



Full wwPDB NMR Structure Validation Report ⓘ

May 29, 2020 – 12:22 am BST

PDB ID : 2N70
Title : Two-fold symmetric structure of the 18-60 construct of S31N M2 from Influenza A in lipid bilayers
Authors : Andreas, L.B.; Reese, M.; Eddy, M.T.; Gelev, V.; Ni, Q.; Miller, E.A.; Emsley, L.; Pintacuda, G.; Chou, J.J.; Griffin, R.G.
Deposited on : 2015-09-01

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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

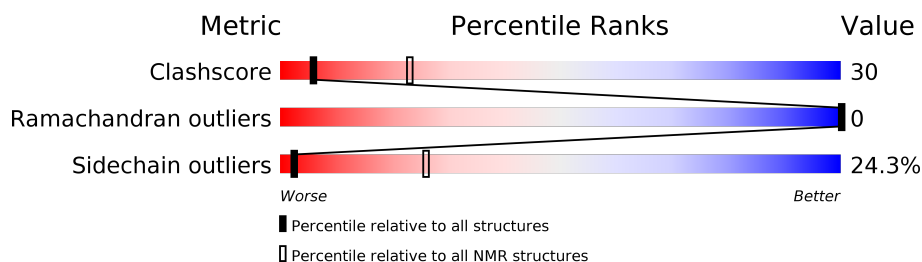
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLID-STATE NMR

The overall completeness of chemical shifts assignment is 28%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	43	
1	B	43	
1	C	43	
1	D	43	

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:130-A:147, B:225-B:246, C:330-C:347, D:425-D:446 (80)	0.24	1

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

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

The models can be grouped into 3 clusters and 4 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2912 atoms, of which 1480 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Matrix protein 2.

Mol	Chain	Residues	Atoms					Trace
1	A	43	Total	C	H	N	O	0
			728	238	370	61	59	
1	B	43	Total	C	H	N	O	0
			728	238	370	61	59	
1	C	43	Total	C	H	N	O	0
			728	238	370	61	59	
1	D	43	Total	C	H	N	O	0
			728	238	370	61	59	

There are 12 discrepancies between the modelled and reference sequences:

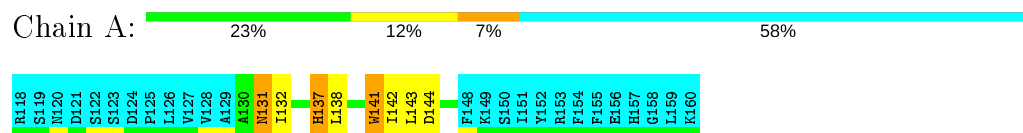
Chain	Residue	Modelled	Actual	Comment	Reference
A	119	SER	CYS	ENGINEERED MUTATION	UNP P63231
A	131	ASN	SER	ENGINEERED MUTATION	UNP P63231
A	150	SER	CYS	ENGINEERED MUTATION	UNP P63231
B	219	SER	CYS	ENGINEERED MUTATION	UNP P63231
B	231	ASN	SER	ENGINEERED MUTATION	UNP P63231
B	250	SER	CYS	ENGINEERED MUTATION	UNP P63231
C	319	SER	CYS	ENGINEERED MUTATION	UNP P63231
C	331	ASN	SER	ENGINEERED MUTATION	UNP P63231
C	350	SER	CYS	ENGINEERED MUTATION	UNP P63231
D	419	SER	CYS	ENGINEERED MUTATION	UNP P63231
D	431	ASN	SER	ENGINEERED MUTATION	UNP P63231
D	450	SER	CYS	ENGINEERED MUTATION	UNP P63231

4 Residue-property plots [i](#)

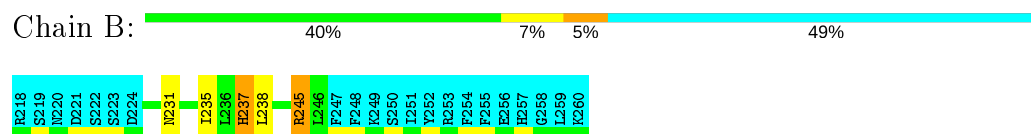
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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.

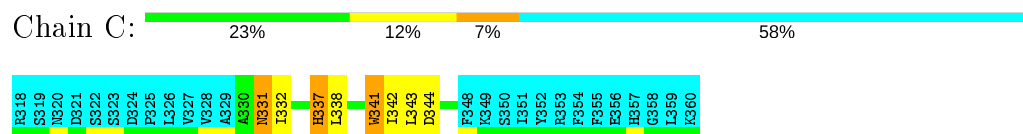
- Molecule 1: Matrix protein 2



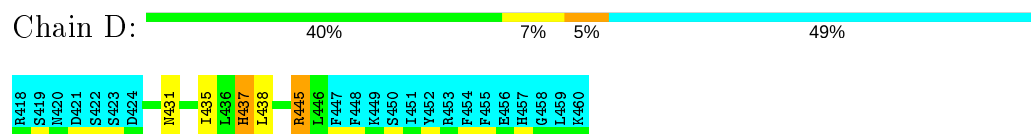
- Molecule 1: Matrix protein 2



- Molecule 1: Matrix protein 2



- Molecule 1: Matrix protein 2

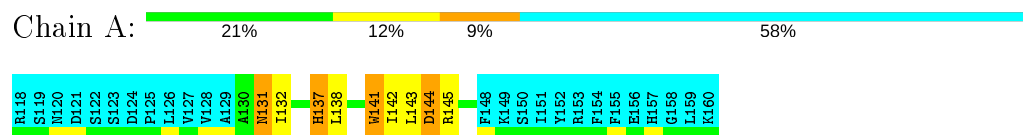


4.2 Scores per residue for each member of the ensemble

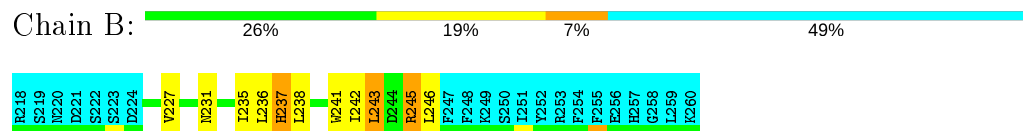
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

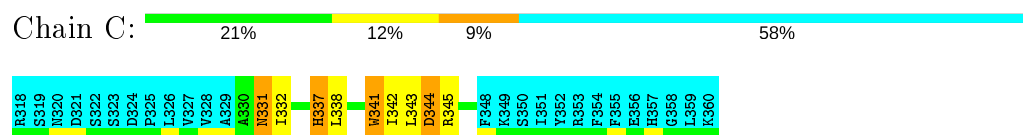
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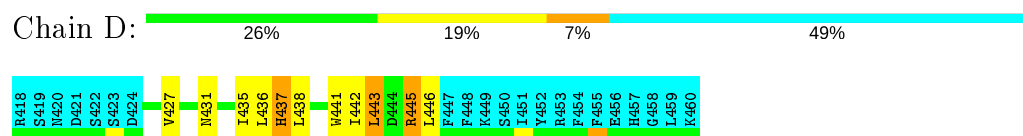
• Molecule 1: Matrix protein 2



• Molecule 1: Matrix protein 2

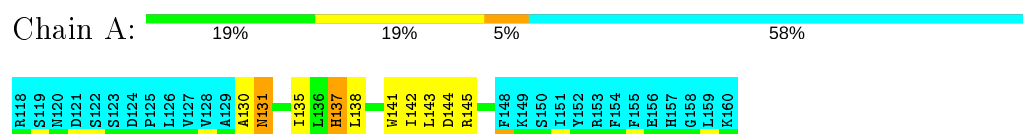


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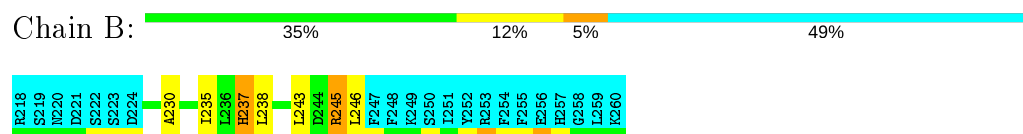


4.2.2 Score per residue for model 2

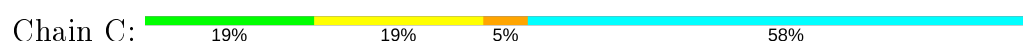
• Molecule 1: Matrix protein 2



• Molecule 1: Matrix protein 2

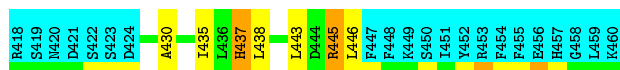
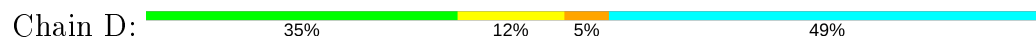


• Molecule 1: Matrix protein 2





- Molecule 1: Matrix protein 2

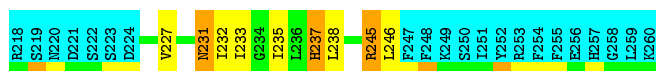


4.2.3 Score per residue for model 3

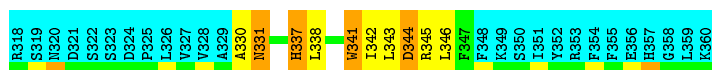
- Molecule 1: Matrix protein 2



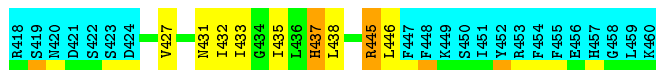
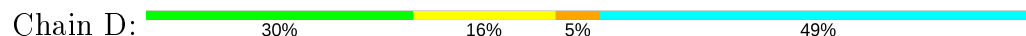
- Molecule 1: Matrix protein 2



- Molecule 1: Matrix protein 2



- Molecule 1: Matrix protein 2

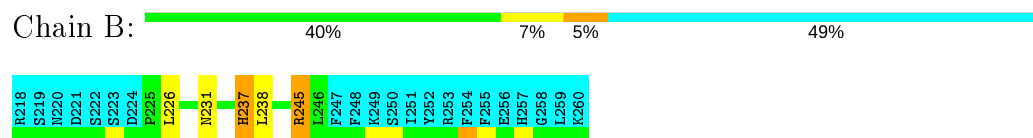


4.2.4 Score per residue for model 4

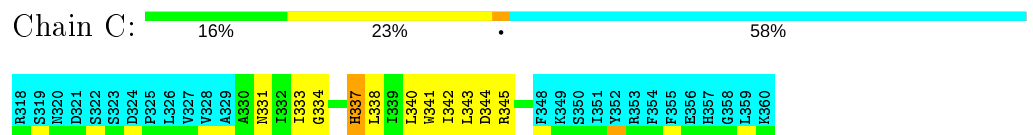
- Molecule 1: Matrix protein 2



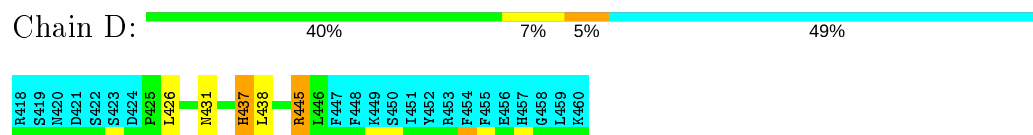
- Molecule 1: Matrix protein 2



- Molecule 1: Matrix protein 2

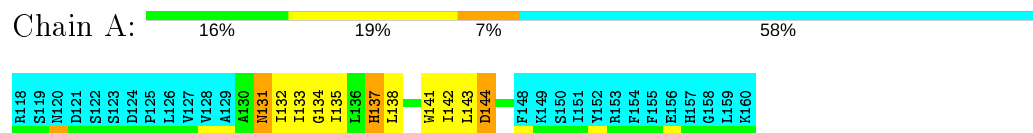


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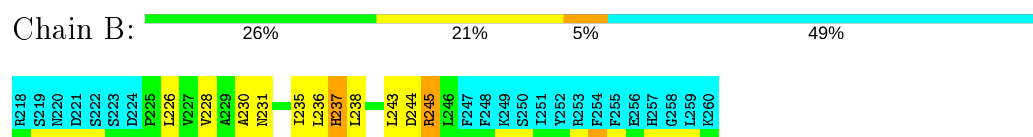


4.2.5 Score per residue for model 5

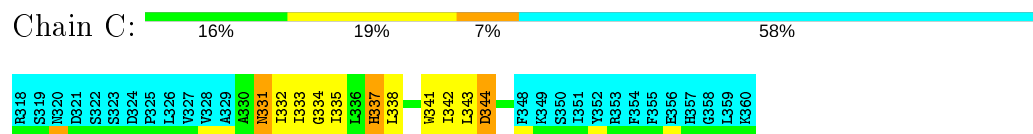
- Molecule 1: Matrix protein 2



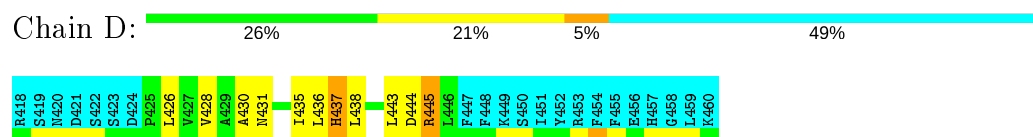
- Molecule 1: Matrix protein 2



- Molecule 1: Matrix protein 2

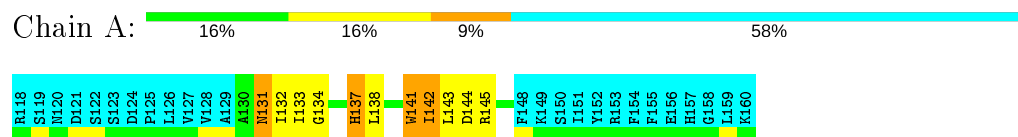


- Molecule 1: Matrix protein 2

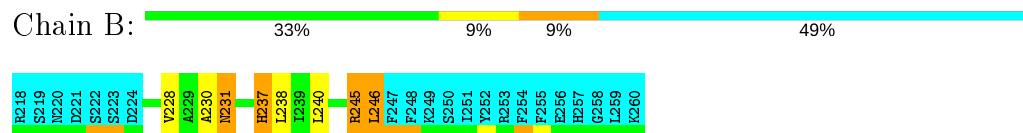


4.2.6 Score per residue for model 6

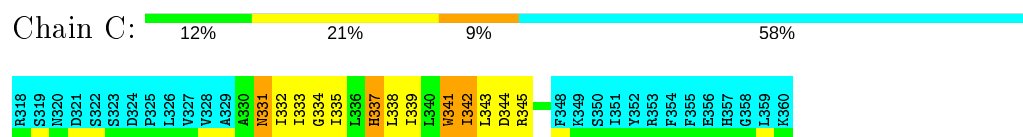
- Molecule 1: Matrix protein 2



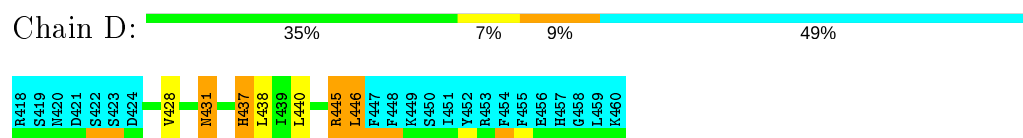
- Molecule 1: Matrix protein 2



- Molecule 1: Matrix protein 2

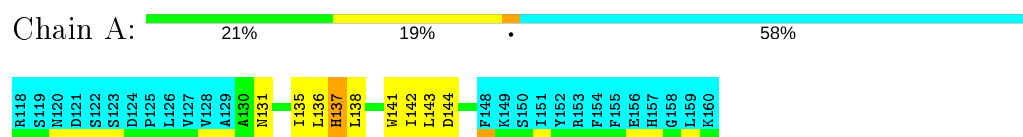


- Molecule 1: Matrix protein 2

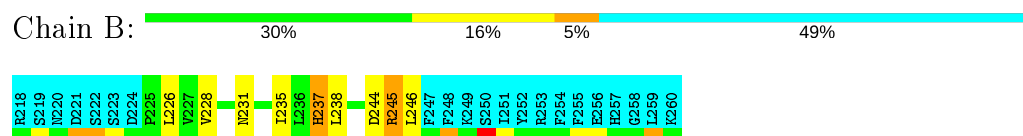


4.2.7 Score per residue for model 7

- Molecule 1: Matrix protein 2

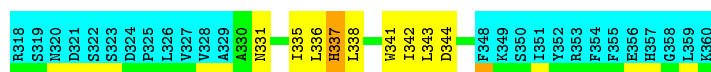


- Molecule 1: Matrix protein 2



- Molecule 1: Matrix protein 2





• Molecule 1: Matrix protein 2

Chain D: 30% 16% 5% 49%



4.2.8 Score per residue for model 8

• Molecule 1: Matrix protein 2

Chain A: 23% 12% 7% 58%



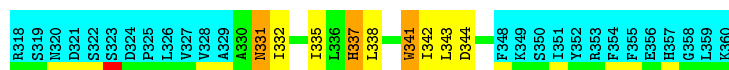
• Molecule 1: Matrix protein 2

Chain B: 35% 12% 5% 49%



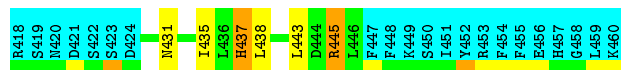
• Molecule 1: Matrix protein 2

Chain C: 21% 14% 7% 58%



• Molecule 1: Matrix protein 2

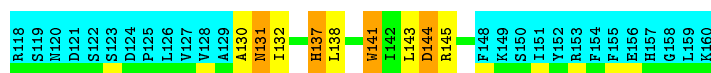
Chain D: 37% 9% 5% 49%



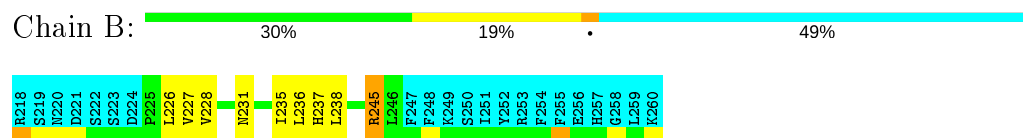
4.2.9 Score per residue for model 9

• Molecule 1: Matrix protein 2

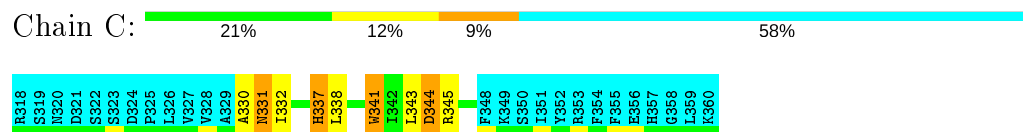
Chain A: 21% 12% 9% 58%



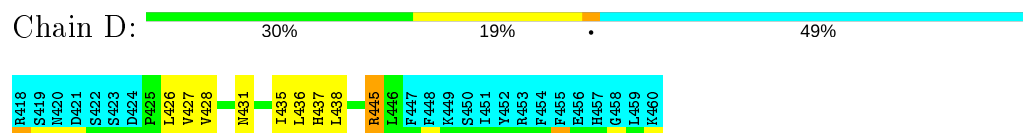
- Molecule 1: Matrix protein 2



- Molecule 1: Matrix protein 2

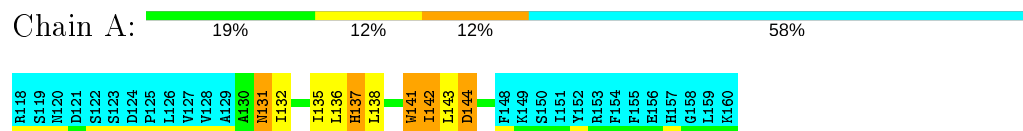


- Molecule 1: Matrix protein 2

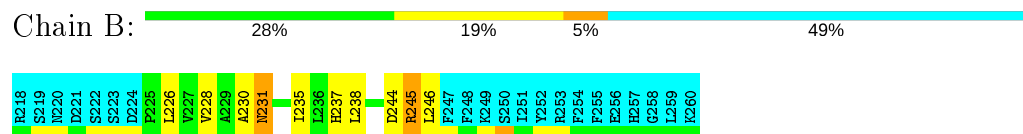


4.2.10 Score per residue for model 10

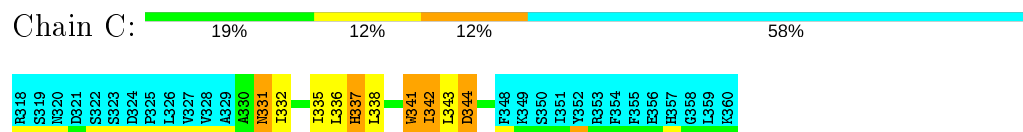
- Molecule 1: Matrix protein 2



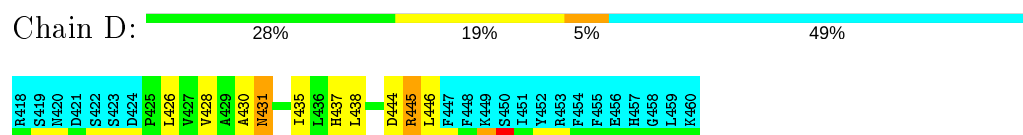
- Molecule 1: Matrix protein 2



- Molecule 1: Matrix protein 2

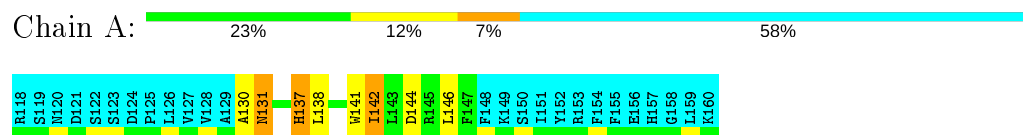


- Molecule 1: Matrix protein 2

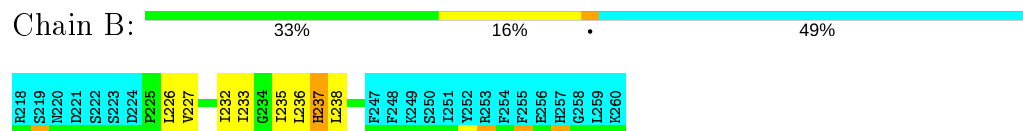


4.2.11 Score per residue for model 11

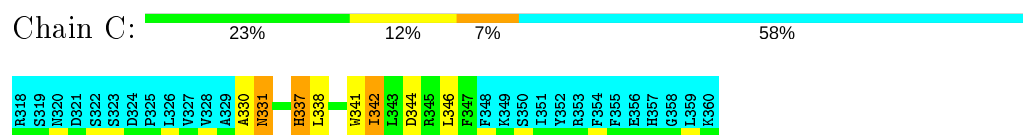
- Molecule 1: Matrix protein 2



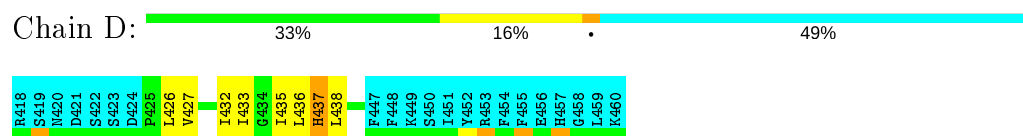
- Molecule 1: Matrix protein 2



- Molecule 1: Matrix protein 2

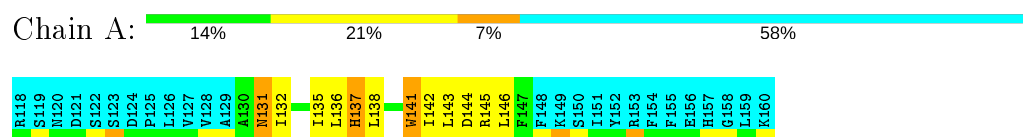


- Molecule 1: Matrix protein 2

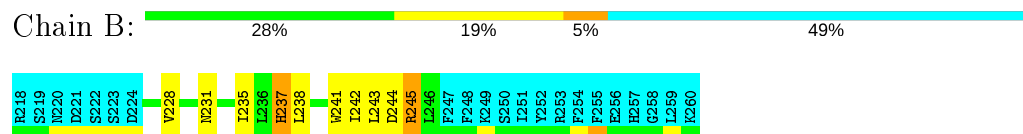


4.2.12 Score per residue for model 12

- Molecule 1: Matrix protein 2

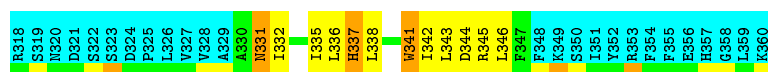


- Molecule 1: Matrix protein 2

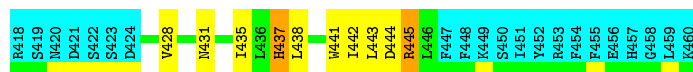


- Molecule 1: Matrix protein 2



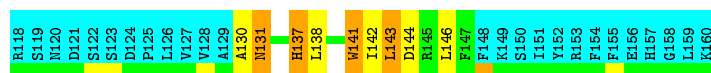


- Molecule 1: Matrix protein 2

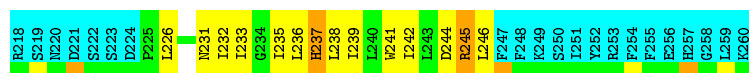


4.2.13 Score per residue for model 13

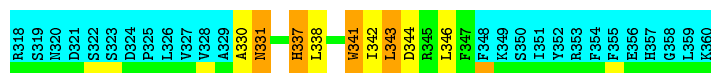
- Molecule 1: Matrix protein 2



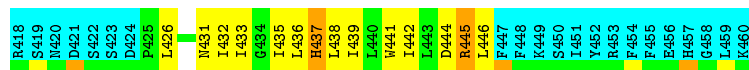
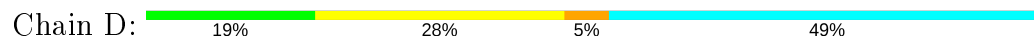
- Molecule 1: Matrix protein 2



- Molecule 1: Matrix protein 2



- Molecule 1: Matrix protein 2

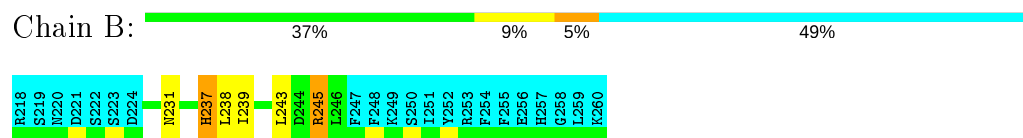


4.2.14 Score per residue for model 14

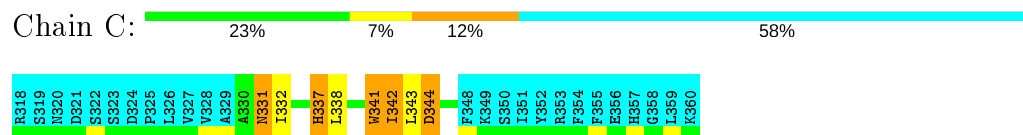
- Molecule 1: Matrix protein 2



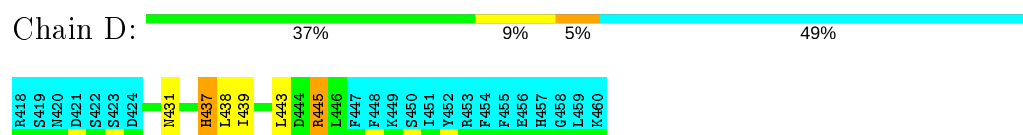
- Molecule 1: Matrix protein 2



- Molecule 1: Matrix protein 2

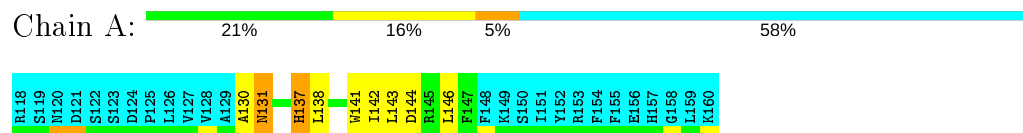


- Molecule 1: Matrix protein 2

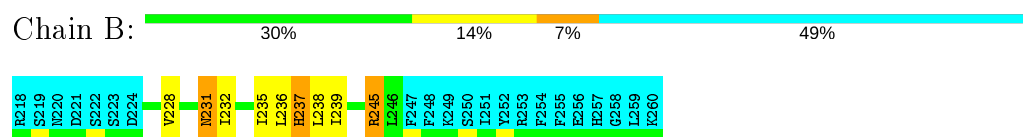


4.2.15 Score per residue for model 15

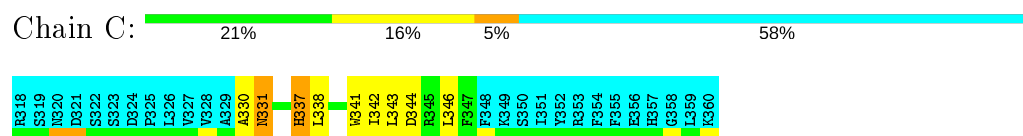
- Molecule 1: Matrix protein 2



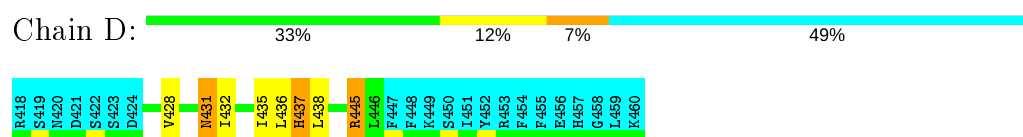
- Molecule 1: Matrix protein 2



- Molecule 1: Matrix protein 2

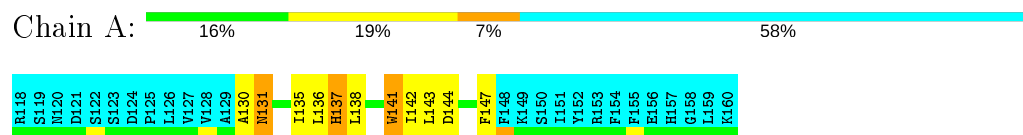


- Molecule 1: Matrix protein 2

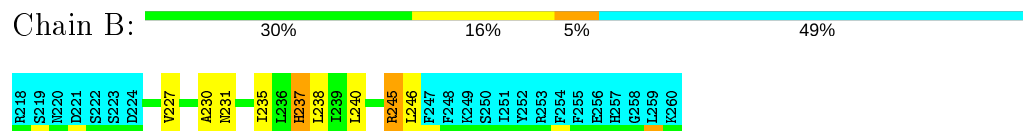


4.2.16 Score per residue for model 16

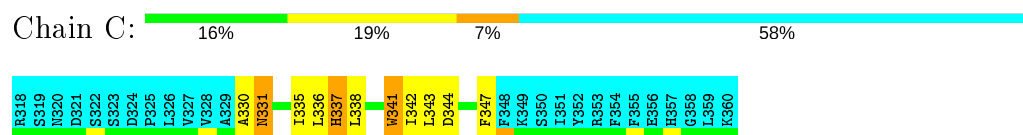
- Molecule 1: Matrix protein 2



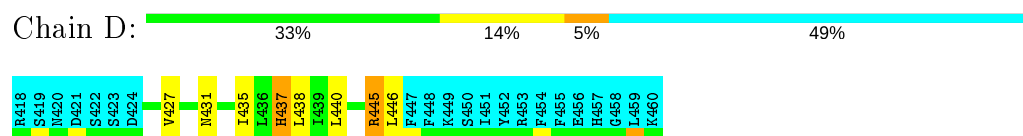
- Molecule 1: Matrix protein 2



- Molecule 1: Matrix protein 2

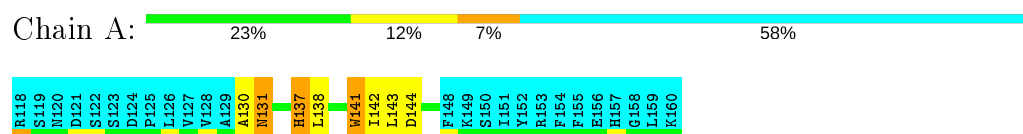


- Molecule 1: Matrix protein 2

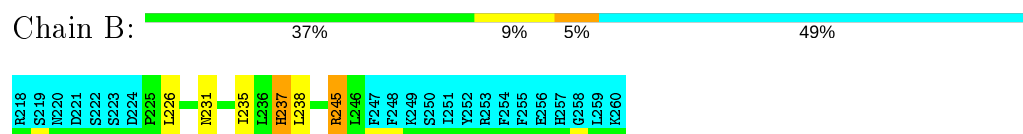


4.2.17 Score per residue for model 17

- Molecule 1: Matrix protein 2

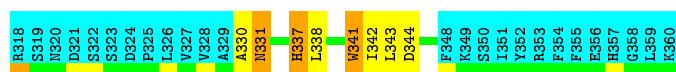


- Molecule 1: Matrix protein 2



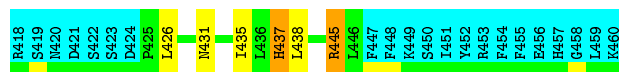
- Molecule 1: Matrix protein 2





- Molecule 1: Matrix protein 2

Chain D: 37% 9% 5% 49%



4.2.18 Score per residue for model 18

- Molecule 1: Matrix protein 2

Chain A: 14% 16% 12% 58%



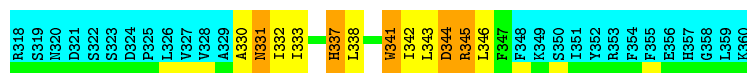
- Molecule 1: Matrix protein 2

Chain B: 35% 9% 7% 49%



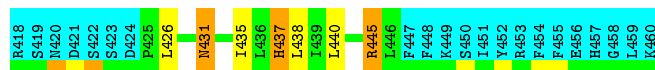
- Molecule 1: Matrix protein 2

Chain C: 14% 16% 12% 58%



- Molecule 1: Matrix protein 2

Chain D: 35% 9% 7% 49%



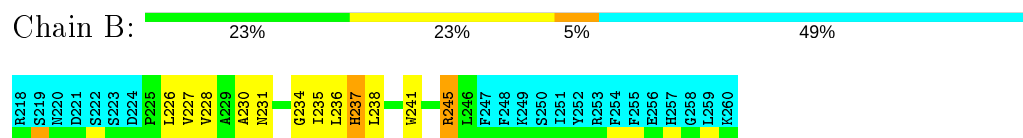
4.2.19 Score per residue for model 19

- Molecule 1: Matrix protein 2

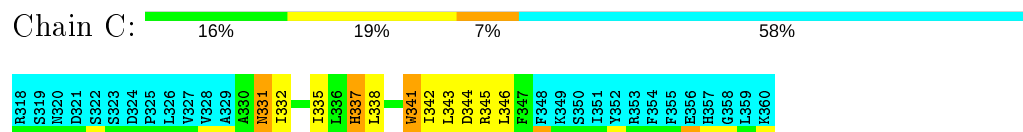
Chain A: 16% 19% 7% 58%



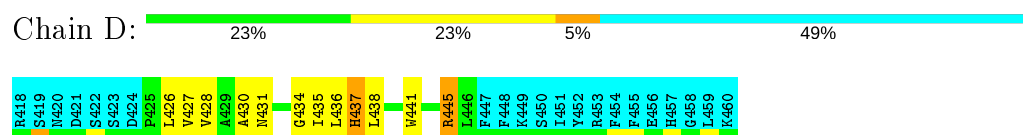
- Molecule 1: Matrix protein 2



- Molecule 1: Matrix protein 2

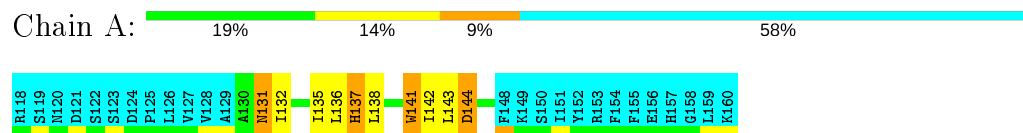


- Molecule 1: Matrix protein 2

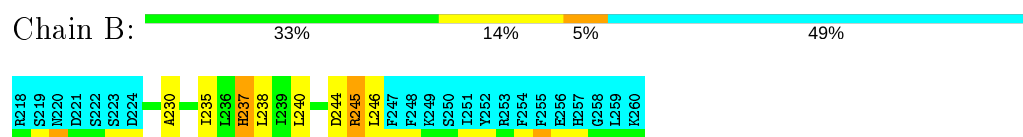


4.2.20 Score per residue for model 20

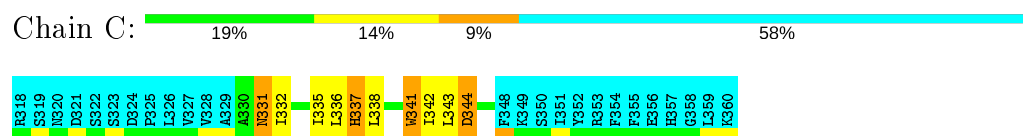
- Molecule 1: Matrix protein 2



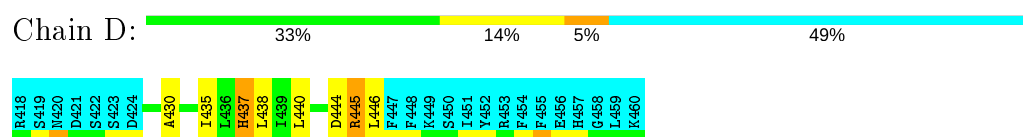
- Molecule 1: Matrix protein 2



- Molecule 1: Matrix protein 2



- Molecule 1: Matrix protein 2



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DGSA-distance geometry simulated annealing*.

Of the 33 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+	structure solution	
X-PLOR NIH	structure solution	
X-PLOR NIH	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)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	399
Number of shifts mapped to atoms	399
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	28%

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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 ⓘ

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	151	167	167	18±4
1	B	174	199	199	13±3
1	C	151	167	167	18±4
1	D	174	199	199	12±3
All	All	13000	14640	14640	820

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:138:LEU:HD21	1:C:337:HIS:CE1	0.85	2.07	14	10
1:A:138:LEU:HD21	1:C:337:HIS:NE2	0.84	1.88	5	19
1:A:137:HIS:CE1	1:C:338:LEU:HD21	0.84	2.07	14	10
1:A:137:HIS:NE2	1:C:338:LEU:HD21	0.83	1.88	5	19
1:A:138:LEU:HD22	1:D:437:HIS:CD2	0.78	2.14	13	9
1:B:237:HIS:CD2	1:C:338:LEU:HD22	0.76	2.15	1	9
1:A:137:HIS:CE1	1:B:238:LEU:HD13	0.74	2.17	18	20
1:B:237:HIS:ND1	1:C:338:LEU:HD22	0.74	1.97	14	10
1:A:138:LEU:HD22	1:D:437:HIS:ND1	0.74	1.98	14	10
1:B:230:ALA:HB1	1:C:335:ILE:HG21	0.73	1.59	19	7
1:A:137:HIS:CD2	1:C:338:LEU:HD11	0.73	2.17	14	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:135:ILE:HG21	1:D:430:ALA:HB1	0.73	1.59	19	5
1:C:337:HIS:CE1	1:D:438:LEU:HD13	0.73	2.19	18	20
1:A:138:LEU:HD11	1:C:337:HIS:CD2	0.72	2.20	14	4
1:B:237:HIS:NE2	1:C:342:ILE:HD13	0.68	2.04	3	3
1:A:137:HIS:ND1	1:B:238:LEU:HD13	0.68	2.04	4	19
1:A:142:ILE:HD13	1:D:437:HIS:NE2	0.67	2.04	3	3
1:C:337:HIS:ND1	1:D:438:LEU:HD13	0.66	2.05	7	19
1:C:330:ALA:HB1	1:D:431:ASN:OD1	0.64	1.93	15	1
1:A:141:TRP:CH2	1:C:341:TRP:CH2	0.63	2.87	17	20
1:A:130:ALA:HB1	1:B:231:ASN:OD1	0.63	1.94	15	2
1:D:437:HIS:CD2	1:D:438:LEU:N	0.63	2.67	2	9
1:B:237:HIS:CD2	1:B:238:LEU:N	0.63	2.67	2	9
1:A:131:ASN:ND2	1:A:132:ILE:N	0.63	2.47	9	1
1:A:141:TRP:CZ3	1:C:341:TRP:CH2	0.62	2.88	10	10
1:A:141:TRP:CH2	1:C:341:TRP:CZ3	0.62	2.87	9	10
1:B:227:VAL:HG11	1:C:331:ASN:HD21	0.62	1.53	16	2
1:C:337:HIS:CG	1:C:338:LEU:N	0.61	2.68	17	18
1:C:331:ASN:ND2	1:C:332:ILE:N	0.61	2.47	9	1
1:A:131:ASN:HD21	1:D:427:VAL:HG11	0.61	1.54	16	2
1:B:237:HIS:ND1	1:C:342:ILE:HD12	0.60	2.12	2	9
1:A:137:HIS:CG	1:A:138:LEU:N	0.59	2.68	12	18
1:A:142:ILE:HD12	1:D:437:HIS:ND1	0.59	2.13	2	9
1:D:437:HIS:ND1	1:D:438:LEU:N	0.58	2.50	18	8
1:B:237:HIS:ND1	1:B:238:LEU:N	0.58	2.51	18	8
1:A:145:ARG:NH1	1:D:441:TRP:CD1	0.56	2.73	19	3
1:A:135:ILE:HG23	1:A:136:LEU:N	0.56	2.16	16	3
1:B:241:TRP:CD1	1:C:345:ARG:NH1	0.56	2.74	12	3
1:C:342:ILE:HG23	1:C:343:LEU:N	0.56	2.15	16	18
1:A:142:ILE:HG23	1:A:143:LEU:N	0.56	2.15	16	18
1:C:335:ILE:HG23	1:C:336:LEU:N	0.54	2.17	16	3
1:B:245:ARG:CG	1:B:245:ARG:HH11	0.54	2.16	9	10
1:B:245:ARG:HH11	1:B:245:ARG:CG	0.54	2.16	4	8
1:D:445:ARG:HH11	1:D:445:ARG:CG	0.54	2.16	4	9
1:B:245:ARG:CG	1:B:245:ARG:NH1	0.54	2.71	8	9
1:B:245:ARG:NH1	1:B:245:ARG:CG	0.54	2.71	18	9
1:B:235:ILE:N	1:B:235:ILE:HD12	0.54	2.18	19	9
1:C:345:ARG:CG	1:C:345:ARG:NH1	0.54	2.71	18	1
1:D:445:ARG:CG	1:D:445:ARG:HH11	0.54	2.16	18	9
1:D:437:HIS:C	1:D:437:HIS:HD1	0.54	2.07	9	1
1:D:435:ILE:HD12	1:D:435:ILE:N	0.53	2.18	19	7
1:A:138:LEU:HD22	1:D:437:HIS:CE1	0.53	2.39	11	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:345:ARG:CG	1:C:345:ARG:HH11	0.53	2.16	18	1
1:A:137:HIS:NE2	1:C:338:LEU:CD2	0.53	2.69	11	5
1:D:445:ARG:CG	1:D:445:ARG:NH1	0.53	2.71	2	12
1:A:145:ARG:HH11	1:A:145:ARG:CG	0.53	2.16	18	1
1:D:445:ARG:NH1	1:D:445:ARG:CG	0.53	2.71	1	6
1:B:227:VAL:HG11	1:C:331:ASN:ND2	0.53	2.18	19	2
1:B:237:HIS:HD1	1:B:237:HIS:C	0.52	2.06	9	1
1:B:237:HIS:CE1	1:C:338:LEU:HD22	0.52	2.38	16	9
1:D:436:LEU:HD23	1:D:436:LEU:O	0.52	2.04	13	1
1:B:237:HIS:C	1:B:237:HIS:ND1	0.52	2.63	9	5
1:A:138:LEU:CD2	1:C:337:HIS:NE2	0.52	2.70	11	7
1:D:435:ILE:N	1:D:435:ILE:HD12	0.52	2.20	5	9
1:B:227:VAL:CG1	1:C:331:ASN:HD21	0.52	2.17	9	4
1:D:437:HIS:C	1:D:437:HIS:ND1	0.52	2.63	9	5
1:A:131:ASN:ND2	1:D:427:VAL:HG11	0.52	2.20	19	2
1:A:138:LEU:HD22	1:D:437:HIS:NE2	0.52	2.19	7	9
1:B:237:HIS:CD2	1:C:342:ILE:HD12	0.51	2.40	14	2
1:C:344:ASP:OD2	1:D:445:ARG:NE	0.51	2.43	16	1
1:B:236:LEU:HD23	1:B:236:LEU:O	0.51	2.04	13	1
1:A:145:ARG:NH1	1:A:145:ARG:CG	0.51	2.71	18	1
1:A:142:ILE:HD13	1:D:437:HIS:CD2	0.51	2.41	17	3
1:C:344:ASP:OD1	1:C:345:ARG:N	0.51	2.43	9	1
1:A:131:ASN:HD21	1:D:427:VAL:CG1	0.51	2.19	9	4
1:A:144:ASP:OD2	1:B:245:ARG:NE	0.51	2.43	16	1
1:A:144:ASP:OD1	1:A:145:ARG:N	0.50	2.43	9	1
1:D:437:HIS:ND1	1:D:437:HIS:C	0.50	2.65	18	4
1:B:237:HIS:CD2	1:C:342:ILE:HD13	0.49	2.42	17	3
1:B:235:ILE:HD12	1:B:235:ILE:N	0.49	2.21	1	7
1:A:131:ASN:CG	1:A:132:ILE:N	0.49	2.66	5	10
1:B:237:HIS:NE2	1:C:338:LEU:HD22	0.49	2.22	7	9
1:B:237:HIS:ND1	1:B:237:HIS:C	0.49	2.65	18	4
1:A:142:ILE:CG2	1:A:143:LEU:N	0.49	2.76	7	17
1:D:431:ASN:CG	1:D:432:ILE:N	0.49	2.66	15	1
1:C:342:ILE:CG2	1:C:343:LEU:N	0.49	2.76	7	17
1:B:231:ASN:CG	1:B:232:ILE:N	0.49	2.66	15	1
1:C:337:HIS:CD2	1:C:338:LEU:N	0.48	2.81	14	1
1:C:331:ASN:CG	1:C:332:ILE:N	0.48	2.66	5	10
1:B:237:HIS:CE1	1:C:338:LEU:CD2	0.48	2.96	17	8
1:B:237:HIS:HE2	1:C:342:ILE:HD13	0.48	1.67	18	2
1:A:144:ASP:OD1	1:B:245:ARG:NH2	0.48	2.46	16	1
1:A:142:ILE:HD12	1:D:437:HIS:CD2	0.48	2.44	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:337:HIS:ND1	1:C:337:HIS:C	0.47	2.67	18	5
1:A:137:HIS:CD2	1:A:138:LEU:N	0.47	2.81	14	1
1:C:344:ASP:OD1	1:D:445:ARG:NH2	0.47	2.46	16	1
1:C:337:HIS:ND1	1:D:438:LEU:HD22	0.47	2.25	14	1
1:B:227:VAL:CG1	1:C:331:ASN:OD1	0.47	2.62	16	2
1:A:138:LEU:CD2	1:D:437:HIS:CE1	0.47	2.98	17	8
1:A:131:ASN:ND2	1:A:131:ASN:C	0.47	2.68	10	2
1:A:137:HIS:C	1:A:137:HIS:ND1	0.47	2.67	18	4
1:A:142:ILE:HD13	1:D:437:HIS:HE2	0.47	1.68	18	3
1:C:331:ASN:ND2	1:C:331:ASN:C	0.47	2.68	10	2
1:A:131:ASN:OD1	1:D:427:VAL:CG1	0.46	2.63	16	2
1:C:333:ILE:HG23	1:C:334:GLY:N	0.46	2.25	6	3
1:A:137:HIS:NE2	1:C:338:LEU:CG	0.46	2.79	14	2
1:A:138:LEU:CG	1:C:337:HIS:NE2	0.46	2.79	14	2
1:A:137:HIS:HE2	1:C:338:LEU:HD21	0.46	1.71	8	3
1:D:426:LEU:N	1:D:426:LEU:HD12	0.46	2.26	7	1
1:A:130:ALA:HB1	1:B:231:ASN:CG	0.46	2.31	18	1
1:A:137:HIS:ND1	1:B:238:LEU:HD22	0.46	2.25	14	1
1:C:330:ALA:HB1	1:D:431:ASN:CG	0.46	2.30	18	1
1:A:133:ILE:HG23	1:A:134:GLY:N	0.46	2.25	6	3
1:A:141:TRP:CG	1:A:142:ILE:N	0.46	2.83	10	2
1:B:228:VAL:O	1:B:231:ASN:N	0.45	2.50	7	8
1:C:341:TRP:CG	1:C:342:ILE:N	0.45	2.83	10	2
1:A:131:ASN:ND2	1:D:431:ASN:OD1	0.45	2.49	18	1
1:B:235:ILE:N	1:B:235:ILE:CD1	0.45	2.80	19	4
1:A:131:ASN:OD1	1:A:132:ILE:N	0.45	2.49	6	1
1:C:331:ASN:OD1	1:C:332:ILE:N	0.45	2.49	6	1
1:A:138:LEU:HD21	1:C:337:HIS:HE2	0.45	1.69	5	4
1:A:141:TRP:C	1:A:141:TRP:CD2	0.45	2.89	16	1
1:D:435:ILE:CD1	1:D:435:ILE:N	0.44	2.80	19	3
1:C:330:ALA:HB1	1:D:431:ASN:ND2	0.44	2.27	18	1
1:C:341:TRP:CE3	1:C:341:TRP:O	0.44	2.70	16	1
1:A:133:ILE:CD1	1:B:235:ILE:HD12	0.44	2.43	18	1
1:D:428:VAL:O	1:D:431:ASN:N	0.44	2.50	7	8
1:D:442:ILE:HG23	1:D:443:LEU:N	0.44	2.28	1	2
1:B:226:LEU:N	1:B:226:LEU:HD12	0.44	2.26	7	1
1:B:242:ILE:HG23	1:B:243:LEU:N	0.44	2.28	1	2
1:B:231:ASN:OD1	1:C:331:ASN:ND2	0.44	2.50	18	1
1:C:337:HIS:C	1:C:337:HIS:ND1	0.43	2.68	8	2
1:A:141:TRP:O	1:A:141:TRP:CE3	0.43	2.71	16	1
1:C:333:ILE:CD1	1:D:435:ILE:HD12	0.43	2.43	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:138:LEU:O	1:A:142:ILE:HG22	0.43	2.14	11	2
1:A:135:ILE:CG2	1:A:136:LEU:N	0.43	2.81	16	1
1:C:335:ILE:CG2	1:C:336:LEU:N	0.43	2.82	16	1
1:A:137:HIS:HE2	1:C:338:LEU:CD2	0.43	2.27	10	2
1:D:438:LEU:O	1:D:441:TRP:N	0.43	2.52	13	1
1:A:137:HIS:CD2	1:C:338:LEU:CD1	0.43	2.98	14	1
1:A:130:ALA:HB1	1:B:231:ASN:ND2	0.43	2.28	18	1
1:D:444:ASP:OD1	1:D:444:ASP:N	0.42	2.52	5	1
1:D:426:LEU:CD1	1:D:426:LEU:N	0.42	2.82	7	1
1:B:226:LEU:N	1:B:226:LEU:CD1	0.42	2.82	7	1
1:C:338:LEU:O	1:C:342:ILE:HG22	0.42	2.15	11	2
1:D:432:ILE:HG23	1:D:433:ILE:N	0.42	2.29	3	3
1:C:337:HIS:HD1	1:D:438:LEU:HD22	0.42	1.74	15	1
1:D:427:VAL:O	1:D:431:ASN:OD1	0.42	2.38	19	1
1:B:232:ILE:HG23	1:B:233:ILE:N	0.42	2.29	3	3
1:B:238:LEU:O	1:B:241:TRP:N	0.42	2.52	13	1
1:A:145:ARG:NH1	1:D:441:TRP:NE1	0.42	2.68	19	1
1:B:235:ILE:CD1	1:B:235:ILE:N	0.42	2.83	5	3
1:B:244:ASP:N	1:B:244:ASP:OD1	0.42	2.52	5	1
1:B:227:VAL:O	1:B:231:ASN:OD1	0.42	2.38	19	1
1:B:241:TRP:NE1	1:C:345:ARG:NH1	0.41	2.69	12	2
1:C:341:TRP:CD2	1:C:341:TRP:C	0.41	2.89	16	1
1:D:437:HIS:CD2	1:D:437:HIS:C	0.41	2.90	5	3
1:A:147:PHE:N	1:A:147:PHE:CD1	0.41	2.89	16	1
1:B:237:HIS:C	1:B:237:HIS:CD2	0.41	2.90	5	1
1:A:138:LEU:CD1	1:C:337:HIS:CD2	0.41	3.00	14	1
1:C:341:TRP:CD1	1:C:342:ILE:N	0.41	2.89	14	1
1:A:137:HIS:HD1	1:B:238:LEU:HD22	0.41	1.75	15	1
1:B:231:ASN:O	1:B:234:GLY:N	0.41	2.54	19	1
1:D:437:HIS:C	1:D:437:HIS:CD2	0.41	2.90	20	1
1:B:243:LEU:HD23	1:B:243:LEU:C	0.41	2.35	2	1
1:C:337:HIS:HD1	1:D:438:LEU:HD13	0.41	1.75	7	2
1:A:131:ASN:C	1:A:131:ASN:ND2	0.41	2.74	12	1
1:C:331:ASN:C	1:C:331:ASN:ND2	0.41	2.74	12	1
1:D:438:LEU:O	1:D:439:ILE:C	0.41	2.59	13	2
1:D:431:ASN:O	1:D:434:GLY:N	0.41	2.54	19	1
1:B:237:HIS:CD2	1:B:237:HIS:C	0.41	2.90	7	3
1:A:137:HIS:ND1	1:A:137:HIS:C	0.41	2.68	3	1
1:C:339:ILE:HD12	1:C:339:ILE:N	0.41	2.31	6	1
1:A:138:LEU:CD2	1:C:337:HIS:HE2	0.41	2.28	10	1
1:A:141:TRP:CD1	1:A:142:ILE:N	0.41	2.89	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:230:ALA:HB1	1:C:335:ILE:HG12	0.41	1.93	16	1
1:B:246:LEU:N	1:B:246:LEU:HD12	0.41	2.31	20	1
1:B:238:LEU:O	1:B:239:ILE:C	0.41	2.59	13	3
1:C:347:PHE:N	1:C:347:PHE:CD1	0.41	2.89	16	1
1:A:141:TRP:CD2	1:A:141:TRP:C	0.41	2.92	19	1
1:D:443:LEU:C	1:D:443:LEU:HD23	0.40	2.35	2	1
1:D:446:LEU:N	1:D:446:LEU:HD12	0.40	2.31	20	1
1:D:435:ILE:N	1:D:435:ILE:CD1	0.40	2.85	9	2

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	18/43 (42%)	17±0 (95±1%)	1±0 (5±1%)	0±0 (0±0%)	100	100
1	B	22/43 (51%)	21±1 (95±4%)	1±1 (5±4%)	0±0 (0±0%)	100	100
1	C	18/43 (42%)	17±0 (95±1%)	1±0 (5±1%)	0±0 (0±0%)	100	100
1	D	22/43 (51%)	21±1 (95±4%)	1±1 (5±4%)	0±0 (0±0%)	100	100
All	All	1600/3440 (47%)	1515 (95%)	85 (5%)	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	16/39 (41%)	12±1 (74±7%)	4±1 (26±7%)	2	22
1	B	19/39 (49%)	15±1 (77±5%)	4±1 (23±5%)	3	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	16/39 (41%)	12±1 (74±7%)	4±1 (26±7%)	2	22
1	D	19/39 (49%)	15±1 (77±5%)	4±1 (23±5%)	3	29
All	All	1400/3120 (45%)	1060 (76%)	340 (24%)	2	26

All 40 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	137	HIS	20
1	A	131	ASN	20
1	C	337	HIS	20
1	C	331	ASN	20
1	B	245	ARG	19
1	D	445	ARG	19
1	D	437	HIS	18
1	B	237	HIS	18
1	C	341	TRP	14
1	A	141	TRP	14
1	D	431	ASN	12
1	B	231	ASN	12
1	D	426	LEU	9
1	C	344	ASP	9
1	A	144	ASP	9
1	B	226	LEU	9
1	B	246	LEU	8
1	D	446	LEU	8
1	A	146	LEU	7
1	C	346	LEU	7
1	D	436	LEU	6
1	B	236	LEU	6
1	B	244	ASP	5
1	A	145	ARG	5
1	C	345	ARG	5
1	D	444	ASP	5
1	B	240	LEU	4
1	A	142	ILE	4
1	B	243	LEU	4
1	C	342	ILE	4
1	D	440	LEU	4
1	D	443	LEU	4
1	C	336	LEU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	136	LEU	2
1	A	143	LEU	2
1	C	343	LEU	2
1	B	242	ILE	1
1	D	442	ILE	1
1	A	140	LEU	1
1	C	340	LEU	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 carbohydrates 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 28% for the well-defined parts and 16% for the entire structure.

7.1 Chemical shift list 1

File name: input_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	399
Number of shifts mapped to atoms	399
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
$^{13}\text{C}_\alpha$	47	-1.05 ± 0.11	Should be applied
$^{13}\text{C}_\beta$	45	0.09 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}'$	47	-0.18 ± 0.10	None needed (< 0.5 ppm)
^{15}N	49	1.60 ± 0.38	Should be applied

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 28%, i.e. 298 atoms were assigned a chemical shift out of a possible 1070. 11 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	147/396 (37%)	36/158 (23%)	74/160 (46%)	37/78 (47%)
Sidechain	125/578 (22%)	18/328 (5%)	104/234 (44%)	3/16 (19%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	26/96 (27%)	4/50 (8%)	16/36 (44%)	6/10 (60%)
Overall	298/1070 (28%)	58/536 (11%)	194/430 (45%)	46/104 (44%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 16%, i.e. 369 atoms were assigned a chemical shift out of a possible 2298. 14 out of 36 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	186/852 (22%)	45/340 (13%)	94/344 (27%)	47/168 (28%)
Sidechain	155/1164 (13%)	21/680 (3%)	130/432 (30%)	4/52 (8%)
Aromatic	28/282 (10%)	4/152 (3%)	18/116 (16%)	6/14 (43%)
Overall	369/2298 (16%)	70/1172 (6%)	242/892 (27%)	57/234 (24%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

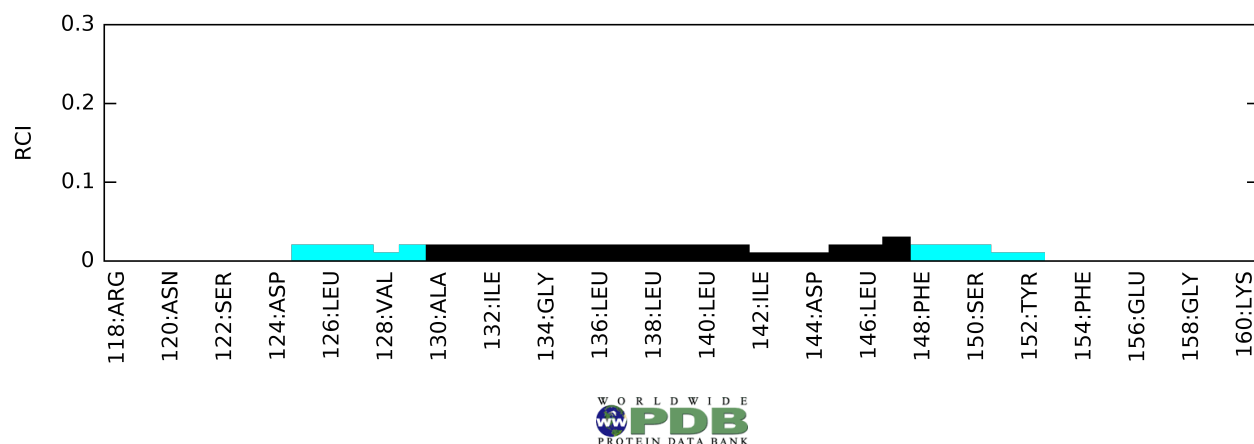
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

The images below report *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.

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:

