU:HD22	0.57	1.76	12	1
1:A:62:ILE:HG23	1:A:76:TYR:HB3	0.57	1.76	14	1
1:A:63:ARG:HB3	1:A:74:HIS:CD2	0.57	2.35	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:91:VAL:HG13	1:A:92:GLU:H	0.56	1.60	4	1
1:A:77:ARG:HG2	1:A:78:ASP:N	0.56	2.16	20	1
1:A:97:LEU:HD12	1:A:107:THR:HB	0.56	1.77	6	1
1:A:61:GLU:HG3	1:A:75:LEU:HD12	0.56	1.76	18	1
1:A:74:HIS:HA	1:A:85:GLU:OE1	0.56	2.00	15	1
1:A:45:LEU:HD12	1:A:113:VAL:HG21	0.56	1.78	8	1
1:A:92:GLU:HB3	1:A:111:PHE:HB3	0.55	1.76	19	1
1:A:28:PHE:HZ	1:A:125:PHE:HB2	0.55	1.61	5	4
1:A:94:THR:HG22	1:A:110:ILE:HG12	0.55	1.76	13	1
1:A:87:ILE:HD11	1:A:94:THR:HG21	0.55	1.77	8	3
1:A:30:VAL:HA	1:A:51:LEU:HD13	0.55	1.78	6	1
1:A:49:CYS:HB3	1:A:125:PHE:CZ	0.55	2.37	2	1
1:A:74:HIS:CE1	1:A:84:GLY:HA3	0.54	2.37	20	1
1:A:64:TRP:HZ3	1:A:121:TYR:HB3	0.54	1.62	15	3
1:A:75:LEU:O	1:A:85:GLU:HG3	0.54	2.03	6	1
1:A:63:ARG:HG3	1:A:124:VAL:HB	0.54	1.79	3	3
1:A:41:LEU:HD12	1:A:140:ILE:HG21	0.54	1.80	19	2
1:A:82:MET:O	1:A:85:GLU:HG3	0.54	2.02	14	4
1:A:51:LEU:HD23	1:A:104:GLY:HA2	0.54	1.79	11	1
1:A:57:ALA:HB1	1:A:60:MET:SD	0.53	2.42	6	1
1:A:97:LEU:HB2	1:A:107:THR:HB	0.53	1.80	18	5
1:A:95:GLU:HG3	1:A:109:ARG:HB2	0.53	1.79	7	1
1:A:118:ASP:HB2	1:A:140:ILE:HB	0.53	1.78	8	3
1:A:85:GLU:HG3	1:A:86:ILE:N	0.53	2.17	17	3
1:A:118:ASP:HB2	1:A:140:ILE:HD13	0.53	1.79	14	2
1:A:53:PRO:HB2	1:A:55:GLN:O	0.53	2.04	8	1
1:A:86:ILE:HG23	1:A:89:LYS:HB2	0.53	1.81	18	2
1:A:63:ARG:HD3	1:A:74:HIS:O	0.53	2.04	6	1
1:A:45:LEU:HD13	1:A:47:LEU:HD21	0.52	1.80	1	4
1:A:121:TYR:CE1	1:A:136:THR:HB	0.52	2.40	2	1
1:A:47:LEU:HD22	1:A:64:TRP:CZ2	0.52	2.39	12	1
1:A:28:PHE:CZ	1:A:125:PHE:HB2	0.52	2.38	5	3
1:A:91:VAL:HG13	1:A:92:GLU:HG2	0.52	1.80	3	1
1:A:66:ARG:CZ	1:A:117:ASP:HA	0.52	2.34	1	1
1:A:49:CYS:HB3	1:A:125:PHE:HZ	0.52	1.65	2	2
1:A:50:GLN:HG2	1:A:105:LYS:HG3	0.52	1.80	5	1
1:A:38:LEU:HA	1:A:139:LYS:HG3	0.52	1.80	7	1
1:A:75:LEU:HG	1:A:76:TYR:N	0.52	2.20	11	1
1:A:82:MET:HG3	1:A:85:GLU:HB3	0.52	1.82	13	1
1:A:93:ARG:HA	1:A:93:ARG:HH11	0.51	1.64	17	1
1:A:61:GLU:HG2	1:A:77:ARG:HB3	0.51	1.82	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:125:PHE:O	1:A:131:TYR:HA	0.51	2.05	13	3
1:A:86:ILE:O	1:A:89:LYS:HB2	0.51	2.04	10	1
1:A:83:PHE:HA	1:A:86:ILE:HG13	0.51	1.81	15	1
1:A:59:HIS:HA	1:A:78:ASP:OD1	0.51	2.05	3	1
1:A:63:ARG:O	1:A:123:CYS:HA	0.51	2.05	5	6
1:A:47:LEU:HB3	1:A:64:TRP:CZ2	0.51	2.40	7	2
1:A:51:LEU:HD11	1:A:125:PHE:CD1	0.51	2.40	15	1
1:A:118:ASP:O	1:A:138:VAL:HB	0.51	2.05	17	3
1:A:61:GLU:HG2	1:A:77:ARG:HA	0.51	1.83	7	1
1:A:60:MET:CG	1:A:127:ASP:HA	0.50	2.36	14	2
1:A:101:ILE:HD11	1:A:125:PHE:CZ	0.50	2.41	14	1
1:A:66:ARG:HB2	1:A:121:TYR:CE1	0.50	2.42	4	1
1:A:49:CYS:HB2	1:A:64:TRP:CH2	0.49	2.42	7	1
1:A:66:ARG:HD3	1:A:117:ASP:HA	0.49	1.83	7	1
1:A:39:ALA:HB2	1:A:45:LEU:HD13	0.49	1.84	14	3
1:A:100:GLY:HA3	1:A:105:LYS:HB2	0.49	1.85	19	1
1:A:45:LEU:HD11	1:A:138:VAL:HG11	0.49	1.83	10	2
1:A:77:ARG:O	1:A:77:ARG:HG2	0.49	2.07	3	2
1:A:36:PRO:HA	1:A:137:GLU:O	0.49	2.07	5	1
1:A:98:LYS:HE2	1:A:101:ILE:HG21	0.49	1.84	6	1
1:A:101:ILE:HD11	1:A:125:PHE:HZ	0.48	1.68	14	1
1:A:74:HIS:HA	1:A:85:GLU:CB	0.48	2.37	18	1
1:A:87:ILE:HD12	1:A:94:THR:HG21	0.48	1.86	17	1
1:A:56:GLN:HG2	1:A:58:GLN:HB2	0.48	1.84	16	1
1:A:118:ASP:HA	1:A:138:VAL:HB	0.48	1.86	1	1
1:A:31:ASN:O	1:A:50:GLN:HB2	0.48	2.08	6	1
1:A:90:TYR:O	1:A:91:VAL:HB	0.48	2.08	15	1
1:A:62:ILE:HG21	1:A:106:VAL:HG11	0.48	1.84	12	1
1:A:51:LEU:O	1:A:53:PRO:HD3	0.48	2.08	9	2
1:A:46:GLU:OE2	1:A:109:ARG:HD2	0.48	2.08	12	1
1:A:45:LEU:HD12	1:A:113:VAL:HB	0.48	1.83	16	1
1:A:115:VAL:HA	1:A:118:ASP:HB3	0.48	1.85	18	2
1:A:74:HIS:HA	1:A:85:GLU:HA	0.48	1.84	8	1
1:A:64:TRP:CE3	1:A:64:TRP:HA	0.48	2.43	20	1
1:A:64:TRP:HA	1:A:122:HIS:O	0.47	2.09	7	1
1:A:41:LEU:HG	1:A:113:VAL:O	0.47	2.09	11	1
1:A:96:LEU:HD13	1:A:108:LEU:HD13	0.47	1.85	17	2
1:A:63:ARG:HB3	1:A:124:VAL:CG1	0.47	2.36	5	1
1:A:93:ARG:HA	1:A:93:ARG:NH1	0.47	2.23	17	1
1:A:47:LEU:HD21	1:A:121:TYR:CZ	0.47	2.44	2	1
1:A:66:ARG:HG2	1:A:121:TYR:HA	0.47	1.86	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:76:TYR:HE2	1:A:87:ILE:HD13	0.47	1.70	12	1
1:A:124:VAL:HA	1:A:132:GLU:O	0.47	2.08	8	3
1:A:77:ARG:HG2	1:A:80:LYS:HB3	0.47	1.86	11	1
1:A:44:ASN:HA	1:A:111:PHE:HA	0.47	1.85	19	1
1:A:47:LEU:O	1:A:107:THR:HA	0.47	2.09	9	4
1:A:33:LEU:HD11	1:A:49:CYS:HA	0.46	1.86	5	1
1:A:124:VAL:HG22	1:A:133:GLU:HG3	0.46	1.86	2	1
1:A:124:VAL:HG22	1:A:133:GLU:HB3	0.46	1.86	16	1
1:A:113:VAL:HG22	1:A:140:ILE:HD11	0.46	1.87	16	2
1:A:121:TYR:HB2	1:A:136:THR:O	0.46	2.10	14	1
1:A:74:HIS:CA	1:A:85:GLU:HB2	0.46	2.40	7	1
1:A:61:GLU:HB3	1:A:126:LYS:HB2	0.46	1.88	15	1
1:A:121:TYR:CD1	1:A:136:THR:HB	0.46	2.46	2	1
1:A:126:LYS:HG2	1:A:131:TYR:HB2	0.46	1.88	3	2
1:A:37:VAL:HG21	1:A:47:LEU:HD23	0.46	1.88	7	2
1:A:38:LEU:HA	1:A:139:LYS:HB2	0.46	1.87	13	1
1:A:51:LEU:N	1:A:51:LEU:HD13	0.46	2.26	19	1
1:A:74:HIS:HB3	1:A:85:GLU:HB3	0.45	1.88	20	1
1:A:91:VAL:HG13	1:A:92:GLU:N	0.45	2.27	19	2
1:A:34:GLU:HA	1:A:134:HIS:HE1	0.45	1.71	16	1
1:A:64:TRP:O	1:A:108:LEU:HD22	0.45	2.12	1	1
1:A:65:PHE:CE1	1:A:87:ILE:HG13	0.45	2.46	2	1
1:A:61:GLU:HG3	1:A:77:ARG:HB3	0.45	1.87	5	1
1:A:94:THR:HA	1:A:109:ARG:O	0.45	2.11	12	1
1:A:66:ARG:HB3	1:A:121:TYR:HD1	0.45	1.72	16	1
1:A:61:GLU:HG3	1:A:77:ARG:HB2	0.45	1.88	16	1
1:A:118:ASP:CA	1:A:138:VAL:HB	0.45	2.42	1	1
1:A:60:MET:HE3	1:A:127:ASP:HB2	0.45	1.89	6	1
1:A:117:ASP:C	1:A:119:GLY:H	0.44	2.16	2	3
1:A:49:CYS:HB3	1:A:125:PHE:CE1	0.44	2.47	3	1
1:A:27:PRO:CB	1:A:130:PHE:HB3	0.44	2.42	5	1
1:A:30:VAL:HG22	1:A:125:PHE:CE2	0.44	2.47	4	1
1:A:117:ASP:HB3	1:A:121:TYR:HE1	0.44	1.71	18	1
1:A:38:LEU:HA	1:A:139:LYS:O	0.44	2.12	5	2
1:A:61:GLU:CG	1:A:77:ARG:HB3	0.44	2.43	5	1
1:A:76:TYR:CE1	1:A:81:ASP:HB3	0.44	2.47	10	1
1:A:48:SER:HA	1:A:106:VAL:O	0.44	2.13	12	1
1:A:28:PHE:CD1	1:A:28:PHE:C	0.44	2.91	18	1
1:A:54:PRO:HD2	1:A:127:ASP:OD2	0.44	2.13	10	1
1:A:90:TYR:CD2	1:A:91:VAL:HG23	0.44	2.48	2	1
1:A:47:LEU:HD23	1:A:110:ILE:HD12	0.44	1.90	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:VAL:HB	1:A:134:HIS:CE1	0.43	2.48	13	2
1:A:97:LEU:HB2	1:A:107:THR:O	0.43	2.13	18	1
1:A:86:ILE:O	1:A:86:ILE:HG23	0.43	2.13	4	3
1:A:35:GLY:O	1:A:136:THR:HG22	0.43	2.13	6	1
1:A:47:LEU:HB3	1:A:64:TRP:CE2	0.43	2.48	10	1
1:A:30:VAL:HG22	1:A:125:PHE:HE2	0.43	1.73	4	1
1:A:94:THR:CG2	1:A:110:ILE:HG12	0.43	2.40	7	1
1:A:92:GLU:OE1	1:A:93:ARG:HD2	0.43	2.14	13	1
1:A:111:PHE:O	1:A:112:ASN:HB3	0.43	2.12	10	3
1:A:28:PHE:HE2	1:A:51:LEU:HD22	0.43	1.74	15	1
1:A:61:GLU:HG2	1:A:77:ARG:CB	0.43	2.43	14	1
1:A:51:LEU:HG	1:A:125:PHE:CD2	0.43	2.48	3	1
1:A:82:MET:H	1:A:85:GLU:CD	0.43	2.16	12	1
1:A:57:ALA:HB1	1:A:60:MET:HB2	0.43	1.90	17	2
1:A:66:ARG:HH21	1:A:116:ASP:HB3	0.43	1.74	5	1
1:A:121:TYR:CZ	1:A:138:VAL:HB	0.42	2.48	2	1
1:A:46:GLU:HA	1:A:108:LEU:O	0.42	2.14	7	1
1:A:31:ASN:HB3	1:A:50:GLN:HB3	0.42	1.91	5	1
1:A:63:ARG:HB2	1:A:124:VAL:HB	0.42	1.89	10	1
1:A:74:HIS:HD2	1:A:85:GLU:HA	0.42	1.74	19	1
1:A:98:LYS:HB2	1:A:98:LYS:HE3	0.42	1.48	2	1
1:A:139:LYS:HA	1:A:139:LYS:HD3	0.42	1.52	6	1
1:A:34:GLU:HA	1:A:134:HIS:CE1	0.42	2.50	16	1
1:A:28:PHE:HD1	1:A:130:PHE:HD1	0.42	1.57	15	1
1:A:117:ASP:OD1	1:A:117:ASP:N	0.42	2.53	13	1
1:A:50:GLN:HG3	1:A:105:LYS:HG3	0.42	1.91	1	1
1:A:65:PHE:O	1:A:122:HIS:HB3	0.42	2.15	3	1
1:A:56:GLN:O	1:A:101:ILE:HG23	0.41	2.14	3	1
1:A:51:LEU:HD13	1:A:51:LEU:N	0.41	2.29	5	1
1:A:114:THR:H	1:A:117:ASP:HB2	0.41	1.75	6	1
1:A:62:ILE:HD11	1:A:64:TRP:CD1	0.41	2.51	1	1
1:A:30:VAL:HG22	1:A:51:LEU:HA	0.41	1.92	10	1
1:A:66:ARG:O	1:A:66:ARG:HG3	0.41	2.15	14	1
1:A:106:VAL:HG21	1:A:125:PHE:HE2	0.41	1.76	15	1
1:A:52:SER:O	1:A:54:PRO:HD3	0.41	2.16	20	2
1:A:56:GLN:H	1:A:56:GLN:NE2	0.41	2.13	16	1
1:A:65:PHE:HB3	1:A:90:TYR:HE2	0.41	1.75	7	1
1:A:35:GLY:HA3	1:A:136:THR:CG2	0.41	2.39	14	1
1:A:62:ILE:HG13	1:A:125:PHE:CE1	0.41	2.50	2	1
1:A:100:GLY:HA2	1:A:103:GLU:OE2	0.41	2.15	3	1
1:A:96:LEU:O	1:A:98:LYS:HE2	0.41	2.16	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:108:LEU:HG	1:A:110:ILE:HG13	0.41	1.93	13	1
1:A:63:ARG:CG	1:A:74:HIS:HB3	0.41	2.46	15	1
1:A:34:GLU:CD	1:A:34:GLU:H	0.41	2.20	17	1
1:A:62:ILE:HG12	1:A:63:ARG:N	0.41	2.31	18	1
1:A:49:CYS:HB2	1:A:64:TRP:NE1	0.41	2.30	19	1
1:A:50:GLN:HA	1:A:104:GLY:O	0.41	2.16	2	2
1:A:139:LYS:HB2	1:A:139:LYS:HE2	0.41	1.66	7	1
1:A:76:TYR:HE2	1:A:98:LYS:HD3	0.41	1.75	9	1
1:A:53:PRO:HG3	1:A:104:GLY:HA3	0.40	1.93	15	1
1:A:140:ILE:HD13	1:A:140:ILE:HA	0.40	1.76	18	1
1:A:95:GLU:HG3	1:A:109:ARG:CB	0.40	2.46	7	1
1:A:51:LEU:HD13	1:A:51:LEU:H	0.40	1.76	19	1
1:A:61:GLU:HG3	1:A:77:ARG:HG3	0.40	1.94	6	1
1:A:66:ARG:HH12	1:A:117:ASP:CG	0.40	2.20	10	1
1:A:66:ARG:CB	1:A:121:TYR:HA	0.40	2.41	16	1
1:A:74:HIS:HB2	1:A:85:GLU:HA	0.40	1.92	1	1
1:A:62:ILE:HG13	1:A:106:VAL:HG21	0.40	1.93	10	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	107/119 (90%)	95±2 (89±2%)	9±2 (9±2%)	3±1 (3±1%)	6	40
All	All	2140/2380 (90%)	1896 (89%)	184 (9%)	60 (3%)	6	40

All 11 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	86	ILE	16
1	A	91	VAL	12
1	A	27	PRO	8
1	A	118	ASP	8
1	A	92	GLU	5

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Mol	Chain	Res	Type	Models (Total)
1	A	119	GLY	4
1	A	74	HIS	2
1	A	112	ASN	2
1	A	75	LEU	1
1	A	35	GLY	1
1	A	36	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	95/106 (90%)	48±5 (51±5%)	47±5 (49±5%)	0	1
All	All	1900/2120 (90%)	960 (51%)	940 (49%)	0	1

All 88 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	88	SER	20
1	A	49	CYS	19
1	A	120	SER	19
1	A	62	ILE	19
1	A	48	SER	18
1	A	141	THR	18
1	A	41	LEU	18
1	A	64	TRP	17
1	A	77	ARG	17
1	A	94	THR	17
1	A	105	LYS	17
1	A	107	THR	17
1	A	75	LEU	17
1	A	51	LEU	16
1	A	82	MET	16
1	A	89	LYS	16
1	A	50	GLN	15
1	A	92	GLU	15
1	A	132	GLU	15

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Mol	Chain	Res	Type	Models (Total)
1	A	66	ARG	14
1	A	80	LYS	14
1	A	96	LEU	14
1	A	103	GLU	14
1	A	106	VAL	14
1	A	130	PHE	14
1	A	29	ILE	13
1	A	60	MET	13
1	A	93	ARG	13
1	A	98	LYS	13
1	A	136	THR	13
1	A	139	LYS	13
1	A	33	LEU	12
1	A	37	VAL	12
1	A	40	SER	12
1	A	56	GLN	12
1	A	109	ARG	12
1	A	122	HIS	12
1	A	134	HIS	12
1	A	135	ILE	12
1	A	28	PHE	12
1	A	52	SER	12
1	A	83	PHE	12
1	A	38	LEU	12
1	A	34	GLU	11
1	A	85	GLU	11
1	A	118	ASP	11
1	A	137	GLU	11
1	A	45	LEU	10
1	A	63	ARG	10
1	A	99	ASP	10
1	A	114	THR	10
1	A	126	LYS	10
1	A	101	ILE	10
1	A	91	VAL	9
1	A	117	ASP	9
1	A	46	GLU	9
1	A	47	LEU	9
1	A	133	GLU	9
1	A	74	HIS	9
1	A	76	TYR	8
1	A	111	PHE	8

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Mol	Chain	Res	Type	Models (Total)
1	A	121	TYR	8
1	A	44	ASN	8
1	A	55	GLN	8
1	A	97	LEU	8
1	A	31	ASN	7
1	A	86	ILE	7
1	A	90	TYR	7
1	A	125	PHE	7
1	A	95	GLU	7
1	A	81	ASP	6
1	A	58	GLN	6
1	A	140	ILE	6
1	A	116	ASP	5
1	A	123	CYS	5
1	A	78	ASP	5
1	A	131	TYR	5
1	A	59	HIS	4
1	A	113	VAL	4
1	A	61	GLU	4
1	A	115	VAL	4
1	A	129	ASP	3
1	A	138	VAL	3
1	A	110	ILE	2
1	A	30	VAL	2
1	A	112	ASN	1
1	A	124	VAL	1
1	A	87	ILE	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 84% for the well-defined parts and 79% 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	1289
Number of shifts mapped to atoms	1289
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	107	0.01 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	95	-0.27 ± 0.21	None needed (< 0.5 ppm)
$^{13}\text{C}'$	107	0.19 ± 0.14	None needed (< 0.5 ppm)
^{15}N	97	-0.41 ± 0.68	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 84%, i.e. 1256 atoms were assigned a chemical shift out of a possible 1488. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	506/543 (93%)	207/223 (93%)	205/216 (95%)	94/104 (90%)
Sidechain	682/805 (85%)	458/521 (88%)	217/256 (85%)	7/28 (25%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	68/140 (49%)	34/68 (50%)	34/63 (54%)	0/9 (0%)
Overall	1256/1488 (84%)	699/812 (86%)	456/535 (85%)	101/141 (72%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 79%, i.e. 1289 atoms were assigned a chemical shift out of a possible 1628. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	524/596 (88%)	213/244 (87%)	214/238 (90%)	97/114 (85%)
Sidechain	697/883 (79%)	468/572 (82%)	221/282 (78%)	8/29 (28%)
Aromatic	68/149 (46%)	34/72 (47%)	34/68 (50%)	0/9 (0%)
Overall	1289/1628 (79%)	715/888 (81%)	469/588 (80%)	105/152 (69%)

7.1.4 Statistically unusual chemical shifts [i](#)

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	108	LEU	HB3	-0.80	-0.26 – 3.31	-6.5
1	A	123	CYS	HB3	0.63	0.69 – 5.10	-5.1
1	A	122	HIS	HB3	1.18	1.18 – 4.91	-5.0

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:

