



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:26 AM UTC

PDB ID : 4C7M / pdb_00004c7m
Title : The crystal structure of TcpB or BtpA TIR domain
Authors : Alaidarous, M.; Ve, T.; Casey, L.W.; Valkov, E.; Ullah, M.O.; Schembri, M.A.;
Mansell, A.; Sweet, M.J.; Kobe, B.
Deposited on : 2013-09-23
Resolution : 2.57 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

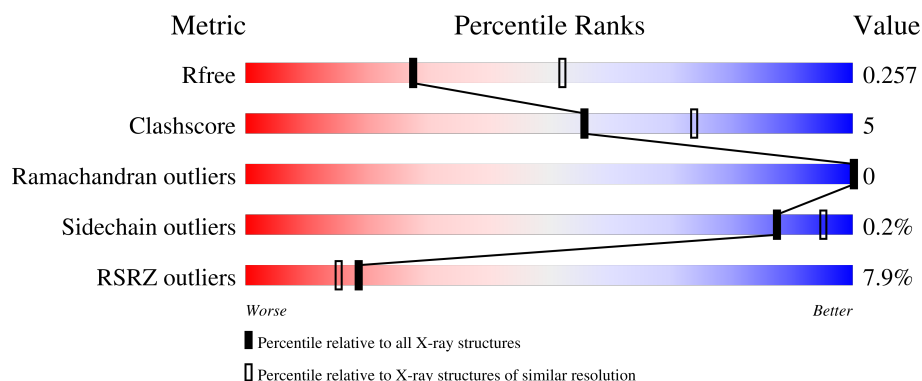
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.57 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}	180053	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)

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	134	11% 79% 19% .
1	B	134	5% 83% 13% .
1	C	134	7% 84% 8% 7%
1	D	134	6% 86% 7% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4069 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 Toll/interleukin-1 receptor domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	132	Total	C	N	O	S	0	0	0
			1042	665	179	197	1			
1	B	128	Total	C	N	O		0	0	0
			1021	656	175	190				
1	C	124	Total	C	N	O		0	0	0
			996	641	171	184				
1	D	125	Total	C	N	O		0	0	0
			1002	646	171	185				

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	117	SER	-	expression tag	UNP A0A4P6KMT3
A	118	ASN	-	expression tag	UNP A0A4P6KMT3
A	119	ALA	-	expression tag	UNP A0A4P6KMT3
B	117	SER	-	expression tag	UNP A0A4P6KMT3
B	118	ASN	-	expression tag	UNP A0A4P6KMT3
B	119	ALA	-	expression tag	UNP A0A4P6KMT3
C	117	SER	-	expression tag	UNP A0A4P6KMT3
C	118	ASN	-	expression tag	UNP A0A4P6KMT3
C	119	ALA	-	expression tag	UNP A0A4P6KMT3
D	117	SER	-	expression tag	UNP A0A4P6KMT3
D	118	ASN	-	expression tag	UNP A0A4P6KMT3
D	119	ALA	-	expression tag	UNP A0A4P6KMT3

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	O	0	0
			4	4		
2	C	1	Total	O	0	0
			1	1		

Continued on next page...

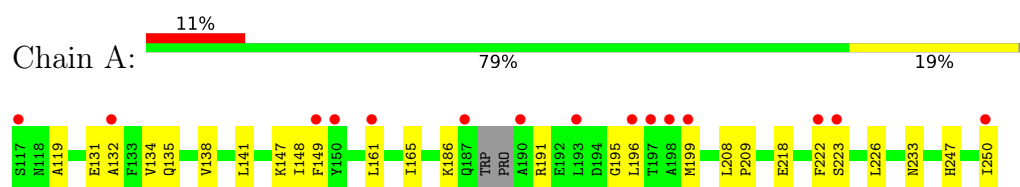
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	3	Total	O	0	0
			3	3		

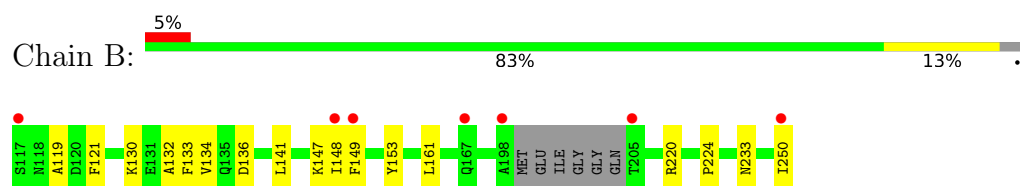
3 Residue-property plots [i](#)

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.

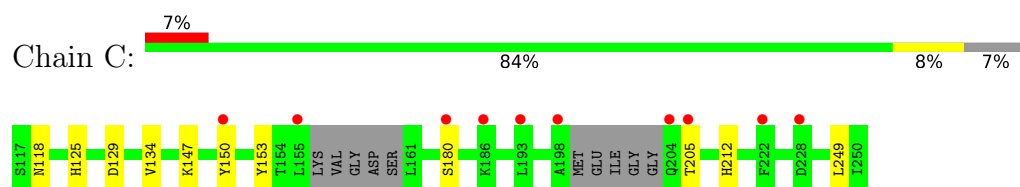
- Molecule 1: Toll/interleukin-1 receptor domain-containing protein



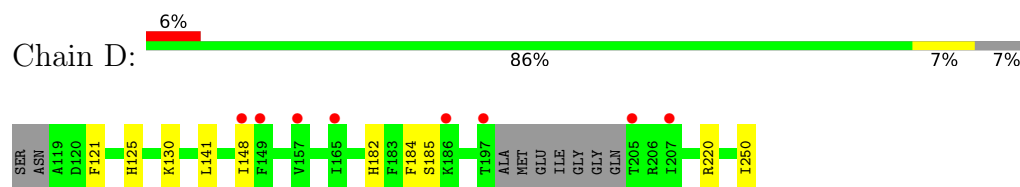
- Molecule 1: Toll/interleukin-1 receptor domain-containing protein



- Molecule 1: Toll/interleukin-1 receptor domain-containing protein



- Molecule 1: Toll/interleukin-1 receptor domain-containing protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.97Å 73.68Å 74.76Å 90.00° 93.29° 90.00°	Depositor
Resolution (Å)	42.42 – 2.57 42.42 – 2.57	Depositor EDS
% Data completeness (in resolution range)	99.9 (42.42-2.57) 99.9 (42.42-2.57)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.58Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.232 , 0.240 0.239 , 0.257	Depositor DCC
R_{free} test set	1009 reflections (5.58%)	wwPDB-VP
Wilson B-factor (Å ²)	51.3	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4069	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.38% 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

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	0.87	0/1059	1.39	4/1424 (0.3%)
1	B	0.80	0/1041	1.35	5/1404 (0.4%)
1	C	0.82	0/1015	1.32	1/1368 (0.1%)
1	D	0.75	0/1022	1.29	4/1378 (0.3%)
All	All	0.81	0/4137	1.34	14/5574 (0.3%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	ALA	N-CA-C	8.77	120.61	111.14
1	C	153	TYR	N-CA-C	7.01	121.43	113.02
1	B	161	LEU	CA-C-N	6.40	129.18	120.54
1	B	161	LEU	C-N-CA	6.40	129.18	120.54
1	D	184	PHE	CA-C-N	6.26	128.96	120.38
1	D	184	PHE	C-N-CA	6.26	128.96	120.38
1	B	233	ASN	CA-CB-CG	5.60	118.20	112.60
1	B	133	PHE	CA-CB-CG	-5.46	108.34	113.80
1	D	220	ARG	CA-C-N	5.27	127.35	120.28
1	D	220	ARG	C-N-CA	5.27	127.35	120.28
1	A	186	LYS	CA-C-N	5.25	131.15	121.70
1	A	186	LYS	C-N-CA	5.25	131.15	121.70
1	A	233	ASN	CA-CB-CG	5.12	117.72	112.60
1	B	153	TYR	N-CA-C	5.08	118.51	112.72

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	1042	0	1047	19	0
1	B	1021	0	1024	9	0
1	C	996	0	997	11	0
1	D	1002	0	1008	4	0
2	A	4	0	0	1	0
2	C	1	0	0	0	0
2	D	3	0	0	0	0
All	All	4069	0	4076	38	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 5.

All (38) 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:B:119:ALA:HB2	1:B:149:PHE:CE2	2.02	0.95
1:A:199:MET:HG3	1:C:205:THR:HG21	1.57	0.84
1:A:119:ALA:HB2	1:A:149:PHE:CE2	2.31	0.66
1:A:218:GLU:O	1:A:222:PHE:HD2	1.81	0.64
1:C:118:ASN:HB3	1:C:147:LYS:HE2	1.80	0.61
1:A:223:SER:OG	1:A:226:LEU:HB2	2.00	0.61
1:A:141:LEU:HB3	1:A:148:ILE:HD11	1.84	0.60
1:A:218:GLU:O	1:A:222:PHE:CD2	2.55	0.59
1:A:199:MET:HG3	1:C:205:THR:CG2	2.29	0.59
1:C:129:ASP:OD2	1:C:180:SER:HB2	2.03	0.58
1:A:147:LYS:HE2	1:A:149:PHE:CZ	2.40	0.56
1:A:131:GLU:O	1:A:135:GLN:HB3	2.07	0.54
1:A:195:GLY:O	1:C:205:THR:HG23	2.08	0.54
1:A:147:LYS:HE2	1:A:149:PHE:HZ	1.73	0.53
1:A:196:LEU:CD2	1:C:249:LEU:HD13	2.38	0.53
1:B:132:ALA:O	1:B:136:ASP:CG	2.52	0.53
1:D:121:PHE:HB2	1:D:148:ILE:HG12	1.92	0.52
1:C:125:HIS:CG	1:C:134:VAL:HG21	2.44	0.51
1:C:125:HIS:CD2	1:C:134:VAL:HG21	2.45	0.51
1:B:220:ARG:HD2	1:B:224:PRO:HA	1.94	0.48
1:A:134:VAL:O	1:A:138:VAL:HG23	2.13	0.48
1:A:161:LEU:O	1:A:165:ILE:HG12	2.14	0.48
1:B:250:ILE:HG22	1:B:250:ILE:O	2.13	0.48
1:A:196:LEU:HD23	1:C:249:LEU:HD13	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:HIS:CD2	1:D:130:LYS:HB2	2.50	0.47
1:B:147:LYS:HE2	1:B:149:PHE:HZ	1.79	0.46
1:A:191:ARG:HG2	2:A:2002:HOH:O	2.16	0.45
1:A:131:GLU:O	1:A:135:GLN:CB	2.65	0.44
1:B:141:LEU:HB3	1:B:148:ILE:CD1	2.48	0.43
1:B:121:PHE:HB2	1:B:148:ILE:HG12	2.01	0.43
1:A:208:LEU:HD12	1:A:209:PRO:HD2	2.01	0.42
1:C:150:TYR:CD1	1:C:150:TYR:C	2.98	0.41
1:B:130:LYS:HA	1:B:134:VAL:HB	2.01	0.41
1:B:147:LYS:HE2	1:B:149:PHE:CZ	2.55	0.41
1:D:141:LEU:HB3	1:D:148:ILE:CD1	2.51	0.41
1:C:180:SER:OG	1:C:212:HIS:HB3	2.20	0.41
1:D:182:HIS:O	1:D:185:SER:HB3	2.21	0.40
1:A:247:HIS:HA	1:A:250:ILE:CD1	2.52	0.40

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	128/134 (96%)	127 (99%)	1 (1%)	0	100	100
1	B	124/134 (92%)	123 (99%)	1 (1%)	0	100	100
1	C	118/134 (88%)	117 (99%)	1 (1%)	0	100	100
1	D	121/134 (90%)	119 (98%)	2 (2%)	0	100	100
All	All	491/536 (92%)	486 (99%)	5 (1%)	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	112/114 (98%)	112 (100%)	0	100	100
1	B	110/114 (96%)	110 (100%)	0	100	100
1	C	107/114 (94%)	107 (100%)	0	100	100
1	D	108/114 (95%)	107 (99%)	1 (1%)	70	85
All	All	437/456 (96%)	436 (100%)	1 (0%)	87	95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	250	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	GLN
1	B	167	GLN
1	C	167	GLN
1	D	167	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 oligosaccharides 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, 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	132/134 (98%)	0.65	15 (11%) 10 8	31, 53, 79, 89	0
1	B	128/134 (95%)	0.65	7 (5%) 30 26	28, 54, 83, 112	0
1	C	124/134 (92%)	0.80	10 (8%) 18 15	36, 57, 88, 106	0
1	D	125/134 (93%)	0.97	8 (6%) 25 21	35, 67, 91, 115	0
All	All	509/536 (94%)	0.77	40 (7%) 18 15	28, 58, 86, 115	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	250	ILE	4.8
1	B	198	ALA	4.3
1	D	186	LYS	3.9
1	D	149	PHE	3.6
1	A	150	TYR	3.3
1	A	187	GLN	3.1
1	D	197	THR	3.1
1	C	180	SER	3.1
1	C	186	LYS	3.0
1	C	193	LEU	2.9
1	A	149	PHE	2.8
1	D	148	ILE	2.7
1	A	198	ALA	2.7
1	A	161	LEU	2.6
1	A	199	MET	2.6
1	D	157	VAL	2.6
1	C	198	ALA	2.6
1	A	196	LEU	2.6
1	C	205	THR	2.6
1	C	150	TYR	2.5
1	A	132	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	155	LEU	2.4
1	B	149	PHE	2.4
1	A	190	ALA	2.4
1	A	197	THR	2.4
1	A	193	LEU	2.4
1	C	222	PHE	2.4
1	A	222	PHE	2.3
1	C	204	GLN	2.3
1	D	165	ILE	2.2
1	B	205	THR	2.2
1	A	223	SER	2.2
1	B	167	GLN	2.1
1	D	207	ILE	2.1
1	A	117	SER	2.1
1	A	250	ILE	2.1
1	C	228	ASP	2.1
1	B	148	ILE	2.0
1	B	117	SER	2.0
1	D	205	THR	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 oligosaccharides 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.