wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 08:25 PM GMT

PDB ID	:	1K5D
Title	:	Crystal structure of Ran-GPPNHP-RanBP1-RanGAP complex
Authors	:	Seewald, M.J.; Koerner, C.; Wittinghofer, A.; Vetter, I.R.
Deposited on	:	2001-10-10
Resolution	:	2.70 Å(reported)

This is a wwPDB X-ray 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
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:

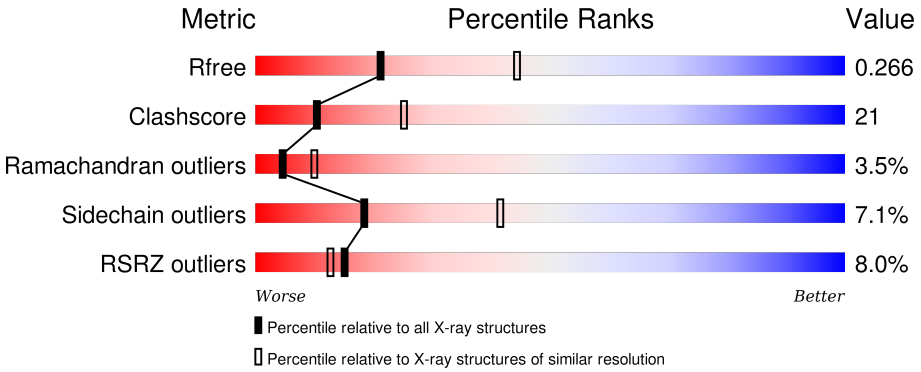
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	216	10% 55% 31% 9% • 5%
1	D	216	9% 56% 30% 8% • 5%
1	G	216	11% 59% 27% 8% • 5%
1	J	216	9% 56% 31% 8% • 5%
2	B	201	12% 34% 30% 7% 27%

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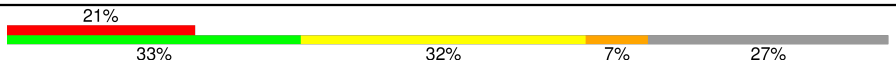
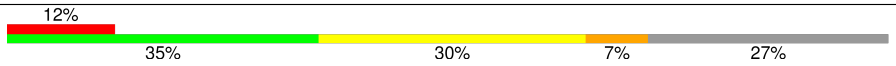
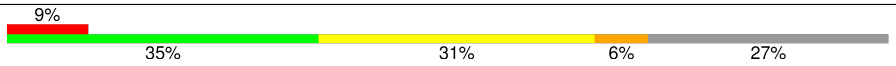
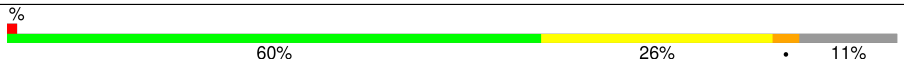
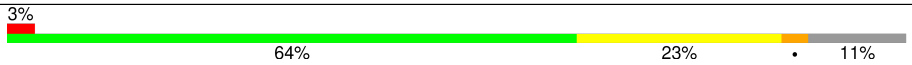
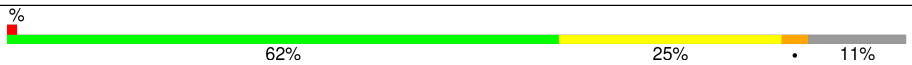
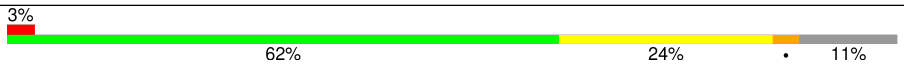
Mol	Chain	Length	Quality of chain
2	E	201	
2	H	201	
2	K	201	
3	C	386	
3	F	386	
3	I	386	
3	L	386	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22738 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called GTP-binding nuclear protein RAN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1652	1067	284	295	6			
1	D	206	Total	C	N	O	S	0	0	0
			1652	1067	284	295	6			
1	G	206	Total	C	N	O	S	0	0	0
			1652	1067	284	295	6			
1	J	206	Total	C	N	O	S	0	0	0
			1652	1067	284	295	6			

- Molecule 2 is a protein called Ran-specific GTPase-activating protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1216	769	214	226	7			
2	E	146	Total	C	N	O	S	0	0	0
			1216	769	214	226	7			
2	H	146	Total	C	N	O	S	0	0	0
			1216	769	214	226	7			
2	K	146	Total	C	N	O	S	0	0	0
			1216	769	214	226	7			

- Molecule 3 is a protein called Ran GTPase activating protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	344	Total	C	N	O	S	0	0	0
			2698	1699	469	522	8			
3	F	344	Total	C	N	O	S	0	0	0
			2698	1699	469	522	8			
3	I	344	Total	C	N	O	S	0	0	0
			2698	1699	469	522	8			
3	L	344	Total	C	N	O	S	0	0	0
			2698	1699	469	522	8			

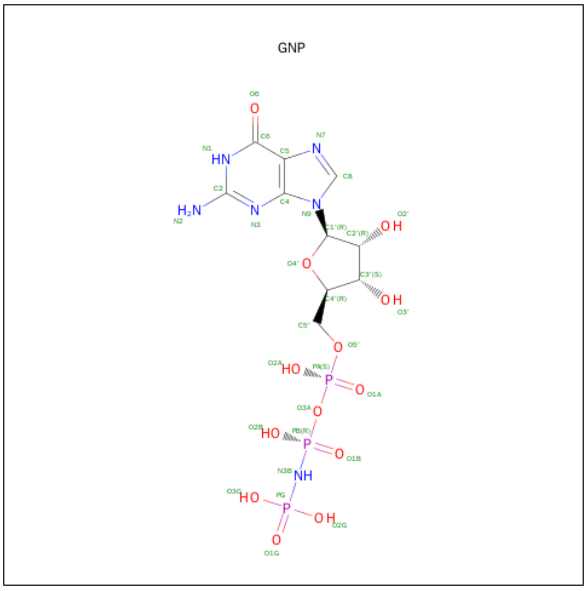
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2	ALA	SER	SEE REMARK 999	UNP P41391
F	2	ALA	SER	SEE REMARK 999	UNP P41391
I	2	ALA	SER	SEE REMARK 999	UNP P41391
L	2	ALA	SER	SEE REMARK 999	UNP P41391

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total Mg 1 1	0	0
4	J	1	Total Mg 1 1	0	0
4	A	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P 32 10 6 13 3	0	0
5	D	1	Total C N O P 32 10 6 13 3	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	G	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
5	J	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

- Molecule 6 is water.

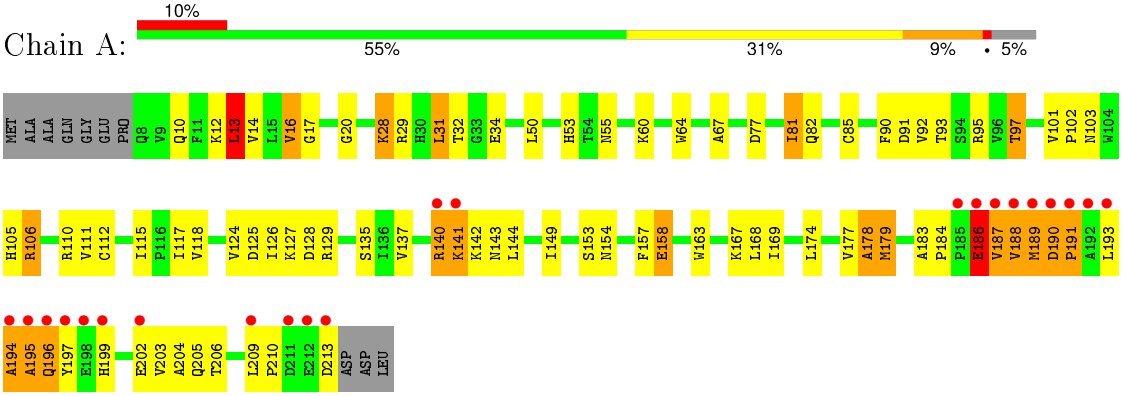
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	24	Total	O	0	0
			24	24		
6	B	3	Total	O	0	0
			3	3		
6	C	71	Total	O	0	0
			71	71		
6	D	29	Total	O	0	0
			29	29		
6	E	2	Total	O	0	0
			2	2		
6	F	47	Total	O	0	0
			47	47		
6	G	25	Total	O	0	0
			25	25		
6	H	5	Total	O	0	0
			5	5		
6	I	53	Total	O	0	0
			53	53		
6	J	31	Total	O	0	0
			31	31		
6	K	4	Total	O	0	0
			4	4		
6	L	48	Total	O	0	0
			48	48		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

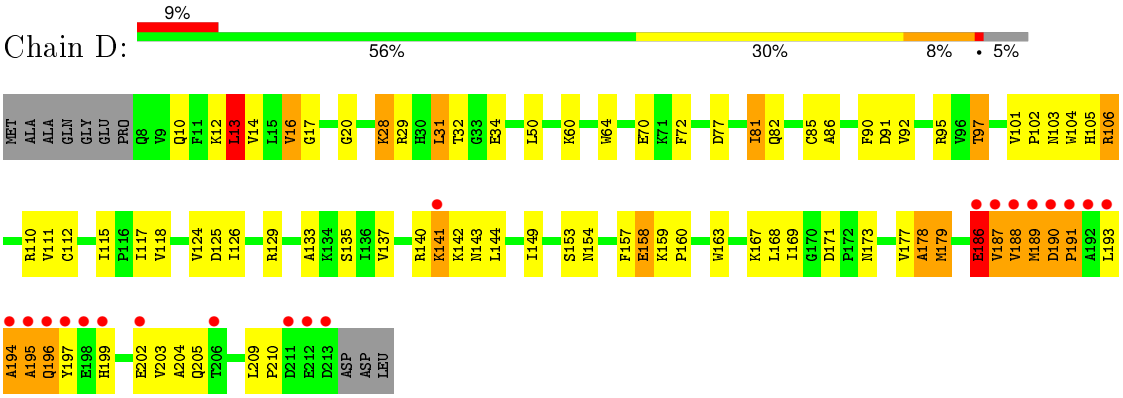
- Molecule 1: GTP-binding nuclear protein RAN

Chain A:



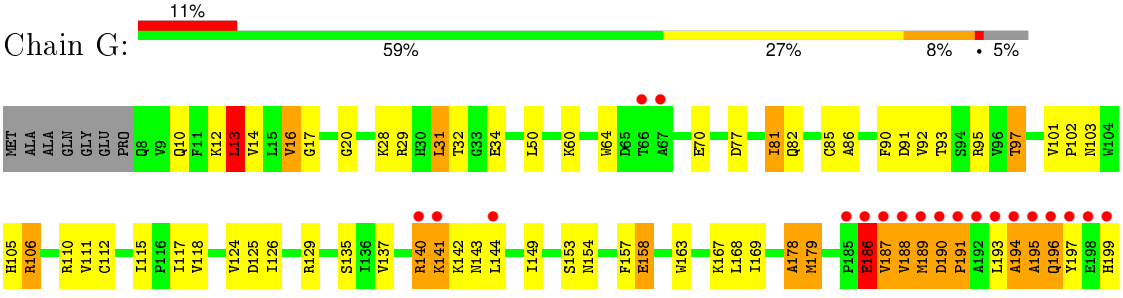
- Molecule 1: GTP-binding nuclear protein RAN

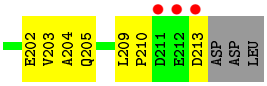
Chain D:



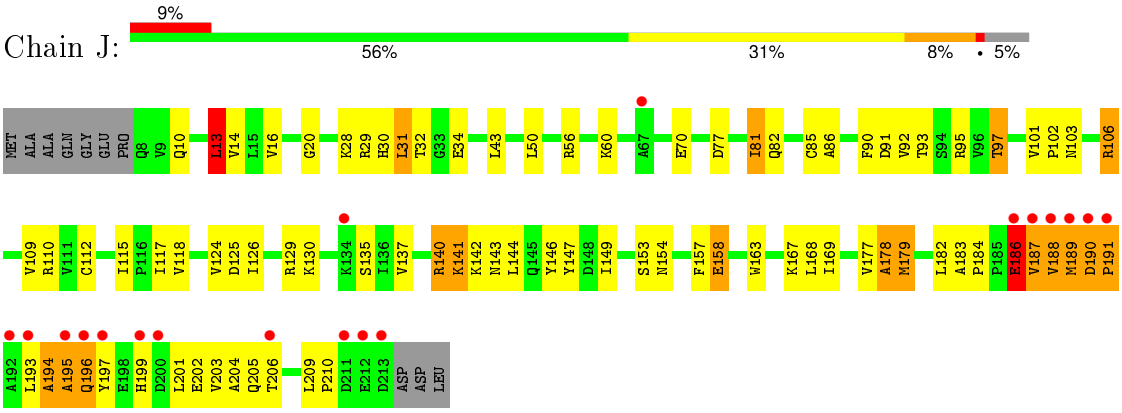
- Molecule 1: GTP-binding nuclear protein RAN

Chain G:

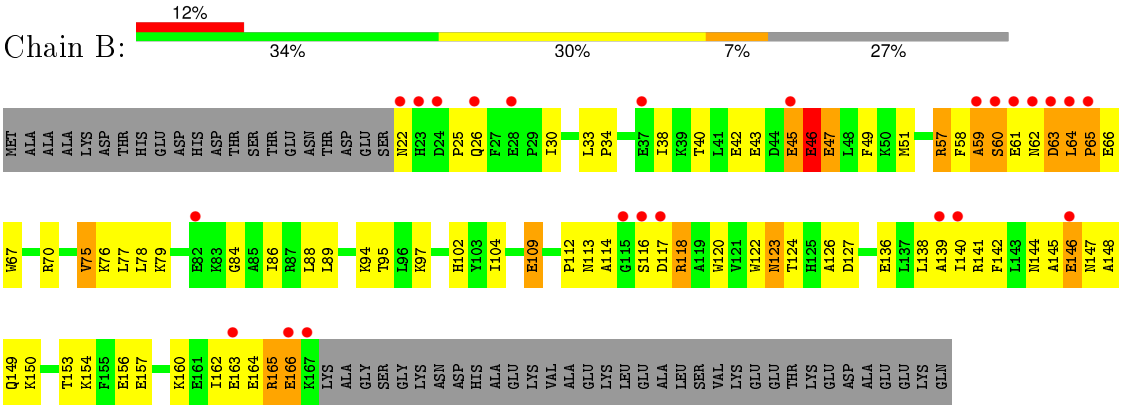




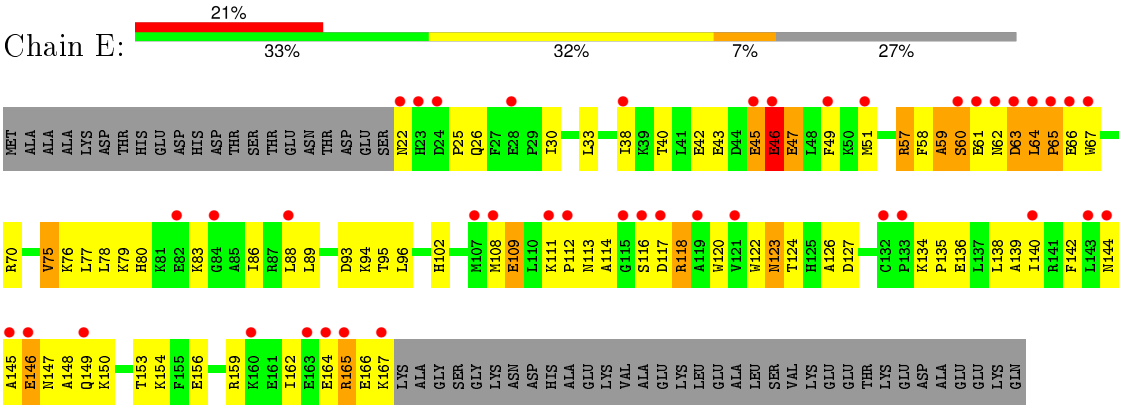
• Molecule 1: GTP-binding nuclear protein RAN



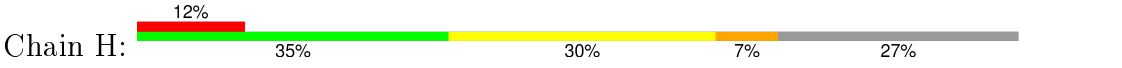
• Molecule 2: Ran-specific GTPase-activating protein

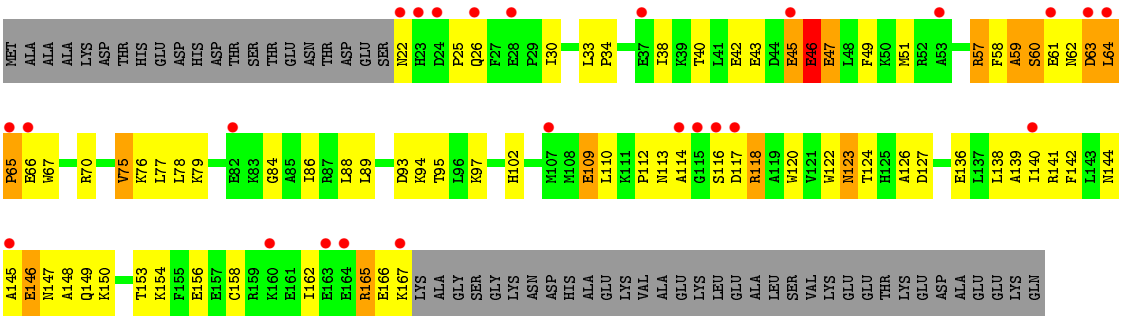


• Molecule 2: Ran-specific GTPase-activating protein



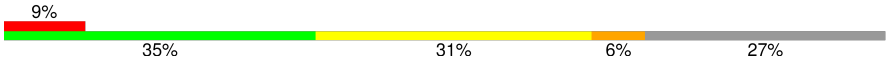
• Molecule 2: Ran-specific GTPase-activating protein

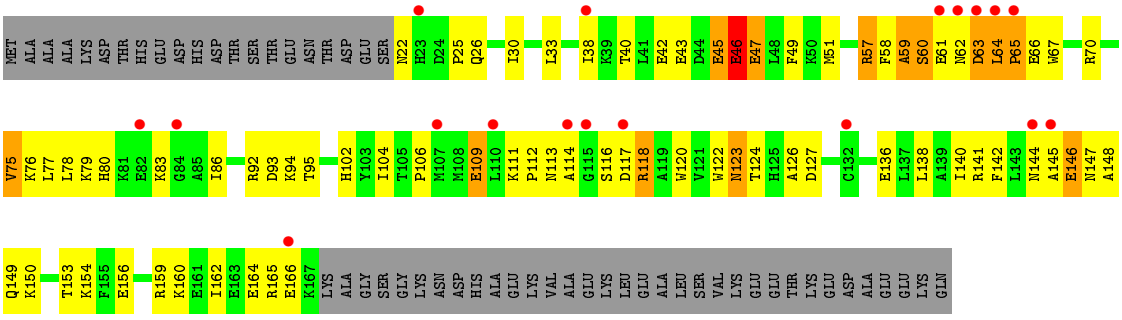




• Molecule 2: Ran-specific GTPase-activating protein

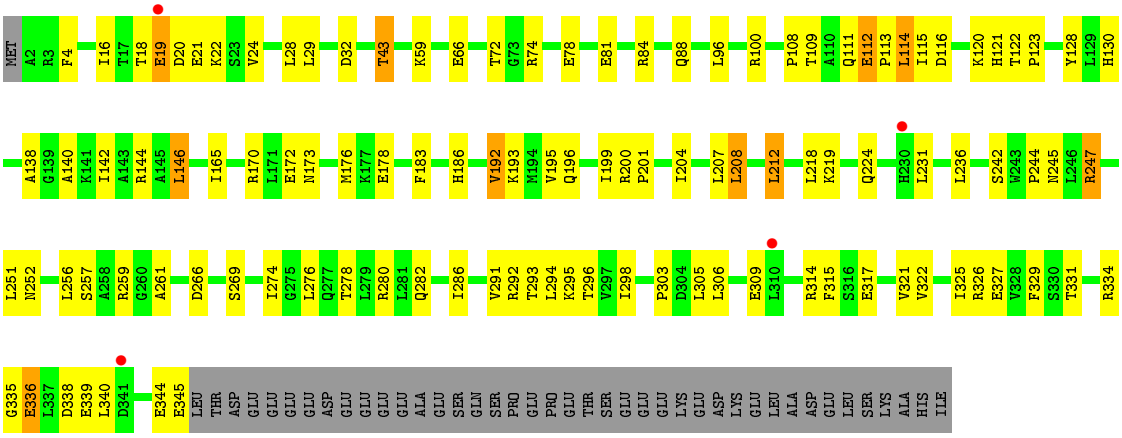
Chain K:





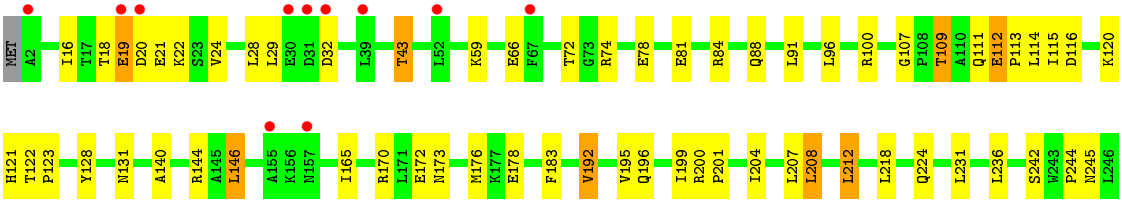
• Molecule 3: Ran GTPase activating protein 1

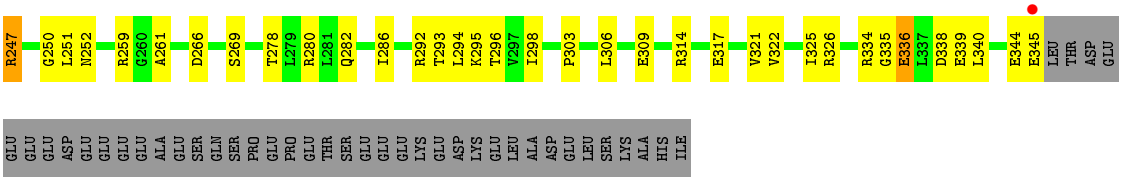
Chain C:



• Molecule 3: Ran GTPase activating protein 1

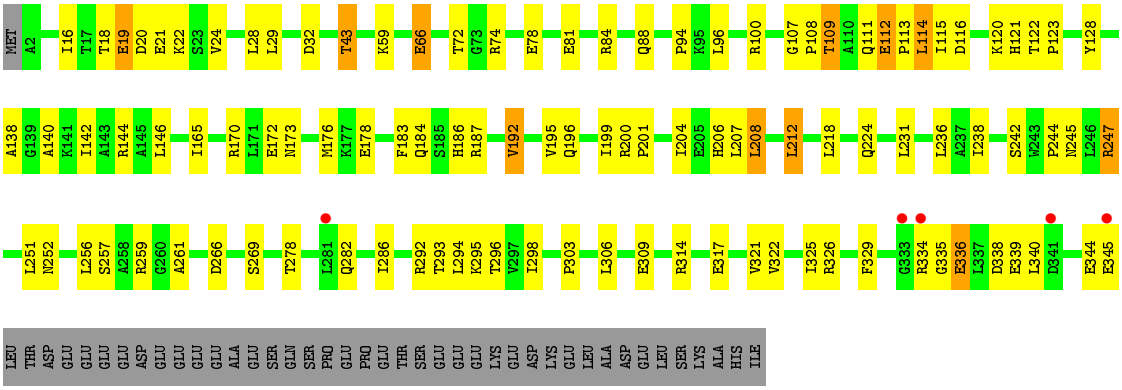
Chain F:





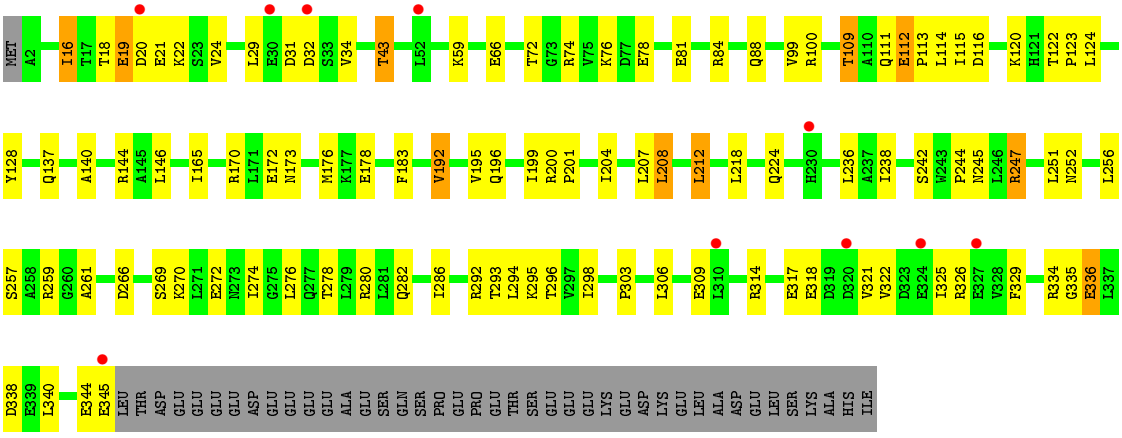
• Molecule 3: Ran GTPase activating protein 1

Chain I:



• Molecule 3: Ran GTPase activating protein 1

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	101.55Å 103.11Å 120.18Å 71.59° 80.55° 67.78°	Depositor
Resolution (Å)	20.00 – 2.70 20.07 – 2.41	Depositor EDS
% Data completeness (in resolution range)	98.0 (20.00-2.70) 87.8 (20.07-2.41)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.22 (at 2.41Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.237 , 0.267 0.237 , 0.266	Depositor DCC
R_{free} test set	11398 reflections (9.93%)	DCC
Wilson B-factor (Å^2)	51.9	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 56.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 159097 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	22738	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.36% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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 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	0.41	0/1693	0.65	1/2296 (0.0%)
1	D	0.41	0/1693	0.64	1/2296 (0.0%)
1	G	0.42	0/1693	0.64	1/2296 (0.0%)
1	J	0.43	0/1693	0.65	1/2296 (0.0%)
2	B	0.36	0/1242	0.62	0/1666
2	E	0.34	0/1242	0.61	0/1666
2	H	0.36	0/1242	0.63	0/1666
2	K	0.36	0/1242	0.62	0/1666
3	C	0.41	0/2737	0.66	0/3697
3	F	0.39	0/2737	0.65	0/3697
3	I	0.39	0/2737	0.66	0/3697
3	L	0.39	0/2737	0.66	0/3697
All	All	0.39	0/22688	0.64	4/30636 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	13	LEU	CA-CB-CG	5.55	128.07	115.30
1	J	13	LEU	CA-CB-CG	5.54	128.03	115.30
1	A	13	LEU	CA-CB-CG	5.28	127.43	115.30
1	D	13	LEU	CA-CB-CG	5.26	127.41	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1652	0	1659	76	0
1	D	1652	0	1659	77	0
1	G	1652	0	1659	71	0
1	J	1652	0	1659	89	0
2	B	1216	0	1208	80	0
2	E	1216	0	1208	85	0
2	H	1216	0	1208	79	0
2	K	1216	0	1208	88	0
3	C	2698	0	2733	103	0
3	F	2698	0	2733	85	0
3	I	2698	0	2733	98	0
3	L	2698	0	2733	93	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
4	G	1	0	0	0	0
4	J	1	0	0	0	0
5	A	32	0	13	2	0
5	D	32	0	13	3	0
5	G	32	0	13	3	0
5	J	32	0	13	6	0
6	A	24	0	0	4	0
6	B	3	0	0	0	0
6	C	71	0	0	17	0
6	D	29	0	0	5	0
6	E	2	0	0	0	0
6	F	47	0	0	7	0
6	G	25	0	0	4	0
6	H	5	0	0	0	0
6	I	53	0	0	8	0
6	J	31	0	0	6	0
6	K	4	0	0	1	0
6	L	48	0	0	5	0
All	All	22738	0	22452	964	0

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 21.

The worst 5 of 964 close contacts within the same asymmetric unit are listed below, sorted by

their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:165:ILE:HA	6:C:445:HOH:O	1.52	1.09
5:J:4250:GNP:PG	6:J:4252:HOH:O	2.14	1.03
1:A:91:ASP:H	1:A:97:THR:HG21	1.22	1.01
1:G:91:ASP:H	1:G:97:THR:HG21	1.21	1.00
1:J:91:ASP:H	1:J:97:THR:HG21	1.23	0.99

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 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 X-ray entries followed by that with respect to entries of similar resolution.

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	204/216 (94%)	174 (85%)	17 (8%)	13 (6%)	2	2
1	D	204/216 (94%)	176 (86%)	15 (7%)	13 (6%)	2	2
1	G	204/216 (94%)	174 (85%)	17 (8%)	13 (6%)	2	2
1	J	204/216 (94%)	175 (86%)	16 (8%)	13 (6%)	2	2
2	B	144/201 (72%)	121 (84%)	15 (10%)	8 (6%)	2	3
2	E	144/201 (72%)	119 (83%)	17 (12%)	8 (6%)	2	3
2	H	144/201 (72%)	121 (84%)	15 (10%)	8 (6%)	2	3
2	K	144/201 (72%)	121 (84%)	15 (10%)	8 (6%)	2	3
3	C	342/386 (89%)	301 (88%)	38 (11%)	3 (1%)	21	49
3	F	342/386 (89%)	302 (88%)	37 (11%)	3 (1%)	21	49
3	I	342/386 (89%)	305 (89%)	34 (10%)	3 (1%)	21	49
3	L	342/386 (89%)	305 (89%)	34 (10%)	3 (1%)	21	49
All	All	2760/3212 (86%)	2394 (87%)	270 (10%)	96 (4%)	4	10

5 of 96 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	ARG
1	A	179	MET
1	A	189	MET
1	A	190	ASP
1	A	191	PRO

5.3.2 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 X-ray entries followed by that with respect to entries of similar resolution.

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	178/185 (96%)	165 (93%)	13 (7%)	17	39
1	D	178/185 (96%)	165 (93%)	13 (7%)	17	39
1	G	178/185 (96%)	165 (93%)	13 (7%)	17	39
1	J	178/185 (96%)	166 (93%)	12 (7%)	20	44
2	B	131/176 (74%)	119 (91%)	12 (9%)	11	25
2	E	131/176 (74%)	119 (91%)	12 (9%)	11	25
2	H	131/176 (74%)	119 (91%)	12 (9%)	11	25
2	K	131/176 (74%)	119 (91%)	12 (9%)	11	25
3	C	295/334 (88%)	277 (94%)	18 (6%)	23	49
3	F	295/334 (88%)	277 (94%)	18 (6%)	23	49
3	I	295/334 (88%)	277 (94%)	18 (6%)	23	49
3	L	295/334 (88%)	277 (94%)	18 (6%)	23	49
All	All	2416/2780 (87%)	2245 (93%)	171 (7%)	18	41

5 of 171 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	146	LEU
1	G	141	LYS
3	L	81	GLU
3	F	196	GLN
1	G	13	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 73 such sidechains are listed below:

Mol	Chain	Res	Type
3	F	206	HIS
1	G	156	ASN
3	L	130	HIS
1	G	30	HIS
2	H	102	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or 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 length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	GNP	A	1250	4	28,34,34	1.52	6 (21%)	33,54,54	2.24	5 (15%)
5	GNP	D	2250	4	28,34,34	1.67	6 (21%)	33,54,54	2.22	7 (21%)
5	GNP	G	3250	4	28,34,34	1.61	4 (14%)	33,54,54	2.24	6 (18%)
5	GNP	J	4250	4	28,34,34	1.69	6 (21%)	33,54,54	2.22	6 (18%)

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
5	GNP	A	1250	4	-	1/12/38/38	0/3/3/3
5	GNP	D	2250	4	-	1/12/38/38	0/3/3/3
5	GNP	G	3250	4	-	1/12/38/38	0/3/3/3
5	GNP	J	4250	4	-	1/12/38/38	0/3/3/3

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	2250	GNP	PG-O2G	-3.95	1.45	1.56
5	D	2250	GNP	PB-O2B	-3.85	1.46	1.56
5	A	1250	GNP	PG-O2G	-3.80	1.46	1.56
5	G	3250	GNP	PG-O2G	-3.77	1.46	1.56
5	G	3250	GNP	PB-O2B	-3.63	1.46	1.56

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	3250	GNP	C5-C6-N1	-8.12	112.48	123.59
5	A	1250	GNP	C5-C6-N1	-8.11	112.50	123.59
5	D	2250	GNP	C5-C6-N1	-8.06	112.58	123.59
5	J	4250	GNP	C5-C6-N1	-7.95	112.72	123.59
5	J	4250	GNP	N3-C2-N1	-3.89	121.51	127.44

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	3250	GNP	O1B-PB-N3B-PG
5	D	2250	GNP	O1B-PB-N3B-PG
5	A	1250	GNP	O1B-PB-N3B-PG
5	J	4250	GNP	O1B-PB-N3B-PG

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1250	GNP	2	0
5	D	2250	GNP	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	3250	GNP	3	0
5	J	4250	GNP	6	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	206/216 (95%)	0.31	22 (10%) 8 6	27, 46, 132, 170	0
1	D	206/216 (95%)	0.50	20 (9%) 10 7	21, 46, 146, 188	0
1	G	206/216 (95%)	0.39	23 (11%) 7 5	28, 49, 127, 168	0
1	J	206/216 (95%)	0.25	19 (9%) 11 9	24, 47, 117, 170	0
2	B	146/201 (72%)	0.69	24 (16%) 2 2	36, 72, 130, 159	0
2	E	146/201 (72%)	1.32	42 (28%) 1 0	41, 88, 138, 159	0
2	H	146/201 (72%)	0.92	25 (17%) 2 1	41, 71, 138, 176	0
2	K	146/201 (72%)	0.58	18 (12%) 5 4	28, 73, 126, 149	0
3	C	344/386 (89%)	-0.12	4 (1%) 81 81	21, 42, 76, 135	0
3	F	344/386 (89%)	-0.08	12 (3%) 48 48	24, 45, 83, 135	0
3	I	344/386 (89%)	-0.09	5 (1%) 76 76	23, 45, 81, 114	0
3	L	344/386 (89%)	-0.03	10 (2%) 55 55	22, 45, 90, 143	0
All	All	2784/3212 (86%)	0.25	224 (8%) 15 13	21, 49, 120, 188	0

The worst 5 of 224 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	189	MET	15.6
1	D	191	PRO	12.1
1	D	192	ALA	11.5
1	G	192	ALA	10.7
1	D	188	VAL	10.6

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	GNP	G	3250	32/32	0.96	0.15	-0.73	37,37,37,37	0
5	GNP	A	1250	32/32	0.96	0.13	-0.81	37,37,37,37	0
4	MG	G	3251	1/1	0.97	0.13	-0.90	36,36,36,36	0
5	GNP	D	2250	32/32	0.98	0.13	-1.04	37,37,37,37	0
5	GNP	J	4250	32/32	0.97	0.12	-1.28	36,36,36,36	0
4	MG	J	4251	1/1	0.98	0.09	-1.82	44,44,44,44	0
4	MG	D	2251	1/1	0.96	0.08	-1.91	44,44,44,44	0
4	MG	A	1251	1/1	0.99	0.07	-2.49	29,29,29,29	0

6.5 Other polymers (i)

There are no such residues in this entry.