Full wwPDB X-ray Structure Validation Report (i)

May 14, 2020 – 09:20 am BST

PDB ID	:	5YWL
Title	:	SsCR_L211H
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Deposited on	:	2017-11-29
Resolution	:	2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 (i)) 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 2.10 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	Percentile Ranks	Value
Rfree		0.247
Clashscore		11
Ramachandran outliers		0.6%
Sidechain outliers		4.2%
RSRZ outliers		6.0%

Worse ← → *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
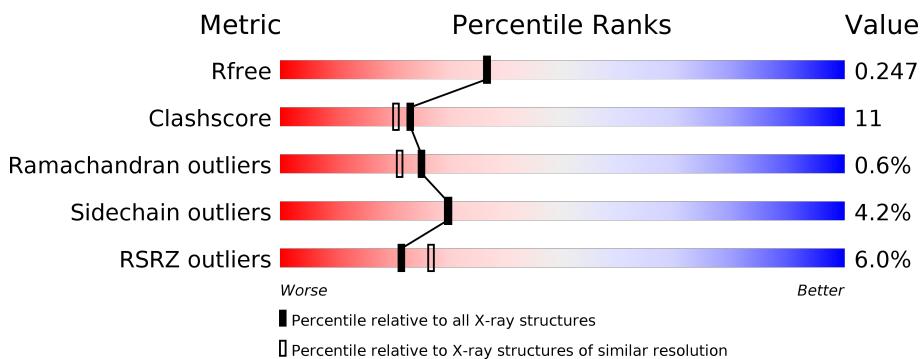
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	334	6% / 80% / 16% / ..

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2835 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 induced by osmotic stress.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2593	1663	422	505	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	211	HIS	LEU	engineered mutation	UNP A3LWG4

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	242	Total	O	0	0
			242	242		

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 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 induced by osmotic stress
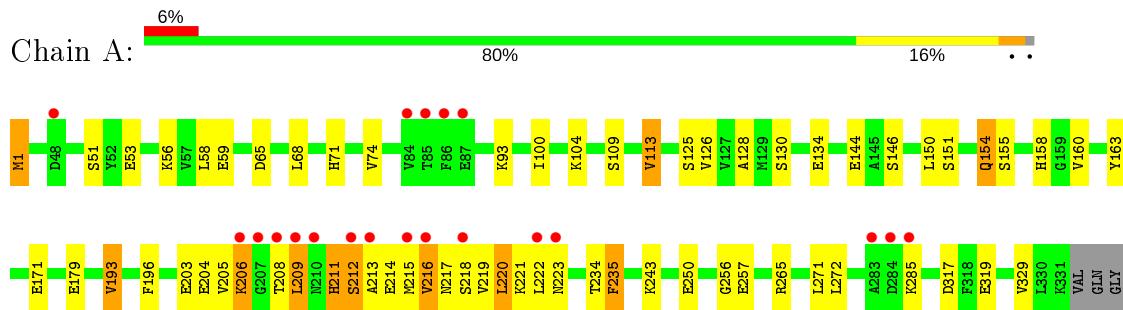
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	47.76Å 53.15Å 140.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.43 – 2.10 34.43 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.6 (34.43-2.10) 97.6 (34.43-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.32 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.206 , 0.265 0.216 , 0.247	Depositor DCC
R_{free} test set	1090 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å^2)	24.8	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 55.5	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	0.92	EDS
Total number of atoms	2835	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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	1.68	19/2646 (0.7%)	0.94	5/3583 (0.1%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	53	GLU	CD-OE1	-6.49	1.18	1.25
1	A	134	GLU	CD-OE2	-6.32	1.18	1.25
1	A	256	GLY	C-O	-6.28	1.13	1.23
1	A	59	GLU	CD-OE2	-6.27	1.18	1.25
1	A	144	GLU	CD-OE1	-6.20	1.18	1.25
1	A	319	GLU	CD-OE2	-6.16	1.18	1.25
1	A	53	GLU	CD-OE2	-5.84	1.19	1.25
1	A	125	SER	CB-OG	-5.76	1.34	1.42
1	A	109	SER	CB-OG	-5.61	1.34	1.42
1	A	250	GLU	CD-OE2	-5.50	1.19	1.25
1	A	171	GLU	CD-OE2	-5.45	1.19	1.25
1	A	257	GLU	CD-OE1	-5.37	1.19	1.25
1	A	128	ALA	C-O	-5.37	1.13	1.23
1	A	146	SER	CB-OG	-5.36	1.35	1.42
1	A	155	SER	CB-OG	-5.28	1.35	1.42
1	A	126	VAL	C-O	-5.27	1.13	1.23
1	A	243	LYS	C-O	-5.10	1.13	1.23
1	A	163	TYR	C-O	-5.09	1.13	1.23
1	A	179	GLU	CD-OE1	-5.01	1.20	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	317	ASP	CB-CG-OD1	5.48	123.24	118.30
1	A	220	LEU	CB-CG-CD1	-5.43	101.77	111.00
1	A	65	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	272	LEU	CB-CG-CD1	-5.21	102.14	111.00
1	A	58	LEU	CB-CG-CD2	-5.09	102.34	111.00

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	2593	0	2596	59	0
2	A	242	0	0	2	0
All	All	2835	0	2596	59	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 11.

All (59) 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:211:HIS:CB	1:A:217:ASN:HB2	1.65	1.24
1:A:211:HIS:HB3	1:A:217:ASN:CB	1.84	1.06
1:A:211:HIS:HB3	1:A:217:ASN:HB2	1.06	1.02
1:A:209:LEU:HA	1:A:329:VAL:HG13	1.44	0.98
1:A:211:HIS:HB2	1:A:214:GLU:HA	1.48	0.95
1:A:211:HIS:CB	1:A:214:GLU:HA	2.01	0.91
1:A:151:SER:OG	1:A:154:GLN:HG2	1.74	0.88
1:A:213:ALA:O	1:A:216:VAL:CG2	2.24	0.85
1:A:211:HIS:O	1:A:211:HIS:ND1	2.10	0.85
1:A:208:THR:O	1:A:209:LEU:HB2	1.78	0.83
1:A:213:ALA:O	1:A:216:VAL:HG22	1.79	0.82
1:A:203:GLU:OE1	1:A:203:GLU:N	2.11	0.80
1:A:211:HIS:O	1:A:214:GLU:CA	2.39	0.71
1:A:211:HIS:O	1:A:214:GLU:HB3	1.92	0.69
1:A:211:HIS:CG	1:A:217:ASN:HB2	2.26	0.69
1:A:211:HIS:CG	1:A:214:GLU:HA	2.28	0.68
1:A:211:HIS:O	1:A:214:GLU:HA	1.95	0.67
1:A:211:HIS:O	1:A:214:GLU:CB	2.43	0.66
1:A:211:HIS:CE1	1:A:214:GLU:HB2	2.30	0.66
1:A:100:ILE:HG22	1:A:104:LYS:HE3	1.79	0.64
1:A:158:HIS:CE1	1:A:160:VAL:HG23	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:VAL:HG21	1:A:271:LEU:CD2	2.32	0.60
1:A:209:LEU:HA	1:A:329:VAL:CG1	2.27	0.58
1:A:211:HIS:C	1:A:214:GLU:HA	2.24	0.58
1:A:214:GLU:O	1:A:217:ASN:N	2.31	0.57
1:A:151:SER:HG	1:A:154:GLN:HG2	1.72	0.54
1:A:219:VAL:HG21	1:A:271:LEU:HD23	1.89	0.54
1:A:211:HIS:HB2	1:A:214:GLU:CA	2.32	0.53
1:A:100:ILE:CG2	1:A:104:LYS:HE3	2.38	0.53
1:A:158:HIS:HE1	1:A:160:VAL:HG23	1.70	0.53
1:A:219:VAL:HA	1:A:222:LEU:HG	1.92	0.52
1:A:218:SER:O	1:A:221:LYS:HG2	2.11	0.51
1:A:211:HIS:ND1	1:A:214:GLU:HB2	2.26	0.50
1:A:212:SER:HA	1:A:214:GLU:N	2.28	0.49
1:A:211:HIS:HD2	1:A:217:ASN:C	2.16	0.49
1:A:196:PHE:CD2	1:A:216:VAL:HG13	2.50	0.47
1:A:213:ALA:O	1:A:216:VAL:HG23	2.13	0.46
1:A:211:HIS:HB2	1:A:217:ASN:HB2	1.79	0.46
1:A:219:VAL:CG2	1:A:271:LEU:HD23	2.46	0.46
1:A:212:SER:HA	1:A:213:ALA:C	2.36	0.46
1:A:150:LEU:HD12	1:A:154:GLN:HG3	1.98	0.45
1:A:205:VAL:HG12	1:A:205:VAL:O	2.16	0.45
1:A:212:SER:CA	1:A:213:ALA:C	2.85	0.45
1:A:217:ASN:HD22	1:A:220:LEU:HB2	1.82	0.45
1:A:196:PHE:CD1	1:A:235:PHE:HB2	2.52	0.45
1:A:211:HIS:CD2	1:A:217:ASN:CB	2.99	0.44
1:A:211:HIS:CG	1:A:214:GLU:CA	2.99	0.44
1:A:204:GLU:O	1:A:206:LYS:N	2.51	0.44
1:A:211:HIS:ND1	1:A:214:GLU:CB	2.82	0.43
1:A:71:HIS:HB3	1:A:74:VAL:HG23	2.00	0.43
1:A:211:HIS:O	1:A:211:HIS:CG	2.69	0.43
1:A:56:LYS:HB3	1:A:56:LYS:HE2	1.88	0.43
1:A:193:VAL:HG11	1:A:234:THR:OG1	2.19	0.42
1:A:206:LYS:HD3	1:A:206:LYS:C	2.41	0.42
1:A:211:HIS:CG	1:A:214:GLU:HB2	2.55	0.41
1:A:68:LEU:HB3	1:A:113:VAL:HG12	2.02	0.41
1:A:1:MET:HG2	2:A:607:HOH:O	2.20	0.41
1:A:223:ASN:HA	1:A:285:LYS:O	2.20	0.41
1:A:265:ARG:HG3	2:A:609:HOH:O	2.20	0.40

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	329/334 (98%)	322 (98%)	5 (2%)	2 (1%)	25	21

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	209	LEU
1	A	193	VAL

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	287/289 (99%)	275 (96%)	12 (4%)	30	30

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	51	SER
1	A	93	LYS
1	A	113	VAL
1	A	130	SER
1	A	154	GLN
1	A	206	LYS
1	A	211	HIS
1	A	212	SER

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Mol	Chain	Res	Type
1	A	215	MET
1	A	216	VAL
1	A	235	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	217	ASN

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 (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(Å²)	Q<0.9
1	A	331/334 (99%)	0.23	20 (6%)	21	27	5, 19, 50, 75	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	86	PHE	9.5
1	A	209	LEU	7.4
1	A	208	THR	6.7
1	A	210	ASN	4.8
1	A	285	LYS	4.0
1	A	207	GLY	3.8
1	A	85	THR	3.6
1	A	84	VAL	3.5
1	A	212	SER	3.1
1	A	215	MET	2.8
1	A	87	GLU	2.8
1	A	218	SER	2.6
1	A	222	LEU	2.6
1	A	213	ALA	2.6
1	A	223	ASN	2.5
1	A	283	ALA	2.2
1	A	284	ASP	2.1
1	A	216	VAL	2.1
1	A	48	ASP	2.0
1	A	206	LYS	2.0

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 carbohydrates 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.