



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 17, 2022 – 09:11 PM EDT

PDB ID : 3WTS
Title : Crystal structure of the complex comprised of ETS1, RUNX1, CBFbeta, and the tcralpha 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

<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
Xtriage (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

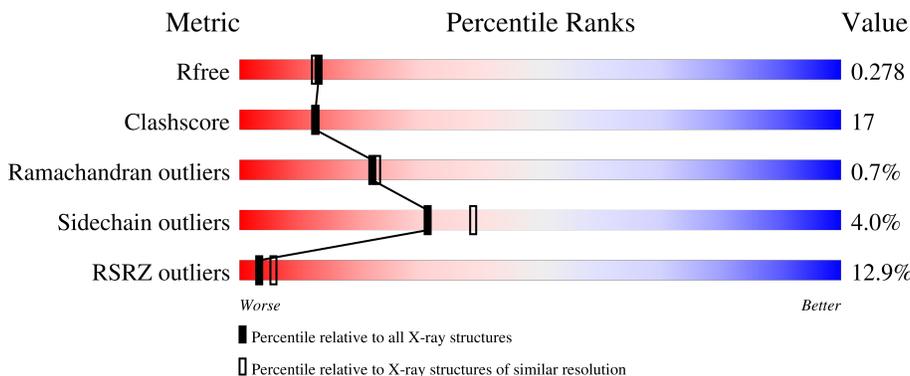
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	205	 43% 13% 42%
1	F	205	 44% 12% 42%
2	B	142	 18% 53% 37% 8%
2	G	142	 10% 65% 25% 9%
3	C	166	 2% 56% 14% 29%

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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

There are 6 unique types of molecules in this entry. The entry contains 7094 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	119	922	579	170	168	5	0	0	0
1	F	118	914	574	169	167	4	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	59	MET	-	expression tag	UNP Q03347
A	94	LYS	LEU	engineered mutation	UNP Q03347
F	59	MET	-	expression tag	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
			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 5'-D(*GP*AP*AP*GP*CP*CP*AP*CP*AP*TP*CP*C P*TP*CP*T)-3'.

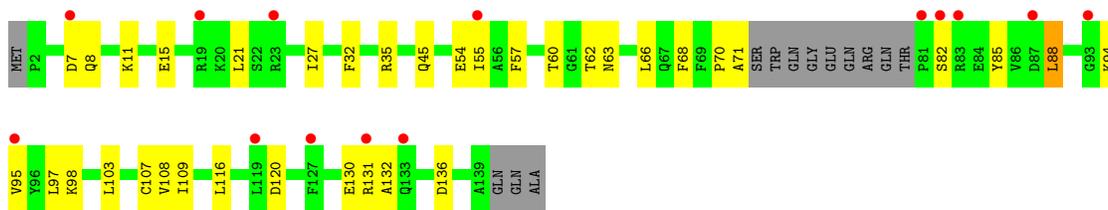
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	15	Total	C	N	O	P	0	0	0
			299	144	54	87	14			
4	I	15	Total	C	N	O	P	0	0	0
			299	144	54	87	14			

- 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'.

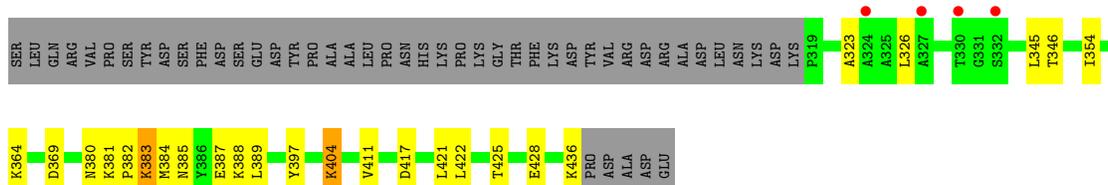
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	15	Total	C	N	O	P	0	0	0
			310	148	59	89	14			
5	J	15	Total	C	N	O	P	0	0	0
			310	148	59	89	14			

- Molecule 6 is water.

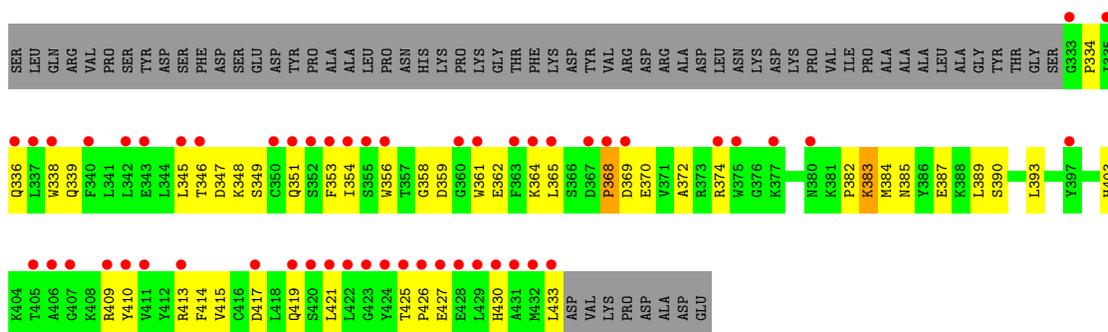
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	18	Total	O	0	0
			18	18		
6	B	3	Total	O	0	0
			3	3		
6	C	16	Total	O	0	0
			16	16		
6	F	13	Total	O	0	0
			13	13		
6	G	3	Total	O	0	0
			3	3		
6	D	7	Total	O	0	0
			7	7		
6	E	14	Total	O	0	0
			14	14		
6	I	2	Total	O	0	0
			2	2		
6	J	11	Total	O	0	0
			11	11		



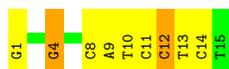
- Molecule 3: Protein C-ets-1



- 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:
80% 20%

A horizontal bar chart for Chain J showing 80% green and 20% yellow.



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.72Å 102.06Å 194.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.99 – 2.35 44.99 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.8 (44.99-2.35) 98.9 (44.99-2.35)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 2.34Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.249 , 0.279 0.249 , 0.278	Depositor DCC
R_{free} test set	6608 reflections (10.13%)	wwPDB-VP
Wilson B-factor (Å ²)	64.1	Xtrriage
Anisotropy	0.140	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7094	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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	0.40	0/941	0.62	0/1278
1	F	0.48	0/933	0.68	0/1268
2	B	0.34	0/1093	0.49	0/1466
2	G	0.36	0/1084	0.50	0/1454
3	C	0.44	0/994	0.58	0/1342
3	H	0.32	0/877	0.43	0/1181
4	D	0.61	0/334	0.94	1/512 (0.2%)
4	I	0.58	0/334	0.88	1/512 (0.2%)
5	E	0.52	0/348	0.82	0/537
5	J	0.47	0/348	0.74	0/537
All	All	0.43	0/7286	0.63	2/10087 (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
4	D	0	2
4	I	0	2
5	E	0	1
All	All	0	5

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	4	DG	N9-C1'-C2'	-5.84	101.50	112.60
4	I	4	DG	N9-C1'-C2'	-5.10	102.91	112.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	12	DC	Sidechain
4	D	4	DG	Sidechain
5	E	113	DT	Sidechain
4	I	4	DG	Sidechain
4	I	9	DA	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	922	0	931	33	0
1	F	914	0	922	23	0
2	B	1071	0	1034	50	0
2	G	1062	0	1026	31	0
3	C	967	0	966	20	0
3	H	853	0	847	47	0
4	D	299	0	170	13	0
4	I	299	0	170	16	0
5	E	310	0	171	2	0
5	J	310	0	171	5	0
6	A	18	0	0	2	0
6	B	3	0	0	0	0
6	C	16	0	0	1	0
6	D	7	0	0	2	0
6	E	14	0	0	0	0
6	F	13	0	0	0	0
6	G	3	0	0	2	0
6	I	2	0	0	0	0
6	J	11	0	0	0	0
All	All	7094	0	6408	224	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 17.

The worst 5 of 224 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:82:ASN:HD21	1:A:118:ARG:HH11	1.14	0.94
1:A:69:ASN:HD21	1:A:95:GLY:H	1.17	0.90
3:H:345:LEU:HB3	3:H:356:TRP:HE1	1.38	0.86
4:I:10:DT:H2''	4:I:11:DC:H5'	1.63	0.79
1:A:69:ASN:ND2	1:A:95:GLY:H	1.80	0.79

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	117/205 (57%)	111 (95%)	6 (5%)	0	100	100
1	F	116/205 (57%)	111 (96%)	5 (4%)	0	100	100
2	B	126/142 (89%)	109 (86%)	16 (13%)	1 (1%)	19	20
2	G	125/142 (88%)	112 (90%)	13 (10%)	0	100	100
3	C	116/166 (70%)	114 (98%)	2 (2%)	0	100	100
3	H	99/166 (60%)	82 (83%)	13 (13%)	4 (4%)	3	1
All	All	699/1026 (68%)	639 (91%)	55 (8%)	5 (1%)	22	23

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	382	PRO
3	H	383	LYS
2	B	116	LEU
3	H	368	PRO
3	H	334	PRO

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	101/180 (56%)	94 (93%)	7 (7%)	15	15
1	F	100/180 (56%)	96 (96%)	4 (4%)	31	39
2	B	113/123 (92%)	110 (97%)	3 (3%)	44	55
2	G	112/123 (91%)	107 (96%)	5 (4%)	27	33
3	C	102/145 (70%)	98 (96%)	4 (4%)	32	40
3	H	91/145 (63%)	89 (98%)	2 (2%)	52	63
All	All	619/896 (69%)	594 (96%)	25 (4%)	31	39

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	96	ASP
1	F	162	TYR
3	H	384	MET
1	F	139	ARG
2	G	7	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	163	HIS
2	G	134	GLN
2	G	67	GLN
3	H	336	GLN
1	A	132	ASN

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	119/205 (58%)	0.63	2 (1%) 70 78	42, 57, 81, 113	0
1	F	118/205 (57%)	0.51	1 (0%) 86 91	38, 51, 71, 94	0
2	B	130/142 (91%)	1.22	26 (20%) 1 2	62, 87, 113, 127	0
2	G	129/142 (90%)	1.01	14 (10%) 5 9	56, 78, 106, 111	0
3	C	118/166 (71%)	0.58	4 (3%) 45 57	38, 58, 87, 95	0
3	H	101/166 (60%)	2.59	53 (52%) 0 0	61, 116, 154, 158	0
4	D	15/15 (100%)	-0.06	0 100 100	46, 51, 60, 61	0
4	I	15/15 (100%)	0.04	0 100 100	50, 61, 75, 78	0
5	E	15/15 (100%)	-0.15	0 100 100	41, 48, 61, 61	0
5	J	15/15 (100%)	-0.06	0 100 100	45, 56, 68, 71	0
All	All	775/1086 (71%)	0.97	100 (12%) 3 5	38, 67, 125, 158	0

The worst 5 of 100 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	433	LEU	9.0
3	H	353	PHE	8.8
3	H	429	LEU	8.2
3	H	421	LEU	8.1
1	A	59	MET	6.8

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 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.