



wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 10:01 am BST

PDB ID : 1YUM
Title : Crystal Structure of Nicotinic Acid Mononucleotide Adenylyltransferase from *Pseudomonas aeruginosa*
Authors : Yoon, H.J.; Kim, H.L.; Mikami, B.; Suh, S.W.
Deposited on : 2005-02-14
Resolution : 1.70 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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 : 2.11
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) : 2.11

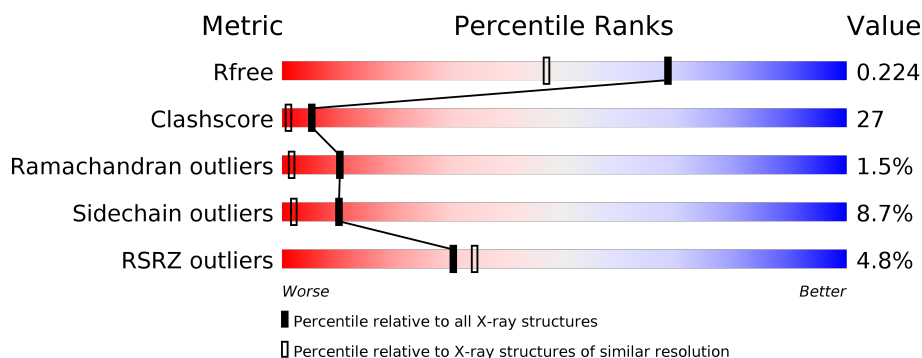
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 ≥ 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	242	<div> <div>4%</div> <div> <div></div> <div>46%</div> <div>36%</div> <div>5% •</div> <div>12%</div> </div> </div>
1	B	242	<div> <div>4%</div> <div> <div></div> <div>51%</div> <div>31%</div> <div>5% •</div> <div>12%</div> </div> </div>
1	C	242	<div> <div>4%</div> <div> <div></div> <div>48%</div> <div>35%</div> <div>• •</div> <div>12%</div> </div> </div>
1	D	242	<div> <div>5%</div> <div> <div></div> <div>50%</div> <div>31%</div> <div>6%</div> <div>12%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CIT	D	3301	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7740 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 'Probable nicotinate-nucleotide adenylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	6	0
			1694	1073	313	302	6			
1	B	212	Total	C	N	O	S	0	5	0
			1682	1067	307	301	7			
1	C	212	Total	C	N	O	S	0	7	0
			1701	1078	315	302	6			
1	D	212	Total	C	N	O	S	0	8	0
			1710	1087	315	302	6			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP Q9HX21
A	-18	GLY	-	EXPRESSION TAG	UNP Q9HX21
A	-17	SER	-	EXPRESSION TAG	UNP Q9HX21
A	-16	SER	-	EXPRESSION TAG	UNP Q9HX21
A	-15	HIS	-	EXPRESSION TAG	UNP Q9HX21
A	-14	HIS	-	EXPRESSION TAG	UNP Q9HX21
A	-13	HIS	-	EXPRESSION TAG	UNP Q9HX21
A	-12	HIS	-	EXPRESSION TAG	UNP Q9HX21
A	-11	HIS	-	EXPRESSION TAG	UNP Q9HX21
A	-10	HIS	-	EXPRESSION TAG	UNP Q9HX21
A	-9	SER	-	EXPRESSION TAG	UNP Q9HX21
A	-8	SER	-	EXPRESSION TAG	UNP Q9HX21
A	-7	GLY	-	EXPRESSION TAG	UNP Q9HX21
A	-6	LEU	-	EXPRESSION TAG	UNP Q9HX21
A	-5	VAL	-	EXPRESSION TAG	UNP Q9HX21
A	-4	PRO	-	EXPRESSION TAG	UNP Q9HX21
A	-3	ARG	-	EXPRESSION TAG	UNP Q9HX21
A	-2	GLY	-	EXPRESSION TAG	UNP Q9HX21
A	-1	SER	-	EXPRESSION TAG	UNP Q9HX21
A	0	HIS	-	EXPRESSION TAG	UNP Q9HX21
A	215	LEU	-	EXPRESSION TAG	UNP Q9HX21

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Chain	Residue	Modelled	Actual	Comment	Reference
A	216	GLU	-	EXPRESSION TAG	UNP Q9HX21
A	217	HIS	-	EXPRESSION TAG	UNP Q9HX21
A	218	HIS	-	EXPRESSION TAG	UNP Q9HX21
A	219	HIS	-	EXPRESSION TAG	UNP Q9HX21
A	220	HIS	-	EXPRESSION TAG	UNP Q9HX21
A	221	HIS	-	EXPRESSION TAG	UNP Q9HX21
A	222	HIS	-	EXPRESSION TAG	UNP Q9HX21
B	-19	MET	-	EXPRESSION TAG	UNP Q9HX21
B	-18	GLY	-	EXPRESSION TAG	UNP Q9HX21
B	-17	SER	-	EXPRESSION TAG	UNP Q9HX21
B	-16	SER	-	EXPRESSION TAG	UNP Q9HX21
B	-15	HIS	-	EXPRESSION TAG	UNP Q9HX21
B	-14	HIS	-	EXPRESSION TAG	UNP Q9HX21
B	-13	HIS	-	EXPRESSION TAG	UNP Q9HX21
B	-12	HIS	-	EXPRESSION TAG	UNP Q9HX21
B	-11	HIS	-	EXPRESSION TAG	UNP Q9HX21
B	-10	HIS	-	EXPRESSION TAG	UNP Q9HX21
B	-9	SER	-	EXPRESSION TAG	UNP Q9HX21
B	-8	SER	-	EXPRESSION TAG	UNP Q9HX21
B	-7	GLY	-	EXPRESSION TAG	UNP Q9HX21
B	-6	LEU	-	EXPRESSION TAG	UNP Q9HX21
B	-5	VAL	-	EXPRESSION TAG	UNP Q9HX21
B	-4	PRO	-	EXPRESSION TAG	UNP Q9HX21
B	-3	ARG	-	EXPRESSION TAG	UNP Q9HX21
B	-2	GLY	-	EXPRESSION TAG	UNP Q9HX21
B	-1	SER	-	EXPRESSION TAG	UNP Q9HX21
B	0	HIS	-	EXPRESSION TAG	UNP Q9HX21
B	215	LEU	-	EXPRESSION TAG	UNP Q9HX21
B	216	GLU	-	EXPRESSION TAG	UNP Q9HX21
B	217	HIS	-	EXPRESSION TAG	UNP Q9HX21
B	218	HIS	-	EXPRESSION TAG	UNP Q9HX21
B	219	HIS	-	EXPRESSION TAG	UNP Q9HX21
B	220	HIS	-	EXPRESSION TAG	UNP Q9HX21
B	221	HIS	-	EXPRESSION TAG	UNP Q9HX21
B	222	HIS	-	EXPRESSION TAG	UNP Q9HX21
C	-19	MET	-	EXPRESSION TAG	UNP Q9HX21
C	-18	GLY	-	EXPRESSION TAG	UNP Q9HX21
C	-17	SER	-	EXPRESSION TAG	UNP Q9HX21
C	-16	SER	-	EXPRESSION TAG	UNP Q9HX21
C	-15	HIS	-	EXPRESSION TAG	UNP Q9HX21
C	-14	HIS	-	EXPRESSION TAG	UNP Q9HX21
C	-13	HIS	-	EXPRESSION TAG	UNP Q9HX21

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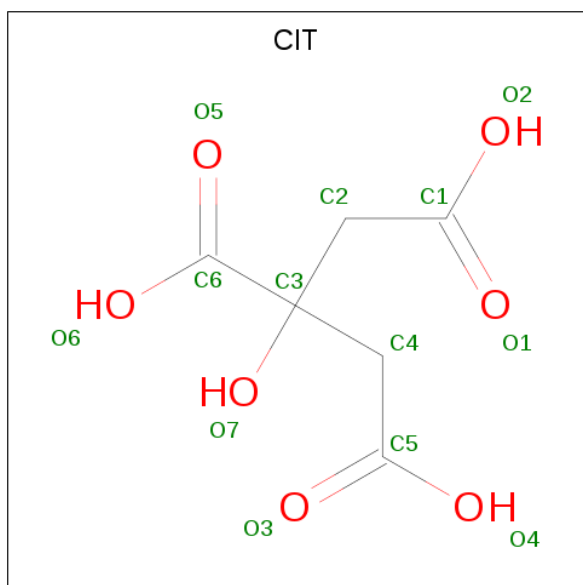
Chain	Residue	Modelled	Actual	Comment	Reference
C	-12	HIS	-	EXPRESSION TAG	UNP Q9HX21
C	-11	HIS	-	EXPRESSION TAG	UNP Q9HX21
C	-10	HIS	-	EXPRESSION TAG	UNP Q9HX21
C	-9	SER	-	EXPRESSION TAG	UNP Q9HX21
C	-8	SER	-	EXPRESSION TAG	UNP Q9HX21
C	-7	GLY	-	EXPRESSION TAG	UNP Q9HX21
C	-6	LEU	-	EXPRESSION TAG	UNP Q9HX21
C	-5	VAL	-	EXPRESSION TAG	UNP Q9HX21
C	-4	PRO	-	EXPRESSION TAG	UNP Q9HX21
C	-3	ARG	-	EXPRESSION TAG	UNP Q9HX21
C	-2	GLY	-	EXPRESSION TAG	UNP Q9HX21
C	-1	SER	-	EXPRESSION TAG	UNP Q9HX21
C	0	HIS	-	EXPRESSION TAG	UNP Q9HX21
C	215	LEU	-	EXPRESSION TAG	UNP Q9HX21
C	216	GLU	-	EXPRESSION TAG	UNP Q9HX21
C	217	HIS	-	EXPRESSION TAG	UNP Q9HX21
C	218	HIS	-	EXPRESSION TAG	UNP Q9HX21
C	219	HIS	-	EXPRESSION TAG	UNP Q9HX21
C	220	HIS	-	EXPRESSION TAG	UNP Q9HX21
C	221	HIS	-	EXPRESSION TAG	UNP Q9HX21
C	222	HIS	-	EXPRESSION TAG	UNP Q9HX21
D	-19	MET	-	EXPRESSION TAG	UNP Q9HX21
D	-18	GLY	-	EXPRESSION TAG	UNP Q9HX21
D	-17	SER	-	EXPRESSION TAG	UNP Q9HX21
D	-16	SER	-	EXPRESSION TAG	UNP Q9HX21
D	-15	HIS	-	EXPRESSION TAG	UNP Q9HX21
D	-14	HIS	-	EXPRESSION TAG	UNP Q9HX21
D	-13	HIS	-	EXPRESSION TAG	UNP Q9HX21
D	-12	HIS	-	EXPRESSION TAG	UNP Q9HX21
D	-11	HIS	-	EXPRESSION TAG	UNP Q9HX21
D	-10	HIS	-	EXPRESSION TAG	UNP Q9HX21
D	-9	SER	-	EXPRESSION TAG	UNP Q9HX21
D	-8	SER	-	EXPRESSION TAG	UNP Q9HX21
D	-7	GLY	-	EXPRESSION TAG	UNP Q9HX21
D	-6	LEU	-	EXPRESSION TAG	UNP Q9HX21
D	-5	VAL	-	EXPRESSION TAG	UNP Q9HX21
D	-4	PRO	-	EXPRESSION TAG	UNP Q9HX21
D	-3	ARG	-	EXPRESSION TAG	UNP Q9HX21
D	-2	GLY	-	EXPRESSION TAG	UNP Q9HX21
D	-1	SER	-	EXPRESSION TAG	UNP Q9HX21
D	0	HIS	-	EXPRESSION TAG	UNP Q9HX21
D	215	LEU	-	EXPRESSION TAG	UNP Q9HX21

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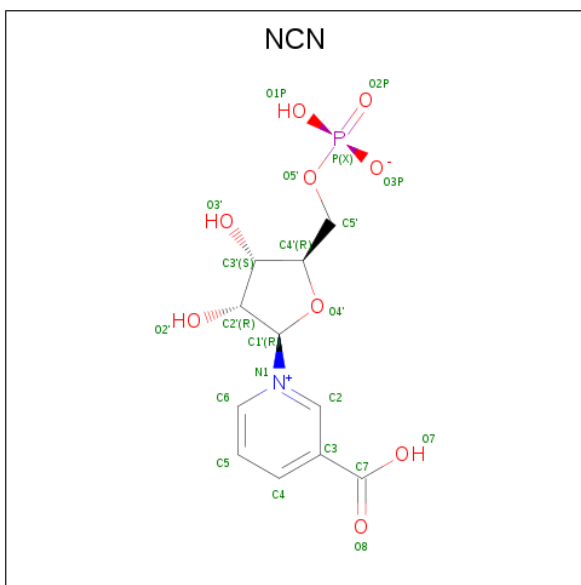
Chain	Residue	Modelled	Actual	Comment	Reference
D	216	GLU	-	EXPRESSION TAG	UNP Q9HX21
D	217	HIS	-	EXPRESSION TAG	UNP Q9HX21
D	218	HIS	-	EXPRESSION TAG	UNP Q9HX21
D	219	HIS	-	EXPRESSION TAG	UNP Q9HX21
D	220	HIS	-	EXPRESSION TAG	UNP Q9HX21
D	221	HIS	-	EXPRESSION TAG	UNP Q9HX21
D	222	HIS	-	EXPRESSION TAG	UNP Q9HX21

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		
2	C	1	Total	C	O	0	0
			13	6	7		
2	D	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is NICOTINATE MONONUCLEOTIDE (three-letter code: NCN) (formula: $C_{11}H_{14}NO_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 22	C 11	N 1	O 9	P 1	0	0
3	B	1	Total 22	C 11	N 1	O 9	P 1	0	0
3	C	1	Total 22	C 11	N 1	O 9	P 1	0	0
3	D	1	Total 22	C 11	N 1	O 9	P 1	0	0

- Molecule 4 is water.

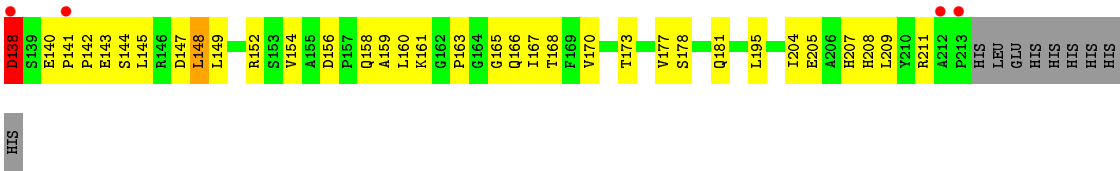
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	164	Total O 164 164	0	0
4	B	215	Total O 215 215	0	0
4	C	225	Total O 225 225	0	0
4	D	209	Total O 209 209	0	0

These plots are drawn for all protein, RNA and DNA 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.

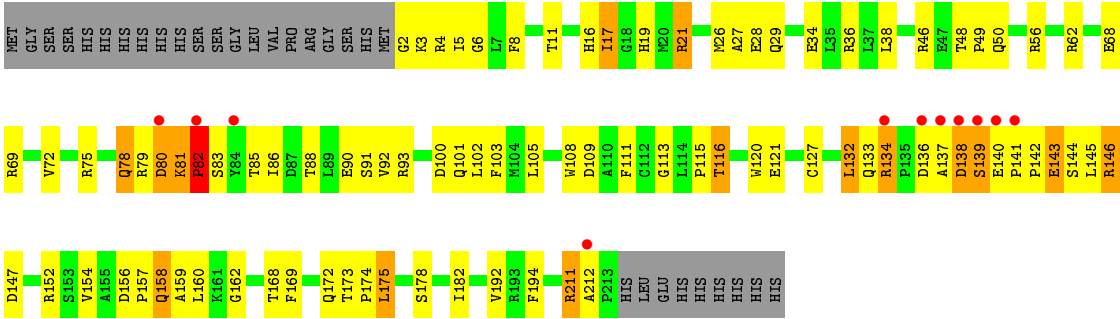
- [illegible]

- [illegible]

- Chain C:
-
- 4% 48% 35% 12%
- MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG ARG GLY SER SER HIS MET G2 K3 R4 L7 F8 G9 G10 T11 H16 I17 R21 M26 A27 E28 Q29 L32 D33 E34 L35 R36 L37 L38 F39 N40 A41 P44 H45 R46 Q50 V51 S52 Q55 M59 V60 E61 R69 V72 D73 P74 R75 E76 L77 Q78 R79 D80 K81 R82 S83 Y84 T85 I86 D87 T88 R93 L96 D99 D100 Q101 L102 L105 W108 F111 C112 G113 L114 P115 T116 R119 W120 E121 A122 L123 L124 V131 L132 Q133 R134 P135 D136 S137



- Molecule 1: 'Probable nicotinate-nucleotide adenylyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.18Å 110.66Å 65.20Å 90.00° 89.99° 90.00°	Depositor
Resolution (Å)	10.00 – 1.70 42.56 – 1.60	Depositor EDS
% Data completeness (in resolution range)	91.3 (10.00-1.70) 93.4 (42.56-1.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.83 (at 1.60Å)	Xtriage
Refinement program	SHELXL-97, SHELXL	Depositor
R, R_{free}	0.191 , 0.251 0.174 , 0.224	Depositor DCC
R_{free} test set	5982 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	18.5	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.487 for -l,k,h 0.488 for h,-k,-l 0.487 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7740	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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: NCN, CIT

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	0.41	0/1763	1.23	8/2402 (0.3%)
1	B	0.41	0/1743	1.22	7/2374 (0.3%)
1	C	0.41	0/1774	1.17	6/2415 (0.2%)
1	D	0.41	0/1791	1.19	10/2438 (0.4%)
All	All	0.41	0/7071	1.20	31/9629 (0.3%)

There are no bond length outliers.

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	134	ARG	NE-CZ-NH1	10.56	125.58	120.30
1	D	21	ARG	NE-CZ-NH2	10.08	125.34	120.30
1	B	21	ARG	NE-CZ-NH1	-9.92	115.34	120.30
1	D	56	ARG	NE-CZ-NH1	9.30	124.95	120.30
1	A	21	ARG	NE-CZ-NH1	-8.54	116.03	120.30

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	1694	0	1692	103	0
1	B	1682	0	1678	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1701	0	1704	109	0
1	D	1710	0	1725	77	0
2	A	13	0	5	3	0
2	B	13	0	5	4	0
2	C	13	0	5	3	0
2	D	13	0	5	6	0
3	A	22	0	12	1	0
3	B	22	0	12	1	0
3	C	22	0	12	2	0
3	D	22	0	11	1	0
4	A	164	0	0	15	0
4	B	215	0	0	15	0
4	C	225	0	0	20	0
4	D	209	0	0	18	0
All	All	7740	0	6866	368	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 27.

The worst 5 of 368 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:79[C]:ARG:NH2	1:A:83:SER:CB	1.90	1.31
1:A:79[C]:ARG:NH2	1:A:83:SER:HB3	1.01	1.30
1:A:79[C]:ARG:CZ	1:A:83:SER:HB3	1.62	1.30
1:B:208:HIS:HB3	1:B:211:ARG:HD3	1.37	1.02
1:B:17[A]:ILE:HG23	1:D:194:PHE:HB3	1.45	0.98

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	217/242 (90%)	202 (93%)	8 (4%)	7 (3%)	4	0
1	B	215/242 (89%)	205 (95%)	7 (3%)	3 (1%)	11	2
1	C	218/242 (90%)	202 (93%)	14 (6%)	2 (1%)	17	5
1	D	220/242 (91%)	208 (94%)	9 (4%)	3 (1%)	11	2
All	All	870/968 (90%)	817 (94%)	38 (4%)	15 (2%)	10	1

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	ASP
1	A	138	ASP
1	B	138	ASP
1	B	139	SER
1	C	82	PRO

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	180/200 (90%)	166 (92%)	14 (8%)	12	3
1	B	178/200 (89%)	166 (93%)	12 (7%)	16	4
1	C	181/200 (90%)	166 (92%)	15 (8%)	11	2
1	D	183/200 (92%)	156 (85%)	27 (15%)	3	0
All	All	722/800 (90%)	654 (91%)	68 (9%)	10	1

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	21	ARG
1	C	138	ASP
1	D	158	GLN
1	C	74	PRO
1	C	82	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	207	HIS
1	C	55	GLN
1	D	133	GLN
1	C	29	GLN
1	C	78	GLN

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 ⓘ

8 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	CIT	C	2301	-	3,12,12	0.73	0	3,17,17	1.50	0
3	NCN	A	302	-	20,23,23	2.56	7 (35%)	27,34,34	3.47	10 (37%)
2	CIT	B	1301	-	3,12,12	1.04	0	3,17,17	1.40	0
3	NCN	D	3302	-	20,23,23	2.67	11 (55%)	27,34,34	3.49	11 (40%)
3	NCN	B	1302	-	20,23,23	2.64	7 (35%)	27,34,34	3.46	10 (37%)
3	NCN	C	2302	-	20,23,23	2.63	6 (30%)	27,34,34	3.18	12 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CIT	D	3301	-	3,12,12	1.15	0	3,17,17	3.43	1 (33%)
2	CIT	A	301	-	3,12,12	0.27	0	3,17,17	1.75	1 (33%)

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	CIT	C	2301	-	-	4/6/16/16	-
3	NCN	A	302	-	-	2/10/30/30	0/2/2/2
2	CIT	B	1301	-	-	6/6/16/16	-
3	NCN	D	3302	-	-	4/10/30/30	0/2/2/2
3	NCN	B	1302	-	-	3/10/30/30	0/2/2/2
3	NCN	C	2302	-	-	3/10/30/30	0/2/2/2
2	CIT	D	3301	-	-	6/6/16/16	-
2	CIT	A	301	-	-	4/6/16/16	-

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1302	NCN	C3-C7	7.94	1.55	1.47
3	C	2302	NCN	C3-C7	7.88	1.55	1.47
3	A	302	NCN	C3-C7	7.75	1.54	1.47
3	D	3302	NCN	C3-C7	7.52	1.54	1.47
3	D	3302	NCN	C6-N1	4.12	1.45	1.35

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	NCN	C4-C3-C7	-12.60	103.44	120.37
3	B	1302	NCN	C4-C3-C7	-11.87	104.43	120.37
3	D	3302	NCN	C4-C3-C7	-11.14	105.40	120.37
3	C	2302	NCN	C4-C3-C7	-8.75	108.62	120.37
3	C	2302	NCN	C5-C4-C3	-6.88	111.92	120.56

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

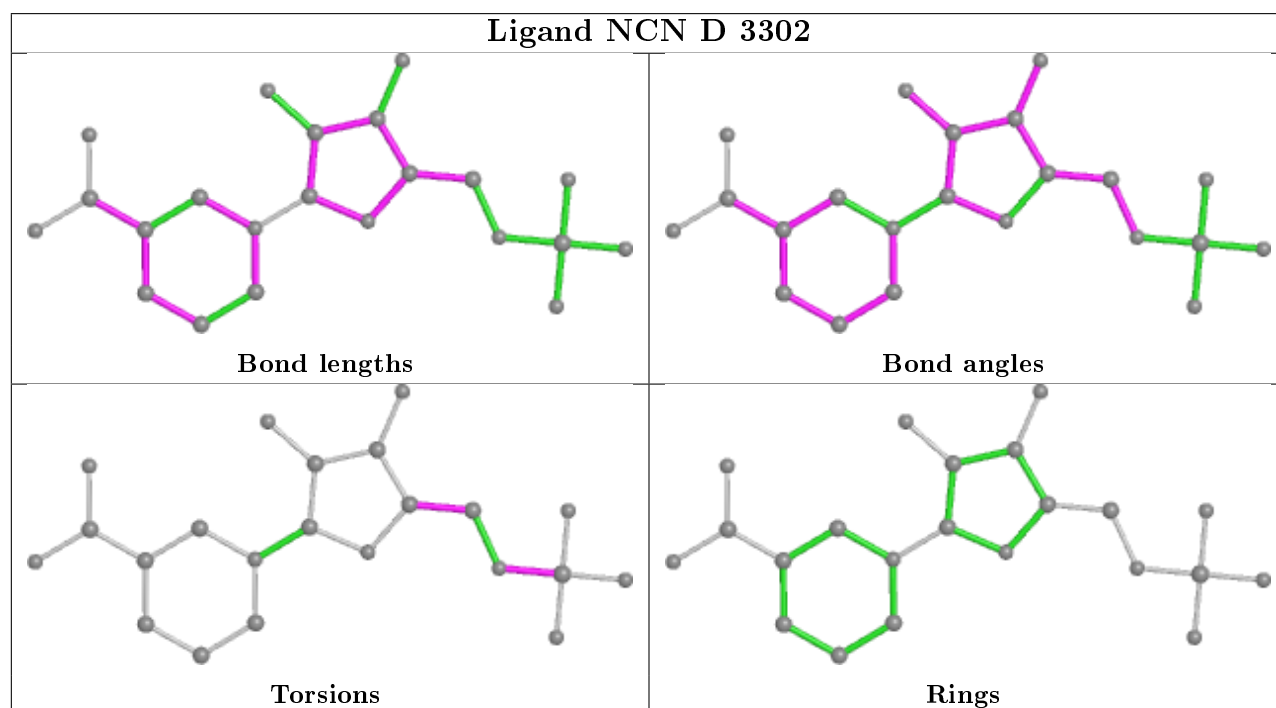
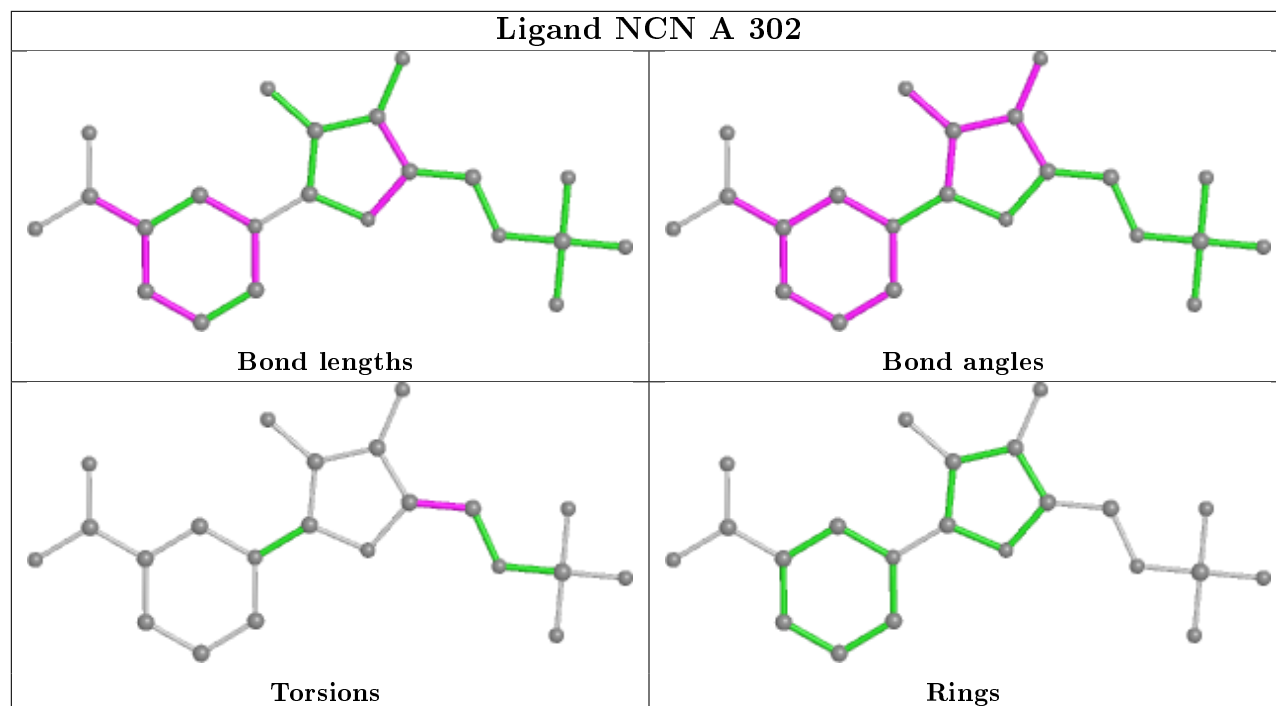
Mol	Chain	Res	Type	Atoms
2	C	2301	CIT	C2-C3-C4-C5
2	C	2301	CIT	O7-C3-C4-C5
2	C	2301	CIT	C6-C3-C4-C5
2	B	1301	CIT	C1-C2-C3-O7
2	B	1301	CIT	C1-C2-C3-C6

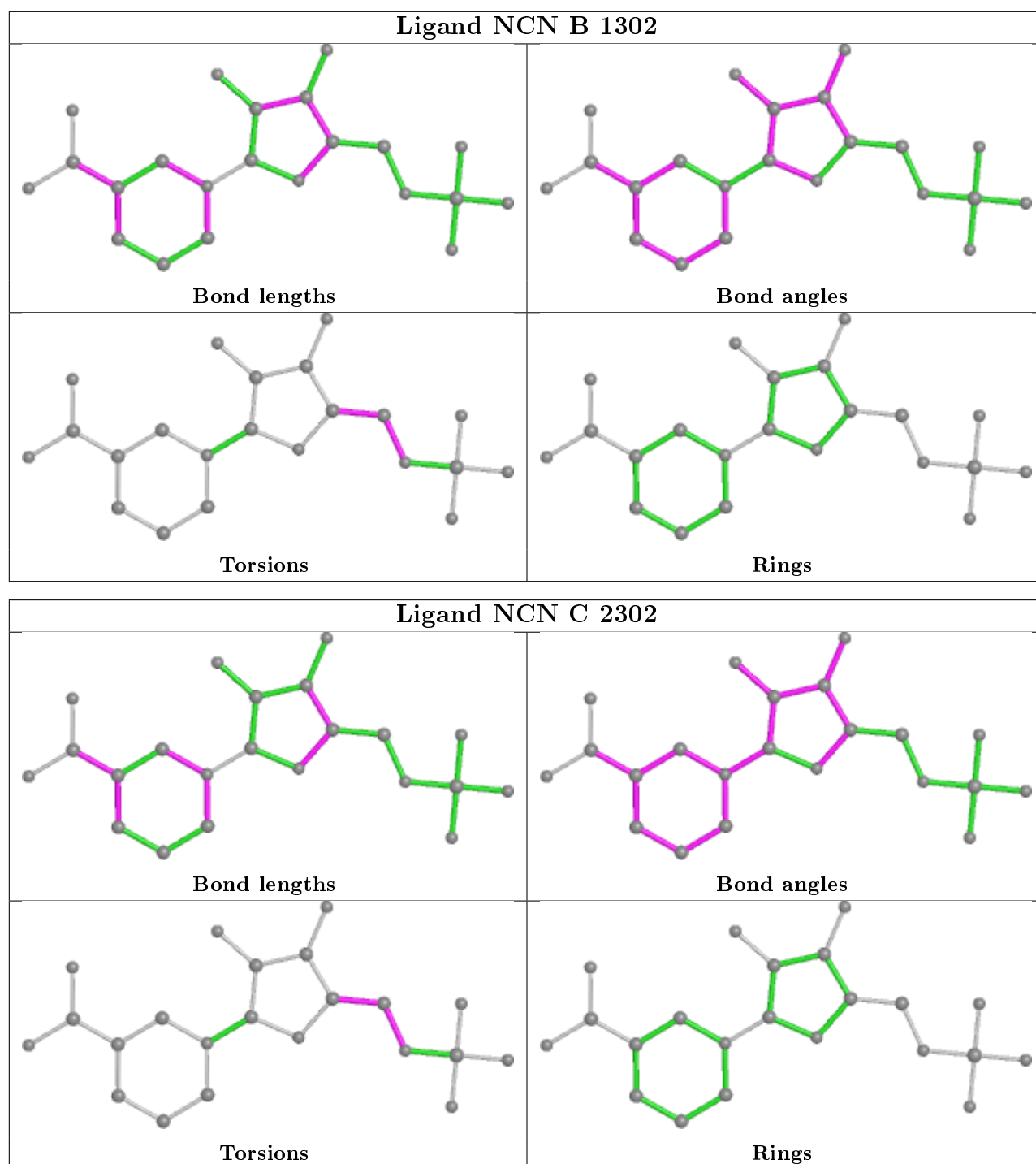
There are no ring outliers.

8 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2301	CIT	3	0
3	A	302	NCN	1	0
2	B	1301	CIT	4	0
3	D	3302	NCN	1	0
3	B	1302	NCN	1	0
3	C	2302	NCN	2	0
2	D	3301	CIT	6	0
2	A	301	CIT	3	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 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, 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	212/242 (87%)	0.20	10 (4%) 31 35	13, 24, 48, 88	1 (0%)
1	B	212/242 (87%)	0.23	10 (4%) 31 35	14, 24, 47, 73	0
1	C	212/242 (87%)	0.28	10 (4%) 31 35	13, 23, 53, 87	0
1	D	212/242 (87%)	0.27	11 (5%) 27 30	12, 24, 52, 97	0
All	All	848/968 (87%)	0.25	41 (4%) 30 34	12, 24, 51, 97	1 (0%)

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	82	PRO	8.1
1	C	82	PRO	8.0
1	B	139	SER	6.3
1	C	138	ASP	6.1
1	C	137	ALA	5.5

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](#)

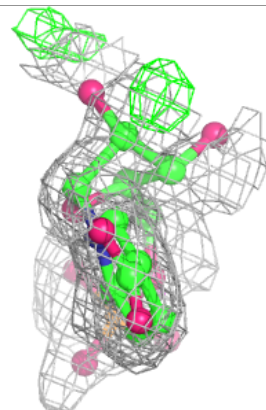
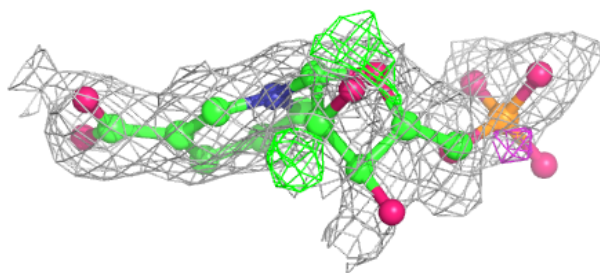
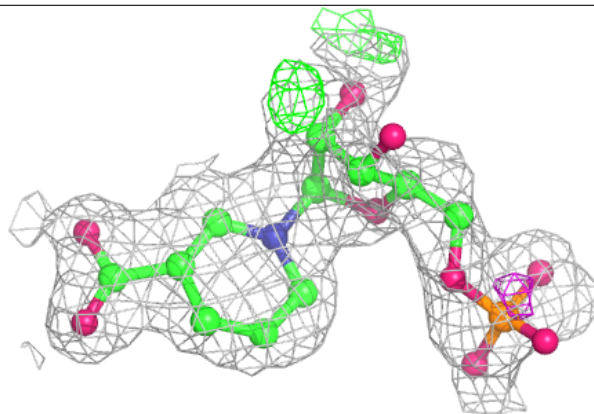
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NCN	D	3302	22/22	0.79	0.16	25,47,75,95	0
2	CIT	B	1301	13/13	0.81	0.27	27,49,79,90	0
3	NCN	B	1302	22/22	0.85	0.18	32,57,83,98	0
2	CIT	A	301	13/13	0.85	0.18	14,45,67,75	0
3	NCN	A	302	22/22	0.87	0.15	25,56,83,89	0
2	CIT	D	3301	13/13	0.89	0.19	18,38,70,76	0
3	NCN	C	2302	22/22	0.89	0.15	18,42,74,81	0
2	CIT	C	2301	13/13	0.91	0.18	15,35,75,79	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.

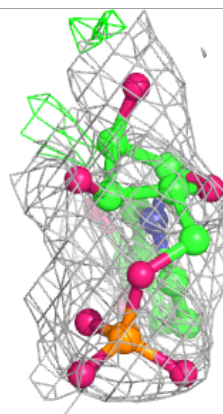
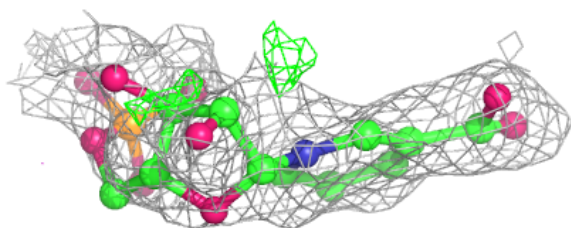
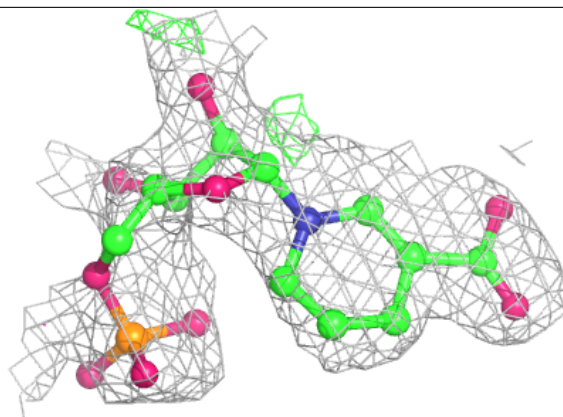
Electron density around NCN D 3302:

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

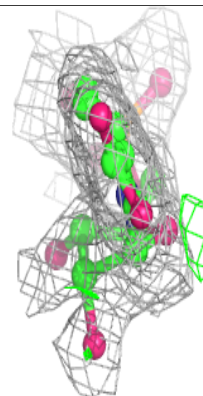
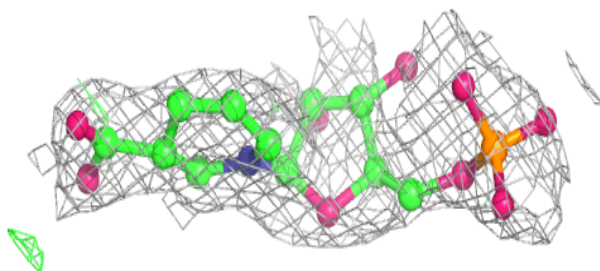
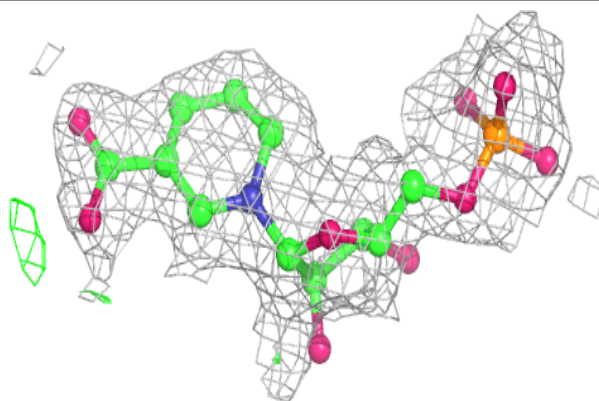


Electron density around NCN B 1302:

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

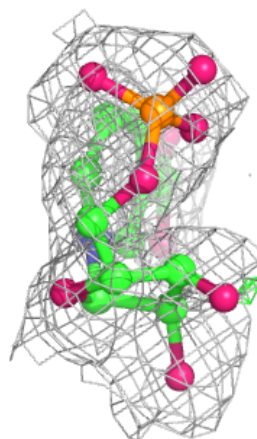
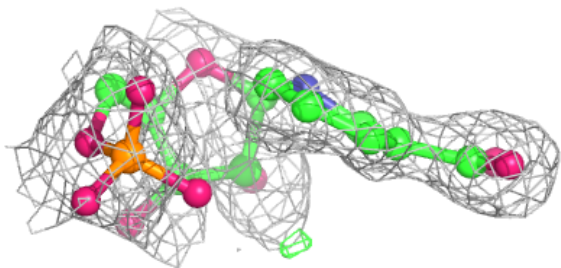
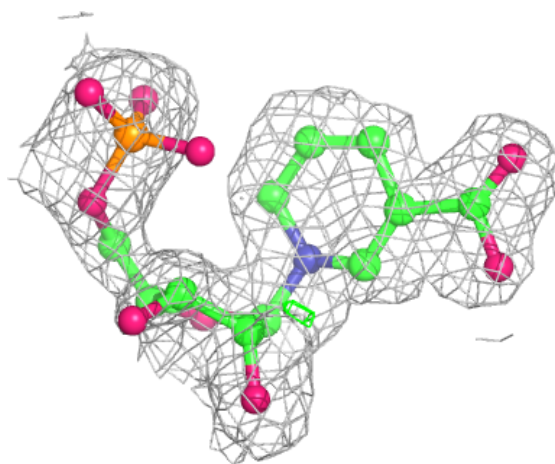
**Electron density around NCN A 302:**

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



Electron density around NCN C 2302:

$2mF_o-DF_c$ (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.