



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:19 PM GMT

PDB ID : 3WTT
Title : Crystal structure of the complex comprised of phosphorylated ETS1, RUNX1, CBFβ, and the tcrα gene enhancer DNA
Authors : Shiina, M.; Hamada, K.; Ogata, K.
Deposited on : 2014-04-21
Resolution : 2.35 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

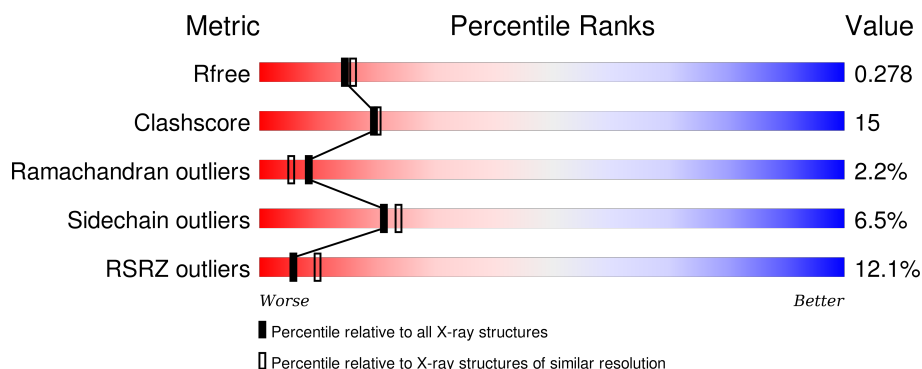
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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 $\leq 5\%$. 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	<div> <div>45%</div> <div>13%</div> <div>42%</div> </div>
1	F	204	<div> <div>50%</div> <div>7%</div> <div>42%</div> </div>
2	B	142	<div> <div>18%</div> <div>50%</div> <div>37%</div> <div>5%</div> <div>8%</div> </div>
2	G	142	<div> <div>13%</div> <div>53%</div> <div>35%</div> <div>8%</div> </div>
3	C	166	<div> <div>56%</div> <div>14%</div> <div>29%</div> </div>

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Mol	Chain	Length	Quality of chain
3	H	166	
4	D	15	
4	I	15	
5	E	15	
5	J	15	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7083 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
1	A	119	Total	C	N	O	S	0	0	0
			919	577	170	168	4			
1	F	118	Total	C	N	O	S	0	0	0
			914	574	169	167	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	94	LYS	LEU	ENGINEERED MUTATION	UNP Q03347
F	94	LYS	LEU	ENGINEERED MUTATION	UNP Q03347

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	131	Total	C	N	O	S	0	0	0
			1078	675	196	201	6			
2	G	130	Total	C	N	O	S	0	0	0
			1071	671	195	199	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	118	Total	C	N	O	S	0	0	0
			967	627	165	171	4			
3	H	93	Total	C	N	O	S	0	0	0
			789	512	137	137	3			

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

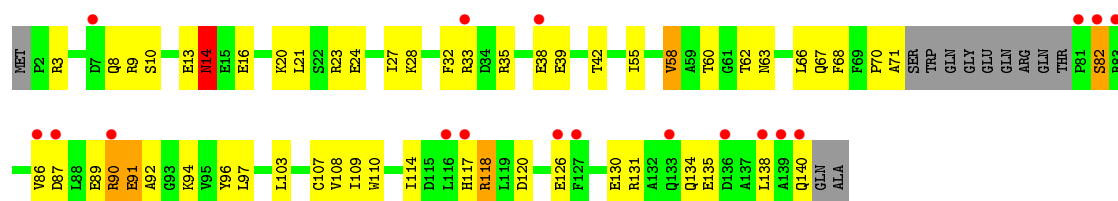
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	15	Total	C	N	O	P	0	0	0
			299	144	54	87	14			
4	I	15	Total	C	N	O	P	0	0	0
			299	144	54	87	14			

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

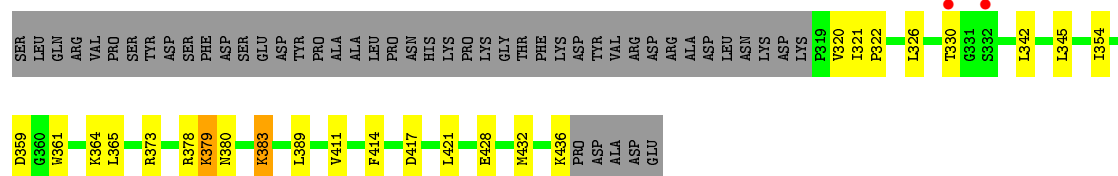
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	15	Total	C	N	O	P	0	0	0
			310	148	59	89	14			
5	J	15	Total	C	N	O	P	0	0	0
			310	148	59	89	14			

- Molecule 6 is water.

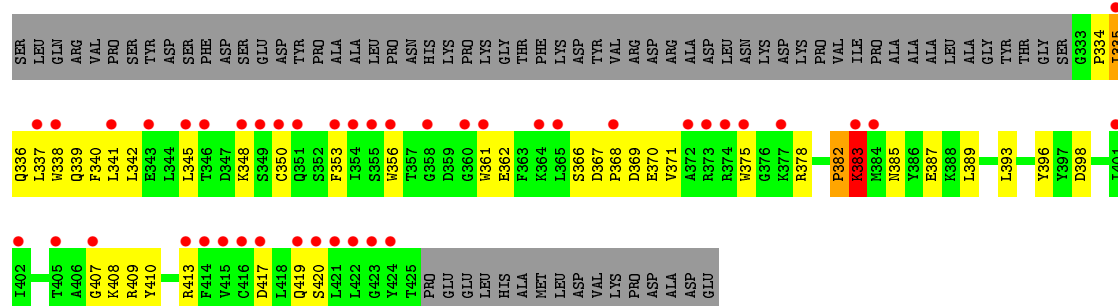
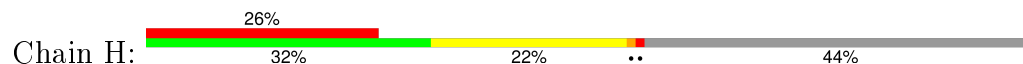
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	19	Total	O	0	0
			19	19		
6	B	5	Total	O	0	0
			5	5		
6	C	18	Total	O	0	0
			18	18		
6	F	24	Total	O	0	0
			24	24		
6	G	11	Total	O	0	0
			11	11		
6	H	2	Total	O	0	0
			2	2		
6	D	9	Total	O	0	0
			9	9		
6	E	18	Total	O	0	0
			18	18		
6	I	4	Total	O	0	0
			4	4		
6	J	17	Total	O	0	0
			17	17		



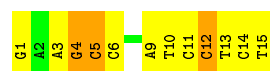
• Molecule 3: Protein C-ets-1



• Molecule 3: Protein C-ets-1



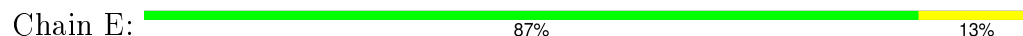
• Molecule 4: 5'-D(*GP*AP*AP*GP*CP*CP*AP*CP*AP*TP*CP*CP*TP*CP*T)-3'



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



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



- Molecule 5: 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	78.62Å 101.72Å 194.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.68 – 2.35 48.68 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.3 (48.68-2.35) 98.4 (48.68-2.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.53 (at 2.34Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.241 , 0.277 0.241 , 0.278	Depositor DCC
R_{free} test set	6531 reflections (10.11%)	DCC
Wilson B-factor (Å ²)	65.6	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 64625 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7083	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.64	0/938	0.79	1/1275 (0.1%)
1	F	0.74	0/933	0.88	0/1268
2	B	0.52	0/1100	0.59	0/1477
2	G	0.59	0/1093	0.64	0/1466
3	C	0.71	0/994	0.76	0/1342
3	H	0.45	0/811	0.53	0/1091
4	D	0.92	0/334	1.13	3/512 (0.6%)
4	I	0.85	0/334	1.10	1/512 (0.2%)
5	E	0.87	0/348	0.91	0/537
5	J	0.79	0/348	0.86	1/537 (0.2%)
All	All	0.67	0/7233	0.78	6/10017 (0.1%)

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	4
4	I	0	4
5	E	0	1
All	All	0	9

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	4	DG	N9-C1'-C2'	-7.67	98.02	112.60
4	I	4	DG	N9-C1'-C2'	-6.95	99.39	112.60
4	D	4	DG	C4'-C3'-O3'	5.56	123.61	109.70
1	A	139	ARG	NE-CZ-NH2	5.29	122.94	120.30
4	D	3	DA	N9-C1'-C2'	5.14	122.38	112.60

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	12	DC	Sidechain
4	D	15	DT	Sidechain
4	D	4	DG	Sidechain
4	D	5	DC	Sidechain
5	E	13	DT	Sidechain

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	919	0	924	27	0
1	F	914	0	922	12	0
2	B	1078	0	1040	48	0
2	G	1071	0	1034	42	0
3	C	967	0	966	20	0
3	H	789	0	785	38	0
4	D	299	0	170	15	0
4	I	299	0	170	7	0
5	E	310	0	171	1	0
5	J	310	0	171	1	0
6	A	19	0	0	2	0
6	B	5	0	0	0	0
6	C	18	0	0	0	0
6	D	9	0	0	1	0
6	E	18	0	0	0	0
6	F	24	0	0	1	0
6	G	11	0	0	0	0
6	H	2	0	0	0	0
6	I	4	0	0	0	0
6	J	17	0	0	0	0
All	All	7083	0	6353	200	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 15.

The worst 5 of 200 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:104:THR:HG22	6:A:317:HOH:O	1.69	0.93
1:A:82:ASN:HD21	1:A:118:ARG:HH11	0.96	0.92
3:H:383:LYS:H	3:H:383:LYS:HD2	1.34	0.90
4:I:11:DC:H1'	4:I:12:DC:H5''	1.59	0.82
1:A:87:ILE:HD12	1:A:87:ILE:O	1.81	0.81

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	117/204 (57%)	112 (96%)	5 (4%)	0	100	100
1	F	116/204 (57%)	111 (96%)	5 (4%)	0	100	100
2	B	127/142 (89%)	111 (87%)	12 (9%)	4 (3%)	5	3
2	G	126/142 (89%)	106 (84%)	14 (11%)	6 (5%)	3	1
3	C	116/166 (70%)	112 (97%)	4 (3%)	0	100	100
3	H	91/166 (55%)	65 (71%)	21 (23%)	5 (6%)	2	0
All	All	693/1024 (68%)	617 (89%)	61 (9%)	15 (2%)	8	5

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	81	PRO
2	G	58	VAL
3	H	335	ILE
2	B	116	LEU
2	G	24	GLU

5.3.2 Protein sidechains ⓘ

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	100/179 (56%)	95 (95%)	5 (5%)	30	37
1	F	100/179 (56%)	96 (96%)	4 (4%)	38	49
2	B	114/123 (93%)	102 (90%)	12 (10%)	8	8
2	G	113/123 (92%)	103 (91%)	10 (9%)	12	12
3	C	102/145 (70%)	98 (96%)	4 (4%)	39	51
3	H	84/145 (58%)	79 (94%)	5 (6%)	24	28
All	All	613/894 (69%)	573 (94%)	40 (6%)	21	24

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	379	LYS
1	F	110	ASP
3	H	383	LYS
3	C	436	LYS
1	F	112	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	134	GLN
2	B	140	GLN
2	G	8	GLN
2	B	14	ASN
2	B	41	GLN

5.3.3 RNA ⓘ

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	119/204 (58%)	0.60	3 (2%) 61 73	42, 58, 84, 96	0
1	F	118/204 (57%)	0.52	2 (1%) 73 83	37, 51, 71, 94	0
2	B	131/142 (92%)	1.26	25 (19%) 2 3	60, 85, 115, 126	0
2	G	130/142 (91%)	0.99	18 (13%) 4 8	56, 77, 107, 119	0
3	C	118/166 (71%)	0.42	2 (1%) 73 83	39, 59, 83, 89	0
3	H	93/166 (56%)	2.20	43 (46%) 0 0	62, 112, 139, 146	0
4	D	15/15 (100%)	-0.06	0 100 100	46, 52, 62, 63	0
4	I	15/15 (100%)	0.04	0 100 100	49, 62, 77, 77	0
5	E	15/15 (100%)	-0.09	0 100 100	43, 49, 60, 65	0
5	J	15/15 (100%)	-0.01	0 100 100	47, 57, 71, 73	0
All	All	769/1084 (70%)	0.88	93 (12%) 6 10	37, 67, 119, 146	0

The worst 5 of 93 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	421	LEU	9.4
2	B	138	LEU	7.9
3	H	360	GLY	7.7
2	B	137	ALA	6.0
3	H	422	LEU	5.8

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.