



wwPDB NMR Structure Validation Summary Report ⓘ

May 29, 2020 – 09:07 am BST

PDB ID : 2MSD
Title : NMR data-driven model of GTPase KRas-GNP tethered to a lipid-bilayer nanodisc
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Deposited on : 2014-07-29

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 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 : 1.8.5 (274361), CSD as541be (2020)
buster-report : 1.1.7 (2018)
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 : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

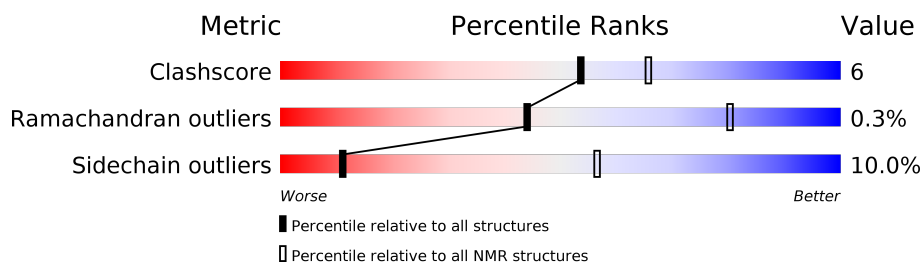
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 0%.

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	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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	200	81% 17% ...
1	C	200	80% 18% ...
2	B	187	76% 14% 8% .

2 Ensemble composition and analysis

This entry contains 10 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:201-A:396, C:401-C:595 (391)	0.26	1
2	B:3-B:172 (170)	0.46	3

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. No single-model clusters were found.

Cluster number	Models
1	3, 6, 7, 10
2	5, 8, 9
3	1, 2, 4

3 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9138 atoms, of which 62 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Apolipoprotein A-I.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	198	1645	1019	22	287	314	3	0
1	C	198	1646	1019	22	287	315	3	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	GLY	-	expression tag	UNP P02647
A	200	PRO	-	expression tag	UNP P02647
C	397	GLY	-	expression tag	UNP P02647
C	398	PRO	-	expression tag	UNP P02647

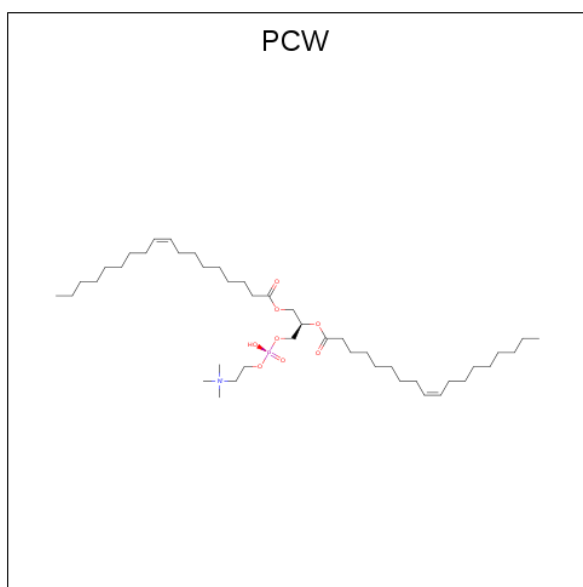
- Molecule 2 is a protein called GTPase KRas.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	185	1494	923	18	257	287	9	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP P01116
B	0	SER	-	expression tag	UNP P01116

- Molecule 3 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: C₄₄H₈₅NO₈P).



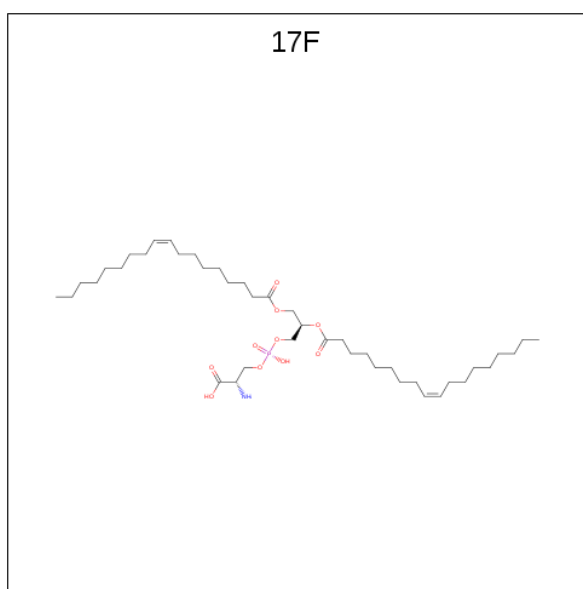
Mol	Chain	Residues	Atoms				
			Total	C	N	O	P
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1

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Mol	Chain	Residues	Atoms				
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1

- Molecule 4 is O-[(S)-({(2R)-2,3-bis[(9Z)-octadec-9-enyloxy]propyl}oxy)(hydroxy)phosphoryl]-L-serine (three-letter code: 17F) (formula: C₄₂H₇₈NO₁₀P).



Mol	Chain	Residues	Atoms				
4	A	1	Total	C	N	O	P
			54	42	1	10	1
4	A	1	Total	C	N	O	P
			54	42	1	10	1
4	A	1	Total	C	N	O	P
			54	42	1	10	1

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Mol	Chain	Residues	Atoms				
			Total	C	N	O	P
4	A	1	Total	C	N	O	P
			54	42	1	10	1
4	A	1	Total	C	N	O	P
			54	42	1	10	1
4	A	1	Total	C	N	O	P
			54	42	1	10	1
4	A	1	Total	C	N	O	P
			54	42	1	10	1
4	A	1	Total	C	N	O	P
			54	42	1	10	1
4	A	1	Total	C	N	O	P
			54	42	1	10	1
4	A	1	Total	C	N	O	P
			54	42	1	10	1
4	A	1	Total	C	N	O	P
			54	42	1	10	1
4	A	1	Total	C	N	O	P
			54	42	1	10	1
4	A	1	Total	C	N	O	P
			54	42	1	10	1
4	A	1	Total	C	N	O	P
			54	42	1	10	1

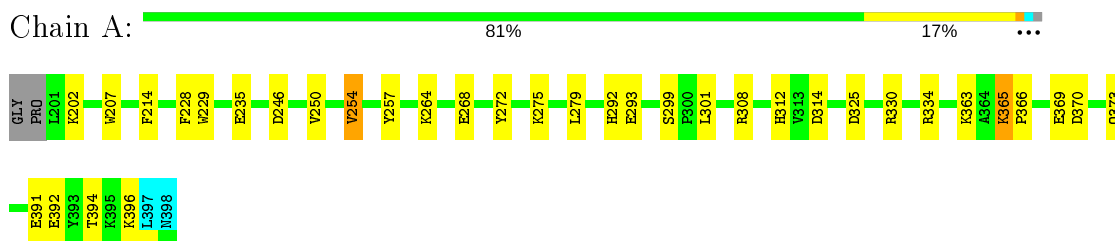
- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).

4 Residue-property plots

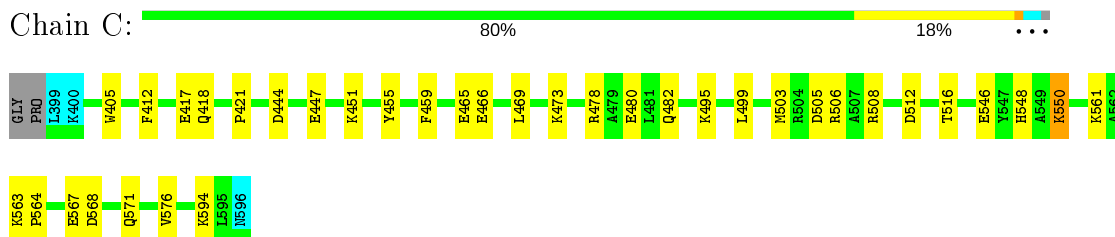
4.1 Average score per residue in the NMR ensemble

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.

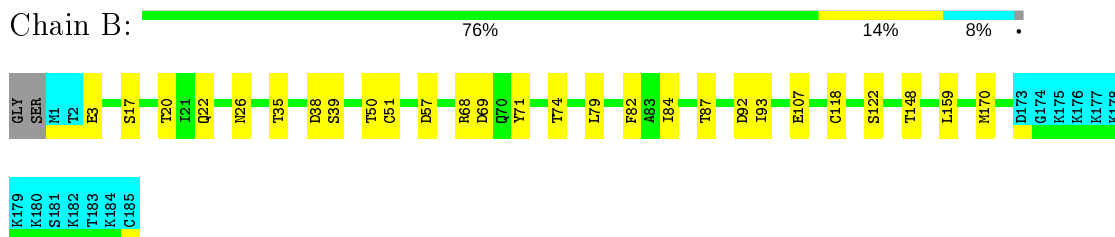
- Molecule 1: Apolipoprotein A-I



- Molecule 1: Apolipoprotein A-I



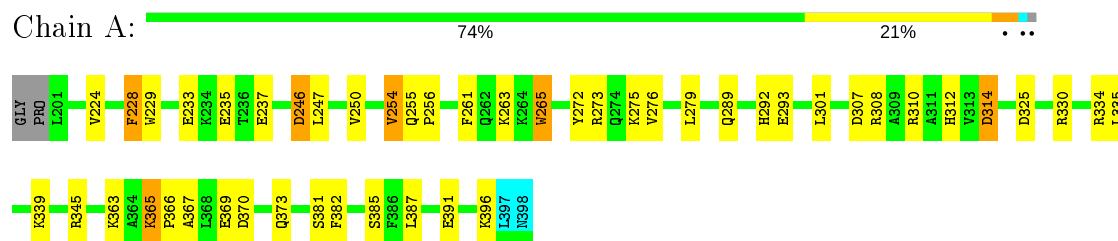
- Molecule 2: GTPase KRas



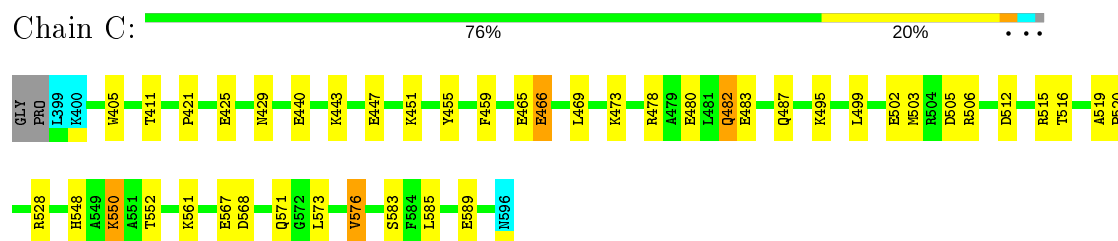
4.2 Residue scores for the representative (medoid) model from the NMR ensemble

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

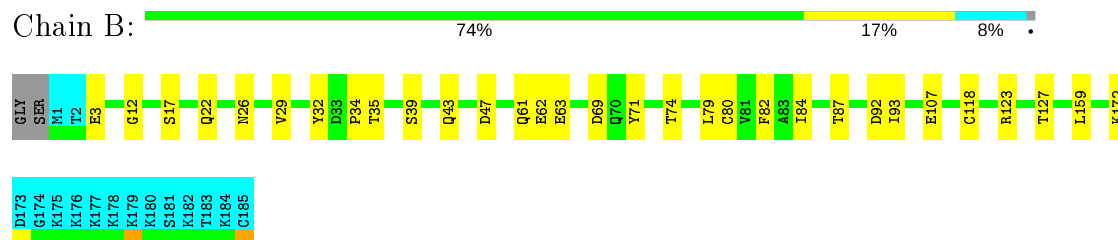
- Molecule 1: Apolipoprotein A-I



- Molecule 1: Apolipoprotein A-I



- Molecule 2: GTPase KRas



5 Refinement protocol and experimental data overview

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

Of the 3000 calculated structures, 10 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
CNS	structure solution	
HADDOCK	structure solution	
CHARMM-GUI	structure solution	
CNS	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)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	44
Number of shifts mapped to atoms	44
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	0%

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: 17F, MG, GNP, PCW

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	A	1607	22	1609	26±6
1	C	1598	22	1597	28±6
2	B	1358	18	1342	13±4
3	A	3456	0	5376	52±4
4	A	864	0	1216	20±5
5	B	32	0	13	1±1
All	All	89160	620	111525	1103

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.

5 of 865 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:308:ARG:CG	1:C:469:LEU:HD11	1.44	1.42	5	2
1:C:465:GLU:O	1:C:469:LEU:CG	1.27	1.82	1	8
1:A:308:ARG:HG2	1:C:469:LEU:CD1	1.27	1.59	5	1
1:C:465:GLU:O	1:C:469:LEU:HG	1.21	1.30	7	10
1:A:391:GLU:O	1:A:395:LYS:HG3	1.10	1.46	6	1

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	195/200 (98%)	191±2 (98±1%)	4±1 (2±1%)	1±1 (0±0%)	32	76
1	C	195/200 (98%)	191±2 (98±1%)	4±2 (2±1%)	1±1 (0±0%)	44	80
2	B	170/187 (91%)	160±2 (94±1%)	10±2 (6±1%)	0±0 (0±0%)	50	82
All	All	5600/5870 (95%)	5416 (97%)	167 (3%)	17 (0%)	44	80

5 of 6 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	365	LYS	8
1	C	563	LYS	5
1	A	366	PRO	1
2	B	34	PRO	1
2	B	117	LYS	1

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	172/175 (98%)	155±2 (90±1%)	17±2 (10±1%)	11	56
1	C	171/175 (98%)	155±2 (91±1%)	16±2 (9±1%)	12	58
2	B	150/165 (91%)	134±3 (90±2%)	16±3 (10±2%)	10	55
All	All	4930/5150 (96%)	4438 (90%)	492 (10%)	11	56

5 of 189 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	254	VAL	10
1	C	550	LYS	9
2	B	122	SER	9
1	A	312	HIS	8
1	C	516	THR	8

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 carbohydrates in this entry.

LIGAND-GEOMETRY INFOmissingINFO

6.6 Other polymers [i](#)

There are no such molecules in this entry.

6.7 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 0% for the well-defined parts and 0% for the entire structure.

7.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping [i](#)

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	44
Number of shifts mapped to atoms	44
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 [i](#)

No chemical shift referencing corrections were calculated (not enough data).

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 0%, i.e. 22 atoms were assigned a chemical shift out of a possible 7198. 0 out of 106 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/2769 (0%)	0/1104 (0%)	0/1122 (0%)	0/543 (0%)
Sidechain	22/3991 (1%)	11/2340 (0%)	11/1446 (1%)	0/205 (0%)
Aromatic	0/438 (0%)	0/244 (0%)	0/194 (0%)	0/0 (—%)
Overall	22/7198 (0%)	11/3688 (0%)	11/2762 (0%)	0/748 (0%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

No *random coil index* (RCI) plot could be generated from the current chemical shift list (`assigned_chem_shift_list_1`). RCI is only applicable to proteins.