



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:16 PM UTC

PDB ID : 1REG / pdb_00001reg
Title : CRYSTAL STRUCTURE OF THE T4 REGA TRANSLATIONAL REGULATOR PROTEIN AT 1.9 ANGSTROMS RESOLUTION
Authors : Kang, C.; Rich, A.
Deposited on : 1995-01-11
Resolution : 1.90 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

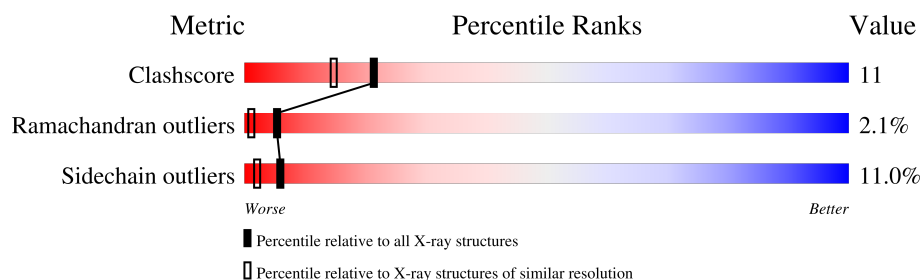
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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))
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	X	122	 60% 28% 11% .
1	Y	122	 48% 38% 9% . .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2111 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 T4 REGA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	122	Total	C	N	O	S	0	0	0
			1026	661	176	182	7			
1	Y	120	Total	C	N	O	S	0	0	0
			1014	655	173	179	7			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	X	44	Total	O	0	0
			44	44		
2	Y	27	Total	O	0	0
			27	27		

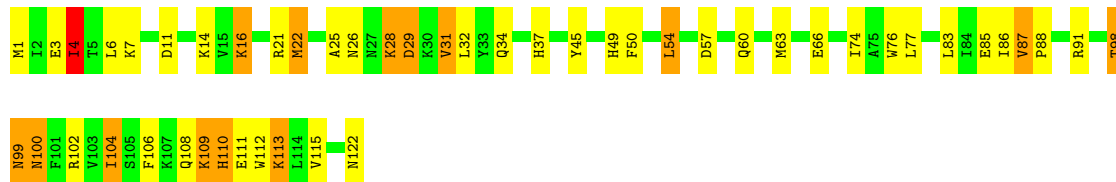
3 Residue-property plots [i](#)

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. 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. 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.

Note EDS was not executed.

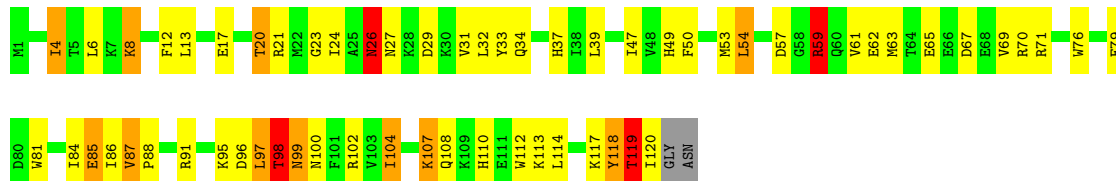
• Molecule 1: T4 REGA

Chain X: 



• Molecule 1: T4 REGA

Chain Y: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.71Å 85.72Å 43.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-1.90)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.0	Depositor
R, R_{free}	0.180 , 0.214	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2111	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

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	X	1.20	5/1046 (0.5%)	1.93	27/1403 (1.9%)
1	Y	1.18	6/1034 (0.6%)	2.13	40/1387 (2.9%)
All	All	1.19	11/2080 (0.5%)	2.03	67/2790 (2.4%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	49	HIS	CD2-NE2	-7.91	1.29	1.37
1	Y	110	HIS	CD2-NE2	-7.58	1.29	1.37
1	X	37	HIS	CD2-NE2	-6.80	1.30	1.37
1	Y	37	HIS	CD2-NE2	-6.72	1.30	1.37
1	Y	110	HIS	CG-ND1	-6.33	1.31	1.38
1	X	49	HIS	CG-ND1	-5.65	1.32	1.38
1	Y	49	HIS	CD2-NE2	-5.49	1.31	1.37
1	X	110	HIS	CD2-NE2	-5.42	1.31	1.37
1	Y	81	TRP	CA-CB	-5.31	1.44	1.53
1	Y	49	HIS	CG-ND1	-5.19	1.32	1.38
1	X	115	VAL	CA-CB	5.18	1.60	1.54

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	99	ASN	N-CA-C	10.53	125.71	110.24
1	X	57	ASP	CA-CB-CG	9.87	122.47	112.60
1	Y	100	ASN	OD1-CG-ND2	-9.11	113.49	122.60
1	Y	24	ILE	N-CA-CB	8.66	119.97	110.53
1	Y	24	ILE	CB-CA-C	-8.60	99.97	111.15
1	Y	110	HIS	CA-CB-CG	-8.14	105.66	113.80
1	X	122	ASN	CA-CB-CG	-8.06	104.54	112.60
1	Y	96	ASP	CA-CB-CG	8.04	120.64	112.60
1	Y	119	THR	CA-C-O	7.83	131.71	120.51
1	X	28	LYS	CA-CB-CG	-7.82	98.47	114.10
1	Y	57	ASP	CA-CB-CG	7.63	120.23	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	108	GLN	OE1-CD-NE2	-7.47	115.13	122.60
1	Y	97	LEU	N-CA-C	-7.46	94.90	110.80
1	X	34	GLN	OE1-CD-NE2	-7.32	115.28	122.60
1	Y	50	PHE	CA-CB-CG	7.30	121.11	113.80
1	X	11	ASP	CA-CB-CG	7.05	119.65	112.60
1	Y	119	THR	O-C-N	7.02	131.92	122.59
1	Y	26	ASN	N-CA-C	-6.96	92.46	107.49
1	Y	99	ASN	O-C-N	6.88	131.32	123.06
1	X	66	GLU	O-C-N	-6.71	115.00	122.12
1	Y	85	GLU	N-CA-C	-6.70	99.30	109.95
1	Y	8	LYS	O-C-N	-6.59	117.20	121.88
1	Y	59	ARG	CB-CG-CD	6.56	126.39	111.30
1	X	34	GLN	CG-CD-NE2	6.55	126.22	116.40
1	Y	86	ILE	N-CA-C	-6.46	99.12	108.36
1	Y	100	ASN	CB-CG-ND2	6.41	126.02	116.40
1	X	122	ASN	OD1-CG-ND2	-6.36	116.24	122.60
1	Y	79	GLU	N-CA-C	-6.32	104.47	111.36
1	Y	27	ASN	OD1-CG-ND2	-6.16	116.44	122.60
1	Y	110	HIS	CB-CG-CD2	-6.15	123.20	131.20
1	X	4	ILE	CA-CB-CG1	-5.97	100.25	110.40
1	Y	34	GLN	OE1-CD-NE2	-5.90	116.70	122.60
1	Y	79	GLU	CA-C-O	-5.83	114.24	120.42
1	X	113	LYS	N-CA-C	-5.82	99.04	108.41
1	Y	112	TRP	CG-CD2-CE3	5.80	139.71	133.90
1	X	87	VAL	CA-C-N	5.74	125.69	119.78
1	X	87	VAL	C-N-CA	5.74	125.69	119.78
1	Y	108	GLN	N-CA-C	-5.65	105.64	112.54
1	Y	27	ASN	CB-CG-ND2	5.64	124.86	116.40
1	Y	96	ASP	CA-C-N	5.61	132.26	121.54
1	Y	96	ASP	C-N-CA	5.61	132.26	121.54
1	Y	107	LYS	CB-CG-CD	5.52	124.01	111.30
1	X	109	LYS	CA-CB-CG	5.50	125.09	114.10
1	X	76	TRP	CE2-CD2-CG	-5.41	100.71	107.20
1	X	112	TRP	CE2-CD2-CG	-5.38	100.74	107.20
1	Y	98	THR	N-CA-CB	5.36	119.55	110.49
1	X	54	LEU	CA-C-N	5.36	127.72	120.65
1	X	54	LEU	C-N-CA	5.36	127.72	120.65
1	X	85	GLU	CA-CB-CG	5.32	124.73	114.10
1	Y	76	TRP	CE2-CD2-CG	-5.28	100.86	107.20
1	Y	69	VAL	N-CA-C	-5.26	105.37	110.42
1	X	49	HIS	CB-CG-CD2	-5.21	124.42	131.20
1	X	4	ILE	N-CA-CB	-5.20	103.70	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	81	TRP	CE2-CD2-CE3	5.19	123.99	118.80
1	Y	112	TRP	CE2-CD2-CG	-5.18	100.98	107.20
1	X	100	ASN	OD1-CG-ND2	-5.17	117.43	122.60
1	Y	67	ASP	N-CA-C	5.15	116.58	111.07
1	X	22	MET	CA-CB-CG	5.14	124.37	114.10
1	X	108	GLN	CA-CB-CG	5.12	124.33	114.10
1	Y	98	THR	N-CA-C	-5.06	100.02	110.80
1	X	122	ASN	CB-CG-ND2	5.03	123.95	116.40
1	Y	120	ILE	N-CA-CB	-5.03	102.94	111.50
1	X	100	ASN	N-CA-C	-5.03	100.98	109.07
1	X	16	LYS	N-CA-CB	-5.02	102.73	110.01
1	Y	47	ILE	N-CA-C	-5.01	101.19	108.36
1	Y	85	GLU	N-CA-CB	5.01	118.87	110.85
1	X	29	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

There are no planarity outliers.

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	X	1026	0	1057	22	0
1	Y	1014	0	1048	25	0
2	X	44	0	0	3	0
2	Y	27	0	0	0	0
All	All	2111	0	2105	45	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 11.

All (45) 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:X:1:MET:N	2:X:150:HOH:O	2.27	0.66
1:Y:17:GLU:O	1:Y:20:THR:HB	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:21:ARG:HD3	1:X:109:LYS:HD3	1.79	0.64
1:Y:39:LEU:HD11	1:Y:53:MET:HE3	1.81	0.63
1:Y:32:LEU:HD22	1:Y:104:ILE:HD13	1.83	0.61
1:Y:31:VAL:HG22	1:Y:113:LYS:HB3	1.84	0.59
1:X:88:PRO:HA	1:Y:95:LYS:HB2	1.85	0.56
1:X:110:HIS:HD2	1:X:111:GLU:HG3	1.70	0.56
1:Y:26:ASN:HD21	1:Y:29:ASP:HB2	1.72	0.55
1:X:26:ASN:HB3	1:X:31:VAL:HG13	1.87	0.55
1:Y:98:THR:HG22	1:Y:99:ASN:H	1.73	0.54
1:X:14:LYS:NZ	1:X:83:LEU:HD22	2.25	0.51
1:X:106:PHE:O	1:X:109:LYS:HG2	2.11	0.51
1:X:50:PHE:O	1:X:54:LEU:HG	2.12	0.50
1:Y:70:ARG:HE	1:Y:99:ASN:HB3	1.76	0.50
1:Y:20:THR:HG22	1:Y:21:ARG:HG3	1.94	0.50
1:Y:117:LYS:O	1:Y:119:THR:N	2.45	0.50
1:Y:4:ILE:HG13	1:Y:85:GLU:O	2.12	0.48
1:Y:20:THR:HG23	1:Y:114:LEU:HD13	1.96	0.48
1:Y:54:LEU:O	1:Y:59:ARG:HB2	2.13	0.48
1:X:22:MET:HE3	1:X:77:LEU:HD23	1.96	0.48
1:X:32:LEU:HD22	1:X:104:ILE:HG12	1.95	0.48
1:Y:4:ILE:HD11	1:Y:84:ILE:HD12	1.96	0.47
1:Y:23:GLY:HA3	1:Y:33:TYR:O	2.13	0.47
1:X:22:MET:HE2	1:X:74:ILE:HG23	1.97	0.46
1:X:91:ARG:HH21	1:Y:91:ARG:HB3	1.80	0.46
1:Y:54:LEU:HD13	1:Y:118:TYR:HD1	1.81	0.46
1:X:26:ASN:HB3	1:X:31:VAL:CG1	2.47	0.44
2:X:142:HOH:O	1:Y:91:ARG:HD2	2.16	0.44
1:X:87:VAL:HA	1:X:88:PRO:HD2	1.83	0.44
1:Y:12:PHE:HD1	1:Y:13:LEU:HD13	1.83	0.44
1:Y:70:ARG:NE	1:Y:99:ASN:HB3	2.32	0.44
1:Y:102:ARG:HG3	1:Y:104:ILE:HD12	2.00	0.43
1:X:3:GLU:HG2	1:X:4:ILE:N	2.34	0.43
1:Y:63:MET:HE1	1:Y:71:ARG:HH12	1.83	0.43
1:X:25:ALA:H	1:X:100:ASN:ND2	2.16	0.42
1:Y:59:ARG:HB3	1:Y:61:VAL:HG23	2.01	0.42
1:X:4:ILE:HG22	1:X:45:TYR:HB2	2.02	0.42
1:X:22:MET:CE	1:X:77:LEU:HD23	2.49	0.42
1:Y:54:LEU:HD13	1:Y:118:TYR:CD1	2.55	0.42
1:X:99:ASN:HB2	2:X:149:HOH:O	2.19	0.41
1:Y:87:VAL:HA	1:Y:88:PRO:HD2	1.89	0.41
1:X:4:ILE:HD11	1:X:86:ILE:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:22:MET:HA	1:X:102:ARG:O	2.21	0.41
1:X:14:LYS:HZ3	1:X:83:LEU:HD22	1.85	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	X	120/122 (98%)	112 (93%)	6 (5%)	2 (2%)	7	2
1	Y	118/122 (97%)	111 (94%)	4 (3%)	3 (2%)	4	1
All	All	238/244 (98%)	223 (94%)	10 (4%)	5 (2%)	5	1

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	99	ASN
1	Y	119	THR
1	Y	98	THR
1	X	98	THR
1	Y	118	TYR

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	X	114/114 (100%)	102 (90%)	12 (10%)	6	2
1	Y	113/114 (99%)	100 (88%)	13 (12%)	5	2
All	All	227/228 (100%)	202 (89%)	25 (11%)	6	2

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	4	ILE
1	X	6	LEU
1	X	7	LYS
1	X	16	LYS
1	X	28	LYS
1	X	29	ASP
1	X	31	VAL
1	X	60	GLN
1	X	63	MET
1	X	98	THR
1	X	104	ILE
1	X	113	LYS
1	Y	4	ILE
1	Y	6	LEU
1	Y	8	LYS
1	Y	20	THR
1	Y	26	ASN
1	Y	54	LEU
1	Y	59	ARG
1	Y	62	GLU
1	Y	65	GLU
1	Y	87	VAL
1	Y	97	LEU
1	Y	104	ILE
1	Y	107	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	60	GLN
1	X	90	GLN
1	X	100	ASN
1	X	108	GLN
1	X	110	HIS

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Mol	Chain	Res	Type
1	Y	34	GLN
1	Y	49	HIS
1	Y	110	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.