Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	1NZS
Title	:	NMR structures of phosphorylated carboxy terminus of bovine rhodopsin in arrestin-bound state
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Deposited on	:	2003-02-19

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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

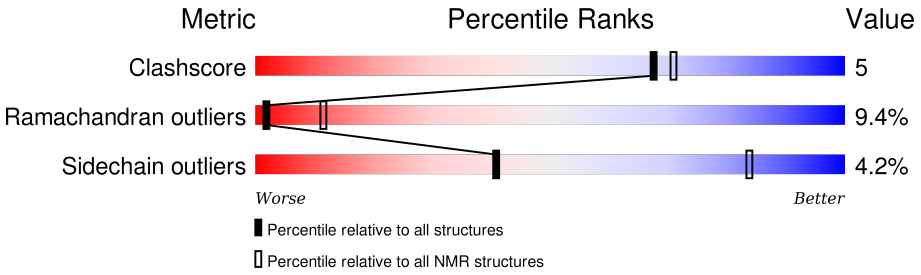
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	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 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	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 <=5%

Mol	Chain	Length	Quality of chain
1	A	19	47% 16% 37%

2 Ensemble composition and analysis

This entry contains 16 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:330-A:333, A:337-A:337, A:339-A:339, A:341-A:341, A:344-A:348 (12)	0.32	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 3 clusters and 7 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 160 atoms, of which 25 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called 19-mer peptide fragment of RHODOPSIN.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
1	A	19	160	78	25	21	36	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	334	SEP	SER	MODIFIED RESIDUE	UNP P02699
A	335	TPO	THR	MODIFIED RESIDUE	UNP P02699
A	336	TPO	THR	MODIFIED RESIDUE	UNP P02699
A	338	SEP	SER	MODIFIED RESIDUE	UNP P02699
A	340	TPO	THR	MODIFIED RESIDUE	UNP P02699
A	342	TPO	THR	MODIFIED RESIDUE	UNP P02699
A	343	SEP	SER	MODIFIED RESIDUE	UNP P02699

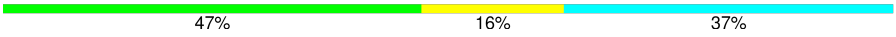
4 Residue-property plots

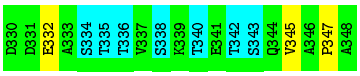
4.1 Average score per residue in the NMR ensemble

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: 19-mer peptide fragment of RHODOPSIN

Chain A:





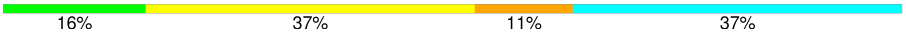
4.2 Scores per residue for each member of the ensemble

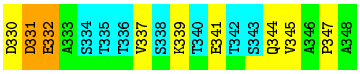
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: 19-mer peptide fragment of RHODOPSIN

Chain A:

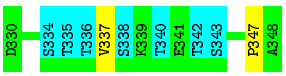




4.2.2 Score per residue for model 2

- Molecule 1: 19-mer peptide fragment of RHODOPSIN

Chain A:



4.2.3 Score per residue for model 3

• Molecule 1: 19-mer peptide fragment of RHODOPSIN

Chain A:

4.2.4 Score per residue for model 4

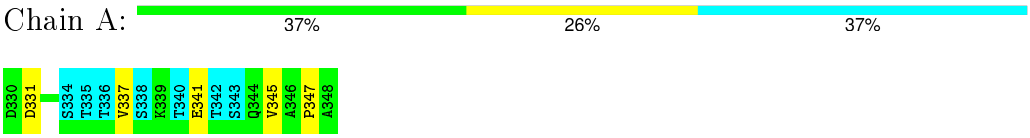
• Molecule 1: 19-mer peptide fragment of RHODOPSIN

Chain A:

4.2.5 Score per residue for model 5

• Molecule 1: 19-mer peptide fragment of RHODOPSIN

Chain A:



4.2.6 Score per residue for model 6

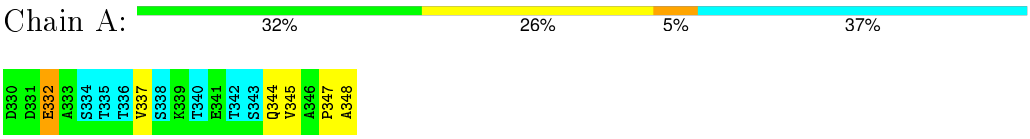
• Molecule 1: 19-mer peptide fragment of RHODOPSIN

Chain A:

4.2.7 Score per residue for model 7

• Molecule 1: 19-mer peptide fragment of RHODOPSIN

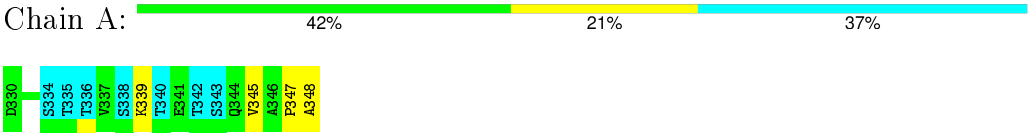
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: 19-mer peptide fragment of RHODOPSIN

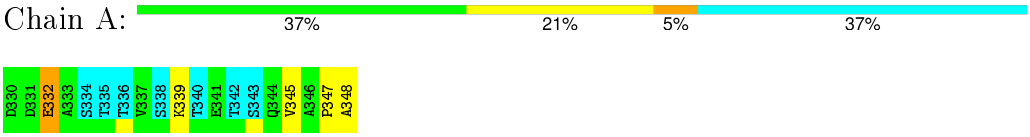
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: 19-mer peptide fragment of RHODOPSIN

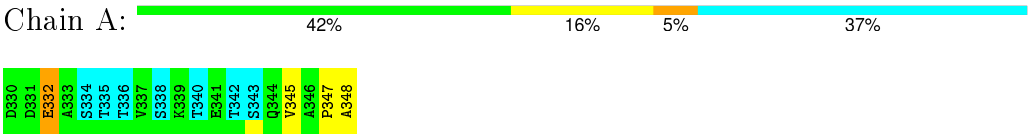
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: 19-mer peptide fragment of RHODOPSIN

Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: 19-mer peptide fragment of RHODOPSIN

Chain A:

4.2.12 Score per residue for model 12

• Molecule 1: 19-mer peptide fragment of RHODOPSIN

Chain A:

4.2.13 Score per residue for model 13

• Molecule 1: 19-mer peptide fragment of RHODOPSIN

Chain A:

4.2.14 Score per residue for model 14

• Molecule 1: 19-mer peptide fragment of RHODOPSIN

Chain A:

4.2.15 Score per residue for model 15

• Molecule 1: 19-mer peptide fragment of RHODOPSIN

Chain A:

4.2.16 Score per residue for model 16

• Molecule 1: 19-mer peptide fragment of RHODOPSIN

Chain A:

5 Refinement protocol and experimental data overview

The models were refined using the following method: *distance geometry, constrained molecular dynamics, simulated annealing.*

Of the 100 calculated structures, 16 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
TINKER	structure solution	3.9
TINKER	refinement	3.9

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

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

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	1.00±1.23	1±4/85 (1.2±4.8%)	1.36±0.91	0±1/107 (0.4±1.4%)
All	All	1.59	17/1360 (1.2%)	1.63	6/1712 (0.4%)

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	331	ASP	CG-OD2	-24.98	0.68	1.25	1	1
1	A	331	ASP	CG-OD1	-23.72	0.70	1.25	1	1
1	A	345	VAL	CB-CG1	-15.85	1.19	1.52	1	1
1	A	345	VAL	CB-CG2	-15.57	1.20	1.52	1	1
1	A	344	GLN	CD-OE1	-10.82	1.00	1.24	1	1
1	A	344	GLN	CG-CD	-10.39	1.27	1.51	1	1
1	A	332	GLU	CD-OE2	-10.18	1.14	1.25	1	1
1	A	332	GLU	CD-OE1	-9.97	1.14	1.25	1	1
1	A	344	GLN	CD-NE2	-9.95	1.07	1.32	1	1
1	A	339	LYS	CE-NZ	-8.23	1.28	1.49	1	1
1	A	341	GLU	CD-OE2	-7.15	1.17	1.25	1	1
1	A	330	ASP	CG-OD2	-6.95	1.09	1.25	1	1
1	A	341	GLU	CD-OE1	-6.78	1.18	1.25	1	1
1	A	330	ASP	CG-OD1	-6.40	1.10	1.25	1	1
1	A	339	LYS	CB-CG	-5.74	1.37	1.52	1	1
1	A	330	ASP	C-O	-5.68	1.12	1.23	1	1
1	A	337	VAL	C-O	-5.08	1.13	1.23	1	1

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	A	331	ASP	CB-CG-OD1	28.07	143.57	118.30	1	1
1	A	331	ASP	CB-CG-OD2	27.11	142.70	118.30	1	1
1	A	331	ASP	OD1-CG-OD2	-26.10	73.72	123.30	1	1
1	A	345	VAL	CG1-CB-CG2	-9.92	95.03	110.90	1	1
1	A	345	VAL	CA-CB-CG1	7.51	122.17	110.90	1	1
1	A	345	VAL	CA-CB-CG2	6.20	120.20	110.90	1	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	89	18	80	1±1
All	All	1424	288	1279	13

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.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:331:ASP:OD2	1:A:331:ASP:CB	1.03	2.07	1	1
1:A:331:ASP:OD1	1:A:331:ASP:CB	1.00	2.10	1	1
1:A:331:ASP:OD1	1:A:331:ASP:CG	0.69	0.70	1	1
1:A:332:GLU:HG3	1:A:344:GLN:HA	0.66	1.68	7	1
1:A:331:ASP:OD2	1:A:331:ASP:CG	0.66	0.67	1	1
1:A:332:GLU:H	1:A:339:LYS:HE3	0.50	1.66	9	1
1:A:345:VAL:HA	1:A:348:ALA:OXT	0.48	2.09	7	5
1:A:341:GLU:O	1:A:345:VAL:HG23	0.47	2.10	5	2

6.3 Torsion angles

6.3.1 Protein backbone

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	10/19 (53%)	8±0 (76±5%)	1±1 (14±9%)	1±1 (9±7%)	2 11
All	All	160/304 (53%)	122 (76%)	23 (14%)	15 (9%)	2 11

All 2 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	347	PRO	11
1	A	337	VAL	4

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	9/9 (100%)	9±0 (96±5%)	0±0 (4±5%)	41 84
All	All	144/144 (100%)	138 (96%)	6 (4%)	41 84

All 3 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	A	332	GLU	3
1	A	339	LYS	2
1	A	331	ASP	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

7 non-standard protein/DNA/RNA residues are 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	SEP	A	334	1	3,5,10	0.61±0.26	0±0 (0±0%)
1	TPO	A	335	1	5,6,11	0.77±0.72	0±0 (1±4%)
1	TPO	A	336	1	5,6,11	0.63±0.32	0±0 (0±0%)
1	SEP	A	338	1	3,5,10	0.80±0.90	0±0 (2±8%)
1	TPO	A	340	1	5,6,11	0.60±0.34	0±0 (0±0%)
1	TPO	A	342	1	5,6,11	0.73±0.82	0±0 (2±9%)
1	SEP	A	343	1	3,5,10	0.87±1.53	0±0 (2±8%)

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	SEP	A	334	1	3,5,14	1.56±0.18	0±0 (0±0%)
1	TPO	A	335	1	5,7,16	1.19±0.30	0±0 (0±0%)
1	TPO	A	336	1	5,7,16	1.32±0.17	0±0 (0±0%)
1	SEP	A	338	1	3,5,14	1.06±0.25	0±0 (0±0%)
1	TPO	A	340	1	5,7,16	1.11±0.18	0±0 (0±0%)
1	TPO	A	342	1	5,7,16	1.26±0.28	0±0 (0±0%)
1	SEP	A	343	1	3,5,14	1.73±0.68	0±0 (2±8%)

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	SEP	A	334	1	-	0±0,2,4,10	0±0,0,0,0
1	TPO	A	335	1	-	0±0,4,6,13	0±0,0,0,0
1	TPO	A	336	1	-	0±0,4,6,13	0±0,0,0,0
1	SEP	A	338	1	-	0±0,2,4,10	0±0,0,0,0
1	TPO	A	340	1	-	0±0,4,6,13	0±0,0,0,0
1	TPO	A	342	1	-	0±0,4,6,13	0±0,0,0,0
1	SEP	A	343	1	-	0±0,2,4,10	0±0,0,0,0

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	343	SEP	OG-CB	11.75	0.91	1.42	1	1
1	A	338	SEP	CB-CA	6.81	1.37	1.53	1	1
1	A	342	TPO	OG1-CB	6.61	1.24	1.43	1	1
1	A	342	TPO	CG2-CB	5.72	1.35	1.51	1	1
1	A	335	TPO	CG2-CB	5.27	1.37	1.51	1	1

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	343	SEP	OG-CB-CA	6.96	127.04	111.19	1	1

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

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided