



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2023 – 01:54 AM EDT

PDB ID : 3B9X  
Title : Crystal structure of the E. coli pyrimidine nucleoside hydrolase YeiK in complex with inosine  
Authors : Iovane, E.; Degano, M.  
Deposited on : 2007-11-07  
Resolution : 2.30 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](mailto: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>.

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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)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

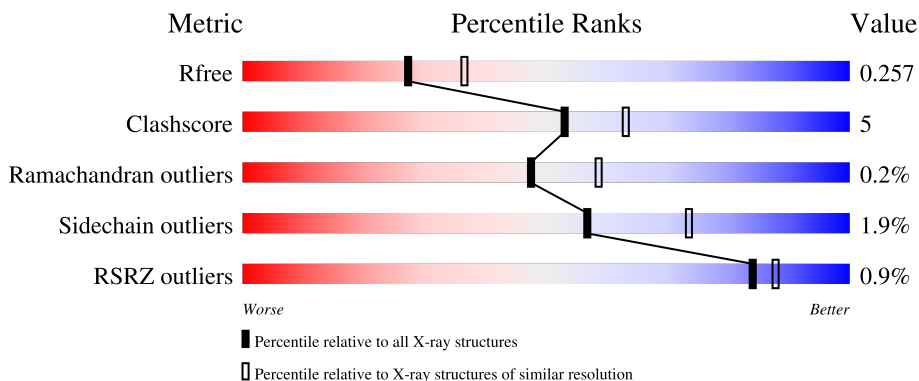
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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  $\geq 3$ , 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	333	84% 8% 7%
1	B	333	80% 10% 9%
1	C	333	2% 77% 8% 15%
1	D	333	% 80% 11% 8%

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 criteria:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
3	NOS	A	401	-	-	X	-
3	NOS	D	401	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9468 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 Pyrimidine-specific ribonucleoside hydrolase rihB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	309	2332	1479	388	445	20	0	1	0
1	B	303	2277	1447	377	433	20	0	0	0
1	C	283	2121	1346	353	403	19	0	0	0
1	D	307	2316	1472	387	437	20	0	1	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P33022
A	-18	GLY	-	expression tag	UNP P33022
A	-17	SER	-	expression tag	UNP P33022
A	-16	SER	-	expression tag	UNP P33022
A	-15	HIS	-	expression tag	UNP P33022
A	-14	HIS	-	expression tag	UNP P33022
A	-13	HIS	-	expression tag	UNP P33022
A	-12	HIS	-	expression tag	UNP P33022
A	-11	HIS	-	expression tag	UNP P33022
A	-10	HIS	-	expression tag	UNP P33022
A	-9	SER	-	expression tag	UNP P33022
A	-8	SER	-	expression tag	UNP P33022
A	-7	GLY	-	expression tag	UNP P33022
A	-6	LEU	-	expression tag	UNP P33022
A	-5	VAL	-	expression tag	UNP P33022
A	-4	PRO	-	expression tag	UNP P33022
A	-3	ARG	-	expression tag	UNP P33022
A	-2	GLY	-	expression tag	UNP P33022
A	-1	SER	-	expression tag	UNP P33022
A	0	HIS	-	expression tag	UNP P33022
A	84	ASP	GLU	SEE REMARK 999	UNP P33022

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	initiating methionine	UNP P33022
B	-18	GLY	-	expression tag	UNP P33022
B	-17	SER	-	expression tag	UNP P33022
B	-16	SER	-	expression tag	UNP P33022
B	-15	HIS	-	expression tag	UNP P33022
B	-14	HIS	-	expression tag	UNP P33022
B	-13	HIS	-	expression tag	UNP P33022
B	-12	HIS	-	expression tag	UNP P33022
B	-11	HIS	-	expression tag	UNP P33022
B	-10	HIS	-	expression tag	UNP P33022
B	-9	SER	-	expression tag	UNP P33022
B	-8	SER	-	expression tag	UNP P33022
B	-7	GLY	-	expression tag	UNP P33022
B	-6	LEU	-	expression tag	UNP P33022
B	-5	VAL	-	expression tag	UNP P33022
B	-4	PRO	-	expression tag	UNP P33022
B	-3	ARG	-	expression tag	UNP P33022
B	-2	GLY	-	expression tag	UNP P33022
B	-1	SER	-	expression tag	UNP P33022
B	0	HIS	-	expression tag	UNP P33022
B	84	ASP	GLU	SEE REMARK 999	UNP P33022
C	-19	MET	-	initiating methionine	UNP P33022
C	-18	GLY	-	expression tag	UNP P33022
C	-17	SER	-	expression tag	UNP P33022
C	-16	SER	-	expression tag	UNP P33022
C	-15	HIS	-	expression tag	UNP P33022
C	-14	HIS	-	expression tag	UNP P33022
C	-13	HIS	-	expression tag	UNP P33022
C	-12	HIS	-	expression tag	UNP P33022
C	-11	HIS	-	expression tag	UNP P33022
C	-10	HIS	-	expression tag	UNP P33022
C	-9	SER	-	expression tag	UNP P33022
C	-8	SER	-	expression tag	UNP P33022
C	-7	GLY	-	expression tag	UNP P33022
C	-6	LEU	-	expression tag	UNP P33022
C	-5	VAL	-	expression tag	UNP P33022
C	-4	PRO	-	expression tag	UNP P33022
C	-3	ARG	-	expression tag	UNP P33022
C	-2	GLY	-	expression tag	UNP P33022
C	-1	SER	-	expression tag	UNP P33022
C	0	HIS	-	expression tag	UNP P33022
C	84	ASP	GLU	SEE REMARK 999	UNP P33022

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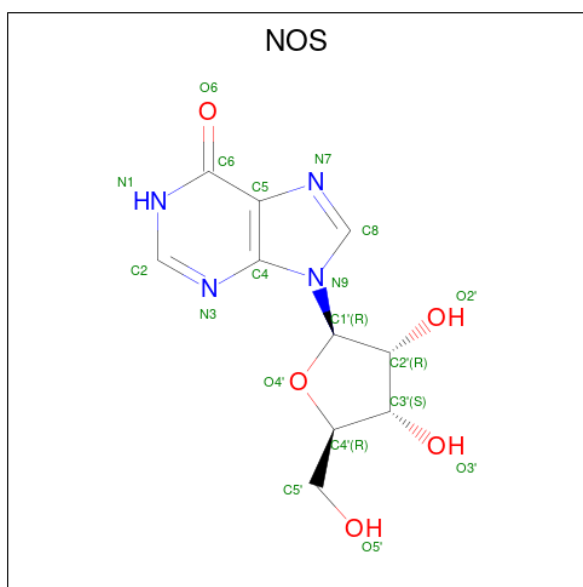
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	initiating methionine	UNP P33022
D	-18	GLY	-	expression tag	UNP P33022
D	-17	SER	-	expression tag	UNP P33022
D	-16	SER	-	expression tag	UNP P33022
D	-15	HIS	-	expression tag	UNP P33022
D	-14	HIS	-	expression tag	UNP P33022
D	-13	HIS	-	expression tag	UNP P33022
D	-12	HIS	-	expression tag	UNP P33022
D	-11	HIS	-	expression tag	UNP P33022
D	-10	HIS	-	expression tag	UNP P33022
D	-9	SER	-	expression tag	UNP P33022
D	-8	SER	-	expression tag	UNP P33022
D	-7	GLY	-	expression tag	UNP P33022
D	-6	LEU	-	expression tag	UNP P33022
D	-5	VAL	-	expression tag	UNP P33022
D	-4	PRO	-	expression tag	UNP P33022
D	-3	ARG	-	expression tag	UNP P33022
D	-2	GLY	-	expression tag	UNP P33022
D	-1	SER	-	expression tag	UNP P33022
D	0	HIS	-	expression tag	UNP P33022
D	84	ASP	GLU	SEE REMARK 999	UNP P33022

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

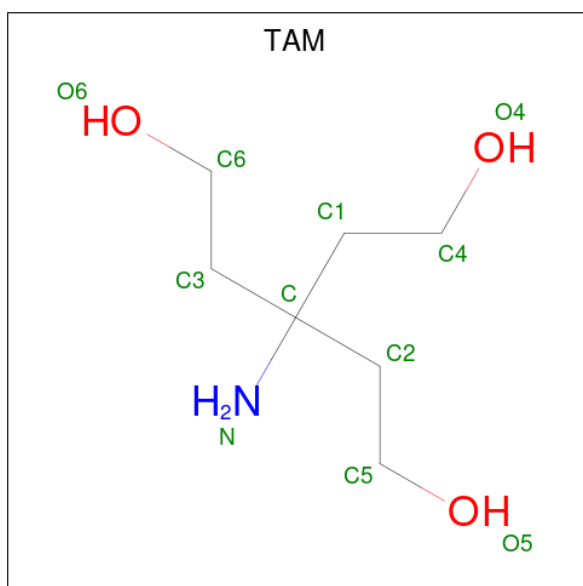
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0

- Molecule 3 is INOSINE (three-letter code: NOS) (formula: C<sub>10</sub>H<sub>12</sub>N<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	Total	C	N	O	0	0
			19	10	4	5		
3	B	1	Total	C	N	O	0	0
			19	10	4	5		
3	C	1	Total	C	N	O	0	0
			19	10	4	5		
3	D	1	Total	C	N	O	0	0
			19	10	4	5		

- Molecule 4 is TRIS(HYDROXYETHYL)AMINOMETHANE (three-letter code: TAM) (formula:  $C_7H_{17}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	N	O	0	0
			11	7	1	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	101	Total	O	0	0
			101	101		
5	B	93	Total	O	0	0
			93	93		
5	C	61	Total	O	0	0
			61	61		
5	D	76	Total	O	0	0
			76	76		







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.11Å 82.41Å 90.16Å 67.90° 79.59° 89.65°	Depositor
Resolution (Å)	81.92 – 2.30 81.98 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.6 (81.92-2.30) 95.6 (81.98-2.30)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.38 (at 2.29Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.201 , 0.255 0.202 , 0.257	Depositor DCC
$R_{free}$ test set	1560 reflections (3.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.1	Xtrriage
Anisotropy	0.465	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 40.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9468	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.47% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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: TAM, CA, NOS

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	0.72	0/2377	0.72	0/3237
1	B	0.74	0/2320	0.71	2/3159 (0.1%)
1	C	0.74	0/2160	0.69	0/2941
1	D	0.71	0/2363	0.69	0/3215
All	All	0.73	0/9220	0.70	2/12552 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4	ARG	NE-CZ-NH2	5.36	122.98	120.30
1	B	118	ASP	CB-CG-OD1	5.08	122.87	118.30

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	2332	0	2337	20	0
1	B	2277	0	2289	24	0
1	C	2121	0	2138	17	0
1	D	2316	0	2336	34	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	19	0	9	7	0
3	B	19	0	10	3	0
3	C	19	0	10	3	0
3	D	19	0	10	7	0
4	D	11	0	17	2	0
5	A	101	0	0	0	0
5	B	93	0	0	3	0
5	C	61	0	0	1	0
5	D	76	0	0	2	0
All	All	9468	0	9156	98	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 5.

All (98) 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:B:227:GLN:HG3	1:B:236:GLY:HA2	1.09	1.04
1:B:143:LYS:HE3	5:B:417:HOH:O	1.60	1.01
1:A:40:ASN:HD21	3:A:401:NOS:H1'	1.29	0.97
1:B:227:GLN:HG3	1:B:236:GLY:CA	1.96	0.95
1:A:231:TYR:HE1	3:A:401:NOS:O6	1.59	0.85
1:D:191:LEU:HD11	1:D:253:ILE:HG23	1.60	0.82
1:B:191:LEU:HD11	1:B:253:ILE:HG23	1.67	0.76
1:A:231:TYR:CE1	3:A:401:NOS:O6	2.39	0.75
1:C:26:HIS:HD2	1:C:28:ALA:H	1.36	0.74
1:A:103:HIS:HD2	1:A:105:VAL:H	1.35	0.72
1:B:103:HIS:HD2	1:B:105:VAL:H	1.36	0.71
1:A:26:HIS:HD2	1:A:28:ALA:H	1.39	0.71
1:B:257:GLU:OE1	5:B:471:HOH:O	2.09	0.70
1:B:227:GLN:CG	1:B:236:GLY:HA2	2.05	0.66
1:A:191:LEU:HD11	1:A:253:ILE:HG23	1.78	0.66
1:C:191:LEU:HD11	1:C:253:ILE:HG23	1.79	0.65
1:C:26:HIS:CD2	1:C:28:ALA:H	2.16	0.64
1:C:103:HIS:HD2	1:C:105:VAL:H	1.44	0.63
1:D:103:HIS:CE1	4:D:402:TAM:H61	2.34	0.62
1:D:52:ASN:ND2	1:D:95:LEU:HG	2.15	0.62
1:B:40:ASN:HD21	3:B:401:NOS:H1'	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:HIS:HD2	1:B:28:ALA:H	1.46	0.62
1:D:103:HIS:HD2	1:D:105:VAL:H	1.47	0.60
1:C:40:ASN:HD21	3:C:401:NOS:H1'	1.65	0.60
1:A:227:GLN:HG3	1:A:236:GLY:HA2	1.85	0.59
1:B:52:ASN:ND2	5:B:459:HOH:O	2.35	0.59
1:A:150:MET:SD	3:A:401:NOS:H5'1	2.43	0.59
1:A:26:HIS:CD2	1:A:28:ALA:H	2.19	0.58
1:D:59:ILE:O	1:D:97:ARG:NH1	2.35	0.58
1:B:26:HIS:CD2	1:B:28:ALA:H	2.21	0.58
1:D:26:HIS:HD2	1:D:28:ALA:H	1.51	0.58
1:B:238:VAL:HG23	1:B:238:VAL:O	2.04	0.57
1:C:164:GLU:OE2	3:C:401:NOS:H5'1	2.05	0.57
1:D:40:ASN:HD21	3:D:401:NOS:H1'	1.68	0.56
1:D:81:ILE:HG21	3:D:401:NOS:C6	2.35	0.55
1:C:198:THR:HB	5:C:428:HOH:O	2.05	0.55
1:D:26:HIS:CD2	1:D:28:ALA:H	2.25	0.55
1:C:103:HIS:CD2	1:C:105:VAL:H	2.25	0.53
1:D:14:HIS:HD2	1:D:219:ILE:HG23	1.74	0.53
1:A:303:GLU:O	1:A:307:ARG:HG3	2.09	0.53
1:B:103:HIS:CD2	1:B:105:VAL:H	2.23	0.53
1:C:87:LEU:O	1:C:87:LEU:HG	2.08	0.52
1:D:81:ILE:HG21	3:D:401:NOS:C5	2.39	0.52
1:A:103:HIS:CD2	1:A:105:VAL:H	2.23	0.52
1:D:231:TYR:HE1	3:D:401:NOS:O6	1.91	0.52
1:C:140:ILE:O	1:C:143:LYS:HB2	2.11	0.51
1:D:103:HIS:CD2	1:D:105:VAL:H	2.27	0.51
1:D:68:PRO:HG3	4:D:402:TAM:O5	2.11	0.51
1:D:14:HIS:CD2	1:D:219:ILE:HG23	2.47	0.50
1:D:51:LEU:HB3	1:D:95:LEU:HD21	1.95	0.49
1:B:87:LEU:O	1:B:87:LEU:HG	2.12	0.49
1:D:90:PRO:HG3	1:D:219:ILE:HG13	1.95	0.49
1:C:12:PRO:HA	1:C:13:GLY:HA3	1.66	0.48
1:A:156:THR:OG1	1:C:277:GLU:OE1	2.31	0.48
1:D:128:SER:O	1:D:132:VAL:HG23	2.14	0.48
1:B:164:GLU:OE2	3:B:401:NOS:H5'1	2.14	0.47
1:D:191:LEU:CD1	1:D:253:ILE:HG23	2.38	0.47
1:B:128:SER:O	1:B:132:VAL:HG23	2.15	0.47
1:B:117:GLY:HA2	1:B:143:LYS:O	2.16	0.46
1:C:135:ARG:HD3	1:C:135:ARG:HA	1.75	0.46
1:D:68:PRO:O	1:D:69:GLN:HG2	2.16	0.46
1:D:75:GLN:N	5:D:443:HOH:O	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:401:NOS:H8	3:C:401:NOS:H2'	1.84	0.45
1:B:140:ILE:O	1:B:143:LYS:HB2	2.15	0.45
1:B:192:THR:HB	1:B:239:HIS:HA	1.98	0.45
1:A:12:PRO:HA	1:A:13:GLY:HA3	1.72	0.45
1:B:47:LEU:HD11	1:B:99:ALA:HB2	1.98	0.45
1:B:191:LEU:CD1	1:B:253:ILE:HG23	2.41	0.45
1:C:191:LEU:CD1	1:C:253:ILE:HG23	2.46	0.44
1:D:74:GLN:HA	5:D:443:HOH:O	2.17	0.44
1:D:12:PRO:HA	1:D:13:GLY:HA3	1.72	0.44
1:A:82:HIS:HE1	3:A:401:NOS:N9	2.16	0.43
1:D:192:THR:HB	1:D:239:HIS:HA	1.99	0.43
1:D:26:HIS:CD2	1:D:28:ALA:HB3	2.53	0.43
1:B:158:ASN:HB2	1:B:231:TYR:CZ	2.54	0.43
1:D:81:ILE:HG22	1:D:82:HIS:ND1	2.34	0.43
3:D:401:NOS:H8	3:D:401:NOS:H2'	1.63	0.43
1:A:105:VAL:O	1:A:109:ILE:HG13	2.19	0.43
1:D:105:VAL:O	1:D:109:ILE:HG13	2.20	0.42
1:D:87:LEU:HG	1:D:87:LEU:O	2.19	0.42
1:A:135:ARG:HD3	1:A:135:ARG:HA	1.81	0.42
1:D:249:ASN:HA	1:D:250:PRO:HD2	1.94	0.42
1:D:235:GLY:O	1:D:237:PRO:HD3	2.18	0.42
1:C:252:GLY:HA3	1:C:297:TRP:CE3	2.55	0.42
1:D:81:ILE:HG13	3:D:401:NOS:C6	2.49	0.42
1:C:192:THR:HB	1:C:239:HIS:HA	2.01	0.42
3:A:401:NOS:H8	3:A:401:NOS:H2'	1.87	0.41
1:A:14:HIS:ND1	1:A:82:HIS:HD2	2.18	0.41
1:A:192:THR:HB	1:A:239:HIS:HA	2.01	0.41
1:B:252:GLY:HA3	1:B:297:TRP:CE3	2.56	0.41
3:B:401:NOS:H8	3:B:401:NOS:H2'	1.79	0.41
1:D:26:HIS:HD2	1:D:28:ALA:HB3	1.86	0.41
1:A:252:GLY:HA3	1:A:297:TRP:CE3	2.56	0.41
1:B:135:ARG:HA	1:B:135:ARG:HD3	1.79	0.41
1:A:40:ASN:ND2	3:A:401:NOS:H1'	2.14	0.41
1:D:252:GLY:HA3	1:D:297:TRP:CE3	2.56	0.41
1:C:156:THR:HG22	1:C:157:GLY:O	2.21	0.41
1:D:231:TYR:CE1	3:D:401:NOS:O6	2.74	0.40

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	308/333 (92%)	296 (96%)	11 (4%)	1 (0%)	41	50
1	B	299/333 (90%)	284 (95%)	14 (5%)	1 (0%)	41	50
1	C	277/333 (83%)	264 (95%)	13 (5%)	0	100	100
1	D	304/333 (91%)	291 (96%)	13 (4%)	0	100	100
All	All	1188/1332 (89%)	1135 (96%)	51 (4%)	2 (0%)	47	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	236	GLY
1	A	39	GLY

### 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	254/274 (93%)	250 (98%)	4 (2%)	62	78
1	B	248/274 (90%)	242 (98%)	6 (2%)	49	66
1	C	232/274 (85%)	229 (99%)	3 (1%)	69	82
1	D	252/274 (92%)	246 (98%)	6 (2%)	49	66
All	All	986/1096 (90%)	967 (98%)	19 (2%)	57	73

All (19) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	69	GLN
1	A	116	ASP
1	A	150	MET
1	A	159	PHE
1	B	69	GLN
1	B	84	ASP
1	B	116	ASP
1	B	128	SER
1	B	150	MET
1	B	190	ASP
1	C	98	GLN
1	C	116	ASP
1	C	150	MET
1	D	69	GLN
1	D	84	ASP
1	D	95	LEU
1	D	116	ASP
1	D	150	MET
1	D	159	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	HIS
1	A	40	ASN
1	A	52	ASN
1	A	82	HIS
1	A	98	GLN
1	A	103	HIS
1	B	26	HIS
1	B	40	ASN
1	B	52	ASN
1	B	103	HIS
1	C	26	HIS
1	C	40	ASN
1	C	52	ASN
1	C	103	HIS
1	C	265	ASN
1	D	26	HIS
1	D	40	ASN
1	D	52	ASN
1	D	82	HIS
1	D	103	HIS

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Mol	Chain	Res	Type
1	D	230	ASN
1	D	265	ASN

### 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 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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
4	TAM	D	402	-	7,10,10	0.47	0	9,12,12	1.42	0
3	NOS	B	401	2	17,21,21	1.14	1 (5%)	17,31,31	1.63	2 (11%)
3	NOS	C	401	2	17,21,21	1.26	2 (11%)	17,31,31	1.53	3 (17%)
3	NOS	D	401	2	17,21,21	1.18	2 (11%)	17,31,31	1.79	4 (23%)
3	NOS	A	401	2	17,21,21	1.29	2 (11%)	17,31,31	2.33	7 (41%)

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
4	TAM	D	402	-	-	8/12/12/12	-
3	NOS	B	401	2	-	2/2/22/22	0/3/3/3
3	NOS	C	401	2	-	2/2/22/22	0/3/3/3
3	NOS	D	401	2	-	2/2/22/22	0/3/3/3
3	NOS	A	401	2	-	0/2/22/22	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	NOS	O4'-C1'	3.54	1.46	1.41
3	C	401	NOS	C2-N3	3.39	1.36	1.29
3	D	401	NOS	C2-N3	2.99	1.35	1.29
3	B	401	NOS	C2-N3	2.80	1.34	1.29
3	A	401	NOS	C2-N3	2.70	1.34	1.29
3	D	401	NOS	O4'-C1'	2.56	1.44	1.41
3	C	401	NOS	C5-C4	2.10	1.48	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	NOS	C3'-C2'-C1'	4.54	107.81	100.98
3	B	401	NOS	C3'-C2'-C1'	4.48	107.72	100.98
3	A	401	NOS	O4'-C4'-C5'	4.12	118.13	109.21
3	C	401	NOS	C3'-C2'-C1'	3.88	106.81	100.98
3	D	401	NOS	C3'-C2'-C1'	3.88	106.81	100.98
3	A	401	NOS	O6-C6-C5	-3.09	118.34	124.37
3	D	401	NOS	O6-C6-C5	-2.97	118.56	124.37
3	A	401	NOS	C5'-C4'-C3'	-2.96	107.95	115.09
3	A	401	NOS	O4'-C1'-C2'	-2.88	102.72	106.93
3	A	401	NOS	C5-C6-N1	2.86	119.00	113.95
3	D	401	NOS	C5-C6-N1	2.75	118.81	113.95
3	C	401	NOS	C5-C6-N1	2.41	118.21	113.95
3	D	401	NOS	C5'-C4'-C3'	-2.17	109.86	115.09
3	B	401	NOS	C8-N7-C5	2.14	107.07	102.99
3	A	401	NOS	C8-N7-C5	2.12	107.03	102.99
3	C	401	NOS	C8-N7-C5	2.09	106.96	102.99

There are no chirality outliers.

All (14) torsion outliers are listed below:

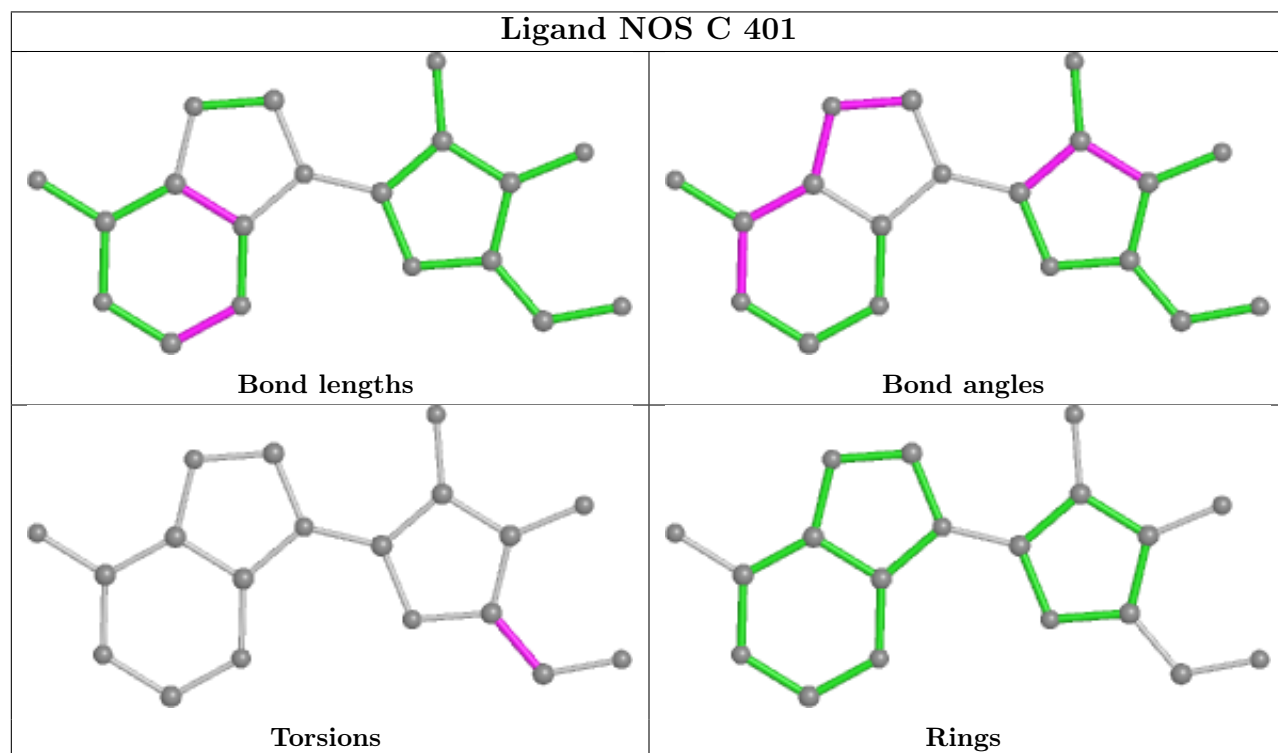
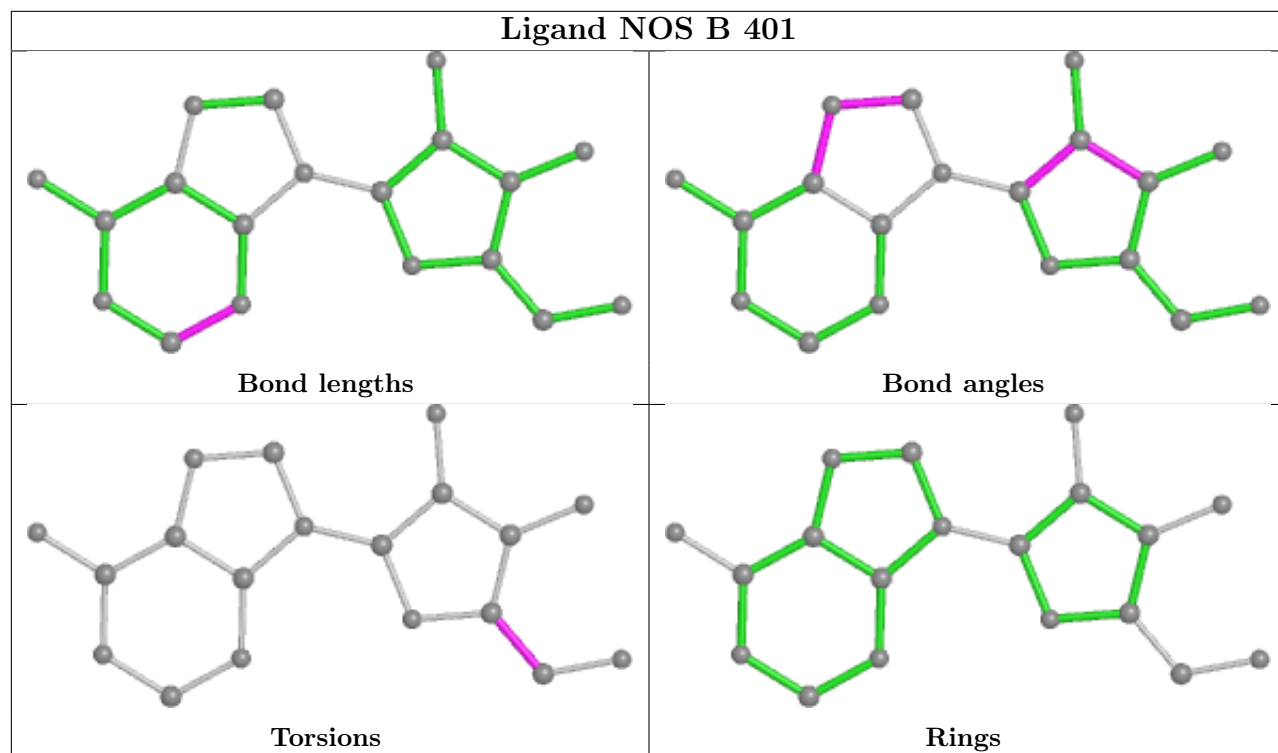
Mol	Chain	Res	Type	Atoms
4	D	402	TAM	C2-C-C1-C4
4	D	402	TAM	C3-C-C1-C4
4	D	402	TAM	N-C-C1-C4
3	C	401	NOS	C3'-C4'-C5'-O5'
3	C	401	NOS	O4'-C4'-C5'-O5'
3	B	401	NOS	C3'-C4'-C5'-O5'
3	B	401	NOS	O4'-C4'-C5'-O5'
4	D	402	TAM	C-C2-C5-O5
3	D	401	NOS	O4'-C4'-C5'-O5'
3	D	401	NOS	C3'-C4'-C5'-O5'
4	D	402	TAM	C-C3-C6-O6
4	D	402	TAM	C1-C-C2-C5
4	D	402	TAM	C3-C-C2-C5
4	D	402	TAM	C1-C-C3-C6

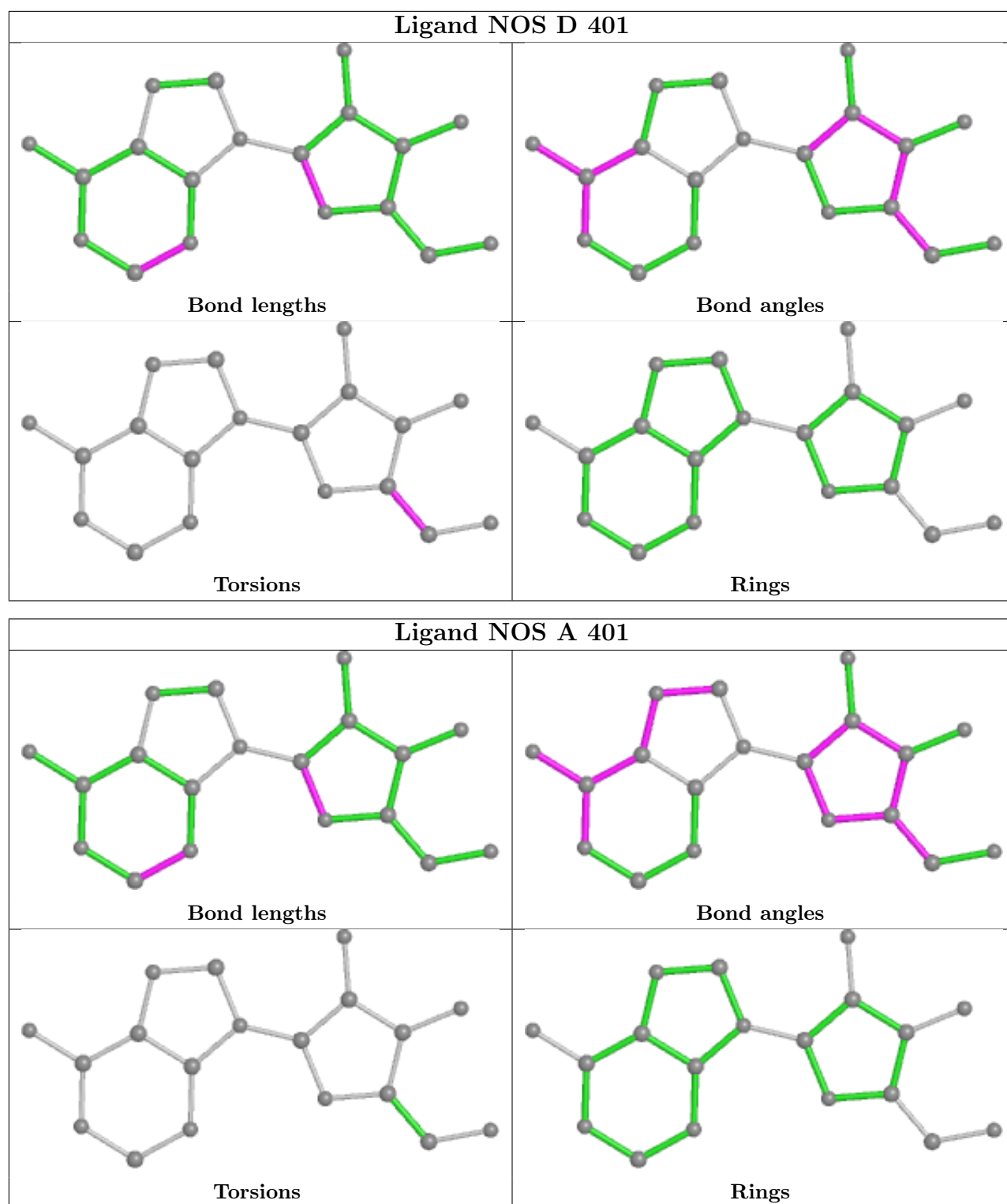
There are no ring outliers.

5 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	402	TAM	2	0
3	B	401	NOS	3	0
3	C	401	NOS	3	0
3	D	401	NOS	7	0
3	A	401	NOS	7	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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	309/333 (92%)	-0.41	0 <a href="#">100</a> <a href="#">100</a>	10, 20, 33, 43	0
1	B	303/333 (90%)	-0.31	1 (0%) <a href="#">94</a> <a href="#">96</a>	10, 21, 43, 67	0
1	C	283/333 (84%)	-0.17	7 (2%) <a href="#">57</a> <a href="#">64</a>	10, 20, 39, 57	0
1	D	307/333 (92%)	-0.31	3 (0%) <a href="#">82</a> <a href="#">86</a>	10, 21, 48, 68	0
All	All	1202/1332 (90%)	-0.30	11 (0%) <a href="#">84</a> <a href="#">88</a>	10, 21, 40, 68	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	209	GLY	3.2
1	B	231	TYR	2.8
1	D	77	VAL	2.6
1	C	86	GLY	2.4
1	D	233	LEU	2.4
1	C	307	ARG	2.2
1	C	59	ILE	2.2
1	C	301	LEU	2.1
1	D	78	ALA	2.1
1	C	296	ASP	2.0
1	C	196	VAL	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.

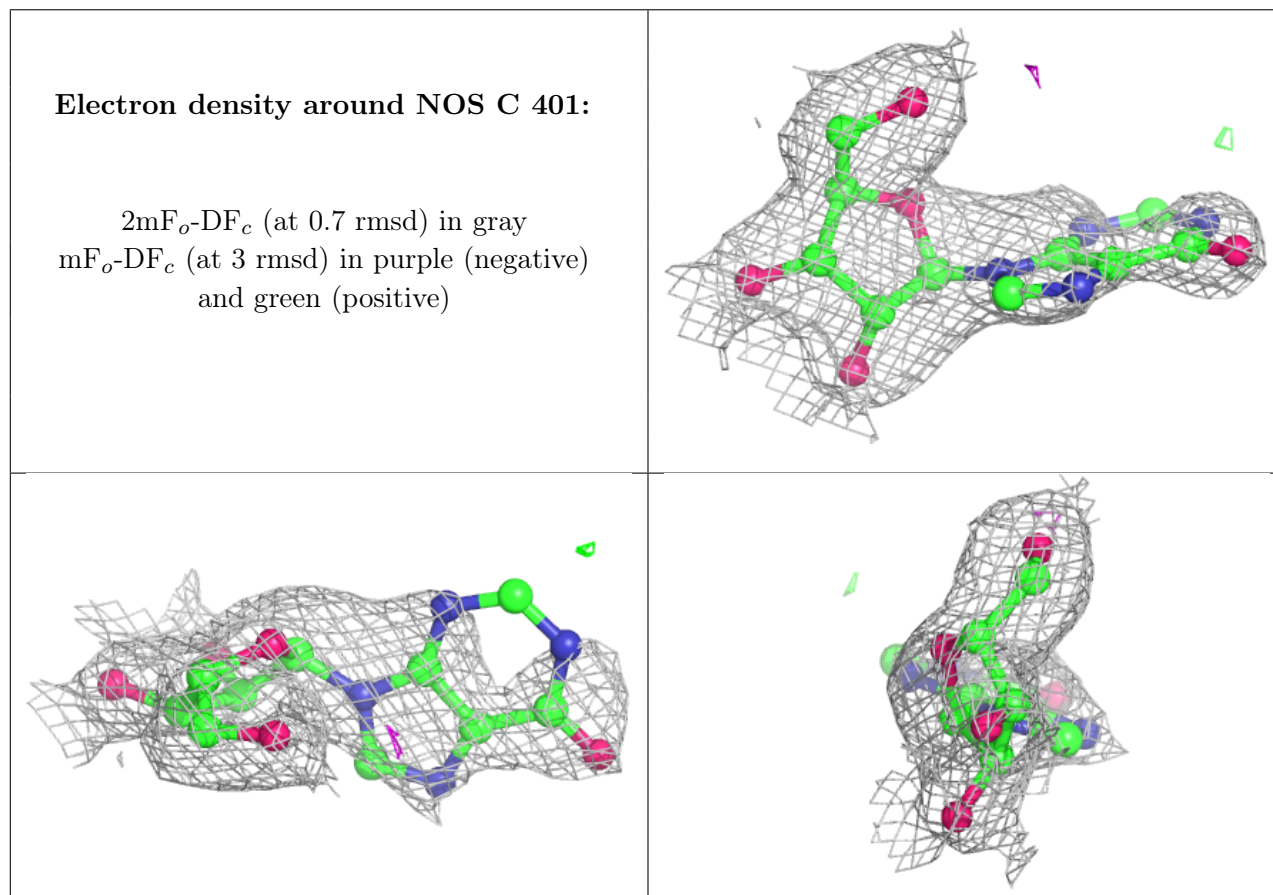


## 6.4 Ligands [i](#)

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<sup>th</sup> 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.

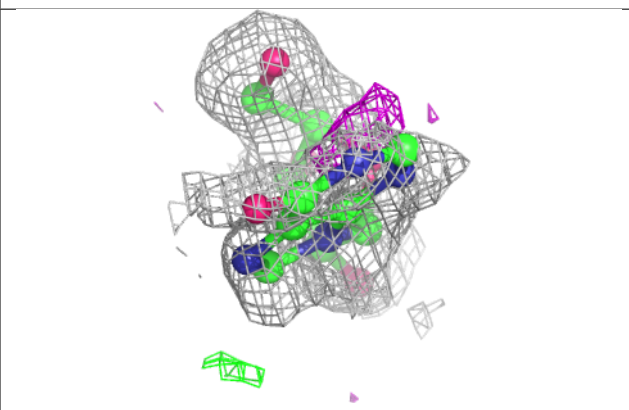
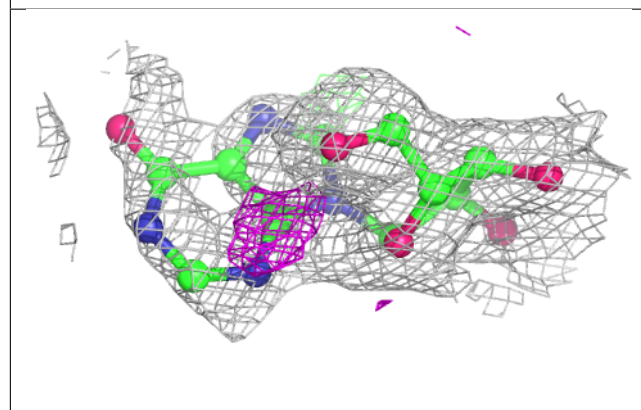
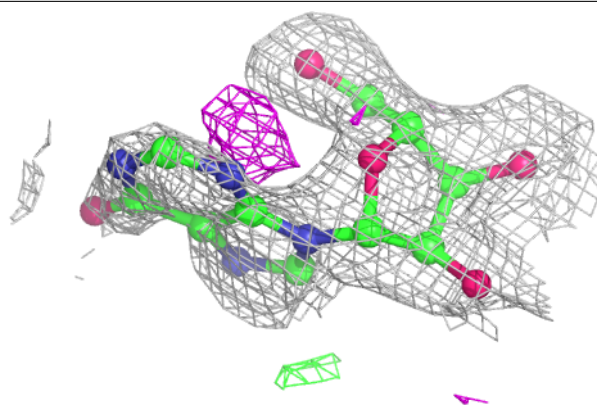
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	TAM	D	402	11/11	0.85	0.19	39,42,45,48	0
3	NOS	C	401	19/19	0.88	0.19	18,43,47,49	10
3	NOS	A	401	19/19	0.89	0.22	20,29,32,34	10
3	NOS	D	401	19/19	0.91	0.26	19,37,46,47	10
3	NOS	B	401	19/19	0.92	0.19	11,31,41,41	10
2	CA	D	400	1/1	0.99	0.04	17,17,17,17	0
2	CA	A	400	1/1	0.99	0.04	15,15,15,15	0
2	CA	B	400	1/1	0.99	0.07	17,17,17,17	0
2	CA	C	400	1/1	1.00	0.06	17,17,17,17	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.

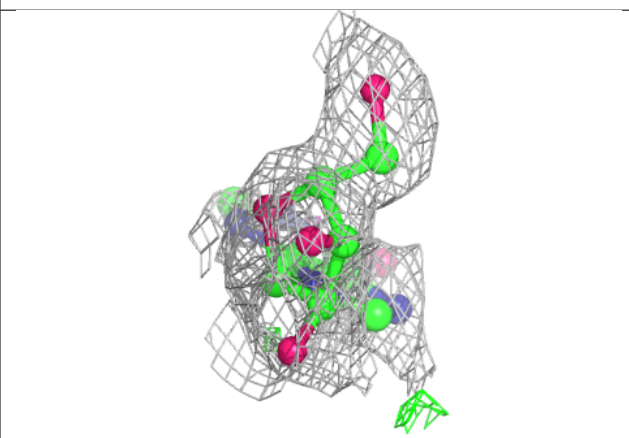
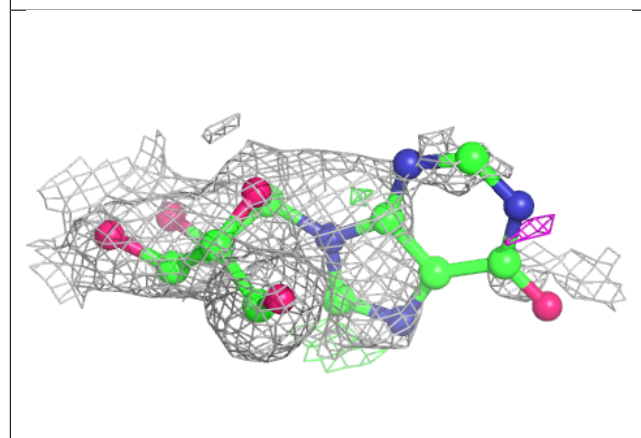
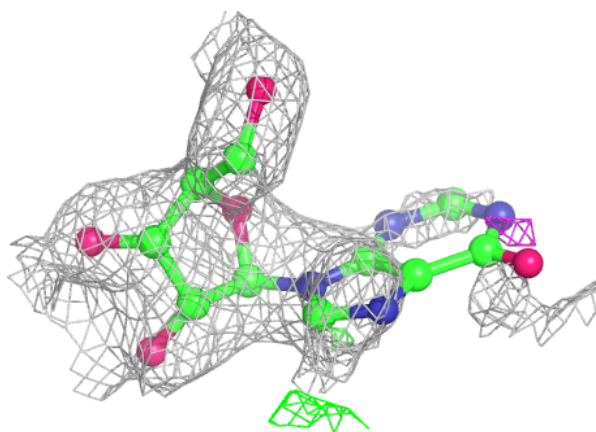


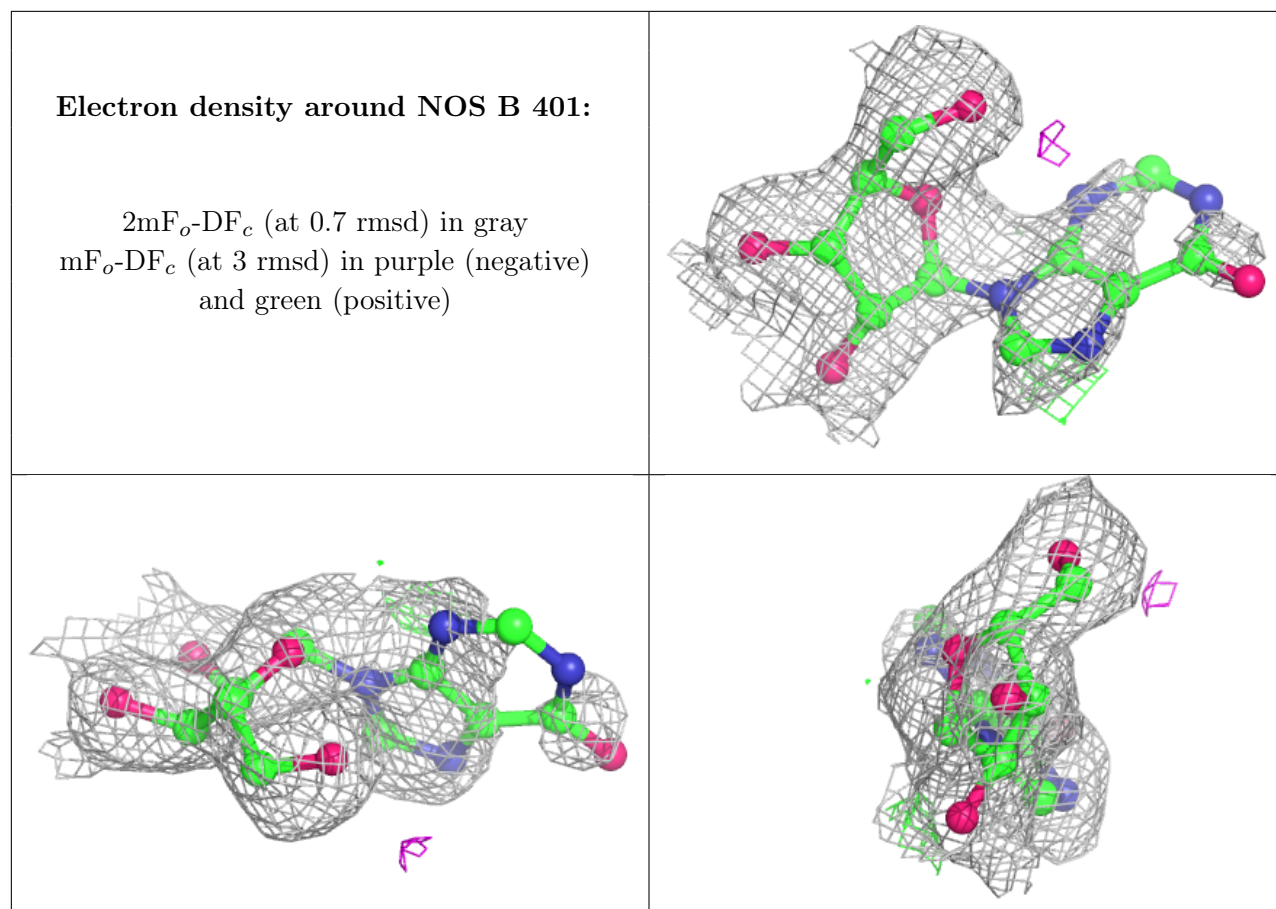
**Electron density around NOS A 401:**

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

**Electron density around NOS D 401:**

$2mF_o-DF_c$  (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.