



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2KS9 / pdb_00002ks9
Title : Solution conformation of substance P in water complexed with NK1R
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Deposited on : 2009-12-31

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:

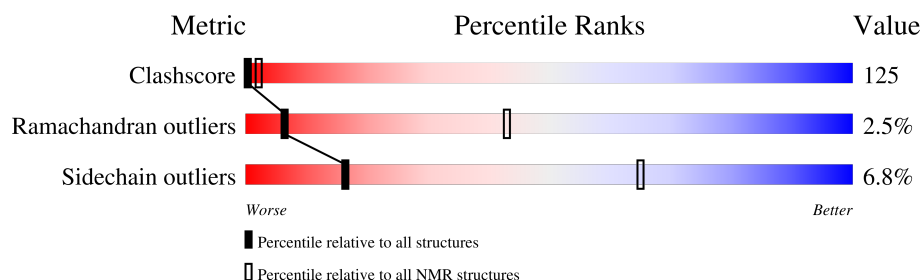
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : 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 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	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	364	
2	B	11	

2 Ensemble composition and analysis

This entry contains 5 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:2-A:361 (360)	0.00	1
2	A:362-A:364, B:365-B:374 (13)	1.91	2

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6061 atoms, of which 3038 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Substance-P receptor.

Mol	Chain	Residues	Atoms						Trace
1	A	363	Total	C	H	N	O	S	0
			5867	1940	2939	464	501	23	

- Molecule 2 is a protein called Substance P.

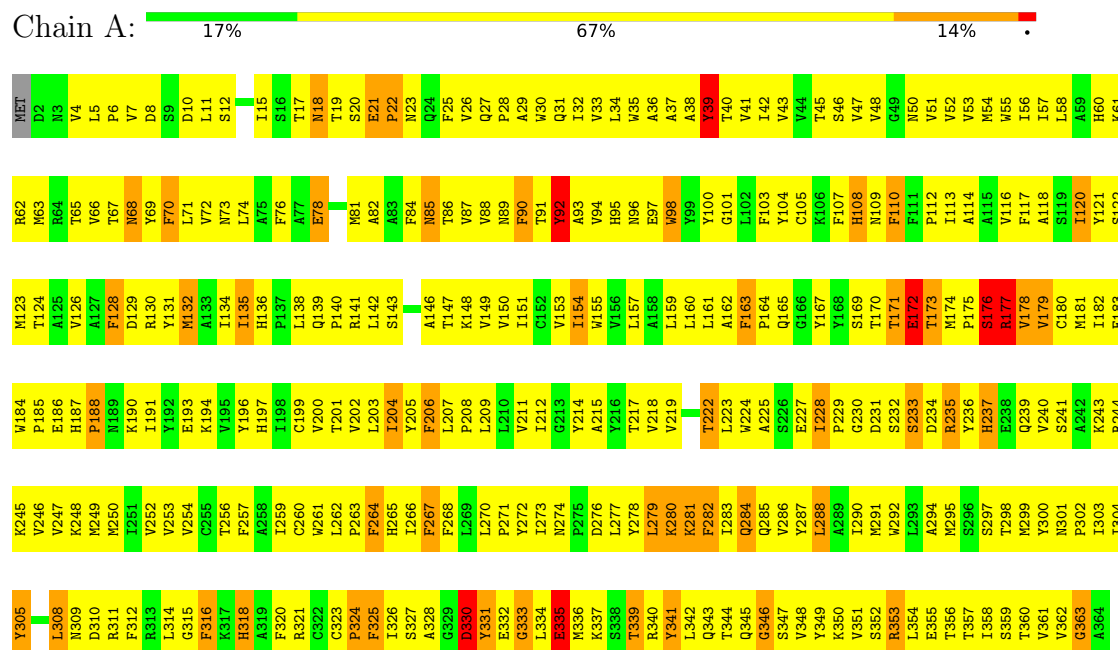
Mol	Chain	Residues	Atoms						Trace
2	B	11	Total	C	H	N	O	S	0
			194	63	99	17	14	1	

4 Residue-property plots

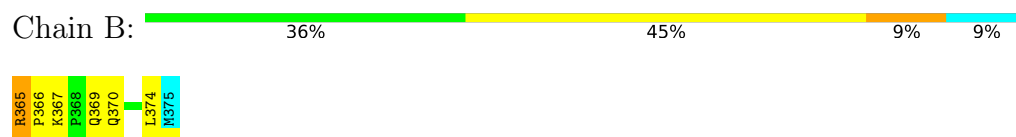
4.1 Average score per residue in the NMR ensemble

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: Substance-P receptor



- Molecule 2: Substance P



4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 1. Colouring as in section 4.1 above.

- Molecule 1: Substance-P receptor

K245	V305	W184	M123	R62	MET
V246	L308	P185	T124	M63	D2
N309	K248	E186	A125	R64	R3
D310	W249	H187	V126	T65	V4
R311	K250	P188	A127	V66	L5
L251	V312	H189	F128	T67	P6
V252	R313	K190	D129	M68	D8
V253	L314	V191	R130	V69	V7
V254	G315	Y192	F131	F70	S9
C255	R316	E193	M132	L71	D10
T256	K317	K194	A133	V72	L11
V257	R318	V195	I134	M73	S12
A258	A319	F196	I135	L74	
F320	V320	H197	H136	A75	I15
R321	C260	I198	P137	F76	S16
C322	W261	V200	L138	A77	T17
C323	L262	V201	O139	E78	N18
F324	P263	T202	P140		T19
F325	F264	L203	R141	M81	S20
L326	H265	L204	L142	A82	E21
S327	T266	T205	S143	A83	P22
A328	F267	F206		F84	N23
C329	F268	L207	A146	M85	O24
S330	L269	P208	T147	T86	F25
V331	P270	L209	K148	M87	V26
E332	T271	L210	V149	V88	Q27
G333	V272	V211	V150	N89	P28
L334	T273	L212	I151	F90	A29
R335	N274	G213	C152	T91	V30
K336	T275	Y214	V153	Y92	Q31
K337	D276	A215	I154	A93	L32
S338	L277	V216	V155	V94	V33
T339	V278	T217	V156	H95	L34
R340	L279	V218	L157	N96	V35
V341	K280	V219	A158	E97	A36
L342	K281		L159	N98	A37
Q343	T282	T222	L161	T99	A38
T344	L283	L223	L162	Y100	Y39
Q345	Q284	W224	F163	G101	T40
G346	Q285	A225	P164	L102	V41
S347	V286	S226	Q165	F103	I42
V348	V287	E227	G166	Y104	V43
V349	L288	L228	V167	C105	V44
K350	A289	P229	V168	L106	T45
V351	L290	G230	S169	F107	S46
S352	M291	D231	T170	H108	V47
R353	W292	S232	T171	N109	V48
L354	L293	S233	E172	F110	G49
E355	A294	D234	T173	F111	N50
T356	M295	R235	M174	P112	V51
T357	S296	V236	P175	T113	V52
L358	S297	H237	P176	A114	V53
S359	T298	E238	S176	A115	M54
T360	M299	Q239	R177	V116	M55
V361	V300	V240	V178	F117	V56
V362	N301	S241	V179	A118	I57
C363	P302	A242	M181	S119	L58
	L303	K243	L182	N120	A59
	T204	P244	F183	V121	H60

Chain B: 27% 55% 9% 9%



5 Refinement protocol and experimental data overview

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

Of the 20 calculated structures, 5 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
XPLOR-NIH	structure solution	2.17.0
AutoDock	structure solution	4.0
XPLOR-NIH	geometry optimization	2.17.0
AutoDock	geometry optimization	4.0
AutoDock	refinement	4.0

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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	1.43±0.00	5±0/3018 (0.2± 0.0%)	1.77±0.00	63±2/4127 (1.5± 0.0%)
2	B	0.69±0.00	0±0/90 (0.0± 0.0%)	1.08±0.00	0±0/121 (0.0± 0.0%)
All	All	1.42	26/15540 (0.2%)	1.75	315/21240 (1.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	2.0±0.0
All	All	0	10

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
1	A	177	ARG	CA-C	-7.89	1.42	1.52	2	5
1	A	171	THR	C-N	6.94	1.43	1.33	3	5
1	A	12	SER	C-N	-6.26	1.28	1.33	1	5
1	A	178	VAL	N-CA	-6.08	1.38	1.46	4	5
1	A	177	ARG	N-CA	-5.37	1.39	1.45	1	5

5 of 65 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
1	A	177	ARG	N-CA-C	13.65	132.03	110.32	4	5
1	A	335	GLU	N-CA-C	-12.29	97.96	111.36	4	5
1	A	22	PRO	N-CA-C	11.60	128.94	113.98	2	5
1	A	163	PHE	CA-CB-CG	-11.39	102.41	113.80	3	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	176	SER	CA-C-N	-9.60	105.66	122.07	2	5

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	176	SER	Peptide	5
1	A	177	ARG	Peptide	5

6.2 Too-close contacts ⓘ

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	2928	2939	2937	751±2
2	B	86	90	87	5±2
All	All	15070	15145	15120	3763

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 125.

5 of 778 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:123:MET:HE2	1:A:123:MET:HA	1.04	1.30	1	5
1:A:334:LEU:HD22	1:A:337:LYS:HA	1.02	1.26	3	5
1:A:17:THR:HG23	1:A:20:SER:H	1.00	1.17	1	5
1:A:161:LEU:HD13	1:A:200:VAL:HG13	0.99	1.27	4	5
1:A:161:LEU:HD12	1:A:204:ILE:HB	0.98	1.31	5	5

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	361/364 (99%)	324±0 (90±0%)	28±0 (8±0%)	9±0 (3±0%)	6	43
2	B	9/11 (82%)	9±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
All	All	1850/1875 (99%)	1665 (90%)	139 (8%)	46 (2%)	6	43

5 of 10 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	172	GLU	5
1	A	188	PRO	5
1	A	222	THR	5
1	A	233	SER	5
1	A	237	HIS	5

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	322/323 (100%)	304±0 (94±0%)	18±0 (6±0%)	21	70
2	B	9/10 (90%)	5±1 (51±17%)	4±1 (49±17%)	0	1
All	All	1655/1665 (99%)	1543 (93%)	112 (7%)	16	65

5 of 25 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	39	TYR	5
1	A	78	GLU	5

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Mol	Chain	Res	Type	Models (Total)
1	A	85	ASN	5
1	A	92	TYR	5
1	A	120	ILE	5

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

No chemical shift data were provided