



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:29 AM UTC

PDB ID : 6AWG / pdb_00006awg
Title : Staphylococcus aureus Type II pantothenate kinase in complex with nucleotides and pantothenate analog Deoxy-N190Pan
Authors : Chen, Y.; Antoshchenko, T.; Strauss, E.; Barnard, L.; Huang, Y.H.
Deposited on : 2017-09-05
Resolution : 2.40 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 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

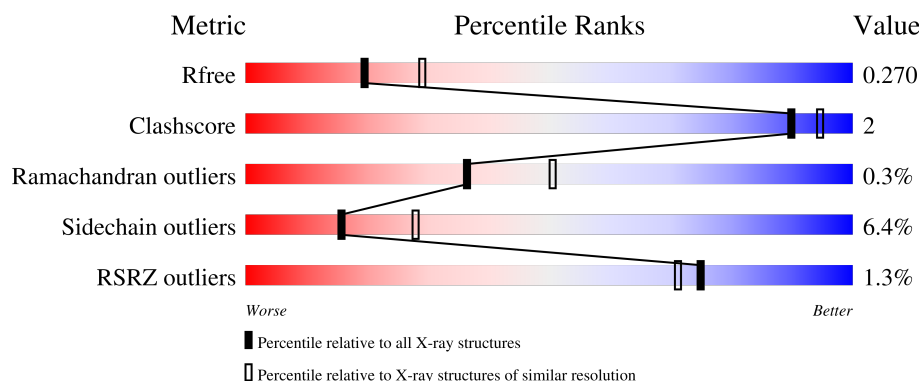
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	266	90% 10%
1	B	266	90% 9% .
1	C	266	3% 90% 9% .
1	D	266	88% 11% .

2 Entry composition [i](#)

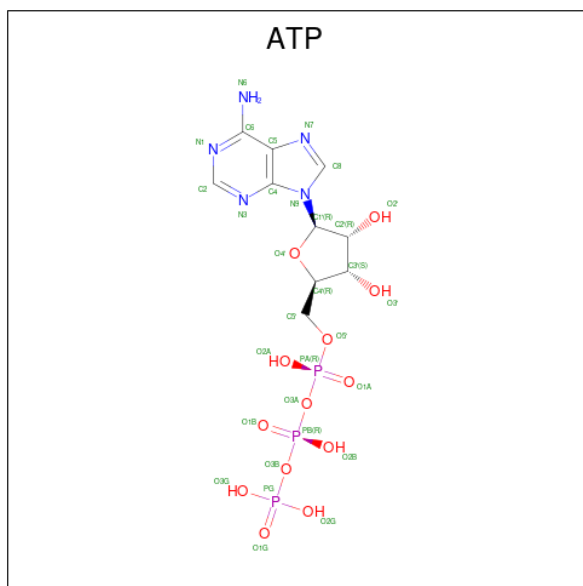
There are 5 unique types of molecules in this entry. The entry contains 8653 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Type II pantothenate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	0	0	0
			2041	1292	350	393	6			
1	B	265	Total	C	N	O	S	0	0	0
			2033	1288	348	391	6			
1	C	266	Total	C	N	O	S	0	0	0
			2041	1292	350	393	6			
1	D	264	Total	C	N	O	S	0	0	0
			2024	1283	347	388	6			

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

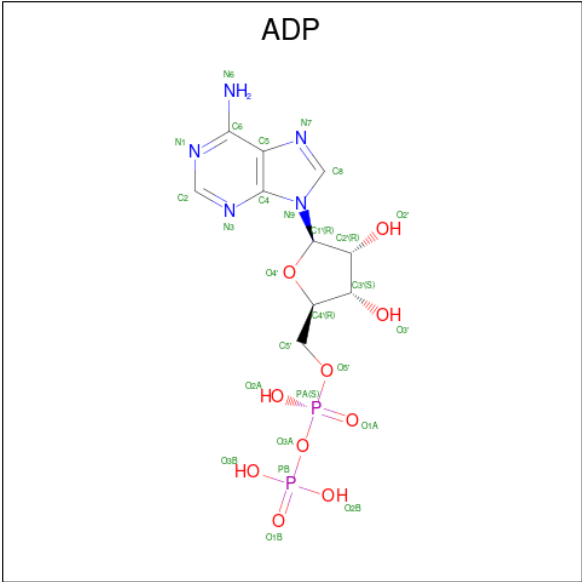


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

-
- Chemical structure of compound 10g, showing a complex molecule with a quaternary carbon, a hydroxyl group, two amide bonds, a benzene ring, and a furan ring. The structure is labeled with atom names (C01, C02, C03, C04, C05, C06, C07, C08, C09, C10, C11, C12, C13, C14, C15, C16, C17, C18, C19, C20, C21, C22, C23, C24, C25) and includes a legend for atom types (C, O, N, H).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 24	C 17	N 2	O 5	0	0
3	B	1	Total 24	C 17	N 2	O 5	0	0
3	C	1	Total 24	C 17	N 2	O 5	0	0
3	D	1	Total 24	C 17	N 2	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	88	Total	O	0	0
			88	88		
5	B	108	Total	O	0	0
			108	108		
5	C	50	Total	O	0	0
			50	50		
5	D	56	Total	O	0	0
			56	56		

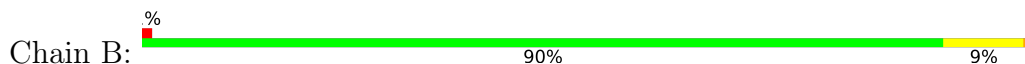
3 Residue-property plots [i](#)

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.

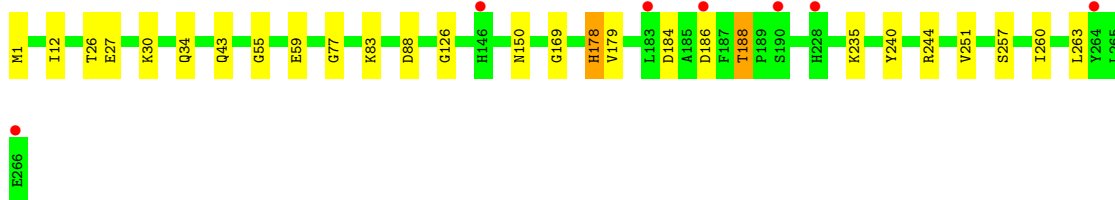
- Molecule 1: Type II pantothenate kinase



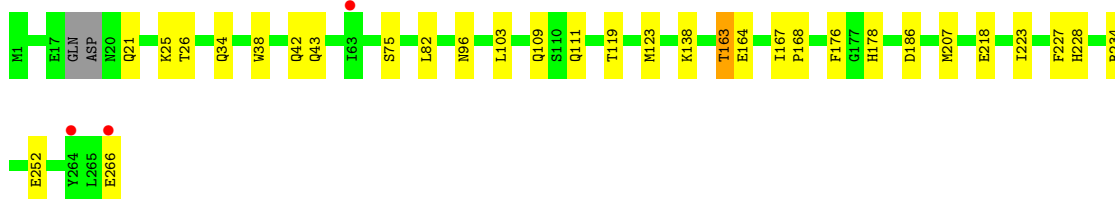
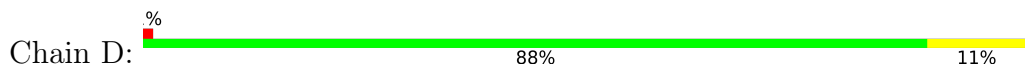
- Molecule 1: Type II pantothenate kinase



- Molecule 1: Type II pantothenate kinase



- Molecule 1: Type II pantothenate kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.65Å 57.17Å 134.54Å 90.00° 100.24° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 50.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.40) 99.8 (50.00-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.192 , 0.267 0.199 , 0.270	Depositor DCC
R_{free} test set	2168 reflections (2.13%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8653	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.47% 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: C0G, ADP, ATP

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	1.07	3/2076 (0.1%)	1.07	3/2813 (0.1%)
1	B	1.02	0/2067	1.15	5/2799 (0.2%)
1	C	0.91	0/2076	1.07	4/2813 (0.1%)
1	D	0.83	0/2058	1.02	0/2787
All	All	0.96	3/8277 (0.0%)	1.08	12/11212 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	23	THR	C-O	-5.66	1.17	1.24
1	A	159	ILE	C-O	-5.36	1.18	1.23
1	A	158	HIS	C-O	-5.30	1.17	1.24

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	186	ASP	N-CA-C	9.40	124.43	111.74
1	B	186	ASP	CA-C-N	-8.96	110.50	122.42
1	B	186	ASP	C-N-CA	-8.96	110.50	122.42
1	B	150	ASN	N-CA-C	6.80	119.53	111.71
1	A	185	ALA	N-CA-C	6.30	118.68	110.43
1	C	184	ASP	N-CA-C	-5.46	102.06	109.54
1	C	150	ASN	N-CA-C	5.34	117.51	111.11
1	B	8	GLY	N-CA-C	5.20	121.08	112.66
1	C	186	ASP	N-CA-C	-5.08	105.39	111.03
1	A	168	PRO	CA-C-N	5.01	126.41	120.14
1	A	168	PRO	C-N-CA	5.01	126.41	120.14
1	C	169	GLY	N-CA-C	5.01	119.94	113.27

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	2041	0	2027	10	0
1	B	2033	0	2020	4	0
1	C	2041	0	2027	8	0
1	D	2024	0	2014	10	0
2	A	31	0	12	1	0
2	C	31	0	12	0	0
3	A	24	0	0	0	0
3	B	24	0	0	0	0
3	C	24	0	0	0	0
3	D	24	0	0	0	0
4	B	27	0	12	0	0
4	D	27	0	12	0	0
5	A	88	0	0	3	0
5	B	108	0	0	2	0
5	C	50	0	0	2	0
5	D	56	0	0	1	0
All	All	8653	0	8136	30	0

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

All (30) 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:185:ALA:HB1	5:B:413:HOH:O	1.15	1.29
1:A:21:GLN:HG3	5:C:408:HOH:O	1.71	0.90
1:A:185:ALA:HB2	5:A:1185:HOH:O	1.85	0.77
1:D:228:HIS:HB3	5:D:453:HOH:O	2.02	0.59
1:C:55:GLY:O	1:C:59:GLU:HG2	2.03	0.59
1:B:185:ALA:CB	5:B:413:HOH:O	2.00	0.57
1:A:185:ALA:HB1	5:A:1184:HOH:O	2.04	0.57
1:D:227:PHE:O	1:D:234:ARG:NH1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:GLN:O	1:A:19:ASP:C	2.48	0.54
1:D:103:LEU:HD11	1:D:207:MET:HB3	1.90	0.53
1:C:188:THR:HG23	5:C:442:HOH:O	2.09	0.52
1:C:126:GLY:HA3	1:D:176:PHE:O	2.10	0.51
1:C:77:GLY:HA3	1:C:257:SER:O	2.14	0.47
1:C:260:ILE:O	1:C:263:LEU:HB2	2.14	0.47
1:B:18:GLN:O	1:B:21:GLN:HB2	2.14	0.46
2:A:1001:ATP:O3G	2:A:1001:ATP:O1B	2.33	0.45
1:D:38:TRP:O	1:D:42:GLN:HG2	2.17	0.45
1:A:126:GLY:HA3	1:B:176:PHE:O	2.18	0.44
1:D:119:THR:HG22	1:D:123:MET:SD	2.57	0.44
1:A:187:PHE:HA	5:A:1157:HOH:O	2.17	0.43
1:D:75:SER:HB2	1:D:111:GLN:HG2	2.00	0.43
1:D:167:ILE:HB	1:D:168:PRO:HD2	2.00	0.43
1:A:155:LYS:HE3	1:A:170:ASP:OD1	2.19	0.43
1:C:55:GLY:HA3	1:D:163:THR:HG21	1.99	0.42
1:A:143:MET:HG2	1:A:190:SER:OG	2.19	0.42
1:C:240:TYR:CZ	1:C:244:ARG:HD3	2.54	0.42
1:A:263:LEU:HD23	1:A:263:LEU:HA	1.93	0.42
1:A:77:GLY:HA3	1:A:257:SER:O	2.20	0.41
1:C:178:HIS:O	1:C:179:VAL:C	2.64	0.41
1:D:96:ASN:HA	1:D:223:ILE:HG13	2.03	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	264/266 (99%)	254 (96%)	10 (4%)	0	100	100
1	B	261/266 (98%)	253 (97%)	7 (3%)	1 (0%)	30	43
1	C	264/266 (99%)	251 (95%)	13 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	260/266 (98%)	249 (96%)	9 (4%)	2 (1%)	16	25
All	All	1049/1064 (99%)	1007 (96%)	39 (4%)	3 (0%)	36	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	21	GLN
1	D	186	ASP
1	B	185	ALA

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	216/216 (100%)	206 (95%)	10 (5%)	24	41
1	B	215/216 (100%)	196 (91%)	19 (9%)	9	15
1	C	216/216 (100%)	203 (94%)	13 (6%)	17	31
1	D	214/216 (99%)	201 (94%)	13 (6%)	17	30
All	All	861/864 (100%)	806 (94%)	55 (6%)	16	28

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	26	THR
1	A	34	GLN
1	A	46	LYS
1	A	59	GLU
1	A	112	ARG
1	A	178	HIS
1	A	186	ASP
1	A	251	VAL
1	A	266	GLU
1	B	22	ARG

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Mol	Chain	Res	Type
1	B	25	LYS
1	B	26	THR
1	B	30	LYS
1	B	41	GLN
1	B	43	GLN
1	B	46	LYS
1	B	83	LYS
1	B	133	GLN
1	B	143	MET
1	B	178	HIS
1	B	184	ASP
1	B	186	ASP
1	B	235	LYS
1	B	243	LEU
1	B	247	LYS
1	B	251	VAL
1	B	252	GLU
1	B	266	GLU
1	C	1	MET
1	C	12	ILE
1	C	26	THR
1	C	27	GLU
1	C	30	LYS
1	C	34	GLN
1	C	43	GLN
1	C	83	LYS
1	C	88	ASP
1	C	178	HIS
1	C	188	THR
1	C	235	LYS
1	C	251	VAL
1	D	25	LYS
1	D	26	THR
1	D	34	GLN
1	D	43	GLN
1	D	82	LEU
1	D	109	GLN
1	D	138	LYS
1	D	163	THR
1	D	164	GLU
1	D	178	HIS
1	D	218	GLU

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Mol	Chain	Res	Type
1	D	252	GLU
1	D	266	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	34	GLN
1	A	53	ASN
1	A	87	HIS
1	A	181	HIS
1	A	182	HIS
1	A	219	ASN
1	B	18	GLN
1	B	42	GLN
1	B	125	GLN
1	B	146	HIS
1	B	219	ASN
1	C	53	ASN
1	C	181	HIS
1	C	182	HIS
1	C	219	ASN
1	D	16	GLN
1	D	66	GLN
1	D	181	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 oligosaccharides 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$
3	C0G	C	302	-	24,25,25	1.45	3 (12%)	34,35,35	1.20	2 (5%)
4	ADP	D	301	-	28,29,29	1.52	5 (17%)	43,45,45	2.11	10 (23%)
2	ATP	A	1001	-	32,33,33	1.25	4 (12%)	48,52,52	2.25	13 (27%)
2	ATP	C	301	-	32,33,33	1.47	5 (15%)	48,52,52	1.95	11 (22%)
3	C0G	D	302	-	24,25,25	1.37	1 (4%)	34,35,35	1.00	1 (2%)
3	C0G	B	302	-	24,25,25	1.72	7 (29%)	34,35,35	1.18	3 (8%)
3	C0G	A	1002	-	24,25,25	1.47	2 (8%)	34,35,35	1.39	6 (17%)
4	ADP	B	301	-	28,29,29	1.40	4 (14%)	43,45,45	2.26	12 (27%)

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
3	C0G	C	302	-	-	0/21/27/27	0/2/2/2
4	ADP	D	301	-	-	2/16/32/32	0/3/3/3
2	ATP	A	1001	-	-	7/22/38/38	0/3/3/3
2	ATP	C	301	-	-	5/22/38/38	0/3/3/3
3	C0G	D	302	-	-	1/21/27/27	0/2/2/2
3	C0G	B	302	-	-	0/21/27/27	0/2/2/2
3	C0G	A	1002	-	-	0/21/27/27	0/2/2/2
4	ADP	B	301	-	-	4/16/32/32	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	ATP	PB-O3B	4.64	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	301	ADP	PA-O3A	4.46	1.64	1.59
3	C	302	C0G	C12-C13	-4.36	1.41	1.51
3	B	302	C0G	C12-C13	-3.94	1.42	1.51
4	D	301	ADP	C5-C4	3.90	1.46	1.39
2	C	301	ATP	C5-C4	3.86	1.46	1.39
3	B	302	C0G	C15-C16	-3.76	1.31	1.39
2	A	1001	ATP	C5-N7	-3.66	1.32	1.39
4	B	301	ADP	C5-C4	3.66	1.45	1.39
3	A	1002	C0G	C15-C16	-3.66	1.32	1.39
3	A	1002	C0G	C12-C13	-3.53	1.43	1.51
3	B	302	C0G	C03-C05	3.43	1.57	1.55
3	D	302	C0G	C12-C13	-3.40	1.43	1.51
4	B	301	ADP	PA-O3A	3.29	1.63	1.59
3	C	302	C0G	C15-C16	-2.60	1.34	1.39
2	C	301	ATP	C5-N7	-2.55	1.34	1.39
4	D	301	ADP	C5-N7	-2.53	1.34	1.39
3	B	302	C0G	C21-C17	-2.49	1.34	1.38
3	B	302	C0G	O24-C05	2.46	1.46	1.42
4	D	301	ADP	C5-C6	2.42	1.47	1.41
3	B	302	C0G	O20-C16	-2.40	1.34	1.38
4	B	301	ADP	C5-N7	-2.33	1.34	1.39
2	C	301	ATP	C5-C6	2.29	1.47	1.41
2	A	1001	ATP	C4-N9	-2.22	1.33	1.37
2	A	1001	ATP	PG-O1G	2.18	1.57	1.50
4	B	301	ADP	C4-N3	2.18	1.38	1.34
2	C	301	ATP	C4-N9	-2.14	1.33	1.37
4	D	301	ADP	C4-N9	-2.12	1.33	1.37
2	A	1001	ATP	C5-C4	2.07	1.42	1.39
3	B	302	C0G	C16-C17	-2.05	1.34	1.39
3	C	302	C0G	C09-C10	2.05	1.55	1.51

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	301	ADP	C5-C4-N3	-7.10	116.94	126.72
4	B	301	ADP	C5-C4-N3	-6.88	117.25	126.72
2	A	1001	ATP	C5-C4-N3	-6.80	117.36	126.72
4	B	301	ADP	N3-C4-N9	6.32	137.92	127.17
2	C	301	ATP	C5-C4-N3	-5.97	118.50	126.72
2	A	1001	ATP	N3-C4-N9	5.85	137.11	127.17
4	D	301	ADP	N3-C4-N9	5.52	136.56	127.17
4	B	301	ADP	N3-C2-N1	-5.46	120.31	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	ATP	C2-N3-C4	5.07	124.21	111.83
2	C	301	ATP	N3-C4-N9	5.04	135.73	127.17
4	B	301	ADP	C2-N3-C4	4.92	123.84	111.83
2	A	1001	ATP	N3-C2-N1	-4.80	121.32	128.58
4	D	301	ADP	C2-N3-C4	4.80	123.55	111.83
2	C	301	ATP	C2-N3-C4	4.51	122.84	111.83
2	C	301	ATP	N3-C2-N1	-4.49	121.78	128.58
4	D	301	ADP	N3-C2-N1	-4.36	121.98	128.58
2	A	1001	ATP	N9-C8-N7	-3.76	108.61	113.94
3	A	1002	C0G	C08-C09-C10	-3.67	106.27	112.39
2	A	1001	ATP	O2A-PA-O3A	3.65	117.15	107.27
2	A	1001	ATP	C4-N9-C8	3.63	109.55	105.74
3	A	1002	C0G	C12-C13-C21	3.61	128.35	120.63
4	B	301	ADP	C4-N9-C8	3.59	109.51	105.74
2	A	1001	ATP	C5-N7-C8	3.54	109.01	103.45
4	D	301	ADP	C4-C5-N7	-3.17	106.96	110.58
2	C	301	ATP	O3G-PG-O2G	3.13	119.54	107.80
4	B	301	ADP	O2A-PA-O3A	3.03	115.46	107.27
2	A	1001	ATP	C4-C5-N7	-2.88	107.29	110.58
2	C	301	ATP	C4-N9-C8	2.79	108.67	105.74
2	A	1001	ATP	O2G-PG-O1G	2.77	121.61	110.83
3	B	302	C0G	O24-C05-C03	2.70	114.16	109.38
4	B	301	ADP	C1'-N9-C8	-2.67	121.17	127.09
4	D	301	ADP	C1'-N9-C8	-2.65	121.22	127.09
3	C	302	C0G	C08-C09-C10	-2.61	108.05	112.39
2	C	301	ATP	C4-C5-N7	-2.55	107.67	110.58
3	A	1002	C0G	O20-C16-C17	2.51	112.83	109.79
2	C	301	ATP	O2A-PA-O1A	2.50	124.07	112.44
3	D	302	C0G	C12-C13-C21	2.46	125.88	120.63
4	B	301	ADP	N9-C8-N7	-2.45	110.45	113.94
2	A	1001	ATP	O2B-PB-O1B	2.43	123.74	112.44
2	C	301	ATP	C6-C5-N7	2.43	136.77	132.09
3	C	302	C0G	C12-C13-C21	2.41	125.77	120.63
4	B	301	ADP	C5-N7-C8	2.40	107.23	103.45
3	B	302	C0G	C08-C09-C10	-2.37	108.44	112.39
3	A	1002	C0G	C14-C13-C21	-2.37	115.28	118.55
4	B	301	ADP	C5-C6-N6	-2.32	117.55	123.29
4	B	301	ADP	C4-C5-N7	-2.30	107.95	110.58
4	D	301	ADP	C5-N7-C8	2.30	107.06	103.45
3	A	1002	C0G	C12-C13-C14	-2.29	116.25	120.94
2	A	1001	ATP	C6-C5-N7	2.29	136.50	132.09
2	A	1001	ATP	C5-C6-N6	-2.24	117.75	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	C0G	O22-C10-C09	-2.23	117.98	122.02
4	D	301	ADP	C2'-C1'-N9	2.23	118.84	113.30
3	A	1002	C0G	C19-O20-C16	-2.18	102.39	105.32
4	D	301	ADP	C6-C5-N7	2.18	136.29	132.09
2	C	301	ATP	C5-N7-C8	2.13	106.80	103.45
4	D	301	ADP	C4-N9-C8	2.06	107.91	105.74
4	B	301	ADP	C6-C5-N7	2.04	136.03	132.09
2	C	301	ATP	N9-C8-N7	-2.01	111.09	113.94

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	ATP	PB-O3B-PG-O3G
2	A	1001	ATP	C5'-O5'-PA-O2A
4	B	301	ADP	C2'-C1'-N9-C4
4	D	301	ADP	C2'-C1'-N9-C4
4	D	301	ADP	C2'-C1'-N9-C8
4	B	301	ADP	C2'-C1'-N9-C8
2	A	1001	ATP	C2'-C1'-N9-C4
2	C	301	ATP	C2'-C1'-N9-C4
2	A	1001	ATP	C2'-C1'-N9-C8
2	C	301	ATP	C2'-C1'-N9-C8
2	A	1001	ATP	PG-O3B-PB-O1B
2	C	301	ATP	PG-O3B-PB-O2B
4	B	301	ADP	PB-O3A-PA-O2A
2	C	301	ATP	PB-O3B-PG-O2G
3	D	302	C0G	C08-C09-C10-O22
2	A	1001	ATP	PG-O3B-PB-O2B
2	A	1001	ATP	PB-O3B-PG-O1G
2	C	301	ATP	PG-O3B-PB-O1B
4	B	301	ADP	PB-O3A-PA-O1A

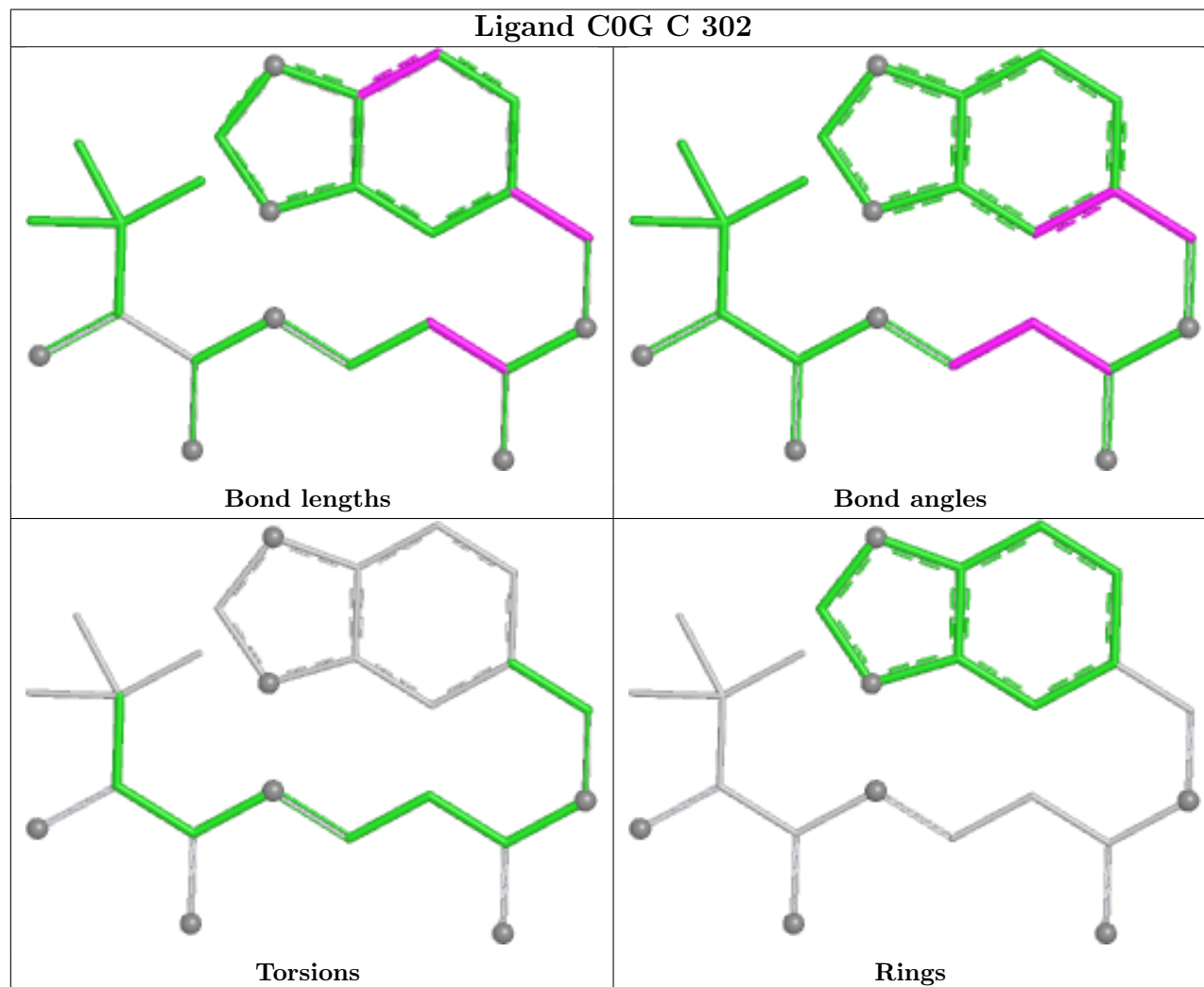
There are no ring outliers.

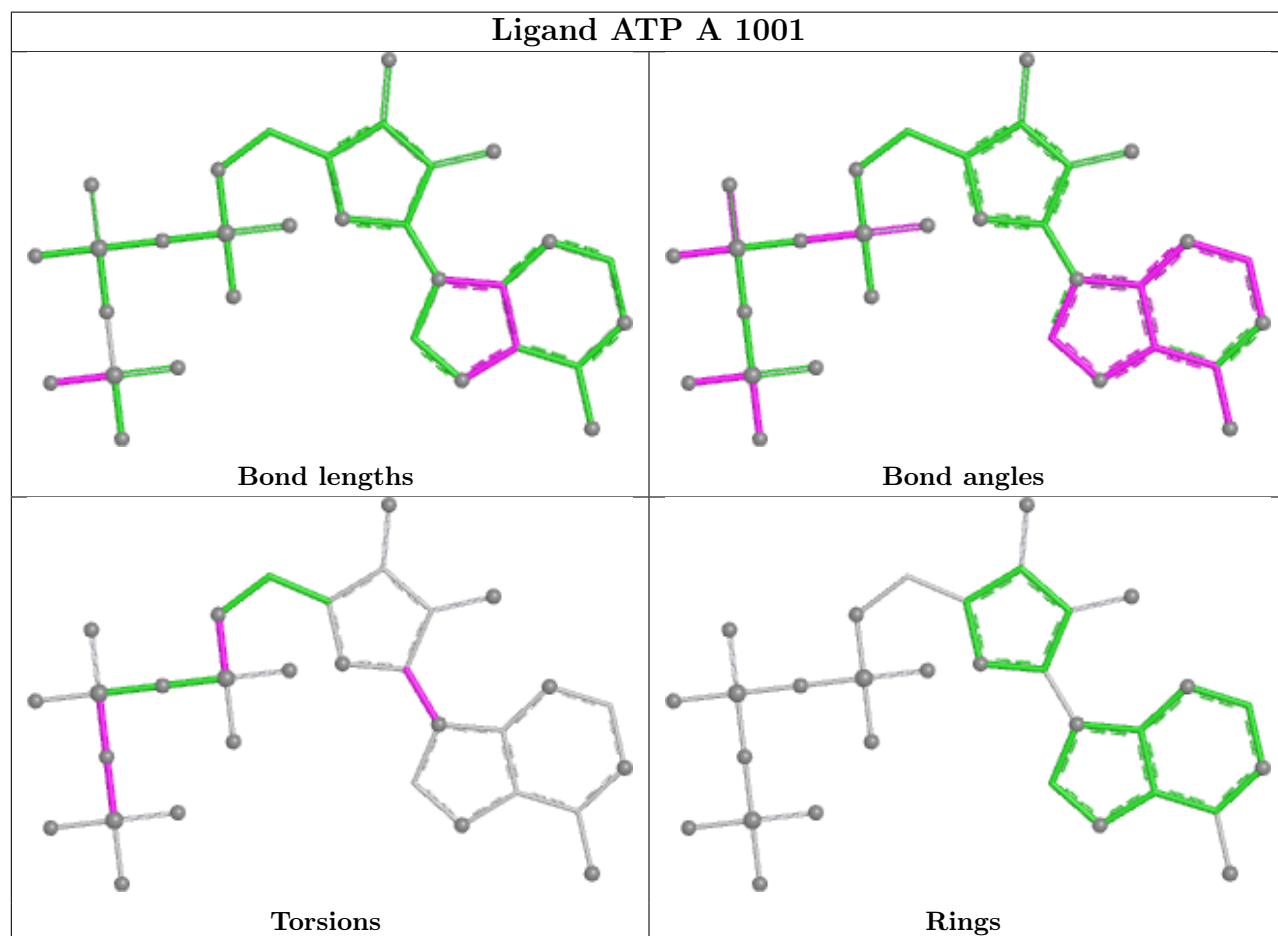
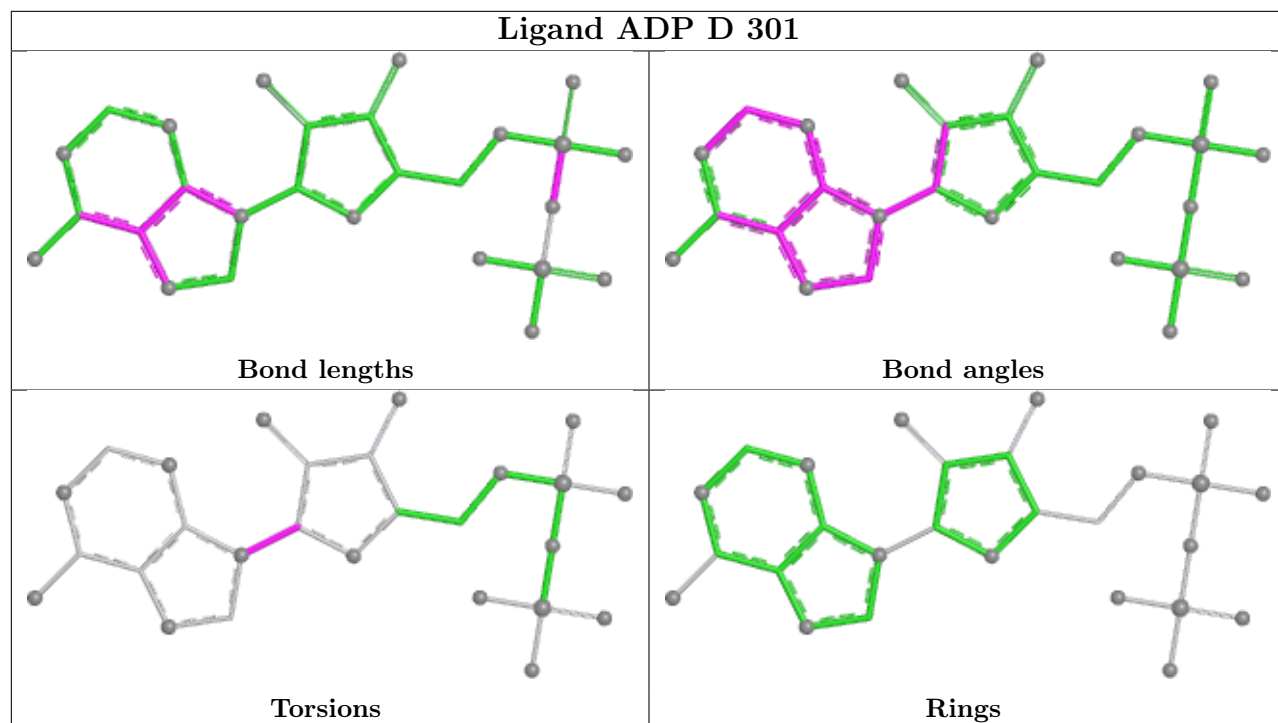
1 monomer is involved in 1 short contact:

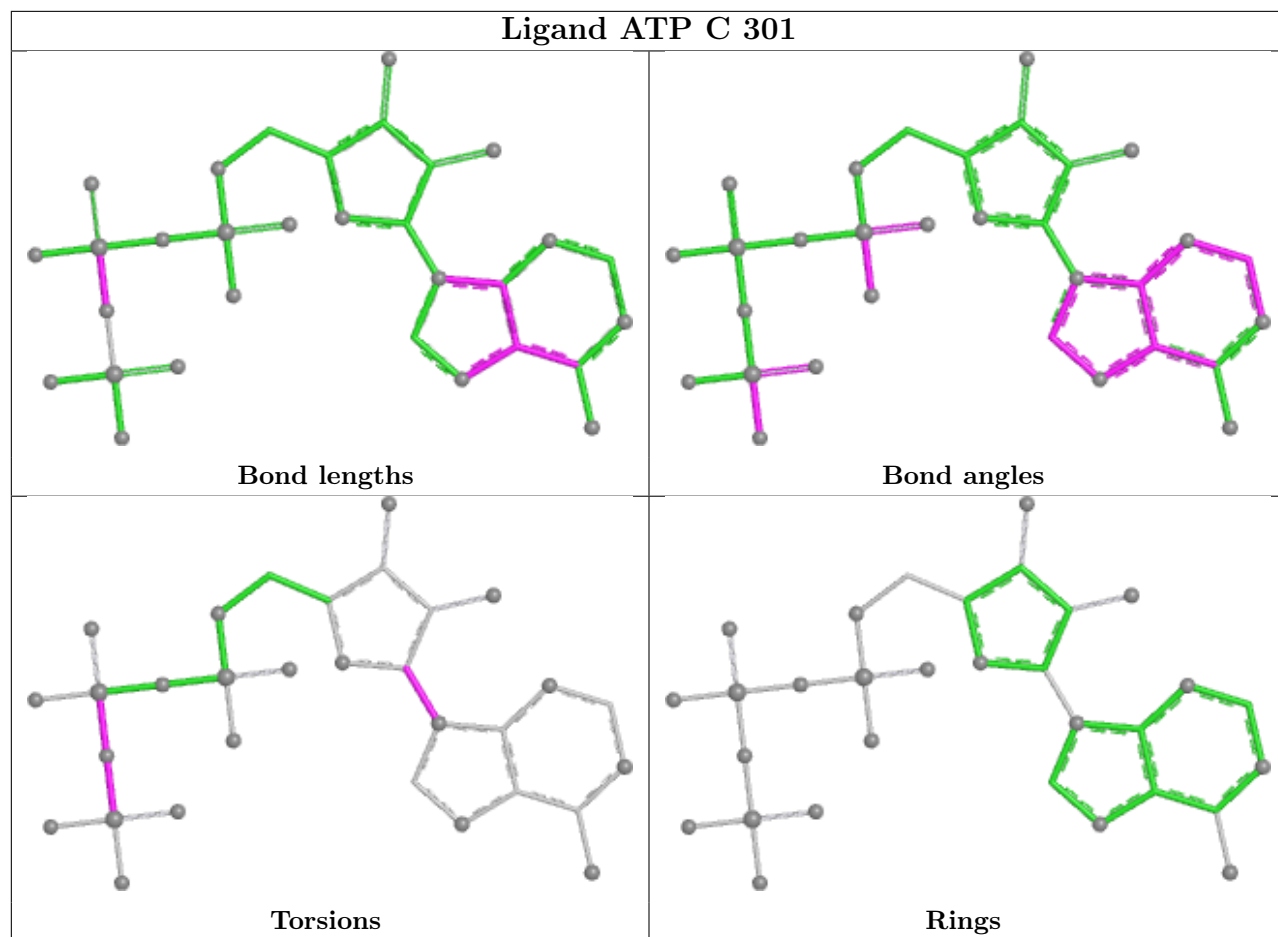
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	ATP	1	0

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

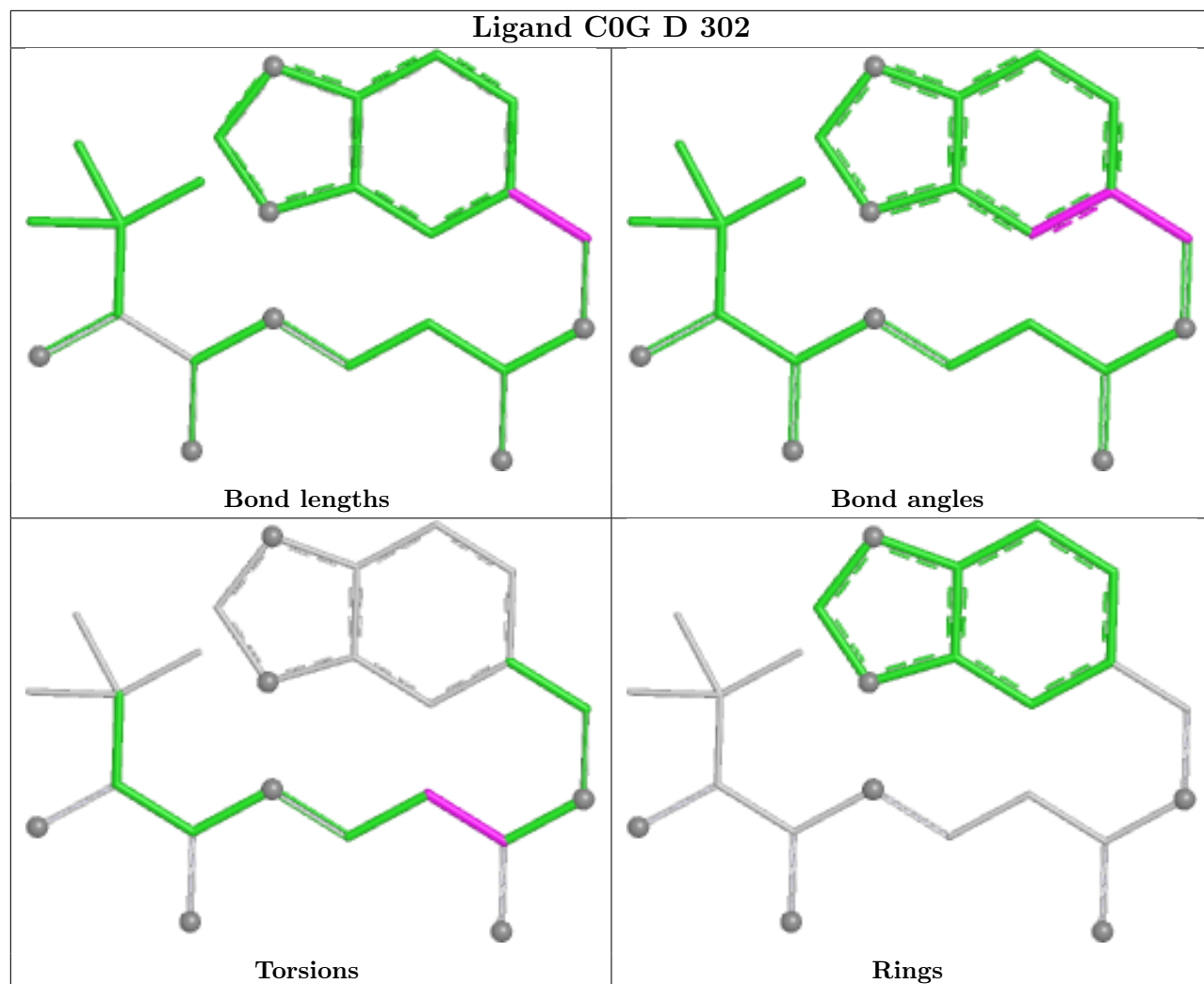
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

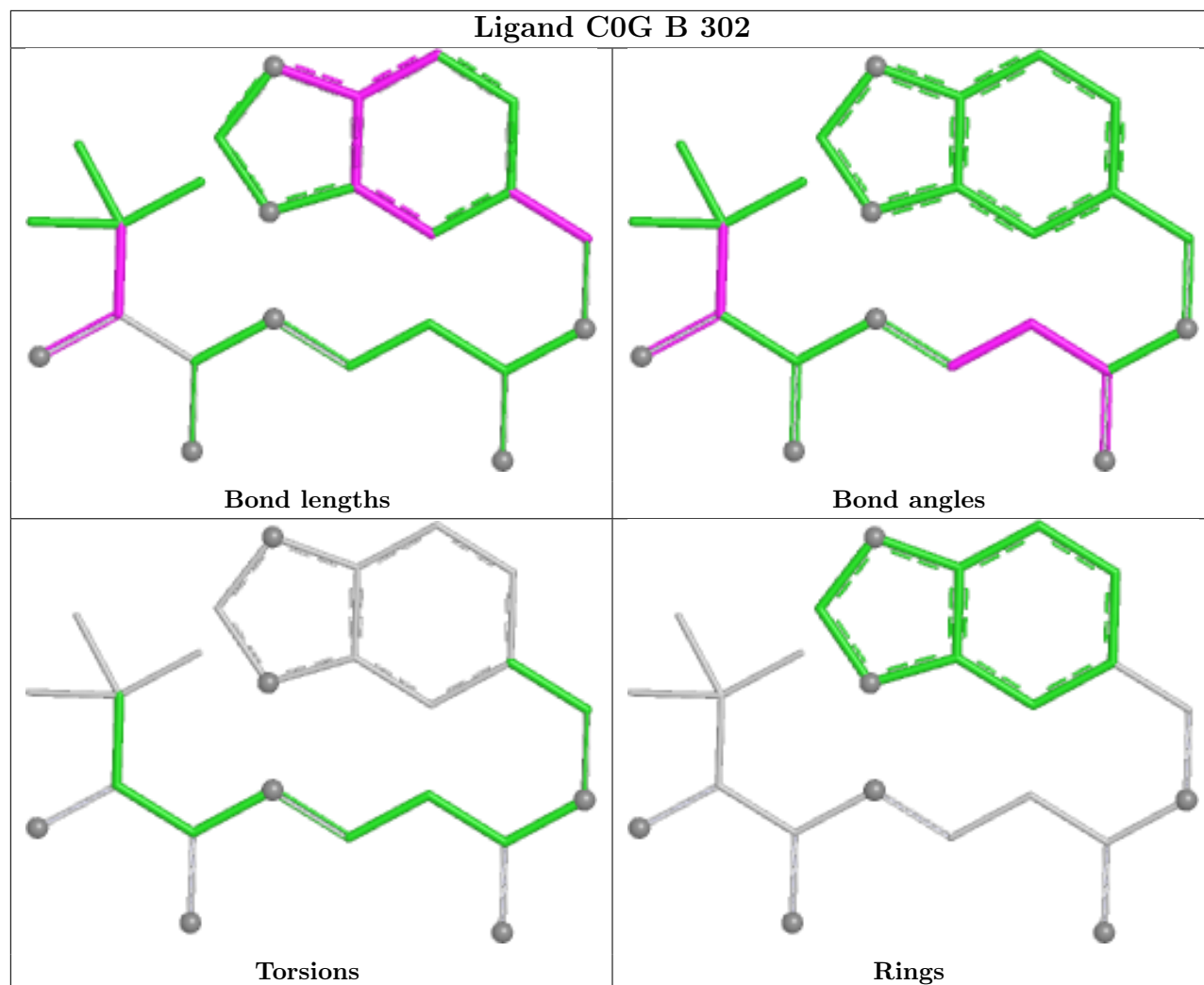


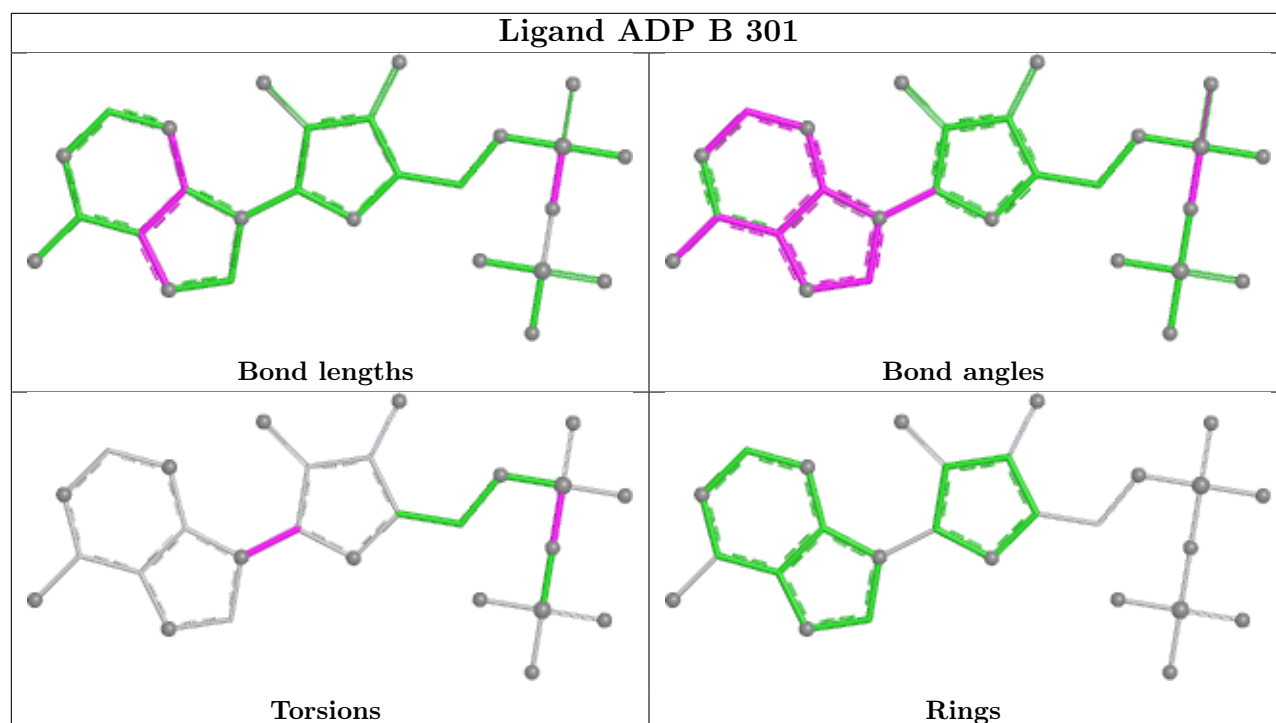
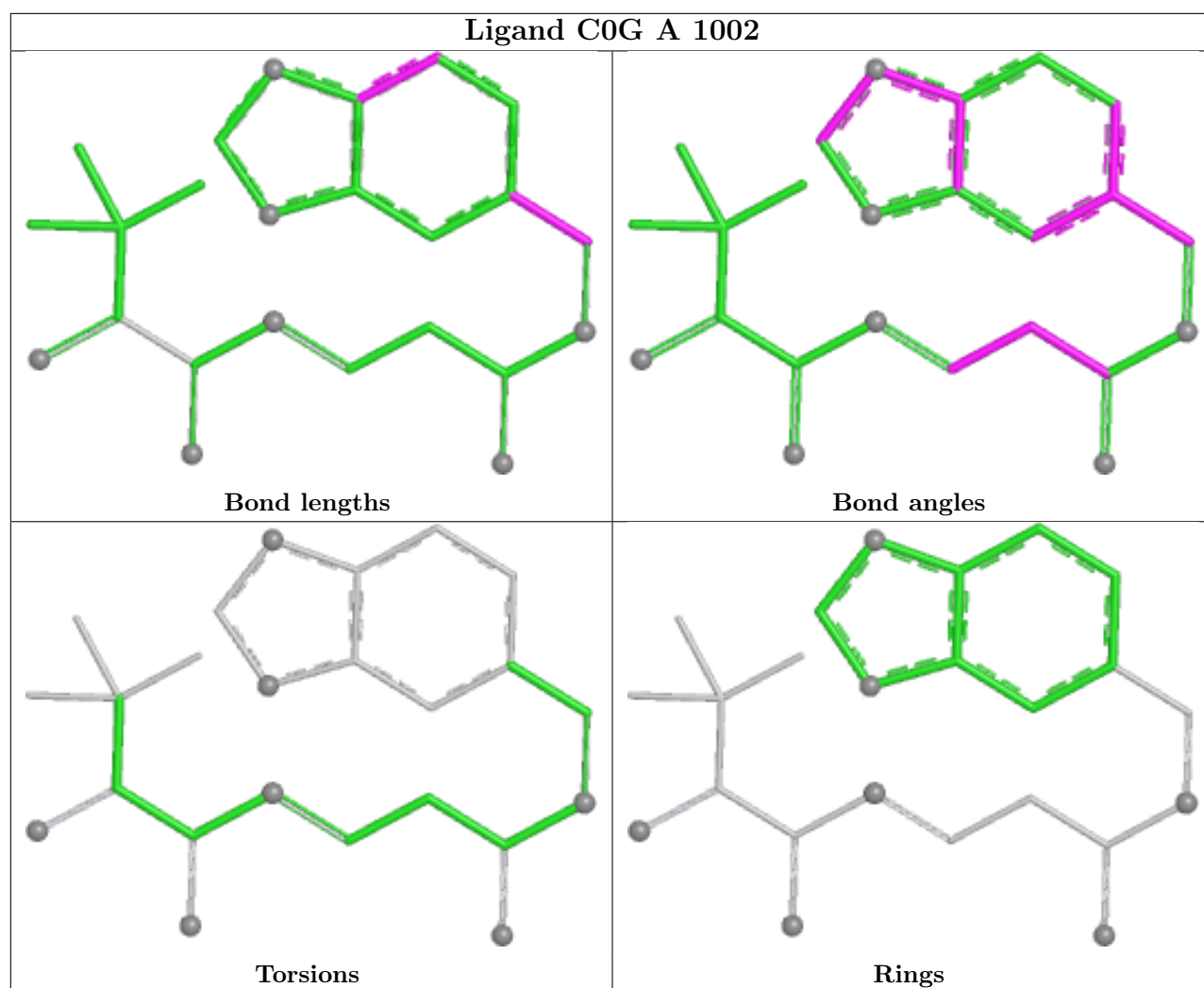




Ligand C0G D 302







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(Å ²)	Q<0.9
1	A	266/266 (100%)	-0.15	2 (0%) 82 80	14, 25, 49, 79	0
1	B	265/266 (99%)	-0.25	2 (0%) 82 80	12, 22, 46, 73	0
1	C	266/266 (100%)	0.29	7 (2%) 57 53	21, 36, 61, 85	0
1	D	264/266 (99%)	0.17	3 (1%) 78 74	19, 36, 75, 94	0
All	All	1061/1064 (99%)	0.02	14 (1%) 75 71	12, 30, 63, 94	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	146	HIS	4.0
1	B	185	ALA	3.5
1	D	264	TYR	3.4
1	D	63	ILE	3.3
1	C	264	TYR	3.3
1	A	264	TYR	3.0
1	C	183	LEU	2.9
1	C	190	SER	2.8
1	B	186	ASP	2.6
1	A	59	GLU	2.5
1	C	186	ASP	2.5
1	C	228	HIS	2.4
1	C	266	GLU	2.4
1	D	266	GLU	2.3

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 [i](#)

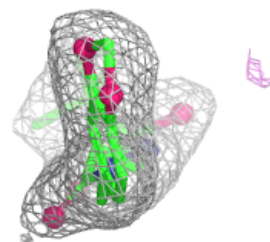
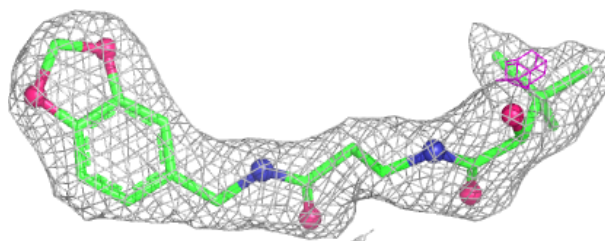
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	C0G	C	302	24/24	0.93	0.08	28,30,33,34	0
2	ATP	C	301	31/31	0.94	0.08	24,34,38,44	3
3	C0G	A	1002	24/24	0.96	0.07	19,22,24,25	0
2	ATP	A	1001	31/31	0.96	0.07	19,24,28,30	3
3	C0G	D	302	24/24	0.96	0.07	21,23,25,25	0
3	C0G	B	302	24/24	0.97	0.06	13,18,21,21	0
4	ADP	D	301	27/27	0.97	0.06	23,27,33,36	0
4	ADP	B	301	27/27	0.98	0.05	17,18,20,20	0

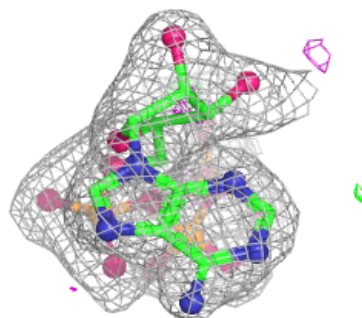
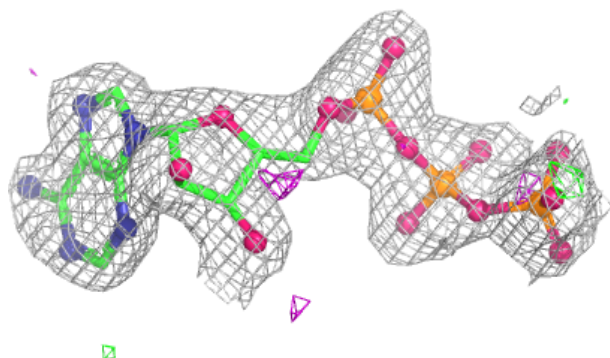
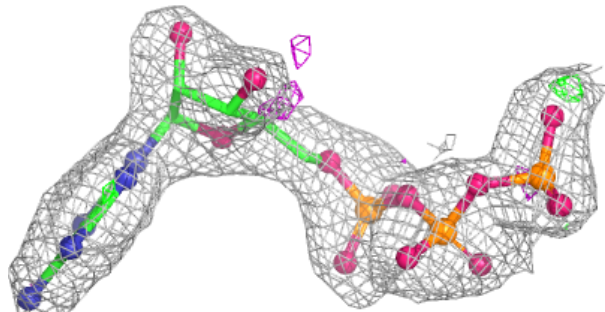
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around C0G C 302:

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

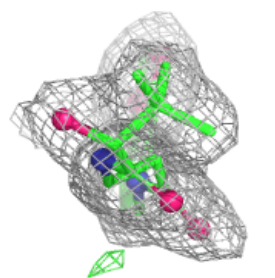
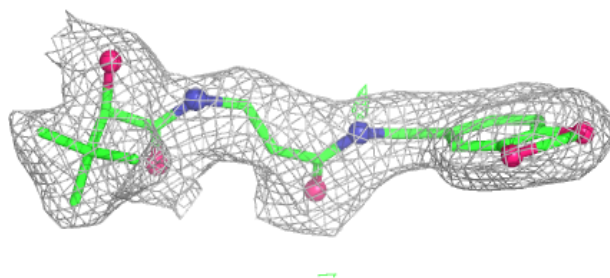
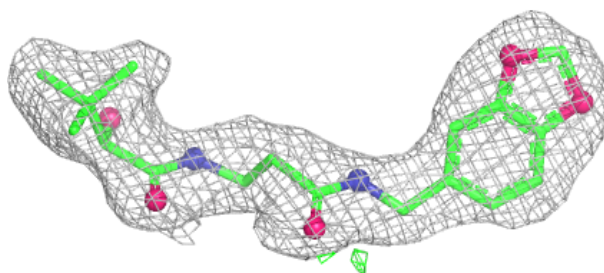
**Electron density around ATP C 301:**

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and green (positive)

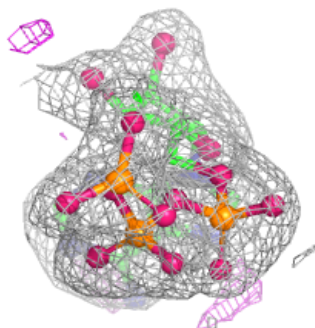
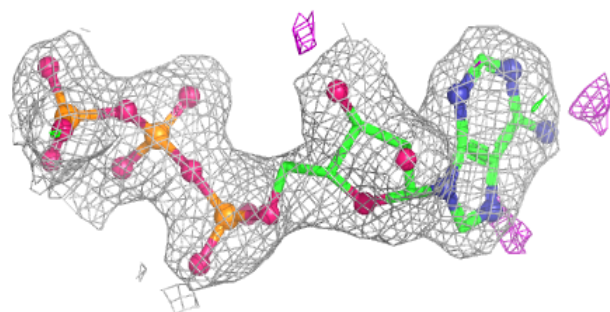
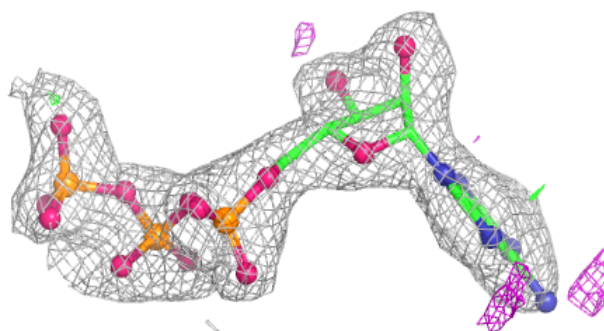


Electron density around C0G A 1002:

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

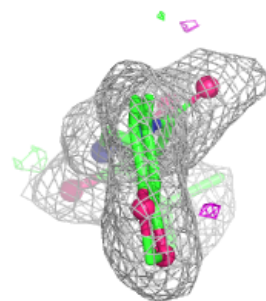
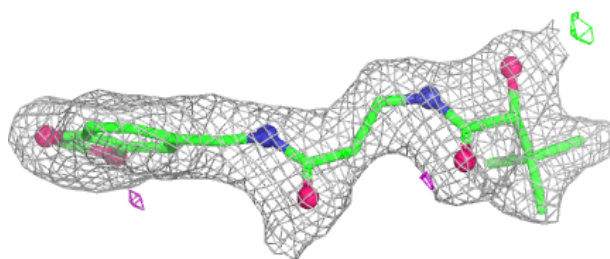
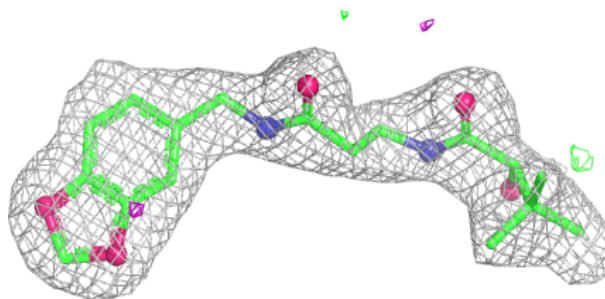
**Electron density around ATP A 1001:**

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

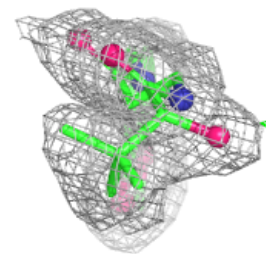
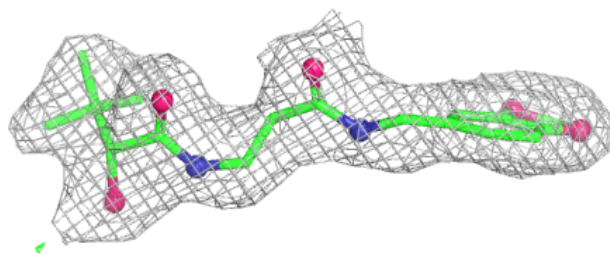
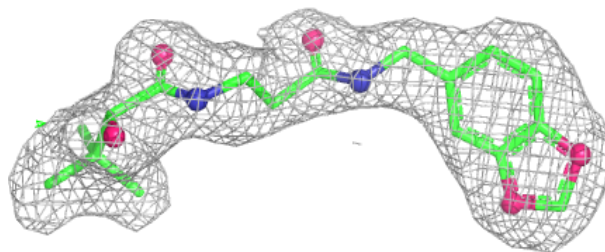


Electron density around C0G D 302:

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

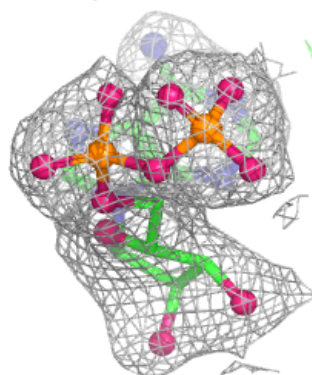
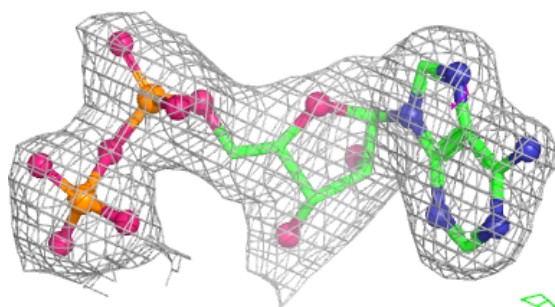
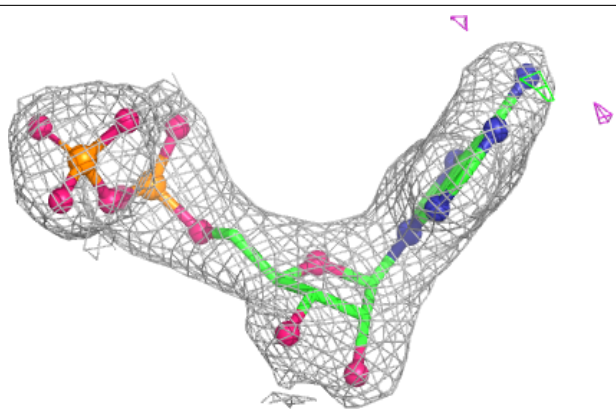
**Electron density around C0G B 302:**

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

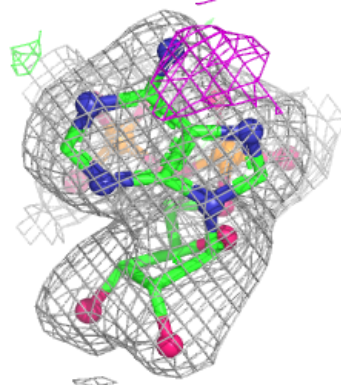
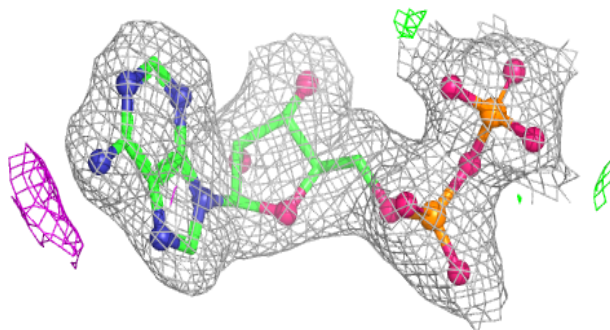
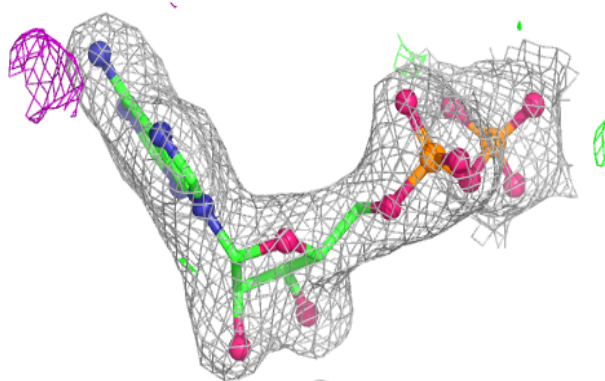


Electron density around ADP D 301:

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

**Electron density around ADP B 301:**

$2mF_o-DF_c$ (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.