

Full wwPDB X-ray Structure Validation Report (i)

May 24, 2020 – 11:43 pm BST

PDB ID	:	1B34
Title	:	CRYSTAL STRUCTURE OF THE D1D2 SUB-COMPLEX FROM THE HU-
		MAN SNRNP CORE DOMAIN
Authors	:	Walke, S.; Young, R.J.; Kambach, C.; Avis, J.M.; De La Fortelle, E.; Li, J.;
		Nagai, K.
Deposited on		
Resolution	:	2.50 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:

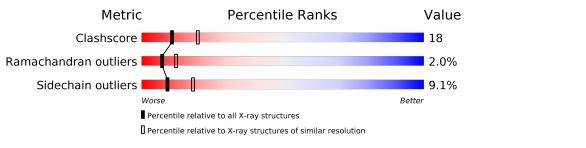
MolProbity : 4.02b-467	
Xtriage (Phenix) : NOT EXECUTED	
\mathbf{EDS} : NOT EXECUTED	
$ \begin{tabular}{lllllllllllllllllllllllllllllllllll$	25 th 2019
Ideal geometry (proteins) : Engh & Huber (2001)	
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)	
Validation Pipeline (wwPDB-VP) : 2.11	

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 2.50 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
Clashscore	141614	$5346 \ (2.50-2.50)$
Ramachandran outliers	138981	5231(2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain					
1	А	119	39%	23%	5%	33%	-	
2	В	118	36%	21%	5% •	37%	_	



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1239 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 (SMALL NUCLEAR RIBONUCLEOPROTEIN SM D1).

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	А	80	Total 633	C 404	N 111	0 115	S 3	0	0	0

• Molecule 2 is a protein called PROTEIN (SMALL NUCLEAR RIBONUCLEOPROTEIN SM D2).

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
2	В	74	Total 586	C 367	N 111	O 103	${ m S}{ m 5}$	0	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	14	Total O 14 14	0	0
3	В	6	Total O 6 6	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. 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. 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.

Note EDS was not executed.

• Molecule 1: PROTEIN (SMALL NUCLEAR RIBONUCLEOPROTEIN SM D1)

Chain A:	39%	23%	o 5%	33%	
MET K2 K2 K5 K5 K6 K6 K6 K6 K6 K6 K6 K6 K6 K6 K6 K6 K6	511 H12 E13 E13 E13 024 024 033 V136 N36 N36 N36 N36 N36 N36 N36 N36 N36	L47 R50 E51 L55 E56 E56	R61 R63 N63 N63 165 165 R66 F68 F68 F68 I69	L70 771 072 072 173 173 176 176 176 177 178	L80 V81 ASP ASP ASP ASP CLU CLU LVS VAL LVS LVS
SER LYS LYS ARG GLU ALA VAL ALA	110 111 111 111 111 111 111 111 111 111	GLY ARG GLY GLY PRO ARG ARG			
• Molecule	2: PROTEIN (SMAL	L NUCLE.	AR RIBON	UCLEOPROT	TEIN SM D2)
Chain B:	36%	21%	5% •	37%	
MET SER LEU LEU LEU ASN PRO LYS	STRA STRA MET PRO PRO PRO PRO CULU CULU CULU CULU CULU CULU CULU CUL	ASM 126 627 628 128 128 128 128 133	Q34 S35 V36 V36 T43 Q41 V42 L43	I 44 N45 C46 N48 N48 N48 N49 K50 K50 K55	F59 D60 R61 R64 R64 K71 E72
M73 TRP THR GLU VAL PRO LYS SER SER	141 142 142 142 142 143 143 143 143 143 143 143 143 143 143	M99 F100 L101 L101 L107 L107 V108	K118		



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 62	Depositor
Cell constants	75.30Å 75.30Å 91.99Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	18.40 - 2.50	Depositor
% Data completeness	99.0 (18.40-2.50)	Depositor
(in resolution range)	33.0 (10.40 2.50)	Depositor
R_{merge}	0.05	Depositor
R _{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.249 , 0.286	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1239	wwPDB-VP
Average B, all atoms $(Å^2)$	40.0	wwPDB-VP



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	Boı	nd lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.96	4/641~(0.6%)	2.02	10/867~(1.2%)	
2	В	0.56	0/590	1.18	2/788~(0.3%)	
All	All	0.80	4/1231~(0.3%)	1.67	12/1655~(0.7%)	

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.

M	ol	Chain	#Chirality outliers	#Planarity outliers
1	1	А	1	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
1	А	13	GLU	C-N	-11.52	1.07	1.34
1	А	79	LEU	CB-CG	10.49	1.82	1.52
1	А	78	THR	CB-CG2	-7.55	1.27	1.52
1	А	79	LEU	C-N	-5.45	1.21	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	77	ASP	CB-CG-OD1	33.66	148.60	118.30
1	А	77	ASP	CB-CG-OD2	-30.00	91.30	118.30
1	А	78	THR	CA-CB-CG2	12.10	129.34	112.40
1	А	66	ARG	NE-CZ-NH2	-9.17	115.72	120.30
1	А	79	LEU	CA-CB-CG	-8.81	95.03	115.30
2	В	47	ARG	NE-CZ-NH2	7.31	123.95	120.30
1	А	50	ARG	NE-CZ-NH2	7.22	123.91	120.30
1	А	12	HIS	CB-CA-C	-6.87	96.67	110.40
1	А	33	ASP	CB-CG-OD1	6.63	124.27	118.30
2	В	34	GLN	CG-CD-OE1	-6.03	109.54	121.60

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	66	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	А	78	THR	OG1-CB-CG2	5.20	121.96	110.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	78	THR	CB

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	56	GLU	Mainchain

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	А	633	0	675	26	1
2	В	586	0	627	29	2
3	А	14	0	0	0	0
3	В	6	0	0	0	0
All	All	1239	0	1302	46	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 18.

All (46) 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:79:LEU:CG	1:A:79:LEU:CB	1.83	1.53
1:A:79:LEU:CG	1:A:79:LEU:CA	2.49	0.90
1:A:36:MET:HE3	2:B:102:ARG:HE	1.50	0.77
2:B:107:ILE:HG22	2:B:108:VAL:HG22	1.74	0.69
1:A:79:LEU:CD1	1:A:79:LEU:CB	2.70	0.69
2:B:29:LEU:O	2:B:33:THR:HG22	1.94	0.67
2:B:39:ASN:O	2:B:55:ARG:NH1	2.27	0.65

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Continued from pre		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:B:30:SER:HA	2:B:33:THR:HG23	1.79	0.63	
1:A:36:MET:CE	2:B:102:ARG:HE	2.11	0.63	
2:B:48:ASN:O	2:B:49:ASN:HB2	1.99	0.63	
1:A:71:PRO:HD2	1:A:74:LEU:HG	1.86	0.57	
1:A:72:ASP:O	2:B:98:LYS:NZ	2.36	0.57	
1:A:76:LEU:HD11	2:B:98:LYS:HD3	1.87	0.57	
1:A:76:LEU:HD21	2:B:98:LYS:HD3	1.89	0.55	
2:B:30:SER:HA	2:B:33:THR:CG2	2.39	0.53	
2:B:26:THR:HG21	2:B:29:LEU:HB2	1.92	0.52	
1:A:6:PHE:CE2	1:A:79:LEU:HB2	2.45	0.52	
1:A:67:TYR:OH	2:B:94:ARG:NH1	2.43	0.52	
2:B:48:ASN:HD22	2:B:50:LYS:NZ	2.10	0.50	
2:B:48:ASN:ND2	2:B:50:LYS:NZ	2.60	0.49	
1:A:79:LEU:HG	1:A:79:LEU:N	2.27	0.49	
1:A:11:SER:O	1:A:12:HIS:HB2	2.13	0.49	
1:A:5:ARG:HA	1:A:8:MET:HE2	1.94	0.49	
1:A:45:MET:CE	1:A:55:LEU:HD11	2.42	0.49	
2:B:72:GLU:OE1	2:B:94:ARG:HD3	2.13	0.48	
1:A:80:LEU:O	1:A:81:VAL:C	2.51	0.48	
1:A:65:ILE:O	2:B:102:ARG:HD3	2.13	0.48	
2:B:60:ASP:OD2	2:B:64:ASN:HB2	2.13	0.48	
2:B:59:PHE:HA	2:B:64:ASN:O	2.16	0.46	
1:A:79:LEU:CD2	1:A:79:LEU:CB	2.83	0.45	
1:A:11:SER:O	1:A:12:HIS:CB	2.64	0.45	
1:A:79:LEU:HG	1:A:79:LEU:CA	2.43	0.44	
2:B:48:ASN:HD22	2:B:50:LYS:HZ1	1.65	0.44	
1:A:61:ARG:HB3	1:A:63:ASN:OD1	2.18	0.44	
1:A:66:ARG:CZ	2:B:50:LYS:HD3	2.48	0.44	
2:B:46:CYS:HB2	2:B:50:LYS:HB2	1.99	0.44	
1:A:4:VAL:O	1:A:8:MET:HG3	2.18	0.43	
2:B:26:THR:HG22	2:B:27:GLY:N	2.32	0.43	
2:B:48:ASN:O	2:B:49:ASN:CB	2.64	0.43	
1:A:67:TYR:HB2	2:B:100:PHE:O	2.19	0.42	
1:A:67:TYR:HE1	1:A:69:ILE:HG13	1.85	0.42	
2:B:42:VAL:HG13	2:B:44:ILE:HG13	2.01	0.42	
2:B:71:LYS:HD2	2:B:71:LYS:N	2.35	0.42	
2:B:26:THR:HG22	2:B:27:GLY:H	1.85	0.41	
1:A:18:GLU:OE2	1:A:66:ARG:NH1	2.54	0.40	
2:B:36:VAL:HG22	2:B:56:VAL:O	2.21	0.40	

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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:51:GLU:OE2	2:B:47:ARG:O[2_654]	1.50	0.70
2:B:34:GLN:OE1	2:B:118:LYS:O[4_765]	2.12	0.08

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	А	78/119~(66%)	71~(91%)	6 (8%)	1 (1%)	12 21
2	В	70/118~(59%)	$61 \ (87\%)$	7 (10%)	2(3%)	4 6
All	All	148/237~(62%)	132~(89%)	13~(9%)	3~(2%)	7 12

All (3) Ramachandran outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
2	В	47	ARG
2	В	27	GLY
1	А	34	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	А	75/101~(74%)	70~(93%)	5(7%)	16 31
2	В	68/110~(62%)	60 (88%)	8 (12%)	5 10
All	All	143/211~(68%)	130~(91%)	13 (9%)	9 18



Mol	Chain	Res	Type
1	А	4	VAL
1	А	24	GLN
1	А	34	VAL
1	А	47	LEU
1	А	74	LEU
2	В	33	THR
2	В	41	GLN
2	В	42	VAL
2	В	47	ARG
2	В	61	ARG
2	В	71	LYS
2	В	93	ASP
2	В	108	VAL

All (13) residues with a non-rotameric sidechain are listed below:

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	64	ASN
2	В	48	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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	А	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	А	13:GLU	С	14:THR	Ν	1.07



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

