



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 02:55 pm BST

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

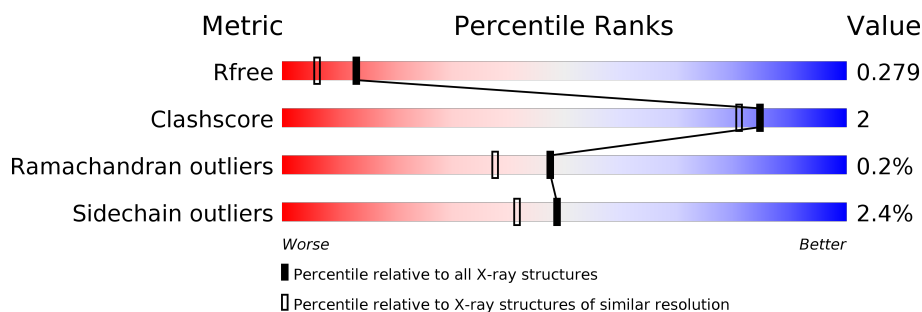
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	91% 6%
1	C	386	80% 14% 6%
1	F	386	88% 6% 6%
2	B	386	89% 5% 6%
2	D	386	89% 5% 6%
2	E	386	87% 7% 6%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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
1	A	364	Total	C	N	O	S	4	0	0
			2785	1768	464	547	6			
1	C	364	Total	C	N	O	S	0	0	0
			2785	1768	464	547	6			
1	F	364	Total	C	N	O	S	0	0	0
			2785	1768	464	547	6			

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

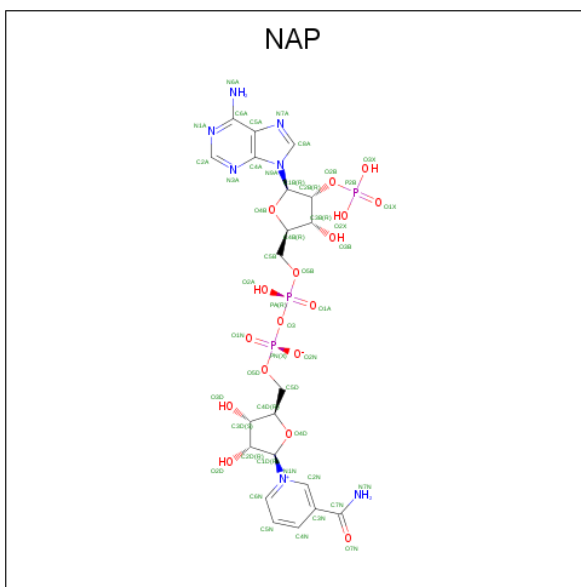
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	364	Total	C	N	O	S	4	0	0
			2788	1768	466	548	6			
2	D	364	Total	C	N	O	S	0	0	0
			2787	1767	466	548	6			
2	E	364	Total	C	N	O	S	0	0	0
			2788	1768	466	548	6			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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: C₂₁H₂₈N₇O₁₇P₃).



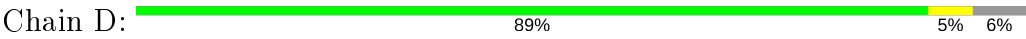
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
4	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
4	E	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 5 is water.

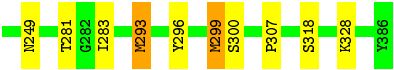
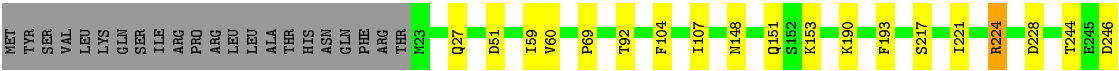
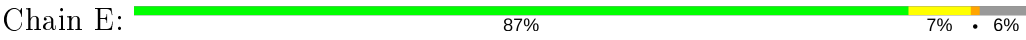
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	296	Total O 296 296	0	0
5	B	234	Total O 234 234	0	0
5	C	183	Total O 183 183	0	0
5	D	318	Total O 318 318	2	0
5	E	206	Total O 206 206	0	0
5	F	283	Total O 283 283	2	0



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 1.97Å)	Xtriage
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 ²)	31.5	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 55.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	18417	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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

All (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
1	C	352	ASP	CB-CG-OD2	6.05	123.75	118.30
1	F	246	ASP	CB-CG-OD2	6.02	123.72	118.30
1	C	379	ASP	CB-CG-OD2	6.00	123.70	118.30
2	B	372	ASP	CB-CG-OD2	5.92	123.63	118.30
1	C	49	ASP	CB-CG-OD2	5.80	123.52	118.30
2	B	199	THR	CA-CB-OG1	5.79	121.17	109.00
2	B	141	ASP	CB-CG-OD2	5.64	123.38	118.30
2	E	224	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	C	51	ASP	CB-CG-OD2	5.53	123.27	118.30
1	F	191	ASP	CB-CG-OD2	5.51	123.26	118.30
2	B	224	ARG	NE-CZ-NH2	-5.47	117.57	120.30
2	D	228	ASP	CB-CG-OD2	5.45	123.20	118.30
1	F	228	ASP	CB-CG-OD2	5.40	123.16	118.30
1	F	51	ASP	CB-CG-OD2	5.37	123.13	118.30
2	B	51	ASP	CB-CG-OD2	5.29	123.06	118.30
2	D	379	ASP	CB-CG-OD2	5.28	123.05	118.30
1	C	361	ASP	CB-CG-OD2	5.22	123.00	118.30
1	C	142	ASP	CB-CG-OD2	5.19	122.97	118.30
2	E	224	ARG	NE-CZ-NH1	5.15	122.88	120.30
2	D	71	ASP	CB-CG-OD2	5.06	122.85	118.30
1	F	141	ASP	CB-CG-OD2	5.01	122.81	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
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.

All (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
1:C:82:LYS:NZ	5:C:1591:HOH:O	2.25	0.69
1:A:221:ILE:HA	3:A:1532:SO4:O3	1.93	0.69
1:C:175:THR:OG1	5:C:1624:HOH:O	2.12	0.68
1:F:334:LYS:CD	5:F:1784:HOH:O	2.44	0.66
1:F:334:LYS:HD3	5:F:1784:HOH:O	1.96	0.66
1:A:236:GLU:OE1	5:A:2472:HOH:O	2.14	0.64
1:C:208:GLN:NE2	5:C:1668:HOH:O	2.31	0.64
3:B:1535:SO4:O2	4:B:3387:NAP:O3B	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:LEU:HD21	1:C:337:THR:HG21	1.83	0.59
1:F:100:ASN:HD22	1:F:128:ASN:H	1.50	0.59
1:F:56:ASN:HD21	1:F:112:ASN:HD22	1.51	0.58
1:C:56:ASN:N	5:C:1556:HOH:O	2.20	0.58
2:D:302:GLN:NE2	5:D:1623:HOH:O	2.29	0.57
2:E:221:ILE:O	2:E:244:THR:HA	2.05	0.57
2:E:69:PRO:HG2	4:E:4387:NAP:H52N	1.87	0.57
1:F:174:LEU:HD22	1:F:337:THR:HG22	1.85	0.57
1:C:61:LYS:HG2	1:C:135:HIS:CD2	2.40	0.56
1:C:333:LEU:O	1:C:337:THR:HG23	2.05	0.56
2:E:299:MET:HE2	4:E:4387:NAP:O4B	2.06	0.55
2:E:249:ASN:ND2	5:E:4531:HOH:O	2.30	0.55
1:C:98:CYS:HB3	1:C:132:TRP:CE3	2.43	0.54
1:A:53:LEU:HD11	1:A:59:ILE:HG23	1.89	0.54
1:F:74:GLN:HE22	1:F:100:ASN:HD21	1.56	0.53
1:C:249:ASN:ND2	5:C:1604:HOH:O	2.29	0.53
2:E:283:ILE:HG13	2:E:293:MET:CE	2.39	0.53
1:A:101:GLU:HG2	1:A:167:ALA:O	2.09	0.52
1:C:383:LEU:HD13	5:C:1639:HOH:O	2.10	0.52
2:D:249:ASN:ND2	5:D:1704:HOH:O	2.28	0.51
2:E:59:ILE:HG22	2:E:107:ILE:HD11	1.93	0.51
2:E:296:TYR:O	4:E:4387:NAP:H2N	2.11	0.50
2:B:68:ASN:HD22	2:B:381:LYS:NZ	2.11	0.49
2:E:281:THR:HG23	2:E:307:PRO:HD3	1.94	0.49
2:D:174:LEU:HD21	2:D:338:LEU:HD13	1.94	0.49
1:F:375:ALA:O	5:F:1798:HOH:O	2.20	0.49
1:C:281:THR:HG23	1:C:307:PRO:HD3	1.94	0.48
2:B:296:TYR:O	4:B:3387:NAP:C2N	2.59	0.47
2:E:299:MET:HG2	4:E:4387:NAP:C5A	2.44	0.47
1:C:345:TYR:CE2	1:C:350:LEU:HD12	2.49	0.46
2:D:281:THR:HG23	2:D:307:PRO:HD3	1.98	0.46
2:D:124:PRO:HD2	5:D:1721:HOH:O	2.16	0.45
1:F:100:ASN:ND2	1:F:128:ASN:H	2.12	0.45
2:E:148:ASN:H	2:E:151:GLN:NE2	2.15	0.45
2:E:60:VAL:HB	2:E:104:PHE:HB3	1.98	0.44
1:C:28:ALA:HA	1:C:133:ARG:HB3	2.00	0.44
1:C:31:TYR:CZ	1:C:96:ALA:HB3	2.52	0.44
1:C:101:GLU:HG2	1:C:167:ALA:O	2.17	0.44
1:C:357:GLU:HA	1:C:383:LEU:O	2.17	0.44
2:D:235:LYS:CE	5:D:1554:HOH:O	2.66	0.43
1:C:148:ASN:HD22	1:C:148:ASN:C	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:318:SER:HB3	1:F:318:SER:HB3	2.01	0.43
1:C:383:LEU:HD21	5:C:1587:HOH:O	2.19	0.43
1:C:165:GLN:HG2	1:C:345:TYR:CE2	2.54	0.43
1:C:343:ALA:O	1:C:347:GLU:HB2	2.19	0.43
3:A:1532:SO4:O1	4:A:2387:NAP:O2B	2.36	0.42
1:C:148:ASN:ND2	1:C:151:GLN:H	2.17	0.42
1:C:148:ASN:HD22	1:C:151:GLN:H	1.66	0.42
2:E:193:PHE:CE2	2:E:217:SER:HB3	2.54	0.42
2:E:299:MET:CE	4:E:4387:NAP:O4B	2.68	0.42
2:E:283:ILE:HG13	2:E:293:MET:HE2	2.02	0.42
1:C:25:THR:HG23	5:C:1628:HOH:O	2.19	0.42
2:E:148:ASN:H	2:E:151:GLN:HE21	1.68	0.42
1:F:361:ASP:HB3	1:F:363:THR:HG23	2.02	0.41
2:B:53:LEU:HD21	2:B:59:ILE:CD1	2.51	0.41
2:E:283:ILE:HG13	2:E:293:MET:HE1	2.03	0.41
1:F:56:ASN:ND2	1:F:112:ASN:HD22	2.17	0.41
1:C:146:LEU:CD2	1:C:342:ILE:HD11	2.51	0.41
1:C:45:SER:HB3	5:C:1628:HOH:O	2.21	0.40
1:C:159:ASN:C	1:C:346:GLU:HB3	2.42	0.40
1:C:369:LEU:HB3	1:C:384:ILE:HD12	2.02	0.40
1:C:278:LYS:NZ	2:D:263:GLN:O	2.54	0.40
1:C:370:TYR:CE2	1:C:384:ILE:HG13	2.57	0.40
3:E:1536:SO4:S	4:E:4387:NAP:O2B	2.78	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	362/386 (94%)	354 (98%)	8 (2%)	0	100	100
1	C	362/386 (94%)	350 (97%)	11 (3%)	1 (0%)	41	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 ⓘ

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

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	LEU
1	A	224	ARG

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Mol	Chain	Res	Type
1	A	300	SER
1	A	328	LYS
1	A	378	LYS
2	B	45	SER
2	B	108	LYS
2	B	114	SER
2	B	224	ARG
2	B	251	ARG
2	B	299	MET
2	B	301	PHE
2	B	330	ASN
2	B	384	ILE
1	C	23	MET
1	C	85	LYS
1	C	107	ILE
1	C	148	ASN
1	C	159	ASN
1	C	168	THR
1	C	224	ARG
1	C	301	PHE
1	C	328	LYS
1	C	331	LYS
1	C	358	THR
1	C	359	LEU
2	D	224	ARG
2	D	301	PHE
2	D	332	GLU
2	D	338	LEU
2	E	27	GLN
2	E	51	ASP
2	E	92	THR
2	E	153	LYS
2	E	190	LYS
2	E	224	ARG
2	E	299	MET
2	E	328	LYS
1	F	155	ASN
1	F	161	LEU
1	F	224	ARG
1	F	299	MET
1	F	301	PHE
1	F	330	ASN

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Mol	Chain	Res	Type
1	F	338	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	73	ASN
1	A	155	ASN
1	A	249	ASN
2	B	68	ASN
2	B	135	HIS
2	B	376	ASN
1	C	148	ASN
1	C	159	ASN
1	C	249	ASN
1	C	340	GLN
2	D	56	ASN
2	D	139	ASN
2	E	27	GLN
2	E	139	ASN
2	E	151	GLN
1	F	56	ASN
1	F	100	ASN
1	F	249	ASN
1	F	330	ASN
1	F	376	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 carbohydrates in this entry.

5.6 Ligand geometry

10 ligands are modelled in this entry.

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

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

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	B	3387	3	-	8/31/67/67	0/5/5/5
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

All (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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	3387	NAP	C2A-N3A	4.35	1.39	1.32
4	A	2387	NAP	C2A-N3A	4.20	1.38	1.32
4	E	4387	NAP	C2A-N3A	4.19	1.38	1.32
3	B	1535	SO4	O1-S	3.15	1.63	1.46
3	B	1535	SO4	O3-S	-2.96	1.23	1.47
3	E	1536	SO4	O4-S	-2.84	1.24	1.47
4	B	3387	NAP	C2A-N1A	2.83	1.39	1.33
4	A	2387	NAP	C2A-N1A	2.59	1.38	1.33
4	E	4387	NAP	P2B-O2B	2.55	1.64	1.59
4	E	4387	NAP	C2A-N1A	2.45	1.38	1.33
4	B	3387	NAP	O4D-C1D	2.18	1.44	1.41

All (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
4	B	3387	NAP	O7N-C7N-C3N	-4.57	114.16	119.63
3	B	1535	SO4	O3-S-O2	4.06	130.52	109.31
4	E	4387	NAP	C6N-N1N-C2N	-3.85	118.46	121.97
3	B	1535	SO4	O4-S-O1	-3.76	89.70	109.31
3	E	1536	SO4	O4-S-O2	-3.74	89.81	109.31
3	E	1536	SO4	O4-S-O3	3.63	124.57	109.06
4	E	4387	NAP	C5D-C4D-C3D	-3.07	103.68	115.18
4	B	3387	NAP	O5B-C5B-C4B	2.96	119.18	108.99
4	B	3387	NAP	C3N-C7N-N7N	2.91	121.24	117.75
4	B	3387	NAP	C6N-N1N-C2N	-2.88	119.34	121.97
4	B	3387	NAP	O5D-C5D-C4D	2.80	118.63	108.99
3	B	1535	SO4	O2-S-O1	-2.76	89.08	109.43
4	E	4387	NAP	C2B-C3B-C4B	2.57	107.57	101.99
4	E	4387	NAP	PN-O3-PA	-2.55	124.07	132.83
4	E	4387	NAP	C3B-C2B-C1B	-2.46	98.26	102.89
4	E	4387	NAP	C5N-C4N-C3N	-2.43	117.47	120.34
4	B	3387	NAP	O5D-PN-O1N	-2.39	99.71	109.07
4	E	4387	NAP	O3B-C3B-C4B	-2.39	104.13	111.05
4	B	3387	NAP	C5D-C4D-C3D	-2.33	106.47	115.18
4	E	4387	NAP	O5D-PN-O1N	-2.23	100.35	109.07
4	B	3387	NAP	O4B-C1B-C2B	-2.22	102.74	106.59
4	E	4387	NAP	O7N-C7N-C3N	-2.21	116.99	119.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	4387	NAP	O2N-PN-O1N	2.20	123.11	112.24
4	A	2387	NAP	O7N-C7N-C3N	-2.19	117.01	119.63
4	E	4387	NAP	O7N-C7N-N7N	2.19	125.69	122.58
4	A	2387	NAP	O2N-PN-O1N	2.13	122.79	112.24
4	A	2387	NAP	C5D-C4D-C3D	-2.08	107.38	115.18

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	3387	NAP	C2B-O2B-P2B-O1X
4	B	3387	NAP	C5D-O5D-PN-O3
4	B	3387	NAP	C5D-O5D-PN-O1N
4	B	3387	NAP	C5D-O5D-PN-O2N
4	B	3387	NAP	O4D-C4D-C5D-O5D
4	B	3387	NAP	C3D-C4D-C5D-O5D
4	E	4387	NAP	C2B-O2B-P2B-O1X
4	E	4387	NAP	C5D-O5D-PN-O3
4	E	4387	NAP	C5D-O5D-PN-O1N
4	E	4387	NAP	C5D-O5D-PN-O2N
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
4	A	2387	NAP	C3D-C4D-C5D-O5D
4	E	4387	NAP	C3D-C4D-C5D-O5D
4	A	2387	NAP	C2B-O2B-P2B-O1X
4	E	4387	NAP	O4D-C4D-C5D-O5D
4	A	2387	NAP	O4B-C4B-C5B-O5B
4	B	3387	NAP	O4B-C4B-C5B-O5B
4	E	4387	NAP	O4B-C4B-C5B-O5B
4	B	3387	NAP	PN-O3-PA-O2A
4	E	4387	NAP	PN-O3-PA-O2A
4	A	2387	NAP	PN-O3-PA-O2A

There are no ring outliers.

6 monomers are involved in 12 short contacts:

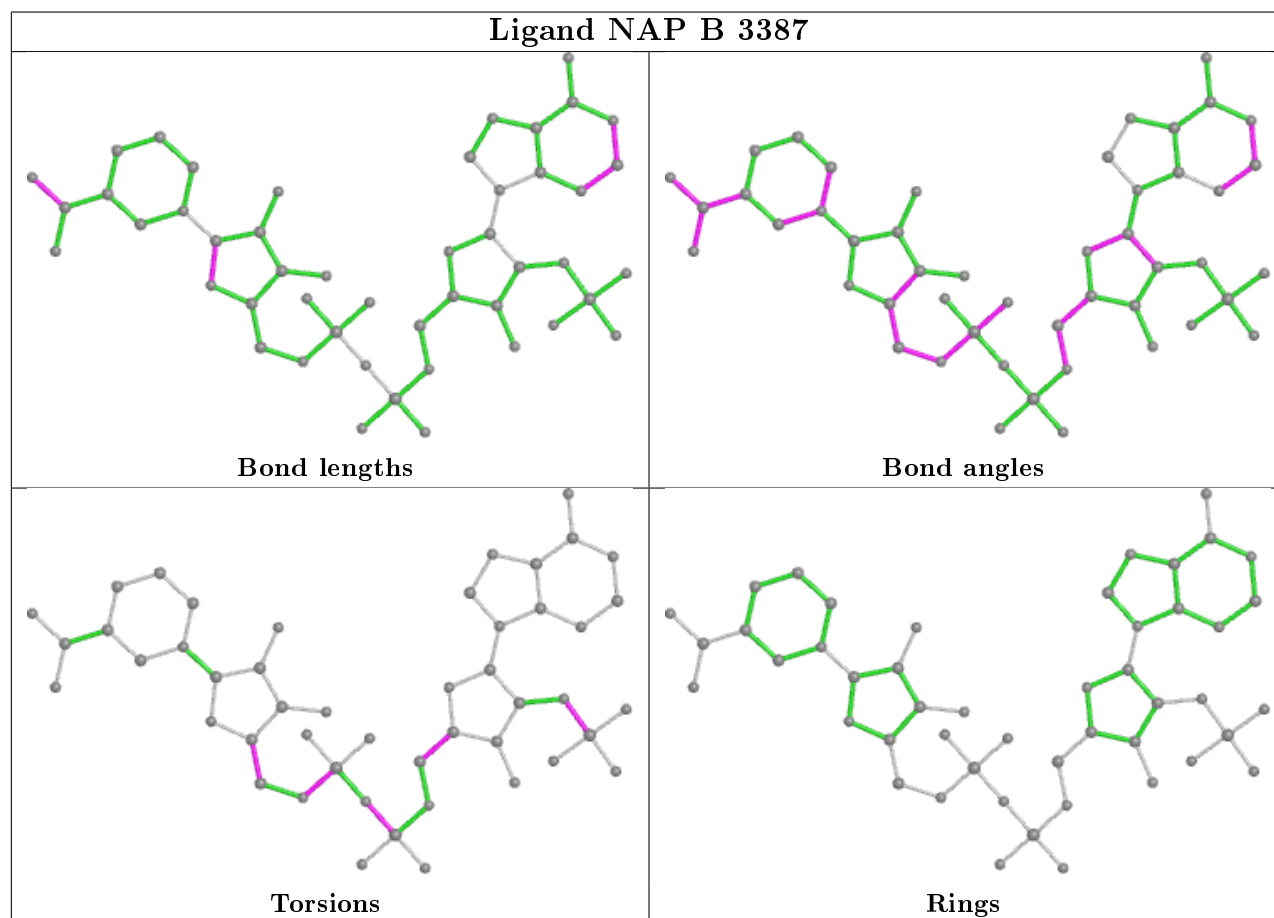
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	3387	NAP	4	0

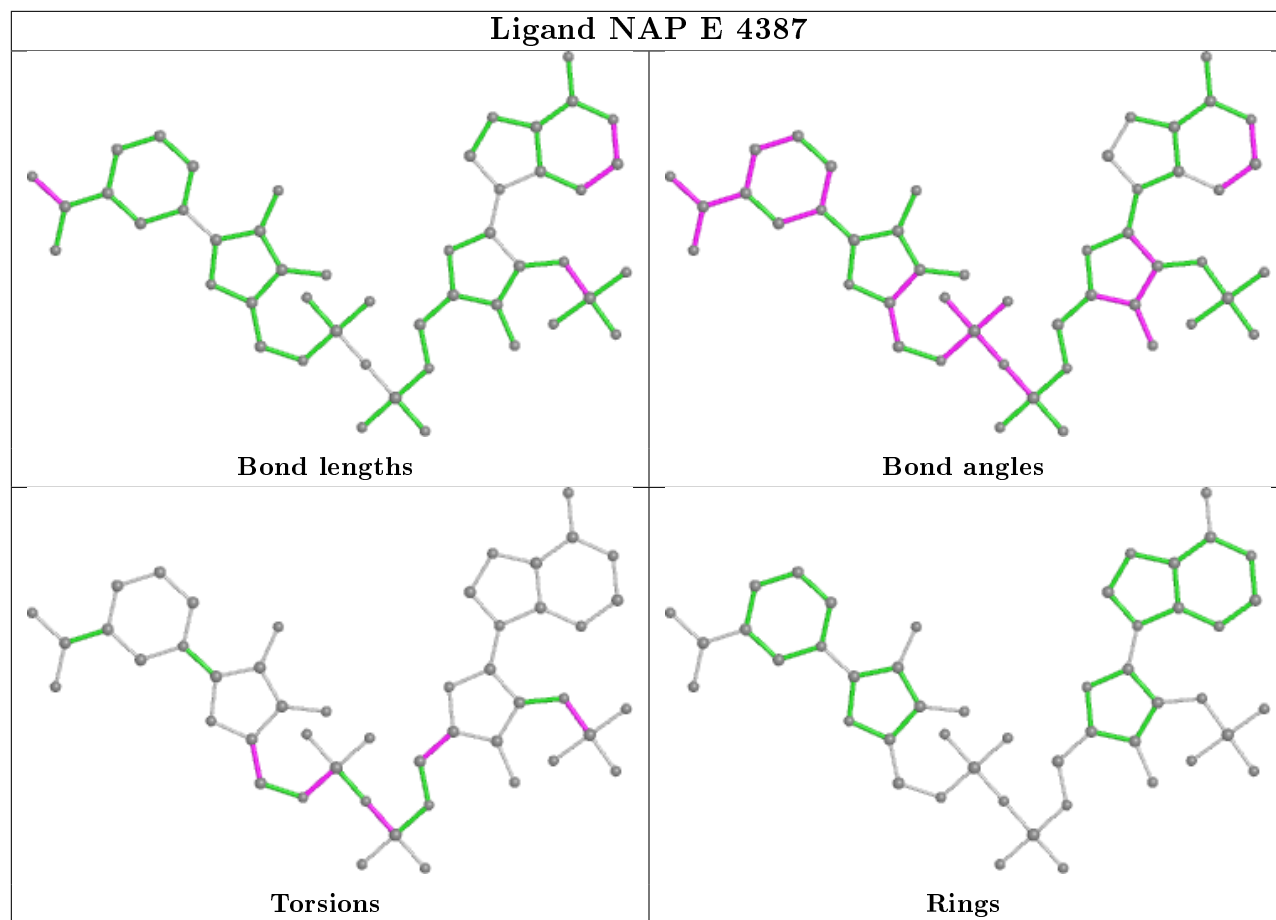
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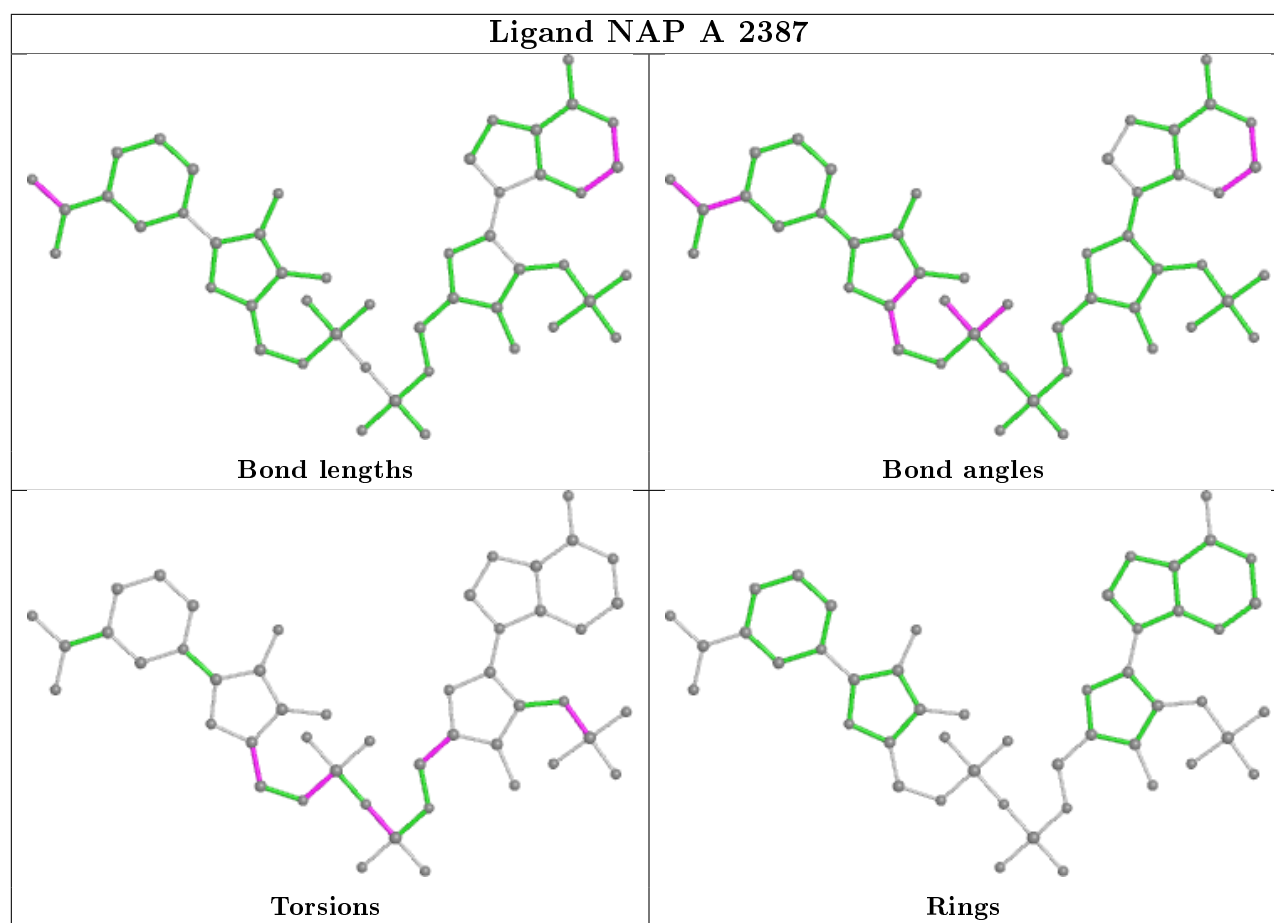
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	4387	NAP	6	0
4	A	2387	NAP	1	0
3	E	1536	SO4	1	0
3	B	1535	SO4	1	0
3	A	1532	SO4	2	0

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 ⓘ

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

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

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

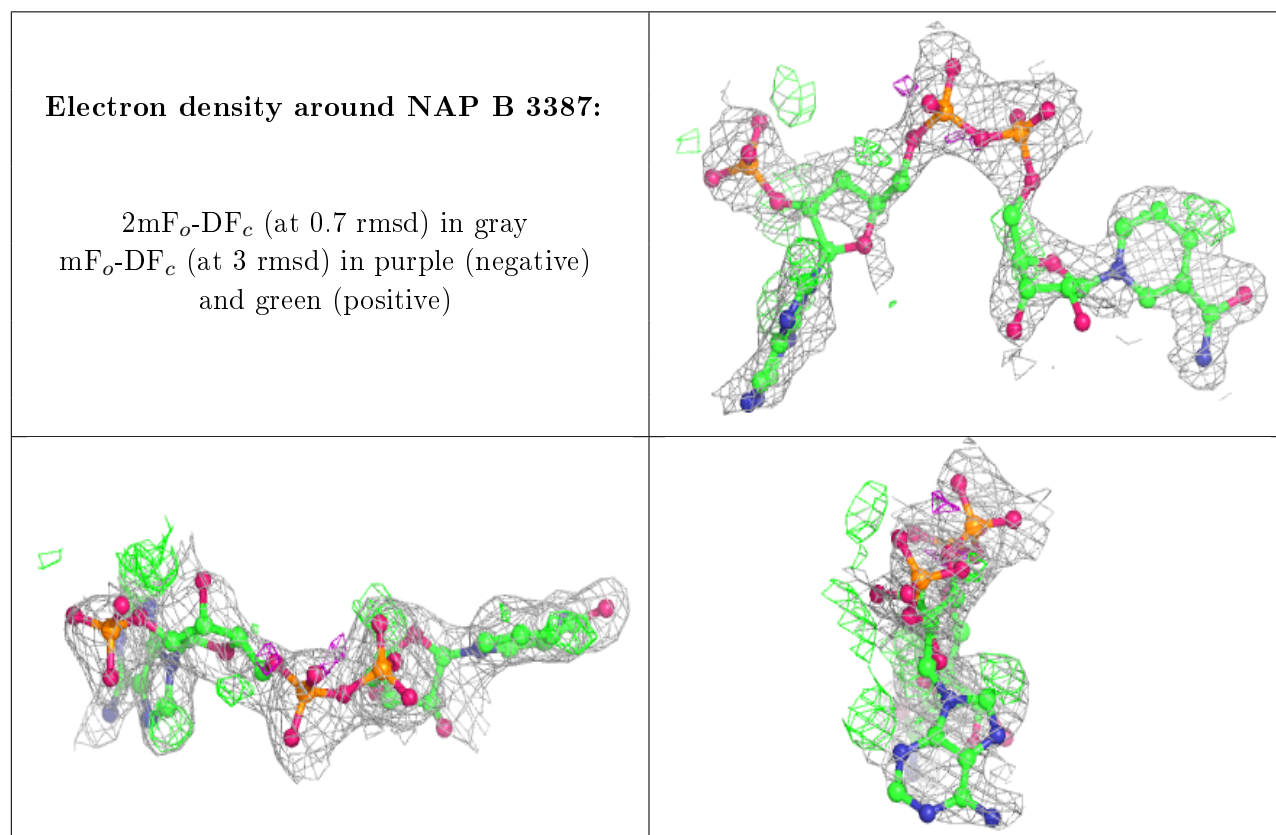
6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

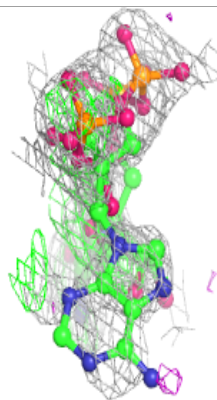
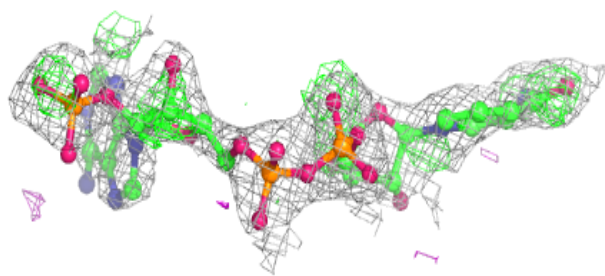
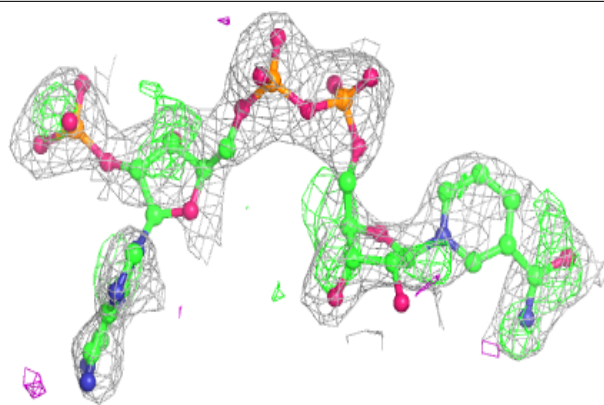
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

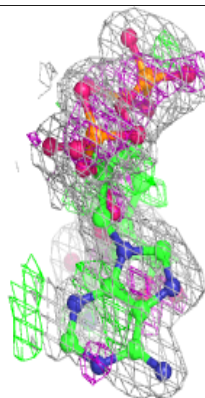
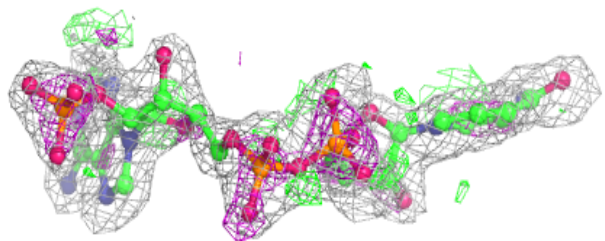
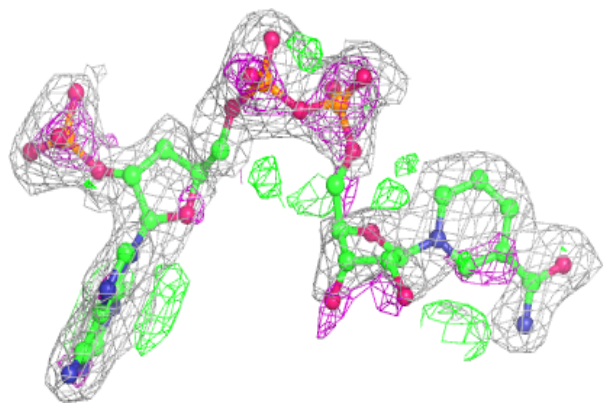


Electron density around NAP E 4387:

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

**Electron density around NAP A 2387:**

$2mF_o-DF_c$ (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.