



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 8, 2025 – 02:14 pm BST

PDB ID : 9S6C / pdb_00009s6c
Title : B12 Binding protein - BtuK1
Authors : Clarke, C.; Banasik, M.; Pickersgill, R.W.
Deposited on : 2025-07-31
Resolution : 1.82 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 : **FAILED**
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

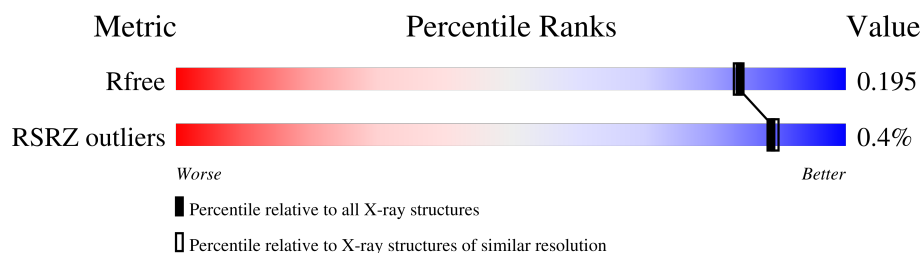
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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}	164625	9242 (1.84-1.80)
RSRZ outliers	164620	9241 (1.84-1.80)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16442 atoms, of which 7582 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 Quinoprotein amine dehydrogenase-like protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	C	337	Total	C	H	N	O	S	0	0	0
			5086	1691	2447	423	515	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	15	GLY	-	expression tag	UNP Q8A7N8

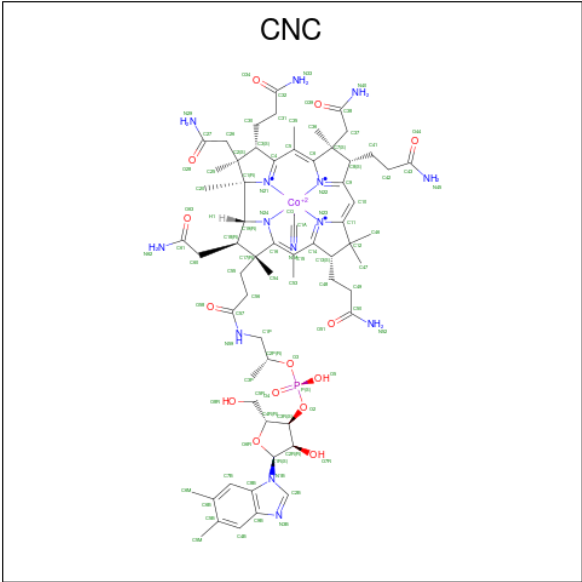
- Molecule 2 is a protein called Quinoprotein amine dehydrogenase-like protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	A	339	Total	C	H	N	O	S	0	0	0
			5119	1702	2462	427	517	11			
2	B	337	Total	C	H	N	O	S	0	0	0
			5094	1694	2451	423	515	11			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	GLY	-	expression tag	UNP Q8A7N8
A	14	HIS	-	expression tag	UNP Q8A7N8
A	15	MET	-	expression tag	UNP Q8A7N8
B	13	GLY	-	expression tag	UNP Q8A7N8
B	14	HIS	-	expression tag	UNP Q8A7N8
B	15	MET	-	expression tag	UNP Q8A7N8

- Molecule 3 is CYANOCOBALAMIN (CCD ID: CNC) (formula: $C_{63}H_{89}CoN_{14}O_{14}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	C	1	Total	C	Co	H	N	O	P	0	0
			167	63	1	74	14	14	1		
3	A	1	Total	C	Co	H	N	O	P	0	0
			167	63	1	74	14	14	1		
3	B	1	Total	C	Co	H	N	O	P	0	0
			167	63	1	74	14	14	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	192	Total O 192 192	0	0
4	A	253	Total O 253 253	0	0
4	B	197	Total O 197 197	0	0

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3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.74Å 129.98Å 164.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.29 – 1.82 14.29 – 1.82	Depositor EDS
% Data completeness (in resolution range)	96.3 (14.29-1.82) 96.3 (14.29-1.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.105)	Depositor
R, R_{free}	0.163 , 0.192 0.164 , 0.195	Depositor DCC
R_{free} test set	6550 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	16442	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 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	$\# Z > 2$
3	CNC	A	401	-	90,103,103	0.89	6 (6%)	139,171,171	1.21	12 (8%)
3	CNC	C	401	-	90,103,103	0.96	6 (6%)	139,171,171	1.37	16 (11%)
3	CNC	B	401	-	90,103,103	0.87	4 (4%)	139,171,171	1.26	15 (10%)

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
3	CNC	B	401	-	1/1/38/38	3/52/235/235	0/3/11/11
3	CNC	A	401	-	1/1/38/38	0/52/235/235	0/3/11/11
3	CNC	C	401	-	-	2/52/235/235	0/3/11/11

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	CNC	C14-N23	3.34	1.40	1.30
3	A	401	CNC	C14-N23	3.32	1.40	1.30
3	B	401	CNC	C14-N23	3.27	1.40	1.30
3	C	401	CNC	C1A-N1A	3.27	1.28	1.14
3	A	401	CNC	C1A-N1A	2.77	1.26	1.14
3	A	401	CNC	C2B-N3B	-2.72	1.29	1.34
3	C	401	CNC	C6-C5	2.72	1.44	1.36
3	B	401	CNC	C19-N24	-2.44	1.44	1.49
3	B	401	CNC	C35-C5	2.38	1.55	1.50
3	C	401	CNC	C2B-N3B	-2.37	1.30	1.34
3	C	401	CNC	C6B-C5B	2.23	1.46	1.40
3	A	401	CNC	C53-C15	2.10	1.55	1.50
3	A	401	CNC	C35-C5	2.09	1.55	1.50
3	C	401	CNC	C53-C15	2.05	1.55	1.50
3	A	401	CNC	C19-N24	-2.03	1.44	1.49
3	B	401	CNC	C53-C15	2.02	1.55	1.50

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	CNC	C3-C4-N21	-5.75	104.76	111.97
3	C	401	CNC	C1-N21-C4	4.90	117.12	109.37
3	A	401	CNC	C1-N21-C4	4.64	116.71	109.37
3	C	401	CNC	C2-C3-C4	4.42	106.66	101.63
3	A	401	CNC	C3-C4-N21	-4.12	106.80	111.97
3	C	401	CNC	C1-C2-C3	-3.99	96.51	101.60
3	B	401	CNC	C1-C19-N24	3.90	112.50	106.33
3	B	401	CNC	C3-C4-N21	-3.74	107.28	111.97
3	B	401	CNC	C1-N21-C4	3.59	115.05	109.37
3	A	401	CNC	C1-C19-N24	3.59	112.01	106.33
3	C	401	CNC	C1-C19-N24	3.32	111.59	106.33
3	C	401	CNC	C60-C18-C19	3.15	121.59	114.09
3	A	401	CNC	C2-C3-C4	3.10	105.15	101.63
3	C	401	CNC	C30-C3-C4	3.02	116.66	109.63
3	A	401	CNC	C18-C60-C61	2.86	121.11	113.97
3	B	401	CNC	C55-C17-C18	-2.81	105.72	111.15
3	C	401	CNC	C18-C60-C61	2.77	120.89	113.97
3	B	401	CNC	C2-C3-C4	2.74	104.75	101.63
3	A	401	CNC	C10-C9-N22	2.74	128.87	125.73
3	A	401	CNC	C60-C18-C19	2.66	120.44	114.09
3	A	401	CNC	O58-C57-C56	-2.57	117.31	122.02
3	C	401	CNC	C25-C2-C1	2.51	117.56	113.78
3	B	401	CNC	C30-C3-C4	2.46	115.35	109.63
3	B	401	CNC	C41-C8-C7	2.45	120.88	114.14
3	B	401	CNC	O2-P-O4	-2.42	100.40	109.47
3	C	401	CNC	O58-C57-C56	-2.41	117.61	122.02
3	C	401	CNC	C3-C4-C5	2.38	127.81	123.81
3	C	401	CNC	C17-C16-C15	2.33	130.27	126.73
3	C	401	CNC	C5-C6-N22	-2.26	120.42	123.88
3	B	401	CNC	C1-C2-C3	-2.24	98.73	101.60
3	A	401	CNC	C1-C2-C3	-2.24	98.74	101.60
3	B	401	CNC	C36-C7-C37	2.22	114.47	110.80
3	B	401	CNC	C42-C41-C8	2.22	121.13	114.73
3	A	401	CNC	C17-C16-C15	2.22	130.10	126.73
3	B	401	CNC	O58-C57-C56	-2.20	118.00	122.02
3	C	401	CNC	C48-C13-C12	2.15	122.64	116.63
3	A	401	CNC	C49-C48-C13	2.14	120.91	114.73
3	C	401	CNC	C13-C14-C15	2.12	127.39	123.81
3	B	401	CNC	C18-C60-C61	2.12	119.26	113.97
3	C	401	CNC	C55-C17-C18	-2.06	107.18	111.15
3	A	401	CNC	C55-C17-C18	-2.04	107.21	111.15
3	B	401	CNC	C5-C4-N21	2.02	127.47	124.19
3	B	401	CNC	C19-N24-C16	2.01	115.22	111.96

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	401	CNC	N24
3	B	401	CNC	N24

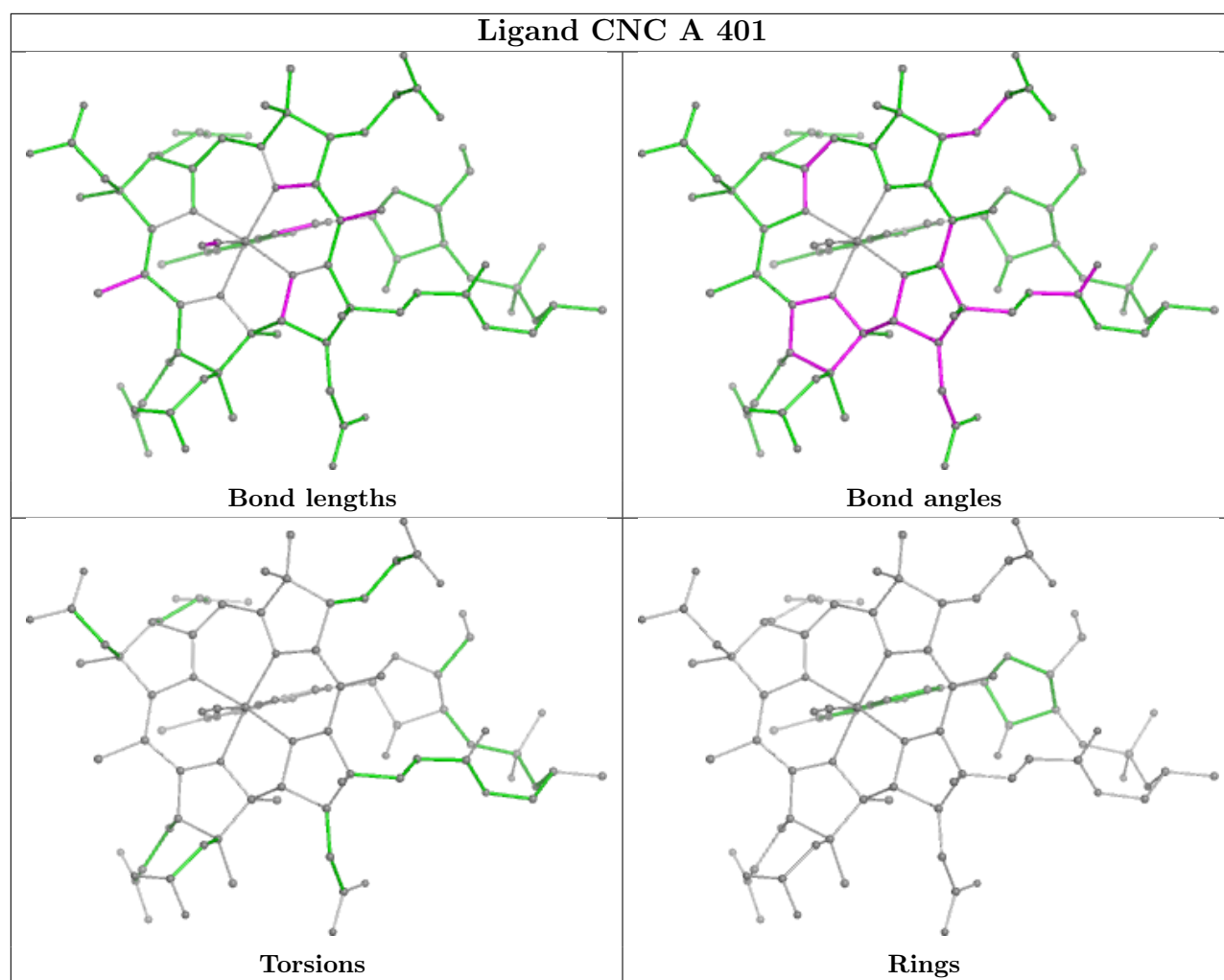
All (5) torsion outliers are listed below:

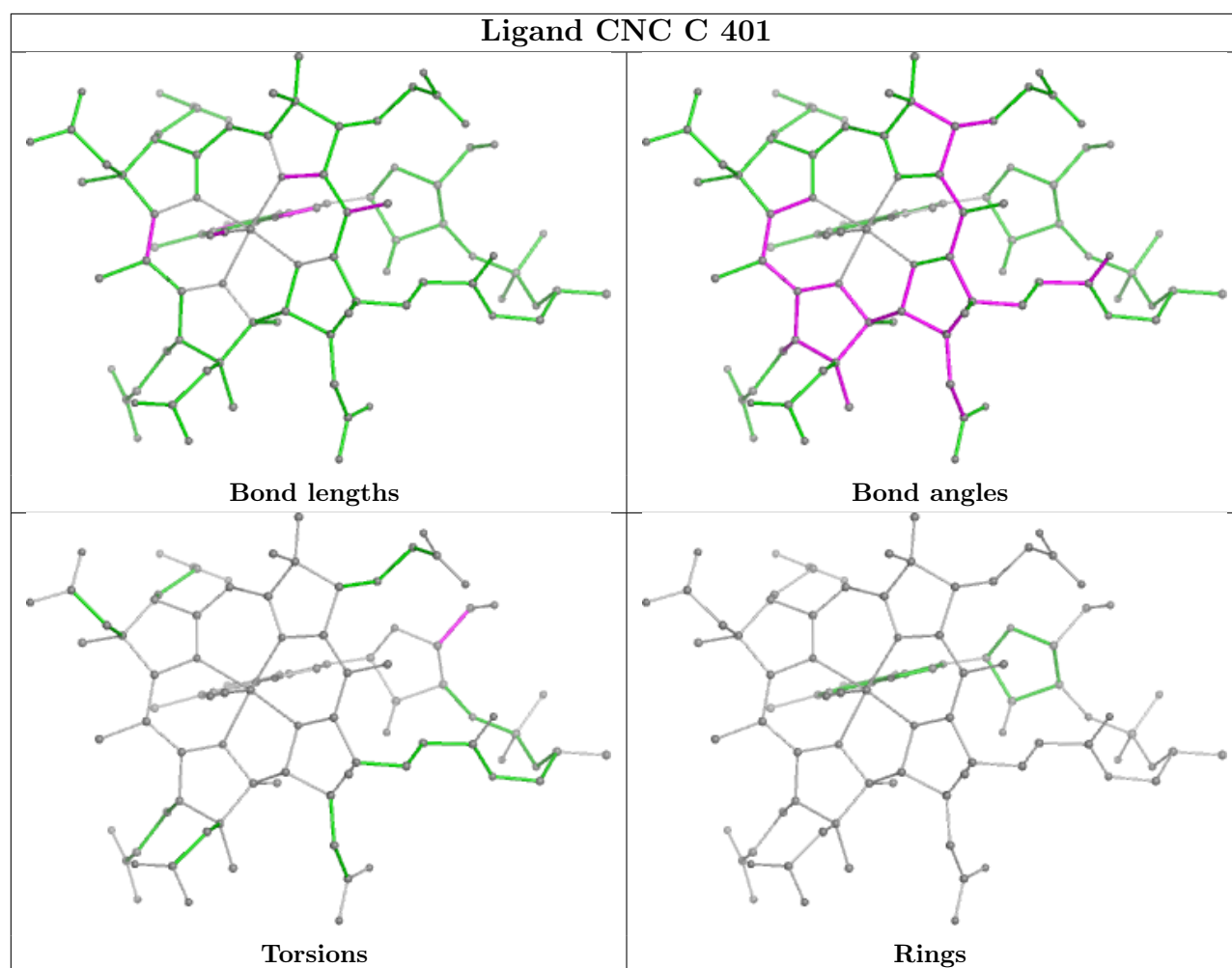
Mol	Chain	Res	Type	Atoms
3	C	401	CNC	O6R-C4R-C5R-O8R
3	C	401	CNC	C3R-C4R-C5R-O8R
3	B	401	CNC	C13-C48-C49-C50
3	B	401	CNC	C41-C42-C43-N45
3	B	401	CNC	C41-C42-C43-O44

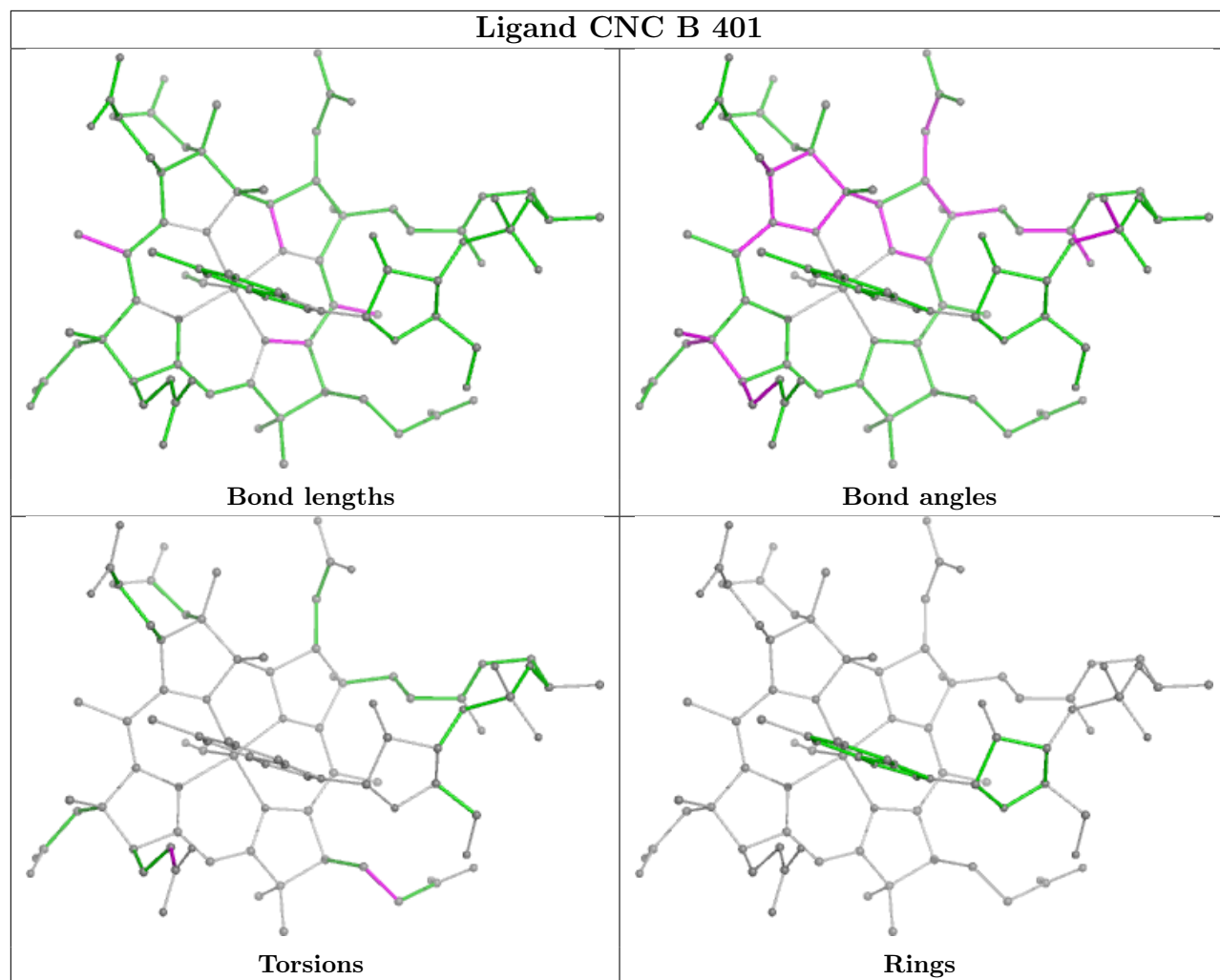
There are no ring outliers.

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.







4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data [i](#)

5.1 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	C	337/337 (100%)	-0.66	0	100 100	20, 33, 58, 72	0
2	A	339/339 (100%)	-0.74	3 (0%)	81 81	18, 29, 50, 72	0
2	B	337/339 (99%)	-0.65	1 (0%)	90 91	20, 34, 53, 87	0
All	All	1013/1015 (99%)	-0.69	4 (0%)	89 89	18, 32, 54, 87	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	13	GLY	2.1
2	B	164	TRP	2.0
2	A	111	ASP	2.0
2	A	182	LEU	2.0

5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 Ligands [i](#)

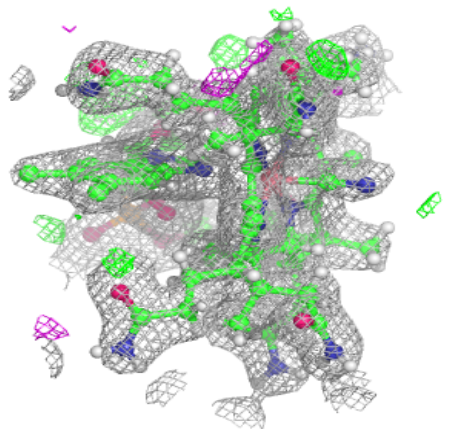
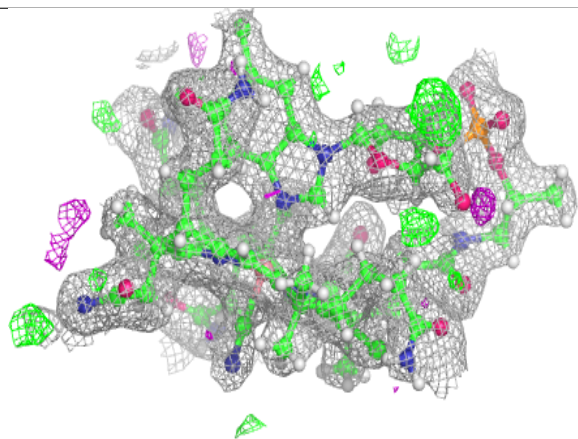
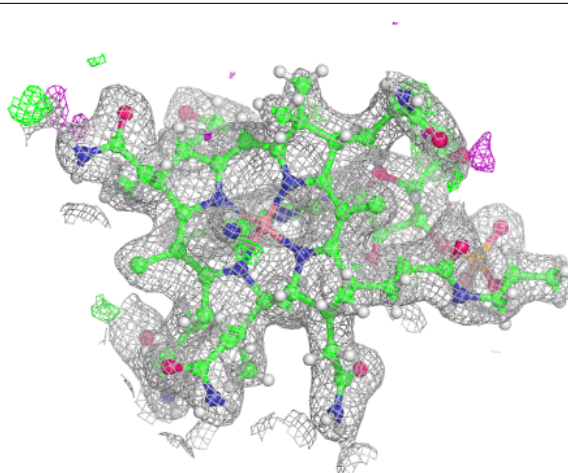
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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	CNC	C	401	93/93	0.98	0.06	23,33,48,57	0
3	CNC	A	401	93/93	0.98	0.05	20,27,37,57	0
3	CNC	B	401	93/93	0.98	0.05	22,25,36,46	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.

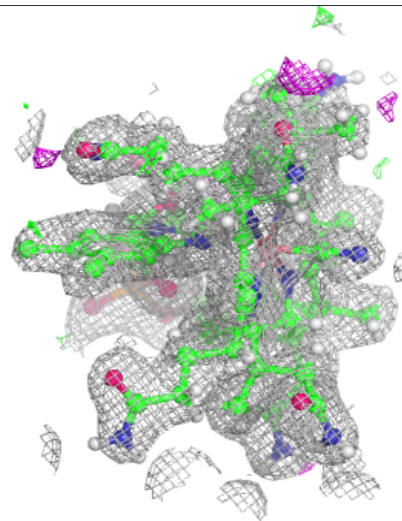
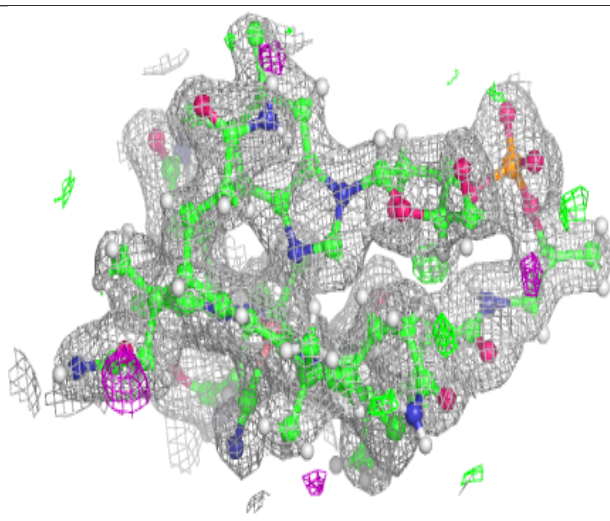
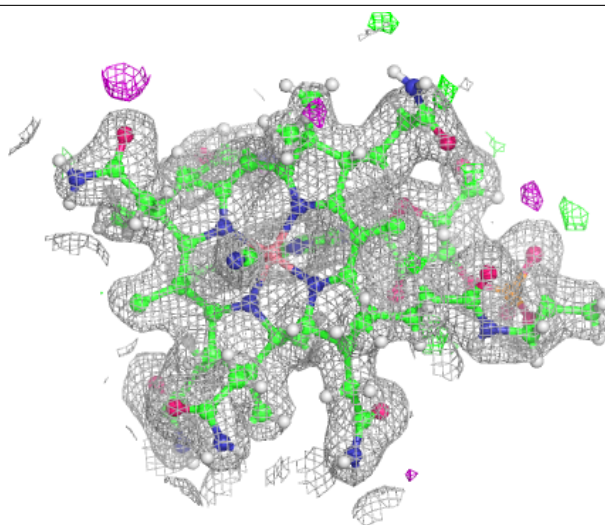
Electron density around CNC C 401:

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



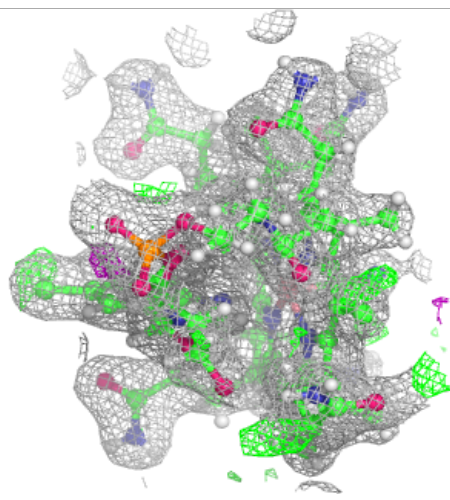
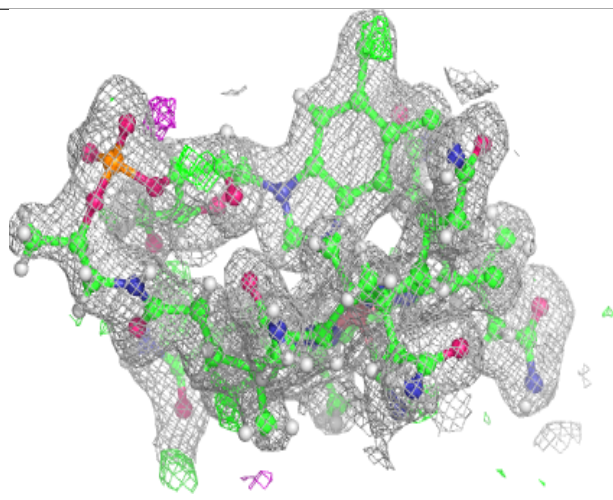
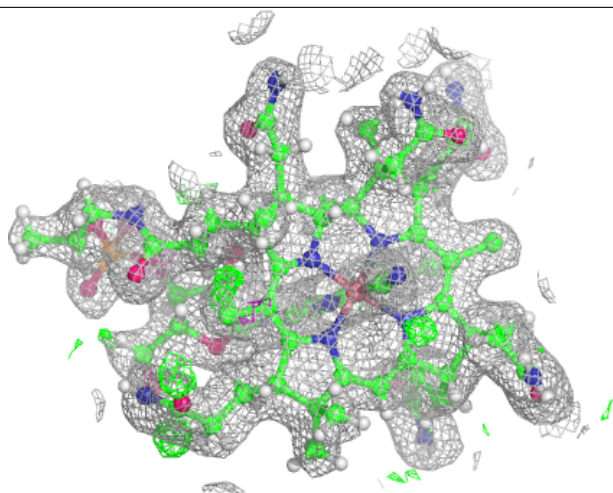
Electron density around CNC A 401:

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



Electron density around CNC B 401:

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



5.5 Other polymers [i](#)

There are no such residues in this entry.