wwPDB X-ray Structure Validation Summary Report (i)

Aug 30, 2023 – 07:52 AM EDT

PDB ID	:	3M06
Title	:	Crystal Structure of TRAF2
Authors	:	Kabaleeswaran, V.; Wu, H.
Deposited on	:	2010-03-02
Resolution	:	2.67 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 (i)) were used in the production of this report:

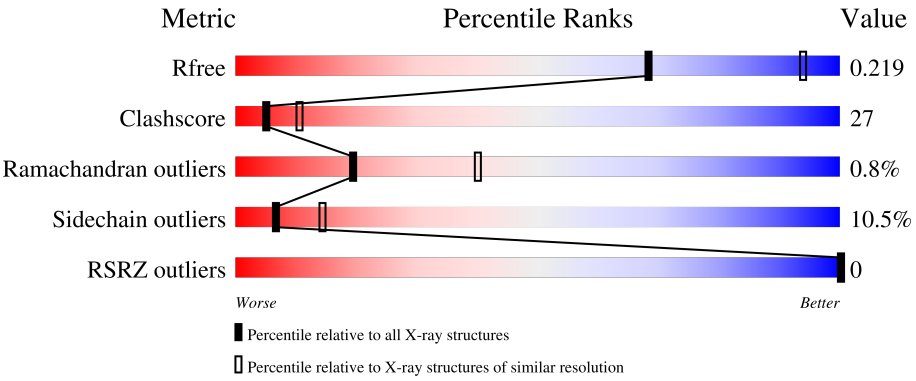
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 2.67 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	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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	72	49% 35% · 14%
1	B	72	51% 33% · 14%
1	C	72	60% 22% · 14%
1	D	72	51% 31% · 14%
1	E	72	46% 35% 6% 14%

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Mol	Chain	Length	Quality of chain
1	F	72	43% 33% 10% 14%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2686 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 TNF receptor-associated factor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	62	Total	C	N	O	S	0	0	0
			447	273	81	90	3			
1	B	62	Total	C	N	O	S	0	0	0
			449	273	83	89	4			
1	C	62	Total	C	N	O	S	0	0	0
			414	253	75	83	3			
1	D	62	Total	C	N	O	S	0	0	0
			453	279	82	88	4			
1	E	62	Total	C	N	O	S	0	0	0
			443	271	78	90	4			
1	F	62	Total	C	N	O	S	0	0	0
			419	257	75	84	3			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	330	LEU	-	expression tag	UNP Q12933
A	331	GLU	-	expression tag	UNP Q12933
A	332	HIS	-	expression tag	UNP Q12933
A	333	HIS	-	expression tag	UNP Q12933
A	334	HIS	-	expression tag	UNP Q12933
A	335	HIS	-	expression tag	UNP Q12933
A	336	HIS	-	expression tag	UNP Q12933
A	337	HIS	-	expression tag	UNP Q12933
B	330	LEU	-	expression tag	UNP Q12933
B	331	GLU	-	expression tag	UNP Q12933
B	332	HIS	-	expression tag	UNP Q12933
B	333	HIS	-	expression tag	UNP Q12933
B	334	HIS	-	expression tag	UNP Q12933
B	335	HIS	-	expression tag	UNP Q12933
B	336	HIS	-	expression tag	UNP Q12933
B	337	HIS	-	expression tag	UNP Q12933
C	330	LEU	-	expression tag	UNP Q12933

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Chain	Residue	Modelled	Actual	Comment	Reference
C	331	GLU	-	expression tag	UNP Q12933
C	332	HIS	-	expression tag	UNP Q12933
C	333	HIS	-	expression tag	UNP Q12933
C	334	HIS	-	expression tag	UNP Q12933
C	335	HIS	-	expression tag	UNP Q12933
C	336	HIS	-	expression tag	UNP Q12933
C	337	HIS	-	expression tag	UNP Q12933
D	330	LEU	-	expression tag	UNP Q12933
D	331	GLU	-	expression tag	UNP Q12933
D	332	HIS	-	expression tag	UNP Q12933
D	333	HIS	-	expression tag	UNP Q12933
D	334	HIS	-	expression tag	UNP Q12933
D	335	HIS	-	expression tag	UNP Q12933
D	336	HIS	-	expression tag	UNP Q12933
D	337	HIS	-	expression tag	UNP Q12933
E	330	LEU	-	expression tag	UNP Q12933
E	331	GLU	-	expression tag	UNP Q12933
E	332	HIS	-	expression tag	UNP Q12933
E	333	HIS	-	expression tag	UNP Q12933
E	334	HIS	-	expression tag	UNP Q12933
E	335	HIS	-	expression tag	UNP Q12933
E	336	HIS	-	expression tag	UNP Q12933
E	337	HIS	-	expression tag	UNP Q12933
F	330	LEU	-	expression tag	UNP Q12933
F	331	GLU	-	expression tag	UNP Q12933
F	332	HIS	-	expression tag	UNP Q12933
F	333	HIS	-	expression tag	UNP Q12933
F	334	HIS	-	expression tag	UNP Q12933
F	335	HIS	-	expression tag	UNP Q12933
F	336	HIS	-	expression tag	UNP Q12933
F	337	HIS	-	expression tag	UNP Q12933

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	13	Total O 13 13	0	0
2	B	8	Total O 8 8	0	0
2	C	9	Total O 9 9	0	0
2	D	10	Total O 10 10	0	0

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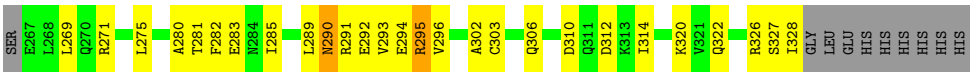
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	10	Total O 10 10	0	0
2	F	11	Total O 11 11	0	0

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: TNF receptor-associated factor 2

Chain A:



• Molecule 1: TNF receptor-associated factor 2

Chain B:

• Molecule 1: TNF receptor-associated factor 2

Chain C:

• Molecule 1: TNF receptor-associated factor 2

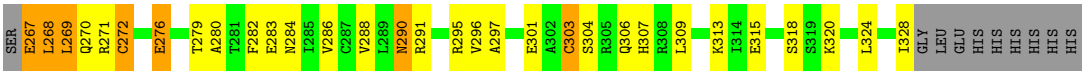
Chain D:

• Molecule 1: TNF receptor-associated factor 2

Chain E:

• Molecule 1: TNF receptor-associated factor 2

Chain F:


SER
E267
L268
L269
Q270
R271
C272
E276
T279
A280
T281
F282
E283
N284
I285
V286
C287
V288
L289
N290
R291
R295
V296
A297
E301
A302
C303
S304
R305
Q306
H307
R308
L309
K313
I314
E315
S318
S319
K320
L324
I328
GLY
LEU
GLU
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	150.71Å 150.71Å 86.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.13 – 2.67 36.12 – 2.67	Depositor EDS
% Data completeness (in resolution range)	99.7 (36.13-2.67) 99.8 (36.12-2.67)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.72 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.1	Depositor
R, R_{free}	0.192 , 0.233 0.225 , 0.219	Depositor DCC
R_{free} test set	1067 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	51.4	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 46.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.466 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.525 for H, K, L 0.475 for K, H, -L	Depositor
Outliers	0 of 20823 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	2686	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.44% 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

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	0.50	0/448	0.66	0/607
1	B	0.48	0/450	0.62	0/609
1	C	0.66	1/415 (0.2%)	0.59	0/566
1	D	0.54	0/454	0.59	0/613
1	E	0.56	0/444	0.63	0/601
1	F	0.74	0/420	0.66	0/571
All	All	0.58	1/2631 (0.0%)	0.62	0/3567

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	272	CYS	CB-SG	-6.30	1.71	1.82

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	447	0	418	26	0
1	B	449	0	420	22	0
1	C	414	0	361	19	0
1	D	453	0	441	31	0
1	E	443	0	408	35	0
1	F	419	0	372	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	13	0	0	0	0
2	B	8	0	0	0	0
2	C	9	0	0	1	0
2	D	10	0	0	1	0
2	E	10	0	0	0	0
2	F	11	0	0	3	0
All	All	2686	0	2420	136	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 27.

The worst 5 of 136 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:286:VAL:HG22	1:F:286:VAL:HG21	1.48	0.95
1:A:295:ARG:HH22	1:F:291:ARG:HH21	1.19	0.87
1:A:275:LEU:HD23	1:B:275:LEU:HD13	1.57	0.86
1:D:275:LEU:HD21	1:F:276:GLU:HB3	1.59	0.84
1:E:304:SER:HA	1:F:303:CYS:HB2	1.62	0.78

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	60/72 (83%)	56 (93%)	4 (7%)	0	100 100
1	B	60/72 (83%)	58 (97%)	2 (3%)	0	100 100
1	C	60/72 (83%)	56 (93%)	4 (7%)	0	100 100
1	D	60/72 (83%)	55 (92%)	5 (8%)	0	100 100
1	E	60/72 (83%)	57 (95%)	2 (3%)	1 (2%)	9 20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	F	60/72 (83%)	53 (88%)	5 (8%)	2 (3%)	4 7
All	All	360/432 (83%)	335 (93%)	22 (6%)	3 (1%)	19 40

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	269	LEU
1	F	269	LEU
1	F	276	GLU

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	45/66 (68%)	40 (89%)	5 (11%)	6 13
1	B	45/66 (68%)	42 (93%)	3 (7%)	16 34
1	C	37/66 (56%)	34 (92%)	3 (8%)	11 25
1	D	47/66 (71%)	43 (92%)	4 (8%)	10 22
1	E	44/66 (67%)	38 (86%)	6 (14%)	3 8
1	F	38/66 (58%)	32 (84%)	6 (16%)	2 5
All	All	256/396 (65%)	229 (90%)	27 (10%)	7 14

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	295	ARG
1	E	288	VAL
1	F	290	ASN
1	E	275	LEU
1	E	301	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	284	ASN
1	E	306	GLN
1	C	284	ASN
1	C	290	ASN
1	C	307	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	62/72 (86%)	-0.52	0	100	100	27, 49, 64, 65	0
1	B	62/72 (86%)	-0.51	0	100	100	30, 47, 68, 69	0
1	C	62/72 (86%)	-0.66	0	100	100	28, 47, 68, 69	0
1	D	62/72 (86%)	-0.46	0	100	100	29, 57, 70, 75	0
1	E	62/72 (86%)	-0.52	0	100	100	21, 51, 73, 75	0
1	F	62/72 (86%)	-0.64	0	100	100	32, 55, 73, 78	0
All	All	372/432 (86%)	-0.55	0	100	100	21, 52, 71, 78	0

There are no RSRZ outliers to report.

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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.