wwPDB X-ray Structure Validation Summary Report (i)

Oct 26, 2024 – 02:47 PM EDT

PDB ID	:	6UY1
Title	:	Crystal structure of the Sth1 bromodomain from Saccharomyces cerevisiae at 2.2 Angstrom resolution
Authors	:	Stavropoulos, P.; Hoelz, A.
Deposited on	:	2019-11-09
Resolution	:	2.21 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:

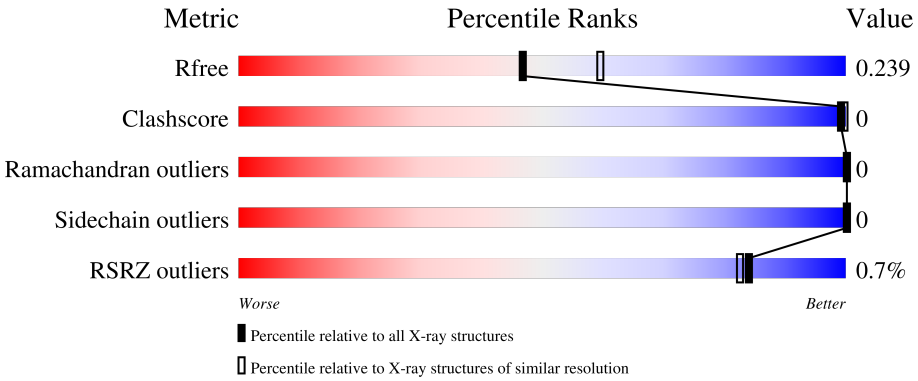
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.21 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}	164625	7167 (2.24-2.20)
Clashscore	180529	8096 (2.24-2.20)
Ramachandran outliers	177936	8010 (2.24-2.20)
Sidechain outliers	177891	8011 (2.24-2.20)
RSRZ outliers	164620	7166 (2.24-2.20)

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	114	96%
1	B	114	96%
1	C	114	96%
1	D	114	97%
1	E	114	96%

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Mol	Chain	Length	Quality of chain
1	F	114	96%
1	G	114	97%
1	H	114	95%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 15429 atoms, of which 7206 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 Nuclear protein STH1/NPS1.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	110	Total	C	H	N	O	S	Se	0	0	0
			1817	592	891	149	180	1	4			
1	B	111	Total	C	H	N	O	S	Se	0	1	0
			1843	600	902	151	185	1	4			
1	C	110	Total	C	H	N	O	S	Se	0	1	0
			1835	596	900	153	182	1	3			
1	D	111	Total	C	H	N	O	S	Se	0	1	0
			1852	601	909	154	183	1	4			
1	E	109	Total	C	H	N	O	S	Se	0	2	0
			1831	595	900	152	179	1	4			
1	F	109	Total	C	H	N	O	S	Se	0	2	0
			1842	598	904	154	182	1	3			
1	G	111	Total	C	H	N	O	S	Se	0	0	0
			1828	595	896	150	182	1	4			
1	H	110	Total	C	H	N	O	S	Se	0	2	0
			1846	600	904	153	185	1	3			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	GLY	-	expression tag	UNP P32597
A	17	PRO	-	expression tag	UNP P32597
A	18	HIS	-	expression tag	UNP P32597
A	19	MSE	-	expression tag	UNP P32597
B	16	GLY	-	expression tag	UNP P32597
B	17	PRO	-	expression tag	UNP P32597
B	18	HIS	-	expression tag	UNP P32597
B	19	MSE	-	expression tag	UNP P32597
C	16	GLY	-	expression tag	UNP P32597
C	17	PRO	-	expression tag	UNP P32597
C	18	HIS	-	expression tag	UNP P32597
C	19	MSE	-	expression tag	UNP P32597
D	16	GLY	-	expression tag	UNP P32597

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Chain	Residue	Modelled	Actual	Comment	Reference
D	17	PRO	-	expression tag	UNP P32597
D	18	HIS	-	expression tag	UNP P32597
D	19	MSE	-	expression tag	UNP P32597
E	16	GLY	-	expression tag	UNP P32597
E	17	PRO	-	expression tag	UNP P32597
E	18	HIS	-	expression tag	UNP P32597
E	19	MSE	-	expression tag	UNP P32597
F	16	GLY	-	expression tag	UNP P32597
F	17	PRO	-	expression tag	UNP P32597
F	18	HIS	-	expression tag	UNP P32597
F	19	MSE	-	expression tag	UNP P32597
G	16	GLY	-	expression tag	UNP P32597
G	17	PRO	-	expression tag	UNP P32597
G	18	HIS	-	expression tag	UNP P32597
G	19	MSE	-	expression tag	UNP P32597
H	16	GLY	-	expression tag	UNP P32597
H	17	PRO	-	expression tag	UNP P32597
H	18	HIS	-	expression tag	UNP P32597
H	19	MSE	-	expression tag	UNP P32597

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total Mg 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	131	Total O 131 131	0	0
3	B	106	Total O 107 107	0	1
3	C	102	Total O 102 102	0	0
3	D	101	Total O 101 101	0	0
3	E	63	Total O 63 63	0	0
3	F	73	Total O 74 74	0	1
3	G	73	Total O 73 73	0	0

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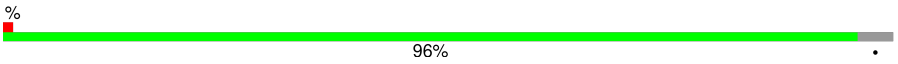
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	83	Total	O	0	0
			83	83		

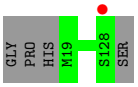
3 Residue-property plots (i)

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: Nuclear protein STH1/NPS1

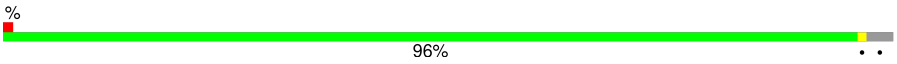
Chain A:

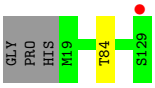




• Molecule 1: Nuclear protein STH1/NPS1

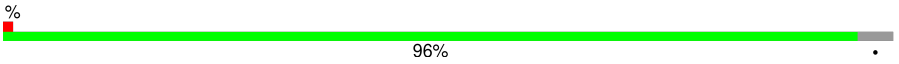
Chain B:

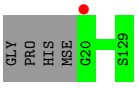




• Molecule 1: Nuclear protein STH1/NPS1

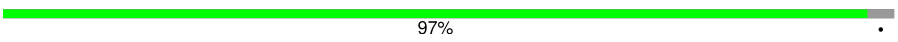
Chain C:





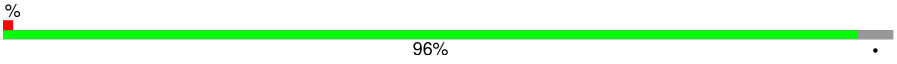
• Molecule 1: Nuclear protein STH1/NPS1

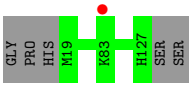
Chain D:



• Molecule 1: Nuclear protein STH1/NPS1

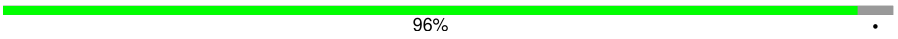
Chain E:

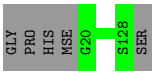




• Molecule 1: Nuclear protein STH1/NPS1

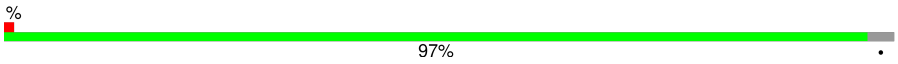
Chain F:

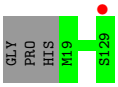




• Molecule 1: Nuclear protein STH1/NPS1

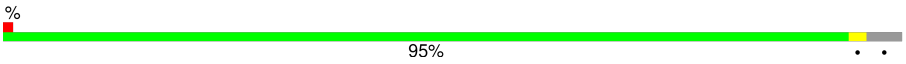
Chain G:

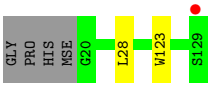




• Molecule 1: Nuclear protein STH1/NPS1

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	76.28Å 76.28Å 98.44Å 90.00° 96.65° 90.00°	Depositor
Resolution (Å)	19.95 – 2.21 19.95 – 2.21	Depositor EDS
% Data completeness (in resolution range)	97.5 (19.95-2.21) 92.4 (19.95-2.21)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.10 (at 2.21Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.184 , 0.228 0.200 , 0.239	Depositor DCC
R_{free} test set	53579 reflections (3.60%)	wwPDB-VP
Wilson B-factor (Å^2)	38.8	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 44.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15429	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.28% 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

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.24	0/945	0.37	0/1269
1	B	0.24	0/960	0.37	0/1289
1	C	0.24	0/954	0.36	0/1281
1	D	0.24	0/962	0.37	0/1291
1	E	0.23	0/957	0.36	0/1285
1	F	0.23	0/957	0.36	0/1285
1	G	0.24	0/951	0.36	0/1277
1	H	0.24	0/961	0.35	0/1291
All	All	0.24	0/7647	0.36	0/10268

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	926	891	890	0	0
1	B	941	902	900	2	0
1	C	935	900	898	0	0
1	D	943	909	907	0	0
1	E	931	900	891	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	938	904	900	0	0
1	G	932	896	895	0	0
1	H	942	904	900	1	0
2	E	1	0	0	0	0
3	A	131	0	0	0	0
3	B	107	0	0	0	0
3	C	102	0	0	0	0
3	D	101	0	0	0	0
3	E	63	0	0	0	0
3	F	74	0	0	0	0
3	G	73	0	0	0	0
3	H	83	0	0	0	0
All	All	8223	7206	7181	3	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 0.

All (3) 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:H:28:LEU:HD13	1:H:123:TRP:CD2	2.36	0.61

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	108/114 (95%)	108 (100%)	0	0	100	100
1	B	110/114 (96%)	109 (99%)	1 (1%)	0	100	100
1	C	109/114 (96%)	105 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	110/114 (96%)	109 (99%)	1 (1%)	0	100	100
1	E	109/114 (96%)	107 (98%)	2 (2%)	0	100	100
1	F	109/114 (96%)	107 (98%)	2 (2%)	0	100	100
1	G	109/114 (96%)	108 (99%)	1 (1%)	0	100	100
1	H	110/114 (96%)	107 (97%)	3 (3%)	0	100	100
All	All	874/912 (96%)	860 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	103/102 (101%)	103 (100%)	0	100	100
1	B	105/102 (103%)	105 (100%)	0	100	100
1	C	104/102 (102%)	104 (100%)	0	100	100
1	D	105/102 (103%)	105 (100%)	0	100	100
1	E	104/102 (102%)	104 (100%)	0	100	100
1	F	104/102 (102%)	104 (100%)	0	100	100
1	G	104/102 (102%)	104 (100%)	0	100	100
1	H	105/102 (103%)	105 (100%)	0	100	100
All	All	834/816 (102%)	834 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes 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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	106/114 (92%)	-0.53	1 (0%)	81	79	36, 49, 73, 110	0
1	B	107/114 (93%)	-0.35	1 (0%)	81	79	30, 52, 86, 132	1 (0%)
1	C	107/114 (93%)	-0.34	1 (0%)	81	79	23, 53, 98, 141	1 (0%)
1	D	107/114 (93%)	-0.47	0	100	100	31, 53, 92, 126	1 (0%)
1	E	105/114 (92%)	-0.00	1 (0%)	79	77	33, 75, 127, 161	1 (0%)
1	F	106/114 (92%)	-0.16	0	100	100	31, 63, 108, 133	2 (1%)
1	G	107/114 (93%)	-0.20	1 (0%)	81	79	40, 69, 113, 150	0
1	H	107/114 (93%)	-0.07	1 (0%)	81	79	35, 68, 115, 143	2 (1%)
All	All	852/912 (93%)	-0.27	6 (0%)	84	82	23, 60, 110, 161	8 (0%)

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	20	GLY	3.1
1	H	129	SER	2.6
1	G	129	SER	2.3
1	B	129	SER	2.2
1	A	128	SER	2.1

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 monosaccharides in this entry.

6.4 Ligands

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. 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	B-factors(Å^2)	Q<0.9
2	MG	E	201	1/1	0.97	0.05	43,43,43,43	0

6.5 Other polymers

There are no such residues in this entry.