

Full wwPDB X-ray Structure Validation Report (i)

May 23, 2020 – 11:33 pm BST

PDB ID : 4YTO

Title: Structure of coiled-coil domain of SYCP1

Authors : park, H.H. Deposited on : 2015-03-18

Resolution : 2.00 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 (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 : 2.11

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)

al geometry (DNA, RNA) : Parkinson et al. (1996)

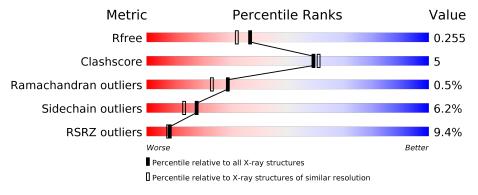
Ideal geometry (DNA, RNA) : Park Validation Pipeline (wwPDB-VP) : 2.11

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 2.00 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\AA)}) \end{array}$
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 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	148	51%	9% •	36%			
1	В	148	5%	9%	• 34%			



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1728 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 Synaptonemal complex protein 1.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	95	Total 772	C 482	- '	O 155	S 3	0	0	0
1	В	97	Total 789	C 493		O 159	S 3	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	802	LEU	-	expression tag	UNP Q15431
A	803	GLU	-	expression tag	UNP Q15431
A	804	HIS	_	expression tag	UNP Q15431
A	805	HIS	-	expression tag	UNP Q15431
A	806	HIS	-	expression tag	UNP Q15431
A	807	HIS	-	expression tag	UNP Q15431
A	808	HIS	-	expression tag	UNP Q15431
A	809	HIS	-	expression tag	UNP Q15431
В	802	LEU	-	expression tag	UNP Q15431
В	803	GLU	-	expression tag	UNP Q15431
В	804	HIS	-	expression tag	UNP Q15431
В	805	HIS	-	expression tag	UNP Q15431
В	806	HIS	-	expression tag	UNP Q15431
В	807	HIS	-	expression tag	UNP Q15431
В	808	HIS	-	expression tag	UNP Q15431
В	809	HIS	-	expression tag	UNP Q15431

• Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0

• Molecule 3 is water.

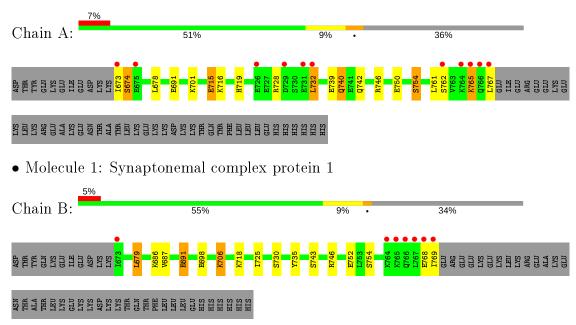
Mol	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
3	A	64	Total O 64 64	0	0
3	В	91	Total O 91 91	0	0



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: Synaptonemal complex protein 1





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants	119.61Å 119.61Å 83.57Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.19 - 2.00	Depositor
Resolution (A)	28.19 - 2.00	EDS
% Data completeness	97.5 (28.19-2.00)	Depositor
(in resolution range)	97.6 (28.19-2.00)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$4.72 \; ({\rm at} \; 1.99 {\rm \AA})$	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.231 , 0.256	Depositor
it, it free	0.236 , 0.255	DCC
R_{free} test set	1978 reflections (4.90%)	wwPDB-VP
Wilson B-factor (\mathring{A}^2)	27.9	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	$0.37 \; , 49.7$	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	0.93	EDS
Total number of atoms	1728	wwPDB-VP
Average B, all atoms $(Å^2)$	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 8.90% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

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	Bo	nd lengths	Bo	nd angles
MIOI	Chain	RMSZ	RMSZ $\# Z > 5$		# Z >5
1	A	1.54	$9/776 \ (1.2\%)$	1.21	3/1032 (0.3%)
1	В	1.61	10/793~(1.3%)	1.12	4/1055 (0.4%)
All	All	1.58	19/1569~(1.2%)	1.17	7/2087 (0.3%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
1	В	768	GLU	CD-OE1	10.42	1.37	1.25
1	В	768	GLU	CD-OE2	7.81	1.34	1.25
1	A	754	SER	CB-OG	-7.80	1.32	1.42
1	В	754	SER	CB-OG	-7.76	1.32	1.42
1	В	698	GLU	CG-CD	7.30	1.62	1.51
1	В	743	SER	CB-OG	-7.10	1.33	1.42
1	В	698	GLU	CD-OE1	6.92	1.33	1.25
1	В	691	GLU	CB-CG	-6.91	1.39	1.52
1	В	691	GLU	CD-OE2	-6.71	1.18	1.25
1	A	691	GLU	CD-OE2	-6.71	1.18	1.25
1	A	739	GLU	CD-OE1	6.48	1.32	1.25
1	A	750	GLU	CD-OE2	6.46	1.32	1.25
1	В	735	TYR	CE1-CZ	-6.41	1.30	1.38
1	A	742	GLN	CB-CG	-5.99	1.36	1.52
1	A	715	GLU	CD-OE1	5.68	1.31	1.25
1	В	743	SER	CA-CB	-5.47	1.44	1.52
1	A	739	GLU	CB-CG	5.25	1.62	1.52
1	A	740	GLN	CG-CD	5.13	1.62	1.51
1	A	691	GLU	CG-CD	5.02	1.59	1.51

All (7) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
1	В	679	LEU	CA-CB-CG	6.37	129.96	115.30
1	В	746	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	A	739	GLU	OE1-CD-OE2	-6.03	116.06	123.30
1	A	746	ARG	NE-CZ-NH1	-5.41	117.60	120.30
1	A	716	LYS	CD-CE-NZ	5.18	123.63	111.70
1	В	698	GLU	CA-CB-CG	5.15	124.74	113.40
1	В	752	GLU	OE1-CD-OE2	-5.12	117.15	123.30

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	772	0	803	12	0
1	В	789	0	820	4	0
2	A	12	0	15	0	0
3	A	64	0	0	5	0
3	В	91	0	0	2	0
All	All	1728	0	1638	15	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 5.

All (15) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{array}{ll} ext{Interatomic} \ ext{distance} \ (ext{\AA}) \end{array}$	$egin{array}{c} ext{Clash} \ ext{overlap } (ext{Å}) \end{array}$
1:A:673:ILE:HG22	1:A:674:SER:H	1.43	0.82
1:A:767:LEU:HD12	3:A:1064:HOH:O	1.81	0.79
1:A:719:HIS:HB3	3:A:1054:HOH:O	1.87	0.73
1:A:673:ILE:HG22	1:A:674:SER:N	2.04	0.71
1:A:673:ILE:CG2	1:A:674:SER:H	2.11	0.63
1:A:740:GLN:CG	3:A:1052:HOH:O	2.59	0.50
1:A:740:GLN:HG2	3:A:1052:HOH:O	2.13	0.48
1:A:767:LEU:CD1	3:A:1064:HOH:O	2.50	0.48

Continued on next page...



Continued	trom	nromanne	naae
-	110116	picolous	puyc

Atom-1	Atom-2	$egin{array}{l} ext{Interatomic} \ ext{distance} \ (ext{Å}) \end{array}$	$egin{array}{c} ext{Clash} \ ext{overlap } (ext{Å}) \end{array}$
1:B:706:LYS:NZ	3:B:905:HOH:O	2.49	0.44
1:A:715:GLU:HG3	1:B:725:ILE:HD13	2.00	0.43
1:B:687:VAL:O	1:B:691:GLU:HG2	2.19	0.43
1:A:701:LYS:HA	1:A:701:LYS:HD3	1.83	0.42
1:B:686:LYS:NZ	3:B:903:HOH:O	2.43	0.41
1:A:728:ARG:NH2	1:A:732:LEU:HD21	2.36	0.41
1:A:765:LYS:HB2	1:A:765:LYS:HE2	1.81	0.41

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	93/148 (63%)	90 (97%)	2 (2%)	1 (1%)	14 8
1	В	95/148 (64%)	95 (100%)	0	0	100 100
All	All	188/296 (64%)	185 (98%)	2 (1%)	1 (0%)	29 23

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Α	674	SER

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	Perce	ntiles
1	A	87/138 (63%)	81 (93%)	6 (7%)	15	11
1	В	89/138 (64%)	84 (94%)	5 (6%)	21	17
All	All	176/276 (64%)	165 (94%)	11 (6%)	18	13

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	678	LEU
1	A	732	LEU
1	A	754	SER
1	A	761	LEU
1	A	762	SER
1	A	765	LYS
1	В	679	LEU
1	В	706	LYS
1	В	718	LYS
1	В	730	SER
1	В	769	ILE

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)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and



the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Т	Chain	Dog	T in le	B	ond leng	${ m gths}$	В	ond ang	gles
MIOI	Type	Chain	Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	A	902	-	5,5,5	1.19	0	5,5,5	1.43	1 (20%)
2	GOL	A	901	_	5,5,5	0.33	0	5,5,5	1.10	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	902	_	-	3/4/4/4	_
2	GOL	A	901	_	-	3/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

\mathbf{Mol}	Chain	${f Res}$	Type	${f Atoms}$	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^o)$
2	A	902	GOL	O1-C1-C2	-2.47	98.34	110.20

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	GOL	O1-C1-C2-C3
2	A	901	GOL	C1-C2-C3-O3
2	A	902	GOL	O1-C1-C2-O2
2	A	901	GOL	O1-C1-C2-O2
2	A	902	GOL	O1-C1-C2-C3
2	A	902	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.



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, 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	${f Analysed}$	<RSRZ $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(A^2)$	$\mathbf{Q}{<}0.9$
1	A	95/148 (64%)	0.45	11 (11%) 4 4	21, 39, 91, 108	0
1	В	97/148 (65%)	0.30	7 (7%) 15 14	20, 41, 81, 103	0
All	All	192/296~(64%)	0.38	18 (9%) 8 8	20, 40, 84, 108	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	768	GLU	7.2
1	В	767	LEU	5.8
1	A	767	LEU	5.2
1	A	764	LYS	4.8
1	A	673	ILE	4.7
1	A	766	GLN	4.7
1	В	769	ILE	4.6
1	В	766	GLN	4.4
1	В	673	ILE	3.7
1	A	765	LYS	3.6
1	A	726	GLU	3.5
1	A	732	LEU	3.4
1	В	765	LYS	3.2
1	A	729	ASP	3.0
1	A	731	GLU	2.9
1	A	762	SER	2.6
1	В	764	LYS	2.6
1	A	675	GLU	2.1

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)

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	${f B-factors}({f A}^2)$	Q<0.9
2	GOL	A	902	6/6	0.86	0.16	43,50,58,75	0
2	GOL	A	901	6/6	0.98	0.09	31,33,36,41	0

6.5 Other polymers (i)

There are no such residues in this entry.

