



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 04:37 am BST

PDB ID : 3NDV  
Title : Crystal structure of the N-terminal beta-aminopeptidase BapA in complex with ampicillin  
Authors : Merz, T.; Heck, T.; Geueke, B.; Kohler, H.-P.E.; Gruetter, M.G.  
Deposited on : 2010-06-08  
Resolution : 1.70 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

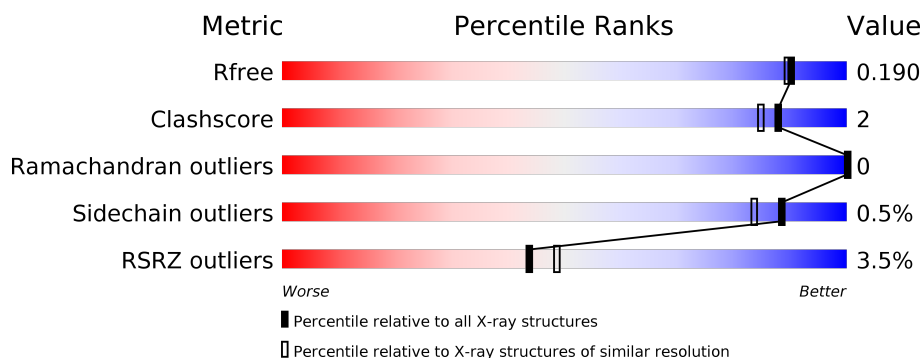
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	373	<div> <div>3%</div> <div> <div></div> <div>94%</div> <div>5%</div> </div> </div>
1	B	373	<div> <div>4%</div> <div> <div></div> <div>94%</div> <div></div> </div> </div>
1	C	373	<div> <div>4%</div> <div> <div></div> <div>93%</div> <div>5%</div> </div> </div>
1	D	373	<div> <div>3%</div> <div> <div></div> <div>93%</div> <div>5%</div> </div> </div>

## 2 Entry composition [i](#)

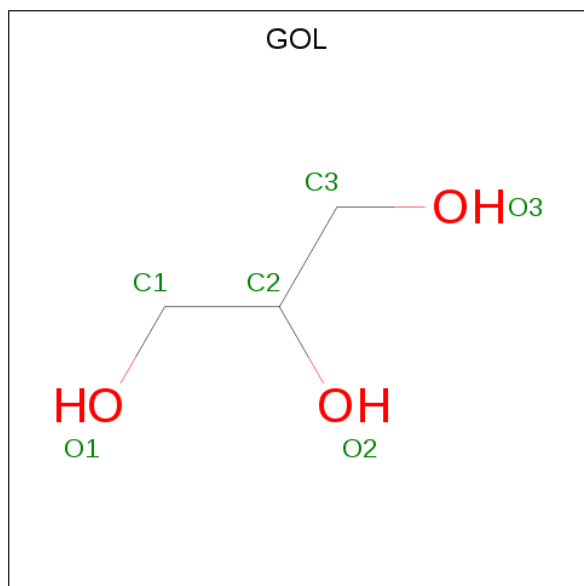
There are 5 unique types of molecules in this entry. The entry contains 11974 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Beta-peptidyl aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	2	0
			2671	1671	485	505	10			
1	B	365	Total	C	N	O	S	0	2	0
			2660	1663	485	502	10			
1	C	366	Total	C	N	O	S	0	3	0
			2680	1675	491	504	10			
1	D	367	Total	C	N	O	S	0	0	0
			2657	1663	481	503	10			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



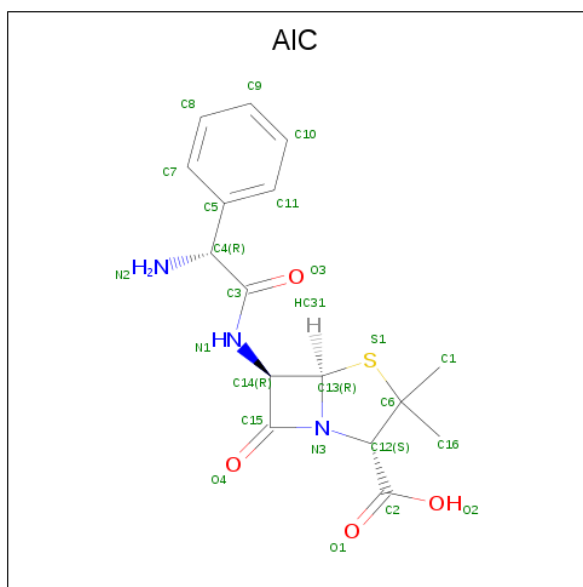
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

*Continued on next page...*

Continued from previous page...

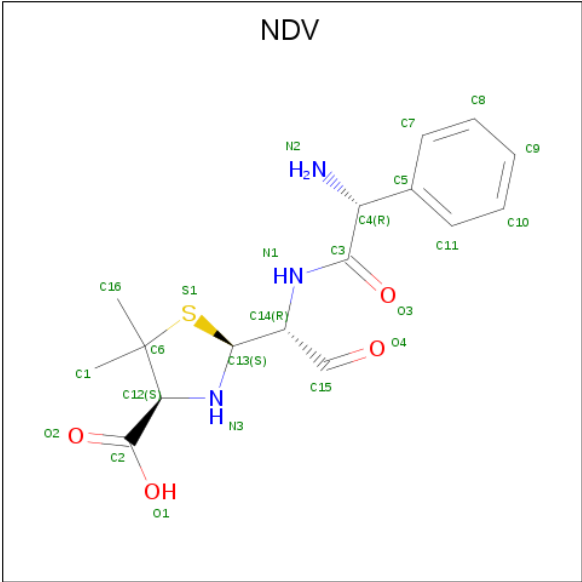
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is (2S,5R,6R)-6-{[(2R)-2-AMINO-2-PHENYLETHANOYL]AMINO}-3,3-DIMETHYL-7-OXO-4-THIA-1-AZABICYCLO[3.2.0]HEPTANE-2-CARBOXYLIC ACID (three-letter code: AIC) (formula: C<sub>16</sub>H<sub>19</sub>N<sub>3</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			24	16	3	4	1		
3	B	1	Total	C	N	O	S	0	0
			24	16	3	4	1		
3	C	1	Total	C	N	O	S	0	0
			24	16	3	4	1		
3	D	1	Total	C	N	O	S	0	0
			24	16	3	4	1		

- Molecule 4 is (2S,4S)-2-[(1R)-1-{[(2R)-2-amino-2-phenylacetyl]amino}-2-oxoethyl]-5,5-dimethyl-1,3-thiazolidine-4-carboxylic acid (three-letter code: NDV) (formula: C<sub>16</sub>H<sub>21</sub>N<sub>3</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			24	16	3	4	1		
4	D	1	Total	C	N	O	S	0	0
			24	16	3	4	1		

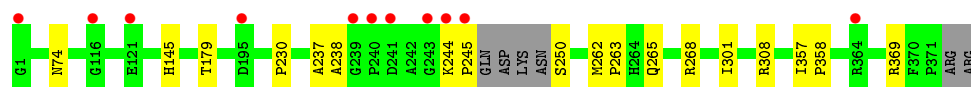
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	291	Total	O	0	0
			291	291		
5	B	302	Total	O	0	0
			302	302		
5	C	264	Total	O	0	0
			264	264		
5	D	281	Total	O	0	0
			281	281		

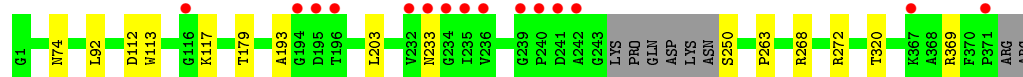
### 3 Residue-property plots [i](#)

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.

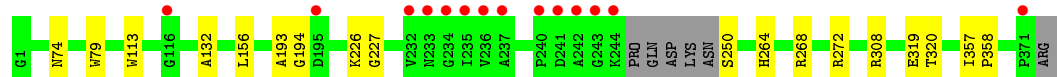
- Molecule 1: Beta-peptidyl aminopeptidase



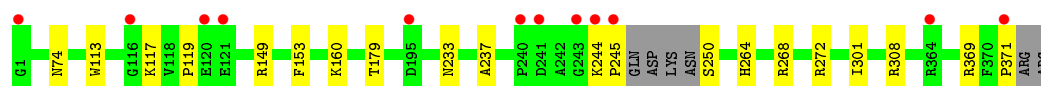
- Molecule 1: Beta-peptidyl aminopeptidase



- Molecule 1: Beta-peptidyl aminopeptidase



- Molecule 1: Beta-peptidyl aminopeptidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.90 Å   96.40 Å   101.50 Å 90.00°   108.40°   90.00°	Depositor
Resolution (Å)	48.84 – 1.70 48.83 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.84-1.70) 98.9 (48.83-1.70)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 1.70 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, $R_{free}$	0.167   ,   0.192 0.164   ,   0.190	Depositor DCC
$R_{free}$ test set	6884 reflections (4.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	11.6	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 58.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11974	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.02% 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: GOL, AIC, NDV

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	0.35	0/2721	0.54	0/3695
1	B	0.34	0/2709	0.52	0/3678
1	C	0.40	0/2729	0.54	0/3703
1	D	0.37	1/2704 (0.0%)	0.54	0/3673
All	All	0.37	1/10863 (0.0%)	0.53	0/14749

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	119	PRO	C-N	-5.10	1.22	1.34

There are no bond angle outliers.

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	2671	0	2689	15	0
1	B	2660	0	2677	12	0
1	C	2680	0	2702	14	0
1	D	2657	0	2672	14	0
2	A	6	0	8	0	0
2	B	12	0	16	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	6	0	8	0	0
3	A	24	0	19	1	0
3	B	24	0	19	1	0
3	C	24	0	19	1	0
3	D	24	0	19	1	0
4	A	24	0	20	1	0
4	D	24	0	20	1	0
5	A	291	0	0	1	0
5	B	302	0	0	0	0
5	C	264	0	0	2	0
5	D	281	0	0	2	0
All	All	11974	0	10888	44	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 2.

All (44) 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:74:ASN:HD21	1:C:268:ARG:HH21	1.10	0.95
1:A:268:ARG:HH21	1:D:74:ASN:HD21	1.16	0.91
1:B:268:ARG:HH21	1:C:74:ASN:HD21	1.18	0.90
1:A:74:ASN:HD21	1:D:268:ARG:HH21	1.14	0.88
1:A:262:MET:H	1:A:265:GLN:HE21	1.44	0.66
1:A:262:MET:H	1:A:265:GLN:NE2	1.96	0.63
1:A:237:ALA:O	4:A:376:NDV:H14	2.01	0.60
1:C:319:GLU:HB2	5:C:867:HOH:O	2.02	0.59
1:A:308:ARG:HD3	5:A:1099:HOH:O	2.01	0.59
1:D:237:ALA:O	4:D:375:NDV:H14	2.05	0.56
1:A:145:HIS:HE1	1:B:112:ASP:OD1	1.88	0.55
1:B:369[B]:ARG:O	1:B:369[B]:ARG:HD2	2.08	0.53
1:A:250:SER:OG	3:A:375:AIC:C3	2.57	0.53
1:A:369[B]:ARG:CZ	1:D:369:ARG:HD2	2.40	0.51
1:C:193:ALA:HB1	1:C:320:THR:HG23	1.92	0.51
1:C:250:SER:OG	3:C:375:AIC:C3	2.59	0.51
1:B:272:ARG:HH12	1:C:74:ASN:ND2	2.11	0.49
1:D:160:LYS:HE2	5:D:483:HOH:O	2.13	0.49
1:B:250:SER:OG	3:B:376:AIC:C3	2.61	0.48
1:D:250:SER:OG	3:D:374:AIC:C3	2.62	0.48
1:C:226:LYS:HD2	1:C:227:GLY:N	2.28	0.48
1:D:244:LYS:HB3	1:D:245:PRO:HD2	1.95	0.47

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:LYS:HB3	1:A:245:PRO:HD2	1.97	0.47
1:C:194:GLY:HA2	1:C:319:GLU:CD	2.36	0.46
1:B:113:TRP:NE1	1:B:117:LYS:HE2	2.31	0.46
1:B:74:ASN:ND2	1:C:272:ARG:HH12	2.14	0.46
1:A:263:PRO:HG2	1:C:264:HIS:CE1	2.52	0.45
1:D:308:ARG:HD3	5:D:1135:HOH:O	2.17	0.44
1:B:263:PRO:HG2	1:D:264:HIS:CE1	2.53	0.43
1:B:92:LEU:N	1:B:92:LEU:HD22	2.33	0.43
1:C:79:TRP:CG	1:C:132:ALA:HB2	2.53	0.43
1:C:357:ILE:HA	1:C:358:PRO:HD3	1.93	0.42
1:A:230:PRO:HD2	1:A:238:ALA:HB3	2.01	0.42
1:A:74:ASN:ND2	1:D:272:ARG:HH12	2.18	0.42
1:D:113:TRP:NE1	1:D:117:LYS:HE2	2.34	0.42
1:B:203:LEU:HD23	1:B:203:LEU:C	2.41	0.41
1:D:301:ILE:N	1:D:301:ILE:HD12	2.34	0.41
1:A:301:ILE:N	1:A:301:ILE:HD12	2.36	0.41
1:A:357:ILE:HA	1:A:358:PRO:HD3	1.95	0.41
1:D:149:ARG:HD2	1:D:153:PHE:CZ	2.56	0.41
1:C:113:TRP:CG	1:C:156:LEU:HD13	2.56	0.41
1:D:369:ARG:C	1:D:371:PRO:HD3	2.40	0.41
1:C:308[A]:ARG:NH2	5:C:817:HOH:O	2.47	0.41
1:B:193:ALA:HB1	1:B:320:THR:HG23	2.03	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	365/373 (98%)	357 (98%)	8 (2%)	0	100	100
1	B	363/373 (97%)	356 (98%)	7 (2%)	0	100	100
1	C	365/373 (98%)	359 (98%)	6 (2%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	363/373 (97%)	355 (98%)	8 (2%)	0	100	100
All	All	1456/1492 (98%)	1427 (98%)	29 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	273/277 (99%)	272 (100%)	1 (0%)	91	87
1	B	271/277 (98%)	269 (99%)	2 (1%)	84	77
1	C	273/277 (99%)	273 (100%)	0	100	100
1	D	271/277 (98%)	269 (99%)	2 (1%)	84	77
All	All	1088/1108 (98%)	1083 (100%)	5 (0%)	88	83

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	179	THR
1	B	179	THR
1	B	233	ASN
1	D	179	THR
1	D	233	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	145	HIS
1	A	220	GLN
1	A	265	GLN
1	B	74	ASN
1	B	220	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	74	ASN
1	D	74	ASN
1	D	212	ASN
1	D	220	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

10 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	GOL	B	374	-	5,5,5	0.30	0	5,5,5	0.52	0
2	GOL	A	374	-	5,5,5	0.31	0	5,5,5	0.50	0
2	GOL	C	374	-	5,5,5	0.29	0	5,5,5	0.60	0
3	AIC	B	376	-	21,26,26	5.24	12 (57%)	31,40,40	2.92	9 (29%)
4	NDV	A	376	-	16,25,25	3.89	4 (25%)	20,36,36	1.54	4 (20%)
2	GOL	B	375	-	5,5,5	0.35	0	5,5,5	0.33	0
4	NDV	D	375	-	16,25,25	3.91	4 (25%)	20,36,36	1.50	3 (15%)
3	AIC	D	374	-	21,26,26	5.24	11 (52%)	31,40,40	2.93	9 (29%)
3	AIC	C	375	-	21,26,26	5.29	11 (52%)	31,40,40	2.92	8 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	AIC	A	375	-	21,26,26	5.24	11 (52%)	31,40,40	2.91	9 (29%)

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	GOL	B	374	-	-	0/4/4/4	-
2	GOL	A	374	-	-	2/4/4/4	-
2	GOL	C	374	-	-	0/4/4/4	-
3	AIC	B	376	-	-	0/12/47/47	0/3/3/3
4	NDV	A	376	-	-	6/12/37/37	0/2/2/2
2	GOL	B	375	-	-	0/4/4/4	-
4	NDV	D	375	-	-	6/12/37/37	0/2/2/2
3	AIC	D	374	-	-	0/12/47/47	0/3/3/3
3	AIC	C	375	-	-	0/12/47/47	0/3/3/3
3	AIC	A	375	-	-	0/12/47/47	0/3/3/3

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	375	AIC	C13-C14	-12.58	1.31	1.56
3	B	376	AIC	C13-C14	-12.50	1.31	1.56
3	A	375	AIC	C13-C14	-12.41	1.31	1.56
3	D	374	AIC	C13-C14	-12.40	1.31	1.56
3	A	375	AIC	C12-N3	-12.28	1.38	1.47
3	D	374	AIC	C12-N3	-12.11	1.38	1.47
3	C	375	AIC	C12-N3	-11.99	1.38	1.47
3	B	376	AIC	C12-N3	-11.78	1.38	1.47
3	C	375	AIC	C13-S1	-11.67	1.62	1.81
3	B	376	AIC	C13-S1	-11.49	1.62	1.81
3	D	374	AIC	C13-S1	-11.43	1.62	1.81
3	A	375	AIC	C13-S1	-11.27	1.62	1.81
4	D	375	NDV	C13-S1	-9.11	1.62	1.84
4	A	376	NDV	C13-S1	-9.05	1.63	1.84
4	D	375	NDV	C6-S1	-8.33	1.68	1.85
4	A	376	NDV	C6-S1	-8.24	1.68	1.85
4	A	376	NDV	C12-N3	7.79	1.57	1.46
4	D	375	NDV	C12-N3	7.77	1.57	1.46
3	D	374	AIC	C13-N3	-6.50	1.32	1.47

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	376	AIC	C13-N3	-6.49	1.32	1.47
3	C	375	AIC	C13-N3	-6.48	1.32	1.47
3	A	375	AIC	C13-N3	-6.40	1.33	1.47
3	B	376	AIC	C14-C15	-4.92	1.42	1.54
4	D	375	NDV	C3-N1	4.84	1.44	1.34
3	A	375	AIC	C3-N1	4.80	1.44	1.34
3	C	375	AIC	C3-N1	4.80	1.44	1.34
3	C	375	AIC	C14-C15	-4.77	1.42	1.54
3	A	375	AIC	C14-C15	-4.75	1.42	1.54
4	A	376	NDV	C3-N1	4.73	1.44	1.34
3	D	374	AIC	C3-N1	4.63	1.44	1.34
3	D	374	AIC	C14-C15	-4.63	1.42	1.54
3	B	376	AIC	C3-N1	4.52	1.44	1.34
3	C	375	AIC	C6-C12	-3.40	1.49	1.56
3	B	376	AIC	C6-C12	-3.39	1.49	1.56
3	A	375	AIC	C6-C12	-3.35	1.49	1.56
3	D	374	AIC	C6-C12	-3.30	1.49	1.56
3	B	376	AIC	C10-C11	3.25	1.45	1.38
3	D	374	AIC	C10-C11	3.15	1.45	1.38
3	B	376	AIC	C7-C5	3.11	1.44	1.39
3	A	375	AIC	C7-C5	3.10	1.44	1.39
3	C	375	AIC	C7-C5	3.09	1.44	1.39
3	D	374	AIC	C7-C5	3.08	1.44	1.39
3	A	375	AIC	C10-C11	3.02	1.45	1.38
3	C	375	AIC	C10-C11	2.96	1.45	1.38
3	C	375	AIC	C11-C5	2.81	1.43	1.39
3	D	374	AIC	C8-C7	2.76	1.44	1.38
3	B	376	AIC	C8-C7	2.72	1.44	1.38
3	C	375	AIC	C8-C7	2.63	1.44	1.38
3	D	374	AIC	C11-C5	2.62	1.43	1.39
3	A	375	AIC	C8-C7	2.57	1.44	1.38
3	B	376	AIC	C11-C5	2.52	1.43	1.39
3	A	375	AIC	C11-C5	2.36	1.42	1.39
3	B	376	AIC	C15-N3	2.19	1.42	1.37

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	374	AIC	C13-N3-C12	10.67	130.55	117.26
3	A	375	AIC	C13-N3-C12	10.61	130.48	117.26
3	C	375	AIC	C13-N3-C12	10.23	130.01	117.26
3	B	376	AIC	C13-N3-C12	9.97	129.68	117.26

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	375	AIC	C13-N3-C15	-5.79	86.44	93.93
3	B	376	AIC	C13-N3-C15	-5.74	86.51	93.93
3	B	376	AIC	O4-C15-N3	5.48	139.49	131.75
3	D	374	AIC	C13-N3-C15	-5.46	86.87	93.93
3	A	375	AIC	C13-N3-C15	-5.43	86.92	93.93
3	D	374	AIC	C14-C13-N3	5.20	94.67	87.98
3	C	375	AIC	C14-C13-N3	5.16	94.61	87.98
3	B	376	AIC	C14-C13-N3	5.13	94.58	87.98
3	C	375	AIC	O4-C15-N3	5.11	138.96	131.75
3	A	375	AIC	C14-C13-N3	4.90	94.29	87.98
3	D	374	AIC	S1-C13-N3	-4.63	98.88	105.10
4	D	375	NDV	C4-C3-N1	4.62	120.40	114.78
3	B	376	AIC	S1-C13-N3	-4.57	98.96	105.10
3	C	375	AIC	S1-C13-N3	-4.48	99.08	105.10
4	A	376	NDV	C4-C3-N1	4.39	120.12	114.78
3	B	376	AIC	C14-C15-N3	-4.33	85.96	91.87
3	A	375	AIC	S1-C13-N3	-4.30	99.32	105.10
3	C	375	AIC	C14-C15-N3	-4.29	86.01	91.87
3	A	375	AIC	C14-C15-N3	-4.29	86.01	91.87
3	D	374	AIC	C14-C15-N3	-4.14	86.21	91.87
3	A	375	AIC	O4-C15-N3	4.07	137.49	131.75
3	D	374	AIC	C6-C12-N3	-3.75	100.83	106.49
3	A	375	AIC	C6-C12-N3	-3.71	100.89	106.49
3	C	375	AIC	C6-C12-N3	-3.65	100.98	106.49
3	D	374	AIC	O4-C15-N3	3.61	136.84	131.75
3	B	376	AIC	C6-C12-N3	-3.41	101.34	106.49
3	B	376	AIC	C14-C13-S1	3.04	124.18	119.40
3	A	375	AIC	C14-C13-S1	2.81	123.81	119.40
3	D	374	AIC	C14-C13-S1	2.64	123.54	119.40
3	C	375	AIC	C14-C13-S1	2.59	123.46	119.40
4	A	376	NDV	C6-S1-C13	2.41	99.16	93.99
3	A	375	AIC	C11-C5-C7	2.36	121.24	118.29
4	D	375	NDV	C6-S1-C13	2.34	99.00	93.99
4	D	375	NDV	O3-C3-N1	-2.20	118.85	122.93
4	A	376	NDV	O3-C3-N1	-2.20	118.85	122.93
3	D	374	AIC	C11-C5-C7	2.17	121.00	118.29
4	A	376	NDV	O4-C15-C14	-2.17	118.79	124.83
3	B	376	AIC	C4-C3-N1	2.02	117.23	114.78

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	376	NDV	O3-C3-N1-C14
4	A	376	NDV	C15-C14-N1-C3
4	D	375	NDV	O3-C3-N1-C14
4	D	375	NDV	C15-C14-N1-C3
4	A	376	NDV	C4-C3-N1-C14
4	D	375	NDV	C4-C3-N1-C14
4	A	376	NDV	C3-C4-C5-C7
4	A	376	NDV	C3-C4-C5-C11
4	D	375	NDV	C3-C4-C5-C7
4	D	375	NDV	C3-C4-C5-C11
2	A	374	GOL	C1-C2-C3-O3
2	A	374	GOL	O2-C2-C3-O3
4	A	376	NDV	C13-C14-N1-C3
4	D	375	NDV	C13-C14-N1-C3

There are no ring outliers.

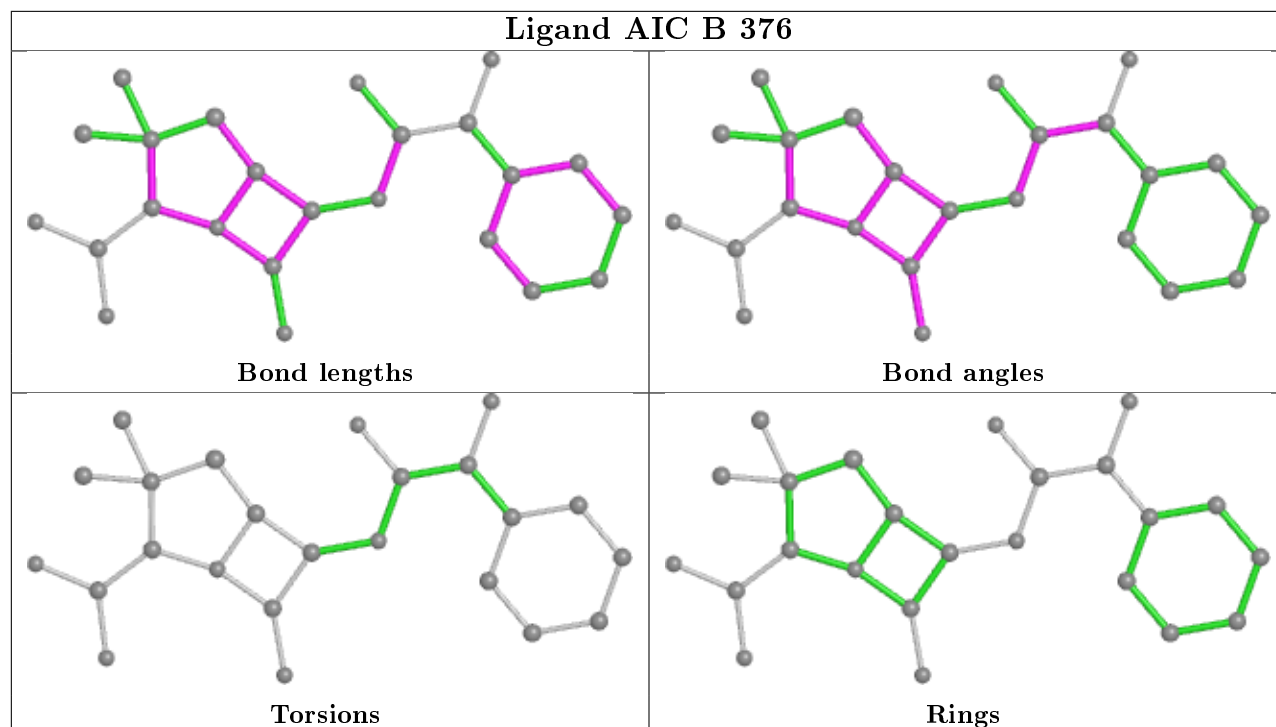
6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	376	AIC	1	0
4	A	376	NDV	1	0
4	D	375	NDV	1	0
3	D	374	AIC	1	0
3	C	375	AIC	1	0
3	A	375	AIC	1	0

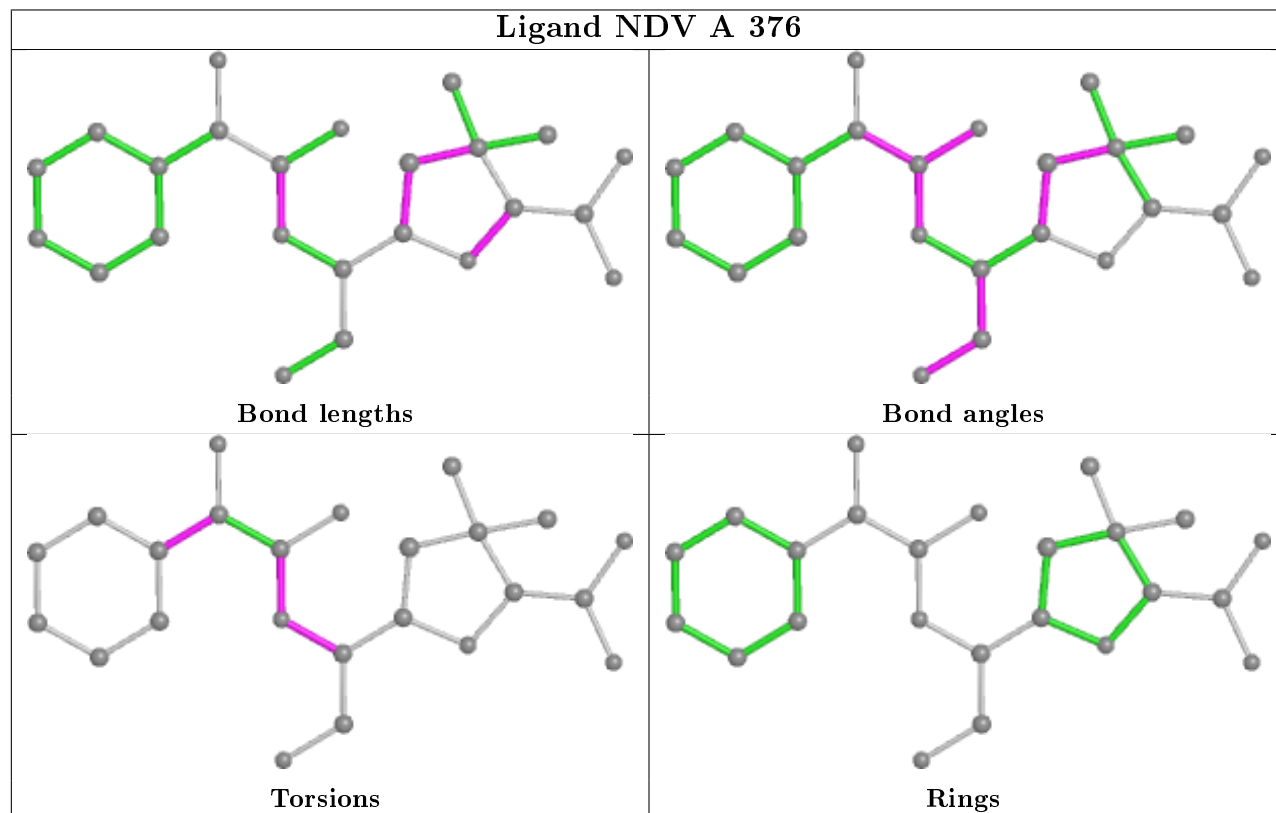
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

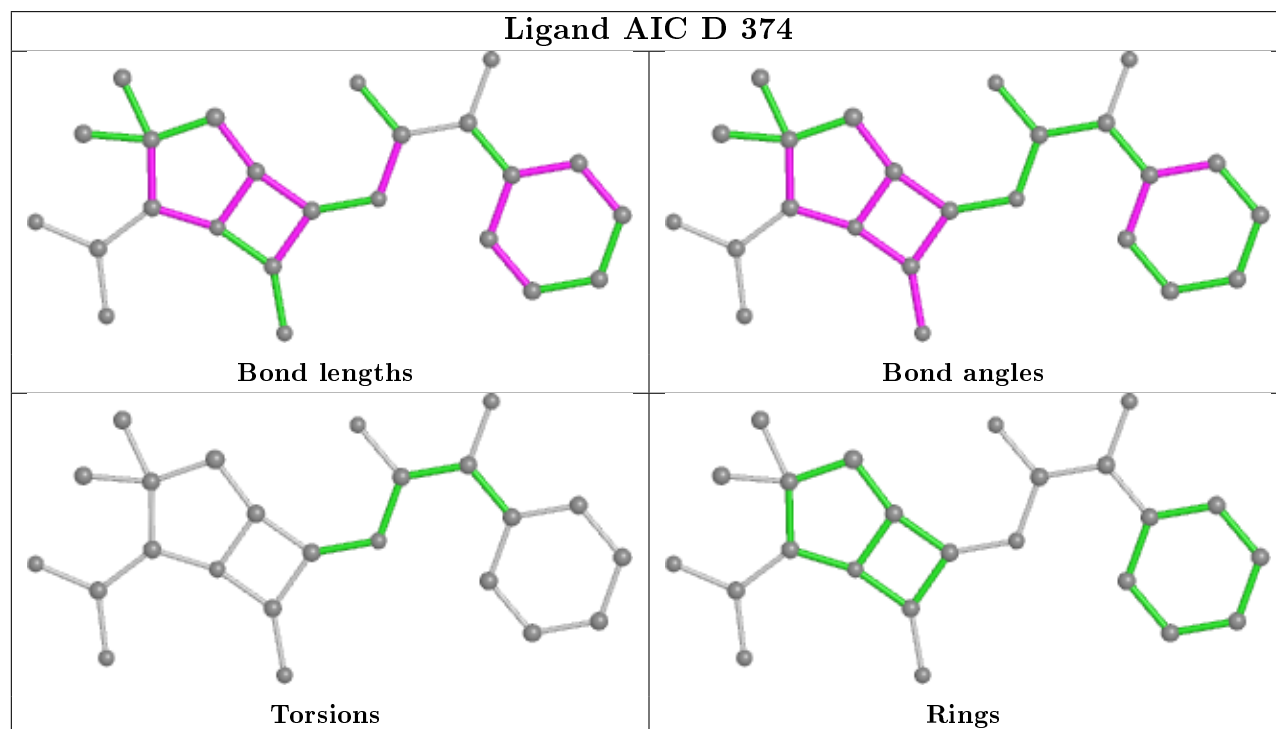
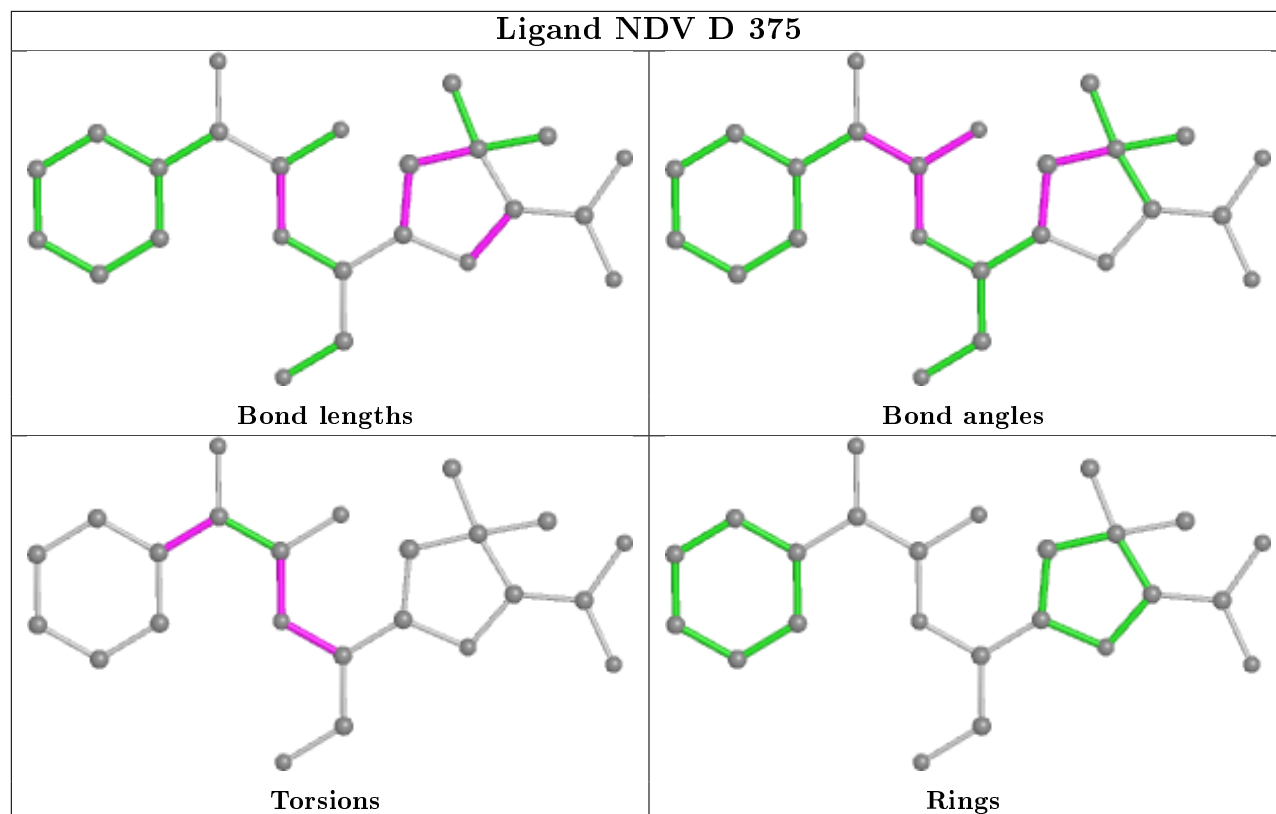


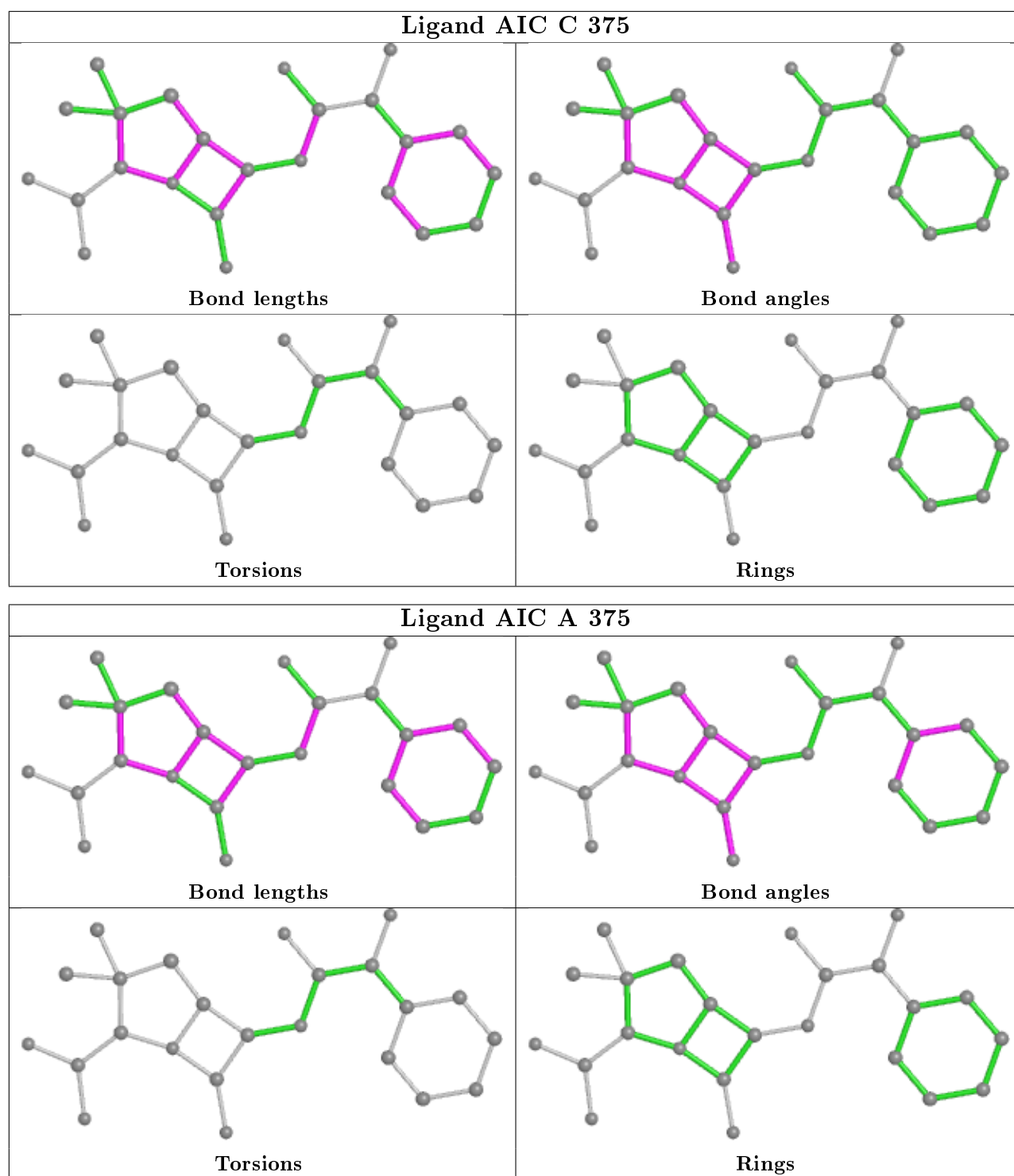
## Ligand AIC B 376



## Ligand NDV A 376







## 5.7 Other polymers ⓘ

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 ⓘ

### 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	367/373 (98%)	-0.29	11 (2%)	50 54	5, 10, 30, 46	0
1	B	365/373 (97%)	-0.10	15 (4%)	37 41	6, 11, 34, 61	0
1	C	366/373 (98%)	-0.11	14 (3%)	40 45	6, 12, 35, 61	0
1	D	367/373 (98%)	-0.26	12 (3%)	46 51	5, 10, 32, 49	0
All	All	1465/1492 (98%)	-0.19	52 (3%)	44 49	5, 11, 33, 61	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	195	ASP	7.5
1	C	235	ILE	7.1
1	B	242	ALA	6.7
1	B	233	ASN	6.7
1	B	235	ILE	5.8
1	C	234	GLY	5.5
1	C	233	ASN	5.4
1	C	242	ALA	5.1
1	B	234	GLY	5.1
1	C	243	GLY	4.8
1	B	240	PRO	4.6
1	C	195	ASP	4.6
1	C	240	PRO	4.4
1	C	236	VAL	4.4
1	D	1	GLY	4.3
1	D	240	PRO	4.2
1	C	371	PRO	3.6
1	A	1	GLY	3.6
1	A	121	GLU	3.5
1	B	232	VAL	3.5
1	D	245	PRO	3.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	240	PRO	3.4
1	C	116	GLY	3.4
1	B	116	GLY	3.3
1	D	116	GLY	3.3
1	A	195	ASP	3.2
1	D	244	LYS	3.2
1	C	241	ASP	3.1
1	D	243	GLY	3.1
1	B	236	VAL	3.1
1	A	364	ARG	3.0
1	B	367	LYS	3.0
1	D	364	ARG	3.0
1	A	244	LYS	3.0
1	C	237	ALA	3.0
1	C	244	LYS	2.9
1	D	195	ASP	2.7
1	A	245	PRO	2.6
1	B	371	PRO	2.6
1	C	232	VAL	2.5
1	B	241	ASP	2.5
1	D	241	ASP	2.4
1	A	239	GLY	2.4
1	B	239	GLY	2.4
1	D	371	PRO	2.3
1	A	243	GLY	2.3
1	B	196	THR	2.2
1	A	241	ASP	2.2
1	D	120	GLU	2.1
1	D	121	GLU	2.1
1	A	116	GLY	2.1
1	B	194	GLY	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

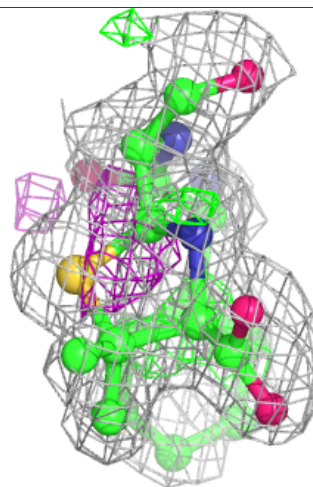
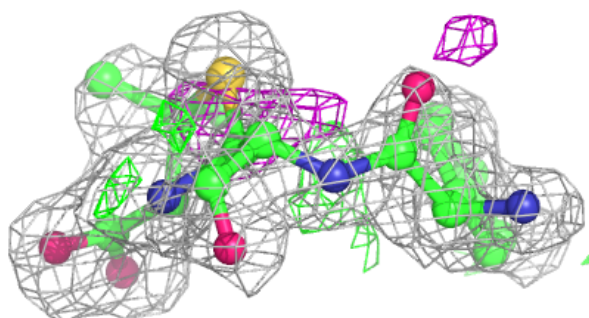
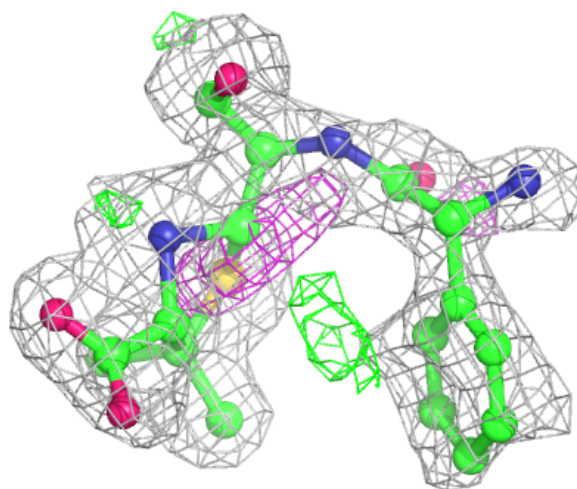
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	NDV	D	375	24/24	0.81	0.21	26,36,45,49	0
4	NDV	A	376	24/24	0.82	0.20	25,35,45,48	0
3	AIC	B	376	24/24	0.92	0.11	8,20,38,45	0
3	AIC	C	375	24/24	0.92	0.11	10,23,39,40	0
3	AIC	D	374	24/24	0.94	0.09	8,18,32,40	0
3	AIC	A	375	24/24	0.95	0.10	8,18,36,41	0
2	GOL	A	374	6/6	0.96	0.07	10,11,12,12	0
2	GOL	B	374	6/6	0.97	0.07	7,9,12,13	0
2	GOL	B	375	6/6	0.97	0.06	10,12,13,15	0
2	GOL	C	374	6/6	0.98	0.07	9,9,10,12	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 NDV D 375:**

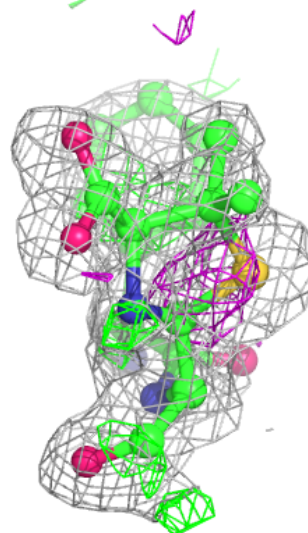
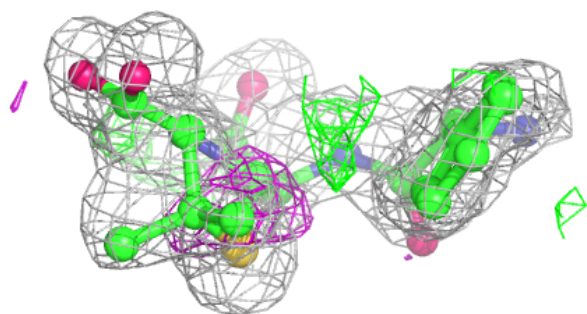
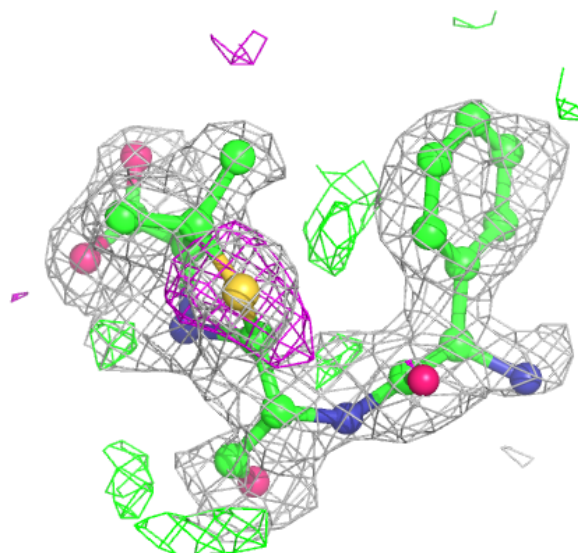
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





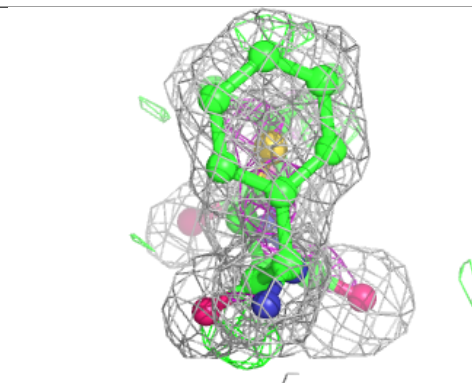
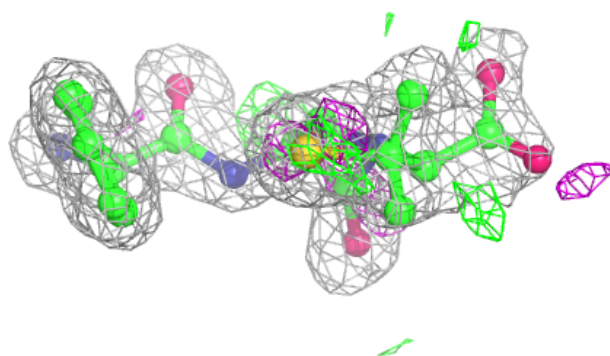
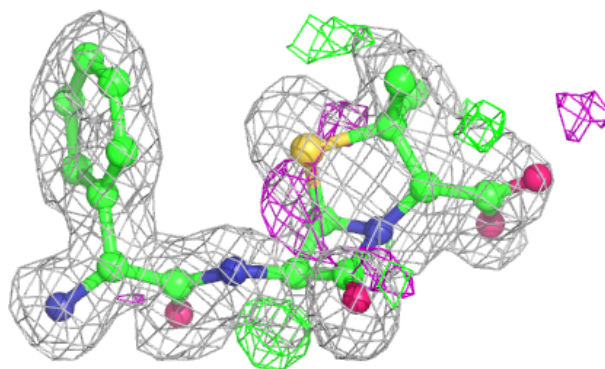
**Electron density around NDV A 376:**

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

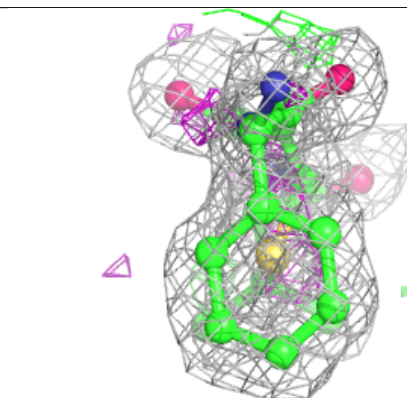
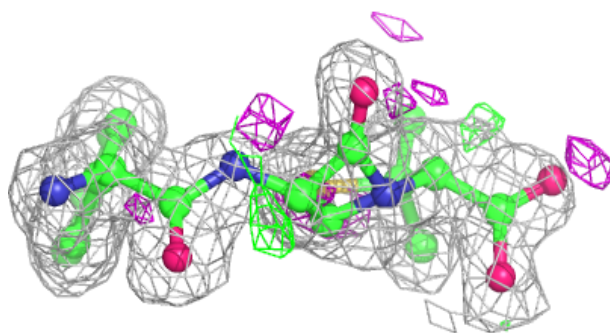
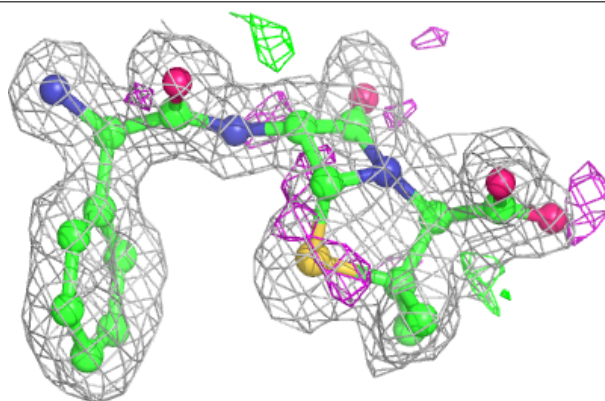


**Electron density around AIC B 376:**

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

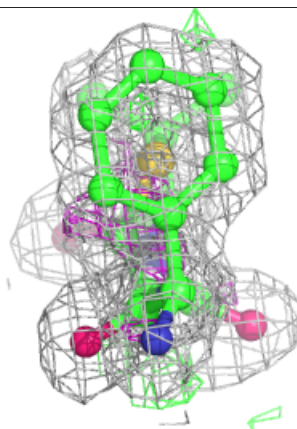
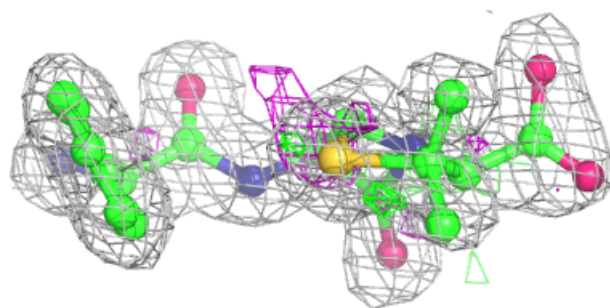
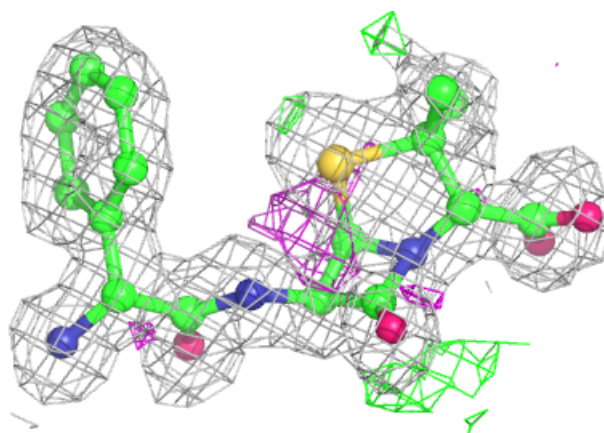
**Electron density around AIC C 375:**

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

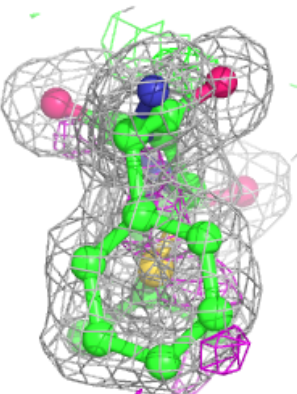
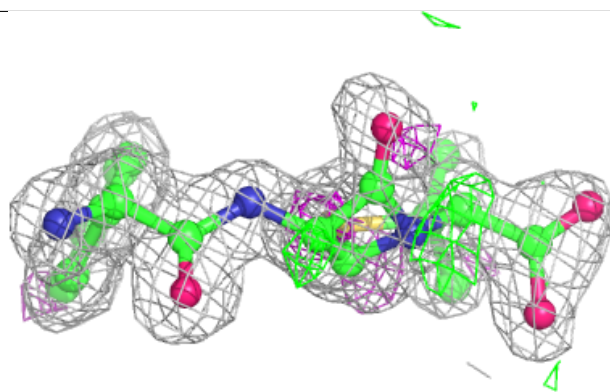
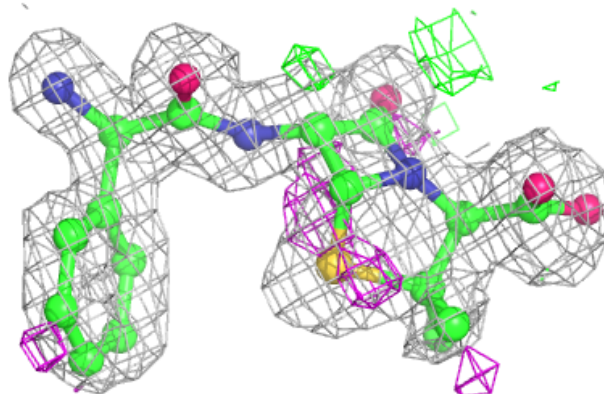


**Electron density around AIC D 374:**

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

**Electron density around AIC A 375:**

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



## 6.5 Other polymers

There are no such residues in this entry.