wwPDB X-ray Structure Validation Summary Report (i)

Nov 10, 2024 – 07:40 PM EST

PDB ID	:	1RCW
Title	:	Crystal structure of CT610 from Chlamydia trachomatis
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Deposited on	:	2003-11-04
Resolution	:	2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

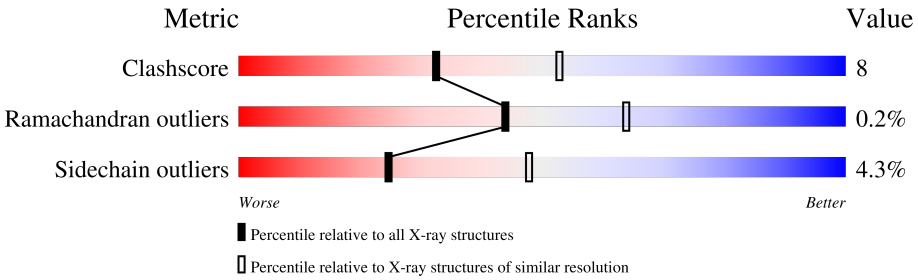
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	FAILED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)

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 <=5%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	231	76% 14% • 8%
1	B	231	78% 13% • 7%
1	C	231	75% 16% • 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5361 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 CT610.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	Se	0	0	0
			1739	1115	284	334	2	4			
1	B	214	Total	C	N	O	S	Se	0	0	0
			1747	1119	285	337	2	4			
1	C	213	Total	C	N	O	S	Se	0	0	0
			1700	1096	276	322	2	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	MSE	MET	modified residue	UNP O84616
A	79	MSE	MET	modified residue	UNP O84616
A	123	MSE	MET	modified residue	UNP O84616
A	191	MSE	MET	modified residue	UNP O84616
B	21	MSE	MET	modified residue	UNP O84616
B	79	MSE	MET	modified residue	UNP O84616
B	123	MSE	MET	modified residue	UNP O84616
B	191	MSE	MET	modified residue	UNP O84616
C	21	MSE	MET	modified residue	UNP O84616
C	79	MSE	MET	modified residue	UNP O84616
C	123	MSE	MET	modified residue	UNP O84616
C	191	MSE	MET	modified residue	UNP O84616

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Fe	0	0
			2	2		
2	B	2	Total	Fe	0	0
			2	2		
2	C	2	Total	Fe	0	0
			2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	71	Total O 71 71	0	0
3	B	72	Total O 72 72	0	0
3	C	26	Total O 26 26	0	0

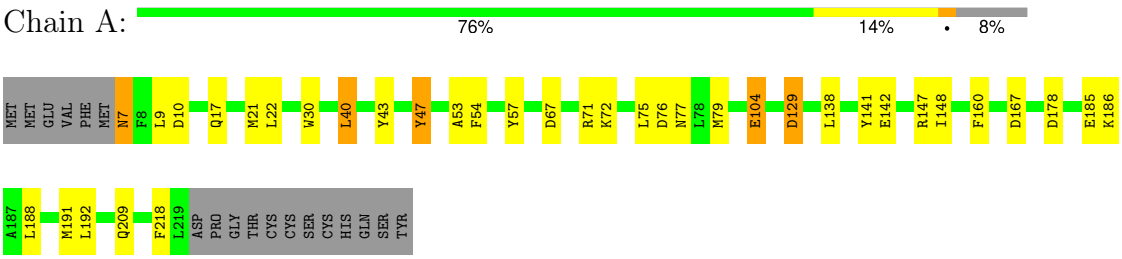
3 Residue-property plots (i)

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 failed to run properly.

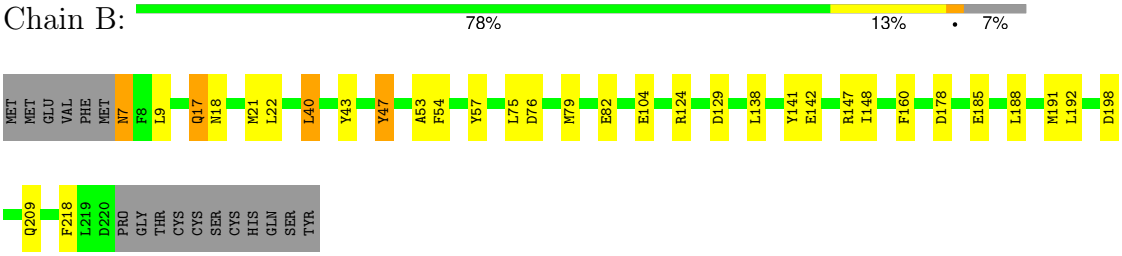
- Molecule 1: CT610

Chain A:



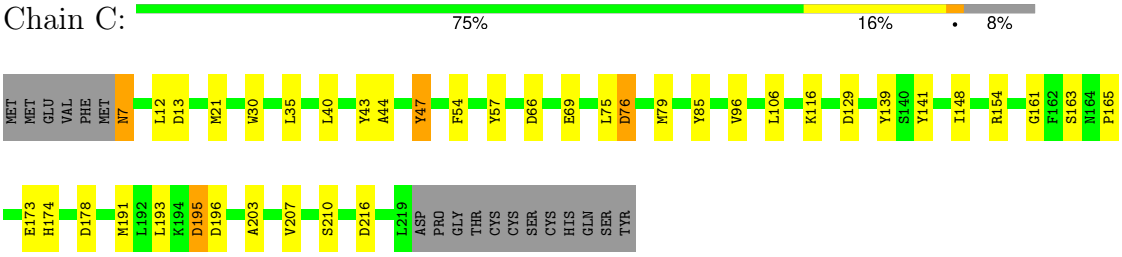
- Molecule 1: CT610

Chain B:



- Molecule 1: CT610

Chain C:



4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	77.55Å 192.97Å 93.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 2.50	Depositor
% Data completeness (in resolution range)	96.8 (29.88-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.79 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.1	Depositor
R, R_{free}	0.191 , 0.258	Depositor
Wilson B-factor (Å^2)	32.2	Xtriage
Anisotropy	0.471	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5361	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.54 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.7189e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

Bond lengths and bond angles in the following residue types are not validated in this section: FE

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	0.82	0/1777	0.90	5/2397 (0.2%)
1	B	0.88	2/1785 (0.1%)	0.93	6/2408 (0.2%)
1	C	0.73	0/1738	0.88	7/2349 (0.3%)
All	All	0.81	2/5300 (0.0%)	0.90	18/7154 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	9	LEU	CG-CD1	-9.62	1.16	1.51
1	B	9	LEU	CG-CD2	-9.01	1.18	1.51

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	9	LEU	CD1-CG-CD2	-10.05	80.34	110.50
1	B	9	LEU	CB-CG-CD2	9.19	126.62	111.00
1	A	10	ASP	CB-CG-OD2	7.07	124.66	118.30
1	B	9	LEU	CB-CG-CD1	6.88	122.70	111.00
1	C	76	ASP	CB-CG-OD2	6.86	124.48	118.30

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	1739	0	1668	33	1
1	B	1747	0	1672	26	1
1	C	1700	0	1616	20	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	71	0	0	9	0
3	B	72	0	0	8	1
3	C	26	0	0	1	0
All	All	5361	0	4956	79	2

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 8.

The worst 5 of 79 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:17:GLN:NE2	3:A:524:HOH:O	1.81	1.09
1:C:43:TYR:OH	1:C:47:TYR:HE1	1.39	1.03
1:A:104:GLU:OE1	3:A:529:HOH:O	1.82	0.97
1:B:43:TYR:OH	1:B:47:TYR:CE1	2.20	0.94
1:A:43:TYR:OH	1:A:47:TYR:CE1	2.26	0.87

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:GLN:NE2	3:B:514:HOH:O[3_654]	1.44	0.76
1:A:104:GLU:OE2	1:C:85:TYR:O[7_544]	1.65	0.55

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	211/231 (91%)	208 (99%)	3 (1%)	0	100	100
1	B	212/231 (92%)	208 (98%)	4 (2%)	0	100	100
1	C	211/231 (91%)	205 (97%)	5 (2%)	1 (0%)	25	44
All	All	634/693 (92%)	621 (98%)	12 (2%)	1 (0%)	44	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	161	GLY

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	182/196 (93%)	175 (96%)	7 (4%)	28	53
1	B	183/196 (93%)	176 (96%)	7 (4%)	28	53
1	C	173/196 (88%)	164 (95%)	9 (5%)	19	39
All	All	538/588 (92%)	515 (96%)	23 (4%)	25	48

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	7	ASN
1	C	69	GLU
1	C	47	TYR
1	C	75	LEU
1	A	209	GLN

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	7	ASN
1	C	7	ASN

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Mol	Chain	Res	Type
1	C	174	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.