wwPDB X-ray Structure Validation Summary Report (i)

Nov 1, 2021 – 02:58 PM EDT

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 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
https://www.wwpdb.org/validation/2017/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:

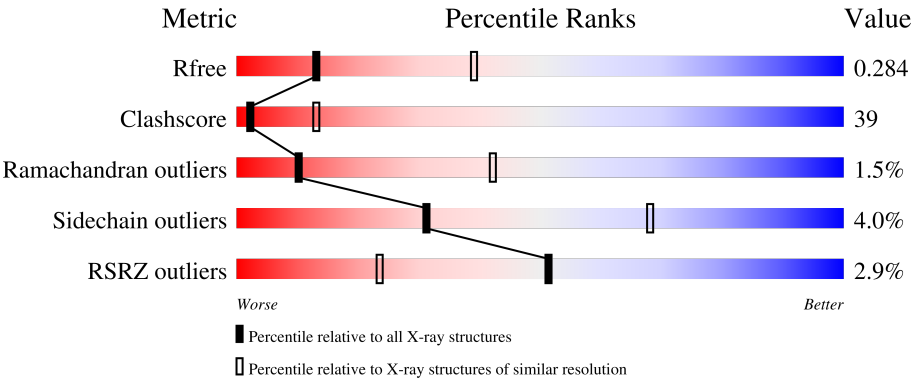
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	135	44% 40% 16%
1	B	135	3% 36% 51% 10%
1	C	135	4% 50% 36% 13%
1	D	135	6% 39% 51% 8%
1	E	135	5% 46% 41% 8%

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Mol	Chain	Length	Quality of chain
1	F	135	42% 48% 8%
1	G	135	27% 51% 19%
1	H	135	26% 52% 21%
1	I	135	3% 19% 62% 16%
1	J	135	4% 21% 54% 21%
1	K	135	40% 44% 13%
1	L	135	41% 41% 16%
1	M	135	39% 46% 13%
1	N	135	5% 27% 53% 18%
1	O	135	41% 47% 8%
1	P	135	44% 39% 16%
1	Q	135	35% 45% 18%
1	R	135	33% 48% 18%
1	S	135	4% 23% 59% 13%
1	T	135	4% 30% 52% 16%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 19270 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 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 mutation	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 mutation	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 mutation	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 mutation	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 mutation	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 mutation	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 mutation	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 mutation	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 mutation	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 mutation	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 mutation	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 mutation	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 mutation	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 mutation	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 mutation	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 mutation	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 mutation	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 mutation	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 mutation	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 mutation	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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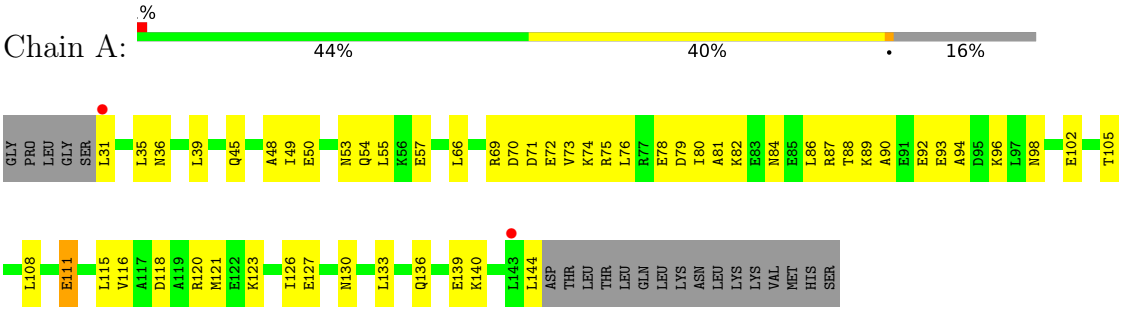
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	R	9	Total O 9 9	0	0
2	S	14	Total O 14 14	0	0
2	T	12	Total O 12 12	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

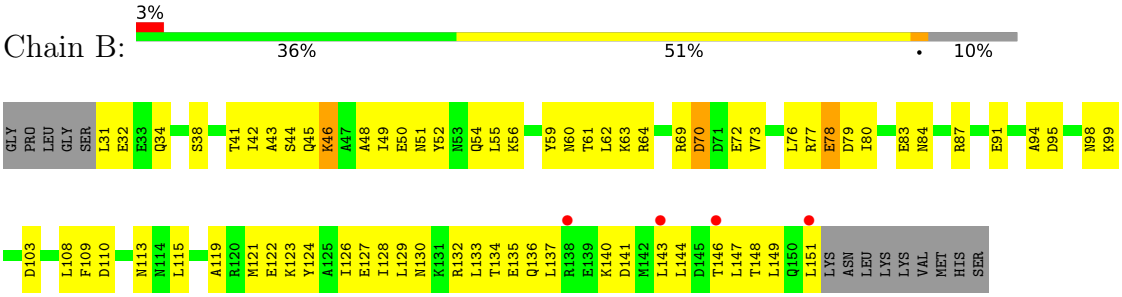
• Molecule 1: Rab guanine nucleotide exchange factor SEC2

Chain A:



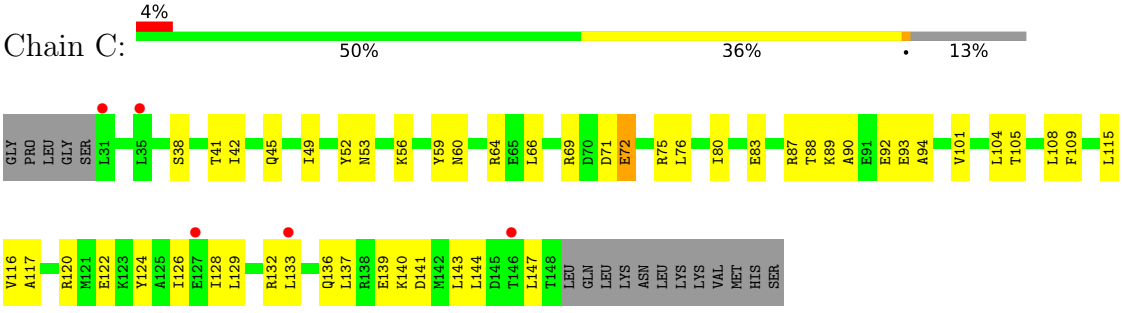
• Molecule 1: Rab guanine nucleotide exchange factor SEC2

Chain B:



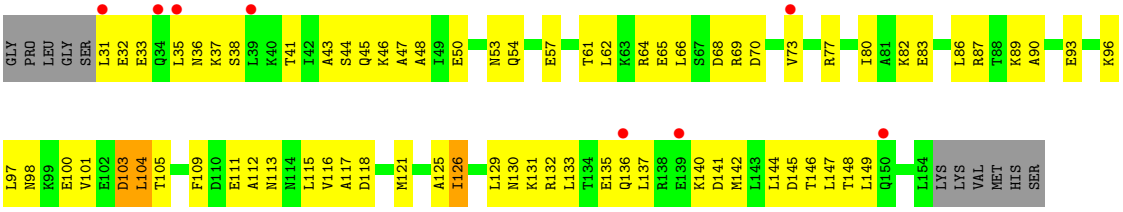
• Molecule 1: Rab guanine nucleotide exchange factor SEC2

Chain C:



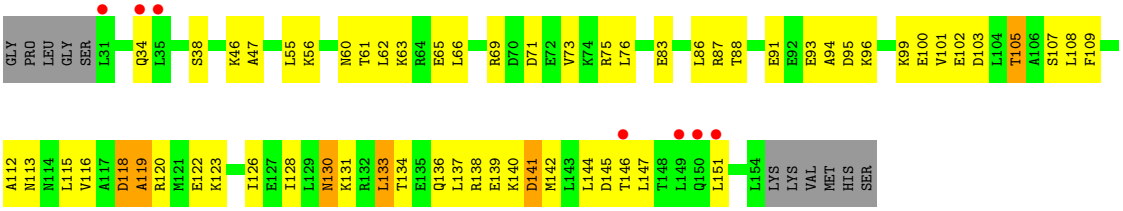
• Molecule 1: Rab guanine nucleotide exchange factor SEC2

Chain D:



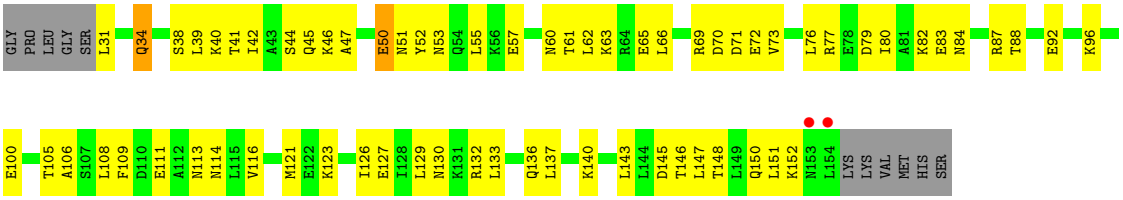
• Molecule 1: Rab guanine nucleotide exchange factor SEC2

Chain E:



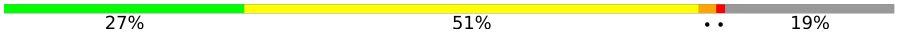
• Molecule 1: Rab guanine nucleotide exchange factor SEC2

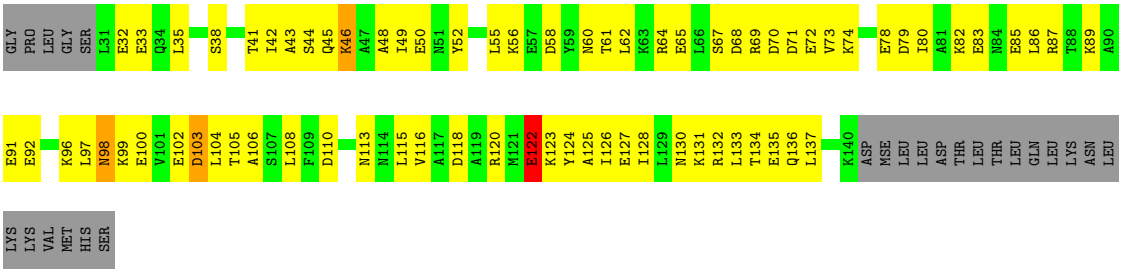
Chain F:



• Molecule 1: Rab guanine nucleotide exchange factor SEC2

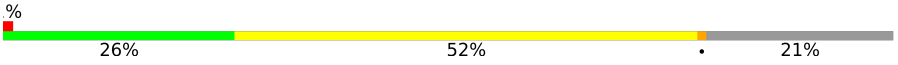
Chain G:

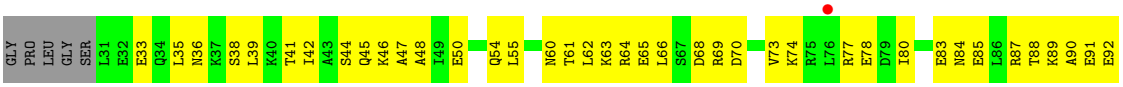


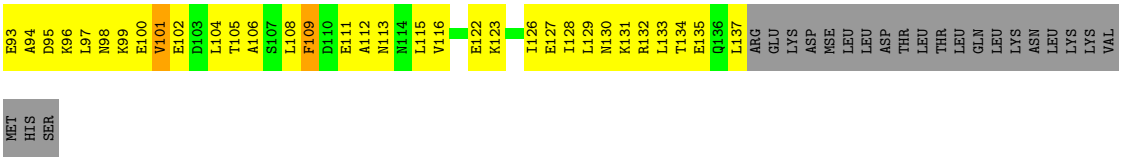


• Molecule 1: Rab guanine nucleotide exchange factor SEC2

Chain H:

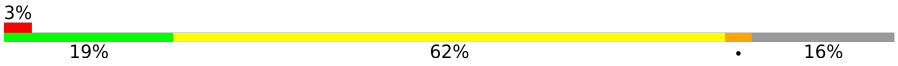


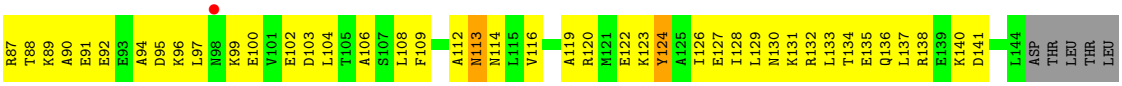




• Molecule 1: Rab guanine nucleotide exchange factor SEC2

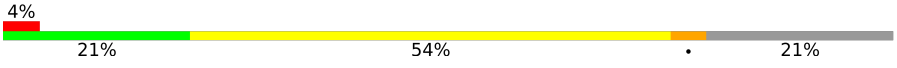
Chain I:





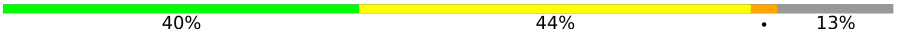
• Molecule 1: Rab guanine nucleotide exchange factor SEC2

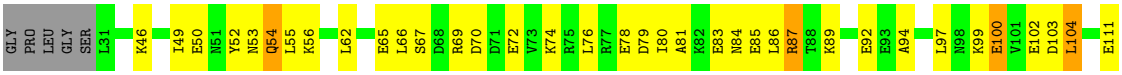
Chain J:

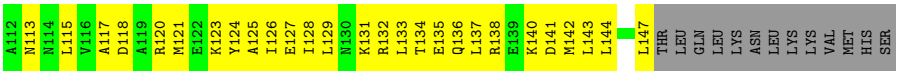


• Molecule 1: Rab guanine nucleotide exchange factor SEC2

Chain K:

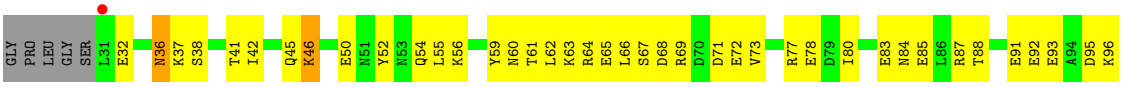


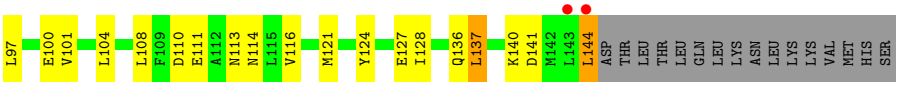




• Molecule 1: Rab guanine nucleotide exchange factor SEC2

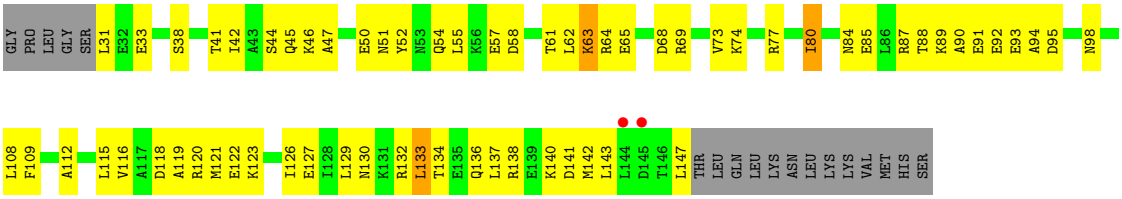
Chain L:





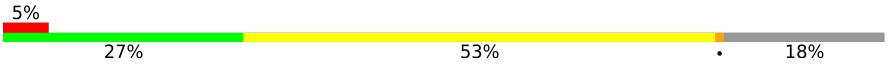
• Molecule 1: Rab guanine nucleotide exchange factor SEC2

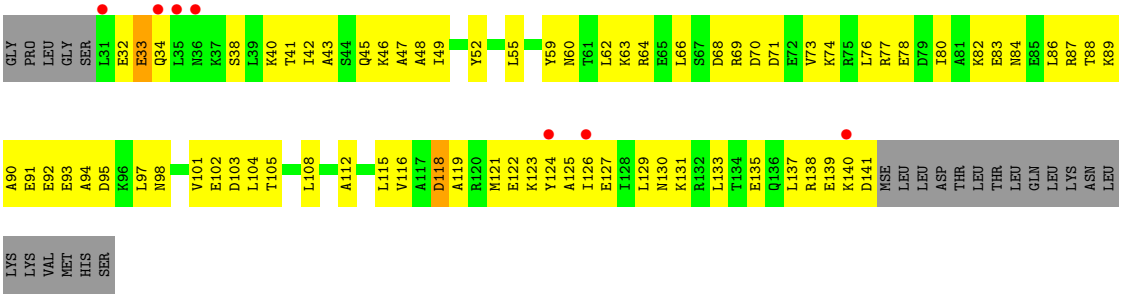
Chain M:



• Molecule 1: Rab guanine nucleotide exchange factor SEC2

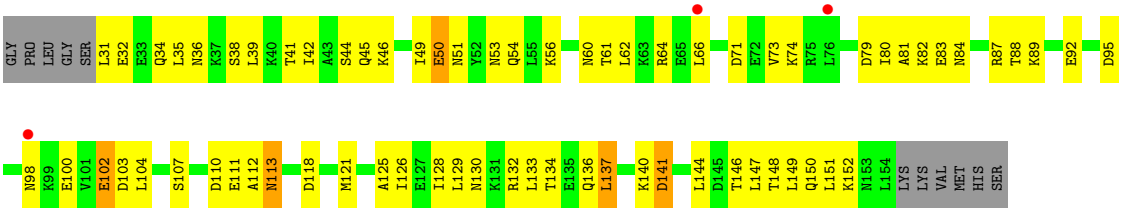
Chain N:





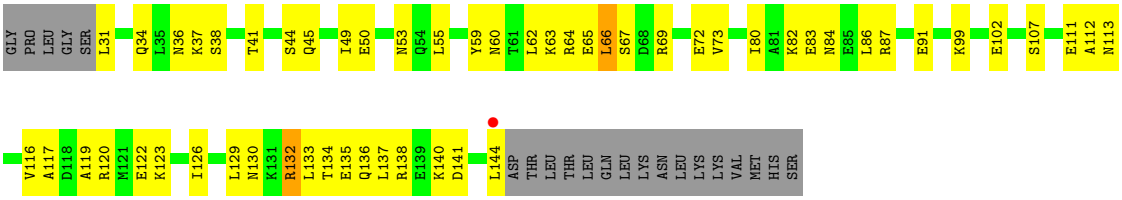
• Molecule 1: Rab guanine nucleotide exchange factor SEC2

Chain O:



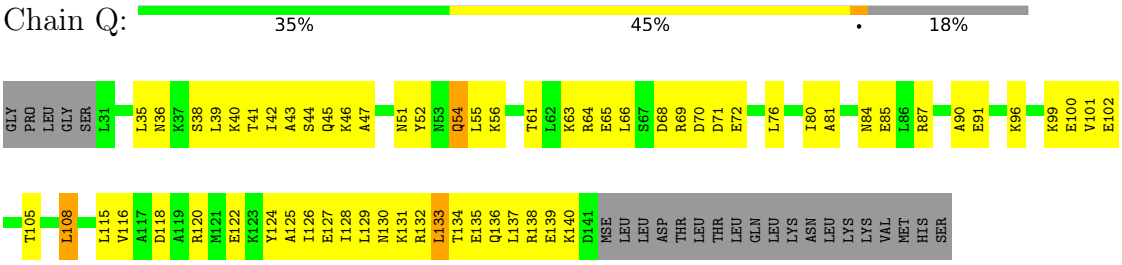
• Molecule 1: Rab guanine nucleotide exchange factor SEC2

Chain P:



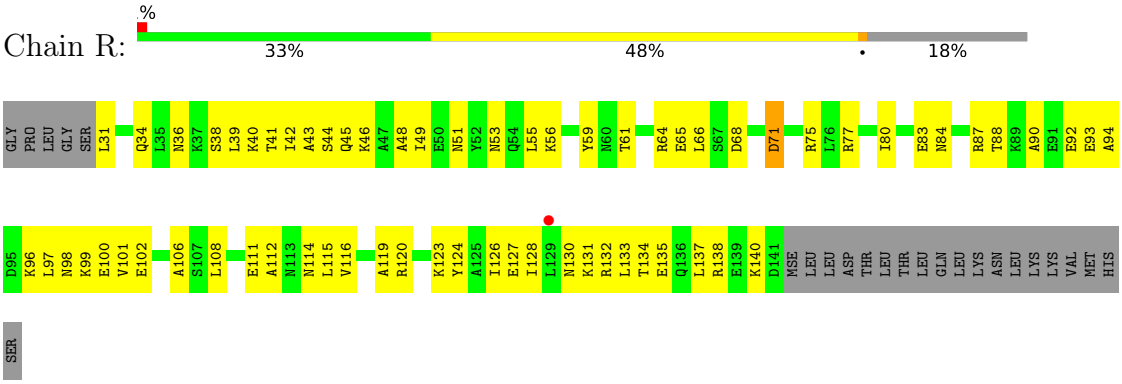
• Molecule 1: Rab guanine nucleotide exchange factor SEC2

Chain Q:



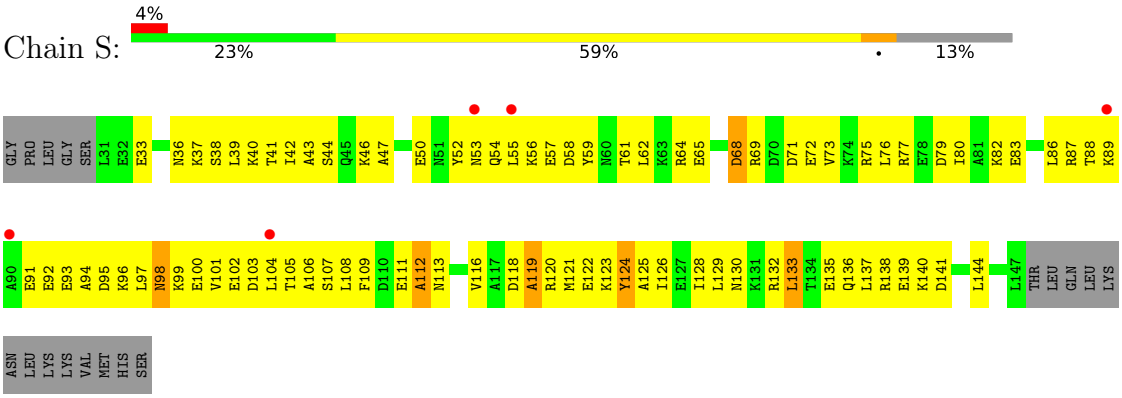
• Molecule 1: Rab guanine nucleotide exchange factor SEC2

Chain R:



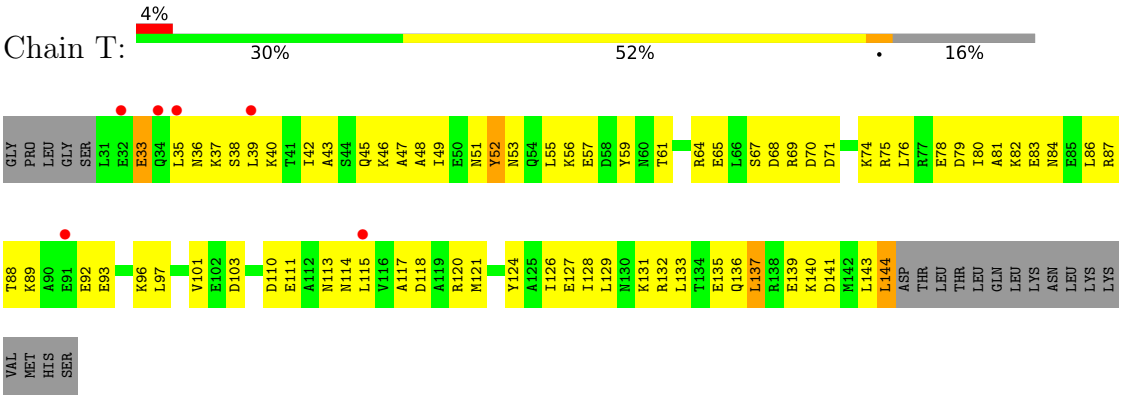
• Molecule 1: Rab guanine nucleotide exchange factor SEC2

Chain S:



• Molecule 1: Rab guanine nucleotide exchange factor SEC2

Chain T:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	2.33 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.229 , 0.285 0.235 , 0.284	Depositor DCC
R_{free} test set	6165 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	80.4	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 124.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.034 for -h,l,k 0.034 for -h,-l,-k 0.499 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	19270	wwPDB-VP
Average B, all atoms (Å^2)	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.*

[1] Intensities estimated from amplitudes.

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

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 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	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
2	P	16	0	0	2	0
2	Q	14	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 39.

The worst 5 of 1488 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)
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 (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	112/135 (83%)	102 (91%)	10 (9%)	0	100 100
1	B	119/135 (88%)	105 (88%)	11 (9%)	3 (2%)	5 28
1	C	116/135 (86%)	105 (90%)	11 (10%)	0	100 100
1	D	122/135 (90%)	108 (88%)	12 (10%)	2 (2%)	9 40
1	E	122/135 (90%)	112 (92%)	7 (6%)	3 (2%)	5 28
1	F	122/135 (90%)	107 (88%)	12 (10%)	3 (2%)	5 28
1	G	108/135 (80%)	89 (82%)	18 (17%)	1 (1%)	17 55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	H	105/135 (78%)	80 (76%)	23 (22%)	2 (2%)	8 36
1	I	112/135 (83%)	96 (86%)	16 (14%)	0	100 100
1	J	105/135 (78%)	86 (82%)	14 (13%)	5 (5%)	2 13
1	K	115/135 (85%)	97 (84%)	17 (15%)	1 (1%)	17 55
1	L	112/135 (83%)	102 (91%)	10 (9%)	0	100 100
1	M	115/135 (85%)	105 (91%)	8 (7%)	2 (2%)	9 39
1	N	109/135 (81%)	88 (81%)	18 (16%)	3 (3%)	5 25
1	O	122/135 (90%)	106 (87%)	12 (10%)	4 (3%)	4 21
1	P	112/135 (83%)	104 (93%)	8 (7%)	0	100 100
1	Q	109/135 (81%)	96 (88%)	12 (11%)	1 (1%)	17 55
1	R	109/135 (81%)	97 (89%)	11 (10%)	1 (1%)	17 55
1	S	115/135 (85%)	102 (89%)	11 (10%)	2 (2%)	9 39
1	T	112/135 (83%)	94 (84%)	16 (14%)	2 (2%)	8 37
All	All	2273/2700 (84%)	1981 (87%)	257 (11%)	35 (2%)	10 42

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 (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	103/120 (86%)	100 (97%)	3 (3%)	42 76
1	B	110/120 (92%)	104 (94%)	6 (6%)	21 57
1	C	107/120 (89%)	105 (98%)	2 (2%)	57 84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	113/120 (94%)	109 (96%)	4 (4%)	36	71
1	E	113/120 (94%)	106 (94%)	7 (6%)	18	52
1	F	113/120 (94%)	109 (96%)	4 (4%)	36	71
1	G	99/120 (82%)	94 (95%)	5 (5%)	24	60
1	H	96/120 (80%)	94 (98%)	2 (2%)	53	82
1	I	103/120 (86%)	96 (93%)	7 (7%)	16	48
1	J	96/120 (80%)	93 (97%)	3 (3%)	40	75
1	K	106/120 (88%)	102 (96%)	4 (4%)	33	69
1	L	103/120 (86%)	98 (95%)	5 (5%)	25	61
1	M	106/120 (88%)	103 (97%)	3 (3%)	43	77
1	N	100/120 (83%)	98 (98%)	2 (2%)	55	83
1	O	113/120 (94%)	105 (93%)	8 (7%)	14	46
1	P	103/120 (86%)	101 (98%)	2 (2%)	57	84
1	Q	100/120 (83%)	96 (96%)	4 (4%)	31	68
1	R	100/120 (83%)	97 (97%)	3 (3%)	41	75
1	S	106/120 (88%)	102 (96%)	4 (4%)	33	69
1	T	103/120 (86%)	98 (95%)	5 (5%)	25	61
All	All	2093/2400 (87%)	2010 (96%)	83 (4%)	31	68

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

Mol	Chain	Res	Type
1	O	36	ASN
1	R	71	ASP
1	O	95	ASP
1	P	66	LEU
1	S	98	ASN

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

Mol	Chain	Res	Type
1	L	54	GLN
1	O	130	ASN
1	L	113	ASN
1	M	114	ASN

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Mol	Chain	Res	Type
1	P	130	ASN

5.3.3 RNA

There are no RNA molecules 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 monosaccharides 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^{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	112/135 (82%)	0.27	2 (1%) 68 40	44, 113, 189, 200	0
1	B	119/135 (88%)	0.32	4 (3%) 45 19	46, 110, 198, 200	0
1	C	116/135 (85%)	0.30	5 (4%) 35 13	77, 151, 200, 200	0
1	D	122/135 (90%)	0.35	8 (6%) 18 5	61, 152, 199, 200	0
1	E	122/135 (90%)	0.46	7 (5%) 23 8	32, 104, 198, 200	0
1	F	122/135 (90%)	0.22	2 (1%) 72 44	20, 108, 193, 200	0
1	G	109/135 (80%)	0.08	0 100 100	69, 128, 187, 200	0
1	H	106/135 (78%)	0.05	1 (0%) 84 63	70, 128, 192, 200	0
1	I	112/135 (82%)	0.23	4 (3%) 42 17	96, 178, 200, 200	0
1	J	106/135 (78%)	0.43	6 (5%) 23 8	65, 168, 199, 200	0
1	K	115/135 (85%)	0.18	0 100 100	15, 115, 193, 200	0
1	L	112/135 (82%)	0.35	3 (2%) 54 26	32, 115, 185, 200	0
1	M	115/135 (85%)	0.19	2 (1%) 70 41	52, 136, 196, 200	0
1	N	110/135 (81%)	0.30	7 (6%) 19 6	38, 142, 192, 200	0
1	O	122/135 (90%)	0.27	3 (2%) 57 29	50, 126, 197, 200	0
1	P	112/135 (82%)	0.20	1 (0%) 84 63	50, 111, 184, 198	0
1	Q	110/135 (81%)	0.01	0 100 100	59, 133, 198, 200	0
1	R	110/135 (81%)	0.14	1 (0%) 84 63	48, 147, 198, 200	0
1	S	115/135 (85%)	0.23	5 (4%) 35 13	108, 177, 200, 200	0
1	T	112/135 (82%)	0.27	6 (5%) 25 9	109, 169, 200, 200	0
All	All	2279/2700 (84%)	0.24	67 (2%) 51 23	15, 138, 199, 200	0

The worst 5 of 67 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	31	LEU	7.0
1	E	146	THR	6.1
1	N	31	LEU	5.5
1	E	34	GLN	5.4
1	D	31	LEU	5.2

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.