



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 10:58 pm GMT

PDB ID : 1EQQ
Title : SINGLE STRANDED DNA BINDING PROTEIN AND SSDNA COMPLEX
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Deposited on : 2000-04-06
Resolution : 3.20 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

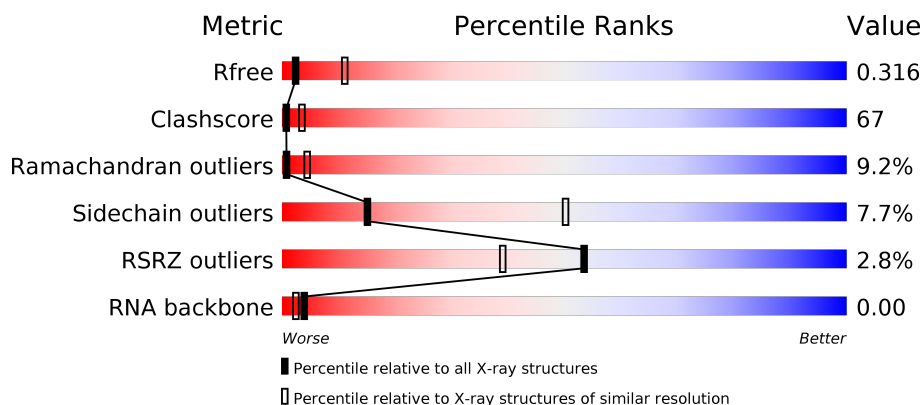
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	100719	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)
RNA backbone	2435	1045 (3.60-2.80)

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. 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 $\leq 5\%$. 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	M	3	
1	N	3	
2	A	178	
2	B	178	

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Mol	Chain	Length	Quality of chain
2	C	178	
2	D	178	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	5MU	M	802	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3737 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 RNA chain called 5'-R*(5MU)P*(5MU)P*(5MU))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	M	3	Total	C	N	O	P	0	0	0
			60	30	6	22	2			
1	N	1	Total	C	N	O		0	0	0
			18	10	2	6				

- Molecule 2 is a protein called SINGLE STRANDED DNA BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	114	Total	C	N	O	S	0	0	0
			884	548	161	171	4			
2	B	120	Total	C	N	O	S	0	0	0
			921	568	171	178	4			
2	C	114	Total	C	N	O	S	0	0	0
			884	548	161	171	4			
2	D	116	Total	C	N	O	S	0	0	0
			904	559	167	174	4			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	20	Total	O	0	0
			20	20		
3	B	15	Total	O	0	0
			15	15		
3	C	17	Total	O	0	0
			17	17		
3	D	13	Total	O	0	0
			13	13		
3	N	1	Total	O	0	0
			1	1		

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: 5'-R*(5MU)P*(5MU)P*(5MU))-3'

Chain M: 




- Molecule 1: 5'-R*(5MU)P*(5MU)P*(5MU))-3'

Chain N: 



- Molecule 2: SINGLE STRANDED DNA BINDING PROTEIN


Chain A: 





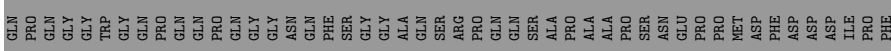


- Molecule 2: SINGLE STRANDED DNA BINDING PROTEIN

Chain B: 







[illegible]

Chain D:

Amino Acid	Percentage
MET	2%
A601	16%
V605	
N606	
K607	
V608	
L610	
V611	
G612	
N613	
G615	
Q616	
D617	
P618	
E619	
V620	
M623	
P624	
N625	
A630	
T633	
L634	
A635	
T636	
E638	
S639	
W640	
R641	
D642	
R643	
A644	
T645	
G646	
E647	
M648	
K649	
E650	
Q651	
T652	
E653	
W654	
R655	
R656	
G657	
V658	
L659	
T660	
G661	
K662	
L663	
A664	
A665	
V666	

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	101.71Å 60.47Å 94.73Å 90.00° 112.60° 90.00°	Depositor
Resolution (Å)	15.00 – 3.20 14.89 – 3.20	Depositor EDS
% Data completeness (in resolution range)	82.5 (15.00-3.20) 82.5 (14.89-3.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	30.25 (at 3.19Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.213 , 0.339 0.233 , 0.316	Depositor DCC
R_{free} test set	396 reflections (5.45%)	DCC
Wilson B-factor (Å ²)	41.4	Xtriage
Anisotropy	0.933	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 61.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.052 for $1/2^*h+3/2^*k, 1/2^*h-1/2^*k, -1/2^*h-1/2^*k-l$ 0.055 for $1/2^*h-3/2^*k, -1/2^*h-1/2^*k, -1/2^*h+1/2^*k-l$	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	3737	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU

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
2	A	0.52	0/897	0.89	3/1210 (0.2%)
2	B	0.51	0/934	0.89	3/1258 (0.2%)
2	C	0.52	0/897	0.89	3/1210 (0.2%)
2	D	0.51	0/917	0.87	3/1236 (0.2%)
All	All	0.51	0/3645	0.88	12/4914 (0.2%)

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	456	ARG	NE-CZ-NH1	13.81	127.20	120.30
2	B	256	ARG	NE-CZ-NH1	13.41	127.01	120.30
2	A	56	ARG	NE-CZ-NH2	13.11	126.85	120.30
2	C	456	ARG	NE-CZ-NH2	-12.96	113.82	120.30
2	D	656	ARG	NE-CZ-NH1	-12.92	113.84	120.30

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	M	60	0	37	16	0
1	N	18	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	884	0	880	145	0
2	B	921	0	912	133	0
2	C	884	0	877	146	0
2	D	904	0	898	132	0
3	A	20	0	0	13	0
3	B	15	0	0	11	0
3	C	17	0	0	6	0
3	D	13	0	0	2	0
3	N	1	0	0	0	0
All	All	3737	0	3617	486	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 67.

The worst 5 of 486 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)
2:A:7:LYS:HE2	2:C:407:LYS:HE2	1.25	1.14
2:C:483:LEU:HD21	2:D:683:LEU:HD21	1.32	1.11
2:B:207:LYS:HE2	2:D:607:LYS:HE2	1.36	1.04
2:A:23:MET:HB2	2:A:24:PRO:HD2	1.33	1.03
2:A:83:LEU:HD21	2:B:283:LEU:HD21	1.50	0.92

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
2	A	112/178 (63%)	82 (73%)	16 (14%)	14 (12%)	0 2
2	B	118/178 (66%)	96 (81%)	14 (12%)	8 (7%)	1 10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	112/178 (63%)	89 (80%)	12 (11%)	11 (10%)	1	4
2	D	114/178 (64%)	93 (82%)	12 (10%)	9 (8%)	1	7
All	All	456/712 (64%)	360 (79%)	54 (12%)	42 (9%)	1	4

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	2	SER
2	A	42	ASP
2	A	92	SER
2	A	113	GLY
2	B	292	SER

5.3.2 Protein sidechains ⓘ

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	
2	A	93/136 (68%)	88 (95%)	5 (5%)	26	65
2	B	95/136 (70%)	88 (93%)	7 (7%)	16	52
2	C	93/136 (68%)	82 (88%)	11 (12%)	6	27
2	D	95/136 (70%)	89 (94%)	6 (6%)	21	59
All	All	376/544 (69%)	347 (92%)	29 (8%)	15	50

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	424	PRO
2	C	443	LYS
2	D	702	VAL
2	C	425	ASN
2	C	450	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	316	GLN
2	C	413	ASN
2	C	476	GLN
2	B	276	GLN
2	D	613	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	M	2/3 (66%)	2 (100%)	0
1	N	0/3	-	-
All	All	2/6 (33%)	2 (100%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	M	802	5MU
1	M	803	5MU

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	5MU	M	801	1	14,19,23	0.99	2 (14%)	16,28,35	4.22	3 (18%)
1	5MU	M	802	1	14,22,23	1.12	2 (14%)	16,32,35	4.23	3 (18%)
1	5MU	M	803	1	14,22,23	1.16	2 (14%)	16,32,35	4.20	3 (18%)
1	5MU	N	900	-	14,19,23	1.01	2 (14%)	16,28,35	4.25	3 (18%)

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
1	5MU	M	801	1	-	0/2/22/26	0/2/2/2
1	5MU	M	802	1	-	0/3/25/26	0/2/2/2
1	5MU	M	803	1	-	0/3/25/26	0/2/2/2
1	5MU	N	900	-	-	0/2/22/26	0/2/2/2

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	803	5MU	C6-C5	-2.29	1.34	1.40
1	N	900	5MU	C6-C5	-2.22	1.34	1.40
1	M	802	5MU	C6-C5	-2.10	1.34	1.40
1	M	801	5MU	C6-C5	-2.10	1.34	1.40
1	N	900	5MU	C4-N3	2.59	1.37	1.33

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	900	5MU	C5-C4-N3	-9.14	115.16	125.24
1	M	802	5MU	C5-C4-N3	-9.12	115.19	125.24
1	M	801	5MU	C5-C4-N3	-9.10	115.20	125.24
1	M	803	5MU	C5-C4-N3	-9.06	115.26	125.24
1	M	803	5MU	C5M-C5-C6	2.05	122.77	118.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	M	801	5MU	6	0
1	M	802	5MU	9	0
1	M	803	5MU	4	0
1	N	900	5MU	1	0

5.5 Carbohydrates

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(Å ²)	Q<0.9
1	M	0/3	-	-	-	-
1	N	0/3	-	-	-	-
2	A	114/178 (64%)	-0.03	6 (5%) 27 15	3, 19, 74, 83	0
2	B	120/178 (67%)	-0.23	2 (1%) 70 57	2, 20, 59, 65	0
2	C	114/178 (64%)	-0.15	2 (1%) 69 55	2, 18, 49, 61	0
2	D	116/178 (65%)	-0.15	3 (2%) 56 41	2, 20, 63, 80	0
All	All	464/718 (64%)	-0.14	13 (2%) 53 39	2, 19, 61, 83	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	646	GLY	4.5
2	D	645	THR	4.4
2	A	48	MET	4.1
2	D	644	ALA	3.7
2	A	2	SER	3.7

6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(Å ²)	Q<0.9
1	5MU	M	803	21/22	0.71	0.32	-	85,87,88,89	0
1	5MU	M	801	18/22	0.77	0.31	-	72,73,75,76	0
1	5MU	M	802	21/22	0.72	0.34	-	73,87,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	5MU	N	900	18/22	0.74	0.38	-	47,48,52,52	0

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.