

wwPDB X-ray Structure Validation Summary Report (i)

Sep 5, 2023 – 02:05 PM EDT

PDB ID : 3UJM

Title : Crystal structure of the NTF2-like domain of the Drosophila melanogaster

Rasputin protein

Authors: Vognsen, T.; Kristensen, O.

Deposited on : 2011-11-08

Resolution : 2.74 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:

Mol Probity : 4.02b-467

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.35

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

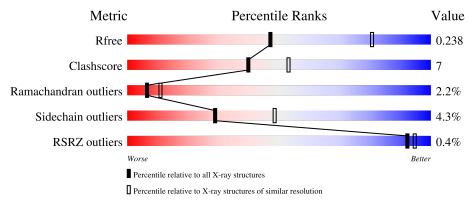
Validation Pipeline (wwPDB-VP) : 2.35

1 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 2.74 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	Similar resolution $(\# \text{Entries, resolution range}(\text{\AA}))$
R_{free}	130704	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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	120	73%	21%	• •
1	В	120	79%	16%	



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1991 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 Rasputin.

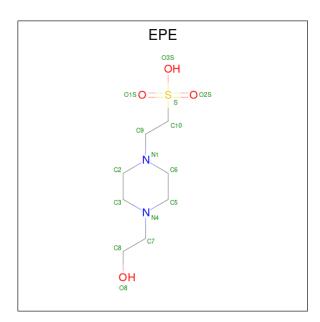
\mathbf{Mol}	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	117	Total 967	C 607		O 175	S	0	1	0
			907	607	102	170	0			
1	B	117	Total	С	N	O	\mathbf{S}	0	0	0
1	D	111	960	602	181	174	3	0		U

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	GLY	-	expression tag	UNP Q9NH72
A	12	SER	-	expression tag	UNP Q9NH72
A	13	HIS	-	expression tag	UNP Q9NH72
A	14	MET	-	expression tag	UNP Q9NH72
В	11	GLY	-	expression tag	UNP Q9NH72
В	12	SER	-	expression tag	UNP Q9NH72
В	13	HIS	-	expression tag	UNP Q9NH72
В	14	MET	-	expression tag	UNP Q9NH72

• Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf			
2	Λ	1	Total	С	N	О	S	0	0	
2	A	1	15	8	2	4	1	0	0	
9	D	1	Total	С	N	О	S	0	0	
2	Б	1	15	8	2	4	1	0	0	

• Molecule 3 is water.

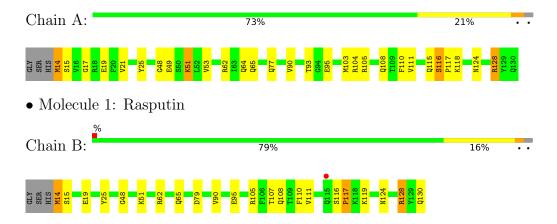
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	20	Total O 20 20	0	0
3	В	14	Total O 14 14	0	0



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: Rasputin





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	39.20Å 80.38Å 39.20Å	Danasitan
a, b, c, α , β , γ	90.00° 92.60° 90.00°	Depositor
Resolution (Å)	39.16 - 2.74	Depositor
Resolution (A)	39.16 - 2.74	EDS
% Data completeness	97.1 (39.16-2.74)	Depositor
(in resolution range)	97.1 (39.16-2.74)	EDS
R_{merge}	0.05	Depositor
$\frac{R_{sym}}{\langle I/\sigma(I)\rangle^{-1}}$	0.05	Depositor
$< I/\sigma(I) > 1$	$2.60 \; (at \; 2.73 \text{Å})$	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.197 , 0.242	Depositor
10, 10 free	0.198 , 0.238	DCC
R_{free} test set	290 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å ²)	53.5	Xtriage
Anisotropy	0.536	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	$0.35 \; , \; 55.2$	EDS
L-test for twinning ²	$< L > = 0.50, < L^2> = 0.34$	Xtriage
	0.049 for l,k,-h	
Estimated twinning fraction	0.056 for h,-k,-l	Xtriage
	0.478 for l,-k,h	
F_o, F_c correlation	0.95	EDS
Total number of atoms	1991	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 8.96% 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: EPE

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	Mol Chain		lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.24	0/990	0.41	0/1336	
1	В	0.23	0/982	0.39	0/1325	
All	All	0.23	0/1972	0.40	0/2661	

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 maintenain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	SER	Peptide

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	967	0	935	17	0
1	В	960	0	929	11	0
2	A	15	0	17	1	0
2	В	15	0	17	1	0
3	A	20	0	0	1	0
3	В	14	0	0	0	0
All	All	1991	0	1898	28	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 7.

The worst 5 of 28 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:A:25:TYR:OH	1:A:108:GLN:NE2	2.18	0.76
1:B:95:GLU:HG2	1:B:105:ARG:HD2	1.80	0.62
1:A:104:ARG:NH2	3:A:302:HOH:O	2.37	0.57
1:B:25:TYR:OH	1:B:108:GLN:OE1	2.14	0.55
1:A:95:GLU:HG2	1:A:105:ARG:HD2	1.90	0.54

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	Percer	ntiles
1	A	116/120 (97%)	107 (92%)	6 (5%)	3 (3%)	5	8
1	В	115/120~(96%)	103 (90%)	10 (9%)	2 (2%)	9	16
All	All	231/240 (96%)	210 (91%)	16 (7%)	5 (2%)	6	11

All (5) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	117	PRO
1	A	116	SER
1	В	116	SER
1	В	117	PRO
1	A	49	GLU

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	A	105/106 (99%)	100 (95%)	5 (5%)	25 44		
1	В	104/106 (98%)	100 (96%)	4 (4%)	33 54		
All	All	209/212 (99%)	200 (96%)	9 (4%)	29 48		

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	107	THR
1	В	128	ARG
1	A	115	GLN
1	A	128	ARG
1	В	14	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	В	56	GLN
1	В	65	GLN
1	В	130	GLN
1	A	91	GLN
1	A	108	GLN

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).

Mal	Type Chain		Chain Res	es Link	Bo	Bond lengths			Bond angles		
Mol T	туре	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
2	EPE	A	201	-	15,15,15	0.82	1 (6%)	18,20,20	1.83	6 (33%)	
2	EPE	В	201	-	15,15,15	0.84	1 (6%)	18,20,20	1.98	6 (33%)	

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.

N	Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
	2	EPE	A	201	-	-	2/9/19/19	0/1/1/1
	2	EPE	В	201	-	-	3/9/19/19	0/1/1/1

All (2) bond length outliers are listed below:

M	ol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(\text{\AA})$
6	2	В	201	EPE	C10-S	2.85	1.81	1.77
6	2	A	201	EPE	C10-S	2.78	1.81	1.77

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



Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
2	A	201	EPE	C5-N4-C3	4.53	119.04	108.83
2	В	201	EPE	C5-N4-C3	4.42	118.77	108.83
2	В	201	EPE	C7-N4-C5	3.92	121.25	111.23
2	В	201	EPE	C7-N4-C3	3.30	119.67	111.23
2	A	201	EPE	C7-N4-C5	3.14	119.26	111.23

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	EPE	C8-C7-N4-C5
2	В	201	EPE	C8-C7-N4-C5
2	A	201	EPE	N4-C7-C8-O8
2	В	201	EPE	N4-C7-C8-O8
2	В	201	EPE	C10-C9-N1-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	EPE	1	0
2	В	201	EPE	1	0

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	$\langle { m RSRZ} \rangle$	$\#\mathrm{RSRZ}{>}2$	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9
1	A	117/120 (97%)	-0.00	0 100 100	30, 59, 98, 112	0
1	В	117/120 (97%)	-0.03	1 (0%) 84 88	29, 58, 94, 113	0
All	All	234/240 (97%)	-0.02	1 (0%) 92 95	29, 59, 97, 113	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	115	GLN	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 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	EPE	В	201	15/15	0.85	0.28	80,90,95,98	0
2	EPE	A	201	15/15	0.88	0.23	75,84,91,91	0



6.5 Other polymers (i)

There are no such residues in this entry.

