



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 01:06 AM UTC

PDB ID : 8YPZ / pdb_00008ypz
Title : Crystal structure of human phosphoribosyl pyrophosphate synthetase 1 (PRPS1) in complex with GDP
Authors : Zhang, L.; Zhang, L.
Deposited on : 2024-03-18
Resolution : 3.00 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 types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

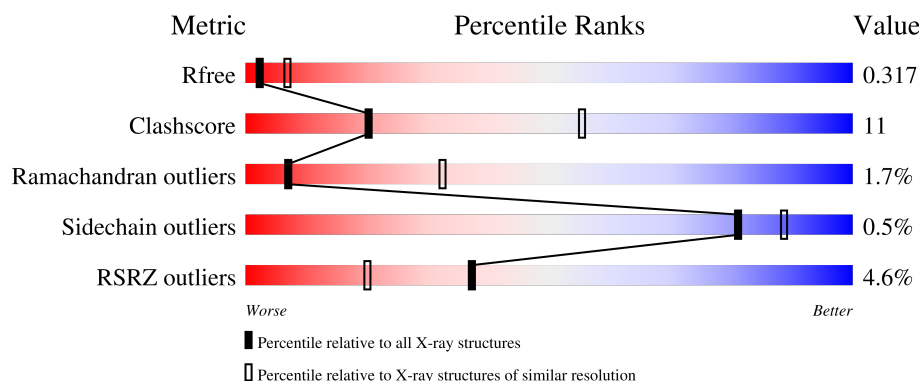
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	318	3% 75% 20% ..
1	B	318	4% 73% 23% ..
1	C	318	4% 76% 21% .
1	D	318	4% 68% 24% . 8%
1	E	318	7% 67% 29% ..

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Mol	Chain	Length	Quality of chain
1	F	318	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PO4	D	1002	-	X	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14526 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.

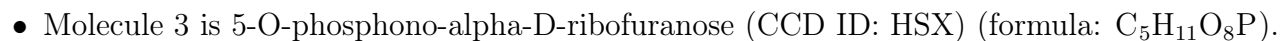
- Molecule 1 is a protein called Ribose-phosphate pyrophosphokinase 1.

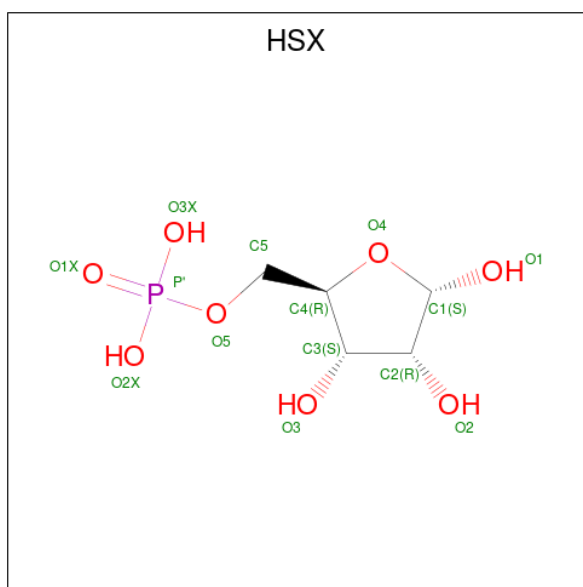
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2360	1481	415	447	17			
1	B	309	Total	C	N	O	S	0	0	0
			2362	1484	415	446	17			
1	C	309	Total	C	N	O	S	0	0	0
			2362	1484	415	446	17			
1	D	294	Total	C	N	O	S	0	0	0
			2245	1407	398	423	17			
1	E	306	Total	C	N	O	S	0	0	0
			2334	1467	409	441	17			
1	F	308	Total	C	N	O	S	0	0	0
			2350	1476	413	444	17			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP P60891
B	1	SER	-	expression tag	UNP P60891
C	1	SER	-	expression tag	UNP P60891
D	1	SER	-	expression tag	UNP P60891
E	1	SER	-	expression tag	UNP P60891
F	1	SER	-	expression tag	UNP P60891

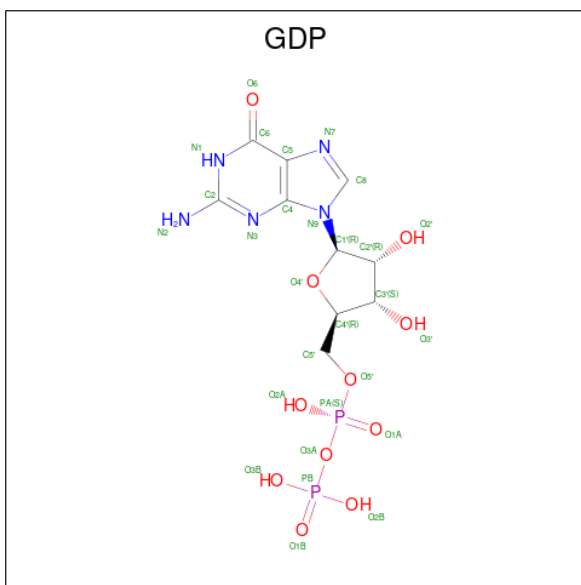
- Molecule 2 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (CCD ID: APC) (formula: C₁₁H₁₈N₅O₁₂P₃).





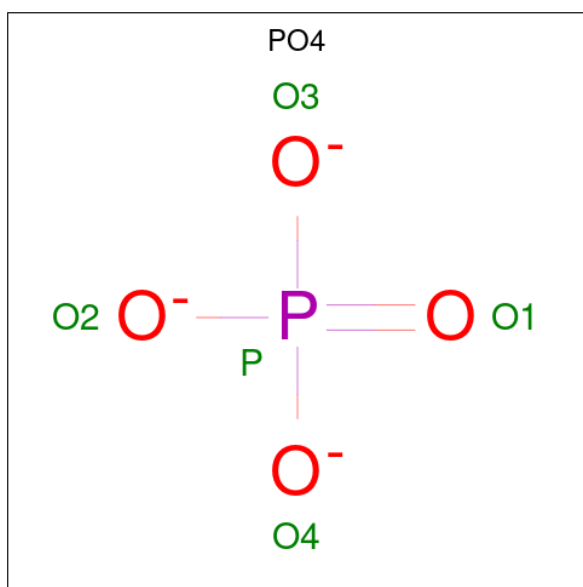
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			14	5	8	1		
3	B	1	Total	C	O	P	0	0
			14	5	8	1		
3	C	1	Total	C	O	P	0	0
			14	5	8	1		
3	E	1	Total	C	O	P	0	0
			14	5	8	1		
3	F	1	Total	C	O	P	0	0
			14	5	8	1		

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 28	C 10	N 5	O 11	P 2	0	0
4	A	1	Total 28	C 10	N 5	O 11	P 2	0	0
4	C	1	Total 24	C 10	N 5	O 8	P 1	0	0
4	C	1	Total 28	C 10	N 5	O 11	P 2	0	0
4	E	1	Total 28	C 10	N 5	O 11	P 2	0	0
4	F	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

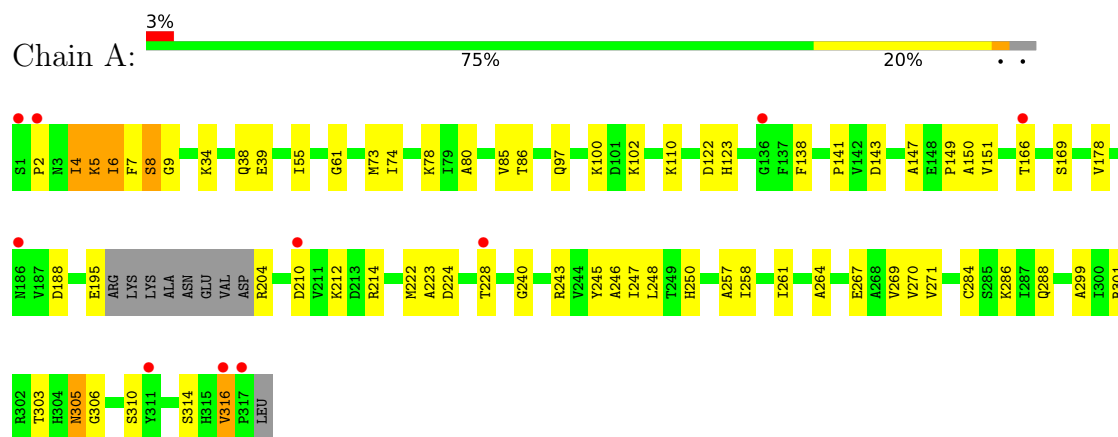
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	15	Total	O	0	0
			15	15		
6	B	11	Total	O	0	0
			11	11		
6	C	12	Total	O	0	0
			12	12		
6	D	6	Total	O	0	0
			6	6		
6	E	7	Total	O	0	0
			7	7		
6	F	12	Total	O	0	0
			12	12		

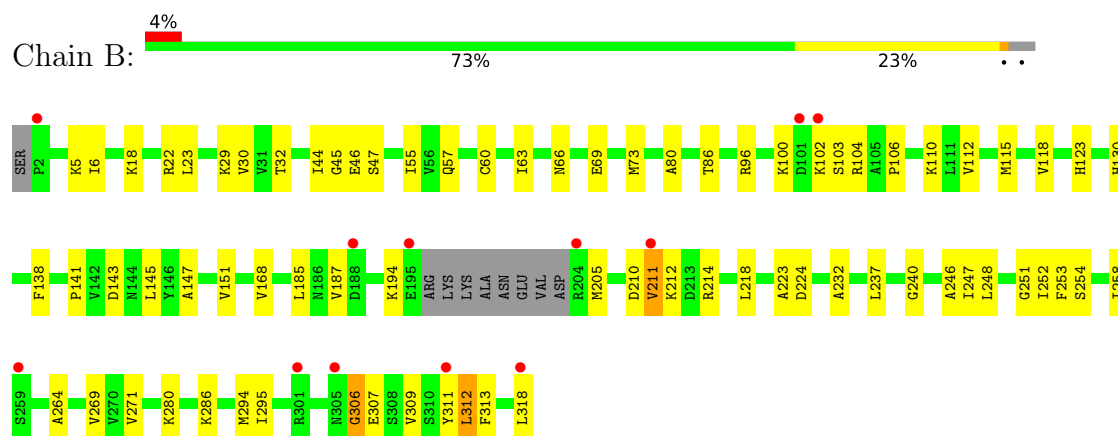
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

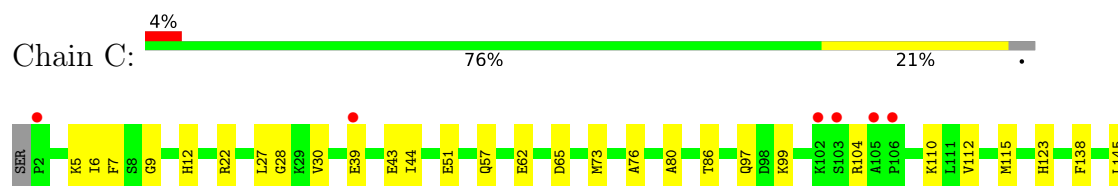
- Molecule 1: Ribose-phosphate pyrophosphokinase 1

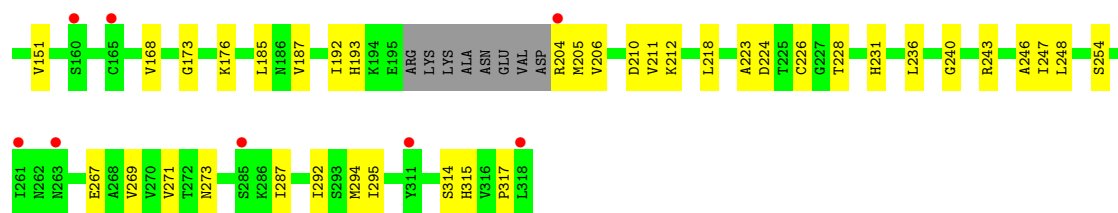


- Molecule 1: Ribose-phosphate pyrophosphokinase 1

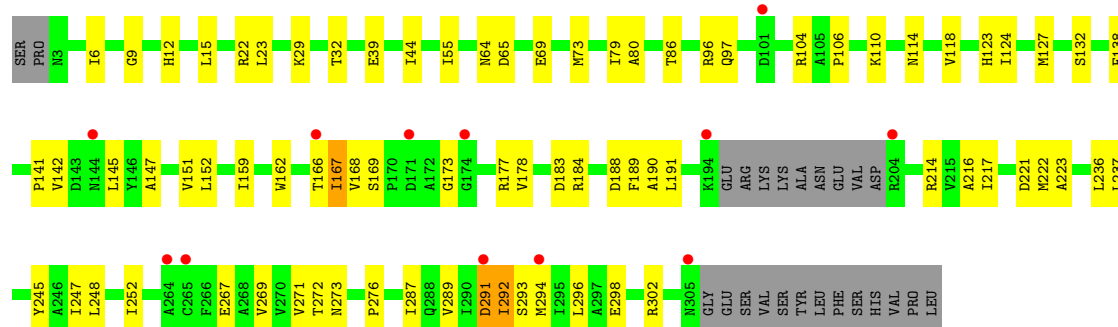


- Molecule 1: Ribose-phosphate pyrophosphokinase 1





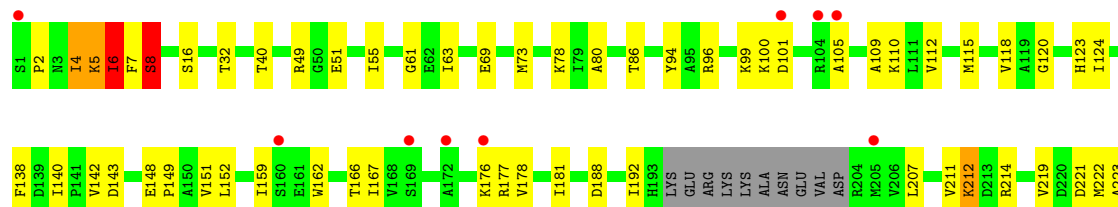
• Molecule 1: Ribose-phosphate pyrophosphokinase 1

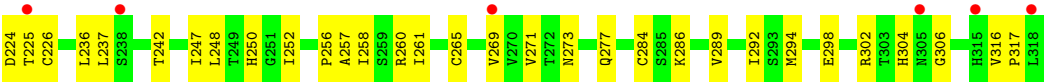


• Molecule 1: Ribose-phosphate pyrophosphokinase 1



• Molecule 1: Ribose-phosphate pyrophosphokinase 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	186.88Å 186.88Å 160.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.70 – 3.00 48.70 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.70-3.00) 97.9 (48.70-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.44 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.17.1-3660	Depositor
R, R_{free}	0.260 , 0.310 0.283 , 0.317	Depositor DCC
R_{free} test set	3108 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	57.4	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.047 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	14526	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.55 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.4739e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: HSX, APC, GDP, PO4

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	0.65	8/2395 (0.3%)	0.57	3/3240 (0.1%)
1	B	0.21	0/2397	0.55	0/3242
1	C	0.22	0/2397	0.51	0/3242
1	D	0.18	0/2275	0.51	0/3075
1	E	0.20	0/2369	0.56	0/3205
1	F	0.77	9/2385 (0.4%)	0.59	2/3228 (0.1%)
All	All	0.45	17/14218 (0.1%)	0.55	5/19232 (0.0%)

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	5	LYS	C-O	-13.80	1.07	1.24
1	F	7	PHE	C-O	-13.79	1.06	1.23
1	A	8	SER	C-O	-13.33	1.07	1.23
1	F	4	ILE	C-O	-11.88	1.10	1.24
1	F	8	SER	C-O	-11.54	1.09	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	ILE	N-CA-C	8.11	119.83	107.99
1	F	6	ILE	CB-CG1-CD1	-5.79	101.64	113.80
1	A	6	ILE	CB-CG1-CD1	-5.50	102.26	113.80
1	A	6	ILE	N-CA-C	5.28	120.33	109.34
1	F	7	PHE	N-CA-C	5.28	118.19	109.85

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	2360	0	2399	46	0
1	B	2362	0	2403	53	0
1	C	2362	0	2403	46	0
1	D	2245	0	2293	58	0
1	E	2334	0	2373	75	0
1	F	2350	0	2391	64	0
2	A	62	0	28	2	0
2	B	31	0	14	1	0
2	C	31	0	14	3	0
2	D	31	0	14	3	0
2	E	31	0	14	1	0
3	A	14	0	0	1	0
3	B	14	0	0	0	0
3	C	14	0	0	5	0
3	E	14	0	0	1	0
3	F	14	0	0	1	0
4	A	56	0	24	11	0
4	C	52	0	24	3	0
4	E	28	0	12	6	0
4	F	28	0	12	5	0
5	A	5	0	0	0	0
5	B	5	0	0	1	0
5	C	5	0	0	0	0
5	D	10	0	0	2	0
5	F	5	0	0	1	0
6	A	15	0	0	1	0
6	B	11	0	0	1	0
6	C	12	0	0	0	0
6	D	6	0	0	0	0
6	E	7	0	0	0	0
6	F	12	0	0	0	0
All	All	14526	0	14418	325	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 11.

The worst 5 of 325 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)
3:C:1002:HSX:O3	3:C:1002:HSX:O1X	1.78	0.99
1:E:316:VAL:HG22	1:E:317:PRO:CD	1.94	0.97
1:E:214:ARG:O	1:E:215:VAL:HG12	1.65	0.97
1:C:223:ALA:HB2	1:C:248:LEU:HD13	1.48	0.93
1:E:316:VAL:HG22	1:E:317:PRO:HD2	1.51	0.91

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	305/318 (96%)	271 (89%)	27 (9%)	7 (2%)	5	25
1	B	305/318 (96%)	273 (90%)	26 (8%)	6 (2%)	6	28
1	C	305/318 (96%)	273 (90%)	27 (9%)	5 (2%)	7	34
1	D	290/318 (91%)	259 (89%)	26 (9%)	5 (2%)	7	32
1	E	302/318 (95%)	268 (89%)	30 (10%)	4 (1%)	9	38
1	F	304/318 (96%)	274 (90%)	26 (9%)	4 (1%)	9	38
All	All	1811/1908 (95%)	1618 (89%)	162 (9%)	31 (2%)	7	32

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	PRO
1	B	194	LYS
1	B	252	ILE
1	B	307	GLU
1	C	12	HIS

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	262/270 (97%)	259 (99%)	3 (1%)	65	83
1	B	262/270 (97%)	261 (100%)	1 (0%)	84	90
1	C	262/270 (97%)	261 (100%)	1 (0%)	84	90
1	D	248/270 (92%)	248 (100%)	0	100	100
1	E	259/270 (96%)	259 (100%)	0	100	100
1	F	261/270 (97%)	259 (99%)	2 (1%)	73	86
All	All	1554/1620 (96%)	1547 (100%)	7 (0%)	81	89

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	318	LEU
1	C	228	THR
1	F	8	SER
1	F	6	ILE
1	A	8	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	75	ASN
1	E	277	GLN
1	D	75	ASN
1	B	158	ASN
1	D	277	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

23 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	APC	C	1001	-	29,33,33	2.06	10 (34%)	44,52,52	2.24	19 (43%)
5	PO4	D	1003	-	4,4,4	0.93	0	6,6,6	0.44	0
5	PO4	A	1006	-	4,4,4	1.00	0	6,6,6	0.38	0
5	PO4	F	3003	-	4,4,4	0.94	0	6,6,6	0.53	0
3	HSX	C	1002	-	14,14,14	2.00	3 (21%)	19,21,21	2.12	3 (15%)
3	HSX	A	1002	-	14,14,14	1.42	2 (14%)	19,21,21	1.51	3 (15%)
2	APC	B	1001	-	29,33,33	1.98	10 (34%)	44,52,52	2.37	23 (52%)
3	HSX	E	1002	-	14,14,14	1.34	1 (7%)	19,21,21	3.59	8 (42%)
4	GDP	A	1004	-	29,30,30	1.21	3 (10%)	45,47,47	1.89	8 (17%)
4	GDP	C	1003	-	26,26,30	1.23	3 (11%)	39,40,47	1.95	7 (17%)
2	APC	A	1005	-	29,33,33	2.02	10 (34%)	44,52,52	2.23	19 (43%)
5	PO4	C	1005	-	4,4,4	1.01	0	6,6,6	0.37	0
4	GDP	E	1003	-	29,30,30	1.30	4 (13%)	45,47,47	1.94	9 (20%)
5	PO4	B	1003	-	4,4,4	0.89	0	6,6,6	0.54	0
4	GDP	A	1003	-	29,30,30	1.21	3 (10%)	45,47,47	1.93	9 (20%)
3	HSX	B	1002	-	14,14,14	1.75	4 (28%)	19,21,21	1.95	6 (31%)
2	APC	D	1001	-	29,33,33	1.96	10 (34%)	44,52,52	2.22	20 (45%)
4	GDP	F	3001	-	29,30,30	1.23	3 (10%)	45,47,47	1.87	6 (13%)
4	GDP	C	1004	-	29,30,30	1.22	4 (13%)	45,47,47	2.02	11 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PO4	D	1002	-	4,4,4	2.20	3 (75%)	6,6,6	1.74	2 (33%)
3	HSX	F	3002	-	14,14,14	1.06	0	19,21,21	1.66	4 (21%)
2	APC	E	1001	-	29,33,33	1.99	10 (34%)	44,52,52	2.26	20 (45%)
2	APC	A	1001	-	29,33,33	1.93	10 (34%)	44,52,52	2.26	20 (45%)

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	APC	C	1001	-	-	6/19/38/38	0/3/3/3
3	HSX	C	1002	-	-	3/6/22/22	0/1/1/1
4	GDP	E	1003	-	-	3/16/32/32	0/3/3/3
3	HSX	A	1002	-	-	5/6/22/22	0/1/1/1
2	APC	B	1001	-	-	5/19/38/38	0/3/3/3
3	HSX	F	3002	-	-	3/6/22/22	0/1/1/1
4	GDP	A	1003	-	-	5/16/32/32	0/3/3/3
3	HSX	B	1002	-	-	3/6/22/22	0/1/1/1
3	HSX	E	1002	-	-	6/6/22/22	0/1/1/1
4	GDP	A	1004	-	-	6/16/32/32	0/3/3/3
2	APC	D	1001	-	-	6/19/38/38	0/3/3/3
2	APC	E	1001	-	-	5/19/38/38	0/3/3/3
4	GDP	C	1003	-	-	3/10/26/32	0/3/3/3
4	GDP	F	3001	-	-	6/16/32/32	0/3/3/3
4	GDP	C	1004	-	-	5/16/32/32	0/3/3/3
2	APC	A	1005	-	-	9/19/38/38	0/3/3/3
2	APC	A	1001	-	-	4/19/38/38	0/3/3/3

The worst 5 of 93 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1001	APC	PB-O3B	4.41	1.63	1.58
3	C	1002	HSX	C1-C2	-4.14	1.48	1.52
3	E	1002	HSX	P'-O1X	3.93	1.62	1.50
3	C	1002	HSX	O4-C1	-3.89	1.38	1.43
2	E	1001	APC	PB-O3B	3.69	1.62	1.58

The worst 5 of 197 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1002	HSX	O5-P'-O1X	-9.03	82.03	106.44
3	E	1002	HSX	O3X-P'-O5	-7.79	86.36	106.67
4	C	1004	GDP	C5-C4-N3	-7.20	116.93	128.39
4	E	1003	GDP	C5-C4-N3	-7.16	117.00	128.39
4	A	1004	GDP	C5-C4-N3	-7.04	117.18	128.39

There are no chirality outliers.

5 of 83 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	APC	C2'-C1'-N9-C8
2	A	1005	APC	PB-C3A-PA-O1A
2	A	1005	APC	PB-C3A-PA-O2A
2	A	1005	APC	PB-C3A-PA-O5'
2	A	1005	APC	C2'-C1'-N9-C8

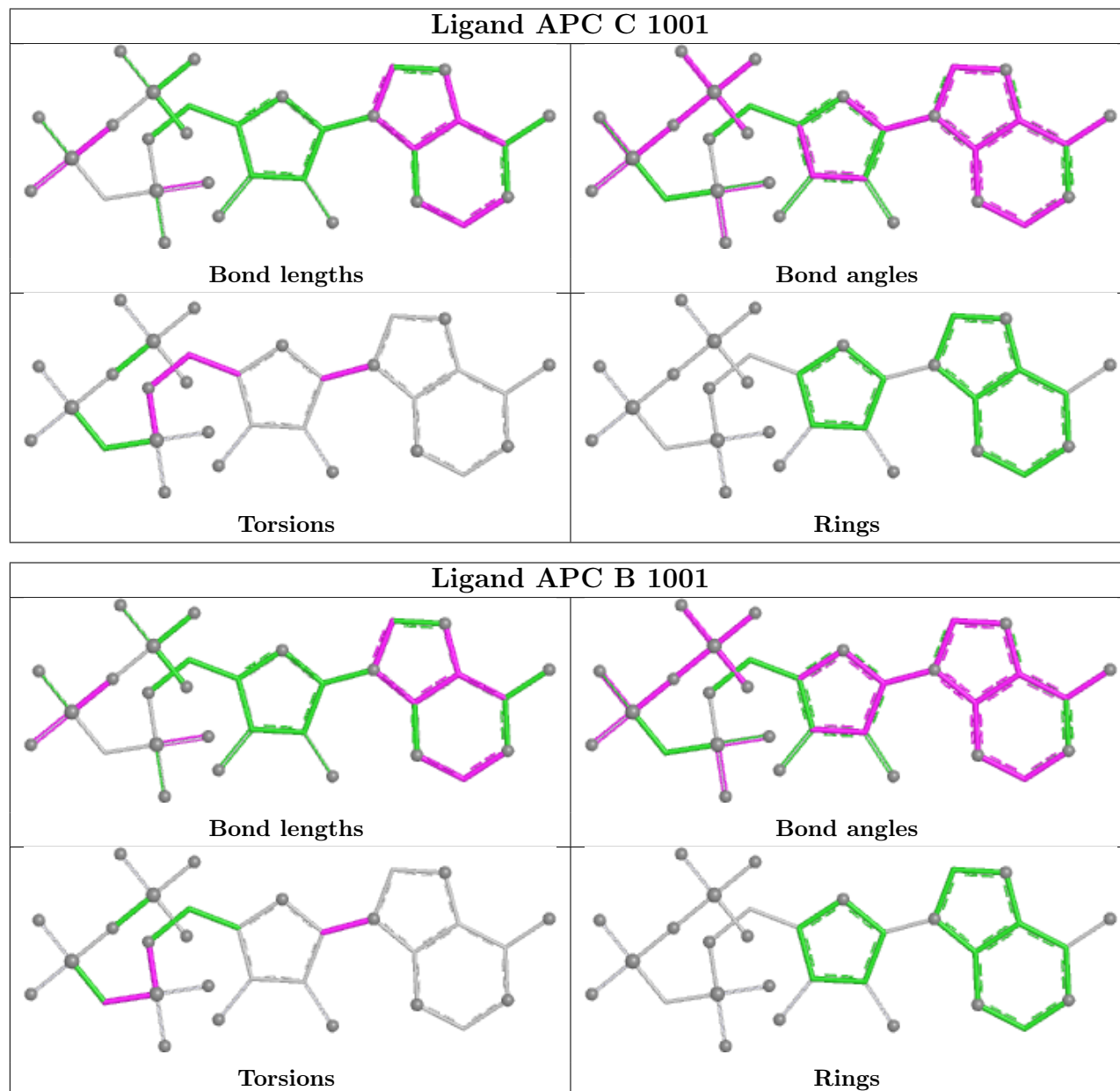
There are no ring outliers.

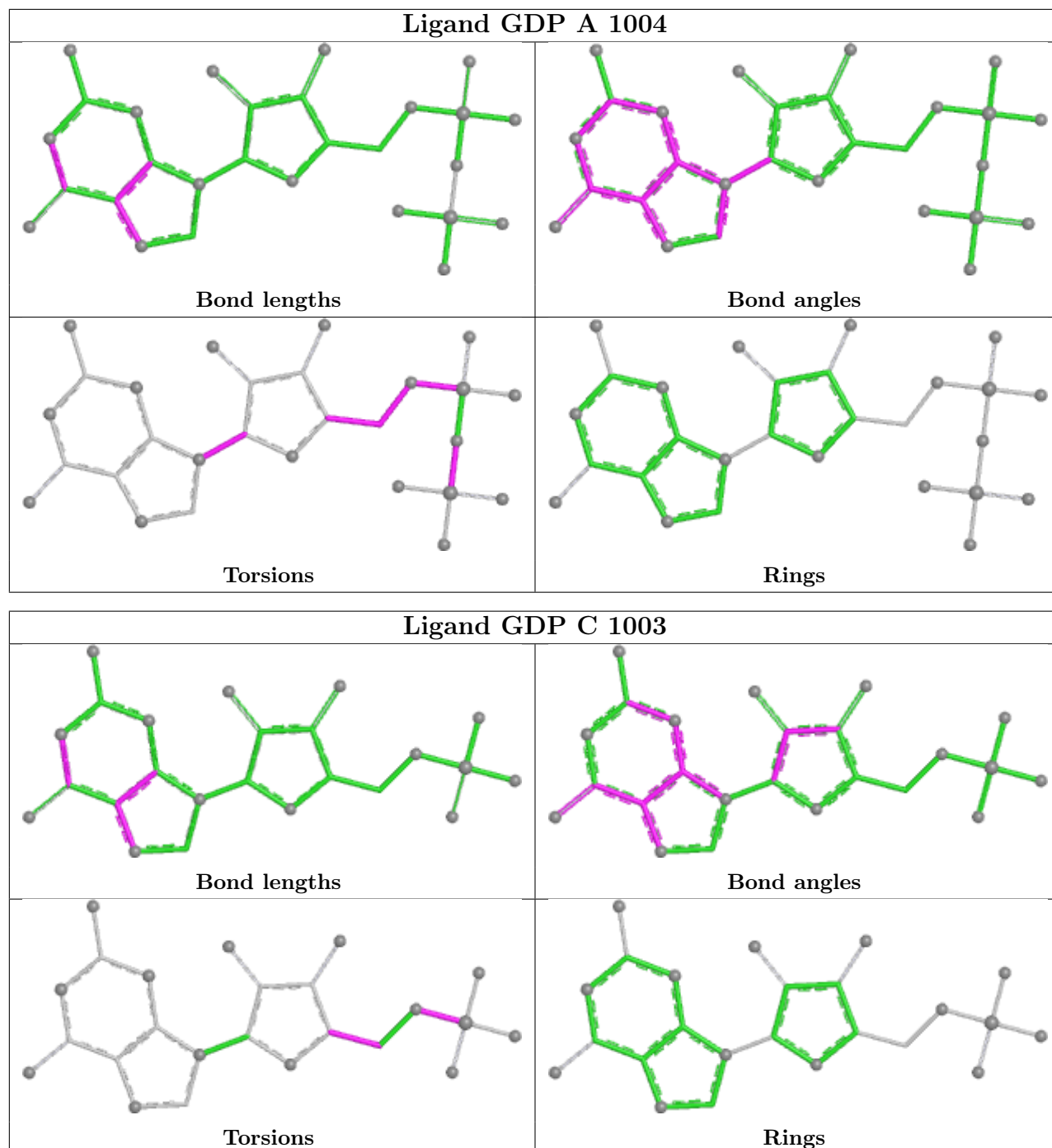
18 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1001	APC	3	0
5	F	3003	PO4	1	0
3	C	1002	HSX	5	0
3	A	1002	HSX	1	0
2	B	1001	APC	1	0
3	E	1002	HSX	1	0
4	A	1004	GDP	7	0
4	C	1003	GDP	1	0
4	E	1003	GDP	6	0
5	B	1003	PO4	1	0
4	A	1003	GDP	4	0
2	D	1001	APC	3	0
4	F	3001	GDP	5	0
4	C	1004	GDP	2	0
5	D	1002	PO4	2	0
3	F	3002	HSX	1	0
2	E	1001	APC	1	0
2	A	1001	APC	2	0

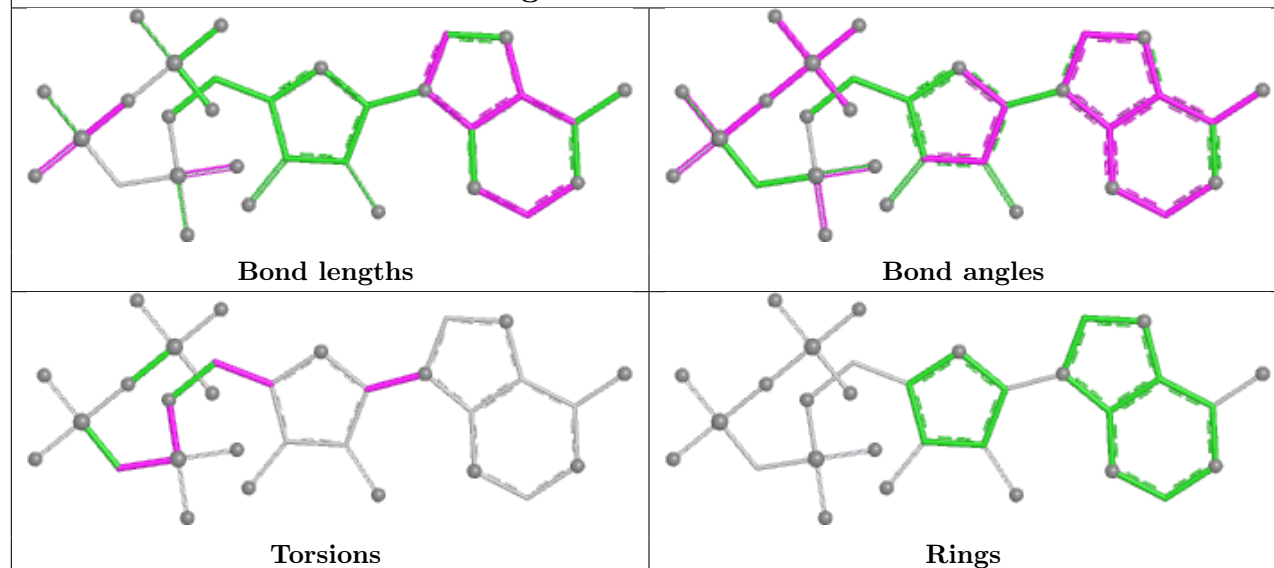
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

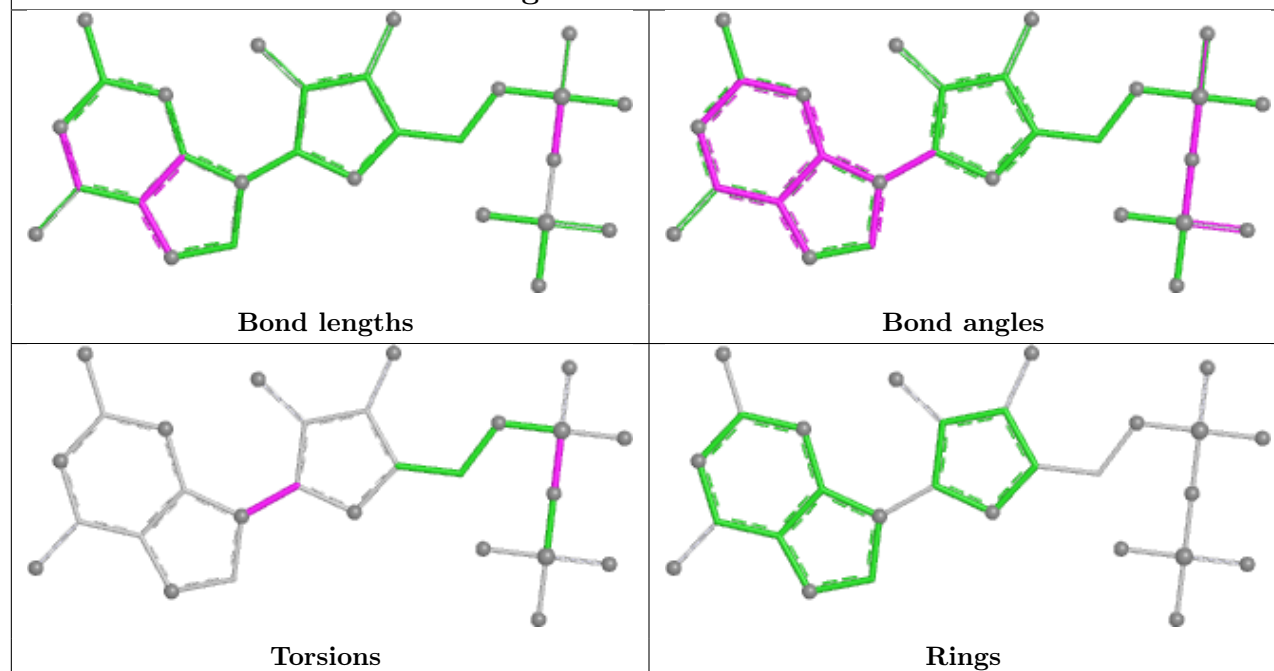


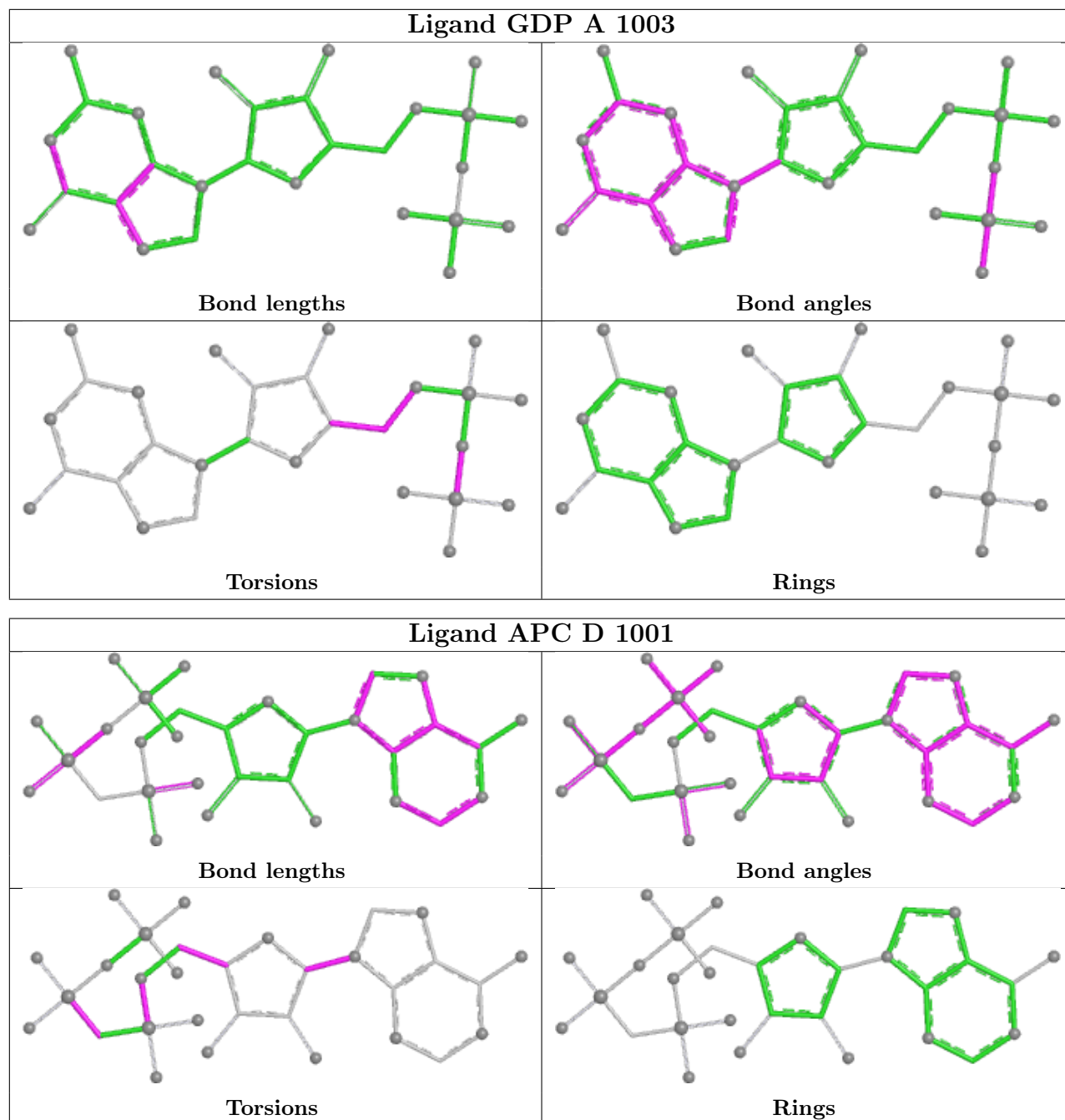


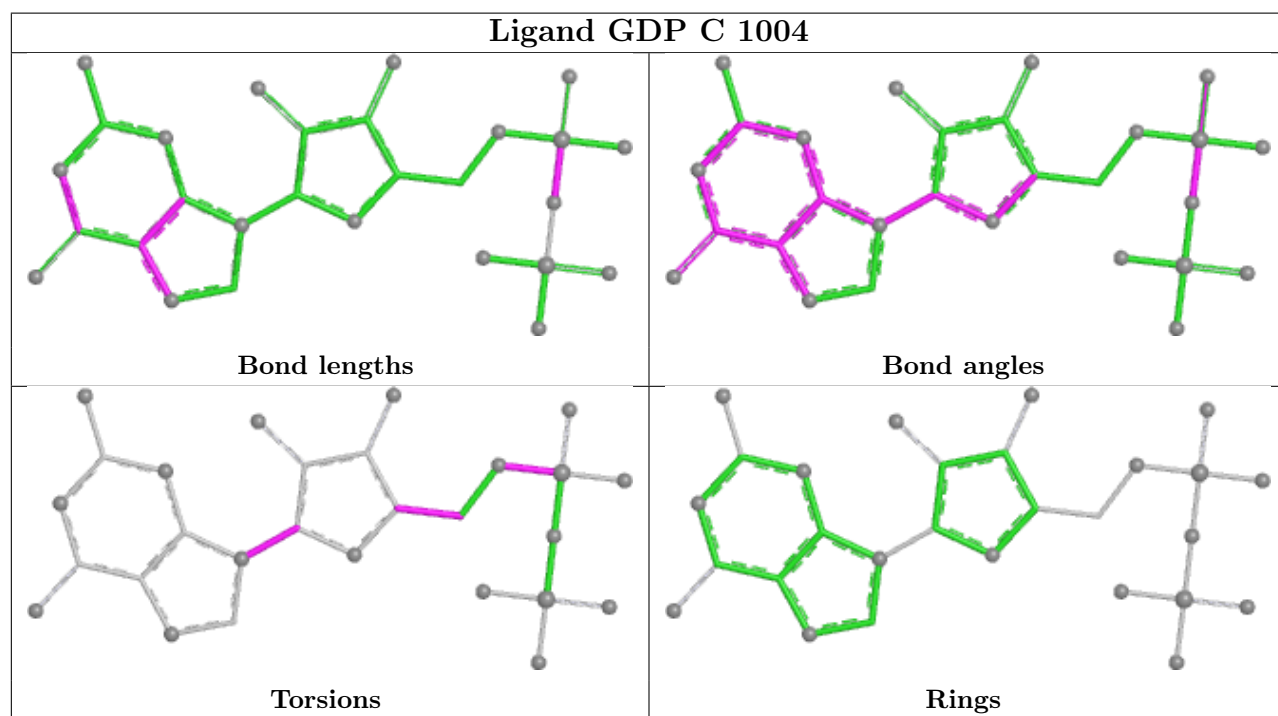
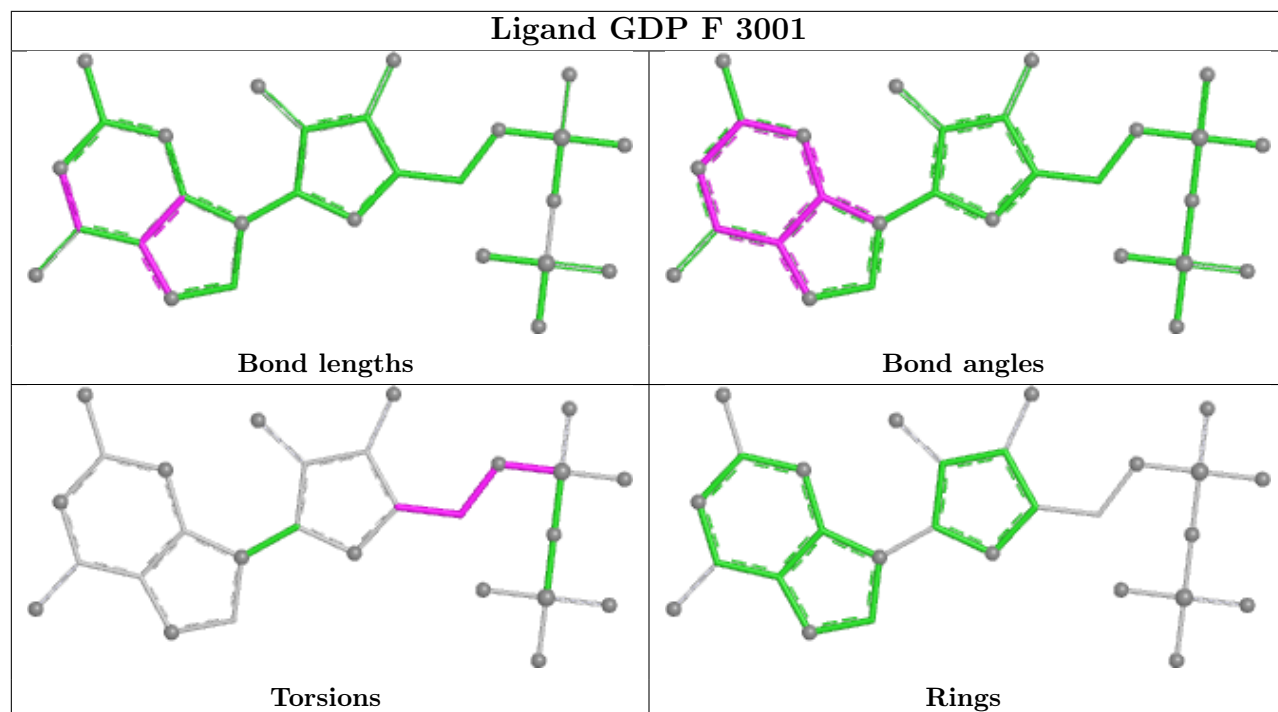
Ligand APC A 1005

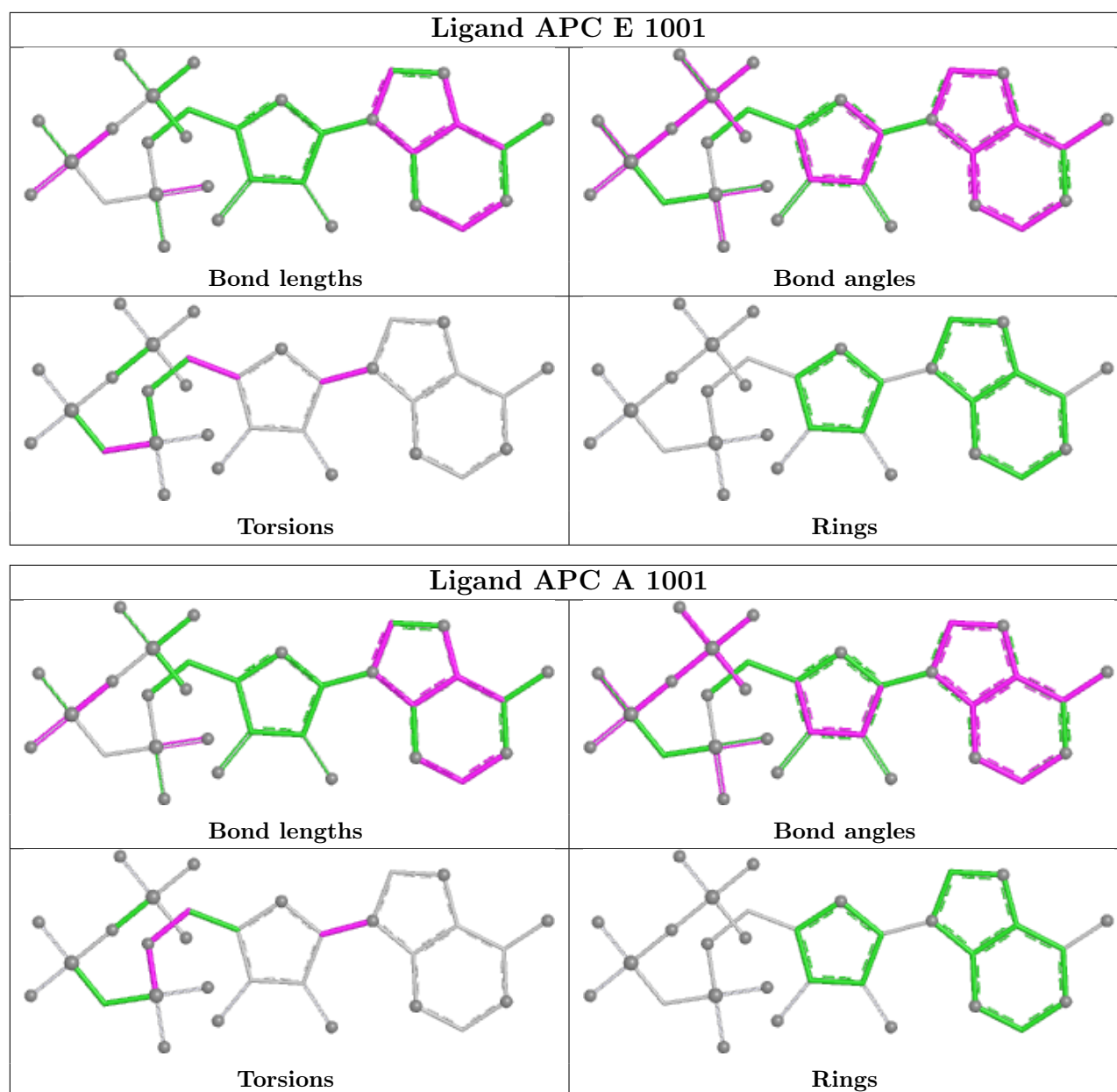


Ligand GDP E 1003









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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(Å²)	Q<0.9
1	A	309/318 (97%)	0.44	10 (3%)	50	29	22, 40, 62, 97	0
1	B	309/318 (97%)	0.26	12 (3%)	43	24	16, 35, 58, 75	0
1	C	309/318 (97%)	0.47	14 (4%)	38	20	21, 35, 59, 76	0
1	D	294/318 (92%)	0.37	12 (4%)	41	23	19, 40, 60, 75	0
1	E	306/318 (96%)	0.65	21 (6%)	23	12	26, 45, 73, 90	0
1	F	308/318 (96%)	0.60	15 (4%)	35	18	19, 37, 59, 73	0
All	All	1835/1908 (96%)	0.47	84 (4%)	37	20	16, 39, 64, 97	0

The worst 5 of 84 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	318	LEU	4.8
1	F	318	LEU	4.2
1	E	166	THR	4.2
1	A	2	PRO	3.9
1	F	1	SER	3.6

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

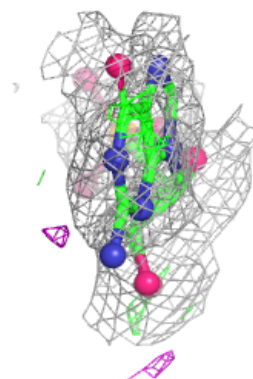
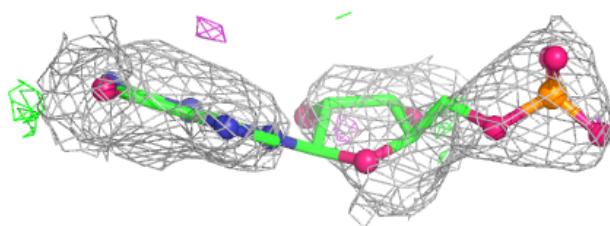
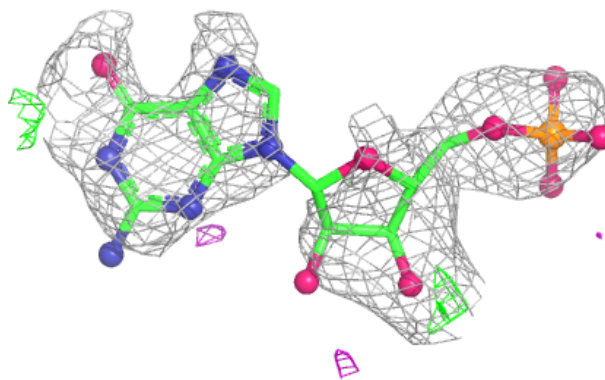
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PO4	D	1003	5/5	0.57	0.21	64,69,90,114	0
4	GDP	C	1003	24/28	0.63	0.22	55,73,87,91	0
3	HSX	A	1002	14/14	0.65	0.20	65,79,108,132	0
3	HSX	B	1002	14/14	0.68	0.19	57,77,107,107	0
4	GDP	E	1003	28/28	0.70	0.29	36,61,134,140	0
3	HSX	E	1002	14/14	0.70	0.18	77,93,103,119	0
3	HSX	C	1002	14/14	0.73	0.17	59,78,90,97	0
4	GDP	A	1004	28/28	0.76	0.20	32,54,74,115	0
3	HSX	F	3002	14/14	0.77	0.14	48,66,82,97	0
4	GDP	F	3001	28/28	0.80	0.20	33,50,75,156	0
4	GDP	C	1004	28/28	0.80	0.20	27,52,88,96	0
2	APC	B	1001	31/31	0.81	0.16	48,63,89,115	0
2	APC	D	1001	31/31	0.82	0.11	43,53,87,88	0
2	APC	A	1005	31/31	0.82	0.13	33,57,97,122	0
2	APC	E	1001	31/31	0.83	0.11	43,65,92,110	0
5	PO4	D	1002	5/5	0.84	0.15	58,67,84,113	0
2	APC	C	1001	31/31	0.84	0.12	33,61,101,103	0
5	PO4	A	1006	5/5	0.85	0.27	43,54,65,113	0
5	PO4	B	1003	5/5	0.85	0.20	53,54,77,96	0
4	GDP	A	1003	28/28	0.86	0.16	23,45,73,89	0
5	PO4	F	3003	5/5	0.86	0.22	47,57,75,94	0
2	APC	A	1001	31/31	0.88	0.11	31,52,92,103	0
5	PO4	C	1005	5/5	0.90	0.30	46,52,95,101	0

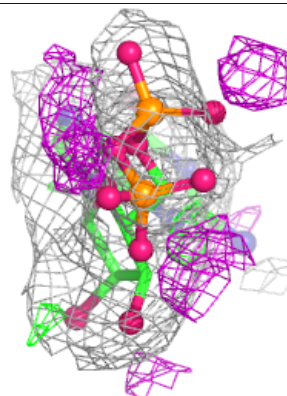
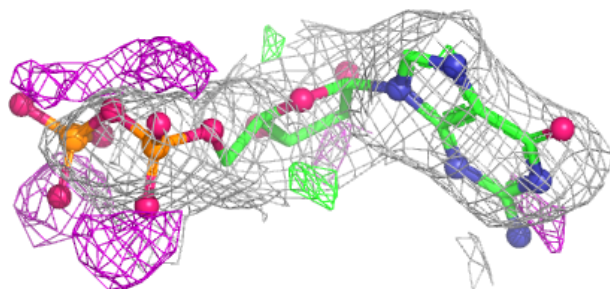
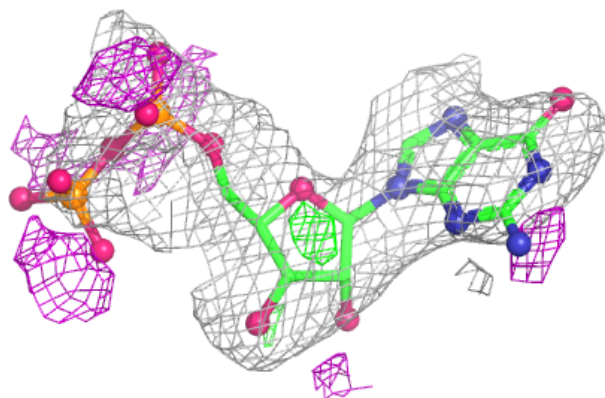
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDP C 1003:

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

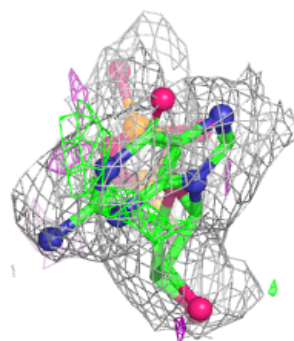
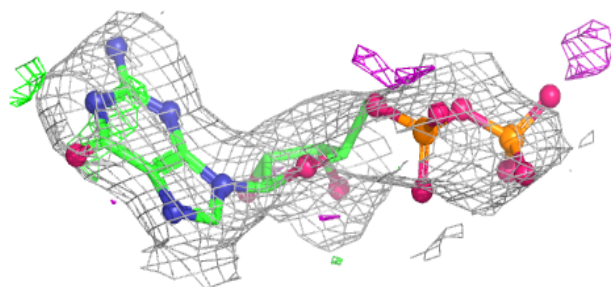
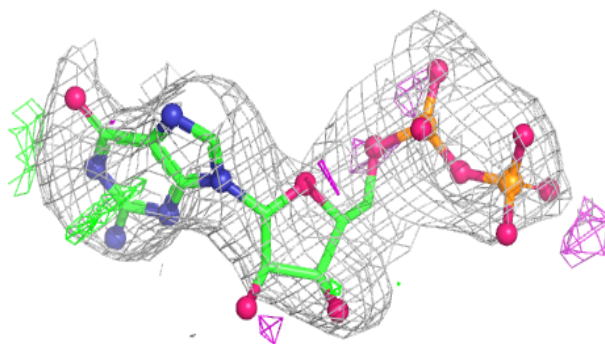
**Electron density around GDP E 1003:**

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

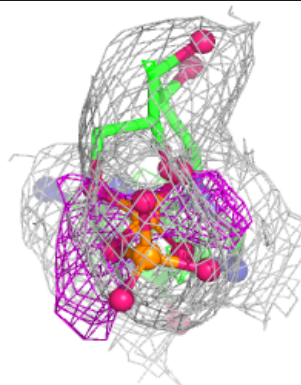
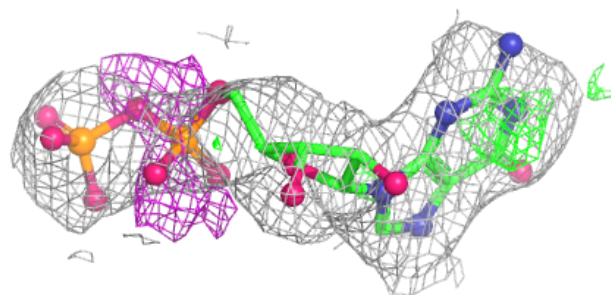
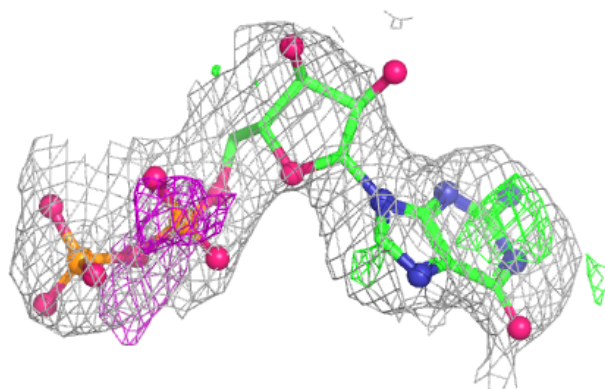


Electron density around GDP A 1004:

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

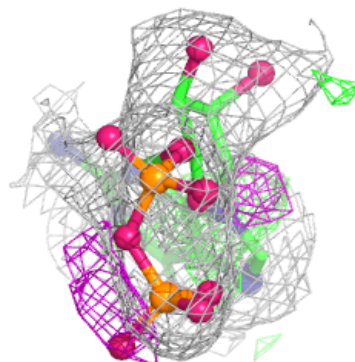
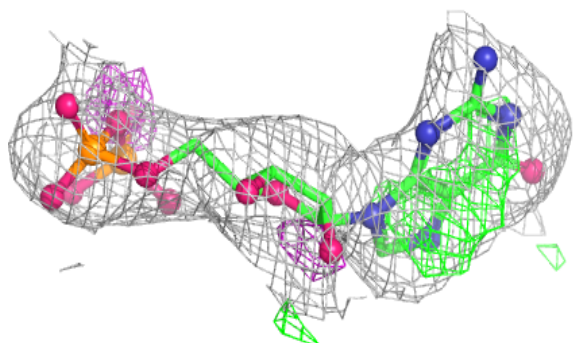
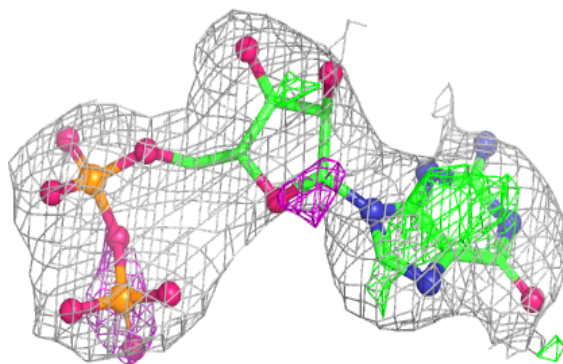
**Electron density around GDP F 3001:**

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

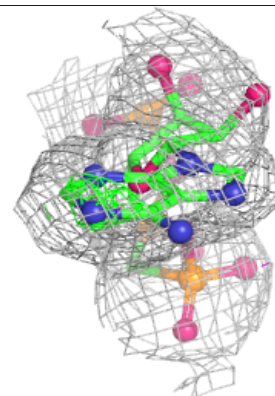
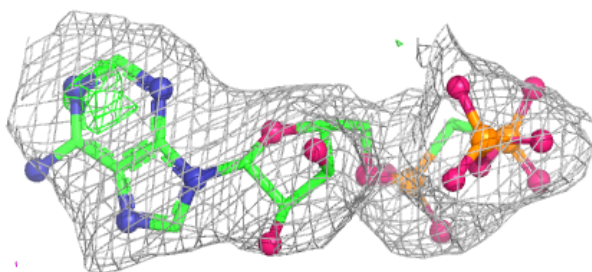
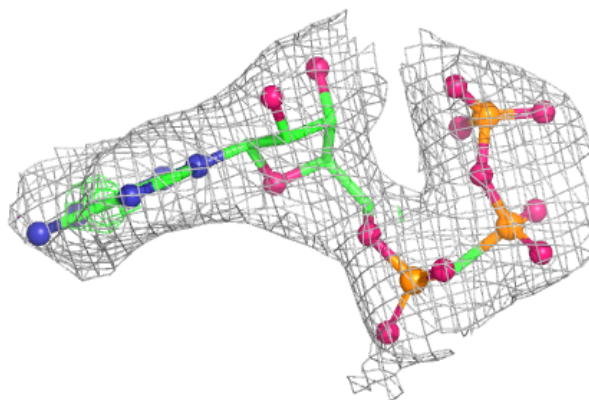


Electron density around GDP C 1004:

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

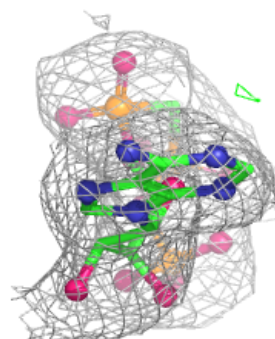
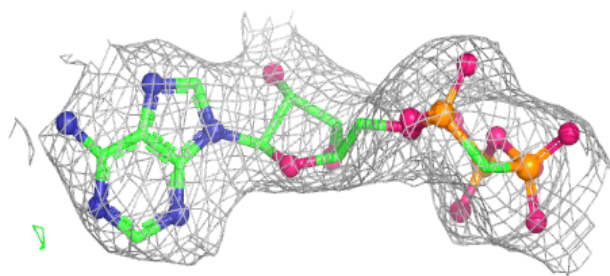
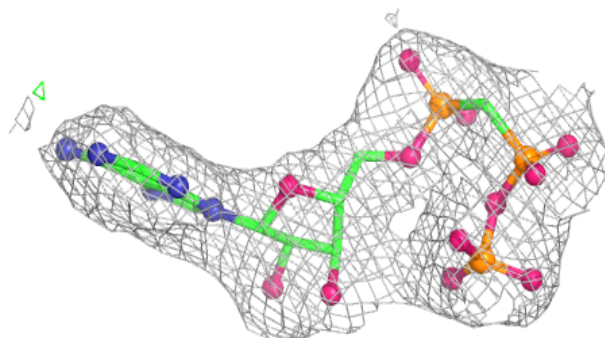
**Electron density around APC B 1001:**

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

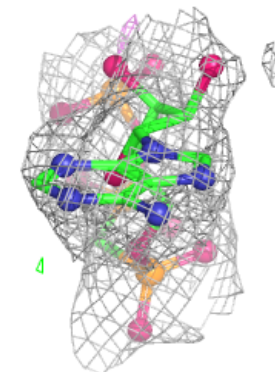
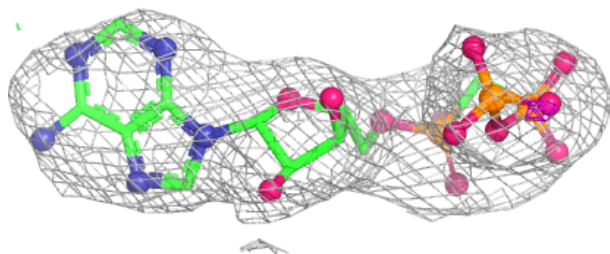
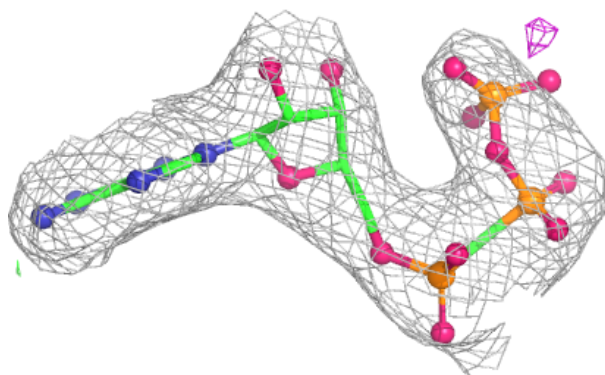


Electron density around APC D 1001:

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

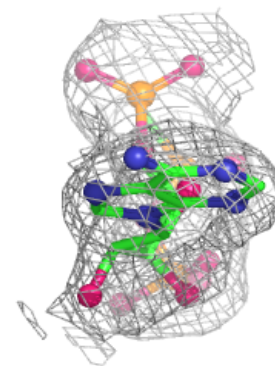
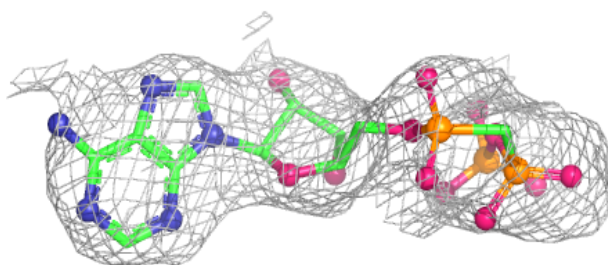
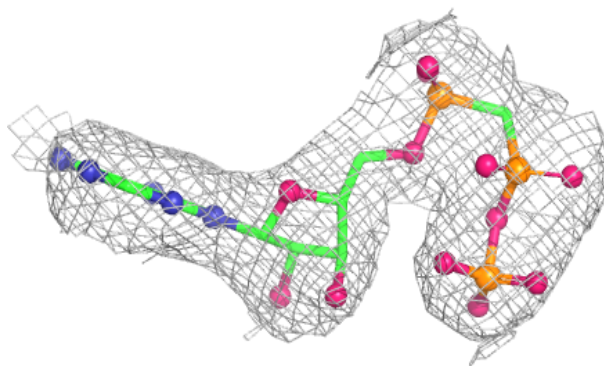
**Electron density around APC A 1005:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
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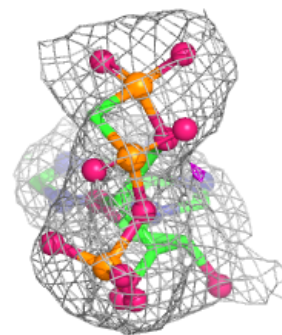
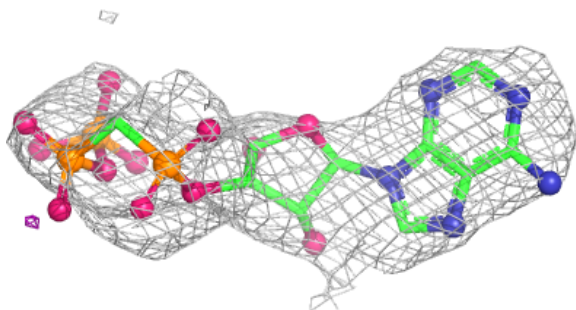
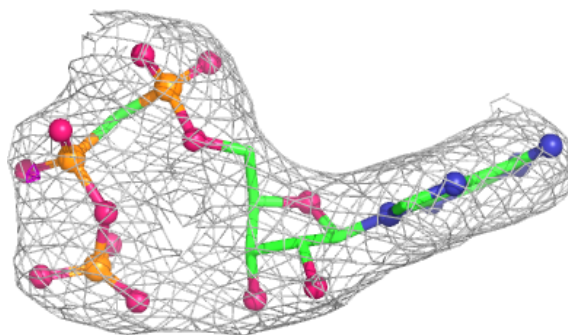


Electron density around APC E 1001:

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

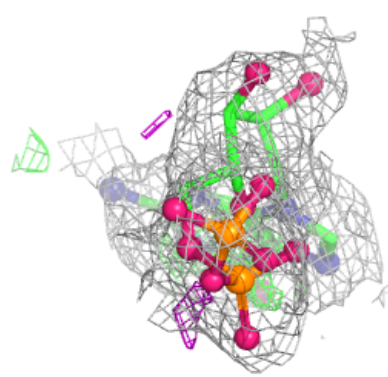
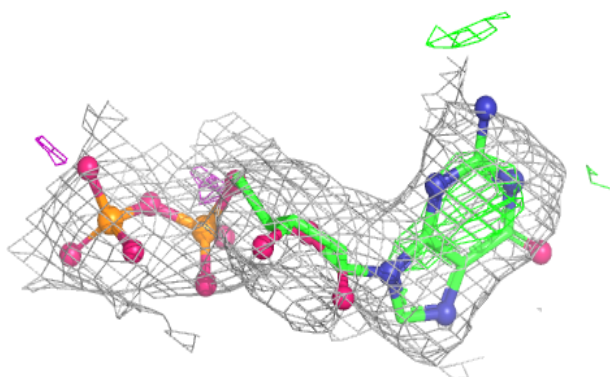
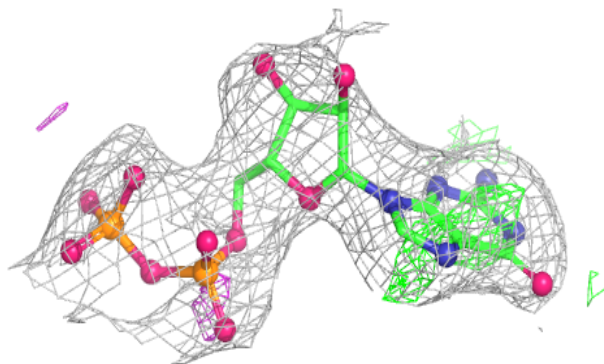
**Electron density around APC C 1001:**

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

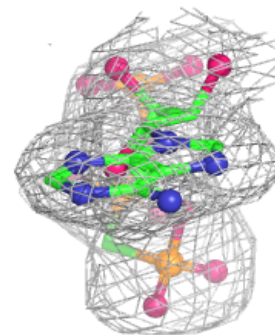
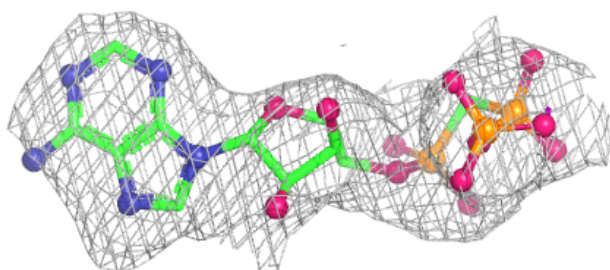
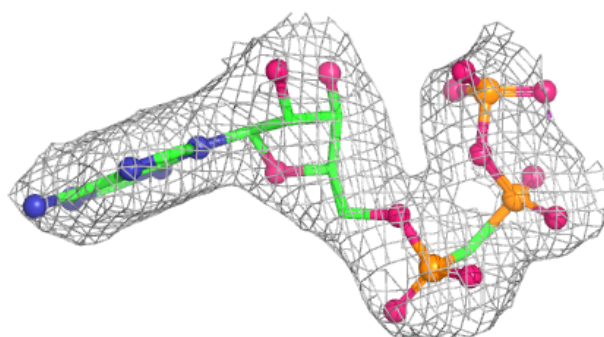


Electron density around GDP A 1003:

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

**Electron density around APC A 1001:**

$2mF_o-DF_c$ (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.