



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 08:08 pm BST

PDB ID : 4JQ4
Title : AKR1C2 complex with indomethacin
Authors : Yosaatmadja, Y.; Flanagan, J.U.; Squire, C.J.
Deposited on : 2013-03-19
Resolution : 1.52 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 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

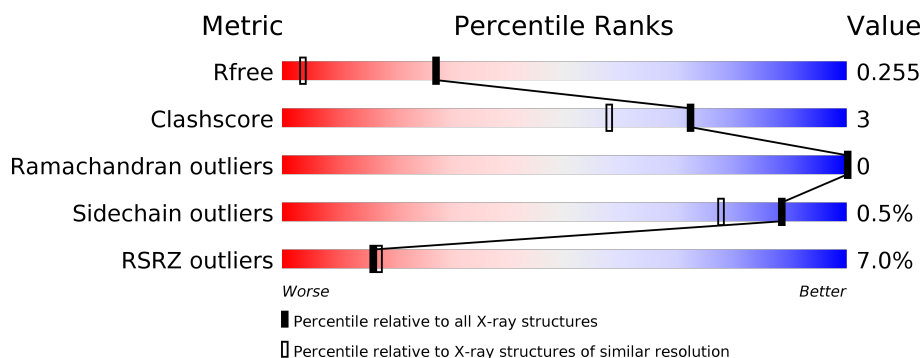
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.52 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	4009 (1.54-1.50)
Clashscore	141614	4249 (1.54-1.50)
Ramachandran outliers	138981	4148 (1.54-1.50)
Sidechain outliers	138945	4146 (1.54-1.50)
RSRZ outliers	127900	3943 (1.54-1.50)

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	331	<div> <div>4%</div> <div>90%</div> <div>5%</div> <div>5%</div> </div>
1	B	331	<div> <div>10%</div> <div>83%</div> <div>11%</div> <div>5%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	A	405	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5622 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.

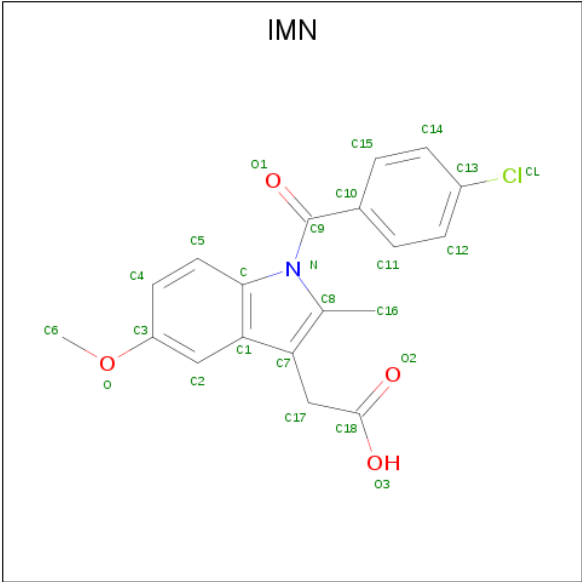
- Molecule 1 is a protein called Aldo-keto reductase family 1 member C2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	1	4	0
			2554	1640	442	461	11			
1	B	314	Total	C	N	O	S	0	4	0
			2510	1615	429	455	11			

There are 16 discrepancies between the modelled and reference sequences:

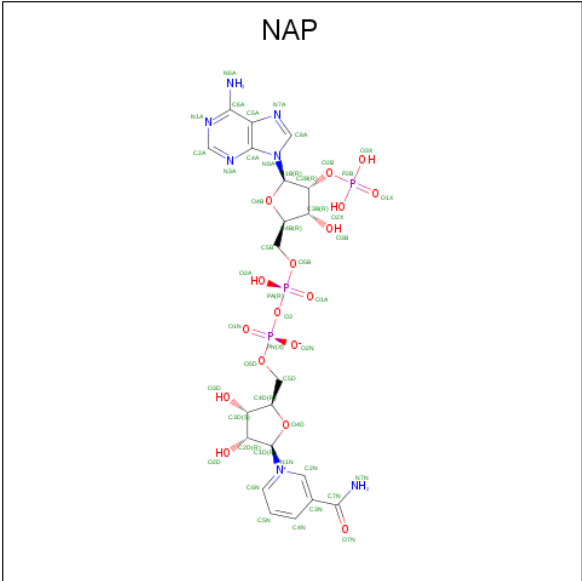
Chain	Residue	Modelled	Actual	Comment	Reference
A	324	LEU	-	EXPRESSION TAG	UNP P52895
A	325	GLU	-	EXPRESSION TAG	UNP P52895
A	326	HIS	-	EXPRESSION TAG	UNP P52895
A	327	HIS	-	EXPRESSION TAG	UNP P52895
A	328	HIS	-	EXPRESSION TAG	UNP P52895
A	329	HIS	-	EXPRESSION TAG	UNP P52895
A	330	HIS	-	EXPRESSION TAG	UNP P52895
A	331	HIS	-	EXPRESSION TAG	UNP P52895
B	324	LEU	-	EXPRESSION TAG	UNP P52895
B	325	GLU	-	EXPRESSION TAG	UNP P52895
B	326	HIS	-	EXPRESSION TAG	UNP P52895
B	327	HIS	-	EXPRESSION TAG	UNP P52895
B	328	HIS	-	EXPRESSION TAG	UNP P52895
B	329	HIS	-	EXPRESSION TAG	UNP P52895
B	330	HIS	-	EXPRESSION TAG	UNP P52895
B	331	HIS	-	EXPRESSION TAG	UNP P52895

- Molecule 2 is INDOMETHACIN (three-letter code: IMN) (formula: C₁₉H₁₆ClNO₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			25	19	1	1	4		
2	B	1	Total	C	Cl	N	O	0	0
			25	19	1	1	4		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



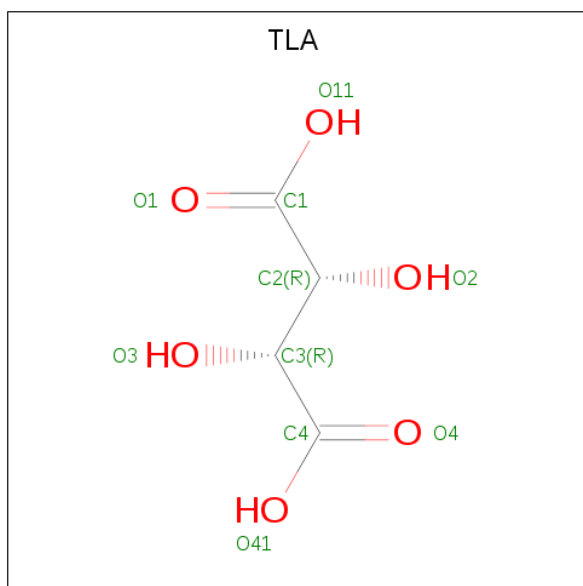
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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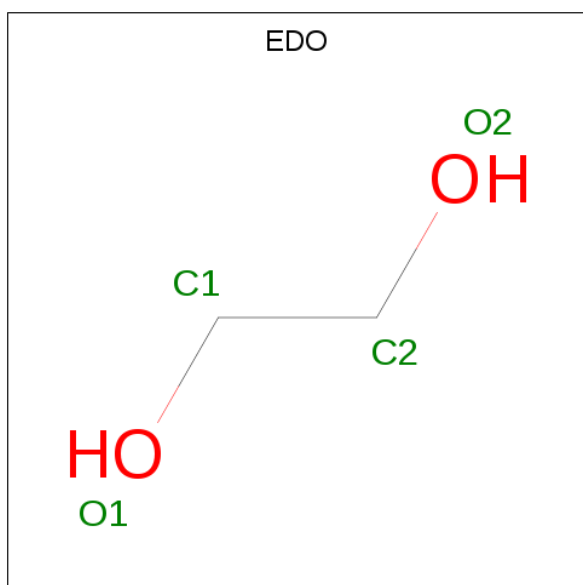
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	B	1	48	21	7	17	3	0	0

- Molecule 4 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: $C_4H_6O_6$).



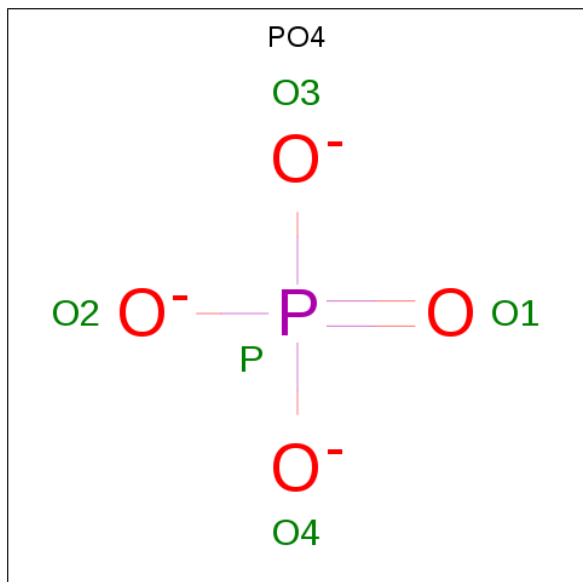
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	10	4	6	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total O P 5 4 1	0	0

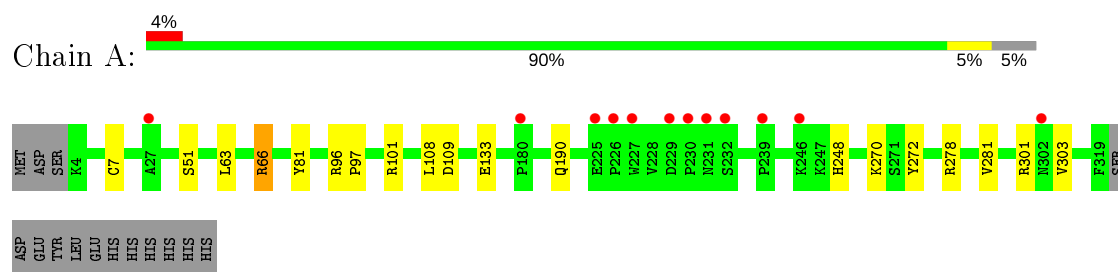
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	194	Total O 194 194	0	0
7	B	179	Total O 179 179	0	0

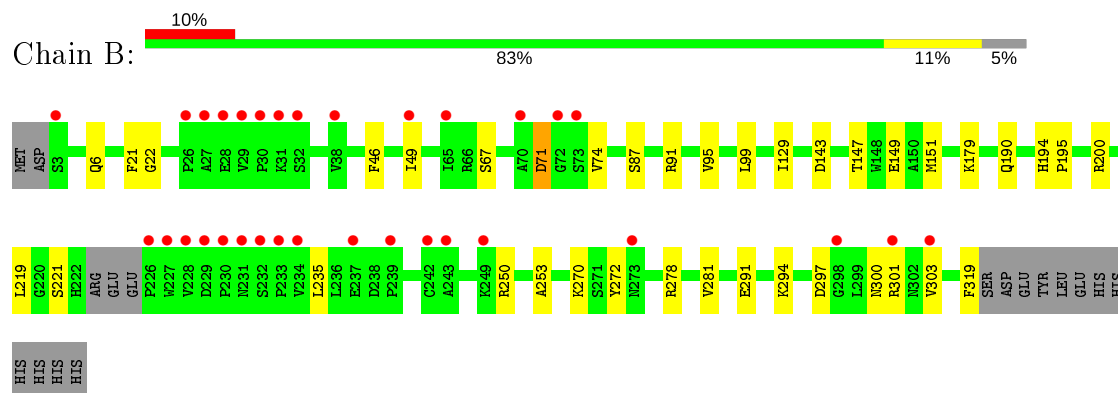
3 Residue-property plots [i](#)

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: Aldo-keto reductase family 1 member C2



- Molecule 1: Aldo-keto reductase family 1 member C2



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	142.45Å 142.45Å 206.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.70 – 1.52 19.70 – 1.52	Depositor EDS
% Data completeness (in resolution range)	98.8 (19.70-1.52) 98.9 (19.70-1.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 1.53Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.197 , 0.251 0.206 , 0.255	Depositor DCC
R_{free} test set	6055 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	18.4	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5622	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, TLA, EDO, NAP, IMN

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	1.00	0/2623	1.08	6/3554 (0.2%)
1	B	1.12	3/2574 (0.1%)	1.08	9/3490 (0.3%)
All	All	1.06	3/5197 (0.1%)	1.08	15/7044 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	91	ARG	C-O	-5.93	1.12	1.23
1	B	87	SER	CB-OG	5.11	1.48	1.42
1	B	46	PHE	CG-CD1	5.04	1.46	1.38

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66[A]	ARG	NE-CZ-NH1	-10.82	114.89	120.30
1	A	66[B]	ARG	NE-CZ-NH1	-10.82	114.89	120.30
1	A	66[A]	ARG	NE-CZ-NH2	10.47	125.54	120.30
1	A	66[B]	ARG	NE-CZ-NH2	10.47	125.54	120.30
1	A	101	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	A	63	LEU	CA-CB-CG	5.91	128.90	115.30
1	B	151	MET	CA-CB-CG	5.47	122.61	113.30
1	B	95	VAL	CG1-CB-CG2	-5.45	102.18	110.90
1	B	319	PHE	CB-CG-CD1	5.36	124.55	120.80
1	B	143	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	B	147	THR	CA-CB-CG2	-5.32	104.95	112.40
1	B	297	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	B	99	LEU	CB-CG-CD2	-5.26	102.06	111.00
1	B	250	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	B	91	ARG	NE-CZ-NH1	-5.02	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2554	0	2578	16	0
1	B	2510	0	2513	18	0
2	A	25	0	15	1	0
2	B	25	0	15	2	0
3	A	48	0	24	2	0
3	B	48	0	25	4	0
4	A	10	0	4	0	0
5	A	12	0	18	5	0
5	B	12	0	18	0	0
6	B	5	0	0	0	0
7	A	194	0	0	3	0
7	B	179	0	0	0	0
All	All	5622	0	5210	35	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (35) 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:66[A]:ARG:HD3	7:A:525:HOH:O	1.79	0.81
1:A:108:LEU:HA	5:A:405:EDO:H22	1.66	0.76
1:A:301:ARG:HG3	1:A:303:VAL:HG23	1.70	0.74
1:B:278:ARG:O	1:B:281:VAL:HG22	1.97	0.65
1:B:67:SER:O	1:B:71:ASP:HB3	1.98	0.62
1:A:190:GLN:OE1	3:A:402:NAP:H2N	2.05	0.56
1:B:301:ARG:HG3	1:B:303:VAL:HG23	1.89	0.55
1:B:270:LYS:HE2	1:B:272:TYR:CD1	2.41	0.54
1:A:270:LYS:O	3:A:402:NAP:H8A	2.08	0.53
1:B:200:ARG:HD3	1:B:200:ARG:O	2.09	0.53
1:B:195:PRO:HD2	1:B:235:LEU:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:LEU:HD23	5:A:405:EDO:H22	1.94	0.49
2:A:401:IMN:H161	2:A:401:IMN:C10	2.43	0.49
1:A:133[B]:GLU:HB2	7:A:654:HOH:O	2.14	0.48
2:B:401:IMN:H161	2:B:401:IMN:C10	2.44	0.48
1:B:270:LYS:O	3:B:402:NAP:H8A	2.14	0.47
1:B:22:GLY:HA3	3:B:402:NAP:H4D	1.97	0.47
1:B:149:GLU:OE2	1:B:179:LYS:NZ	2.38	0.47
1:B:21:PHE:HB3	1:B:49[A]:ILE:HD13	1.96	0.46
1:A:109:ASP:H	5:A:405:EDO:C1	2.28	0.45
1:A:270:LYS:HE2	1:A:272:TYR:CD1	2.52	0.45
1:B:270:LYS:HB2	3:B:402:NAP:H52N	1.98	0.45
1:B:195:PRO:O	1:B:300:ASN:HA	2.18	0.43
1:B:194:HIS:HB2	1:B:195:PRO:CD	2.49	0.43
1:A:109:ASP:OD2	5:A:405:EDO:H11	2.19	0.42
1:A:109:ASP:H	5:A:405:EDO:H11	1.84	0.42
1:A:248:HIS:HE1	7:A:693:HOH:O	2.02	0.42
1:A:96:ARG:HB3	1:A:97:PRO:HD3	2.02	0.42
1:B:190:GLN:OE1	3:B:402:NAP:H2N	2.20	0.42
1:A:51:SER:HB3	1:A:81:TYR:OH	2.20	0.42
1:B:129:ILE:HD11	2:B:401:IMN:C14	2.50	0.42
1:B:291:GLU:OE2	1:B:294:LYS:HE3	2.20	0.41
1:A:278:ARG:O	1:A:281[A]:VAL:HG22	2.20	0.41
1:B:219:LEU:HD22	1:B:253:ALA:HB1	2.02	0.41
1:A:7:CYS:O	1:B:6[A]:GLN:HG2	2.21	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	318/331 (96%)	312 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	314/331 (95%)	303 (96%)	11 (4%)	0	100	100
All	All	632/662 (96%)	615 (97%)	17 (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	281/293 (96%)	281 (100%)	0	100	100
1	B	273/293 (93%)	270 (99%)	3 (1%)	73	52
All	All	554/586 (94%)	551 (100%)	3 (0%)	88	78

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	71	ASP
1	B	74	VAL
1	B	221	SER

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](#)

12 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	$\# Z > 2$
5	EDO	A	405	-	3,3,3	0.87	0	2,2,2	0.90	0
4	TLA	A	403	-	3,9,9	0.47	0	6,12,12	0.94	0
2	IMN	B	401	-	21,27,27	2.08	7 (33%)	26,39,39	1.24	2 (7%)
5	EDO	B	404	-	3,3,3	1.15	0	2,2,2	0.88	0
5	EDO	B	405	-	3,3,3	0.42	0	2,2,2	1.18	0
2	IMN	A	401	-	21,27,27	2.24	10 (47%)	26,39,39	1.78	6 (23%)
6	PO4	B	406	-	4,4,4	0.70	0	6,6,6	0.47	0
5	EDO	A	404	-	3,3,3	0.94	0	2,2,2	0.92	0
3	NAP	A	402	-	45,52,52	2.48	13 (28%)	56,80,80	1.33	7 (12%)
3	NAP	B	402	-	45,52,52	2.46	13 (28%)	56,80,80	1.76	11 (19%)
5	EDO	A	406	-	3,3,3	0.26	0	2,2,2	0.96	0
5	EDO	B	403	-	3,3,3	0.95	0	2,2,2	0.14	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
5	EDO	A	405	-	-	1/1/1/1	-
4	TLA	A	403	-	-	0/4/12/12	-
2	IMN	B	401	-	-	2/8/14/14	0/3/3/3
5	EDO	B	404	-	-	0/1/1/1	-
5	EDO	B	405	-	-	1/1/1/1	-
2	IMN	A	401	-	-	2/8/14/14	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	404	-	-	0/1/1/1	-
3	NAP	A	402	-	-	2/31/67/67	0/5/5/5
3	NAP	B	402	-	-	4/31/67/67	0/5/5/5
5	EDO	A	406	-	-	1/1/1/1	-
5	EDO	B	403	-	-	0/1/1/1	-

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	NAP	O4D-C1D	9.47	1.54	1.41
3	A	402	NAP	C2A-N3A	6.58	1.42	1.32
3	A	402	NAP	O4D-C1D	6.42	1.50	1.41
3	A	402	NAP	C3N-C7N	-5.96	1.41	1.50
3	B	402	NAP	C2A-N3A	5.56	1.41	1.32
3	A	402	NAP	O3B-C3B	-5.53	1.30	1.43
3	A	402	NAP	O4D-C4D	4.74	1.55	1.45
3	B	402	NAP	PA-O5B	4.68	1.78	1.59
2	A	401	IMN	C10-C9	-4.53	1.42	1.50
3	B	402	NAP	C2N-N1N	4.49	1.40	1.35
2	B	401	IMN	C10-C9	-4.48	1.42	1.50
3	B	402	NAP	C3N-C7N	-4.48	1.43	1.50
3	A	402	NAP	C2D-C1D	4.34	1.60	1.53
2	A	401	IMN	C16-C8	4.27	1.58	1.49
3	B	402	NAP	C2A-N1A	4.11	1.41	1.33
2	B	401	IMN	C-N	-3.89	1.33	1.39
2	B	401	IMN	C2-C1	-3.83	1.34	1.42
3	A	402	NAP	C2A-N1A	3.18	1.39	1.33
2	A	401	IMN	C2-C1	-3.15	1.35	1.42
3	A	402	NAP	C6N-N1N	3.07	1.42	1.35
2	A	401	IMN	C2-C3	3.02	1.42	1.37
3	B	402	NAP	O4B-C1B	2.97	1.45	1.41
3	A	402	NAP	O7N-C7N	2.87	1.29	1.24
2	B	401	IMN	C5-C	-2.78	1.35	1.41
2	A	401	IMN	C5-C	-2.72	1.35	1.41
2	B	401	IMN	C8-C7	-2.70	1.33	1.39
3	B	402	NAP	PN-O5D	2.65	1.70	1.59
3	B	402	NAP	C6N-N1N	2.63	1.41	1.35
2	A	401	IMN	C13-CL	2.62	1.80	1.74
3	B	402	NAP	C7N-N7N	2.42	1.37	1.33
3	A	402	NAP	C3D-C4D	2.42	1.59	1.53
2	B	401	IMN	C13-CL	-2.35	1.69	1.74
3	B	402	NAP	O3D-C3D	2.33	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	IMN	O-C6	2.32	1.49	1.42
2	A	401	IMN	C8-C7	-2.21	1.34	1.39
2	A	401	IMN	C5-C4	2.18	1.41	1.36
3	B	402	NAP	P2B-O2B	2.12	1.63	1.59
2	A	401	IMN	C-N	-2.12	1.36	1.39
3	A	402	NAP	O3D-C3D	-2.11	1.38	1.43
3	B	402	NAP	C5A-C4A	-2.08	1.35	1.40
3	A	402	NAP	PN-O1N	-2.07	1.43	1.50
3	A	402	NAP	O2D-C2D	2.06	1.47	1.43
2	B	401	IMN	C2-C3	2.01	1.40	1.37

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	NAP	N3A-C2A-N1A	-6.53	118.47	128.68
3	B	402	NAP	O2A-PA-O5B	-4.95	84.75	107.75
2	A	401	IMN	C16-C8-N	4.08	127.52	122.37
2	A	401	IMN	C17-C7-C8	-4.04	122.85	126.41
3	A	402	NAP	N3A-C2A-N1A	-3.87	122.64	128.68
3	B	402	NAP	O2A-PA-O1A	3.80	131.03	112.24
3	B	402	NAP	C6N-N1N-C2N	-3.68	118.61	121.97
2	B	401	IMN	C18-C17-C7	-3.53	109.09	115.96
3	B	402	NAP	O2N-PN-O5D	3.51	124.05	107.75
3	A	402	NAP	C5N-C4N-C3N	3.40	124.37	120.34
2	A	401	IMN	C18-C17-C7	-3.39	109.36	115.96
3	B	402	NAP	O2N-PN-O1N	3.25	128.30	112.24
3	A	402	NAP	O2N-PN-O1N	2.90	126.58	112.24
2	A	401	IMN	C6-O-C3	-2.66	111.73	117.51
3	B	402	NAP	C2D-C3D-C4D	-2.54	97.71	102.64
3	B	402	NAP	C3N-C2N-N1N	2.47	122.84	120.43
2	A	401	IMN	C14-C13-CL	2.39	123.10	119.35
3	A	402	NAP	O7N-C7N-C3N	2.37	122.47	119.63
3	A	402	NAP	C2N-C3N-C4N	-2.36	115.58	118.26
3	A	402	NAP	O2A-PA-O5B	-2.36	96.79	107.75
3	B	402	NAP	C3D-C2D-C1D	2.36	104.53	100.98
2	A	401	IMN	C2-C1-C	2.28	122.38	119.65
3	B	402	NAP	C1B-N9A-C4A	-2.25	122.69	126.64
3	A	402	NAP	O2B-P2B-O1X	-2.20	100.89	109.39
3	B	402	NAP	O5B-PA-O1A	-2.15	100.67	109.07
2	B	401	IMN	C16-C8-N	2.14	125.07	122.37

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	402	NAP	PA-O3-PN-O5D
3	B	402	NAP	C5D-O5D-PN-O2N
5	B	405	EDO	O1-C1-C2-O2
5	A	406	EDO	O1-C1-C2-O2
3	A	402	NAP	PA-O3-PN-O5D
2	B	401	IMN	C11-C10-C9-N
3	B	402	NAP	C5D-O5D-PN-O3
3	B	402	NAP	PN-O3-PA-O2A
3	A	402	NAP	C4D-C5D-O5D-PN
2	B	401	IMN	C15-C10-C9-N
2	A	401	IMN	C15-C10-C9-N
2	A	401	IMN	C4-C3-O-C6
5	A	405	EDO	O1-C1-C2-O2

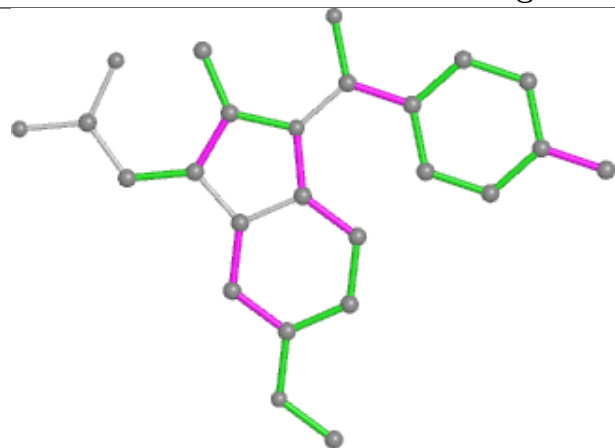
There are no ring outliers.

5 monomers are involved in 14 short contacts:

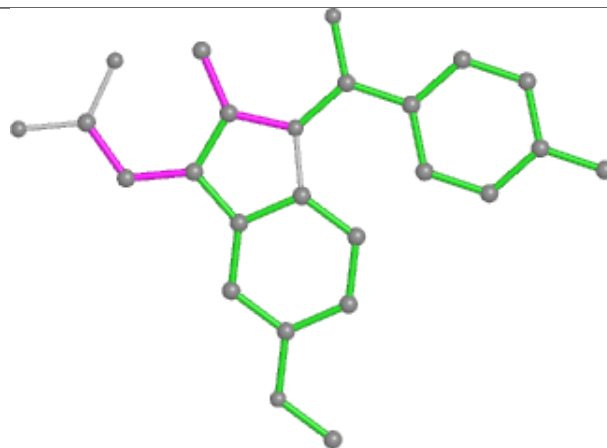
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	405	EDO	5	0
2	B	401	IMN	2	0
2	A	401	IMN	1	0
3	A	402	NAP	2	0
3	B	402	NAP	4	0

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.

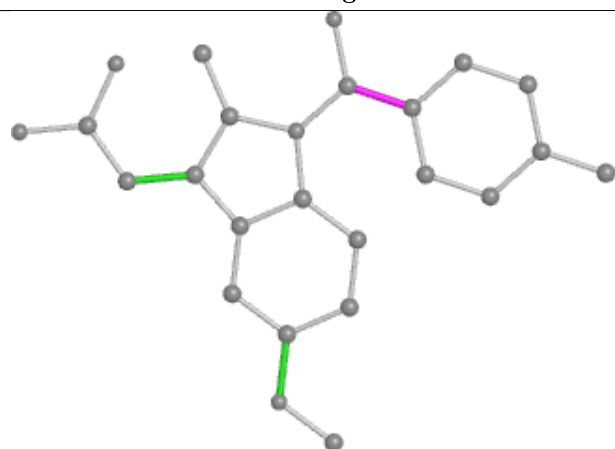
Ligand IMN B 401



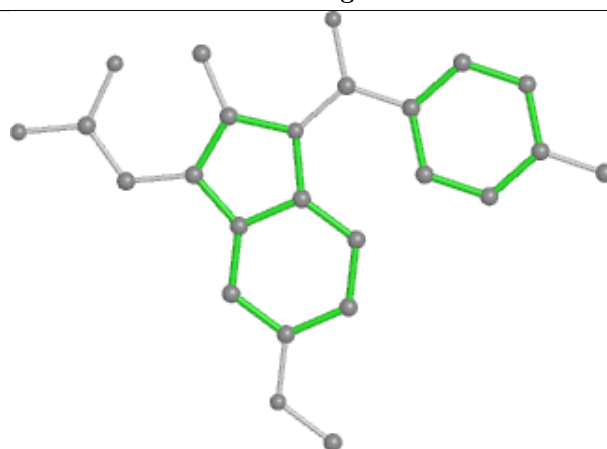
Bond lengths



Bond angles

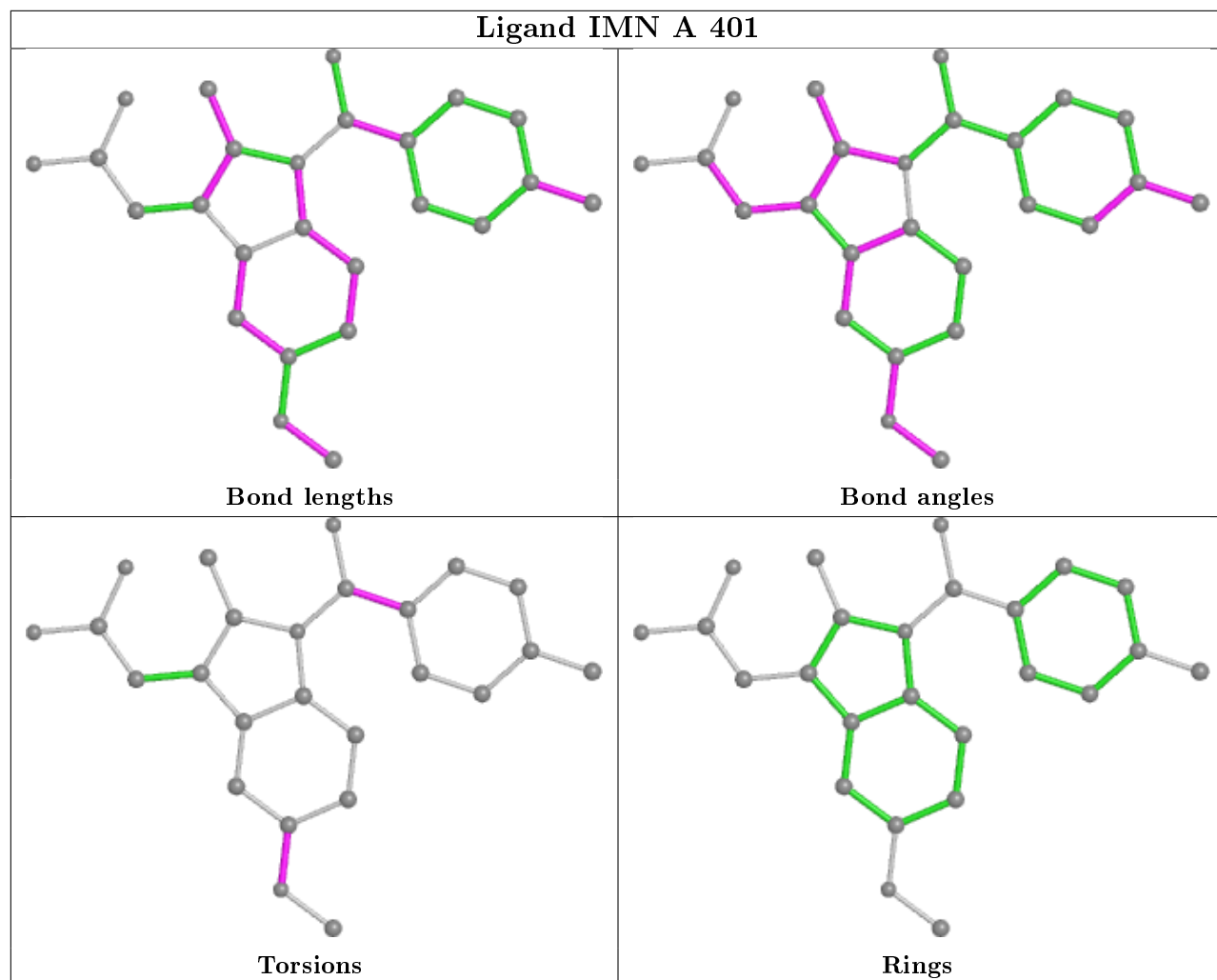


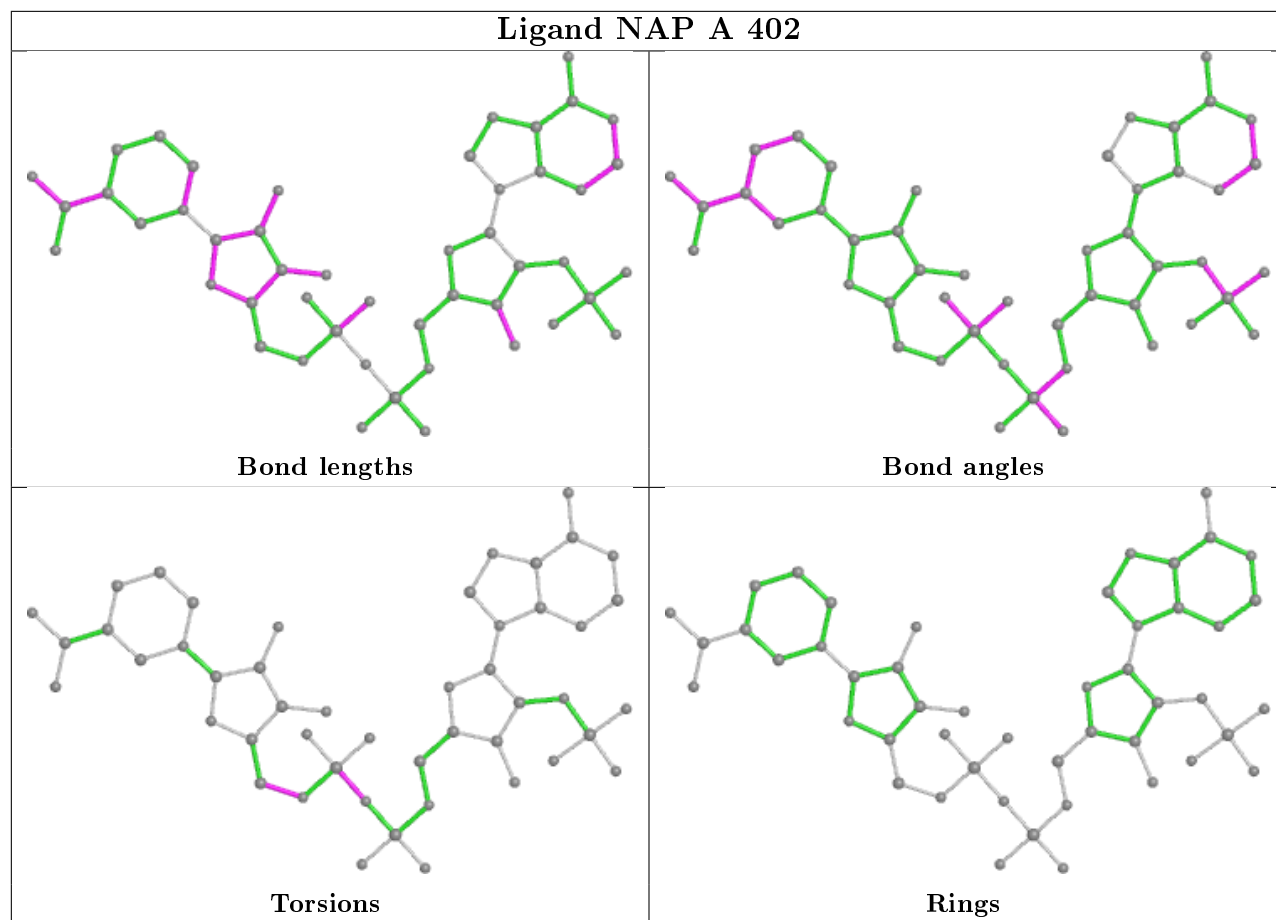
Torsions

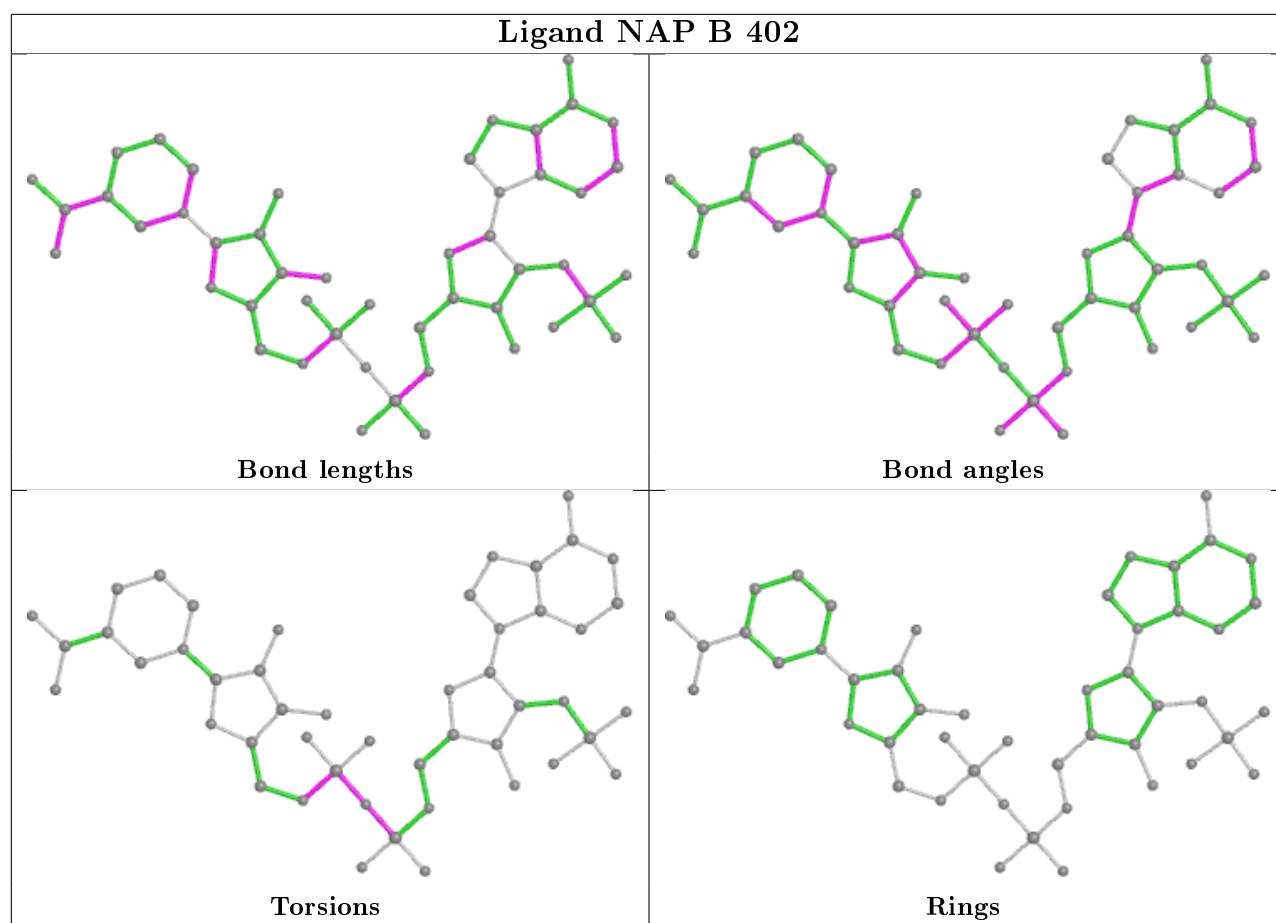


Rings

Ligand IMN A 401







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, 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	316/331 (95%)	-0.04	12 (3%) 40 45	14, 23, 42, 58	9 (2%)
1	B	314/331 (94%)	0.23	32 (10%) 6 6	9, 23, 54, 77	5 (1%)
All	All	630/662 (95%)	0.10	44 (6%) 16 17	9, 23, 49, 77	14 (2%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	29	VAL	5.8
1	B	230	PRO	5.0
1	B	226	PRO	4.7
1	B	228	VAL	4.5
1	A	231	ASN	4.5
1	B	227	TRP	4.5
1	A	227	TRP	4.4
1	A	302	ASN	4.4
1	A	230	PRO	4.2
1	B	26	PRO	4.2
1	B	27	ALA	4.1
1	B	231	ASN	4.1
1	B	30	PRO	4.0
1	B	232	SER	3.7
1	B	229	ASP	3.5
1	A	226	PRO	3.4
1	A	27	ALA	3.4
1	B	234	VAL	3.4
1	B	70	ALA	3.4
1	A	229	ASP	3.2
1	B	303	VAL	3.1
1	A	225	GLU	3.1
1	B	28	GLU	3.1
1	A	232	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	237	GLU	3.0
1	B	233	PRO	2.9
1	B	31	LYS	2.9
1	B	242	CYS	2.8
1	B	298	GLY	2.8
1	B	32	SER	2.8
1	A	180	PRO	2.7
1	B	3	SER	2.6
1	B	249	LYS	2.6
1	B	301	ARG	2.6
1	B	65	ILE	2.6
1	B	38	VAL	2.3
1	B	72	GLY	2.3
1	A	239	PRO	2.3
1	B	243	ALA	2.2
1	A	246	LYS	2.2
1	B	239	PRO	2.2
1	B	273	ASN	2.2
1	B	49[A]	ILE	2.1
1	B	73	SER	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	IMN	B	401	25/25	0.78	0.16	33,50,73,81	0
4	TLA	A	403	10/10	0.82	0.16	40,45,56,57	0
2	IMN	A	401	25/25	0.88	0.10	24,31,54,65	0

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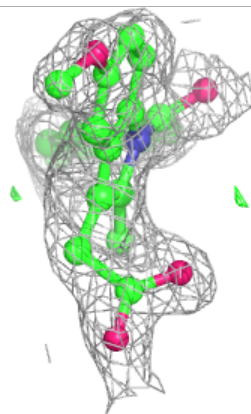
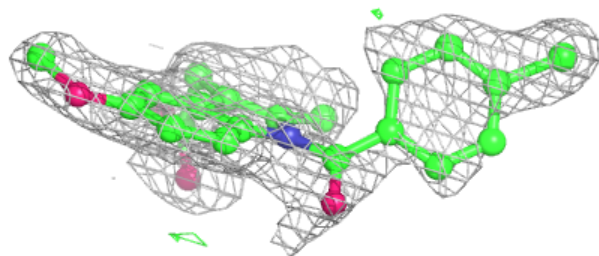
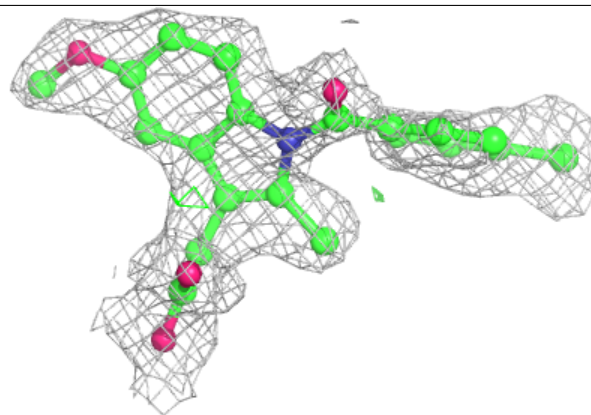
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	EDO	B	404	4/4	0.89	0.10	25,26,29,29	0
5	EDO	B	405	4/4	0.90	0.24	35,39,42,46	0
6	PO4	B	406	5/5	0.92	0.24	53,58,72,75	5
3	NAP	B	402	48/48	0.94	0.13	20,41,58,65	0
5	EDO	A	406	4/4	0.94	0.09	36,42,42,43	0
5	EDO	A	405	4/4	0.95	0.07	20,32,34,52	0
5	EDO	B	403	4/4	0.96	0.07	19,21,22,25	0
3	NAP	A	402	48/48	0.97	0.07	15,23,29,39	0
5	EDO	A	404	4/4	0.97	0.08	17,18,22,23	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.

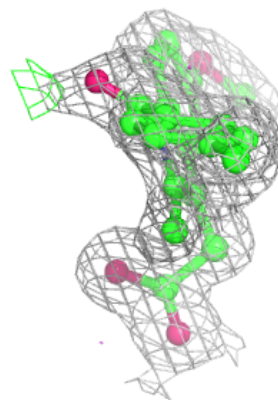
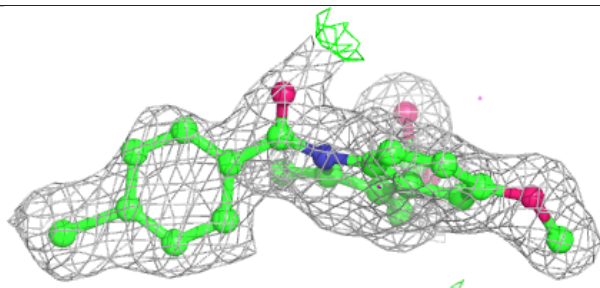
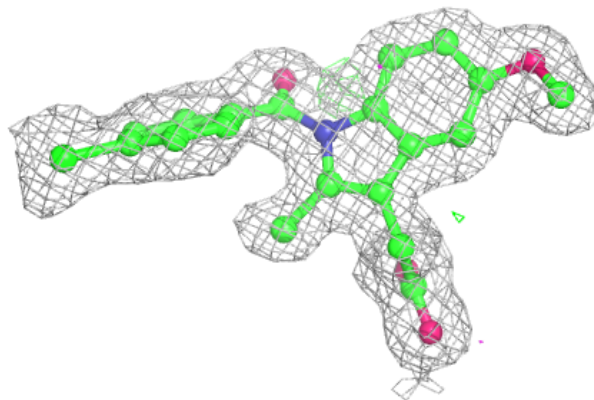
Electron density around IMN B 401:

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

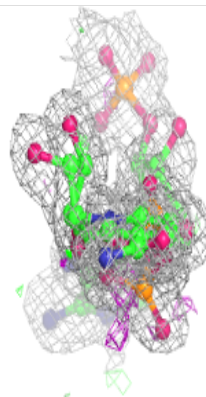
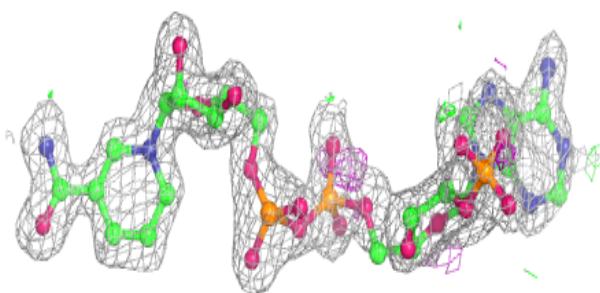
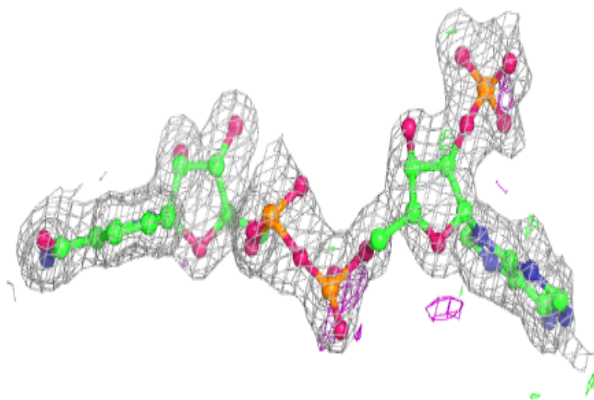


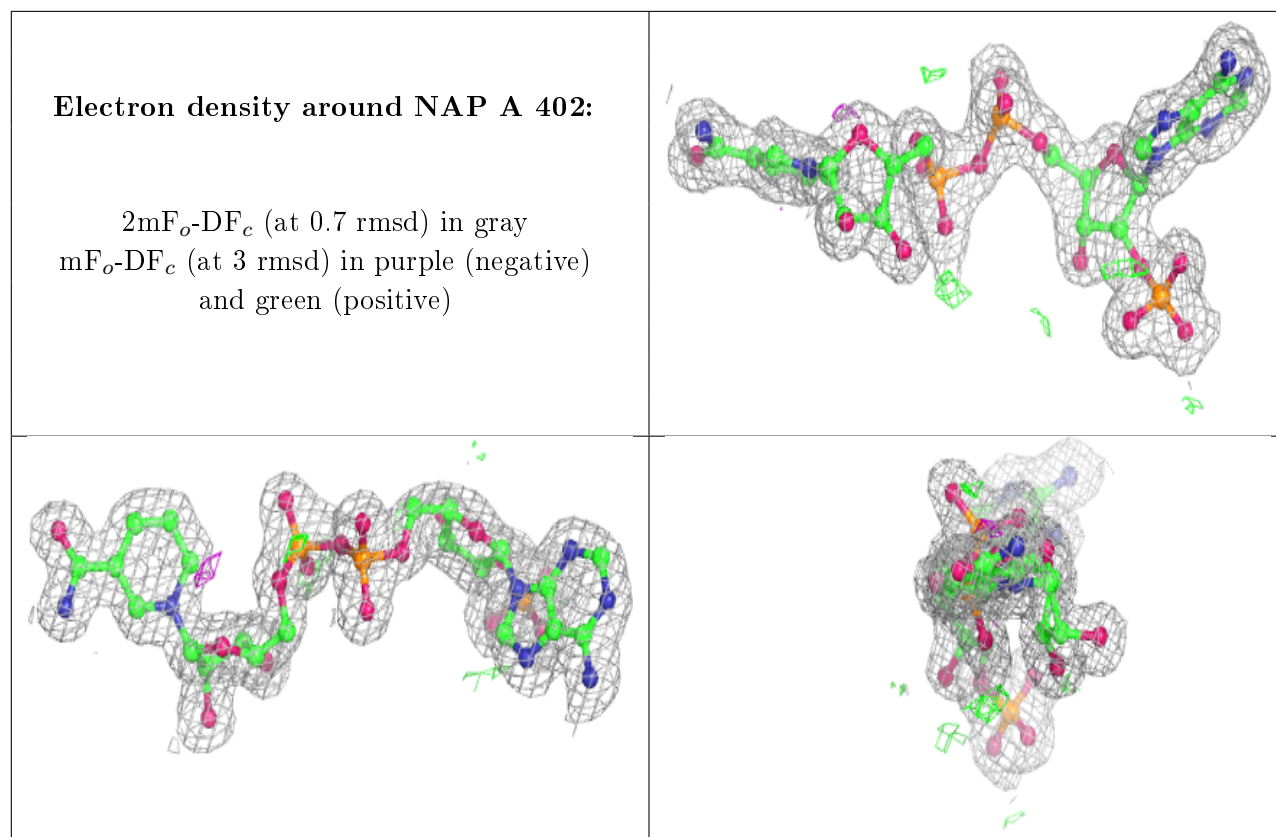
Electron density around IMN A 401:

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

**Electron density around NAP 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.