



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:03 AM GMT

PDB ID : 2VRC  
Title : CRYSTAL STRUCTURE OF THE CITROBACTER SP. TRIPHENYL-METHANE REDUCTASE COMPLEXED WITH NADP(H)  
Authors : Kim, Y.; Park, H.J.; Kwak, S.N.; Lee, J.S.; Oh, T.K.; Kim, M.H.  
Deposited on : 2008-03-31  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

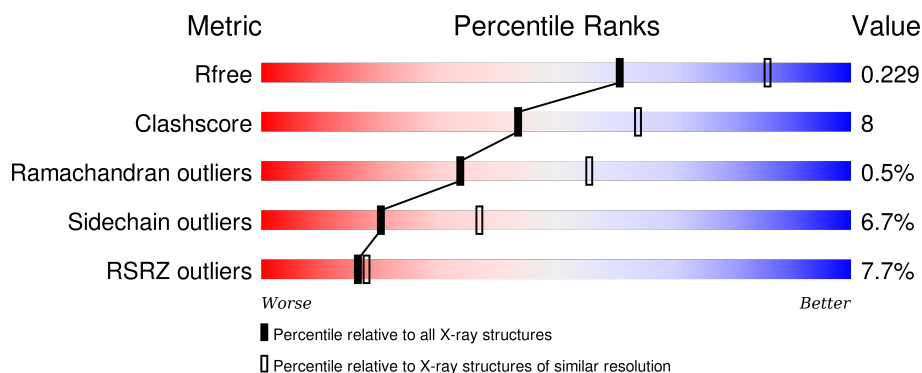
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	287	<div> <div>3%</div> <div>85%</div> <div>11%</div> <div>..</div> </div>
1	B	287	<div> <div>3%</div> <div>82%</div> <div>16%</div> <div>..</div> </div>
1	C	287	<div> <div>14%</div> <div>74%</div> <div>21%</div> <div>..</div> </div>
2	D	287	<div> <div>10%</div> <div>81%</div> <div>16%</div> <div>..</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8912 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 TRIPHENYLMETHANE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	Se	0	1	0
			2170	1379	367	422	2			
1	B	285	Total	C	N	O	Se	0	1	0
			2168	1376	367	423	2			
1	C	285	Total	C	N	O	Se	0	0	0
			2162	1373	366	421	2			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	PHE	MET	CONFLICT	UNP Q2TNI4
A	21	MSE	LEU	ENGINEERED MUTATION	UNP Q2TNI4
A	22	ALA	LYS	ENGINEERED MUTATION	UNP Q2TNI4
A	23	ALA	LYS	ENGINEERED MUTATION	UNP Q2TNI4
A	156	THR	ILE	CONFLICT	UNP Q2TNI4
A	235	MSE	LEU	ENGINEERED MUTATION	UNP Q2TNI4
B	1	PHE	MET	CONFLICT	UNP Q2TNI4
B	21	MSE	LEU	ENGINEERED MUTATION	UNP Q2TNI4
B	22	ALA	LYS	ENGINEERED MUTATION	UNP Q2TNI4
B	23	ALA	LYS	ENGINEERED MUTATION	UNP Q2TNI4
B	156	THR	ILE	CONFLICT	UNP Q2TNI4
B	235	MSE	LEU	ENGINEERED MUTATION	UNP Q2TNI4
C	1	PHE	MET	CONFLICT	UNP Q2TNI4
C	21	MSE	LEU	ENGINEERED MUTATION	UNP Q2TNI4
C	22	ALA	LYS	ENGINEERED MUTATION	UNP Q2TNI4
C	23	ALA	LYS	ENGINEERED MUTATION	UNP Q2TNI4
C	156	THR	ILE	CONFLICT	UNP Q2TNI4
C	235	MSE	LEU	ENGINEERED MUTATION	UNP Q2TNI4

- Molecule 2 is a protein called TRIPHENYLMETHANE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	285	Total	C	N	O	Se	0	1	0
			2170	1376	368	424	2			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	PHE	MET	CONFLICT	UNP Q2TNI4
D	21	MSE	LEU	ENGINEERED MUTATION	UNP Q2TNI4
D	22	ALA	LYS	ENGINEERED MUTATION	UNP Q2TNI4
D	23	ALA	LYS	ENGINEERED MUTATION	UNP Q2TNI4
D	128	THR	ILE	CONFLICT	UNP Q2TNI4
D	156	THR	ILE	CONFLICT	UNP Q2TNI4
D	235	MSE	LEU	ENGINEERED MUTATION	UNP Q2TNI4

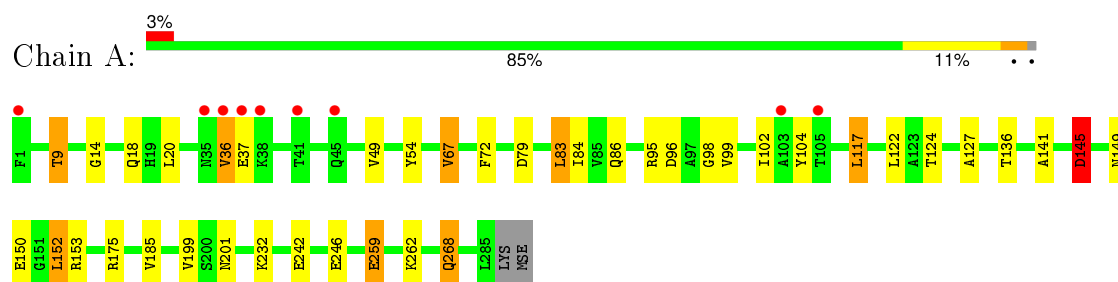
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	76	Total	O	0	0
			76	76		
3	B	80	Total	O	0	0
			80	80		
3	C	34	Total	O	0	0
			34	34		
3	D	52	Total	O	0	0
			52	52		

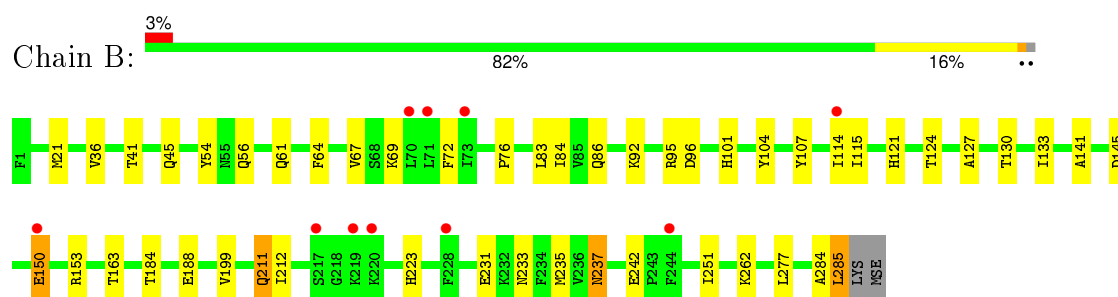
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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.

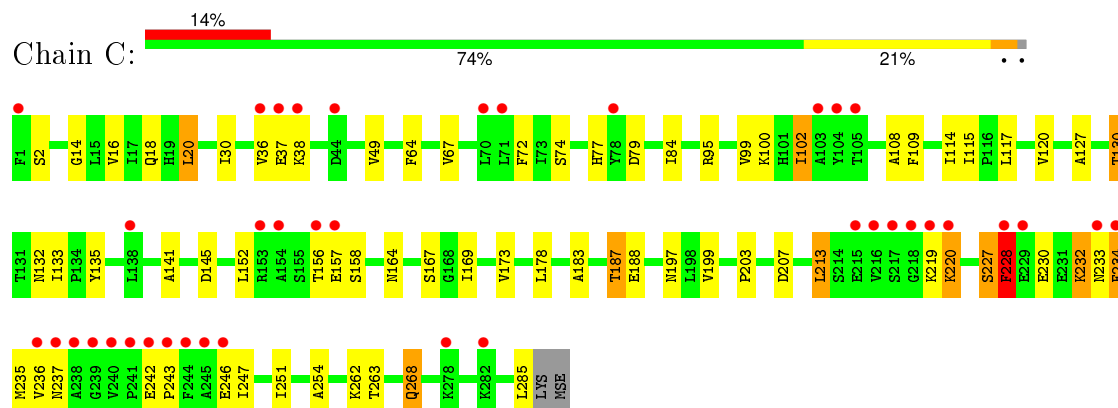
#### • Molecule 1: TRIPHENYLMETHANE REDUCTASE



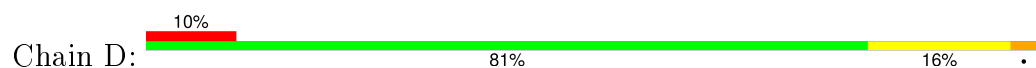
#### • Molecule 1: TRIPHENYLMETHANE REDUCTASE

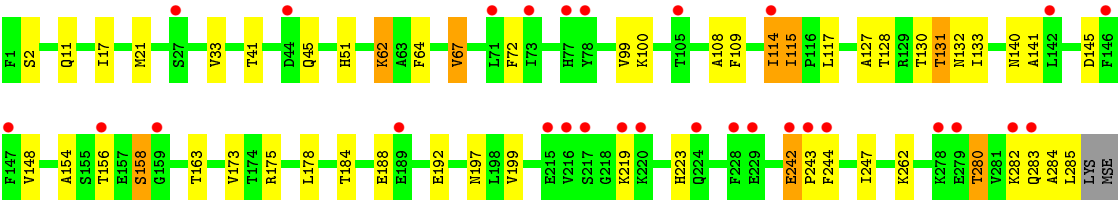


#### • Molecule 1: TRIPHENYLMETHANE REDUCTASE



#### • Molecule 2: TRIPHENYLMETHANE REDUCTASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.96Å 76.95Å 272.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.36 – 2.50 29.15 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.36-2.50) 95.9 (29.15-2.50)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	82.19 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.190 , 0.239 0.183 , 0.229	Depositor DCC
$R_{free}$ test set	2747 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.6	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 52.9	EDS
Estimated twinning fraction	0.033 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	1 of 53943 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8912	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.69	0/2208	0.77	4/3003 (0.1%)
1	B	0.65	0/2206	0.68	0/3000
1	C	0.58	1/2200 (0.0%)	0.68	1/2992 (0.0%)
2	D	0.60	0/2208	0.66	0/3003
All	All	0.63	1/8822 (0.0%)	0.70	5/11998 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	37	GLU	CB-CG	-7.27	1.38	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	228	PHE	CB-CA-C	-13.66	83.07	110.40
1	A	117[A]	LEU	CA-CB-CG	7.76	133.15	115.30
1	A	117[B]	LEU	CA-CB-CG	7.76	133.15	115.30
1	A	79	ASP	CB-CG-OD1	5.67	123.40	118.30
1	A	145	ASP	CB-CG-OD1	-5.34	113.49	118.30

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	A	2170	0	2171	25	0
1	B	2168	0	2165	41	0
1	C	2162	0	2161	47	0
2	D	2170	0	2164	41	0
3	A	76	0	0	2	0
3	B	80	0	0	4	0
3	C	34	0	0	1	0
3	D	52	0	0	2	0
All	All	8912	0	8661	141	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 8.

The worst 5 of 141 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:C:228:PHE:O	1:C:228:PHE:CD2	1.69	1.45
1:B:284:ALA:O	1:B:285:LEU:HD12	1.41	1.20
1:B:284:ALA:C	1:B:285:LEU:HD12	1.76	1.03
1:B:284:ALA:C	1:B:285:LEU:CD1	2.30	1.00
1:C:228:PHE:HD2	1:C:228:PHE:O	1.21	0.94

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	284/287 (99%)	278 (98%)	6 (2%)	0	100	100
1	B	284/287 (99%)	277 (98%)	7 (2%)	0	100	100
1	C	283/287 (99%)	264 (93%)	14 (5%)	5 (2%)	11	18
2	D	284/287 (99%)	273 (96%)	10 (4%)	1 (0%)	39	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1135/1148 (99%)	1092 (96%)	37 (3%)	6 (0%)	34 55

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	228	PHE
1	C	156	THR
1	C	220	LYS
1	C	234	PHE
1	C	38	LYS

### 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	231/229 (101%)	213 (92%)	18 (8%)	16 29
1	B	231/229 (101%)	221 (96%)	10 (4%)	35 61
1	C	230/229 (100%)	209 (91%)	21 (9%)	12 22
2	D	231/229 (101%)	217 (94%)	14 (6%)	23 42
All	All	923/916 (101%)	860 (93%)	63 (7%)	20 36

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	20	LEU
1	C	158	SER
2	D	145	ASP
1	C	72	PHE
1	C	102	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	61	GLN
1	C	164	ASN
2	D	86	GLN
1	C	86	GLN
1	C	197	ASN

### 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 carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	283/287 (98%)	0.23	9 (3%) 51 56	23, 34, 50, 61	0
1	B	283/287 (98%)	0.21	10 (3%) 48 53	23, 35, 52, 60	0
1	C	283/287 (98%)	0.60	39 (13%) 4 4	35, 46, 77, 88	0
2	D	283/287 (98%)	0.39	29 (10%) 9 9	28, 41, 63, 67	0
All	All	1132/1148 (98%)	0.36	87 (7%) 16 18	23, 39, 63, 88	0

The worst 5 of 87 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	243	PRO	6.8
2	D	216	VAL	6.6
1	C	244	PHE	5.9
1	C	242	GLU	5.4
1	A	37	GLU	4.9

### 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 carbohydrates 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.