

wwPDB X-ray Structure Validation Summary Report (i)

Sep 26, 2023 – 08:57 PM EDT

PDB ID : 6D8L

Title: Group I self-splicing intron P4-P6 domain mutant U131A (without isopropanol

soaking)

Authors : Shoffner, G.M. Deposited on : 2018-04-26

Resolution : 3.14 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 Xtriage (Phenix): 1.13

EDS : 2.35.1

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)

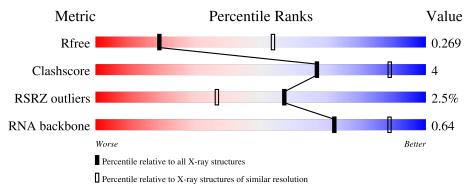
Validation Pipeline (wwPDB-VP) : 2.35.1

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 3.14 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.



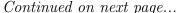
Whole archive Similar resolution Metric (#Entries)(#Entries, resolution range(Å)) \mathbf{R}_{free} 130704 1626 (3.18-3.10) Clashscore 141614 1735 (3.18-3.10) RSRZ outliers 127900 1588 (3.18-3.10) RNA backbone 3102 1000 (3.46-2.82)

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	158	65%	30%				
1	В	158	73%	22%				

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
2	MG	A	301	-	-	-	X





Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	A	305	-	-	-	X
2	MG	A	307	-	-	-	X
2	MG	A	308	-	-	-	X
2	MG	A	312	-	-	-	X
2	MG	В	305	-	-	-	X
2	MG	В	309	-	-	-	X



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6795 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 Group I self-splicing intron.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	A	158	Total 3385	C 1512	N 619	O 1096	P 158	41	0	0
1	В	158	Total 3385	C 1512	N 619	O 1096	P 158	68	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	G	A	conflict	GB 10832
A	131	A	U	engineered mutation	GB 10832
В	103	G	A	conflict	GB 10832
В	131	A	U	engineered mutation	GB 10832

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	12	Total Mg 12 12	0	0
2	В	10	Total Mg 10 10	0	0

• Molecule 3 is water.

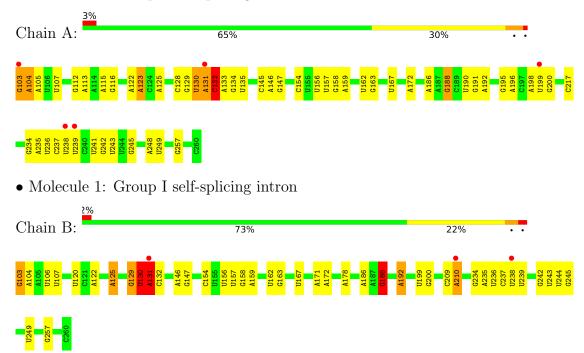
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total O 2 2	0	0
3	В	1	Total O 1 1	0	0



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: Group I self-splicing intron





4 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 21 21 21	Depositor	
Cell constants	75.48Å 132.95Å 147.54Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	67.20 - 3.14	Depositor	
Resolution (A)	67.20 - 3.14	EDS	
% Data completeness	95.8 (67.20-3.14)	Depositor	
(in resolution range)	95.9 (67.20-3.14)	EDS	
R_{merge}	(Not available)	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	2.64 (at 3.13Å)	Xtriage	
Refinement program	PHENIX 1.12_2829	Depositor	
D D.	0.250 , 0.270	Depositor	
R, R_{free}	0.249 , 0.269	DCC	
R_{free} test set	2553 reflections (10.00%)	wwPDB-VP	
Wilson B-factor (Å ²)	108.2	Xtriage	
Anisotropy	0.599	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.25, 79.2	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	0.94	EDS	
Total number of atoms	6795	wwPDB-VP	
Average B, all atoms (Å ²)	121.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.55% 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: 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	Bo	nd lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z >5	
1	A	0.31	1/3790 (0.0%)	0.84	3/5906 (0.1%)	
1	В	0.34	1/3790 (0.0%)	0.84	11/5906 (0.2%)	
All	All	0.32	$2/7580 \ (0.0\%)$	0.84	14/11812 (0.1%)	

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(ext{\AA})$
1	A	103	G	OP3-P	-10.19	1.49	1.61
1	В	103	G	OP3-P	-10.15	1.49	1.61

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
1	A	245	G	O4'-C1'-N9	8.22	114.77	108.20
1	В	129	G	P-O3'-C3'	7.37	128.55	119.70
1	A	131	A	P-O3'-C3'	7.23	128.37	119.70
1	В	131	A	P-O3'-C3'	6.69	127.73	119.70
1	В	192	A	O4'-C1'-N9	6.68	113.54	108.20

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	3385	0	1704	24	0
1	В	3385	0	1704	13	0
2	A	12	0	0	0	0
2	В	10	0	0	0	0
3	A	2	0	0	0	0
3	В	1	0	0	0	0
All	All	6795	0	3408	37	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 4.

The worst 5 of 37 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:123:A:H2	1:A:198:A:H62	1.37	0.72	
1:A:103:G:H3'	1:A:257:G:H21	1.63	0.63	
1:B:120:U:O2'	1:B:125:A:N6	2.30	0.63	
1:A:103:G:C2'	1:A:104:A:H5'	2.35	0.57	
1:A:103:G:O2'	1:A:104:A:H5'	2.06	0.55	

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein molecules in this entry.

5.3.2 Protein sidechains (i)

There are no protein molecules in this entry.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	157/158 (99%)	25 (15%)	3 (1%)
1	В	157/158 (99%)	24 (15%)	2 (1%)
All	All	314/316 (99%)	49 (15%)	5 (1%)



5 of 49 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	104	A
1	A	105	A
1	A	107	U
1	A	122	A
1	A	123	A

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	130	U
1	A	131	A
1	A	199	U
1	В	129	G
1	В	131	A

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 22 ligands modelled in this entry, 22 are 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 (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	Analysed	<RSRZ $>$	# RSRZ > 2		>2	$OWAB(\AA^2)$	Q < 0.9
1	A	158/158 (100%)	-0.23	5 (3%)	47	26	86, 118, 177, 236	4 (2%)
1	В	158/158 (100%)	-0.18	3 (1%)	66	48	80, 112, 177, 253	6 (3%)
All	All	316/316 (100%)	-0.21	8 (2%)	57	37	80, 114, 177, 253	10 (3%)

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	238	U	7.2
1	A	131	A	4.6
1	В	210	A	3.1
1	A	238	U	3.0
1	В	131	A	2.8

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 monosaccharides 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	MG	A	312	1/1	0.55	0.87	94,94,94,94	0
2	MG	A	307	1/1	0.59	0.43	110,110,110,110	0
2	MG	A	305	1/1	0.67	0.49	88,88,88,88	0
2	MG	A	306	1/1	0.67	0.23	90,90,90,90	0
2	MG	A	301	1/1	0.68	0.51	89,89,89,89	0
2	MG	В	309	1/1	0.71	0.98	81,81,81,81	0
2	MG	A	310	1/1	0.75	0.22	103,103,103,103	0
2	MG	A	308	1/1	0.77	0.94	106,106,106,106	0
2	MG	В	305	1/1	0.80	0.84	84,84,84,84	0
2	MG	A	304	1/1	0.83	0.41	91,91,91,91	0
2	MG	A	311	1/1	0.85	0.58	104,104,104,104	0
2	MG	A	309	1/1	0.87	0.09	104,104,104,104	0
2	MG	В	310	1/1	0.89	0.81	62,62,62,62	0
2	MG	В	304	1/1	0.92	0.38	94,94,94,94	0
2	MG	В	307	1/1	0.93	0.82	80,80,80,80	0
2	MG	В	303	1/1	0.93	0.36	97,97,97,97	0
2	MG	В	306	1/1	0.93	0.49	93,93,93,93	0
2	MG	В	301	1/1	0.94	0.54	88,88,88,88	0
2	MG	В	308	1/1	0.95	0.32	84,84,84,84	0
2	MG	A	302	1/1	0.98	0.35	74,74,74,74	0
2	MG	В	302	1/1	0.98	0.39	70,70,70,70	0
2	MG	A	303	1/1	0.99	0.41	100,100,100,100	0

6.5 Other polymers (i)

There are no such residues in this entry.

