



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 03:03 pm BST

PDB ID : 5KVS  
Title : Substrate Analog and NADP<sup>+</sup> bound structure of Irp3, a ThiazolinyI Imine Reductase from *Yersinia enterocolitica*  
Authors : Meneely, K.M.; Lamb, A.L.  
Deposited on : 2016-07-15  
Resolution : 1.28 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.

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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)  
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

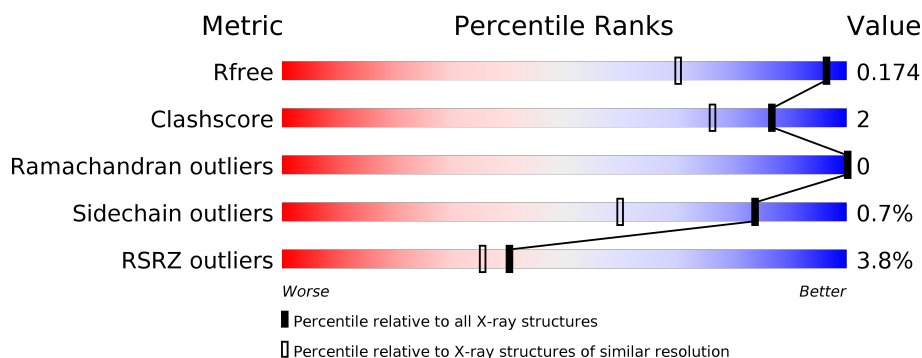
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.28 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	1850 (1.30-1.26)
Clashscore	141614	1926 (1.30-1.26)
Ramachandran outliers	138981	1860 (1.30-1.26)
Sidechain outliers	138945	1859 (1.30-1.26)
RSRZ outliers	127900	1807 (1.30-1.26)

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  $\geq 3$ , 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	385	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>5%</div> <div>8%</div> </div> </div>
1	B	385	<div> <div>5%</div> <div> <div></div> <div>86%</div> <div>5%</div> <div>8%</div> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12210 atoms, of which 5824 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 Irp3 protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	353	Total	C	H	N	O	S	0	21	0
			5770	1834	2893	517	508	18			
1	B	354	Total	C	H	N	O	S	0	11	0
			5661	1802	2824	516	500	19			

There are 40 discrepancies between the modelled and reference sequences:

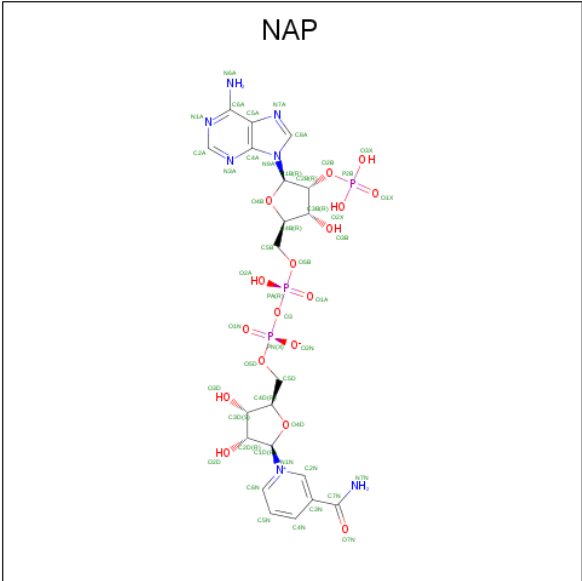
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP O54512
A	-18	GLY	-	expression tag	UNP O54512
A	-17	SER	-	expression tag	UNP O54512
A	-16	SER	-	expression tag	UNP O54512
A	-15	HIS	-	expression tag	UNP O54512
A	-14	HIS	-	expression tag	UNP O54512
A	-13	HIS	-	expression tag	UNP O54512
A	-12	HIS	-	expression tag	UNP O54512
A	-11	HIS	-	expression tag	UNP O54512
A	-10	HIS	-	expression tag	UNP O54512
A	-9	SER	-	expression tag	UNP O54512
A	-8	SER	-	expression tag	UNP O54512
A	-7	GLY	-	expression tag	UNP O54512
A	-6	LEU	-	expression tag	UNP O54512
A	-5	VAL	-	expression tag	UNP O54512
A	-4	PRO	-	expression tag	UNP O54512
A	-3	ARG	-	expression tag	UNP O54512
A	-2	GLY	-	expression tag	UNP O54512
A	-1	SER	-	expression tag	UNP O54512
A	0	HIS	-	expression tag	UNP O54512
B	-19	MET	-	initiating methionine	UNP O54512
B	-18	GLY	-	expression tag	UNP O54512
B	-17	SER	-	expression tag	UNP O54512
B	-16	SER	-	expression tag	UNP O54512
B	-15	HIS	-	expression tag	UNP O54512

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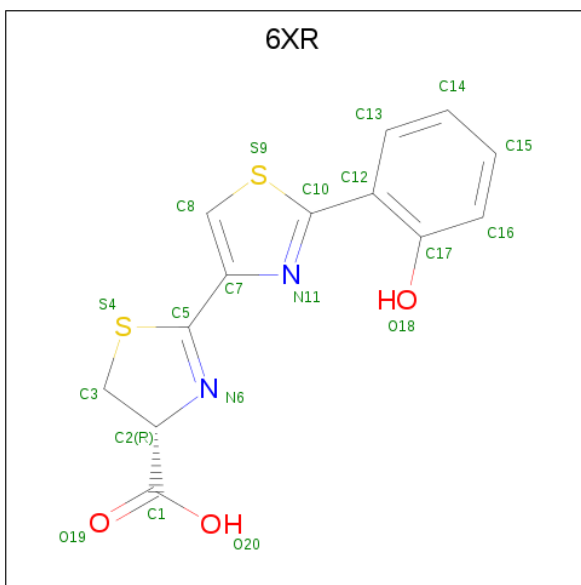
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP O54512
B	-13	HIS	-	expression tag	UNP O54512
B	-12	HIS	-	expression tag	UNP O54512
B	-11	HIS	-	expression tag	UNP O54512
B	-10	HIS	-	expression tag	UNP O54512
B	-9	SER	-	expression tag	UNP O54512
B	-8	SER	-	expression tag	UNP O54512
B	-7	GLY	-	expression tag	UNP O54512
B	-6	LEU	-	expression tag	UNP O54512
B	-5	VAL	-	expression tag	UNP O54512
B	-4	PRO	-	expression tag	UNP O54512
B	-3	ARG	-	expression tag	UNP O54512
B	-2	GLY	-	expression tag	UNP O54512
B	-1	SER	-	expression tag	UNP O54512
B	0	HIS	-	expression tag	UNP O54512

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
2	B	1	Total	C	H	N	O	P	0	1
			146	42	50	14	34	6		

- Molecule 3 is (4 {R})-2-[2-(2-hydroxyphenyl)-1,3-thiazol-4-yl]-4,5-dihydro-1,3-thiazole-4-carboxylic acid (three-letter code: 6XR) (formula: C<sub>13</sub>H<sub>10</sub>N<sub>2</sub>O<sub>3</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	S	0	0
			29	13	9	2	3	2		
3	B	1	Total	C	H	N	O	S	0	0
			29	13	9	2	3	2		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 5 is FORMIC ACID (three-letter code: FMT) (formula:  $\text{CH}_2\text{O}_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			4	1	1	2		
5	B	1	Total	C	H	O	0	0
			4	1	1	2		


- Molecule 6 is water.

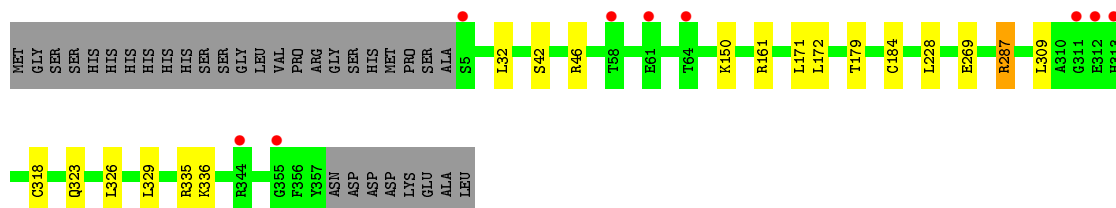
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	261	Total	O	0	0
			261	261		
6	B	213	Total	O	0	0
			213	213		

### 3 Residue-property plots [i](#)


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.

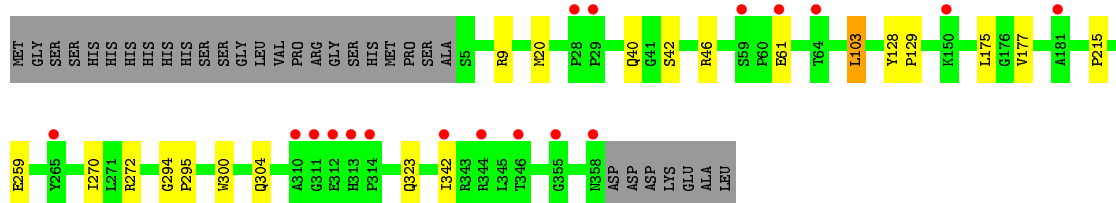
- Molecule 1: Irp3 protein

Chain A: 



- Molecule 1: Irp3 protein

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	41.39Å 148.55Å 65.40Å 90.00° 95.30° 90.00°	Depositor
Resolution (Å)	36.04 – 1.28 36.04 – 1.28	Depositor EDS
% Data completeness (in resolution range)	96.7 (36.04-1.28) 96.7 (36.04-1.28)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.78 (at 1.28Å)	Xtriage
Refinement program	PHENIX (1.10_2155), REFMAC	Depositor
R, $R_{free}$	0.162 , 0.174 0.162 , 0.174	Depositor DCC
$R_{free}$ test set	9896 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.3	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.45 , 47.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	12210	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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: FMT, EDO, NAP, 6XR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.45	0/3019	0.68	3/4116 (0.1%)
1	B	0.39	0/2949	0.62	1/4019 (0.0%)
All	All	0.42	0/5968	0.65	4/8135 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	A	287[A]	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	A	287[B]	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	B	103	LEU	CA-CB-CG	5.87	128.81	115.30

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	2877	2893	2895	12	3
1	B	2837	2824	2826	14	2
2	A	48	25	24	2	0
2	B	96	50	46	3	0
3	A	20	9	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	20	9	0	1	0
4	A	4	6	6	0	0
4	B	4	6	6	0	0
5	A	3	1	1	0	0
5	B	3	1	1	0	0
6	A	261	0	0	3	1
6	B	213	0	0	3	1
All	All	6386	5824	5805	25	4

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 2.

All (25) 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)
2:B:401[A]:NAP:N7N	3:B:402:6XR:O19	1.93	1.02
1:B:9[A]:ARG:NH1	6:B:501:HOH:O	2.13	0.81
1:A:287[B]:ARG:NH1	6:A:501:HOH:O	2.20	0.71
1:B:20[A]:MET:HE3	1:B:295:PRO:HD3	1.85	0.59
1:A:179[A]:THR:HG21	1:A:326:LEU:HA	1.88	0.55
1:A:287[B]:ARG:NH2	1:B:270:ILE:O	2.39	0.55
1:A:184[A]:CYS:SG	1:A:336:LYS:HG3	2.47	0.54
1:A:171[A]:LEU:CD2	1:A:228[A]:LEU:HD23	2.38	0.53
1:B:42[B]:SER:OG	2:B:401[B]:NAP:O3X	2.27	0.52
1:A:287[B]:ARG:HH22	1:B:272:ARG:HG2	1.76	0.51
1:B:300:TRP:O	1:B:304[A]:GLN:HG2	2.12	0.50
1:B:40:GLN:NE2	6:B:505:HOH:O	2.33	0.46
1:A:150:LYS:HG3	6:A:562:HOH:O	2.16	0.46
1:B:20[A]:MET:CE	1:B:294:GLY:HA3	2.47	0.44
1:A:42[B]:SER:OG	2:A:401:NAP:O1X	2.35	0.43
1:A:318[B]:CYS:HA	1:A:323:GLN:NE2	2.33	0.43
1:A:335:ARG:NH2	6:A:505:HOH:O	2.48	0.43
1:B:128:TYR:OH	2:B:401[A]:NAP:N7N	2.49	0.43
1:A:179[A]:THR:HG23	1:A:329:LEU:HD22	2.01	0.42
1:B:20[A]:MET:CE	1:B:295:PRO:HD3	2.48	0.42
1:A:42[B]:SER:HG	2:A:401:NAP:P2B	2.43	0.41
1:B:323:GLN:NE2	6:B:510:HOH:O	2.53	0.41
1:B:175:LEU:HB3	1:B:177:VAL:HG23	2.03	0.41
1:B:215:PRO:CD	1:B:342:ILE:HG23	2.51	0.41
1:B:128:TYR:N	1:B:129:PRO:CD	2.85	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ARG:HH21	6:B:701:HOH:O[2_645]	1.54	0.06
1:B:9[B]:ARG:NH2	1:B:259:GLU:OE1[2_655]	2.16	0.04
1:A:309:LEU:O	1:B:46:ARG:HH22[2_646]	1.57	0.03
1:A:269:GLU:OE2	6:A:651:HOH:O[2_656]	2.18	0.02

## 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	372/385 (97%)	363 (98%)	9 (2%)	0	100	100
1	B	363/385 (94%)	351 (97%)	12 (3%)	0	100	100
All	All	735/770 (96%)	714 (97%)	21 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	319/325 (98%)	317 (99%)	2 (1%)	86	64
1	B	310/325 (95%)	308 (99%)	2 (1%)	86	64
All	All	629/650 (97%)	625 (99%)	4 (1%)	84	64

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LEU
1	A	172	LEU
1	B	61	GLU
1	B	103	LEU

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

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

9 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	NAP	B	401[B]	-	45,52,52	4.21	12 (26%)	56,80,80	2.03	4 (7%)
5	FMT	B	404	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	404	-	0,2,2	0.00	-	0,1,1	0.00	-
2	NAP	B	401[A]	-	45,52,52	4.40	12 (26%)	56,80,80	2.19	7 (12%)
2	NAP	A	401	-	45,52,52	3.92	12 (26%)	56,80,80	1.81	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EDO	A	403	-	3,3,3	0.31	0	2,2,2	0.59	0
3	6XR	B	402	-	17,22,22	1.40	4 (23%)	13,31,31	1.47	1 (7%)
3	6XR	A	402	-	17,22,22	1.22	2 (11%)	13,31,31	1.44	2 (15%)
4	EDO	B	403	-	3,3,3	0.30	0	2,2,2	0.57	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	B	401[B]	-	-	6/31/67/67	0/5/5/5
2	NAP	B	401[A]	-	-	10/31/67/67	0/5/5/5
2	NAP	A	401	-	-	5/31/67/67	0/5/5/5
4	EDO	A	403	-	-	0/1/1/1	-
3	6XR	B	402	-	-	0/2/21/21	0/3/3/3
3	6XR	A	402	-	-	0/2/21/21	0/3/3/3
4	EDO	B	403	-	-	0/1/1/1	-

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401[A]	NAP	C2D-C1D	-16.36	1.28	1.53
2	B	401[B]	NAP	C2D-C1D	-16.21	1.29	1.53
2	B	401[A]	NAP	O4B-C1B	14.49	1.61	1.41
2	B	401[A]	NAP	O4D-C1D	14.35	1.61	1.41
2	A	401	NAP	C2D-C1D	-13.86	1.32	1.53
2	B	401[B]	NAP	O4D-C1D	13.61	1.60	1.41
2	B	401[B]	NAP	O4B-C1B	13.23	1.59	1.41
2	A	401	NAP	O4D-C1D	12.99	1.59	1.41
2	A	401	NAP	O4B-C1B	12.59	1.58	1.41
2	B	401[A]	NAP	O4D-C4D	-7.14	1.29	1.45
2	B	401[B]	NAP	C7N-N7N	6.07	1.44	1.33
2	B	401[B]	NAP	O4D-C4D	-6.07	1.31	1.45
2	A	401	NAP	C7N-N7N	6.04	1.44	1.33
2	B	401[A]	NAP	O4B-C4B	-5.95	1.31	1.45
2	A	401	NAP	O4D-C4D	-5.50	1.32	1.45
2	A	401	NAP	O4B-C4B	-5.27	1.33	1.45
2	B	401[B]	NAP	O4B-C4B	-5.18	1.33	1.45
2	B	401[A]	NAP	C7N-N7N	5.16	1.42	1.33
2	A	401	NAP	C2A-N3A	3.87	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAP	O2D-C2D	3.53	1.51	1.43
2	B	401[A]	NAP	C2A-N3A	3.32	1.37	1.32
2	B	401[B]	NAP	C2A-N3A	3.30	1.37	1.32
2	B	401[A]	NAP	O2D-C2D	3.27	1.50	1.43
2	B	401[B]	NAP	O2D-C2D	3.21	1.50	1.43
3	B	402	6XR	C3-S4	-3.00	1.75	1.81
3	B	402	6XR	C5-S4	-2.89	1.66	1.77
2	B	401[A]	NAP	O3D-C3D	-2.83	1.36	1.43
2	A	401	NAP	O3D-C3D	-2.79	1.36	1.43
2	B	401[A]	NAP	O3B-C3B	-2.76	1.36	1.43
2	B	401[B]	NAP	O3B-C3B	-2.70	1.36	1.43
3	A	402	6XR	C5-S4	-2.59	1.67	1.77
2	B	401[B]	NAP	O3D-C3D	-2.56	1.36	1.43
3	B	402	6XR	C10-N11	2.56	1.35	1.31
3	A	402	6XR	C3-S4	-2.49	1.76	1.81
2	B	401[A]	NAP	C6A-N6A	2.43	1.42	1.34
2	A	401	NAP	O3B-C3B	-2.39	1.37	1.43
2	B	401[B]	NAP	C5A-C4A	-2.33	1.34	1.40
2	B	401[B]	NAP	C6A-N6A	2.33	1.42	1.34
2	B	401[A]	NAP	C5A-C4A	-2.31	1.34	1.40
2	A	401	NAP	C5A-C4A	-2.22	1.35	1.40
2	A	401	NAP	C6A-N6A	2.17	1.42	1.34
3	B	402	6XR	C8-S9	2.16	1.74	1.70

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401[A]	NAP	C5A-C6A-N6A	11.29	137.50	120.35
2	B	401[B]	NAP	C5A-C6A-N6A	10.45	136.24	120.35
2	A	401	NAP	C5A-C6A-N6A	8.54	133.33	120.35
2	B	401[A]	NAP	N6A-C6A-N1A	-7.75	102.48	118.57
2	B	401[B]	NAP	N6A-C6A-N1A	-7.00	104.04	118.57
2	A	401	NAP	N6A-C6A-N1A	-5.45	107.27	118.57
2	B	401[A]	NAP	N3A-C2A-N1A	-5.30	120.40	128.68
2	B	401[B]	NAP	N3A-C2A-N1A	-5.01	120.85	128.68
2	A	401	NAP	N3A-C2A-N1A	-4.90	121.01	128.68
3	B	402	6XR	C7-C5-N6	4.28	126.55	124.27
3	A	402	6XR	C3-C2-N6	-3.69	103.61	109.80
2	B	401[A]	NAP	C2N-C3N-C4N	2.78	121.41	118.26
2	B	401[A]	NAP	O7N-C7N-C3N	2.68	122.84	119.63
2	A	401	NAP	O4D-C1D-C2D	-2.55	103.19	106.93
2	B	401[A]	NAP	C2N-N1N-C1D	-2.55	113.46	119.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NAP	C2N-C3N-C4N	2.47	121.06	118.26
3	A	402	6XR	C7-C5-N6	-2.17	123.11	124.27
2	B	401[B]	NAP	C2N-C3N-C4N	2.16	120.70	118.26
2	B	401[A]	NAP	C1B-N9A-C4A	-2.08	122.99	126.64
2	A	401	NAP	C3D-C2D-C1D	2.03	104.03	100.98

There are no chirality outliers.

All (21) torsion outliers are listed below:

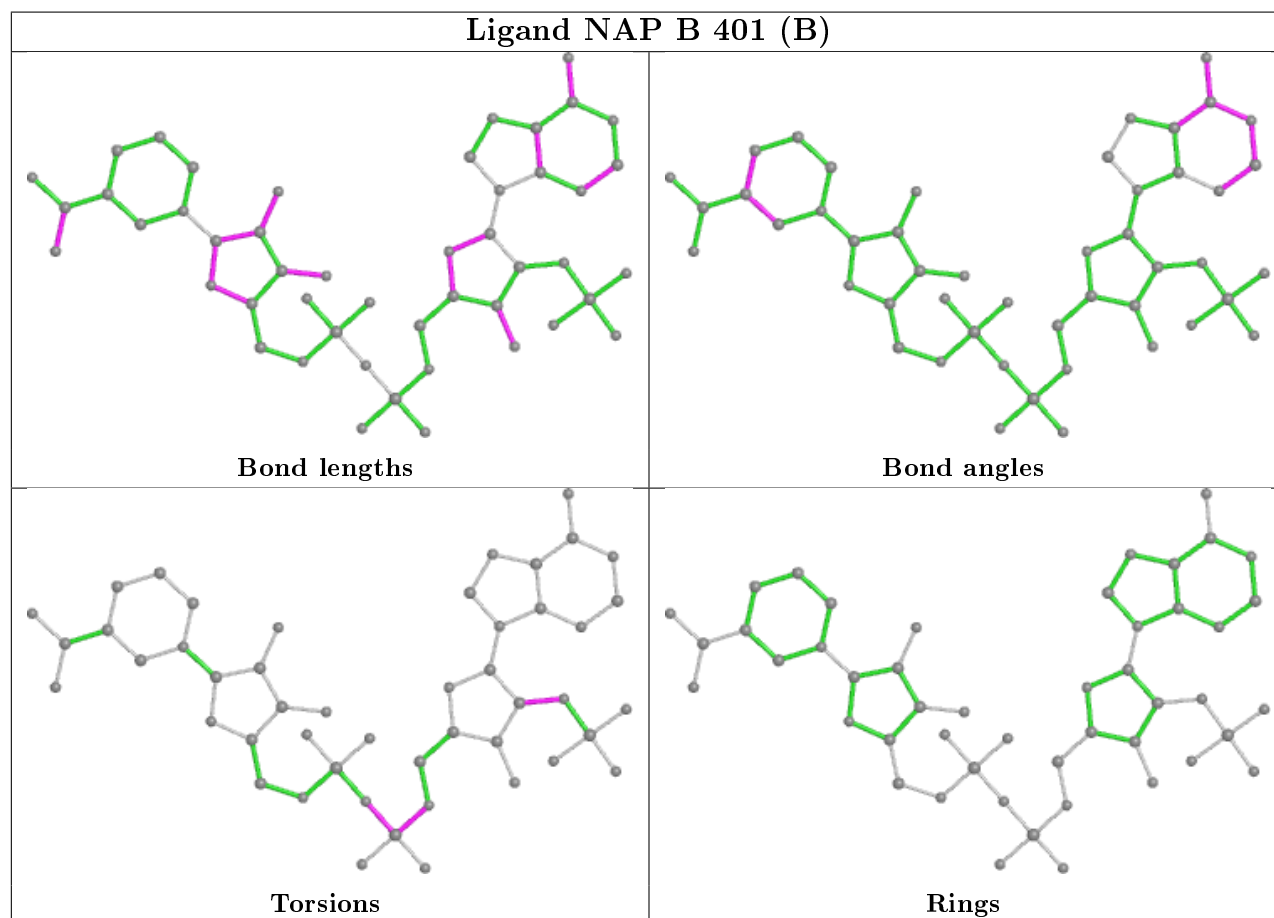
Mol	Chain	Res	Type	Atoms
2	B	401[B]	NAP	C5B-O5B-PA-O1A
2	B	401[B]	NAP	C5B-O5B-PA-O2A
2	B	401[B]	NAP	C3B-C2B-O2B-P2B
2	B	401[A]	NAP	C5B-O5B-PA-O1A
2	B	401[A]	NAP	C5B-O5B-PA-O2A
2	B	401[A]	NAP	O4D-C1D-N1N-C2N
2	B	401[A]	NAP	O4D-C1D-N1N-C6N
2	B	401[A]	NAP	C2D-C1D-N1N-C2N
2	B	401[A]	NAP	C2D-C1D-N1N-C6N
2	A	401	NAP	C5B-O5B-PA-O1A
2	A	401	NAP	C5B-O5B-PA-O2A
2	B	401[A]	NAP	C3B-C2B-O2B-P2B
2	A	401	NAP	C3B-C2B-O2B-P2B
2	B	401[B]	NAP	C1B-C2B-O2B-P2B
2	A	401	NAP	C1B-C2B-O2B-P2B
2	B	401[B]	NAP	PN-O3-PA-O5B
2	B	401[A]	NAP	PN-O3-PA-O5B
2	B	401[A]	NAP	C1B-C2B-O2B-P2B
2	B	401[B]	NAP	C5B-O5B-PA-O3
2	B	401[A]	NAP	C5B-O5B-PA-O3
2	A	401	NAP	C5B-O5B-PA-O3

There are no ring outliers.

4 monomers are involved in 5 short contacts:

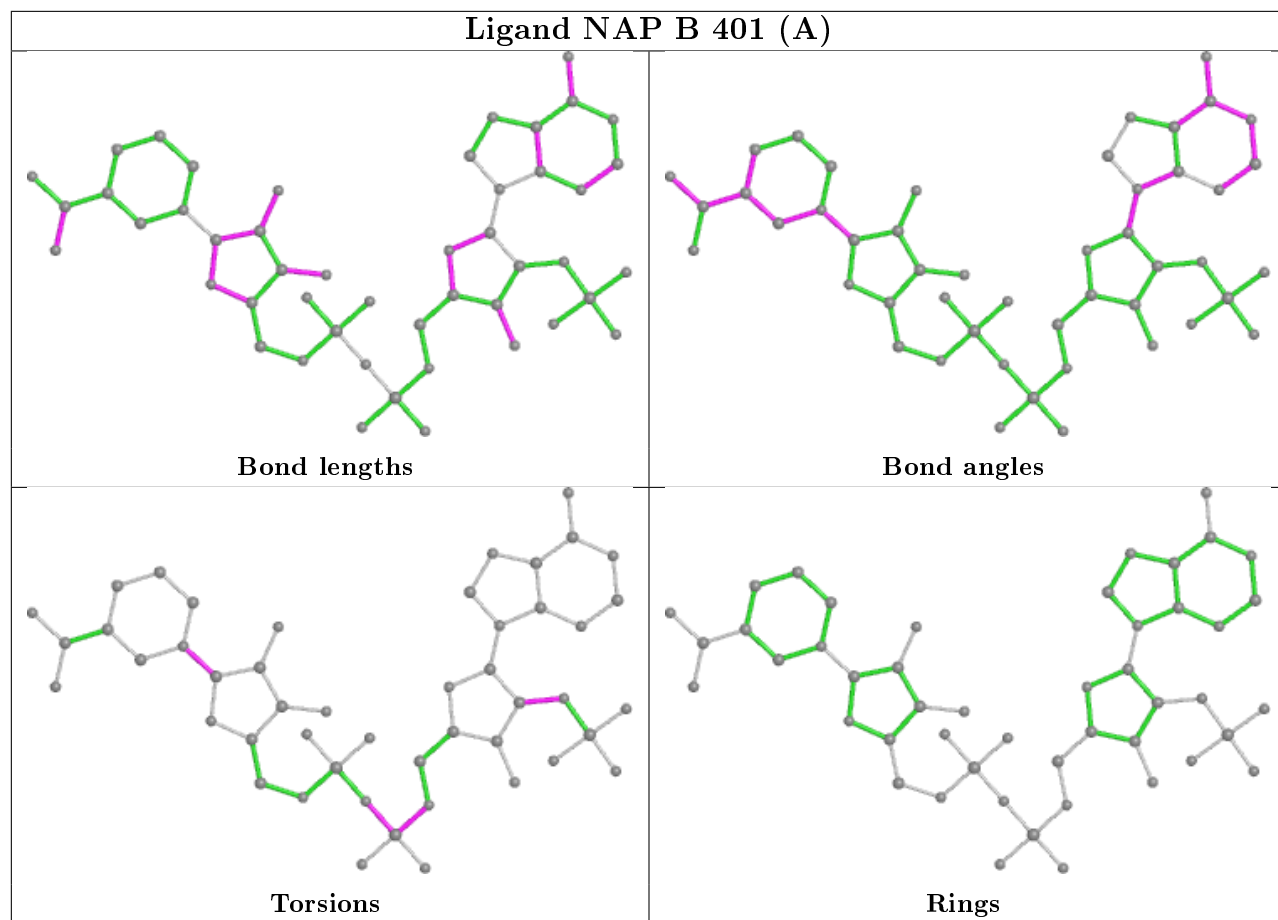
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401[B]	NAP	1	0
2	B	401[A]	NAP	2	0
2	A	401	NAP	2	0
3	B	402	6XR	1	0

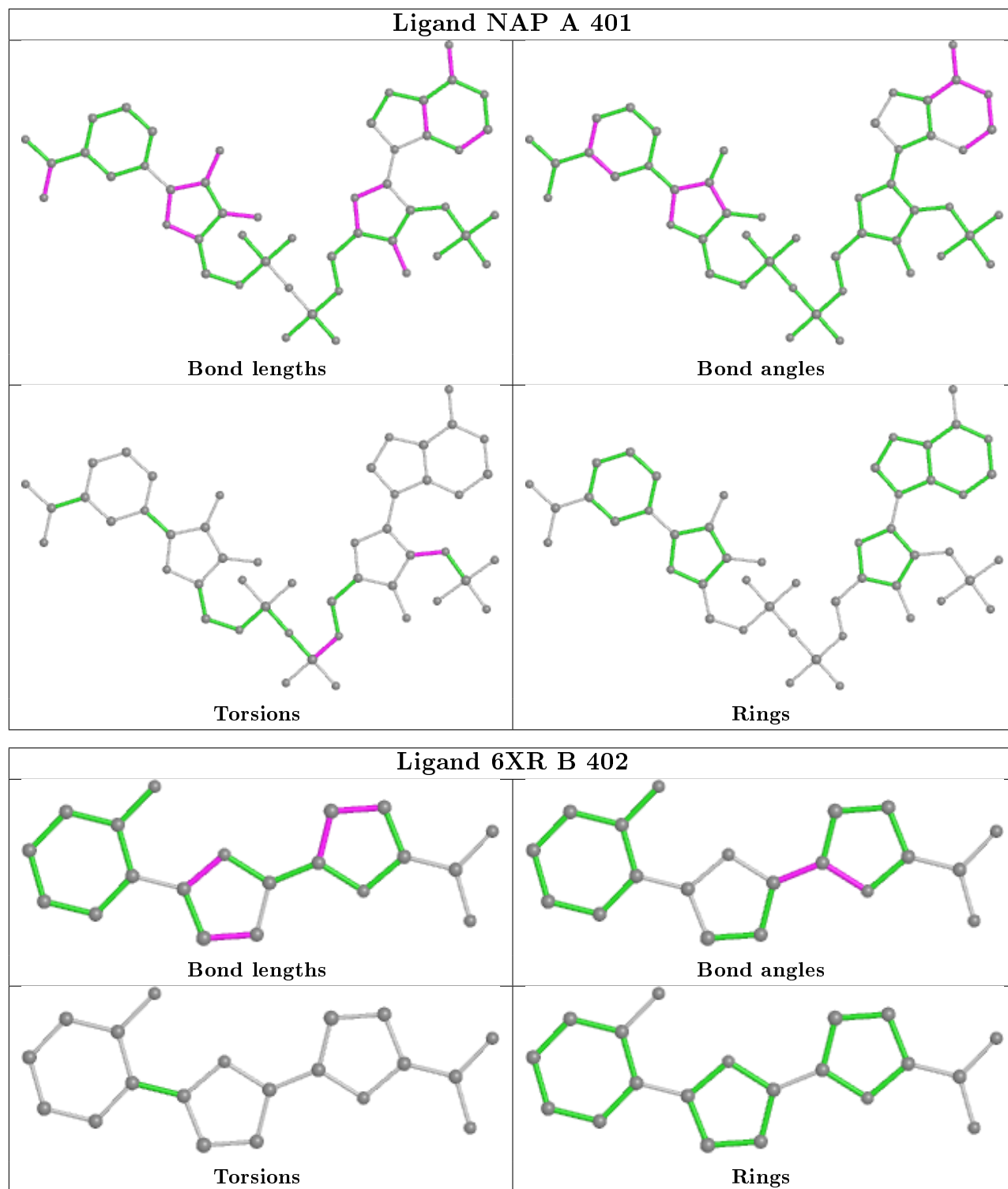
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

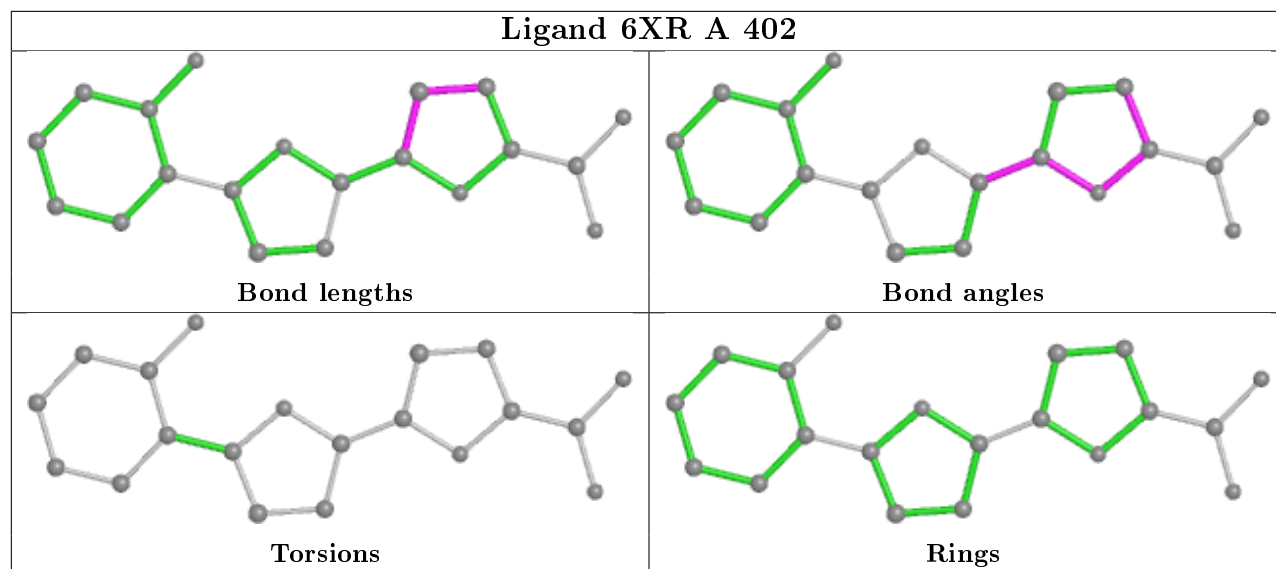




## Ligand NAP B 401 (A)







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	353/385 (91%)	0.06	9 (2%) 57 53	10, 16, 33, 50	0
1	B	354/385 (91%)	0.10	18 (5%) 28 24	10, 19, 35, 49	0
All	All	707/770 (91%)	0.08	27 (3%) 40 35	10, 18, 35, 50	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	64	THR	4.1
1	B	313	HIS	3.9
1	B	344	ARG	3.8
1	A	313	HIS	3.8
1	B	314	PRO	3.7
1	A	344	ARG	3.6
1	A	61	GLU	3.6
1	A	64	THR	3.2
1	B	358	ASN	3.0
1	B	311	GLY	3.0
1	B	355	GLY	2.9
1	B	28	PRO	2.9
1	B	61	GLU	2.9
1	B	59	SER	2.9
1	B	342	ILE	2.8
1	B	150	LYS	2.8
1	A	355	GLY	2.8
1	B	29	PRO	2.7
1	A	311	GLY	2.7
1	B	310	ALA	2.6
1	B	312	GLU	2.3
1	A	312	GLU	2.3
1	A	5	SER	2.2
1	B	346	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	58[A]	THR	2.1
1	B	181	ALA	2.1
1	B	265	TYR	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

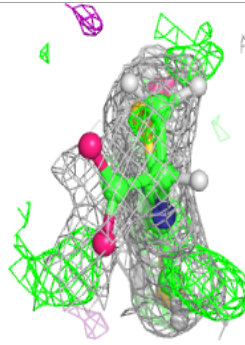
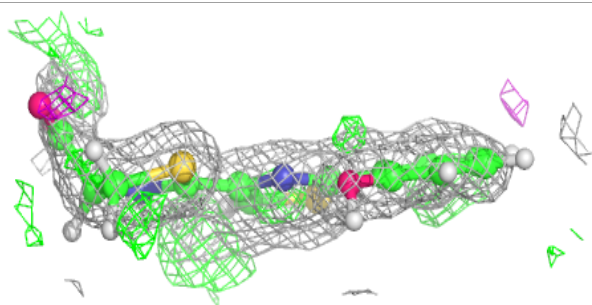
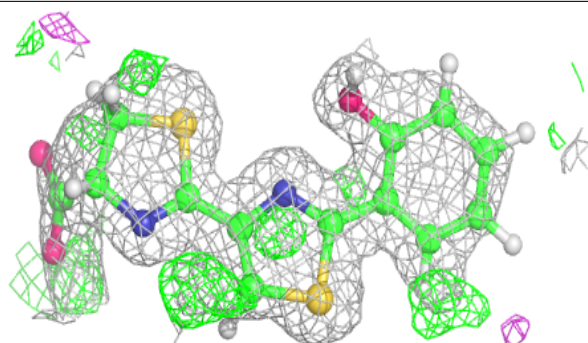
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	6XR	B	402	20/20	0.89	0.19	18,26,38,44	29
5	FMT	A	404	3/3	0.93	0.09	25,28,29,35	0
5	FMT	B	404	3/3	0.93	0.08	25,26,28,30	0
4	EDO	B	403	4/4	0.93	0.09	19,28,36,36	0
2	NAP	B	401[B]	48/48	0.95	0.10	15,22,39,40	73
2	NAP	B	401[A]	48/48	0.95	0.10	14,22,29,36	73
3	6XR	A	402	20/20	0.96	0.10	15,20,29,33	29
4	EDO	A	403	4/4	0.96	0.06	20,29,40,40	0
2	NAP	A	401	48/48	0.98	0.06	13,19,30,42	0

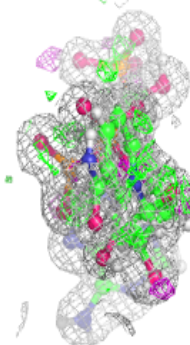
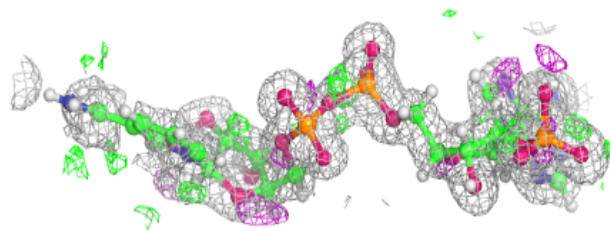
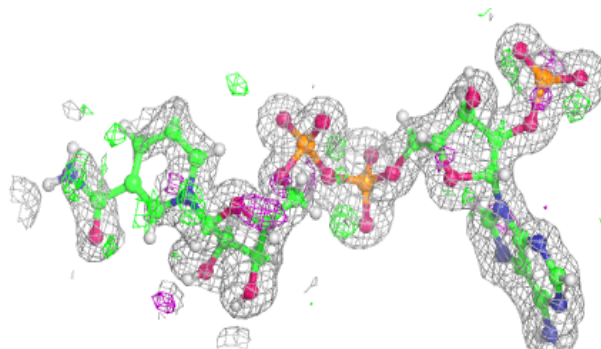
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 6XR B 402:**

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

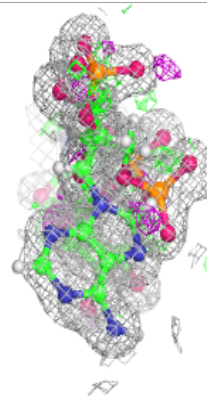
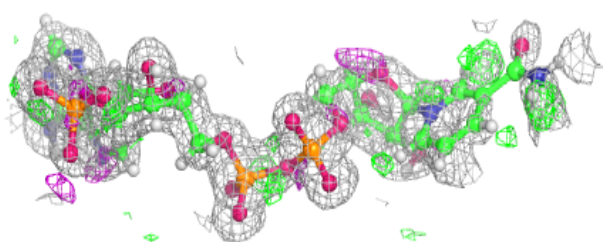
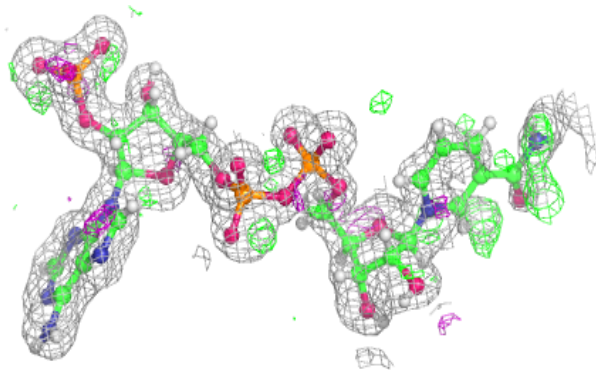
**Electron density around NAP B 401 (B):**

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

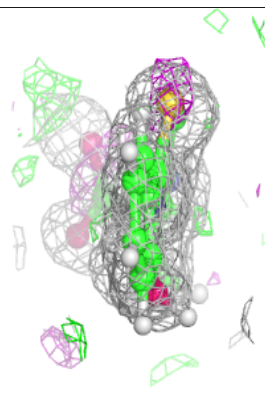
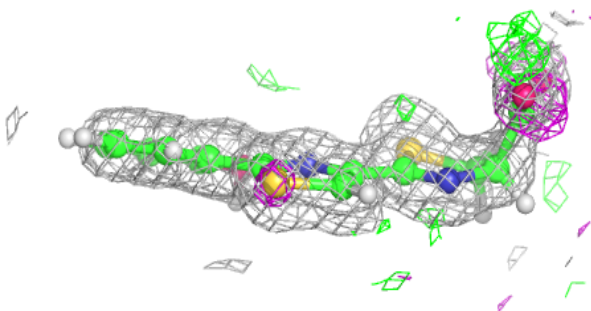
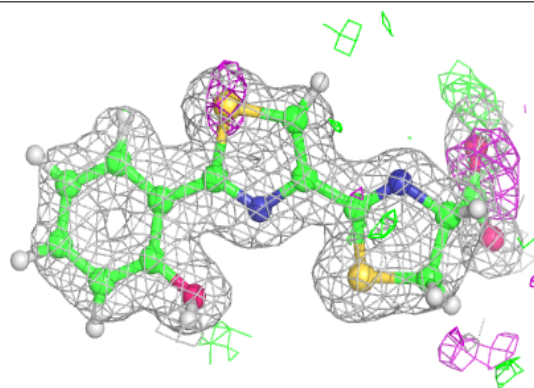


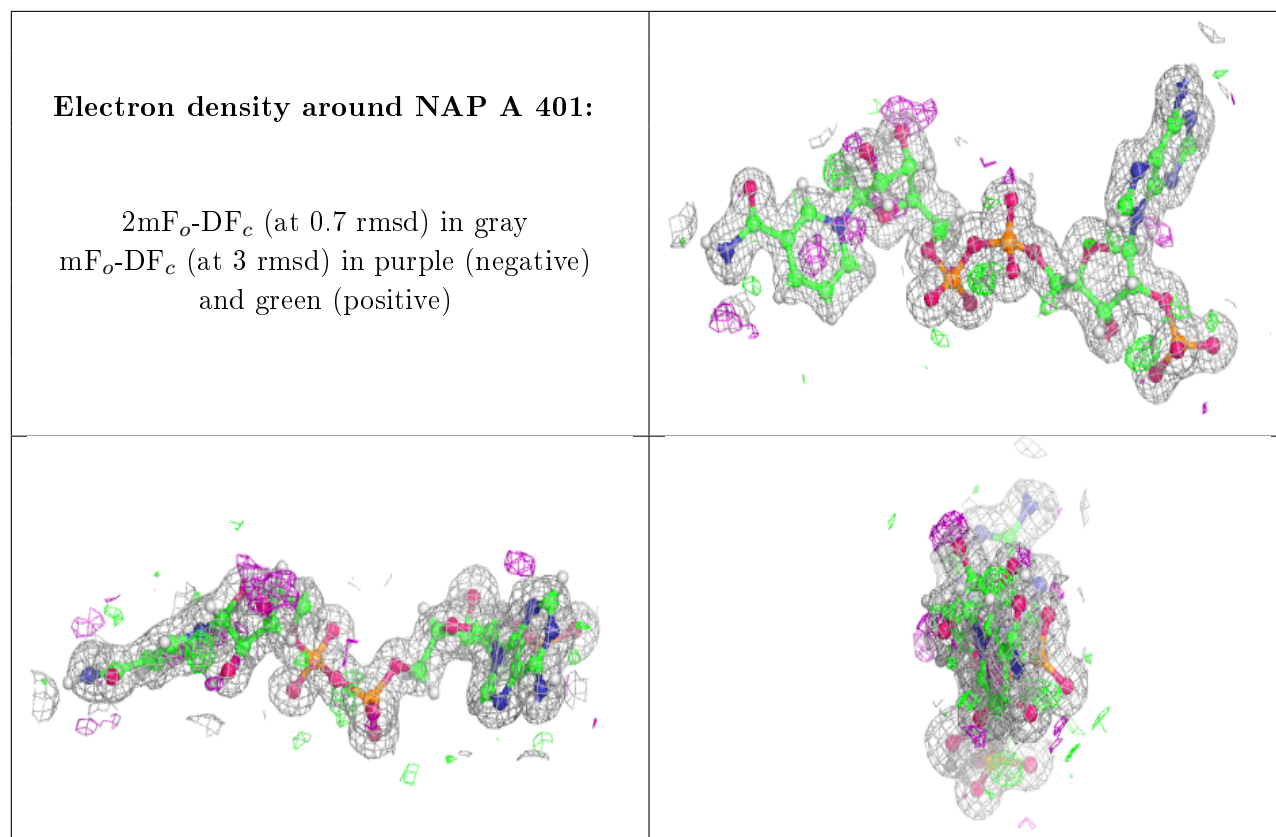
**Electron density around NAP B 401 (A):**

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

**Electron density around 6XR A 402:**

$2mF_o-DF_c$  (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.