Full wwPDB X-ray Structure Validation Report ⓘ

Jan 10, 2017 – 09:18 PM EST

PDB ID	:	5HBZ
Title	:	Structure of EAV NSP11 K170A mutant at 3.10A
Authors	:	Zhang, M.F.; Chen, Z.Z.
Deposited on	:	2016-01-04
Resolution	:	3.10 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
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)	:	rb-20028442

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 3.10 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.
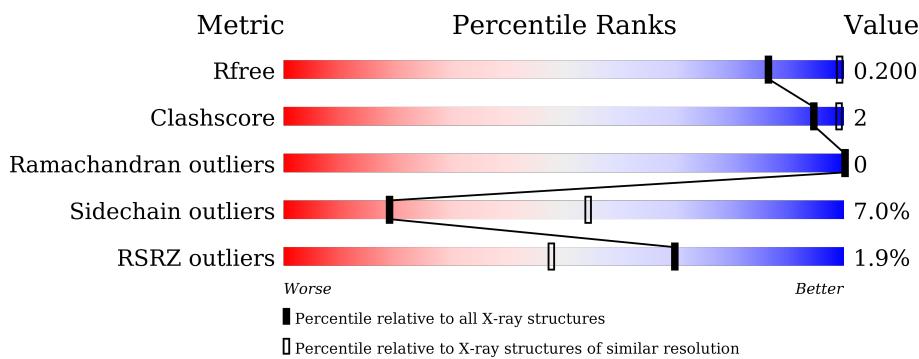
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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 <=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	221	
1	B	221	
1	C	221	
1	D	221	
1	E	221	
1	F	221	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 9946 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 Non-structural protein 11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total 1694	C 1090	N 281	O 312	S 11	0	0	0
1	B	219	Total 1675	C 1078	N 277	O 309	S 11	0	0	0
1	C	219	Total 1686	C 1084	N 279	O 312	S 11	0	0	0
1	D	209	Total 1626	C 1051	N 267	O 297	S 11	0	0	0
1	E	209	Total 1625	C 1050	N 265	O 299	S 11	0	0	0
1	F	211	Total 1640	C 1058	N 267	O 304	S 11	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLU	-	expression tag	UNP P19811
A	0	SER	-	expression tag	UNP P19811
A	170	ALA	LYS	engineered mutation	UNP P19811
B	-1	GLU	-	expression tag	UNP P19811
B	0	SER	-	expression tag	UNP P19811
B	170	ALA	LYS	engineered mutation	UNP P19811
C	-1	GLU	-	expression tag	UNP P19811
C	0	SER	-	expression tag	UNP P19811
C	170	ALA	LYS	engineered mutation	UNP P19811
D	-1	GLU	-	expression tag	UNP P19811
D	0	SER	-	expression tag	UNP P19811
D	170	ALA	LYS	engineered mutation	UNP P19811
E	-1	GLU	-	expression tag	UNP P19811
E	0	SER	-	expression tag	UNP P19811
E	170	ALA	LYS	engineered mutation	UNP P19811
F	-1	GLU	-	expression tag	UNP P19811
F	0	SER	-	expression tag	UNP P19811

Continued on next page...

Continued from previous page...

| Chain	Residue	Modelled	Actual	Comment	Reference
F	170	ALA	LYS	engineered mutation	UNP P19811

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 errors 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: Non-structural protein 11
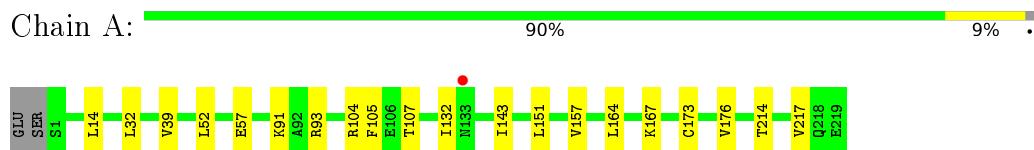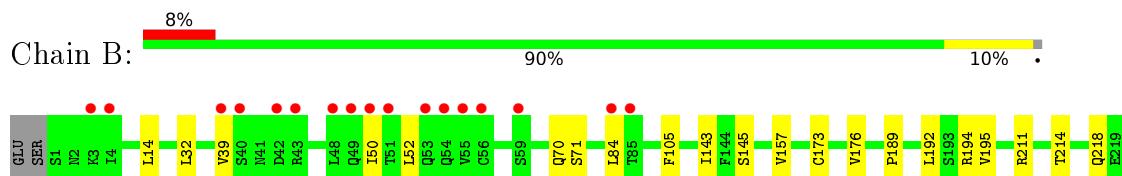
Chain A:

- Molecule 1: Non-structural protein 11

Chain B:

- Molecule 1: Non-structural protein 11

Chain C:

- Molecule 1: Non-structural protein 11

Chain D:

- Molecule 1: Non-structural protein 11

Chain E:

- Molecule 1: Non-structural protein 11

Chain F:
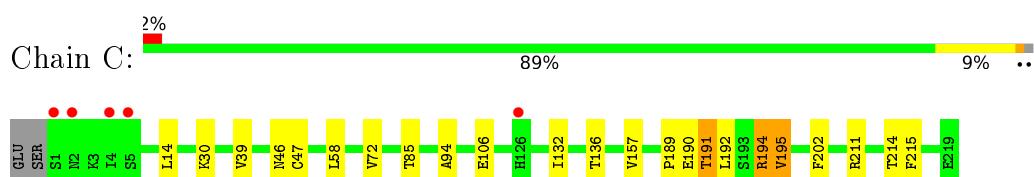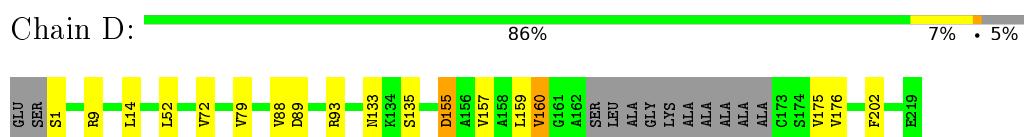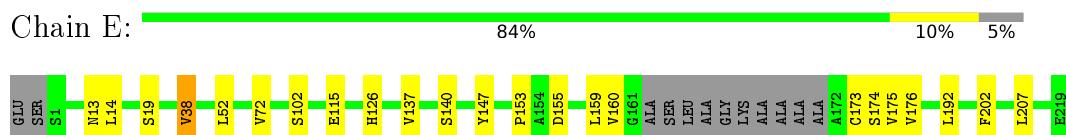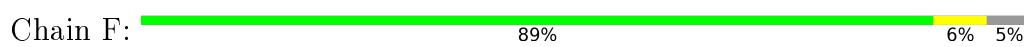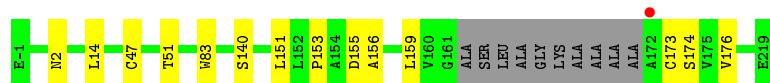
4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	248.27Å 248.27Å 226.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.10 48.55 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.7 (50.00-3.10) 96.7 (48.55-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.00 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.195 , 0.199 0.198 , 0.200	Depositor DCC
R_{free} test set	2361 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	75.1	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 33.8	EDS
L-test for twinning[2]	$<\|L\|> = 0.50$, $<L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9946	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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 (i)

5.1 Standard geometry (i)

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	0.45	0/1746	0.68	0/2385
1	B	0.44	0/1726	0.66	0/2362
1	C	0.46	0/1738	0.66	0/2377
1	D	0.48	0/1677	0.71	0/2289
1	E	0.46	0/1676	0.69	0/2289
1	F	0.47	0/1691	0.69	1/2309 (0.0%)
All	All	0.46	0/10254	0.68	1/14011 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	156	ALA	N-CA-C	-5.27	96.76	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	145	SER	Peptide
1	D	155	ASP	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	1694	0	1640	4	0
1	B	1675	0	1604	2	0
1	C	1686	0	1618	11	0
1	D	1626	0	1557	7	0
1	E	1625	0	1556	11	0
1	F	1640	0	1567	2	0
All	All	9946	0	9542	34	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 2.

All (34) 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:D:9:ARG:HD3	1:D:160:VAL:HG21	1.50	0.94
1:C:189:PRO:HD2	1:C:211:ARG:HG3	1.56	0.88
1:E:13:ASN:HD21	1:E:160:VAL:HG11	1.62	0.65
1:D:9:ARG:CD	1:D:160:VAL:HG11	2.28	0.64
1:D:159:LEU:O	1:D:160:VAL:HG13	2.02	0.59
1:C:195:VAL:HG22	1:E:137:VAL:HG21	1.84	0.59
1:D:14:LEU:HD13	1:D:202:PHE:CG	2.40	0.57
1:C:189:PRO:HG2	1:C:191:THR:O	2.05	0.57
1:D:9:ARG:HD2	1:D:160:VAL:HG11	1.88	0.55
1:E:13:ASN:HD21	1:E:160:VAL:CG1	2.20	0.54
1:E:14:LEU:HD13	1:E:202:PHE:CG	2.43	0.53
1:C:214:THR:HG22	1:C:215:PHE:N	2.24	0.53
1:C:58:LEU:HD22	1:C:94:ALA:HB2	1.91	0.52
1:C:214:THR:OG1	1:E:192:LEU:HD13	2.10	0.51
1:A:132:ILE:HD11	1:A:164:LEU:HB2	1.93	0.50
1:C:195:VAL:CG2	1:E:137:VAL:HG21	2.41	0.50
1:F:140:SER:HA	1:F:174:SER:O	2.13	0.48
1:D:9:ARG:HD3	1:D:160:VAL:CG2	2.34	0.47
1:F:153:PRO:C	1:F:155:ASP:H	2.18	0.47
1:E:19:SER:HA	1:E:38:VAL:HG22	1.97	0.47
1:A:104:ARG:HA	1:A:107:THR:HG22	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:PRO:HD2	1:B:211:ARG:HG3	1.99	0.45
1:C:14:LEU:HD11	1:C:202:PHE:CE1	2.52	0.44
1:C:72:VAL:HG21	1:C:106:GLU:HG3	1.99	0.44
1:C:194:ARG:HG3	1:C:195:VAL:N	2.32	0.44
1:A:105:PHE:CD2	1:A:143:ILE:HD12	2.53	0.43
1:B:105:PHE:CD2	1:B:143:ILE:HD12	2.54	0.43
1:A:132:ILE:HD12	1:A:164:LEU:HD22	1.99	0.43
1:D:9:ARG:CD	1:D:160:VAL:HG21	2.35	0.42
1:E:140:SER:HA	1:E:174:SER:O	2.19	0.42
1:E:159:LEU:O	1:E:160:VAL:HG22	2.19	0.42
1:E:153:PRO:C	1:E:155:ASP:H	2.23	0.41
1:E:126:HIS:HE2	1:E:147:TYR:HH	1.68	0.41
1:C:214:THR:HG22	1:C:215:PHE:H	1.86	0.41

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	
1	A	217/221 (98%)	209 (96%)	8 (4%)	0	100	100
1	B	217/221 (98%)	207 (95%)	10 (5%)	0	100	100
1	C	217/221 (98%)	207 (95%)	10 (5%)	0	100	100
1	D	205/221 (93%)	188 (92%)	17 (8%)	0	100	100
1	E	205/221 (93%)	191 (93%)	14 (7%)	0	100	100
1	F	207/221 (94%)	191 (92%)	16 (8%)	0	100	100
All	All	1268/1326 (96%)	1193 (94%)	75 (6%)	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	182/186 (98%)	168 (92%)	14 (8%)	16	50
1	B	178/186 (96%)	162 (91%)	16 (9%)	12	41
1	C	180/186 (97%)	167 (93%)	13 (7%)	18	53
1	D	175/186 (94%)	161 (92%)	14 (8%)	15	48
1	E	175/186 (94%)	166 (95%)	9 (5%)	29	66
1	F	177/186 (95%)	168 (95%)	9 (5%)	29	66
All	All	1067/1116 (96%)	992 (93%)	75 (7%)	19	54

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	32	LEU
1	A	39	VAL
1	A	52	LEU
1	A	57	GLU
1	A	91	LYS
1	A	93	ARG
1	A	151	LEU
1	A	157	VAL
1	A	167	LYS
1	A	173	CYS
1	A	176	VAL
1	A	214	THR
1	A	217	VAL
1	B	14	LEU
1	B	32	LEU
1	B	39	VAL
1	B	50	ILE
1	B	52	LEU
1	B	70	GLN
1	B	71	SER
1	B	84	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	157	VAL
1	B	173	CYS
1	B	176	VAL
1	B	192	LEU
1	B	194	ARG
1	B	195	VAL
1	B	214	THR
1	B	218	GLN
1	C	30	LYS
1	C	39	VAL
1	C	46	ASN
1	C	47	CYS
1	C	85	THR
1	C	132	ILE
1	C	136	THR
1	C	157	VAL
1	C	190	GLU
1	C	191	THR
1	C	192	LEU
1	C	194	ARG
1	C	195	VAL
1	D	1	SER
1	D	52	LEU
1	D	72	VAL
1	D	79	VAL
1	D	88	VAL
1	D	89	ASP
1	D	93	ARG
1	D	133	ASN
1	D	135	SER
1	D	155	ASP
1	D	157	VAL
1	D	160	VAL
1	D	175	VAL
1	D	176	VAL
1	E	38	VAL
1	E	52	LEU
1	E	72	VAL
1	E	102	SER
1	E	115	GLU
1	E	173	CYS
1	E	175	VAL

Continued on next page...

Full wwPDB X-ray Structure Validation Report

Continued from previous page...

Mol	Chain	Res	Type
1	E	176	VAL
1	E	207	LEU
1	F	2	ASN
1	F	14	LEU
1	F	47	CYS
1	F	51	THR
1	F	83	TRP
1	F	151	LEU
1	F	159	LEU
1	F	173	CYS
1	F	176	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	13	ASN
1	F	2	ASN
1	F	218	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 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	A	219/221 (99%)	0.10	1 (0%)	91	83	50, 65, 89, 121	0
1	B	219/221 (99%)	0.46	17 (7%)	16	5	57, 83, 111, 124	0
1	C	219/221 (99%)	0.21	5 (2%)	64	40	54, 74, 103, 117	0
1	D	209/221 (94%)	0.04	0	100	100	50, 65, 90, 117	0
1	E	209/221 (94%)	0.05	0	100	100	48, 70, 103, 156	0
1	F	211/221 (95%)	0.18	1 (0%)	91	83	45, 68, 104, 148	0
All	All	1286/1326 (96%)	0.17	24 (1%)	70	48	45, 71, 104, 156	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	40	SER	4.2
1	B	42	ASP	3.3
1	B	55	VAL	3.0
1	B	4	ILE	3.0
1	C	1	SER	2.9
1	B	53	GLN	2.8
1	B	43	ARG	2.8
1	B	51	THR	2.8
1	B	85	THR	2.7
1	B	49	GLN	2.7
1	C	5	SER	2.7
1	B	50	ILE	2.6
1	B	39	VAL	2.6
1	B	59	SER	2.6
1	B	3	LYS	2.4
1	B	56	CYS	2.4
1	F	172	ALA	2.3
1	C	126	HIS	2.3
1	C	2	ASN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	48	LEU	2.2
1	A	133	ASN	2.2
1	B	84	LEU	2.1
1	C	4	ILE	2.1
1	B	54	GLN	2.0

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 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.