



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 14, 2020 – 12:04 pm BST

PDB ID : 2C6Q
Title : Crystal structure of human guanosine monophosphate reductase 2 GMPR2 in complex with IMP and NADPH
Authors : Kursula, P.; Stenmark, P.; Arrowsmith, C.; Berglund, H.; Edwards, A.; Ehn, M.; Graslund, S.; Hammarstrom, M.; Hallberg, B.M.; Kotenyova, T.; Nilsson-Ehle, P.; Ogg, D.; Persson, C.; Sagemark, J.; Schuler, H.; Sundstrom, M.; Thorsell, A.; Weigelt, J.; Nordlund, P.
Deposited on : 2005-11-11
Resolution : 1.70 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

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

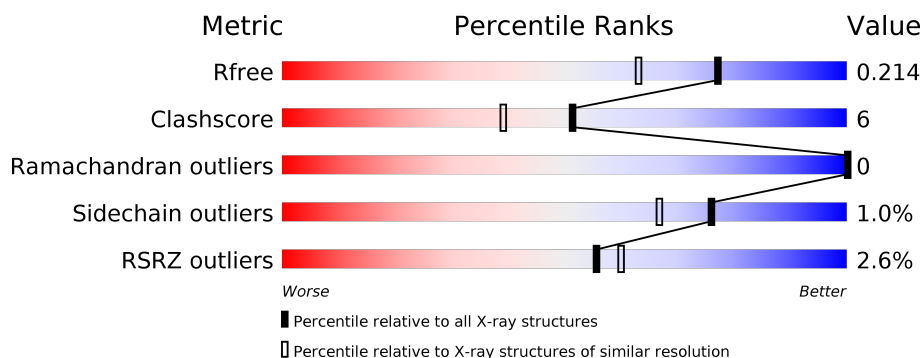
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	351	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>7%</div> <div>7%</div> </div> </div>
1	B	351	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>7%</div> <div>6%</div> </div> </div>
1	C	351	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>9%</div> <div>7%</div> </div> </div>
1	D	351	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>8%</div> <div>7%</div> </div> </div>
1	E	351	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>6%</div> <div>7%</div> </div> </div>
1	F	351	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>8%</div> <div>7%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	351	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>82%</div><div>9%</div><div>9%</div></div></div>
1	H	351	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>83%</div><div>11%</div><div>7%</div></div></div>

2 Entry composition

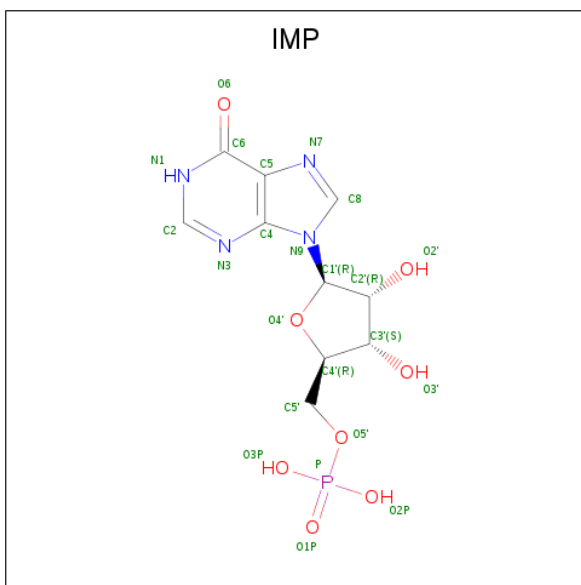
There are 4 unique types of molecules in this entry. The entry contains 23052 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GMP REDUCTASE 2.

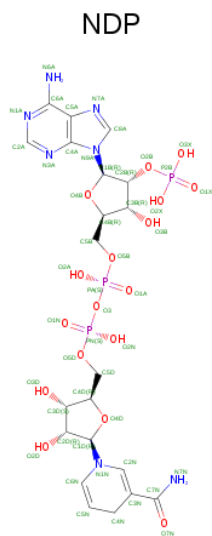
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	0	0
			2494	1573	430	473	18			
1	B	329	Total	C	N	O	S	0	1	0
			2507	1580	432	476	19			
1	C	328	Total	C	N	O	S	0	1	0
			2505	1579	434	474	18			
1	D	328	Total	C	N	O	S	0	0	0
			2494	1573	430	473	18			
1	E	328	Total	C	N	O	S	0	4	0
			2519	1586	434	480	19			
1	F	328	Total	C	N	O	S	0	0	0
			2494	1573	430	473	18			
1	G	321	Total	C	N	O	S	0	0	0
			2444	1542	420	464	18			
1	H	328	Total	C	N	O	S	0	2	0
			2506	1579	432	476	19			

- Molecule 2 is INOSINIC ACID (three-letter code: IMP) (formula: C₁₀H₁₃N₄O₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	E	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	F	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	G	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	H	1	Total	C	N	O	P	0	0
			23	10	4	8	1		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	302	Total O 302 302	0	0
4	B	285	Total O 285 285	0	0
4	C	335	Total O 335 335	0	0
4	D	305	Total O 305 305	0	0
4	E	352	Total O 352 352	0	0

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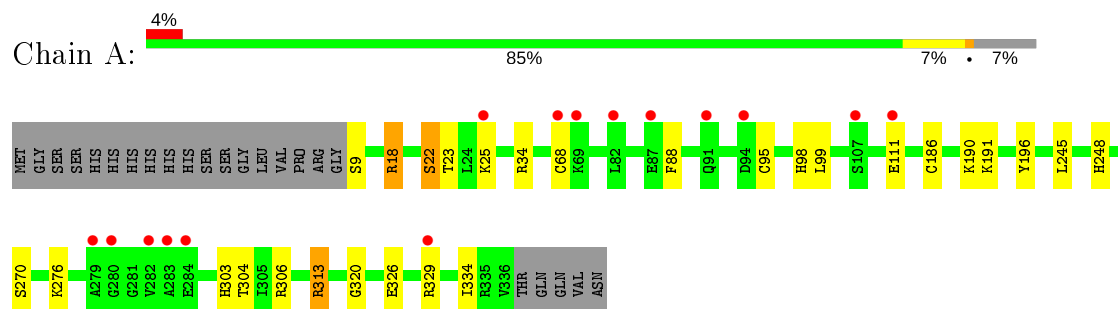
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	346	Total 346	O 346	0	0
4	G	304	Total 304	O 304	0	0
4	H	340	Total 340	O 340	0	0

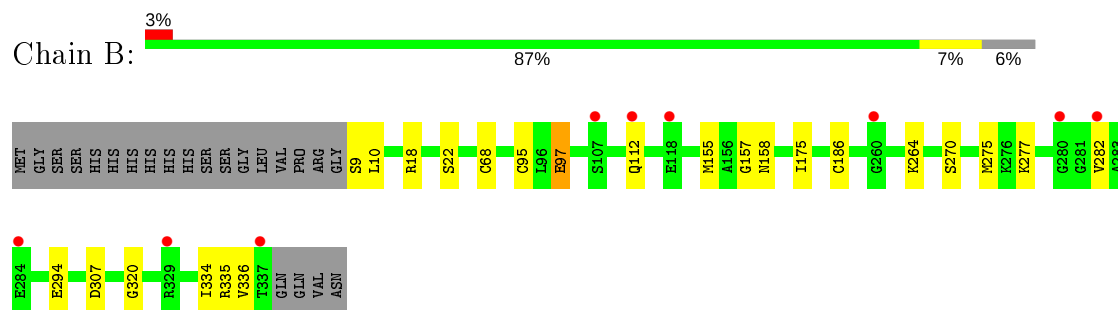
3 Residue-property plots [i](#)

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.

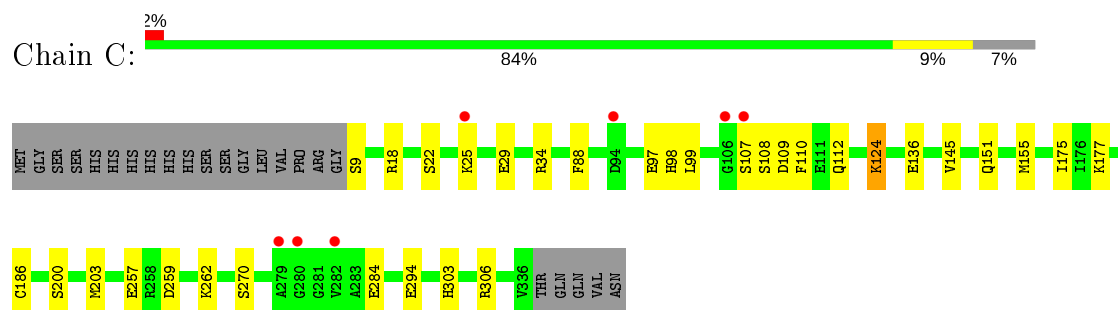
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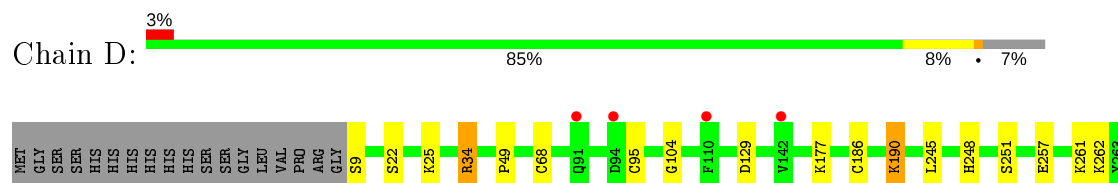
• Molecule 1: GMP REDUCTASE 2



• Molecule 1: GMP REDUCTASE 2

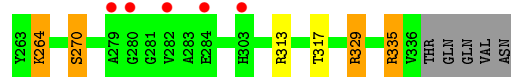
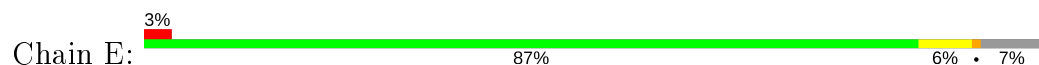


• Molecule 1: GMP REDUCTASE 2

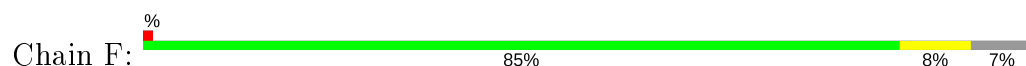




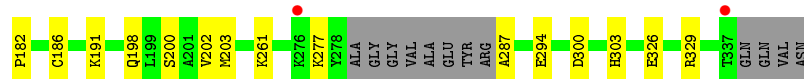
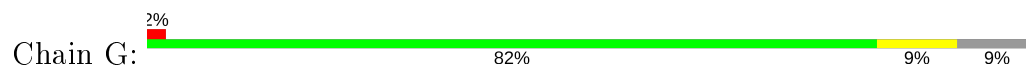
• Molecule 1: GMP REDUCTASE 2



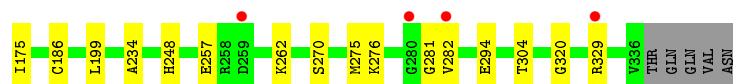
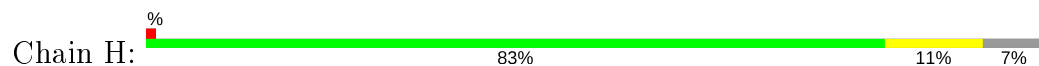
• Molecule 1: GMP REDUCTASE 2



• Molecule 1: GMP REDUCTASE 2



• Molecule 1: GMP REDUCTASE 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	131.68Å 141.37Å 164.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.70 10.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (10.00-1.70) 99.9 (10.00-1.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.22 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.163 , 0.206 0.174 , 0.214	Depositor DCC
R_{free} test set	16715 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	17.0	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	23052	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% 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: NDP, IMP

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	0.79	0/2539	0.80	3/3414 (0.1%)
1	B	0.80	0/2552	0.81	1/3432 (0.0%)
1	C	0.87	0/2550	0.87	3/3428 (0.1%)
1	D	0.84	0/2539	0.82	2/3414 (0.1%)
1	E	0.89	1/2564 (0.0%)	0.87	2/3448 (0.1%)
1	F	0.87	1/2539 (0.0%)	0.87	3/3414 (0.1%)
1	G	0.84	0/2487	0.86	5/3343 (0.1%)
1	H	0.89	0/2551	0.84	2/3430 (0.1%)
All	All	0.85	2/20321 (0.0%)	0.84	21/27323 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	270	SER	CB-OG	-6.01	1.34	1.42
1	F	68	CYS	CB-SG	-5.97	1.72	1.81

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	34	ARG	NE-CZ-NH1	8.97	124.79	120.30
1	H	34	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	D	34	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	G	34	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	F	335	ARG	NE-CZ-NH1	6.77	123.69	120.30

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	2494	0	2494	23	0
1	B	2507	0	2505	22	0
1	C	2505	0	2506	27	0
1	D	2494	0	2494	28	0
1	E	2519	0	2512	24	0
1	F	2494	0	2494	29	0
1	G	2444	0	2447	26	0
1	H	2506	0	2502	32	0
2	A	23	0	11	3	0
2	B	23	0	11	6	0
2	C	23	0	11	6	0
2	D	23	0	11	4	0
2	E	23	0	11	3	0
2	F	23	0	11	6	0
2	G	23	0	11	3	0
2	H	23	0	11	2	0
3	A	48	0	26	3	0
3	B	48	0	26	6	0
3	C	48	0	26	6	0
3	D	48	0	26	2	0
3	E	48	0	26	3	0
3	F	48	0	26	9	0
3	H	48	0	26	4	0
4	A	302	0	0	10	0
4	B	285	0	0	6	0
4	C	335	0	0	14	0
4	D	305	0	0	5	0
4	E	352	0	0	9	1
4	F	346	0	0	10	1
4	G	304	0	0	10	0
4	H	340	0	0	7	0
All	All	23052	0	20224	222	1

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 6.

The worst 5 of 222 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:CYS:SG	2:D:1337:IMP:H2	1.31	1.65
1:G:186:CYS:SG	2:G:1338:IMP:H2	1.49	1.52
1:A:186:CYS:SG	2:A:1337:IMP:H2	1.57	1.43
1:F:186:CYS:SG	2:F:1337:IMP:H2	1.68	1.31
1:C:186:CYS:SG	2:C:1337:IMP:H2	1.69	1.31

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:2329:HOH:O	4:F:2148:HOH:O[4_445]	2.17	0.03

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	326/351 (93%)	320 (98%)	6 (2%)	0	100	100
1	B	328/351 (93%)	321 (98%)	7 (2%)	0	100	100
1	C	327/351 (93%)	324 (99%)	3 (1%)	0	100	100
1	D	326/351 (93%)	321 (98%)	5 (2%)	0	100	100
1	E	330/351 (94%)	325 (98%)	5 (2%)	0	100	100
1	F	326/351 (93%)	320 (98%)	6 (2%)	0	100	100
1	G	317/351 (90%)	311 (98%)	6 (2%)	0	100	100
1	H	328/351 (93%)	323 (98%)	5 (2%)	0	100	100
All	All	2608/2808 (93%)	2565 (98%)	43 (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	267/287 (93%)	264 (99%)	3 (1%)	73	63
1	B	269/287 (94%)	266 (99%)	3 (1%)	73	63
1	C	268/287 (93%)	265 (99%)	3 (1%)	73	63
1	D	267/287 (93%)	266 (100%)	1 (0%)	91	87
1	E	271/287 (94%)	268 (99%)	3 (1%)	73	63
1	F	267/287 (93%)	264 (99%)	3 (1%)	73	63
1	G	264/287 (92%)	261 (99%)	3 (1%)	73	63
1	H	269/287 (94%)	267 (99%)	2 (1%)	84	77
All	All	2142/2296 (93%)	2121 (99%)	21 (1%)	76	67

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	190	LYS
1	E	329	ARG
1	G	148	ARG
1	C	177	LYS
1	G	177	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	137	HIS
1	F	43	GLN
1	G	303	HIS
1	D	248	HIS
1	H	43	GLN

5.3.3 RNA ⓘ

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](#)

15 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	IMP	H	1337	-	21,25,25	1.39	4 (19%)	23,38,38	1.66	3 (13%)
3	NDP	B	1340	-	45,52,52	1.74	5 (11%)	53,80,80	1.61	6 (11%)
3	NDP	D	1338	-	45,52,52	1.84	7 (15%)	53,80,80	1.72	7 (13%)
2	IMP	E	1337	-	21,25,25	1.66	5 (23%)	23,38,38	1.73	4 (17%)
2	IMP	A	1337	-	21,25,25	1.42	2 (9%)	23,38,38	1.76	4 (17%)
3	NDP	C	1338	-	45,52,52	1.60	5 (11%)	53,80,80	1.34	3 (5%)
2	IMP	C	1337	-	21,25,25	1.45	3 (14%)	23,38,38	1.81	5 (21%)
3	NDP	A	1338	-	45,52,52	1.80	4 (8%)	53,80,80	2.03	9 (16%)
3	NDP	E	1338	-	45,52,52	1.77	7 (15%)	53,80,80	1.67	11 (20%)
3	NDP	F	1338	-	45,52,52	1.69	7 (15%)	53,80,80	1.39	5 (9%)
2	IMP	D	1337	1	21,25,25	1.57	3 (14%)	23,38,38	1.67	3 (13%)
2	IMP	F	1337	-	21,25,25	1.27	2 (9%)	23,38,38	1.84	3 (13%)
2	IMP	G	1338	-	21,25,25	1.48	2 (9%)	23,38,38	1.63	3 (13%)
3	NDP	H	1338	-	45,52,52	1.65	6 (13%)	53,80,80	1.76	13 (24%)
2	IMP	B	1339	-	21,25,25	1.34	3 (14%)	23,38,38	1.68	4 (17%)

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	IMP	H	1337	-	-	0/6/26/26	0/3/3/3
3	NDP	B	1340	-	-	4/30/77/77	0/5/5/5
3	NDP	D	1338	-	-	6/30/77/77	0/5/5/5
2	IMP	E	1337	-	-	0/6/26/26	0/3/3/3
2	IMP	A	1337	-	-	0/6/26/26	0/3/3/3
3	NDP	C	1338	-	-	10/30/77/77	0/5/5/5
2	IMP	C	1337	-	-	0/6/26/26	0/3/3/3
3	NDP	A	1338	-	-	5/30/77/77	0/5/5/5
3	NDP	E	1338	-	-	7/30/77/77	0/5/5/5
3	NDP	F	1338	-	-	8/30/77/77	0/5/5/5
2	IMP	D	1337	1	-	0/6/26/26	0/3/3/3
2	IMP	F	1337	-	-	0/6/26/26	0/3/3/3
2	IMP	G	1338	-	-	0/6/26/26	0/3/3/3
3	NDP	H	1338	-	-	5/30/77/77	0/5/5/5
2	IMP	B	1339	-	-	0/6/26/26	0/3/3/3

The worst 5 of 65 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1338	NDP	O7N-C7N	7.98	1.43	1.24
3	A	1338	NDP	O7N-C7N	7.81	1.43	1.24
3	B	1340	NDP	O7N-C7N	7.57	1.42	1.24
3	E	1338	NDP	O7N-C7N	7.26	1.41	1.24
3	H	1338	NDP	O7N-C7N	7.12	1.41	1.24

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1338	NDP	C1D-N1N-C2N	-9.52	105.25	121.11
3	H	1338	NDP	C1D-N1N-C2N	-6.51	110.27	121.11
3	E	1338	NDP	C1D-N1N-C2N	-6.40	110.45	121.11
3	D	1338	NDP	C1D-N1N-C2N	-6.27	110.67	121.11
3	B	1340	NDP	C1D-N1N-C2N	-6.16	110.86	121.11

There are no chirality outliers.

5 of 45 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1340	NDP	C2B-O2B-P2B-O3X

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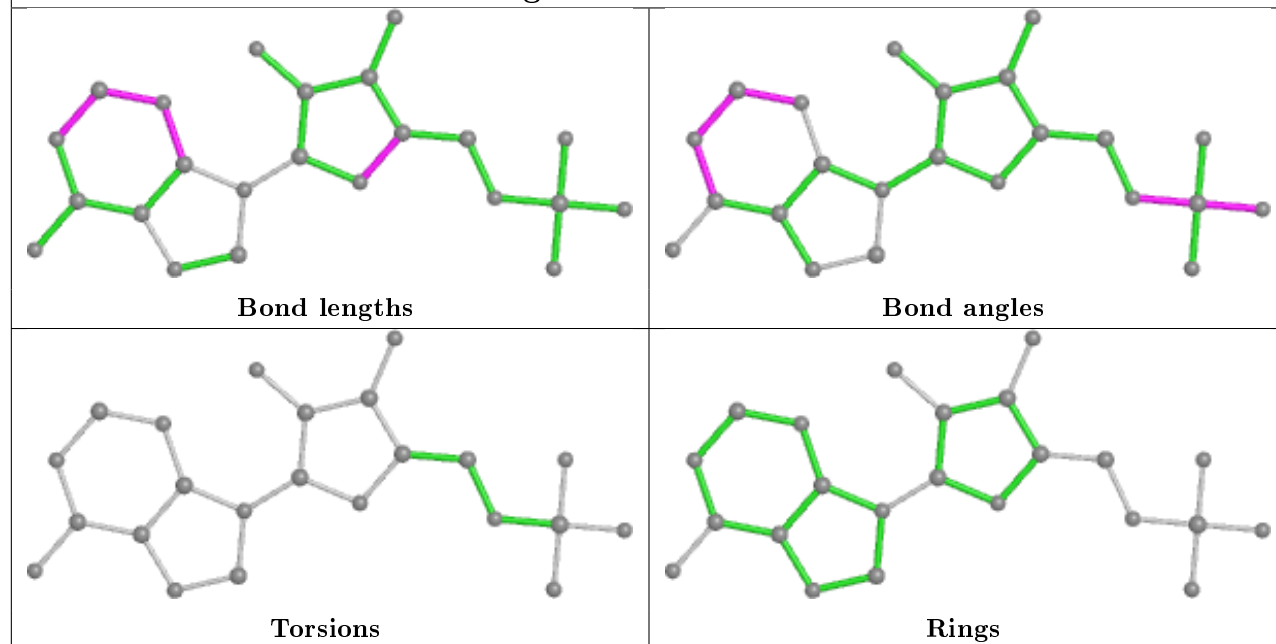
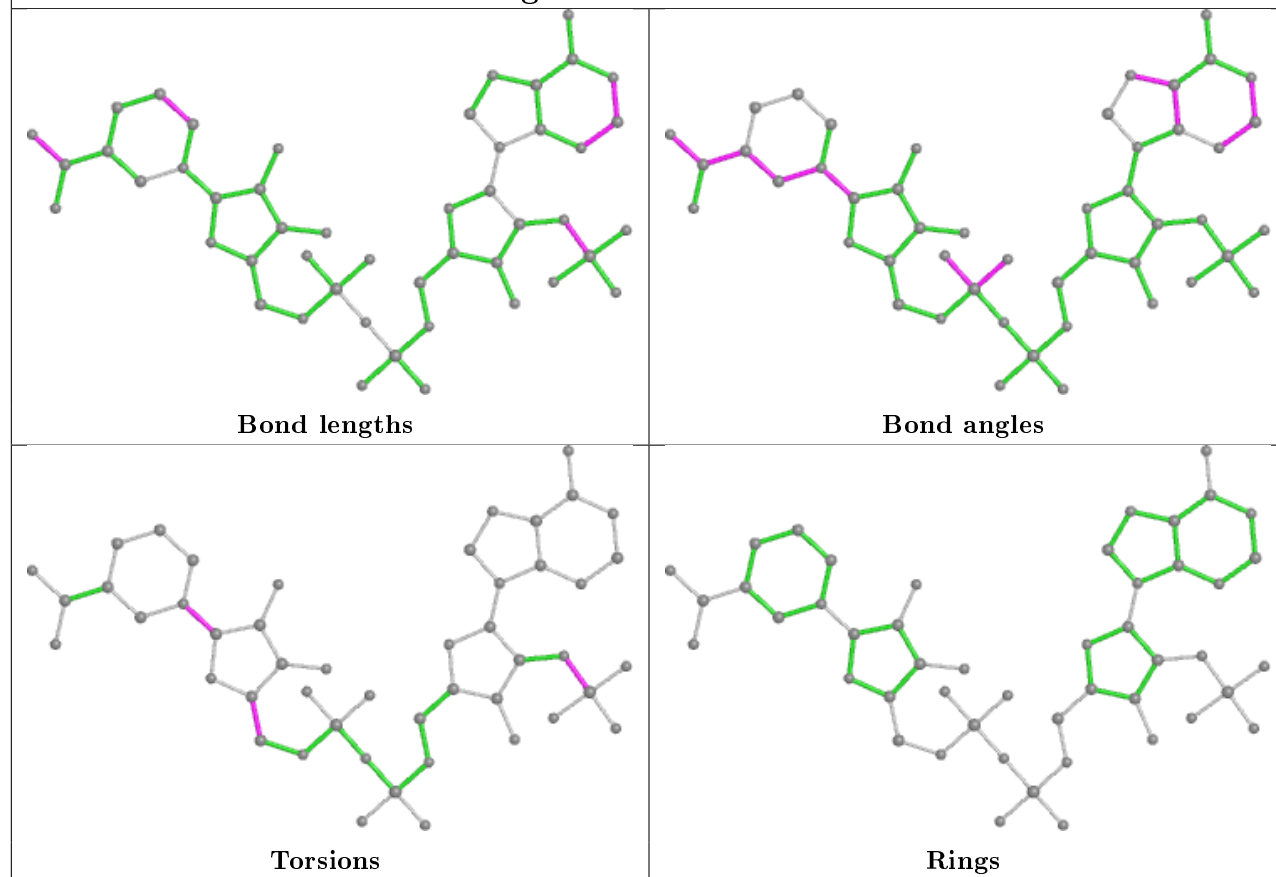
Mol	Chain	Res	Type	Atoms
3	B	1340	NDP	O4D-C4D-C5D-O5D
3	C	1338	NDP	C5D-O5D-PN-O3
3	C	1338	NDP	C5D-O5D-PN-O2N
3	A	1338	NDP	C2B-O2B-P2B-O3X

There are no ring outliers.

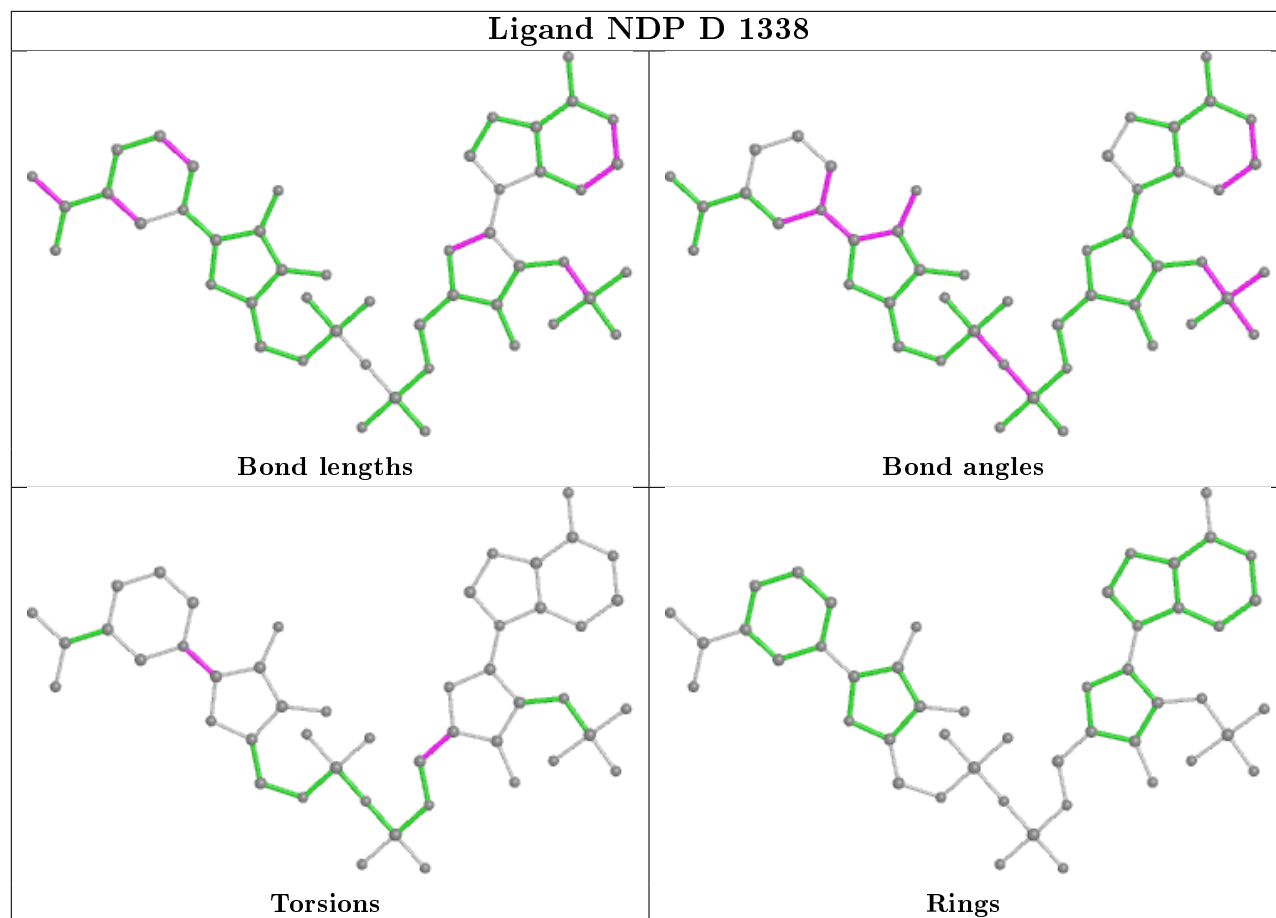
15 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1337	IMP	2	0
3	B	1340	NDP	6	0
3	D	1338	NDP	2	0
2	E	1337	IMP	3	0
2	A	1337	IMP	3	0
3	C	1338	NDP	6	0
2	C	1337	IMP	6	0
3	A	1338	NDP	3	0
3	E	1338	NDP	3	0
3	F	1338	NDP	9	0
2	D	1337	IMP	4	0
2	F	1337	IMP	6	0
2	G	1338	IMP	3	0
3	H	1338	NDP	4	0
2	B	1339	IMP	6	0

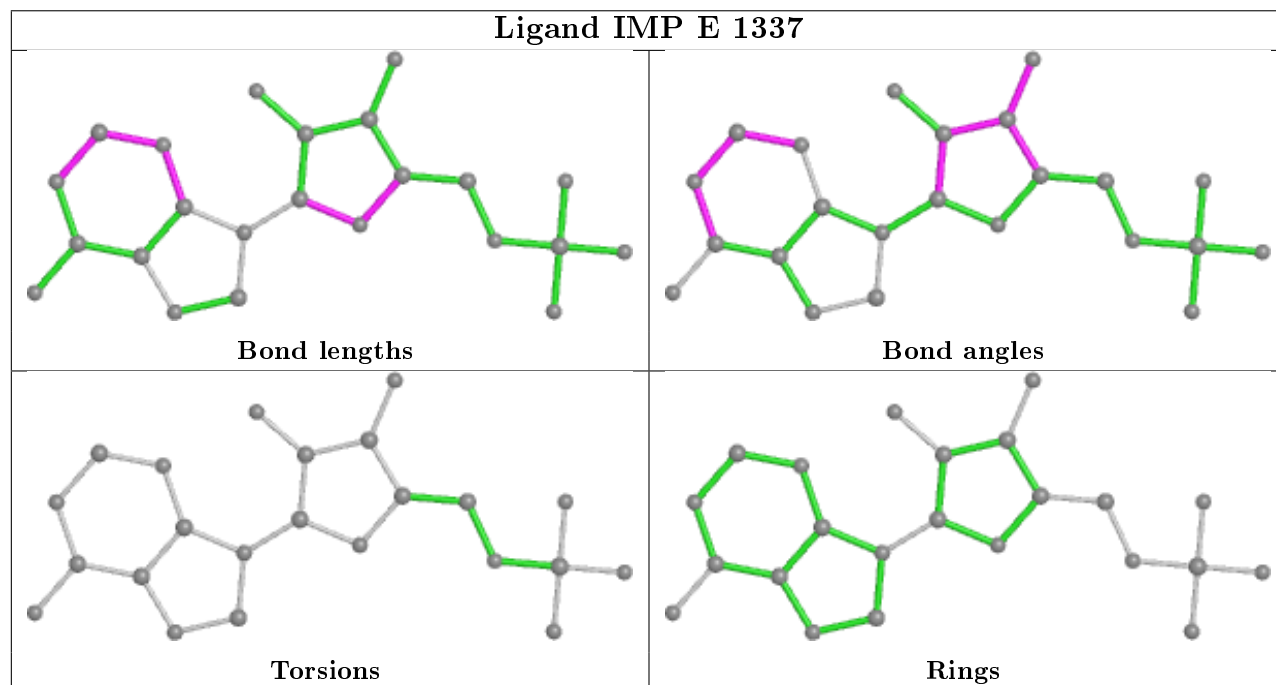
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand IMP H 1337**Ligand NDP B 1340**

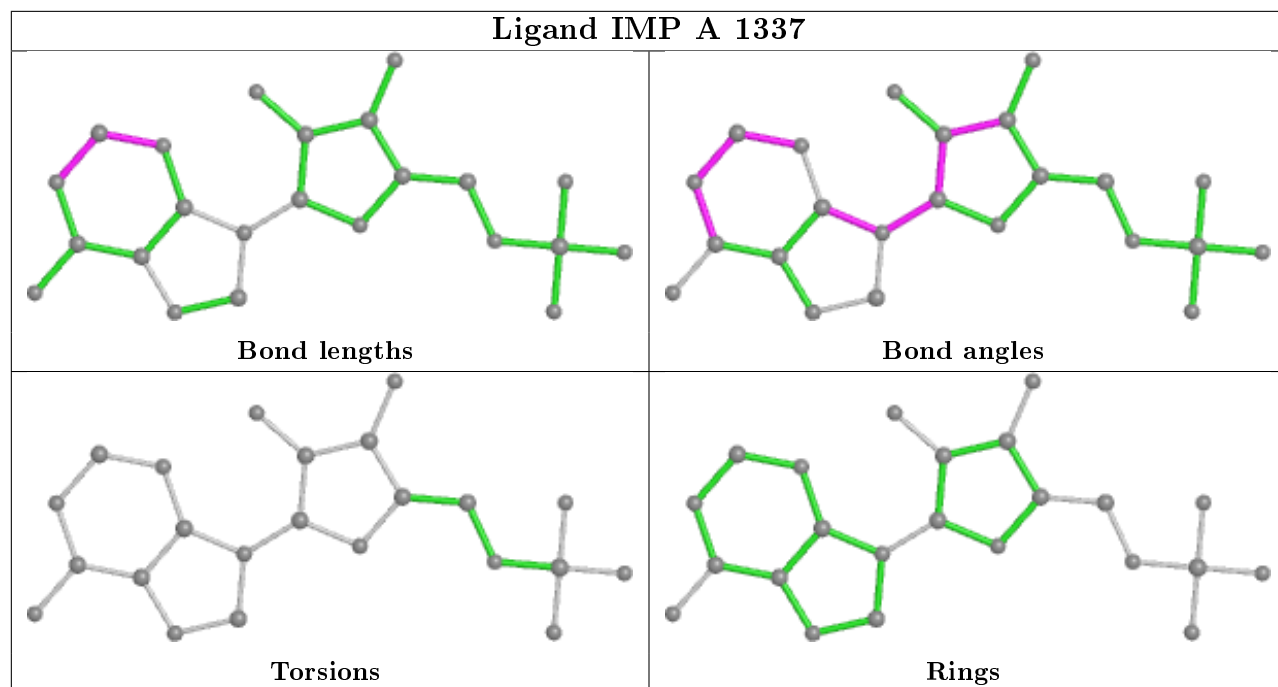
Ligand NDP D 1338



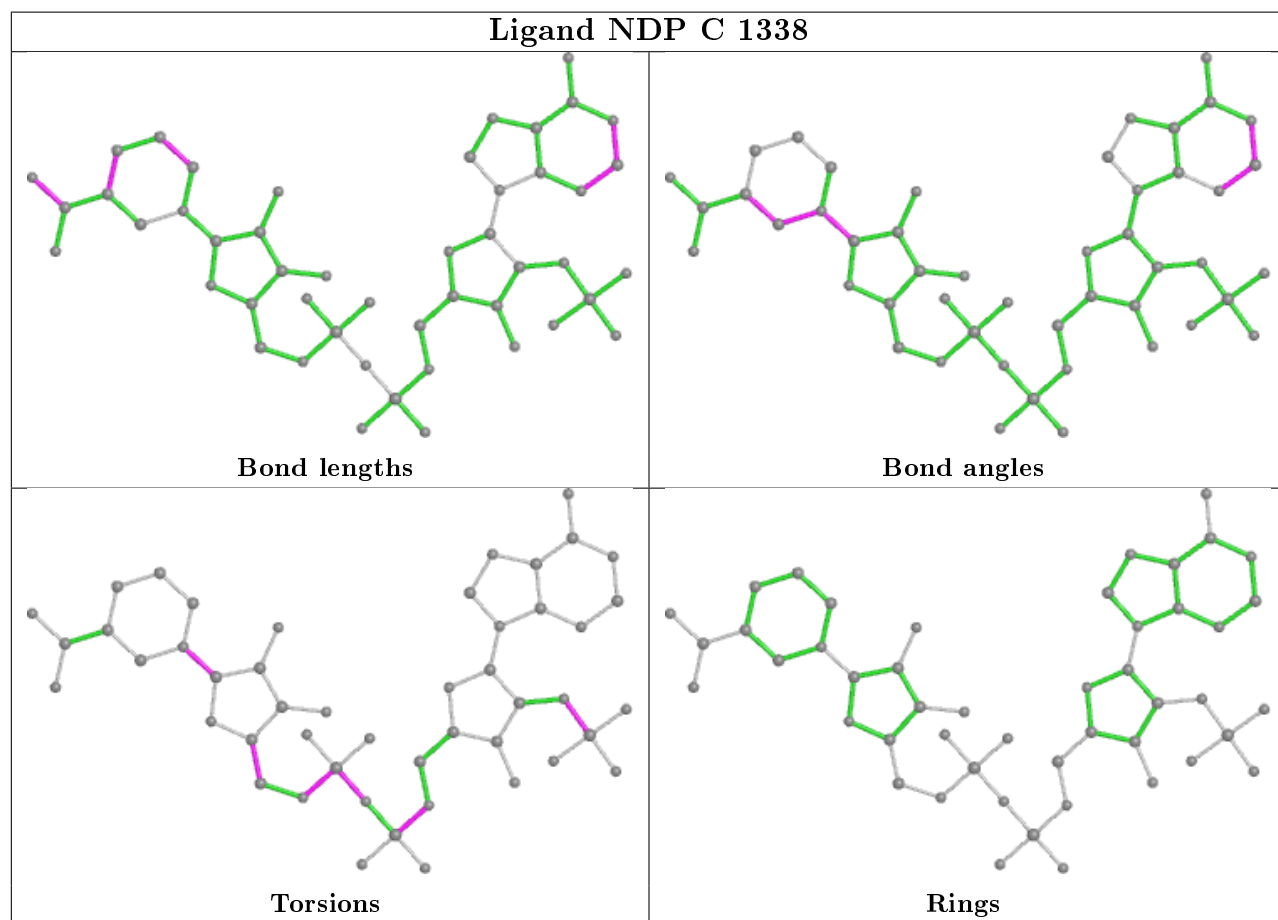
Ligand IMP E 1337



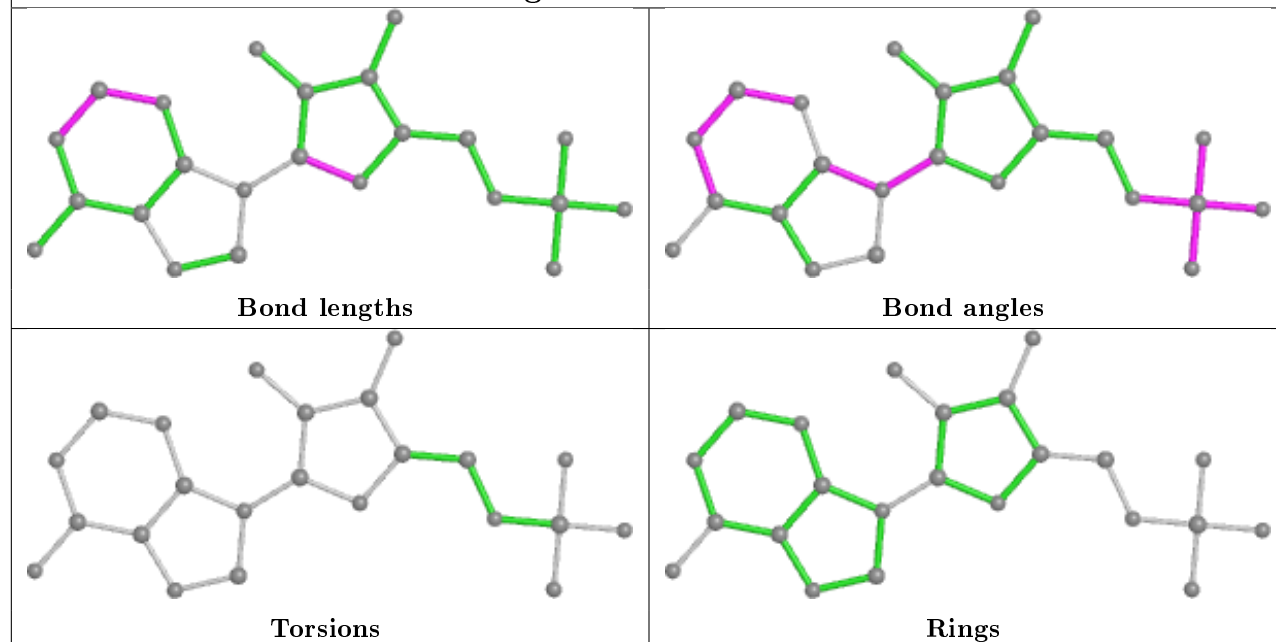
Ligand IMP A 1337



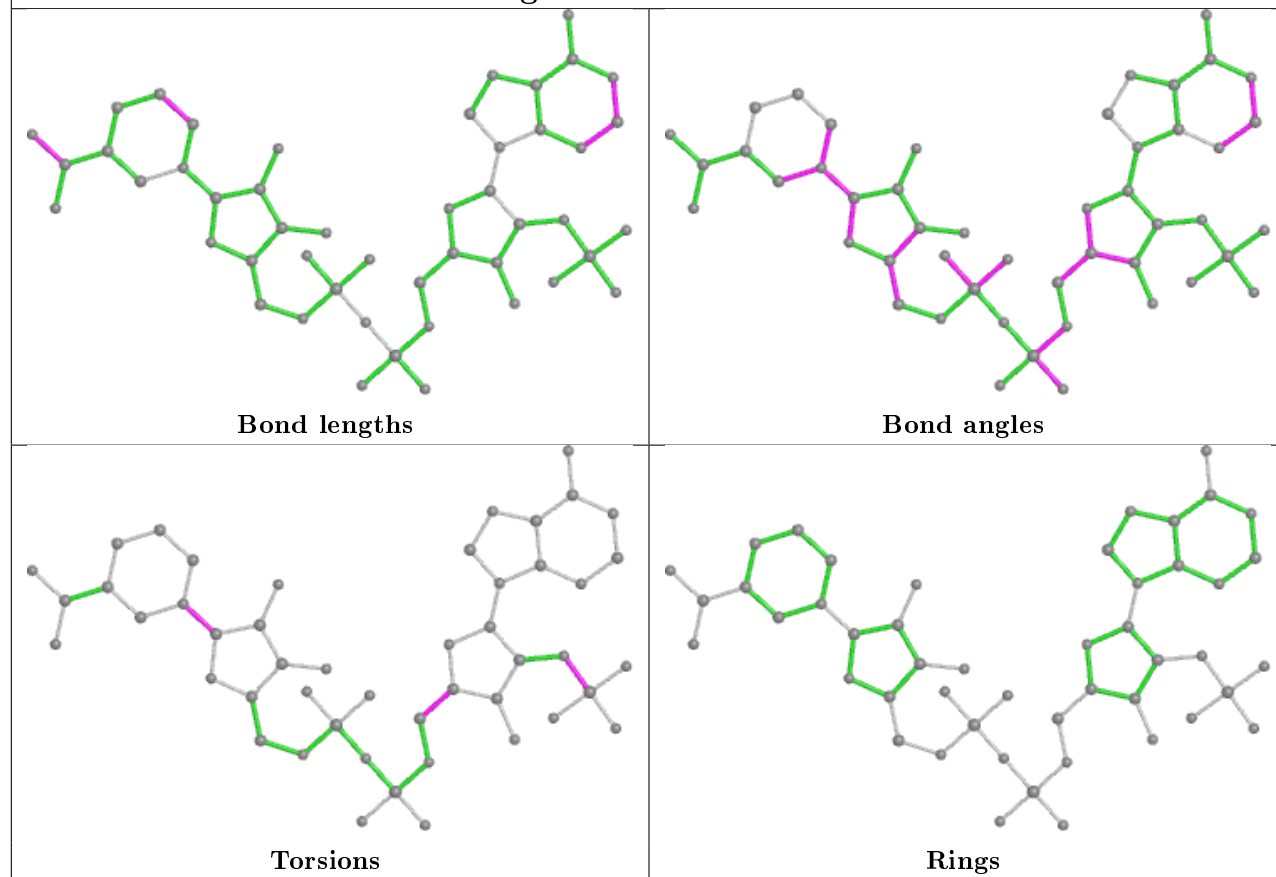
Ligand NDP C 1338

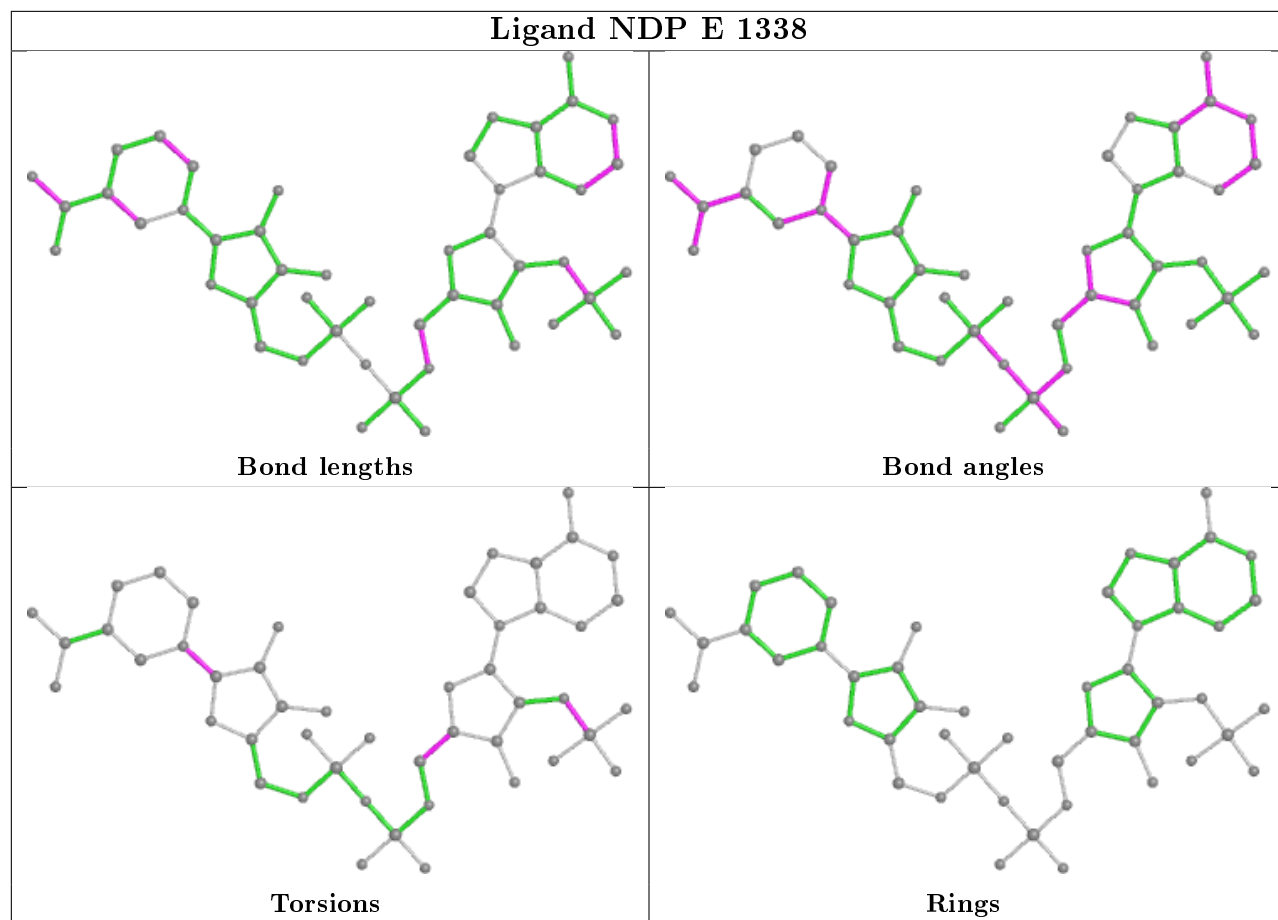


Ligand IMP C 1337

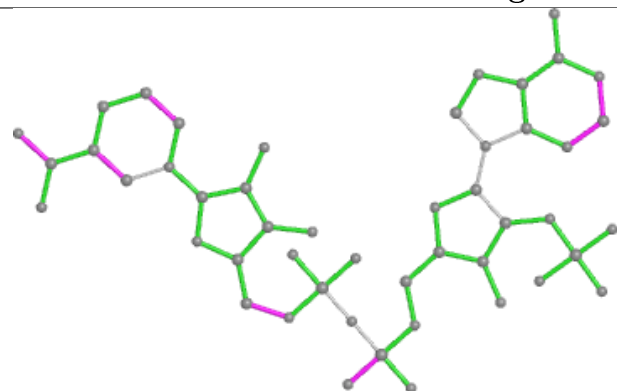


Ligand NDP A 1338

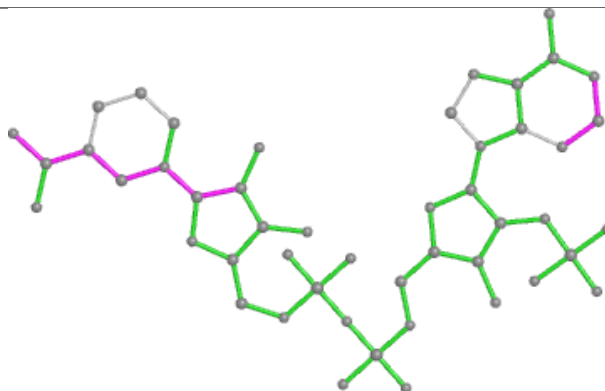




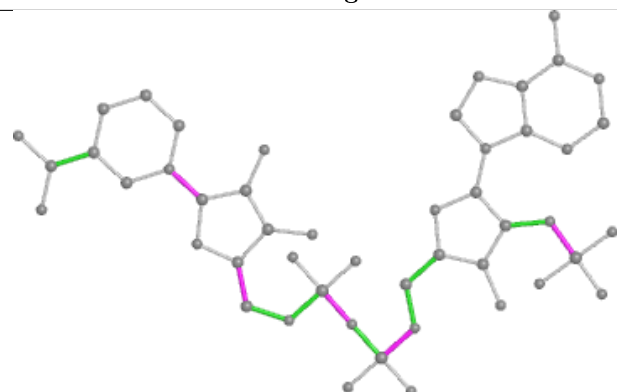
Ligand NDP F 1338



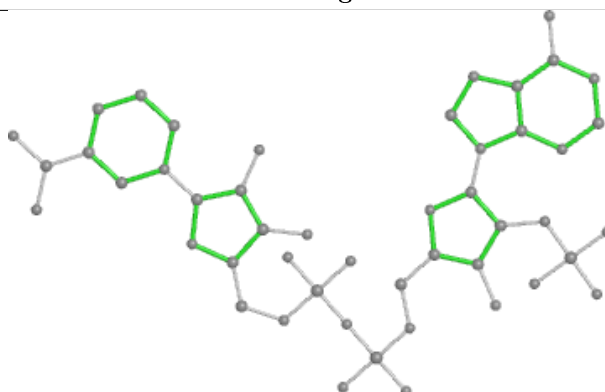
Bond lengths



Bond angles

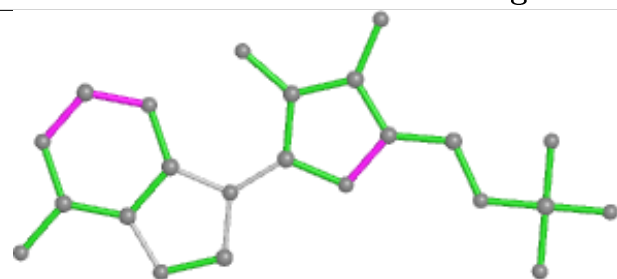


Torsions

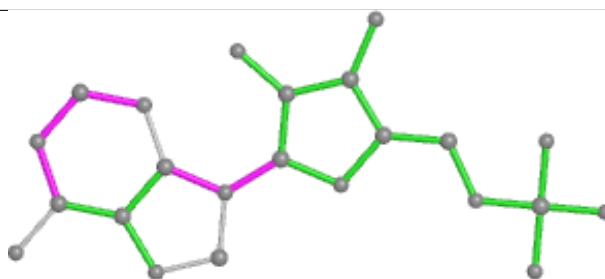


Rings

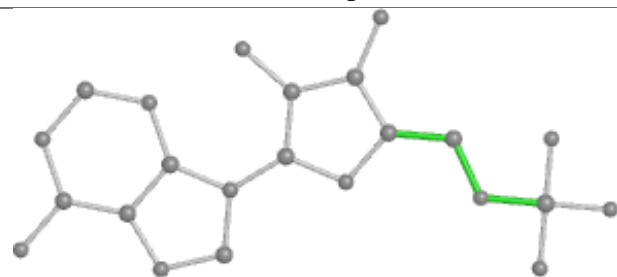
Ligand IMP D 1337



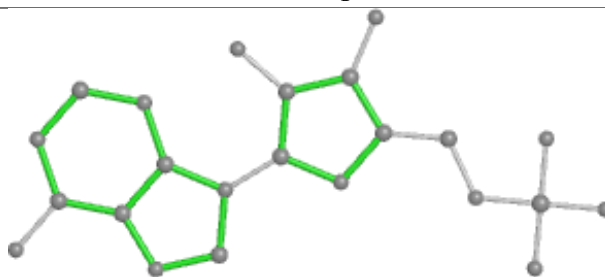
Bond lengths



Bond angles

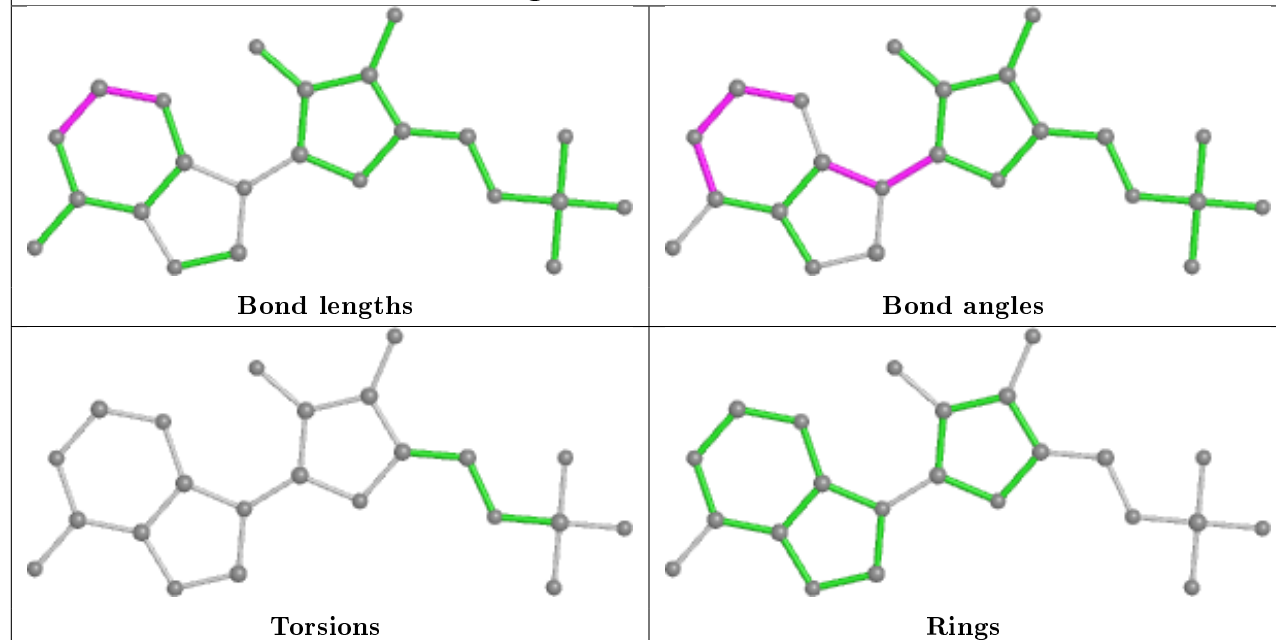


Torsions

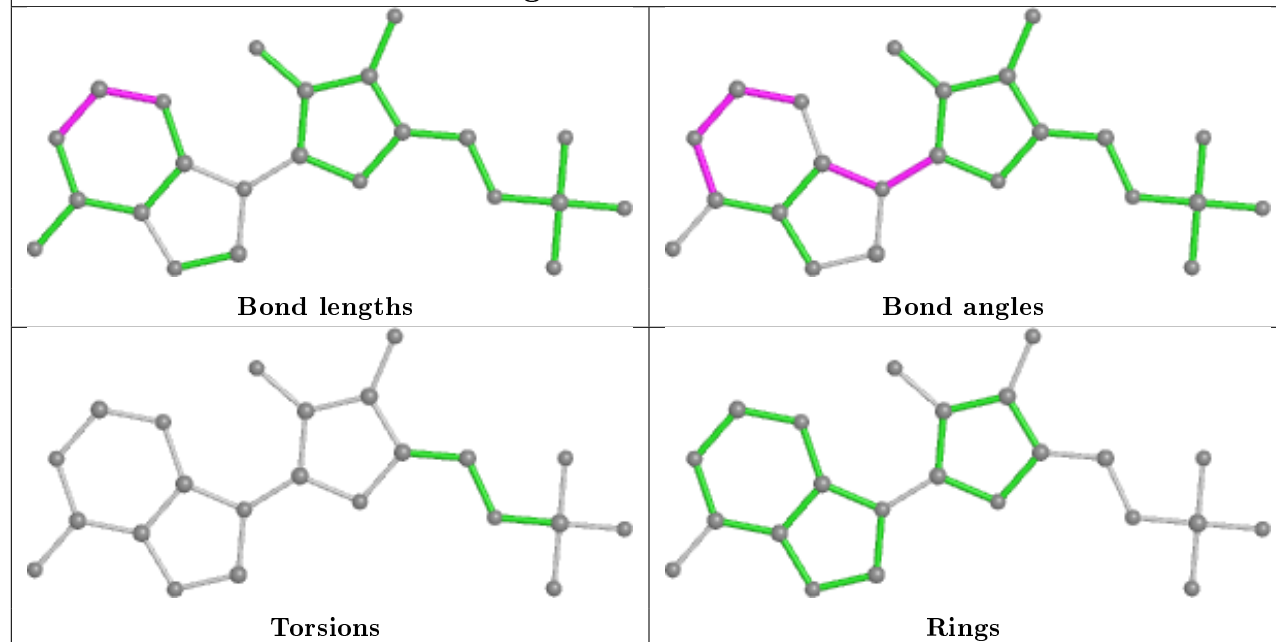


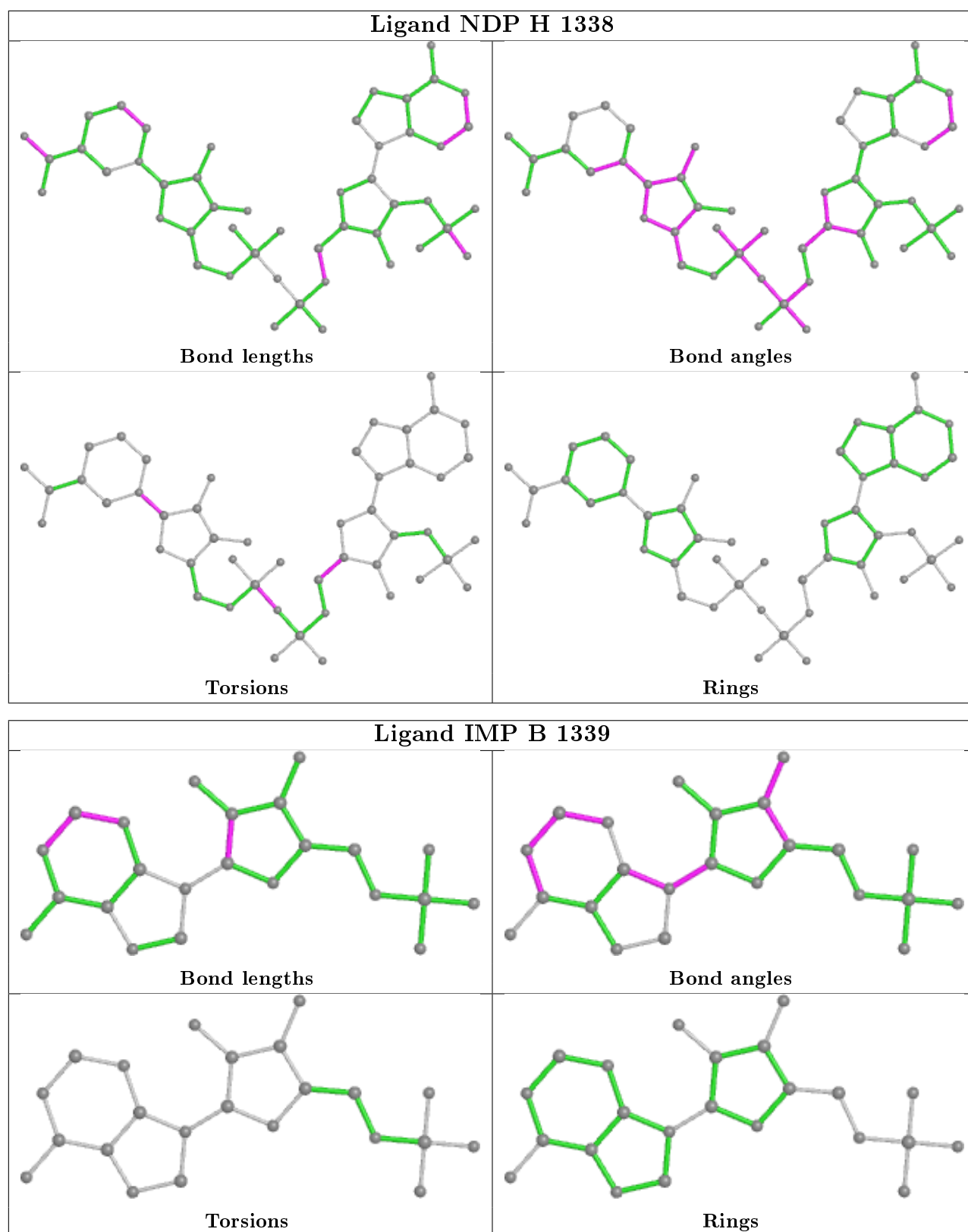
Rings

Ligand IMP F 1337



Ligand IMP G 1338





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	328/351 (93%)	0.32	15 (4%) 32 36	19, 25, 35, 45	0
1	B	329/351 (93%)	0.27	9 (2%) 54 58	19, 25, 35, 46	0
1	C	328/351 (93%)	0.23	7 (2%) 63 67	19, 24, 37, 50	0
1	D	328/351 (93%)	0.27	10 (3%) 50 54	18, 25, 35, 44	0
1	E	328/351 (93%)	0.21	10 (3%) 50 54	20, 25, 36, 45	0
1	F	328/351 (93%)	0.26	5 (1%) 73 77	19, 25, 35, 42	0
1	G	321/351 (91%)	0.31	8 (2%) 57 61	19, 25, 34, 47	0
1	H	328/351 (93%)	0.15	5 (1%) 73 77	20, 25, 34, 45	0
All	All	2618/2808 (93%)	0.25	69 (2%) 56 60	18, 25, 35, 50	0

The worst 5 of 69 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	280	GLY	8.2
1	A	280	GLY	7.6
1	E	280	GLY	6.2
1	D	279	ALA	6.0
1	C	107	SER	5.4

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

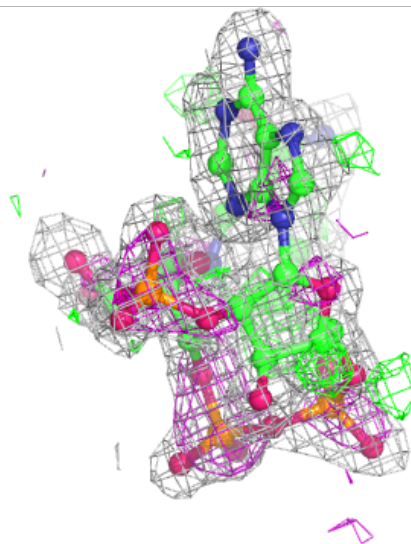
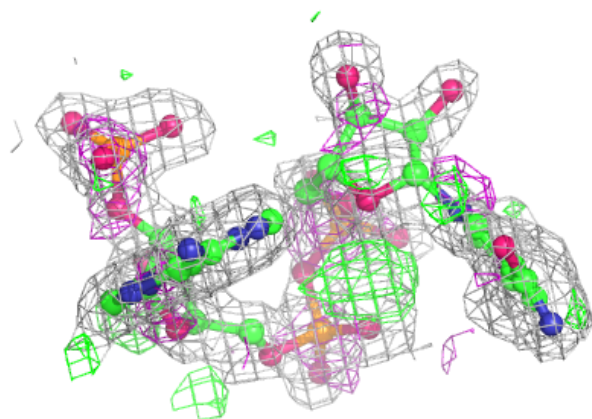
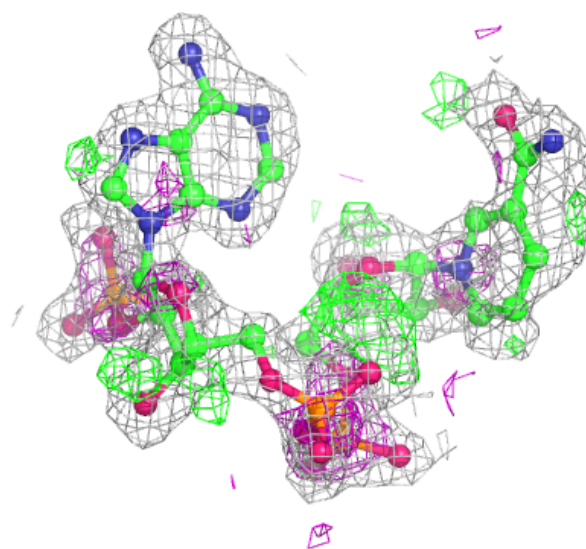
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NDP	E	1338	48/48	0.86	0.21	26,35,45,47	0
3	NDP	C	1338	48/48	0.87	0.20	27,39,57,62	0
3	NDP	D	1338	48/48	0.87	0.22	22,40,54,58	0
3	NDP	A	1338	48/48	0.89	0.19	24,38,50,52	0
3	NDP	H	1338	48/48	0.89	0.17	23,34,43,45	0
3	NDP	F	1338	48/48	0.90	0.16	23,33,50,57	0
3	NDP	B	1340	48/48	0.92	0.18	20,38,61,68	0
2	IMP	F	1337	23/23	0.97	0.07	20,23,28,32	0
2	IMP	G	1338	23/23	0.97	0.07	19,24,27,31	0
2	IMP	A	1337	23/23	0.97	0.06	22,24,27,31	0
2	IMP	B	1339	23/23	0.97	0.07	19,23,26,30	0
2	IMP	H	1337	23/23	0.98	0.06	21,23,27,29	0
2	IMP	E	1337	23/23	0.98	0.06	19,23,26,32	0
2	IMP	C	1337	23/23	0.98	0.07	19,23,29,33	0
2	IMP	D	1337	23/23	0.98	0.06	19,23,26,29	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.

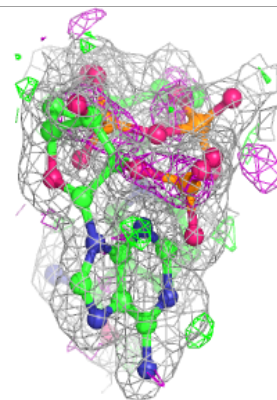
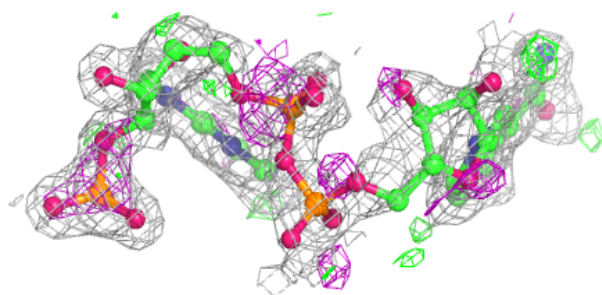
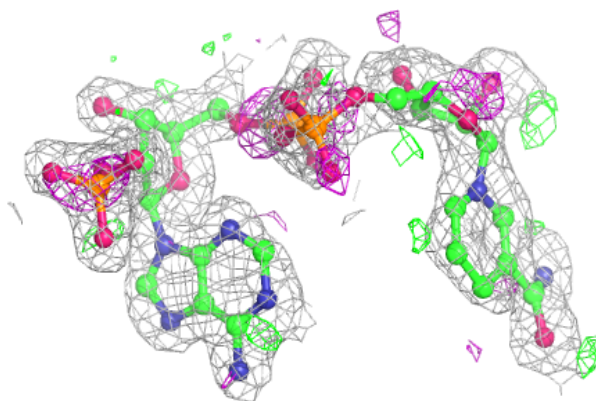
Electron density around NDP E 1338:

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



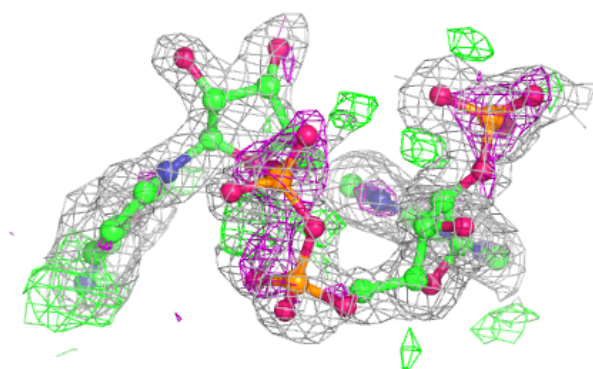
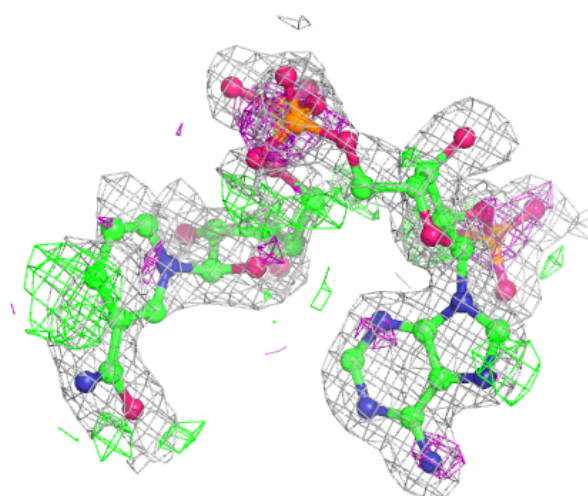
Electron density around NDP C 1338:

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



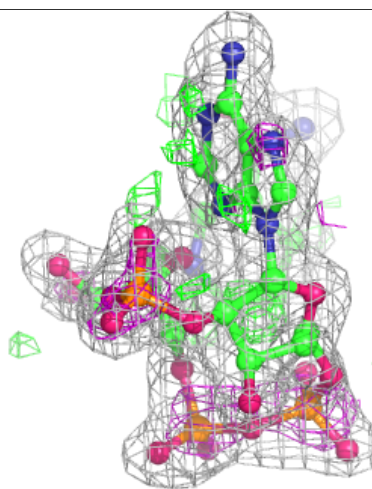
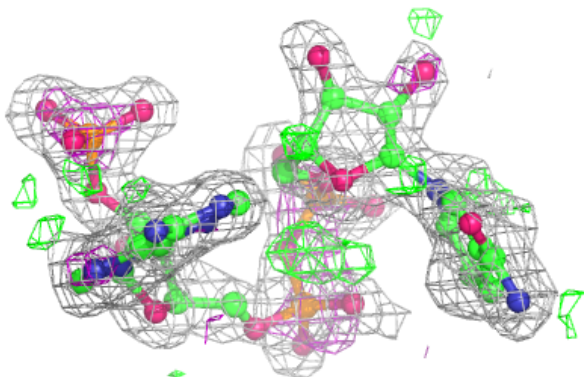
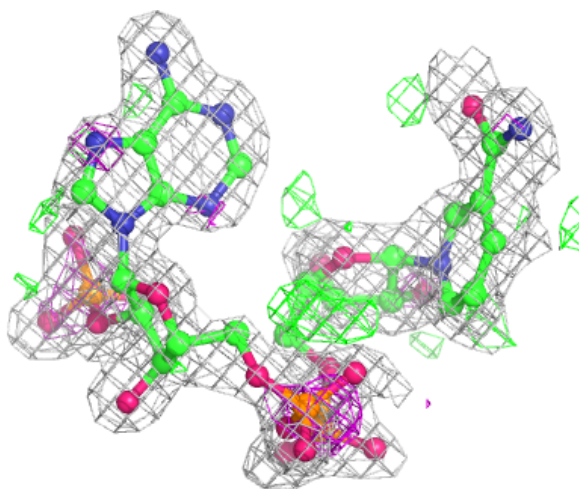
Electron density around NDP D 1338:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



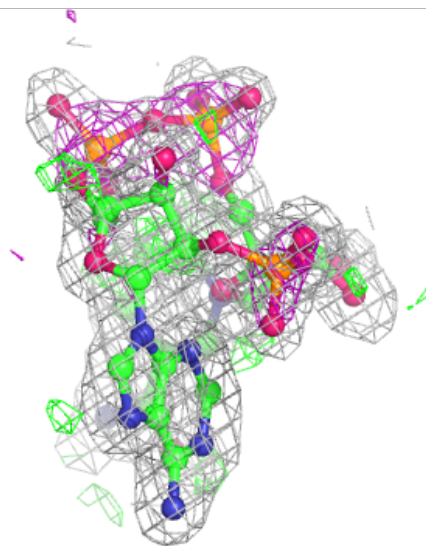
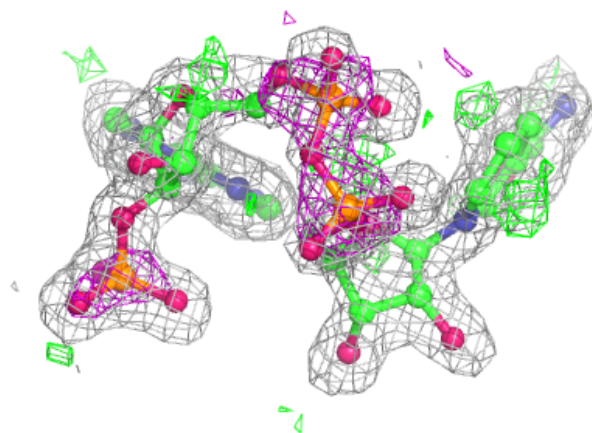
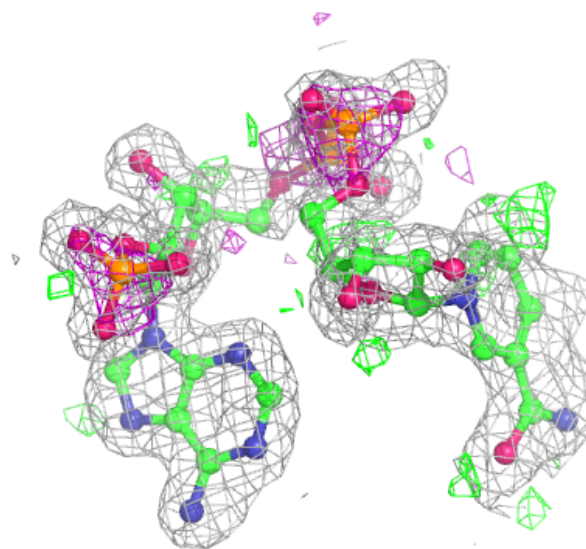
Electron density around NDP A 1338:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



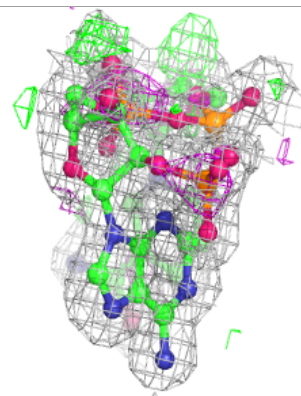
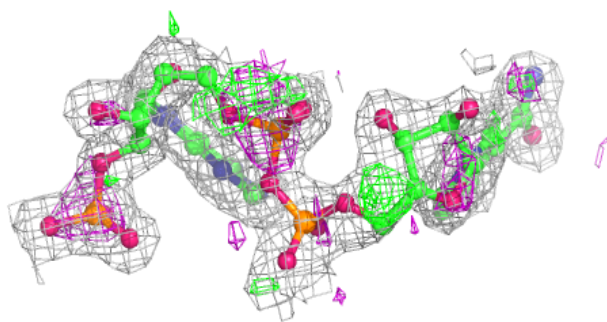
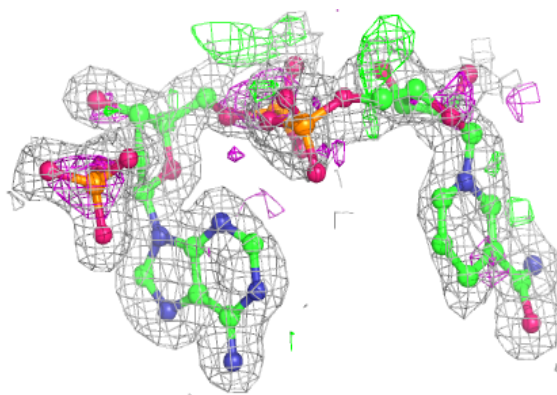
Electron density around NDP H 1338:

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and green (positive)

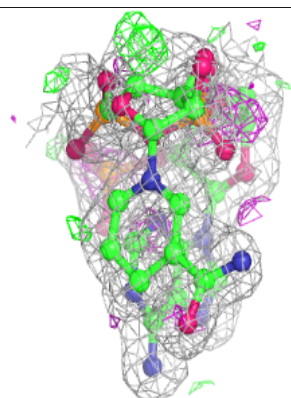
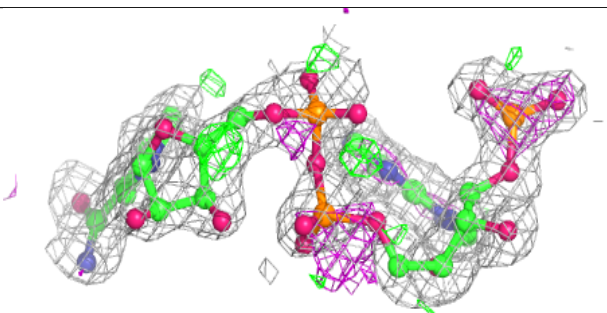
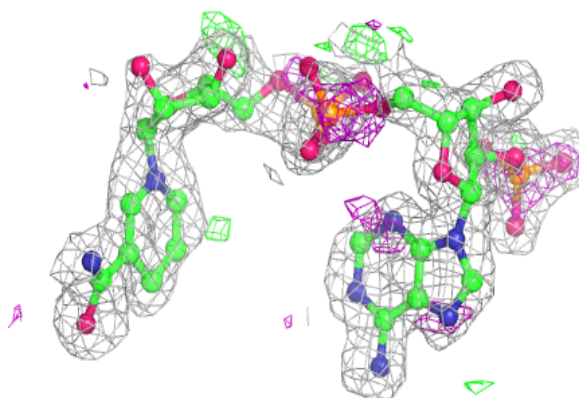


Electron density around NDP F 1338:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

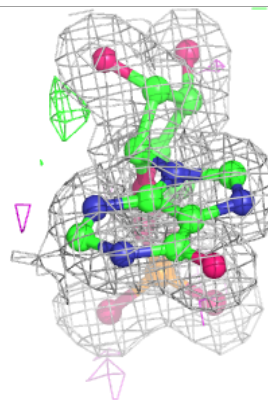
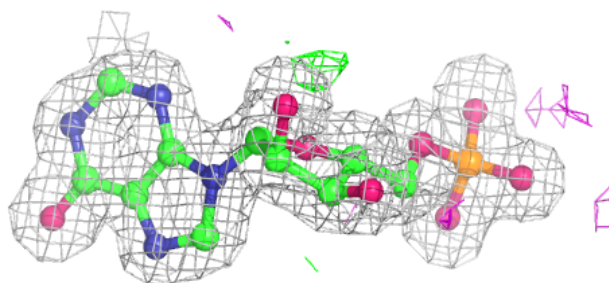
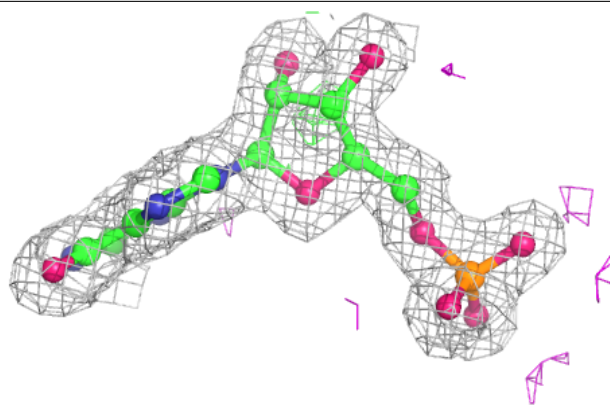
**Electron density around NDP B 1340:**

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and green (positive)

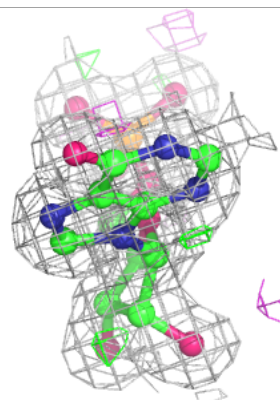
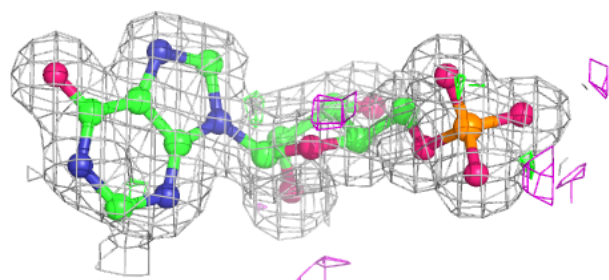
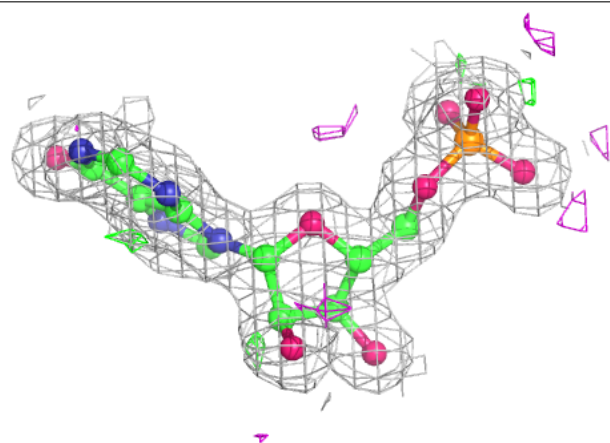


Electron density around IMP F 1337:

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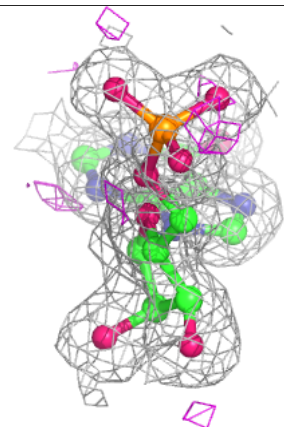
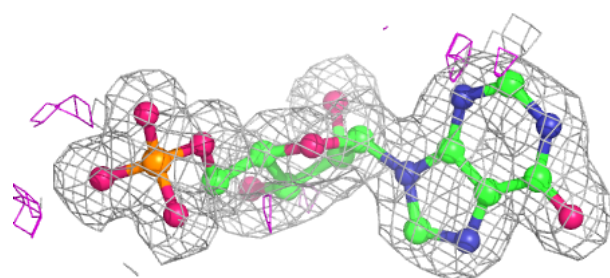
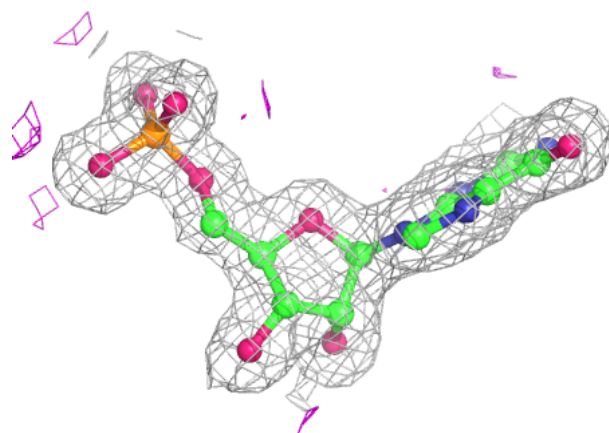
**Electron density around IMP G 1338:**

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and green (positive)

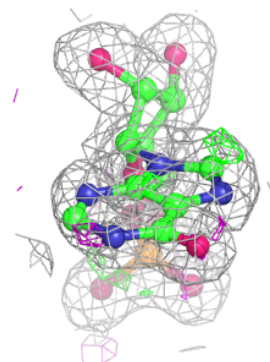
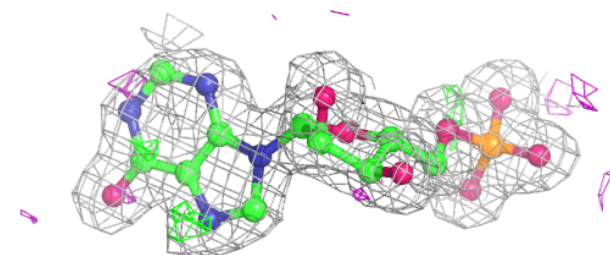
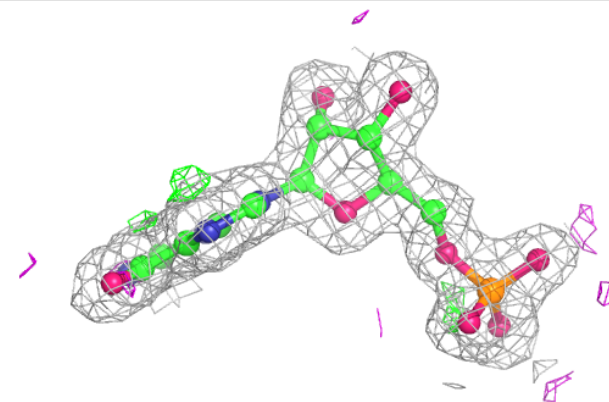


Electron density around IMP A 1337:

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and green (positive)

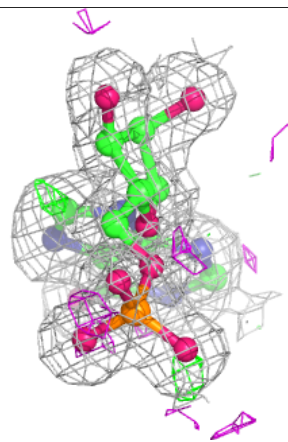
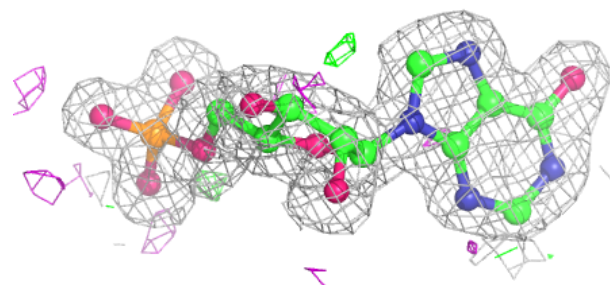
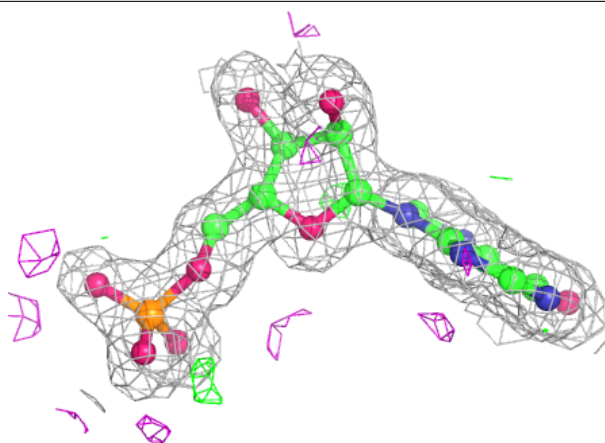
**Electron density around IMP B 1339:**

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



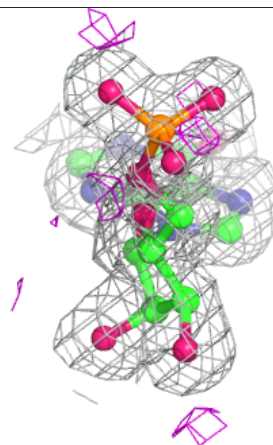
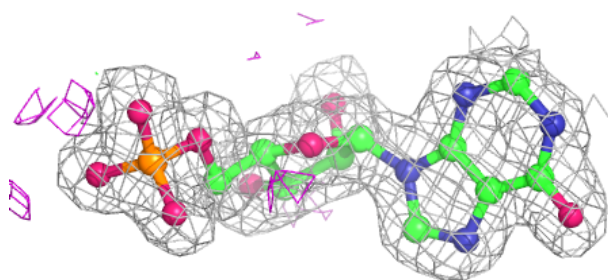
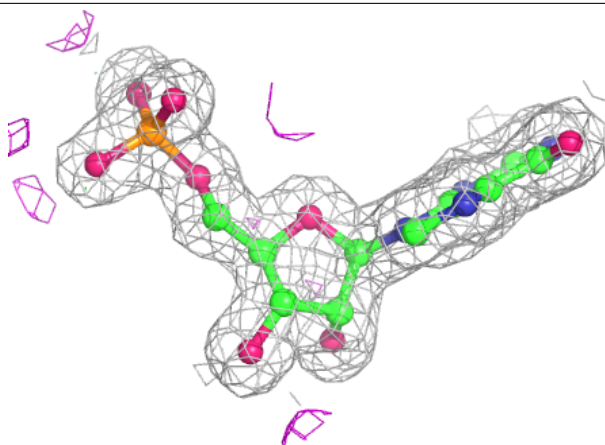
Electron density around IMP H 1337:

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



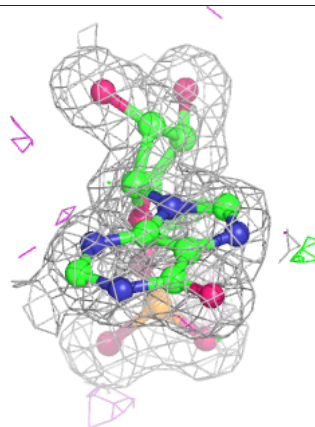
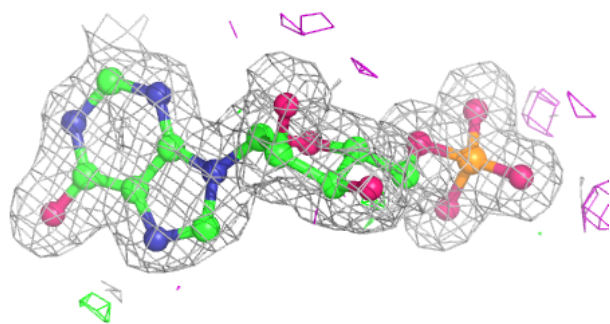
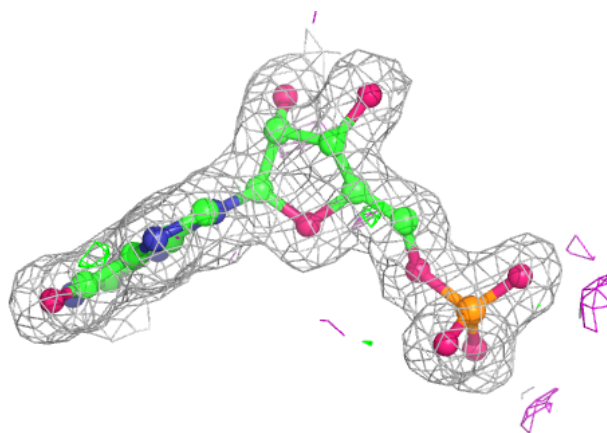
Electron density around IMP E 1337:

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



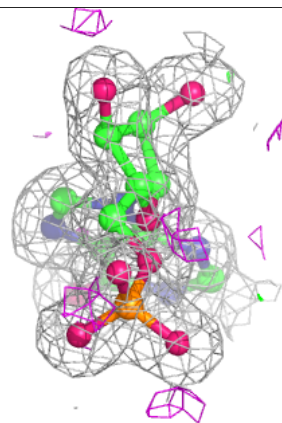
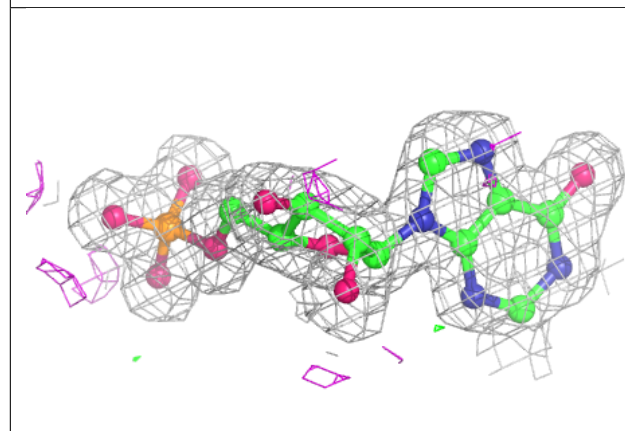
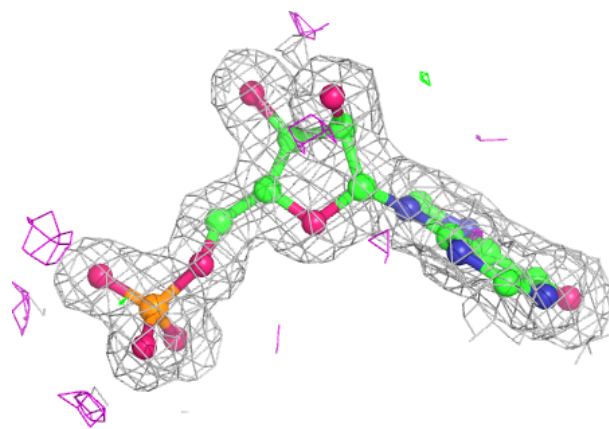
Electron density around IMP C 1337:

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



Electron density around IMP D 1337:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.