Full wwPDB NMR Structure Validation Report (i)

Apr 21, 2024 – 05:42 PM EDT

PDB ID	:	2KJ3
Title	:	High-resolution structure of the HET-s(218-289) prion in its amyloid form obtained by solid-state NMR
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Deposited on	:	2009-05-20

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 (i) 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 (i)) were used in the production of this report:

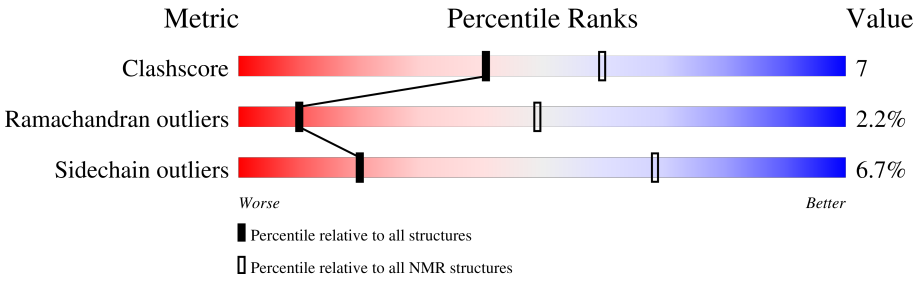
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLID-STATE NMR

The overall completeness of chemical shifts assignment was not calculated.

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	79	56% 10% 34%
1	B	79	52% 16% 32%
1	C	79	59% 6% 34%

2 Ensemble composition and analysis (i)

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

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:225-A:249, A:261-A:287, B:225-B:250, B:260-B:287, C:225-C:249, C:261-C:287 (158)	1.18	13

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

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

The models can be grouped into 3 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3606 atoms, of which 1779 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Small s protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	79	1202	371	593	123	114	1	0
1	B	79	1202	371	593	123	114	1	0
1	C	79	1202	371	593	123	114	1	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	217	MET	-	initiating methionine	UNP Q03689
A	290	HIS	-	expression tag	UNP Q03689
A	291	HIS	-	expression tag	UNP Q03689
A	292	HIS	-	expression tag	UNP Q03689
A	293	HIS	-	expression tag	UNP Q03689
A	294	HIS	-	expression tag	UNP Q03689
A	295	HIS	-	expression tag	UNP Q03689
B	217	MET	-	initiating methionine	UNP Q03689
B	290	HIS	-	expression tag	UNP Q03689
B	291	HIS	-	expression tag	UNP Q03689
B	292	HIS	-	expression tag	UNP Q03689
B	293	HIS	-	expression tag	UNP Q03689
B	294	HIS	-	expression tag	UNP Q03689
B	295	HIS	-	expression tag	UNP Q03689
C	217	MET	-	initiating methionine	UNP Q03689
C	290	HIS	-	expression tag	UNP Q03689
C	291	HIS	-	expression tag	UNP Q03689
C	292	HIS	-	expression tag	UNP Q03689
C	293	HIS	-	expression tag	UNP Q03689
C	294	HIS	-	expression tag	UNP Q03689
C	295	HIS	-	expression tag	UNP Q03689

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: Small s protein

Chain A: 56% 10% 34%

M217 K218 I219 D220 A221 I222 V223 G224 E235 R236 A237 R238 L250 H251 G252 G253 I254 R255 I256 S257 D258 Q259 T260 E265 G278 N279 E280 K284 W287 D288 N289 H290 H291 H292 H293 H294 H295

• Molecule 1: Small s protein

Chain B: 52% 16% 32%

M217 K218 I219 D220 A221 I222 V223 G224 K229 E235 R236 A237 R238 V239 Q240 L241 G242 H251 G252 G253 I254 R255 I256 S257 D258 Q259 E265 V275 G278 N279 E280 K284 W287 D288 N289 H290 H291 H292 H293 H294 H295

• Molecule 1: Small s protein

Chain C: 59% 6% 34%

M217 K218 I219 D220 A221 I222 V223 G224 K229 E235 R236 A237 R238 L250 H251 G252 G253 I254 R255 I256 S257 D258 Q259 T260 W287 D288 N289 H290 H291 H292 H293 H294 H295

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

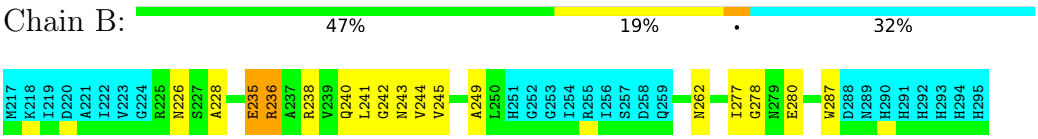
• Molecule 1: Small s protein

Chain A: 53% 11% • 34%

M217 K218 I219 D220 A221 I222 V223 G224 R225 N226 E235 R236 V239 G242 L250 H251 G252 G253 I254 R255 I256 S257 D258 Q259 T260 T261 N262 S263 V264 V275 L276 I277 G278 D288 N289 H290 H291 H292 H293 H294 H295

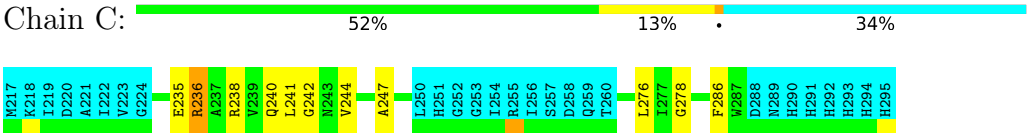
- Molecule 1: Small s protein

Chain B:



- Molecule 1: Small s protein

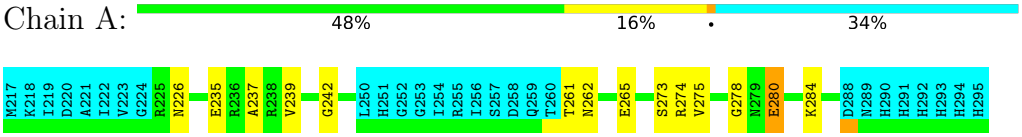
Chain C:



4.2.2 Score per residue for model 2

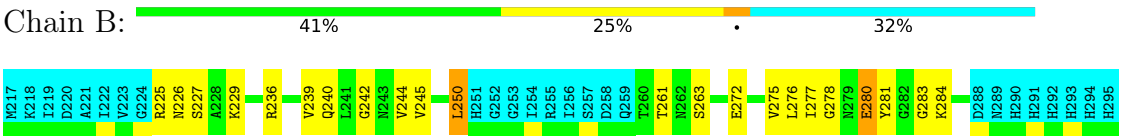
- Molecule 1: Small s protein

Chain A:



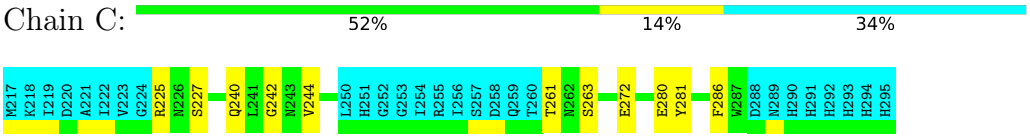
- Molecule 1: Small s protein

Chain B:



- Molecule 1: Small s protein

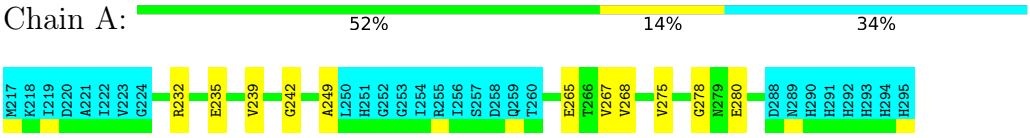
Chain C:



4.2.3 Score per residue for model 3

- Molecule 1: Small s protein

Chain A:



- Molecule 1: Small s protein

Chain B: 44% 24% 32%

M217 K218 I219 D220 A221 I222 V223 G224 R225 K229 D230 I231 E235 R236 Q240 L241 G242 A247 L250 H251 G252 G253 I254 R255 I256 S257 D258 Q259 S263 V264 E265 E272 V275 L276 I277 G278 N279 E280 K284 W287 D288 N289 H290 H291 H292 H293 H294 H295

- Molecule 1: Small s protein

Chain C: 49% 14% • 34%

M217 K218 I219 D220 A221 I222 V223 G224 S227 A228 K229 E235 R236 A237 R238 L241 G242 L250 H251 G252 G253 I254 R255 I256 S257 D258 Q259 T260 E265 G278 N279 E280 K284 G285 F286 W287 D288 N289 H290 H291 H292 H293 H294 H295

4.2.4 Score per residue for model 4

- Molecule 1: Small s protein

Chain A: 51% 14% • 34%

M217 K218 I219 D220 A221 I222 V223 G224 K229 E235 R238 V244 A249 L250 H251 G252 G253 I254 R255 I256 S257 D258 Q259 T260 V264 E265 G269 S273 K284 G285 F286 W287 D288 N289 H290 H291 H292 H293 H294 H295

- Molecule 1: Small s protein

Chain B: 46% 22% • 32%

M217 K218 I219 D220 A221 I222 V223 G224 A228 K229 T233 E234 E235 R236 A237 R238 V244 A247 H251 G252 G253 I254 R255 I256 S257 D258 Q259 V264 E265 E272 S273 R274 G283 K284 G285 F286 W287 D288 N289 H290 H291 H292 H293 H294 H295

- Molecule 1: Small s protein

Chain C: 46% 18% • 34%

M217 K218 I219 D220 A221 I222 V223 G224 A228 K229 R232 E235 R236 A237 R238 V239 V244 L250 H251 G252 G253 I254 R255 I256 S257 D258 Q259 T260 E265 V268 R274 V275 E280 G285 F286 W287 D288 N289 H290 H291 H292 H293 H294 H295

4.2.5 Score per residue for model 5

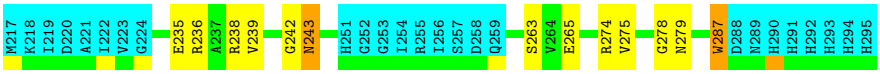
- Molecule 1: Small s protein

Chain A: 49% 15% • 34%

M217 K218 I219 D220 A221 I222 V223 G224 R225 N226 T233 E234 E235 R238 V239 A249 L250 H251 G252 G253 I254 R255 I256 S257 D258 Q259 T260 S263 K270 R274 V275 N279 G282 W287 D288 N289 H290 H291 H292 H293 H294 H295

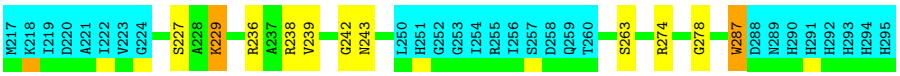
- Molecule 1: Small s protein

Chain B: 52% 14% • 32%



• Molecule 1: Small s protein

Chain C:



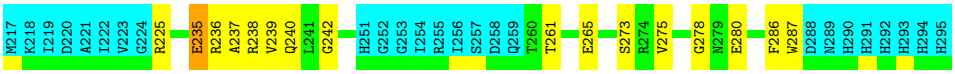
4.2.6 Score per residue for model 6

• Molecule 1: Small s protein

Chain A:

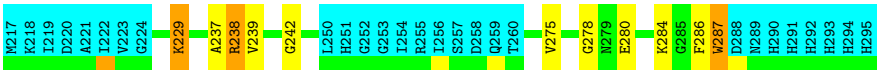
• Molecule 1: Small s protein

Chain B:



• Molecule 1: Small s protein

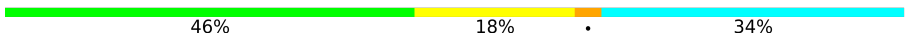
Chain C:

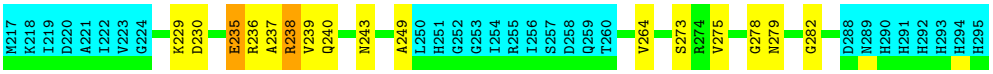


4.2.7 Score per residue for model 7

• Molecule 1: Small s protein

Chain A:





• Molecule 1: Small s protein

Chain B:

• Molecule 1: Small s protein

Chain C: 48% 13% 5% 34%

M217 K218 I219 D220 A221 I222 V223 G224 A228 K229 E235 R236 A237 R238 N243 A249 L250 H251 G252 G253 I254 R255 I256 S257 D258 Q259 T260 G271 E272 S273 R274 N279 G282 G283 K284 D288 N289 H290 H291 H292 H293 H294 H295

4.2.8 Score per residue for model 8

• Molecule 1: Small s protein

Chain A: 57% 8% • 34%

M217 K218 I219 D220 A221 I222 V223 G224 R225 K229 L250 H251 G252 G253 I254 R255 I256 S257 D258 Q259 T260 E272 S273 E280 K284 W287 D288 N289 H290 H291 H292 H293 H294 H295

• Molecule 1: Small s protein

Chain B: 53% 11% • 32%

M217 K218 I219 D220 A221 I222 V223 G224 K229 T233 E234 E235 R236 A237 R238 H251 G252 G253 I254 R255 I256 S257 D258 Q259 K270 G271 E272 S273 R274 Y281 K284 W287 D288 N289 H290 H291 H292 H293 H294 H295

• Molecule 1: Small s protein

Chain C: 51% 11% • 34%

M217 K218 I219 D220 A221 I222 V223 G224 R225 K229 T233 E234 E235 R236 A237 R238 V245 L250 H251 G252 G253 I254 R255 I256 S257 D258 Q259 T260 E272 K284 G285 F286 W287 D288 N289 H290 H291 H292 H293 H294 H295

4.2.9 Score per residue for model 9

• Molecule 1: Small s protein

Chain A: 53% 13% 34%

M217 K218 I219 D220 A221 I222 V223 G224 R232 E235 R236 A237 R238 A249 L250 H251 G252 G253 I254 R255 I256 S257 D258 Q259 T260 V264 V268 L276 G283 K284 D288 N289 H290 H291 H292 H293 H294 H295

• Molecule 1: Small s protein

Chain B: 44% 22% • 32%

W217 K218 I219 D220 A221 I222 V223 G224 A228 K229 R232 T233 R236 V239 Q240 A247 A248 A249 L250 H251 G252 G253 I254 R255 I256 S257 D258 Q259 T260 V264 E265 V268 R274 V275 L276 K284 G285 F286 W287 D288 N289 H290 H291 H292 H293 H294 H295

• Molecule 1: Small s protein

Chain C: 51% 11% • 34%

M217 K218 I219 D220 A221 I222 V223 G224 A228 K229 E235 R236 A237 R238 V239 Q240 A247 L250 H251 G252 G253 I254 R255 I256 S257 D258 Q259 T260 E265 G271 G285 F286 W287 D288 N289 H290 H291 H292 H293 H294 H295

4.2.10 Score per residue for model 10

- Molecule 1: Small s protein

Chain A: 47% 19% 34%

M217 K218 I219 D220 A221 I222 V223 G224 E235 R236 A237 R238 A249 L250 H251 G252 G253 I254 R255 I256 S257 D258 Q259 T260 T261 N262 S263 V264 E265 S273 R274 G278 N279 E280 Y281 G282 G283 K284 W287 D288 N289 H290 H291 H292 H293 H294 H295

- Molecule 1: Small s protein

Chain B: 47% 19% •• 32%

M217 K218 I219 D220 A221 I222 V223 G224 R225 N226 S227 A228 K229 R232 E235 R236 A237 G242 L250 H251 G252 G253 I254 R255 I256 S257 D258 Q259 T260 T261 N262 S263 V264 E272 S273 R274 E280 Y281 W287 D288 N289 H290 H291 H292 H293 H294 H295

- Molecule 1: Small s protein

Chain C: 54% 10% • 34%

M217 K218 I219 D220 A221 I222 V223 G224 R225 A228 K229 E235 R238 V245 L250 H251 G252 G253 I254 R255 I256 S257 D258 Q259 T260 E265 E280 K284 D288 N289 H290 H291 H292 H293 H294 H295

4.2.11 Score per residue for model 11

- Molecule 1: Small s protein

Chain A: 46% 18% •• 34%

M217 K218 I219 D220 A221 I222 V223 G224 R225 R232 T233 E234 E235 R236 A237 R238 L250 H251 G252 G253 I254 R255 I256 S257 D258 Q259 T260 T261 N262 E265 V268 E272 S273 R274 E280 K284 G285 F286 W287 D288 N289 H290 H291 H292 H293 H294 H295

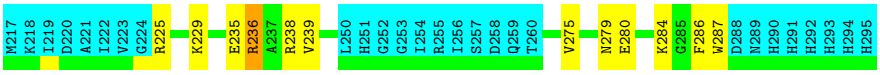
- Molecule 1: Small s protein

Chain B: 51% 15% • 32%

M217 K218 I219 D220 A221 I222 V223 G224 R225 N226 K229 E235 R236 A237 R238 V239 H251 G252 G253 I254 R255 I256 S257 D258 Q259 T260 S273 R274 V275 N279 E280 K284 G285 F286 W287 D288 N289 H290 H291 H292 H293 H294 H295

- Molecule 1: Small s protein

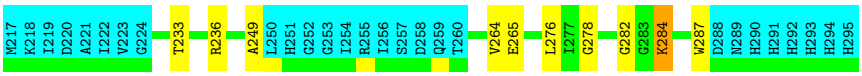
Chain C: 51% 14% • 34%



4.2.12 Score per residue for model 12

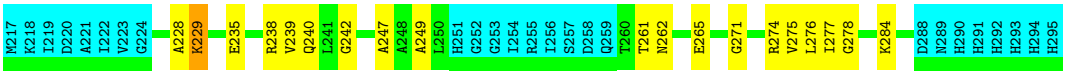
- Molecule 1: Small s protein

Chain A:



- Molecule 1: Small s protein

Chain B:



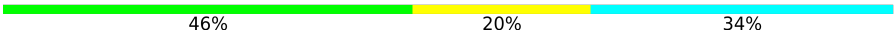
- Molecule 1: Small s protein

Chain C:

4.2.13 Score per residue for model 13 (medoid)

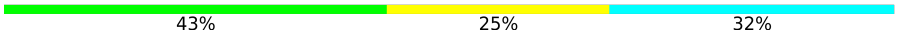
- Molecule 1: Small s protein

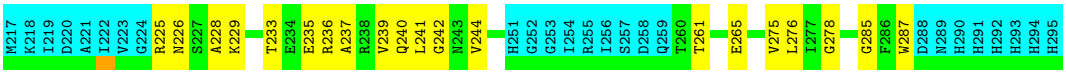
Chain A:



- Molecule 1: Small s protein

Chain B:





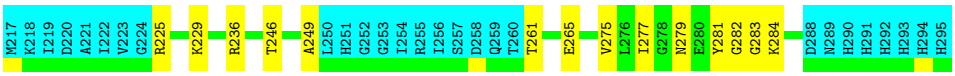
- Molecule 1: Small s protein

Chain C:

4.2.14 Score per residue for model 14

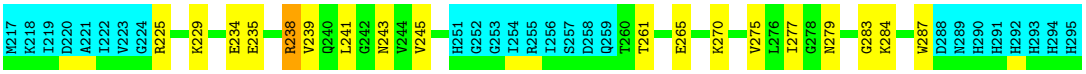
- Molecule 1: Small s protein

Chain A: 48% 18% 34%



- Molecule 1: Small s protein

Chain B: 46% 22% • 32%



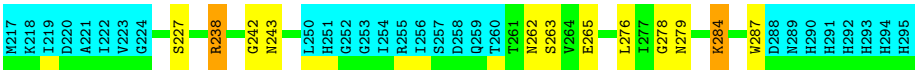
- Molecule 1: Small s protein

Chain C: 51% 14% • 34%

4.2.15 Score per residue for model 15

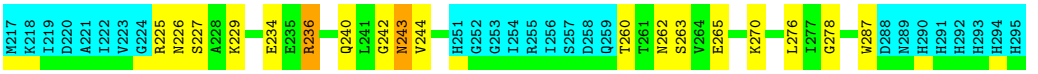
- Molecule 1: Small s protein

Chain A: 51% 13% • 34%



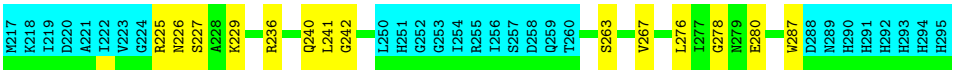
- Molecule 1: Small s protein

Chain B: 46% 20% • 32%



- Molecule 1: Small s protein

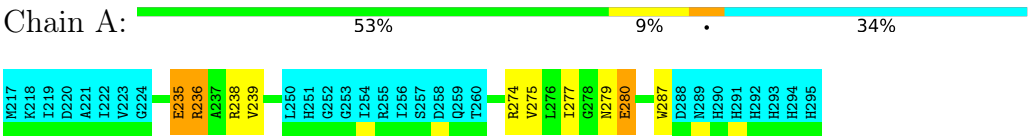
Chain C: 48% 18% 34%



4.2.16 Score per residue for model 16

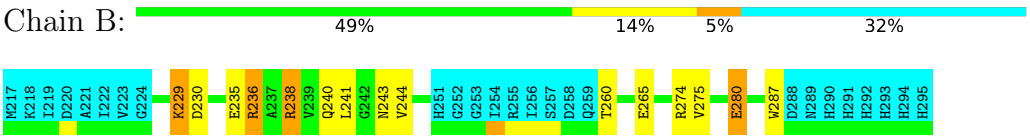
- Molecule 1: Small s protein

Chain A:



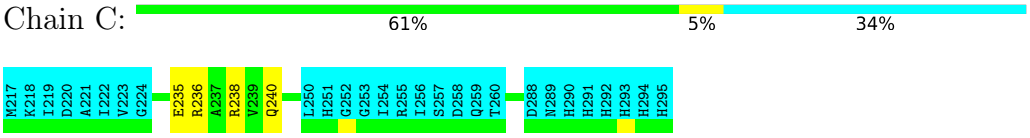
- Molecule 1: Small s protein

Chain B:



- Molecule 1: Small s protein

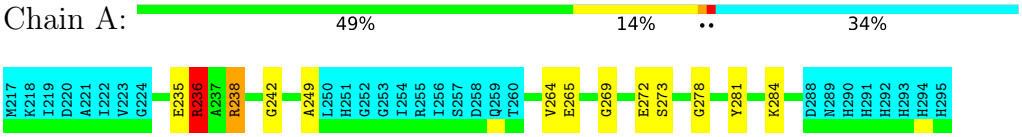
Chain C:



4.2.17 Score per residue for model 17

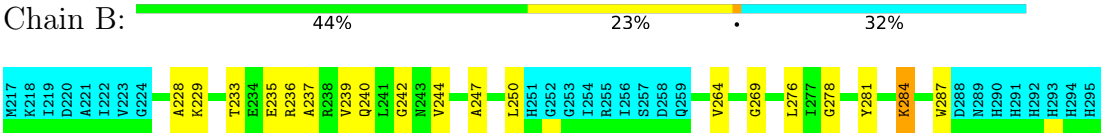
- Molecule 1: Small s protein

Chain A:



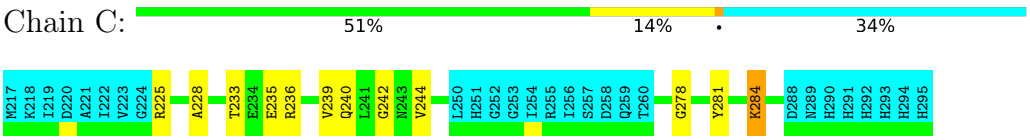
- Molecule 1: Small s protein

Chain B:



- Molecule 1: Small s protein

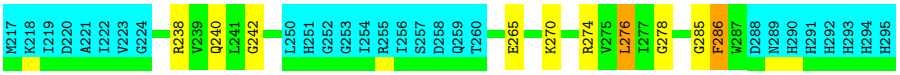
Chain C:



4.2.18 Score per residue for model 18

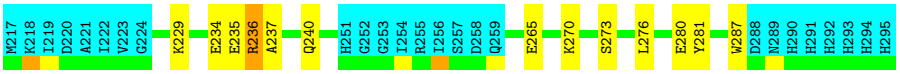
- Molecule 1: Small s protein

Chain A: 53% 10% • 34%



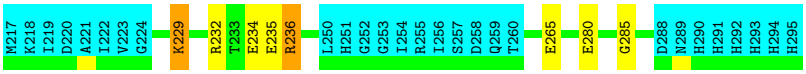
- Molecule 1: Small s protein

Chain B: 52% 15% • 32%



- Molecule 1: Small s protein

Chain C: 56% 8% • 34%



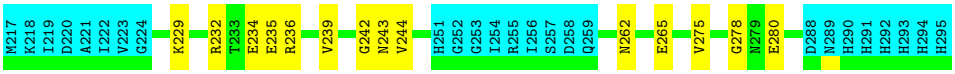
4.2.19 Score per residue for model 19

- Molecule 1: Small s protein

Chain A: 53% 11% • 34%

- Molecule 1: Small s protein

Chain B: 51% 18% 32%



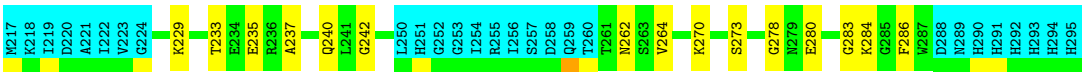
- Molecule 1: Small s protein

Chain C: 52% 13% • 34%

4.2.20 Score per residue for model 20

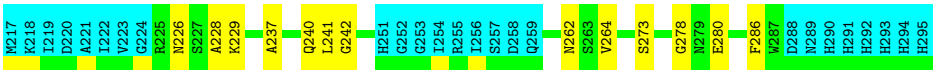
- Molecule 1: Small s protein

Chain A: 47% 19% 34%



- Molecule 1: Small s protein

Chain B: 52% 16% 32%



- Molecule 1: Small s protein

Chain C: 48% 16% • 34%

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing, TORSION ANGLE DYNAMICS.*

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
CYANA	structure calculation	
CNS	refinement	

No chemical shift data was provided. 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.

6 Model quality (i)

6.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.93±0.04	0±0/397 (0.0± 0.0%)	0.72±0.04	0±0/535 (0.0± 0.0%)
1	B	1.02±0.04	0±0/412 (0.0± 0.0%)	0.77±0.04	0±0/556 (0.0± 0.0%)
1	C	0.98±0.03	0±0/397 (0.0± 0.0%)	0.75±0.04	0±0/535 (0.0± 0.0%)
All	All	0.98	0/24120 (0.0%)	0.75	2/32520 (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	B	0.0±0.0	0.3±0.6
1	A	0.0±0.0	0.4±0.8
1	C	0.0±0.0	0.4±0.7
All	All	0	22

There are no bond-length outliers.

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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	B	232	ARG	CD-NE-CZ	5.51	131.31	123.60	10	1
1	A	225	ARG	NE-CZ-NH1	5.41	123.00	120.30	11	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)
1	C	236	ARG	Sidechain	4
1	A	238	ARG	Sidechain	4

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Mol	Chain	Res	Type	Group	Models (Total)
1	B	274	ARG	Sidechain	3
1	C	238	ARG	Sidechain	2
1	B	238	ARG	Sidechain	2
1	A	274	ARG	Sidechain	2
1	C	225	ARG	Sidechain	1
1	B	232	ARG	Sidechain	1
1	A	225	ARG	Sidechain	1
1	A	236	ARG	Sidechain	1
1	C	232	ARG	Sidechain	1

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	393	394	394	7±2
1	B	408	412	412	11±3
1	C	393	394	394	6±2
All	All	23880	24000	24000	357

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 7.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:239:VAL:HG12	1:A:275:VAL:HB	0.76	1.57	5	2
1:B:239:VAL:HG12	1:B:275:VAL:HB	0.62	1.70	11	4
1:C:244:VAL:HG11	1:C:285:GLY:HA3	0.61	1.73	4	1
1:B:276:LEU:HB3	1:B:287:TRP:CH2	0.60	2.31	13	1
1:B:274:ARG:O	1:C:238:ARG:HA	0.60	1.97	16	2
1:B:240:GLN:HB2	1:B:286:PHE:CE2	0.59	2.33	6	1
1:B:242:GLY:O	1:B:278:GLY:HA3	0.59	1.98	13	10
1:A:265:GLU:HB3	1:B:229:LYS:O	0.58	1.98	11	5
1:B:244:VAL:HG11	1:B:285:GLY:HA3	0.58	1.75	4	1
1:B:277:ILE:HG22	1:C:241:LEU:HB3	0.57	1.75	3	2
1:A:267:VAL:HG12	1:B:231:ILE:HD12	0.57	1.76	3	1
1:C:276:LEU:HB3	1:C:287:TRP:CH2	0.57	2.34	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:278:GLY:O	1:B:242:GLY:HA3	0.57	2.00	7	7
1:B:262:ASN:HA	1:C:226:ASN:O	0.56	2.01	15	2
1:B:233:THR:HG21	1:B:239:VAL:HG22	0.56	1.76	9	1
1:B:264:VAL:HA	1:C:228:ALA:O	0.55	2.02	20	6
1:C:229:LYS:HB2	1:C:265:GLU:O	0.55	2.01	4	1
1:B:284:LYS:O	1:B:284:LYS:HD2	0.55	2.02	17	1
1:A:264:VAL:HA	1:B:228:ALA:O	0.55	2.01	1	9
1:B:232:ARG:NH1	1:B:232:ARG:HB2	0.55	2.17	10	1
1:B:225:ARG:O	1:B:261:THR:HA	0.54	2.02	6	1
1:C:242:GLY:O	1:C:278:GLY:HA3	0.54	2.02	6	8
1:A:270:LYS:O	1:B:234:GLU:HA	0.54	2.02	18	1
1:A:265:GLU:HB2	1:B:229:LYS:O	0.53	2.04	3	6
1:A:287:TRP:CH2	1:B:240:GLN:HB2	0.53	2.39	16	2
1:A:276:LEU:HG	1:B:240:GLN:OE1	0.53	2.03	9	1
1:A:242:GLY:O	1:A:278:GLY:HA3	0.53	2.04	13	9
1:A:249:ALA:HB2	1:A:282:GLY:N	0.53	2.19	5	1
1:A:261:THR:O	1:B:225:ARG:HA	0.53	2.03	13	2
1:A:233:THR:HB	1:A:237:ALA:CB	0.53	2.34	11	1
1:C:284:LYS:HD2	1:C:284:LYS:O	0.52	2.04	17	1
1:B:240:GLN:HB2	1:B:286:PHE:CD1	0.52	2.39	20	1
1:B:279:ASN:HA	1:C:243:ASN:O	0.52	2.05	5	2
1:A:262:ASN:HA	1:B:226:ASN:O	0.52	2.05	1	5
1:A:274:ARG:O	1:B:238:ARG:HA	0.52	2.04	16	2
1:A:273:SER:HA	1:B:237:ALA:O	0.52	2.05	20	5
1:C:238:ARG:O	1:C:274:ARG:HA	0.52	2.05	12	5
1:C:227:SER:O	1:C:263:SER:HA	0.51	2.04	2	4
1:A:237:ALA:HA	1:A:273:SER:O	0.51	2.05	2	3
1:C:229:LYS:HB3	1:C:265:GLU:O	0.51	2.05	18	6
1:B:287:TRP:CH2	1:C:240:GLN:HB2	0.51	2.40	15	2
1:B:237:ALA:HA	1:B:273:SER:O	0.51	2.06	18	5
1:A:277:ILE:HG23	1:B:241:LEU:HD12	0.51	1.82	13	3
1:B:249:ALA:HA	1:C:247:ALA:HB2	0.51	1.81	1	3
1:C:249:ALA:HB2	1:C:282:GLY:HA2	0.51	1.83	7	1
1:A:236:ARG:HD2	1:A:272:GLU:OE2	0.51	2.05	11	1
1:B:273:SER:HA	1:C:237:ALA:O	0.50	2.05	4	3
1:B:276:LEU:HG	1:C:240:GLN:OE1	0.50	2.07	9	2
1:C:240:GLN:HG2	1:C:244:VAL:CG2	0.50	2.37	2	4
1:A:285:GLY:HA3	1:A:287:TRP:CZ3	0.50	2.41	19	1
1:B:265:GLU:HB3	1:C:229:LYS:O	0.50	2.07	18	3
1:B:233:THR:HB	1:B:237:ALA:HB3	0.50	1.84	13	1
1:C:236:ARG:N	1:C:236:ARG:HD3	0.49	2.22	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:270:LYS:O	1:C:234:GLU:HA	0.49	2.07	18	2
1:A:287:TRP:HA	1:A:287:TRP:CE3	0.49	2.42	5	1
1:C:239:VAL:HG12	1:C:275:VAL:HB	0.49	1.82	11	1
1:B:235:GLU:C	1:B:236:ARG:HD3	0.49	2.28	7	3
1:B:240:GLN:CG	1:B:276:LEU:HD13	0.49	2.37	12	6
1:A:235:GLU:HB3	1:A:236:ARG:NH1	0.49	2.23	7	3
1:A:249:ALA:HA	1:B:247:ALA:HB2	0.49	1.83	12	5
1:B:272:GLU:HB3	1:C:236:ARG:H	0.49	1.68	4	1
1:A:233:THR:HG21	1:A:239:VAL:HG13	0.49	1.84	5	1
1:A:279:ASN:HA	1:B:243:ASN:O	0.49	2.07	5	3
1:B:249:ALA:HB2	1:B:282:GLY:HA2	0.49	1.83	7	1
1:B:238:ARG:O	1:B:274:ARG:HA	0.49	2.08	4	2
1:A:269:GLY:HA2	1:B:233:THR:O	0.49	2.08	4	1
1:C:243:ASN:HA	1:C:279:ASN:O	0.49	2.08	7	1
1:B:277:ILE:HG23	1:C:241:LEU:HD12	0.48	1.85	14	2
1:B:278:GLY:O	1:C:242:GLY:HA3	0.48	2.08	20	2
1:B:284:LYS:HB3	1:B:287:TRP:O	0.48	2.07	9	1
1:A:276:LEU:HB3	1:A:287:TRP:CH2	0.48	2.43	13	1
1:B:239:VAL:HA	1:B:275:VAL:O	0.48	2.08	6	3
1:B:243:ASN:HD22	1:B:244:VAL:N	0.48	2.06	15	1
1:B:232:ARG:HB2	1:B:232:ARG:HH11	0.48	1.68	10	1
1:A:235:GLU:C	1:A:236:ARG:HD2	0.48	2.29	16	1
1:B:232:ARG:HD3	1:B:234:GLU:OE2	0.48	2.08	19	1
1:B:243:ASN:OD1	1:B:245:VAL:HG23	0.48	2.09	1	1
1:C:225:ARG:O	1:C:261:THR:HA	0.48	2.09	2	1
1:B:235:GLU:C	1:B:236:ARG:HD2	0.48	2.29	16	3
1:C:284:LYS:HB2	1:C:287:TRP:O	0.48	2.09	8	1
1:B:236:ARG:N	1:B:236:ARG:HD3	0.47	2.24	11	2
1:B:261:THR:O	1:C:225:ARG:HA	0.47	2.10	2	3
1:B:287:TRP:HA	1:B:287:TRP:CE3	0.47	2.44	5	1
1:A:232:ARG:O	1:A:268:VAL:HA	0.47	2.10	3	3
1:C:286:PHE:HB3	1:C:287:TRP:CE3	0.47	2.44	9	1
1:C:240:GLN:CG	1:C:276:LEU:HD13	0.47	2.40	15	3
1:A:246:THR:OG1	1:A:282:GLY:HA3	0.47	2.08	14	1
1:A:244:VAL:HG11	1:A:285:GLY:HA3	0.47	1.86	4	1
1:C:237:ALA:HA	1:C:273:SER:O	0.47	2.10	7	1
1:C:235:GLU:C	1:C:236:ARG:HD2	0.47	2.31	8	2
1:B:229:LYS:HB3	1:B:265:GLU:O	0.46	2.10	14	7
1:C:284:LYS:HA	1:C:287:TRP:NE1	0.46	2.25	3	1
1:C:235:GLU:C	1:C:236:ARG:HD3	0.46	2.31	1	2
1:C:280:GLU:HG2	1:C:287:TRP:NE1	0.46	2.24	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:284:LYS:NZ	1:C:284:LYS:HB2	0.46	2.25	10	1
1:B:244:VAL:CG1	1:B:285:GLY:HA3	0.46	2.40	4	1
1:B:263:SER:O	1:C:227:SER:HA	0.46	2.11	2	3
1:A:243:ASN:ND2	1:A:279:ASN:HD22	0.46	2.08	15	1
1:C:284:LYS:HA	1:C:287:TRP:O	0.46	2.11	6	1
1:B:240:GLN:HG3	1:B:276:LEU:HD13	0.46	1.87	13	2
1:A:262:ASN:OD1	1:B:226:ASN:HB3	0.46	2.11	13	1
1:B:236:ARG:HD3	1:B:236:ARG:N	0.46	2.25	1	1
1:B:240:GLN:HG2	1:B:244:VAL:CG2	0.46	2.41	2	4
1:B:265:GLU:HB2	1:C:229:LYS:O	0.46	2.11	9	4
1:B:232:ARG:O	1:B:268:VAL:HA	0.46	2.11	9	1
1:A:249:ALA:HB2	1:A:282:GLY:HA2	0.45	1.88	12	4
1:C:240:GLN:HG3	1:C:276:LEU:HD13	0.45	1.87	12	1
1:A:281:TYR:HA	1:B:245:VAL:O	0.45	2.10	14	1
1:B:275:VAL:HG13	1:C:239:VAL:HG23	0.45	1.89	5	1
1:B:284:LYS:HB2	1:B:287:TRP:O	0.45	2.11	17	1
1:B:280:GLU:O	1:C:244:VAL:HA	0.45	2.12	2	2
1:B:243:ASN:HA	1:B:279:ASN:O	0.45	2.11	7	1
1:A:226:ASN:HA	1:A:262:ASN:O	0.45	2.12	2	2
1:C:235:GLU:HB3	1:C:236:ARG:NH1	0.45	2.26	1	2
1:A:280:GLU:O	1:B:244:VAL:HA	0.45	2.12	2	3
1:B:281:TYR:HA	1:C:245:VAL:O	0.45	2.12	10	1
1:B:283:GLY:O	1:B:284:LYS:HE2	0.45	2.12	4	1
1:A:226:ASN:OD1	1:B:242:GLY:HA2	0.45	2.11	5	1
1:C:230:ASP:O	1:C:266:THR:HA	0.45	2.12	20	1
1:B:284:LYS:HA	1:B:287:TRP:NE1	0.44	2.26	3	1
1:C:287:TRP:CE3	1:C:287:TRP:HA	0.44	2.46	5	1
1:B:261:THR:CG2	1:C:225:ARG:HG2	0.44	2.42	12	1
1:B:262:ASN:ND2	1:C:226:ASN:HB3	0.44	2.27	12	1
1:A:240:GLN:HB2	1:A:286:PHE:CD1	0.44	2.47	20	1
1:B:240:GLN:HG3	1:B:276:LEU:CD1	0.44	2.42	9	1
1:A:239:VAL:HA	1:A:275:VAL:O	0.44	2.12	3	4
1:A:239:VAL:HG22	1:A:275:VAL:CG2	0.44	2.42	13	1
1:B:227:SER:O	1:B:263:SER:HA	0.44	2.12	15	2
1:A:283:GLY:O	1:A:284:LYS:HG2	0.44	2.12	9	1
1:B:283:GLY:O	1:C:286:PHE:HA	0.44	2.12	2	1
1:B:229:LYS:HB2	1:B:265:GLU:O	0.44	2.13	4	1
1:A:275:VAL:HG12	1:B:239:VAL:CG1	0.44	2.42	14	1
1:A:284:LYS:HA	1:A:287:TRP:NE1	0.44	2.28	8	1
1:B:281:TYR:CD1	1:C:245:VAL:HG13	0.43	2.48	8	1
1:A:225:ARG:HG2	1:A:225:ARG:HH11	0.43	1.73	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:234:GLU:O	1:B:270:LYS:HA	0.43	2.13	14	1
1:A:269:GLY:HA2	1:B:233:THR:OG1	0.43	2.14	17	1
1:A:227:SER:O	1:A:263:SER:HA	0.43	2.13	15	1
1:B:262:ASN:HD21	1:C:241:LEU:HG	0.43	1.74	15	1
1:B:272:GLU:HB2	1:C:235:GLU:O	0.43	2.13	3	1
1:C:284:LYS:HA	1:C:287:TRP:CD1	0.43	2.49	3	1
1:B:274:ARG:HB3	1:B:286:PHE:CE1	0.43	2.49	9	1
1:A:274:ARG:HB3	1:A:287:TRP:CE3	0.43	2.49	10	1
1:B:284:LYS:HA	1:B:287:TRP:CD1	0.43	2.49	8	1
1:B:274:ARG:HB3	1:B:287:TRP:CE3	0.43	2.48	10	1
1:B:229:LYS:HE2	1:B:265:GLU:OE2	0.43	2.14	16	1
1:A:285:GLY:HA3	1:A:287:TRP:CE3	0.43	2.49	19	1
1:B:280:GLU:HG2	1:B:287:TRP:CZ2	0.42	2.49	1	1
1:A:285:GLY:HA2	1:B:287:TRP:CD1	0.42	2.48	18	1
1:C:239:VAL:HA	1:C:275:VAL:O	0.42	2.14	6	2
1:B:226:ASN:HD21	1:B:277:ILE:HG22	0.42	1.75	2	1
1:C:233:THR:HG22	1:C:239:VAL:HG21	0.42	1.91	17	1
1:C:232:ARG:O	1:C:268:VAL:HA	0.42	2.14	4	2
1:A:276:LEU:HD23	1:A:287:TRP:CH2	0.42	2.50	15	1
1:A:229:LYS:HB3	1:A:265:GLU:O	0.42	2.15	19	1
1:A:283:GLY:C	1:A:284:LYS:HD2	0.42	2.35	20	1
1:B:234:GLU:HB2	1:B:270:LYS:HE3	0.42	1.91	15	1
1:C:240:GLN:HG2	1:C:244:VAL:HG23	0.42	1.91	2	1
1:B:239:VAL:HG23	1:B:275:VAL:HB	0.42	1.90	14	1
1:A:276:LEU:HB2	1:A:286:PHE:CZ	0.42	2.50	18	1
1:A:233:THR:OG1	1:A:237:ALA:HB1	0.42	2.15	20	1
1:B:226:ASN:HA	1:B:262:ASN:O	0.41	2.15	10	1
1:C:276:LEU:HD12	1:C:287:TRP:CZ3	0.41	2.50	14	1
1:B:269:GLY:HA2	1:C:233:THR:OG1	0.41	2.15	17	1
1:B:287:TRP:CZ2	1:C:238:ARG:HB2	0.41	2.51	6	1
1:A:243:ASN:HA	1:A:279:ASN:O	0.41	2.14	7	1
1:C:233:THR:HB	1:C:237:ALA:HB3	0.41	1.91	13	1
1:C:240:GLN:HB2	1:C:286:PHE:CD1	0.41	2.50	20	1
1:A:229:LYS:HB2	1:A:265:GLU:O	0.41	2.15	4	1
1:A:280:GLU:HB2	1:B:240:GLN:NE2	0.41	2.30	16	1
1:A:276:LEU:HB3	1:A:287:TRP:CZ2	0.41	2.50	12	1
1:A:229:LYS:HE2	1:A:265:GLU:O	0.41	2.16	14	1
1:B:276:LEU:HB3	1:C:240:GLN:OE1	0.41	2.16	2	1
1:B:240:GLN:HB2	1:B:286:PHE:CD2	0.41	2.49	6	1
1:B:233:THR:HG22	1:B:239:VAL:HG21	0.41	1.93	17	1
1:A:279:ASN:OD1	1:B:243:ASN:HB3	0.41	2.15	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:246:THR:OG1	1:C:282:GLY:HA3	0.41	2.16	14	1
1:A:233:THR:CG2	1:A:239:VAL:HG13	0.41	2.45	5	1
1:B:272:GLU:HB3	1:C:235:GLU:O	0.41	2.16	10	1
1:A:275:VAL:HG12	1:B:239:VAL:HB	0.41	1.93	13	1
1:B:260:THR:HB	1:C:225:ARG:O	0.41	2.15	15	1
1:A:277:ILE:HG22	1:B:241:LEU:HB3	0.41	1.91	16	1
1:C:283:GLY:C	1:C:284:LYS:HD2	0.41	2.36	20	1
1:A:249:ALA:HB2	1:A:282:GLY:HA3	0.41	1.92	10	1
1:C:276:LEU:HD12	1:C:286:PHE:CB	0.40	2.46	1	1
1:B:261:THR:HG23	1:C:225:ARG:HB3	0.40	1.93	10	1
1:B:239:VAL:HG12	1:B:275:VAL:HG22	0.40	1.91	12	1
1:A:240:GLN:HB3	1:A:276:LEU:HD22	0.40	1.92	18	1
1:A:261:THR:HB	1:B:225:ARG:HD2	0.40	1.94	2	1
1:B:226:ASN:OD1	1:B:262:ASN:HB3	0.40	2.16	1	1
1:B:245:VAL:HG21	1:B:250:LEU:O	0.40	2.15	2	1
1:B:287:TRP:CZ2	1:C:286:PHE:HD1	0.40	2.34	3	1
1:B:280:GLU:HB2	1:C:240:GLN:NE2	0.40	2.31	16	1
1:A:236:ARG:HD3	1:A:272:GLU:OE2	0.40	2.17	17	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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	52/79 (66%)	46±2 (88±3%)	5±1 (10±3%)	1±1 (2±2%)	10	49
1	B	54/79 (68%)	46±1 (86±3%)	6±2 (12±3%)	1±1 (3±2%)	8	44
1	C	52/79 (66%)	46±1 (88±3%)	6±1 (11±3%)	1±1 (2±2%)	12	54
All	All	3160/4740 (67%)	2753 (87%)	337 (11%)	70 (2%)	10	49

All 19 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	235	GLU	13

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Mol	Chain	Res	Type	Models (Total)
1	A	235	GLU	13
1	C	235	GLU	10
1	A	284	LYS	6
1	B	284	LYS	4
1	B	250	LEU	3
1	C	271	GLY	3
1	C	286	PHE	2
1	B	271	GLY	2
1	C	285	GLY	2
1	B	285	GLY	2
1	A	286	PHE	2
1	C	284	LYS	2
1	B	272	GLU	1
1	A	287	TRP	1
1	B	286	PHE	1
1	A	283	GLY	1
1	B	283	GLY	1
1	B	287	TRP	1

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	40/63 (63%)	37±1 (94±3%)	3±1 (6±3%)	21	69
1	B	42/63 (67%)	39±2 (93±4%)	3±2 (7±4%)	19	68
1	C	40/63 (63%)	37±2 (93±4%)	3±2 (7±4%)	19	68
All	All	2440/3780 (65%)	2276 (93%)	164 (7%)	20	68

All 52 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	B	236	ARG	14
1	C	236	ARG	11
1	A	238	ARG	11
1	C	229	LYS	11
1	A	280	GLU	9

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Mol	Chain	Res	Type	Models (Total)
1	A	236	ARG	8
1	B	280	GLU	8
1	C	238	ARG	8
1	A	284	LYS	7
1	C	280	GLU	6
1	B	229	LYS	6
1	B	238	ARG	5
1	C	286	PHE	3
1	C	287	TRP	3
1	A	229	LYS	3
1	A	225	ARG	3
1	B	272	GLU	2
1	B	284	LYS	2
1	C	272	GLU	2
1	B	225	ARG	2
1	B	275	VAL	2
1	A	287	TRP	2
1	B	287	TRP	2
1	A	270	LYS	2
1	B	243	ASN	2
1	C	279	ASN	2
1	B	260	THR	2
1	A	233	THR	2
1	B	286	PHE	1
1	A	230	ASP	1
1	A	240	GLN	1
1	C	274	ARG	1
1	A	272	GLU	1
1	B	233	THR	1
1	B	274	ARG	1
1	C	233	THR	1
1	B	232	ARG	1
1	B	279	ASN	1
1	C	225	ARG	1
1	C	270	LYS	1
1	C	267	VAL	1
1	B	230	ASP	1
1	B	250	LEU	1
1	B	281	TYR	1
1	C	281	TYR	1
1	C	284	LYS	1
1	A	276	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	262	ASN	1
1	B	262	ASN	1
1	B	241	LEU	1
1	C	240	GLN	1
1	C	241	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 monosaccharides 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 (i)

No chemical shift data were provided