



Full wwPDB X-ray Structure Validation 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 Full wwPDB X-ray Structure Validation 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 ⓘ 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 ⓘ](#)) 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

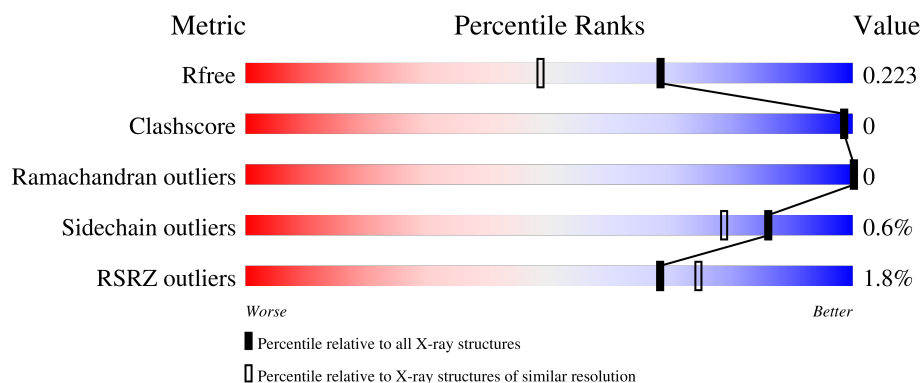
1 Overall quality at a glance

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 ≥ 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 style="width: 100%; height: 10px; background-color: red; position: relative;"> % <div style="position: absolute; top: 0; left: 0; width: 36%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 0; left: 36%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: 0; left: 63%; height: 10px; background-color: grey;"></div> </div> <div>36% 63%</div> </div>
1	B	1174	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <div style="position: absolute; top: 0; left: 0; width: 38%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 0; left: 38%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: 0; left: 61%; height: 10px; background-color: grey;"></div> </div> <div>38% 61%</div> </div>
1	C	1174	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <div style="position: absolute; top: 0; left: 0; width: 36%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 0; left: 36%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: 0; left: 63%; height: 10px; background-color: grey;"></div> </div> <div>36% 63%</div> </div>

2 Entry composition ⓘ

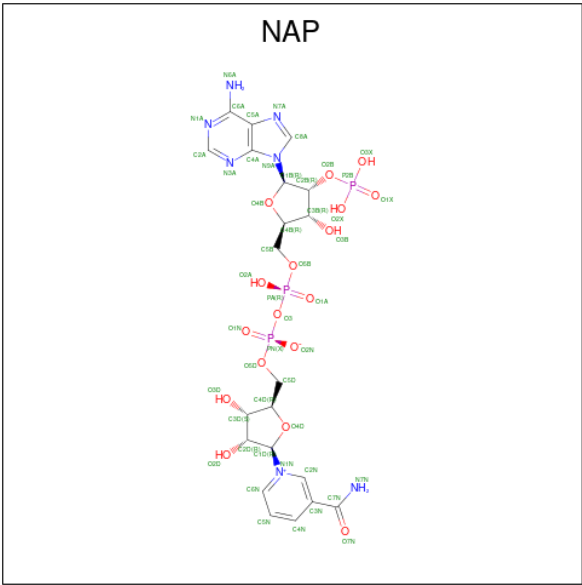
There are 3 unique types of molecules in this entry. The entry contains 11491 atoms, of which 0 are hydrogens and 0 are deuteriums.

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			

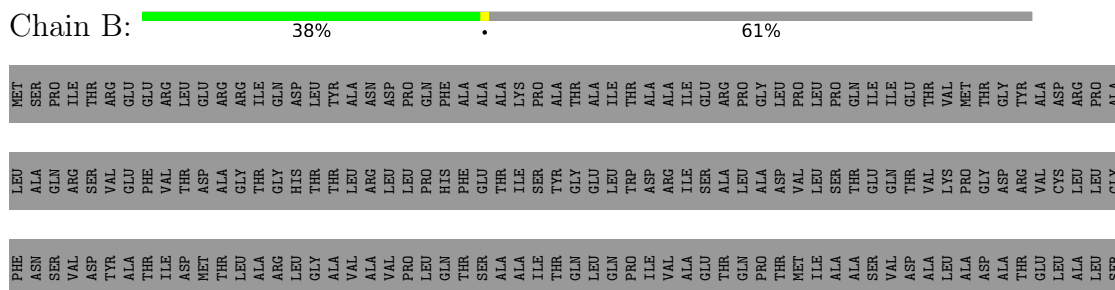
- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	24.8	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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.

All (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
1	B	1103	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	B	1107	ASP	CB-CG-OD2	5.71	123.44	118.30
1	B	1103	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	B	1137	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	C	1030	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	B	1108	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	863	ASP	CB-CG-OD1	5.27	123.05	118.30
1	C	1030	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	C	1000	ASP	CB-CG-OD1	5.15	122.94	118.30
1	C	863	ASP	CB-CG-OD1	5.13	122.91	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	3371	0	3326	6	0
1	B	3527	0	3462	4	0
1	C	3354	0	3313	1	0
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.

All (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
1:B:760:ILE:HG12	1:B:906:ARG:HG2	1.98	0.45
1:A:1093:ASP:O	1:A:1096:GLN:HG3	2.17	0.45
1:A:760:ILE:HG12	1:A:906:ARG:HG2	2.00	0.44
1:C:1062:MET:SD	1:C:1133:ALA:HB3	2.57	0.44
1:B:1129:ARG:NH2	3:B:1303:HOH:O	2.44	0.42

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	826	ASP
1	C	1096	GLN
1	A	892	GLN
1	A	922	ILE
1	A	1144	GLU

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Mol	Chain	Res	Type
1	B	916	TYR

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

All (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
2	B	1201	NAP	C2A-N3A	2.33	1.35	1.32
2	A	1601	NAP	C5A-C4A	2.23	1.46	1.40

All (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
2	B	1201	NAP	N3A-C2A-N1A	-3.45	123.29	128.68
2	C	1201	NAP	C3N-C7N-N7N	3.10	121.47	117.75
2	C	1201	NAP	C1B-N9A-C4A	-2.86	121.62	126.64
2	A	1601	NAP	C2A-N1A-C6A	2.85	123.62	118.75
2	A	1601	NAP	C1B-N9A-C4A	-2.72	121.87	126.64
2	C	1201	NAP	C2A-N1A-C6A	2.69	123.36	118.75
2	B	1201	NAP	O3D-C3D-C2D	-2.62	105.72	112.04
2	B	1201	NAP	PN-O3-PA	-2.53	124.16	132.83
2	B	1201	NAP	C4A-C5A-N7A	-2.51	106.78	109.40
2	C	1201	NAP	O2A-PA-O1A	2.45	124.37	112.24
2	A	1601	NAP	O7N-C7N-C3N	-2.25	116.94	119.63
2	B	1201	NAP	O3X-P2B-O2X	2.19	116.00	107.64
2	A	1601	NAP	N6A-C6A-N1A	2.15	123.04	118.57
2	A	1601	NAP	C4N-C3N-C7N	-2.09	115.45	121.04
2	B	1201	NAP	O2A-PA-O1A	2.06	122.41	112.24
2	A	1601	NAP	O2N-PN-O1N	2.02	122.25	112.24

There are no chirality outliers.

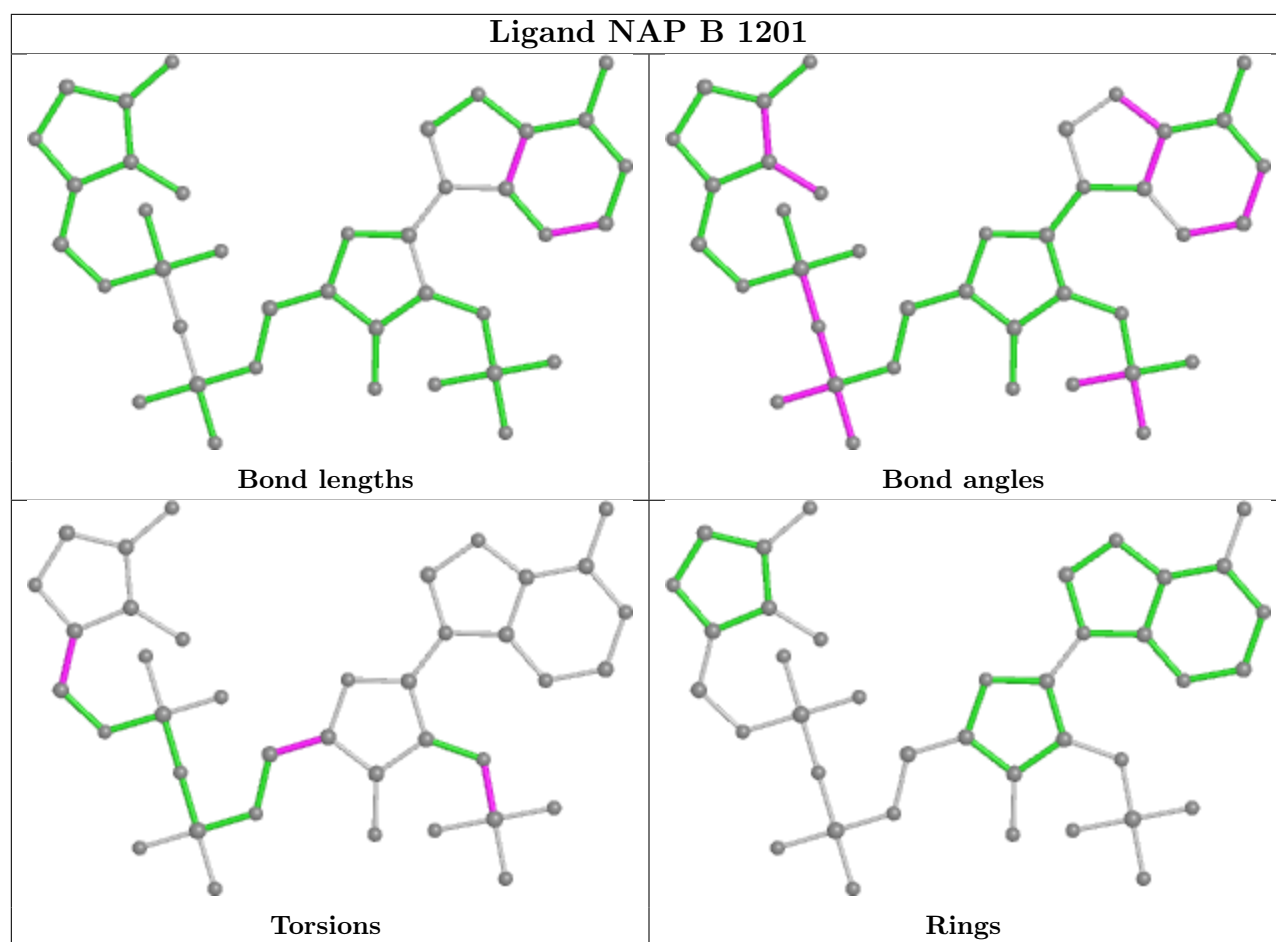
All (16) torsion outliers are listed below:

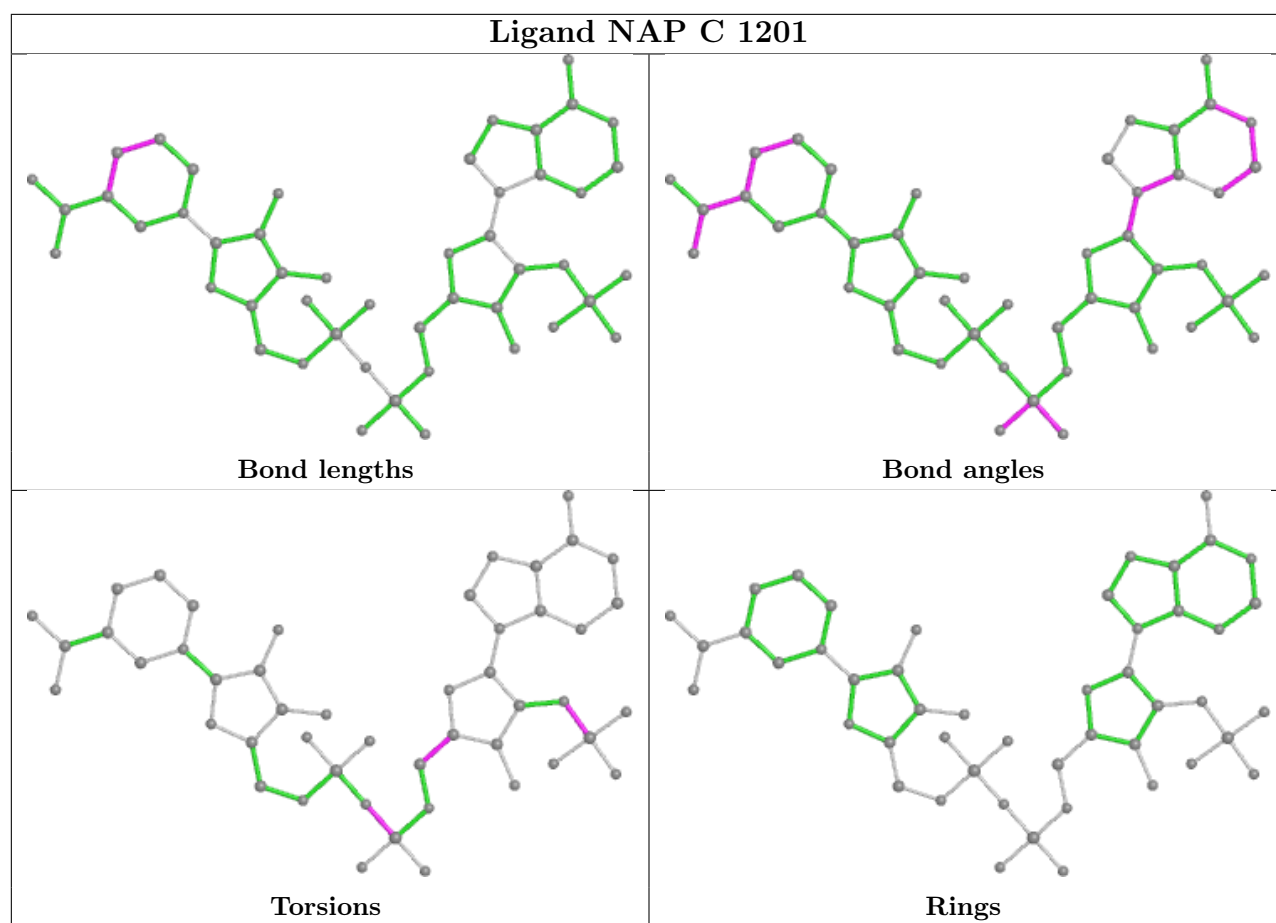
Mol	Chain	Res	Type	Atoms
2	A	1601	NAP	C5D-O5D-PN-O1N
2	A	1601	NAP	PN-O3-PA-O1A
2	A	1601	NAP	C5D-O5D-PN-O3
2	A	1601	NAP	C5D-O5D-PN-O2N
2	A	1601	NAP	PN-O3-PA-O2A
2	C	1201	NAP	PN-O3-PA-O1A
2	A	1601	NAP	C2B-O2B-P2B-O1X
2	C	1201	NAP	C2B-O2B-P2B-O2X
2	A	1601	NAP	C2B-O2B-P2B-O2X
2	B	1201	NAP	C2B-O2B-P2B-O2X
2	B	1201	NAP	C2B-O2B-P2B-O3X
2	A	1601	NAP	O4B-C4B-C5B-O5B
2	B	1201	NAP	O4B-C4B-C5B-O5B
2	C	1201	NAP	PN-O3-PA-O2A
2	C	1201	NAP	O4B-C4B-C5B-O5B
2	B	1201	NAP	O4D-C4D-C5D-O5D

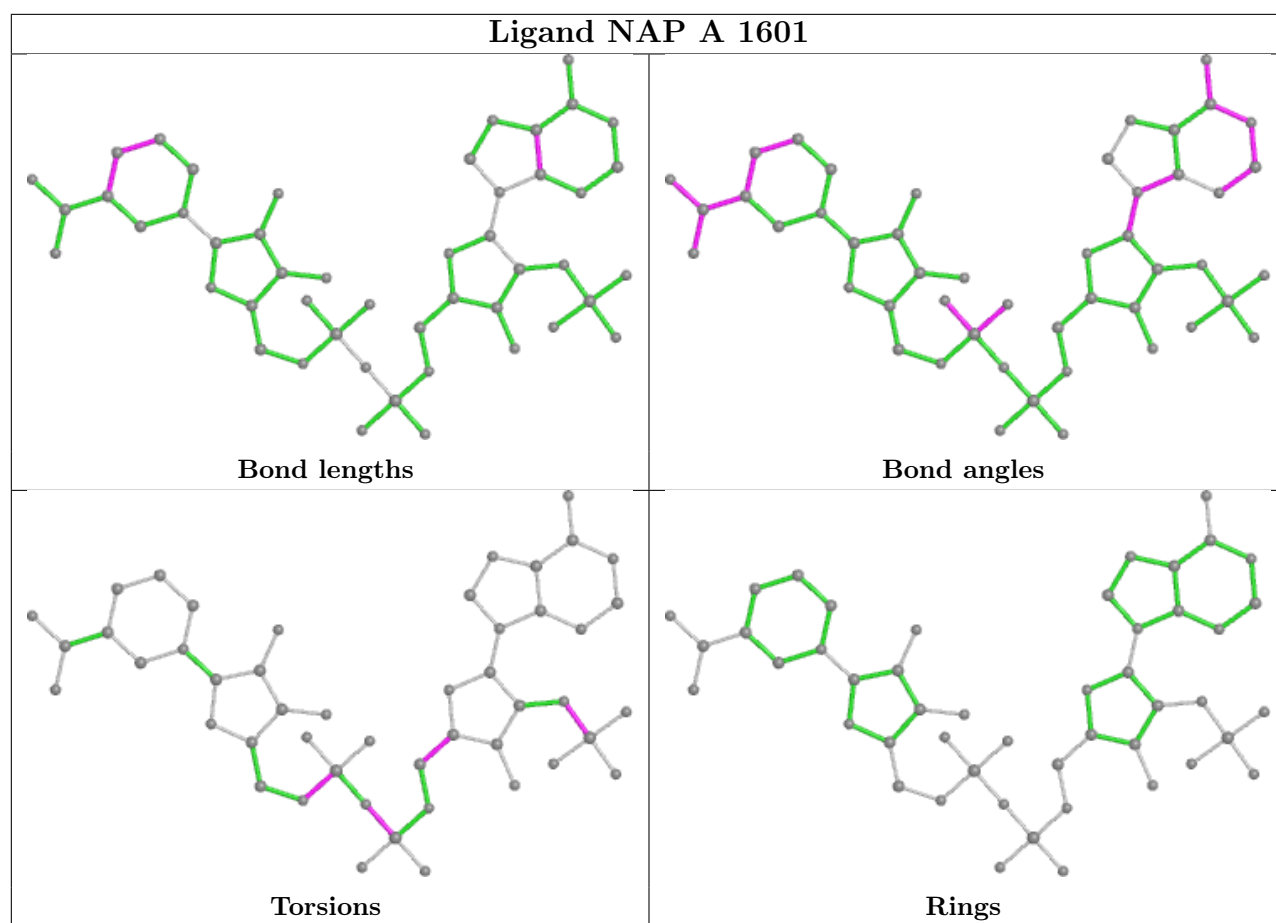
There are no ring outliers.

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

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	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

All (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
1	C	952	TYR	3.4
1	A	747	THR	3.4
1	A	951	SER	3.1
1	C	1126	ARG	3.1
1	A	1122	ARG	2.9
1	A	1126	ARG	2.8
1	B	865	GLN	2.8
1	B	816	LYS	2.7
1	A	775	ASN	2.5
1	B	1025	ASP	2.4
1	C	1119	HIS	2.4
1	A	1120	ASN	2.4
1	A	1119	HIS	2.4
1	A	1117	LEU	2.3
1	C	1027	ALA	2.3
1	C	779	ARG	2.1
1	A	1023	ALA	2.1
1	A	949	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	948	VAL	2.1

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](#)

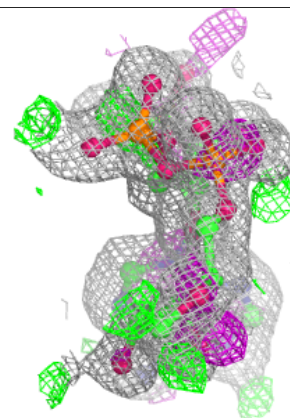
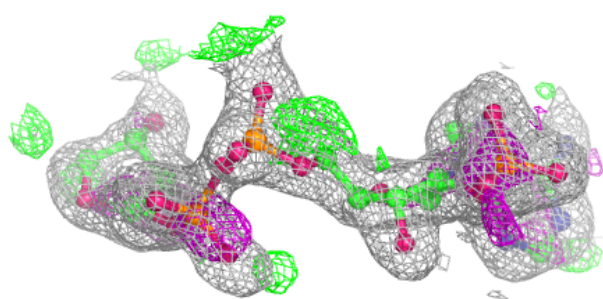
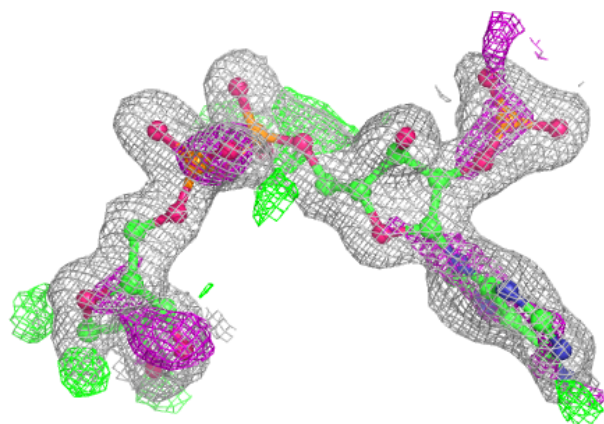
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\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

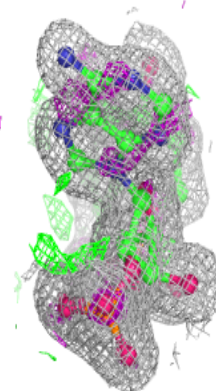
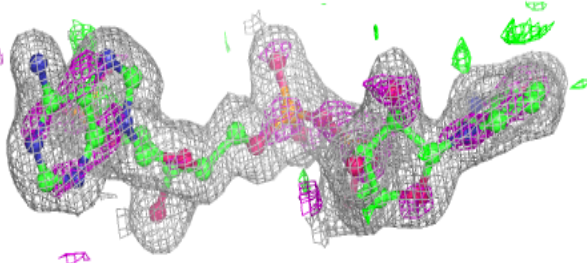
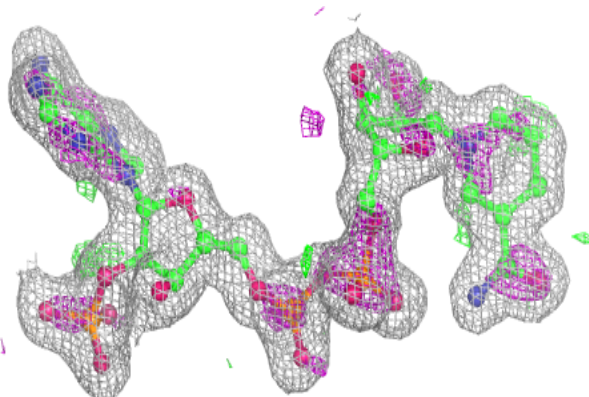
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

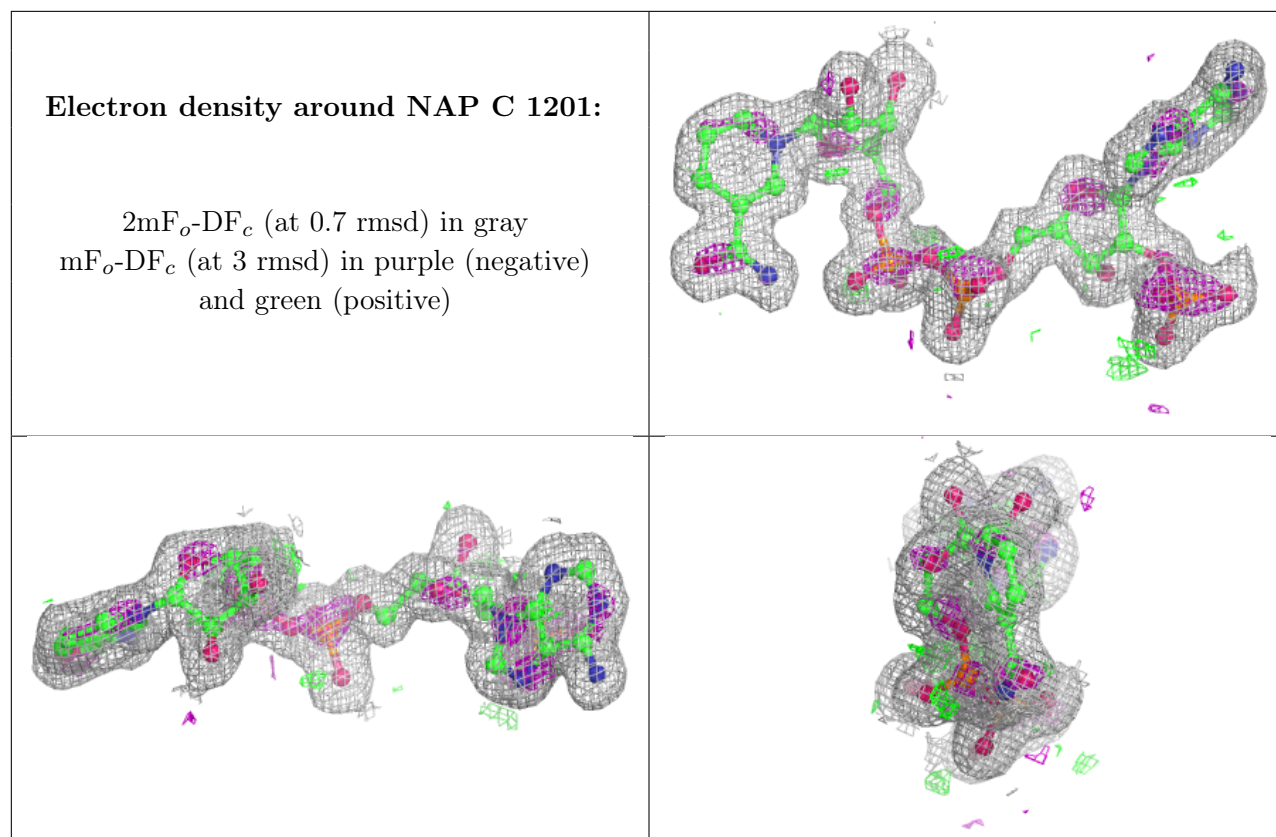
Electron density around NAP B 1201:

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

**Electron density around NAP 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.