WORLDWIDE
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PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 10:58 PM EDT

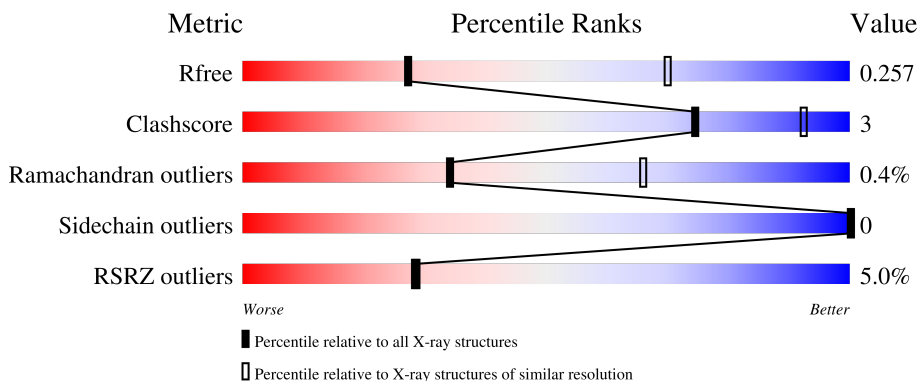|		
PDB ID	:	7RTC
Title	:	Crystal structure of the ARM domain from Drosophila SARM1 in complex with NaMN
Authors	:	Gu, W.; Ve, T.; Kobe, B.
Deposited on	:	2021-08-13
Resolution	:	3.31 Å(reported)

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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 3.31 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	Percentile Ranks	Value
Rfree		0.257
Clashscore		3
Ramachandran outliers		0.4%
Sidechain outliers		0
RSRZ outliers		5.0%

Worse — *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1089 (3.36-3.28)
Clashscore	141614	1137 (3.36-3.28)
Ramachandran outliers	138981	1115 (3.36-3.28)
Sidechain outliers	138945	1114 (3.36-3.28)
RSRZ outliers	127900	1059 (3.36-3.28)

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.

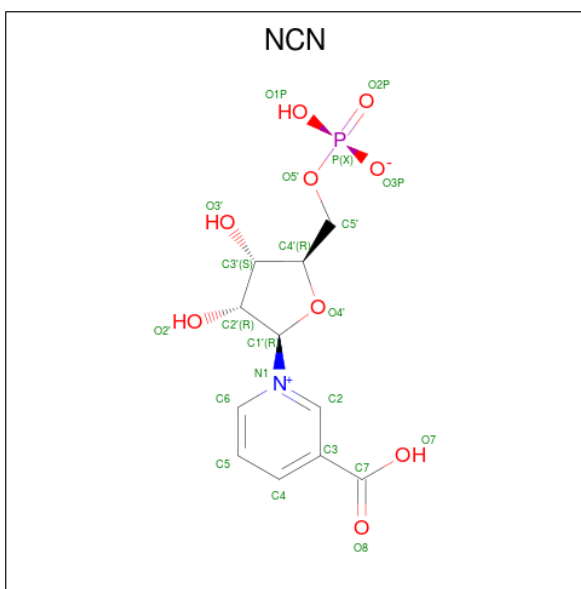| Mol	Chain	Length	Quality of chain
1	A	364	3% / 85% 6% 9%
1	B	364	4% / 85% 6% 9%
1	C	364	6% / 83% 8% 9%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 15431 atoms, of which 7682 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(+) hydrolase sarm1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	331	Total	C	H	N	O	S	0	0	0
			5111	1601	2550	459	483	18			
1	B	331	Total	C	H	N	O	S	0	0	0
			5113	1601	2552	459	483	18			
1	C	331	Total	C	H	N	O	S	0	0	0
			5105	1601	2544	459	483	18			

- Molecule 2 is NICOTINATE MONONUCLEOTIDE (three-letter code: NCN) (formula: $C_{11}H_{14}NO_9P$) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			34	11	12	1	9	1		
2	B	1	Total	C	H	N	O	P	0	0
			34	11	12	1	9	1		
2	C	1	Total	C	H	N	O	P	0	0
			34	11	12	1	9	1		

3 Residue-property plots ⓘ

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.
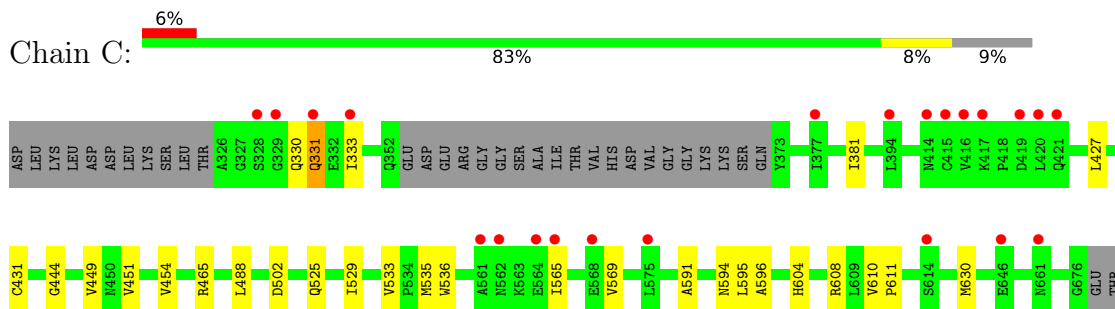
- Molecule 1: NAD(+) hydrolase sarm1
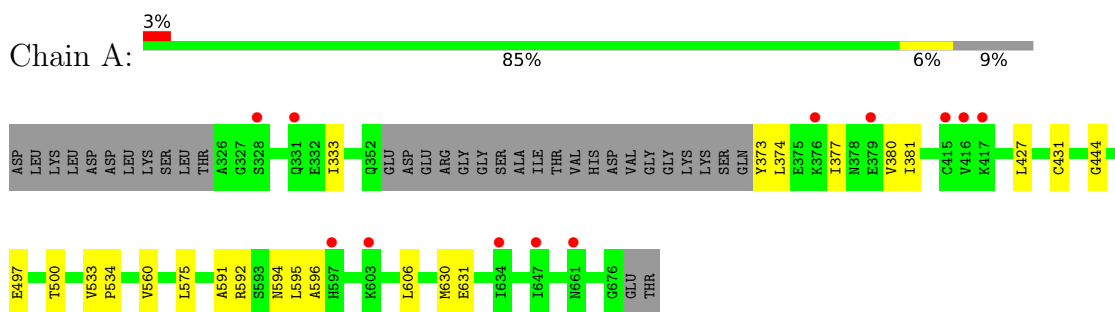
- Molecule 1: NAD(+) hydrolase sarm1
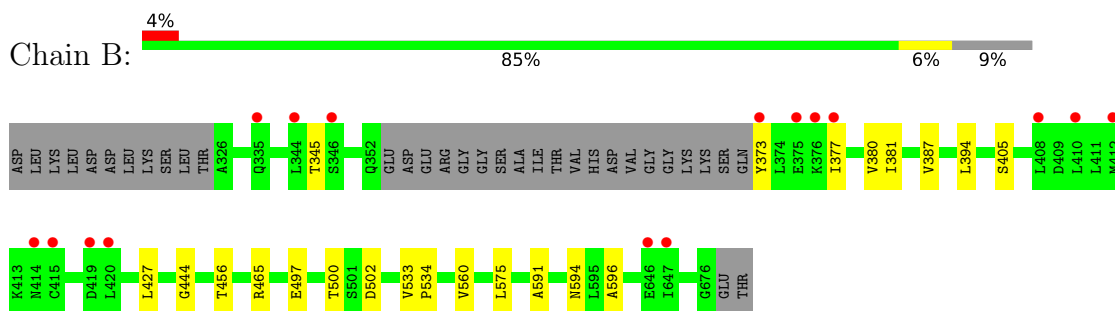
- Molecule 1: NAD(+) hydrolase sarm1

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	67.12Å 102.82Å 100.20Å 90.00° 103.84° 90.00°	Depositor
Resolution (Å)	39.41 – 3.31 39.41 – 3.31	Depositor EDS
% Data completeness (in resolution range)	92.0 (39.41-3.31) 92.0 (39.41-3.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 3.32Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.238 , 0.257 0.238 , 0.257	Depositor DCC
R_{free} test set	934 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	79.0	Xtriage
Anisotropy	0.551	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 35.3	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	15431	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.33% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: NCN

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	0.28	0/2603	0.44	0/3517
1	B	0.28	0/2603	0.43	0/3517
1	C	0.28	0/2603	0.43	0/3517
All	All	0.28	0/7809	0.43	0/10551

There are no bond length outliers.

There are no bond angle outliers.

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	2561	2550	2551	16	0
1	B	2561	2552	2551	12	0
1	C	2561	2544	2551	23	0
2	A	22	12	12	0	0
2	B	22	12	12	0	0
2	C	22	12	12	0	0
All	All	7749	7682	7689	50	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 3.

All (50) 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:331:GLN:HG2	1:C:333:ILE:HD11	1.73	0.70
1:C:591:ALA:O	1:C:596:ALA:HB2	1.98	0.64
1:C:330:GLN:O	1:C:331:GLN:HB3	2.00	0.61
1:B:591:ALA:O	1:B:596:ALA:HB2	2.03	0.58
1:C:331:GLN:HG2	1:C:333:ILE:CD1	2.34	0.57
1:A:591:ALA:O	1:A:596:ALA:HB2	2.04	0.57
1:A:591:ALA:HB2	1:A:630:MET:CG	2.36	0.55
1:C:535:MET:O	1:C:536:TRP:HB2	2.07	0.55
1:C:330:GLN:O	1:C:331:GLN:CB	2.57	0.52
1:A:333:ILE:HG23	1:A:333:ILE:O	2.10	0.51
1:C:465:ARG:NE	1:C:502:ASP:OD2	2.42	0.51
1:B:465:ARG:NE	1:B:502:ASP:OD2	2.41	0.51
1:B:345:THR:HG22	1:B:405:SER:HB3	1.94	0.50
1:A:592:ARG:NH2	1:B:456:THR:O	2.45	0.50
1:C:533:VAL:O	1:C:535:MET:O	2.30	0.50
1:C:333:ILE:HG22	1:C:333:ILE:O	2.12	0.48
1:C:565:ILE:O	1:C:569:VAL:HG23	2.13	0.48
1:A:381:ILE:HD13	1:A:431:CYS:SG	2.54	0.47
1:C:381:ILE:HD12	1:C:427:LEU:HD11	1.97	0.47
1:C:381:ILE:HD13	1:C:431:CYS:SG	2.55	0.47
1:C:591:ALA:HB2	1:C:630:MET:CG	2.45	0.47
1:B:560:VAL:HG11	1:B:575:LEU:HD11	1.96	0.47
1:C:604:HIS:O	1:C:608:ARG:HG2	2.16	0.46
1:A:560:VAL:HG11	1:A:575:LEU:HD11	1.98	0.46
1:A:606:LEU:HD21	1:A:631:GLU:HG3	1.98	0.46
1:A:377:ILE:O	1:A:380:VAL:HG12	2.16	0.45
1:A:591:ALA:O	1:A:594:ASN:O	2.34	0.45
1:A:533:VAL:N	1:A:534:PRO:HD2	2.31	0.45
1:C:529:ILE:HD11	1:C:569:VAL:HG22	1.98	0.45
1:A:591:ALA:HB2	1:A:630:MET:HG3	1.99	0.45
1:C:591:ALA:O	1:C:594:ASN:O	2.35	0.45
1:C:594:ASN:O	1:C:595:LEU:HG	2.17	0.44
1:B:497:GLU:O	1:B:500:THR:HG22	2.17	0.44
1:A:591:ALA:HB2	1:A:630:MET:HG2	2.00	0.43
1:B:387:VAL:HG21	1:B:394:LEU:HD22	2.00	0.43
1:A:497:GLU:O	1:A:500:THR:HG22	2.19	0.43
1:C:525:GLN:HB3	1:C:565:ILE:HD13	2.01	0.42
1:C:591:ALA:HB2	1:C:630:MET:HG3	2.02	0.42
1:A:373:TYR:CD2	1:A:374:LEU:HD13	2.55	0.42
1:C:529:ILE:HD11	1:C:569:VAL:CG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:TYR:CD2	1:B:373:TYR:O	2.73	0.41
1:B:377:ILE:HA	1:B:380:VAL:HG12	2.01	0.41
1:A:594:ASN:O	1:A:595:LEU:HG	2.20	0.41
1:A:381:ILE:HD12	1:A:427:LEU:HD11	2.03	0.41
1:B:533:VAL:N	1:B:534:PRO:HD2	2.36	0.40
1:B:591:ALA:O	1:B:594:ASN:O	2.39	0.40
1:C:449:VAL:HG11	1:C:488:LEU:HB2	2.04	0.40
1:B:381:ILE:HD12	1:B:427:LEU:HD11	2.04	0.40
1:C:451:VAL:HA	1:C:454:VAL:HG22	2.03	0.40
1:C:610:VAL:N	1:C:611:PRO:HD2	2.36	0.40

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	327/364 (90%)	311 (95%)	15 (5%)	1 (0%)	41	71
1	B	327/364 (90%)	312 (95%)	14 (4%)	1 (0%)	41	71
1	C	327/364 (90%)	304 (93%)	21 (6%)	2 (1%)	25	57
All	All	981/1092 (90%)	927 (94%)	50 (5%)	4 (0%)	34	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	331	GLN
1	A	444	GLY
1	B	444	GLY
1	C	444	GLY

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	280/308 (91%)	280 (100%)	0	100	100
1	B	280/308 (91%)	280 (100%)	0	100	100
1	C	280/308 (91%)	280 (100%)	0	100	100
All	All	840/924 (91%)	840 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

3 ligands are modelled in this entry.

There are no bond length outliers.
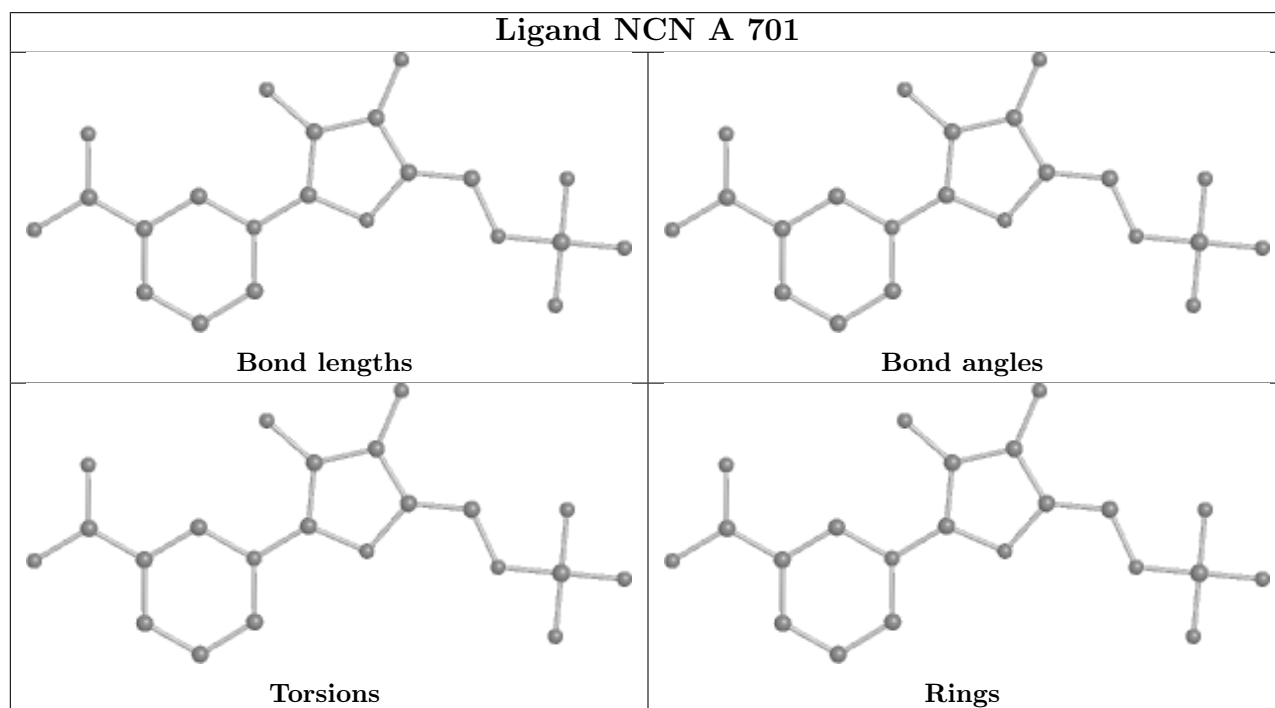
There are no bond angle outliers.
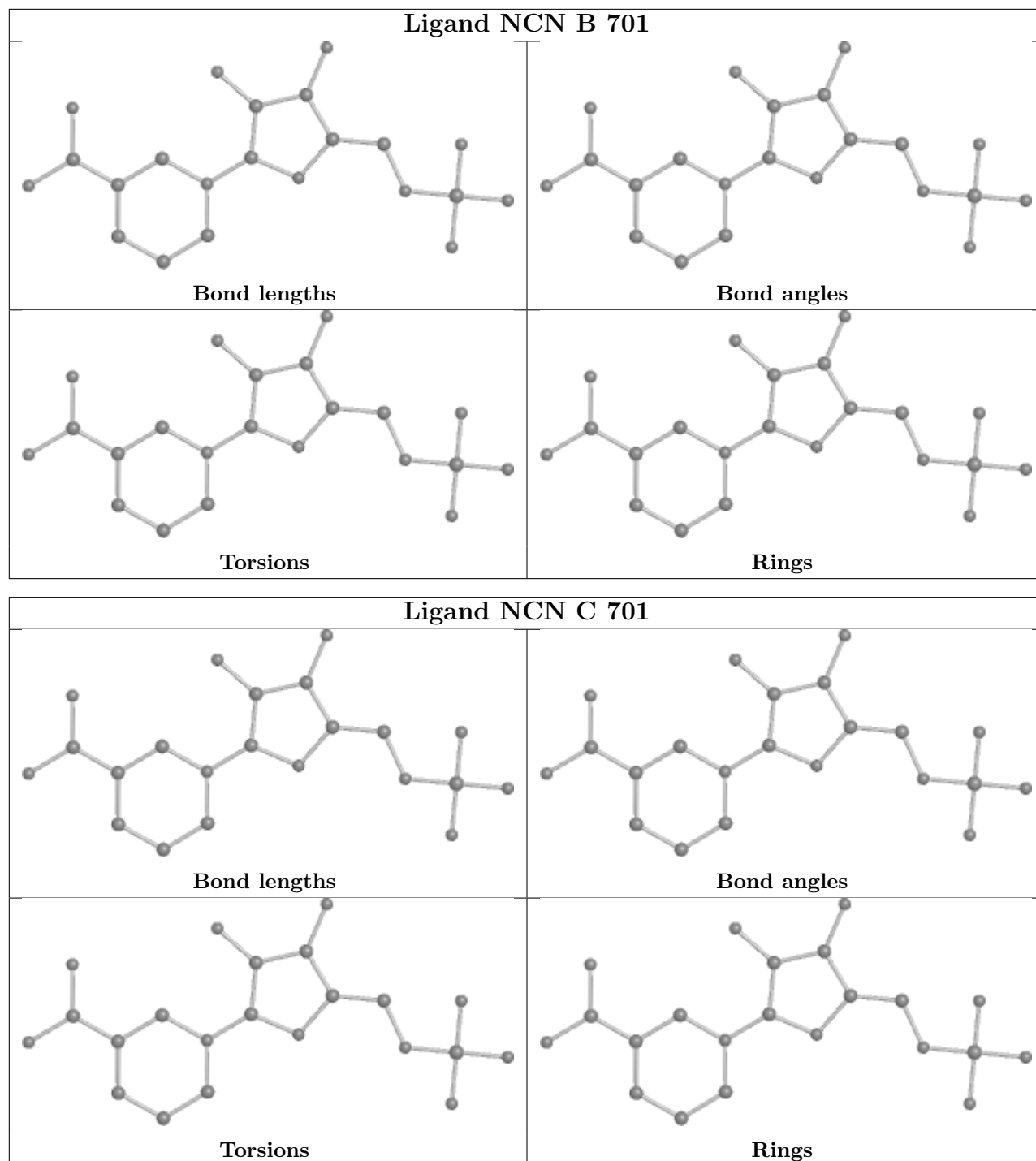
There are no chirality outliers.

There are no torsion outliers.

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 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 NCN A 701

Bond lengths — Bond angles — Torsions — Rings

Ligand NCN B 701

Bond lengths	Bond angles

Torsions	Rings

Ligand NCN C 701

Bond lengths	Bond angles

Torsions	Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	331/364 (90%)	0.36	12 (3%)	42	41	60, 73, 91, 113	0
1	B	331/364 (90%)	0.33	16 (4%)	30	30	61, 74, 91, 103	0
1	C	331/364 (90%)	0.48	22 (6%)	18	19	63, 75, 96, 113	0
All	All	993/1092 (90%)	0.39	50 (5%)	28	28	60, 74, 92, 113	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	414	ASN	5.4
1	C	331	GLN	4.5
1	C	333	ILE	4.1
1	C	561	ALA	4.0
1	B	373	TYR	3.9
1	A	415	CYS	3.9
1	A	328	SER	3.9
1	C	415	CYS	3.7
1	A	331	GLN	3.7
1	C	329	GLY	3.7
1	C	575	LEU	3.3
1	C	421	GLN	3.3
1	B	408	LEU	3.3
1	C	646	GLU	3.2
1	B	419	ASP	3.1
1	A	597	HIS	3.1
1	C	419	ASP	3.1
1	A	416	VAL	3.1
1	C	416	VAL	3.0
1	C	562	ASN	2.9
1	B	646	GLU	2.9
1	C	420	LEU	2.9
1	B	412	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	328	SER	2.9
1	C	394	LEU	2.9
1	A	417	LYS	2.8
1	B	415	CYS	2.8
1	C	417	LYS	2.6
1	A	379	GLU	2.6
1	C	564	GLU	2.6
1	B	376	LYS	2.5
1	B	344	LEU	2.4
1	B	410	LEU	2.4
1	A	661	ASN	2.4
1	C	661	ASN	2.3
1	A	647	ILE	2.3
1	C	568	GLU	2.3
1	B	377	ILE	2.3
1	A	376	LYS	2.3
1	B	414	ASN	2.2
1	A	603	LYS	2.2
1	C	565	ILE	2.2
1	B	647	ILE	2.1
1	C	377	ILE	2.1
1	C	614	SER	2.1
1	B	335	GLN	2.1
1	B	375	GLU	2.0
1	A	634	ILE	2.0
1	B	346	SER	2.0
1	B	420	LEU	2.0

6.2　Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3　Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4　Ligands ⓘ

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(Å^2)	Q<0.9
2	NCN	C	701	22/22	0.88	0.22	75,80,96,99	0
2	NCN	A	701	22/22	0.90	0.24	74,80,98,102	0
2	NCN	B	701	22/22	0.91	0.27	71,79,96,99	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.
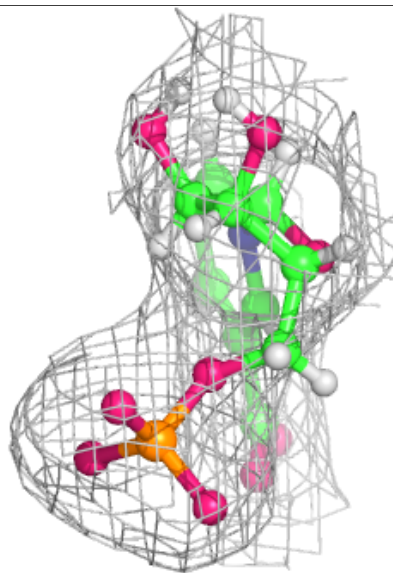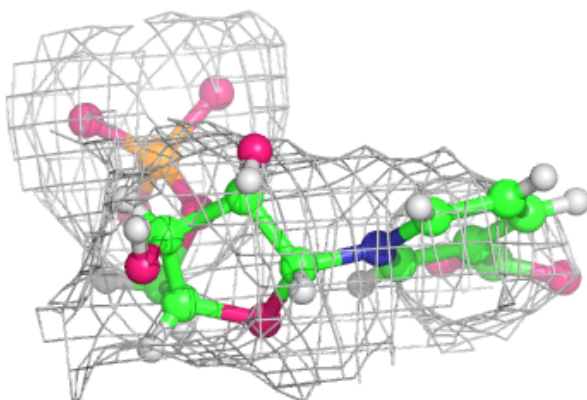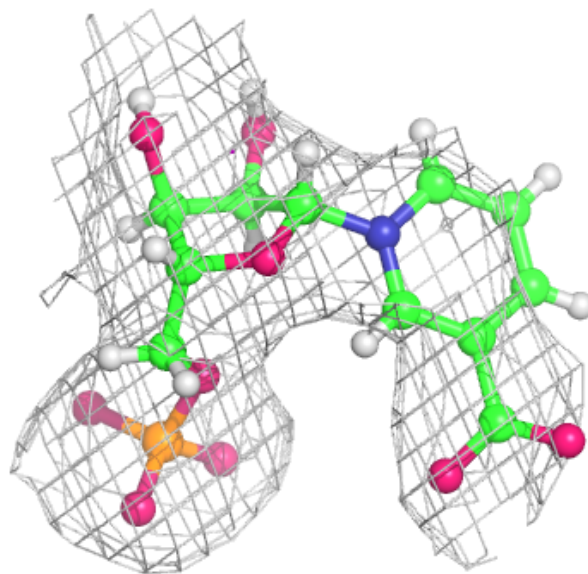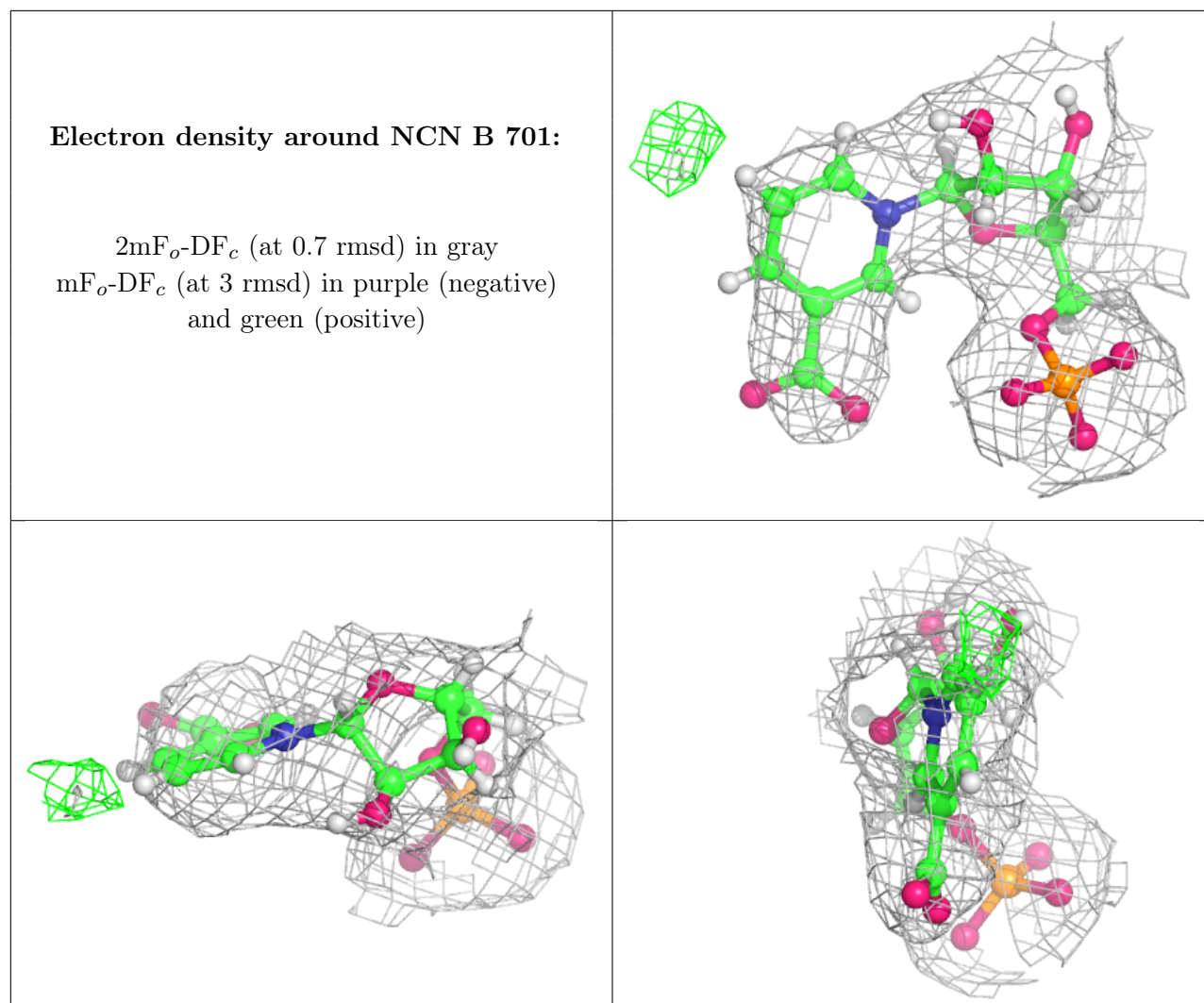
Electron density around NCN C 701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
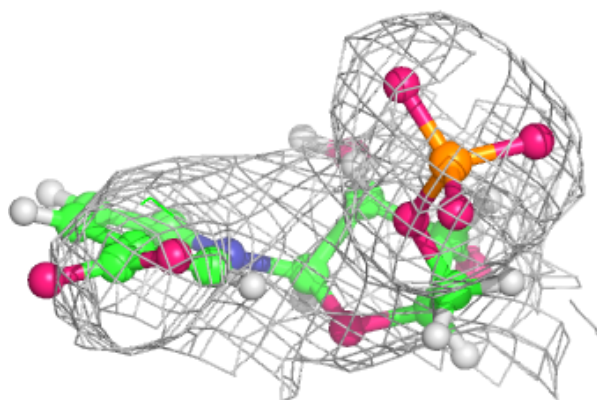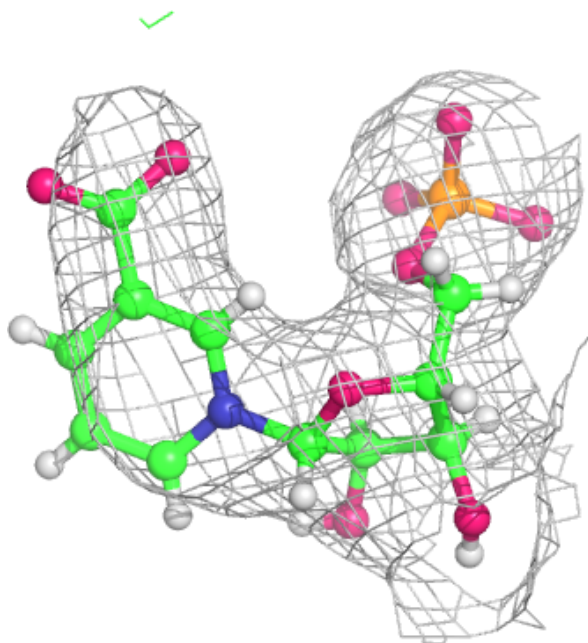
Electron density around NCN A 701:

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

Electron density around NCN B 701:

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.