

Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2K5K
Title	:	Solution structure of RhR2 from Rhodobacter Sphaeroides. Northeast Struc-
		tural Genomics Consortium
Authors	:	Lee, H.; Bansal, S.; Chen, C.X.; Jiang, M.; Maglaqui, M.; Xiao, R.; Liu, J.;
		Baran, M.C.; Swapna, G.; Acton, T.B.; Rost, B.; Montelione, G.T.; Preste-
		gard, J.H.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2008-06-28

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

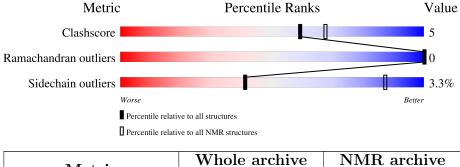
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $SOLUTION\ NMR$

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)	${f NMR} \ {f archive} \ (\#{f Entries})$
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	٨	70			
	А	70	14%	74%	11%



2 Ensemble composition and analysis (i)

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: *fewest violations*.

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:15-A:24 (10)	0.21	5										

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

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

NmrClust was unable to cluster the ensemble.

Error message: Inconsistent models



3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1006 atoms, of which 506 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called uncharacterized protein RhR2.

Mol	Chain	Residues		Atoms									
1	٨	69	Total	С	Η	Ν	Ο	S	0				
	A	62	1006	309	506	96	93	2	0				

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	63	LEU	-	expression tag	UNP Q3IYU5
A	64	GLU	-	expression tag	UNP Q3IYU5
А	65	HIS	-	expression tag	UNP Q3IYU5
А	66	HIS	-	expression tag	UNP Q3IYU5
А	67	HIS	-	expression tag	UNP Q3IYU5
А	68	HIS	-	expression tag	UNP Q3IYU5
А	69	HIS	-	expression tag	UNP Q3IYU5
A	70	HIS	_	expression tag	UNP Q3IYU5



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: uncharacterized protein RhR2

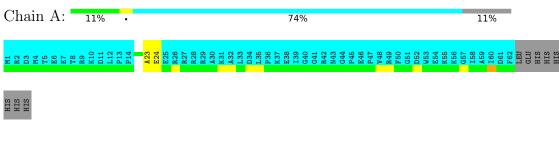
Chain	А			1	4%	, D													74	%												1	1%	6					
M1 R2 M4 R5	EG	E7 70	R9	K10	D11	P13	P14	с7.1 В 26	R28	A30 V 24	იო	L33	D34	L35	P36	K37	E38 139	040 140	G41	R42	G44	E46 D47	141 V48	R49	F50	G51	ι Ω	W D 3	K56		A59 7 20	160 D61	F62		HIS	HIS	н	HIS	н.
HIS																																							

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: uncharacterized protein RhR2



4.2.2 Score per residue for model 2

• Molecule 1: uncharacterized protein RhR2

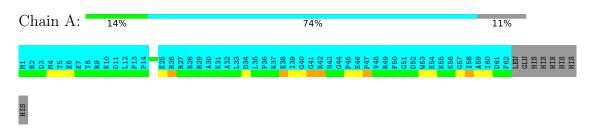
Chain A: 13% · 74% 11%



HIS HIS HIS

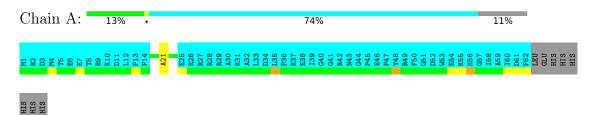
4.2.3 Score per residue for model 3

\bullet Molecule 1: uncharacterized protein RhR2



4.2.4 Score per residue for model 4

 \bullet Molecule 1: uncharacterized protein RhR2



4.2.5 Score per residue for model 5 (medoid)

• Molecule 1: uncharacterized protein RhR2

Chain A:	11%	••		74%		11%
M1 R2 D3 T5 E6 E7	T8 R9 D11	P13 P14 L17	L20 E25 R26 R27 R28	K29 K31 A30 L33 L33 L33 C34 C33 K33 K37 K37 K37 K33 K33 K33 K33 K33 K	641 842 844 945 945 844 945 747 849 849 849 849 849 850	U53 E54 K55 K56 K56 K56 A56 D61 D61 F62 LEU H10 H10
HIS HIS HIS HIS HIS						

4.2.6 Score per residue for model 6

 \bullet Molecule 1: uncharacterized protein RhR2





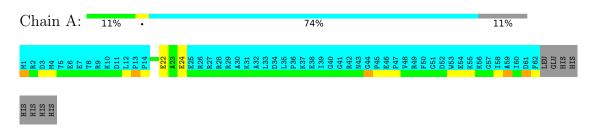
4.2.7 Score per residue for model 7

• Molecule 1: uncharacterized protein RhR2



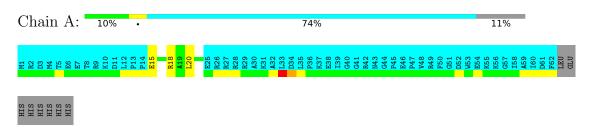
4.2.8 Score per residue for model 8

• Molecule 1: uncharacterized protein RhR2



4.2.9 Score per residue for model 9

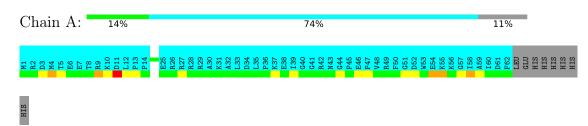
• Molecule 1: uncharacterized protein RhR2





4.2.10 Score per residue for model 10

 \bullet Molecule 1: uncharacterized protein RhR2





5 Refinement protocol and experimental data overview (i)

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

Of the 50 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
CYANA	structure solution	2.1
X-PLOR NIH	refinement	

No chemical shift data was provided.



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	А	74	73	73	1±1
All	All	740	730	730	7

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 5.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Moo	dels
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:17:LEU:HD22	1:A:17:LEU:N	0.51	2.21	5	1
1:A:17:LEU:N	1:A:17:LEU:CD2	0.50	2.74	5	1
1:A:20:LEU:HD13	1:A:20:LEU:O	0.49	2.07	5	1
1:A:17:LEU:CD2	1:A:17:LEU:N	0.47	2.78	7	1
1:A:17:LEU:N	1:A:17:LEU:HD22	0.44	2.27	7	1
1:A:18:ARG:C	1:A:20:LEU:N	0.41	2.73	9	1
1:A:22:GLU:C	1:A:24:GLU:N	0.40	2.75	8	1

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

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



Mol	Chain	Analysed	Favoured Allowed		Outliers	Percentiles	
1	А	10/70~(14%)	10 ± 0 (97 $\pm5\%$)	$0{\pm}0$ ($3{\pm}5\%$)	0±0 (0±0%)	100 100	
All	All	100/700~(14%)	97~(97%)	3(3%)	0 (0%)	100 100	

entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

There are no Ramachandran outliers.

6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed and the total number of residues.

Mol	Chain	hain Analysed Rotameric		Outliers	Outliers Percentile	
1	А	6/58~(10%)	6 ± 0 (97 $\pm7\%$)	$0{\pm}0~(3{\pm}7\%)$	41	87
All	All	60/580~(10%)	58~(97%)	2~(3%)	41	87

All 2 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	А	18	ARG	1
1	А	20	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

