



Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 05:22 AM BST

PDB ID : 2RS9
Title : Solution structure of the bromodomain of human BRPF1 in complex with histone H4K5ac peptide
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Deposited on : 2011-12-08

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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

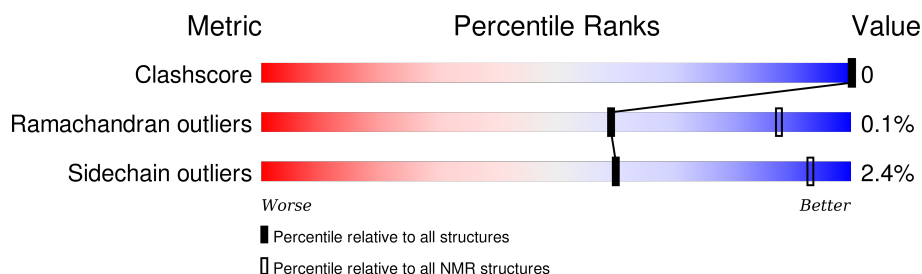
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 92%.

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	10	100%
2	B	121	88% 12%

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	B:47-B:153 (107)	0.22	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 4 clusters and 7 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2063 atoms, of which 1027 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Acetylated lysine 5 of peptide from Histone H4.

Mol	Chain	Residues	Atoms					Trace
1	A	10	Total	C	H	N	O	0
			140	39	73	15	13	

- Molecule 2 is a protein called Peregrin.

Mol	Chain	Residues	Atoms					Trace
2	B	121	Total	C	H	N	O	S
			1923	611	954	167	187	4

There are 13 discrepancies between the modelled and reference sequences:

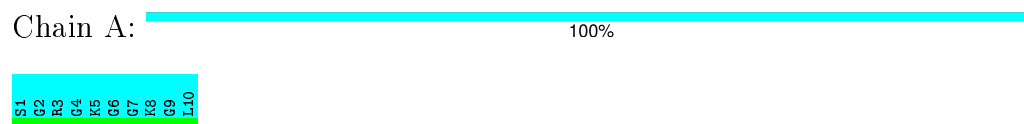
Chain	Residue	Modelled	Actual	Comment	Reference
B	41	GLY	-	EXPRESSION TAG	UNP P55201
B	42	SER	-	EXPRESSION TAG	UNP P55201
B	43	SER	-	EXPRESSION TAG	UNP P55201
B	44	GLY	-	EXPRESSION TAG	UNP P55201
B	45	SER	-	EXPRESSION TAG	UNP P55201
B	46	SER	-	EXPRESSION TAG	UNP P55201
B	47	GLY	-	EXPRESSION TAG	UNP P55201
B	156	SER	-	EXPRESSION TAG	UNP P55201
B	157	GLY	-	EXPRESSION TAG	UNP P55201
B	158	PRO	-	EXPRESSION TAG	UNP P55201
B	159	SER	-	EXPRESSION TAG	UNP P55201
B	160	SER	-	EXPRESSION TAG	UNP P55201
B	161	GLY	-	EXPRESSION TAG	UNP P55201

4 Residue-property plots

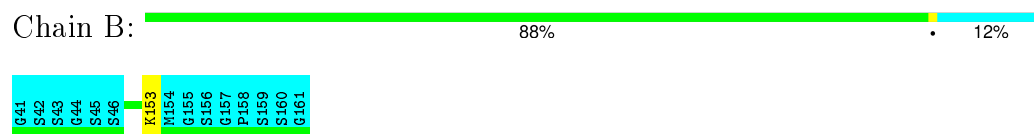
4.1 Average score per residue in the NMR ensemble

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: Acetylated lysine 5 of peptide from Histone H4



- Molecule 2: Peregrin

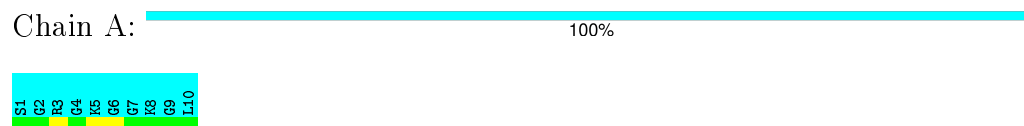


4.2 Scores per residue for each member of the ensemble

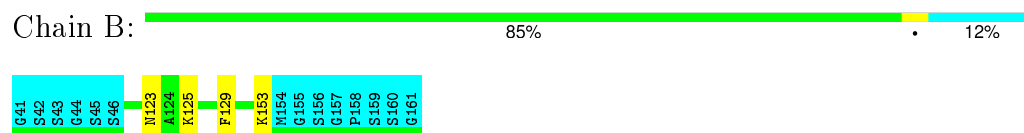
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Acetylated lysine 5 of peptide from Histone H4

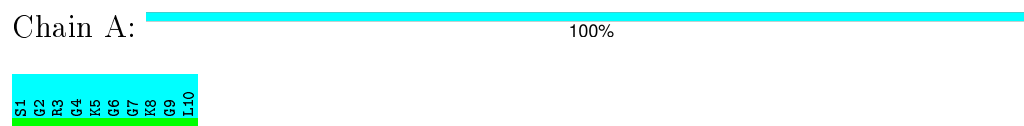


- Molecule 2: Peregrin

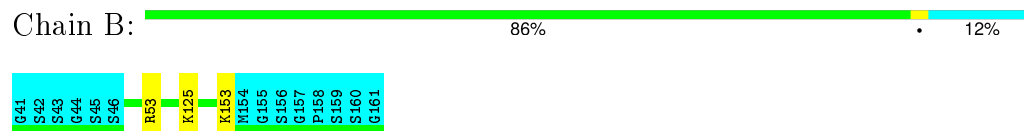


4.2.2 Score per residue for model 2

- Molecule 1: Acetylated lysine 5 of peptide from Histone H4

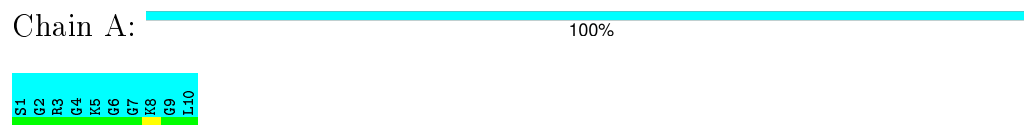


- Molecule 2: Peregrin

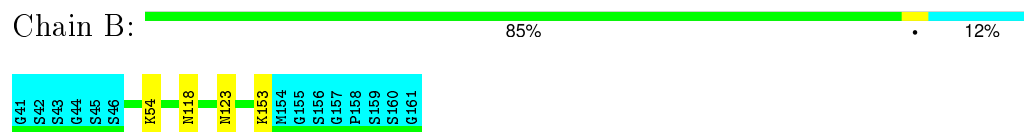


4.2.3 Score per residue for model 3

- Molecule 1: Acetylated lysine 5 of peptide from Histone H4



- Molecule 2: Peregrin

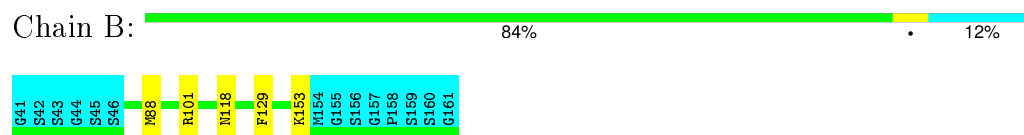


4.2.4 Score per residue for model 4

- Molecule 1: Acetylated lysine 5 of peptide from Histone H4

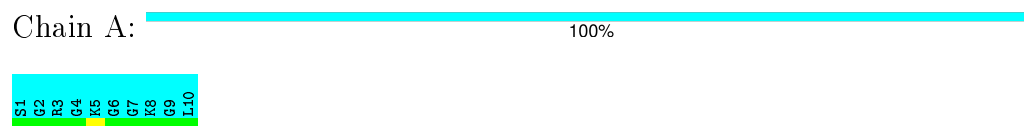


- Molecule 2: Peregrin

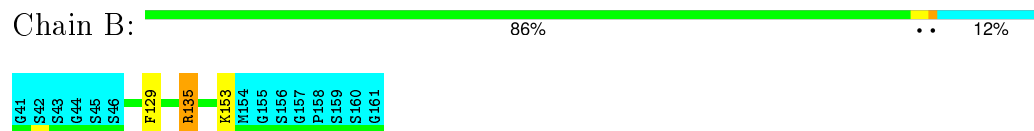


4.2.5 Score per residue for model 5

- Molecule 1: Acetylated lysine 5 of peptide from Histone H4

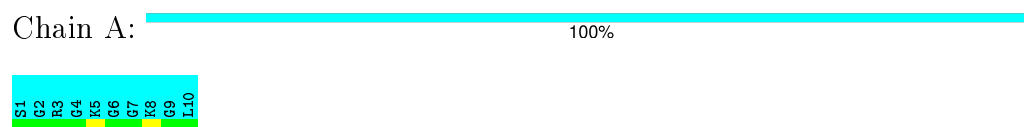


- Molecule 2: Peregrin

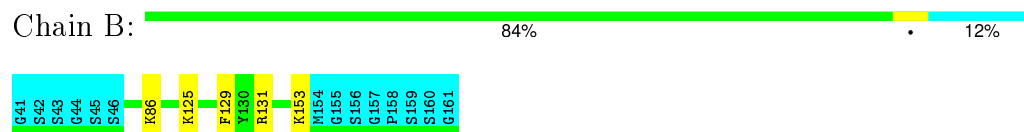


4.2.6 Score per residue for model 6

- Molecule 1: Acetylated lysine 5 of peptide from Histone H4

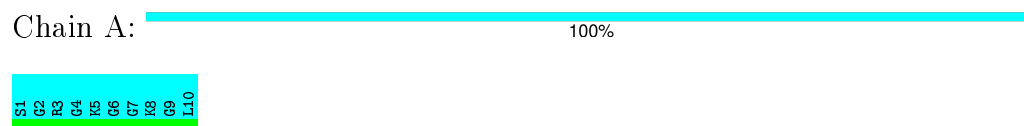


- Molecule 2: Peregrin

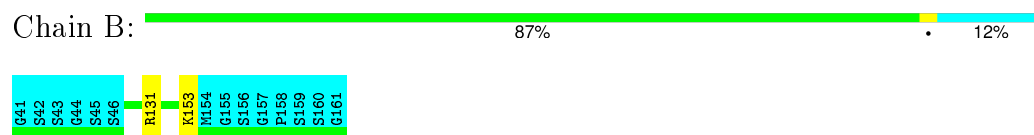


4.2.7 Score per residue for model 7

- Molecule 1: Acetylated lysine 5 of peptide from Histone H4

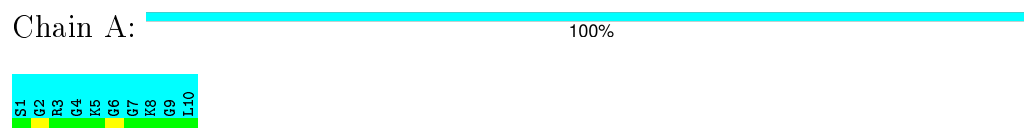


- Molecule 2: Peregrin

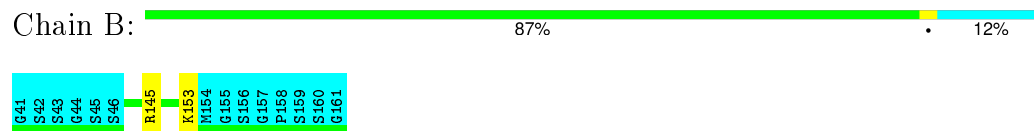


4.2.8 Score per residue for model 8

- Molecule 1: Acetylated lysine 5 of peptide from Histone H4

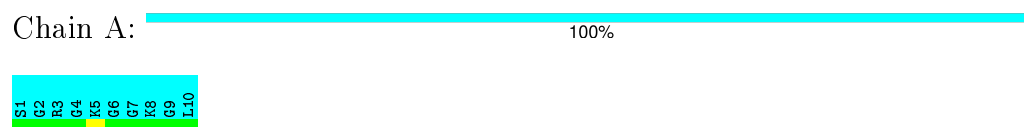


- Molecule 2: Peregrin

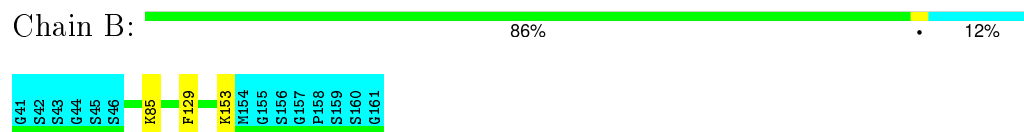


4.2.9 Score per residue for model 9

- Molecule 1: Acetylated lysine 5 of peptide from Histone H4

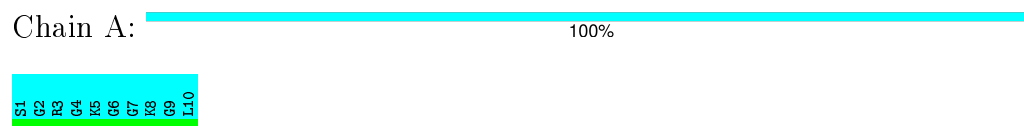


- Molecule 2: Peregrin

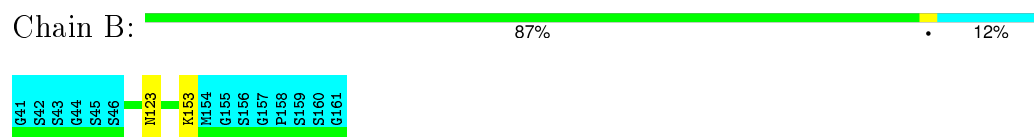


4.2.10 Score per residue for model 10

- Molecule 1: Acetylated lysine 5 of peptide from Histone H4



- Molecule 2: Peregrin




4.2.11 Score per residue for model 11

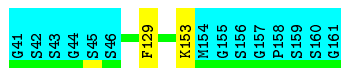
- Molecule 1: Acetylated lysine 5 of peptide from Histone H4

Chain A:  100%



- Molecule 2: Peregrin

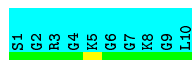
Chain B:  87%  12%





4.2.12 Score per residue for model 12

- Molecule 1: Acetylated lysine 5 of peptide from Histone H4

Chain A:  100%



- Molecule 2: Peregrin

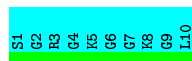
Chain B:  84%  12%





4.2.13 Score per residue for model 13

- Molecule 1: Acetylated lysine 5 of peptide from Histone H4

Chain A:  100%



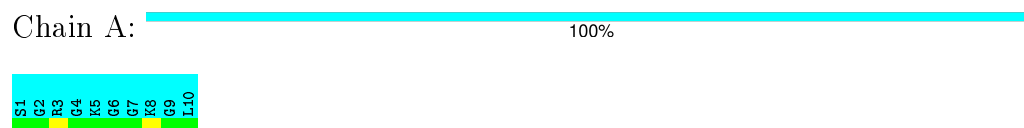
- Molecule 2: Peregrin

Chain B:  86%  12%

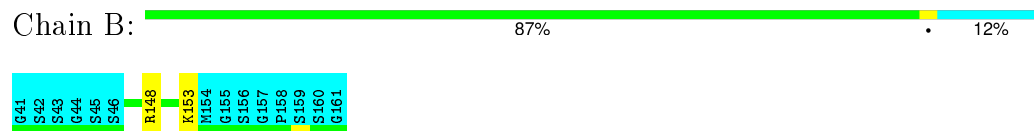


4.2.14 Score per residue for model 14

- Molecule 1: Acetylated lysine 5 of peptide from Histone H4

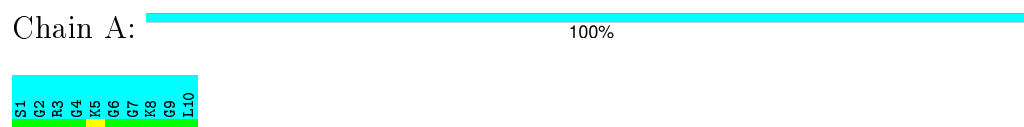


- Molecule 2: Peregrin

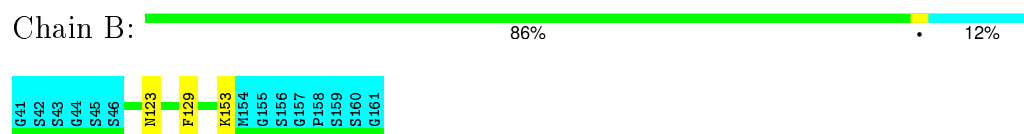


4.2.15 Score per residue for model 15

- Molecule 1: Acetylated lysine 5 of peptide from Histone H4

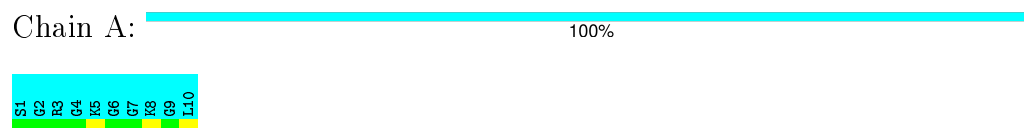


- Molecule 2: Peregrin

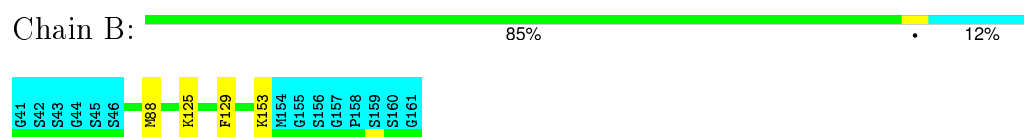


4.2.16 Score per residue for model 16

- Molecule 1: Acetylated lysine 5 of peptide from Histone H4

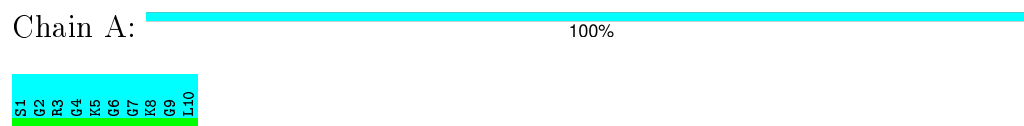


- Molecule 2: Peregrin

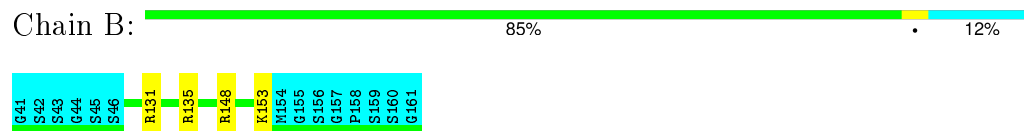


4.2.17 Score per residue for model 17

- Molecule 1: Acetylated lysine 5 of peptide from Histone H4

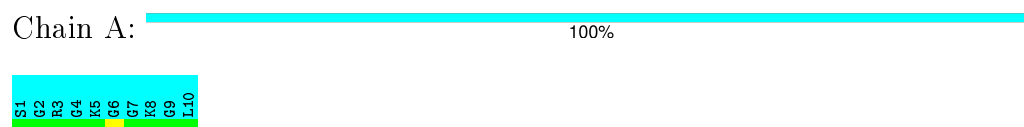


- Molecule 2: Peregrin

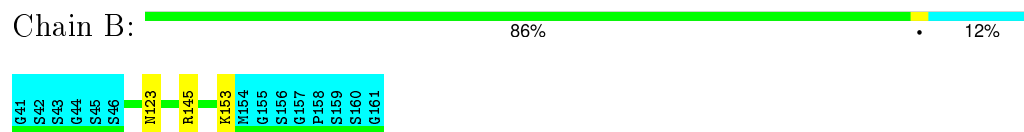


4.2.18 Score per residue for model 18

- Molecule 1: Acetylated lysine 5 of peptide from Histone H4

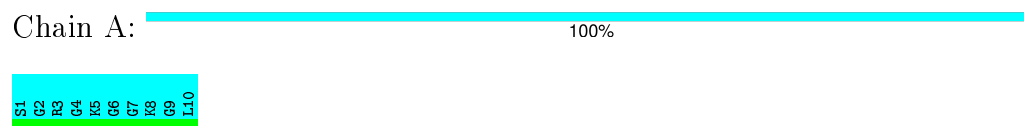


- Molecule 2: Peregrin

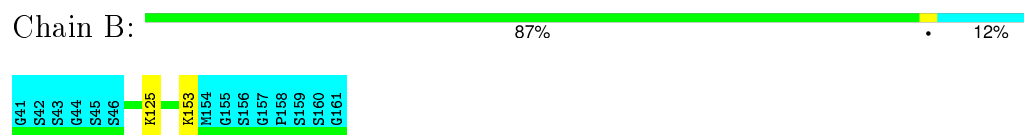


4.2.19 Score per residue for model 19

- Molecule 1: Acetylated lysine 5 of peptide from Histone H4



- Molecule 2: Peregrin





4.2.20 Score per residue for model 20

- Molecule 1: Acetylated lysine 5 of peptide from Histone H4

Chain A:  100%

S1	G2	R3	G4	K5	G6	G7	K8	G9	L10
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- Molecule 2: Peregrin

Chain B:  88%  12%

G41	S42	S43	G44	S45	S46	K153	M154	G155	S156	G157	P158	S159	S160	G161
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5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics, molecular dynamics*.

Of the 100 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 solution	2.1
AMBER	refinement	5
CYANA	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)	2rs9_cs.str
Number of chemical shift lists	1
Total number of shifts	1599
Number of shifts mapped to atoms	1599
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	92%

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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ALY

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
2	B	0.71±0.00	0±0/909 (0.0±0.0%)	0.88±0.01	0±1/1224 (0.0±0.1%)
All	All	0.71	0/18180 (0.0%)	0.88	8/24480 (0.0%)

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(°)	Ideal(°)	Models	
								Worst	Total
2	B	148	ARG	NE-CZ-NH2	-6.24	117.18	120.30	14	2
2	B	131	ARG	NE-CZ-NH1	5.85	123.22	120.30	6	1
2	B	148	ARG	NE-CZ-NH1	5.48	123.04	120.30	14	2
2	B	101	ARG	NE-CZ-NH1	5.30	122.95	120.30	12	1
2	B	53	ARG	NE-CZ-NH1	5.20	122.90	120.30	2	1
2	B	135	ARG	NE-CZ-NH1	5.17	122.88	120.30	5	1

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	0	0	0	0±0
2	B	891	886	886	0±0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes
All	All	17820	17720	17720	-

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 -.

There are no clashes.

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	0	-	-	-	-
2	B	107/121 (88%)	103±1 (96±1%)	4±1 (3±1%)	0±0 (0±0%)	59 88
All	All	2140/2620 (82%)	2064 (96%)	74 (3%)	2 (0%)	59 88

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
2	B	125	LYS	2

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	0	-	-	-
2	B	96/105 (91%)	94±1 (98±1%)	2±1 (2±1%)	60 93
All	All	1920/2180 (88%)	1873 (98%)	47 (2%)	60 93

All 13 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)
2	B	153	LYS	20
2	B	123	ASN	7
2	B	118	ASN	3
2	B	125	LYS	3
2	B	135	ARG	2
2	B	145	ARG	2
2	B	88	MET	2
2	B	101	ARG	2
2	B	131	ARG	2
2	B	86	LYS	1
2	B	85	LYS	1
2	B	54	LYS	1
2	B	149	ARG	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
1	ALY	A	5	1	9,11,12	0.59±0.04	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
1	ALY	A	5	1	10,12,14	1.28±0.32	0±0 (1±3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	ALY	A	5	1	-	0±0,8,10,12	0±0,0,0,0

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	5	ALY	CE-NZ-CH	5.68	132.14	122.38	1	2

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 92% for the well-defined parts and 89% for the entire structure.

7.1 Chemical shift list 1

File name: 2rs9_cs.str

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	1599
Number of shifts mapped to atoms	1599
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
$^{13}\text{C}_\alpha$	119	-0.20 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	111	0.49 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}'$	119	-0.44 ± 0.13	None needed (< 0.5 ppm)
^{15}N	111	0.54 ± 0.21	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 92%, i.e. 1310 atoms were assigned a chemical shift out of a possible 1419. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	524/527 (99%)	210/210 (100%)	214/214 (100%)	100/103 (97%)
Sidechain	670/773 (87%)	417/454 (92%)	234/275 (85%)	19/44 (43%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	116/119 (97%)	62/64 (97%)	54/54 (100%)	0/1 (0%)
Overall	1310/1419 (92%)	689/728 (95%)	502/543 (92%)	119/148 (80%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 89%, i.e. 1438 atoms were assigned a chemical shift out of a possible 1613. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	595/640 (93%)	246/255 (96%)	238/260 (92%)	111/125 (89%)
Sidechain	727/854 (85%)	462/505 (91%)	246/301 (82%)	19/48 (40%)
Aromatic	116/119 (97%)	62/64 (97%)	54/54 (100%)	0/1 (0%)
Overall	1438/1613 (89%)	770/824 (93%)	538/615 (87%)	130/174 (75%)

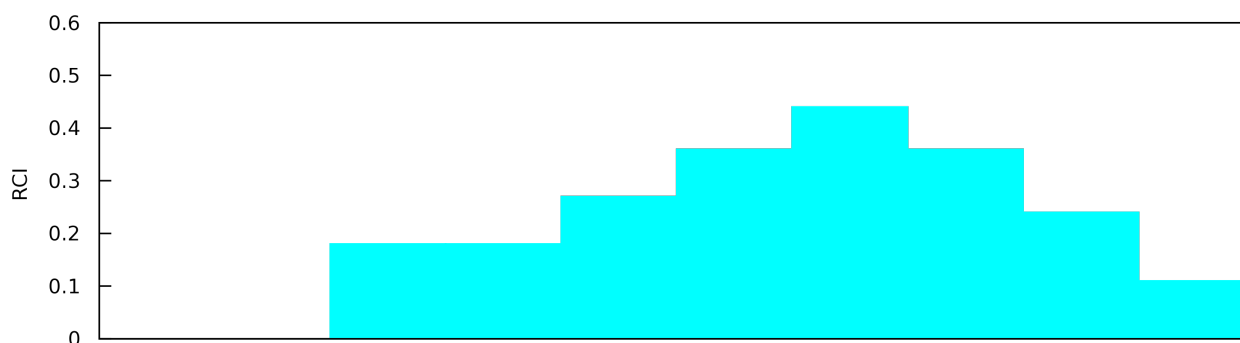
7.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots ⓘ

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:

