Full wwPDB X-ray Structure Validation Report (i)

Jun 27, 2022 – 10:06 am BST

PDB ID	:	7R4M
Title	:	Crystal structure of mitochondrial NAD kinase
Authors	:	Labesse, G.; Mary, C.; Gelin, M.; Lionne, C.
Deposited on	:	2022-02-08
Resolution	:	2.29 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 (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:

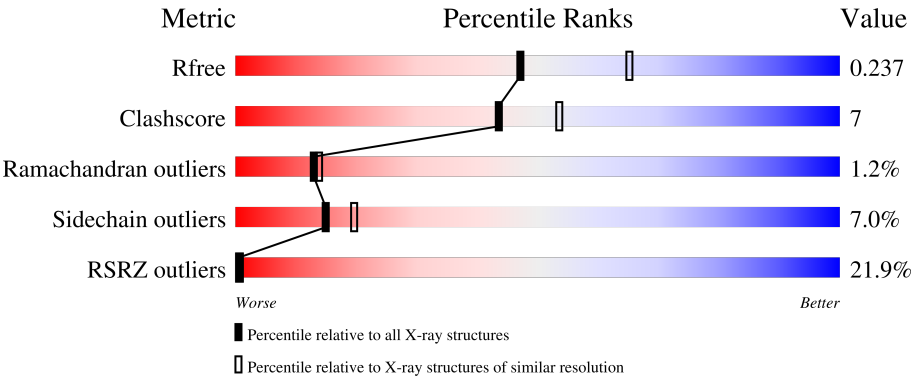
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 2.29 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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% 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	391	19% 70% 13% • 14%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2869 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.

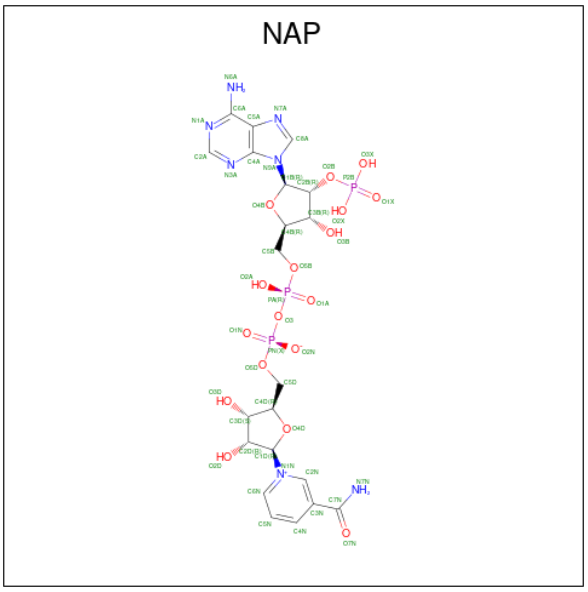
- Molecule 1 is a protein called NAD kinase 2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	2	0
			2668	1672	484	502	10			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	52	MET	-	initiating methionine	UNP Q4G0N4
A	53	GLY	-	expression tag	UNP Q4G0N4
A	54	HIS	-	expression tag	UNP Q4G0N4
A	55	HIS	-	expression tag	UNP Q4G0N4
A	56	HIS	-	expression tag	UNP Q4G0N4
A	57	HIS	-	expression tag	UNP Q4G0N4
A	58	HIS	-	expression tag	UNP Q4G0N4
A	59	HIS	-	expression tag	UNP Q4G0N4
A	60	GLY	-	expression tag	UNP Q4G0N4

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

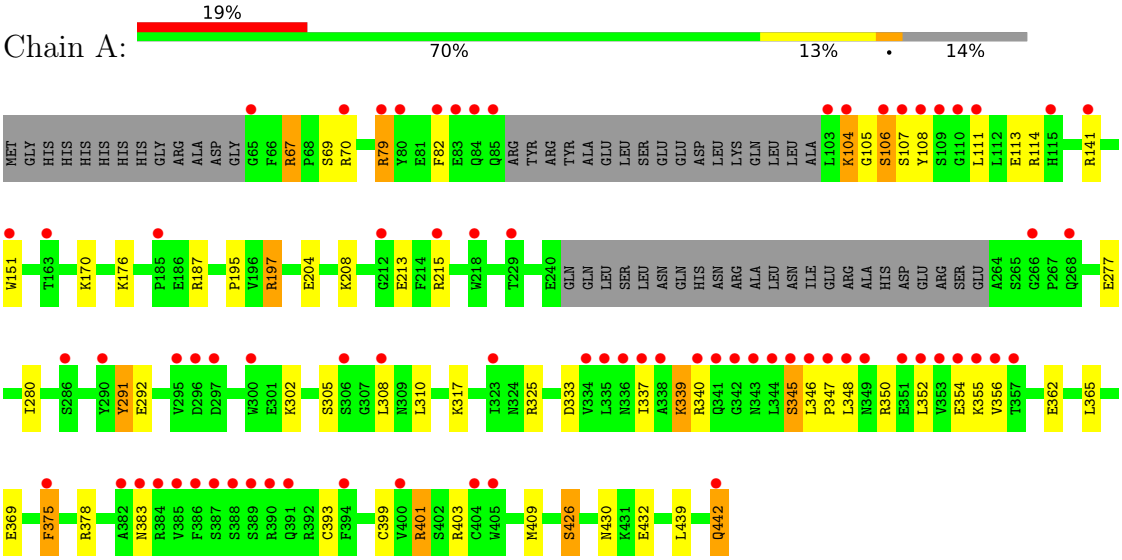
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	152	Total	O	0	0
			152	152		

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 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 (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: NAD kinase 2, mitochondrial



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	68.47Å 68.47Å 223.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.59 – 2.29 48.42 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.4 (40.59-2.29) 99.4 (48.42-2.29)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.51 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.19.1	Depositor
R, R_{free}	0.201 , 0.243 0.194 , 0.237	Depositor DCC
R_{free} test set	2050 reflections (8.31%)	wwPDB-VP
Wilson B-factor (Å^2)	49.7	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	2869	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: NAP, CA

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	0.45	0/2725	0.65	2/3685 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	79[A]	ARG	CA-C-O	5.04	130.68	120.10
1	A	79[B]	ARG	CA-C-O	5.04	130.68	120.10

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	2668	0	2620	34	0
2	A	48	0	24	2	0
3	A	1	0	0	0	0
4	A	152	0	0	2	1
All	All	2869	0	2644	36	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 7.

All (36) 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:442:GLN:O	4:A:601:HOH:O	1.57	1.19
2:A:501:NAP:C4D	2:A:501:NAP:O4D	1.65	1.09
1:A:67:ARG:HD2	1:A:67:ARG:C	2.00	0.81
1:A:280:ILE:HG12	1:A:409:MET:HG2	1.67	0.77
1:A:375:PHE:HE1	1:A:393:CYS:SG	2.22	0.63
1:A:348:LEU:HA	1:A:352:LEU:HD23	1.79	0.63
1:A:352:LEU:O	1:A:356:VAL:HG12	2.03	0.58
1:A:317:LYS:HG3	1:A:365:LEU:HD22	1.83	0.58
1:A:70:ARG:HG2	1:A:151:TRP:CZ2	2.39	0.57
1:A:197:ARG:NH2	1:A:204:GLU:OE2	2.37	0.55
1:A:291:TYR:CE1	1:A:308:LEU:HD21	2.41	0.55
1:A:375:PHE:CE1	1:A:393:CYS:SG	3.01	0.53
1:A:195:PRO:CB	1:A:442:GLN:HB3	2.39	0.52
1:A:107:SER:HA	1:A:111:LEU:HD13	1.89	0.52
2:A:501:NAP:O4D	2:A:501:NAP:C5D	2.49	0.52
1:A:292:GLU:HG2	1:A:302:LYS:HG2	1.93	0.50
1:A:399:CYS:SG	1:A:426:SER:HB3	2.52	0.49
1:A:114:ARG:NE	1:A:187:ARG:HG3	2.28	0.49
1:A:195:PRO:HB3	1:A:442:GLN:HB3	1.94	0.48
1:A:439:LEU:HA	1:A:439:LEU:HD23	1.71	0.47
1:A:401:ARG:HD2	1:A:403:ARG:NH2	2.29	0.47
1:A:170:LYS:NZ	4:A:609:HOH:O	2.47	0.46
1:A:291:TYR:OH	1:A:305:SER:OG	2.31	0.45
1:A:430:ASN:OD1	1:A:432:GLU:HG2	2.16	0.45
1:A:104:LYS:HE2	1:A:104:LYS:HB2	1.80	0.45
1:A:333:ASP:O	1:A:337:ILE:HG13	2.18	0.44
1:A:345:SER:OG	1:A:346:LEU:N	2.49	0.44
1:A:305:SER:HB2	1:A:378:ARG:O	2.19	0.43
1:A:350:ARG:NH1	1:A:354:GLU:OE2	2.52	0.42
1:A:339:LYS:O	1:A:340:ARG:C	2.58	0.42
1:A:176:LYS:HE2	1:A:176:LYS:HB2	1.90	0.41
1:A:106:SER:O	1:A:106:SER:OG	2.30	0.41
1:A:208:LYS:HG2	1:A:213:GLU:HB2	2.02	0.41
1:A:350:ARG:O	1:A:354:GLU:HG3	2.20	0.41
1:A:310:LEU:HG	1:A:375:PHE:HB2	2.04	0.40
1:A:215:ARG:NH2	1:A:369:GLU:OE2	2.52	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)
4:A:601:HOH:O	4:A:718:HOH:O[6_445]	2.13	0.07

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	334/391 (85%)	311 (93%)	19 (6%)	4 (1%)	13 14

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	383	ASN
1	A	108	TYR
1	A	105	GLY
1	A	347	PRO

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	288/342 (84%)	266 (92%)	22 (8%)	13 16

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ARG
1	A	69	SER

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Mol	Chain	Res	Type
1	A	79[A]	ARG
1	A	79[B]	ARG
1	A	82	PHE
1	A	104	LYS
1	A	106	SER
1	A	113	GLU
1	A	141[A]	ARG
1	A	141[B]	ARG
1	A	197	ARG
1	A	277	GLU
1	A	291	TYR
1	A	325	ARG
1	A	339	LYS
1	A	345	SER
1	A	355	LYS
1	A	362	GLU
1	A	375	PHE
1	A	401	ARG
1	A	426	SER
1	A	442	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	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)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	501	3	45,52,52	3.31	14 (31%)	56,80,80	1.38	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	A	501	3	-	7/31/67/67	0/5/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	NAP	O4D-C4D	9.29	1.65	1.45
2	A	501	NAP	C3B-C4B	-8.23	1.32	1.53
2	A	501	NAP	C3D-C4D	-8.19	1.32	1.53
2	A	501	NAP	O4B-C4B	7.04	1.60	1.45
2	A	501	NAP	O4B-C1B	-5.46	1.33	1.41
2	A	501	NAP	C7N-N7N	5.43	1.43	1.33
2	A	501	NAP	O4D-C1D	-5.42	1.33	1.41
2	A	501	NAP	O2D-C2D	-4.91	1.31	1.43
2	A	501	NAP	P2B-O2B	4.54	1.67	1.59
2	A	501	NAP	O3B-C3B	3.73	1.51	1.43
2	A	501	NAP	P2B-O1X	3.59	1.62	1.50
2	A	501	NAP	C6A-N6A	3.06	1.45	1.34
2	A	501	NAP	PA-O5B	2.57	1.69	1.59
2	A	501	NAP	C2A-N1A	-2.31	1.29	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	NAP	N3A-C2A-N1A	-3.86	122.65	128.68
2	A	501	NAP	C5N-C4N-C3N	-3.75	115.91	120.34
2	A	501	NAP	PN-O3-PA	-3.57	120.58	132.83
2	A	501	NAP	C2N-C3N-C4N	3.32	122.03	118.26
2	A	501	NAP	C4A-C5A-N7A	-2.93	106.35	109.40
2	A	501	NAP	C2B-C3B-C4B	2.37	107.15	101.99
2	A	501	NAP	C3D-C2D-C1D	2.28	104.40	100.98
2	A	501	NAP	C3N-C7N-N7N	2.26	120.47	117.75
2	A	501	NAP	O7N-C7N-C3N	-2.09	117.13	119.63

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NAP	C5B-O5B-PA-O1A
2	A	501	NAP	PN-O3-PA-O5B
2	A	501	NAP	C2B-O2B-P2B-O1X
2	A	501	NAP	C3B-C2B-O2B-P2B
2	A	501	NAP	C1B-C2B-O2B-P2B
2	A	501	NAP	C5B-O5B-PA-O3
2	A	501	NAP	C2B-O2B-P2B-O3X

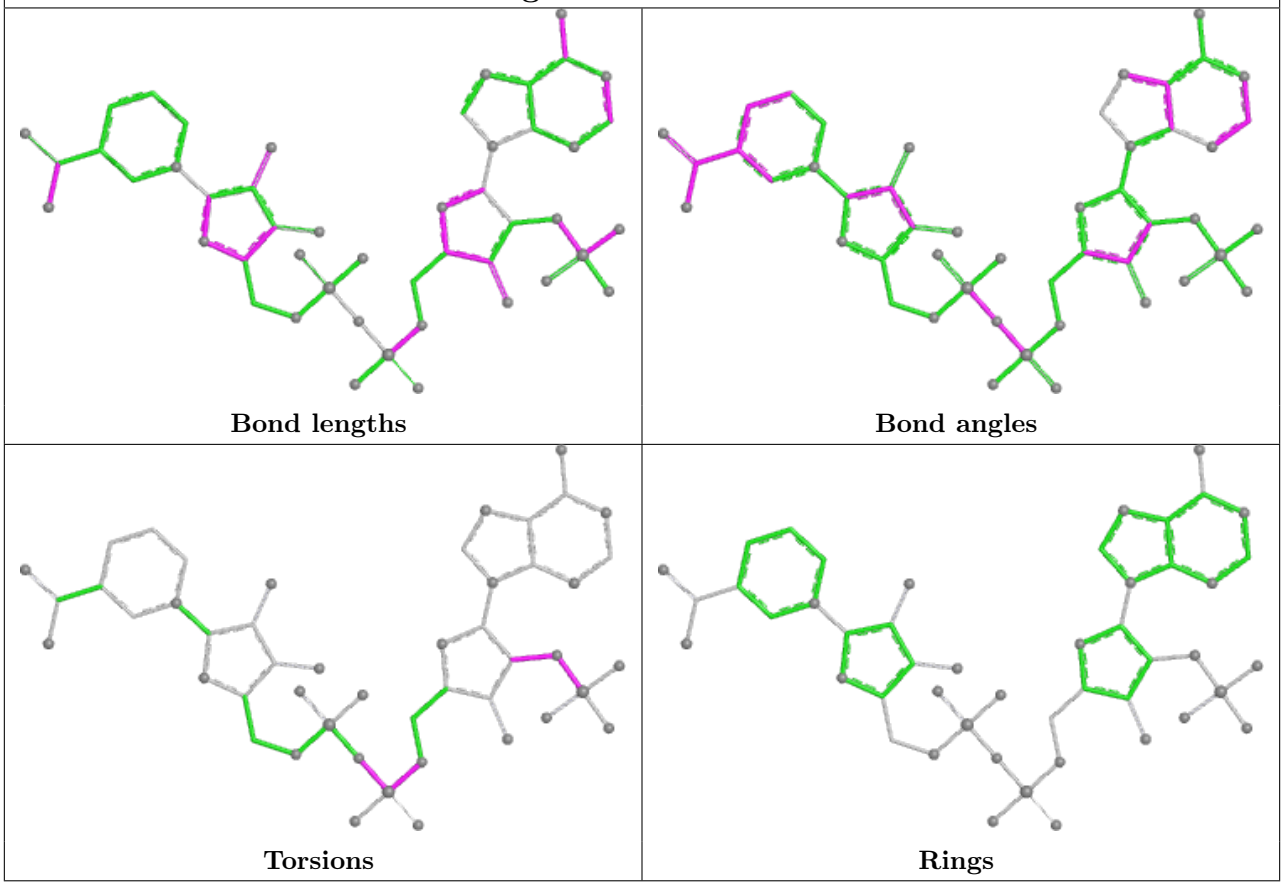
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NAP	2	0

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 then 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.

Ligand NAP A 501



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, 95^{th} 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	338/391 (86%)	1.63	74 (21%) 0 1	40, 54, 119, 140	51 (15%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	108	TYR	11.3
1	A	344	LEU	8.7
1	A	343	ASN	8.7
1	A	345	SER	7.6
1	A	352	LEU	7.5
1	A	109	SER	7.5
1	A	356	VAL	7.4
1	A	342	GLY	6.9
1	A	348	LEU	6.3
1	A	346	LEU	6.2
1	A	82	PHE	6.0
1	A	337	ILE	5.9
1	A	340	ARG	5.9
1	A	338	ALA	5.7
1	A	336	ASN	4.9
1	A	442	GLN	4.8
1	A	341	GLN	4.8
1	A	266	GLY	4.7
1	A	85	GLN	4.5
1	A	107	SER	4.4
1	A	391	GLN	4.3
1	A	103	LEU	4.3
1	A	110	GLY	4.3
1	A	84	GLN	4.0
1	A	388	SER	4.0
1	A	335	LEU	3.8
1	A	80	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	355	LYS	3.6
1	A	394	PHE	3.5
1	A	386	PHE	3.5
1	A	65	GLY	3.5
1	A	83	GLU	3.3
1	A	297	ASP	3.2
1	A	300	TRP	3.2
1	A	354	GLU	3.2
1	A	349	ASN	3.2
1	A	104	LYS	3.2
1	A	115	HIS	3.1
1	A	353	VAL	3.0
1	A	347	PRO	3.0
1	A	357	THR	2.9
1	A	351	GLU	2.8
1	A	385	VAL	2.8
1	A	290	TYR	2.8
1	A	106	SER	2.8
1	A	268	GLN	2.7
1	A	308	LEU	2.7
1	A	405	TRP	2.7
1	A	111	LEU	2.6
1	A	387	SER	2.5
1	A	215	ARG	2.5
1	A	382	ALA	2.5
1	A	163	THR	2.4
1	A	229	THR	2.4
1	A	296	ASP	2.4
1	A	375	PHE	2.4
1	A	306	SER	2.4
1	A	383	ASN	2.3
1	A	212	GLY	2.3
1	A	79[A]	ARG	2.3
1	A	218	TRP	2.3
1	A	295	VAL	2.3
1	A	70	ARG	2.2
1	A	384	ARG	2.2
1	A	404	CYS	2.2
1	A	151	TRP	2.2
1	A	334	VAL	2.2
1	A	389	SER	2.1
1	A	390	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	185	PRO	2.1
1	A	141[A]	ARG	2.0
1	A	400	VAL	2.0
1	A	286	SER	2.0
1	A	323	ILE	2.0

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)

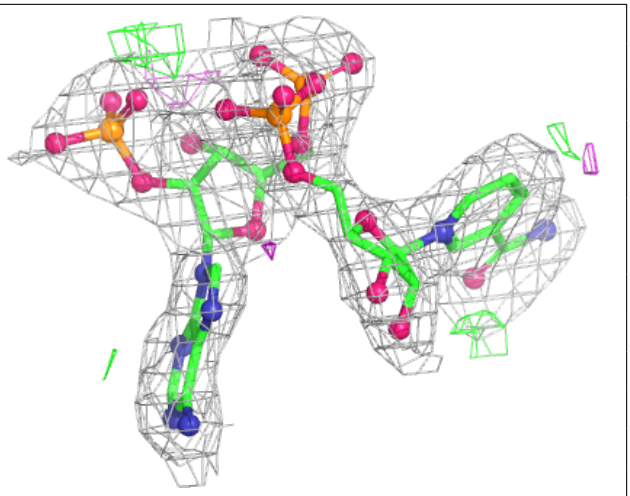
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

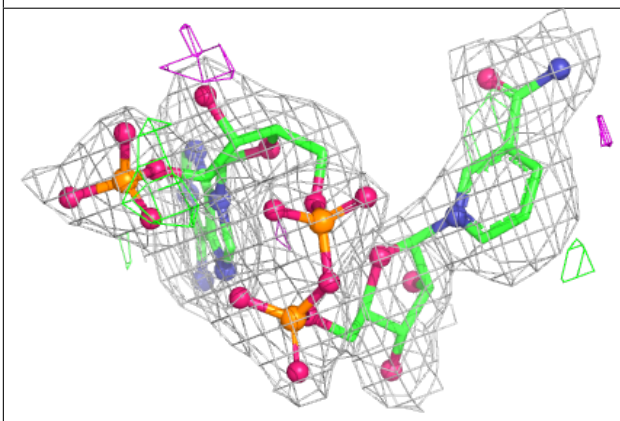
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAP	A	501	48/48	0.89	0.20	34,45,49,51	0
3	CA	A	502	1/1	0.90	0.17	47,47,47,47	0

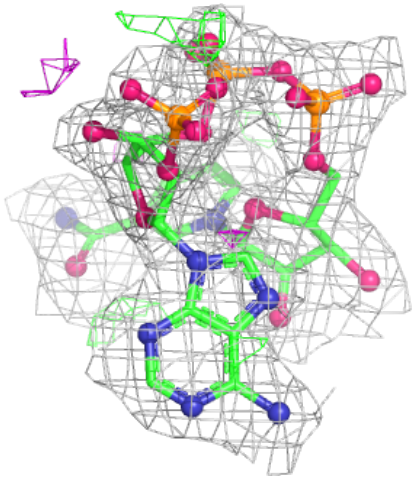
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP A 501:

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

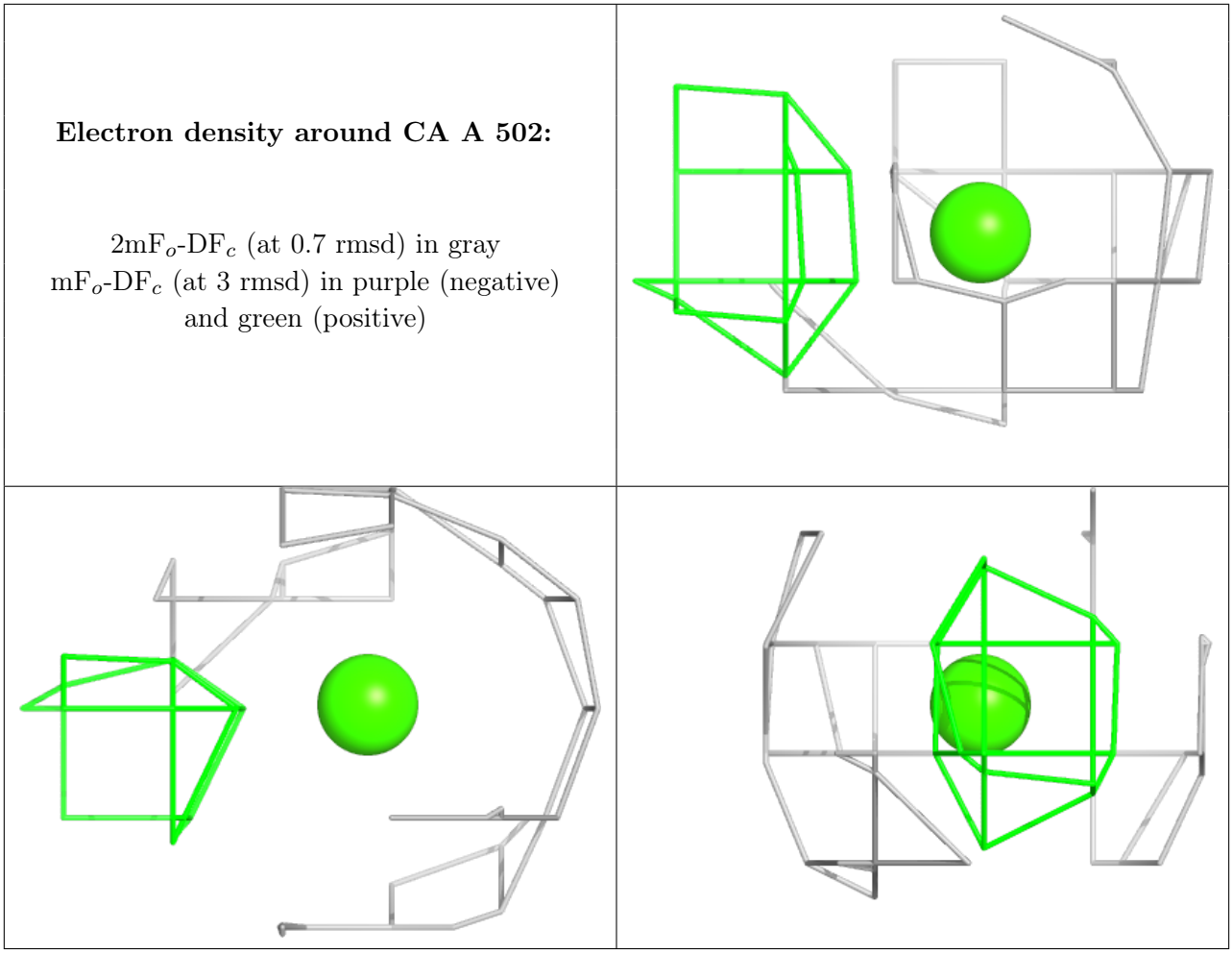






Electron density around CA A 502:

$2mF_o$-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.