



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 03:03 PM UTC

PDB ID : 6MPP / pdb_00006mpp
BMRB ID : 27632
Title : HLA-A*01:01 complex with NRAS Q61K peptide by NMR
Authors : Flores-Solis, D.; McShan, A.C.; Sgourakis, N.G.
Deposited on : 2018-10-08

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

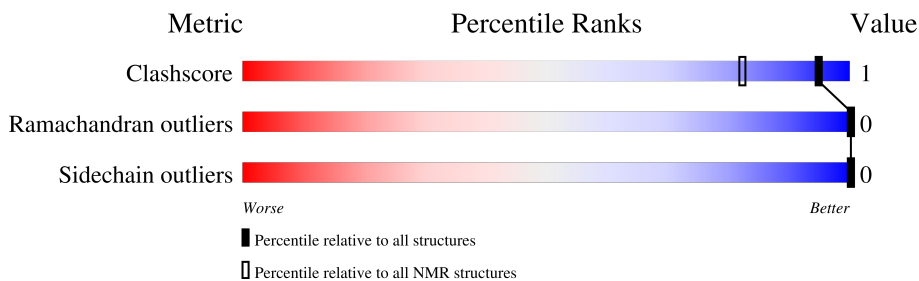
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 30%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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

Mol	Chain	Length	Quality of chain
1	A	279	
2	B	10	
3	C	100	

2 Ensemble composition and analysis

This entry contains 10 models. Model 5 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:1-A:274, B:1-B:3, B:8-B:10, C:1-C:100 (380)	0.08	5

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 1 clusters. No single-model clusters were found.

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

3 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6110 atoms, of which 2966 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called HLA class I histocompatibility antigen, A-1 alpha chain.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	A	274	4313	1383	2086	408	426	10	0

- Molecule 2 is a protein called NRAS Q61K peptide.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
2	B	10	157	50	77	11	19	0

- Molecule 3 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
3	C	100	1640	533	803	141	159	4	0

There is a discrepancy between the modelled and reference sequences:

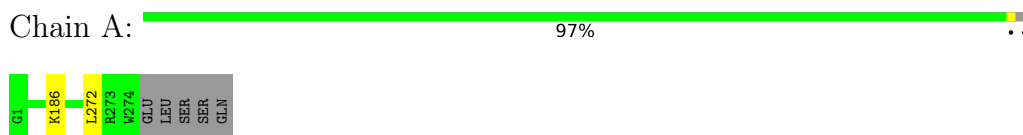
Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	initiating methionine	UNP P61769

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.

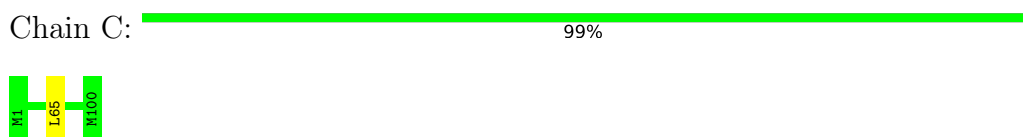
- Molecule 1: HLA class I histocompatibility antigen, A-1 alpha chain



- Molecule 2: NRAS Q61K peptide



- Molecule 3: Beta-2-microglobulin

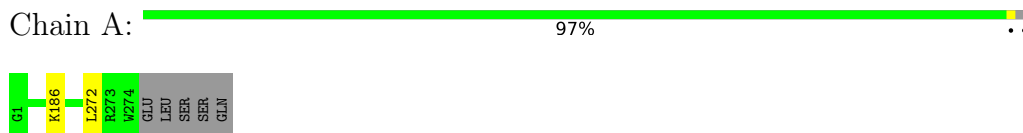


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

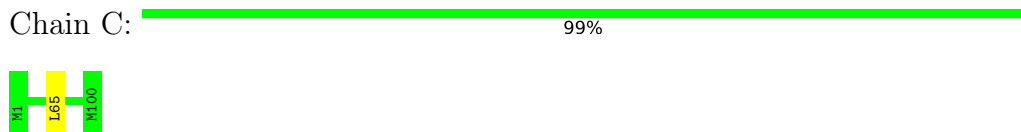
- Molecule 1: HLA class I histocompatibility antigen, A-1 alpha chain



- Molecule 2: NRAS Q61K peptide

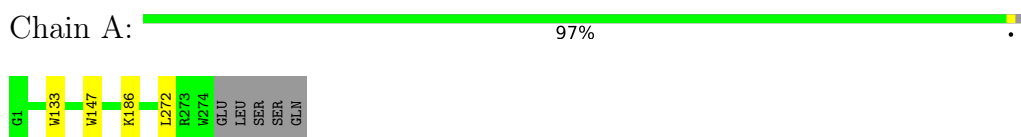


- Molecule 3: Beta-2-microglobulin



4.2.2 Score per residue for model 2

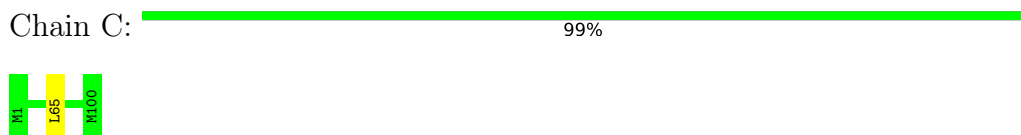
- Molecule 1: HLA class I histocompatibility antigen, A-1 alpha chain



- Molecule 2: NRAS Q61K peptide

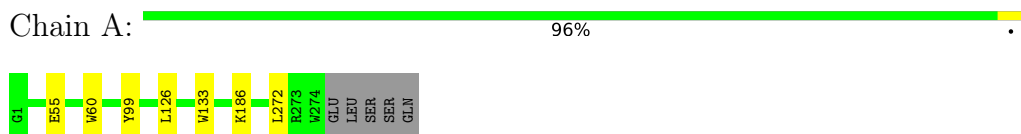


- Molecule 3: Beta-2-microglobulin



4.2.3 Score per residue for model 3

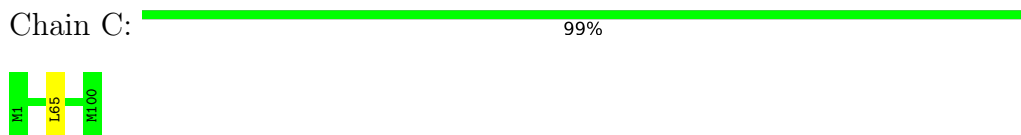
- Molecule 1: HLA class I histocompatibility antigen, A-1 alpha chain



- Molecule 2: NRAS Q61K peptide

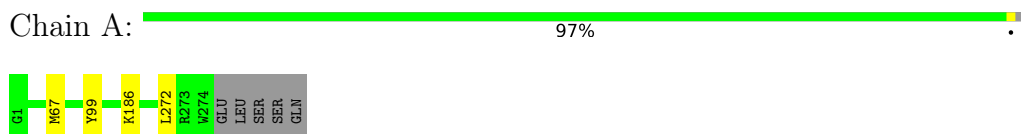


- Molecule 3: Beta-2-microglobulin



4.2.4 Score per residue for model 4

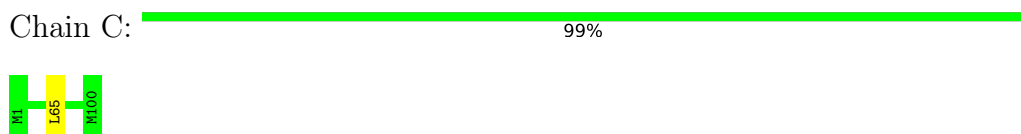
- Molecule 1: HLA class I histocompatibility antigen, A-1 alpha chain



- Molecule 2: NRAS Q61K peptide

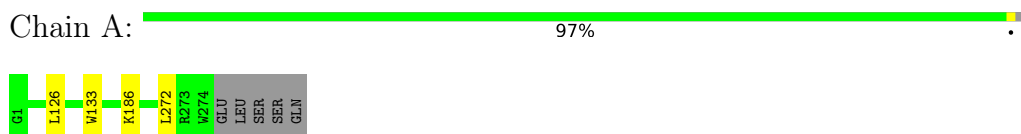


- Molecule 3: Beta-2-microglobulin



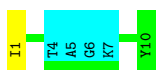
4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: HLA class I histocompatibility antigen, A-1 alpha chain



- Molecule 2: NRAS Q61K peptide





- Molecule 3: Beta-2-microglobulin

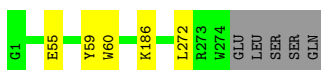
Chain C: 99%



4.2.6 Score per residue for model 6

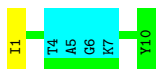
- Molecule 1: HLA class I histocompatibility antigen, A-1 alpha chain

Chain A: 96%



- Molecule 2: NRAS Q61K peptide

Chain B: 50% 10% 40%



- Molecule 3: Beta-2-microglobulin

Chain C: 99%



4.2.7 Score per residue for model 7

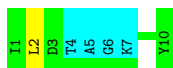
- Molecule 1: HLA class I histocompatibility antigen, A-1 alpha chain

Chain A: 97%

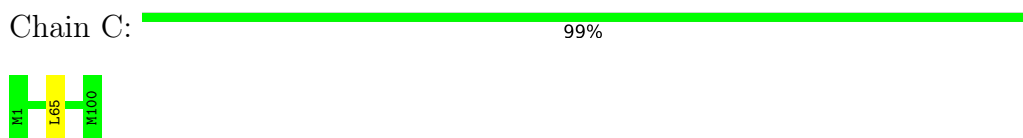


- Molecule 2: NRAS Q61K peptide

Chain B: 50% 10% 40%

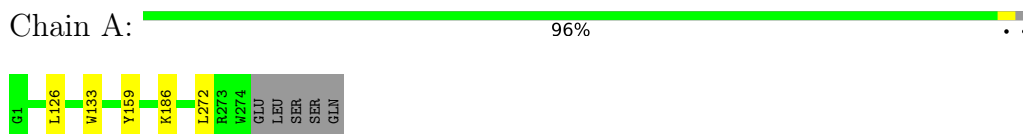


- Molecule 3: Beta-2-microglobulin



4.2.8 Score per residue for model 8

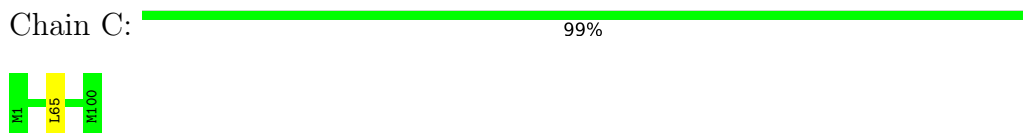
- Molecule 1: HLA class I histocompatibility antigen, A-1 alpha chain



- Molecule 2: NRAS Q61K peptide

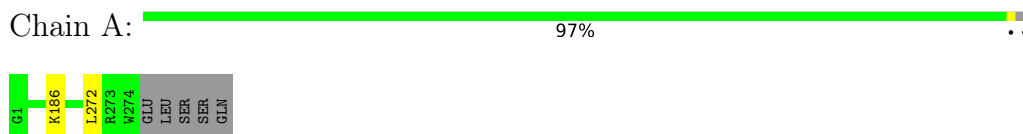


- Molecule 3: Beta-2-microglobulin



4.2.9 Score per residue for model 9

- Molecule 1: HLA class I histocompatibility antigen, A-1 alpha chain



- Molecule 2: NRAS Q61K peptide



- Molecule 3: Beta-2-microglobulin

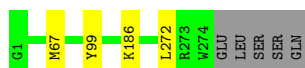
Chain C:  99%



4.2.10 Score per residue for model 10

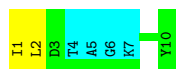
- Molecule 1: HLA class I histocompatibility antigen, A-1 alpha chain

Chain A:  97%



- Molecule 2: NRAS Q61K peptide

Chain B:  40% 20% 40%



- Molecule 3: Beta-2-microglobulin

Chain C:  99%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *distance geometry*.

Of the 50000 calculated structures, 10 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
CS-ROSETTA	refinement	
CS-ROSETTA	structure calculation	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1603
Number of shifts mapped to atoms	1571
Number of unparsed shifts	0
Number of shifts with mapping errors	32
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	30%

6 Model quality i

6.1 Standard geometry i

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 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	2227	2086	2086	4±1
2	B	55	49	49	1±1
3	C	837	803	803	2±0
All	All	31190	29380	29380	67

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:1:ILE:O	2:B:1:ILE:HG23	0.70	1.85	9	1
1:A:67:MET:HE2	1:A:67:MET:HA	0.62	1.70	4	3
2:B:1:ILE:O	2:B:1:ILE:HG13	0.62	1.92	10	1
2:B:1:ILE:O	2:B:1:ILE:HG22	0.57	1.99	6	2
1:A:159:TYR:OH	2:B:1:ILE:O	0.55	2.21	8	1
2:B:2:LEU:C	2:B:2:LEU:HD12	0.54	2.27	10	4
1:A:186:LYS:HD2	1:A:186:LYS:N	0.54	2.17	4	10
2:B:1:ILE:O	2:B:1:ILE:CG2	0.53	2.57	9	2
1:A:99:TYR:CD1	1:A:99:TYR:C	0.50	2.90	10	4
3:C:65:LEU:HD23	3:C:65:LEU:N	0.49	2.23	4	10
1:A:133:TRP:CZ2	1:A:147:TRP:CE3	0.47	3.03	2	1
1:A:272:LEU:HD12	1:A:272:LEU:N	0.47	2.25	4	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:2:LEU:HD12	2:B:2:LEU:O	0.47	2.10	10	1
1:A:55:GLU:OE2	1:A:60:TRP:CD1	0.46	2.69	6	2
3:C:65:LEU:N	3:C:65:LEU:CD2	0.45	2.79	1	10
1:A:126:LEU:HB2	1:A:133:TRP:CZ3	0.43	2.48	8	3
1:A:55:GLU:CD	1:A:59:TYR:CB	0.40	2.94	6	1
1:A:55:GLU:CD	1:A:59:TYR:HB2	0.40	2.42	6	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	272/279 (97%)	263±0 (97±0%)	9±0 (3±0%)	0±0 (0±0%)	100	100
2	B	4/10 (40%)	4±0 (92±11%)	0±0 (8±11%)	0±0 (0±0%)	100	100
3	C	98/100 (98%)	94±0 (96±0%)	4±0 (4±0%)	0±0 (0±0%)	100	100
All	All	3740/3890 (96%)	3607 (96%)	133 (4%)	0 (0%)	100	100

There are no Ramachandran outliers.

6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	231/236 (98%)	231±0 (100±0%)	0±0 (0±0%)	100	100
2	B	6/8 (75%)	6±0 (100±0%)	0±0 (0±0%)	100	100
3	C	95/95 (100%)	95±0 (100±0%)	0±0 (0±0%)	100	100
All	All	3320/3390 (98%)	3320 (100%)	0 (0%)	100	100

There are no protein residues with a non-rotameric sidechain to report.

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [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 30% for the well-defined parts and 30% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *starfile V3.txt*

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	1603
Number of shifts mapped to atoms	1571
Number of unparsed shifts	0
Number of shifts with mapping errors	32
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	14

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

- No matching atom found in the structure. All 32 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	275	GLU	H	7.36	0.018	1
1	A	275	GLU	C	175.186	0.000	1
1	A	275	GLU	CA	54.869	0.000	1
1	A	275	GLU	CB	31.112	0.040	1
1	A	275	GLU	N	125.689	0.028	1
1	A	276	LEU	H	7.493	0.020	1
1	A	276	LEU	HD11	0.81	0.000	.
1	A	276	LEU	HD12	0.81	0.000	.
1	A	276	LEU	HD13	0.81	0.000	.
1	A	276	LEU	HD21	0.864	0.001	.
1	A	276	LEU	HD22	0.864	0.001	.
1	A	276	LEU	HD23	0.864	0.001	.
1	A	276	LEU	C	177.188	0.000	1
1	A	276	LEU	CA	54.769	0.023	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	276	LEU	CB	41.908	0.033	1
1	A	276	LEU	CD1	23.734	0.000	.
1	A	276	LEU	CD2	24.584	0.006	.
1	A	276	LEU	N	122.926	0.015	1
1	A	277	SER	H	8.127	0.019	1
1	A	277	SER	C	174.52	0.000	1
1	A	277	SER	CA	57.786	0.000	1
1	A	277	SER	CB	63.943	0.000	1
1	A	277	SER	N	116.933	0.030	1
1	A	278	SER	H	8.207	0.020	1
1	A	278	SER	C	173.944	0.000	1
1	A	278	SER	CA	57.722	0.003	1
1	A	278	SER	CB	63.903	0.023	1
1	A	278	SER	N	118.258	0.046	1
1	A	279	GLN	H	8.214	0.019	1
1	A	279	GLN	CA	53.193	0.000	1
1	A	279	GLN	CB	29.131	0.000	1
1	A	279	GLN	N	123.686	0.035	1

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
$^{13}\text{C}_\alpha$	251	0.27 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	228	-0.21 ± 0.18	None needed (< 0.5 ppm)
$^{13}\text{C}'$	241	-0.01 ± 0.04	None needed (< 0.5 ppm)
^{15}N	251	-0.20 ± 0.26	None needed (< 0.5 ppm)

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 30%, i.e. 1543 atoms were assigned a chemical shift out of a possible 5224. 0 out of 44 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	969/1887 (51%)	244/766 (32%)	483/760 (64%)	242/361 (67%)
Sidechain	568/2809 (20%)	279/1801 (15%)	289/871 (33%)	0/137 (0%)
Aromatic	6/528 (1%)	5/261 (2%)	0/243 (0%)	1/24 (4%)
Overall	1543/5224 (30%)	528/2828 (19%)	772/1874 (41%)	243/522 (47%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 30%, i.e. 1571 atoms were assigned a chemical shift out of a possible 5268. 0 out of 44 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	982/1908 (51%)	253/775 (33%)	483/768 (63%)	246/365 (67%)
Sidechain	583/2832 (21%)	294/1816 (16%)	289/878 (33%)	0/138 (0%)
Aromatic	6/528 (1%)	5/261 (2%)	0/243 (0%)	1/24 (4%)
Overall	1571/5268 (30%)	552/2852 (19%)	772/1889 (41%)	247/527 (47%)

7.1.4 Statistically unusual chemical shifts [i](#)

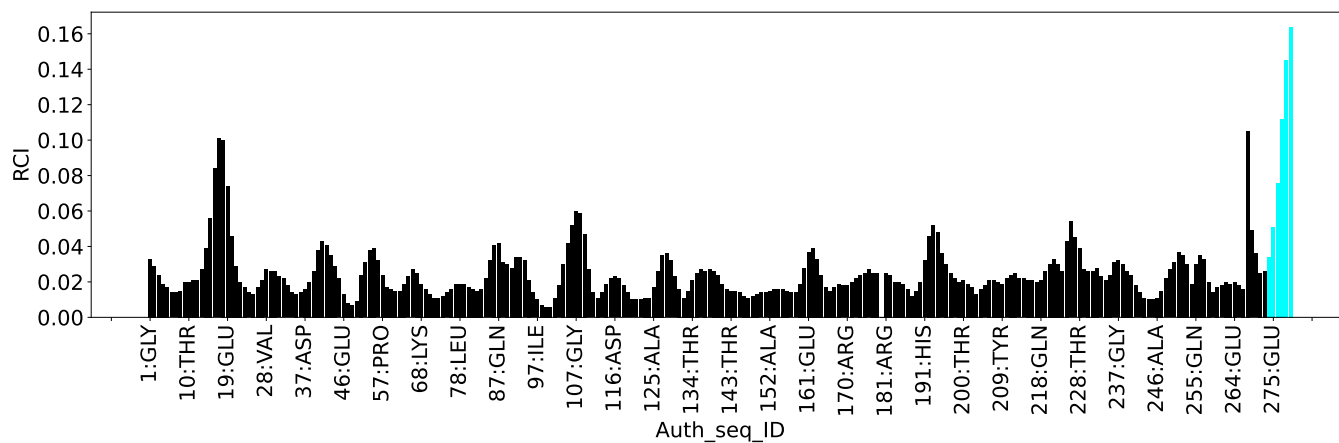
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	117	ALA	HB1	-0.86	0.14 – 2.58	-9.1
1	A	117	ALA	HB2	-0.86	0.14 – 2.58	-9.1
1	A	117	ALA	HB3	-0.86	0.14 – 2.58	-9.1
1	A	47	PRO	CA	52.62	55.85 – 70.84	-7.2
1	A	120	GLY	C	185.64	164.92 – 182.89	6.5
1	A	132	SER	C	185.27	166.15 – 183.14	6.2
1	A	112	GLY	C	184.36	164.92 – 182.89	5.8
1	A	100	GLY	C	184.09	164.92 – 182.89	5.7
1	A	211	ALA	HB1	0.04	0.14 – 2.58	-5.4
1	A	211	ALA	HB2	0.04	0.14 – 2.58	-5.4
1	A	211	ALA	HB3	0.04	0.14 – 2.58	-5.4
1	A	188	HIS	C	185.51	165.57 – 184.97	5.3
1	A	124	ILE	C	185.60	166.59 – 185.34	5.1
1	A	101	CYS	C	185.18	164.77 – 184.97	5.1

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. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:

