



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 06:56 AM UTC

PDB ID : 2MAK / pdb_00002mak
BMRB ID : 19363
Title : Solution structure of the STIM1 CC1-CC2 homodimer in complex with two
Orai1 C-terminal domains.
Authors : Stathopoulos, P.B.; Ikura, M.
Deposited on : 2013-07-12

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

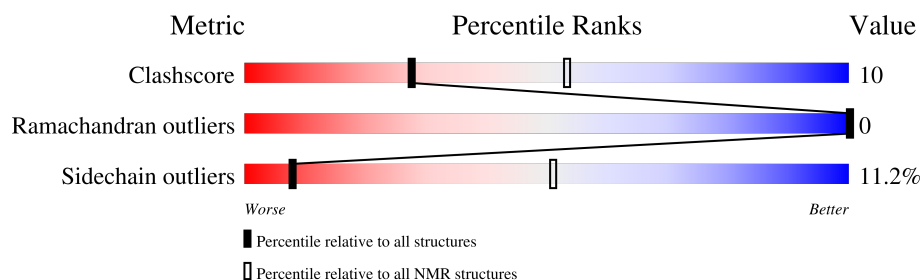
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 43%.

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	82	61% 17% 18%
1	C	82	61% 16% 5% 18%
2	B	23	61% 30% 9%
2	D	23	57% 30% 13%

2 Ensemble composition and analysis

This entry contains 20 models. Model 3 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:316-A:382, B:0-B:0, B:272-B:291, C:316-C:382, D:0-D:0, D:272-D:290 (175)	0.54	3

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 4 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3454 atoms, of which 1714 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Stromal interaction molecule 1.

Mol	Chain	Residues	Atoms						Trace
1	A	82	Total	C	H	N	O	S	0
			1372	428	689	123	131	1	
1	C	82	Total	C	H	N	O	S	0
			1372	428	689	123	131	1	

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q13586
A	-4	SER	-	expression tag	UNP Q13586
A	-3	HIS	-	expression tag	UNP Q13586
A	-2	MET	-	expression tag	UNP Q13586
A	-1	ALA	-	expression tag	UNP Q13586
A	0	SER	-	expression tag	UNP Q13586
C	-5	GLY	-	expression tag	UNP Q13586
C	-4	SER	-	expression tag	UNP Q13586
C	-3	HIS	-	expression tag	UNP Q13586
C	-2	MET	-	expression tag	UNP Q13586
C	-1	ALA	-	expression tag	UNP Q13586
C	0	SER	-	expression tag	UNP Q13586

- Molecule 2 is a protein called Calcium release-activated calcium channel protein 1.

Mol	Chain	Residues	Atoms					Trace
2	B	23	Total	C	H	N	O	0
			355	111	168	36	40	
2	D	23	Total	C	H	N	O	0
			355	111	168	36	40	

There are 4 discrepancies between the modelled and reference sequences:

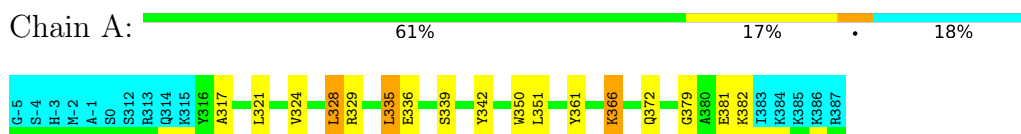
Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP Q96D31
B	0	SER	-	expression tag	UNP Q96D31
D	-1	GLY	-	expression tag	UNP Q96D31
D	0	SER	-	expression tag	UNP Q96D31

4 Residue-property plots

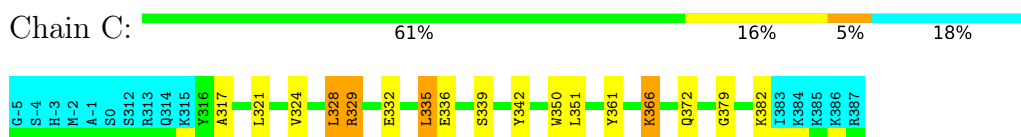
4.1 Average score per residue in the NMR ensemble

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: Stromal interaction molecule 1



- Molecule 1: Stromal interaction molecule 1



- Molecule 2: Calcium release-activated calcium channel protein 1



- Molecule 2: Calcium release-activated calcium channel protein 1

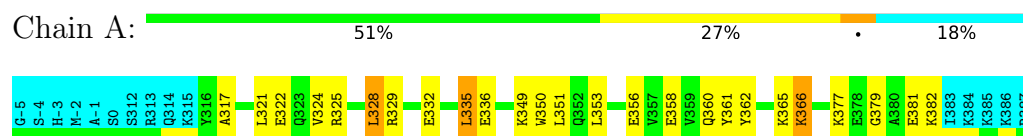


4.2 Scores per residue for each member of the ensemble

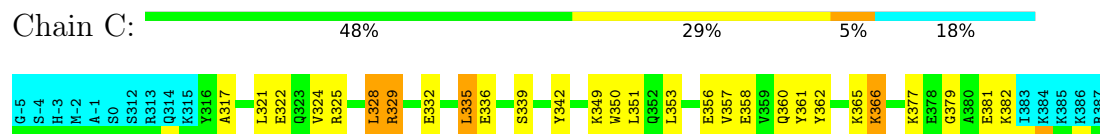
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

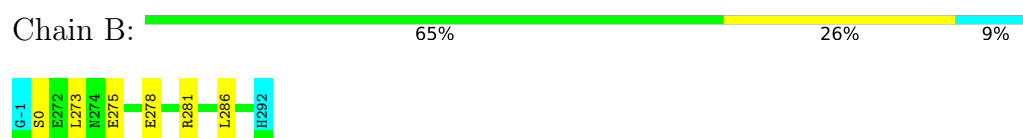
- Molecule 1: Stromal interaction molecule 1



- Molecule 1: Stromal interaction molecule 1



- Molecule 2: Calcium release-activated calcium channel protein 1

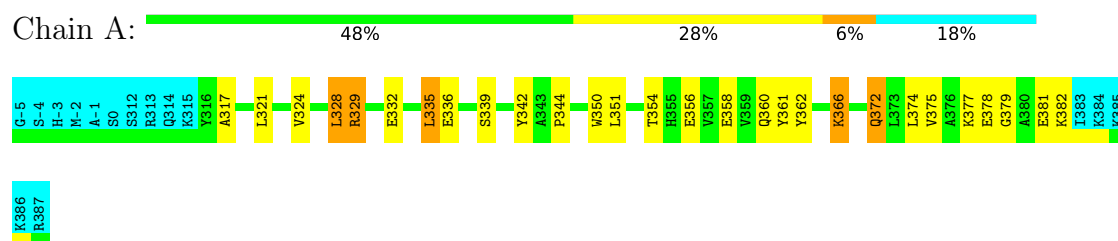


- Molecule 2: Calcium release-activated calcium channel protein 1

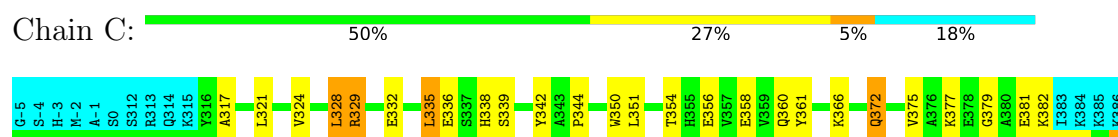


4.2.2 Score per residue for model 2

- Molecule 1: Stromal interaction molecule 1



- Molecule 1: Stromal interaction molecule 1





- Molecule 2: Calcium release-activated calcium channel protein 1

Chain B: 57% 35% 9%



- Molecule 2: Calcium release-activated calcium channel protein 1

Chain D: 43% 39% 13%



4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Stromal interaction molecule 1

Chain A: 55% 22% 5% 18%



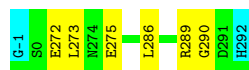
- Molecule 1: Stromal interaction molecule 1

Chain C: 55% 23% 18%



- Molecule 2: Calcium release-activated calcium channel protein 1

Chain B: 65% 26% 9%



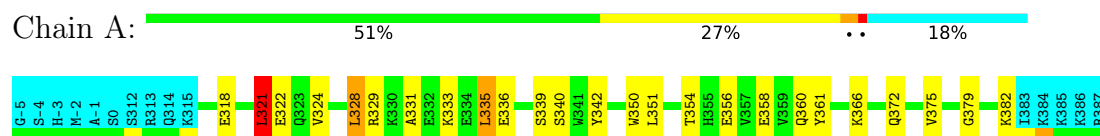
- Molecule 2: Calcium release-activated calcium channel protein 1

Chain D: 74% 13% 13%

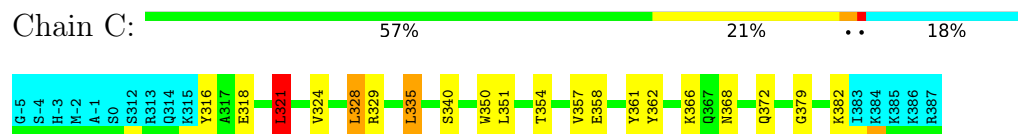


4.2.4 Score per residue for model 4

- Molecule 1: Stromal interaction molecule 1



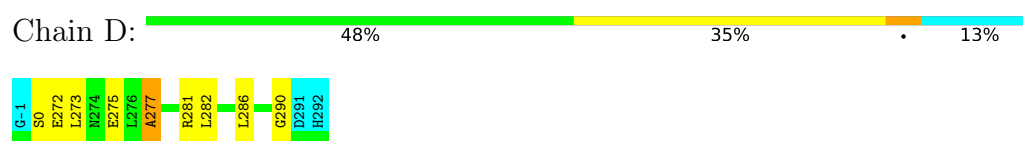
- Molecule 1: Stromal interaction molecule 1



- Molecule 2: Calcium release-activated calcium channel protein 1

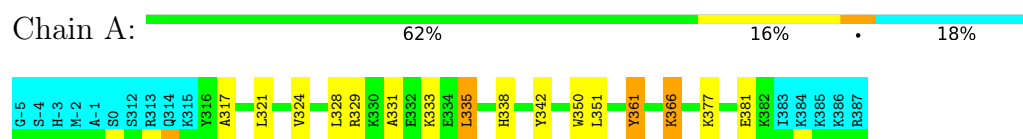


- Molecule 2: Calcium release-activated calcium channel protein 1

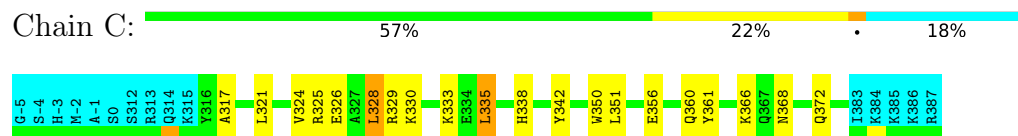


4.2.5 Score per residue for model 5

- Molecule 1: Stromal interaction molecule 1



- Molecule 1: Stromal interaction molecule 1



- Molecule 2: Calcium release-activated calcium channel protein 1





- Molecule 2: Calcium release-activated calcium channel protein 1

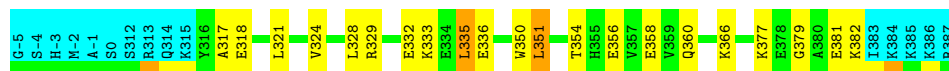


4.2.6 Score per residue for model 6

- Molecule 1: Stromal interaction molecule 1



- Molecule 1: Stromal interaction molecule 1



- Molecule 2: Calcium release-activated calcium channel protein 1



- Molecule 2: Calcium release-activated calcium channel protein 1

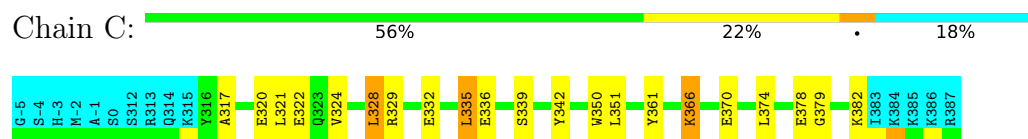


4.2.7 Score per residue for model 7

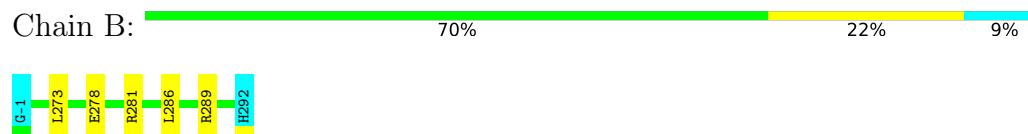
- Molecule 1: Stromal interaction molecule 1



- Molecule 1: Stromal interaction molecule 1



- Molecule 2: Calcium release-activated calcium channel protein 1

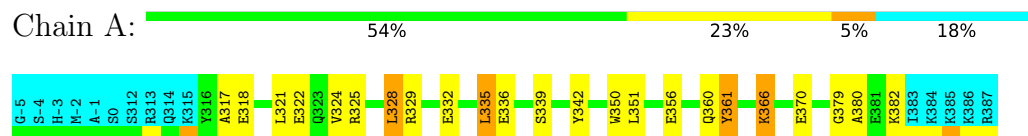


- Molecule 2: Calcium release-activated calcium channel protein 1

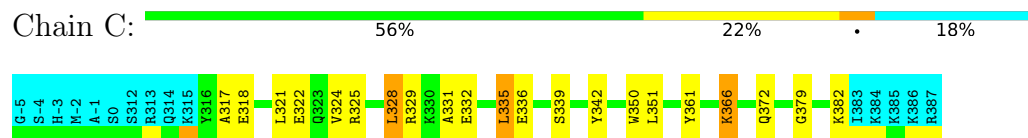


4.2.8 Score per residue for model 8

- Molecule 1: Stromal interaction molecule 1



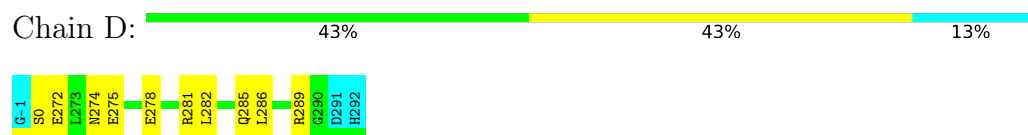
- Molecule 1: Stromal interaction molecule 1



- Molecule 2: Calcium release-activated calcium channel protein 1

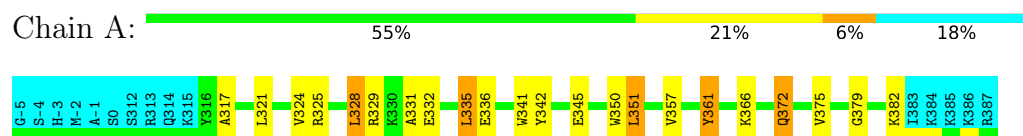


- Molecule 2: Calcium release-activated calcium channel protein 1

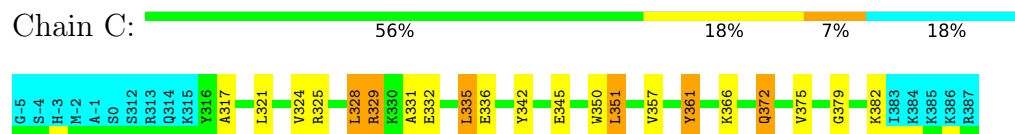


4.2.9 Score per residue for model 9

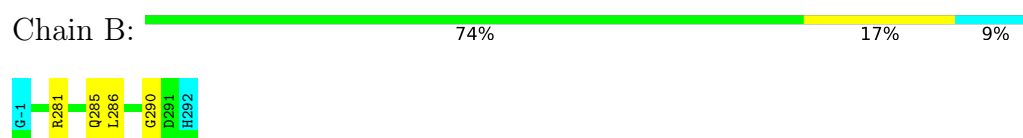
- Molecule 1: Stromal interaction molecule 1



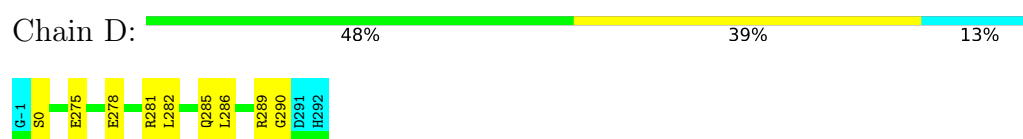
- Molecule 1: Stromal interaction molecule 1



- Molecule 2: Calcium release-activated calcium channel protein 1

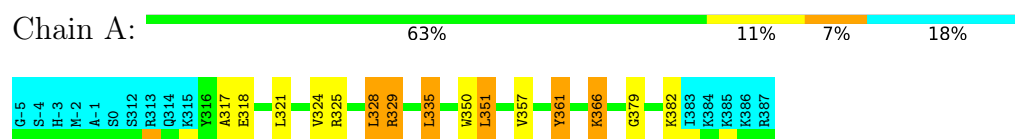


- Molecule 2: Calcium release-activated calcium channel protein 1

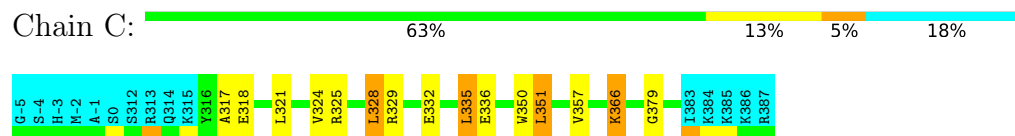


4.2.10 Score per residue for model 10

- Molecule 1: Stromal interaction molecule 1

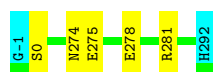


- Molecule 1: Stromal interaction molecule 1



- Molecule 2: Calcium release-activated calcium channel protein 1





- Molecule 2: Calcium release-activated calcium channel protein 1

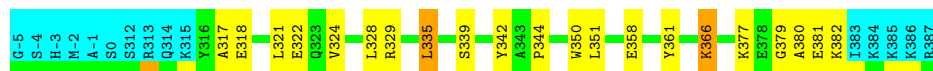


4.2.11 Score per residue for model 11

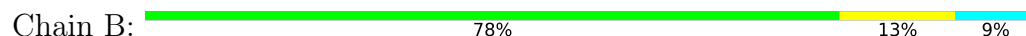
- Molecule 1: Stromal interaction molecule 1



- Molecule 1: Stromal interaction molecule 1



- Molecule 2: Calcium release-activated calcium channel protein 1



- Molecule 2: Calcium release-activated calcium channel protein 1

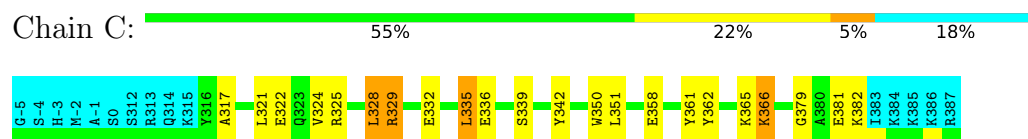


4.2.12 Score per residue for model 12

- Molecule 1: Stromal interaction molecule 1



- Molecule 1: Stromal interaction molecule 1



- Molecule 2: Calcium release-activated calcium channel protein 1

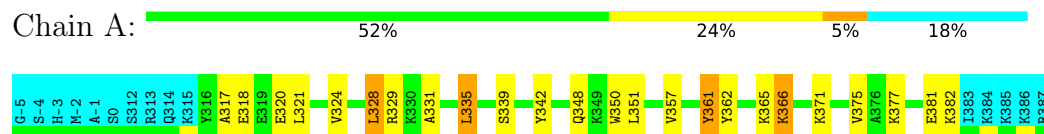


- Molecule 2: Calcium release-activated calcium channel protein 1

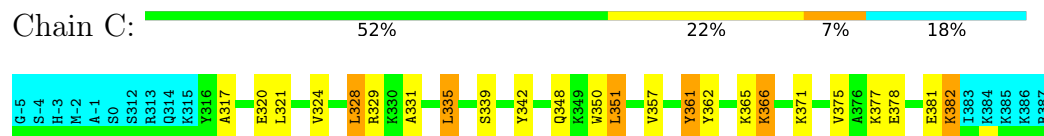


4.2.13 Score per residue for model 13

- Molecule 1: Stromal interaction molecule 1



- Molecule 1: Stromal interaction molecule 1



- Molecule 2: Calcium release-activated calcium channel protein 1

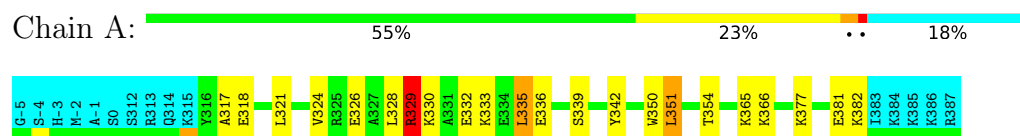


- Molecule 2: Calcium release-activated calcium channel protein 1

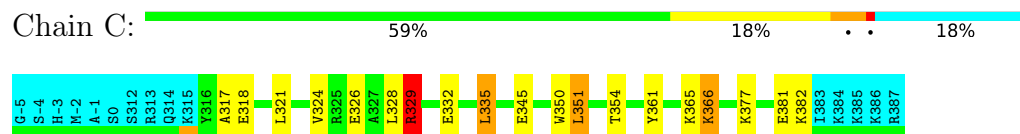


4.2.14 Score per residue for model 14

- Molecule 1: Stromal interaction molecule 1



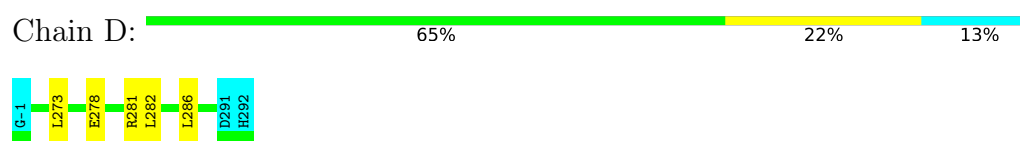
- Molecule 1: Stromal interaction molecule 1



- Molecule 2: Calcium release-activated calcium channel protein 1

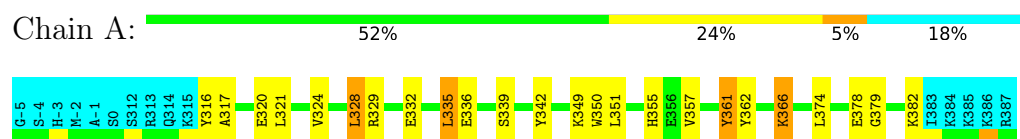


- Molecule 2: Calcium release-activated calcium channel protein 1

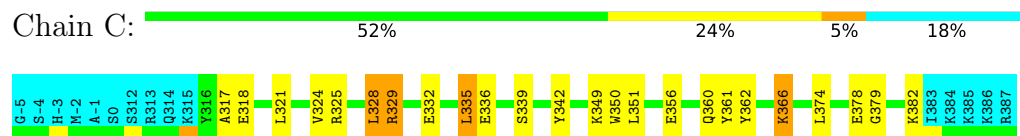


4.2.15 Score per residue for model 15

- Molecule 1: Stromal interaction molecule 1



- Molecule 1: Stromal interaction molecule 1

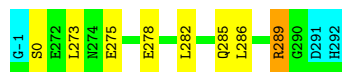


- Molecule 2: Calcium release-activated calcium channel protein 1





- Molecule 2: Calcium release-activated calcium channel protein 1



4.2.16 Score per residue for model 16

- Molecule 1: Stromal interaction molecule 1



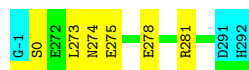
- Molecule 1: Stromal interaction molecule 1



- Molecule 2: Calcium release-activated calcium channel protein 1

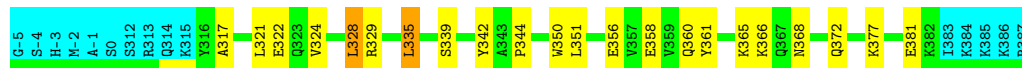


- Molecule 2: Calcium release-activated calcium channel protein 1



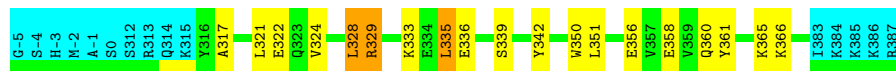
4.2.17 Score per residue for model 17

- Molecule 1: Stromal interaction molecule 1



- Molecule 1: Stromal interaction molecule 1

Chain C: 



- Molecule 2: Calcium release-activated calcium channel protein 1

Chain B: 



- Molecule 2: Calcium release-activated calcium channel protein 1

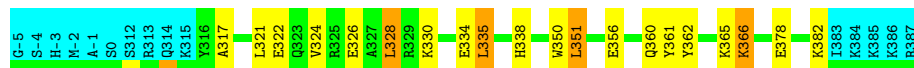
Chain D: 



4.2.18 Score per residue for model 18

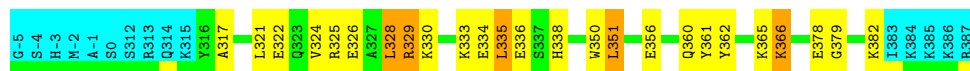
- Molecule 1: Stromal interaction molecule 1

Chain A: 



- Molecule 1: Stromal interaction molecule 1

Chain C: 



- Molecule 2: Calcium release-activated calcium channel protein 1

Chain B: 



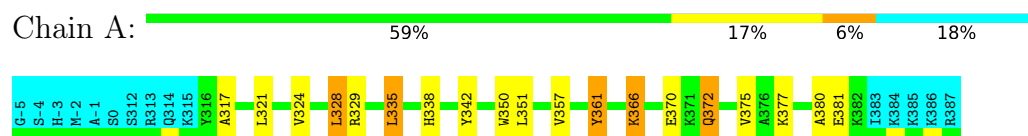
- Molecule 2: Calcium release-activated calcium channel protein 1

Chain D: 

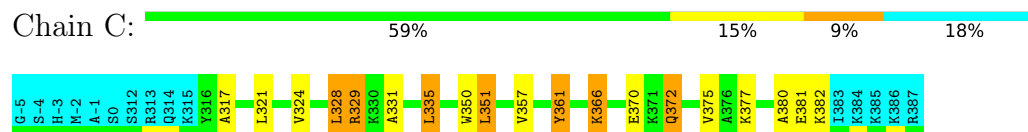


4.2.19 Score per residue for model 19

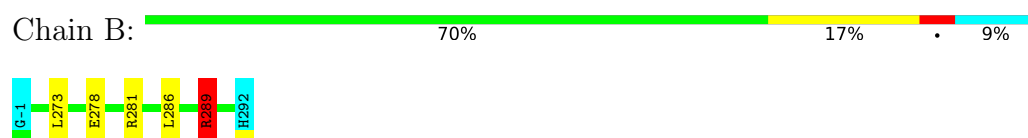
- Molecule 1: Stromal interaction molecule 1



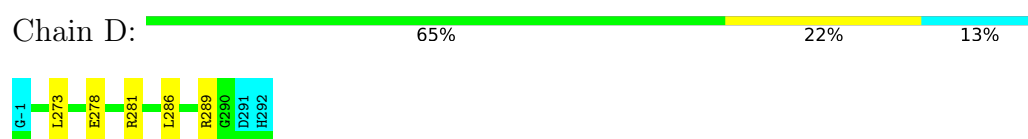
- Molecule 1: Stromal interaction molecule 1



- Molecule 2: Calcium release-activated calcium channel protein 1

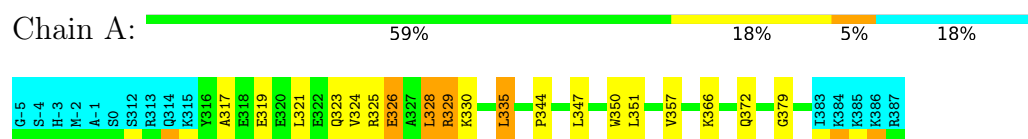


- Molecule 2: Calcium release-activated calcium channel protein 1

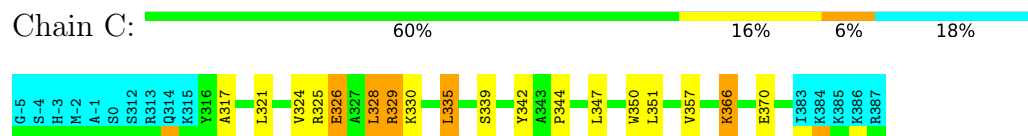


4.2.20 Score per residue for model 20

- Molecule 1: Stromal interaction molecule 1



- Molecule 1: Stromal interaction molecule 1



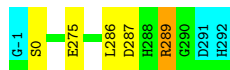
- Molecule 2: Calcium release-activated calcium channel protein 1





- Molecule 2: Calcium release-activated calcium channel protein 1

Chain D:
65% 17% • 13%



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
TALOS	geometry optimization	
CYANA	structure solution	3.0
CNS	refinement	
CNS	geometry optimization	

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	1245
Number of shifts mapped to atoms	1245
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	43%

6 Model quality

6.1 Standard geometry

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	1.05±0.04	0±0/573 (0.0± 0.1%)	1.03±0.03	0±0/772 (0.0± 0.0%)
1	C	1.05±0.04	0±0/573 (0.0± 0.1%)	1.03±0.03	0±0/772 (0.0± 0.0%)
2	B	1.28±0.04	0±0/174 (0.0± 0.1%)	1.10±0.05	0±0/234 (0.0± 0.0%)
2	D	1.26±0.05	0±0/166 (0.0± 0.1%)	1.11±0.05	0±0/223 (0.0± 0.0%)
All	All	1.11	7/29720 (0.0%)	1.05	3/40020 (0.0%)

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	C	0.0±0.0	0.1±0.4
1	A	0.0±0.0	0.1±0.3
2	B	0.0±0.0	0.1±0.4
2	D	0.0±0.0	0.1±0.4
All	All	0	11

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	372	GLN	N-CA	-6.52	1.38	1.46	20	1
1	C	372	GLN	N-CA	-5.30	1.40	1.46	8	1
1	A	322	GLU	C-O	5.15	1.30	1.24	4	1
2	B	277	ALA	CA-C	-5.14	1.46	1.52	4	1
1	C	365	LYS	C-O	-5.13	1.17	1.24	16	1
2	D	277	ALA	CA-C	-5.03	1.46	1.52	4	1
1	A	365	LYS	C-O	-5.03	1.17	1.24	16	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)	Models	
								Worst	Total
1	C	321	LEU	N-CA-CB	5.63	118.49	110.16	4	1
1	C	372	GLN	N-CA-CB	-5.35	102.25	110.01	8	1
1	A	321	LEU	N-CA-CB	5.26	117.95	110.16	4	1

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	289	ARG	Sidechain	3
1	C	329	ARG	Sidechain	3
2	D	289	ARG	Sidechain	3
1	A	329	ARG	Sidechain	2

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	562	551	551	13 $\pm$ 3
1	C	562	551	551	13 $\pm$ 3
2	B	172	156	156	3 $\pm$ 1
2	D	164	152	152	3 $\pm$ 1
All	All	29200	28200	28200	559

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 10.

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

Atom-1	Atom-2	Clash($\text{\AA}$)	Distance($\text{\AA}$)	Models	
				Worst	Total
1:A:358:GLU:HA	1:A:361:TYR:CE2	0.74	2.18	12	7
1:C:358:GLU:HA	1:C:361:TYR:CE2	0.73	2.19	17	7
1:A:335:LEU:HG	1:A:350:TRP:CG	0.66	2.25	7	20
1:A:317:ALA:O	1:A:321:LEU:HG	0.64	1.92	7	19
1:C:372:GLN:HA	1:C:375:VAL:HG12	0.63	1.69	19	4
1:C:317:ALA:O	1:C:321:LEU:HG	0.62	1.93	9	19
1:A:320:GLU:HG3	1:C:324:VAL:HG23	0.62	1.72	7	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:335:LEU:HG	1:C:350:TRP:CG	0.61	2.30	17	20
2:D:0:SER:O	2:D:275:GLU:HG2	0.59	1.98	10	15
1:A:326:GLU:O	1:A:330:LYS:HB2	0.59	1.98	18	3
1:A:377:LYS:O	1:A:381:GLU:HG2	0.59	1.98	14	10
1:A:372:GLN:HA	1:A:375:VAL:HG12	0.58	1.74	9	5
1:C:332:GLU:O	1:C:336:GLU:HG2	0.58	1.98	12	10
1:A:366:LYS:O	1:A:370:GLU:HG2	0.57	1.98	7	3
2:B:277:ALA:O	2:B:281:ARG:HG2	0.57	1.99	4	1
2:B:0:SER:O	2:B:275:GLU:HG2	0.57	2.00	18	12
1:C:326:GLU:O	1:C:330:LYS:HB2	0.57	1.98	18	3
1:C:349:LYS:O	1:C:353:LEU:HG	0.57	1.99	1	1
1:C:339:SER:HA	1:C:342:TYR:CE1	0.56	2.35	2	12
1:A:329:ARG:N	1:A:329:ARG:HD2	0.56	2.15	14	4
1:C:324:VAL:O	1:C:328:LEU:HB3	0.56	2.00	14	20
1:A:324:VAL:O	1:A:328:LEU:HB3	0.56	2.00	14	20
1:C:377:LYS:O	1:C:381:GLU:HG2	0.56	2.00	14	7
2:D:277:ALA:O	2:D:281:ARG:HG2	0.56	2.00	4	1
1:C:329:ARG:HD2	1:C:329:ARG:N	0.56	2.16	14	5
1:A:332:GLU:O	1:A:336:GLU:HG2	0.56	2.00	12	9
1:A:324:VAL:HG11	1:C:324:VAL:HG21	0.56	1.77	7	1
2:B:285:GLN:O	2:B:289:ARG:HB2	0.55	2.02	12	3
1:A:349:LYS:O	1:A:353:LEU:HG	0.55	2.02	1	1
1:C:362:TYR:O	1:C:366:LYS:HD2	0.54	2.02	18	6
1:C:371:LYS:O	1:C:375:VAL:HG23	0.54	2.02	13	1
1:C:366:LYS:O	1:C:370:GLU:HG2	0.54	2.03	7	3
1:A:321:LEU:HD13	1:C:357:VAL:HG21	0.53	1.79	9	5
1:A:339:SER:HA	1:A:342:TYR:CE1	0.53	2.38	3	11
2:B:278:GLU:O	2:B:282:LEU:HG	0.53	2.04	17	5
1:C:378:GLU:O	1:C:382:LYS:HD3	0.53	2.04	18	1
1:A:329:ARG:NE	1:C:361:TYR:HB2	0.52	2.20	19	2
2:B:278:GLU:O	2:B:281:ARG:HG2	0.52	2.04	2	14
1:A:357:VAL:HG21	1:C:321:LEU:HD13	0.52	1.80	9	4
1:A:333:LYS:HA	1:A:336:GLU:CD	0.52	2.29	4	1
2:D:278:GLU:O	2:D:281:ARG:HG2	0.52	2.05	2	13
2:D:278:GLU:O	2:D:282:LEU:HG	0.51	2.04	8	6
1:C:378:GLU:O	1:C:382:LYS:HG3	0.51	2.05	7	1
1:A:361:TYR:HB2	1:C:329:ARG:NE	0.51	2.20	10	1
1:A:333:LYS:HA	1:A:336:GLU:OE2	0.51	2.05	14	1
1:C:362:TYR:CZ	1:C:366:LYS:HD3	0.51	2.40	3	1
1:C:366:LYS:HA	1:C:366:LYS:HE2	0.50	1.82	7	5
1:A:357:VAL:HG13	1:C:325:ARG:HB2	0.50	1.83	10	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:378:GLU:HB3	1:A:382:LYS:HE2	0.50	1.82	7	1
1:A:335:LEU:HG	1:A:350:TRP:CD2	0.50	2.42	20	15
1:A:324:VAL:HG21	1:C:324:VAL:HG11	0.50	1.83	7	1
1:A:361:TYR:HB2	1:C:329:ARG:HE	0.50	1.66	10	1
1:A:329:ARG:HE	1:C:361:TYR:HB2	0.50	1.66	19	2
1:A:340:SER:HA	2:B:290:GLY:CA	0.50	2.36	4	1
1:A:366:LYS:HA	1:A:366:LYS:HE2	0.50	1.84	19	5
1:A:351:LEU:HG	2:B:281:ARG:HB3	0.50	1.83	9	3
1:A:319:GLU:O	1:A:323:GLN:HG2	0.50	2.07	20	1
2:B:289:ARG:HD3	2:B:291:ASP:O	0.49	2.07	12	1
1:A:374:LEU:O	1:A:378:GLU:HG2	0.49	2.07	2	1
1:A:338:HIS:HB3	1:A:342:TYR:CE2	0.49	2.43	5	2
1:C:338:HIS:HB3	1:C:342:TYR:CE2	0.49	2.43	5	1
1:A:362:TYR:O	1:A:366:LYS:HD2	0.49	2.06	3	6
1:A:362:TYR:CZ	1:A:366:LYS:HD3	0.49	2.42	3	1
1:A:325:ARG:HB2	1:C:357:VAL:HG13	0.49	1.83	10	1
2:D:285:GLN:O	2:D:289:ARG:HB2	0.49	2.06	12	3
2:D:0:SER:O	2:D:274:ASN:HB3	0.49	2.07	10	1
2:B:281:ARG:O	2:B:285:GLN:HG2	0.49	2.08	11	3
1:A:361:TYR:O	1:A:365:LYS:HG2	0.49	2.08	13	3
1:A:329:ARG:HD3	1:C:361:TYR:HB2	0.48	1.85	2	1
1:A:371:LYS:O	1:A:375:VAL:HG23	0.48	2.08	13	1
1:A:356:GLU:O	1:A:360:GLN:HG2	0.48	2.09	6	7
1:C:335:LEU:HG	1:C:350:TRP:CD1	0.48	2.43	7	1
1:C:333:LYS:O	1:C:336:GLU:HG2	0.48	2.09	17	1
1:C:322:GLU:O	1:C:325:ARG:HB3	0.48	2.09	8	5
1:C:356:GLU:O	1:C:360:GLN:HG2	0.48	2.09	6	7
1:A:329:ARG:HH11	1:A:329:ARG:HG3	0.48	1.69	14	2
1:C:379:GLY:O	1:C:382:LYS:HB3	0.48	2.09	9	1
2:B:0:SER:O	2:B:274:ASN:HB3	0.48	2.09	10	1
1:A:342:TYR:O	2:B:290:GLY:HA3	0.47	2.08	3	4
1:A:324:VAL:HG23	1:C:320:GLU:HG3	0.47	1.85	7	1
1:A:379:GLY:O	1:A:382:LYS:HB3	0.47	2.08	9	2
1:A:329:ARG:HH12	1:A:332:GLU:CD	0.47	2.17	14	1
1:C:351:LEU:HG	2:D:281:ARG:HB3	0.47	1.86	9	5
1:A:322:GLU:O	1:A:325:ARG:HB3	0.47	2.09	8	3
1:C:361:TYR:O	1:C:365:LYS:HG2	0.47	2.09	13	3
1:C:329:ARG:HH11	1:C:329:ARG:HG3	0.47	1.69	14	1
1:A:361:TYR:HB2	1:C:329:ARG:HD3	0.46	1.86	9	5
1:A:368:ASN:O	1:A:372:GLN:HG3	0.46	2.10	17	1
1:A:324:VAL:HG11	1:C:324:VAL:HG11	0.46	1.87	4	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:354:THR:O	1:A:358:GLU:HB2	0.46	2.10	6	1
1:C:368:ASN:O	1:C:372:GLN:HG2	0.46	2.11	4	2
1:C:342:TYR:O	2:D:290:GLY:HA3	0.46	2.11	3	4
1:A:334:GLU:O	1:A:338:HIS:HB2	0.46	2.11	18	2
1:C:361:TYR:C	1:C:361:TYR:CD1	0.46	2.94	18	1
1:C:340:SER:HA	2:D:290:GLY:CA	0.46	2.41	4	1
1:A:365:LYS:HD2	1:C:329:ARG:CZ	0.46	2.40	12	1
1:C:374:LEU:O	1:C:378:GLU:HG2	0.45	2.10	7	2
1:A:351:LEU:HG	2:B:281:ARG:CB	0.45	2.42	14	3
1:C:348:GLN:HA	1:C:348:GLN:OE1	0.45	2.11	13	1
1:A:379:GLY:HA3	2:D:287:ASP:OD2	0.45	2.10	20	1
1:A:358:GLU:HA	1:A:361:TYR:CD2	0.45	2.46	17	4
1:A:321:LEU:HD12	1:A:322:GLU:N	0.45	2.27	8	5
1:C:381:GLU:HG3	1:C:382:LYS:HD3	0.45	1.88	12	1
1:C:351:LEU:HG	2:D:281:ARG:CB	0.45	2.41	14	5
1:C:361:TYR:CD1	1:C:362:TYR:N	0.45	2.85	4	2
1:C:378:GLU:C	1:C:382:LYS:HD3	0.44	2.37	18	1
1:A:357:VAL:HG22	1:C:325:ARG:NH2	0.44	2.27	20	1
1:A:354:THR:HA	1:C:321:LEU:HD21	0.44	1.89	14	2
1:C:358:GLU:HA	1:C:361:TYR:CD2	0.44	2.47	4	4
1:C:366:LYS:HA	1:C:366:LYS:CE	0.44	2.42	19	3
1:C:361:TYR:CD1	1:C:361:TYR:C	0.44	2.96	9	3
1:C:354:THR:O	1:C:358:GLU:HB2	0.44	2.12	6	1
2:B:281:ARG:HG3	2:B:282:LEU:N	0.44	2.28	4	1
2:D:281:ARG:HG3	2:D:282:LEU:N	0.44	2.28	4	1
1:C:374:LEU:O	1:C:378:GLU:HG3	0.43	2.12	15	1
1:A:331:ALA:O	1:A:335:LEU:HB2	0.43	2.13	13	4
1:A:378:GLU:HA	1:A:381:GLU:OE2	0.43	2.14	12	1
1:A:329:ARG:NH2	1:C:365:LYS:HE3	0.43	2.28	14	1
2:B:272:GLU:OE2	2:B:276:LEU:HD12	0.43	2.14	18	1
1:A:316:TYR:O	1:A:320:GLU:HG2	0.43	2.14	15	1
1:A:329:ARG:CZ	1:C:365:LYS:HE3	0.43	2.44	17	1
1:A:335:LEU:HG	1:A:350:TRP:CD1	0.43	2.49	7	1
1:A:378:GLU:O	1:A:382:LYS:HG3	0.43	2.13	7	2
1:A:344:PRO:HB3	2:B:289:ARG:HG2	0.42	1.90	2	3
1:A:321:LEU:HD21	1:C:354:THR:HA	0.42	1.91	14	3
1:C:344:PRO:HB3	2:D:289:ARG:HG2	0.42	1.90	20	3
2:B:287:ASP:OD2	1:C:379:GLY:HA3	0.42	2.14	4	1
1:C:325:ARG:O	1:C:329:ARG:HB2	0.42	2.13	20	1
1:C:331:ALA:O	1:C:335:LEU:HB2	0.42	2.14	9	5
1:A:361:TYR:CD1	1:A:361:TYR:C	0.42	2.97	11	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:365:LYS:HE3	1:C:329:ARG:NH2	0.42	2.30	14	2
1:A:366:LYS:HZ2	2:D:272:GLU:CD	0.42	2.23	2	1
1:A:329:ARG:HG2	1:C:364:ILE:HG21	0.42	1.92	3	1
1:C:334:GLU:O	1:C:338:HIS:HB2	0.42	2.15	18	1
2:D:281:ARG:O	2:D:285:GLN:HG2	0.42	2.14	11	3
1:A:360:GLN:O	1:A:364:ILE:HG13	0.42	2.15	3	1
1:A:331:ALA:HB2	1:C:316:TYR:CE1	0.42	2.49	4	1
1:A:374:LEU:O	1:A:378:GLU:HG3	0.42	2.15	15	1
1:A:348:GLN:HA	1:A:348:GLN:OE1	0.42	2.15	13	1
1:A:342:TYR:CE1	1:A:346:ALA:HB3	0.42	2.50	16	1
1:A:381:GLU:HG3	1:A:382:LYS:HD3	0.42	1.92	16	1
1:A:321:LEU:HD23	1:C:328:LEU:HD13	0.42	1.92	17	1
1:A:366:LYS:HA	1:A:366:LYS:CE	0.42	2.45	19	2
1:C:338:HIS:CD2	1:C:342:TYR:HE2	0.42	2.33	2	1
1:A:325:ARG:O	1:A:329:ARG:HB2	0.42	2.15	20	1
2:B:272:GLU:HA	2:B:275:GLU:CG	0.41	2.45	3	1
1:C:339:SER:HA	1:C:342:TYR:CZ	0.41	2.50	8	1
1:C:333:LYS:HA	1:C:336:GLU:OE2	0.41	2.16	18	1
1:A:361:TYR:CD1	1:A:362:TYR:N	0.41	2.88	2	1
1:C:321:LEU:HD12	1:C:322:GLU:N	0.41	2.29	7	5
1:A:325:ARG:NH2	1:C:357:VAL:HG22	0.41	2.31	20	1
1:C:329:ARG:HH12	1:C:332:GLU:CD	0.41	2.22	14	1
1:A:321:LEU:C	1:C:357:VAL:HG11	0.41	2.41	4	1
1:C:378:GLU:O	1:C:382:LYS:HE3	0.41	2.16	13	1
2:B:272:GLU:CD	1:C:366:LYS:HZ2	0.41	2.23	14	1
1:A:355:HIS:NE2	2:B:274:ASN:HA	0.41	2.31	15	1
1:A:336:GLU:CD	1:C:372:GLN:HE21	0.41	2.23	3	1
1:A:354:THR:HA	1:C:321:LEU:CD2	0.40	2.47	2	1
1:A:321:LEU:CD2	1:C:354:THR:HA	0.40	2.46	2	2
1:A:372:GLN:HA	1:A:375:VAL:CG1	0.40	2.47	6	1
1:A:358:GLU:CD	1:C:365:LYS:HZ3	0.40	2.25	12	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	67/82 (82%)	66±1 (99±1%)	1±1 (1±1%)	0±0 (0±0%)	100	100
1	C	67/82 (82%)	66±1 (99±1%)	1±1 (1±1%)	0±0 (0±0%)	100	100
2	B	21/23 (91%)	20±1 (96±3%)	1±1 (4±3%)	0±0 (0±0%)	100	100
2	D	20/23 (87%)	19±1 (95±3%)	1±1 (5±3%)	0±0 (0±0%)	100	100
All	All	3500/4200 (83%)	3434 (98%)	66 (2%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	58/71 (82%)	52±1 (89±2%)	6±1 (11±2%)	8	52
1	C	58/71 (82%)	51±1 (89±2%)	7±1 (11±2%)	8	51
2	B	18/19 (95%)	16±1 (89±5%)	2±1 (11±5%)	8	52
2	D	17/19 (89%)	15±1 (87±5%)	2±1 (13±5%)	6	47
All	All	3020/3600 (84%)	2681 (89%)	339 (11%)	8	51

All 46 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	335	LEU	20
1	A	351	LEU	20
1	A	366	LYS	20
1	C	335	LEU	20
1	C	351	LEU	20
1	C	366	LYS	20
1	C	328	LEU	17
1	C	329	ARG	17
1	A	328	LEU	16
2	B	273	LEU	16
2	D	273	LEU	16
2	D	286	LEU	16
1	A	329	ARG	15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
2	B	286	LEU	14
1	C	382	LYS	11
1	A	382	LYS	10
1	A	361	TYR	9
1	C	361	TYR	9
2	D	272	GLU	5
2	D	289	ARG	4
2	B	289	ARG	4
1	A	372	GLN	3
1	C	372	GLN	3
2	B	285	GLN	3
2	D	285	GLN	3
1	A	333	LYS	2
1	C	325	ARG	2
1	C	333	LYS	2
2	B	272	GLU	2
1	A	320	GLU	2
1	C	320	GLU	2
1	C	326	GLU	2
1	A	321	LEU	1
1	C	321	LEU	1
1	A	325	ARG	1
1	A	345	GLU	1
1	C	345	GLU	1
1	A	349	LYS	1
1	C	349	LYS	1
1	A	322	GLU	1
1	A	338	HIS	1
1	C	322	GLU	1
1	C	338	HIS	1
1	A	326	GLU	1
1	A	347	LEU	1
1	C	347	LEU	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 [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 43% for the well-defined parts and 42% 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	1010
Number of shifts mapped to atoms	1010
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	82	-0.36 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	80	0.28 ± 0.04	None needed (< 0.5 ppm)
$^{13}\text{C}'$	77	-0.29 ± 0.08	None needed (< 0.5 ppm)
^{15}N	77	0.07 ± 0.17	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 34%, i.e. 835 atoms were assigned a chemical shift out of a possible 2481. 0 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	330/875 (38%)	133/352 (38%)	132/350 (38%)	65/173 (38%)
Sidechain	467/1424 (33%)	318/908 (35%)	149/454 (33%)	0/62 (0%)

Continued on next page...

Continued from previous page...

	Total	¹ H	¹³ C	¹⁵ N
Aromatic	38/182 (21%)	19/90 (21%)	17/82 (21%)	2/10 (20%)
Overall	835/2481 (34%)	470/1350 (35%)	298/886 (34%)	67/245 (27%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 34%, i.e. 1010 atoms were assigned a chemical shift out of a possible 2972. 0 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	397/1054 (38%)	161/426 (38%)	159/420 (38%)	77/208 (37%)
Sidechain	575/1708 (34%)	391/1088 (36%)	184/536 (34%)	0/84 (0%)
Aromatic	38/210 (18%)	19/106 (18%)	17/90 (19%)	2/14 (14%)
Overall	1010/2972 (34%)	571/1620 (35%)	360/1046 (34%)	79/306 (26%)

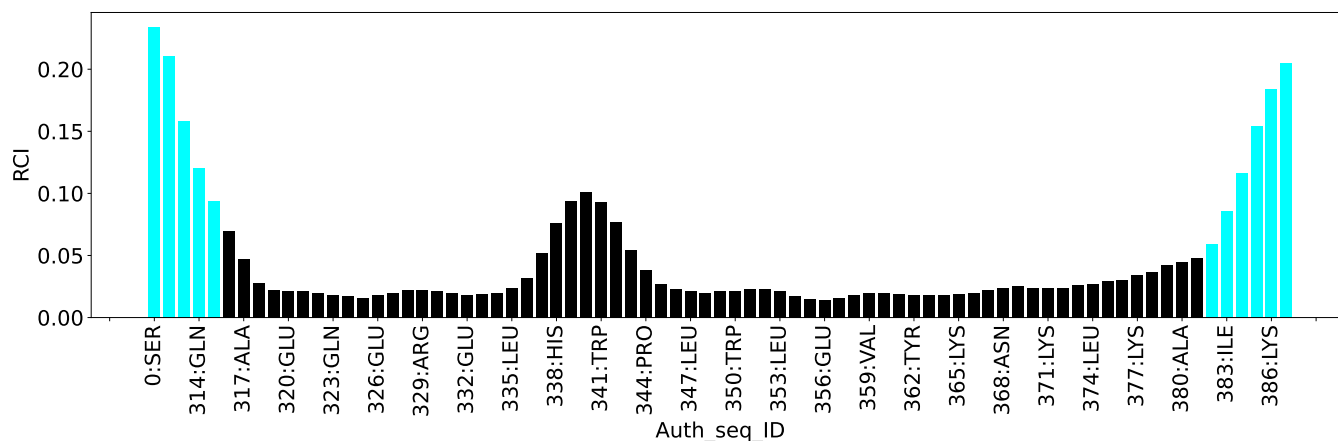
7.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

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: *assigned_chem_shift_list_2*

7.2.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	235
Number of shifts mapped to atoms	235
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.2.2 Chemical shift referencing

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

7.2.3 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 9%, i.e. 223 atoms were assigned a chemical shift out of a possible 2481. 0 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	85/875 (10%)	43/352 (12%)	21/350 (6%)	21/173 (12%)
Sidechain	138/1424 (10%)	94/908 (10%)	41/454 (9%)	3/62 (5%)
Aromatic	0/182 (0%)	0/90 (0%)	0/82 (0%)	0/10 (0%)
Overall	223/2481 (9%)	137/1350 (10%)	62/886 (7%)	24/245 (10%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 8%, i.e. 234 atoms were assigned a chemical shift out of a possible 2972. 0 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	93/1054 (9%)	47/426 (11%)	23/420 (5%)	23/208 (11%)
Sidechain	141/1708 (8%)	96/1088 (9%)	42/536 (8%)	3/84 (4%)
Aromatic	0/210 (0%)	0/106 (0%)	0/90 (0%)	0/14 (0%)
Overall	234/2972 (8%)	143/1620 (9%)	65/1046 (6%)	26/306 (8%)

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:

