



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 15, 2020 – 04:24 PM EDT

PDB ID : 7K35  
Title : EQADH-NADH-4-METHYLBENZYL ALCOHOL, p21  
Authors : Plapp, B.V.; Ramaswamy, S.  
Deposited on : 2020-09-10  
Resolution : 1.20 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 : 2.14.4  
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) : 2.14.4

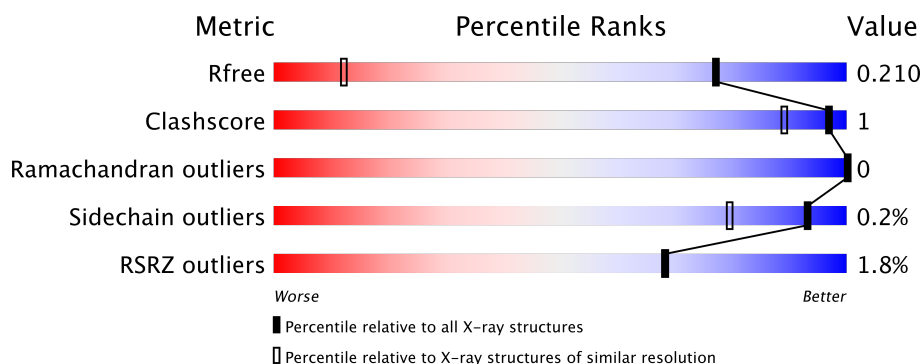
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.20 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	1223 (1.22-1.18)
Clashscore	141614	1286 (1.22-1.18)
Ramachandran outliers	138981	1240 (1.22-1.18)
Sidechain outliers	138945	1239 (1.22-1.18)
RSRZ outliers	127900	1200 (1.22-1.18)

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	374	<div> <div>2%</div> <div>98%</div> <div>.</div> </div>
1	B	374	<div> <div>2%</div> <div>98%</div> <div>.</div> </div>
1	C	374	<div> <div>%</div> <div>96%</div> <div>.</div> </div>
1	D	374	<div> <div>2%</div> <div>98%</div> <div>.</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12848 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.

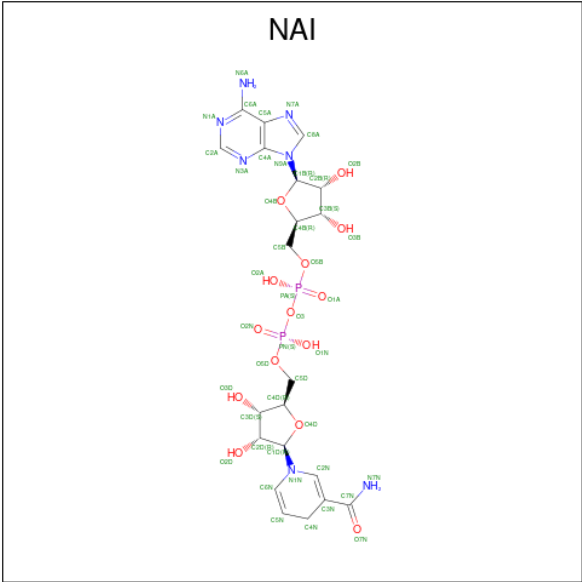
- Molecule 1 is a protein called Alcohol dehydrogenase E chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	12	0
			2827	1797	477	527	26			
1	B	374	Total	C	N	O	S	0	19	0
			2856	1812	483	537	24			
1	C	374	Total	C	N	O	S	0	11	0
			2832	1798	481	529	24			
1	D	374	Total	C	N	O	S	0	12	0
			2832	1799	477	530	26			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

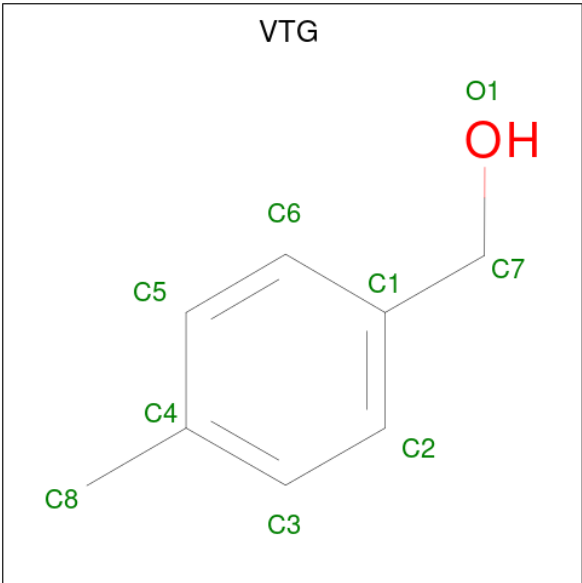
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		

- Molecule 3 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C<sub>21</sub>H<sub>29</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by author).



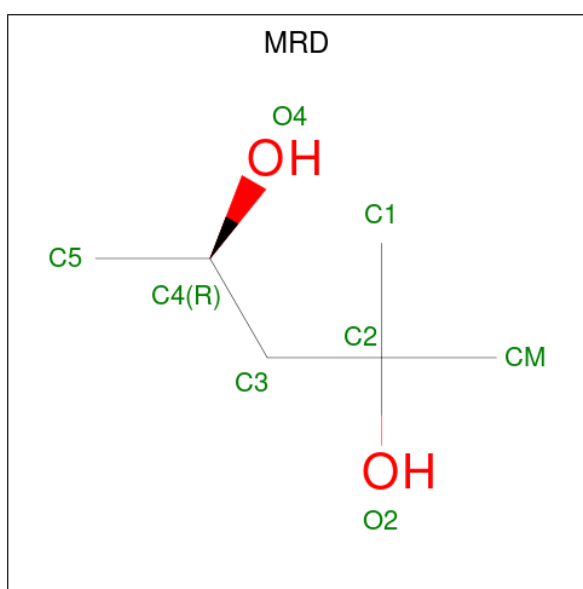
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is (4-methylphenyl)methanol (three-letter code: VTG) (formula: C<sub>8</sub>H<sub>10</sub>O) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 9 8 1	0	0
4	B	1	Total C O 9 8 1	0	0
4	C	1	Total C O 9 8 1	0	0
4	D	1	Total C O 9 8 1	0	0

- Molecule 5 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 8 6 2	0	0
5	C	1	Total C O 8 6 2	0	1

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	283	Total O 286 286	0	8
6	B	306	Total O 308 308	0	5
6	C	339	Total O 344 344	0	13

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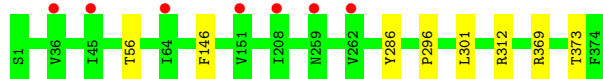
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	320	Total 327	O 327	0	13

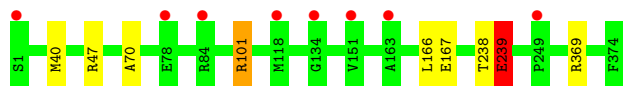
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Alcohol dehydrogenase E chain



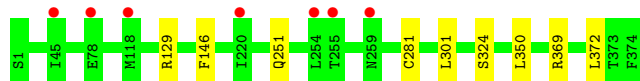
- Molecule 1: Alcohol dehydrogenase E chain



- Molecule 1: Alcohol dehydrogenase E chain



- Molecule 1: Alcohol dehydrogenase E chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.22Å 180.22Å 86.86Å 90.00° 106.12° 90.00°	Depositor
Resolution (Å)	19.96 – 1.20 19.96 – 1.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.96-1.20) 99.2 (19.96-1.20)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.44 (at 1.20Å)	Xtriage
Refinement program	REFMAC 5.8.0266	Depositor
R, $R_{free}$	0.176 , 0.210 0.177 , 0.210	Depositor DCC
$R_{free}$ test set	2399 reflections (0.53%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.1	Xtriage
Anisotropy	0.598	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 47.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	12848	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 66.14 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.3356e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: MRD, ZN, NAI, VTG

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	0.84	0/2929	1.01	3/3954 (0.1%)
1	B	0.87	3/2986 (0.1%)	1.01	3/4028 (0.1%)
1	C	0.89	3/2929 (0.1%)	1.03	4/3954 (0.1%)
1	D	0.86	1/2929 (0.0%)	1.02	4/3955 (0.1%)
All	All	0.87	7/11773 (0.1%)	1.01	14/15891 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	239	GLU	CD-OE2	12.22	1.39	1.25
1	C	239	GLU	CD-OE2	7.05	1.33	1.25
1	C	48	SER	CA-CB	-6.23	1.43	1.52
1	C	177	SER	CA-CB	-5.88	1.44	1.52
1	D	324	SER	CA-CB	-5.15	1.45	1.52
1	B	167[A]	GLU	CD-OE2	5.11	1.31	1.25
1	B	167[B]	GLU	CD-OE2	5.11	1.31	1.25

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	369	ARG	NE-CZ-NH2	-6.81	116.89	120.30
1	D	146	PHE	CB-CG-CD2	-6.45	116.28	120.80
1	D	129	ARG	NE-CZ-NH1	6.27	123.43	120.30
1	B	369	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	C	312	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	D	129	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	C	369	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	C	149	TYR	CB-CG-CD1	-5.29	117.82	121.00
1	A	146	PHE	CB-CG-CD2	-5.28	117.10	120.80
1	A	369	ARG	NE-CZ-NH2	-5.22	117.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	146	PHE	CB-CG-CD1	5.11	124.38	120.80
1	A	312	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	B	101	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	B	47	ARG	NE-CZ-NH1	-5.04	117.78	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	2827	0	2884	4	0
1	B	2856	0	2886	9	0
1	C	2832	0	2898	4	0
1	D	2832	0	2898	3	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	44	0	27	0	0
3	B	44	0	27	0	0
3	C	44	0	27	0	0
3	D	44	0	27	0	0
4	A	9	0	0	0	0
4	B	9	0	0	0	0
4	C	9	0	0	0	0
4	D	9	0	0	0	0
5	B	8	0	14	2	0
5	C	8	0	14	1	0
6	A	286	0	0	1	0
6	B	308	0	0	1	0
6	C	344	0	0	0	0
6	D	327	0	0	0	0
All	All	12848	0	11702	20	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 1.

All (20) 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:D:251:GLN:HA	1:D:281[B]:CYS:SG	2.15	0.86
1:B:40[B]:MET:HE3	1:B:40[B]:MET:HA	1.74	0.68
1:B:239:GLU:CG	5:B:405:MRD:HMC1	2.36	0.56
1:B:101:ARG:NH2	6:B:502:HOH:O	2.41	0.52
1:B:239:GLU:HG2	5:B:405:MRD:HMC1	1.91	0.51
1:C:238:THR:C	1:C:239:GLU:HG3	2.33	0.49
1:B:238:THR:C	1:B:239:GLU:HG3	2.33	0.48
1:C:100:CYS:HB2	1:C:112:LEU:HD12	1.98	0.45
1:B:70:ALA:HB1	1:B:166:LEU:HD22	1.98	0.45
1:A:286:TYR:OH	1:B:101:ARG:NE	2.51	0.44
1:C:243:PRO:HA	1:C:250:ILE:HD13	2.02	0.42
1:D:301:LEU:HD12	1:D:301:LEU:C	2.39	0.42
1:A:301:LEU:C	1:A:301:LEU:HD12	2.40	0.42
1:B:40[B]:MET:HA	1:B:40[B]:MET:CE	2.40	0.41
5:C:405[A]:MRD:H5C3	5:C:405[A]:MRD:H1C1	2.01	0.41
1:C:350:LEU:O	1:C:372:LEU:HA	2.21	0.41
1:A:56:THR:HG23	1:A:296:PRO:HA	2.02	0.41
1:A:373[A]:THR:HG23	6:A:589[A]:HOH:O	2.21	0.41
1:B:238:THR:O	1:B:239:GLU:HG3	2.21	0.41
1:D:350:LEU:O	1:D:372:LEU:HA	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	384/374 (103%)	370 (96%)	14 (4%)	0	100	100
1	B	390/374 (104%)	377 (97%)	13 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	383/374 (102%)	370 (97%)	13 (3%)	0	100	100
1	D	384/374 (103%)	374 (97%)	10 (3%)	0	100	100
All	All	1541/1496 (103%)	1491 (97%)	50 (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	319/308 (104%)	319 (100%)	0	100	100
1	B	325/308 (106%)	324 (100%)	1 (0%)	92	79
1	C	319/308 (104%)	318 (100%)	1 (0%)	92	79
1	D	319/308 (104%)	319 (100%)	0	100	100
All	All	1282/1232 (104%)	1280 (100%)	2 (0%)	93	79

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	239	GLU
1	C	239	GLU

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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
4	VTG	B	404	2	9,9,9	1.08	1 (11%)	11,11,11	0.93	1 (9%)
3	NAI	A	403	-	42,48,48	1.96	12 (28%)	47,73,73	1.71	9 (19%)
4	VTG	C	404	2	9,9,9	1.14	2 (22%)	11,11,11	1.74	2 (18%)
4	VTG	A	404	2	9,9,9	1.63	3 (33%)	11,11,11	1.07	1 (9%)
3	NAI	C	403	-	42,48,48	1.93	13 (30%)	47,73,73	2.26	15 (31%)
5	MRD	B	405	-	7,7,7	0.22	0	9,10,10	0.64	0
3	NAI	D	403	-	42,48,48	1.83	10 (23%)	47,73,73	2.00	14 (29%)
5	MRD	C	405[A]	-	7,7,7	0.23	0	9,10,10	0.84	0
3	NAI	B	403	-	42,48,48	1.65	7 (16%)	47,73,73	1.68	11 (23%)
4	VTG	D	404	2	9,9,9	1.16	1 (11%)	11,11,11	0.85	1 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	VTG	B	404	2	-	0/2/2/2	0/1/1/1
3	NAI	A	403	-	-	5/25/72/72	0/5/5/5
4	VTG	C	404	2	-	0/2/2/2	0/1/1/1
4	VTG	A	404	2	-	0/2/2/2	0/1/1/1
3	NAI	C	403	-	-	5/25/72/72	0/5/5/5
5	MRD	B	405	-	-	0/5/5/5	-
3	NAI	D	403	-	-	3/25/72/72	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MRD	C	405[A]	-	-	1/5/5/5	-
3	NAI	B	403	-	-	3/25/72/72	0/5/5/5
4	VTG	D	404	2	-	1/2/2/2	0/1/1/1

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	403	NAI	C2A-N3A	5.80	1.41	1.32
3	B	403	NAI	C2A-N3A	5.15	1.40	1.32
3	C	403	NAI	C2A-N3A	4.94	1.40	1.32
3	D	403	NAI	C2A-N3A	4.83	1.39	1.32
3	C	403	NAI	C6N-N1N	4.68	1.49	1.37
3	D	403	NAI	C4A-N3A	4.51	1.41	1.35
3	C	403	NAI	C2A-N1A	4.11	1.41	1.33
3	B	403	NAI	C6N-C5N	-4.06	1.26	1.33
3	D	403	NAI	C8A-N7A	-3.99	1.27	1.34
3	B	403	NAI	C8A-N7A	-3.92	1.27	1.34
3	A	403	NAI	C2A-N1A	-3.92	1.26	1.33
3	A	403	NAI	C6A-N1A	-3.77	1.20	1.37
3	A	403	NAI	C6N-N1N	3.74	1.46	1.37
3	A	403	NAI	C4N-C5N	3.43	1.57	1.48
3	D	403	NAI	C2A-N1A	3.43	1.40	1.33
3	C	403	NAI	O4D-C4D	-3.35	1.37	1.45
3	C	403	NAI	C6N-C5N	-3.32	1.27	1.33
3	B	403	NAI	C4N-C3N	-3.14	1.43	1.49
4	A	404	VTG	C6-C5	-2.94	1.33	1.38
3	D	403	NAI	PA-O1A	-2.88	1.40	1.50
3	C	403	NAI	C7N-C3N	-2.78	1.42	1.48
3	D	403	NAI	O7N-C7N	-2.78	1.17	1.24
3	D	403	NAI	C6N-C5N	-2.67	1.28	1.33
4	B	404	VTG	C6-C5	-2.65	1.33	1.38
3	C	403	NAI	O4B-C1B	2.60	1.44	1.41
3	D	403	NAI	O4B-C1B	2.56	1.44	1.41
3	C	403	NAI	O2D-C2D	-2.53	1.37	1.43
3	C	403	NAI	C5A-C4A	2.51	1.47	1.40
3	A	403	NAI	C4A-N3A	-2.47	1.32	1.35
3	A	403	NAI	C1D-N1N	-2.47	1.39	1.46
3	C	403	NAI	C4N-C3N	-2.47	1.45	1.49
3	A	403	NAI	C4N-C3N	-2.39	1.45	1.49
4	A	404	VTG	C5-C4	-2.32	1.32	1.38
4	A	404	VTG	C3-C2	-2.30	1.34	1.38
3	C	403	NAI	C4A-N3A	-2.29	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	404	VTG	C5-C4	-2.29	1.32	1.38
3	A	403	NAI	C8A-N7A	-2.28	1.30	1.34
4	D	404	VTG	C3-C2	-2.27	1.34	1.38
3	A	403	NAI	O4D-C1D	2.26	1.47	1.42
3	B	403	NAI	C4N-C5N	2.19	1.54	1.48
3	B	403	NAI	O4B-C1B	2.19	1.44	1.41
3	C	403	NAI	O3D-C3D	2.17	1.48	1.43
3	A	403	NAI	C6A-N6A	-2.16	1.26	1.34
3	D	403	NAI	O2D-C2D	-2.08	1.38	1.43
3	A	403	NAI	O4B-C4B	-2.07	1.40	1.45
3	C	403	NAI	C6A-N1A	-2.06	1.28	1.37
3	B	403	NAI	PA-O1A	-2.04	1.43	1.50
3	D	403	NAI	PN-O5D	2.03	1.67	1.59
4	C	404	VTG	C2-C1	-2.00	1.34	1.38

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	403	NAI	N3A-C2A-N1A	-7.63	116.75	128.68
3	D	403	NAI	N3A-C2A-N1A	-7.27	117.32	128.68
3	B	403	NAI	C1B-N9A-C4A	-5.95	116.18	126.64
3	D	403	NAI	C2A-N1A-C6A	5.85	128.76	118.75
3	A	403	NAI	N3A-C2A-N1A	-5.02	120.83	128.68
3	B	403	NAI	N3A-C2A-N1A	-4.89	121.04	128.68
3	C	403	NAI	C3N-C7N-N7N	4.28	125.28	117.67
3	C	403	NAI	C1D-N1N-C2N	4.13	127.99	121.11
3	C	403	NAI	C3N-C2N-N1N	4.01	128.81	123.10
3	A	403	NAI	C1D-N1N-C2N	3.94	127.67	121.11
3	A	403	NAI	C2D-C1D-N1N	3.92	123.12	113.30
3	C	403	NAI	C2D-C1D-N1N	3.70	122.58	113.30
4	C	404	VTG	C2-C3-C4	-3.65	116.49	121.38
3	C	403	NAI	C2A-N1A-C6A	3.62	124.94	118.75
3	C	403	NAI	C4A-C5A-N7A	3.60	113.15	109.40
3	A	403	NAI	C2A-N1A-C6A	3.57	124.86	118.75
3	C	403	NAI	C5A-C6A-N6A	-3.44	115.13	120.35
3	A	403	NAI	C3N-C2N-N1N	3.31	127.82	123.10
3	C	403	NAI	PN-O3-PA	3.28	144.09	132.83
3	B	403	NAI	O4B-C1B-C2B	-3.24	102.18	106.93
4	C	404	VTG	C5-C6-C1	-3.15	116.69	121.03
3	A	403	NAI	C1B-N9A-C4A	-3.10	121.19	126.64
3	C	403	NAI	O7N-C7N-N7N	-3.05	115.75	122.88
3	D	403	NAI	O3D-C3D-C4D	2.99	119.69	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	403	NAI	O4D-C1D-C2D	-2.94	100.22	106.64
3	B	403	NAI	C2A-N1A-C6A	2.81	123.56	118.75
3	D	403	NAI	C1B-N9A-C4A	-2.80	121.72	126.64
3	C	403	NAI	C3D-C2D-C1D	-2.78	96.14	101.43
3	B	403	NAI	O2A-PA-O1A	2.64	125.31	112.24
3	A	403	NAI	O4B-C1B-C2B	-2.57	103.17	106.93
3	C	403	NAI	N6A-C6A-N1A	2.57	123.92	118.57
3	D	403	NAI	O2A-PA-O1A	2.55	124.87	112.24
3	D	403	NAI	C4A-C5A-N7A	-2.54	106.75	109.40
3	C	403	NAI	O2D-C2D-C3D	2.48	119.85	111.82
3	B	403	NAI	C3D-C2D-C1D	-2.45	96.77	101.43
3	A	403	NAI	O2B-C2B-C3B	2.42	119.65	111.82
3	D	403	NAI	O4D-C1D-N1N	2.40	112.75	108.06
4	B	404	VTG	O1-C7-C1	2.39	120.84	112.03
4	A	404	VTG	C6-C5-C4	2.32	124.50	121.38
3	C	403	NAI	C1B-N9A-C4A	-2.32	122.56	126.64
3	D	403	NAI	C1D-N1N-C6N	-2.28	115.92	120.83
3	C	403	NAI	O4B-C1B-C2B	-2.23	103.67	106.93
3	D	403	NAI	C5A-C6A-N1A	-2.20	115.38	120.35
3	D	403	NAI	O7N-C7N-C3N	-2.19	116.76	120.90
3	B	403	NAI	O3D-C3D-C4D	2.19	117.38	111.05
3	D	403	NAI	N6A-C6A-N1A	2.17	123.07	118.57
3	B	403	NAI	C4A-C5A-N7A	-2.16	107.14	109.40
3	B	403	NAI	C5A-C6A-N6A	2.13	123.59	120.35
3	D	403	NAI	C2D-C1D-N1N	2.12	118.63	113.30
3	A	403	NAI	O4D-C4D-C3D	2.10	109.26	105.11
3	B	403	NAI	PN-O3-PA	-2.07	125.72	132.83
3	B	403	NAI	C3B-C2B-C1B	2.05	104.06	100.98
3	D	403	NAI	O4B-C1B-C2B	-2.04	103.94	106.93
4	D	404	VTG	O1-C7-C1	2.02	119.46	112.03

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	403	NAI	C2D-C1D-N1N-C2N
3	B	403	NAI	C2D-C1D-N1N-C2N
3	A	403	NAI	C2D-C1D-N1N-C2N
3	D	403	NAI	O4D-C1D-N1N-C2N
3	C	403	NAI	C5B-O5B-PA-O3
3	A	403	NAI	O4D-C1D-N1N-C2N
3	C	403	NAI	O4D-C1D-N1N-C2N

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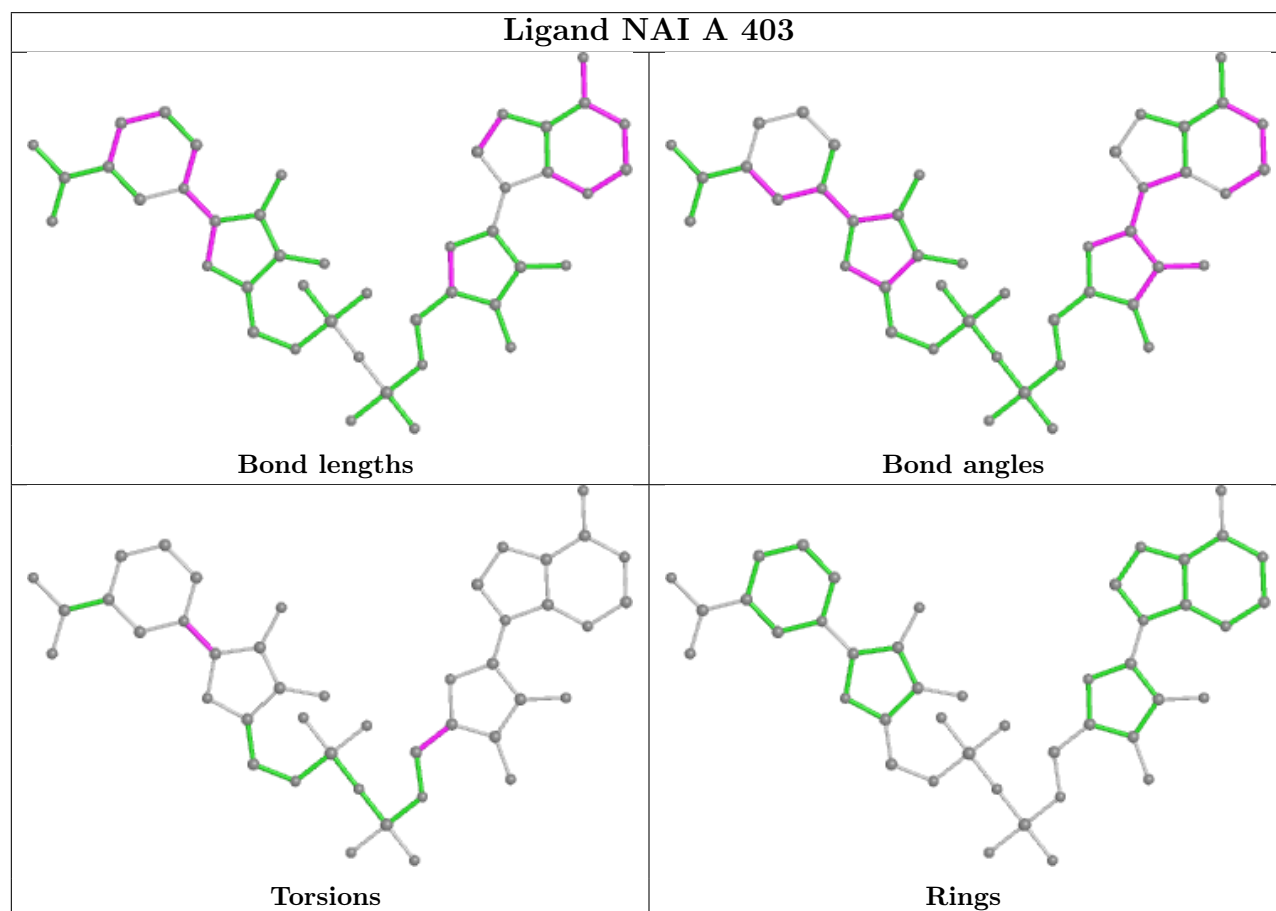
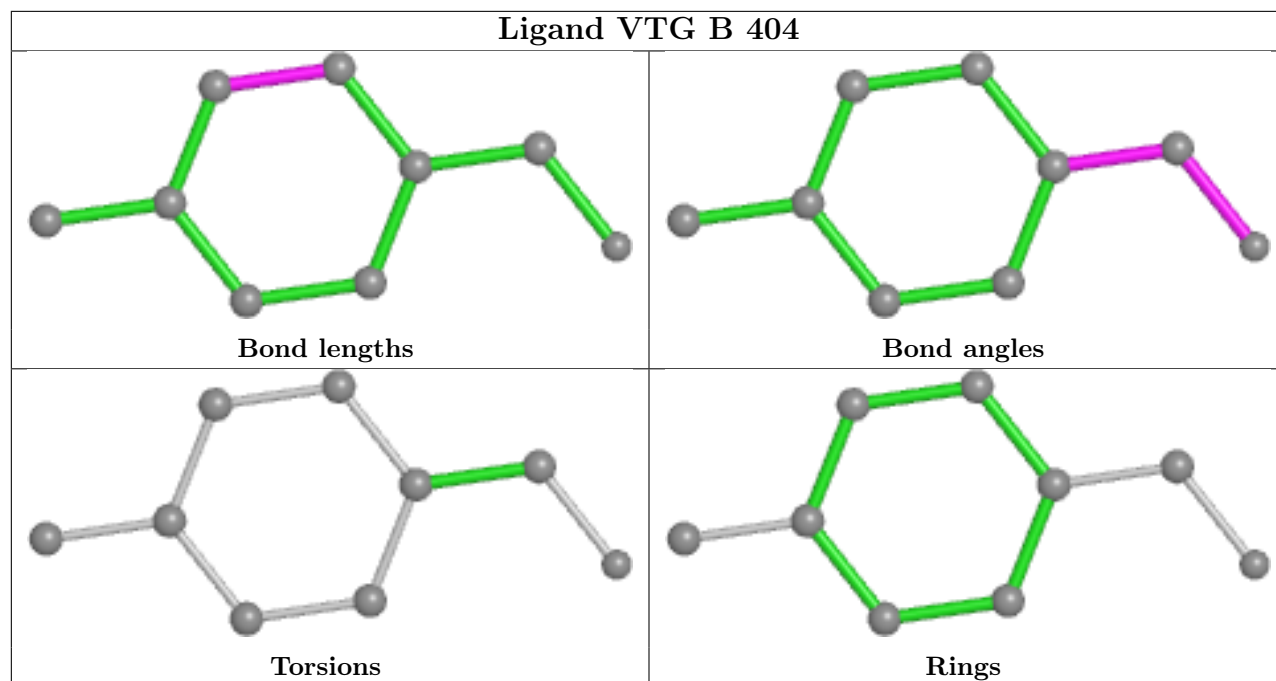
Mol	Chain	Res	Type	Atoms
3	B	403	NAI	O4D-C1D-N1N-C2N
3	C	403	NAI	C2D-C1D-N1N-C2N
3	A	403	NAI	O4D-C1D-N1N-C6N
3	A	403	NAI	C2D-C1D-N1N-C6N
3	C	403	NAI	O4D-C1D-N1N-C6N
3	A	403	NAI	O4B-C4B-C5B-O5B
3	C	403	NAI	O4B-C4B-C5B-O5B
3	D	403	NAI	O4B-C4B-C5B-O5B
3	B	403	NAI	O4B-C4B-C5B-O5B
5	C	405[A]	MRD	C2-C3-C4-C5
4	D	404	VTG	C6-C1-C7-O1

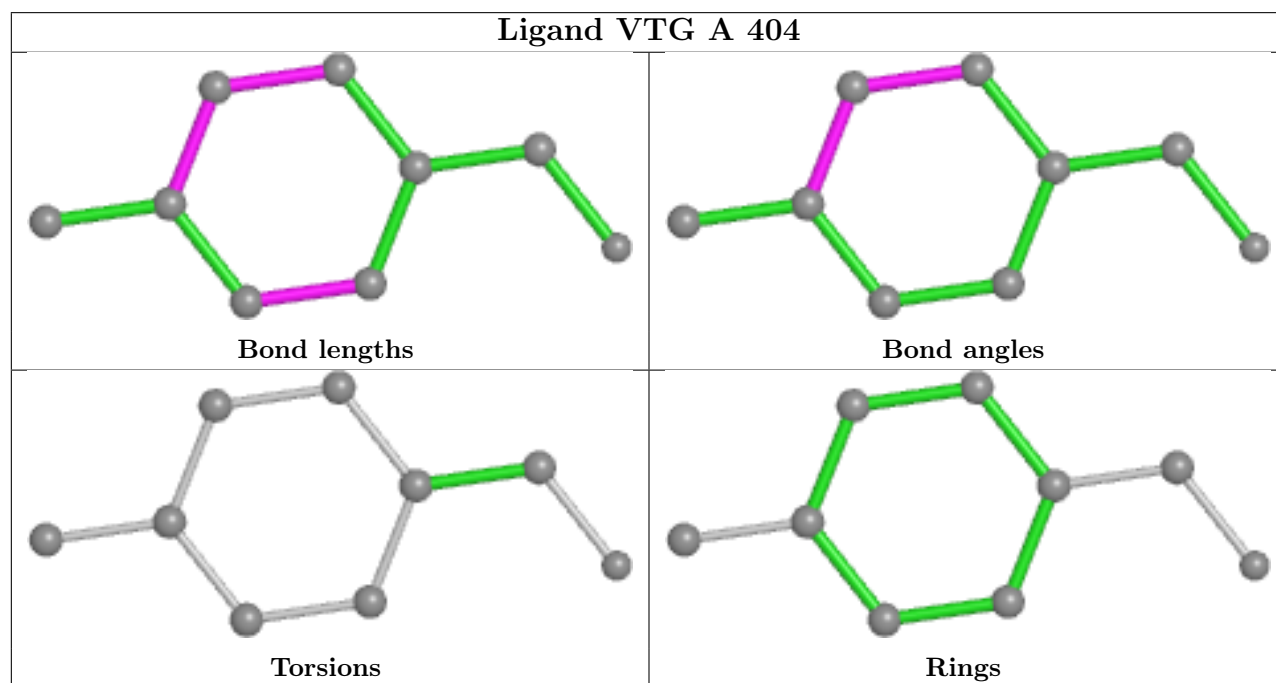
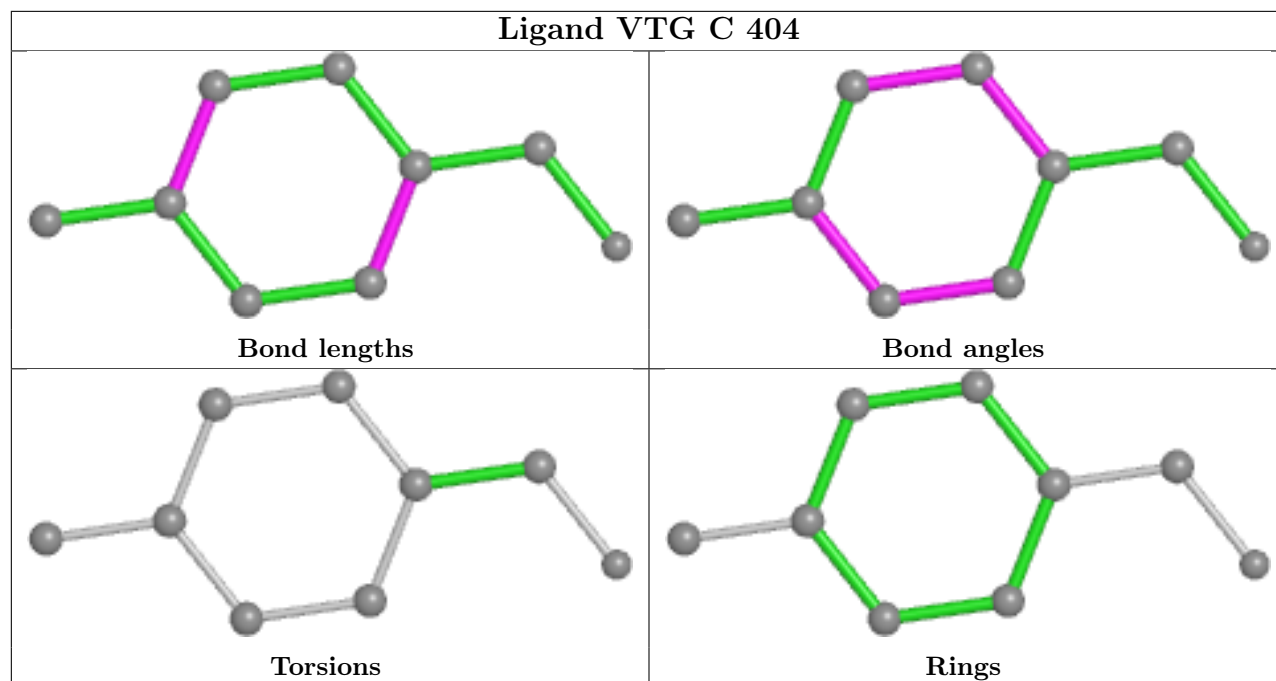
There are no ring outliers.

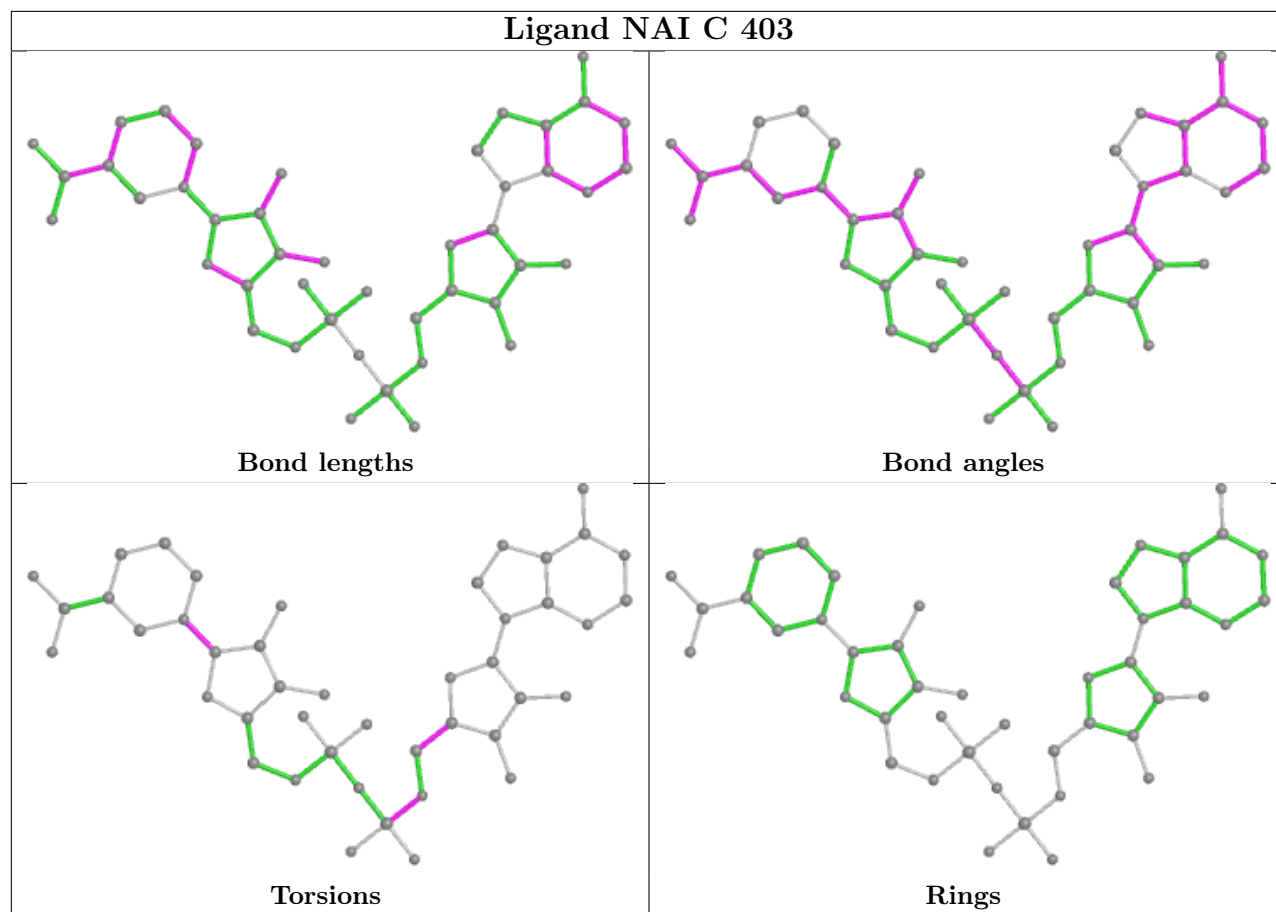
2 monomers are involved in 3 short contacts:

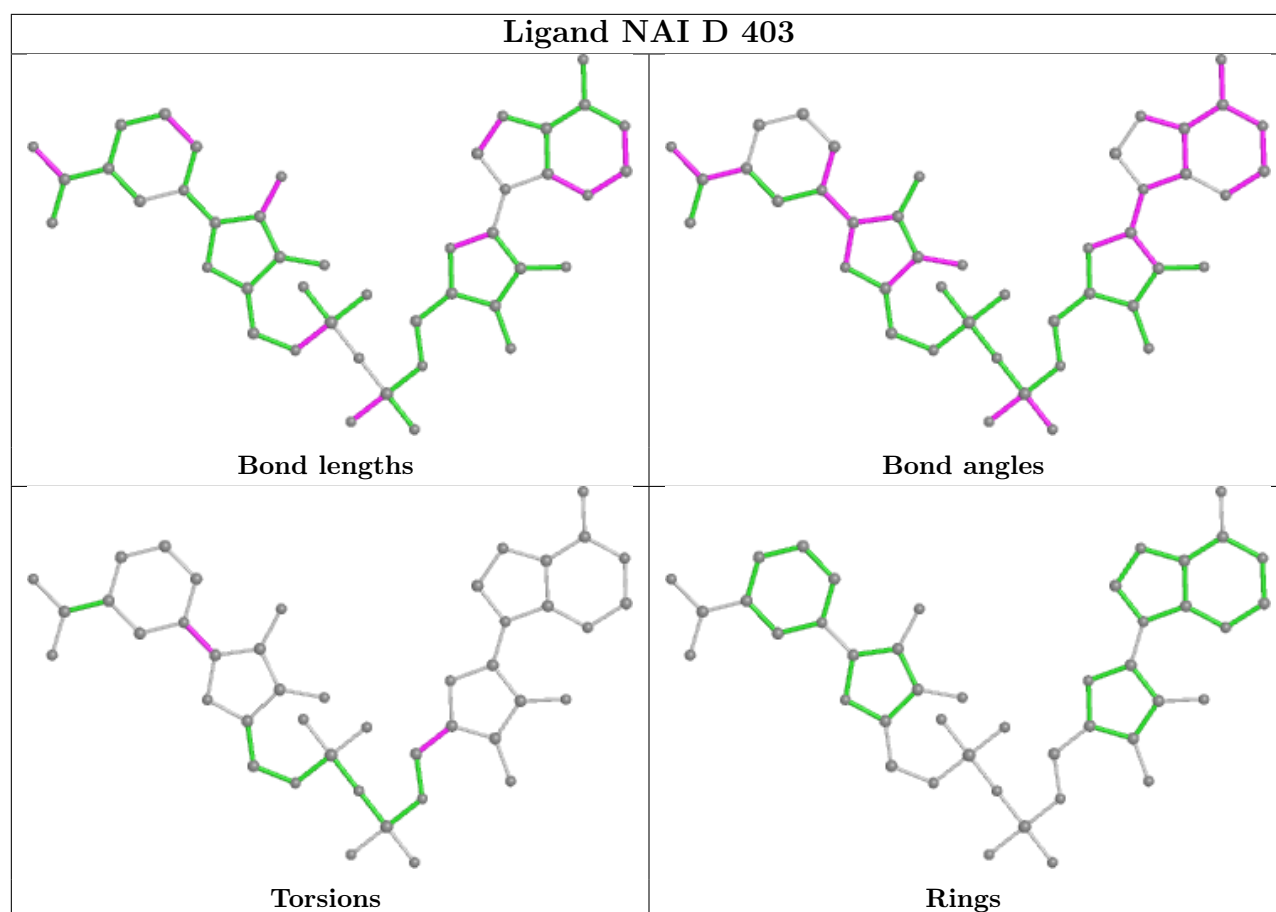
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	405	MRD	2	0
5	C	405[A]	MRD	1	0

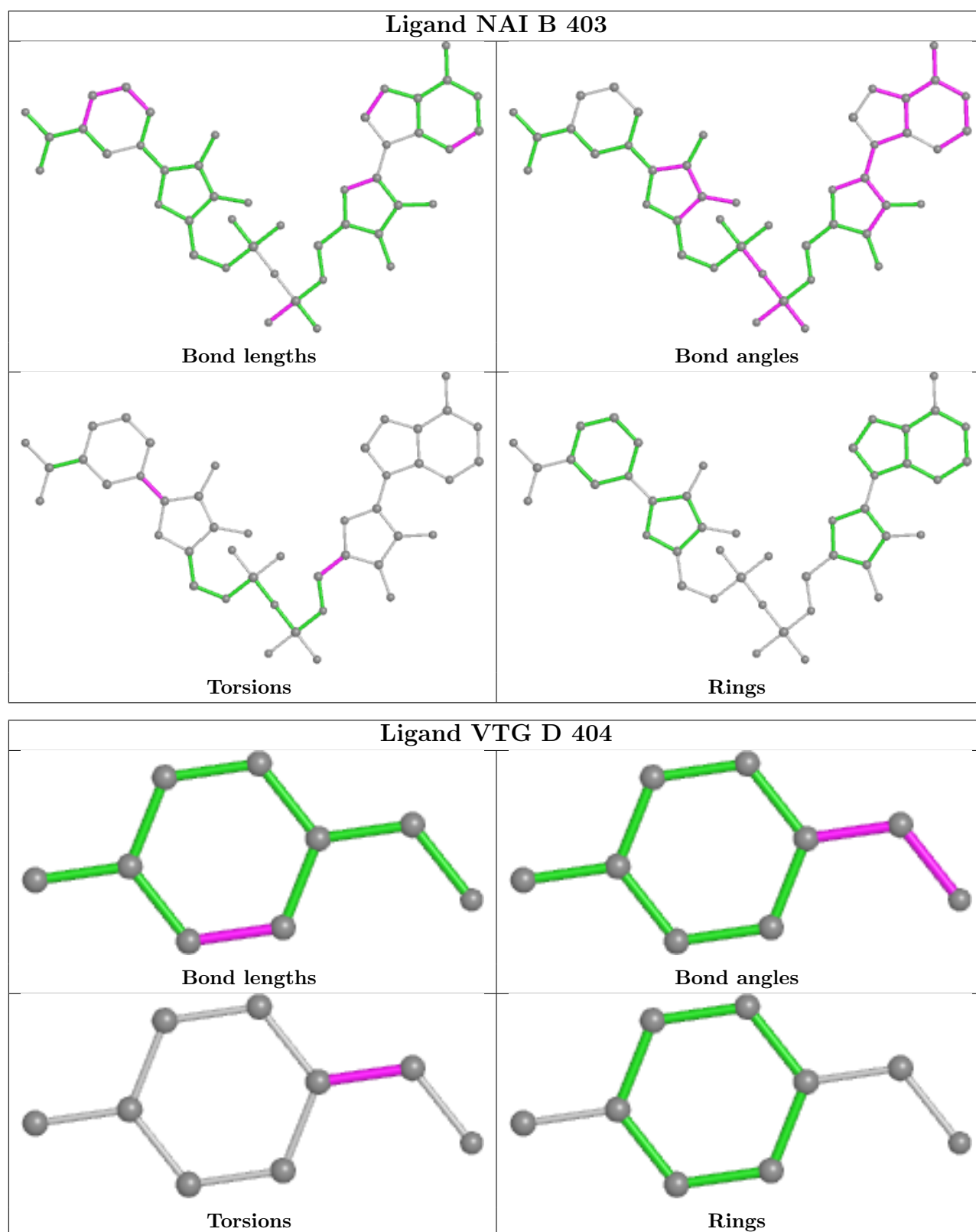
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











## 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	374/374 (100%)	0.21	7 (1%) 66 67	17, 23, 35, 48	0
1	B	374/374 (100%)	0.18	8 (2%) 63 63	17, 23, 35, 54	0
1	C	374/374 (100%)	0.24	5 (1%) 77 77	17, 23, 34, 50	0
1	D	374/374 (100%)	0.20	7 (1%) 66 67	18, 23, 35, 45	0
All	All	1496/1496 (100%)	0.21	27 (1%) 68 68	17, 23, 35, 54	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	151	VAL	3.3
1	D	259	ASN	3.2
1	B	163	ALA	2.9
1	A	36	VAL	2.8
1	C	151	VAL	2.7
1	B	78	GLU	2.4
1	A	64	ILE	2.4
1	B	1	SER	2.4
1	D	254	LEU	2.4
1	B	84	ARG	2.4
1	C	64	ILE	2.3
1	C	107	GLU	2.3
1	B	118	MET	2.3
1	B	249	PRO	2.3
1	A	262	VAL	2.3
1	D	78	GLU	2.3
1	A	259	ASN	2.2
1	A	208	ILE	2.2
1	D	45	ILE	2.2
1	D	255	THR	2.2
1	A	45	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	151	VAL	2.1
1	D	118	MET	2.1
1	C	78	GLU	2.1
1	D	220	ILE	2.1
1	B	134	GLY	2.1
1	C	291	ILE	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	MRD	C	405[A]	8/8	0.89	0.15	39,45,50,50	8
5	MRD	B	405	8/8	0.94	0.12	36,41,47,48	0
3	NAI	C	403	44/44	0.95	0.08	15,20,25,33	0
4	VTG	C	404	9/9	0.95	0.07	21,23,25,31	0
3	NAI	A	403	44/44	0.96	0.07	15,20,26,31	0
4	VTG	A	404	9/9	0.96	0.06	20,21,24,25	0
4	VTG	B	404	9/9	0.96	0.06	22,23,24,26	0
4	VTG	D	404	9/9	0.96	0.07	21,22,25,29	0
3	NAI	B	403	44/44	0.97	0.06	17,19,25,30	0
3	NAI	D	403	44/44	0.97	0.06	17,20,25,34	0
2	ZN	D	402	1/1	0.99	0.03	21,21,21,21	0
2	ZN	C	402	1/1	0.99	0.03	22,22,22,22	0
2	ZN	B	401	1/1	0.99	0.06	23,23,23,23	0
2	ZN	C	401	1/1	0.99	0.06	23,23,23,23	0
2	ZN	D	401	1/1	0.99	0.06	23,23,23,23	0
2	ZN	A	401	1/1	0.99	0.05	23,23,23,23	0
2	ZN	B	402	1/1	0.99	0.02	22,22,22,22	0

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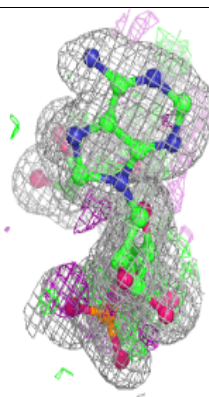
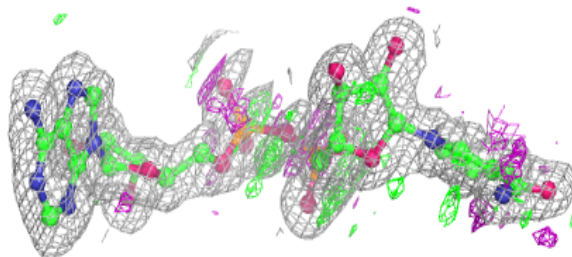
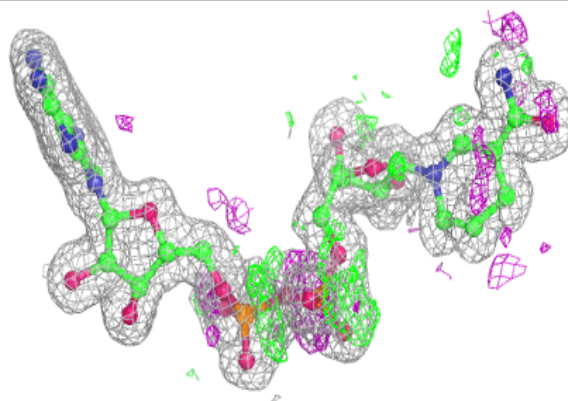
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	A	402	1/1	0.99	0.03	20,20,20,20	0

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.

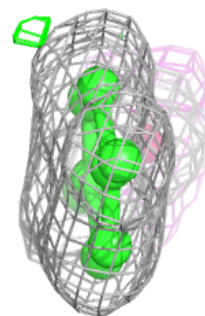
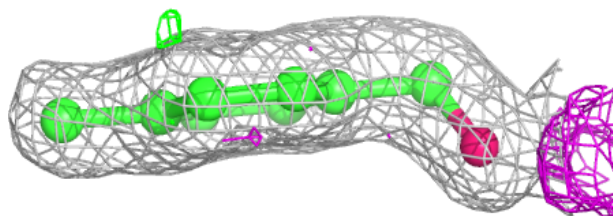
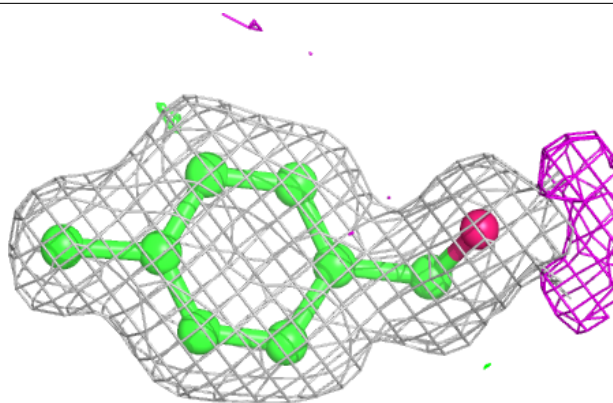
**Electron density around NAI C 403:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

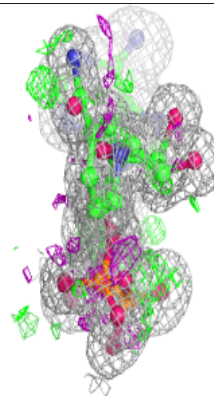
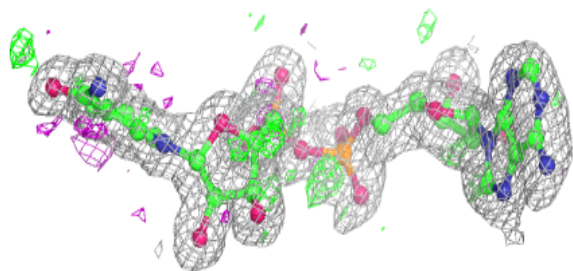
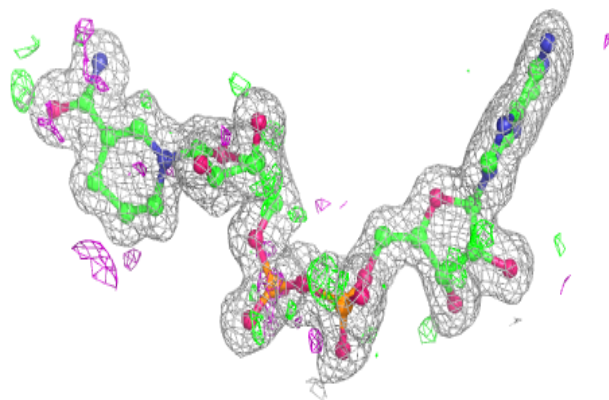


**Electron density around VTG C 404:**

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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
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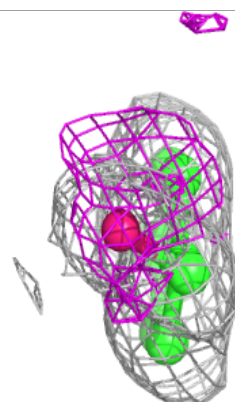
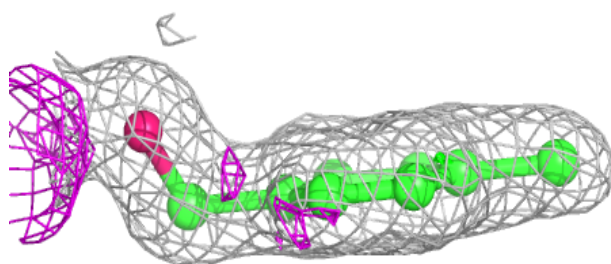
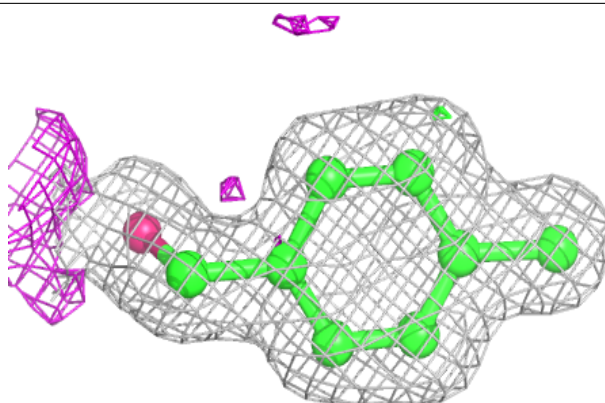
**Electron density around NAI A 403:**

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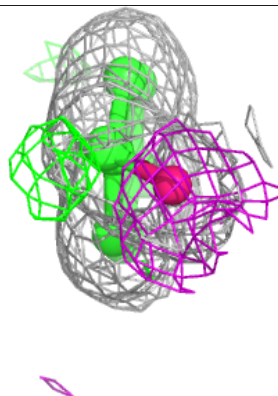
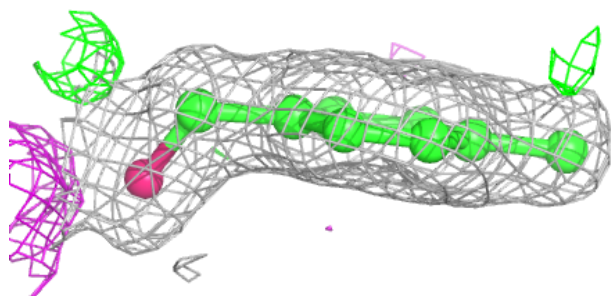
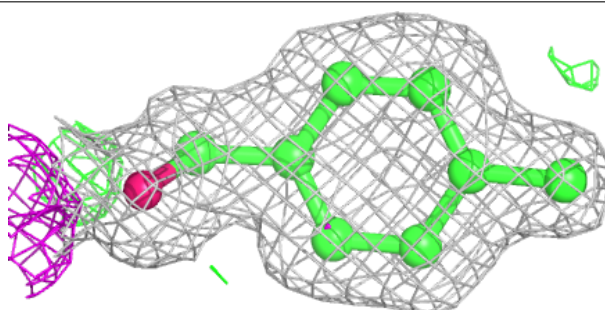


**Electron density around VTG A 404:**

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and green (positive)

**Electron density around VTG B 404:**

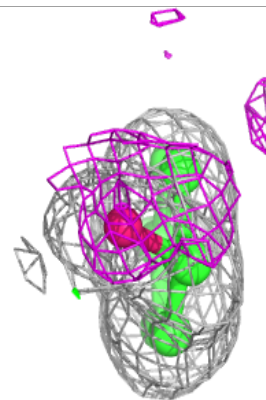
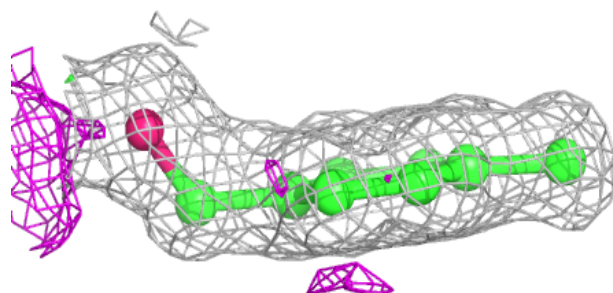
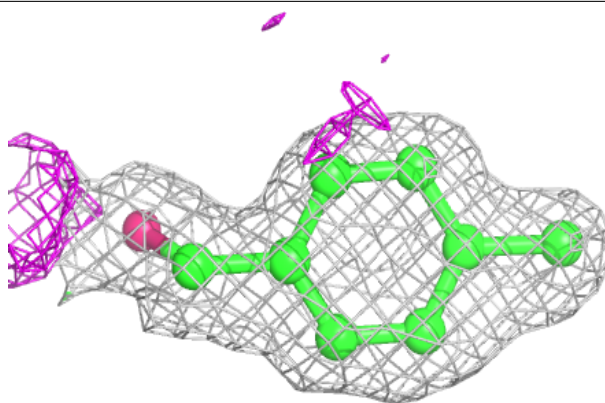
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



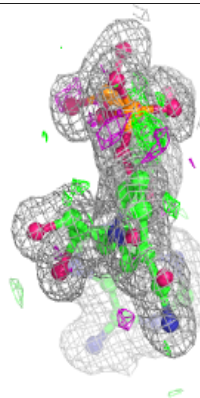
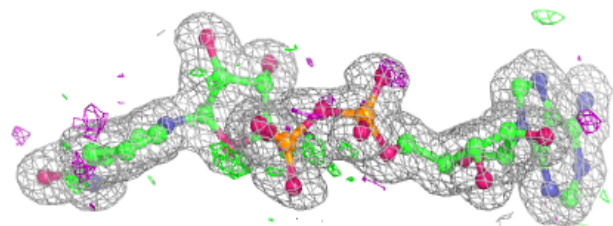
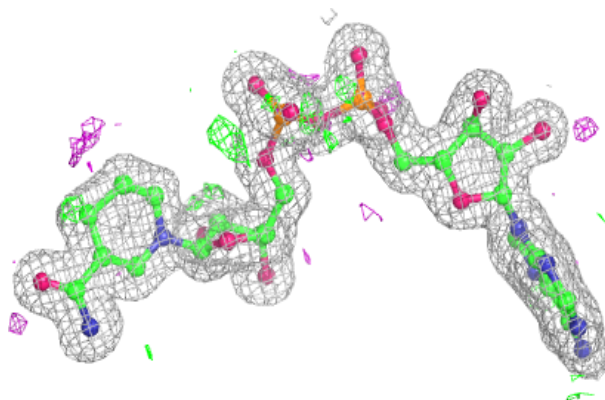


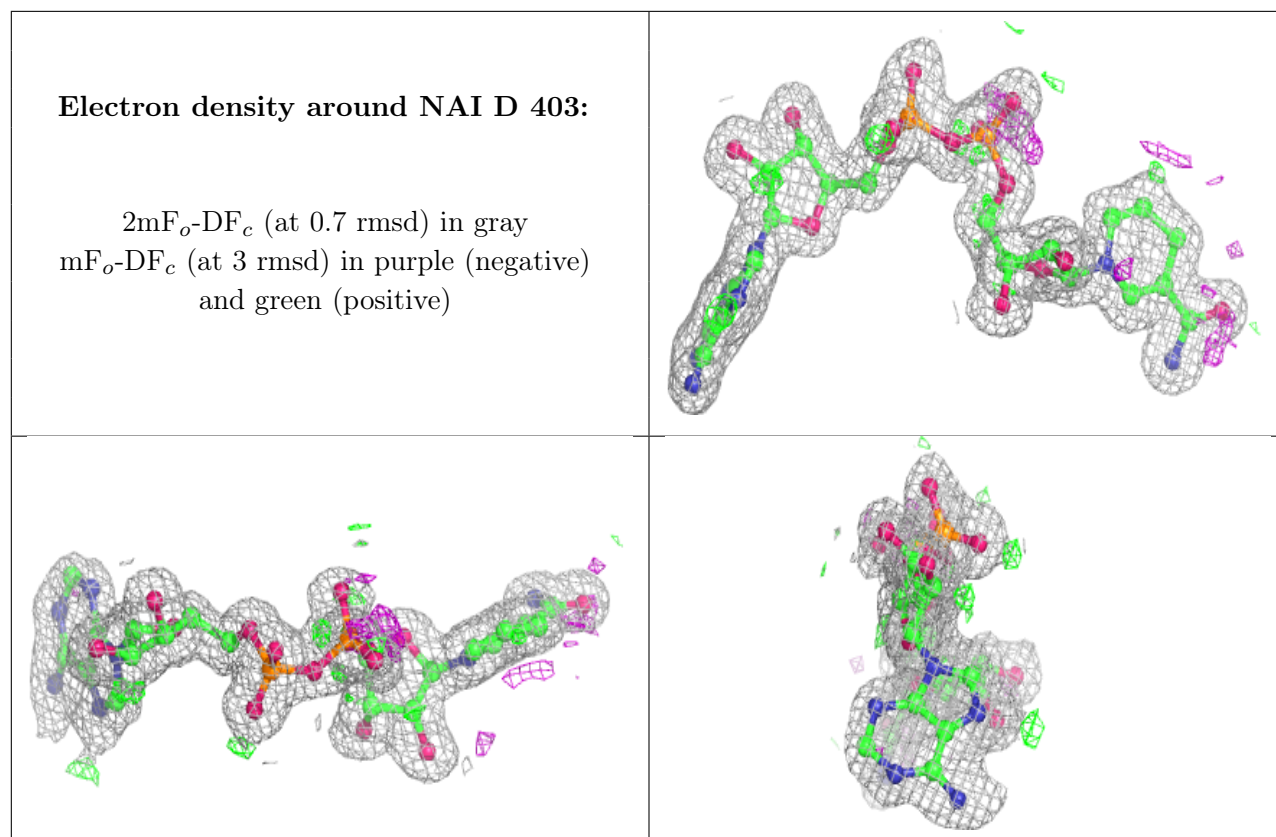
**Electron density around VTG D 404:**

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

**Electron density around NAI B 403:**

$2mF_o-DF_c$  (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.