

wwPDB X-ray Structure Validation Summary Report (i)

Oct 25, 2022 - 07:19 PM EDT

PDB ID	:	5SUG
Title	:	PanDDA analysis group deposition – $Aar2/RNaseH$ in complex with fragment
		P03H05 from the F2X-Universal Library
Authors	:	Barthel, T.; Wollenhaupt, J.; Lima, G.M.A.; Wahl, M.C.; Weiss, M.S.
Deposited on	:	2022-08-26
Resolution	:	1.53 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:

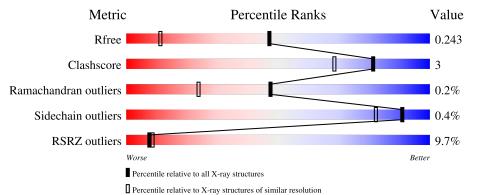
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.53 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	$\begin{array}{c} \textbf{Whole archive} \\ \textbf{(\#Entries)} \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	2556 (1.56-1.52)
Clashscore	141614	2634(1.56-1.52)
Ramachandran outliers	138981	2580 (1.56-1.52)
Sidechain outliers	138945	2577 (1.56-1.52)
RSRZ outliers	127900	2524 (1.56-1.52)

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	А	258	8%	% 8'	%			
2	В	308	90%	8%	•			

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
3	W1E	А	2101	-	-	-	Х
3	W1E	В	401	-	-	-	Х



5SUG

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9261 atoms, of which 4524 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 Pre-mRNA-splicing factor 8.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	А	237	Total 4068	C 1287	Н 2060	N 336	O 373	S 12	0	21	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	1833	GLY	-	expression tag	UNP P33334
А	1834	ALA	-	expression tag	UNP P33334
А	1835	MET	-	expression tag	UNP P33334

• Molecule 2 is a protein called A1 cistron-splicing factor AAR2.

Μ	ol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
2	2	В	300	Total 5044	C 1654	Н 2464	N 421	O 485	S 20	11	17	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	-3	GLY	-	expression tag	UNP P32357
В	-2	ALA	-	expression tag	UNP P32357
В	-1	MET	-	expression tag	UNP P32357
В	0	ALA	-	expression tag	UNP P32357
В	166	SER	LEU	conflict	UNP P32357
В	167	SER	LYS	conflict	UNP P32357
В	?	-	LEU	deletion	UNP P32357
В	?	-	GLN	deletion	UNP P32357
В	?	-	LYS	deletion	UNP P32357
В	?	-	ALA	deletion	UNP P32357
В	?	-	GLY	deletion	UNP P32357
В	?	-	SER	deletion	UNP P32357
В	?	-	LYS	deletion	UNP P32357

Continued on next page...

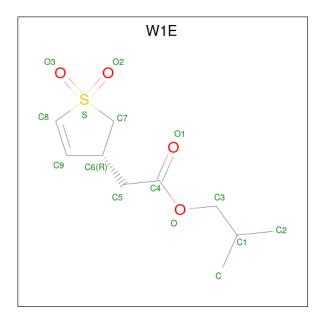


FC	ΤT	0
22	U	G

eenteenta	Contributed from proceedes page								
Chain	Residue	Modelled	Actual	Comment	Reference				
В	?	-	MET	deletion	UNP P32357				
В	?	-	GLU	deletion	UNP P32357				
В	?	-	ALA	deletion	UNP P32357				
В	?	-	LYS	deletion	UNP P32357				
В	?	-	ASN	deletion	UNP P32357				
В	?	-	GLU	deletion	UNP P32357				
В	170	SER	ASP	conflict	UNP P32357				

Continued from previous page..

• Molecule 3 is 2-methylpropyl [(3R)-1,1-dioxo-2,3-dihydro-1H-1lambda 6 -thiophen-3-yl]acet ate (three-letter code: W1E) (formula: $C_{10}H_{16}O_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total C O S 15 10 4 1	0	0
3	В	1	Total C O S 15 10 4 1	0	0

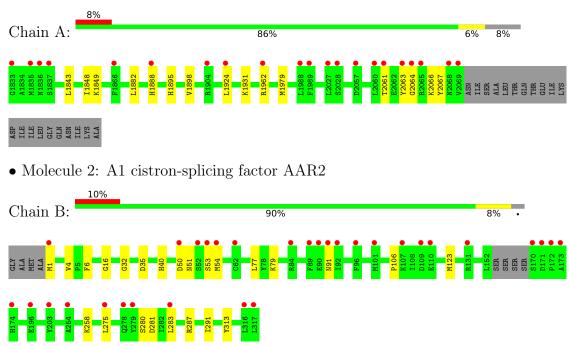
• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	60	Total O 60 60	0	0
4	В	59	Total O 59 59	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: Pre-mRNA-splicing factor 8



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	88.62Å 81.88Å 93.53Å	Depositor
a, b, c, α , β , γ	90.00° 108.49° 90.00°	Depositor
Resolution (Å)	44.35 - 1.53	Depositor
Resolution (A)	44.59 - 1.53	EDS
% Data completeness	97.6(44.35 - 1.53)	Depositor
(in resolution range)	97.7 (44.59 - 1.53)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$0.81 (at 1.52 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
D D.	0.205 , 0.236	Depositor
R, R_{free}	0.215 , 0.243	DCC
R_{free} test set	2095 reflections $(2.23%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	36.6	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.41 , 49.6	EDS
L-test for twinning ²	$ \langle L \rangle = 0.51, \langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9261	wwPDB-VP
Average B, all atoms $(Å^2)$	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.58% of the height of the origin peak. No significant pseudotranslation is detected.

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.



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: W1E

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	А	0.55	1/2149~(0.0%)	0.66	0/2911
2	В	0.51	0/2739	0.67	2/3699~(0.1%)
All	All	0.53	1/4888~(0.0%)	0.67	2/6610~(0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
1	А	1924	LEU	C-N	9.47	1.52	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	В	123[A]	MET	CG-SD-CE	5.93	109.69	100.20
2	В	123[B]	MET	CG-SD-CE	5.93	109.69	100.20

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	А	2008	2060	1974	9	0
2	В	2580	2464	2398	15	0
3	А	15	0	0	0	0

Continued on next page...



001111	Continued from pretious page								
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes			
3	В	15	0	0	0	0			
4	А	60	0	0	3	0			
4	В	59	0	0	2	0			
All	All	4737	4524	4372	24	0			

Continued from previous page...

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 3.

The worst 5 of 24 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:2063:TYR:O	4:A:2201:HOH:O	2.14	0.65
1:A:1882:LEU:HD12	1:A:1888:HIS:O	2.00	0.60
1:A:2061:THR:O	1:A:2064:GLY:N	2.34	0.60
2:B:258:LYS:HD2	2:B:258:LYS:H	1.70	0.57
2:B:1:MET:HB3	2:B:35:ASP:HA	1.90	0.53

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	Perce	ntiles
1	А	258/258~(100%)	251 (97%)	7 (3%)	0	100	100
2	В	315/308~(102%)	306~(97%)	8~(2%)	1 (0%)	41	19
All	All	573/566~(101%)	557 (97%)	15 (3%)	1 (0%)	47	24

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	В	106	PRO



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	Analysed Rotameric Out		Percentiles
1	А	237/233~(102%)	233~(98%)	4 (2%)	60 31
2	В	294/284~(104%)	294 (100%)	0	100 100
All	All	531/517~(103%)	527~(99%)	4 (1%)	91 64

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	1962	ARG
1	А	1979[A]	MET
1	А	1979[B]	MET
1	А	1979[C]	MET

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

Mol	Chain	Res	Type
2	В	70	GLN
2	В	91	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 monosaccharides 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 Type C	Chain Res	Res Link	Bond lengths			Bond angles				
IVIOI	Mol Type Cha	Chain	an res		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
3	W1E	В	401	-	$12,\!15,\!15$	2.25	3 (25%)	$10,\!21,\!21$	2.34	2 (20%)
3	W1E	А	2101	-	$12,\!15,\!15$	2.41	3 (25%)	10,21,21	2.12	2 (20%)

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
3	W1E	В	401	-	-	0/9/20/20	0/1/1/1
3	W1E	А	2101	-	-	2/9/20/20	0/1/1/1

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	А	2101	W1E	O2-S	-5.12	1.40	1.44
3	В	401	W1E	O3-S	-5.07	1.40	1.44
3	А	2101	W1E	O3-S	-4.91	1.40	1.44
3	В	401	W1E	O2-S	-3.95	1.41	1.44
3	В	401	W1E	C7-S	-3.69	1.73	1.78

The worst 5 of 6 bond length outliers are listed below:

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	В	401	W1E	O-C4-C5	6.06	121.89	111.14
3	А	2101	W1E	O-C4-C5	5.64	121.14	111.14
3	В	401	W1E	O-C4-O1	-3.21	115.50	123.59
3	А	2101	W1E	O-C4-O1	-3.06	115.86	123.59

There are no chirality outliers.



Mol	Chain	Res	Type	Atoms
3	А	2101	W1E	C-C1-C3-O
3	А	2101	W1E	C2-C1-C3-O

All (2) torsion outliers are listed below:

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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	237/258~(91%)	0.76	21 (8%) 9 11	33, 42, 75, 94	0
2	В	300/308~(97%)	0.89	31 (10%) 6 7	33, 44, 78, 100	0
All	All	537/566~(94%)	0.83	52 (9%) 7 9	33, 43, 76, 100	0

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	1989	PHE	7.8
1	А	2069	VAL	7.6
2	В	1	MET	7.5
2	В	173	ALA	6.9
2	В	92	ILE	6.7

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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
3	W1E	В	401	15/15	0.37	0.67	20,20,20,20	15
3	W1E	А	2101	15/15	0.57	0.51	20,20,20,20	15

6.5 Other polymers (i)

There are no such residues in this entry.

