



Full wwPDB NMR Structure Validation Report ⓘ

Mar 26, 2026 – 01:46 AM UTC

PDB ID : 2LB1 / pdb_00002lb1
BMRB ID : 17543
Title : Structure of the second domain of human Smurf1 in complex with a human Smad1 derived peptide
Authors : Macias, M.J.; Aragon, E.; Goerner, N.; Zaromytidou, A.; Xi, Q.; Escobedo, A.; Massague, J.
Deposited on : 2011-03-22

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

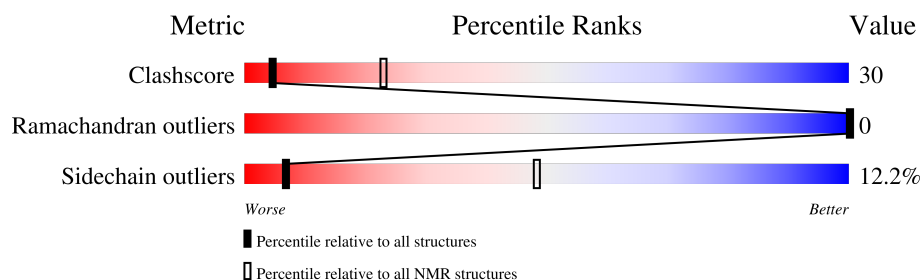
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 40%.

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	36	
2	B	15	

2 Ensemble composition and analysis

This entry contains 20 models. Model 20 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:282-A:313, B:221-B:231 (43)	0.56	20

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 1 single-model cluster was found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 754 atoms, of which 369 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called E3 ubiquitin-protein ligase SMURF1.

Mol	Chain	Residues	Atoms					Trace
1	A	35	Total	C	H	N	O	0
			564	181	279	53	51	

- Molecule 2 is a protein called Mothers against decapentaplegic homolog 1.

Mol	Chain	Residues	Atoms					Trace
2	B	14	Total	C	H	N	O	1
			190	65	90	14	21	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	234	NH2	-	insertion	UNP Q15797

4 Residue-property plots [i](#)

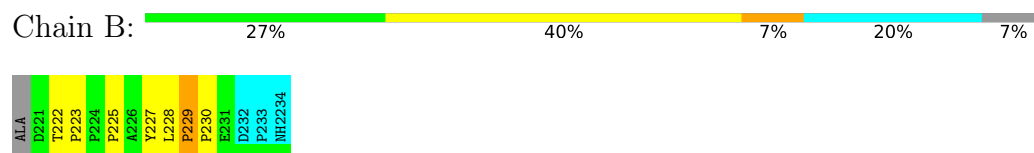
4.1 Average score per residue in the NMR ensemble

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: E3 ubiquitin-protein ligase SMURF1



- Molecule 2: Mothers against decapentaplegic homolog 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: E3 ubiquitin-protein ligase SMURF1

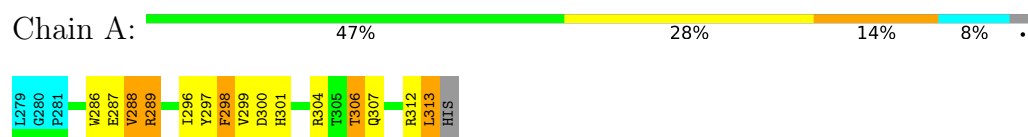


- Molecule 2: Mothers against decapentaplegic homolog 1

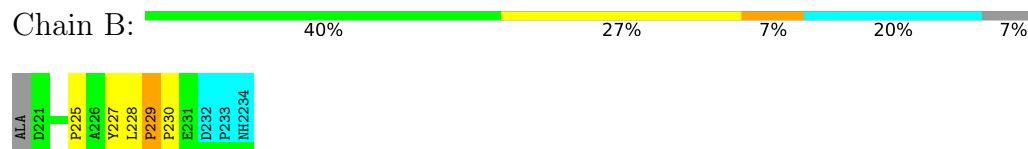


4.2.2 Score per residue for model 2

- Molecule 1: E3 ubiquitin-protein ligase SMURF1



- Molecule 2: Mothers against decapentaplegic homolog 1

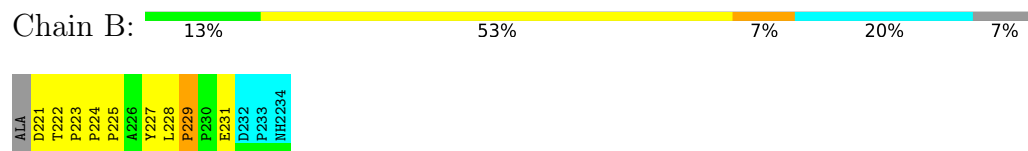


4.2.3 Score per residue for model 3

- Molecule 1: E3 ubiquitin-protein ligase SMURF1

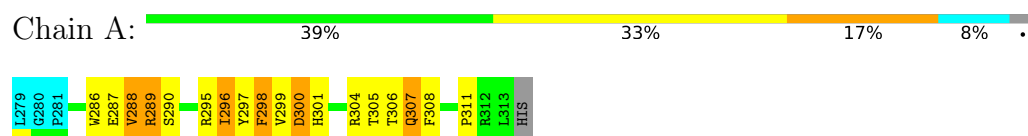


- Molecule 2: Mothers against decapentaplegic homolog 1



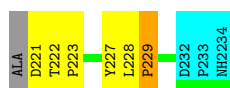
4.2.4 Score per residue for model 4

- Molecule 1: E3 ubiquitin-protein ligase SMURF1



- Molecule 2: Mothers against decapentaplegic homolog 1





4.2.5 Score per residue for model 5

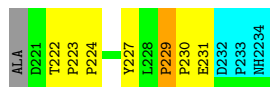
- Molecule 1: E3 ubiquitin-protein ligase SMURF1

Chain A:



- Molecule 2: Mothers against decapentaplegic homolog 1

Chain B:



4.2.6 Score per residue for model 6

- Molecule 1: E3 ubiquitin-protein ligase SMURF1

Chain A:



- Molecule 2: Mothers against decapentaplegic homolog 1

Chain B:



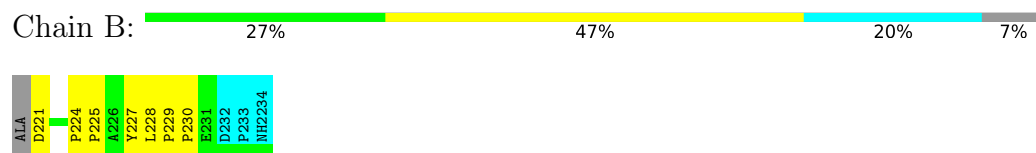
4.2.7 Score per residue for model 7

- Molecule 1: E3 ubiquitin-protein ligase SMURF1

Chain A:

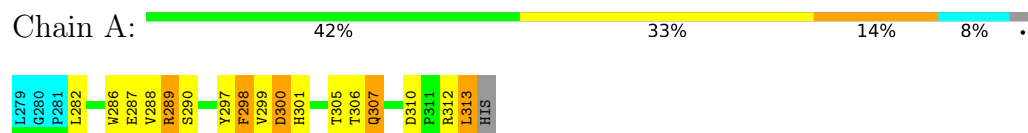


- Molecule 2: Mothers against decapentaplegic homolog 1

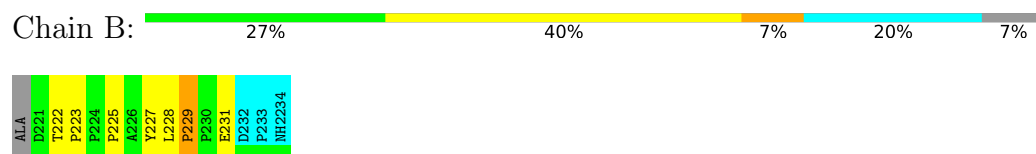


4.2.8 Score per residue for model 8

- Molecule 1: E3 ubiquitin-protein ligase SMURF1



- Molecule 2: Mothers against decapentaplegic homolog 1

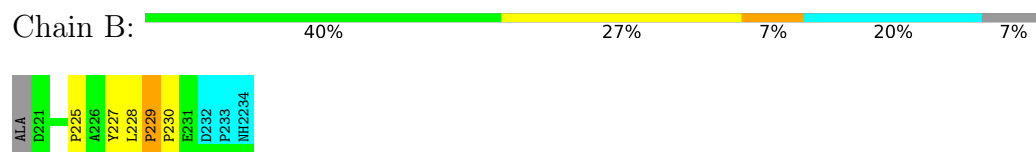


4.2.9 Score per residue for model 9

- Molecule 1: E3 ubiquitin-protein ligase SMURF1



- Molecule 2: Mothers against decapentaplegic homolog 1



4.2.10 Score per residue for model 10

- Molecule 1: E3 ubiquitin-protein ligase SMURF1

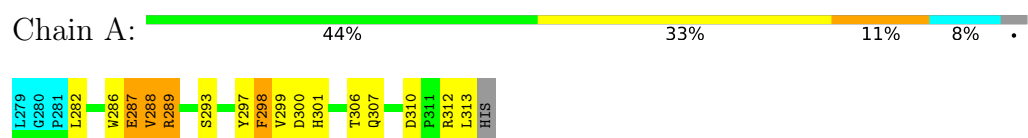


- Molecule 2: Mothers against decapentaplegic homolog 1

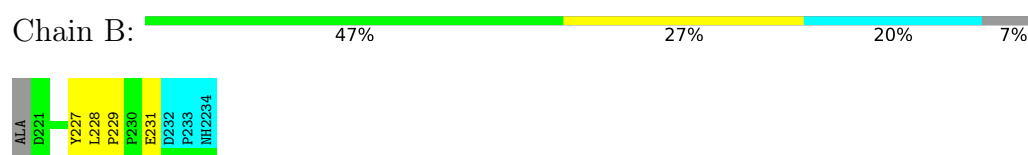


4.2.11 Score per residue for model 11

- Molecule 1: E3 ubiquitin-protein ligase SMURF1



- Molecule 2: Mothers against decapentaplegic homolog 1

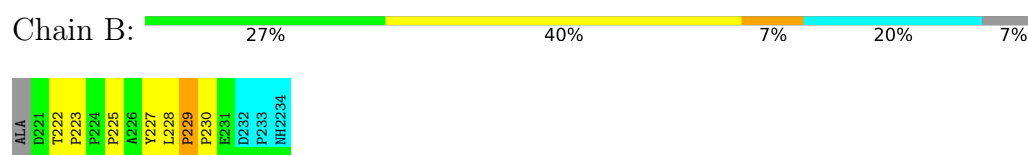


4.2.12 Score per residue for model 12

- Molecule 1: E3 ubiquitin-protein ligase SMURF1



- Molecule 2: Mothers against decapentaplegic homolog 1



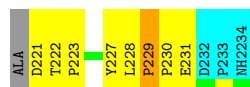
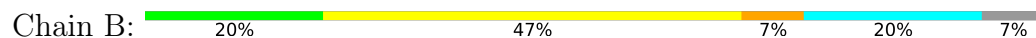
4.2.13 Score per residue for model 13

- Molecule 1: E3 ubiquitin-protein ligase SMURF1





- Molecule 2: Mothers against decapentaplegic homolog 1



4.2.14 Score per residue for model 14

- Molecule 1: E3 ubiquitin-protein ligase SMURF1



- Molecule 2: Mothers against decapentaplegic homolog 1

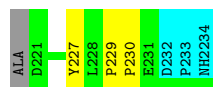


4.2.15 Score per residue for model 15

- Molecule 1: E3 ubiquitin-protein ligase SMURF1

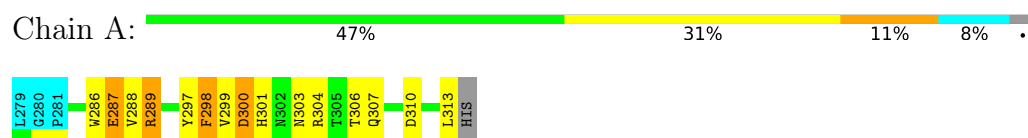


- Molecule 2: Mothers against decapentaplegic homolog 1

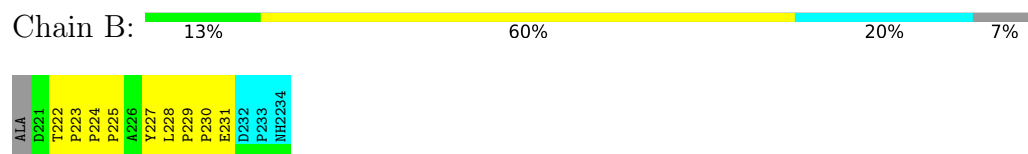


4.2.16 Score per residue for model 16

- Molecule 1: E3 ubiquitin-protein ligase SMURF1



- Molecule 2: Mothers against decapentaplegic homolog 1

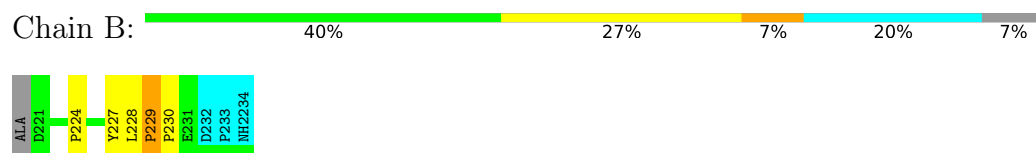


4.2.17 Score per residue for model 17

- Molecule 1: E3 ubiquitin-protein ligase SMURF1



- Molecule 2: Mothers against decapentaplegic homolog 1



4.2.18 Score per residue for model 18

- Molecule 1: E3 ubiquitin-protein ligase SMURF1



- Molecule 2: Mothers against decapentaplegic homolog 1



4.2.19 Score per residue for model 19

- Molecule 1: E3 ubiquitin-protein ligase SMURF1

Chain A: 50% 25% 14% 8% .



- Molecule 2: Mothers against decapentaplegic homolog 1

Chain B: 13% 53% 7% 20% 7%



4.2.20 Score per residue for model 20 (medoid)

- Molecule 1: E3 ubiquitin-protein ligase SMURF1

Chain A: 47% 33% 8% 8% .



- Molecule 2: Mothers against decapentaplegic homolog 1

Chain B: 20% 53% 20% 7%



5 Refinement protocol and experimental data overview

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

Of the 300 calculated structures, 20 were deposited, based on the following criterion: *structures with acceptable covalent geometry*.

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

Software name	Classification	Version
CNS	structure solution	1.3
CNS	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	2
Total number of shifts	260
Number of shifts mapped to atoms	251
Number of unparsed shifts	0
Number of shifts with mapping errors	9
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	40%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NH2

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	0.66±0.03	0±0/274 (0.0± 0.0%)	0.90±0.02	1±0/374 (0.3± 0.0%)
2	B	0.61±0.05	0±0/90 (0.0± 0.0%)	0.98±0.06	0±0/129 (0.0± 0.0%)
All	All	0.65	0/7280 (0.0%)	0.92	20/10060 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.1±0.3
2	B	0.0±0.0	0.9±0.2
All	All	0	21

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	298	PHE	CA-CB-CG	-7.28	106.52	113.80	19	20

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
2	B	229	PRO	Peptide	19
1	A	289	ARG	Sidechain	2

6.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	266	256	255	20±3
2	B	84	77	76	8±3
All	All	7000	6660	6620	415

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 30.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:289:ARG:HD2	1:A:297:TYR:HE1	0.83	1.31	11	17
1:A:289:ARG:HD2	1:A:297:TYR:CE1	0.74	2.17	11	18
1:A:288:VAL:HG23	1:A:296:ILE:HD11	0.74	1.57	2	4
2:B:222:THR:HB	2:B:223:PRO:HD2	0.73	1.58	13	7
1:A:299:VAL:HG12	2:B:227:TYR:HA	0.71	1.61	1	17
1:A:299:VAL:HG21	2:B:228:LEU:O	0.69	1.87	14	16
1:A:298:PHE:HB2	1:A:307:GLN:HB2	0.68	1.64	2	3
1:A:289:ARG:HG2	2:B:230:PRO:HA	0.68	1.64	9	8
1:A:307:GLN:HE21	1:A:307:GLN:HA	0.68	1.48	15	2
1:A:287:GLU:HG2	1:A:301:HIS:CE1	0.66	2.26	17	20
1:A:298:PHE:O	1:A:306:THR:HA	0.65	1.91	7	19
1:A:286:TRP:HE3	1:A:298:PHE:CE1	0.64	2.10	2	20
1:A:298:PHE:CB	1:A:307:GLN:HG2	0.64	2.22	8	1
1:A:286:TRP:CE3	1:A:298:PHE:CE1	0.63	2.87	20	20
1:A:288:VAL:HB	1:A:296:ILE:HD11	0.61	1.71	18	2
1:A:306:THR:HB	2:B:224:PRO:HB2	0.61	1.73	16	7
1:A:298:PHE:HB2	1:A:307:GLN:HG2	0.61	1.72	8	1
1:A:282:LEU:HD22	1:A:312:ARG:HD2	0.59	1.72	7	2
1:A:299:VAL:HB	2:B:227:TYR:HB2	0.59	1.74	3	8
1:A:313:LEU:H	1:A:313:LEU:HD13	0.59	1.57	19	2
1:A:286:TRP:HE3	1:A:298:PHE:CZ	0.58	2.16	14	20
1:A:301:HIS:HD2	2:B:227:TYR:CD2	0.58	2.17	5	17
1:A:301:HIS:CE1	2:B:229:PRO:HB3	0.58	2.33	13	11
1:A:282:LEU:HB2	1:A:312:ARG:HD3	0.58	1.74	9	2
1:A:305:THR:HG23	1:A:307:GLN:HE22	0.57	1.60	8	1
2:B:222:THR:OG1	2:B:223:PRO:HD2	0.57	1.99	19	5

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:288:VAL:HG12	1:A:298:PHE:CE1	0.55	2.36	18	7
1:A:299:VAL:CG1	2:B:227:TYR:HA	0.55	2.32	18	8
1:A:300:ASP:OD2	1:A:305:THR:HG22	0.54	2.01	8	2
1:A:304:ARG:HG3	2:B:227:TYR:CE1	0.54	2.36	3	2
1:A:301:HIS:HD2	2:B:227:TYR:CD1	0.54	2.20	6	3
1:A:299:VAL:HG23	1:A:299:VAL:O	0.52	2.05	2	11
1:A:300:ASP:OD2	1:A:303:ASN:HB2	0.52	2.05	7	4
1:A:286:TRP:CE3	1:A:298:PHE:CZ	0.51	2.99	4	20
1:A:288:VAL:HG12	1:A:298:PHE:CZ	0.51	2.41	19	6
2:B:222:THR:CB	2:B:223:PRO:HD2	0.51	2.33	13	1
1:A:299:VAL:O	1:A:299:VAL:HG23	0.50	2.07	17	3
1:A:297:TYR:CE2	2:B:225:PRO:HG2	0.50	2.42	2	2
1:A:308:PHE:CZ	2:B:221:ASP:HB2	0.50	2.42	7	1
1:A:289:ARG:HE	2:B:231:GLU:HG2	0.50	1.67	16	3
1:A:300:ASP:O	1:A:304:ARG:HA	0.49	2.07	19	4
1:A:295:ARG:HD3	2:B:221:ASP:OD1	0.49	2.06	3	2
1:A:289:ARG:HE	2:B:231:GLU:CD	0.49	2.16	11	2
1:A:286:TRP:CZ3	1:A:311:PRO:HD3	0.49	2.43	10	1
1:A:306:THR:HG21	2:B:225:PRO:O	0.49	2.07	3	2
1:A:308:PHE:CE2	2:B:222:THR:O	0.49	2.66	1	2
1:A:287:GLU:HG3	2:B:230:PRO:HG3	0.48	1.86	15	3
1:A:310:ASP:HB3	1:A:313:LEU:HD21	0.48	1.84	15	1
1:A:299:VAL:CB	2:B:227:TYR:HB2	0.48	2.37	3	2
1:A:301:HIS:HA	2:B:227:TYR:CE2	0.48	2.43	19	2
1:A:300:ASP:HB3	1:A:305:THR:HG22	0.48	1.84	6	1
1:A:295:ARG:HD3	2:B:221:ASP:OD2	0.48	2.09	6	1
1:A:282:LEU:HD22	1:A:312:ARG:HH11	0.47	1.69	11	1
1:A:289:ARG:HB2	1:A:299:VAL:CG2	0.47	2.40	12	8
1:A:298:PHE:HB2	1:A:307:GLN:O	0.47	2.08	20	4
1:A:310:ASP:OD2	1:A:313:LEU:HG	0.47	2.10	16	2
1:A:297:TYR:CD2	2:B:225:PRO:HD2	0.47	2.44	14	9
1:A:288:VAL:HG21	1:A:312:ARG:NH1	0.46	2.26	2	1
1:A:289:ARG:HB3	1:A:297:TYR:CE1	0.46	2.45	3	2
1:A:287:GLU:HB2	1:A:299:VAL:O	0.46	2.10	4	1
1:A:288:VAL:HG21	1:A:312:ARG:HH11	0.46	1.71	2	1
1:A:306:THR:CG2	2:B:224:PRO:HB2	0.46	2.41	5	2
1:A:313:LEU:N	1:A:313:LEU:HD13	0.45	2.26	6	1
1:A:286:TRP:CE3	1:A:298:PHE:CD1	0.45	3.05	10	3
2:B:222:THR:HB	2:B:223:PRO:CD	0.45	2.42	3	4
1:A:304:ARG:HG3	2:B:227:TYR:CE2	0.45	2.47	2	1
1:A:308:PHE:CZ	2:B:221:ASP:HB3	0.45	2.47	4	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:306:THR:HG22	2:B:224:PRO:HB2	0.45	1.87	3	1
1:A:289:ARG:HB2	1:A:299:VAL:HG22	0.45	1.88	5	1
1:A:310:ASP:HB3	1:A:313:LEU:HD12	0.44	1.87	14	1
1:A:289:ARG:NH2	2:B:231:GLU:O	0.44	2.51	5	2
1:A:285:GLY:HA3	1:A:302:ASN:ND2	0.44	2.28	20	1
1:A:288:VAL:HG23	1:A:288:VAL:O	0.43	2.13	19	3
1:A:313:LEU:HD13	1:A:313:LEU:N	0.43	2.26	19	1
1:A:300:ASP:HB3	1:A:305:THR:HB	0.43	1.90	19	1
1:A:301:HIS:HE1	2:B:229:PRO:HB3	0.43	1.73	14	2
1:A:289:ARG:HB2	1:A:299:VAL:HG21	0.43	1.90	10	1
1:A:301:HIS:NE2	2:B:229:PRO:HA	0.42	2.30	4	1
1:A:301:HIS:CD2	2:B:227:TYR:CE2	0.41	3.08	12	1
1:A:296:ILE:HD13	1:A:297:TYR:N	0.41	2.31	3	3
1:A:310:ASP:OD2	1:A:313:LEU:HD13	0.41	2.16	8	1
1:A:307:GLN:HE21	1:A:307:GLN:CA	0.41	2.28	4	1
2:B:224:PRO:HA	2:B:225:PRO:HD3	0.41	1.82	3	1
2:B:231:GLU:O	2:B:231:GLU:HG3	0.41	2.16	3	1
1:A:301:HIS:HD2	2:B:227:TYR:HD2	0.41	1.57	7	1
1:A:301:HIS:CD2	2:B:227:TYR:CE1	0.40	3.09	6	1
2:B:231:GLU:HG3	2:B:231:GLU:O	0.40	2.17	19	1
1:A:289:ARG:HH21	2:B:231:GLU:CD	0.40	2.25	20	1
1:A:288:VAL:O	1:A:288:VAL:HG23	0.40	2.16	6	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	31/36 (86%)	29±1 (92±2%)	2±1 (8±2%)	0±0 (0±0%)	100	100
2	B	10/15 (67%)	9±1 (92±6%)	1±1 (8±6%)	0±0 (0±0%)	100	100
All	All	820/1020 (80%)	757 (92%)	63 (8%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	30/33 (91%)	25±1 (84±4%)	5±1 (16±4%)	4	40
2	B	10/12 (83%)	10±0 (100±0%)	0±0 (0±0%)	100	100
All	All	800/900 (89%)	702 (88%)	98 (12%)	7	48

All 13 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	300	ASP	19
1	A	289	ARG	18
1	A	288	VAL	16
1	A	287	GLU	8
1	A	296	ILE	8
1	A	313	LEU	7
1	A	305	THR	6
1	A	307	GLN	6
1	A	290	SER	5
1	A	295	ARG	2
1	A	306	THR	1
1	A	293	SER	1
1	A	304	ARG	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

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 40% for the well-defined parts and 38% 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	193
Number of shifts mapped to atoms	189
Number of unparsed shifts	0
Number of shifts with mapping errors	4
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

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

- No matching atom found in the structure. All 4 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	314	HIS	H	7.599	0.003	1
1	A	314	HIS	HA	4.14	0.000	1
1	A	314	HIS	HB2	2.927	0.000	2
1	A	314	HIS	HB3	2.766	0.000	2

7.1.2 Chemical shift referencing

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

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 30%, i.e. 180 atoms were assigned a chemical

shift out of a possible 593. 0 out of 6 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	61/201 (30%)	61/80 (76%)	0/86 (0%)	0/35 (0%)
Sidechain	103/334 (31%)	103/216 (48%)	0/103 (0%)	0/15 (0%)
Aromatic	16/58 (28%)	16/28 (57%)	0/27 (0%)	0/3 (0%)
Overall	180/593 (30%)	180/324 (56%)	0/216 (0%)	0/53 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 29%, i.e. 188 atoms were assigned a chemical shift out of a possible 650. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	65/223 (29%)	65/89 (73%)	0/96 (0%)	0/38 (0%)
Sidechain	107/369 (29%)	107/239 (45%)	0/115 (0%)	0/15 (0%)
Aromatic	16/58 (28%)	16/28 (57%)	0/27 (0%)	0/3 (0%)
Overall	188/650 (29%)	188/356 (53%)	0/238 (0%)	0/56 (0%)

7.1.4 Statistically unusual chemical shifts ⓘ

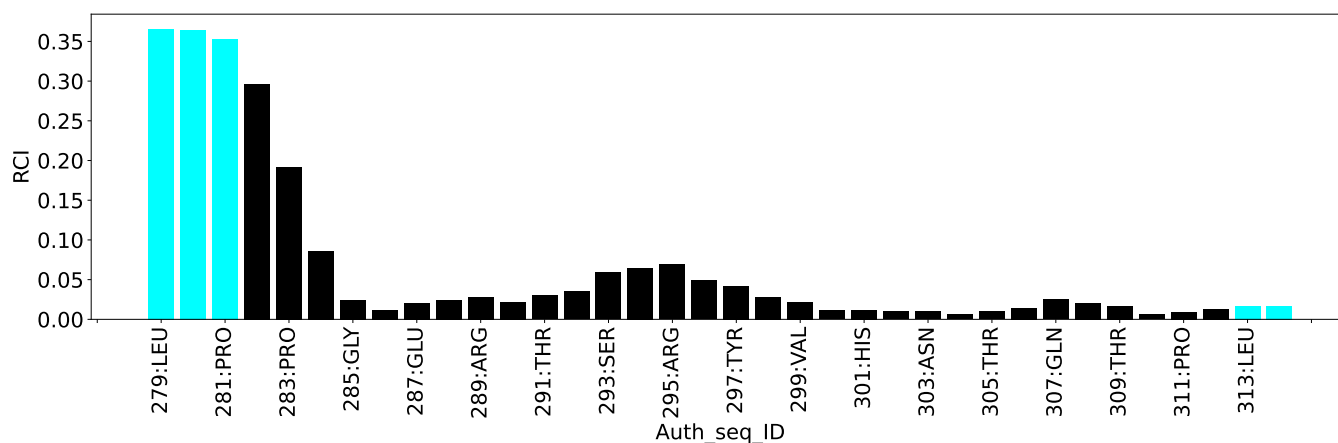
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	300	ASP	HB3	-0.23	1.32 – 4.00	-10.8
1	A	310	ASP	HA	2.51	3.04 – 6.12	-6.7
1	A	311	PRO	HG3	-0.03	0.33 – 3.48	-6.2
1	A	289	ARG	HG3	-0.10	0.15 – 2.94	-5.9
1	A	311	PRO	HG2	0.28	0.41 – 3.45	-5.4
1	A	304	ARG	HA	2.00	2.06 – 6.51	-5.2

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:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *peptide_cs*

7.2.1 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	67
Number of shifts mapped to atoms	62
Number of unparsed shifts	0
Number of shifts with mapping errors	5
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 5 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2	B	220	ALA	H	8.202	0.000	1
2	B	220	ALA	HA	4.049	0.000	1
2	B	220	ALA	HB1	1.133	0.000	1
2	B	220	ALA	HB2	1.133	0.000	1
2	B	220	ALA	HB3	1.133	0.000	1

7.2.2 Chemical shift referencing [i](#)

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

7.2.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 10%, i.e. 58 atoms were assigned a chemical shift out of a possible 593. 0 out of 6 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	16/201 (8%)	16/80 (20%)	0/86 (0%)	0/35 (0%)
Sidechain	40/334 (12%)	40/216 (19%)	0/103 (0%)	0/15 (0%)
Aromatic	2/58 (3%)	2/28 (7%)	0/27 (0%)	0/3 (0%)
Overall	58/593 (10%)	58/324 (18%)	0/216 (0%)	0/53 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 10%, i.e. 62 atoms were assigned a chemical shift out of a possible 650. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	18/223 (8%)	18/89 (20%)	0/96 (0%)	0/38 (0%)
Sidechain	42/369 (11%)	42/239 (18%)	0/115 (0%)	0/15 (0%)
Aromatic	2/58 (3%)	2/28 (7%)	0/27 (0%)	0/3 (0%)
Overall	62/650 (10%)	62/356 (17%)	0/238 (0%)	0/56 (0%)

7.2.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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 B:

