



wwPDB X-ray Structure Validation Summary Report

Aug 17, 2022 – 04:15 PM EDT

PDB ID : 3WTW
Title : Crystal structure of the complex comprised of ETS1(K167A), RUNX1, CBF-BETA, and the tcralpha gene enhancer DNA
Authors : Shiina, M.; Hamada, K.; Ogata, K.
Deposited on : 2014-04-21
Resolution : 2.90 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  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](#) ) were used in the production of this report:

MolProbity : 4.02b-467
Xtrriage (Phenix) : 1.13
EDS : 2.29
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) : 2.29

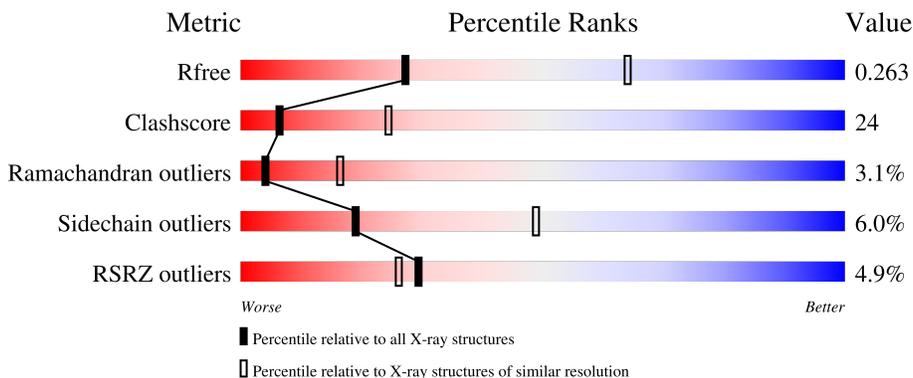
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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.



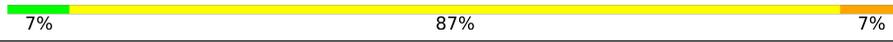
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 $\leq 5\%$. 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	204	
1	F	204	
2	B	142	
2	G	142	
3	C	166	

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Mol	Chain	Length	Quality of chain
3	H	166	 <p>19% 21% 33% 7% 39%</p>
4	D	15	 <p>20% 80%</p>
4	I	15	 <p>7% 87% 7%</p>
5	E	15	 <p>87% 13%</p>
5	J	15	 <p>93% 7%</p>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7014 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 Runt-related transcription factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	118	910	571	168	167	4	0	0	0
1	F	119	921	577	172	168	4	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	94	LYS	LEU	engineered mutation	UNP Q03347
A	167	ALA	LYS	engineered mutation	UNP Q03347
F	94	LYS	LEU	engineered mutation	UNP Q03347
F	167	ALA	LYS	engineered mutation	UNP Q03347

- Molecule 2 is a protein called Core-binding factor subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	130	1071	671	195	199	6	0	0	0
2	G	129	1062	666	193	197	6	0	0	0

- Molecule 3 is a protein called Protein C-ets-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	118	967	627	165	171	4	0	0	0
3	H	101	853	553	147	149	4	0	0	0

- Molecule 4 is a DNA chain called DNA (5'-D(*GP*AP*AP*GP*CP*CP*AP*CP*AP*TP*CP*CP*TP*CP*T)-3').

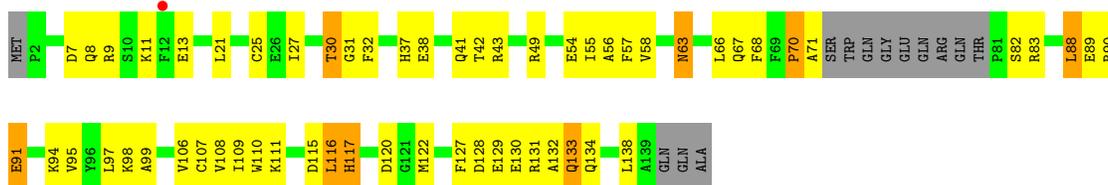
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	15	Total	C	N	O	P	0	0	0
			299	144	54	87	14			
4	I	15	Total	C	N	O	P	0	0	0
			299	144	54	87	14			

- Molecule 5 is a DNA chain called DNA (5'-D(*AP*GP*AP*GP*GP*AP*TP*GP*TP*GP*GP*CP*TP*TP*C)-3').

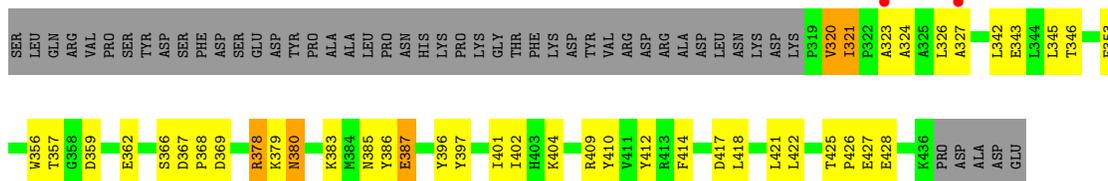
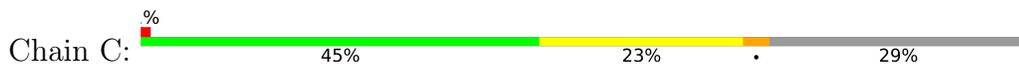
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	15	Total	C	N	O	P	0	0	0
			310	148	59	89	14			
5	J	15	Total	C	N	O	P	0	0	0
			310	148	59	89	14			

- Molecule 6 is water.

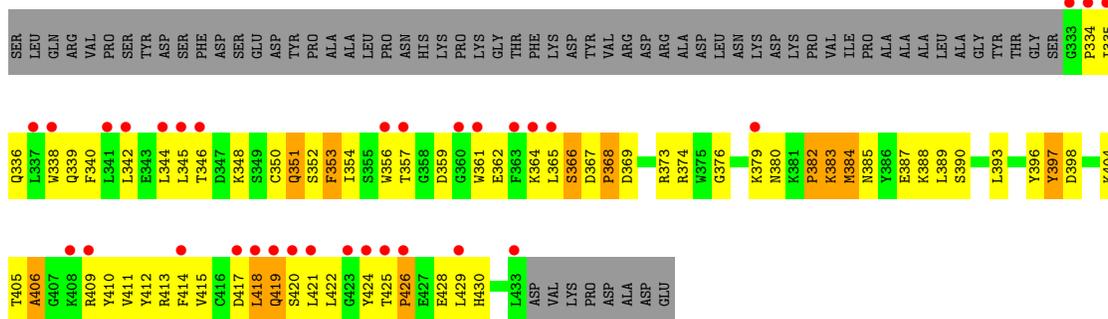
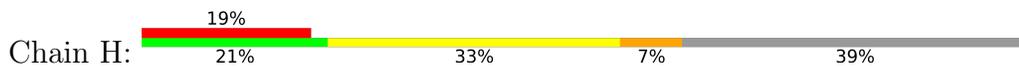
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	O	0	0
			1	1		
6	B	1	Total	O	0	0
			1	1		
6	C	3	Total	O	0	0
			3	3		
6	F	5	Total	O	0	0
			5	5		
6	G	1	Total	O	0	0
			1	1		
6	E	1	Total	O	0	0
			1	1		



• Molecule 3: Protein C-ets-1



• Molecule 3: Protein C-ets-1



• Molecule 4: DNA (5'-D(*GP*AP*AP*GP*CP*CP*AP*CP*AP*TP*CP*CP*TP*CP*T)-3')



• Molecule 4: DNA (5'-D(*GP*AP*AP*GP*CP*CP*AP*CP*AP*TP*CP*CP*TP*CP*T)-3')



- Molecule 5: DNA (5'-D(*AP*GP*AP*GP*GP*AP*TP*GP*TP*GP*GP*CP*TP*TP*C)-3')

Chain E:  87% 13%



- Molecule 5: DNA (5'-D(*AP*GP*AP*GP*GP*AP*TP*GP*TP*GP*GP*CP*TP*TP*C)-3')

Chain J:  93% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.50Å 100.61Å 194.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.36 – 2.90 42.36 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.9 (42.36-2.90) 98.0 (42.36-2.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.60 (at 2.90Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.219 , 0.264 0.218 , 0.263	Depositor DCC
R_{free} test set	3414 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å ²)	77.0	Xtrriage
Anisotropy	0.301	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 56.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7014	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

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	0.58	1/929 (0.1%)	0.71	0/1264
1	F	0.62	0/940	0.79	0/1278
2	B	0.44	0/1093	0.57	0/1466
2	G	0.50	0/1084	0.62	0/1454
3	C	0.57	0/994	0.67	0/1342
3	H	0.42	0/877	0.52	0/1181
4	D	0.69	0/334	0.90	0/512
4	I	0.73	0/334	0.92	0/512
5	E	0.71	0/348	0.81	0/537
5	J	0.72	0/348	0.84	0/537
All	All	0.57	1/7281 (0.0%)	0.70	0/10083

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
4	D	0	3
4	I	0	2
5	E	0	1
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	81	CYS	CB-SG	-5.17	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	4	DG	Sidechain
4	D	5	DC	Sidechain
4	D	6	DC	Sidechain
5	E	13	DT	Sidechain
4	I	4	DG	Sidechain

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	910	0	914	34	0
1	F	921	0	927	37	0
2	B	1071	0	1034	65	0
2	G	1062	0	1026	51	0
3	C	967	0	966	34	0
3	H	853	0	847	81	0
4	D	299	0	170	14	0
4	I	299	0	170	17	0
5	E	310	0	171	1	0
5	J	310	0	171	1	0
6	A	1	0	0	0	0
6	B	1	0	0	1	0
6	C	3	0	0	0	0
6	E	1	0	0	0	0
6	F	5	0	0	1	0
6	G	1	0	0	0	0
All	All	7014	0	6396	321	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 24.

The worst 5 of 321 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)
3:C:385:ASN:HD21	3:C:387:GLU:HB2	1.22	1.01
1:A:82:ASN:HD21	1:A:118:ARG:HH11	1.04	0.89
2:B:8:GLN:HE21	2:B:107:CYS:H	1.16	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:THR:H	2:B:104:ASN:HD21	1.20	0.87
1:A:109:ASN:HD21	1:A:111:GLU:HB2	1.39	0.86

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	116/204 (57%)	108 (93%)	6 (5%)	2 (2%)	9 31
1	F	117/204 (57%)	109 (93%)	7 (6%)	1 (1%)	17 48
2	B	126/142 (89%)	99 (79%)	24 (19%)	3 (2%)	6 22
2	G	125/142 (88%)	107 (86%)	13 (10%)	5 (4%)	3 11
3	C	116/166 (70%)	109 (94%)	6 (5%)	1 (1%)	17 48
3	H	99/166 (60%)	68 (69%)	21 (21%)	10 (10%)	0 1
All	All	699/1024 (68%)	600 (86%)	77 (11%)	22 (3%)	4 16

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	320	VAL
3	H	366	SER
3	H	382	PRO
2	B	15	GLU
2	B	116	LEU

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	99/178 (56%)	92 (93%)	7 (7%)	14	40
1	F	100/178 (56%)	94 (94%)	6 (6%)	19	49
2	B	113/123 (92%)	109 (96%)	4 (4%)	36	70
2	G	112/123 (91%)	104 (93%)	8 (7%)	14	40
3	C	102/145 (70%)	96 (94%)	6 (6%)	19	49
3	H	91/145 (63%)	85 (93%)	6 (7%)	16	44
All	All	617/892 (69%)	580 (94%)	37 (6%)	19	49

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	117	HIS
3	H	419	GLN
2	G	120	ASP
3	H	353	PHE
3	C	369	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	112	ASN
1	F	155	ASN
1	F	127	GLN
2	G	8	GLN
2	B	8	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](#)

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	118/204 (57%)	0.04	0 100 100	57, 77, 94, 111	0
1	F	119/204 (58%)	0.00	1 (0%) 86 86	51, 66, 86, 132	0
2	B	130/142 (91%)	0.39	2 (1%) 73 73	80, 105, 131, 136	0
2	G	129/142 (90%)	0.21	1 (0%) 86 86	68, 89, 117, 122	0
3	C	118/166 (71%)	0.15	2 (1%) 70 69	52, 72, 104, 115	0
3	H	101/166 (60%)	1.49	32 (31%) 0 0	77, 131, 172, 180	0
4	D	15/15 (100%)	-0.27	0 100 100	59, 67, 79, 80	0
4	I	15/15 (100%)	-0.28	0 100 100	61, 72, 90, 92	0
5	E	15/15 (100%)	-0.37	0 100 100	55, 67, 81, 85	0
5	J	15/15 (100%)	-0.30	0 100 100	59, 69, 92, 98	0
All	All	775/1084 (71%)	0.30	38 (4%) 29 26	51, 82, 143, 180	0

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	360	GLY	7.7
3	H	345	LEU	6.0
1	F	178	ARG	5.2
3	H	424	TYR	5.0
3	H	333	GLY	4.7

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.