



wwPDB NMR Structure Validation Summary Report ⓘ

Mar 11, 2018 – 05:10 pm GMT

PDB ID : 2LMQ
Title : Structural Model for a 40-residue Beta-Amyloid Fibril with Three-Fold Symmetry, Negative Stagger
Authors : Tycko, R.; Paravastu, A.
Deposited on : 2011-12-09

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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 : 20171227.v01 (using entries in the PDB archive December 27th 2017)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk31020
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

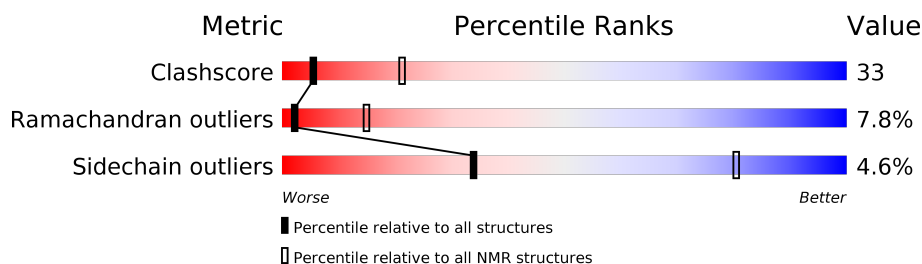
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLID-STATE NMR

The overall completeness of chemical shifts assignment is 1%.

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	136327	12091
Ramachandran outliers	132723	10835
Sidechain outliers	132532	10811

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	40	43% 25% 13% 20%
1	B	40	23% 55% • 20%
1	C	40	35% 45% 20%
1	D	40	23% 48% • 8% 20%
1	E	40	30% 45% • • 20%
1	F	40	30% 30% 20% 20%
1	G	40	40% 25% 15% 20%
1	H	40	35% 43% • 20%
1	I	40	35% 45% 20%

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Mol	Chain	Length	Quality of chain
1	J	40	
1	K	40	
1	L	40	
1	M	40	
1	N	40	
1	O	40	
1	P	40	
1	Q	40	
1	R	40	

2 Ensemble composition and analysis

This entry contains 10 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:11-A:23, A:27-A:40, B:9-B:40, C:9-C:40, D:12- D:40, E:9-E:39, F:11-F:23, F:30-F:40, G:12-G:23, G:27-G:40, H:9-H:40, I:9- I:40, J:9-J:40, K:9-K:39, L:11-L:39, M:11-M:40, N:9- N:40, O:9-O:40, P:12-P:40, Q:9-Q:40, R:9-R:40 (544)	1.55	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 2 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 7, 9, 10
2	5, 6, 8

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 8550 atoms, of which 4266 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Beta-amyloid protein 40.

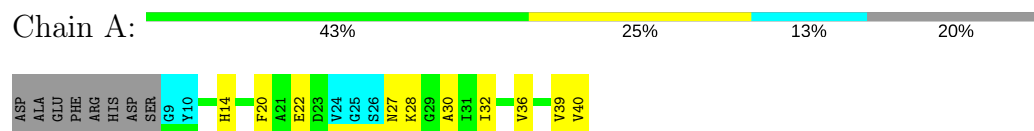
Mol	Chain	Residues	Atoms						Trace
1	A	32	Total	C	H	N	O	S	0
			475	154	237	40	43	1	
1	B	32	Total	C	H	N	O	S	0
			475	154	237	40	43	1	
1	C	32	Total	C	H	N	O	S	0
			475	154	237	40	43	1	
1	D	32	Total	C	H	N	O	S	0
			475	154	237	40	43	1	
1	E	32	Total	C	H	N	O	S	0
			475	154	237	40	43	1	
1	F	32	Total	C	H	N	O	S	0
			475	154	237	40	43	1	
1	G	32	Total	C	H	N	O	S	0
			475	154	237	40	43	1	
1	H	32	Total	C	H	N	O	S	0
			475	154	237	40	43	1	
1	I	32	Total	C	H	N	O	S	0
			475	154	237	40	43	1	
1	J	32	Total	C	H	N	O	S	0
			475	154	237	40	43	1	
1	K	32	Total	C	H	N	O	S	0
			475	154	237	40	43	1	
1	L	32	Total	C	H	N	O	S	0
			475	154	237	40	43	1	
1	M	32	Total	C	H	N	O	S	0
			475	154	237	40	43	1	
1	N	32	Total	C	H	N	O	S	0
			475	154	237	40	43	1	
1	O	32	Total	C	H	N	O	S	0
			475	154	237	40	43	1	
1	P	32	Total	C	H	N	O	S	0
			475	154	237	40	43	1	
1	Q	32	Total	C	H	N	O	S	0
			475	154	237	40	43	1	
1	R	32	Total	C	H	N	O	S	0
			475	154	237	40	43	1	

4 Residue-property plots [i](#)

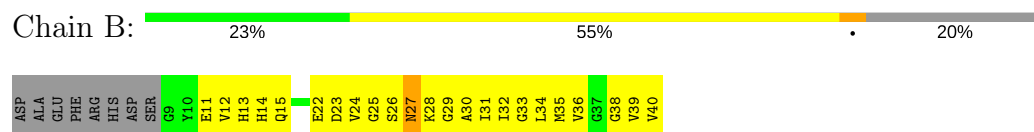
4.1 Average score per residue in the NMR ensemble

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.

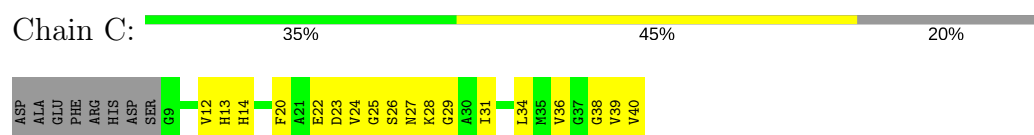
- Molecule 1: Beta-amyloid protein 40



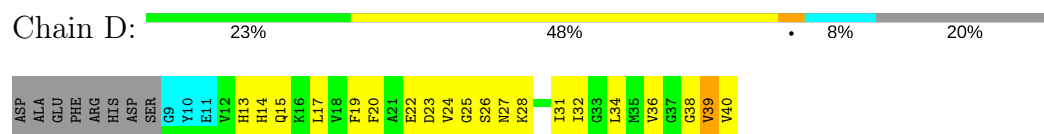
- Molecule 1: Beta-amyloid protein 40



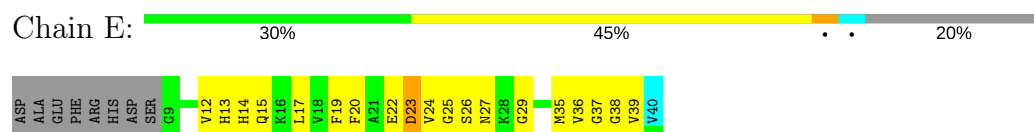
- Molecule 1: Beta-amyloid protein 40



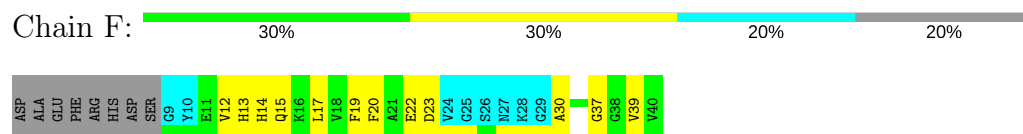
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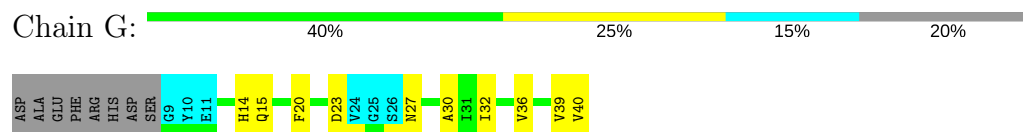
- Molecule 1: Beta-amyloid protein 40



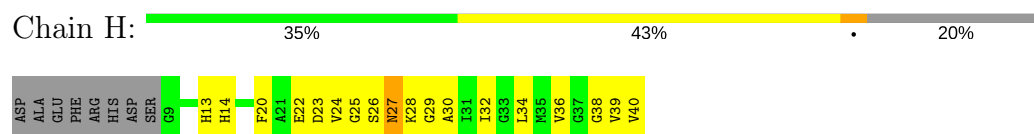
- Molecule 1: Beta-amyloid protein 40



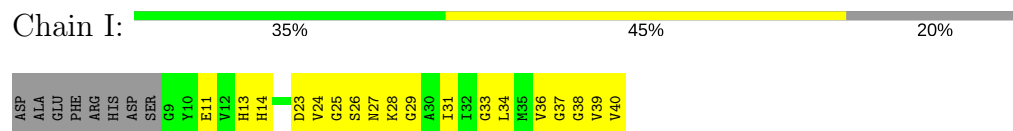
- Molecule 1: Beta-amyloid protein 40



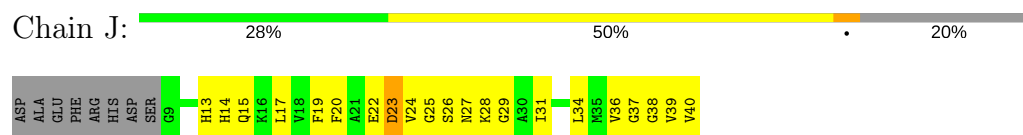
- Molecule 1: Beta-amyloid protein 40



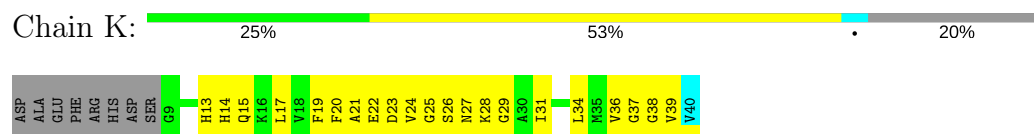
- Molecule 1: Beta-amyloid protein 40



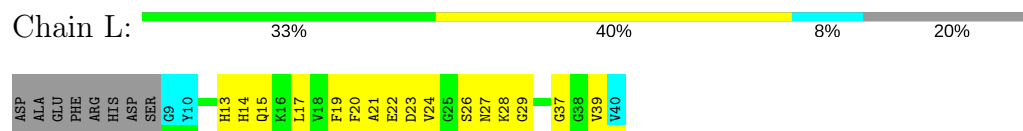
- Molecule 1: Beta-amyloid protein 40



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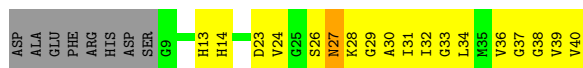


- Molecule 1: Beta-amyloid protein 40

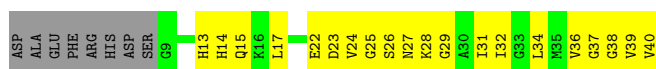




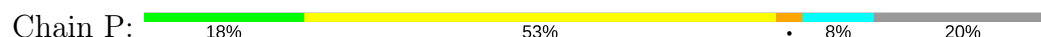
- Molecule 1: Beta-amyloid protein 40



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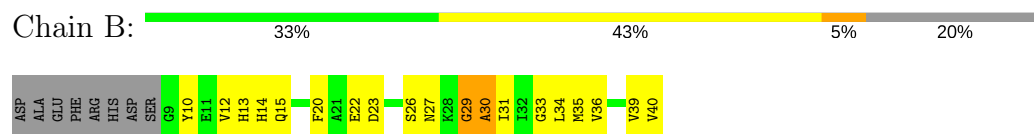
4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 1. Colouring as in section 4.1 above.

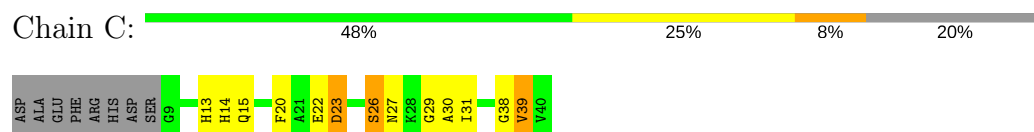
- Molecule 1: Beta-amyloid protein 40



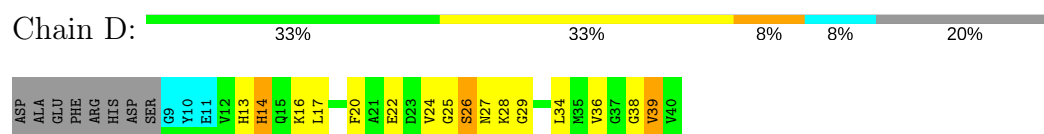
• Molecule 1: Beta-amyloid protein 40



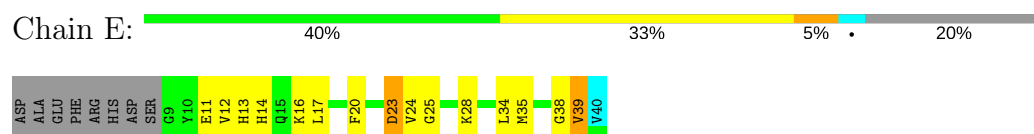
• Molecule 1: Beta-amyloid protein 40



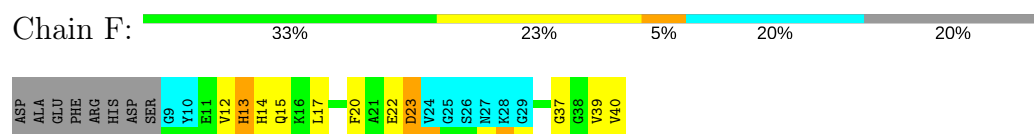
• Molecule 1: Beta-amyloid protein 40



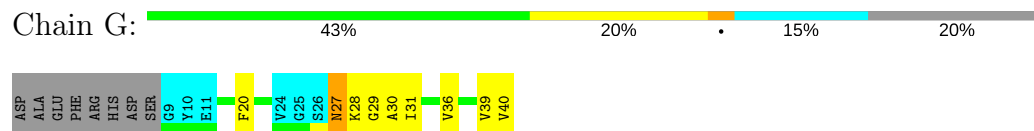
• Molecule 1: Beta-amyloid protein 40



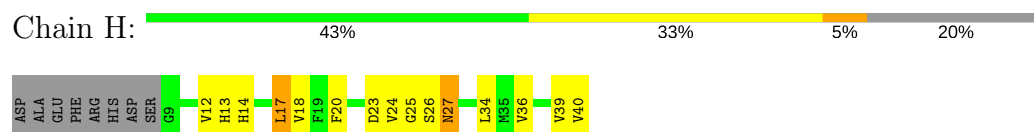
• Molecule 1: Beta-amyloid protein 40



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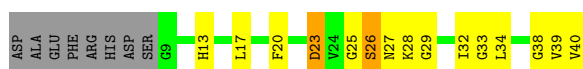


• Molecule 1: Beta-amyloid protein 40



• Molecule 1: Beta-amyloid protein 40





- Molecule 1: Beta-amyloid protein 40



- Molecule 1: Beta-amyloid protein 40



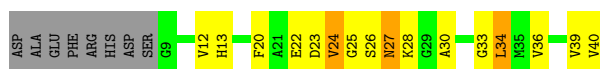
- Molecule 1: Beta-amyloid protein 40



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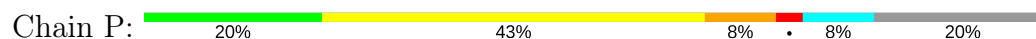
- Molecule 1: Beta-amyloid protein 40



- Molecule 1: Beta-amyloid protein 40

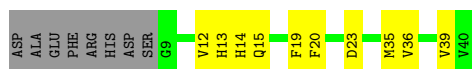


- Molecule 1: Beta-amyloid protein 40



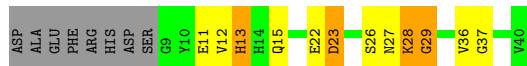
- Molecule 1: Beta-amyloid protein 40

Chain Q:  55% 25% 20%



- Molecule 1: Beta-amyloid protein 40

Chain R:  50% 20% 10% 20%



5 Refinement protocol and experimental data overview

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

Of the 40 calculated structures, 10 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
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)	2lmq_cs.str
Number of chemical shift lists	1
Total number of shifts	90
Number of shifts mapped to atoms	90
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	1%

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 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	0.67±0.02	0±0/208 (0.0±0.0%)	0.82±0.03	0±0/277 (0.0±0.0%)
1	B	0.70±0.03	0±0/242 (0.0±0.0%)	0.84±0.04	0±0/323 (0.0±0.0%)
1	C	0.73±0.01	0±0/242 (0.0±0.0%)	0.85±0.04	0±0/323 (0.0±0.0%)
1	D	0.66±0.02	0±0/216 (0.0±0.0%)	0.83±0.04	0±0/288 (0.0±0.0%)
1	E	0.73±0.02	0±0/235 (0.0±0.0%)	0.83±0.06	0±0/316 (0.0±0.0%)
1	F	0.71±0.04	0±0/187 (0.0±0.0%)	0.78±0.05	0±0/250 (0.0±0.0%)
1	G	0.61±0.01	0±0/199 (0.0±0.0%)	0.81±0.03	0±0/265 (0.0±0.0%)
1	H	0.69±0.03	0±0/242 (0.0±0.0%)	0.84±0.04	0±0/323 (0.0±0.0%)
1	I	0.76±0.03	0±0/242 (0.0±0.0%)	0.90±0.08	0±0/323 (0.0±0.0%)
1	J	0.74±0.02	0±0/242 (0.0±0.0%)	0.92±0.06	0±0/323 (0.0±0.1%)
1	K	0.73±0.02	0±0/235 (0.0±0.0%)	0.82±0.05	0±0/316 (0.0±0.0%)
1	L	0.69±0.02	0±0/218 (0.0±0.0%)	0.76±0.02	0±0/293 (0.0±0.0%)
1	M	0.64±0.01	0±0/225 (0.0±0.0%)	0.80±0.03	0±0/300 (0.0±0.0%)
1	N	0.69±0.02	0±0/242 (0.0±0.0%)	0.82±0.03	0±0/323 (0.0±0.0%)
1	O	0.73±0.03	0±0/242 (0.0±0.0%)	0.88±0.06	0±0/323 (0.0±0.0%)
1	P	0.67±0.03	0±0/216 (0.0±0.0%)	0.88±0.04	0±0/288 (0.0±0.0%)
1	Q	0.71±0.02	0±0/242 (0.0±0.0%)	0.81±0.05	0±0/323 (0.0±0.0%)
1	R	0.68±0.02	0±0/242 (0.0±0.0%)	0.78±0.02	0±0/323 (0.0±0.0%)
All	All	0.70	0/41170 (0.0%)	0.84	1/55000 (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	I	0.0±0.0	0.1±0.3
All	All	0	1

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)	Models	
								Worst	Total
1	J	24	VAL	CA-C-N	5.56	127.32	116.20	2	1

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	I	28	LYS	Mainchain	1

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	205	208	208	11 \pm 3
1	B	238	237	236	25 \pm 6
1	C	238	237	236	28 \pm 2
1	D	213	219	219	30 \pm 6
1	E	230	228	227	25 \pm 6
1	F	184	186	186	16 \pm 5
1	G	196	202	202	9 \pm 2
1	H	238	237	236	22 \pm 7
1	I	238	237	236	25 \pm 6
1	J	238	237	236	33 \pm 7
1	K	230	228	227	31 \pm 8
1	L	214	216	216	16 \pm 5
1	M	222	225	225	11 \pm 3
1	N	238	237	236	20 \pm 6
1	O	238	237	236	30 \pm 6
1	P	213	219	219	32 \pm 6
1	Q	238	237	236	24 \pm 3
1	R	238	237	236	16 \pm 3
All	All	40490	40640	40530	2686

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 33.

5 of 2149 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:H:27:ASN:O	1:H:29:GLY:N	1.09	1.84	6	1
1:H:39:VAL:HG12	1:N:31:ILE:HD12	0.92	1.39	10	1
1:N:34:LEU:HD23	1:N:35:MET:N	0.86	1.86	6	1
1:C:27:ASN:O	1:C:29:GLY:N	0.86	2.07	6	1
1:A:36:VAL:HG11	1:C:17:LEU:HD11	0.85	1.45	2	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	26/40 (65%)	21±1 (80±4%)	5±1 (17±4%)	1±1 (3±3%)	9	44
1	B	30/40 (75%)	24±2 (78±5%)	4±2 (13±6%)	3±1 (8±4%)	2	13
1	C	30/40 (75%)	23±1 (78±3%)	4±1 (14±3%)	2±1 (8±3%)	2	14
1	D	28/40 (70%)	20±2 (73±6%)	6±2 (20±6%)	2±1 (7±2%)	2	17
1	E	30/40 (75%)	23±1 (76±3%)	4±2 (12±6%)	4±1 (12±4%)	1	7
1	F	23/40 (58%)	20±1 (87±4%)	2±1 (8±5%)	1±1 (5±3%)	4	24
1	G	25/40 (62%)	19±1 (78±5%)	4±1 (18±5%)	1±1 (5±4%)	5	27
1	H	30/40 (75%)	24±1 (79±4%)	4±2 (12±5%)	3±2 (8±5%)	2	13
1	I	30/40 (75%)	24±1 (78±5%)	4±1 (14±5%)	2±1 (8±4%)	2	14
1	J	30/40 (75%)	24±1 (79±5%)	4±2 (14±6%)	2±1 (7±4%)	2	17
1	K	30/40 (75%)	24±1 (78±3%)	3±1 (11±2%)	3±1 (11±3%)	1	8
1	L	29/40 (72%)	22±2 (76±6%)	4±2 (15±6%)	3±2 (10±5%)	1	10
1	M	29/40 (72%)	21±1 (74±3%)	6±1 (19±4%)	2±1 (7±4%)	2	16
1	N	30/40 (75%)	23±1 (77±5%)	5±1 (17±4%)	2±1 (6±2%)	3	21
1	O	30/40 (75%)	23±2 (76±7%)	5±2 (16±6%)	2±1 (8±4%)	2	14
1	P	28/40 (70%)	22±2 (78±6%)	4±2 (14±6%)	2±1 (8±4%)	2	14
1	Q	30/40 (75%)	23±1 (76±5%)	5±2 (16±6%)	2±1 (7±3%)	2	16
1	R	30/40 (75%)	23±2 (78±5%)	4±1 (12±4%)	3±1 (10±4%)	1	10
All	All	5180/7200 (72%)	4015 (78%)	759 (15%)	406 (8%)	2	15

5 of 141 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	L	28	LYS	7
1	E	26	SER	7
1	C	29	GLY	6
1	R	28	LYS	6
1	E	23	ASP	6

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	21/31 (68%)	20±0 (97±2%)	1±0 (3±2%)	49	90
1	B	24/31 (77%)	23±1 (95±5%)	1±1 (5±5%)	31	78
1	C	24/31 (77%)	23±1 (95±3%)	1±1 (5±3%)	34	80
1	D	22/31 (71%)	21±1 (93±6%)	2±1 (7±6%)	22	69
1	E	23/31 (74%)	22±1 (96±4%)	1±1 (4±4%)	36	82
1	F	19/31 (61%)	18±1 (93±4%)	1±1 (7±4%)	22	69
1	G	20/31 (65%)	20±0 (98±2%)	0±0 (2±2%)	70	95
1	H	24/31 (77%)	23±1 (95±4%)	1±1 (5±4%)	34	80
1	I	24/31 (77%)	23±1 (95±4%)	1±1 (5±4%)	31	78
1	J	24/31 (77%)	22±1 (92±5%)	2±1 (8±5%)	19	66
1	K	23/31 (74%)	22±1 (95±5%)	1±1 (5±5%)	32	79
1	L	22/31 (71%)	21±1 (95±4%)	1±1 (5±4%)	34	81
1	M	23/31 (74%)	23±0 (99±2%)	0±0 (1±2%)	73	96
1	N	24/31 (77%)	23±1 (95±3%)	1±1 (5±3%)	34	80
1	O	24/31 (77%)	23±1 (95±2%)	1±1 (5±3%)	31	78
1	P	22/31 (71%)	20±1 (92±6%)	2±1 (8±6%)	17	63
1	Q	24/31 (77%)	23±1 (98±3%)	1±1 (2±3%)	54	92
1	R	24/31 (77%)	23±1 (97±2%)	1±1 (3±3%)	45	88
All	All	4110/5580 (74%)	3920 (95%)	190 (5%)	34	80

5 of 115 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	P	36	VAL	5
1	A	14	HIS	5
1	F	17	LEU	5
1	J	23	ASP	4
1	F	13	HIS	4

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 i

The completeness of assignment taking into account all chemical shift lists is 1% for the well-defined parts and 1% for the entire structure.

7.1 Chemical shift list 1

File name: 2lmq_cs.str

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping i

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

Total number of shifts	90
Number of shifts mapped to atoms	90
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 i

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	32	0.39 ± 0.51	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	26	-0.83 ± 0.41	Should be applied
$^{13}\text{C}'$	32	1.25 ± 0.24	Should be applied
^{15}N	0	—	None (insufficient data)

7.1.3 Completeness of resonance assignments i

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 1%, i.e. 77 atoms were assigned a chemical shift out of a possible 6211. 0 out of 138 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	54/2720 (2%)	0/1088 (0%)	54/1088 (5%)	0/544 (0%)
Sidechain	23/2827 (1%)	0/1612 (0%)	23/1145 (2%)	0/70 (0%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	0/664 (0%)	0/368 (0%)	0/260 (0%)	0/36 (0%)
Overall	77/6211 (1%)	0/3068 (0%)	77/2493 (3%)	0/650 (0%)

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 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.

Random coil index (RCI) for chain A:

