



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 11:31 PM BST

PDB ID : 2KE5
Title : Solution structure and dynamics of the small GTPase Ralb in its active conformation: significance for effector protein binding
Authors : Fenwick, R.; Prasannan, S.; Campbell, L.J.; Nietlispach, D.; Evetts, K.A.; Camonis, J.; Mott, H.R.; Owen, D.
Deposited on : 2009-01-23

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 ⓘ 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 : 1.7.1 (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

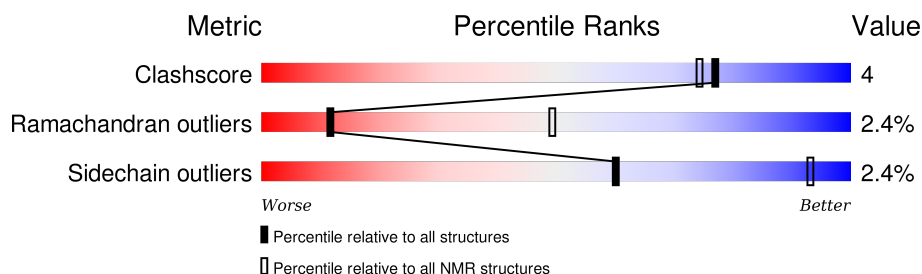
1 Overall quality at a glance

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	174	 85% 10% 5%

2 Ensemble composition and analysis ⓘ

This entry contains 50 models. Model 39 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:12-A:71, A:78-A:182 (165)	0.39	39

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 are 4 unique types of molecules in this entry. The entry contains 2844 atoms, of which 1409 are hydrogens and 0 are deuteriums.

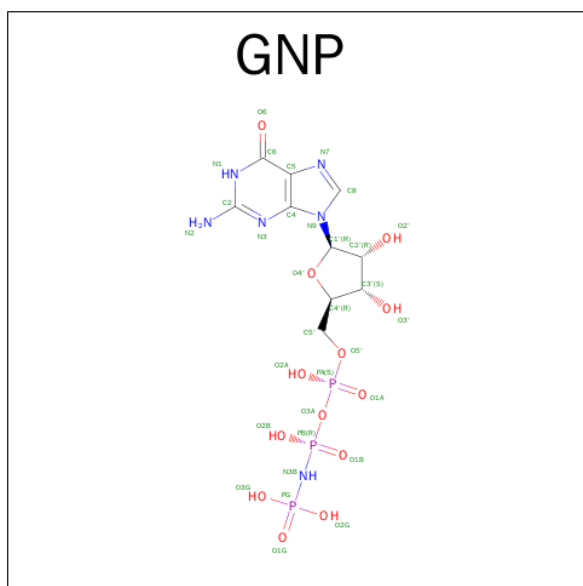
- Molecule 1 is a protein called Ras-related protein Ral-B.

Mol	Chain	Residues	Atoms						Trace
1	A	174	Total	C	H	N	O	S	0
			2792	884	1392	235	277	4	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	72	LEU	GLN	ENGINEERED	UNP P11234

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					
2	A	1	Total	C	H	N	O	P
			45	10	13	6	13	3

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	
3	A	1	Total	Mg
			1	1

- Molecule 4 is water.

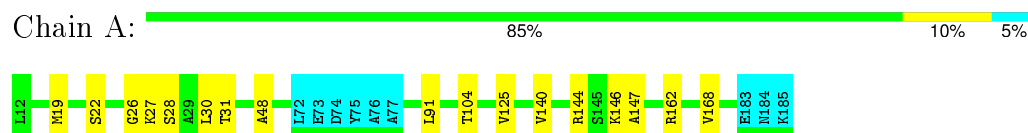
Mol	Chain	Residues	Atoms		
4	A	2	Total	H	O
			6	4	2

4 Residue-property plots [i](#)

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: Ras-related protein Ral-B

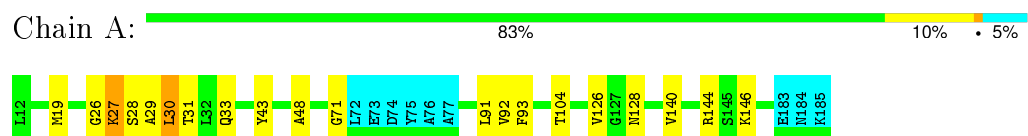


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

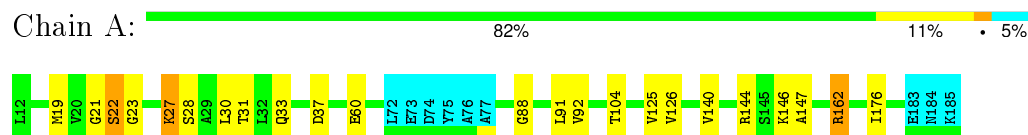
4.2.1 Score per residue for model 1

- Molecule 1: Ras-related protein Ral-B



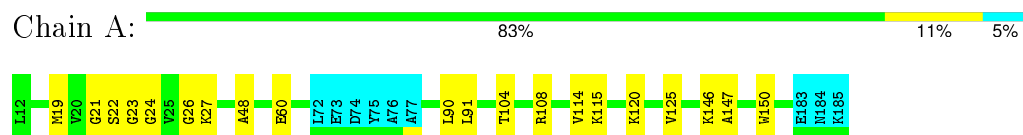
4.2.2 Score per residue for model 2

- Molecule 1: Ras-related protein Ral-B



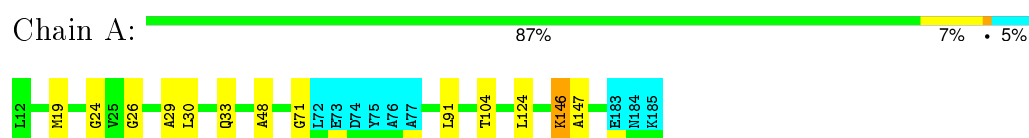
4.2.3 Score per residue for model 3

- Molecule 1: Ras-related protein Ral-B



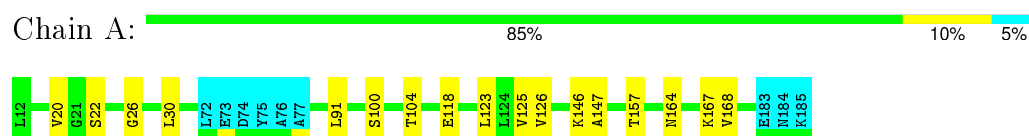
4.2.4 Score per residue for model 4

- Molecule 1: Ras-related protein Ral-B



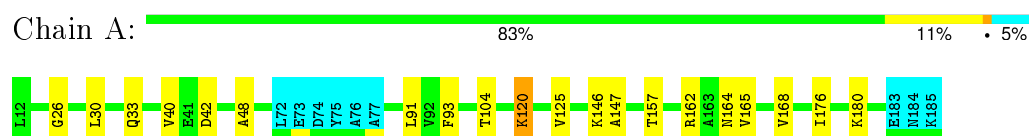
4.2.5 Score per residue for model 5

- Molecule 1: Ras-related protein Ral-B



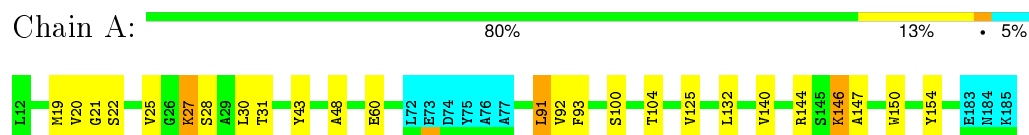
4.2.6 Score per residue for model 6

- Molecule 1: Ras-related protein Ral-B



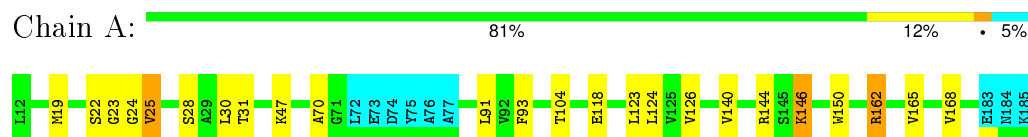
4.2.7 Score per residue for model 7

- Molecule 1: Ras-related protein Ral-B



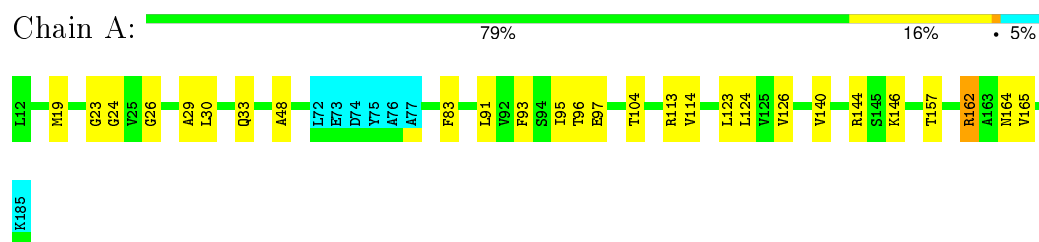
4.2.8 Score per residue for model 8

- Molecule 1: Ras-related protein Ral-B



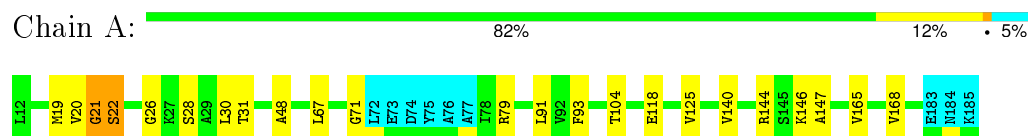
4.2.9 Score per residue for model 9

- Molecule 1: Ras-related protein Ral-B



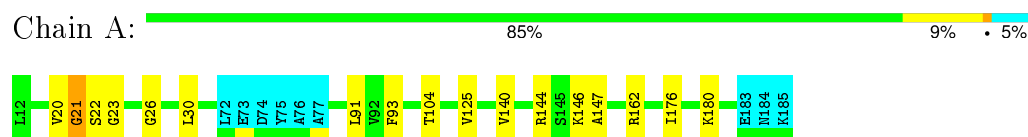
4.2.10 Score per residue for model 10

- Molecule 1: Ras-related protein Ral-B



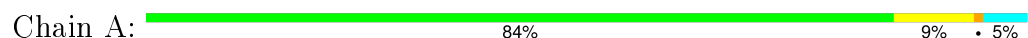
4.2.11 Score per residue for model 11

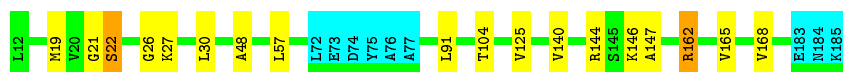
- Molecule 1: Ras-related protein Ral-B



4.2.12 Score per residue for model 12

- Molecule 1: Ras-related protein Ral-B





4.2.13 Score per residue for model 13

- Molecule 1: Ras-related protein Ral-B

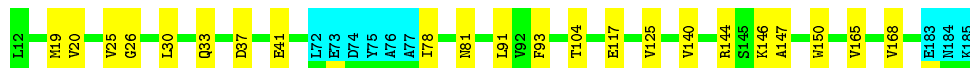
Chain A: 84% 11% 5%



4.2.14 Score per residue for model 14

- Molecule 1: Ras-related protein Ral-B

Chain A: 82% 13% 5%



4.2.15 Score per residue for model 15

- Molecule 1: Ras-related protein Ral-B

Chain A: 86% 8% 5%



4.2.16 Score per residue for model 16


- Molecule 1: Ras-related protein Ral-B

Chain A: 84% 10% 5%



4.2.17 Score per residue for model 17


- Molecule 1: Ras-related protein Ral-B

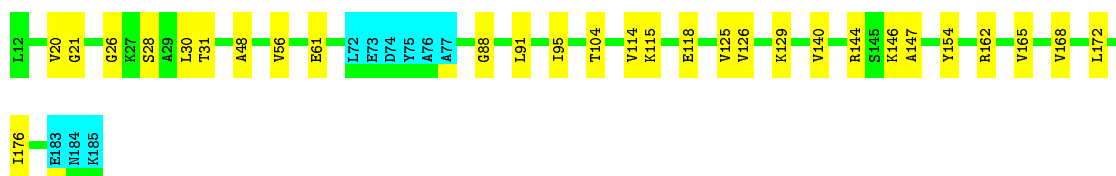
Chain A:  84% 9% 5%



4.2.18 Score per residue for model 18

- Molecule 1: Ras-related protein Ral-B

Chain A:  78% 17% 5%



4.2.19 Score per residue for model 19

- Molecule 1: Ras-related protein Ral-B

Chain A:  82% 13% 5%



4.2.20 Score per residue for model 20


- Molecule 1: Ras-related protein Ral-B

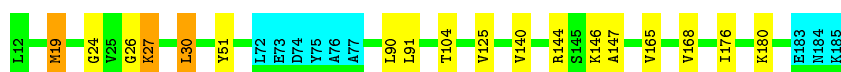
Chain A:  79% 15% 5%



4.2.21 Score per residue for model 21

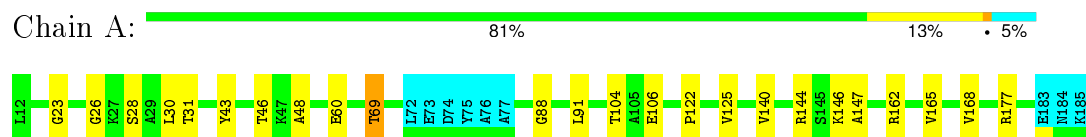
- Molecule 1: Ras-related protein Ral-B

Chain A:  84% 9% 5%



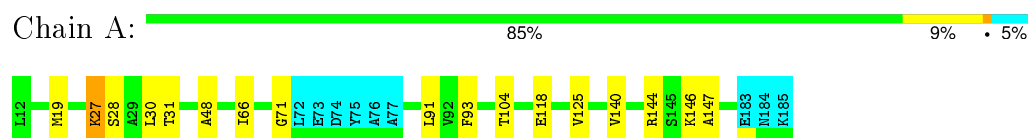
4.2.22 Score per residue for model 22

- Molecule 1: Ras-related protein Ral-B



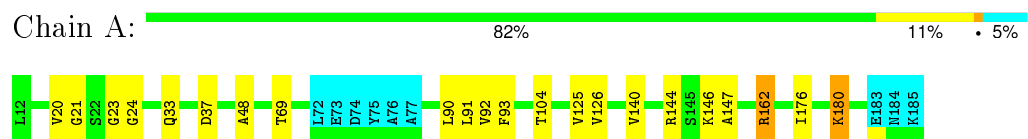
4.2.23 Score per residue for model 23

- Molecule 1: Ras-related protein Ral-B



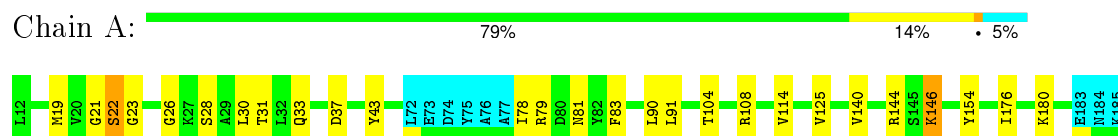
4.2.24 Score per residue for model 24

- Molecule 1: Ras-related protein Ral-B



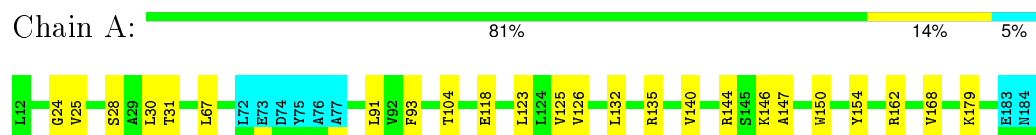
4.2.25 Score per residue for model 25

- Molecule 1: Ras-related protein Ral-B



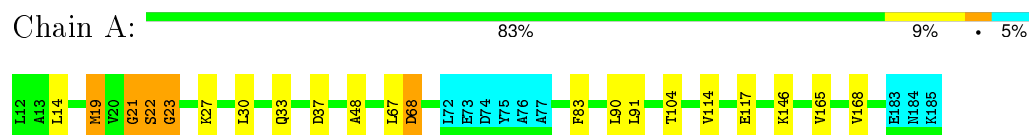
4.2.26 Score per residue for model 26

- Molecule 1: Ras-related protein Ral-B



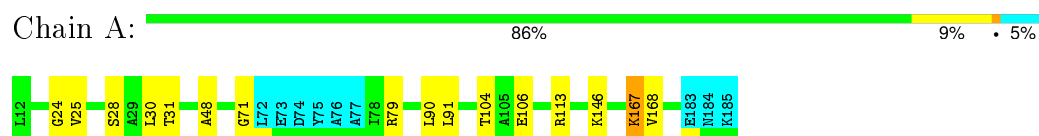
4.2.27 Score per residue for model 27

- Molecule 1: Ras-related protein Ral-B



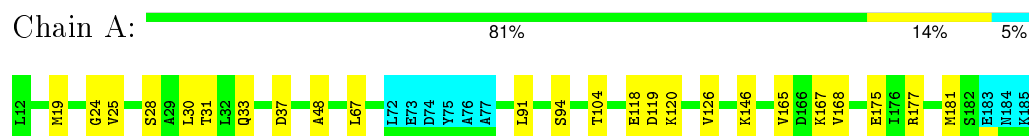
4.2.28 Score per residue for model 28

- Molecule 1: Ras-related protein Ral-B



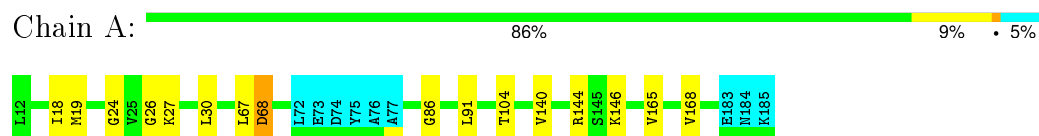
4.2.29 Score per residue for model 29

- Molecule 1: Ras-related protein Ral-B



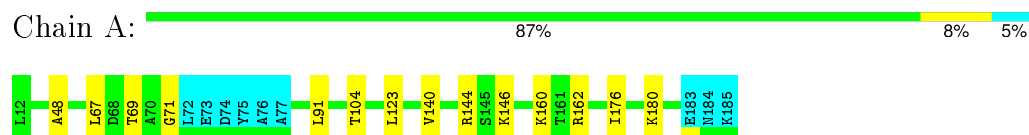
4.2.30 Score per residue for model 30

- Molecule 1: Ras-related protein Ral-B



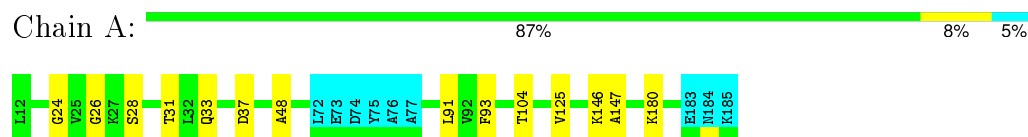
4.2.31 Score per residue for model 31

- Molecule 1: Ras-related protein Ral-B



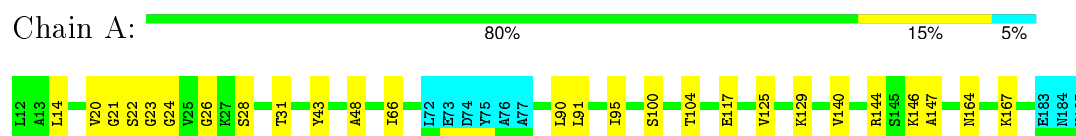
4.2.32 Score per residue for model 32

- Molecule 1: Ras-related protein Ral-B



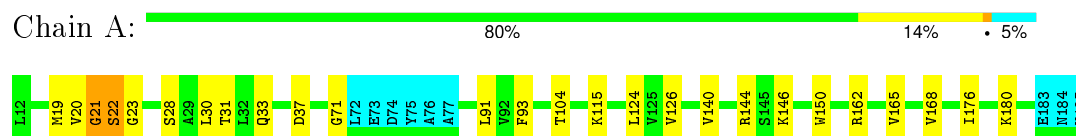
4.2.33 Score per residue for model 33

- Molecule 1: Ras-related protein Ral-B



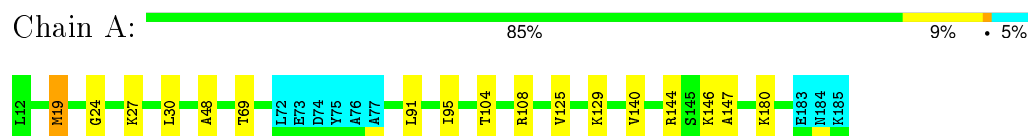
4.2.34 Score per residue for model 34

- Molecule 1: Ras-related protein Ral-B



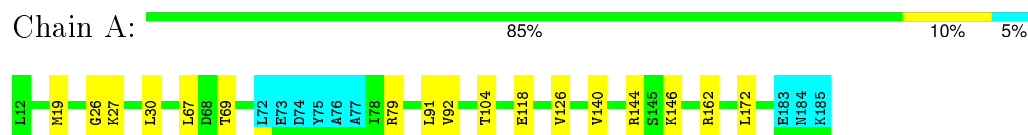
4.2.35 Score per residue for model 35

- Molecule 1: Ras-related protein Ral-B



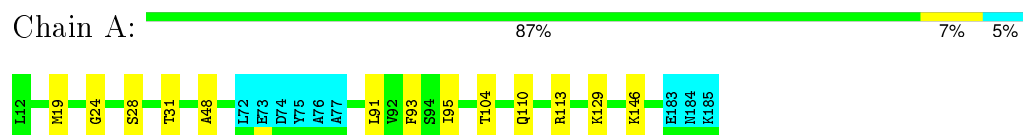
4.2.36 Score per residue for model 36

- Molecule 1: Ras-related protein Ral-B



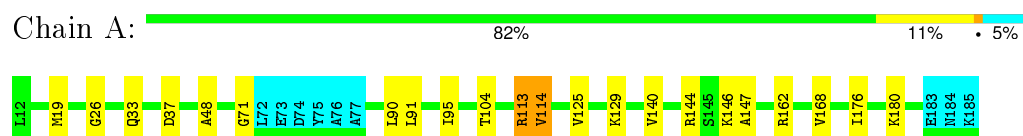
4.2.37 Score per residue for model 37

- Molecule 1: Ras-related protein Ral-B



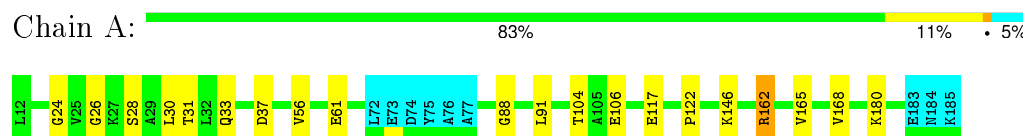
4.2.38 Score per residue for model 38

- Molecule 1: Ras-related protein Ral-B



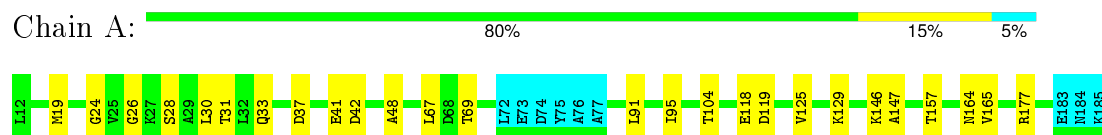
4.2.39 Score per residue for model 39 (medoid)

- Molecule 1: Ras-related protein Ral-B



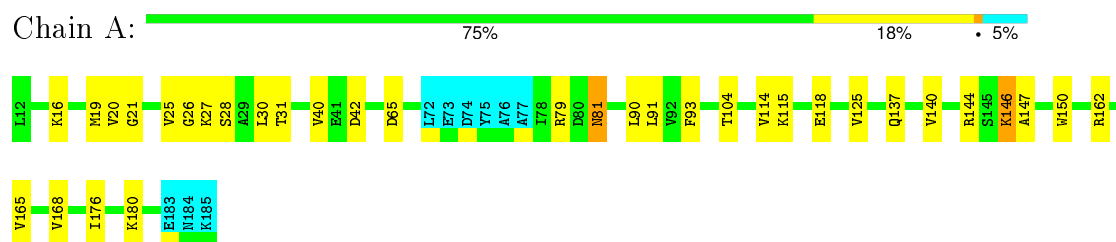
4.2.42 Score per residue for model 42

- Molecule 1: Ras-related protein Ral-B



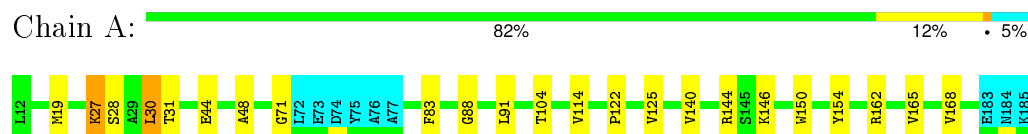
4.2.43 Score per residue for model 43

- Molecule 1: Ras-related protein Ral-B



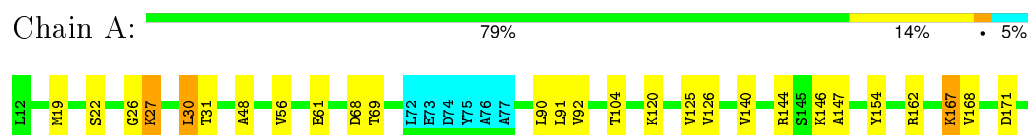
4.2.44 Score per residue for model 44

- Molecule 1: Ras-related protein Ral-B



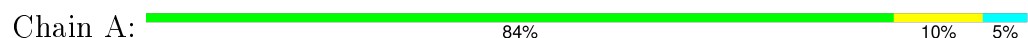
4.2.45 Score per residue for model 45

- Molecule 1: Ras-related protein Ral-B



4.2.46 Score per residue for model 46

- Molecule 1: Ras-related protein Ral-B





4.2.47 Score per residue for model 47

- Molecule 1: Ras-related protein Ral-B

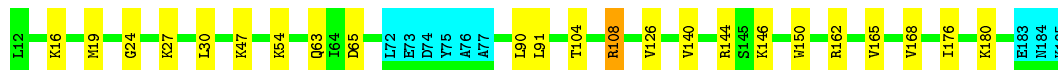
Chain A: 81% 12% • 5%



4.2.48 Score per residue for model 48

- Molecule 1: Ras-related protein Ral-B

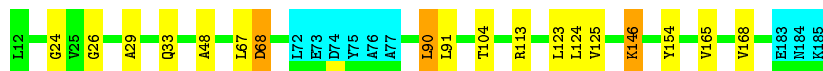
Chain A: 82% 13% • 5%



4.2.49 Score per residue for model 49

- Molecule 1: Ras-related protein Ral-B

Chain A: 84% 9% • 5%



4.2.50 Score per residue for model 50

- Molecule 1: Ras-related protein Ral-B

Chain A: 81% 12% • 5%



5 Refinement protocol and experimental data overview ⓘ

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

Of the 100 calculated structures, 50 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	refinement	1.1

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: GNP, MG

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 ⓘ

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	1326	1327	1322	9±3
2	A	32	13	13	1±1
All	All	68050	67200	66750	501

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 4.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:125:VAL:HG11	1:A:147:ALA:HB1	0.71	1.63	43	25
1:A:22:SER:N	1:A:104:THR:HG22	0.67	2.05	33	14
1:A:90:LEU:HD21	1:A:168:VAL:HG21	0.62	1.72	38	2
1:A:100:SER:O	1:A:104:THR:HG23	0.59	1.97	33	3
1:A:30:LEU:HD22	1:A:30:LEU:H	0.59	1.57	21	14
1:A:91:LEU:HD21	1:A:104:THR:HB	0.58	1.74	40	33
1:A:93:PHE:HB3	1:A:104:THR:HG21	0.56	1.77	8	19
1:A:30:LEU:H	1:A:30:LEU:HD22	0.56	1.59	16	19
1:A:92:VAL:HG23	1:A:126:VAL:HG13	0.55	1.77	1	4
1:A:22:SER:H	1:A:104:THR:HG22	0.54	1.59	33	1
1:A:91:LEU:HD11	1:A:104:THR:HB	0.53	1.80	11	44

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:LYS:HD2	1:A:27:LYS:H	0.53	1.64	1	2
1:A:165:VAL:O	1:A:168:VAL:HG22	0.52	2.04	34	21
1:A:27:LYS:H	1:A:27:LYS:HD2	0.52	1.65	47	1
1:A:157:THR:HG22	1:A:164:ASN:HB2	0.51	1.83	42	5
1:A:67:LEU:HD13	1:A:68:ASP:N	0.51	2.21	47	5
1:A:123:LEU:HG	1:A:124:LEU:N	0.51	2.21	49	3
1:A:125:VAL:HG11	1:A:147:ALA:CB	0.50	2.36	16	12
1:A:126:VAL:HG11	1:A:168:VAL:HG11	0.50	1.84	9	8
1:A:113:ARG:HG3	1:A:114:VAL:N	0.49	2.23	38	1
1:A:95:ILE:HG12	1:A:129:LYS:HB3	0.49	1.84	18	5
1:A:33:GLN:HE21	1:A:162:ARG:HG2	0.49	1.68	9	1
1:A:19:MET:HB3	1:A:27:LYS:HB3	0.49	1.85	21	5
1:A:92:VAL:HG22	1:A:126:VAL:HG12	0.48	1.85	2	1
1:A:19:MET:HB3	1:A:27:LYS:HB2	0.47	1.83	45	3
1:A:176:ILE:O	1:A:180:LYS:HB3	0.47	2.09	48	13
1:A:125:VAL:HG13	1:A:154:TYR:HA	0.47	1.85	18	2
1:A:33:GLN:HB2	1:A:165:VAL:HG21	0.47	1.86	41	3
1:A:29:ALA:O	1:A:33:GLN:HG2	0.47	2.09	49	5
1:A:132:LEU:HD12	1:A:132:LEU:N	0.46	2.25	15	2
1:A:30:LEU:HD11	1:A:92:VAL:HG11	0.46	1.87	7	1
1:A:140:VAL:O	1:A:144:ARG:HG3	0.46	2.10	19	33
1:A:83:PHE:HB3	1:A:114:VAL:HG21	0.46	1.87	27	3
1:A:27:LYS:H	1:A:27:LYS:HD3	0.46	1.70	7	1
1:A:172:LEU:HD22	1:A:172:LEU:O	0.46	2.11	19	2
1:A:19:MET:SD	1:A:90:LEU:HD23	0.46	2.51	45	1
1:A:28:SER:O	1:A:31:THR:HB	0.46	2.10	18	26
1:A:146:LYS:HD2	1:A:146:LYS:O	0.46	2.11	4	2
1:A:88:GLY:HA3	1:A:176:ILE:HD11	0.46	1.88	19	4
1:A:19:MET:HG3	1:A:27:LYS:HB2	0.46	1.87	12	3
1:A:88:GLY:HA2	1:A:122:PRO:HG2	0.46	1.88	22	3
1:A:146:LYS:HZ3	1:A:150:TRP:HE1	0.45	1.53	20	1
1:A:19:MET:HG3	1:A:27:LYS:HB3	0.45	1.89	27	4
1:A:146:LYS:NZ	1:A:150:TRP:NE1	0.45	2.65	43	1
1:A:164:ASN:O	1:A:167:LYS:HB3	0.45	2.11	33	1
1:A:30:LEU:HD12	1:A:165:VAL:HG23	0.45	1.88	42	2
1:A:126:VAL:HB	1:A:168:VAL:HG11	0.45	1.89	5	1
1:A:108:ARG:NE	1:A:150:TRP:NE1	0.45	2.64	3	1
1:A:24:GLY:O	1:A:25:VAL:HG22	0.45	2.12	8	1
1:A:146:LYS:HE3	1:A:150:TRP:CZ2	0.45	2.46	40	8
2:A:500:GNP:O3A	2:A:500:GNP:O1G	0.44	2.35	18	10
1:A:92:VAL:HG13	1:A:126:VAL:HG13	0.44	1.89	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:LYS:HD2	1:A:63:GLN:HG2	0.44	1.89	48	1
1:A:25:VAL:HG21	1:A:93:PHE:HA	0.44	1.88	7	3
1:A:176:ILE:HG23	1:A:180:LYS:HD3	0.43	1.89	16	1
1:A:20:VAL:HG22	1:A:21:GLY:N	0.43	2.27	20	12
1:A:18:ILE:HD11	1:A:86:GLY:HA3	0.43	1.89	30	1
1:A:22:SER:HB2	1:A:100:SER:HA	0.43	1.89	5	1
1:A:83:PHE:HB2	1:A:114:VAL:HG11	0.43	1.91	46	2
1:A:125:VAL:HG22	1:A:154:TYR:HD1	0.43	1.73	49	5
1:A:40:VAL:HG12	1:A:42:ASP:H	0.43	1.72	43	2
1:A:146:LYS:NZ	1:A:147:ALA:HA	0.43	2.29	4	1
1:A:56:VAL:HA	1:A:61:GLU:HA	0.43	1.90	19	4
1:A:31:THR:HG23	1:A:66:ILE:HG21	0.43	1.91	23	2
1:A:132:LEU:HD23	1:A:135:ARG:HD3	0.43	1.91	15	1
1:A:27:LYS:HD3	1:A:27:LYS:H	0.43	1.73	2	1
1:A:20:VAL:HB	1:A:91:LEU:HA	0.43	1.91	5	1
2:A:500:GNP:O1G	2:A:500:GNP:O3A	0.43	2.37	20	7
1:A:16:LYS:HG2	1:A:65:ASP:HB3	0.43	1.91	48	2
2:A:500:GNP:O1B	2:A:500:GNP:O3G	0.43	2.37	37	6
1:A:78:ILE:HA	1:A:81:ASN:ND2	0.43	2.29	25	1
1:A:176:ILE:HA	1:A:180:LYS:HB2	0.43	1.91	24	1
1:A:25:VAL:HG13	1:A:94:SER:OG	0.42	2.13	29	1
1:A:67:LEU:O	1:A:68:ASP:HB3	0.42	2.15	47	1
1:A:33:GLN:O	1:A:37:ASP:HA	0.42	2.15	25	13
1:A:40:VAL:HG22	1:A:42:ASP:H	0.42	1.74	6	1
2:A:500:GNP:O3G	2:A:500:GNP:O1B	0.42	2.38	14	5
1:A:95:ILE:HG13	1:A:96:THR:N	0.42	2.30	9	1
1:A:20:VAL:HG13	1:A:91:LEU:HA	0.42	1.91	14	1
1:A:26:GLY:O	1:A:30:LEU:HD22	0.42	2.15	17	1
1:A:146:LYS:O	1:A:146:LYS:HD2	0.42	2.15	49	1
1:A:110:GLN:HA	1:A:113:ARG:HG3	0.42	1.92	37	1
1:A:177:ARG:HA	1:A:177:ARG:NE	0.42	2.30	41	1
1:A:81:ASN:N	1:A:81:ASN:HD22	0.42	2.13	43	1
1:A:114:VAL:HG23	1:A:115:LYS:HG2	0.42	1.92	3	4
1:A:132:LEU:HD13	1:A:135:ARG:HD2	0.42	1.90	40	1
1:A:113:ARG:HA	1:A:113:ARG:NE	0.41	2.30	49	2
1:A:95:ILE:HD11	1:A:129:LYS:O	0.41	2.15	35	1
1:A:165:VAL:O	1:A:168:VAL:HG12	0.41	2.15	27	1
1:A:122:PRO:HG3	1:A:180:LYS:HD2	0.41	1.92	47	1
1:A:114:VAL:HG23	1:A:115:LYS:N	0.41	2.30	20	1
1:A:132:LEU:HB3	1:A:135:ARG:HB2	0.41	1.92	26	1
1:A:78:ILE:HA	1:A:81:ASN:HD22	0.41	1.76	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:161:THR:C	1:A:162:ARG:HG3	0.41	2.34	50	1
1:A:98:HIS:O	1:A:102:THR:HG22	0.41	2.15	20	1
1:A:90:LEU:CD1	1:A:168:VAL:HG21	0.41	2.45	27	1
1:A:120:LYS:N	1:A:120:LYS:HD2	0.41	2.31	6	1
1:A:167:LYS:HG3	1:A:168:VAL:N	0.41	2.31	45	2
1:A:22:SER:HB2	1:A:104:THR:HG23	0.41	1.93	10	1
1:A:165:VAL:HG13	1:A:166:ASP:N	0.41	2.31	17	1
1:A:90:LEU:HD23	1:A:124:LEU:O	0.41	2.16	49	1
1:A:31:THR:HG21	1:A:68:ASP:HB3	0.41	1.91	45	1
1:A:21:GLY:O	1:A:23:GLY:N	0.41	2.54	27	1
1:A:108:ARG:NH1	1:A:150:TRP:HB3	0.40	2.31	48	1
1:A:16:LYS:HB2	1:A:86:GLY:HA2	0.40	1.92	20	1
1:A:24:GLY:HA2	2:A:500:GNP:HNB3	0.40	1.76	28	1
1:A:119:ASP:C	1:A:120:LYS:HD2	0.40	2.37	29	1
1:A:46:THR:HG21	1:A:69:THR:H	0.40	1.77	22	1
1:A:25:VAL:HG11	1:A:93:PHE:HA	0.40	1.93	26	1
1:A:177:ARG:O	1:A:181:MET:HB2	0.40	2.17	29	1

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	164/174 (94%)	150±2 (91±2%)	10±3 (6±2%)	4±1 (2±1%)	12	49
All	All	8200/8700 (94%)	7496 (91%)	509 (6%)	195 (2%)	12	49

All 18 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	26	GLY	33
1	A	48	ALA	31
1	A	162	ARG	25
1	A	24	GLY	19
1	A	71	GLY	12

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Mol	Chain	Res	Type	Models (Total)
1	A	23	GLY	12
1	A	118	GLU	11
1	A	22	SER	10
1	A	21	GLY	10
1	A	69	THR	8
1	A	43	TYR	8
1	A	68	ASP	4
1	A	70	ALA	3
1	A	41	GLU	3
1	A	119	ASP	2
1	A	25	VAL	2
1	A	19	MET	1
1	A	42	ASP	1

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	144/151 (95%)	140±1 (98±1%)	4±1 (2±1%)	60	93
All	All	7200/7550 (95%)	7024 (98%)	176 (2%)	60	93

All 39 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	146	LYS	45
1	A	19	MET	19
1	A	90	LEU	10
1	A	27	LYS	10
1	A	162	ARG	10
1	A	30	LEU	8
1	A	67	LEU	6
1	A	123	LEU	5
1	A	167	LYS	5
1	A	60	GLU	4
1	A	180	LYS	4
1	A	177	ARG	4

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Mol	Chain	Res	Type	Models (Total)
1	A	124	LEU	4
1	A	117	GLU	4
1	A	14	LEU	3
1	A	91	LEU	3
1	A	108	ARG	3
1	A	120	LYS	3
1	A	106	GLU	3
1	A	47	LYS	2
1	A	97	GLU	2
1	A	113	ARG	2
1	A	57	LEU	1
1	A	51	TYR	1
1	A	44	GLU	1
1	A	115	LYS	1
1	A	12	LEU	1
1	A	175	GLU	1
1	A	137	GLN	1
1	A	128	ASN	1
1	A	118	GLU	1
1	A	179	LYS	1
1	A	81	ASN	1
1	A	164	ASN	1
1	A	172	LEU	1
1	A	171	ASP	1
1	A	129	LYS	1
1	A	114	VAL	1
1	A	160	LYS	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	GNP	A	500	3	29,34,34	1.30±0.02	0±0 (0±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	Bond angles		
					Counts	RMSZ	#Z>2
2	GNP	A	500	3	26,54,54	1.33±0.02	0±0 (0±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	GNP	A	500	3	-	0±0,13,38,38	0±0,3,3,3

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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