



Full wwPDB X-ray Structure Validation Report

Sep 26, 2014 – 04:00 PM EDT

PDB ID : 4QAS
Title : 1.27 Å resolution structure of CT263-D161N (MTAN) from Chlamydia trachomatis
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Deposited on : 2014-05-05
Resolution : 1.25 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

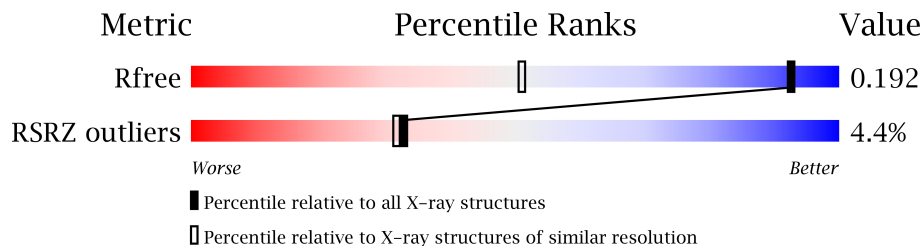
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : **FAILED**
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23828
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23828

1 Overall quality at a glance

The reported resolution of this entry is 1.25 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}	66092	1021 (1.30-1.22)
RSRZ outliers	66119	1021 (1.30-1.22)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6479 atoms, of which 3085 are hydrogens and 0 are deuterium.

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 CT263.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	197	Total	C	H	N	O	S	0	7	0
			3150	1026	1585	244	288	7			
1	B	187	Total	C	H	N	O	S	0	6	0
			2972	967	1500	229	268	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	EXPRESSION TAG	UNP B0B7H9
A	-3	SER	-	EXPRESSION TAG	UNP B0B7H9
A	-2	THR	-	EXPRESSION TAG	UNP B0B7H9
A	-1	GLY	-	EXPRESSION TAG	UNP B0B7H9
A	0	SER	-	EXPRESSION TAG	UNP B0B7H9
A	161	ASN	ASP	ENGINEERED MUTATION	UNP B0B7H9
B	-4	GLY	-	EXPRESSION TAG	UNP B0B7H9
B	-3	SER	-	EXPRESSION TAG	UNP B0B7H9
B	-2	THR	-	EXPRESSION TAG	UNP B0B7H9
B	-1	GLY	-	EXPRESSION TAG	UNP B0B7H9
B	0	SER	-	EXPRESSION TAG	UNP B0B7H9
B	161	ASN	ASP	ENGINEERED MUTATION	UNP B0B7H9

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	193	Total	O	0	0
			193	193		
3	B	159	Total	O	0	0
			159	159		

3 Residue-property plots

MolProbity failed to run properly - this section will therefore be empty.

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	65.44Å 104.15Å 58.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.37 – 1.25 55.41 – 1.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (33.37-1.25) 99.9 (55.41-1.25)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 1.25Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.174 , 0.192 0.174 , 0.192	Depositor DCC
R_{free} test set	5516 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	16.3	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 44.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 110328 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6479	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

MolProbity failed to run properly - this section will therefore be empty.

5.2 Close contacts ⓘ

MolProbity failed to run properly - this section will therefore be empty.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

MolProbity failed to run properly - this section will therefore be empty.

5.3.2 Protein sidechains ⓘ

MolProbity failed to run properly - this section will therefore be empty.

5.3.3 RNA ⓘ

MolProbity failed to run properly - this section will therefore be empty.

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	201	-	4,4,4	0.18	0	6,6,6	0.09	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	201	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	197/201 (98%)	0.01	7 (3%) 41 41	12, 21, 53, 88	0
1	B	187/201 (93%)	-0.01	10 (5%) 25 25	13, 20, 56, 108	0
All	All	384/402 (95%)	0.00	17 (4%) 33 32	12, 21, 55, 108	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	196	VAL	7.9
1	B	194	ILE	5.2
1	B	96	PRO	5.1
1	A	124	TYR	4.6
1	B	95	THR	4.5
1	A	123	PRO	3.5
1	B	193	PHE	3.4
1	B	102	GLU	2.8
1	B	125	ARG	2.6
1	A	126	ASP	2.6
1	A	50	TYR	2.3
1	A	0	SER	2.2
1	B	126	ASP	2.2
1	B	124	TYR	2.2
1	B	128	PHE	2.2
1	B	123	PRO	2.1
1	A	1	MET	2.0

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 carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	A	201	5/5	0.14	0.94	68,76,84,84	0

6.5 Other polymers

There are no such residues in this entry.