



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2L6X / pdb_00002l6x
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Title : Solution NMR Structure of Proteorhodopsin.
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Membrane Protein Structures by Solution NMR (MPSbyNMR)
Deposited on : 2010-11-29

This is a wwPDB NMR Structure Validation Summary 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
Mogul : 2022.3.0, CSD as543be (2022)
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

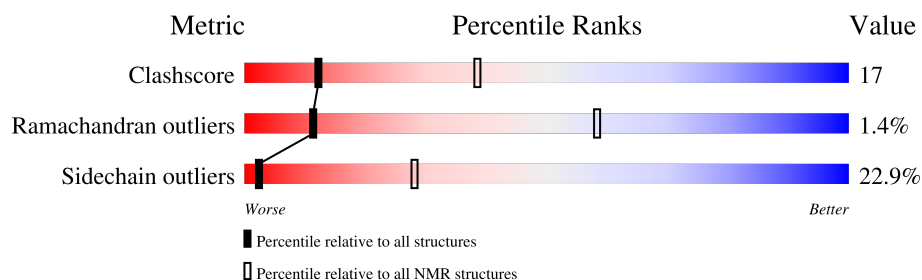
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 63%.

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	243	

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	A:23-A:169, A:178-A:208, A:215-A:247 (211)	0.99	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 3 single-model clusters were found.

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

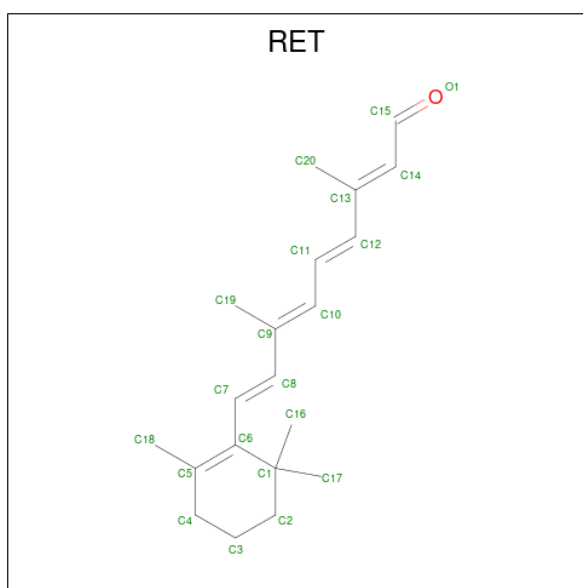
- Molecule 1 is a protein called Green-light absorbing proteorhodopsin.

Mol	Chain	Residues	Atoms						Trace
1	A	235	Total	C	H	N	O	S	0
			3621	1211	1804	276	317	13	

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MET	-	initiating methionine	UNP Q9F7P4
A	250	PRO	-	expression tag	UNP Q9F7P4
A	251	GLY	-	expression tag	UNP Q9F7P4
A	252	GLY	-	expression tag	UNP Q9F7P4
A	253	GLY	-	expression tag	UNP Q9F7P4
A	254	SER	-	expression tag	UNP Q9F7P4
A	255	HIS	-	expression tag	UNP Q9F7P4
A	256	HIS	-	expression tag	UNP Q9F7P4
A	257	HIS	-	expression tag	UNP Q9F7P4
A	258	HIS	-	expression tag	UNP Q9F7P4
A	259	HIS	-	expression tag	UNP Q9F7P4
A	260	HIS	-	expression tag	UNP Q9F7P4

- Molecule 2 is RETINAL (CCD ID: RET) (formula: $C_{20}H_{28}O$).



Mol	Chain	Residues	Atoms		
			Total	C	H
2	A	1	48	20	28

5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure solution	3.0
CYANA	refinement	3.0

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	2004
Number of shifts mapped to atoms	1998
Number of unparsed shifts	0
Number of shifts with mapping errors	6
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	63%

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: RET

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	0.27±0.00	0±0/1725 (0.0± 0.0%)	0.66±0.01	1±0/2361 (0.0± 0.0%)
All	All	0.27	0/34500 (0.0%)	0.66	19/47220 (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	230	ASN	CA-C-O	6.32	126.75	119.35	13	19

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	1671	1675	1672	57±8
2	A	20	28	27	2±2
All	All	33820	34060	33980	1156

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 17.

5 of 507 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:113:LEU:HD11	1:A:182:VAL:HG13	0.99	1.35	1	8
1:A:101:THR:HG22	1:A:105:LEU:HD23	0.96	1.38	16	4
1:A:229:VAL:HG13	1:A:233:LEU:HD13	0.95	1.34	15	2
1:A:84:ILE:HD11	1:A:216:ALA:HB1	0.94	1.39	17	1
1:A:113:LEU:HD12	1:A:182:VAL:HG13	0.92	1.40	17	3

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	211/243 (87%)	195±3 (92±1%)	13±2 (6±1%)	3±1 (1±1%)	11	58
All	All	4220/4860 (87%)	3896 (92%)	265 (6%)	59 (1%)	11	58

5 of 13 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	118	ASN	17
1	A	178	ALA	13
1	A	147	ALA	10
1	A	247	SER	4
1	A	207	GLY	4

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	172/192 (90%)	133±4 (77±2%)	39±4 (23±2%)	2	28
All	All	3440/3840 (90%)	2652 (77%)	788 (23%)	2	28

5 of 121 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	179	SER	20
1	A	57	LYS	16
1	A	135	LEU	16
1	A	146	MET	16
1	A	132	LEU	15

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](#)

1 ligand 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
2	RET	A	301	1	20,20,21	2.18±0.00	6±0 (30±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	Counts	Bond angles	
						RMSZ	#Z>2
2	RET	A	301	1	27,27,28	2.94±0.01	12±0 (44±0%)

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
2	RET	A	301	1	-	0±0,13,30,31	0±0,1,1,1

5 of 6 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
2	A	301	RET	C2-C3	6.32	1.37	1.52	17	20
2	A	301	RET	C8-C9	3.81	1.54	1.46	6	20
2	A	301	RET	C17-C1	3.64	1.46	1.53	13	20
2	A	301	RET	C19-C9	3.00	1.56	1.50	14	20
2	A	301	RET	C4-C5	2.11	1.54	1.51	5	20

5 of 12 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	A	301	RET	C17-C1-C6	7.43	121.89	110.24	1	20
2	A	301	RET	C18-C5-C6	6.03	117.91	124.48	10	20
2	A	301	RET	C1-C6-C5	5.37	115.30	122.64	4	20
2	A	301	RET	C1-C6-C7	5.07	129.39	115.65	7	20
2	A	301	RET	C2-C1-C6	4.91	117.57	110.44	7	20

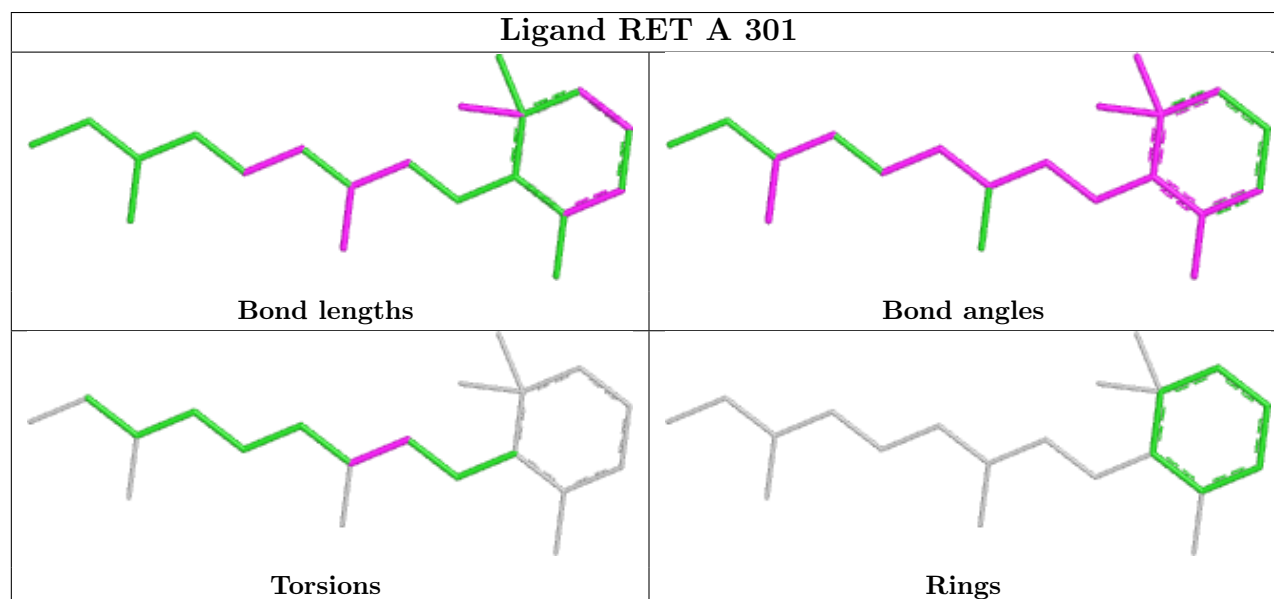
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 63% for the well-defined parts and 63% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

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	2004
Number of shifts mapped to atoms	1998
Number of unparsed shifts	0
Number of shifts with mapping errors	6
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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

- No matching atom found in the structure. First 5 (of 6) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	214	LYR	H	8.335	0.020	1
1	A	214	LYR	HA	4.815	0.020	1
1	A	214	LYR	C	177.081	0.400	1
1	A	214	LYR	CA	58.884	0.400	1
1	A	214	LYR	CB	34.757	0.400	1
1	A	214	LYR	N	113.027	0.400	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	222	-0.99 ± 0.23	Should be checked
$^{13}\text{C}_\beta$	175	0.09 ± 0.07	None needed (< 0.5 ppm)

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Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}'$	213	-0.21 ± 0.14	None needed (< 0.5 ppm)
^{15}N	214	1.20 ± 0.21	Should be applied

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 63%, i.e. 1853 atoms were assigned a chemical shift out of a possible 2930. 0 out of 45 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	948/1061 (89%)	360/433 (83%)	394/422 (93%)	194/206 (94%)
Sidechain	819/1475 (56%)	530/993 (53%)	289/456 (63%)	0/26 (0%)
Aromatic	86/394 (22%)	39/190 (21%)	39/192 (20%)	8/12 (67%)
Overall	1853/2930 (63%)	929/1616 (57%)	722/1070 (67%)	202/244 (83%)

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	201	PRO	CB	37.86	26.06 – 37.61	5.2

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:

