wwPDB X-ray Structure Validation Summary Report (i)

Oct 11, 2023 – 07:28 AM EDT

PDB ID	:	6WW6
Title	:	Crystal structure of EutV bound to RNA
Authors	:	Ataide, S.F.; Walshe, J.L.
Deposited on	:	2020-05-07
Resolution	:	3.80 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:

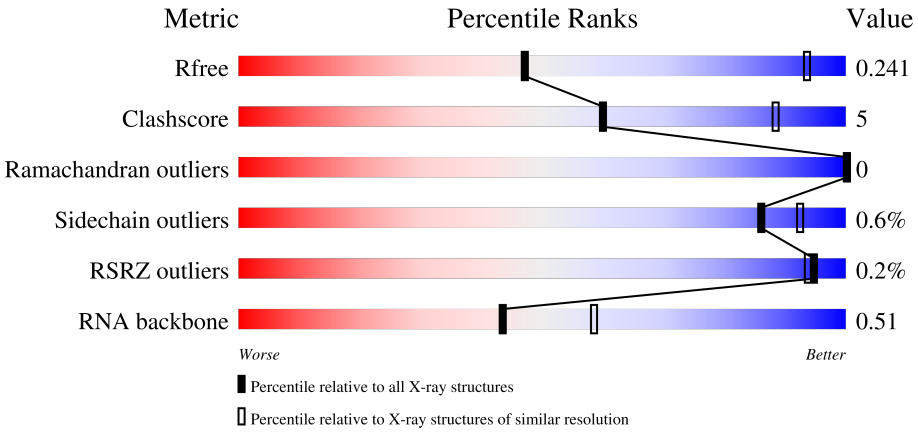
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.80 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}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)
RNA backbone	3102	1036 (4.60-3.00)

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	192	95%
1	B	192	92% 8%
2	C	54	2% 26% 6% 67%
2	D	54	19% 13% 69%

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Mol	Chain	Length	Quality of chain
2	E	54	
2	F	54	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4480 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 Response regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	190	Total	C	N	O	S	0	0	0
			1486	938	247	292	9			
1	B	192	Total	C	N	O	S	0	0	0
			1502	946	249	298	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP A0A1Q1FU69
A	0	ASN	-	expression tag	UNP A0A1Q1FU69
B	-1	SER	-	expression tag	UNP A0A1Q1FU69
B	0	ASN	-	expression tag	UNP A0A1Q1FU69

- Molecule 2 is a RNA chain called eutP P2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	17	Total	C	N	O	P	0	17	0
			367	164	72	114	17			
2	F	17	Total	C	N	O	P	0	17	0
			364	163	67	117	17			
2	D	17	Total	C	N	O	P	0	17	0
			364	163	67	117	17			
2	C	18	Total	C	N	O	P	0	18	0
			389	174	77	120	18			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	G	-	expression tag	GB 295112306
E	-1	G	-	expression tag	GB 295112306
F	-2	G	-	expression tag	GB 295112306
F	-1	G	-	expression tag	GB 295112306

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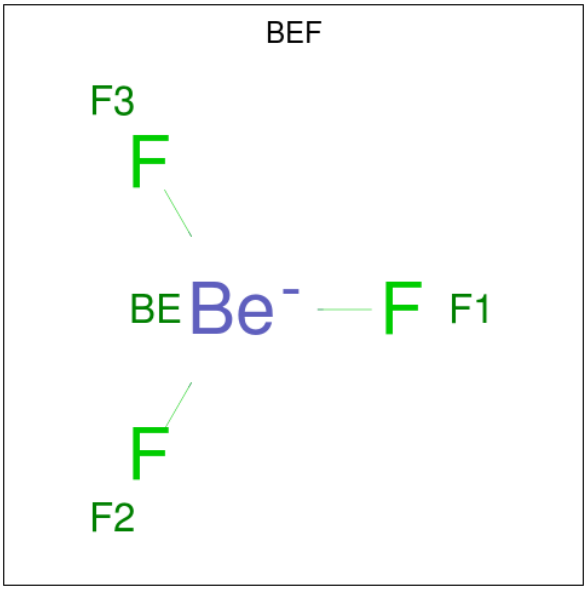
Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	G	-	expression tag	GB 295112306
D	-1	G	-	expression tag	GB 295112306
C	-2	G	-	expression tag	GB 295112306
C	-1	G	-	expression tag	GB 295112306

- Molecule 3 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3).



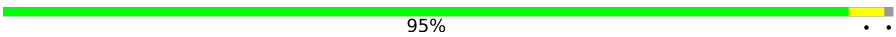
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Be	F	0	0
			4	1	3		
3	B	1	Total	Be	F	0	0
			4	1	3		

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: Response regulator

Chain A:



• Molecule 1: Response regulator

Chain B:

• Molecule 2: eutP P2

Chain E:

• Molecule 2: eutP P2

Chain F:

• Molecule 2: eutP P2

Chain D:

• Molecule 2: eutP P2

Chain C:


G
G
G
A
A
U
C
A
G
A
A
A
C
A
C
A
A
U
G
G
C
G
U
G
U
U
U
U
A
A
A
C
A
A30
A39
G40
G41
A42
G43
A47
A
G
A
C

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41 3 2	Depositor
Cell constants a, b, c, α, β, γ	258.48Å 258.48Å 258.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.19 – 3.80 47.19 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (47.19-3.80) 99.4 (47.19-3.80)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 3.77Å)	Xtriage
Refinement program	PHENIX dev_3758	Depositor
R, R_{free}	0.233 , 0.241 0.233 , 0.241	Depositor DCC
R_{free} test set	729 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	128.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 97.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4480	wwPDB-VP
Average B, all atoms (Å^2)	158.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical 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.

5 Model quality

5.1 Standard geometry

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

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	$\#\|Z\| > 5$
1	A	0.38	0/1497	0.64	0/2010
1	B	0.41	0/1513	0.65	0/2030
2	C	0.24	0/436	0.75	0/678
2	D	0.19	0/407	0.74	0/632
2	E	0.19	0/411	0.71	0/639
2	F	0.23	0/407	0.78	0/632
All	All	0.34	0/4671	0.68	0/6621

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1486	0	1563	10	0
1	B	1502	0	1574	11	1
2	C	389	0	163	2	0
2	D	364	0	150	3	0
2	E	367	0	152	6	0
2	F	364	0	156	5	0
3	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	4	0	0	1	0
All	All	4480	0	3758	30	1

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 5.

The worst 5 of 30 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:F:18[B]:C:O2'	2:F:19[B]:G:OP2	1.91	0.88
1:B:177:ARG:HB2	1:B:177:ARG:NH2	1.92	0.84
1:A:172:MET:HG2	2:E:43[B]:G:N3	1.96	0.80
2:E:32[B]:U:O4	2:E:47[B]:A:N6	2.16	0.79
1:A:164:TYR:OH	2:E:39[B]:A:OP1	2.07	0.63

All (1) 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:B:64:LYS:NZ	1:B:155:GLU:OE2[5_555]	1.95	0.25

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	A	188/192 (98%)	183 (97%)	5 (3%)	0	100	100
1	B	190/192 (99%)	186 (98%)	4 (2%)	0	100	100
All	All	378/384 (98%)	369 (98%)	9 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	167/169 (99%)	167 (100%)	0	100 100
1	B	169/169 (100%)	167 (99%)	2 (1%)	71 84
All	All	336/338 (99%)	334 (99%)	2 (1%)	86 92

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	81	LEU
1	B	101	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	17/54 (31%)	3 (17%)	1 (5%)
2	D	16/54 (29%)	2 (12%)	0
2	E	16/54 (29%)	2 (12%)	0
2	F	16/54 (29%)	3 (18%)	0
All	All	65/216 (30%)	10 (15%)	1 (1%)

5 of 10 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	E	40[B]	G
2	E	41[B]	G
2	F	16[B]	G
2	F	17[B]	G
2	F	19[B]	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	C	42[A]	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)

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	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	BEF	B	201	1	0,3,3	-	-	-		
3	BEF	A	201	1	0,3,3	-	-	-		

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	201	BEF	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

6.1 Protein, DNA and RNA chains

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	OWAB(Å^2)	Q<0.9
1	A	190/192 (98%)	-0.20	0 100 100	83, 124, 180, 225	0
1	B	192/192 (100%)	-0.27	0 100 100	86, 125, 164, 203	0
2	C	18/54 (33%)	0.43	1 (5%) 24 20	158, 195, 296, 303	17 (94%)
2	D	17/54 (31%)	-0.10	0 100 100	165, 200, 289, 300	17 (100%)
2	E	17/54 (31%)	-0.09	0 100 100	165, 200, 296, 304	17 (100%)
2	F	17/54 (31%)	0.33	0 100 100	155, 191, 287, 302	17 (100%)
All	All	451/600 (75%)	-0.18	1 (0%) 95 94	83, 130, 225, 304	68 (15%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	30[A]	A	2.6

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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	B-factors(Å^2)	Q<0.9
3	BEF	A	201	4/4	0.89	0.14	177,179,185,190	0
3	BEF	B	201	4/4	0.95	0.10	134,136,142,147	0

6.5 Other polymers (i)

There are no such residues in this entry.