wwPDB X-ray Structure Validation Summary Report (i)

May 17, 2020 – 08:51 am BST

PDB ID	:	5LSB
Title	:	Crystal structure of yeast Hsh49p in complex with Cus1p binding domain.
Authors	:	van Roon, A.M.; Obayashi, E.; Sposito, B.; Oubridge, C.; Nagai, K.
Deposited on	:	2016-08-24
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
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:

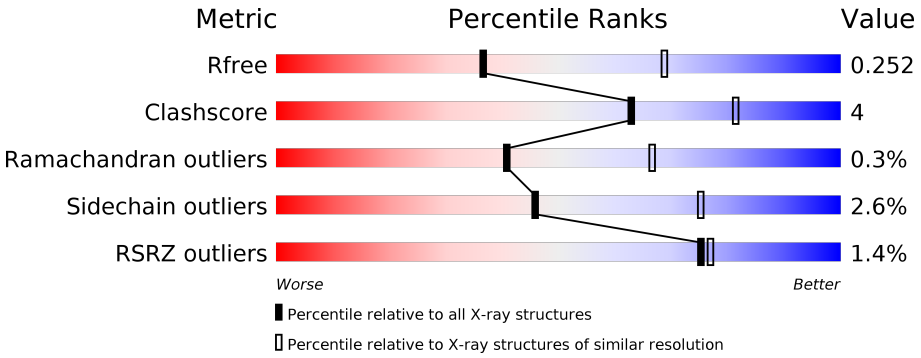
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 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	215	73% 9% 18%
1	C	215	72% 7% 18%
1	F	215	69% 10% 19%
2	B	84	67% 7% 26%
2	D	84	70% 26%
2	H	84	73% 26%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5799 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 Protein HSH49.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	176	Total	C	N	O	S	0	0	0
			1451	943	243	263	2			
1	C	176	Total	C	N	O	S	0	0	0
			1451	943	243	263	2			
1	F	174	Total	C	N	O	S	0	0	0
			1439	937	240	260	2			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q99181
A	0	GLY	-	expression tag	UNP Q99181
A	1	SER	-	expression tag	UNP Q99181
C	-1	GLY	-	expression tag	UNP Q99181
C	0	GLY	-	expression tag	UNP Q99181
C	1	SER	-	expression tag	UNP Q99181
F	-1	GLY	-	expression tag	UNP Q99181
F	0	GLY	-	expression tag	UNP Q99181
F	1	SER	-	expression tag	UNP Q99181

- Molecule 2 is a protein called Cold sensitive U2 snRNA suppressor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	62	Total	C	N	O	S	0	0	0
			484	312	83	85	4			
2	D	62	Total	C	N	O	S	0	0	0
			484	312	83	85	4			
2	H	62	Total	C	N	O	S	0	0	0
			484	312	83	85	4			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	285	MET	-	initiating methionine	UNP Q02554
B	286	ALA	-	expression tag	UNP Q02554
B	287	VAL	-	expression tag	UNP Q02554
B	288	GLY	-	expression tag	UNP Q02554
B	289	SER	-	expression tag	UNP Q02554
D	285	MET	-	initiating methionine	UNP Q02554
D	286	ALA	-	expression tag	UNP Q02554
D	287	VAL	-	expression tag	UNP Q02554
D	288	GLY	-	expression tag	UNP Q02554
D	289	SER	-	expression tag	UNP Q02554
H	285	MET	-	initiating methionine	UNP Q02554
H	286	ALA	-	expression tag	UNP Q02554
H	287	VAL	-	expression tag	UNP Q02554
H	288	GLY	-	expression tag	UNP Q02554
H	289	SER	-	expression tag	UNP Q02554

- Molecule 3 is water.

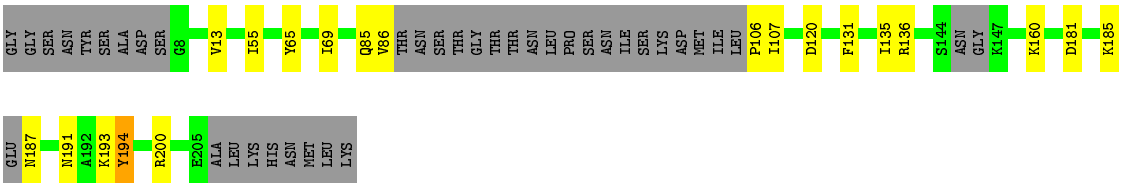
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total O 2 2	0	0
3	C	1	Total O 1 1	0	0
3	F	1	Total O 1 1	0	0
3	H	2	Total O 2 2	0	0

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 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.

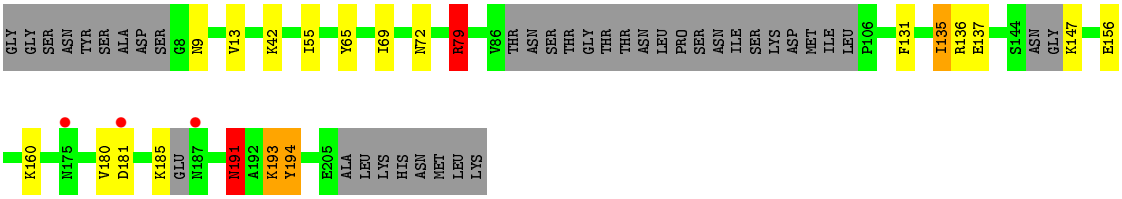
- Molecule 1: Protein HSH49

Chain A:



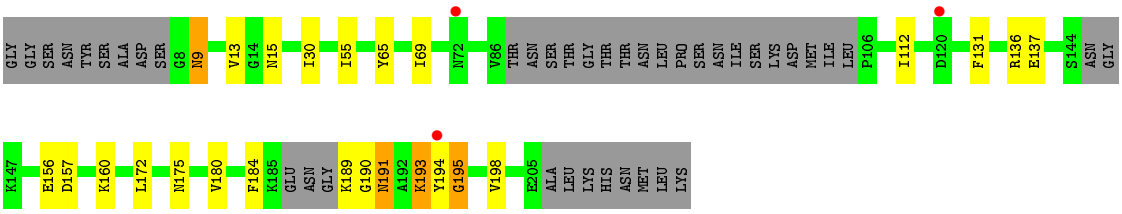
- Molecule 1: Protein HSH49

Chain C:



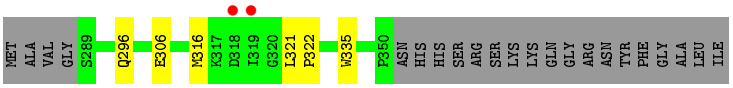
- Molecule 1: Protein HSH49

Chain F:



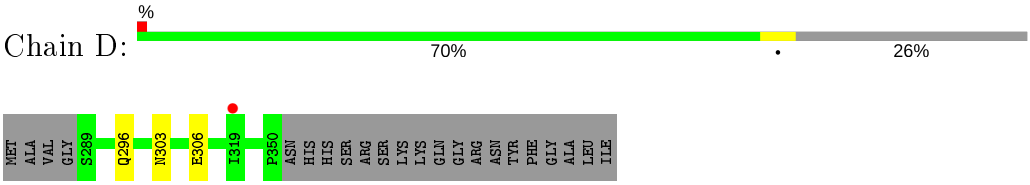
- Molecule 2: Cold sensitive U2 snRNA suppressor 1

Chain B:



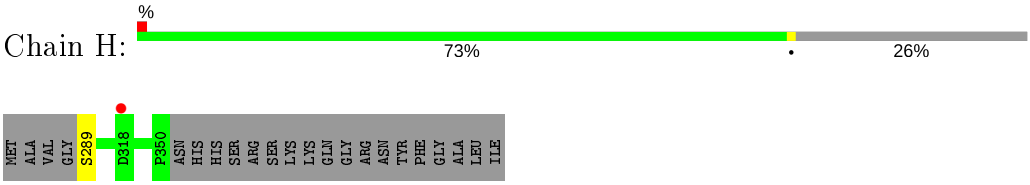
• Molecule 2: Cold sensitive U2 snRNA suppressor 1

Chain D:



• Molecule 2: Cold sensitive U2 snRNA suppressor 1

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	142.08Å 142.08Å 40.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.52 – 2.70 35.52 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (35.52-2.70) 100.0 (35.52-2.70)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.18 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.184 , 0.233 0.212 , 0.252	Depositor DCC
R_{free} test set	1301 reflections (5.20%)	wwPDB-VP
Wilson B-factor (Å^2)	29.7	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 31.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.012 for -h,-k,l 0.005 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
Reported twinning fraction	0.638 for H, K, L \ 0.362 for -K, -H, -L \	Depositor
Outliers	0 of 24999 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	5799	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.49% 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	0/1475	0.73	0/1982
1	C	0.47	0/1475	0.74	1/1982 (0.1%)
1	F	0.48	0/1463	0.74	2/1966 (0.1%)
2	B	0.51	0/496	0.77	1/672 (0.1%)
2	D	0.49	0/496	0.67	0/672
2	H	0.48	0/496	0.66	0/672
All	All	0.50	0/5901	0.73	4/7946 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	335	TRP	CA-CB-CG	6.70	126.44	113.70
1	C	79	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	F	184	PHE	N-CA-C	5.63	126.21	111.00
1	F	195	GLY	N-CA-C	-5.28	99.90	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	194	TYR	Peptide

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Mol	Chain	Res	Type	Group
1	C	194	TYR	Peptide

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	1451	0	1480	8	0
1	C	1451	0	1480	14	0
1	F	1439	0	1471	20	0
2	B	484	0	502	7	0
2	D	484	0	502	1	0
2	H	484	0	502	1	0
3	A	2	0	0	0	0
3	C	1	0	0	0	0
3	F	1	0	0	0	0
3	H	2	0	0	0	0
All	All	5799	0	5937	50	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 4.

The worst 5 of 50 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:C:185:LYS:HE2	1:C:194:TYR:OH	1.50	1.11
1:F:172:LEU:HD11	1:F:175:ASN:HA	1.43	0.98
1:F:190:GLY:N	1:F:194:TYR:CE2	2.39	0.91
1:C:136:ARG:NH1	1:C:137:GLU:O	2.12	0.83
1:F:136:ARG:NH1	1:F:137:GLU:O	2.13	0.81

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	168/215 (78%)	162 (96%)	6 (4%)	0	100 100
1	C	168/215 (78%)	160 (95%)	7 (4%)	1 (1%)	25 50
1	F	166/215 (77%)	157 (95%)	8 (5%)	1 (1%)	25 50
2	B	60/84 (71%)	59 (98%)	1 (2%)	0	100 100
2	D	60/84 (71%)	59 (98%)	1 (2%)	0	100 100
2	H	60/84 (71%)	58 (97%)	2 (3%)	0	100 100
All	All	682/897 (76%)	655 (96%)	25 (4%)	2 (0%)	41 66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	191	ASN
1	F	191	ASN

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	156/189 (82%)	151 (97%)	5 (3%)	39 68
1	C	156/189 (82%)	149 (96%)	7 (4%)	27 55
1	F	155/189 (82%)	152 (98%)	3 (2%)	57 82
2	B	53/70 (76%)	53 (100%)	0	100 100
2	D	53/70 (76%)	52 (98%)	1 (2%)	57 82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	H	53/70 (76%)	53 (100%)	0	100 100
All	All	626/777 (81%)	610 (97%)	16 (3%)	46 75

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	79	ARG
1	C	135	ILE
2	D	303	ASN
1	C	42	LYS
1	F	9	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

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

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	176/215 (81%)	-0.24	0	100	100	14, 24, 38, 51	1 (0%)
1	C	176/215 (81%)	0.06	3 (1%)	70	72	17, 31, 52, 67	1 (0%)
1	F	174/215 (80%)	0.08	3 (1%)	70	72	22, 32, 52, 61	1 (0%)
2	B	62/84 (73%)	-0.06	2 (3%)	47	48	10, 23, 41, 56	0
2	D	62/84 (73%)	-0.12	1 (1%)	72	74	16, 27, 45, 59	0
2	H	62/84 (73%)	-0.04	1 (1%)	72	74	23, 36, 57, 69	0
All	All	712/897 (79%)	-0.04	10 (1%)	75	77	10, 29, 50, 69	3 (0%)

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	194	TYR	4.6
1	C	175	ASN	4.0
2	B	318	ASP	2.8
2	H	318	ASP	2.7
2	B	319	ILE	2.4

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 (i)

There are no such residues in this entry.