



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2023 – 06:11 AM EDT

PDB ID : 1N9G  
Title : Mitochondrial 2-enoyl thioester reductase Etr1p/Etr2p heterodimer from *Candida tropicalis*  
Authors : Torkko, J.M.; Koivuranta, K.T.; Kastaniotis, A.J.; Airenne, T.T.; Glumoff, T.; Ilves, M.; Hartig, A.; Gurvitz, A.; Hiltunen, J.K.  
Deposited on : 2002-11-25  
Resolution : 1.98 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.35  
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) : 2.35

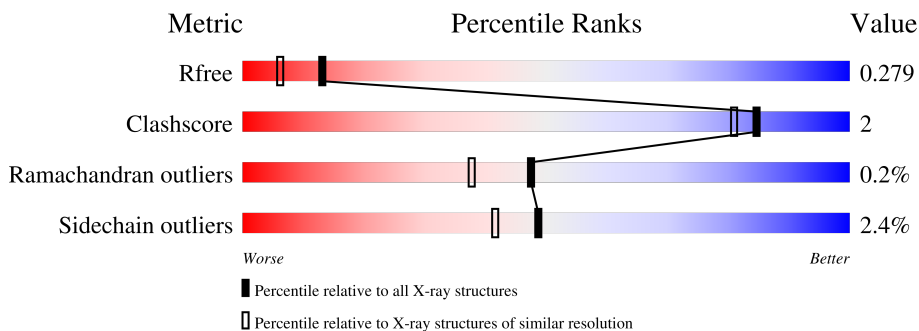
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.98 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)

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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	386	
1	C	386	
1	F	386	
2	B	386	
2	D	386	
2	E	386	

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
3	SO4	A	1532	-	-	X	-
3	SO4	B	1535	-	X	-	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18417 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 2,4-dienoyl-CoA reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	364	2785	1768	464	547	6	4	0	0
1	C	364	2785	1768	464	547	6	0	0	0
1	F	364	2785	1768	464	547	6	0	0	0

- Molecule 2 is a protein called 2,4-dienoyl-CoA reductase.

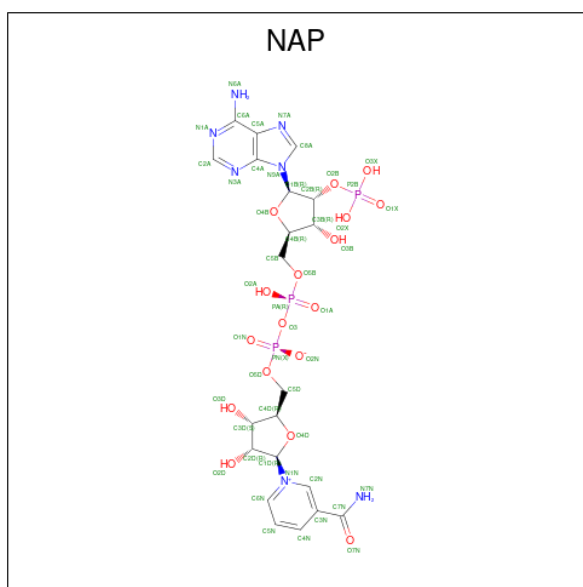
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	364	2788	1768	466	548	6	4	0	0
2	D	364	2787	1767	466	548	6	0	0	0
2	E	364	2788	1768	466	548	6	0	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 4 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
			Total	C	N	O	P		
4	A	1	48	21	7	17	3	0	0
4	B	1	48	21	7	17	3	0	0
4	E	1	48	21	7	17	3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	296	296	296	0	0
5	B	234	234	234	0	0
5	C	183	183	183	0	0
5	D	318	318	318	2	0
5	E	206	206	206	0	0
5	F	283	283	283	2	0

### 3 Residue-property plots


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. 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. 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.

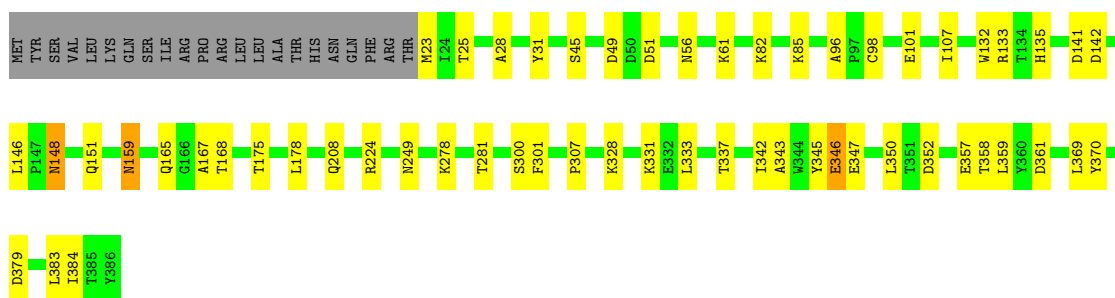
- Molecule 1: 2,4-dienoyl-CoA reductase

Chain A:  91% 6%




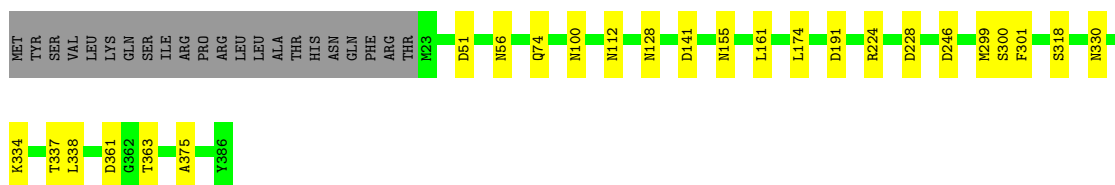
- Molecule 1: 2,4-dienoyl-CoA reductase

Chain C:  80% 14% 6%




- Molecule 1: 2,4-dienoyl-CoA reductase

Chain F:  88% 6% 6%



- Molecule 2: 2,4-dienoyl-CoA reductase

Chain B:  89% 5% 6%





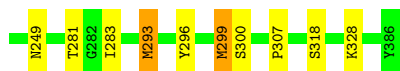
- Molecule 2: 2,4-dienoyl-CoA reductase

Chain D: 89% 5% 6%



- Molecule 2: 2,4-dienoyl-CoA reductase

Chain E: 87% 7% 6%





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	229.45Å 95.50Å 164.23Å 90.00° 124.71° 90.00°	Depositor
Resolution (Å)	19.43 – 1.98 19.41 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.43-1.98) 99.8 (19.41-1.98)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.45 (at 1.97Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.195 , 0.235 0.257 , 0.279	Depositor DCC
$R_{free}$ test set	10101 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.5	Xtrriage
Anisotropy	0.114	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 55.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	18417	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% 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: SO4, 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	0.58	2/2844 (0.1%)	0.74	1/3865 (0.0%)
1	C	0.58	0/2844	0.76	7/3865 (0.2%)
1	F	0.58	0/2844	0.75	5/3865 (0.1%)
2	B	0.61	2/2847 (0.1%)	0.74	5/3870 (0.1%)
2	D	0.60	0/2846	0.78	4/3869 (0.1%)
2	E	0.55	1/2847 (0.0%)	0.76	4/3870 (0.1%)
All	All	0.58	5/17072 (0.0%)	0.75	26/23204 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
2	B	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	199	THR	CB-OG1	-14.07	1.15	1.43
1	A	296	TYR	C-O	-8.21	1.07	1.23
2	E	293	MET	SD-CE	-6.81	1.39	1.77
1	A	269	LYS	C-O	-5.43	1.13	1.23
2	B	293	MET	SD-CE	-5.14	1.49	1.77

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	372	ASP	CB-CG-OD2	9.18	126.56	118.30
1	C	141	ASP	CB-CG-OD2	8.68	126.11	118.30
2	E	228	ASP	CB-CG-OD2	7.20	124.78	118.30
1	A	246	ASP	CB-CG-OD2	6.78	124.40	118.30
2	E	246	ASP	CB-CG-OD2	6.13	123.82	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	299	MET	Peptide
1	C	346	GLU	Peptide

## 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	2785	0	2767	4	0
1	C	2785	0	2767	30	0
1	F	2785	0	2767	11	0
2	B	2788	0	2767	6	0
2	D	2787	0	2764	8	0
2	E	2788	0	2767	17	0
3	A	5	0	0	2	0
3	B	5	0	0	1	0
3	C	5	0	0	0	0
3	D	10	0	0	0	0
3	E	5	0	0	1	0
3	F	5	0	0	0	0
4	A	48	0	25	1	0
4	B	48	0	25	4	0
4	E	48	0	25	6	0
5	A	296	0	0	1	0
5	B	234	0	0	1	0
5	C	183	0	0	9	0
5	D	318	0	0	4	0
5	E	206	0	0	1	0
5	F	283	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	18417	0	16674	77	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 77 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:C:159:ASN:HB2	1:C:346:GLU:HB3	1.59	0.85
2:B:300:SER:HB3	5:B:3487:HOH:O	1.80	0.82
2:B:296:TYR:O	4:B:3387:NAP:H2N	1.85	0.76
2:B:69:PRO:HG2	4:B:3387:NAP:H52N	1.68	0.74
2:D:56:ASN:HD21	2:D:112:ASN:HD22	1.36	0.73

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	362/386 (94%)	354 (98%)	8 (2%)	0	100	100
1	C	362/386 (94%)	350 (97%)	11 (3%)	1 (0%)	41	29
1	F	362/386 (94%)	351 (97%)	10 (3%)	1 (0%)	41	29
2	B	362/386 (94%)	353 (98%)	8 (2%)	1 (0%)	41	29
2	D	362/386 (94%)	351 (97%)	10 (3%)	1 (0%)	41	29
2	E	362/386 (94%)	350 (97%)	11 (3%)	1 (0%)	41	29
All	All	2172/2316 (94%)	2109 (97%)	58 (3%)	5 (0%)	47	38

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	300	SER
2	E	300	SER
1	F	300	SER
2	B	301	PHE
1	C	300	SER

### 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	306/327 (94%)	301 (98%)	5 (2%)	62 56
1	C	306/327 (94%)	294 (96%)	12 (4%)	32 19
1	F	306/327 (94%)	299 (98%)	7 (2%)	50 44
2	B	307/328 (94%)	298 (97%)	9 (3%)	42 31
2	D	306/328 (93%)	302 (99%)	4 (1%)	69 64
2	E	307/328 (94%)	299 (97%)	8 (3%)	46 37
All	All	1838/1965 (94%)	1793 (98%)	45 (2%)	49 41

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	332	GLU
2	E	224	ARG
2	D	338	LEU
2	E	92	THR
2	E	328	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	139	ASN
1	F	100	ASN
1	F	376	ASN
1	F	249	ASN

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Mol	Chain	Res	Type
1	F	56	ASN

### 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](#)

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAP	A	2387	1	45,52,52	1.66	3 (6%)	56,80,80	1.27	4 (7%)
3	SO4	F	1537	-	4,4,4	0.27	0	6,6,6	0.20	0
4	NAP	B	3387	3	45,52,52	1.85	4 (8%)	56,80,80	1.61	9 (16%)
3	SO4	D	1531	-	4,4,4	0.19	0	6,6,6	0.27	0
3	SO4	D	1533	-	4,4,4	0.27	0	6,6,6	0.55	0
3	SO4	E	1536	4	4,4,4	1.43	1 (25%)	6,6,6	2.16	2 (33%)
3	SO4	A	1532	-	4,4,4	0.28	0	6,6,6	0.35	0
3	SO4	C	1534	-	4,4,4	0.26	0	6,6,6	0.43	0
4	NAP	E	4387	3	45,52,52	1.71	4 (8%)	56,80,80	1.56	12 (21%)
3	SO4	B	1535	4	4,4,4	4.47	4 (100%)	6,6,6	4.14	5 (83%)

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	NAP	E	4387	3	-	8/31/67/67	0/5/5/5
4	NAP	A	2387	1	-	9/31/67/67	0/5/5/5
4	NAP	B	3387	3	-	8/31/67/67	0/5/5/5

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	3387	NAP	O7N-C7N	9.44	1.42	1.24
4	A	2387	NAP	O7N-C7N	8.49	1.40	1.24
4	E	4387	NAP	O7N-C7N	8.45	1.40	1.24
3	B	1535	SO4	O4-S	-6.39	0.95	1.47
3	B	1535	SO4	O2-S	-4.53	1.21	1.46

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1535	SO4	O4-S-O3	6.52	136.89	109.06
4	A	2387	NAP	N3A-C2A-N1A	-5.65	119.85	128.68
4	E	4387	NAP	N3A-C2A-N1A	-5.55	120.01	128.68
4	B	3387	NAP	N3A-C2A-N1A	-5.52	120.05	128.68
3	B	1535	SO4	O4-S-O2	-4.67	84.95	109.31

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2387	NAP	C2B-O2B-P2B-O2X
4	A	2387	NAP	C5D-O5D-PN-O3
4	A	2387	NAP	C5D-O5D-PN-O1N
4	A	2387	NAP	C5D-O5D-PN-O2N
4	A	2387	NAP	O4D-C4D-C5D-O5D

There are no ring outliers.

6 monomers are involved in 12 short contacts:

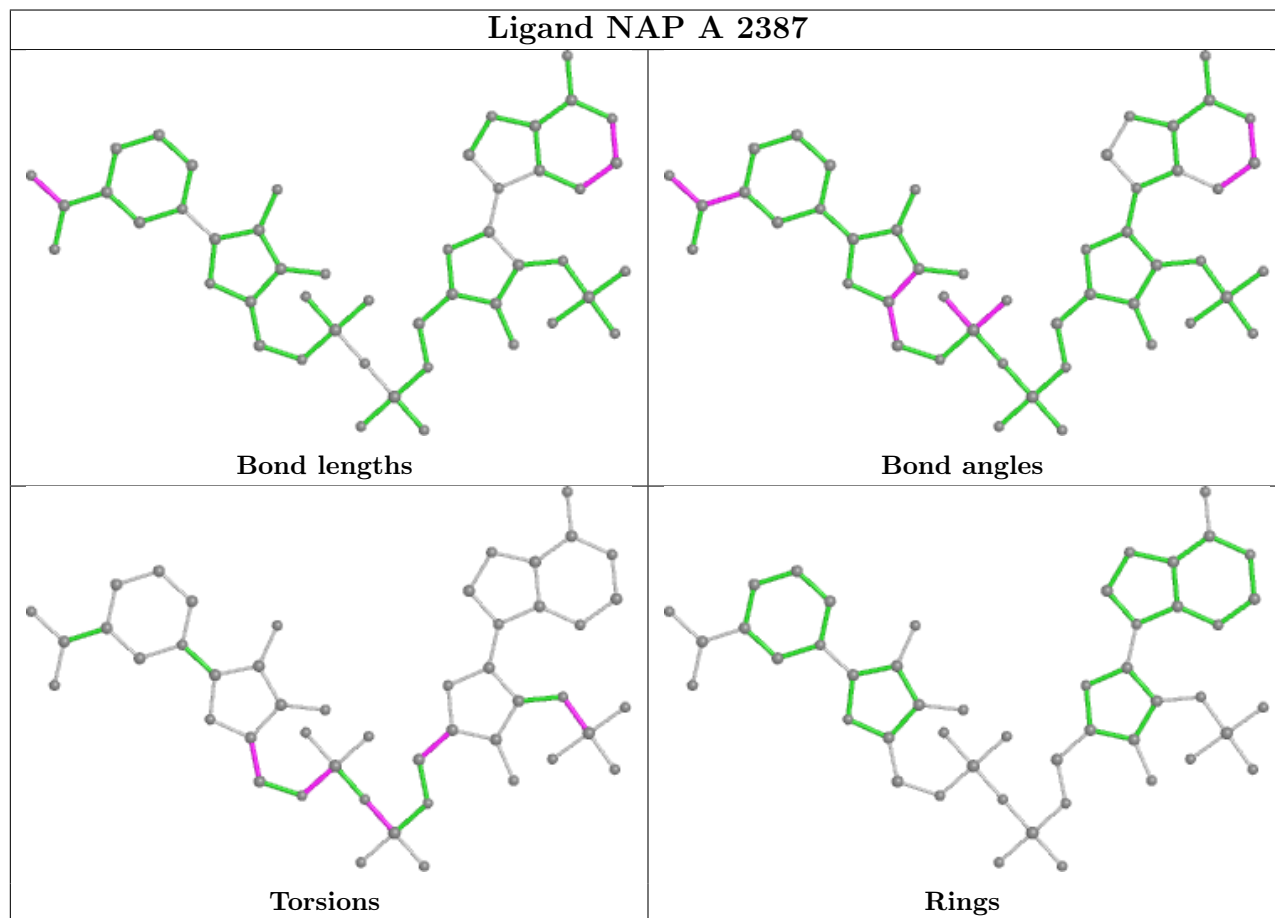
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2387	NAP	1	0

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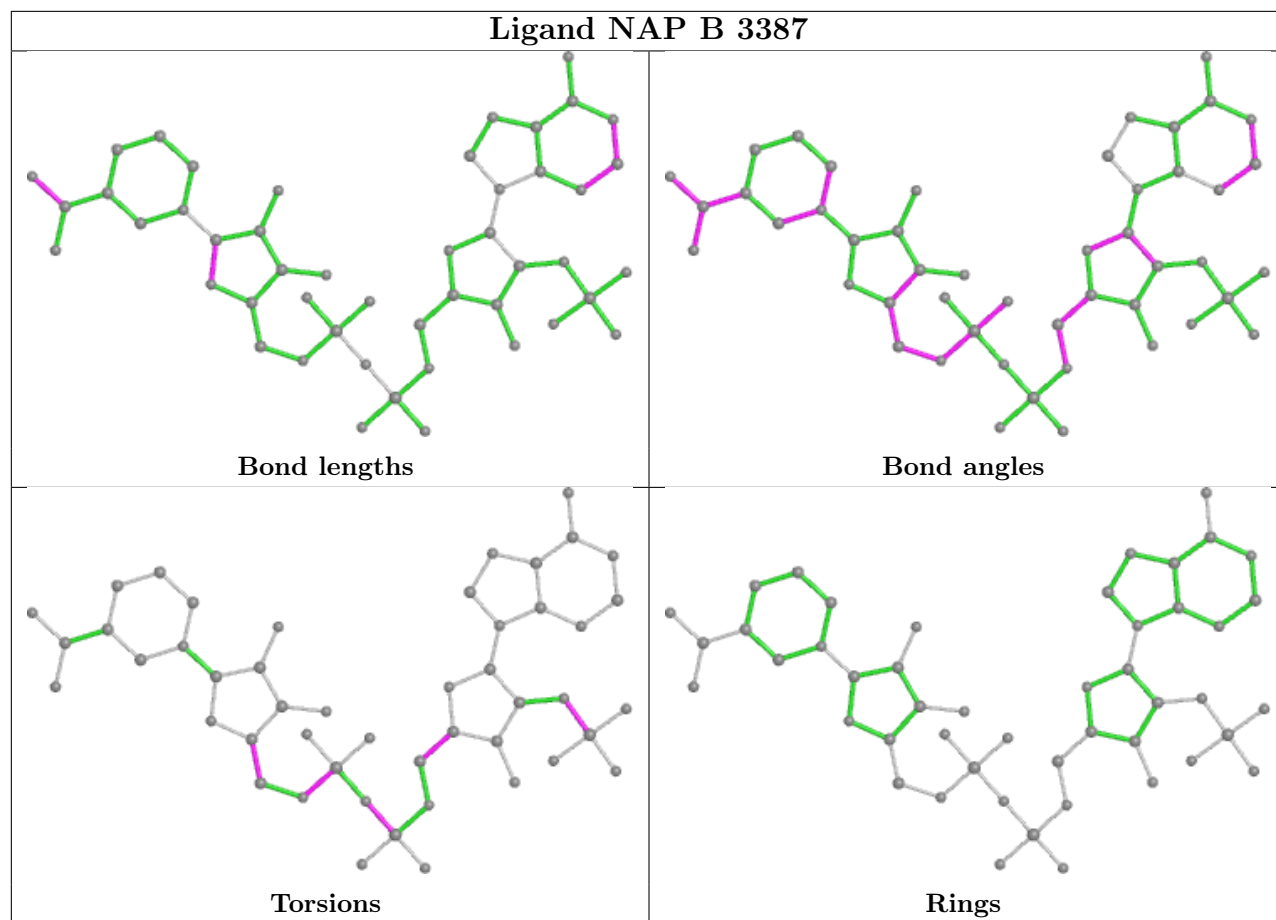
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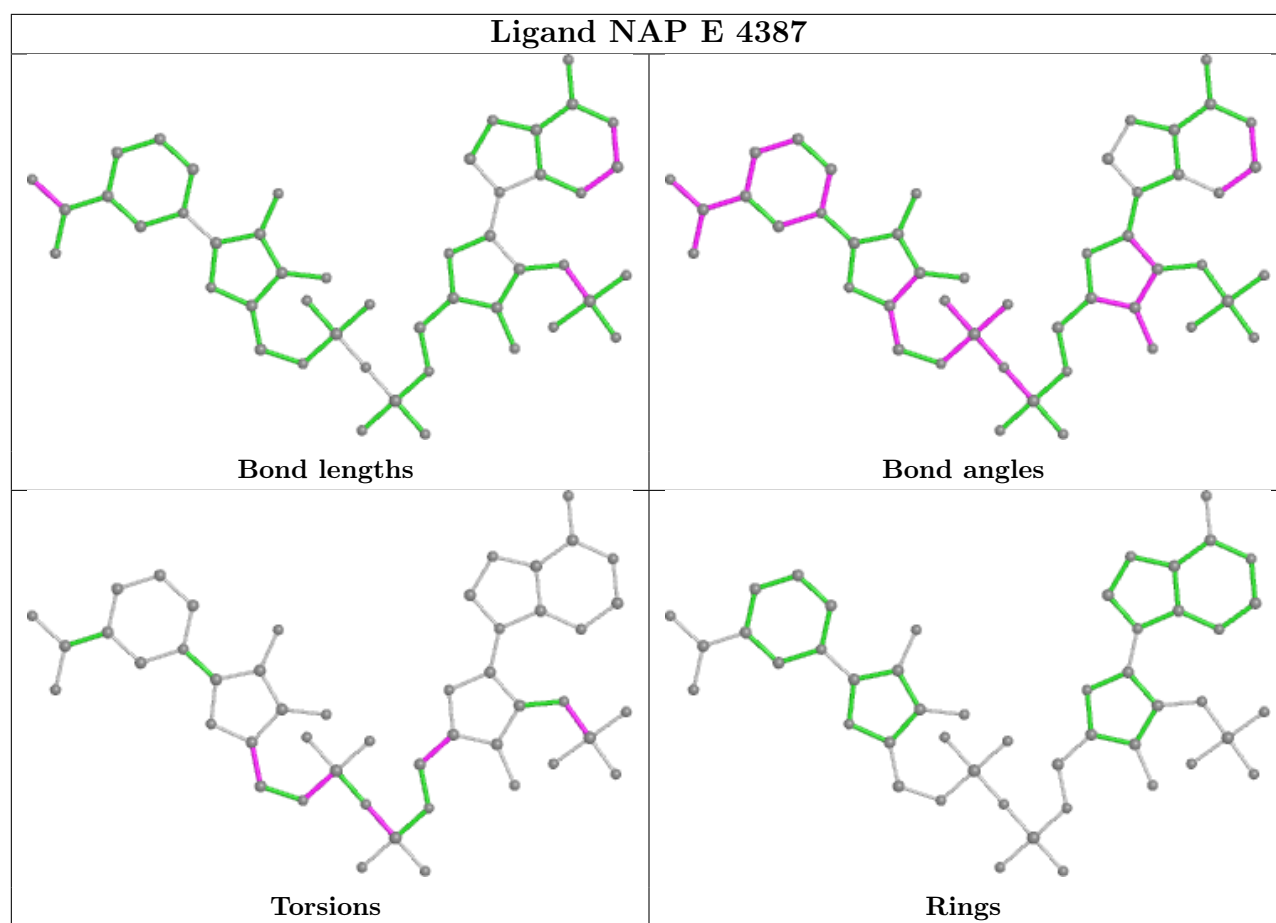
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	3387	NAP	4	0
3	E	1536	SO4	1	0
3	A	1532	SO4	2	0
4	E	4387	NAP	6	0
3	B	1535	SO4	1	0

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 [\(i\)](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

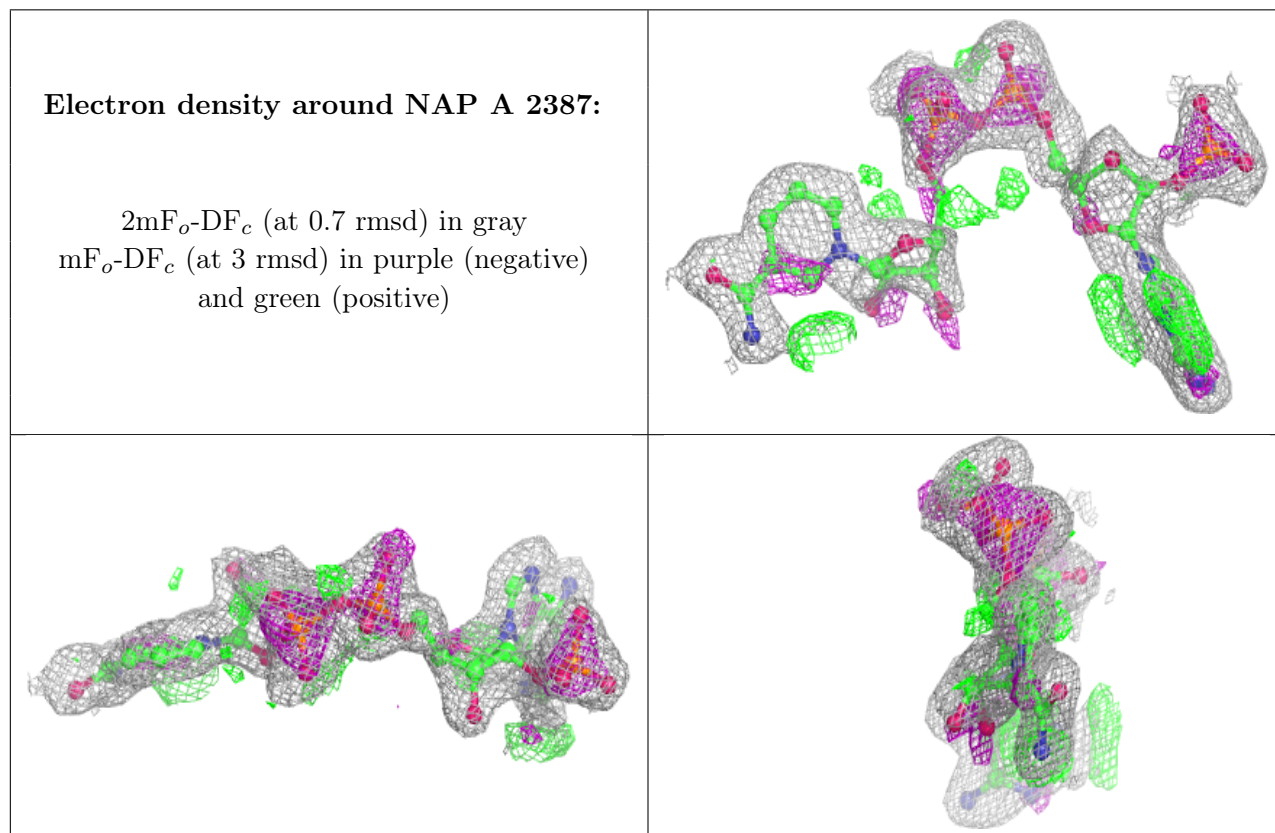
### 6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands [i](#)

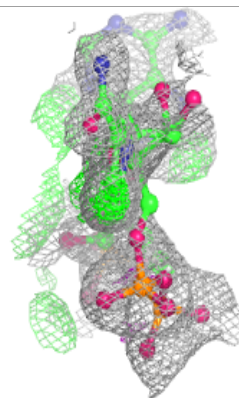
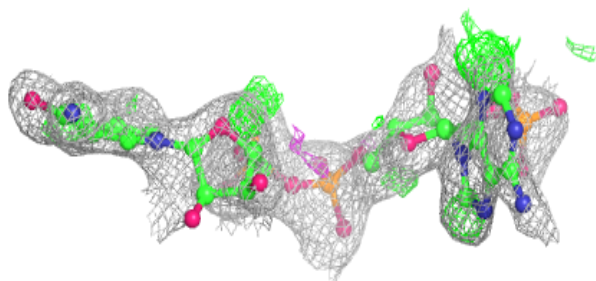
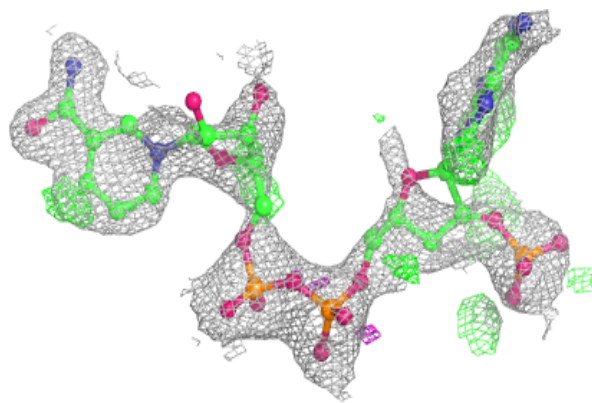
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

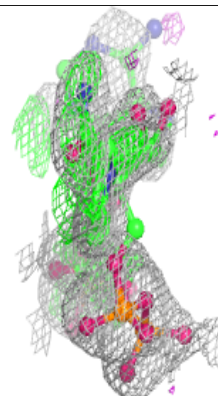
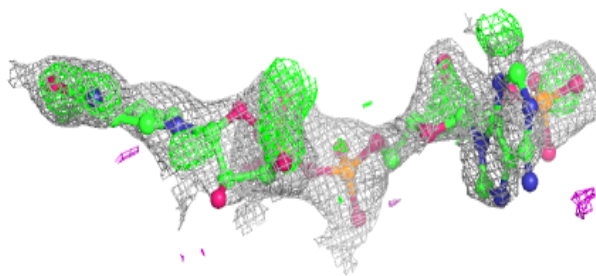
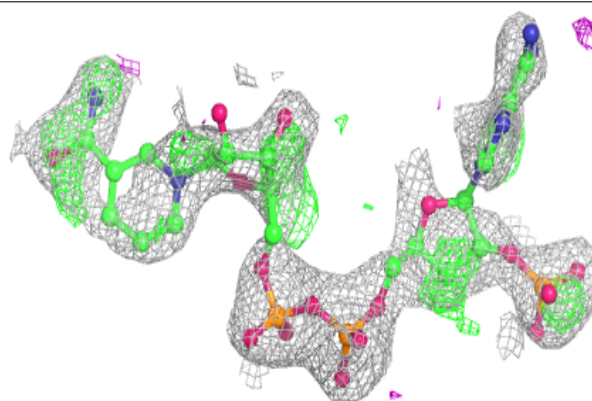


**Electron density around NAP B 3387:**

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

**Electron density around NAP E 4387:**

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



## 6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.