



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 03:47 PM GMT

PDB ID : 2E7S  
Title : Crystal structure of the yeast Sec2p GEF domain  
Authors : Fukai, S.; Sato, Y.; Nureki, O.  
Deposited on : 2007-01-12  
Resolution : 3.00 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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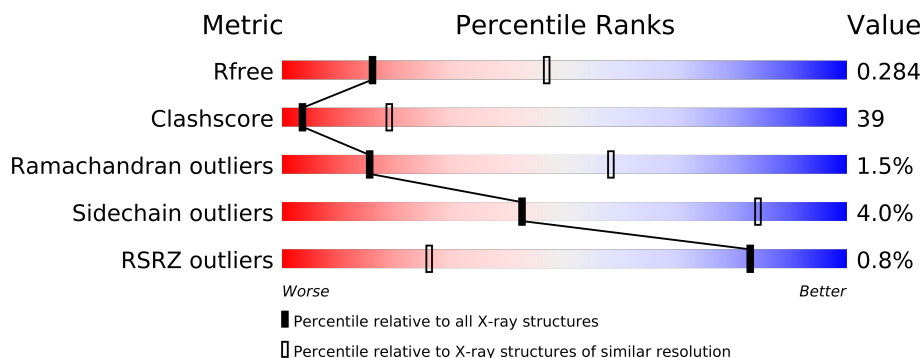
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.00 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.



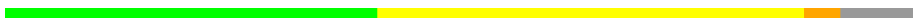
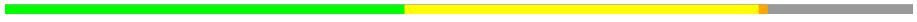
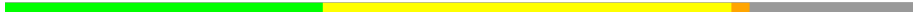

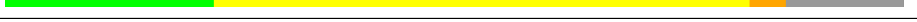

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	135	
1	B	135	
1	C	135	
1	D	135	
1	E	135	
1	F	135	
1	G	135	
1	H	135	
1	I	135	
1	J	135	
1	K	135	
1	L	135	
1	M	135	
1	N	135	

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Mol	Chain	Length	Quality of chain
1	O	135	
1	P	135	
1	Q	135	
1	R	135	
1	S	135	
1	T	135	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19270 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Rab guanine nucleotide exchange factor SEC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	114	Total	C	N	O	Se	0	0	0
			938	575	164	197	2			
1	B	121	Total	C	N	O	Se	0	0	0
			993	610	172	209	2			
1	C	118	Total	C	N	O	Se	0	0	0
			968	593	168	205	2			
1	D	124	Total	C	N	O	Se	0	0	0
			1018	626	177	213	2			
1	E	124	Total	C	N	O	Se	0	0	0
			1018	626	177	213	2			
1	F	124	Total	C	N	O	Se	0	0	0
			1018	626	177	213	2			
1	G	110	Total	C	N	O	Se	0	0	0
			906	554	160	191	1			
1	H	107	Total	C	N	O	Se	0	0	0
			877	537	153	186	1			
1	I	114	Total	C	N	O	Se	0	0	0
			938	575	164	197	2			
1	J	107	Total	C	N	O	Se	0	0	0
			877	537	153	186	1			
1	K	117	Total	C	N	O	Se	0	0	0
			961	589	167	203	2			
1	L	114	Total	C	N	O	Se	0	0	0
			938	575	164	197	2			
1	M	117	Total	C	N	O	Se	0	0	0
			961	589	167	203	2			
1	N	111	Total	C	N	O	Se	0	0	0
			914	558	161	194	1			
1	O	124	Total	C	N	O	Se	0	0	0
			1018	626	177	213	2			
1	P	114	Total	C	N	O	Se	0	0	0
			938	575	164	197	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	111	Total	C	N	O	Se	0	0	0
			914	558	161	194	1			
1	R	111	Total	C	N	O	Se	0	0	0
			914	558	161	194	1			
1	S	117	Total	C	N	O	Se	0	0	0
			961	589	167	203	2			
1	T	114	Total	C	N	O	Se	0	0	0
			938	575	164	197	2			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	GLY	-	EXPRESSION TAG	UNP P17065
A	27	PRO	-	EXPRESSION TAG	UNP P17065
A	28	LEU	-	EXPRESSION TAG	UNP P17065
A	29	GLY	-	EXPRESSION TAG	UNP P17065
A	30	SER	-	EXPRESSION TAG	UNP P17065
A	115	LEU	MET	ENGINEERED	UNP P17065
B	26	GLY	-	EXPRESSION TAG	UNP P17065
B	27	PRO	-	EXPRESSION TAG	UNP P17065
B	28	LEU	-	EXPRESSION TAG	UNP P17065
B	29	GLY	-	EXPRESSION TAG	UNP P17065
B	30	SER	-	EXPRESSION TAG	UNP P17065
B	115	LEU	MET	ENGINEERED	UNP P17065
C	26	GLY	-	EXPRESSION TAG	UNP P17065
C	27	PRO	-	EXPRESSION TAG	UNP P17065
C	28	LEU	-	EXPRESSION TAG	UNP P17065
C	29	GLY	-	EXPRESSION TAG	UNP P17065
C	30	SER	-	EXPRESSION TAG	UNP P17065
C	115	LEU	MET	ENGINEERED	UNP P17065
D	26	GLY	-	EXPRESSION TAG	UNP P17065
D	27	PRO	-	EXPRESSION TAG	UNP P17065
D	28	LEU	-	EXPRESSION TAG	UNP P17065
D	29	GLY	-	EXPRESSION TAG	UNP P17065
D	30	SER	-	EXPRESSION TAG	UNP P17065
D	115	LEU	MET	ENGINEERED	UNP P17065
E	26	GLY	-	EXPRESSION TAG	UNP P17065
E	27	PRO	-	EXPRESSION TAG	UNP P17065
E	28	LEU	-	EXPRESSION TAG	UNP P17065
E	29	GLY	-	EXPRESSION TAG	UNP P17065
E	30	SER	-	EXPRESSION TAG	UNP P17065
E	115	LEU	MET	ENGINEERED	UNP P17065
F	26	GLY	-	EXPRESSION TAG	UNP P17065

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Chain	Residue	Modelled	Actual	Comment	Reference
F	27	PRO	-	EXPRESSION TAG	UNP P17065
F	28	LEU	-	EXPRESSION TAG	UNP P17065
F	29	GLY	-	EXPRESSION TAG	UNP P17065
F	30	SER	-	EXPRESSION TAG	UNP P17065
F	115	LEU	MET	ENGINEERED	UNP P17065
G	26	GLY	-	EXPRESSION TAG	UNP P17065
G	27	PRO	-	EXPRESSION TAG	UNP P17065
G	28	LEU	-	EXPRESSION TAG	UNP P17065
G	29	GLY	-	EXPRESSION TAG	UNP P17065
G	30	SER	-	EXPRESSION TAG	UNP P17065
G	115	LEU	MET	ENGINEERED	UNP P17065
H	26	GLY	-	EXPRESSION TAG	UNP P17065
H	27	PRO	-	EXPRESSION TAG	UNP P17065
H	28	LEU	-	EXPRESSION TAG	UNP P17065
H	29	GLY	-	EXPRESSION TAG	UNP P17065
H	30	SER	-	EXPRESSION TAG	UNP P17065
H	115	LEU	MET	ENGINEERED	UNP P17065
I	26	GLY	-	EXPRESSION TAG	UNP P17065
I	27	PRO	-	EXPRESSION TAG	UNP P17065
I	28	LEU	-	EXPRESSION TAG	UNP P17065
I	29	GLY	-	EXPRESSION TAG	UNP P17065
I	30	SER	-	EXPRESSION TAG	UNP P17065
I	115	LEU	MET	ENGINEERED	UNP P17065
J	26	GLY	-	EXPRESSION TAG	UNP P17065
J	27	PRO	-	EXPRESSION TAG	UNP P17065
J	28	LEU	-	EXPRESSION TAG	UNP P17065
J	29	GLY	-	EXPRESSION TAG	UNP P17065
J	30	SER	-	EXPRESSION TAG	UNP P17065
J	115	LEU	MET	ENGINEERED	UNP P17065
K	26	GLY	-	EXPRESSION TAG	UNP P17065
K	27	PRO	-	EXPRESSION TAG	UNP P17065
K	28	LEU	-	EXPRESSION TAG	UNP P17065
K	29	GLY	-	EXPRESSION TAG	UNP P17065
K	30	SER	-	EXPRESSION TAG	UNP P17065
K	115	LEU	MET	ENGINEERED	UNP P17065
L	26	GLY	-	EXPRESSION TAG	UNP P17065
L	27	PRO	-	EXPRESSION TAG	UNP P17065
L	28	LEU	-	EXPRESSION TAG	UNP P17065
L	29	GLY	-	EXPRESSION TAG	UNP P17065
L	30	SER	-	EXPRESSION TAG	UNP P17065
L	115	LEU	MET	ENGINEERED	UNP P17065
M	26	GLY	-	EXPRESSION TAG	UNP P17065

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Chain	Residue	Modelled	Actual	Comment	Reference
M	27	PRO	-	EXPRESSION TAG	UNP P17065
M	28	LEU	-	EXPRESSION TAG	UNP P17065
M	29	GLY	-	EXPRESSION TAG	UNP P17065
M	30	SER	-	EXPRESSION TAG	UNP P17065
M	115	LEU	MET	ENGINEERED	UNP P17065
N	26	GLY	-	EXPRESSION TAG	UNP P17065
N	27	PRO	-	EXPRESSION TAG	UNP P17065
N	28	LEU	-	EXPRESSION TAG	UNP P17065
N	29	GLY	-	EXPRESSION TAG	UNP P17065
N	30	SER	-	EXPRESSION TAG	UNP P17065
N	115	LEU	MET	ENGINEERED	UNP P17065
O	26	GLY	-	EXPRESSION TAG	UNP P17065
O	27	PRO	-	EXPRESSION TAG	UNP P17065
O	28	LEU	-	EXPRESSION TAG	UNP P17065
O	29	GLY	-	EXPRESSION TAG	UNP P17065
O	30	SER	-	EXPRESSION TAG	UNP P17065
O	115	LEU	MET	ENGINEERED	UNP P17065
P	26	GLY	-	EXPRESSION TAG	UNP P17065
P	27	PRO	-	EXPRESSION TAG	UNP P17065
P	28	LEU	-	EXPRESSION TAG	UNP P17065
P	29	GLY	-	EXPRESSION TAG	UNP P17065
P	30	SER	-	EXPRESSION TAG	UNP P17065
P	115	LEU	MET	ENGINEERED	UNP P17065
Q	26	GLY	-	EXPRESSION TAG	UNP P17065
Q	27	PRO	-	EXPRESSION TAG	UNP P17065
Q	28	LEU	-	EXPRESSION TAG	UNP P17065
Q	29	GLY	-	EXPRESSION TAG	UNP P17065
Q	30	SER	-	EXPRESSION TAG	UNP P17065
Q	115	LEU	MET	ENGINEERED	UNP P17065
R	26	GLY	-	EXPRESSION TAG	UNP P17065
R	27	PRO	-	EXPRESSION TAG	UNP P17065
R	28	LEU	-	EXPRESSION TAG	UNP P17065
R	29	GLY	-	EXPRESSION TAG	UNP P17065
R	30	SER	-	EXPRESSION TAG	UNP P17065
R	115	LEU	MET	ENGINEERED	UNP P17065
S	26	GLY	-	EXPRESSION TAG	UNP P17065
S	27	PRO	-	EXPRESSION TAG	UNP P17065
S	28	LEU	-	EXPRESSION TAG	UNP P17065
S	29	GLY	-	EXPRESSION TAG	UNP P17065
S	30	SER	-	EXPRESSION TAG	UNP P17065
S	115	LEU	MET	ENGINEERED	UNP P17065
T	26	GLY	-	EXPRESSION TAG	UNP P17065

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Chain	Residue	Modelled	Actual	Comment	Reference
T	27	PRO	-	EXPRESSION TAG	UNP P17065
T	28	LEU	-	EXPRESSION TAG	UNP P17065
T	29	GLY	-	EXPRESSION TAG	UNP P17065
T	30	SER	-	EXPRESSION TAG	UNP P17065
T	115	LEU	MET	ENGINEERED	UNP P17065

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	17	Total O 17 17	0	0
2	B	14	Total O 14 14	0	0
2	C	12	Total O 12 12	0	0
2	D	11	Total O 11 11	0	0
2	E	17	Total O 17 17	0	0
2	F	9	Total O 9 9	0	0
2	G	12	Total O 12 12	0	0
2	H	10	Total O 10 10	0	0
2	I	6	Total O 6 6	0	0
2	J	11	Total O 11 11	0	0
2	K	20	Total O 20 20	0	0
2	L	17	Total O 17 17	0	0
2	M	14	Total O 14 14	0	0
2	N	16	Total O 16 16	0	0
2	O	11	Total O 11 11	0	0
2	P	16	Total O 16 16	0	0
2	Q	14	Total O 14 14	0	0

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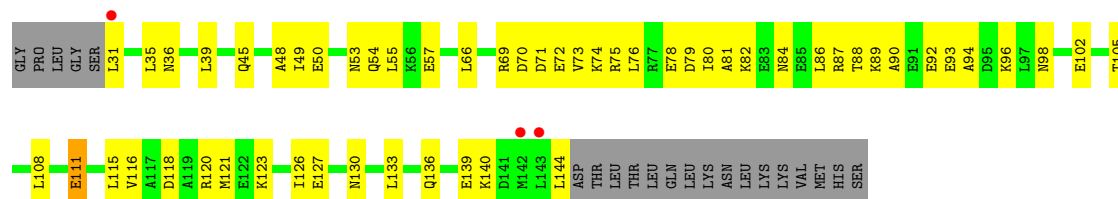
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	R	9	Total 9	O 9	0	0
2	S	14	Total 14	O 14	0	0
2	T	12	Total 12	O 12	0	0

### 3 Residue-property plots

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.

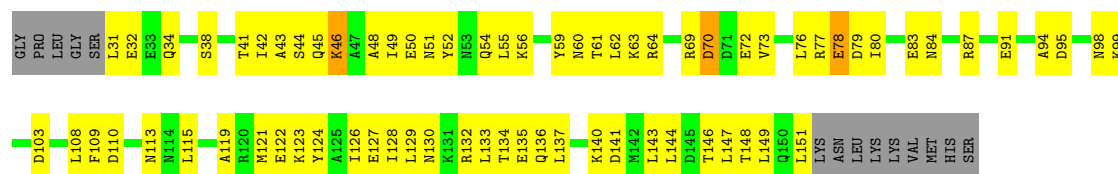
- Molecule 1: Rab guanine nucleotide exchange factor SEC2

Chain A: 



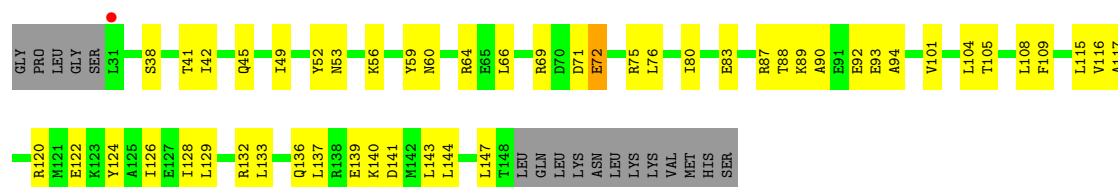
- Molecule 1: Rab guanine nucleotide exchange factor SEC2

Chain B: 



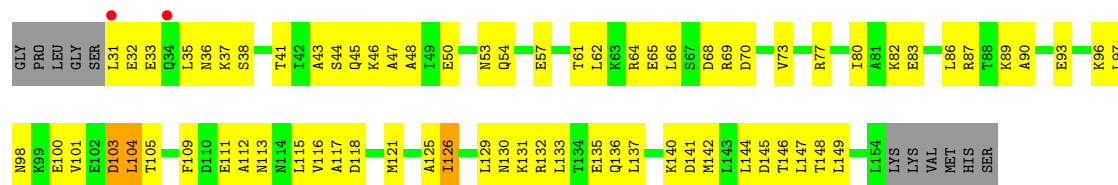
- Molecule 1: Rab guanine nucleotide exchange factor SEC2

Chain C: 



- Molecule 1: Rab guanine nucleotide exchange factor SEC2

Chain D: 



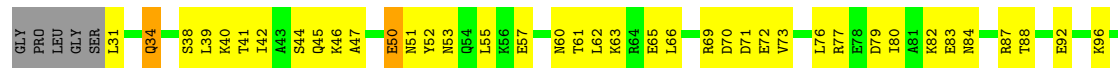
- Molecule 1: Rab guanine nucleotide exchange factor SEC2

Chain E: 



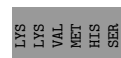
- Molecule 1: Rab guanine nucleotide exchange factor SEC2

Chain F: 



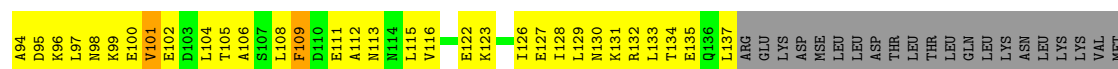
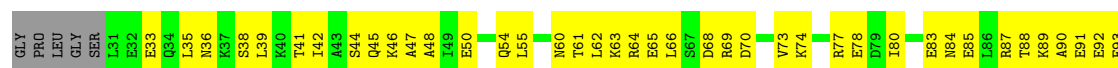
- Molecule 1: Rab guanine nucleotide exchange factor SEC2

Chain G: 



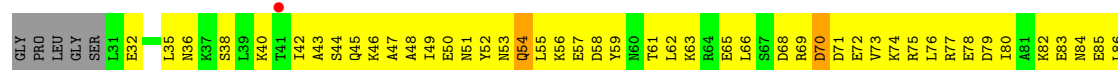
- Molecule 1: Rab guanine nucleotide exchange factor SEC2

Chain H: 



- Molecule 1: Rab guanine nucleotide exchange factor SEC2

Chain I: 



GLN  
LEU  
LYS  
ASN  
LEU  
LYS  
VAL  
MET  
HIS  
SER

- Molecule 1: Rab guanine nucleotide exchange factor SEC2

Chain J: 

GLY PRO LEU GLY SER L31 E32 E33 Q34 N36 K37 S38 L39 K40 T41 I42 I43 S44 Q45 K46 A47 V116 V117 I49 E50 N51 N52 N53 Q54 L55 K56 Y69 N60 T61 L62 K63 R64 E65 L66 S67 T134 E135 Q136 L137 ARG GLU LYS ASP MSE LEU LEU ASP THR LEU THR LEU GLN LEU LYS ASN

LEU  
LYS  
LYS  
VAL  
MET  
HIS  
SER

- Molecule 1: Rab guanine nucleotide exchange factor SEC2

Chain K: 

GLY PRO LEU GLY SER L31 K46 L49 E50 N51 Y52 N53 Q54 K56 L62 E65 L66 S67 D68 R69 D70 D71 E72 K73 L74 K75 L76 R77 E78 D79 I80 K81 K82 E83 N84 E85 L86 T88 K89 E92 E93 A94 L97 N98 K99 E100 V101 E102 D103 L104 E111 A112 N113 N114 L115 V116 A117 D118 A119 R120 M121 E122 K123 Y124 A125 L126 E127 L128 L129 M130 K131 R132 L133 T134 E135 Q136 L137 R138 E139 K140 D141 M142 M143 L144 L147 THR LEU LEU GLN LEU LYS ASN LEU LYS VAL MET HIS SER

- Molecule 1: Rab guanine nucleotide exchange factor SEC2

Chain L: 

GLY PRO LEU GLY SER L31 E32 N36 S38 T41 I42 Q45 K46 E50 N51 Y52 N53 Q54 L55 K56 Y69 N60 T61 L62 K63 R64 E65 S67 D68 R69 D70 D71 E72 V73 R77 E78 D79 I80 E83 N84 E85 L86 R87 T88 E91 E92 E93 A94 D95 K96 L97 E100 L104 L108 F109 D110 E111 A112 N113 M114 L115 V116 L118 M121 Y124 E127 L128 Q136 L137 K140 D141 M142 L143 L144 ASP THR LEU THR LEU GLN LEU LYS ASN LEU LYS VAL MET HIS SER

- Molecule 1: Rab guanine nucleotide exchange factor SEC2

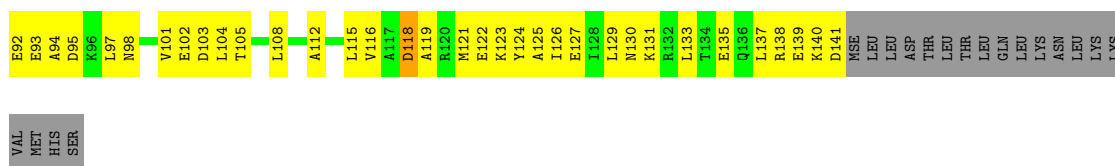
Chain M: 

GLY PRO LEU GLY SER L31 E32 E33 S38 T41 I42 A43 S44 Q45 K46 A47 E50 N51 Y52 N53 Q54 L55 K56 E57 D58 T61 L62 K63 R64 E65 D68 R69 V73 K74 R77 I80 N84 E85 L86 R87 T88 K89 E91 E92 E93 A94 D95 N98 L108 F109 A112 L115 V116 A117 D118 R119 M121 E122 K123 L126 E127 L128 I129 M130 K131 R132 L133 T134 E135 Q136 L137 R138 E139 K140 D141 M142 L143 L147 THR LEU LEU GLN LEU LYS ASN LEU LYS VAL MET HIS SER

- Molecule 1: Rab guanine nucleotide exchange factor SEC2

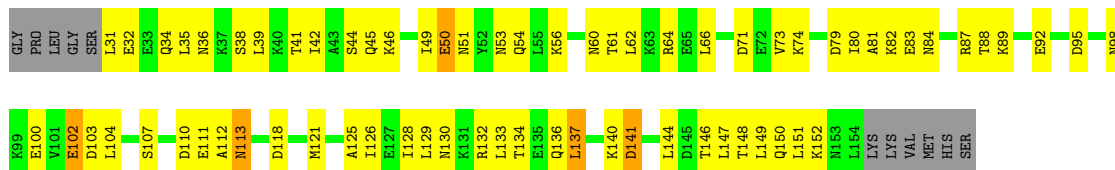
Chain N: 

GLY PRO LEU GLY SER L31 E32 E33 Q34 S38 L39 K40 T41 I42 A43 S44 Q45 K46 A47 Y52 L55 Y69 N60 T61 L62 K63 R64 E65 S67 D68 R69 D70 D71 E72 V73 K74 R75 L76 R77 E78 D79 I80 A81 K82 E83 N84 E85 L86 R87 T88 K89 A90 E91



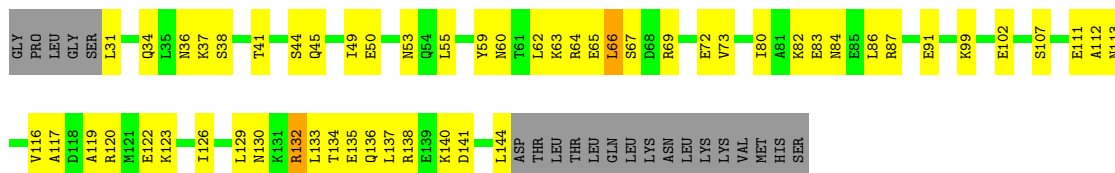
- Molecule 1: Rab guanine nucleotide exchange factor SEC2

Chain O:



- Molecule 1: Rab guanine nucleotide exchange factor SEC2

Chain P:



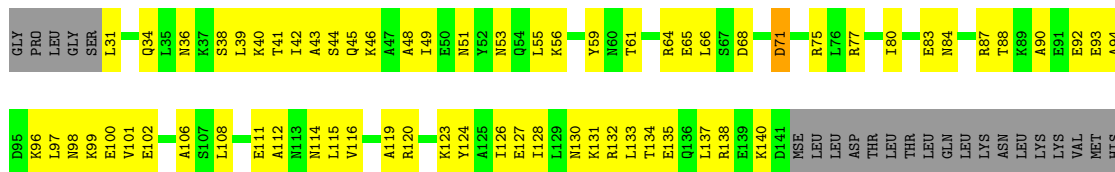
- Molecule 1: Rab guanine nucleotide exchange factor SEC2

Chain Q:



- Molecule 1: Rab guanine nucleotide exchange factor SEC2

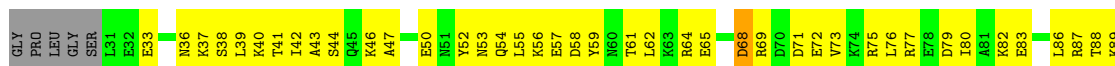
Chain R:

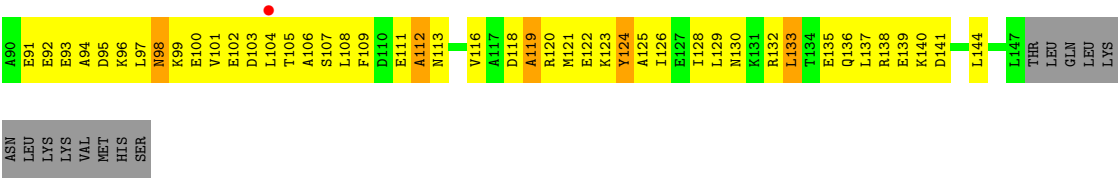


SER

- Molecule 1: Rab guanine nucleotide exchange factor SEC2

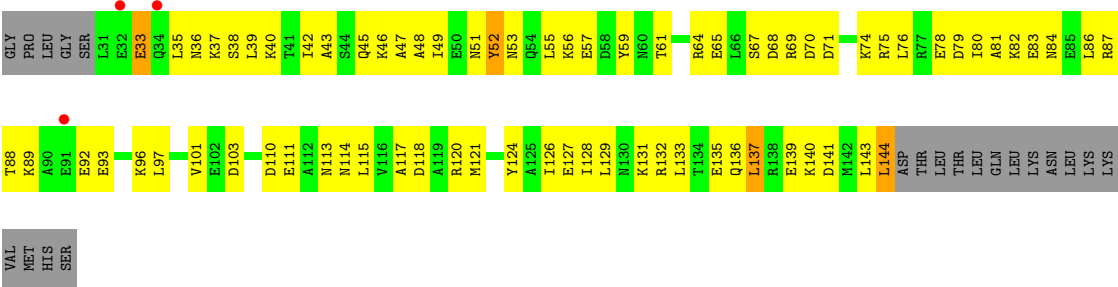
Chain S:





● Molecule 1: Rab guanine nucleotide exchange factor SEC2

Chain T:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.94Å 176.57Å 181.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 49.90 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.00) 99.4 (49.90-3.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.33 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.229 , 0.285 0.236 , 0.284	Depositor DCC
$R_{free}$ test set	6165 reflections (5.10%)	DCC
Wilson B-factor (Å <sup>2</sup> )	80.4	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 121.6	EDS
Estimated twinning fraction	0.034 for -h,l,k 0.034 for -h,-l,-k 0.499 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	2 of 127163 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	19270	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	136.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.44% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

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	0.53	0/939	0.63	0/1252
1	B	0.53	0/994	0.64	0/1328
1	C	0.42	0/969	0.57	0/1294
1	D	0.47	0/1019	0.59	0/1361
1	E	0.59	0/1019	0.66	0/1361
1	F	0.64	0/1019	0.69	0/1361
1	G	0.51	0/908	0.59	0/1212
1	H	0.49	0/879	0.62	0/1175
1	I	0.39	0/939	0.58	0/1252
1	J	0.44	0/879	0.59	0/1175
1	K	0.66	1/962 (0.1%)	0.66	0/1284
1	L	0.60	0/939	0.62	0/1252
1	M	0.45	0/962	0.63	0/1284
1	N	0.48	0/916	0.61	0/1223
1	O	0.54	0/1019	0.64	0/1361
1	P	0.56	0/939	0.64	0/1252
1	Q	0.50	0/916	0.61	0/1223
1	R	0.46	0/916	0.57	0/1223
1	S	0.39	0/962	0.58	0/1284
1	T	0.39	0/939	0.59	0/1252
All	All	0.51	1/19034 (0.0%)	0.62	0/25409

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	54	GLN	CG-CD	5.78	1.64	1.51

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.



## 5.2 Close contacts ⓘ

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	938	0	945	61	0
1	B	993	0	1004	74	0
1	C	968	0	974	67	0
1	D	1018	0	1034	92	0
1	E	1018	0	1034	83	0
1	F	1018	0	1034	88	0
1	G	906	0	910	108	0
1	H	877	0	878	114	0
1	I	938	0	945	136	0
1	J	877	0	878	122	0
1	K	961	0	967	78	0
1	L	938	0	945	89	0
1	M	961	0	967	80	0
1	N	914	0	914	89	0
1	O	1018	0	1034	84	0
1	P	938	0	945	90	0
1	Q	914	0	914	98	0
1	R	914	0	914	95	0
1	S	961	0	967	115	0
1	T	938	0	945	94	0
2	A	17	0	0	3	0
2	B	14	0	0	9	0
2	C	12	0	0	2	0
2	D	11	0	0	5	0
2	E	17	0	0	5	0
2	F	9	0	0	2	0
2	G	12	0	0	9	0
2	H	10	0	0	3	0
2	I	6	0	0	2	0
2	J	11	0	0	8	0
2	K	20	0	0	1	0
2	L	17	0	0	10	0
2	M	14	0	0	8	0
2	N	16	0	0	4	0
2	O	11	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	16	0	0	2	0
2	Q	14	0	0	3	0
2	R	9	0	0	4	0
2	S	14	0	0	6	0
2	T	12	0	0	3	0
All	All	19270	0	19148	1488	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 39.

The worst 5 of 1488 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:73:VAL:HG21	1:J:69:ARG:HD2	1.31	1.13
1:Q:126:ILE:HD13	1:R:126:ILE:HG21	1.32	1.10
1:M:133:LEU:HD12	1:N:133:LEU:HD22	1.33	1.09
1:L:110:ASP:HA	1:L:113:ASN:HD22	1.14	1.08
1:Q:133:LEU:HD22	1:R:133:LEU:HB2	1.32	1.08

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 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 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	112/135 (83%)	102 (91%)	10 (9%)	0	100	100
1	B	119/135 (88%)	105 (88%)	11 (9%)	3 (2%)	9	40
1	C	116/135 (86%)	105 (90%)	11 (10%)	0	100	100
1	D	122/135 (90%)	108 (88%)	12 (10%)	2 (2%)	14	56
1	E	122/135 (90%)	112 (92%)	7 (6%)	3 (2%)	9	40
1	F	122/135 (90%)	107 (88%)	12 (10%)	3 (2%)	9	40
1	G	108/135 (80%)	89 (82%)	18 (17%)	1 (1%)	25	73
1	H	105/135 (78%)	80 (76%)	23 (22%)	2 (2%)	12	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	112/135 (83%)	96 (86%)	16 (14%)	0	100	100
1	J	105/135 (78%)	86 (82%)	14 (13%)	5 (5%)	4	20
1	K	115/135 (85%)	97 (84%)	17 (15%)	1 (1%)	25	73
1	L	112/135 (83%)	102 (91%)	10 (9%)	0	100	100
1	M	115/135 (85%)	105 (91%)	8 (7%)	2 (2%)	14	54
1	N	109/135 (81%)	88 (81%)	18 (16%)	3 (3%)	8	37
1	O	122/135 (90%)	106 (87%)	12 (10%)	4 (3%)	6	32
1	P	112/135 (83%)	104 (93%)	8 (7%)	0	100	100
1	Q	109/135 (81%)	96 (88%)	12 (11%)	1 (1%)	25	73
1	R	109/135 (81%)	97 (89%)	11 (10%)	1 (1%)	25	73
1	S	115/135 (85%)	102 (89%)	11 (10%)	2 (2%)	14	54
1	T	112/135 (83%)	94 (84%)	16 (14%)	2 (2%)	13	53
All	All	2273/2700 (84%)	1981 (87%)	257 (11%)	35 (2%)	15	58

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	32	GLU
1	O	113	ASN
1	T	52	TYR
1	D	104	LEU
1	E	119	ALA

### 5.3.2 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 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	103/120 (86%)	100 (97%)	3 (3%)	55	90
1	B	110/120 (92%)	104 (94%)	6 (6%)	30	73
1	C	107/120 (89%)	105 (98%)	2 (2%)	69	94
1	D	113/120 (94%)	109 (96%)	4 (4%)	48	87
1	E	113/120 (94%)	106 (94%)	7 (6%)	26	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	113/120 (94%)	109 (96%)	4 (4%)	48	87
1	G	99/120 (82%)	94 (95%)	5 (5%)	33	76
1	H	96/120 (80%)	94 (98%)	2 (2%)	66	94
1	I	103/120 (86%)	96 (93%)	7 (7%)	22	63
1	J	96/120 (80%)	93 (97%)	3 (3%)	52	89
1	K	106/120 (88%)	102 (96%)	4 (4%)	44	85
1	L	103/120 (86%)	98 (95%)	5 (5%)	35	78
1	M	106/120 (88%)	103 (97%)	3 (3%)	56	91
1	N	100/120 (83%)	98 (98%)	2 (2%)	68	94
1	O	113/120 (94%)	105 (93%)	8 (7%)	21	61
1	P	103/120 (86%)	101 (98%)	2 (2%)	69	94
1	Q	100/120 (83%)	96 (96%)	4 (4%)	42	84
1	R	100/120 (83%)	97 (97%)	3 (3%)	53	90
1	S	106/120 (88%)	102 (96%)	4 (4%)	44	85
1	T	103/120 (86%)	98 (95%)	5 (5%)	35	78
All	All	2093/2400 (87%)	2010 (96%)	83 (4%)	42	84

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	114	ASN
1	K	100	GLU
1	S	124	TYR
1	I	124	TYR
1	J	118	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 83 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	53	ASN
1	I	60	ASN
1	Q	84	ASN
1	G	60	ASN
1	H	113	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

### 5.8 Polymer linkage issues

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	114/135 (84%)	0.15	3 (2%) 53 10	44, 114, 190, 200	0
1	B	121/135 (89%)	0.16	0 100 100	46, 110, 198, 200	0
1	C	118/135 (87%)	0.15	1 (0%) 83 26	77, 154, 200, 200	0
1	D	124/135 (91%)	0.18	2 (1%) 68 16	61, 152, 199, 200	0
1	E	124/135 (91%)	0.24	3 (2%) 56 11	32, 107, 198, 200	0
1	F	124/135 (91%)	0.08	0 100 100	20, 108, 193, 200	0
1	G	110/135 (81%)	0.01	0 100 100	69, 129, 190, 200	0
1	H	107/135 (79%)	-0.00	0 100 100	70, 128, 192, 200	0
1	I	114/135 (84%)	0.10	1 (0%) 81 24	96, 178, 200, 200	0
1	J	107/135 (79%)	0.24	1 (0%) 81 24	65, 166, 199, 200	0
1	K	117/135 (86%)	0.06	0 100 100	15, 116, 194, 200	0
1	L	114/135 (84%)	0.20	2 (1%) 65 14	32, 115, 191, 200	0
1	M	117/135 (86%)	0.08	0 100 100	52, 136, 198, 200	0
1	N	111/135 (82%)	0.15	1 (0%) 81 24	38, 142, 192, 200	0
1	O	124/135 (91%)	0.13	0 100 100	50, 126, 198, 200	0
1	P	114/135 (84%)	0.09	0 100 100	50, 111, 187, 200	0
1	Q	111/135 (82%)	-0.03	0 100 100	59, 133, 198, 200	0
1	R	111/135 (82%)	0.06	0 100 100	48, 147, 198, 200	0
1	S	117/135 (86%)	0.11	1 (0%) 81 24	108, 178, 200, 200	0
1	T	114/135 (84%)	0.13	3 (2%) 53 10	109, 169, 200, 200	0
All	All	2313/2700 (85%)	0.12	18 (0%) 83 26	15, 138, 199, 200	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	31	LEU	4.4
1	E	34	GLN	3.3
1	N	31	LEU	3.3
1	D	31	LEU	3.3
1	E	146	THR	3.1

## 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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.