



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2021 – 06:07 PM EST

PDB ID : 7JNS  
Title : Ternary complex crystal structure of secondary alcohol dehydrogenases from the *Thermoanaerobacter ethanolicus* mutants C295 and I86A provides better understanding of catalytic mechanism  
Authors : Dinh, T.; Phillips, R.; Rahn, K.  
Deposited on : 2020-08-05  
Resolution : 2.34 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	:	2.17
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)	:	2.17

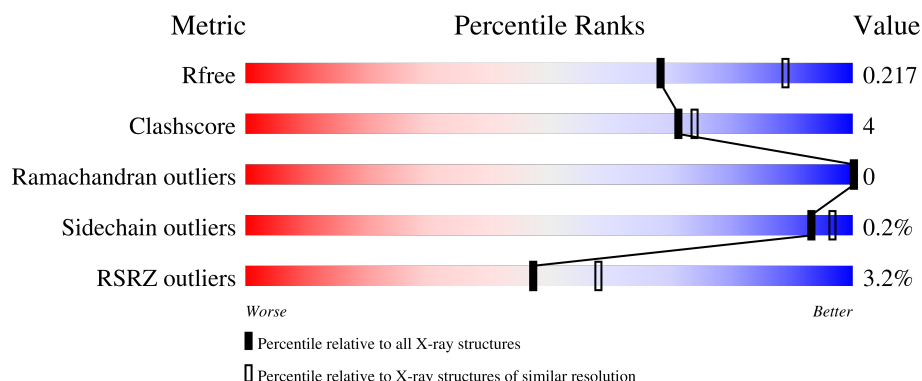
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.34 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	352	<div> <div>8%</div> <div> <div></div> <div>91%</div> <div>9%</div> </div> </div>
1	B	352	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>9%</div> </div> </div>
1	C	352	<div> <div>3%</div> <div> <div></div> <div>91%</div> <div>9%</div> </div> </div>
1	D	352	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>9%</div> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11011 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 Secondary-alcohol dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	0	0
			2623	1679	452	474	18			
1	B	352	Total	C	N	O	S	0	1	0
			2647	1695	456	477	19			
1	C	352	Total	C	N	O	S	0	0	0
			2640	1690	455	476	19			
1	D	352	Total	C	N	O	S	0	3	0
			2654	1704	455	476	19			

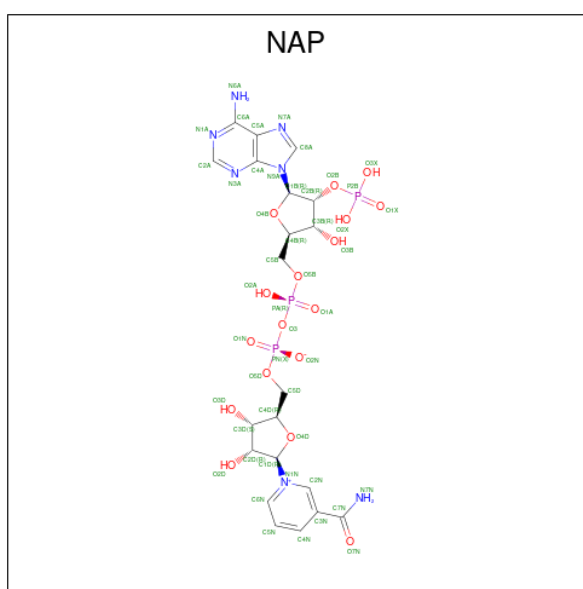
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	86	ALA	ILE	engineered mutation	UNP P77990
A	91	ARG	TRP	conflict	UNP P77990
A	313	ARG	PRO	conflict	UNP P77990
A	325	ARG	GLN	conflict	UNP P77990
B	86	ALA	ILE	engineered mutation	UNP P77990
B	91	ARG	TRP	conflict	UNP P77990
B	313	ARG	PRO	conflict	UNP P77990
B	325	ARG	GLN	conflict	UNP P77990
C	86	ALA	ILE	engineered mutation	UNP P77990
C	91	ARG	TRP	conflict	UNP P77990
C	313	ARG	PRO	conflict	UNP P77990
C	325	ARG	GLN	conflict	UNP P77990
D	86	ALA	ILE	engineered mutation	UNP P77990
D	91	ARG	TRP	conflict	UNP P77990
D	313	ARG	PRO	conflict	UNP P77990
D	325	ARG	GLN	conflict	UNP P77990

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

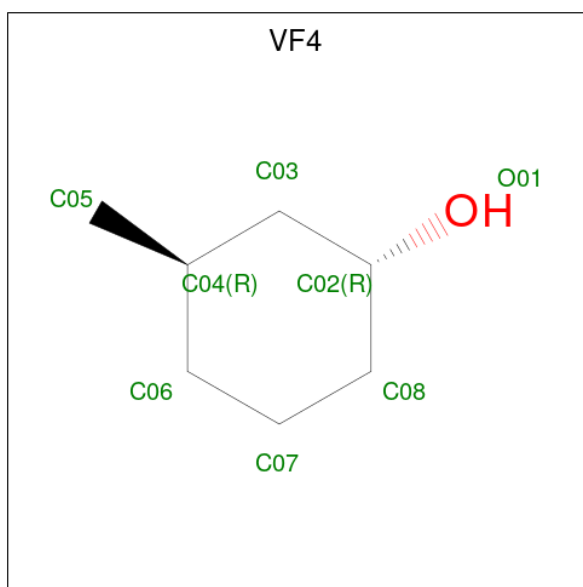
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is (1R,3S)-3-methylcyclohexan-1-ol (three-letter code: VF4) (formula:  $C_7H_{14}O$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	7	1		
4	B	1	Total	C	O	0	0
			8	7	1		
4	D	1	Total	C	O	0	0
			8	7	1		

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	K	0	0
			1	1		
5	B	1	Total	K	0	0
			1	1		
5	C	1	Total	K	0	0
			1	1		
5	D	1	Total	K	0	0
			1	1		

- Molecule 6 is water.

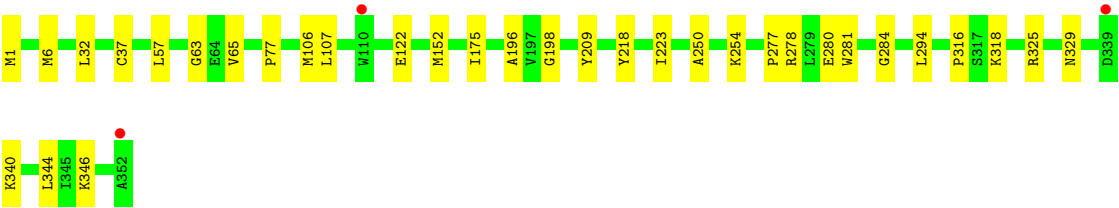
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	38	Total	O	0	0
			38	38		
6	B	64	Total	O	0	0
			64	64		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	57	Total	O	0	0
			57	57		
6	D	64	Total	O	0	0
			64	64		







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.82Å 122.85Å 165.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.53 – 2.34 68.53 – 2.34	Depositor EDS
% Data completeness (in resolution range)	73.2 (68.53-2.34) 73.2 (68.53-2.34)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.41 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, $R_{free}$	0.178 , 0.217 0.178 , 0.217	Depositor DCC
$R_{free}$ test set	2000 reflections (3.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.7	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.0	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	11011	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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: VF4, K, ZN, NAP

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	0.25	0/2681	0.47	0/3629
1	B	0.26	0/2705	0.48	0/3660
1	C	0.26	0/2698	0.49	0/3650
1	D	0.26	0/2721	0.48	0/3682
All	All	0.26	0/10805	0.48	0/14621

There are no bond length outliers.

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	2623	0	2656	17	0
1	B	2647	0	2689	20	0
1	C	2640	0	2681	21	0
1	D	2654	0	2712	19	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	48	0	23	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	48	0	23	1	0
3	C	48	0	24	1	0
3	D	48	0	23	1	0
4	A	8	0	0	0	0
4	B	8	0	0	0	0
4	D	8	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	38	0	0	0	0
6	B	64	0	0	1	0
6	C	57	0	0	2	0
6	D	64	0	0	1	0
All	All	11011	0	10831	76	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 4.

All (76) 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:65:VAL:HG12	1:D:77:PRO:HA	1.76	0.68
1:B:189:ARG:NH2	1:C:189:ARG:O	2.30	0.65
1:D:1:MET:N	6:D:502:HOH:O	2.36	0.59
1:A:175:ILE:HG12	1:A:198:GLY:HA3	1.84	0.58
1:B:254:LYS:HG2	1:B:280:GLU:HG2	1.86	0.58
1:C:254:LYS:HG2	1:C:280:GLU:HG2	1.86	0.58
1:D:254:LYS:HG2	1:D:280:GLU:HG2	1.87	0.56
1:A:254:LYS:HG2	1:A:280:GLU:HG2	1.86	0.55
1:D:1:MET:HG3	1:D:122:GLU:HB2	1.89	0.54
1:D:6:MET:HB2	1:D:57:LEU:HD21	1.89	0.54
1:B:107:LEU:HD22	1:B:294:LEU:HD13	1.91	0.51
1:A:110:TRP:NE1	1:A:112:PHE:O	2.44	0.51
1:A:43:THR:HG23	1:A:49:ILE:HG12	1.92	0.50
1:B:218:TYR:HE1	1:B:223:ILE:HD11	1.77	0.50
1:D:107:LEU:HD22	1:D:294:LEU:HD13	1.94	0.50
1:D:250:ALA:HA	1:D:277:PRO:HD3	1.93	0.50
1:A:3:GLY:N	1:A:17:LYS:HZ3	2.09	0.49
1:D:281:TRP:CE3	1:D:284:GLY:HA2	2.47	0.49
1:A:12:VAL:HG13	1:A:44:VAL:HG11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:ARG:O	1:B:329:ASN:ND2	2.47	0.48
1:D:218:TYR:HB3	1:D:223[B]:ILE:HD11	1.95	0.48
1:B:336:LEU:HG	1:B:344:LEU:HD22	1.94	0.48
1:C:258:PRO:HG3	1:D:106:MET:HE2	1.94	0.48
3:B:402:NAP:H6N	3:B:402:NAP:H2D	1.60	0.48
1:C:236:VAL:O	1:C:257:LYS:HG3	2.14	0.48
1:B:281:TRP:CE3	1:B:284:GLY:HA2	2.49	0.47
1:A:62:VAL:HG11	1:A:136:LEU:HD22	1.96	0.47
1:D:32:LEU:HG	1:D:63:GLY:HA2	1.96	0.47
1:A:101:GLN:HB3	1:A:294:LEU:HD23	1.96	0.47
1:C:152:MET:HE1	1:C:316:PRO:HG3	1.96	0.47
1:C:282:GLY:HA3	1:C:286:ALA:HB2	1.97	0.47
1:A:281:TRP:CE3	1:A:284:GLY:HA2	2.50	0.47
1:C:187:LYS:NZ	6:C:504:HOH:O	2.38	0.47
1:A:146:VAL:HG13	1:A:147:MET:HE2	1.96	0.46
1:C:250:ALA:HA	1:C:277:PRO:HD3	1.96	0.46
1:D:325:ARG:O	1:D:329:ASN:ND2	2.49	0.46
1:B:175:ILE:HG21	1:B:196:ALA:HB1	1.98	0.46
1:B:101:GLN:HB3	1:B:294:LEU:HD23	1.98	0.46
1:C:281:TRP:CE3	1:C:284:GLY:HA2	2.51	0.46
1:B:175:ILE:HG12	1:B:198:GLY:HA3	1.97	0.46
1:A:282:GLY:HA3	1:A:286:ALA:HB2	1.97	0.45
3:D:402:NAP:H6N	3:D:402:NAP:H2D	1.62	0.45
3:A:402:NAP:H6N	3:A:402:NAP:H2D	1.59	0.45
1:C:234:LYS:O	1:C:257:LYS:HG2	2.16	0.45
1:C:271:GLY:O	1:D:278:ARG:NE	2.34	0.45
1:B:152:MET:HE1	1:B:316:PRO:HG3	1.99	0.45
1:C:101:GLN:HB3	1:C:294:LEU:HD23	1.98	0.45
1:D:340:LYS:HG2	1:D:344:LEU:HD23	1.99	0.45
1:B:282:GLY:HA3	1:B:286:ALA:HB2	1.99	0.45
1:C:175:ILE:HG21	1:C:196:ALA:HB1	1.99	0.44
1:D:175:ILE:HG21	1:D:196:ALA:HB1	1.99	0.44
1:C:325:ARG:O	1:C:329:ASN:ND2	2.51	0.44
1:D:152:MET:HE1	1:D:316:PRO:HG3	1.99	0.43
1:C:336:LEU:HD23	1:C:336:LEU:HA	1.83	0.43
1:B:165:GLU:OE1	1:C:304:ARG:NH1	2.51	0.43
1:B:38:THR:HG22	1:B:340:LYS:NZ	2.34	0.43
1:C:175:ILE:HG12	1:C:198:GLY:HA3	2.00	0.43
1:C:329:ASN:ND2	6:C:508:HOH:O	2.51	0.42
1:A:248:ILE:HD12	1:A:248:ILE:HA	1.89	0.42
1:B:2:LYS:HA	1:B:16:GLU:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:37:CYS:HA	1:D:346:LYS:HZ2	1.84	0.42
1:D:175:ILE:HG12	1:D:198:GLY:HA3	2.01	0.42
1:A:20:PRO:HG2	1:A:28:ILE:HD12	2.02	0.42
1:A:278:ARG:HD2	1:B:268:PHE:O	2.19	0.42
1:A:280:GLU:OE1	1:A:280:GLU:N	2.52	0.42
1:B:20:PRO:HG2	1:B:28:ILE:HD12	2.01	0.42
1:A:107:LEU:HD22	1:A:294:LEU:HD13	2.01	0.42
1:C:7:LEU:HD12	1:C:11:LYS:HG2	2.01	0.41
1:C:151:MET:SD	1:C:177:PRO:HB2	2.61	0.41
3:C:402:NAP:H2D	3:C:402:NAP:H6N	1.64	0.41
1:B:318:LYS:HE3	6:B:535:HOH:O	2.21	0.41
1:B:248:ILE:HD12	1:B:248:ILE:HA	1.90	0.41
1:D:209:TYR:CE2	1:D:318:LYS:HG3	2.55	0.41
1:B:146:VAL:HG13	1:B:147:MET:HE2	2.02	0.41
1:C:1:MET:HG2	1:C:17:LYS:O	2.21	0.41
1:A:341:PRO:HD2	1:A:344:LEU:HB3	2.04	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	348/352 (99%)	334 (96%)	14 (4%)	0	100	100
1	B	351/352 (100%)	340 (97%)	11 (3%)	0	100	100
1	C	350/352 (99%)	339 (97%)	11 (3%)	0	100	100
1	D	353/352 (100%)	342 (97%)	11 (3%)	0	100	100
All	All	1402/1408 (100%)	1355 (97%)	47 (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	271/273 (99%)	270 (100%)	1 (0%)	91	95
1	B	274/273 (100%)	274 (100%)	0	100	100
1	C	273/273 (100%)	272 (100%)	1 (0%)	91	95
1	D	276/273 (101%)	276 (100%)	0	100	100
All	All	1094/1092 (100%)	1092 (100%)	2 (0%)	93	96

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

Mol	Chain	Res	Type
1	A	106	MET
1	C	106	MET

Sometimes 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 15 ligands modelled in this entry, 8 are monoatomic - leaving 7 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	$\# Z  > 2$
3	NAP	C	402	-	45,52,52	4.60	16 (35%)	56,80,80	1.85	8 (14%)
3	NAP	D	402	-	45,52,52	4.61	16 (35%)	56,80,80	1.85	9 (16%)
4	VF4	A	403	-	8,8,8	0.52	0	10,10,10	0.98	1 (10%)
4	VF4	D	403	-	8,8,8	0.48	0	10,10,10	2.02	4 (40%)
3	NAP	A	402	-	45,52,52	4.65	18 (40%)	56,80,80	1.79	8 (14%)
4	VF4	B	403	-	8,8,8	0.48	0	10,10,10	1.28	1 (10%)
3	NAP	B	402	-	45,52,52	4.61	17 (37%)	56,80,80	1.79	9 (16%)

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
3	NAP	C	402	-	-	17/31/67/67	0/5/5/5
3	NAP	D	402	-	-	16/31/67/67	0/5/5/5
4	VF4	A	403	-	-	-	0/1/1/1
4	VF4	D	403	-	-	-	0/1/1/1
3	NAP	A	402	-	-	15/31/67/67	0/5/5/5
4	VF4	B	403	-	-	-	0/1/1/1
3	NAP	B	402	-	-	16/31/67/67	0/5/5/5

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	NAP	C2D-C1D	-14.98	1.31	1.53
3	B	402	NAP	O4D-C1D	14.95	1.61	1.41
3	D	402	NAP	C2D-C1D	-14.91	1.31	1.53
3	A	402	NAP	C2D-C1D	-14.91	1.31	1.53
3	A	402	NAP	O4D-C1D	14.91	1.61	1.41
3	D	402	NAP	O4D-C1D	14.90	1.61	1.41
3	A	402	NAP	O4B-C1B	14.85	1.61	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	NAP	O4D-C1D	14.83	1.61	1.41
3	B	402	NAP	C2D-C1D	-14.82	1.31	1.53
3	D	402	NAP	O4B-C1B	14.66	1.61	1.41
3	B	402	NAP	O4B-C1B	14.62	1.61	1.41
3	C	402	NAP	O4B-C1B	14.51	1.61	1.41
3	C	402	NAP	C7N-N7N	8.94	1.50	1.33
3	B	402	NAP	C7N-N7N	8.93	1.50	1.33
3	A	402	NAP	C7N-N7N	8.92	1.50	1.33
3	D	402	NAP	C7N-N7N	8.90	1.50	1.33
3	A	402	NAP	O4D-C4D	-5.91	1.31	1.45
3	A	402	NAP	O4B-C4B	-5.89	1.31	1.45
3	C	402	NAP	O4D-C4D	-5.84	1.31	1.45
3	C	402	NAP	O4B-C4B	-5.83	1.32	1.45
3	D	402	NAP	O4D-C4D	-5.81	1.32	1.45
3	B	402	NAP	O4B-C4B	-5.79	1.32	1.45
3	B	402	NAP	O4D-C4D	-5.78	1.32	1.45
3	D	402	NAP	O4B-C4B	-5.74	1.32	1.45
3	A	402	NAP	C6A-N6A	5.35	1.53	1.34
3	D	402	NAP	C6A-N6A	5.18	1.53	1.34
3	C	402	NAP	C6A-N6A	5.18	1.53	1.34
3	B	402	NAP	C6A-N6A	5.15	1.52	1.34
3	A	402	NAP	P2B-O2B	4.43	1.67	1.59
3	B	402	NAP	C3N-C7N	4.39	1.57	1.50
3	D	402	NAP	C3N-C7N	4.34	1.57	1.50
3	A	402	NAP	C3N-C7N	4.31	1.57	1.50
3	C	402	NAP	C3N-C7N	4.31	1.57	1.50
3	D	402	NAP	P2B-O2B	4.04	1.66	1.59
3	C	402	NAP	P2B-O2B	3.96	1.66	1.59
3	B	402	NAP	P2B-O2B	3.90	1.66	1.59
3	D	402	NAP	O2D-C2D	3.76	1.51	1.43
3	A	402	NAP	O2D-C2D	3.72	1.51	1.43
3	B	402	NAP	O2D-C2D	3.70	1.51	1.43
3	C	402	NAP	O2D-C2D	3.70	1.51	1.43
3	C	402	NAP	O3D-C3D	-3.18	1.35	1.43
3	A	402	NAP	O3D-C3D	-3.18	1.35	1.43
3	B	402	NAP	O3D-C3D	-3.17	1.35	1.43
3	D	402	NAP	O3D-C3D	-3.15	1.35	1.43
3	D	402	NAP	PA-O5B	2.86	1.70	1.59
3	B	402	NAP	PA-O5B	2.82	1.70	1.59
3	A	402	NAP	PA-O5B	2.79	1.70	1.59
3	C	402	NAP	PA-O5B	2.74	1.70	1.59
3	A	402	NAP	O3B-C3B	-2.65	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	NAP	O3B-C3B	-2.61	1.36	1.43
3	B	402	NAP	O3B-C3B	-2.61	1.36	1.43
3	C	402	NAP	O3B-C3B	-2.52	1.37	1.43
3	B	402	NAP	C5A-C4A	-2.50	1.34	1.40
3	C	402	NAP	C5A-C4A	-2.47	1.34	1.40
3	A	402	NAP	C5A-C4A	-2.45	1.34	1.40
3	D	402	NAP	C5A-C4A	-2.43	1.34	1.40
3	D	402	NAP	C2N-N1N	2.34	1.37	1.35
3	B	402	NAP	C2N-N1N	2.33	1.37	1.35
3	A	402	NAP	C2A-N1A	2.26	1.38	1.33
3	C	402	NAP	C2N-N1N	2.22	1.37	1.35
3	A	402	NAP	C2N-N1N	2.20	1.37	1.35
3	A	402	NAP	C2A-N3A	2.18	1.35	1.32
3	C	402	NAP	C2A-N1A	2.13	1.37	1.33
3	B	402	NAP	C2A-N3A	2.12	1.35	1.32
3	B	402	NAP	C2A-N1A	2.10	1.37	1.33
3	D	402	NAP	C2A-N1A	2.05	1.37	1.33
3	A	402	NAP	O2B-C2B	2.03	1.51	1.44

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	402	NAP	C5A-C6A-N6A	8.12	132.69	120.35
3	C	402	NAP	C5A-C6A-N6A	8.08	132.63	120.35
3	B	402	NAP	C5A-C6A-N6A	7.74	132.11	120.35
3	A	402	NAP	C5A-C6A-N6A	7.70	132.06	120.35
3	B	402	NAP	N3A-C2A-N1A	-5.67	119.81	128.68
3	C	402	NAP	N3A-C2A-N1A	-5.62	119.90	128.68
3	A	402	NAP	N3A-C2A-N1A	-5.61	119.91	128.68
3	D	402	NAP	N3A-C2A-N1A	-5.55	120.01	128.68
3	D	402	NAP	N6A-C6A-N1A	-5.42	107.33	118.57
3	C	402	NAP	N6A-C6A-N1A	-5.37	107.42	118.57
3	B	402	NAP	N6A-C6A-N1A	-5.19	107.79	118.57
3	C	402	NAP	C1B-N9A-C4A	-5.19	117.52	126.64
3	D	402	NAP	C1B-N9A-C4A	-4.98	117.89	126.64
3	A	402	NAP	N6A-C6A-N1A	-4.93	108.34	118.57
3	B	402	NAP	C1B-N9A-C4A	-4.72	118.34	126.64
4	D	403	VF4	C03-C04-C06	4.08	115.84	109.41
3	A	402	NAP	C1B-N9A-C4A	-4.01	119.59	126.64
4	B	403	VF4	C04-C03-C02	-3.19	108.21	112.02
3	A	402	NAP	PN-O3-PA	-3.17	121.95	132.83
4	A	403	VF4	C04-C03-C02	-2.65	108.86	112.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	403	VF4	C03-C02-C08	-2.65	107.39	110.55
3	B	402	NAP	PN-O3-PA	-2.54	124.12	132.83
3	C	402	NAP	PN-O3-PA	-2.43	124.47	132.83
4	D	403	VF4	C05-C04-C06	-2.38	106.91	112.09
3	B	402	NAP	C3D-C2D-C1D	2.29	104.42	100.98
3	D	402	NAP	PN-O3-PA	-2.25	125.09	132.83
3	D	402	NAP	C6N-N1N-C2N	-2.22	119.95	121.97
4	D	403	VF4	C07-C06-C04	2.20	118.15	111.67
3	A	402	NAP	C3D-C2D-C1D	2.19	104.27	100.98
3	D	402	NAP	C3D-C2D-C1D	2.18	104.25	100.98
3	B	402	NAP	C3N-C7N-N7N	2.15	120.33	117.75
3	B	402	NAP	O7N-C7N-N7N	-2.15	119.53	122.58
3	C	402	NAP	C6N-N1N-C2N	-2.12	120.04	121.97
3	D	402	NAP	O7N-C7N-N7N	-2.11	119.58	122.58
3	C	402	NAP	C3N-C7N-N7N	2.11	120.28	117.75
3	D	402	NAP	C3N-C7N-N7N	2.02	120.17	117.75
3	A	402	NAP	O7N-C7N-N7N	-2.01	119.72	122.58
3	B	402	NAP	C6N-N1N-C2N	-2.01	120.14	121.97
3	C	402	NAP	O7N-C7N-N7N	-2.00	119.73	122.58
3	A	402	NAP	C3N-C7N-N7N	2.00	120.16	117.75

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	NAP	O4B-C4B-C5B-O5B
3	A	402	NAP	C2B-O2B-P2B-O1X
3	A	402	NAP	C5D-O5D-PN-O3
3	A	402	NAP	C5D-O5D-PN-O1N
3	A	402	NAP	O4D-C4D-C5D-O5D
3	A	402	NAP	O4D-C1D-N1N-C2N
3	A	402	NAP	O4D-C1D-N1N-C6N
3	A	402	NAP	C2D-C1D-N1N-C2N
3	A	402	NAP	C2D-C1D-N1N-C6N
3	B	402	NAP	C5D-O5D-PN-O3
3	B	402	NAP	C5D-O5D-PN-O1N
3	B	402	NAP	O4D-C1D-N1N-C2N
3	B	402	NAP	O4D-C1D-N1N-C6N
3	B	402	NAP	C2D-C1D-N1N-C2N
3	B	402	NAP	C2D-C1D-N1N-C6N
3	C	402	NAP	C5D-O5D-PN-O3
3	C	402	NAP	O4D-C4D-C5D-O5D

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Mol	Chain	Res	Type	Atoms
3	C	402	NAP	O4D-C1D-N1N-C2N
3	C	402	NAP	O4D-C1D-N1N-C6N
3	C	402	NAP	C2D-C1D-N1N-C2N
3	C	402	NAP	C2D-C1D-N1N-C6N
3	D	402	NAP	C5D-O5D-PN-O1N
3	D	402	NAP	C5D-O5D-PN-O2N
3	D	402	NAP	O4D-C1D-N1N-C2N
3	D	402	NAP	O4D-C1D-N1N-C6N
3	D	402	NAP	C2D-C1D-N1N-C2N
3	D	402	NAP	C2D-C1D-N1N-C6N
3	A	402	NAP	C3B-C4B-C5B-O5B
3	B	402	NAP	O4B-C4B-C5B-O5B
3	B	402	NAP	C3B-C4B-C5B-O5B
3	B	402	NAP	O4D-C4D-C5D-O5D
3	C	402	NAP	O4B-C4B-C5B-O5B
3	C	402	NAP	C3B-C4B-C5B-O5B
3	D	402	NAP	O4B-C4B-C5B-O5B
3	D	402	NAP	C3B-C4B-C5B-O5B
3	D	402	NAP	C3D-C4D-C5D-O5D
3	A	402	NAP	C3D-C4D-C5D-O5D
3	B	402	NAP	C3D-C4D-C5D-O5D
3	C	402	NAP	C3D-C4D-C5D-O5D
3	C	402	NAP	C1B-C2B-O2B-P2B
3	D	402	NAP	C1B-C2B-O2B-P2B
3	A	402	NAP	C3B-C2B-O2B-P2B
3	C	402	NAP	C3B-C2B-O2B-P2B
3	D	402	NAP	C3B-C2B-O2B-P2B
3	D	402	NAP	O4D-C4D-C5D-O5D
3	A	402	NAP	C1B-C2B-O2B-P2B
3	A	402	NAP	PA-O3-PN-O5D
3	B	402	NAP	PN-O3-PA-O5B
3	B	402	NAP	PA-O3-PN-O5D
3	C	402	NAP	PN-O3-PA-O5B
3	C	402	NAP	PA-O3-PN-O5D
3	D	402	NAP	PN-O3-PA-O5B
3	D	402	NAP	PA-O3-PN-O5D
3	B	402	NAP	C2B-O2B-P2B-O1X
3	C	402	NAP	C2B-O2B-P2B-O1X
3	C	402	NAP	C5D-O5D-PN-O1N
3	B	402	NAP	C3B-C2B-O2B-P2B
3	B	402	NAP	C1B-C2B-O2B-P2B
3	A	402	NAP	PN-O3-PA-O5B

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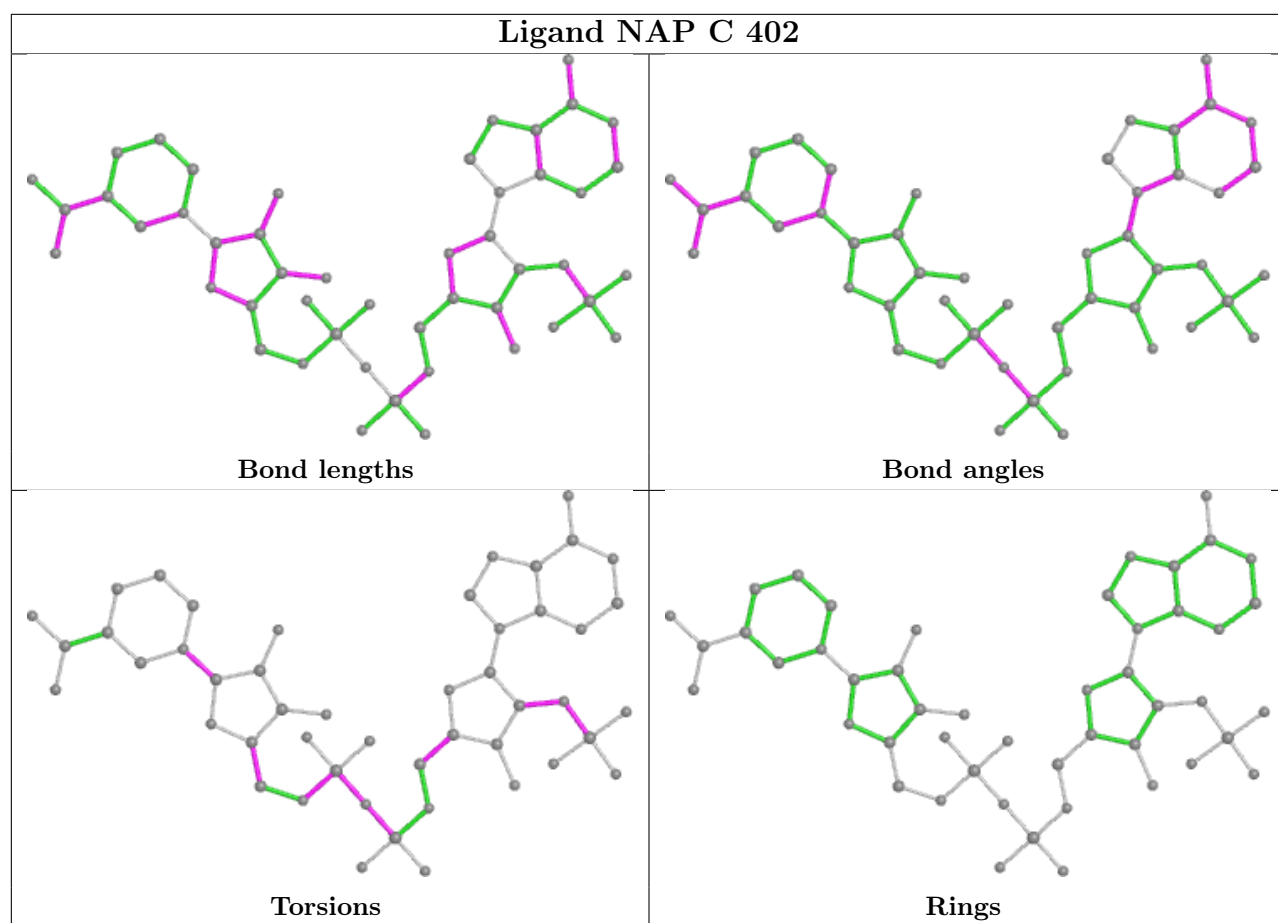
Mol	Chain	Res	Type	Atoms
3	D	402	NAP	C2B-O2B-P2B-O1X
3	B	402	NAP	C2B-O2B-P2B-O2X
3	C	402	NAP	C2B-O2B-P2B-O2X
3	D	402	NAP	C5D-O5D-PN-O3
3	C	402	NAP	C5D-O5D-PN-O2N

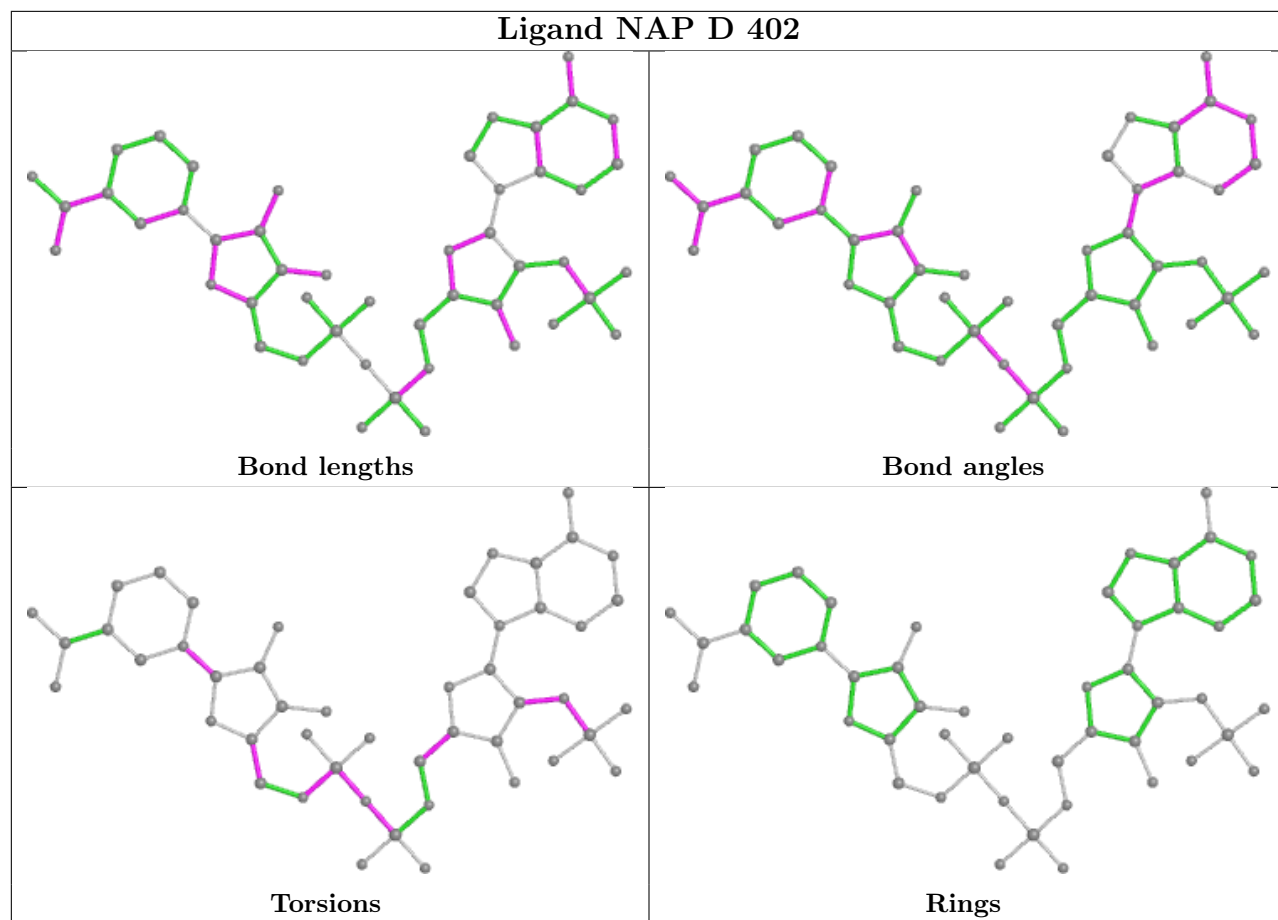
There are no ring outliers.

4 monomers are involved in 4 short contacts:

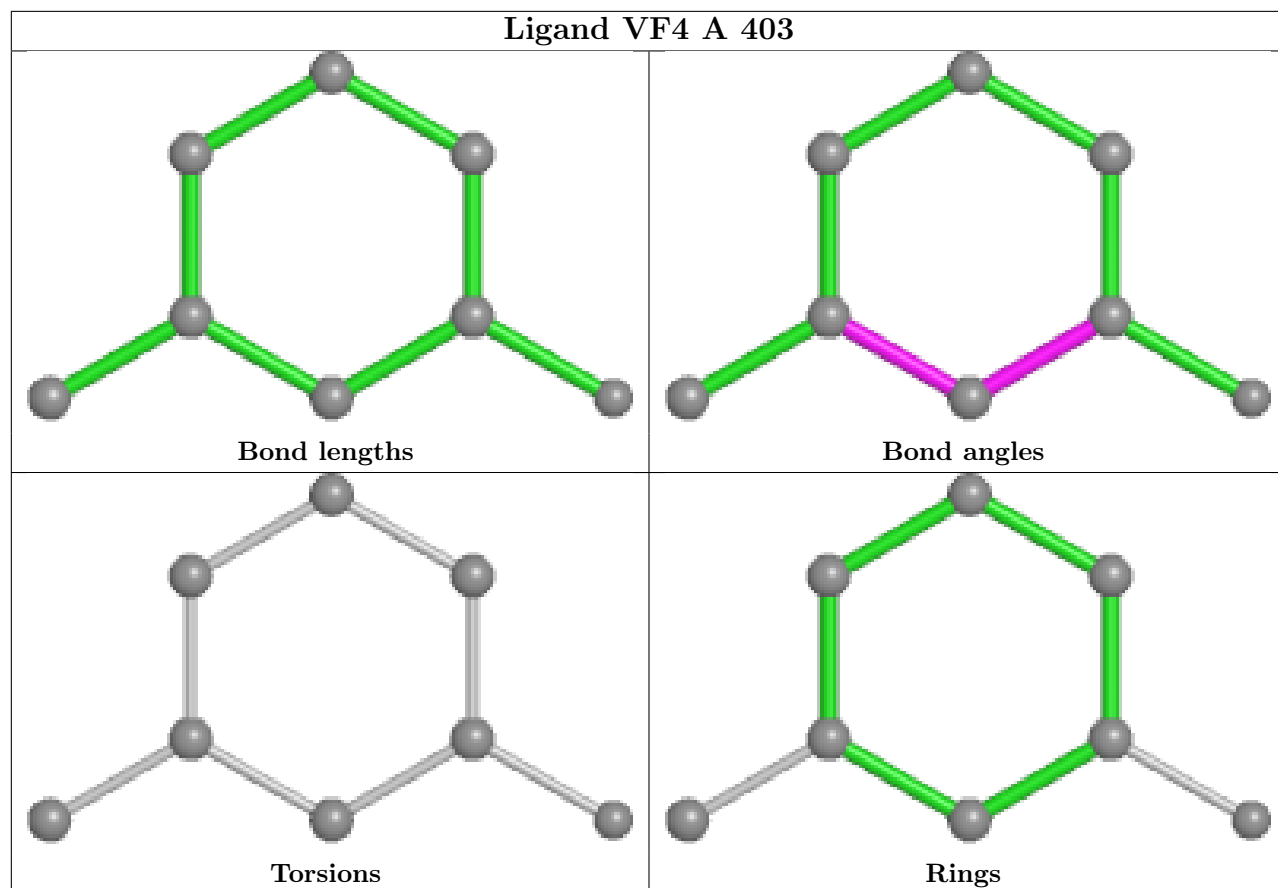
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	402	NAP	1	0
3	D	402	NAP	1	0
3	A	402	NAP	1	0
3	B	402	NAP	1	0

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.

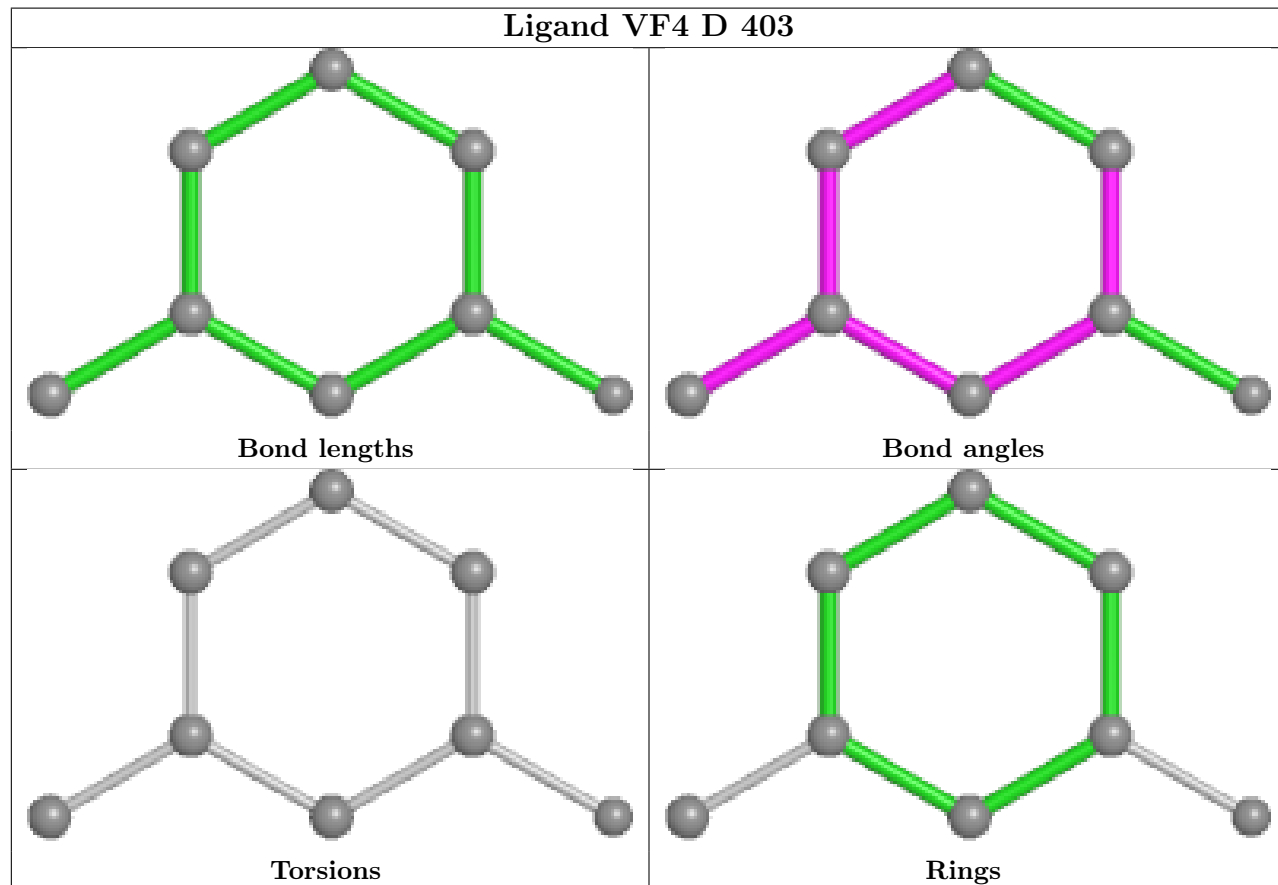


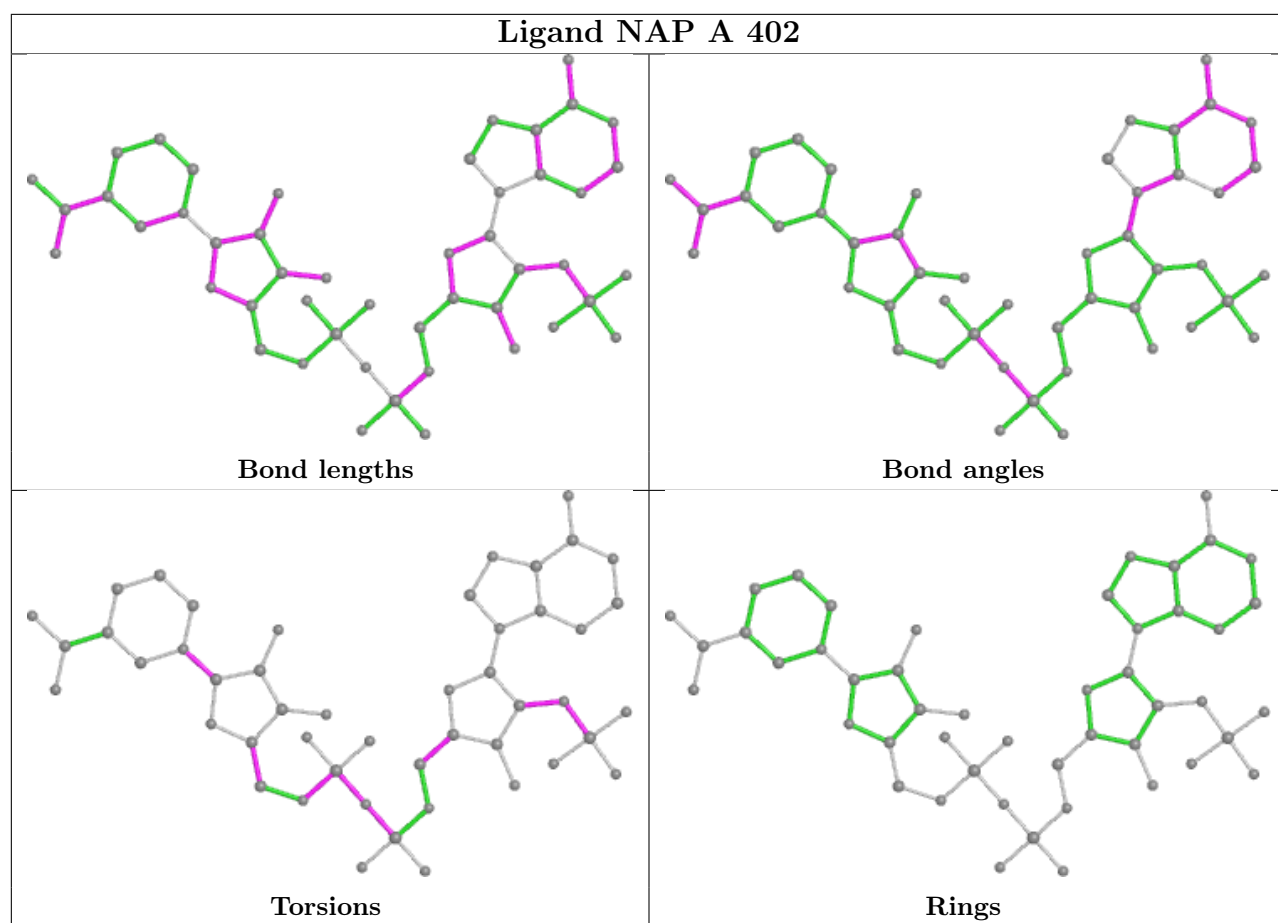


## Ligand VF4 A 403

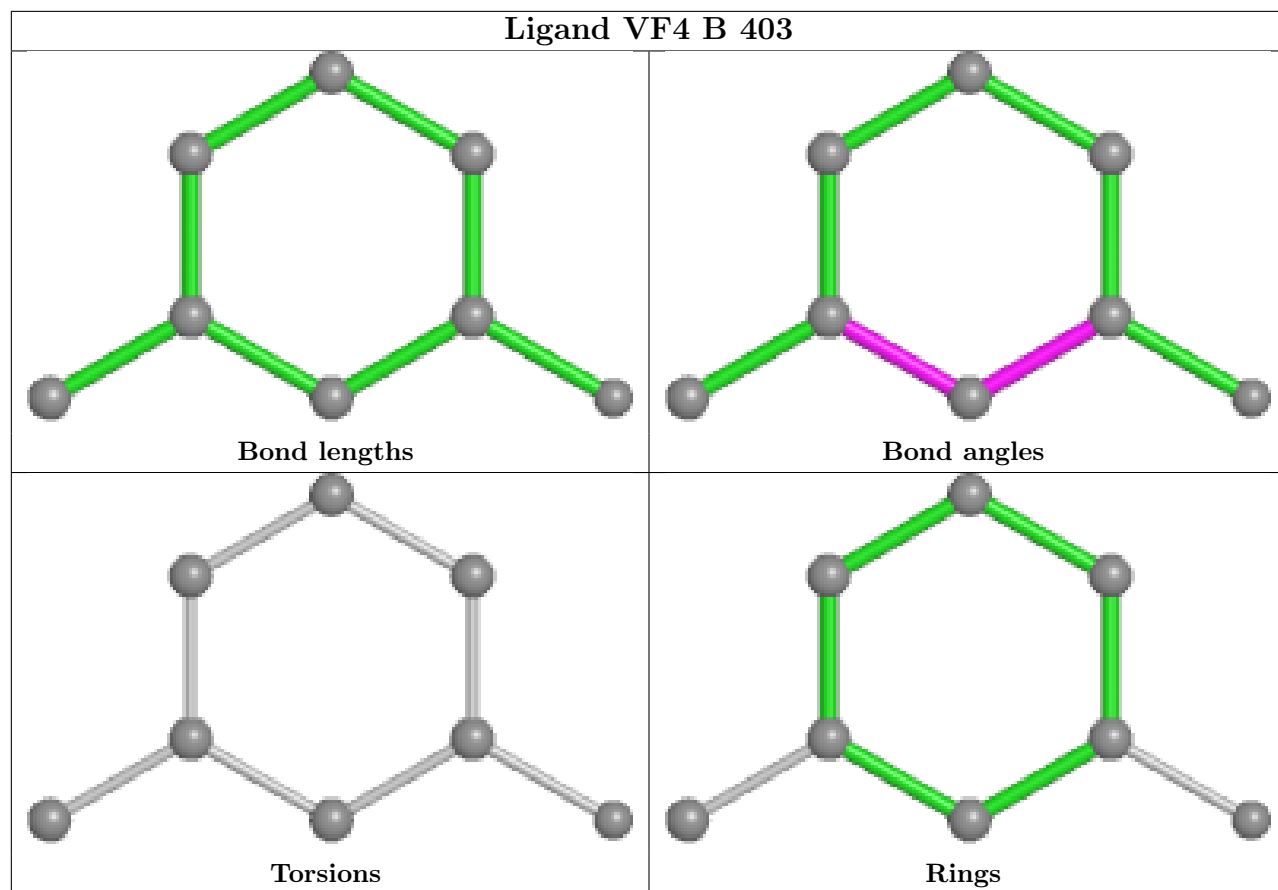


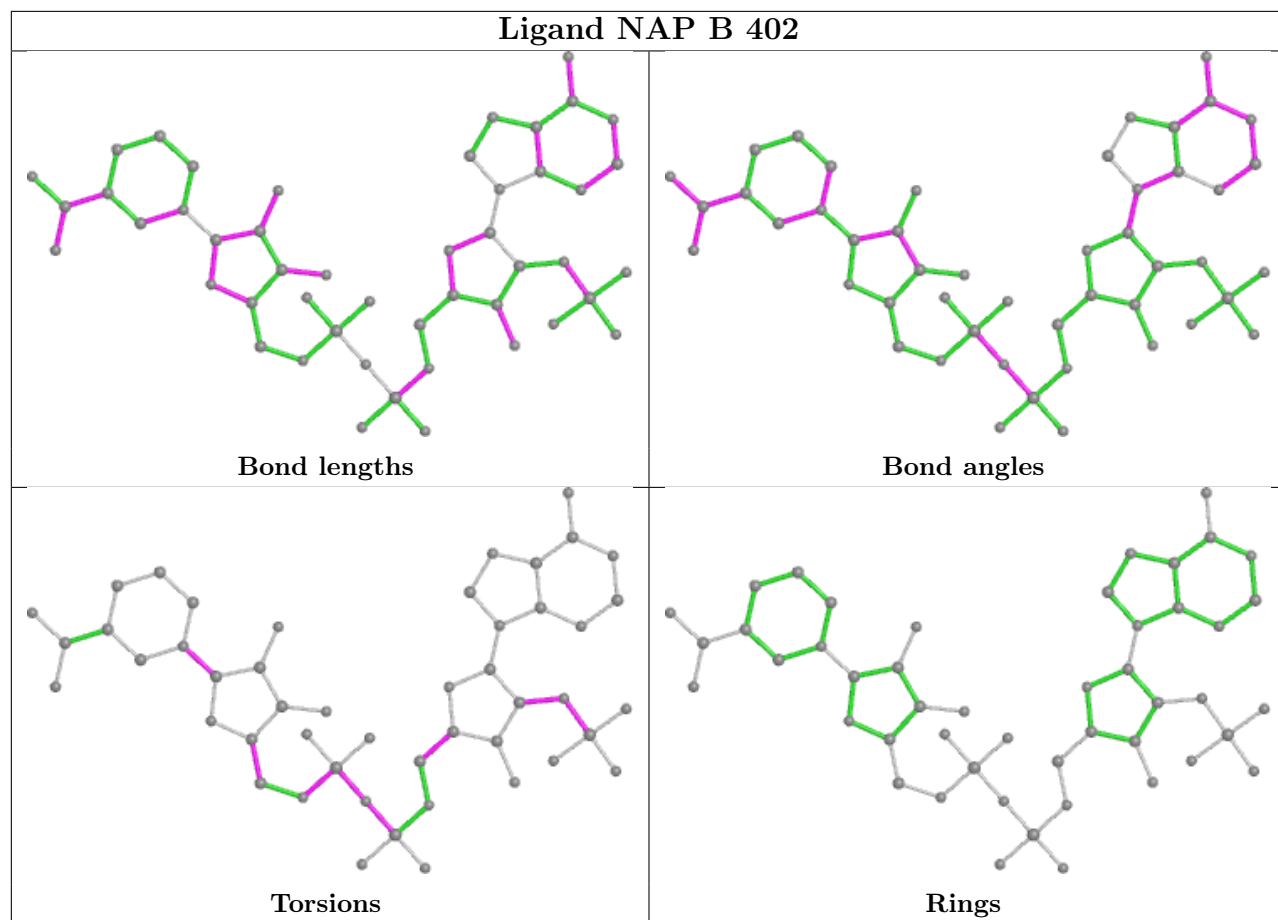
## Ligand VF4 D 403











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	350/352 (99%)	0.51	29 (8%)	11 17	38, 68, 117, 140	0
1	B	352/352 (100%)	0.13	4 (1%)	80 86	34, 51, 82, 133	0
1	C	352/352 (100%)	0.14	9 (2%)	56 64	29, 52, 94, 126	0
1	D	352/352 (100%)	0.08	3 (0%)	84 89	33, 49, 71, 114	0
All	All	1406/1408 (99%)	0.21	45 (3%)	47 58	29, 53, 100, 140	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	352	ALA	7.3
1	A	14	TRP	6.3
1	B	218	TYR	5.7
1	A	45	PHE	5.5
1	A	352	ALA	5.4
1	A	7	LEU	5.0
1	A	49	ILE	4.7
1	B	352	ALA	4.5
1	A	4	PHE	4.3
1	A	218	TYR	4.2
1	A	335	MET	4.0
1	B	219	LYS	3.5
1	A	12	VAL	3.4
1	A	327	PHE	3.4
1	C	15	ILE	3.1
1	A	9	ILE	3.1
1	C	49	ILE	3.0
1	A	334	PHE	3.0
1	A	15	ILE	2.9
1	A	51	GLU	2.9
1	A	351	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	339	ASP	2.7
1	A	325	ARG	2.7
1	A	120	PHE	2.6
1	A	336	LEU	2.6
1	A	342	LYS	2.6
1	A	220	ASP	2.6
1	A	53	HIS	2.5
1	D	110	TRP	2.5
1	B	54	ASN	2.5
1	C	48	ALA	2.5
1	A	62	VAL	2.4
1	A	21	ALA	2.4
1	C	221	GLY	2.3
1	C	2	LYS	2.3
1	D	339	ASP	2.3
1	A	64	GLU	2.2
1	C	340	LYS	2.1
1	C	327	PHE	2.1
1	A	63	GLY	2.1
1	A	324	PHE	2.1
1	C	352	ALA	2.1
1	A	56	ILE	2.0
1	A	332	LYS	2.0
1	C	339	ASP	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](#)

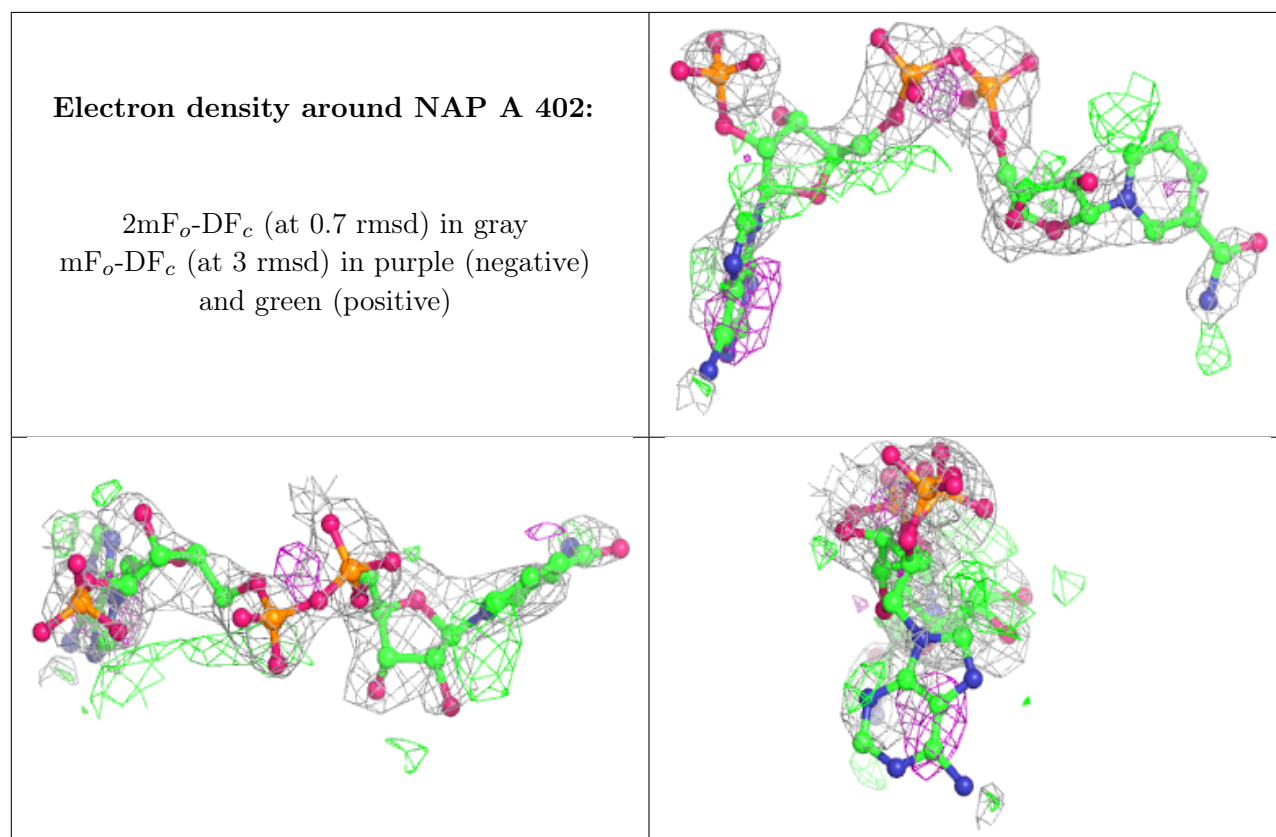
There are no monosaccharides in this entry.

## 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.

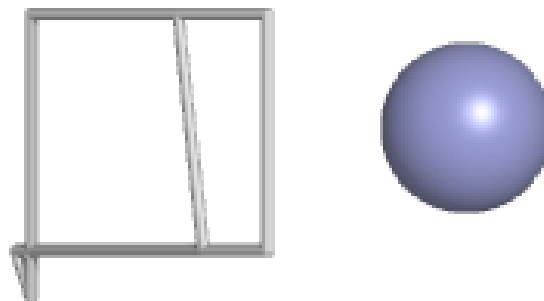
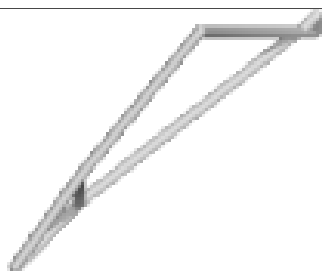
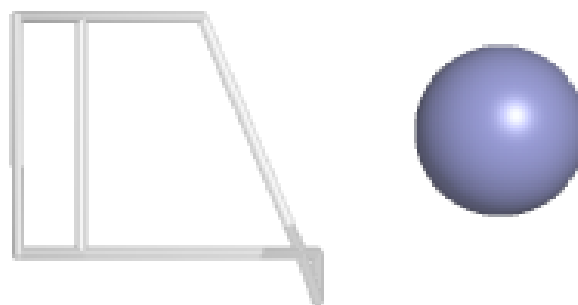
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAP	A	402	48/48	0.73	0.32	56,82,99,109	48
2	ZN	A	401	1/1	0.81	0.11	79,79,79,79	1
3	NAP	B	402	48/48	0.84	0.25	47,66,87,101	48
4	VF4	B	403	8/8	0.84	0.38	59,66,72,78	8
2	ZN	B	401	1/1	0.85	0.14	55,55,55,55	1
4	VF4	A	403	8/8	0.87	0.36	73,85,94,95	0
4	VF4	D	403	8/8	0.88	0.27	50,62,69,72	8
3	NAP	D	402	48/48	0.91	0.24	43,67,78,91	48
2	ZN	D	401	1/1	0.91	0.13	54,54,54,54	1
5	K	B	404	1/1	0.91	0.09	55,55,55,55	0
3	NAP	C	402	48/48	0.92	0.20	45,63,80,86	48
5	K	A	404	1/1	0.94	0.10	62,62,62,62	0
2	ZN	C	401	1/1	0.94	0.15	58,58,58,58	1
5	K	C	403	1/1	0.96	0.12	52,52,52,52	0
5	K	D	404	1/1	0.96	0.10	55,55,55,55	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.



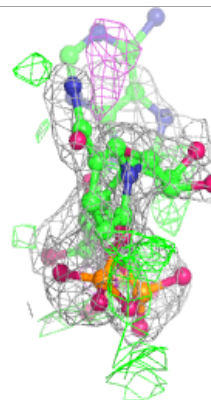
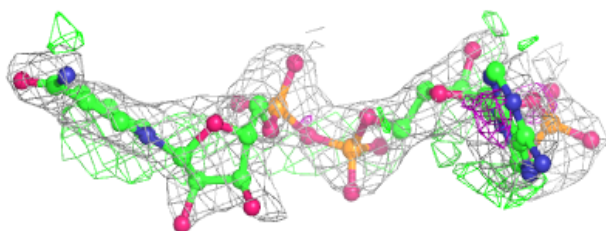
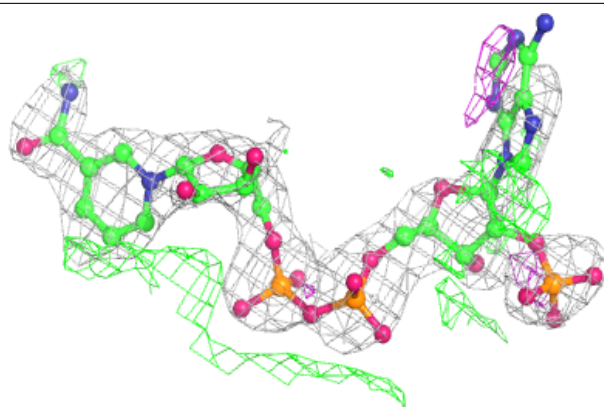
**Electron density around ZN A 401:**

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



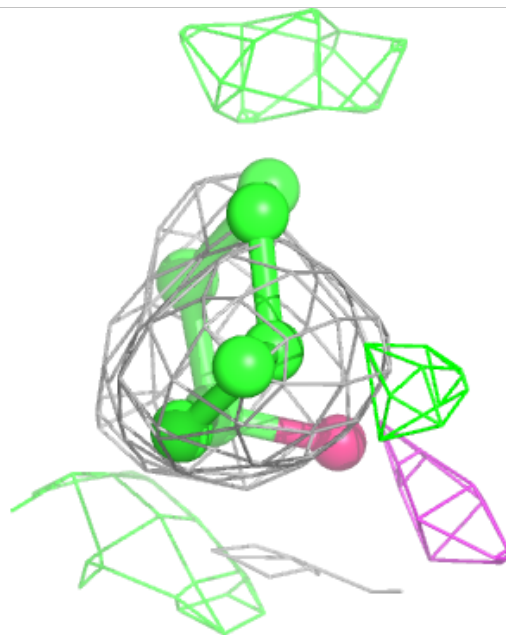
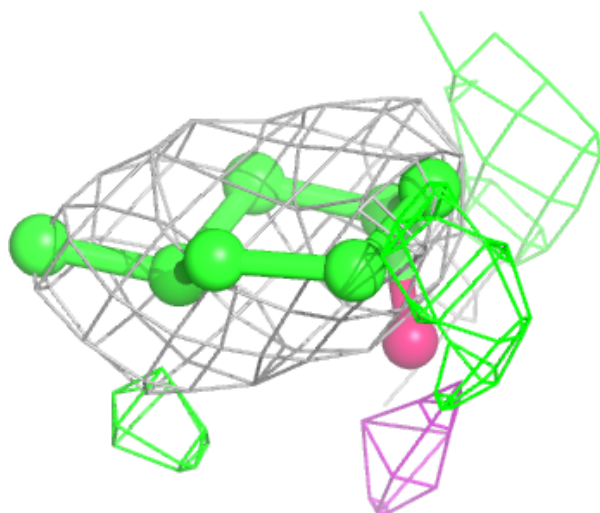
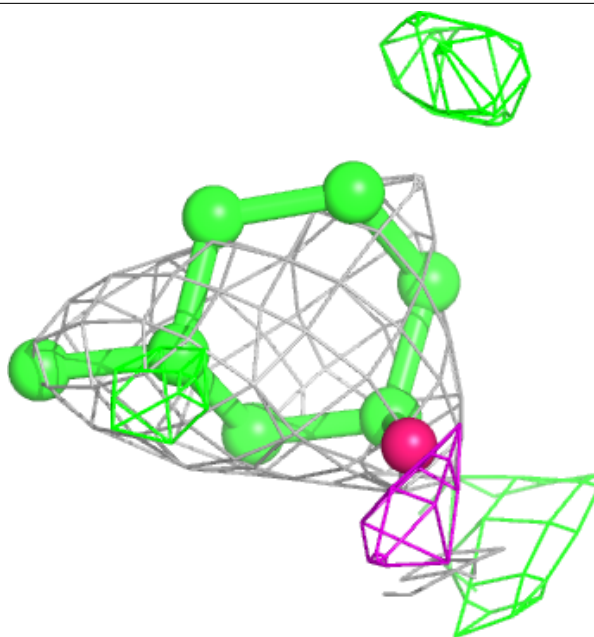
**Electron density around NAP B 402:**

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



**Electron density around VF4 B 403:**

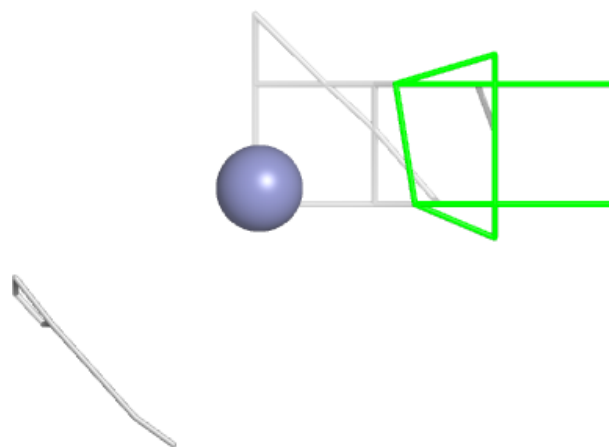
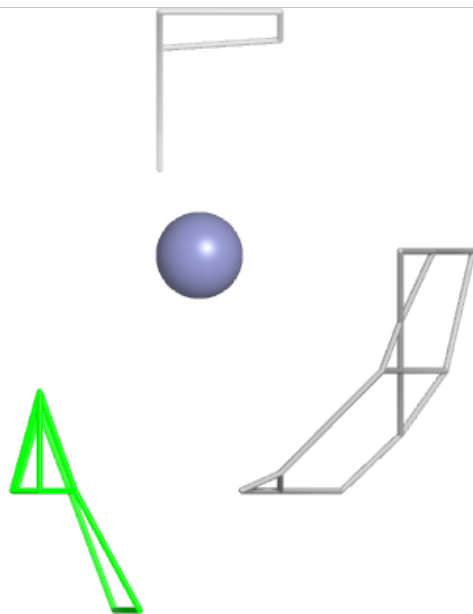
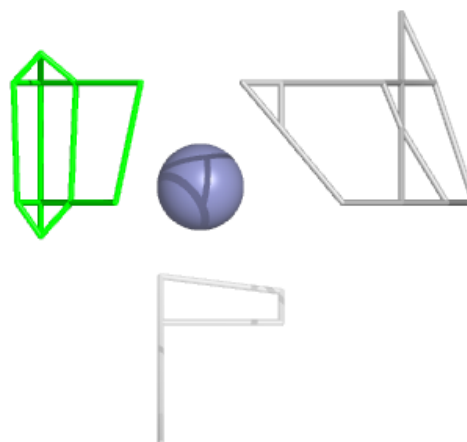
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





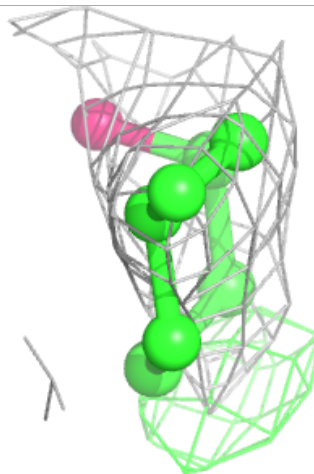
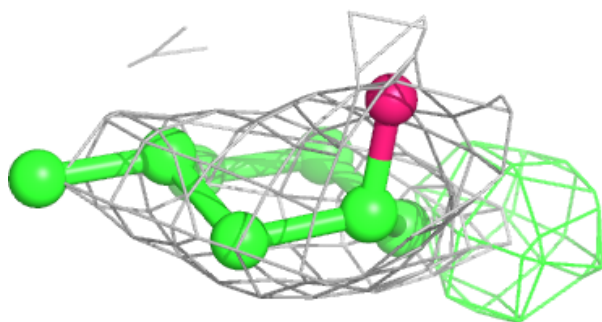
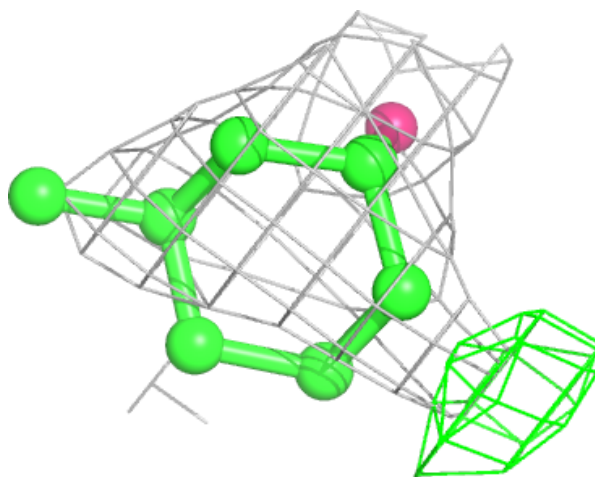
**Electron density around ZN B 401:**

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



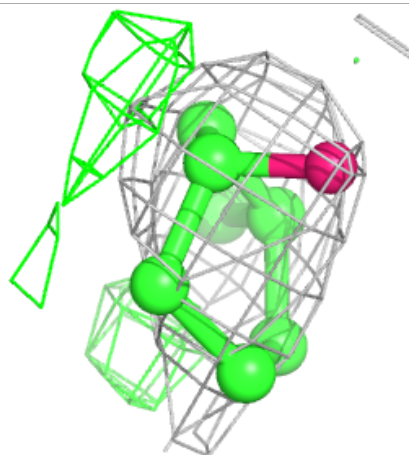
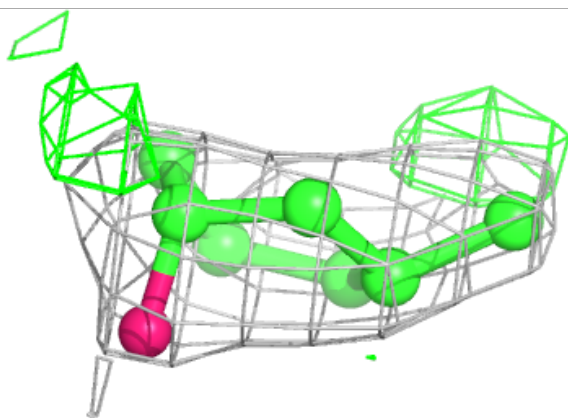
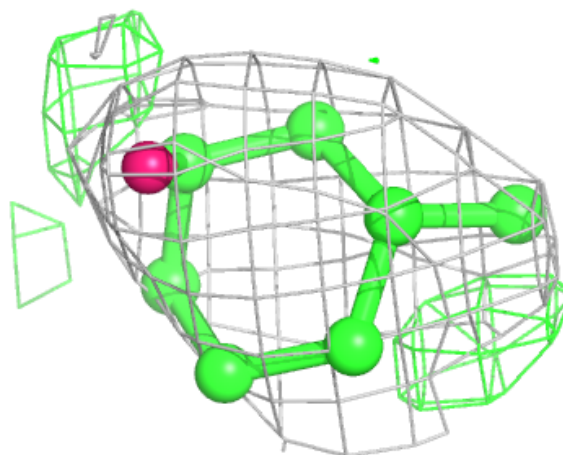
**Electron density around VF4 A 403:**

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



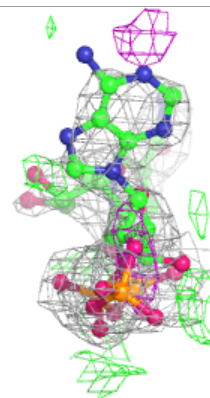
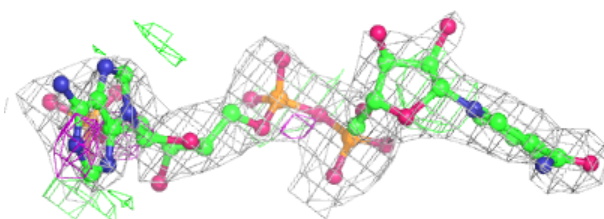
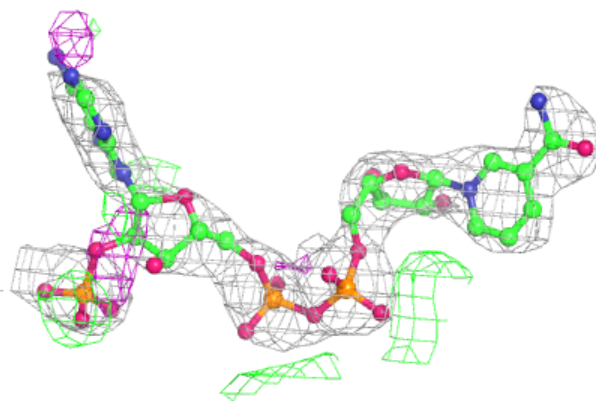
**Electron density around VF4 D 403:**

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

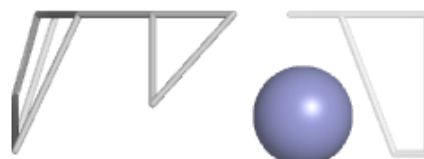
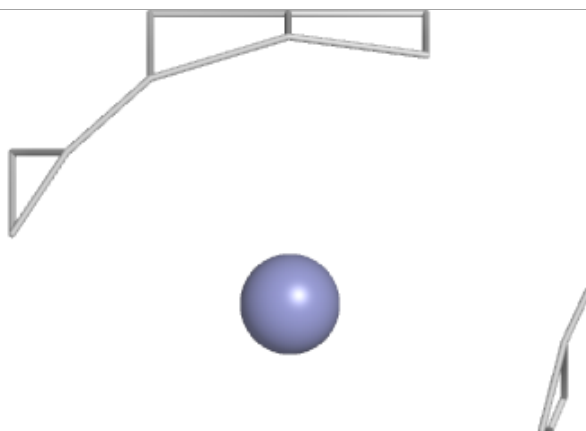
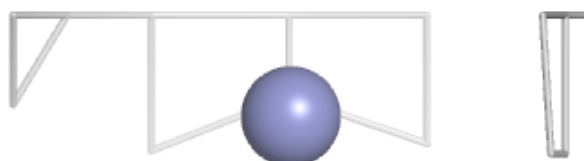


**Electron density around NAP D 402:**

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

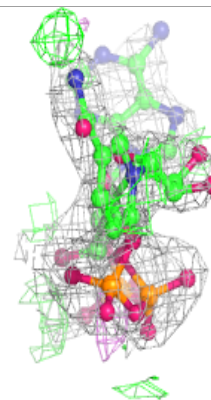
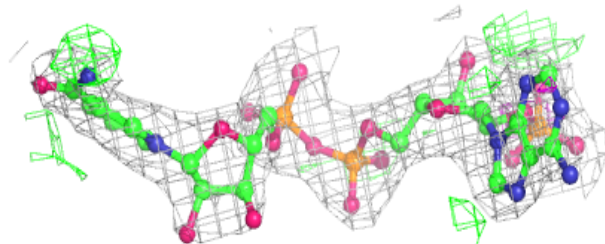
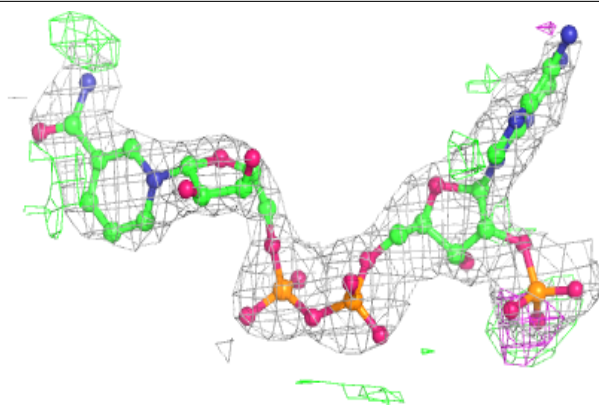
**Electron density around ZN D 401:**

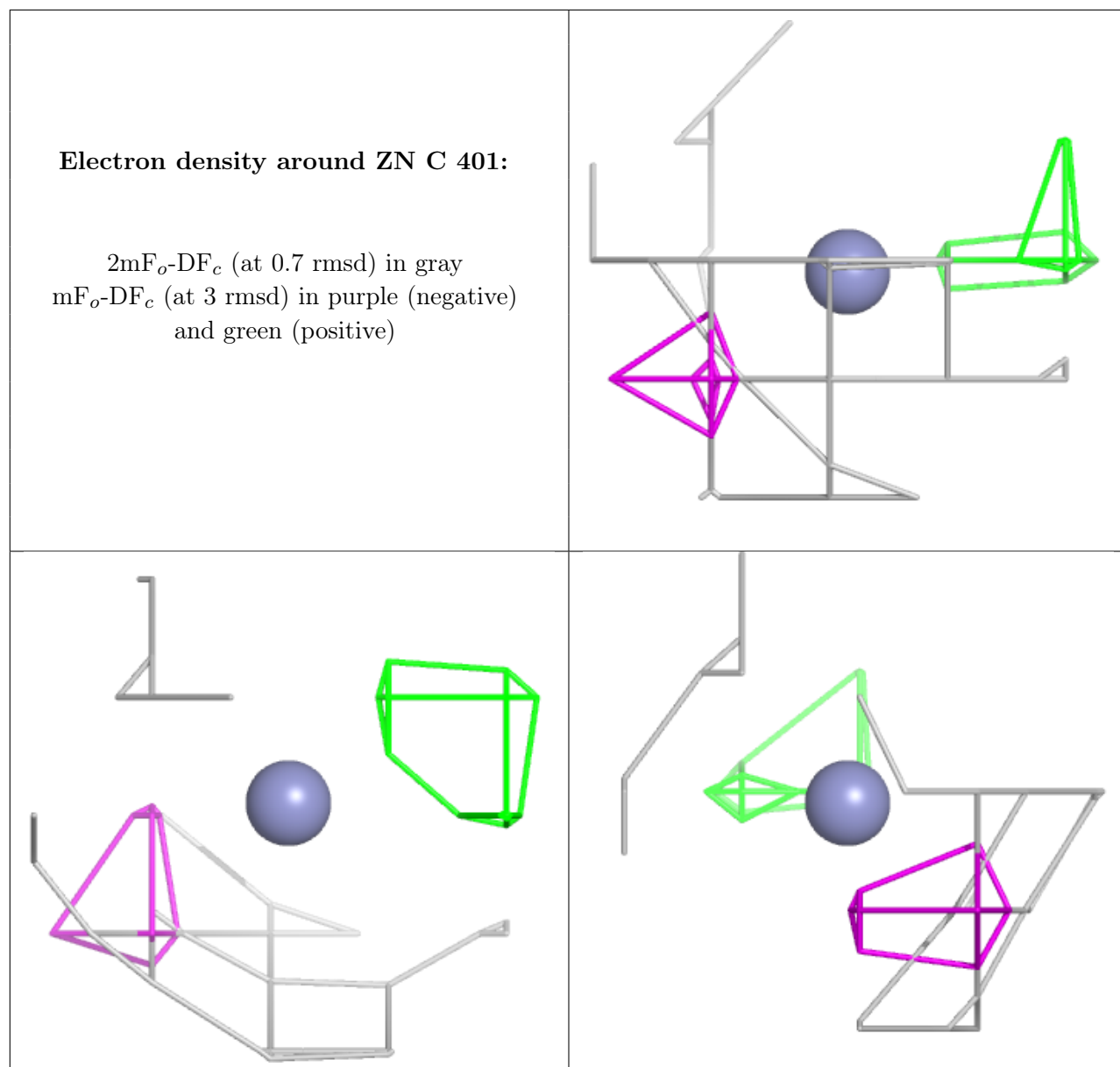
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around NAP C 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 ⓘ

There are no such residues in this entry.