



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:34 AM UTC

PDB ID : 3ZQF / pdb_00003zqf
Title : Structure of Tetracycline repressor in complex with antiinducer peptide-TAP1
Authors : Sevvana, M.; Goeke, D.; Stoeckle, C.; Kaspar, D.; Grubmueller, S.; Goetz, C.;
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Deposited on : 2011-06-09
Resolution : 2.56 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

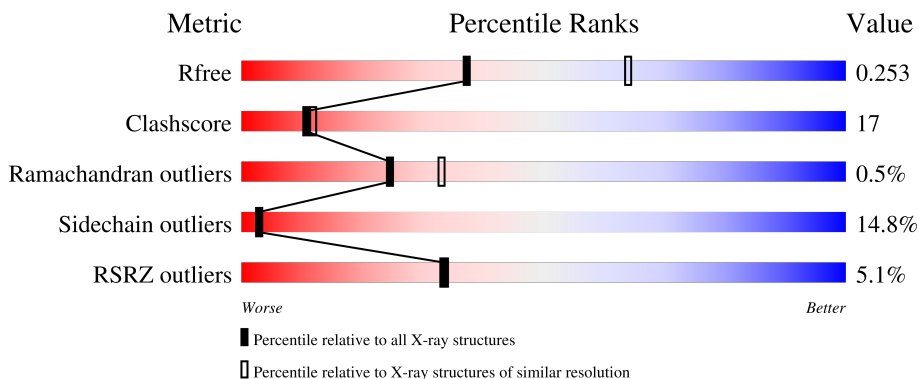
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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	208	4% 51% 28% 7% 12%
2	C	16	6% 44% 25% 12% 19%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1558 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 TETRACYCLINE REPRESSOR PROTEIN CLASS B FROM TRANSPOSON TN10, TETRACYCLINE REPRESSOR PROTEIN CLASS D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	183	Total	C	N	O	S	0	0	0
			1462	928	263	270	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68	SER	CYS	engineered mutation	UNP P04483
A	88	ASN	CYS	engineered mutation	UNP P04483
A	121	THR	CYS	engineered mutation	UNP P04483
A	144	SER	CYS	engineered mutation	UNP P04483

- Molecule 2 is a protein called ANTI-INDUCER PEPTIDE TAP1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	13	Total	C	N	O	0	0	0
			91	55	22	14			

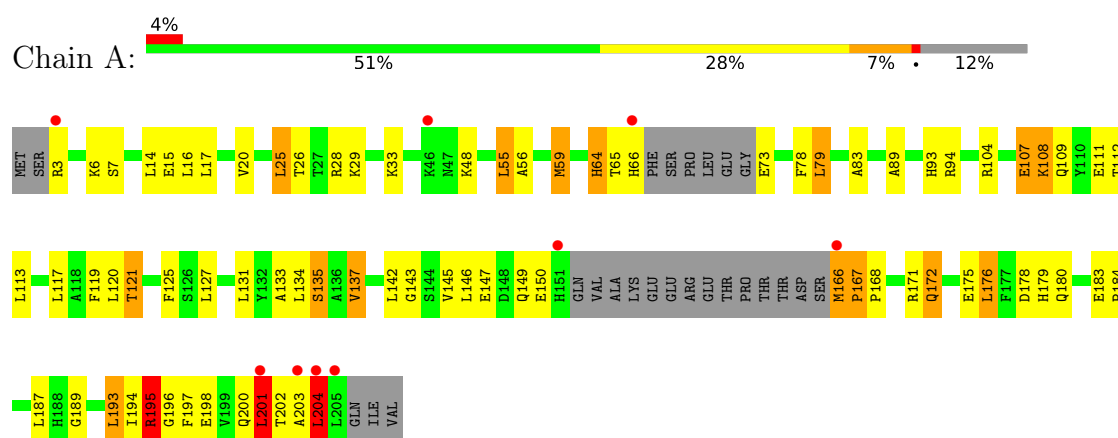
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	O	0	0
			5	5		

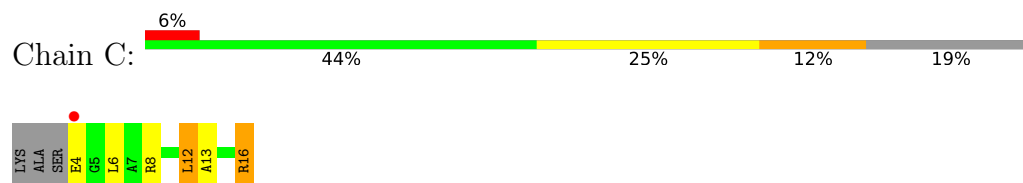
3 Residue-property plots [i](#)

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: TETRACYCLINE REPRESSOR PROTEIN CLASS B FROM TRANSPOSON TN10, TETRACYCLINE REPRESSOR PROTEIN CLASS D



- Molecule 2: ANTI-INDUCER PEPTIDE TAP1



4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	68.65Å 68.65Å 182.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.18 – 2.56 32.18 – 2.56	Depositor EDS
% Data completeness (in resolution range)	100.0 (32.18-2.56) 99.6 (32.18-2.56)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.57Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.206 , 0.247 0.217 , 0.253	Depositor DCC
R_{free} test set	673 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	68.5	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 61.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.062 for -h,k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	1558	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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	1.40	5/1489 (0.3%)	1.63	24/2011 (1.2%)
2	C	1.10	0/90	1.43	0/119
All	All	1.39	5/1579 (0.3%)	1.62	24/2130 (1.1%)

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
1	A	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	167	PRO	CA-C	7.02	1.55	1.51
1	A	204	LEU	N-CA	6.13	1.53	1.46
1	A	194	ILE	N-CA	-6.04	1.39	1.46
1	A	202	THR	CA-C	5.44	1.59	1.52
1	A	135	SER	N-CA	-5.42	1.39	1.46

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	MET	CA-C-N	17.09	132.14	119.66
1	A	166	MET	C-N-CA	17.09	132.14	119.66
1	A	167	PRO	CA-C-N	13.70	133.49	119.24
1	A	167	PRO	C-N-CA	13.70	133.49	119.24
1	A	167	PRO	N-CA-C	11.44	121.45	110.47
1	A	104	ARG	CA-C-N	7.58	127.34	119.76
1	A	104	ARG	C-N-CA	7.58	127.34	119.76
1	A	65	THR	N-CA-C	-7.35	102.07	113.02
1	A	172	GLN	N-CA-C	-7.29	103.86	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	LEU	N-CA-C	6.47	122.05	111.37
1	A	178	ASP	N-CA-C	-6.29	104.33	111.07
1	A	56	ALA	N-CA-C	-6.26	104.38	111.14
1	A	179	HIS	CA-C-N	-6.23	112.47	122.24
1	A	179	HIS	C-N-CA	-6.23	112.47	122.24
1	A	149	GLN	N-CA-C	6.14	120.45	113.15
1	A	204	LEU	CA-C-N	5.99	132.48	121.70
1	A	204	LEU	C-N-CA	5.99	132.48	121.70
1	A	137	VAL	CB-CA-C	-5.87	104.22	112.14
1	A	195	ARG	CA-CB-CG	-5.54	103.02	114.10
1	A	89	ALA	N-CA-C	-5.28	105.43	111.14
1	A	189	GLY	N-CA-C	-5.26	106.42	112.73
1	A	187	LEU	N-CA-C	5.25	117.41	111.11
1	A	111	GLU	N-CA-C	-5.24	105.26	110.97
1	A	204	LEU	N-CA-C	5.05	117.56	110.23

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	166	MET	Peptide

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	1462	0	1457	48	0
2	C	91	0	99	7	0
3	A	5	0	0	0	0
All	All	1558	0	1556	52	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.

All (52) 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:25:LEU:C	1:A:25:LEU:HD23	1.87	0.99
1:A:204:LEU:H	1:A:204:LEU:HD23	1.44	0.81
1:A:180:GLN:HB2	1:A:184:PRO:HG3	1.63	0.78
1:A:25:LEU:HD23	1:A:25:LEU:O	1.84	0.77
2:C:4:GLU:C	2:C:6:LEU:H	2.00	0.68
1:A:117:LEU:O	1:A:121:THR:OG1	2.11	0.68
1:A:59:MET:HE3	1:A:93:HIS:HB2	1.78	0.65
1:A:83:ALA:HB2	1:A:137:VAL:CG1	2.28	0.63
1:A:172:GLN:O	1:A:176:LEU:HB2	1.99	0.62
1:A:200:GLN:HA	1:A:200:GLN:OE1	1.98	0.61
1:A:119:PHE:CD2	1:A:120:LEU:HD23	2.37	0.60
1:A:59:MET:CE	1:A:93:HIS:HB2	2.33	0.59
1:A:25:LEU:C	1:A:25:LEU:CD2	2.66	0.58
1:A:193:LEU:HD22	1:A:197:PHE:CZ	2.40	0.56
1:A:112:THR:HG22	2:C:16:ARG:HG2	1.88	0.56
1:A:107:GLU:HG3	1:A:108:LYS:N	2.20	0.55
1:A:3:ARG:O	1:A:3:ARG:HD2	2.08	0.54
1:A:78:PHE:O	1:A:79:LEU:C	2.48	0.54
1:A:16:LEU:O	1:A:20:VAL:HG22	2.11	0.51
1:A:64:HIS:HD2	2:C:16:ARG:O	1.92	0.51
2:C:4:GLU:C	2:C:6:LEU:N	2.67	0.51
1:A:59:MET:HE3	1:A:93:HIS:ND1	2.26	0.50
1:A:171:ARG:NH1	1:A:175:GLU:HB2	2.27	0.50
1:A:146:LEU:HD23	1:A:146:LEU:HA	1.77	0.47
1:A:25:LEU:O	1:A:48:LYS:HE2	2.14	0.47
1:A:109:GLN:HB3	2:C:13:ALA:O	2.15	0.46
1:A:201:LEU:HA	1:A:201:LEU:HD22	1.44	0.46
1:A:59:MET:HE3	1:A:93:HIS:CB	2.44	0.46
1:A:55:LEU:HD12	1:A:55:LEU:HA	1.84	0.45
1:A:14:LEU:HD23	1:A:55:LEU:HG	1.98	0.45
1:A:15:GLU:OE1	1:A:33:LYS:NZ	2.47	0.45
1:A:6:LYS:O	1:A:7:SER:C	2.59	0.44
1:A:120:LEU:O	1:A:125:PHE:HB2	2.18	0.44
1:A:176:LEU:O	1:A:180:GLN:HG2	2.18	0.44
1:A:134:LEU:HD23	1:A:134:LEU:HA	1.62	0.43
1:A:171:ARG:HH12	1:A:175:GLU:HB2	1.84	0.43
1:A:133:ALA:O	1:A:137:VAL:HG23	2.18	0.43
1:A:134:LEU:O	1:A:135:SER:C	2.58	0.43
2:C:6:LEU:O	2:C:6:LEU:HG	2.18	0.42
1:A:193:LEU:HD22	1:A:197:PHE:CE2	2.55	0.42
1:A:183:GLU:N	1:A:184:PRO:HD2	2.35	0.42
1:A:145:VAL:O	1:A:146:LEU:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:PRO:CB	1:A:168:PRO:HD2	2.50	0.41
1:A:204:LEU:H	1:A:204:LEU:CD2	2.14	0.41
1:A:142:LEU:O	1:A:143:GLY:C	2.61	0.41
1:A:26:THR:OG1	1:A:29:LYS:HG3	2.21	0.41
1:A:195:ARG:O	1:A:196:GLY:C	2.62	0.41
1:A:113:LEU:HD12	1:A:113:LEU:HA	1.77	0.41
1:A:3:ARG:O	1:A:3:ARG:CG	2.68	0.41
1:A:131:LEU:HA	1:A:131:LEU:HD23	1.80	0.40
1:A:16:LEU:O	1:A:17:LEU:C	2.64	0.40
2:C:12:LEU:HD13	2:C:12:LEU:HA	1.89	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	177/208 (85%)	165 (93%)	11 (6%)	1 (1%)	21	28
2	C	11/16 (69%)	10 (91%)	1 (9%)	0	100	100
All	All	188/224 (84%)	175 (93%)	12 (6%)	1 (0%)	24	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	ALA

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	155/179 (87%)	134 (86%)	21 (14%)	4	3
2	C	7/10 (70%)	4 (57%)	3 (43%)	0	0
All	All	162/189 (86%)	138 (85%)	24 (15%)	3	3

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	28	ARG
1	A	55	LEU
1	A	59	MET
1	A	64	HIS
1	A	66	HIS
1	A	73	GLU
1	A	79	LEU
1	A	94	ARG
1	A	107	GLU
1	A	108	LYS
1	A	121	THR
1	A	127	LEU
1	A	147	GLU
1	A	150	GLU
1	A	176	LEU
1	A	193	LEU
1	A	195	ARG
1	A	198	GLU
1	A	201	LEU
1	A	204	LEU
2	C	8	ARG
2	C	12	LEU
2	C	16	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	82	ASN
1	A	151	HIS

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 [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	183/208 (87%)	0.09	9 (4%) 35 35	51, 79, 116, 136	0
2	C	13/16 (81%)	0.43	1 (7%) 19 19	77, 85, 100, 110	0
All	All	196/224 (87%)	0.11	10 (5%) 33 34	51, 80, 116, 136	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	205	LEU	4.9
1	A	166	MET	4.8
1	A	203	ALA	4.7
2	C	4	GLU	3.8
1	A	204	LEU	3.7
1	A	151	HIS	3.1
1	A	66	HIS	2.4
1	A	3	ARG	2.4
1	A	201	LEU	2.1
1	A	46	LYS	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.