



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 11:19 pm BST

PDB ID : 1NYT  
Title : SHIKIMATE DEHYDROGENASE AroE COMPLEXED WITH NADP+  
Authors : Roszak, A.W.; Lapthorn, A.J.  
Deposited on : 2003-02-13  
Resolution : 1.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

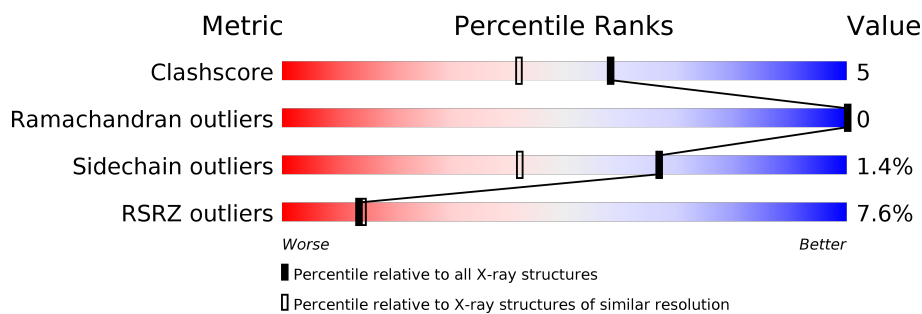
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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))
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	271	<div> <div>6%</div> <div> <div></div> <div>95%</div> <div>5%</div> </div> </div>
1	B	271	<div> <div>3%</div> <div> <div></div> <div>93%</div> <div>7%</div> </div> </div>
1	C	271	<div> <div>10%</div> <div> <div></div> <div>93%</div> <div>7%</div> <div></div> </div> </div>
1	D	271	<div> <div>12%</div> <div> <div></div> <div>93%</div> <div>6%</div> <div></div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	1404	-	-	X	-
2	SO4	C	1423	-	-	X	-
4	DTV	A	1405	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9929 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 Shikimate 5-dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	6	0
			2088	1331	358	391	8			
1	B	271	Total	C	N	O	S	0	8	0
			2090	1329	359	393	9			
1	C	269	Total	C	N	O	S	0	6	0
			2066	1314	355	388	9			
1	D	270	Total	C	N	O	S	0	10	0
			2082	1323	355	395	9			

- Molecule 2 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



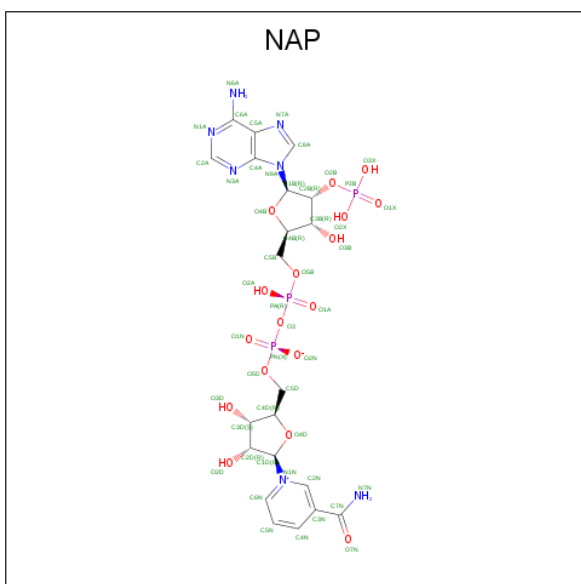
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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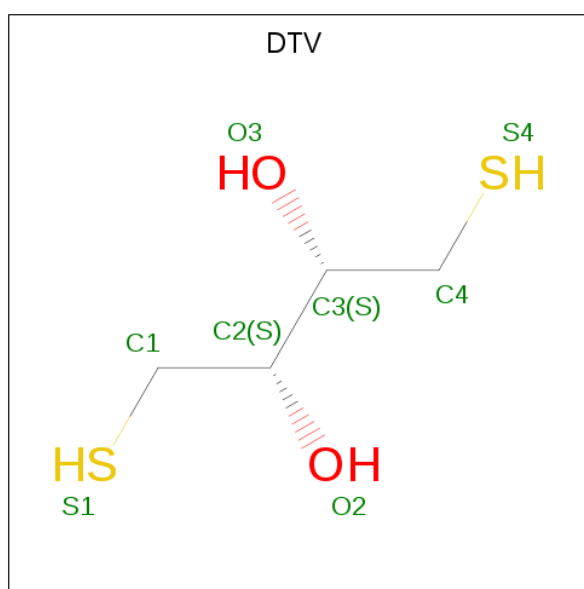
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	C	1	Total 5	O 4	S 1	0	0
2	C	1	Total 5	O 4	S 1	0	0
2	C	1	Total 5	O 4	S 1	0	0
2	C	1	Total 5	O 4	S 1	0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

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ).



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

- Molecule 4 is (2S,3S)-1,4-DIMERCAPTOBUTANE-2,3-DIOL (three-letter code: DTV) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			8	4	2	2		

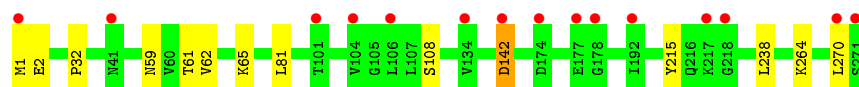
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	365	Total	O	0	0
			365	365		
5	B	391	Total	O	0	0
			391	391		
5	C	302	Total	O	0	0
			302	302		
5	D	275	Total	O	0	0
			275	275		

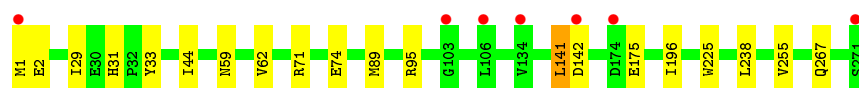
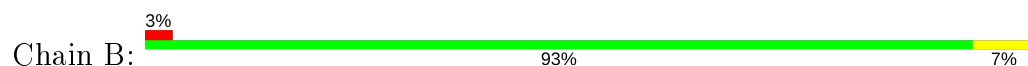
### 3 Residue-property plots [i](#)

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.

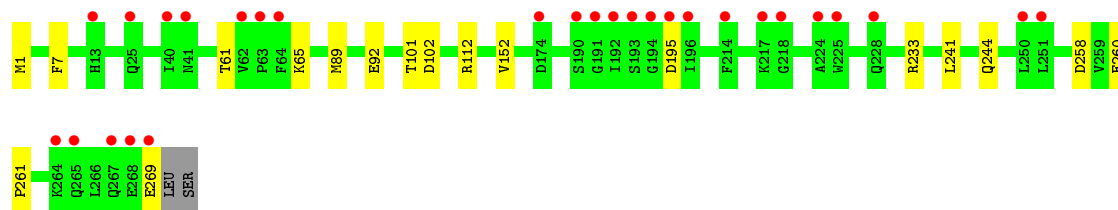
- Molecule 1: Shikimate 5-dehydrogenase



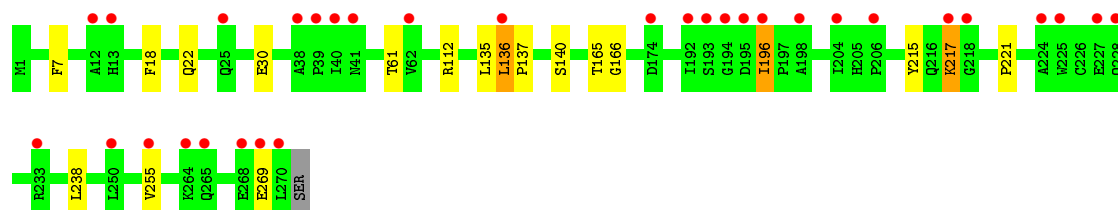
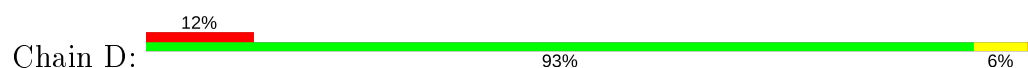
- Molecule 1: Shikimate 5-dehydrogenase



- Molecule 1: Shikimate 5-dehydrogenase



- Molecule 1: Shikimate 5-dehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.52Å 140.02Å 102.71Å 90.00° 122.07° 90.00°	Depositor
Resolution (Å)	38.92 – 1.50 38.92 – 1.50	Depositor EDS
% Data completeness (in resolution range)	93.1 (38.92-1.50) 93.1 (38.92-1.50)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.29 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.1.27	Depositor
R, $R_{free}$	0.132 , 0.169 0.164 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.7	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 54.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.087 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	9929	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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: NAP, SO4, DTV

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	0.82	0/2162	0.85	1/2934 (0.0%)
1	B	0.83	1/2174 (0.0%)	0.84	0/2949
1	C	0.79	0/2139	0.90	7/2901 (0.2%)
1	D	0.76	0/2175	0.88	2/2954 (0.1%)
All	All	0.80	1/8650 (0.0%)	0.87	10/11738 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	175	GLU	CD-OE1	6.85	1.33	1.25

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	112	ARG	NE-CZ-NH2	-9.12	115.74	120.30
1	D	112	ARG	NE-CZ-NH2	-8.73	115.93	120.30
1	D	112	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	C	112	ARG	NE-CZ-NH1	7.29	123.94	120.30
1	C	233	ARG	NE-CZ-NH2	7.04	123.82	120.30
1	C	258[A]	ASP	CB-CG-OD2	6.08	123.77	118.30
1	C	258[B]	ASP	CB-CG-OD2	6.08	123.77	118.30
1	A	142	ASP	CB-CG-OD2	5.71	123.44	118.30
1	C	195	ASP	CB-CG-OD2	5.23	123.01	118.30
1	C	102	ASP	CB-CG-OD1	5.09	122.88	118.30

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	2088	0	2086	27	0
1	B	2090	0	2086	14	0
1	C	2066	0	2057	15	0
1	D	2082	0	2064	19	0
2	A	20	0	0	4	0
2	B	20	0	0	0	0
2	C	20	0	0	2	0
2	D	10	0	0	0	0
3	A	48	0	25	6	0
3	B	48	0	25	0	0
3	C	48	0	25	0	0
3	D	48	0	25	0	0
4	A	8	0	10	12	0
5	A	365	0	0	9	0
5	B	391	0	0	4	0
5	C	302	0	0	6	0
5	D	275	0	0	8	0
All	All	9929	0	8403	82	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 5.

All (82) 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)
5:A:1671:HOH:O	1:C:89[B]:MET:HE1	1.05	1.21
2:A:1404:SO4:O3	5:A:1681:HOH:O	1.59	1.20
1:D:140[A]:SER:OG	5:D:1601:HOH:O	1.63	1.15
5:A:1671:HOH:O	1:C:89[B]:MET:CE	1.68	1.08
1:A:215[B]:TYR:CE2	1:A:238[B]:LEU:HD21	1.93	1.02
1:D:30[A]:GLU:OE2	5:D:1626:HOH:O	1.76	1.02
1:A:215[B]:TYR:CD2	1:A:238[B]:LEU:CD2	2.44	1.01
1:A:215[B]:TYR:CE2	1:A:238[B]:LEU:CD2	2.46	0.98
1:B:89[B]:MET:CE	5:D:1499:HOH:O	2.12	0.96
1:A:215[B]:TYR:CD2	1:A:238[B]:LEU:HD21	2.01	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:LEU:HD11	1:C:92:GLU:HG3	1.55	0.87
1:A:215[B]:TYR:CD2	1:A:238[B]:LEU:HD23	2.14	0.83
1:C:152[B]:VAL:HG13	5:C:1708:HOH:O	1.78	0.82
1:D:217:LYS:H	1:D:217:LYS:HD3	1.46	0.79
1:D:196[A]:ILE:HD11	1:D:221:PRO:O	1.84	0.78
2:A:1404:SO4:O2	4:A:1405:DTV:H3	1.84	0.78
2:A:1404:SO4:S	5:A:1681:HOH:O	2.31	0.76
1:A:108[A]:SER:OG	5:A:1527:HOH:O	2.02	0.76
1:B:89[B]:MET:HE1	5:D:1499:HOH:O	1.81	0.75
1:A:215[B]:TYR:CE2	1:A:238[B]:LEU:HD23	2.22	0.74
1:C:152[B]:VAL:CG1	5:C:1708:HOH:O	2.34	0.74
3:A:1401:NAP:C4N	4:A:1405:DTV:H4C1	2.19	0.73
1:D:196[A]:ILE:HG23	5:D:1625:HOH:O	1.92	0.70
1:A:61:THR:OG1	4:A:1405:DTV:S4	2.25	0.68
1:A:61:THR:HG1	4:A:1405:DTV:H4	0.79	0.68
1:C:241:LEU:HD11	5:C:1480:HOH:O	1.94	0.68
1:A:65:LYS:HZ1	4:A:1405:DTV:H2	1.59	0.66
5:B:1578:HOH:O	1:D:255[B]:VAL:HG13	1.96	0.64
1:B:59[B]:ASN:ND2	5:B:1775:HOH:O	2.31	0.64
1:D:136:LEU:HD13	1:D:165:THR:HG21	1.81	0.62
1:C:89[A]:MET:CE	5:C:1626:HOH:O	2.47	0.62
1:A:215[B]:TYR:HE2	1:A:238[B]:LEU:HD21	1.61	0.61
1:A:2[A]:GLU:OE1	1:A:32:PRO:CB	2.49	0.61
1:B:89[B]:MET:HE3	5:D:1499:HOH:O	1.87	0.60
1:B:62:VAL:HG13	5:B:1815:HOH:O	2.01	0.59
1:A:215[A]:TYR:OH	5:A:1724:HOH:O	2.00	0.59
1:A:81:LEU:CD1	1:C:92:GLU:HG3	2.29	0.58
1:D:7:PHE:O	1:D:61[A]:THR:HG22	2.03	0.58
1:B:29:ILE:O	1:B:29:ILE:HG22	2.04	0.57
1:D:217:LYS:CD	1:D:217:LYS:H	2.12	0.56
1:D:166:GLY:HA2	5:D:1641:HOH:O	2.04	0.56
1:A:238[B]:LEU:HD11	1:A:270:LEU:HD12	1.86	0.56
1:B:31:HIS:HE1	5:D:1528:HOH:O	1.88	0.56
1:B:141:LEU:O	1:B:142:ASP:HB3	2.04	0.55
1:A:1:MET:O	1:A:1:MET:HG2	2.06	0.55
1:C:61:THR:OG1	2:C:1423:SO4:O2	2.24	0.54
2:A:1404:SO4:O2	4:A:1405:DTV:H1C2	2.08	0.53
1:A:62[A]:VAL:HG13	5:A:1523:HOH:O	2.08	0.53
1:D:215:TYR:CB	1:D:238:LEU:HD22	2.39	0.52
1:C:101:THR:O	1:C:244:GLN:HG2	2.09	0.51
1:A:59:ASN:HB3	4:A:1405:DTV:S1	2.50	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:LEU:HB3	1:D:137:PRO:HD3	1.93	0.51
1:D:196[A]:ILE:HD11	1:D:221:PRO:C	2.30	0.51
1:B:238:LEU:HD23	1:B:267[A]:GLN:HG3	1.93	0.50
1:A:238[B]:LEU:HD11	1:A:270:LEU:CD1	2.43	0.49
3:A:1401:NAP:C5N	4:A:1405:DTV:H4C1	2.43	0.49
1:B:44:ILE:HD12	1:B:71:ARG:HB2	1.94	0.49
3:A:1401:NAP:C5N	4:A:1405:DTV:C4	2.92	0.48
1:A:2[A]:GLU:OE1	1:A:32:PRO:HB2	2.14	0.47
1:D:215:TYR:HB2	1:D:238:LEU:CD2	2.44	0.47
1:A:142:ASP:HA	5:A:1705:HOH:O	2.15	0.47
1:C:260:GLU:HB2	1:C:261:PRO:HD3	1.97	0.47
1:C:65[A]:LYS:HE3	2:C:1423:SO4:O1	2.15	0.47
1:B:74:GLU:OE2	1:B:95:ARG:NH2	2.49	0.46
1:B:141:LEU:O	1:B:142:ASP:CB	2.64	0.45
1:D:136:LEU:CD1	1:D:165:THR:HG21	2.47	0.45
1:D:215:TYR:CG	1:D:238:LEU:HD22	2.52	0.44
1:B:59[B]:ASN:CG	5:B:1775:HOH:O	2.55	0.44
1:A:65:LYS:NZ	4:A:1405:DTV:H4C2	2.33	0.44
1:A:62[B]:VAL:HG13	3:A:1401:NAP:O3	2.16	0.44
3:A:1401:NAP:C4N	4:A:1405:DTV:C4	2.94	0.43
3:A:1401:NAP:C3N	4:A:1405:DTV:H4C1	2.49	0.43
1:A:264:LYS:HG3	5:A:1759:HOH:O	2.18	0.42
1:C:152[A]:VAL:HG12	5:C:1708:HOH:O	2.18	0.42
1:D:215:TYR:CB	1:D:238:LEU:CD2	2.97	0.42
1:C:92:GLU:HG2	5:C:1529:HOH:O	2.21	0.41
1:D:18:PHE:O	1:D:22:GLN:HG2	2.21	0.40
1:C:7:PHE:O	1:C:61:THR:HG22	2.21	0.40
1:B:196:ILE:CD1	1:B:225:TRP:CD1	3.04	0.40
1:A:2[A]:GLU:OE1	1:A:32:PRO:HB3	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	275/271 (102%)	270 (98%)	5 (2%)	0	100	100
1	B	277/271 (102%)	269 (97%)	8 (3%)	0	100	100
1	C	273/271 (101%)	266 (97%)	7 (3%)	0	100	100
1	D	278/271 (103%)	274 (99%)	4 (1%)	0	100	100
All	All	1103/1084 (102%)	1079 (98%)	24 (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	223/217 (103%)	223 (100%)	0	100	100
1	B	225/217 (104%)	219 (97%)	6 (3%)	44	15
1	C	220/217 (101%)	218 (99%)	2 (1%)	78	61
1	D	224/217 (103%)	217 (97%)	7 (3%)	40	11
All	All	892/868 (103%)	877 (98%)	15 (2%)	67	33

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1	MET
1	B	2	GLU
1	B	33	TYR
1	B	141	LEU
1	B	255[A]	VAL
1	B	255[B]	VAL
1	C	1	MET
1	C	269	GLU
1	D	135	LEU
1	D	136	LEU
1	D	196[A]	ILE
1	D	196[B]	ILE
1	D	217	LYS

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Mol	Chain	Res	Type
1	D	269[A]	GLU
1	D	269[B]	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	B	169	GLN
1	C	25	GLN
1	C	228	GLN
1	C	267	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

19 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	$\# Z  > 2$
4	DTV	A	1405	-	7,7,7	0.83	0	4,8,8	2.25	2 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	A	1402	-	4,4,4	0.36	0	6,6,6	0.33	0
3	NAP	C	1421	-	45,52,52	1.59	4 (8%)	56,80,80	1.77	10 (17%)
3	NAP	B	1411	-	45,52,52	1.41	4 (8%)	56,80,80	1.57	5 (8%)
2	SO4	A	1403	-	4,4,4	0.22	0	6,6,6	0.66	0
2	SO4	C	1426	-	4,4,4	0.36	0	6,6,6	0.68	0
2	SO4	C	1422	-	4,4,4	0.26	0	6,6,6	0.13	0
2	SO4	D	1433	-	4,4,4	0.15	0	6,6,6	0.46	0
2	SO4	B	1412	-	4,4,4	0.21	0	6,6,6	0.26	0
2	SO4	A	1404	-	4,4,4	0.35	0	6,6,6	0.62	0
2	SO4	C	1425	-	4,4,4	0.45	0	6,6,6	0.75	0
2	SO4	B	1413	-	4,4,4	0.42	0	6,6,6	0.95	0
2	SO4	B	1434	-	4,4,4	0.15	0	6,6,6	0.76	0
3	NAP	D	1431	-	45,52,52	1.48	6 (13%)	56,80,80	1.58	8 (14%)
2	SO4	B	1414	-	4,4,4	0.46	0	6,6,6	0.79	0
2	SO4	A	1424	-	4,4,4	0.32	0	6,6,6	0.60	0
2	SO4	D	1432	-	4,4,4	0.17	0	6,6,6	0.23	0
2	SO4	C	1423	-	4,4,4	0.25	0	6,6,6	0.64	0
3	NAP	A	1401	-	45,52,52	1.22	3 (6%)	56,80,80	1.51	6 (10%)

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	1421	-	-	3/31/67/67	0/5/5/5
4	DTV	A	1405	-	-	4/8/8/8	-
3	NAP	B	1411	-	-	1/31/67/67	0/5/5/5
3	NAP	D	1431	-	-	1/31/67/67	0/5/5/5
3	NAP	A	1401	-	-	1/31/67/67	0/5/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1421	NAP	O7N-C7N	7.07	1.37	1.24
3	D	1431	NAP	O7N-C7N	6.27	1.36	1.24
3	A	1401	NAP	O7N-C7N	4.93	1.33	1.24
3	B	1411	NAP	O7N-C7N	4.93	1.33	1.24
3	B	1411	NAP	C2A-N3A	4.80	1.39	1.32
3	C	1421	NAP	C2A-N3A	4.65	1.39	1.32
3	D	1431	NAP	C2A-N3A	3.57	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1401	NAP	C2A-N3A	3.27	1.37	1.32
3	D	1431	NAP	C2A-N1A	3.23	1.39	1.33
3	C	1421	NAP	C2A-N1A	2.82	1.39	1.33
3	B	1411	NAP	C2A-N1A	2.71	1.39	1.33
3	B	1411	NAP	P2B-O2B	2.52	1.64	1.59
3	D	1431	NAP	P2B-O2B	2.44	1.63	1.59
3	D	1431	NAP	C2N-N1N	2.29	1.37	1.35
3	D	1431	NAP	C7N-N7N	2.27	1.37	1.33
3	A	1401	NAP	C2A-N1A	2.08	1.37	1.33
3	C	1421	NAP	P2B-O2B	2.04	1.63	1.59

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1421	NAP	C3N-C7N-N7N	7.52	126.77	117.75
3	B	1411	NAP	N3A-C2A-N1A	-6.12	119.11	128.68
3	C	1421	NAP	N3A-C2A-N1A	-6.10	119.15	128.68
3	D	1431	NAP	C3N-C7N-N7N	5.58	124.45	117.75
3	A	1401	NAP	O7N-C7N-C3N	-5.57	112.96	119.63
3	D	1431	NAP	N3A-C2A-N1A	-5.32	120.37	128.68
3	B	1411	NAP	C3N-C7N-N7N	5.26	124.06	117.75
3	C	1421	NAP	O7N-C7N-C3N	-5.10	113.52	119.63
3	A	1401	NAP	C3N-C7N-N7N	4.57	123.24	117.75
3	A	1401	NAP	N3A-C2A-N1A	-4.44	121.73	128.68
3	B	1411	NAP	O7N-C7N-C3N	-4.39	114.37	119.63
3	D	1431	NAP	O7N-C7N-C3N	-3.98	114.87	119.63
4	A	1405	DTV	O3-C3-C2	3.76	117.45	109.72
3	D	1431	NAP	C2N-C3N-C4N	3.46	122.19	118.26
3	B	1411	NAP	C2N-C3N-C4N	3.28	121.97	118.26
3	A	1401	NAP	O4D-C1D-C2D	-3.17	102.29	106.93
3	C	1421	NAP	O4D-C1D-C2D	-2.55	103.20	106.93
3	D	1431	NAP	C3N-C2N-N1N	-2.53	117.95	120.43
3	C	1421	NAP	C3B-C2B-C1B	-2.42	98.33	102.89
3	C	1421	NAP	O2N-PN-O1N	2.41	124.16	112.24
4	A	1405	DTV	C3-C4-S4	2.35	121.31	114.47
3	D	1431	NAP	O3X-P2B-O2X	2.32	116.50	107.64
3	D	1431	NAP	PN-O3-PA	-2.32	124.87	132.83
3	D	1431	NAP	C5N-C4N-C3N	-2.26	117.67	120.34
3	B	1411	NAP	PN-O3-PA	-2.19	125.31	132.83
3	C	1421	NAP	C1B-N9A-C4A	-2.17	122.83	126.64
3	C	1421	NAP	C6N-N1N-C2N	-2.10	120.06	121.97
3	C	1421	NAP	PN-O3-PA	-2.08	125.70	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1421	NAP	O7N-C7N-N7N	-2.03	119.70	122.58
3	A	1401	NAP	C2A-N1A-C6A	2.03	122.22	118.75
3	A	1401	NAP	O2N-PN-O1N	2.03	122.26	112.24

There are no chirality outliers.

All (10) torsion outliers are listed below:

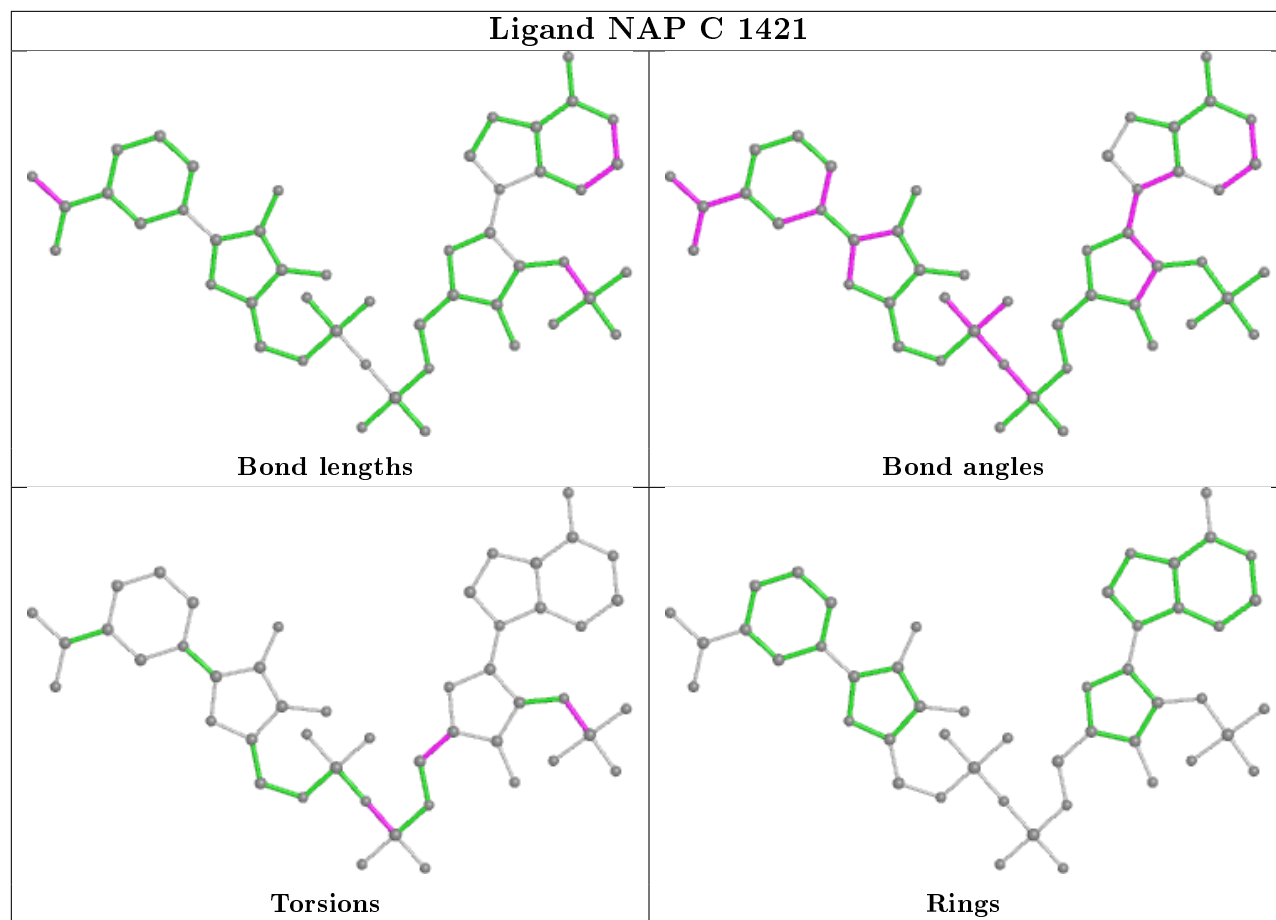
Mol	Chain	Res	Type	Atoms
4	A	1405	DTV	S1-C1-C2-O2
4	A	1405	DTV	S1-C1-C2-C3
4	A	1405	DTV	C2-C3-C4-S4
4	A	1405	DTV	O3-C3-C4-S4
3	C	1421	NAP	C2B-O2B-P2B-O2X
3	B	1411	NAP	O4B-C4B-C5B-O5B
3	A	1401	NAP	O4B-C4B-C5B-O5B
3	C	1421	NAP	PN-O3-PA-O1A
3	C	1421	NAP	O4B-C4B-C5B-O5B
3	D	1431	NAP	O4B-C4B-C5B-O5B

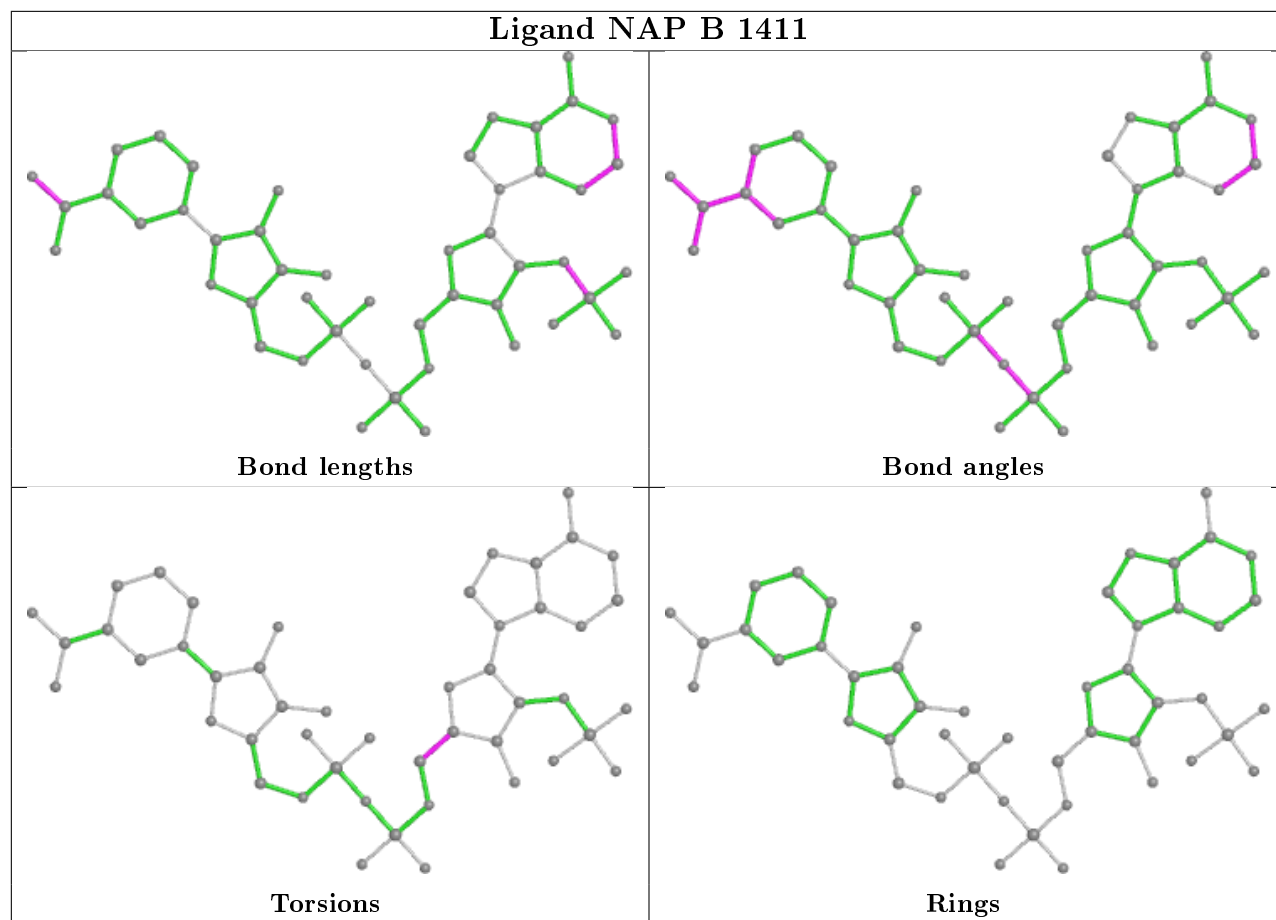
There are no ring outliers.

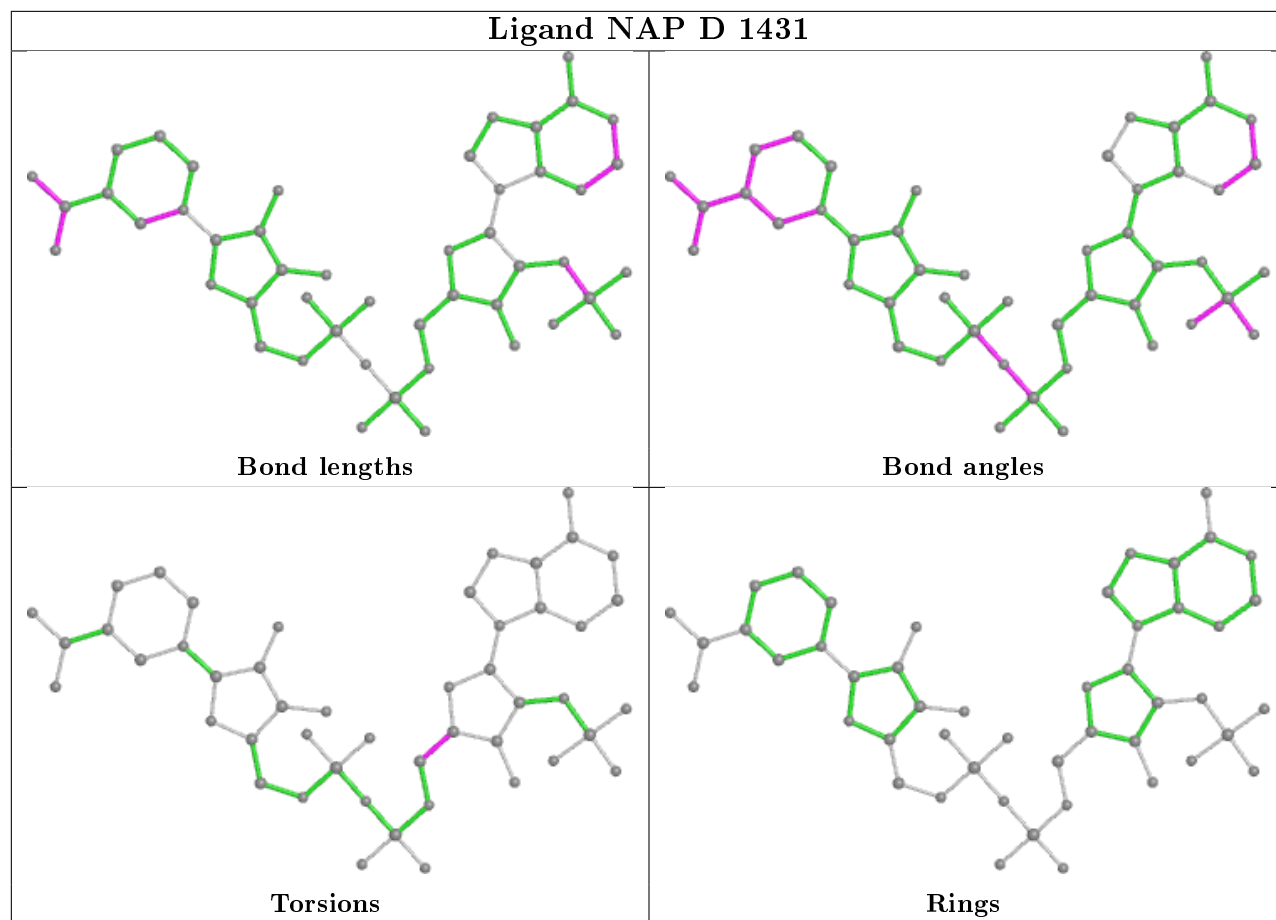
4 monomers are involved in 17 short contacts:

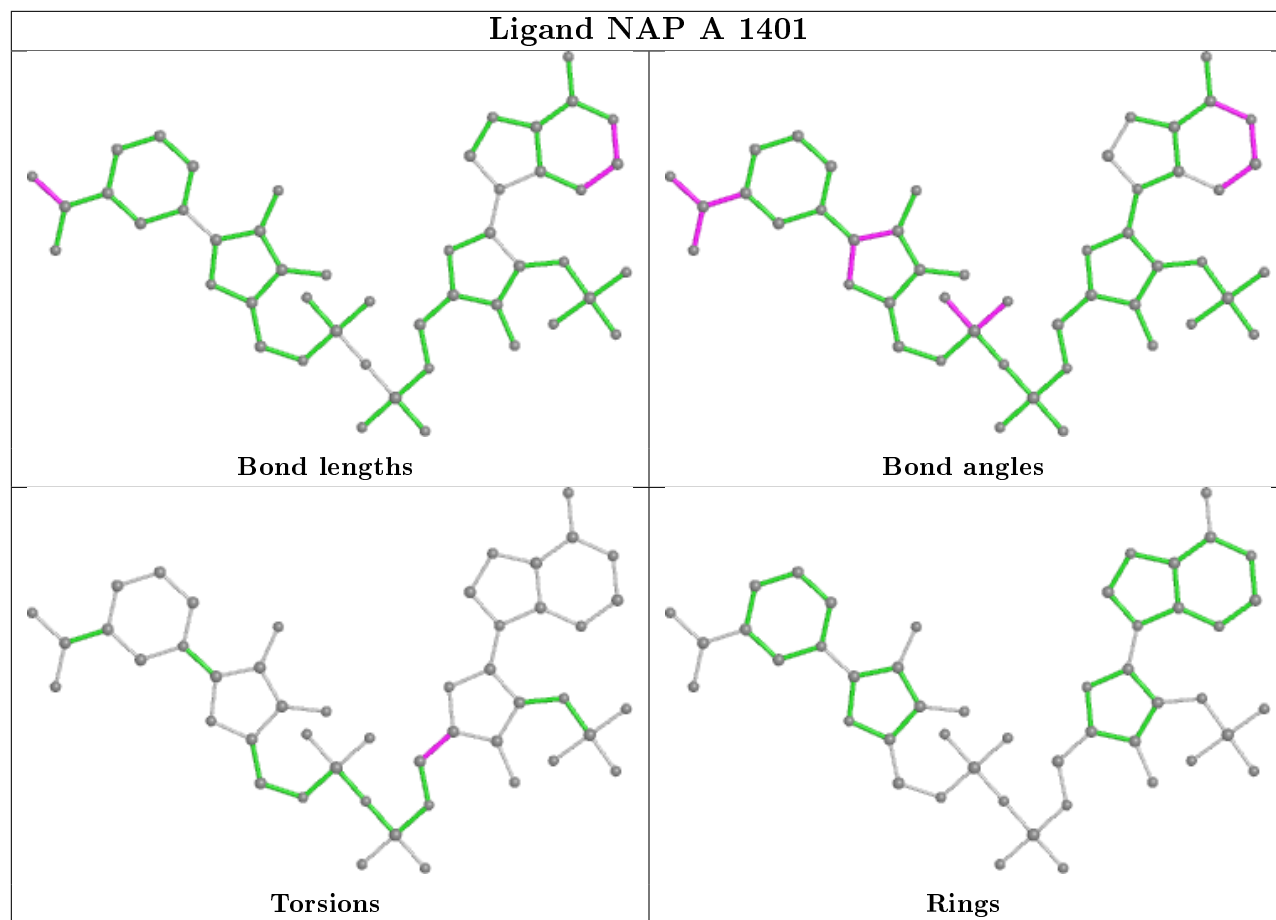
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1405	DTV	12	0
2	A	1404	SO4	4	0
2	C	1423	SO4	2	0
3	A	1401	NAP	6	0

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 [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	271/271 (100%)	0.15	15 (5%) 25 27	6, 11, 23, 42	0
1	B	271/271 (100%)	0.11	7 (2%) 56 61	6, 11, 24, 43	0
1	C	269/271 (99%)	0.49	28 (10%) 6 6	7, 14, 28, 53	0
1	D	270/271 (99%)	0.49	32 (11%) 4 4	7, 16, 29, 54	0
All	All	1081/1084 (99%)	0.31	82 (7%) 13 14	6, 13, 27, 54	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	270	LEU	10.3
1	B	1	MET	7.5
1	C	268	GLU	7.0
1	C	192	ILE	6.2
1	A	1	MET	6.2
1	A	270	LEU	5.6
1	D	268	GLU	5.6
1	A	192	ILE	5.3
1	C	41	ASN	4.7
1	C	196	ILE	4.7
1	D	192	ILE	4.3
1	C	193	SER	4.3
1	C	40	ILE	4.2
1	D	13	HIS	4.2
1	C	217	LYS	4.1
1	C	218	GLY	4.0
1	C	194	GLY	4.0
1	D	40	ILE	3.9
1	D	194	GLY	3.9
1	C	13	HIS	3.9
1	C	228	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	225	TRP	3.7
1	C	224	ALA	3.7
1	C	195	ASP	3.6
1	D	264	LYS	3.6
1	D	12	ALA	3.6
1	C	191	GLY	3.6
1	D	228	GLN	3.5
1	C	63	PRO	3.5
1	D	41[A]	ASN	3.4
1	A	271	SER	3.4
1	D	206	PRO	3.3
1	D	174	ASP	3.3
1	A	174	ASP	3.3
1	D	217	LYS	3.1
1	C	190	SER	3.0
1	C	267	GLN	3.0
1	C	174	ASP	2.9
1	D	62	VAL	2.9
1	C	25	GLN	2.8
1	C	225	TRP	2.8
1	C	264	LYS	2.8
1	B	106	LEU	2.8
1	A	106	LEU	2.8
1	B	271	SER	2.8
1	A	217	LYS	2.7
1	D	233	ARG	2.7
1	D	218	GLY	2.7
1	B	103	GLY	2.7
1	C	265	GLN	2.6
1	C	62	VAL	2.6
1	B	142	ASP	2.6
1	D	269[A]	GLU	2.6
1	C	214	PHE	2.5
1	B	134	VAL	2.5
1	D	224	ALA	2.4
1	D	38	ALA	2.4
1	D	198	ALA	2.4
1	A	134	VAL	2.4
1	D	204	ILE	2.4
1	D	255[A]	VAL	2.3
1	C	269	GLU	2.3
1	D	136	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	174	ASP	2.3
1	A	142	ASP	2.3
1	D	265	GLN	2.3
1	C	250	LEU	2.2
1	D	250	LEU	2.2
1	A	104	VAL	2.2
1	A	218	GLY	2.2
1	C	64	PHE	2.1
1	A	178	GLY	2.1
1	D	193	SER	2.1
1	D	39	PRO	2.1
1	C	251	LEU	2.1
1	A	41	ASN	2.1
1	A	177	GLU	2.1
1	A	101	THR	2.1
1	D	227	GLU	2.0
1	D	195	ASP	2.0
1	D	25	GLN	2.0
1	D	196[A]	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	B	1434	5/5	0.85	0.22	26,26,28,29	5
2	SO4	C	1423	5/5	0.85	0.32	20,25,27,30	5
2	SO4	C	1426	5/5	0.86	0.21	23,27,28,34	5
4	DTV	A	1405	8/8	0.89	0.48	10,22,23,23	8

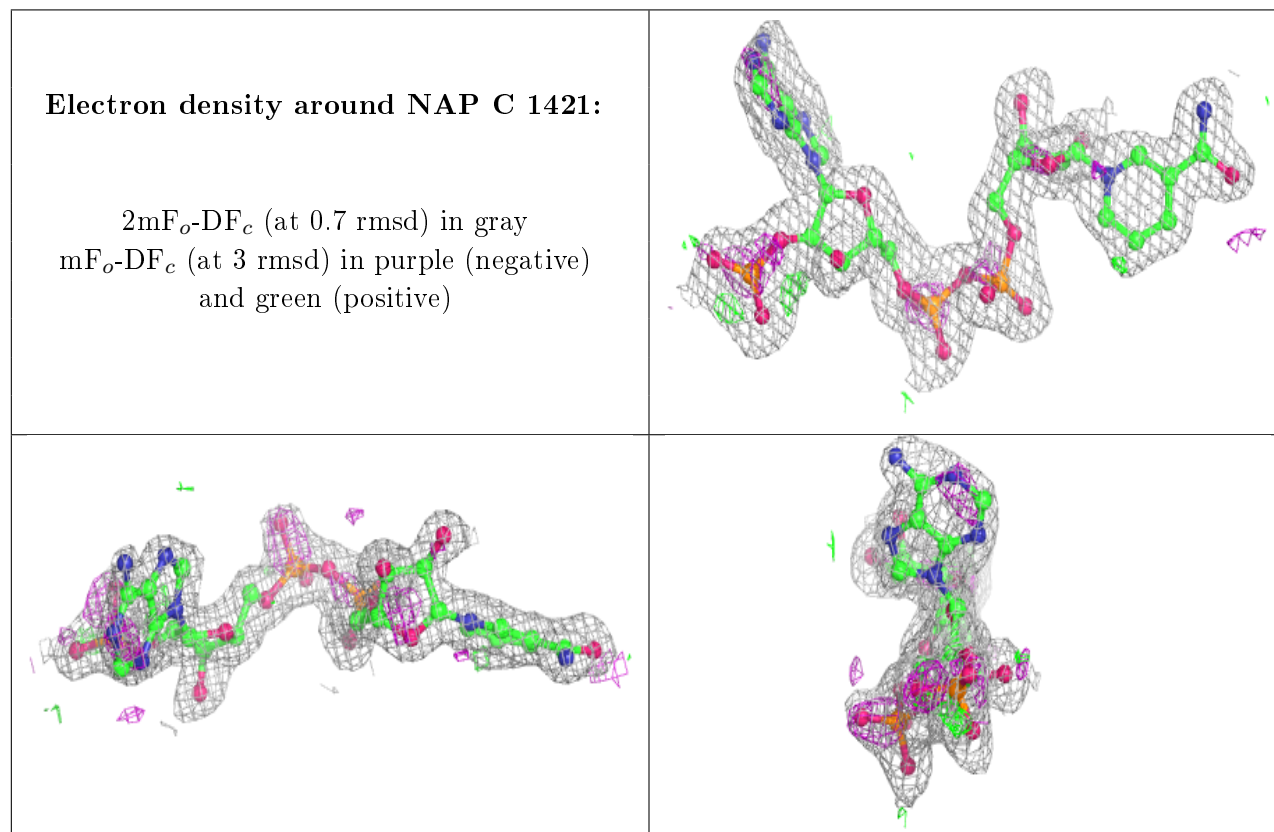
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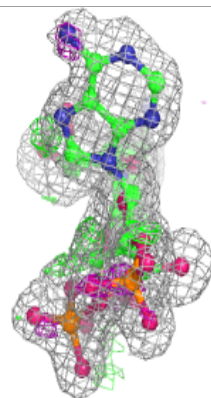
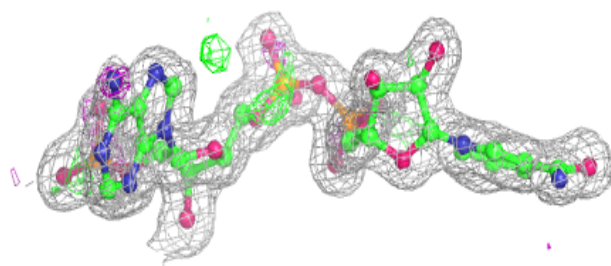
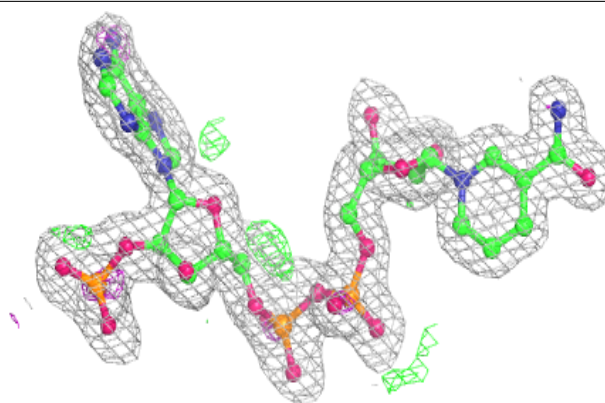
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	D	1433	5/5	0.90	0.19	32,33,35,35	5
3	NAP	C	1421	48/48	0.90	0.14	14,24,31,33	0
2	SO4	A	1402	5/5	0.90	0.22	21,24,26,27	5
2	SO4	D	1432	5/5	0.91	0.12	27,28,31,31	5
2	SO4	A	1424	5/5	0.93	0.11	23,24,26,26	5
2	SO4	B	1412	5/5	0.95	0.10	24,25,25,27	5
3	NAP	D	1431	48/48	0.95	0.09	13,17,21,23	0
2	SO4	B	1414	5/5	0.95	0.27	16,17,21,25	5
2	SO4	C	1425	5/5	0.96	0.23	23,27,28,29	5
2	SO4	C	1422	5/5	0.96	0.07	21,21,25,25	5
2	SO4	A	1404	5/5	0.96	0.23	22,23,26,30	5
2	SO4	A	1403	5/5	0.98	0.12	22,24,28,30	0
3	NAP	B	1411	48/48	0.98	0.07	7,10,13,15	0
3	NAP	A	1401	48/48	0.98	0.07	8,11,14,17	0
2	SO4	B	1413	5/5	0.99	0.10	20,21,26,28	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.

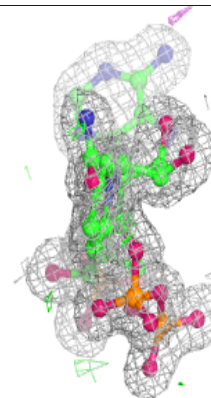
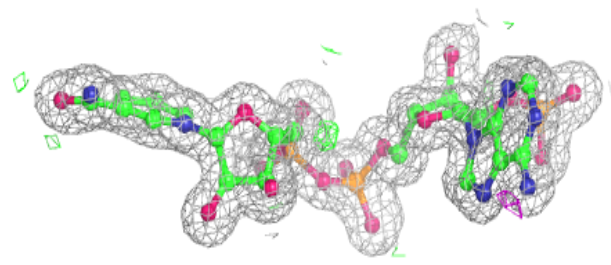
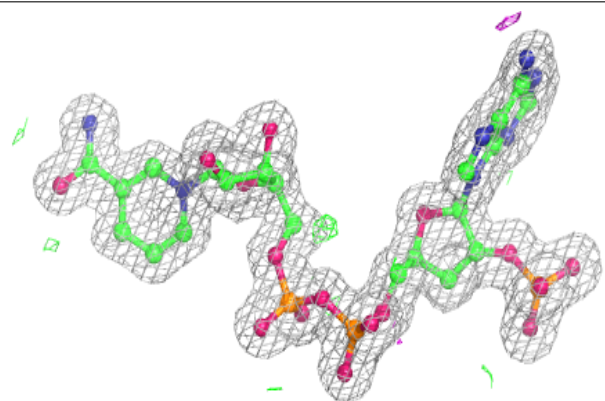


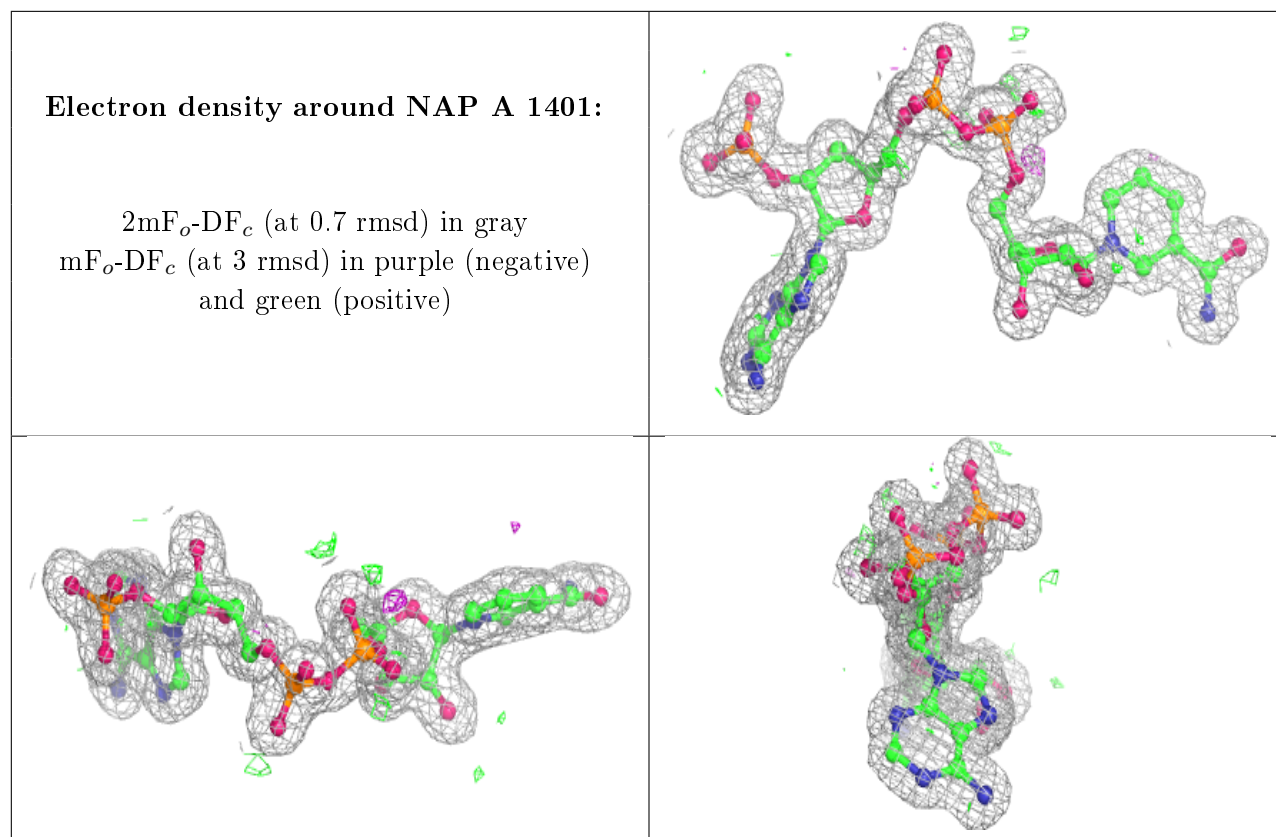
**Electron density around NAP D 1431:**

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

**Electron density around NAP B 1411:**

$2mF_o-DF_c$  (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.