



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:47 AM UTC

PDB ID : 3ORE / pdb_00003ore
Title : Crystal structure of TTHA0988 in space group P6522
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RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2010-09-07
Resolution : 2.90 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)	:	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

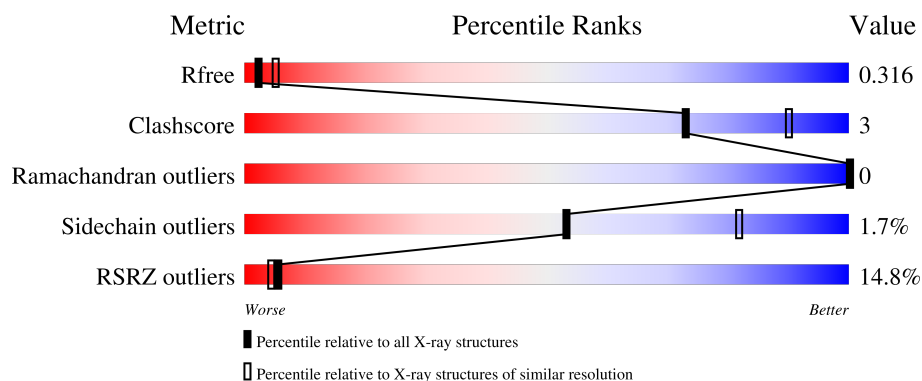
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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 $\leq 5\%$. 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	494	9% 89% 8% .
1	B	494	13% 49% . 47%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5454 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 Putative uncharacterized protein TTHA0988.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	0	0
			3588	2326	644	616	2			
1	B	263	Total	C	N	O	S	0	0	0
			1866	1204	337	323	2			

4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	142.07Å 142.07Å 259.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.87 – 2.90 47.87 – 2.90	Depositor EDS
% Data completeness (in resolution range)	91.7 (47.87-2.90) 91.7 (47.87-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.51 (at 2.91Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.285 , 0.316 0.288 , 0.316	Depositor DCC
R_{free} test set	1625 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	60.7	Xtriage
Anisotropy	0.497	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 59.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	5454	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% 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	0.41	0/3692	0.66	0/5048
1	B	0.44	0/1916	0.67	0/2614
All	All	0.42	0/5608	0.66	0/7662

There are no bond length outliers.

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	3588	0	3634	23	0
1	B	1866	0	1828	12	0
All	All	5454	0	5462	35	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 3.

All (35) 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:342:VAL:HG11	1:A:349:ALA:HB1	1.46	0.95
1:A:342:VAL:HG11	1:A:349:ALA:CB	2.06	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:LEU:HD11	1:A:367:LEU:HD12	1.61	0.81
1:A:151:ALA:HB2	1:A:170:LEU:HD23	1.65	0.78
1:A:214:LEU:HD11	1:A:234:VAL:HG21	1.67	0.75
1:A:392:LEU:HD11	1:A:480:LEU:HD21	1.70	0.72
1:A:214:LEU:CD2	1:A:342:VAL:HG22	2.26	0.64
1:B:255:ALA:HB3	1:B:256:PRO:HD3	1.82	0.61
1:B:455:VAL:HG11	1:B:480:LEU:HD13	1.81	0.61
1:A:135:LEU:HD12	1:A:136:PRO:HD2	1.82	0.61
1:B:301:LEU:HD11	1:B:324:ARG:CZ	2.35	0.57
1:B:301:LEU:HD11	1:B:324:ARG:NH2	2.19	0.56
1:A:115:TYR:CE1	1:A:127:ALA:HB3	2.42	0.54
1:B:330:VAL:HG11	1:B:484:ARG:HB3	1.90	0.54
1:B:342:VAL:HG11	1:B:349:ALA:HB1	1.89	0.53
1:B:442:LEU:HG	1:B:477:LEU:HD11	1.91	0.53
1:B:228:PRO:HD3	1:B:363:ALA:HB2	1.93	0.51
1:A:22:LEU:HD21	1:A:192:GLY:HA3	1.93	0.50
1:A:127:ALA:HB1	1:A:128:GLU:HA	1.93	0.50
1:A:59:ARG:CZ	1:A:63:LEU:HD11	2.41	0.49
1:B:457:LEU:HD22	1:B:477:LEU:HD21	1.95	0.48
1:A:175:LEU:HD12	1:A:200:ALA:HB3	1.94	0.48
1:A:386:LEU:HD12	1:A:387:PRO:HD2	1.96	0.48
1:A:5:PHE:CE1	1:A:7:LEU:HD11	2.50	0.46
1:A:78:VAL:HG21	1:A:189:LEU:HD23	1.99	0.44
1:A:5:PHE:HE1	1:A:7:LEU:HD11	1.84	0.43
1:B:455:VAL:HG11	1:B:480:LEU:CD1	2.48	0.42
1:A:24:LEU:HD22	1:A:64:LEU:HD22	2.02	0.42
1:A:407:ALA:HB3	1:A:430:VAL:HG13	2.01	0.42
1:A:441:PRO:CD	1:A:468:LYS:HD2	2.50	0.42
1:A:213:LEU:HD11	1:A:357:ILE:HG22	2.02	0.41
1:A:423:VAL:HG12	1:A:425:LEU:CD1	2.51	0.41
1:B:265:VAL:HG13	1:B:292:ALA:HB2	2.03	0.40
1:B:223:LEU:O	1:B:223:LEU:HD12	2.21	0.40
1:A:214:LEU:HD23	1:A:342:VAL:HG13	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	475/494 (96%)	455 (96%)	20 (4%)	0	100	100
1	B	255/494 (52%)	241 (94%)	14 (6%)	0	100	100
All	All	730/988 (74%)	696 (95%)	34 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	357/381 (94%)	353 (99%)	4 (1%)	65	88
1	B	172/381 (45%)	167 (97%)	5 (3%)	37	71
All	All	529/762 (69%)	520 (98%)	9 (2%)	53	82

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ASP
1	A	100	LEU
1	A	273	LEU
1	A	405	PHE
1	B	230	LEU
1	B	241	LEU
1	B	273	LEU
1	B	301	LEU

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Mol	Chain	Res	Type
1	B	477	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

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	481/494 (97%)	0.58	45 (9%) 14 12	37, 57, 92, 108	0
1	B	263/494 (53%)	1.33	65 (24%) 2 1	50, 86, 151, 172	0
All	All	744/988 (75%)	0.85	110 (14%) 5 4	37, 64, 127, 172	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	434	GLU	10.0
1	B	241	LEU	7.4
1	B	221	PRO	6.9
1	B	403	GLU	6.7
1	A	327	GLY	6.6
1	B	448	PRO	6.3
1	B	244	HIS	5.8
1	B	463	LEU	5.6
1	B	398	PRO	5.2
1	B	430	VAL	4.9
1	A	372	LEU	4.6
1	B	242	GLY	4.6
1	B	358	GLY	4.4
1	A	493	SER	4.4
1	A	67	LEU	4.2
1	B	465	GLY	4.1
1	A	11	GLU	4.1
1	A	94	SER	4.0
1	A	407	ALA	4.0
1	B	461	GLY	3.9
1	A	140	HIS	3.9
1	A	404	ALA	3.9
1	B	396	PRO	3.7
1	B	231	MET	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	269	ALA	3.4
1	B	453	PRO	3.4
1	B	355	GLY	3.4
1	A	431	PRO	3.3
1	A	406	ARG	3.3
1	A	2	VAL	3.3
1	B	492	THR	3.3
1	B	247	LEU	3.2
1	A	492	THR	3.2
1	B	286	LEU	3.1
1	B	429	GLU	3.1
1	B	407	ALA	3.1
1	A	137	ARG	3.1
1	B	245	LEU	3.1
1	B	389	ALA	3.0
1	B	462	SER	3.0
1	A	62	ARG	3.0
1	A	397	GLY	3.0
1	A	426	LEU	3.0
1	A	87	GLU	3.0
1	B	394	LEU	2.9
1	B	401	ALA	2.9
1	B	269	ALA	2.9
1	A	268	GLY	2.9
1	B	395	LEU	2.9
1	B	379	ARG	2.8
1	B	353	LEU	2.8
1	B	263	ARG	2.8
1	B	373	ARG	2.8
1	A	9	PHE	2.8
1	B	466	TYR	2.8
1	B	356	ARG	2.7
1	B	240	PHE	2.7
1	B	404	ALA	2.7
1	A	405	PHE	2.7
1	B	234	VAL	2.7
1	A	429	GLU	2.7
1	A	57	ARG	2.6
1	A	328	PRO	2.6
1	B	343	ARG	2.6
1	A	374	PRO	2.6
1	A	403	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	467	ALA	2.6
1	B	402	GLY	2.5
1	A	417	ARG	2.5
1	B	287	ARG	2.5
1	B	361	LEU	2.5
1	B	493	SER	2.5
1	A	375	VAL	2.5
1	B	230	LEU	2.4
1	A	430	VAL	2.4
1	B	243	GLY	2.4
1	B	376	ARG	2.4
1	B	357	ILE	2.4
1	B	346	LEU	2.4
1	A	432	GLY	2.4
1	B	411	GLY	2.4
1	B	285	ALA	2.4
1	A	425	LEU	2.4
1	B	431	PRO	2.4
1	A	3	ARG	2.3
1	B	400	PHE	2.3
1	A	416	ALA	2.3
1	B	468	LYS	2.3
1	A	259	ARG	2.3
1	A	305	GLU	2.3
1	A	412	PRO	2.3
1	A	468	LYS	2.2
1	A	490	HIS	2.2
1	A	452	ARG	2.2
1	A	388	GLU	2.2
1	B	444	GLY	2.1
1	A	384	ARG	2.1
1	B	248	ALA	2.1
1	B	456	LEU	2.1
1	A	185	THR	2.1
1	B	249	ARG	2.1
1	B	342	VAL	2.1
1	B	314	LEU	2.1
1	A	76	ARG	2.1
1	B	406	ARG	2.1
1	B	399	GLN	2.0
1	B	421	VAL	2.0
1	A	394	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	340	LEU	2.0
1	B	433	GLY	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.