wwPDB X-ray Structure Validation Summary Report (i)

Jun 24, 2024 – 09:14 AM EDT

PDB ID	:	6Y31
Title	:	NG domain of human SRP54 T117 deletion mutant
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Deposited on	:	2020-02-17
Resolution	:	4.00 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

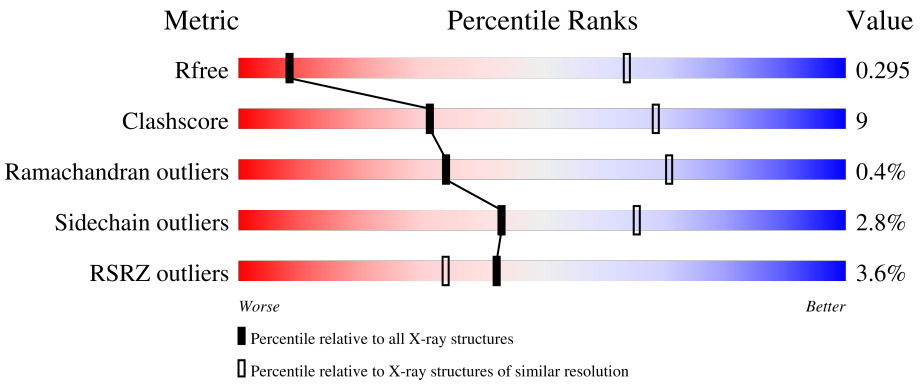
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 4.00 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	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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	303	4% 75% 18% • •
1	B	303	2% 82% 15% • •
1	C	303	4% 83% 12% • •
1	D	303	4% 81% 17% •

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 9043 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 Signal recognition particle 54 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	290	2236	1424	378	421	13	0	0	0
1	B	295	2269	1445	383	428	13	0	0	0
1	C	295	2269	1445	383	428	13	0	0	0
1	D	295	2269	1445	383	428	13	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP P61011
A	-6	GLY	-	expression tag	UNP P61011
A	-5	HIS	-	expression tag	UNP P61011
A	-4	HIS	-	expression tag	UNP P61011
A	-3	HIS	-	expression tag	UNP P61011
A	-2	HIS	-	expression tag	UNP P61011
A	-1	HIS	-	expression tag	UNP P61011
A	0	HIS	-	expression tag	UNP P61011
A	?	-	THR	deletion	UNP P61011
B	-7	MET	-	initiating methionine	UNP P61011
B	-6	GLY	-	expression tag	UNP P61011
B	-5	HIS	-	expression tag	UNP P61011
B	-4	HIS	-	expression tag	UNP P61011
B	-3	HIS	-	expression tag	UNP P61011
B	-2	HIS	-	expression tag	UNP P61011
B	-1	HIS	-	expression tag	UNP P61011
B	0	HIS	-	expression tag	UNP P61011
B	?	-	THR	deletion	UNP P61011
C	-7	MET	-	initiating methionine	UNP P61011
C	-6	GLY	-	expression tag	UNP P61011
C	-5	HIS	-	expression tag	UNP P61011

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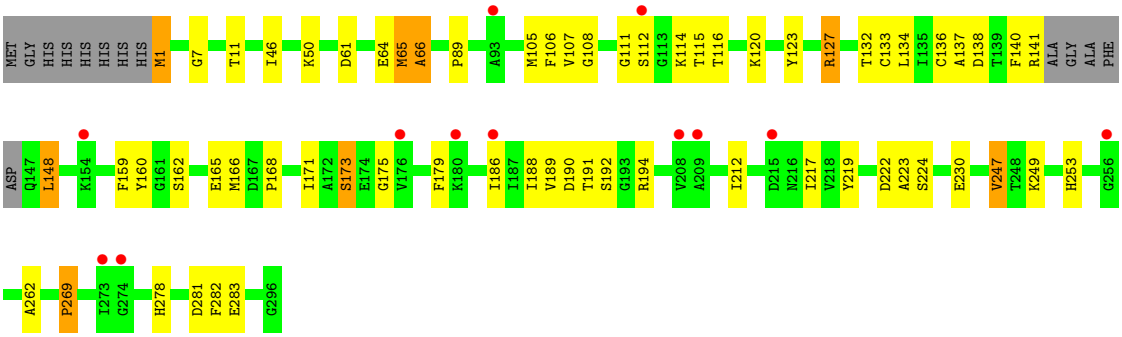
Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	HIS	-	expression tag	UNP P61011
C	-3	HIS	-	expression tag	UNP P61011
C	-2	HIS	-	expression tag	UNP P61011
C	-1	HIS	-	expression tag	UNP P61011
C	0	HIS	-	expression tag	UNP P61011
C	?	-	THR	deletion	UNP P61011
D	-7	MET	-	initiating methionine	UNP P61011
D	-6	GLY	-	expression tag	UNP P61011
D	-5	HIS	-	expression tag	UNP P61011
D	-4	HIS	-	expression tag	UNP P61011
D	-3	HIS	-	expression tag	UNP P61011
D	-2	HIS	-	expression tag	UNP P61011
D	-1	HIS	-	expression tag	UNP P61011
D	0	HIS	-	expression tag	UNP P61011
D	?	-	THR	deletion	UNP P61011

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.

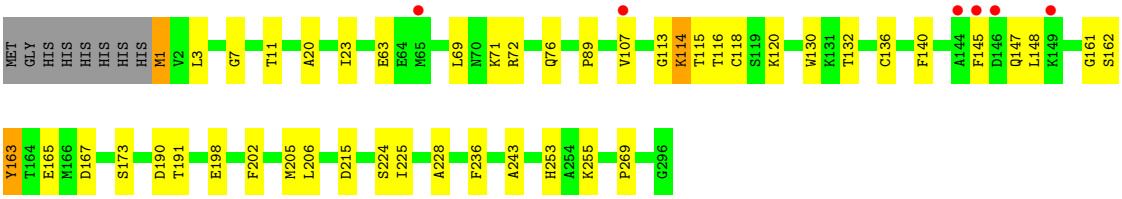
• Molecule 1: Signal recognition particle 54 kDa protein

Chain A:



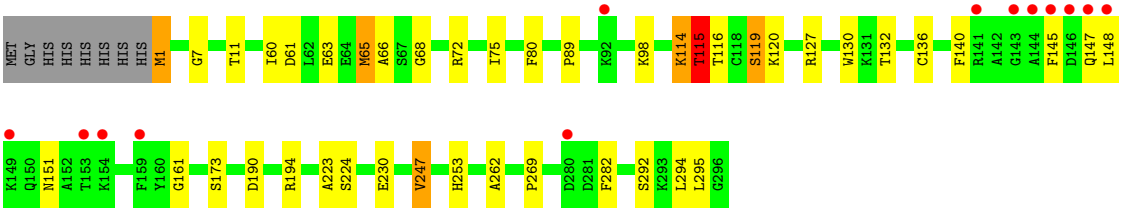
• Molecule 1: Signal recognition particle 54 kDa protein

Chain B:



• Molecule 1: Signal recognition particle 54 kDa protein

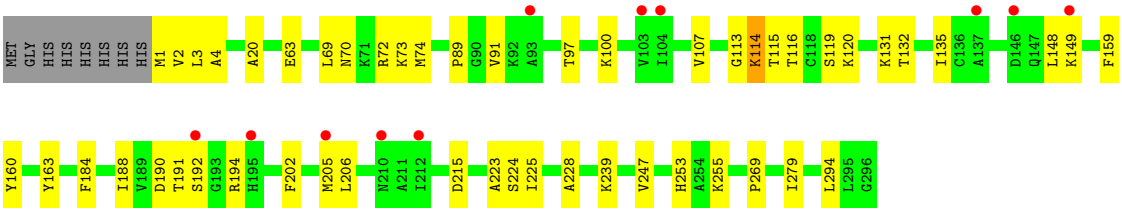
Chain C:



• Molecule 1: Signal recognition particle 54 kDa protein

Chain D:

4%
81%
17%


MET GLY HIS HIS HIS HIS HIS M1 V2 L3 A4 A20 E63 L69 N70 K71 R72 K73 M74 P89 G90 V91 K92 A93 T97 K100 V103 I104 V107 G113 K114 T115 T116 C118 S119 K120 K131 T132 I135 C136 A137 D146 Q147 L148 K149 F159
Y160 Y163 F184 I188 V189 D190 T191 S192 G193 R194 H195 F202 M205 L206 N210 A211 I212 D215 A223 S224 I225 A228 K239 V247 H253 A254 K255 P269 I279 L294 L295 G296

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	87.36Å 50.61Å 181.63Å 90.00° 99.39° 90.00°	Depositor
Resolution (Å)	45.72 – 4.00 48.70 – 4.40	Depositor EDS
% Data completeness (in resolution range)	94.7 (45.72-4.00) 79.3 (48.70-4.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.55 (at 4.45Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.311 , 0.331 0.312 , 0.295	Depositor DCC
R_{free} test set	488 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å^2)	104.3	Xtriage
Anisotropy	0.557	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 85.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.80	EDS
Total number of atoms	9043	wwPDB-VP
Average B, all atoms (Å^2)	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.55% 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 (i)

5.1 Standard geometry (i)

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	0.37	0/2268	0.71	2/3054 (0.1%)
1	B	0.33	0/2303	0.65	2/3103 (0.1%)
1	C	0.30	0/2303	0.56	2/3103 (0.1%)
1	D	0.31	0/2303	0.60	0/3103
All	All	0.33	0/9177	0.63	6/12363 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	69	LEU	CA-CB-CG	11.57	141.92	115.30
1	C	115	THR	N-CA-C	-6.25	94.11	111.00
1	A	64	GLU	N-CA-C	-5.70	95.60	111.00
1	B	163	TYR	CB-CG-CD1	-5.67	117.60	121.00
1	C	114	LYS	C-N-CA	5.09	134.44	121.70

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	2236	0	2308	57	2
1	B	2269	0	2335	41	0
1	C	2269	0	2335	27	2
1	D	2269	0	2335	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9043	0	9313	165	2

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 9.

The worst 5 of 165 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:A:115:THR:HG21	1:A:148:LEU:HD13	1.33	1.09
1:C:115:THR:OG1	1:C:147:GLN:NE2	1.93	1.01
1:A:111:GLY:O	1:A:249:LYS:NZ	1.98	0.96
1:A:140:PHE:HB3	1:A:162:SER:HB3	1.44	0.95
1:B:114:LYS:NZ	1:B:191:THR:OG1	2.00	0.94

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:GLU:OE2	1:C:68:GLY:N[2_646]	2.03	0.17
1:A:281:ASP:OD2	1:C:72:ARG:NH2[2_646]	2.17	0.03

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	286/303 (94%)	278 (97%)	7 (2%)	1 (0%)	41	75
1	B	293/303 (97%)	286 (98%)	6 (2%)	1 (0%)	41	75
1	C	293/303 (97%)	287 (98%)	4 (1%)	2 (1%)	22	61
1	D	293/303 (97%)	285 (97%)	7 (2%)	1 (0%)	41	75
All	All	1165/1212 (96%)	1136 (98%)	24 (2%)	5 (0%)	34	71

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	115	THR
1	A	66	ALA
1	B	114	LYS
1	C	66	ALA
1	D	114	LYS

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	243/252 (96%)	236 (97%)	7 (3%)	42	65
1	B	245/252 (97%)	239 (98%)	6 (2%)	49	69
1	C	245/252 (97%)	236 (96%)	9 (4%)	34	60
1	D	245/252 (97%)	240 (98%)	5 (2%)	55	73
All	All	978/1008 (97%)	951 (97%)	27 (3%)	43	65

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	63	GLU
1	C	127	ARG
1	D	132	THR
1	C	119	SER
1	C	132	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	147	GLN
1	C	151	ASN
1	C	232	GLN
1	D	147	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	290/303 (95%)	0.20	12 (4%)	37	30	90, 135, 214, 244	0
1	B	295/303 (97%)	0.02	6 (2%)	65	56	78, 135, 188, 206	0
1	C	295/303 (97%)	0.10	13 (4%)	34	28	80, 127, 211, 247	0
1	D	295/303 (97%)	0.09	11 (3%)	41	32	74, 129, 224, 247	0
All	All	1175/1212 (96%)	0.10	42 (3%)	42	34	74, 132, 215, 247	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	145	PHE	5.6
1	C	148	LEU	4.4
1	C	146	ASP	4.3
1	C	144	ALA	4.2
1	B	146	ASP	4.2

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.