



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 04:09 pm BST

PDB ID : 3LZ6
Title : Guinea Pig 11beta hydroxysteroid dehydrogenase with PF-877423
Authors : Pauly, T.A.
Deposited on : 2010-03-01
Resolution : 1.84 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

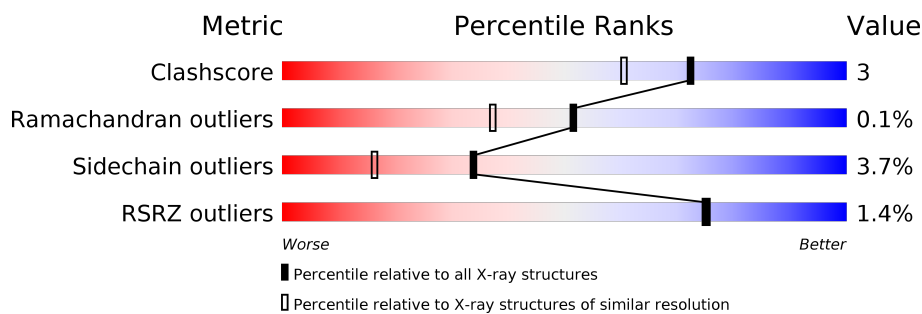
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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 $\leq 5\%$. 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	263	<div> <div>2%</div> <div>90%</div> <div>9%</div> <div>.</div> </div>
1	B	263	<div> <div>2%</div> <div>90%</div> <div>10%</div> </div>
1	C	263	<div> <div>91%</div> <div>8%</div> <div>.</div> </div>
1	D	263	<div> <div>2%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 8730 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 Corticosteroid 11-beta-dehydrogenase isozyme 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			2018	1296	337	370	15			
1	B	263	Total	C	N	O	S	0	0	0
			2018	1296	337	370	15			
1	C	263	Total	C	N	O	S	0	0	0
			2018	1296	337	370	15			
1	D	263	Total	C	N	O	S	0	0	0
			2018	1296	337	370	15			

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



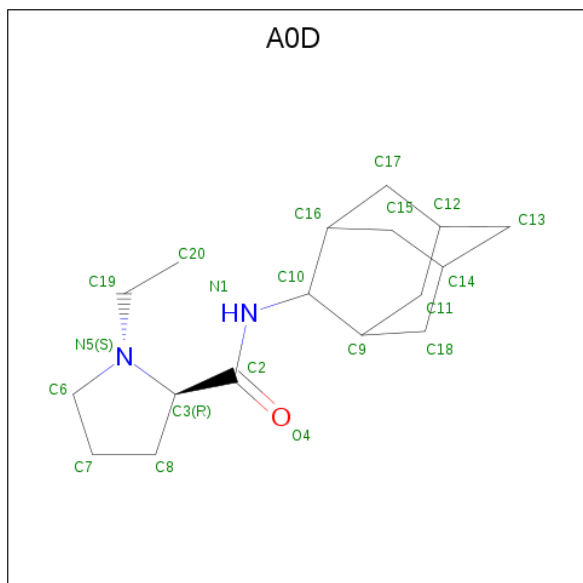
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	B	1	Total	C	N	O	P	0
			48	21	7	17	3	

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

- Molecule 3 is N-adamantan-2-yl-1-ethyl-D-prolinamide (three-letter code: A0D) (formula: $C_{17}H_{28}N_2O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			20	17	2	1		
3	B	1	Total	C	N	O	0	0
			20	17	2	1		
3	C	1	Total	C	N	O	0	0
			20	17	2	1		
3	D	1	Total	C	N	O	0	0
			20	17	2	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	101	Total	O	0	0
			101	101		
4	B	92	Total	O	0	0
			92	92		
4	C	84	Total	O	0	0
			84	84		

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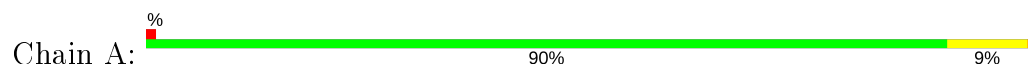
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	109	Total	O	0	0
			109	109		

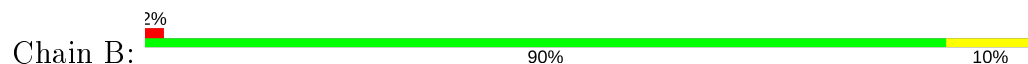
3 Residue-property plots [i](#)

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: Corticosteroid 11-beta-dehydrogenase isozyme 1



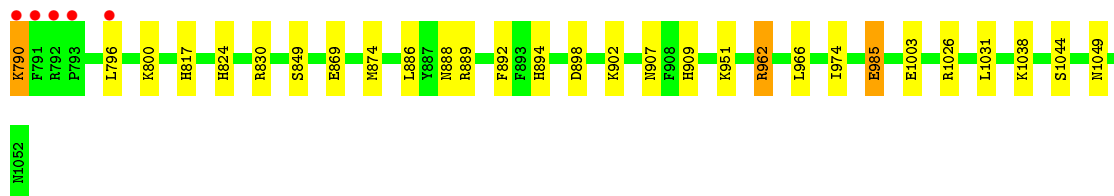
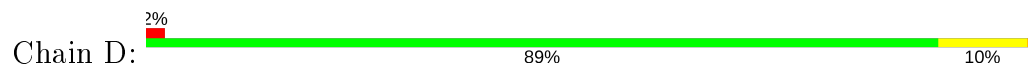
- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1



- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1



- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.40 Å 83.90 Å 179.96 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.29 – 1.84 48.80 – 1.84	Depositor EDS
% Data completeness (in resolution range)	95.7 (91.29-1.84) 89.1 (48.80-1.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 1.84 Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.207 , 0.251 0.221 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	19.6	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8730	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, A0D

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	1.01	2/2057 (0.1%)	1.04	4/2777 (0.1%)
1	B	0.94	1/2057 (0.0%)	1.07	8/2777 (0.3%)
1	C	0.96	0/2057	1.04	5/2777 (0.2%)
1	D	1.06	5/2057 (0.2%)	1.05	7/2777 (0.3%)
All	All	0.99	8/8228 (0.1%)	1.05	24/11108 (0.2%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	888	ASN	CB-CG	8.10	1.69	1.51
1	D	985	GLU	CG-CD	8.09	1.64	1.51
1	B	497	VAL	C-O	7.93	1.38	1.23
1	A	14	VAL	CB-CG1	5.96	1.65	1.52
1	A	38	VAL	CB-CG1	5.39	1.64	1.52
1	D	985	GLU	CB-CG	5.21	1.62	1.52
1	D	985	GLU	CD-OE2	-5.07	1.20	1.25
1	D	951	LYS	CD-CE	5.06	1.64	1.51

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	436	ARG	NE-CZ-NH2	-20.48	110.06	120.30
1	A	173	ARG	NE-CZ-NH2	-19.57	110.52	120.30
1	C	699	ARG	NE-CZ-NH2	-19.25	110.68	120.30
1	D	962	ARG	NE-CZ-NH2	-18.93	110.83	120.30
1	B	436	ARG	NE-CZ-NH1	17.18	128.89	120.30
1	A	173	ARG	NE-CZ-NH1	16.40	128.50	120.30
1	C	699	ARG	NE-CZ-NH1	15.61	128.11	120.30
1	D	962	ARG	NE-CZ-NH1	10.85	125.72	120.30
1	D	985	GLU	OE1-CD-OE2	-10.12	111.15	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	497	VAL	N-CA-C	8.29	133.39	111.00
1	D	962	ARG	CG-CD-NE	-7.07	96.96	111.80
1	A	173	ARG	CD-NE-CZ	6.56	132.79	123.60
1	C	699	ARG	CD-NE-CZ	6.42	132.59	123.60
1	B	372	ASP	CB-CG-OD2	6.34	124.01	118.30
1	B	497	VAL	CB-CA-C	-5.84	100.29	111.40
1	B	436	ARG	CD-NE-CZ	5.80	131.72	123.60
1	C	596	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	177	LEU	CA-CB-CG	5.53	128.01	115.30
1	C	699	ARG	CG-CD-NE	-5.50	100.24	111.80
1	B	333	ASP	CB-CG-OD2	5.41	123.17	118.30
1	B	436	ARG	CG-CD-NE	-5.31	100.66	111.80
1	D	830	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	D	898	ASP	CB-CG-OD2	5.14	122.93	118.30
1	D	962	ARG	CD-NE-CZ	5.00	130.60	123.60

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	2018	0	2053	9	0
1	B	2018	0	2050	14	0
1	C	2018	0	2050	17	0
1	D	2018	0	2050	12	0
2	A	48	0	25	1	0
2	B	48	0	25	2	0
2	C	48	0	25	3	0
2	D	48	0	25	0	0
3	A	20	0	27	0	0
3	B	20	0	28	5	0
3	C	20	0	28	6	0
3	D	20	0	27	0	0
4	A	101	0	0	0	0
4	B	92	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	84	0	0	2	0
4	D	109	0	0	0	0
All	All	8730	0	8413	57	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 3.

All (57) 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:B:360:LEU:H	1:B:381:ASN:HD21	1.16	0.88
1:D:886:LEU:H	1:D:907:ASN:HD21	1.26	0.83
1:C:623:LEU:H	1:C:644:ASN:HD21	1.27	0.82
1:D:800:LYS:HE2	1:D:874:MET:O	1.81	0.80
1:C:625:ASN:HD21	1:C:636:ASN:ND2	1.81	0.78
1:C:625:ASN:HD21	1:C:636:ASN:CG	1.88	0.76
1:B:526:ASN:O	4:B:2286:HOH:O	2.10	0.69
1:B:368:HIS:CE1	1:B:370:GLU:OE2	2.46	0.68
1:C:724:ALA:HA	3:C:2006:A0D:H13A	1.78	0.65
1:B:368:HIS:NE2	1:B:370:GLU:OE2	2.32	0.63
1:B:360:LEU:H	1:B:381:ASN:ND2	1.91	0.62
1:C:623:LEU:H	1:C:644:ASN:ND2	1.97	0.62
1:C:625:ASN:ND2	1:C:636:ASN:ND2	2.48	0.61
1:B:509:PRO:HA	1:B:512:LYS:HE2	1.84	0.59
1:A:28:HIS:HE1	1:A:214:GLU:O	1.85	0.58
1:D:800:LYS:CE	1:D:874:MET:O	2.51	0.58
1:B:455:LEU:N	3:B:2005:A0D:H7A	2.19	0.57
1:D:886:LEU:HD11	1:D:902:LYS:HE2	1.86	0.57
2:B:2001:NAP:C7N	3:B:2005:A0D:H17A	2.35	0.57
1:D:886:LEU:H	1:D:907:ASN:ND2	1.99	0.56
1:B:335:THR:O	1:B:339:GLU:HG3	2.04	0.56
1:C:625:ASN:ND2	1:C:636:ASN:HD21	2.04	0.56
1:D:892:PHE:HB2	1:D:894:HIS:HE1	1.69	0.56
1:C:529:ARG:NH1	4:C:2380:HOH:O	2.38	0.56
1:D:790:LYS:HG2	1:D:790:LYS:O	2.06	0.54
1:C:638:ARG:HA	1:D:909:HIS:HE1	1.73	0.53
1:C:561:HIS:CE1	1:C:585:ALA:HB1	2.44	0.53
1:D:962:ARG:HD3	1:D:974:ILE:O	2.08	0.53
1:C:555:LEU:HA	1:C:558:MET:HE3	1.93	0.51
1:C:554:HIS:HE1	1:C:740:GLU:O	1.94	0.50
3:B:2005:A0D:H17	3:B:2005:A0D:C2	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2002:NAP:C3N	3:C:2006:A0D:H17A	2.41	0.50
1:A:95:HIS:CE1	1:A:122:PHE:CE1	3.00	0.48
2:C:2002:NAP:C7N	3:C:2006:A0D:H17A	2.43	0.48
2:B:2001:NAP:C3N	3:B:2005:A0D:H17A	2.43	0.48
1:A:197:THR:HG21	2:A:2000:NAP:O1A	2.13	0.47
1:A:192:LEU:HD13	1:A:210:ALA:HB2	1.95	0.47
3:C:2006:A0D:C2	3:C:2006:A0D:H17	2.36	0.46
1:A:151:THR:HG21	1:B:433:SER:HB2	1.99	0.45
1:C:733:LEU:HD11	1:D:1049:ASN:HB2	1.99	0.45
1:B:368:HIS:CD2	1:B:370:GLU:OE2	2.70	0.45
3:B:2005:A0D:H16	3:B:2005:A0D:O4	2.18	0.44
1:C:554:HIS:HD2	4:C:2193:HOH:O	2.01	0.44
1:A:131:PRO:O	1:A:135:GLN:HG3	2.18	0.43
3:C:2006:A0D:H16	3:C:2006:A0D:O4	2.18	0.43
1:B:494:MET:O	1:B:494:MET:HE3	2.18	0.43
1:A:239:VAL:N	1:A:240:PRO:CD	2.81	0.43
1:D:817:HIS:HE1	1:D:1003:GLU:O	2.02	0.42
1:A:150:ILE:HG22	1:B:511:ARG:HG3	2.00	0.42
1:B:314:ALA:O	1:B:318:GLU:HG3	2.19	0.42
1:B:287:GLU:HG3	1:B:476:LYS:HG3	2.02	0.42
1:A:99:ASN:HD22	1:A:99:ASN:N	2.18	0.41
1:C:699:ARG:HD3	1:C:711:ILE:HB	2.01	0.41
1:D:824:HIS:ND1	1:D:849:SER:HB2	2.36	0.41
2:C:2002:NAP:C4N	3:C:2006:A0D:H17A	2.50	0.41
1:C:786:ASN:HD22	1:C:786:ASN:C	2.24	0.41
1:C:561:HIS:CE1	1:C:585:ALA:CB	3.04	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	261/263 (99%)	251 (96%)	9 (3%)	1 (0%)	34	20
1	B	261/263 (99%)	252 (97%)	9 (3%)	0	100	100
1	C	261/263 (99%)	252 (97%)	9 (3%)	0	100	100
1	D	261/263 (99%)	252 (97%)	9 (3%)	0	100	100
All	All	1044/1052 (99%)	1007 (96%)	36 (3%)	1 (0%)	51	37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	ALA

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	214/214 (100%)	206 (96%)	8 (4%)	34	16
1	B	214/214 (100%)	209 (98%)	5 (2%)	50	34
1	C	214/214 (100%)	205 (96%)	9 (4%)	30	12
1	D	214/214 (100%)	204 (95%)	10 (5%)	26	10
All	All	856/856 (100%)	824 (96%)	32 (4%)	34	16

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LYS
1	A	99	ASN
1	A	114	SER
1	A	178	VAL
1	A	192	LEU
1	A	218	LEU
1	A	237	ARG
1	A	260	ASN
1	B	264	LYS
1	B	307	GLU

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Mol	Chain	Res	Type
1	B	362	ASN
1	B	363	ARG
1	B	505	LEU
1	C	529	ARG
1	C	568	SER
1	C	625	ASN
1	C	626	ARG
1	C	685	SER
1	C	706	LYS
1	C	718	LEU
1	C	744	LEU
1	C	786	ASN
1	D	790	LYS
1	D	796	LEU
1	D	869	GLU
1	D	889	ARG
1	D	966	LEU
1	D	985	GLU
1	D	1026	ARG
1	D	1031	LEU
1	D	1038	LYS
1	D	1044	SER

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	28	HIS
1	A	47	GLN
1	A	83	ASN
1	A	94	ASN
1	A	99	ASN
1	A	120	HIS
1	A	182	ASN
1	A	260	ASN
1	B	357	ASN
1	B	373	ASN
1	B	381	ASN
1	C	554	HIS
1	C	620	ASN
1	C	625	ASN
1	C	631	HIS
1	C	644	ASN

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Mol	Chain	Res	Type
1	C	786	ASN
1	D	817	HIS
1	D	899	ASN
1	D	907	ASN
1	D	909	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

8 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	$\# Z > 2$
2	NAP	D	2003	-	45,52,52	1.32	2 (4%)	56,80,80	1.74	14 (25%)
2	NAP	C	2002	-	45,52,52	1.53	4 (8%)	56,80,80	1.81	14 (25%)
3	A0D	B	2005	-	23,23,23	2.58	11 (47%)	33,34,34	2.33	13 (39%)
3	A0D	C	2006	-	23,23,23	2.58	11 (47%)	33,34,34	2.32	13 (39%)
2	NAP	B	2001	-	45,52,52	1.43	4 (8%)	56,80,80	1.88	18 (32%)
2	NAP	A	2000	-	45,52,52	1.36	2 (4%)	56,80,80	1.92	15 (26%)
3	A0D	D	2007	-	23,23,23	3.29	6 (26%)	33,34,34	2.17	11 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A0D	A	2004	-	23,23,23	3.75	13 (56%)	33,34,34	3.21	20 (60%)

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
2	NAP	D	2003	-	-	7/31/67/67	0/5/5/5
2	NAP	C	2002	-	-	4/31/67/67	0/5/5/5
3	A0D	B	2005	-	-	2/10/48/48	0/5/4/4
3	A0D	C	2006	-	-	2/10/48/48	0/5/4/4
2	NAP	B	2001	-	-	3/31/67/67	0/5/5/5
2	NAP	A	2000	-	-	3/31/67/67	0/5/5/5
3	A0D	D	2007	-	-	3/10/48/48	0/5/4/4
3	A0D	A	2004	-	-	0/10/48/48	0/5/4/4

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2004	A0D	C16-C10	-12.02	1.22	1.53
3	D	2007	A0D	C16-C10	-11.45	1.24	1.53
3	D	2007	A0D	C8-C3	-7.48	1.35	1.53
3	C	2006	A0D	C17-C16	-7.13	1.36	1.53
3	B	2005	A0D	C17-C16	-7.13	1.36	1.53
2	B	2001	NAP	C4A-N3A	6.99	1.45	1.35
3	A	2004	A0D	O4-C2	6.70	1.36	1.23
2	C	2002	NAP	C4A-N3A	6.56	1.44	1.35
2	A	2000	NAP	C4A-N3A	6.53	1.44	1.35
2	D	2003	NAP	C4A-N3A	6.19	1.44	1.35
3	A	2004	A0D	C17-C12	-5.15	1.39	1.52
3	C	2006	A0D	C16-C10	-4.62	1.41	1.53
3	B	2005	A0D	C16-C10	-4.62	1.41	1.53
3	D	2007	A0D	C11-C12	-4.51	1.41	1.52
3	A	2004	A0D	C11-C9	-4.29	1.43	1.53
3	A	2004	A0D	C9-C10	4.21	1.64	1.53
3	A	2004	A0D	C2-N1	3.86	1.42	1.34
3	B	2005	A0D	C18-C9	3.38	1.61	1.53
3	C	2006	A0D	C18-C9	3.34	1.61	1.53
3	C	2006	A0D	C11-C9	-3.30	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2005	A0D	C11-C9	-3.27	1.45	1.53
3	B	2005	A0D	C18-C14	3.23	1.61	1.52
3	C	2006	A0D	C18-C14	3.22	1.61	1.52
3	C	2006	A0D	O4-C2	3.19	1.29	1.23
3	D	2007	A0D	C11-C9	3.18	1.60	1.53
3	B	2005	A0D	O4-C2	3.16	1.29	1.23
3	C	2006	A0D	C3-C2	-3.11	1.45	1.52
3	B	2005	A0D	C3-C2	-3.10	1.45	1.52
3	B	2005	A0D	C13-C14	-3.02	1.44	1.52
3	C	2006	A0D	C13-C14	-2.99	1.45	1.52
3	A	2004	A0D	C10-N1	2.95	1.50	1.45
3	A	2004	A0D	C11-C12	-2.91	1.45	1.52
3	A	2004	A0D	C15-C14	-2.91	1.45	1.52
3	D	2007	A0D	C2-N1	-2.75	1.27	1.34
3	A	2004	A0D	C8-C3	2.63	1.60	1.53
2	C	2002	NAP	O4D-C1D	2.52	1.44	1.41
3	A	2004	A0D	C15-C16	-2.49	1.47	1.53
2	C	2002	NAP	O4D-C4D	-2.49	1.39	1.45
3	D	2007	A0D	C13-C12	2.44	1.59	1.52
2	B	2001	NAP	P2B-O2B	2.34	1.63	1.59
2	D	2003	NAP	C2A-N3A	2.30	1.35	1.32
3	B	2005	A0D	C9-C10	-2.27	1.47	1.53
3	C	2006	A0D	C9-C10	-2.27	1.47	1.53
2	B	2001	NAP	C3N-C7N	-2.24	1.47	1.50
3	A	2004	A0D	C6-N5	-2.23	1.41	1.47
3	B	2005	A0D	C2-N1	2.17	1.38	1.34
3	C	2006	A0D	C2-N1	2.16	1.38	1.34
3	A	2004	A0D	C18-C9	-2.15	1.48	1.53
2	A	2000	NAP	C7N-N7N	2.12	1.37	1.33
3	C	2006	A0D	C17-C12	-2.08	1.47	1.52
3	B	2005	A0D	C17-C12	-2.06	1.47	1.52
2	C	2002	NAP	O3D-C3D	2.03	1.47	1.43
2	B	2001	NAP	C5A-C4A	-2.01	1.35	1.40

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2004	A0D	C8-C3-C2	-7.23	95.79	111.22
3	A	2004	A0D	C16-C10-N1	-6.96	98.73	112.00
2	A	2000	NAP	N3A-C2A-N1A	-6.53	118.48	128.68
3	A	2004	A0D	C13-C12-C11	-5.63	99.01	109.65
3	A	2004	A0D	C9-C10-N1	5.48	122.43	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2006	A0D	C16-C10-N1	-5.43	101.66	112.00
3	B	2005	A0D	C16-C10-N1	-5.42	101.67	112.00
2	C	2002	NAP	N3A-C2A-N1A	-5.36	120.30	128.68
2	B	2001	NAP	N3A-C2A-N1A	-5.22	120.53	128.68
3	C	2006	A0D	C15-C16-C10	5.17	119.49	109.56
3	B	2005	A0D	C15-C16-C10	5.17	119.49	109.56
3	D	2007	A0D	C8-C3-N5	4.93	115.77	104.98
3	A	2004	A0D	C17-C12-C11	4.89	118.87	109.65
3	B	2005	A0D	C18-C9-C11	-4.50	101.33	109.05
3	C	2006	A0D	C18-C9-C11	-4.49	101.34	109.05
3	C	2006	A0D	C15-C14-C13	-4.30	101.52	109.65
2	D	2003	NAP	O2B-C2B-C1B	4.29	125.55	110.10
3	B	2005	A0D	C15-C14-C13	-4.29	101.56	109.65
3	D	2007	A0D	C18-C14-C15	-4.29	101.56	109.65
3	A	2004	A0D	C17-C16-C10	4.05	117.34	109.56
3	A	2004	A0D	C18-C9-C10	-3.96	101.95	109.56
2	D	2003	NAP	N3A-C2A-N1A	-3.90	122.58	128.68
3	D	2007	A0D	C16-C10-N1	-3.87	104.62	112.00
2	C	2002	NAP	C3N-C7N-N7N	3.87	122.39	117.75
3	D	2007	A0D	C15-C16-C10	3.87	117.00	109.56
2	A	2000	NAP	O7N-C7N-C3N	-3.85	115.03	119.63
3	A	2004	A0D	C17-C12-C13	-3.85	102.39	109.65
2	D	2003	NAP	C4A-C5A-N7A	-3.83	105.41	109.40
2	C	2002	NAP	O2B-C2B-C1B	3.80	123.78	110.10
2	A	2000	NAP	O3X-P2B-O2X	3.79	122.11	107.64
3	A	2004	A0D	C18-C9-C11	3.71	115.41	109.05
2	C	2002	NAP	C4A-C5A-N7A	-3.63	105.62	109.40
2	A	2000	NAP	O2B-C2B-C1B	3.56	122.93	110.10
3	A	2004	A0D	C8-C3-N5	-3.52	97.29	104.98
2	A	2000	NAP	C3D-C2D-C1D	3.51	106.26	100.98
2	A	2000	NAP	O3B-C3B-C4B	-3.50	100.93	111.05
3	D	2007	A0D	C15-C14-C13	3.47	116.19	109.65
2	C	2002	NAP	O7N-C7N-C3N	-3.42	115.54	119.63
3	B	2005	A0D	C6-N5-C3	3.42	113.44	106.54
3	C	2006	A0D	C6-N5-C3	3.41	113.43	106.54
2	B	2001	NAP	C5B-C4B-C3B	-3.30	102.80	115.18
2	A	2000	NAP	C4A-C5A-N7A	-3.24	106.02	109.40
2	B	2001	NAP	O3B-C3B-C2B	-3.19	102.09	111.17
2	D	2003	NAP	O3D-C3D-C2D	-3.19	101.51	111.82
2	C	2002	NAP	O2D-C2D-C3D	3.14	121.98	111.82
2	A	2000	NAP	O3D-C3D-C4D	-3.09	102.13	111.05
3	B	2005	A0D	C19-N5-C3	-3.08	104.59	112.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2006	A0D	C19-N5-C3	-3.06	104.63	112.88
3	A	2004	A0D	C9-C18-C14	-3.06	104.74	110.17
2	C	2002	NAP	O2D-C2D-C1D	3.02	122.01	110.85
3	D	2007	A0D	C19-N5-C3	-3.02	104.75	112.88
2	B	2001	NAP	O3D-C3D-C2D	-3.00	102.10	111.82
2	D	2003	NAP	C6N-N1N-C2N	2.99	124.70	121.97
3	A	2004	A0D	C18-C14-C13	2.97	115.25	109.65
3	D	2007	A0D	C7-C6-N5	-2.95	99.35	104.15
2	B	2001	NAP	O2B-C2B-C1B	2.94	120.69	110.10
2	D	2003	NAP	C3N-C7N-N7N	2.93	121.27	117.75
2	C	2002	NAP	C2A-N1A-C6A	2.93	123.76	118.75
3	B	2005	A0D	C17-C16-C15	2.92	114.06	109.05
2	B	2001	NAP	O4B-C1B-C2B	2.92	111.65	106.59
2	B	2001	NAP	C4A-C5A-N7A	-2.92	106.36	109.40
3	D	2007	A0D	C6-N5-C3	-2.90	100.68	106.54
3	C	2006	A0D	C17-C16-C15	2.90	114.02	109.05
2	B	2001	NAP	O4B-C4B-C3B	2.88	110.81	105.11
2	B	2001	NAP	O3B-C3B-C4B	-2.86	102.79	111.05
2	C	2002	NAP	C2D-C3D-C4D	2.82	108.11	102.64
2	A	2000	NAP	O2D-C2D-C1D	2.81	121.21	110.85
2	B	2001	NAP	C3N-C7N-N7N	2.80	121.11	117.75
3	D	2007	A0D	C7-C8-C3	-2.78	98.36	104.18
2	B	2001	NAP	O7N-C7N-C3N	-2.78	116.31	119.63
3	A	2004	A0D	C15-C14-C13	-2.78	104.40	109.65
2	B	2001	NAP	C6N-N1N-C2N	2.75	124.48	121.97
3	D	2007	A0D	C2-C3-N5	2.65	115.87	112.36
2	A	2000	NAP	C5N-C4N-C3N	-2.60	117.27	120.34
3	A	2004	A0D	C14-C13-C12	2.58	115.36	109.89
3	A	2004	A0D	C9-C11-C12	2.56	114.71	110.17
3	D	2007	A0D	C10-N1-C2	-2.54	119.38	123.21
3	B	2005	A0D	C16-C15-C14	-2.49	105.74	110.17
3	B	2005	A0D	C18-C14-C15	2.49	114.34	109.65
3	C	2006	A0D	C16-C15-C14	-2.48	105.76	110.17
3	C	2006	A0D	C18-C14-C15	2.48	114.32	109.65
3	B	2005	A0D	C16-C17-C12	-2.48	105.77	110.17
3	A	2004	A0D	C16-C17-C12	-2.47	105.78	110.17
2	C	2002	NAP	O3B-C3B-C2B	-2.45	104.19	111.17
3	C	2006	A0D	C16-C17-C12	-2.44	105.83	110.17
2	B	2001	NAP	C3N-C2N-N1N	-2.43	118.05	120.43
2	B	2001	NAP	PN-O3-PA	-2.43	124.50	132.83
2	D	2003	NAP	O7N-C7N-C3N	-2.41	116.75	119.63
2	D	2003	NAP	O3B-C3B-C2B	-2.38	104.42	111.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2000	NAP	C2B-C3B-C4B	2.37	107.13	101.99
2	B	2001	NAP	C2B-C3B-C4B	2.36	107.11	101.99
2	A	2000	NAP	O3D-C3D-C2D	-2.32	104.31	111.82
2	D	2003	NAP	C3D-C2D-C1D	2.32	104.47	100.98
3	A	2004	A0D	C16-C15-C14	-2.29	106.09	110.17
2	C	2002	NAP	C5B-C4B-C3B	-2.26	106.70	115.18
3	A	2004	A0D	C18-C14-C15	-2.26	105.39	109.65
2	B	2001	NAP	C4N-C3N-C7N	-2.23	115.06	121.04
2	D	2003	NAP	O3X-P2B-O2B	-2.23	96.00	105.99
2	A	2000	NAP	O2A-PA-O1A	2.23	123.25	112.24
3	C	2006	A0D	C17-C16-C10	-2.23	105.29	109.56
3	B	2005	A0D	C17-C16-C10	-2.22	105.30	109.56
2	B	2001	NAP	C2N-C3N-C7N	2.19	125.81	119.46
2	A	2000	NAP	O7N-C7N-N7N	2.16	125.64	122.58
2	D	2003	NAP	C3N-C2N-N1N	-2.15	118.33	120.43
3	B	2005	A0D	O4-C2-N1	2.13	126.88	122.93
2	D	2003	NAP	O2A-PA-O1A	2.13	122.75	112.24
2	B	2001	NAP	O3X-P2B-O1X	2.12	119.00	110.68
3	C	2006	A0D	O4-C2-N1	2.12	126.86	122.93
2	D	2003	NAP	C2B-C3B-C4B	2.12	106.59	101.99
3	B	2005	A0D	C9-C11-C12	-2.11	106.41	110.17
2	A	2000	NAP	O4D-C1D-C2D	-2.10	103.86	106.93
2	C	2002	NAP	C5A-C6A-N6A	2.09	123.53	120.35
3	C	2006	A0D	C9-C11-C12	-2.09	106.45	110.17
2	C	2002	NAP	O2X-P2B-O1X	2.09	118.86	110.68
3	A	2004	A0D	O4-C2-C3	-2.05	115.53	120.63
3	A	2004	A0D	C15-C16-C10	2.04	113.49	109.56
2	C	2002	NAP	O2B-P2B-O1X	-2.04	101.53	109.39
2	D	2003	NAP	O3B-C3B-C4B	-2.03	105.18	111.05

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2003	NAP	C5D-O5D-PN-O2N
2	D	2003	NAP	C1B-C2B-O2B-P2B
3	D	2007	A0D	O4-C2-N1-C10
2	A	2000	NAP	PN-O3-PA-O1A
3	D	2007	A0D	O4-C2-C3-C8
3	D	2007	A0D	C20-C19-N5-C6
2	D	2003	NAP	C5D-O5D-PN-O3
2	D	2003	NAP	PN-O3-PA-O2A

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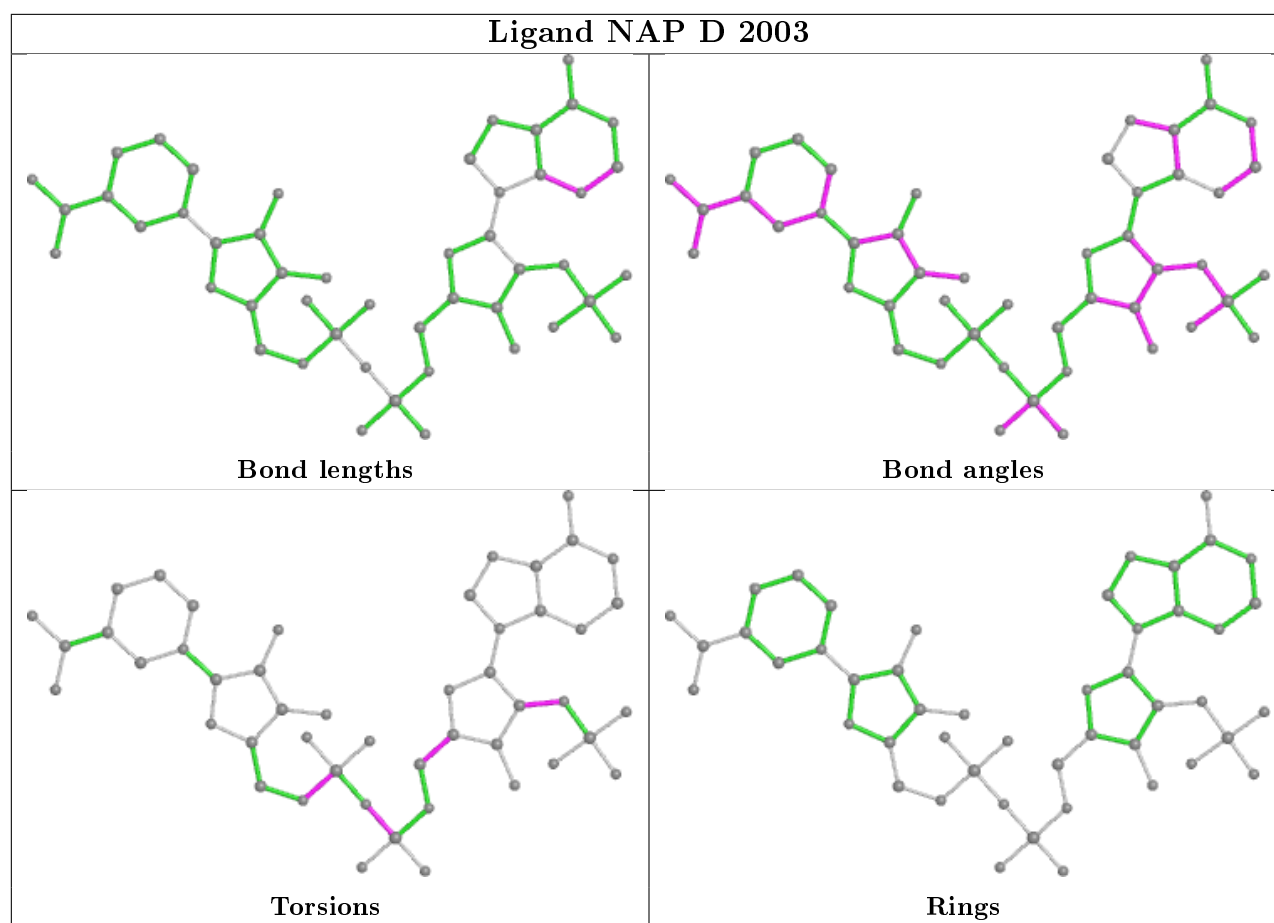
Mol	Chain	Res	Type	Atoms
2	C	2002	NAP	PN-O3-PA-O1A
2	B	2001	NAP	PN-O3-PA-O2A
2	D	2003	NAP	C5D-O5D-PN-O1N
2	D	2003	NAP	PN-O3-PA-O1A
2	C	2002	NAP	PN-O3-PA-O2A
2	A	2000	NAP	PN-O3-PA-O2A
2	C	2002	NAP	C1B-C2B-O2B-P2B
2	B	2001	NAP	O4B-C4B-C5B-O5B
2	C	2002	NAP	O4B-C4B-C5B-O5B
2	D	2003	NAP	O4B-C4B-C5B-O5B
3	B	2005	A0D	C9-C10-N1-C2
3	B	2005	A0D	C16-C10-N1-C2
3	C	2006	A0D	C9-C10-N1-C2
3	C	2006	A0D	C16-C10-N1-C2
2	A	2000	NAP	O4B-C4B-C5B-O5B
2	B	2001	NAP	C5D-O5D-PN-O1N

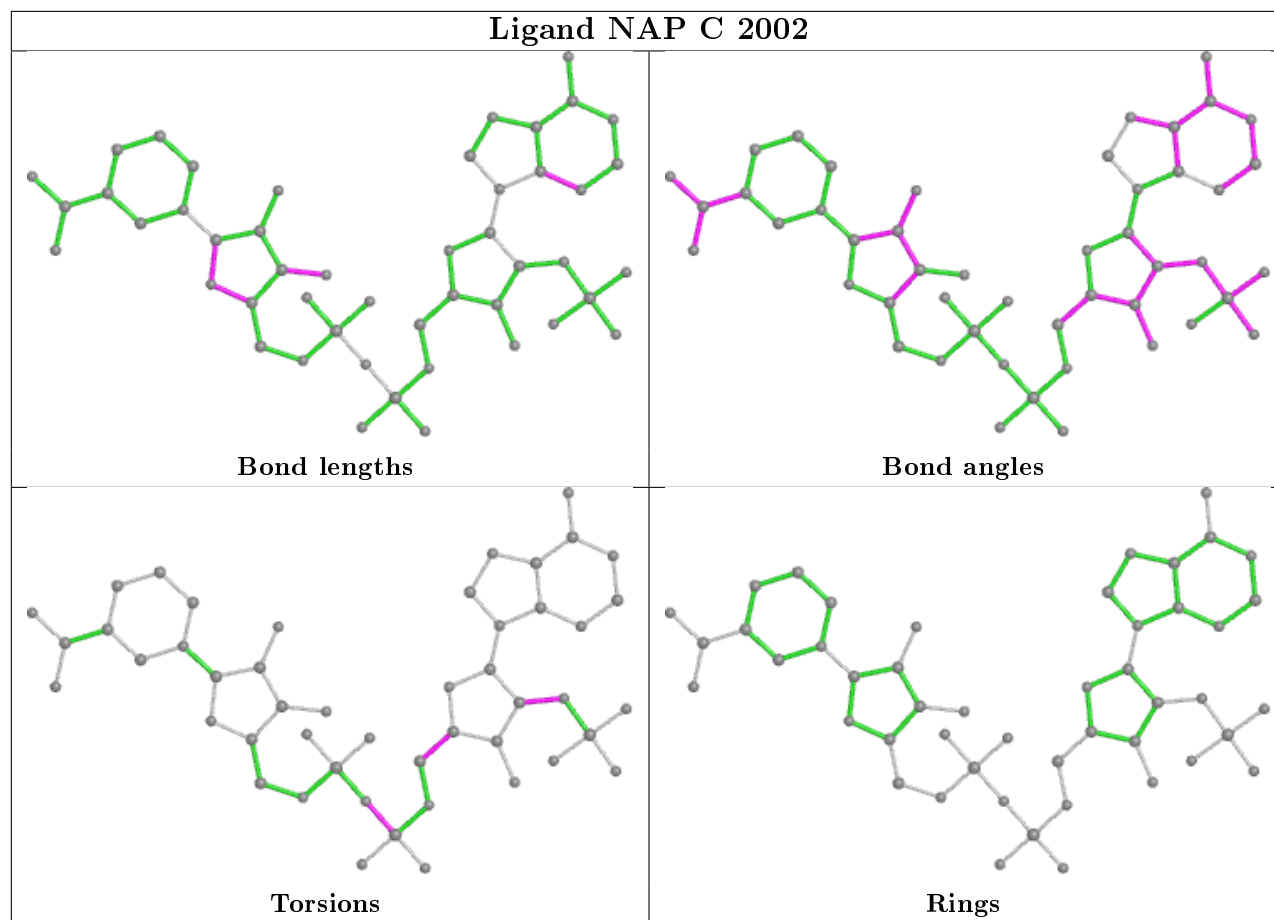
There are no ring outliers.

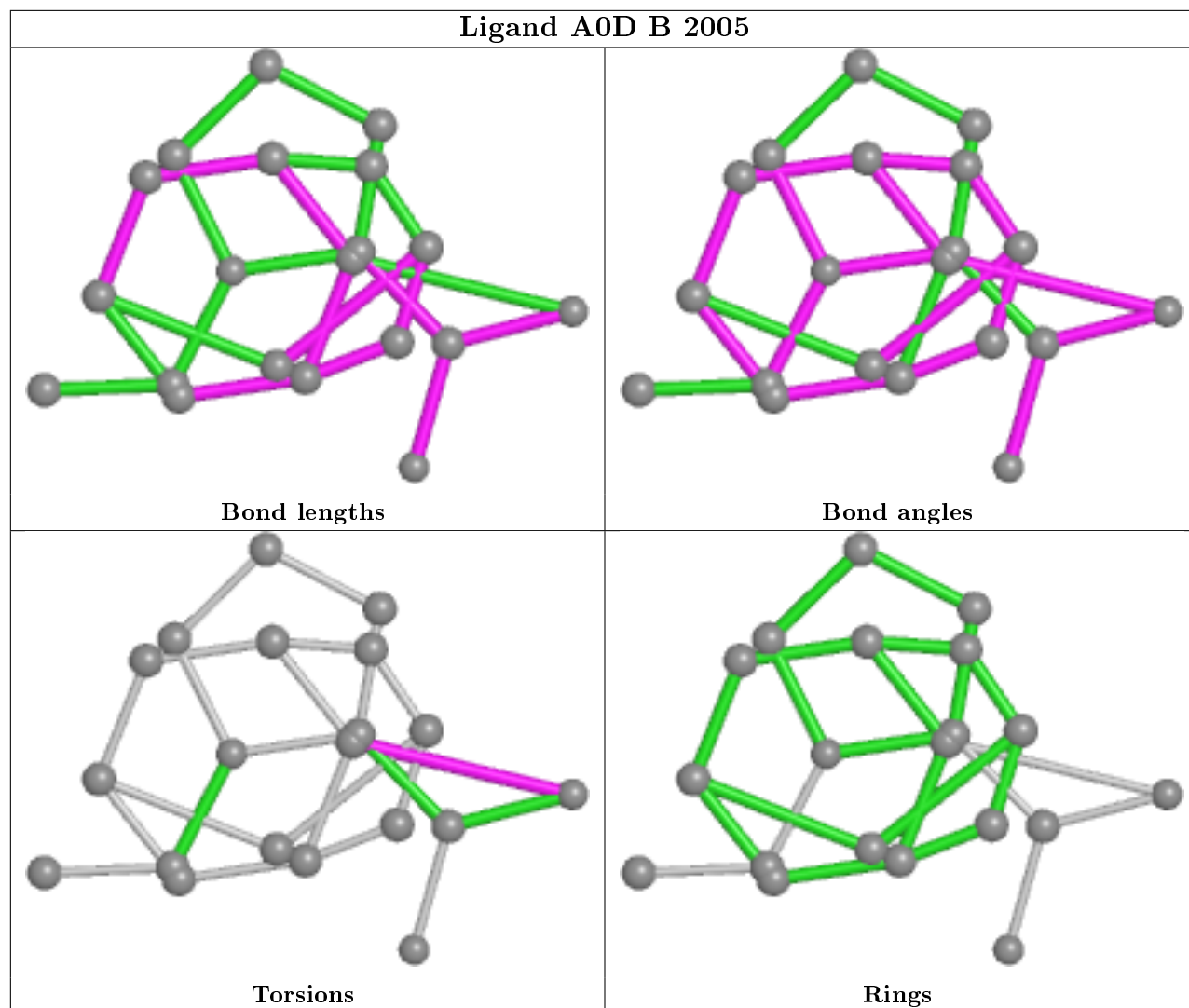
5 monomers are involved in 12 short contacts:

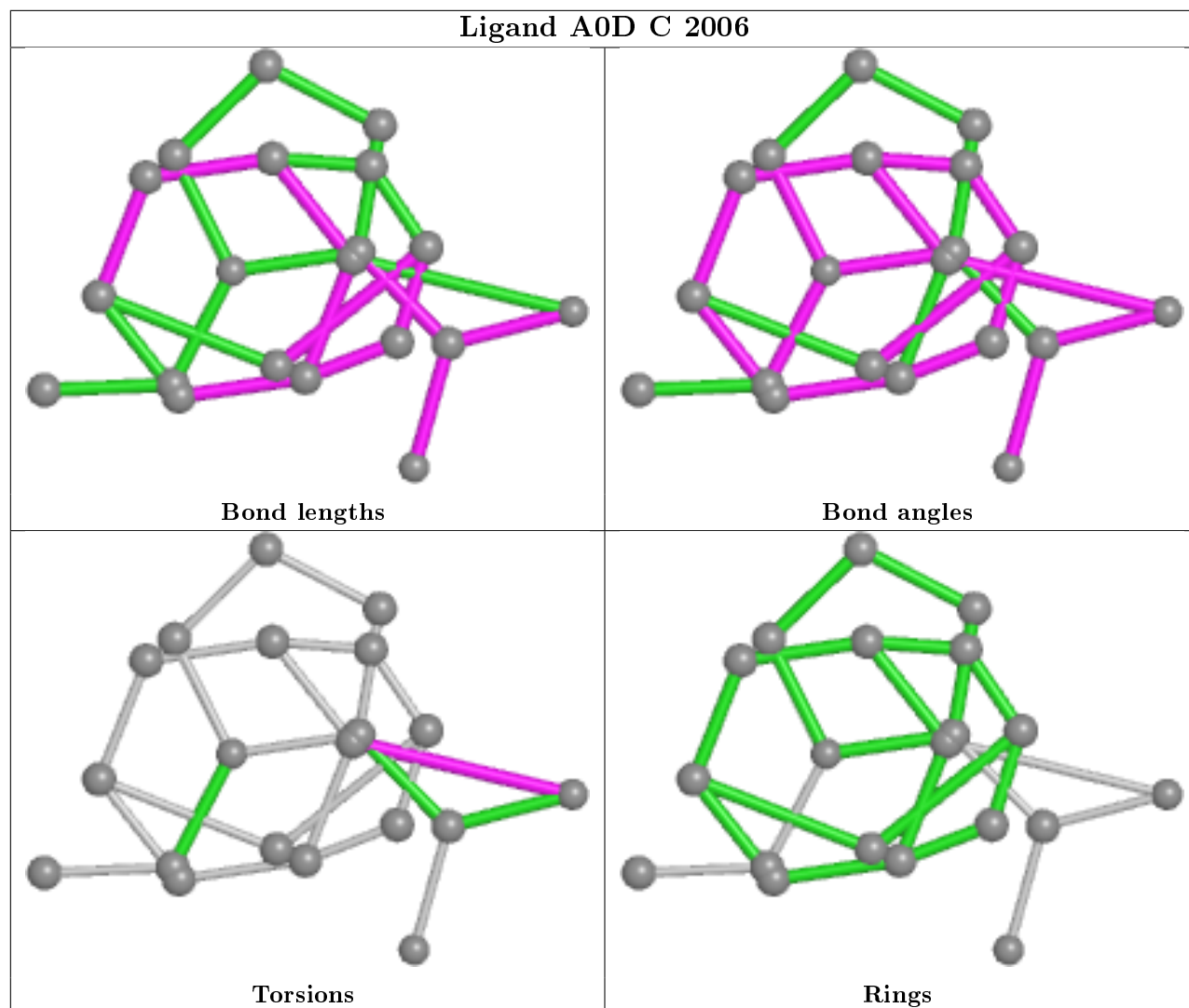
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2002	NAP	3	0
3	B	2005	A0D	5	0
3	C	2006	A0D	6	0
2	B	2001	NAP	2	0
2	A	2000	NAP	1	0

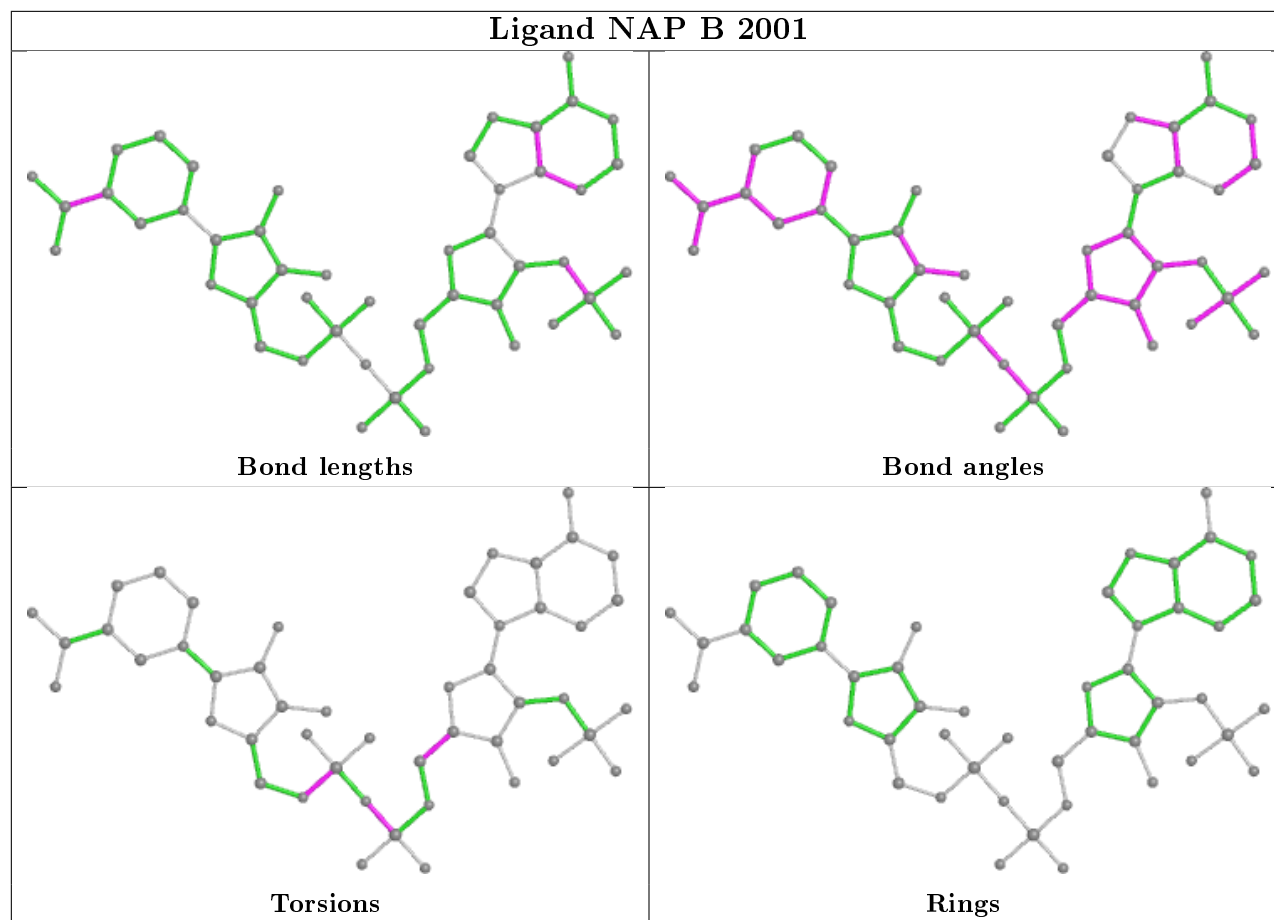
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

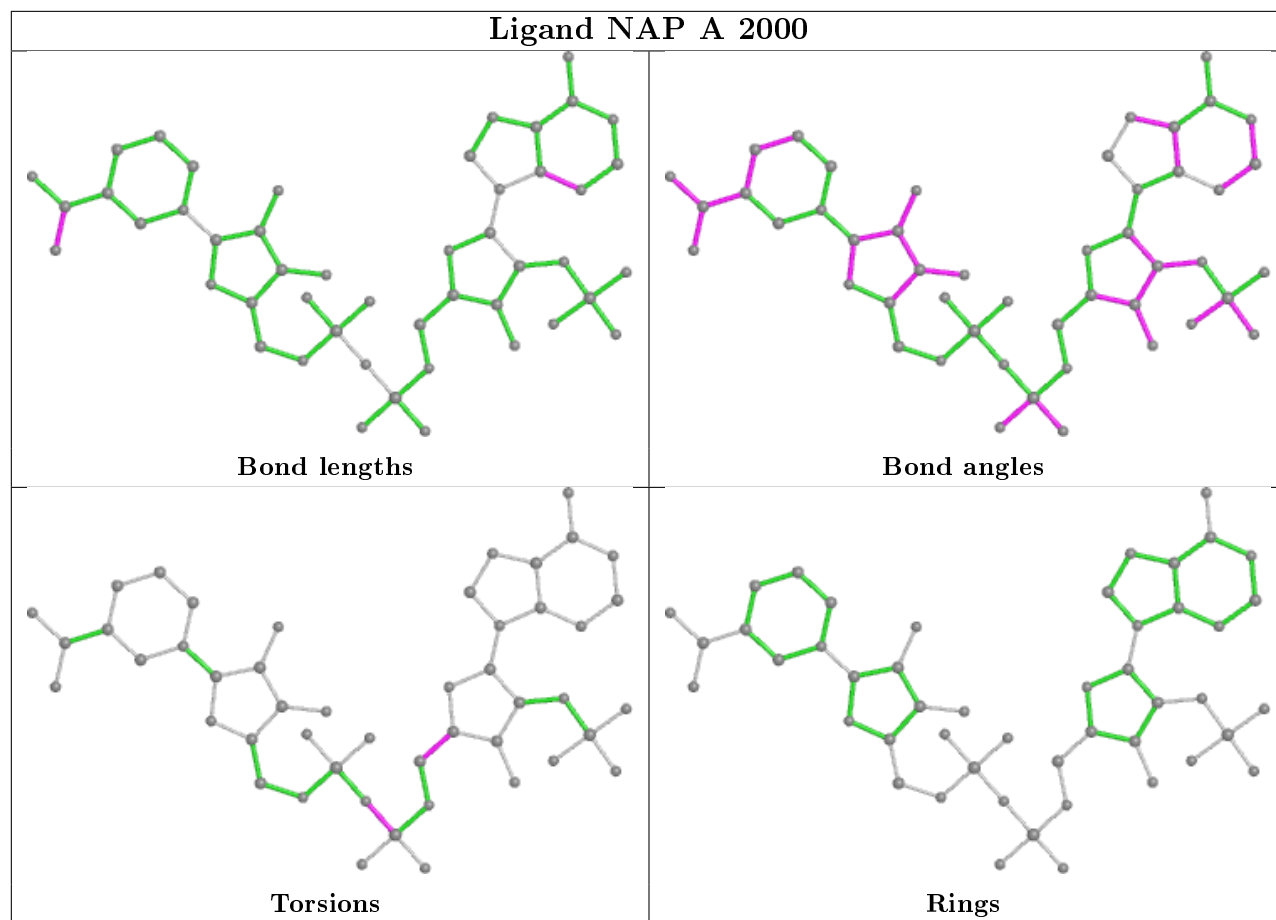


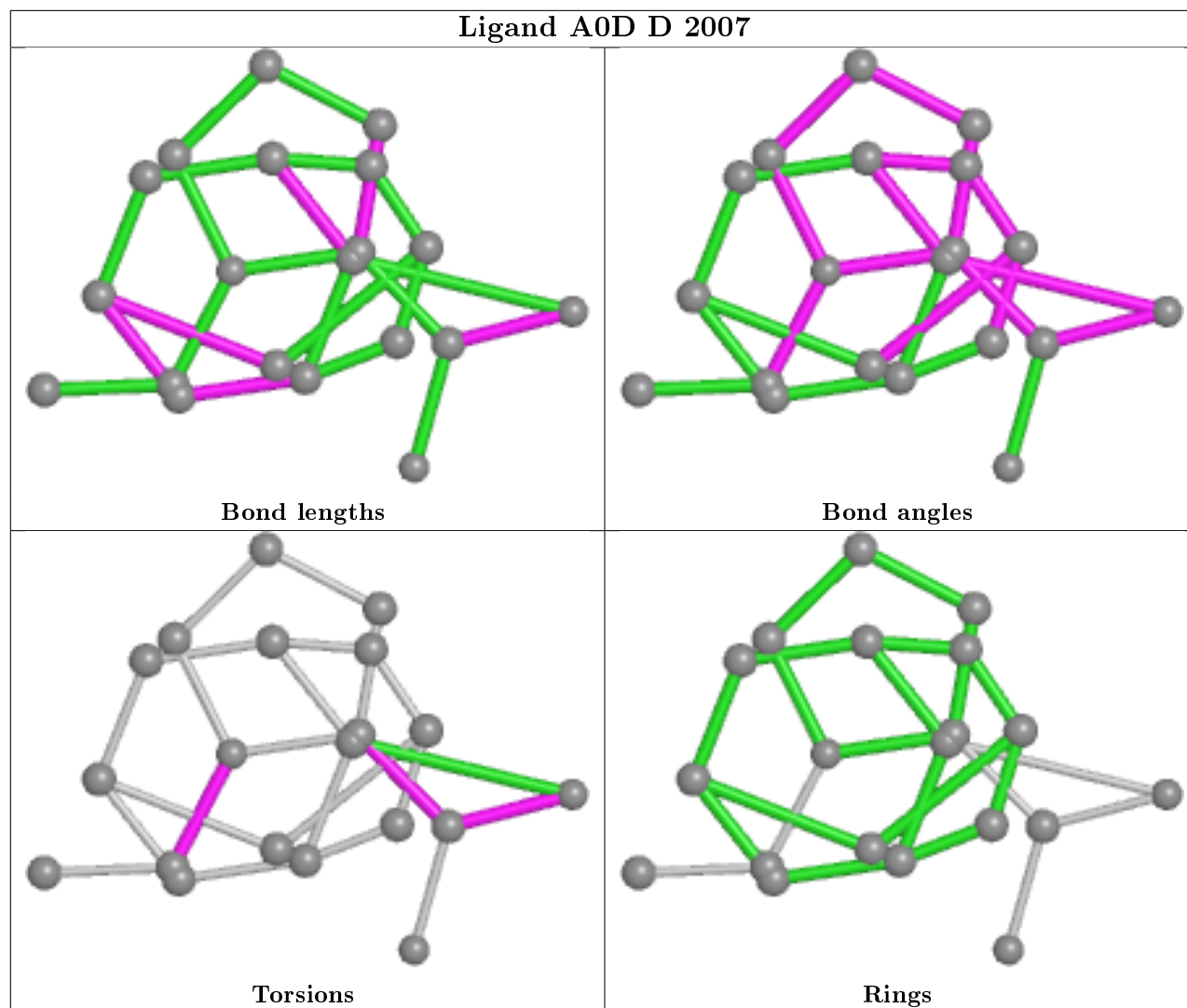


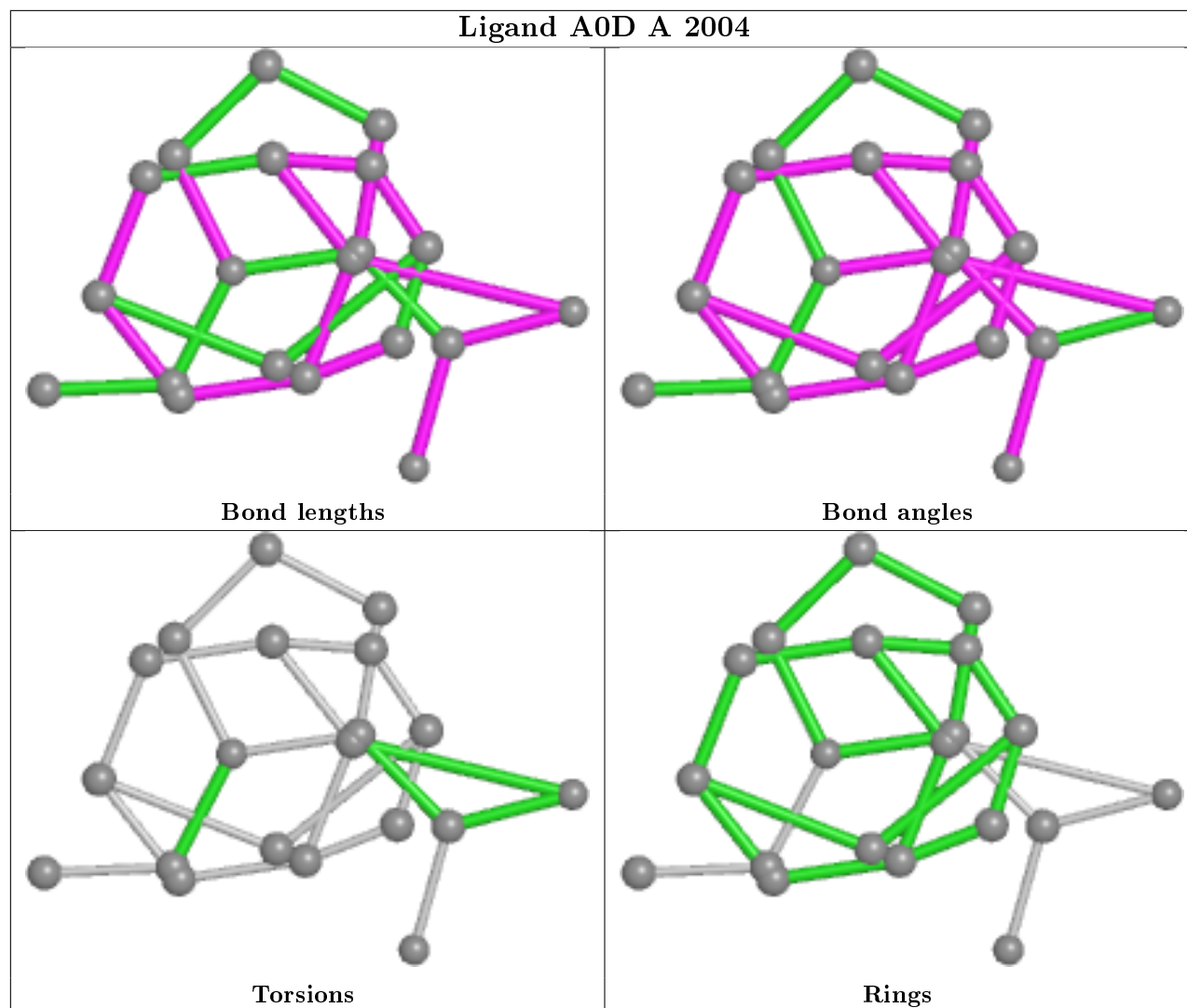












5.7 Other polymers [i](#)

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, 95th 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 ²)	Q<0.9
1	A	263/263 (100%)	-0.04	3 (1%) 80 80	15, 23, 33, 43	0
1	B	263/263 (100%)	0.11	6 (2%) 60 58	15, 25, 36, 46	0
1	C	263/263 (100%)	0.08	1 (0%) 92 92	14, 26, 37, 44	0
1	D	263/263 (100%)	-0.06	5 (1%) 66 65	14, 21, 33, 42	0
All	All	1052/1052 (100%)	0.02	15 (1%) 75 75	14, 23, 35, 46	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	98	TYR	4.5
1	D	793	PRO	3.0
1	D	790	LYS	3.0
1	D	792	ARG	2.8
1	B	363	ARG	2.8
1	B	361	TYR	2.5
1	B	264	LYS	2.3
1	B	271	GLN	2.3
1	B	313	VAL	2.2
1	A	177	LEU	2.1
1	C	568	SER	2.1
1	D	791	PHE	2.1
1	A	1	LYS	2.1
1	B	266	ARG	2.0
1	D	796	LEU	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

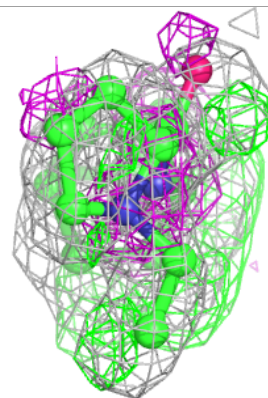
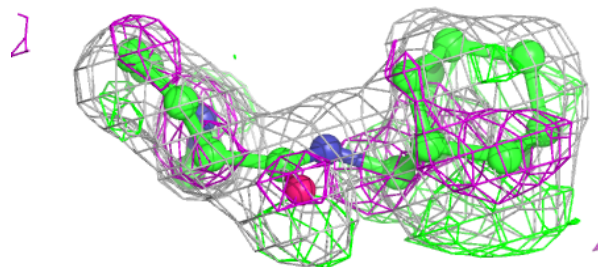
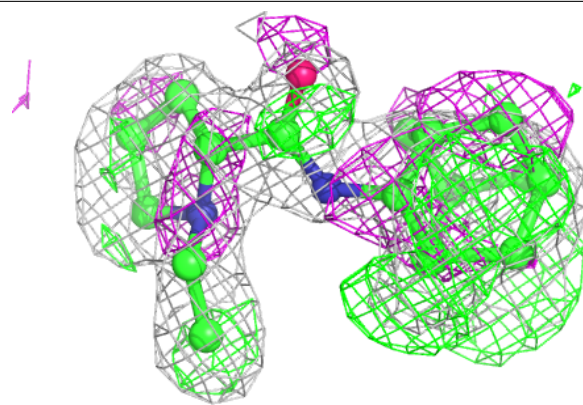
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	A0D	B	2005	20/20	0.60	0.26	2,16,23,23	0
3	A0D	C	2006	20/20	0.76	0.19	2,16,23,23	0
3	A0D	A	2004	20/20	0.79	0.21	2,7,16,16	0
3	A0D	D	2007	20/20	0.80	0.20	2,13,23,29	0
2	NAP	C	2002	48/48	0.97	0.09	15,23,29,31	0
2	NAP	A	2000	48/48	0.98	0.09	12,17,22,24	0
2	NAP	D	2003	48/48	0.98	0.08	12,15,18,20	0
2	NAP	B	2001	48/48	0.98	0.09	13,18,24,27	0

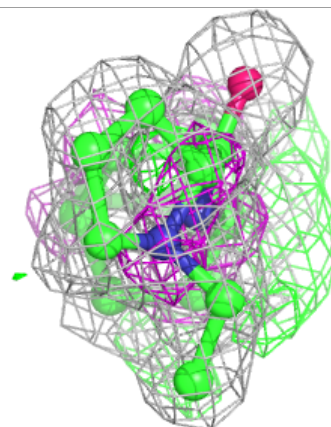
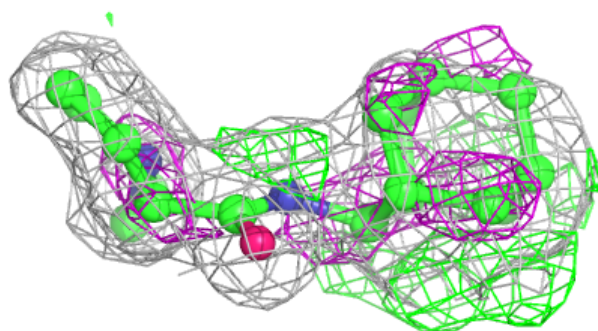
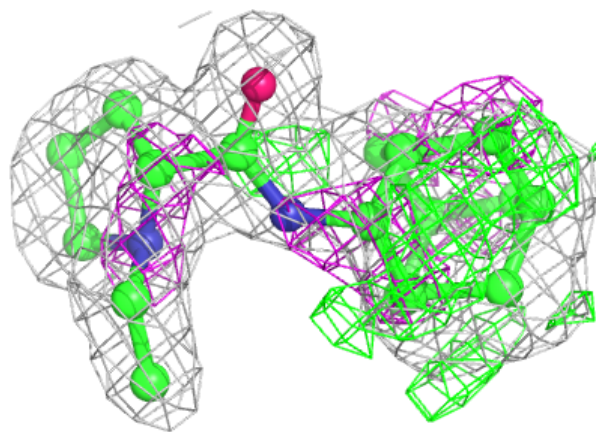
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around A0D B 2005:

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

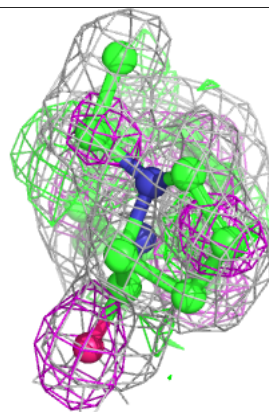
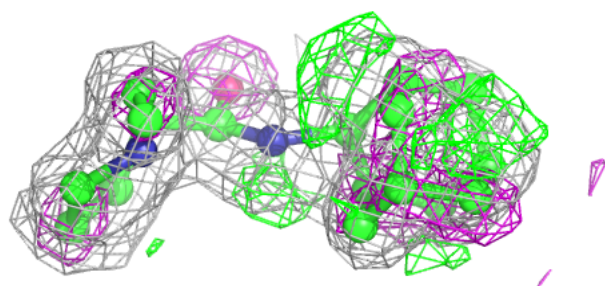
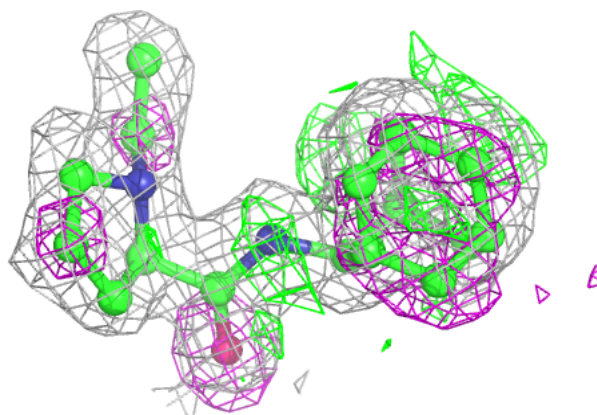
**Electron density around A0D C 2006:**

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

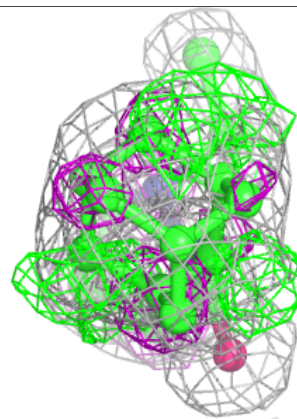
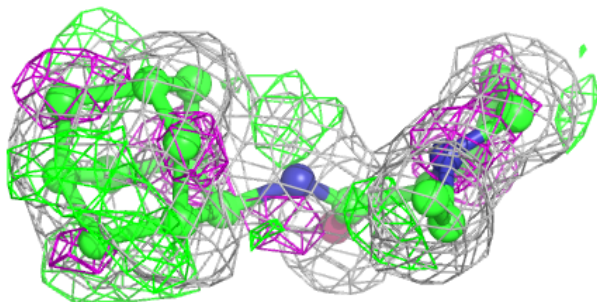
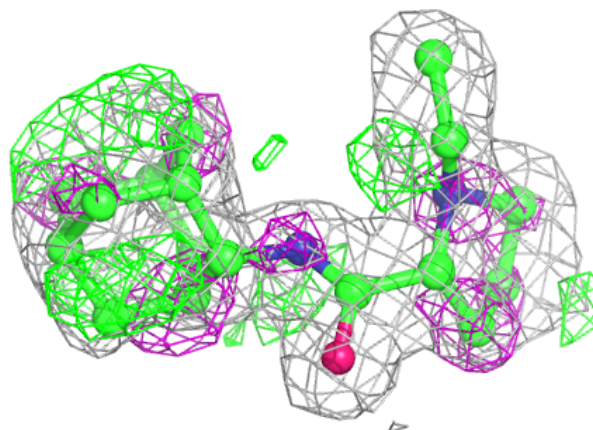


Electron density around A0D A 2004:

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

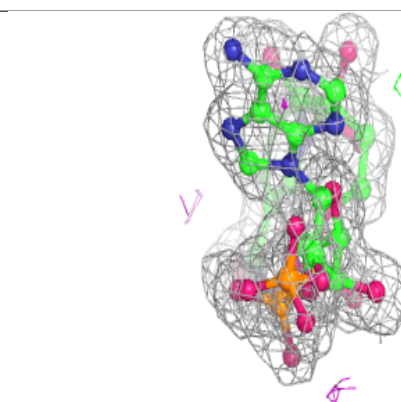
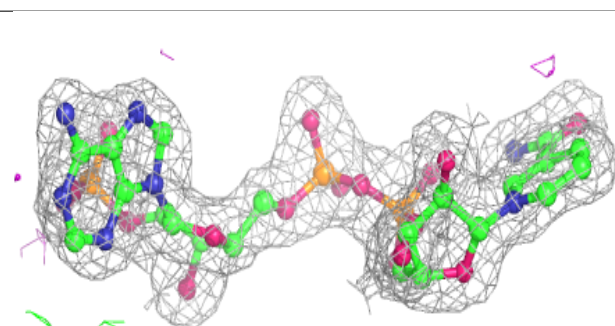
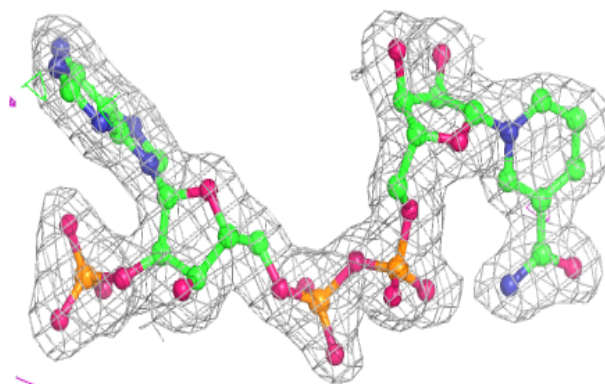
**Electron density around A0D D 2007:**

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

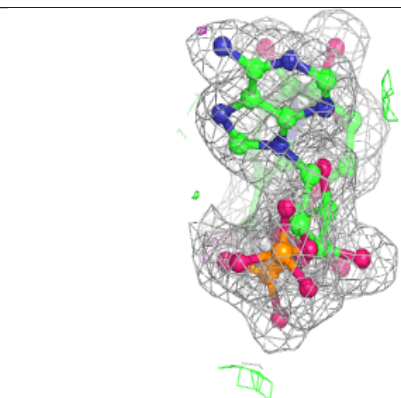
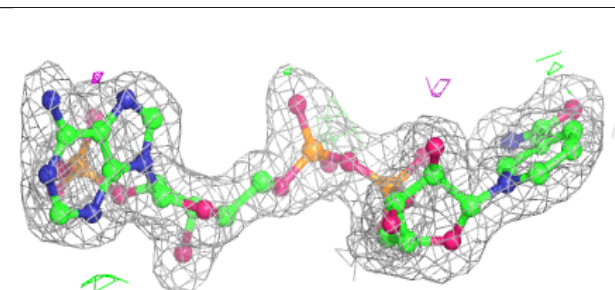
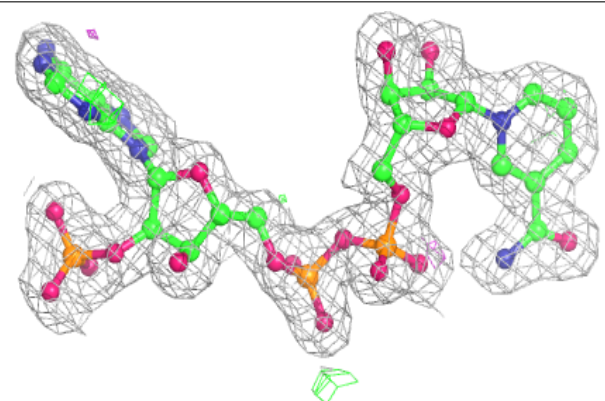


Electron density around NAP C 2002:

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

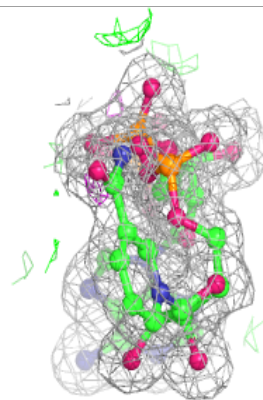
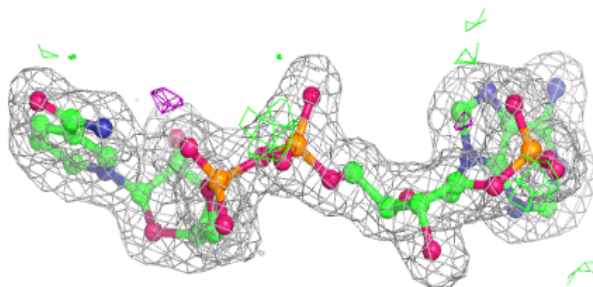
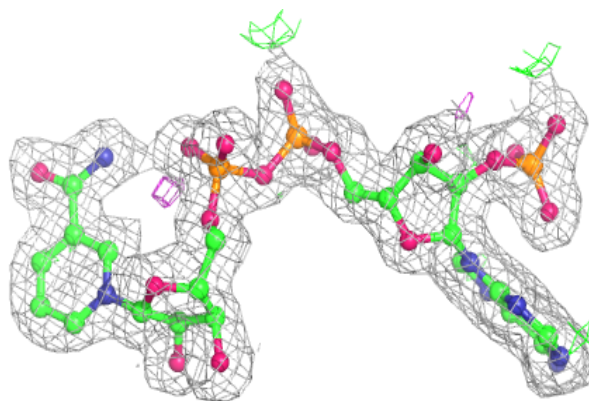
**Electron density around NAP A 2000:**

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

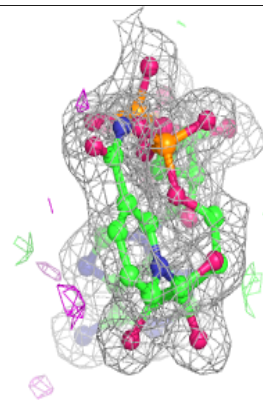
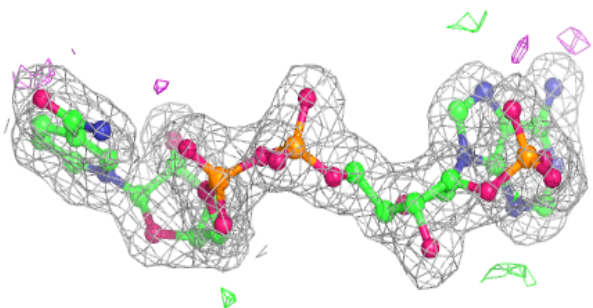
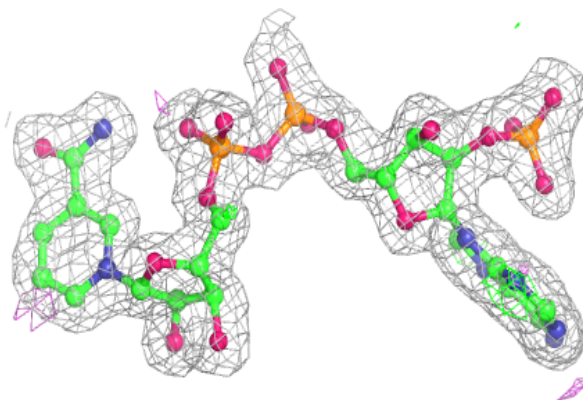


Electron density around NAP D 2003:

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

**Electron density around NAP B 2001:**

$2mF_o-DF_c$ (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.