



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2017 – 01:36 AM EDT

PDB ID : 5MSP  
Title : Structure of the unmodified PCP-R didomain of carboxylic acid reductase (CAR) from Segniliparus rugosus in complex with NADP, F2221 form  
Authors : Gahloth, D.; Leys, D.  
Deposited on : unknown  
Resolution : 2.41 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](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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20029824

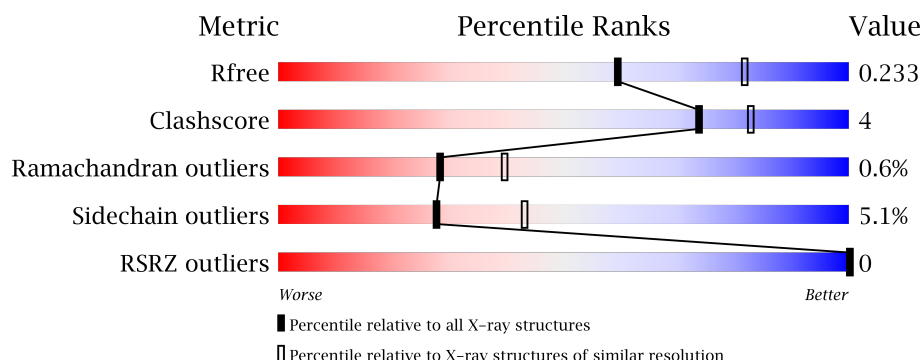
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


The reported resolution of this entry is 2.41 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))
$R_{free}$	100719	3709 (2.44-2.40)
Clashscore	112137	4241 (2.44-2.40)
Ramachandran outliers	110173	4178 (2.44-2.40)
Sidechain outliers	110143	4179 (2.44-2.40)
RSRZ outliers	101464	3740 (2.44-2.40)

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	1188	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3987 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 Thioester reductase domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	512	Total	C	N	O	S	0	0	0
			3911	2483	682	745	1			

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			40	15	6	16	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	36	Total	0	0
			36		



- Molecule 1: Thioester reductase domain-containing protein



E1121	
Q1125	
H1126	
S1127	
V1128	
L1132	
D1143	
D1171	
L1187	
LEU	

## 4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.37Å 137.68Å 202.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	101.04 – 2.41 101.04 – 2.41	Depositor EDS
% Data completeness (in resolution range)	99.2 (101.04-2.41) 99.3 (101.04-2.41)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.57 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.179 , 0.227 0.189 , 0.233	Depositor DCC
$R_{free}$ test set	1728 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	61.6	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 36.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.027 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	3987	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

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

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	0.88	2/3996 (0.1%)	0.95	17/5437 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	669	PRO	N-CA	8.91	1.62	1.47
1	A	968	ASN	CA-C	5.12	1.66	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	806	ARG	NE-CZ-NH2	-8.58	116.01	120.30
1	A	999	MET	CG-SD-CE	8.44	113.71	100.20
1	A	968	ASN	N-CA-C	7.25	130.58	111.00
1	A	1171	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	A	806	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	A	1018	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	1044	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	A	1042	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	A	838	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	A	942	VAL	N-CA-C	-5.71	95.57	111.00
1	A	838	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	A	1044	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	A	676	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	962	ILE	N-CA-C	5.22	125.10	111.00
1	A	1187	LEU	N-CA-C	-5.08	97.30	111.00
1	A	749	ARG	C-N-CD	5.03	138.96	128.40
1	A	883	ARG	NE-CZ-NH1	5.02	122.81	120.30

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	3911	0	3863	30	0
2	A	40	0	19	0	0
3	A	36	0	0	0	1
All	All	3987	0	3882	30	1

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 4.

All (30) 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:694:HIS:CE1	1:A:830:LYS:NZ	2.30	0.99
1:A:749:ARG:HH11	1:A:749:ARG:HG2	1.36	0.91
1:A:877:ARG:NH1	1:A:880:ASP:OD2	2.08	0.86
1:A:694:HIS:HE1	1:A:830:LYS:NZ	1.77	0.80
1:A:793:ARG:NH1	1:A:819:GLN:O	2.20	0.75
1:A:694:HIS:CE1	1:A:830:LYS:HZ2	2.05	0.65
1:A:694:HIS:CE1	1:A:830:LYS:HZ1	2.14	0.64
1:A:744:SER:OG	1:A:745:SER:N	2.32	0.62
1:A:751:THR:HG23	1:A:754:SER:H	1.63	0.62
1:A:749:ARG:NH1	1:A:749:ARG:HG2	2.09	0.60
1:A:1046:HIS:HD2	1:A:1081:ASP:OD1	1.90	0.54
1:A:743:ARG:HH11	1:A:743:ARG:CB	2.21	0.52
1:A:1044:ARG:HD3	1:A:1143:ASP:OD2	2.10	0.52
1:A:798:THR:HG22	1:A:799:GLY:N	2.24	0.52
1:A:694:HIS:HE1	1:A:830:LYS:HZ1	1.51	0.51
1:A:997:SER:HB2	1:A:1000:ILE:HD11	1.93	0.50
1:A:943:GLU:HG3	1:A:944:PRO:HD2	1.95	0.49
1:A:839:LEU:O	1:A:842:VAL:HG22	2.13	0.49
1:A:1046:HIS:CD2	1:A:1081:ASP:OD1	2.67	0.46
1:A:833:LYS:HG2	1:A:833:LYS:H	1.51	0.46
1:A:795:VAL:HG21	1:A:812:TRP:CE3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1077:ASN:C	1:A:1077:ASN:OD1	2.56	0.43
1:A:749:ARG:NH1	1:A:749:ARG:CG	2.73	0.43
1:A:761:THR:O	1:A:962:ILE:HG12	2.19	0.42
1:A:1018:ARG:HG2	1:A:1126:HIS:O	2.20	0.41
1:A:999:MET:HG2	1:A:1047:TYR:OH	2.21	0.41
1:A:782:ALA:HA	1:A:785:LEU:HD22	2.03	0.40
1:A:793:ARG:HD3	1:A:793:ARG:HA	1.71	0.40
1:A:798:THR:CG2	1:A:869:PHE:CE2	3.04	0.40
1:A:752:PHE:CD1	1:A:752:PHE:C	2.93	0.40

All (1) 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)
3:A:1327:HOH:O	3:A:1327:HOH:O[3_656]	1.77	0.43

## 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	506/1188 (43%)	480 (95%)	23 (4%)	3 (1%)	28	40

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1038	ALA
1	A	945	SER
1	A	958	ALA

### 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	409/947 (43%)	388 (95%)	21 (5%)	28	43

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	690	ASP
1	A	696	SER
1	A	743	ARG
1	A	764	ARG
1	A	790	SER
1	A	824	VAL
1	A	825	VAL
1	A	839	LEU
1	A	901	VAL
1	A	942	VAL
1	A	944	PRO
1	A	959	VAL
1	A	1010	LEU
1	A	1100	SER
1	A	1103	ASP
1	A	1117	ARG
1	A	1121	GLU
1	A	1125	GLN
1	A	1128	VAL
1	A	1132	LEU
1	A	1187	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	675	GLN
1	A	1046	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 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	NAP	A	1201	-	36,43,52	0.97	1 (2%)	42,67,80	1.69	7 (16%)

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	NAP	A	1201	-	-	0/23/59/67	0/4/4/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	NAP	P2B-O2X	-2.28	1.45	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	A	1201	NAP	N3A-C2A-N1A	-6.58	123.13	128.86
2	A	1201	NAP	C1B-N9A-C4A	-3.53	120.53	126.64
2	A	1201	NAP	O4D-C1D-C2D	-2.50	101.56	104.74
2	A	1201	NAP	C4A-C5A-N7A	-2.25	107.23	109.41
2	A	1201	NAP	C3B-C2B-C1B	-2.04	98.76	102.75
2	A	1201	NAP	O2D-C2D-C1D	2.34	117.85	109.96
2	A	1201	NAP	O3X-P2B-O2X	3.47	121.61	107.61

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 [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	512/1188 (43%)	0.00	0 100 100	44, 63, 95, 134	0

There are no RSRZ outliers to report.

### 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](#)

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, 95<sup>th</sup> 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAP	A	1201	40/48	0.99	0.15	0.24	39,53,60,62	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.