



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 17, 2024 – 12:37 AM EDT

PDB ID : 5MSU  
Title : Structure of the R domain of carboxylic acid reductase (CAR) from *Mycobacterium marinum* in complex with NADP, P21 form  
Authors : Gahloth, D.; Leys, D.  
Deposited on : 2017-01-05  
Resolution : 1.74 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

<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>.

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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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

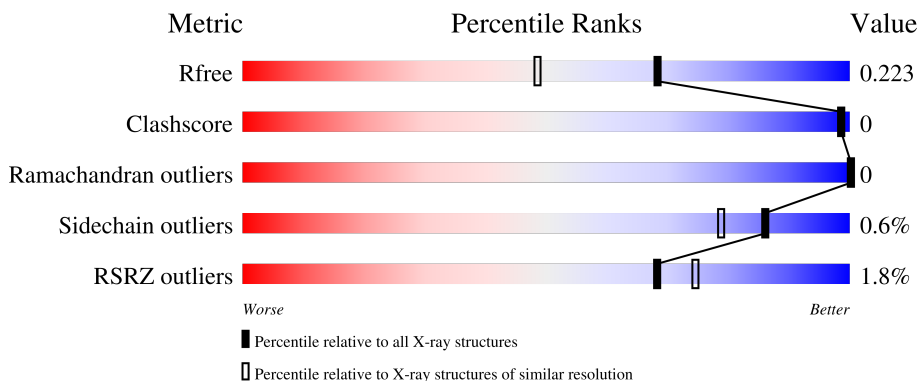
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.74 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))
$R_{free}$	130704	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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  $\geq 3$ , 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	1174	<div> <div> <div></div> <div>36%</div> <div></div> </div> <div> <div></div> <div>63%</div> <div></div> </div> </div>
1	B	1174	<div> <div> <div></div> <div>38%</div> <div></div> </div> <div> <div></div> <div>61%</div> <div></div> </div> </div>
1	C	1174	<div> <div> <div></div> <div>36%</div> <div></div> </div> <div> <div></div> <div>63%</div> <div></div> </div> </div>

## 2 Entry composition [i](#)

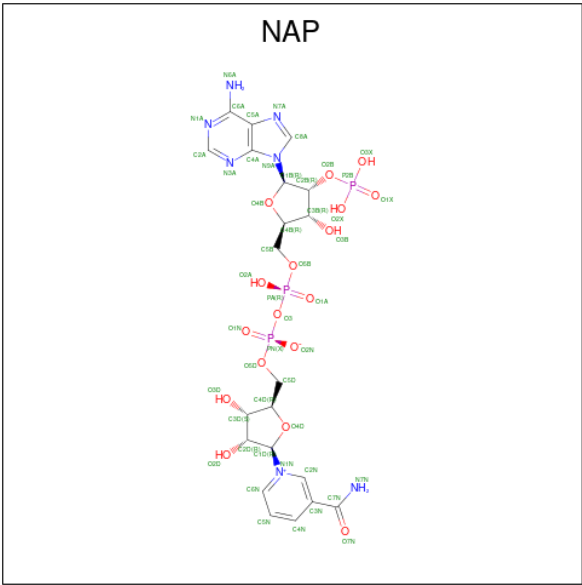
There are 3 unique types of molecules in this entry. The entry contains 11491 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Carboxylic acid reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	434	Total	C	N	O	S	0	0	0
			3354	2125	588	632	9			
1	A	436	Total	C	N	O	S	0	0	0
			3371	2134	590	638	9			
1	B	459	Total	C	N	O	S	0	0	0
			3527	2227	617	674	9			

- 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	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			39	15	5	16	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	370	Total 370	O 370	0	0
3	A	310	Total 310	O 310	0	0
3	B	424	Total 424	O 424	0	0



- Molecule 1: Carboxylic acid reductase

TYR	THR	GLY	PHE	GLY	ASP	ARG	ASP	GLN	VAL	ASP	GLY	ASN	LEU	MET
VAL	GLU	ASN	ASP	MET	GLY	GLN	GLY	GLN	VAL	VAL	GLY	ASN	ALA	SER
GLU	GLU	SER	ALA	ILE	ALA	SER	ILE	ILE	ILE	ALA	ILE	ILE	PRO	PRO
ALA	ASN	ALA	ASP	LEU	ALA	LEU	ASP	LEU	ASP	ASP	THR	VAL	ARG	ILE
ALA	GLY	ARG	GLY	ILE	ARG	THR	VAL	GLY	THR	SER	ARG	TYR	VAL	ARG
ARG	LEU	ALA	PHE	ASP	GLY	TYR	ASP	ALA	VAL	GLY	VAL	ALA	GLU	ARG
LEU	LEU	TYR	TYR	GLY	LEU	LEU	ALA	THR	LEU	LEU	VAL	THR	GLU	GLU
THR	THR	LEU	THR	ALA	LEU	ARG	ALA	THR	ALA	ALA	LEU	THR	GLU	GLU
GLY	GLY	LEU	GLY	ILE	ALA	CYS	ILE	THR	ALA	LEU	VAL	THR	LEU	ARG
SER	ILE	ALA	GLY	ARG	GLY	ASN	GLY	ASN	LEU	LEU	PHE	ASP	THR	LEU
ASP	ILE	VAL	ASP	ARG	GLN	GLY	ILE	GLY	ILE	ILE	MET	THR	ASP	GLU
VAL	LYS	ILE	ILE	PRO	VAL	GLY	THR	GLY	TYR	THR	HIS	THR	ALA	ARG
GLN	LEU	VAL	MET	ALA	LYS	THR	VAL	THR	THR	THR	HIS	LEU	GLY	ARG
PRO	ALA	PRO	GLU	VAL	ALA	ALA	ALA	ALA	SER	SER	ARG	ALA	THR	ILE
ASP	ARG	THR	GLU	LEU	GLY	TYR	GLY	TYR	GLY	GLY	GLN	ARG	GLN	GLN
ALA	PRO	GLN	VAL	ASP	ILE	PHE	ILE	PHE	SER	SER	VAL	LEU	HIS	ASP
SER	ILE	ALA	GLY	ARG	ALA	ASN	GLY	ASN	LEU	GLY	ASP	MET	THR	GLU
THR	GLY	VAL	ASP	ARG	GLN	GLY	THR	VAL	THR	GLY	ALA	ALA	PRO	MET
VAL	LYS	ILE	ILE	PRO	VAL	ALA	ASN	ALA	GLY	GLY	ALA	ALA	PRO	GLY
GLN	LEU	VAL	MET	ALA	LYS	THR	ASN	ALA	GLY	GLY	ALA	VAL	THR	TYR
PRO	ALA	PRO	GLU	VAL	LYS	GLU	ASP	LYS	ALA	ALA	HIS	VAL	LEU	ALA
ASP	ARG	THR	GLU	GLU	VAL	PHE	VAL	ASP	PRO	PRO	ARG	VAL	LEU	ASN
ALA	PRO	GLN	VAL	VAL	THR	THR	GLY	LEU	GLY	GLY	VAL	THR	LEU	ASN
SER	GLY	GLY	GLY	ASP	GLY	THR	ASP	THR	THR	THR	GLN	THR	LEU	GLN
ASN	GLN	ALA	PRO	TYR	GLY	TYR	GLY	ASP	ALA	ALA	VAL	THR	LEU	THR
GLY	LEU	ALA	PRO	LYS	ASN	ALA	ASN	LEU	VAL	ASN	ALA	THR	SER	PRO
GLN	LYS	LEU	GLU	LYS	ASN	ALA	LEU	LEU	ALA	ASN	THR	THR	TYR	ALA
VAL	LYS	LEU	GLU	VAL	ASN	GLN	VAL	LEU	VAL	VAL	ALA	GLN	THR	ALA
T747	HIS	ASP	PHE	VAL	VAL	THR	THR	PHE	ARG	ARG	ALA	GLN	GLU	ASN
T747	HIS	ASP	PHE	VAL	VAL	THR	THR	PHE	ARG	ARG	ALA	GLN	GLU	ASN
R779	GLY	GLY	GLY	PRO	GLY	THR	GLY	ASP	ALA	ALA	VAL	THR	LEU	GLN
D826	GLY	VAL	VAL	ASP	GLY	THR	GLY	THR	THR	THR	GLY	THR	LEU	GLN
D863	LEU	ALA	ALA	THR	THR	THR	THR	THR	THR	THR	THR	THR	LEU	GLN
R906	GLY	GLY	GLY	VAL	GLY	THR	THR	THR	THR	THR	THR	THR	LEU	GLN
Y952	SER	SER	SER	LEU	LEU	THR	THR	THR	THR	THR	THR	THR	LEU	GLN
D1000	ASN	ASN	THR	GLY	ASP	GLY	ASP	VAL	VAL	VAL	ALA	GLN	GLU	ALA
A1023	LEU	HIS	GLY	GLN	ILE	GLN	ILE	THR	THR	THR	THR	THR	LEU	ALA
ALA	HIS	GLY	GLY	GLN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	LEU	ALA
ASP	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	LEU	ALA
A1027	PHE	ILE	PHE	VAL	MET	PHE	PHE	THR	THR	THR	THR	THR	LEU	ALA
GLY	ASP	LYS	THR	VAL	LYS	VAL	VAL	VAL	PHE	PHE	ALA	GLN	LEU	ALA
R1030														

- Molecule 1: Carboxylic acid reductase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.54Å 58.95Å 135.56Å 90.00° 105.92° 90.00°	Depositor
Resolution (Å)	130.36 – 1.74 50.33 – 1.74	Depositor EDS
% Data completeness (in resolution range)	99.7 (130.36-1.74) 99.8 (50.33-1.74)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.75 (at 1.74Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.188 , 0.213 0.202 , 0.223	Depositor DCC
$R_{free}$ test set	7843 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.8	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 35.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11491	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 3.67% 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	0.44	0/3445	0.72	1/4694 (0.0%)
1	B	0.47	0/3602	0.76	7/4909 (0.1%)
1	C	0.44	0/3427	0.75	7/4667 (0.1%)
All	All	0.45	0/10474	0.74	15/14270 (0.1%)

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1108	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	C	906	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	C	906	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	B	985	MET	CG-SD-CE	6.20	110.12	100.20
1	C	1150	ASP	CB-CG-OD1	5.88	123.59	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	3371	0	3326	6	0
1	B	3527	0	3462	4	0
1	C	3354	0	3313	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	48	0	25	0	0
2	B	39	0	18	0	0
2	C	48	0	25	0	0
3	A	310	0	0	1	0
3	B	424	0	0	1	0
3	C	370	0	0	0	0
All	All	11491	0	10169	10	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 0.

The worst 5 of 10 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:1129:ARG:NH2	3:A:1701:HOH:O	1.97	0.81
1:A:922:ILE:O	1:A:922:ILE:HD13	2.02	0.59
1:A:872:ASP:OD2	1:B:770:ARG:HD2	2.04	0.57
1:B:1093:ASP:OD2	1:B:1097:ARG:NH2	2.44	0.50
1:A:1062:MET:SD	1:A:1133:ALA:HB3	2.56	0.46

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	432/1174 (37%)	426 (99%)	6 (1%)	0	100	100
1	B	455/1174 (39%)	447 (98%)	8 (2%)	0	100	100
1	C	428/1174 (36%)	422 (99%)	6 (1%)	0	100	100
All	All	1315/3522 (37%)	1295 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	352/946 (37%)	349 (99%)	3 (1%)	78	67
1	B	366/946 (39%)	365 (100%)	1 (0%)	92	89
1	C	350/946 (37%)	348 (99%)	2 (1%)	86	79
All	All	1068/2838 (38%)	1062 (99%)	6 (1%)	86	79

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	922	ILE
1	A	1144	GLU
1	B	916	TYR
1	C	1096	GLN
1	C	826	ASP

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

Mol	Chain	Res	Type
1	C	971	HIS
1	B	1143	GLN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

3 ligands are 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	B	1201	-	36,42,52	0.99	2 (5%)	43,65,80	1.24	6 (13%)
2	NAP	C	1201	-	45,52,52	1.30	2 (4%)	56,80,80	1.55	6 (10%)
2	NAP	A	1601	-	45,52,52	1.46	3 (6%)	56,80,80	1.61	9 (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	B	1201	-	-	4/23/56/67	0/4/4/5
2	NAP	C	1201	-	-	4/31/67/67	0/5/5/5
2	NAP	A	1601	-	-	8/31/67/67	0/5/5/5

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1601	NAP	C4N-C3N	7.02	1.51	1.39
2	C	1201	NAP	C4N-C3N	6.65	1.50	1.39
2	A	1601	NAP	C5N-C4N	3.17	1.45	1.38
2	B	1201	NAP	C5A-C4A	2.59	1.47	1.40
2	C	1201	NAP	C5N-C4N	2.53	1.44	1.38

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1201	NAP	C5N-C4N-C3N	-5.87	113.40	120.34
2	A	1601	NAP	C5N-C4N-C3N	-5.85	113.42	120.34
2	A	1601	NAP	C3N-C7N-N7N	4.45	123.09	117.75
2	C	1201	NAP	N3A-C2A-N1A	-4.21	122.09	128.68
2	A	1601	NAP	N3A-C2A-N1A	-3.91	122.57	128.68

There are no chirality outliers.

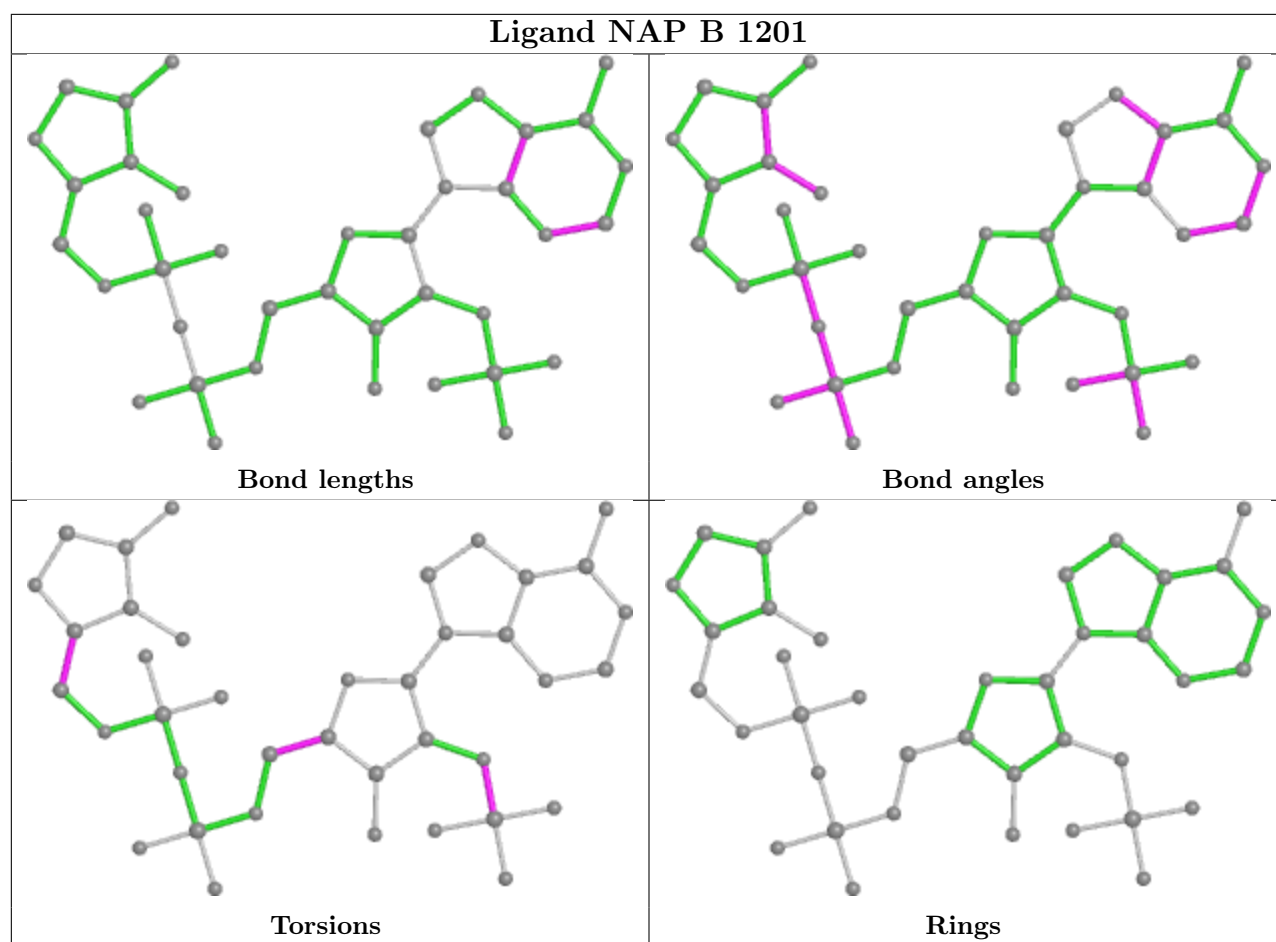
5 of 16 torsion outliers are listed below:

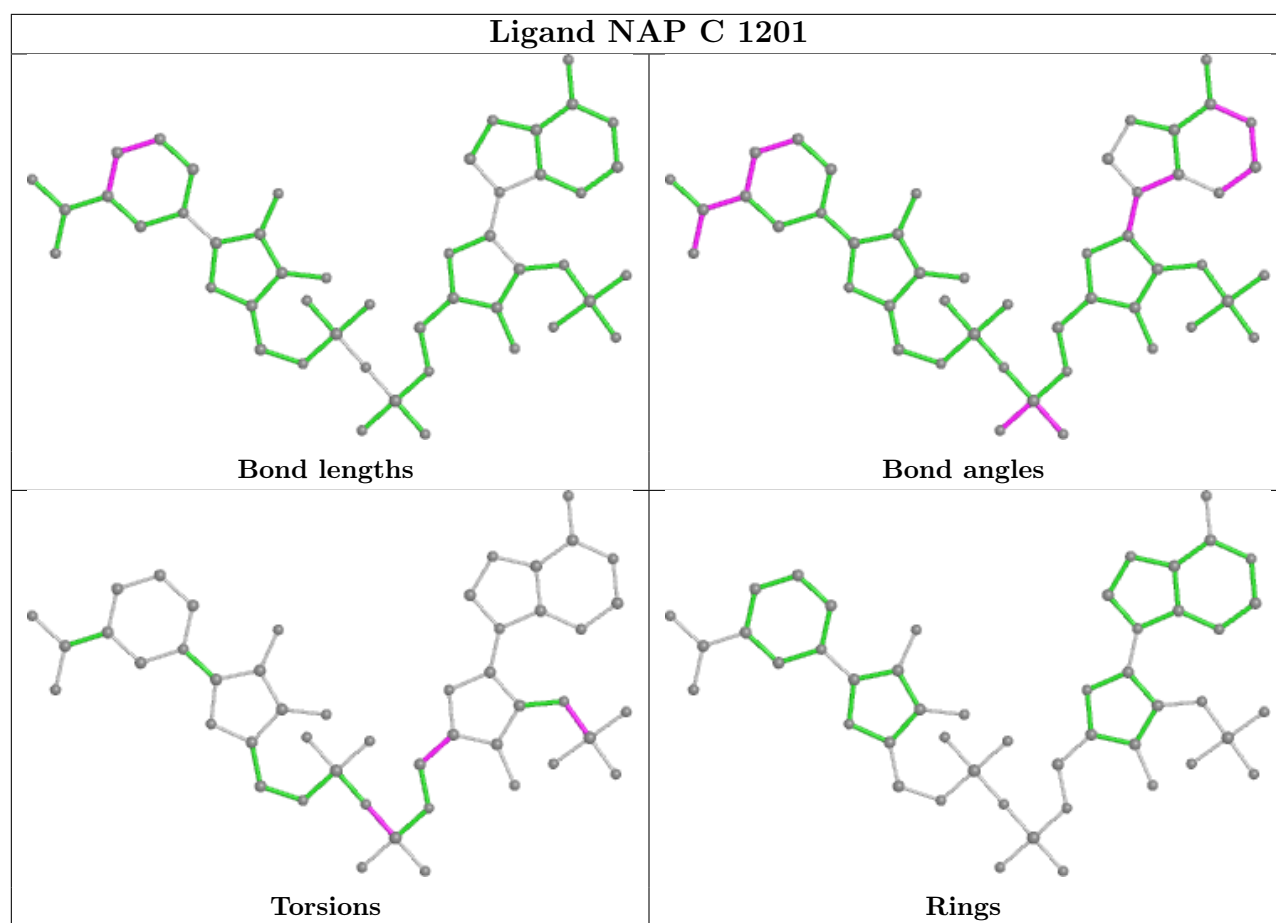
Mol	Chain	Res	Type	Atoms
2	A	1601	NAP	C5D-O5D-PN-O1N
2	A	1601	NAP	PN-O3-PA-O1A
2	A	1601	NAP	C5D-O5D-PN-O3
2	A	1601	NAP	C5D-O5D-PN-O2N
2	A	1601	NAP	PN-O3-PA-O2A

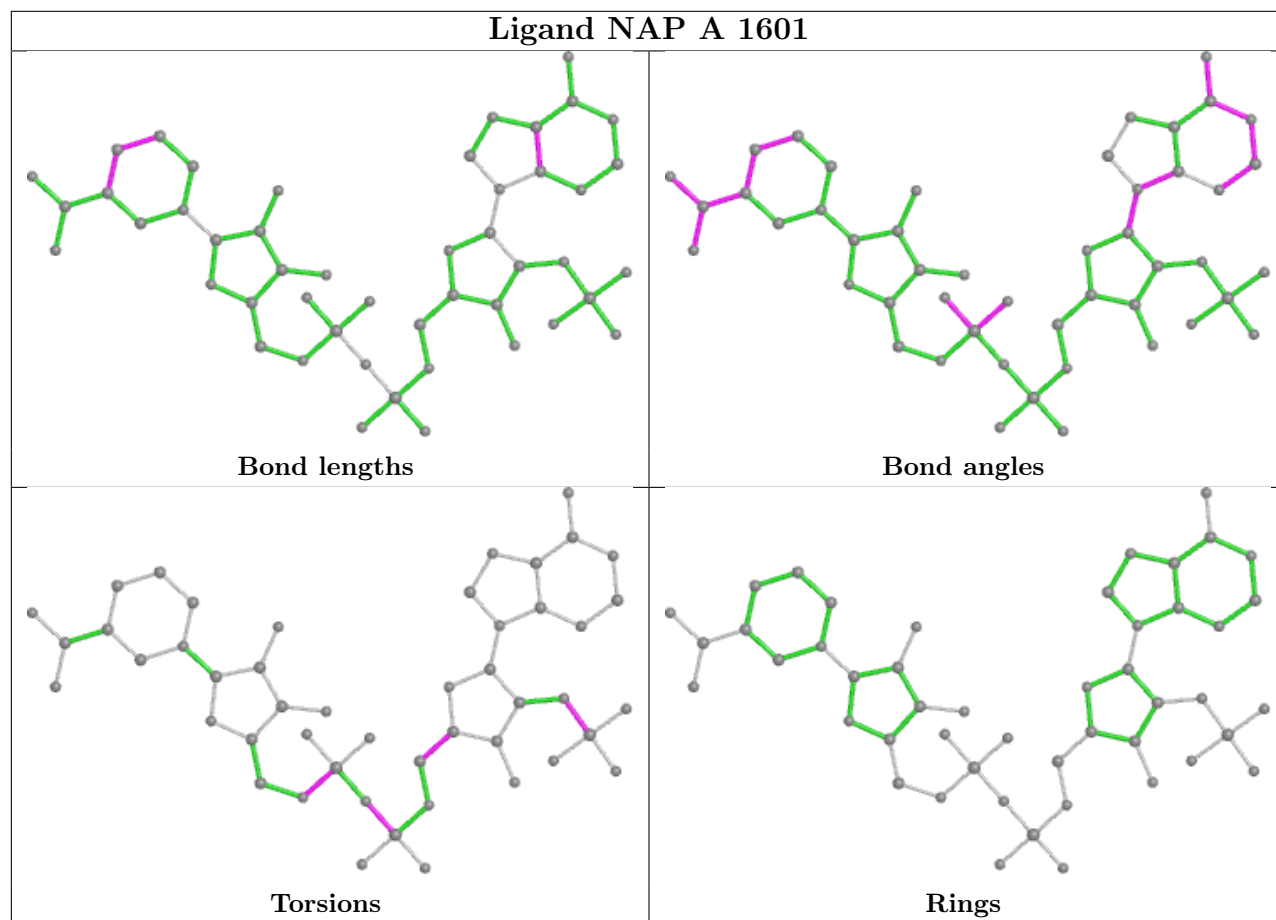
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 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	436/1174 (37%)	0.36	15 (3%) 45 51	20, 43, 75, 104	0
1	B	459/1174 (39%)	0.20	4 (0%) 84 88	19, 40, 67, 85	0
1	C	434/1174 (36%)	0.14	5 (1%) 79 84	18, 36, 64, 82	0
All	All	1329/3522 (37%)	0.23	24 (1%) 68 74	18, 39, 70, 104	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	952	TYR	5.4
1	A	1024	ALA	4.1
1	A	950	ASP	4.1
1	A	777	GLN	3.6
1	B	731	SER	3.4

### 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 monosaccharides in this entry.

### 6.4 Ligands [i](#)

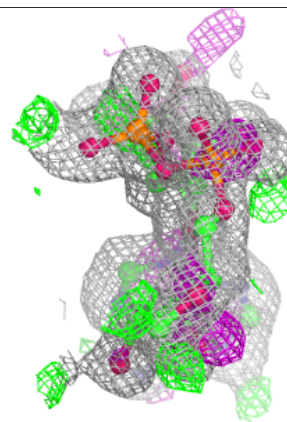
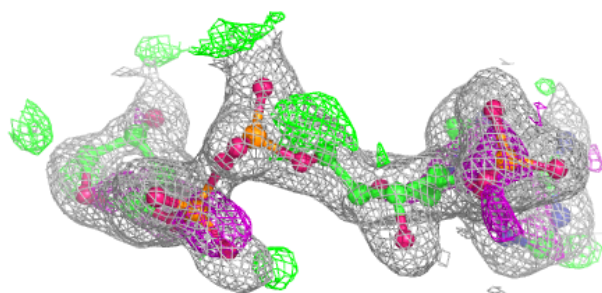
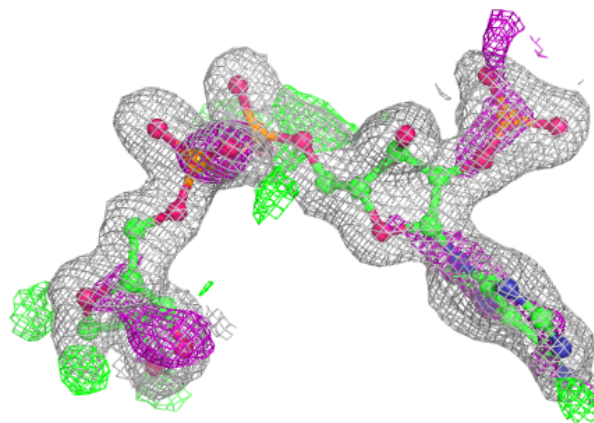
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAP	B	1201	39/48	0.89	0.19	23,30,35,39	8
2	NAP	A	1601	48/48	0.97	0.07	17,21,24,26	0
2	NAP	C	1201	48/48	0.98	0.06	16,18,21,24	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

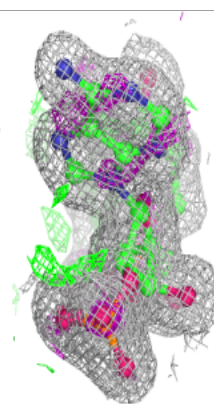
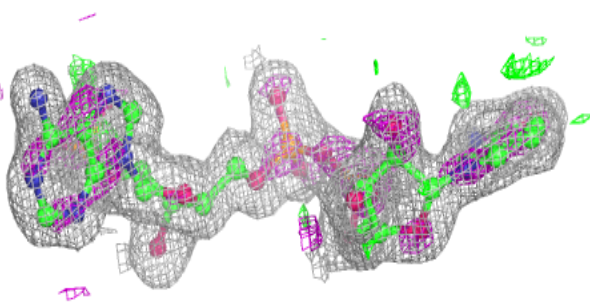
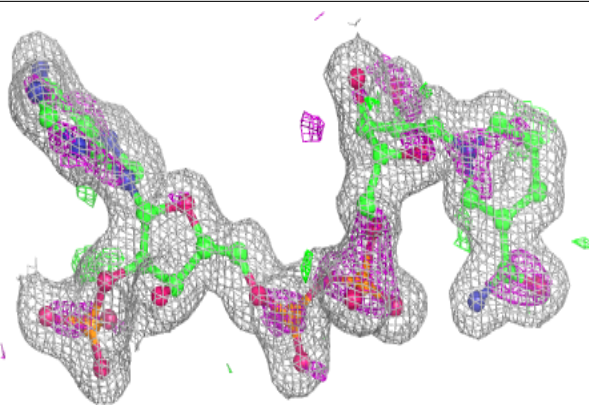
**Electron density around NAP B 1201:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
 mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
 and green (positive)

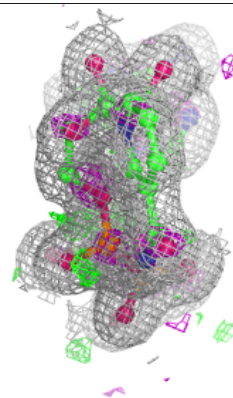
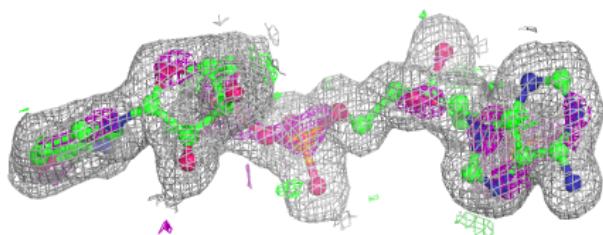
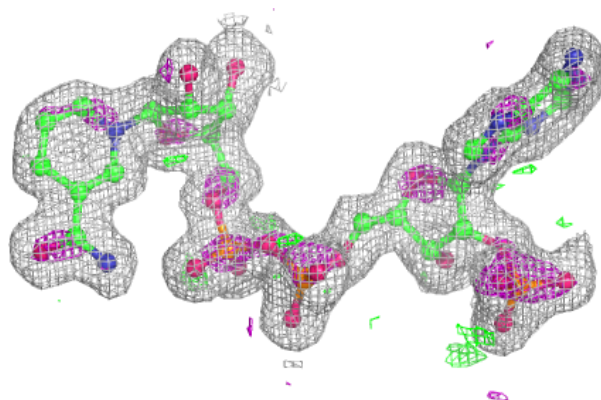


**Electron density around NAP A 1601:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around NAP C 1201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.