



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:54 PM UTC

PDB ID : 8BV3 / pdb_00008bv3
Title : Bacillus subtilis DnaA domain III structure
Authors : Pintar, S.; Hubbard, J.A.
Deposited on : 2022-12-01
Resolution : 2.38 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

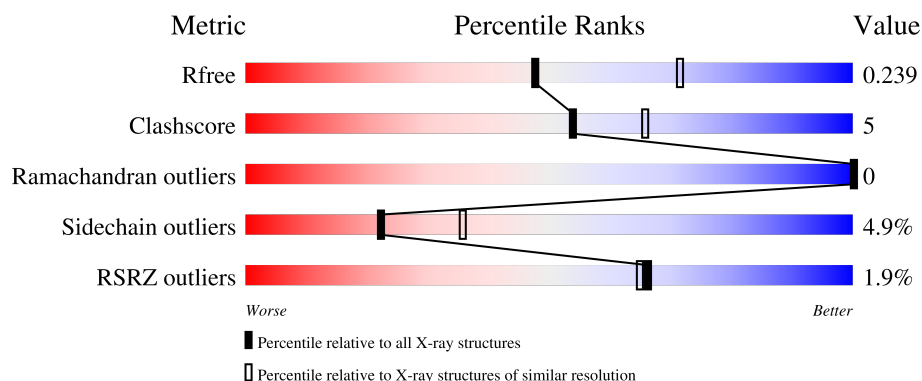
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	243	2% 83% 13% ..
1	B	243	3% 74% 21% ..
1	C	243	81% 16% .
1	D	243	% 81% 14% ..
1	E	243	2% 81% 14% ..

2 Entry composition [i](#)

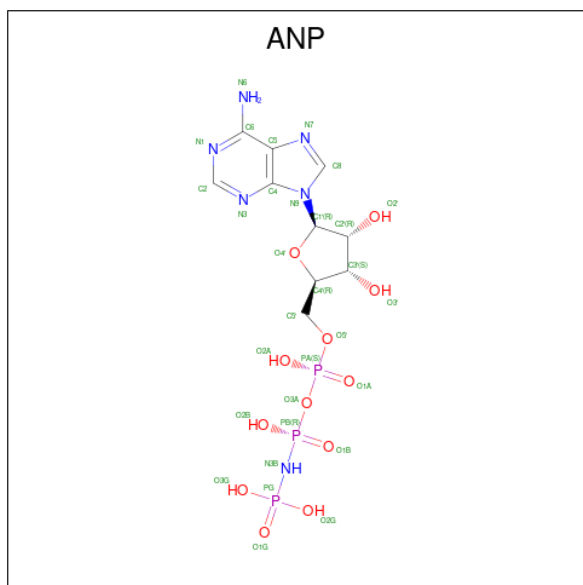
There are 5 unique types of molecules in this entry. The entry contains 9656 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Chromosomal replication initiator protein DnaA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	235	Total	C	N	O	S	0	0	0
			1873	1194	323	353	3			
1	B	235	Total	C	N	O	S	0	0	0
			1873	1194	323	353	3			
1	C	235	Total	C	N	O	S	0	0	0
			1873	1194	323	353	3			
1	D	235	Total	C	N	O	S	0	0	0
			1873	1194	323	353	3			
1	E	235	Total	C	N	O	S	0	0	0
			1873	1194	323	353	3			

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	K	0	0
			1	1		
3	B	2	Total	K	0	0
			2	2		
3	C	3	Total	K	0	0
			3	3		
3	D	2	Total	K	0	0
			2	2		
3	E	1	Total	K	0	0
			1	1		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		

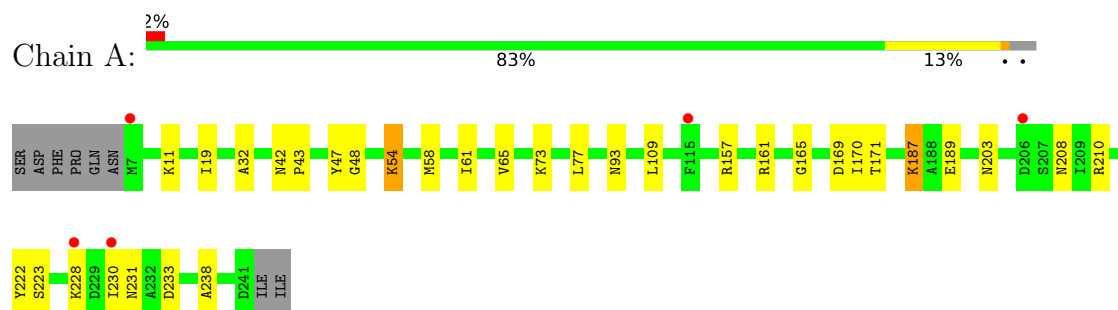
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	14	Total 14	O 14	0	0
5	B	29	Total 29	O 29	0	0
5	C	36	Total 36	O 36	0	0
5	D	29	Total 29	O 29	0	0
5	E	14	Total 14	O 14	0	0

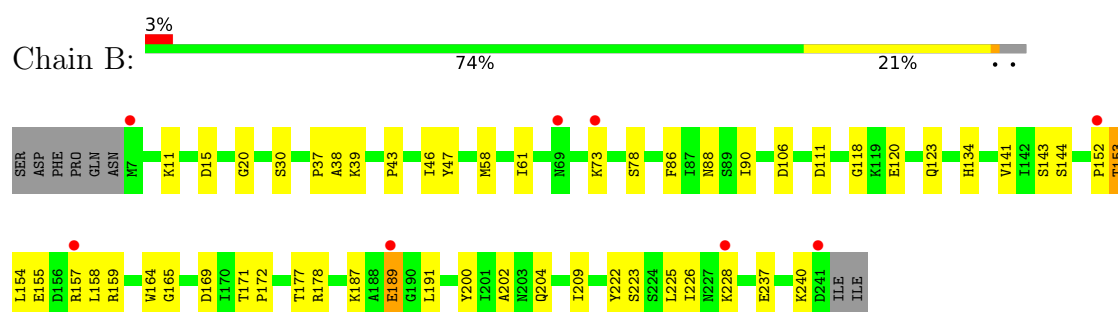
3 Residue-property plots [i](#)

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.

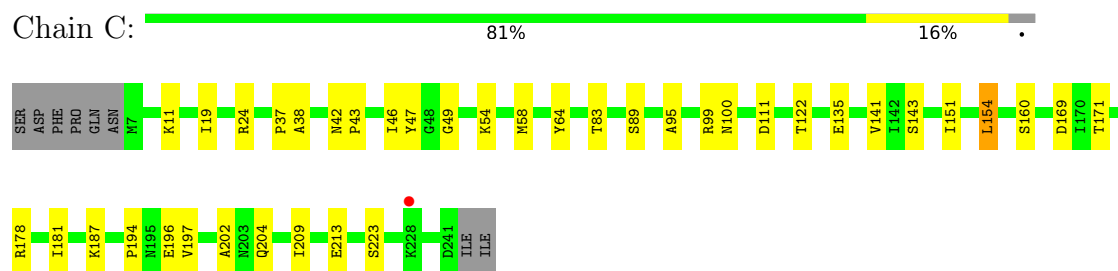
- Molecule 1: Chromosomal replication initiator protein DnaA



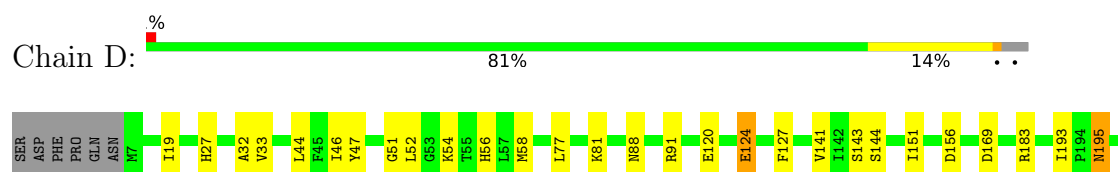
- Molecule 1: Chromosomal replication initiator protein DnaA

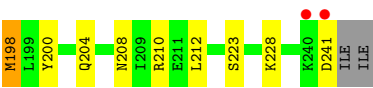


- Molecule 1: Chromosomal replication initiator protein DnaA

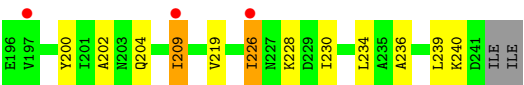
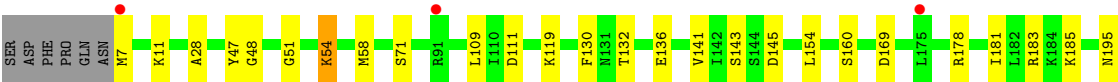
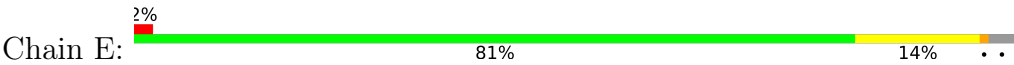


- Molecule 1: Chromosomal replication initiator protein DnaA





● Molecule 1: Chromosomal replication initiator protein DnaA



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	81.58Å 81.58Å 223.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	74.40 – 2.38 74.40 – 2.38	Depositor EDS
% Data completeness (in resolution range)	85.3 (74.40-2.38) 85.2 (74.40-2.38)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.191 , 0.239 0.191 , 0.239	Depositor DCC
R_{free} test set	2720 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	42.6	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 30.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.005 for -h,-k,l 0.044 for h,-h-k,-l 0.028 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9656	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% 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: MG, ANP, K

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	1.11	0/1911	1.51	3/2589 (0.1%)
1	B	1.06	0/1911	1.41	5/2589 (0.2%)
1	C	1.08	0/1911	1.48	6/2589 (0.2%)
1	D	1.08	2/1911 (0.1%)	1.45	4/2589 (0.2%)
1	E	1.05	0/1911	1.50	6/2589 (0.2%)
All	All	1.08	2/9555 (0.0%)	1.47	24/12945 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	56	HIS	CE1-NE2	6.35	1.38	1.32
1	D	151	ILE	N-CA	5.04	1.50	1.46

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	195	ASN	CA-CB-CG	-6.01	106.59	112.60
1	D	120	GLU	CB-CG-CD	6.00	122.81	112.60
1	E	119	LYS	CA-C-N	5.73	128.75	120.38
1	E	119	LYS	C-N-CA	5.73	128.75	120.38
1	B	20	GLY	CA-C-O	-5.64	114.97	121.46
1	A	32	ALA	CA-C-N	5.50	127.59	120.56
1	A	32	ALA	C-N-CA	5.50	127.59	120.56
1	C	49	GLY	CA-C-N	5.49	127.94	120.63
1	C	49	GLY	C-N-CA	5.49	127.94	120.63
1	B	88	ASN	CB-CA-C	-5.48	102.27	110.88
1	C	171	THR	CB-CA-C	5.47	117.28	108.91
1	B	120	GLU	CB-CG-CD	5.39	121.76	112.60
1	C	19	ILE	CA-C-N	5.36	126.94	122.17
1	C	19	ILE	C-N-CA	5.36	126.94	122.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	32	ALA	CA-C-N	5.19	127.10	120.56
1	D	32	ALA	C-N-CA	5.19	127.10	120.56
1	E	145	ASP	N-CA-C	-5.18	106.96	113.28
1	E	28	ALA	CA-C-N	5.18	127.17	120.44
1	E	28	ALA	C-N-CA	5.18	127.17	120.44
1	E	130	PHE	N-CA-C	-5.17	105.54	111.07
1	B	106	ASP	N-CA-C	-5.10	107.19	113.41
1	B	177	THR	CA-CB-OG1	-5.03	102.05	109.60
1	C	89	SER	N-CA-C	-5.02	105.94	111.71
1	A	171	THR	CB-CA-C	5.01	116.58	108.91

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1873	0	1867	12	0
1	B	1873	0	1867	25	0
1	C	1873	0	1867	17	0
1	D	1873	0	1867	19	0
1	E	1873	0	1867	21	0
2	A	31	0	13	0	0
2	B	31	0	13	0	0
2	C	31	0	13	1	0
2	D	31	0	13	2	0
2	E	31	0	13	3	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	3	0	0	0	0
3	D	2	0	0	0	0
3	E	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	1	0	0	0	0
5	A	14	0	0	0	0
5	B	29	0	0	0	0
5	C	36	0	0	0	0
5	D	29	0	0	0	0
5	E	14	0	0	0	0
All	All	9656	0	9400	92	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 5.

All (92) 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:E:48:GLY:O	1:E:54:LYS:HE3	1.94	0.67
1:B:200:TYR:O	1:B:204:GLN:HG2	1.97	0.65
1:D:54:LYS:NZ	2:D:301:ANP:O2G	2.29	0.65
1:D:58:MET:HE3	1:D:141:VAL:HG12	1.80	0.64
1:B:86:PHE:CZ	1:B:90:ILE:HD11	2.32	0.63
1:D:88:ASN:OD1	1:D:91:ARG:NH2	2.31	0.62
1:B:226:ILE:HD12	1:B:228:LYS:HD2	1.82	0.62
1:E:226:ILE:HD11	1:E:234:LEU:HD11	1.82	0.61
1:E:226:ILE:HG13	1:E:228:LYS:HB2	1.83	0.61
1:D:54:LYS:HE3	2:D:301:ANP:O2B	2.02	0.60
1:E:54:LYS:NZ	2:E:301:ANP:O2B	2.35	0.59
1:C:47:TYR:CZ	1:C:169:ASP:HB3	2.38	0.59
1:D:200:TYR:O	1:D:204:GLN:HG2	2.02	0.59
1:E:181:ILE:HG21	1:E:209:ILE:HD13	1.85	0.58
1:B:189:GLU:HB3	1:B:191:LEU:HG	1.85	0.58
1:C:54:LYS:HE3	2:C:301:ANP:O2B	2.05	0.56
1:E:51:GLY:O	1:E:209:ILE:HG23	2.05	0.55
1:D:46:ILE:O	1:D:143:SER:HA	2.07	0.55
1:B:178:ARG:NH1	1:B:202:ALA:O	2.36	0.55
1:B:152:PRO:C	1:B:154:LEU:H	2.16	0.54
1:E:178:ARG:NH1	1:E:202:ALA:O	2.40	0.54
1:E:209:ILE:HG12	2:E:301:ANP:C1'	2.38	0.54
1:A:48:GLY:O	1:A:54:LYS:HE2	2.08	0.53
1:D:198:MET:HA	1:D:198:MET:HE2	1.90	0.53
1:E:200:TYR:O	1:E:204:GLN:HG2	2.08	0.53
1:A:208:ASN:OD1	1:A:210:ARG:HB2	2.09	0.53
1:B:111:ASP:OD1	1:B:143:SER:OG	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:111:ASP:HA	1:E:143:SER:OG	2.10	0.51
1:D:47:TYR:HA	1:D:144:SER:O	2.11	0.51
1:C:181:ILE:HD13	1:C:209:ILE:HG12	1.94	0.50
1:E:47:TYR:CZ	1:E:169:ASP:HB3	2.46	0.50
1:B:134:HIS:CD2	1:B:164:TRP:CH2	2.99	0.49
1:D:124:GLU:O	1:D:127:PHE:HB3	2.13	0.49
1:A:77:LEU:HD23	1:A:77:LEU:N	2.28	0.49
1:B:123:GLN:OE1	1:B:155:GLU:HG3	2.13	0.48
1:D:47:TYR:CZ	1:D:169:ASP:HB3	2.47	0.48
1:B:47:TYR:CZ	1:B:169:ASP:HB3	2.48	0.48
1:C:58:MET:HE3	1:C:141:VAL:HG12	1.96	0.48
1:E:109:LEU:HD23	1:E:141:VAL:HB	1.94	0.48
1:D:193:ILE:HG21	1:D:198:MET:HE3	1.96	0.46
1:D:210:ARG:HD2	1:E:160:SER:OG	2.15	0.46
1:C:194:PRO:HB2	1:C:197:VAL:HG23	1.97	0.46
1:D:33:VAL:HG21	1:D:44:LEU:HD22	1.99	0.45
1:A:231:ASN:OD1	1:A:233:ASP:HB2	2.17	0.45
1:C:178:ARG:NH1	1:C:202:ALA:O	2.50	0.45
1:D:208:ASN:OD1	1:D:210:ARG:HB2	2.16	0.45
1:E:181:ILE:CG2	1:E:209:ILE:HD13	2.48	0.44
1:C:111:ASP:OD1	1:C:143:SER:OG	2.35	0.44
1:C:151:ILE:HB	1:C:154:LEU:HD22	1.99	0.44
1:B:118:GLY:N	1:B:153:THR:OG1	2.44	0.43
1:D:195:ASN:N	1:D:195:ASN:OD1	2.51	0.43
1:C:209:ILE:O	1:C:213:GLU:HG3	2.18	0.43
1:A:61:ILE:O	1:A:65:VAL:HG23	2.18	0.43
1:B:47:TYR:O	1:B:169:ASP:HA	2.18	0.43
1:E:58:MET:HE3	1:E:141:VAL:HG12	1.99	0.43
1:B:30:SER:HB3	1:B:61:ILE:HD11	2.00	0.43
1:B:58:MET:HE3	1:B:141:VAL:HG12	2.01	0.43
1:B:46:ILE:O	1:B:143:SER:HA	2.18	0.43
1:B:225:LEU:HD11	1:C:24:ARG:HG2	2.01	0.43
1:B:37:PRO:O	1:B:38:ALA:HB3	2.18	0.43
1:D:77:LEU:HB2	1:D:81:LYS:HD2	2.01	0.43
1:E:132:THR:O	1:E:136:GLU:HG3	2.20	0.42
1:E:219:VAL:HG23	1:E:239:LEU:HD21	2.00	0.42
1:D:19:ILE:HD11	1:D:27:HIS:CE1	2.54	0.42
1:B:237:GLU:OE2	1:B:240:LYS:HD2	2.19	0.42
1:C:95:ALA:O	1:C:99:ARG:HG3	2.18	0.42
1:A:157:ARG:O	1:A:161:ARG:HD2	2.19	0.42
1:C:64:TYR:CD1	1:C:64:TYR:C	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:PRO:O	1:C:38:ALA:HB3	2.20	0.42
1:E:200:TYR:CE2	1:E:236:ALA:HA	2.55	0.41
1:A:42:ASN:HA	1:A:43:PRO:HA	1.79	0.41
1:A:47:TYR:CZ	1:A:169:ASP:HB3	2.55	0.41
1:B:171:THR:HB	1:B:172:PRO:CD	2.50	0.41
1:D:51:GLY:O	1:D:52:LEU:HD23	2.20	0.41
1:C:46:ILE:O	1:C:143:SER:HA	2.20	0.41
1:B:134:HIS:HD2	1:B:164:TRP:CH2	2.37	0.41
1:B:222:TYR:CE2	1:B:226:ILE:HD13	2.56	0.41
1:E:185:LYS:HE3	1:E:209:ILE:HD11	2.03	0.41
1:B:47:TYR:HA	1:B:144:SER:O	2.20	0.41
1:C:42:ASN:HA	1:C:43:PRO:HA	1.96	0.41
1:A:43:PRO:O	1:A:165:GLY:HA3	2.20	0.41
1:B:43:PRO:O	1:B:165:GLY:HA3	2.20	0.41
1:C:83:THR:OG1	1:C:122:THR:HG21	2.21	0.41
1:B:153:THR:O	1:B:154:LEU:C	2.64	0.41
1:E:183:ARG:NH2	1:E:195:ASN:OD1	2.43	0.41
1:A:58:MET:HE2	1:A:109:LEU:HB3	2.01	0.40
1:D:47:TYR:O	1:D:169:ASP:HA	2.21	0.40
1:A:187:LYS:HA	1:A:187:LYS:HE3	2.04	0.40
1:A:222:TYR:CD2	1:A:238:ALA:HB2	2.57	0.40
1:B:158:LEU:O	1:B:159:ARG:C	2.63	0.40
1:E:209:ILE:HG12	2:E:301:ANP:N9	2.35	0.40
1:C:47:TYR:CE1	1:C:169:ASP:HB3	2.57	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	233/243 (96%)	219 (94%)	14 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	233/243 (96%)	220 (94%)	13 (6%)	0	100	100
1	C	233/243 (96%)	223 (96%)	10 (4%)	0	100	100
1	D	233/243 (96%)	221 (95%)	12 (5%)	0	100	100
1	E	233/243 (96%)	219 (94%)	14 (6%)	0	100	100
All	All	1165/1215 (96%)	1102 (95%)	63 (5%)	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	202/210 (96%)	190 (94%)	12 (6%)	18	28
1	B	202/210 (96%)	191 (95%)	11 (5%)	20	32
1	C	202/210 (96%)	193 (96%)	9 (4%)	24	39
1	D	202/210 (96%)	194 (96%)	8 (4%)	28	44
1	E	202/210 (96%)	193 (96%)	9 (4%)	24	39
All	All	1010/1050 (96%)	961 (95%)	49 (5%)	22	36

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	19	ILE
1	A	54	LYS
1	A	73	LYS
1	A	93	ASN
1	A	170	ILE
1	A	187	LYS
1	A	189	GLU
1	A	203	ASN
1	A	223	SER

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Mol	Chain	Res	Type
1	A	228	LYS
1	A	230	ILE
1	B	11	LYS
1	B	15	ASP
1	B	39	LYS
1	B	73	LYS
1	B	78	SER
1	B	153	THR
1	B	157	ARG
1	B	187	LYS
1	B	189	GLU
1	B	209	ILE
1	B	223	SER
1	C	11	LYS
1	C	100	ASN
1	C	135	GLU
1	C	154	LEU
1	C	160	SER
1	C	187	LYS
1	C	196	GLU
1	C	204	GLN
1	C	223	SER
1	D	124	GLU
1	D	156	ASP
1	D	183	ARG
1	D	198	MET
1	D	212	LEU
1	D	223	SER
1	D	228	LYS
1	D	241	ASP
1	E	7	MET
1	E	11	LYS
1	E	54	LYS
1	E	71	SER
1	E	154	LEU
1	E	209	ILE
1	E	226	ILE
1	E	230	ILE
1	E	240	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	203	ASN
1	B	27	HIS
1	B	134	HIS
1	B	195	ASN
1	B	227	ASN
1	C	100	ASN
1	C	134	HIS
1	D	27	HIS
1	D	93	ASN
1	E	203	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 14 are monoatomic - leaving 5 for Mogul analysis.

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	ANP	D	301	4	33,33,33	1.59	3 (9%)	45,52,52	0.95	2 (4%)
2	ANP	B	301	4	33,33,33	1.60	3 (9%)	45,52,52	1.03	2 (4%)
2	ANP	C	301	4	33,33,33	1.58	3 (9%)	45,52,52	1.36	4 (8%)
2	ANP	E	301	4	33,33,33	1.52	3 (9%)	45,52,52	1.07	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ANP	A	301	4	33,33,33	1.35	4 (12%)	45,52,52	1.52	6 (13%)

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	ANP	D	301	4	-	5/18/38/38	0/3/3/3
2	ANP	B	301	4	-	3/18/38/38	0/3/3/3
2	ANP	C	301	4	-	3/18/38/38	0/3/3/3
2	ANP	E	301	4	-	4/18/38/38	0/3/3/3
2	ANP	A	301	4	-	3/18/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	ANP	PG-O1G	7.69	1.57	1.46
2	D	301	ANP	PG-O1G	7.65	1.57	1.46
2	B	301	ANP	PG-O1G	7.54	1.57	1.46
2	E	301	ANP	PG-O1G	6.78	1.56	1.46
2	A	301	ANP	PG-O1G	5.37	1.54	1.46
2	A	301	ANP	PB-O1B	3.24	1.51	1.46
2	E	301	ANP	PB-O1B	3.06	1.50	1.46
2	B	301	ANP	PB-O1B	3.02	1.50	1.46
2	C	301	ANP	PB-O1B	2.96	1.50	1.46
2	D	301	ANP	PB-O1B	2.89	1.50	1.46
2	E	301	ANP	PB-O2B	-2.48	1.50	1.56
2	D	301	ANP	PB-O2B	-2.24	1.50	1.56
2	A	301	ANP	PB-O2B	-2.18	1.51	1.56
2	A	301	ANP	PB-O3A	2.13	1.61	1.59
2	C	301	ANP	PB-O2B	-2.12	1.51	1.56
2	B	301	ANP	PG-O3G	-2.05	1.51	1.56

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	ANP	O1B-PB-N3B	5.47	119.83	111.77
2	A	301	ANP	O2G-PG-O1G	-5.36	100.02	113.45
2	A	301	ANP	O2B-PB-O1B	4.75	120.06	109.87
2	C	301	ANP	O2B-PB-O1B	4.27	119.03	109.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	ANP	O2A-PA-O3A	4.02	118.15	107.27
2	B	301	ANP	O2B-PB-O1B	4.01	118.46	109.87
2	E	301	ANP	O2B-PB-O1B	4.00	118.45	109.87
2	B	301	ANP	O2G-PG-O1G	-3.68	104.21	113.45
2	D	301	ANP	O2B-PB-O1B	3.26	116.86	109.87
2	E	301	ANP	O2G-PG-O1G	-2.90	106.17	113.45
2	A	301	ANP	O2G-PG-O3G	2.72	114.90	107.59
2	A	301	ANP	O1B-PB-N3B	2.72	115.77	111.77
2	A	301	ANP	O3A-PA-O1A	-2.63	102.79	110.70
2	E	301	ANP	O1G-PG-N3B	-2.21	108.51	111.77
2	C	301	ANP	O2A-PA-O1A	2.21	122.72	112.44
2	C	301	ANP	O2G-PG-O1G	-2.13	108.11	113.45
2	D	301	ANP	O2A-PA-O1A	2.09	122.15	112.44

There are no chirality outliers.

All (18) torsion outliers are listed below:

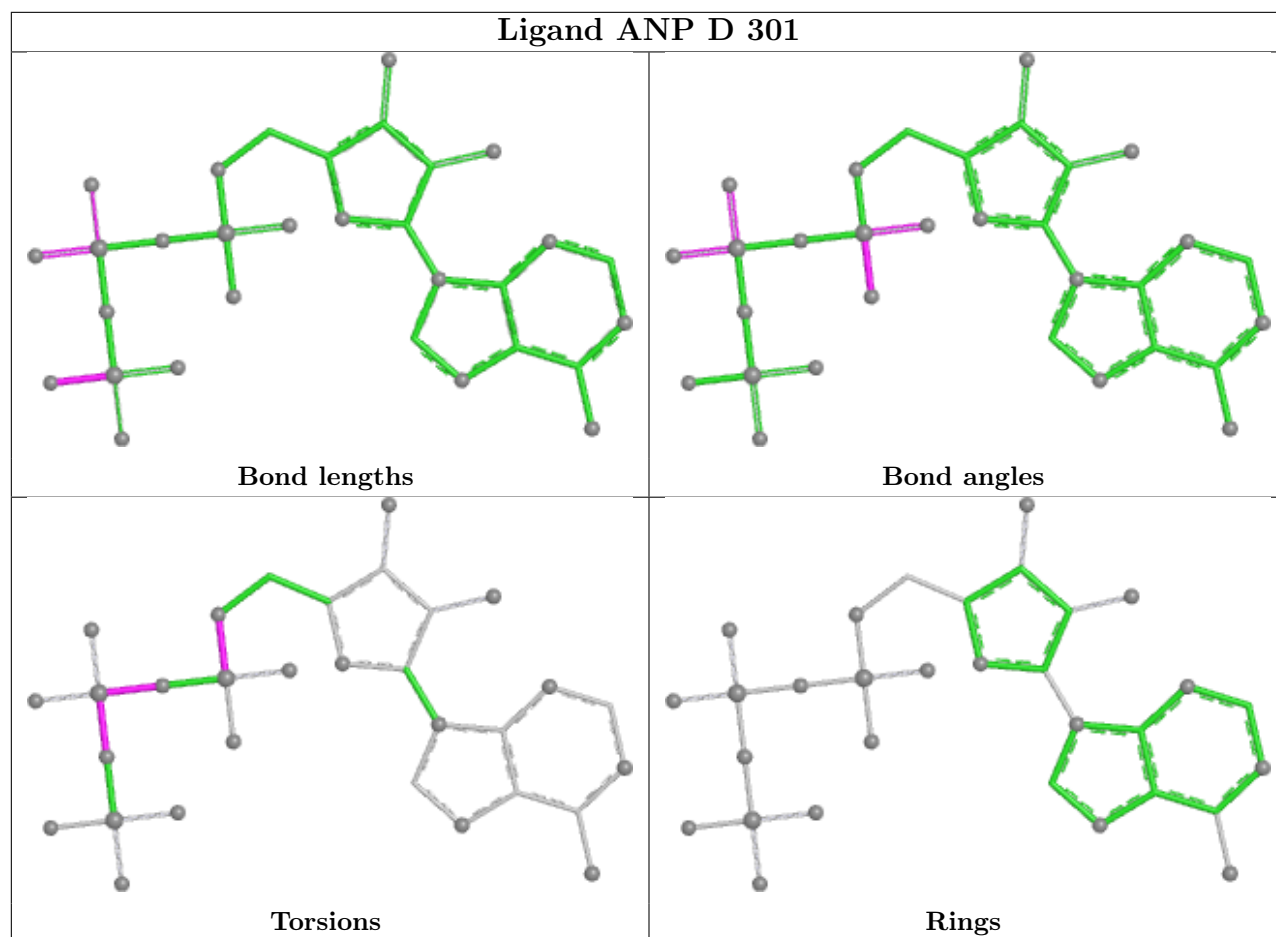
Mol	Chain	Res	Type	Atoms
2	A	301	ANP	PG-N3B-PB-O1B
2	B	301	ANP	PG-N3B-PB-O1B
2	B	301	ANP	PA-O3A-PB-O2B
2	C	301	ANP	PG-N3B-PB-O1B
2	C	301	ANP	PA-O3A-PB-O2B
2	D	301	ANP	PG-N3B-PB-O1B
2	D	301	ANP	PA-O3A-PB-O2B
2	D	301	ANP	C5'-O5'-PA-O1A
2	E	301	ANP	PG-N3B-PB-O1B
2	E	301	ANP	PG-N3B-PB-O3A
2	E	301	ANP	PA-O3A-PB-O2B
2	D	301	ANP	C5'-O5'-PA-O3A
2	A	301	ANP	PA-O3A-PB-O1B
2	B	301	ANP	PA-O3A-PB-O1B
2	C	301	ANP	PA-O3A-PB-O1B
2	D	301	ANP	PA-O3A-PB-O1B
2	E	301	ANP	PA-O3A-PB-O1B
2	A	301	ANP	PG-N3B-PB-O3A

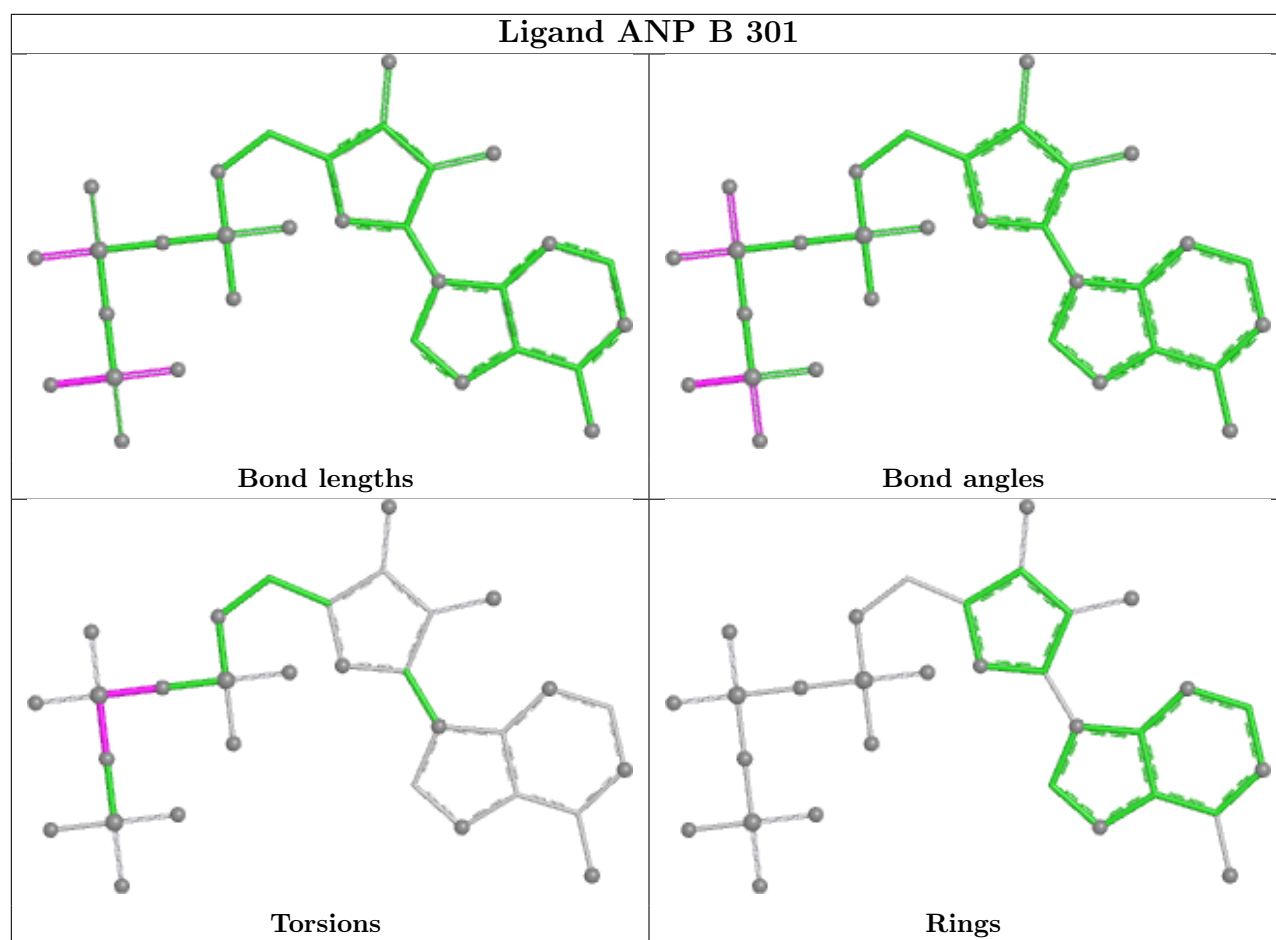
There are no ring outliers.

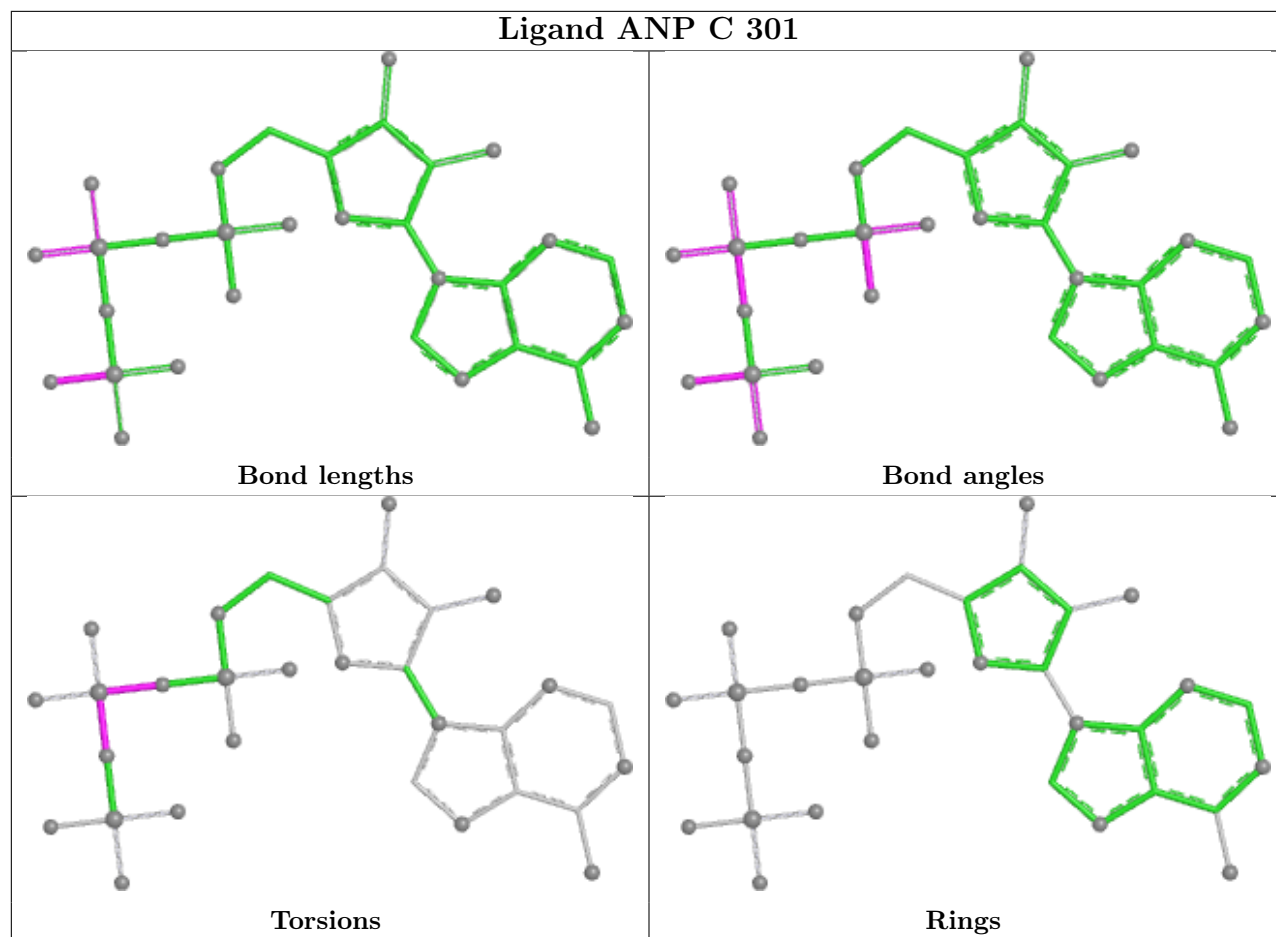
3 monomers are involved in 6 short contacts:

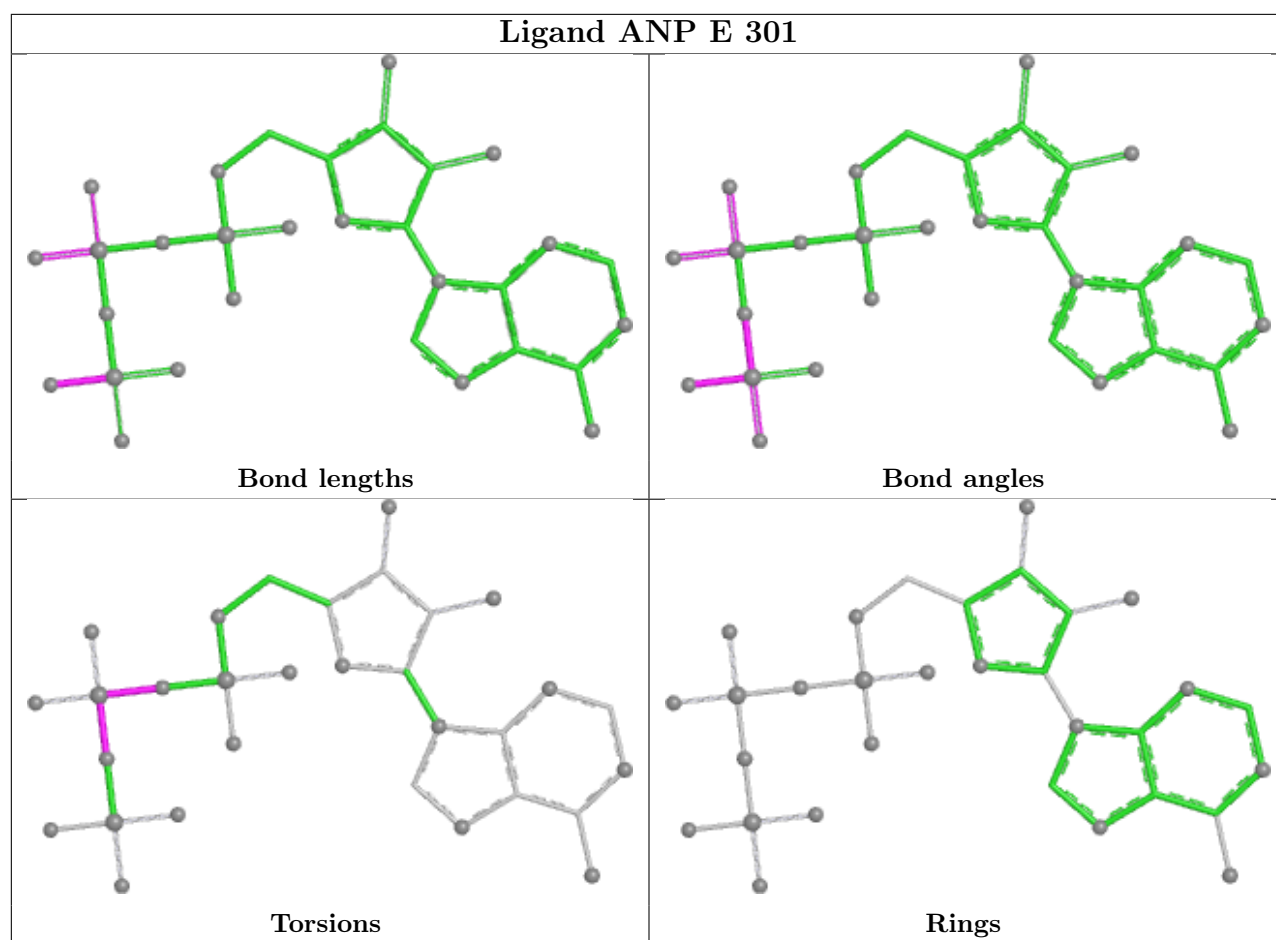
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	ANP	2	0
2	C	301	ANP	1	0
2	E	301	ANP	3	0

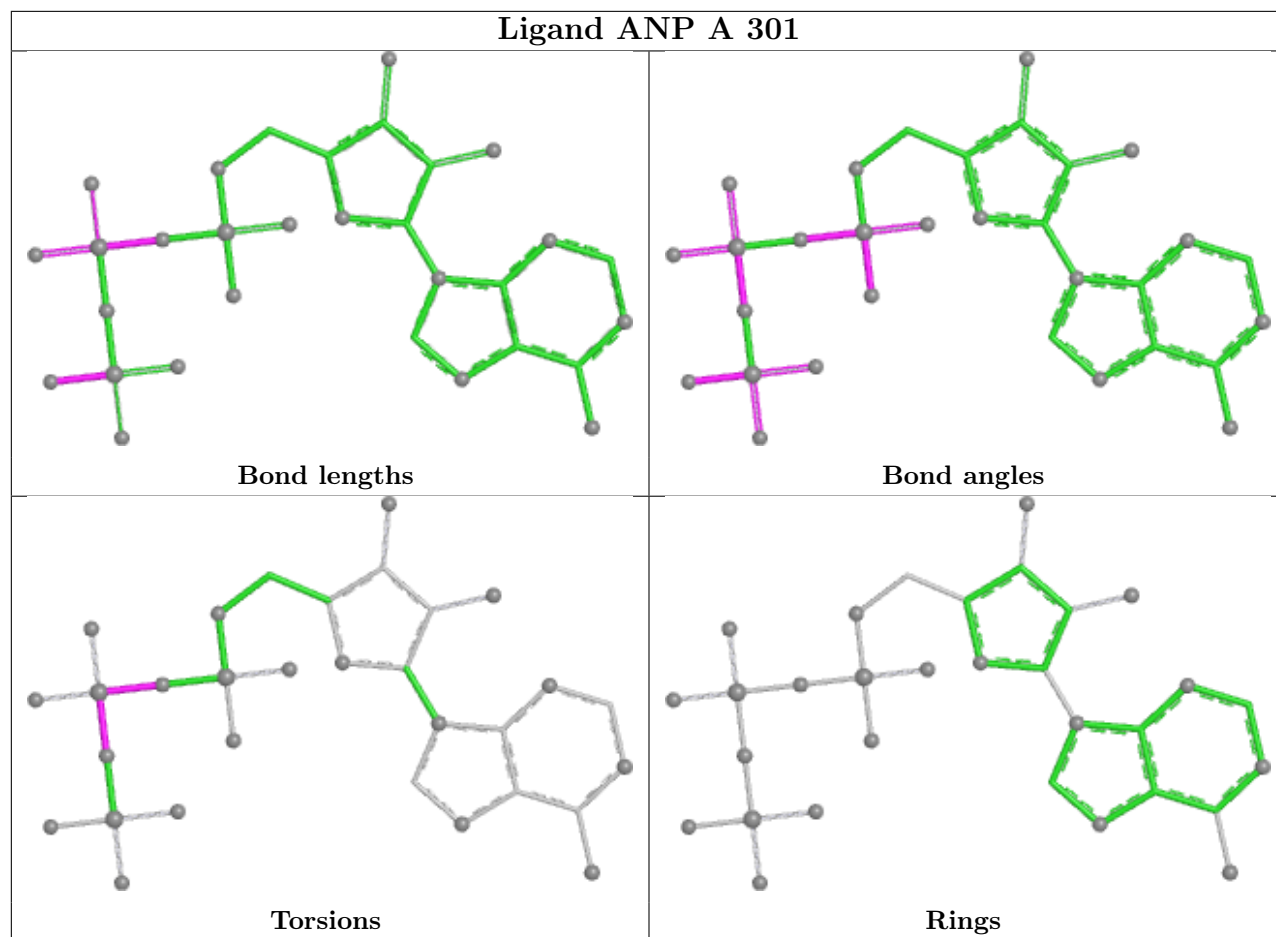
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	235/243 (96%)	0.31	5 (2%) 63 62	37, 54, 80, 92	0
1	B	235/243 (96%)	0.08	8 (3%) 48 48	28, 45, 73, 86	0
1	C	235/243 (96%)	-0.10	1 (0%) 88 88	26, 42, 75, 93	0
1	D	235/243 (96%)	-0.08	2 (0%) 81 80	32, 45, 66, 89	0
1	E	235/243 (96%)	0.17	6 (2%) 57 56	29, 50, 78, 91	0
All	All	1175/1215 (96%)	0.08	22 (1%) 66 65	26, 48, 76, 93	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	7	MET	3.5
1	E	175	LEU	3.3
1	B	228	LYS	3.3
1	C	228	LYS	2.9
1	A	206	ASP	2.7
1	E	7	MET	2.5
1	B	73	LYS	2.5
1	A	230	ILE	2.5
1	B	241	ASP	2.5
1	E	91	ARG	2.4
1	D	240	LYS	2.4
1	E	197	VAL	2.4
1	B	157	ARG	2.3
1	E	209	ILE	2.3
1	E	226	ILE	2.2
1	B	69	ASN	2.2
1	A	115	PHE	2.2
1	D	241	ASP	2.2
1	B	189	GLU	2.1
1	B	152	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	228	LYS	2.0
1	A	7	MET	2.0

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.

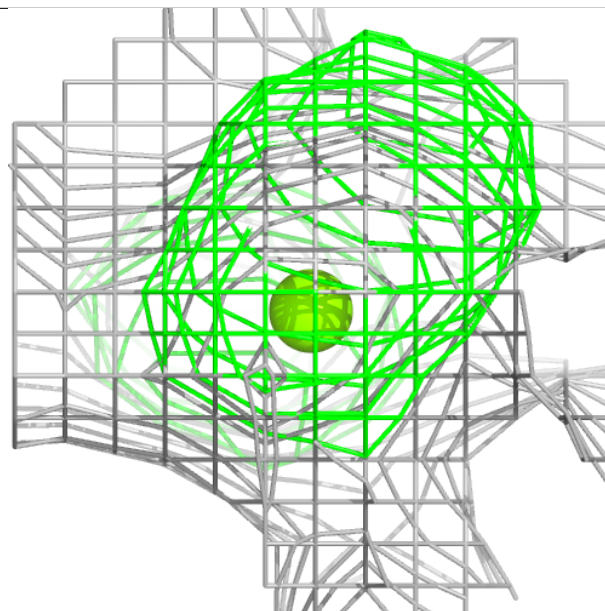
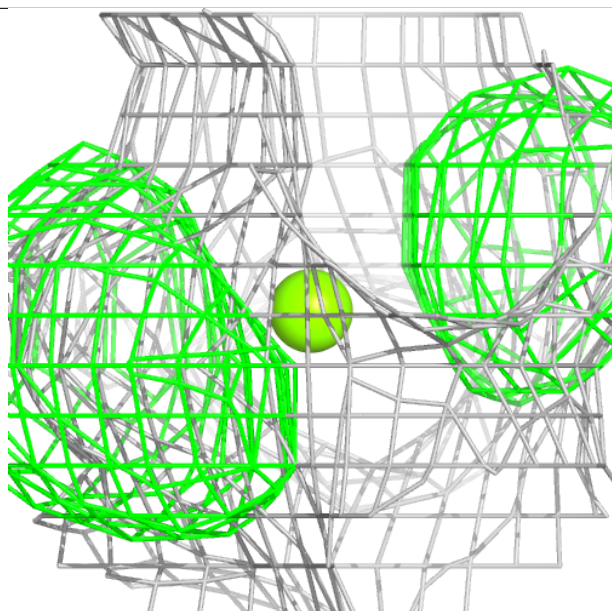
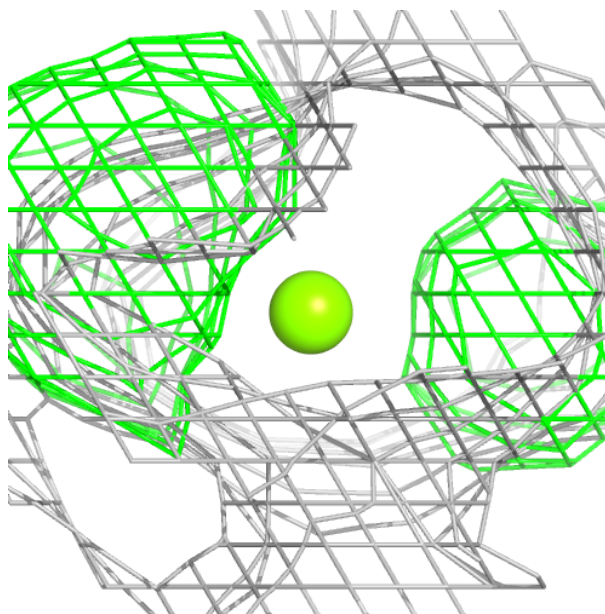
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	K	B	302	1/1	0.93	0.10	72,72,72,72	0
3	K	D	303	1/1	0.94	0.07	73,73,73,73	0
4	MG	E	303	1/1	0.95	0.09	30,30,30,30	0
3	K	C	303	1/1	0.96	0.07	55,55,55,55	0
3	K	C	304	1/1	0.96	0.07	67,67,67,67	0
2	ANP	A	301	31/31	0.97	0.06	39,46,52,58	0
3	K	B	303	1/1	0.97	0.06	64,64,64,64	0
4	MG	A	303	1/1	0.97	0.06	30,30,30,30	0
4	MG	C	305	1/1	0.97	0.07	30,30,30,30	0
2	ANP	E	301	31/31	0.97	0.06	33,42,57,68	0
3	K	A	302	1/1	0.98	0.04	48,48,48,48	0
2	ANP	D	301	31/31	0.98	0.05	29,35,49,56	0
4	MG	D	304	1/1	0.98	0.06	30,30,30,30	0
2	ANP	C	301	31/31	0.98	0.05	30,37,47,48	0
3	K	C	302	1/1	0.99	0.03	34,34,34,34	0
4	MG	B	304	1/1	0.99	0.06	30,30,30,30	0
3	K	D	302	1/1	0.99	0.04	45,45,45,45	0
2	ANP	B	301	31/31	0.99	0.04	22,26,35,45	0
3	K	E	302	1/1	0.99	0.05	47,47,47,47	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.

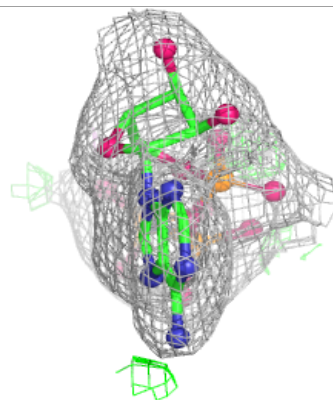
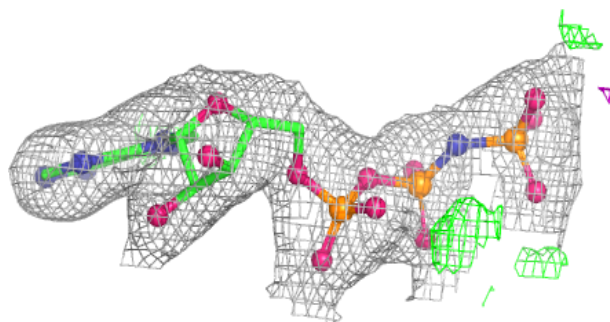
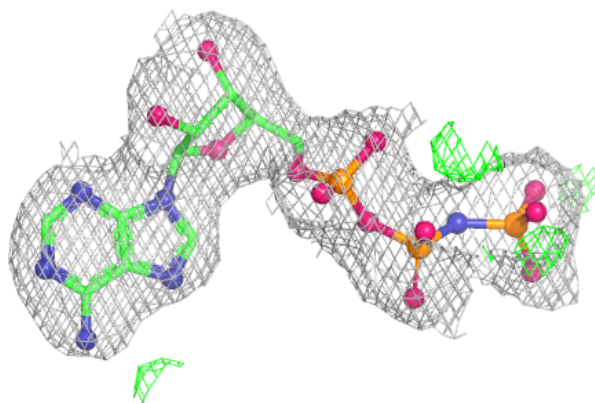
Electron density around MG E 303:

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



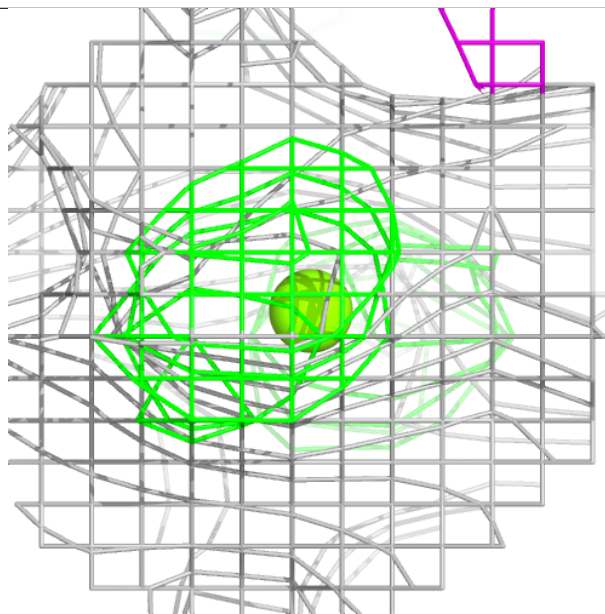
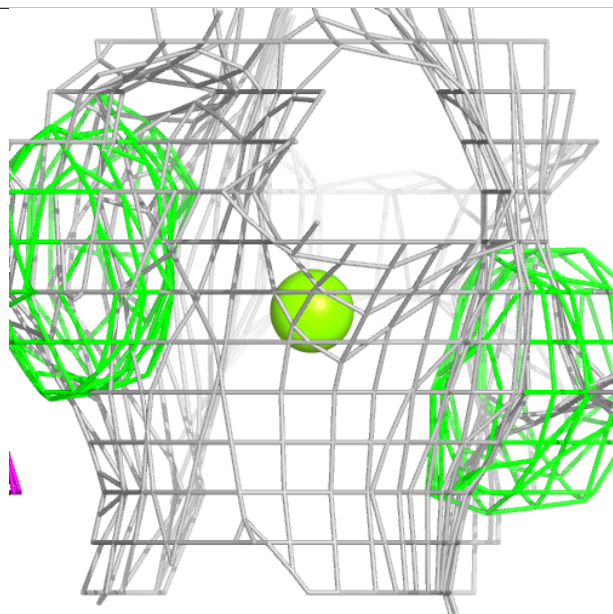
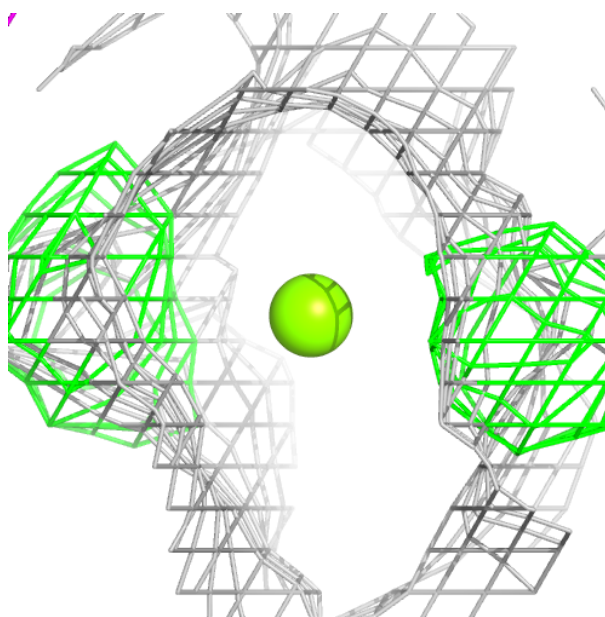
Electron density around ANP A 301:

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



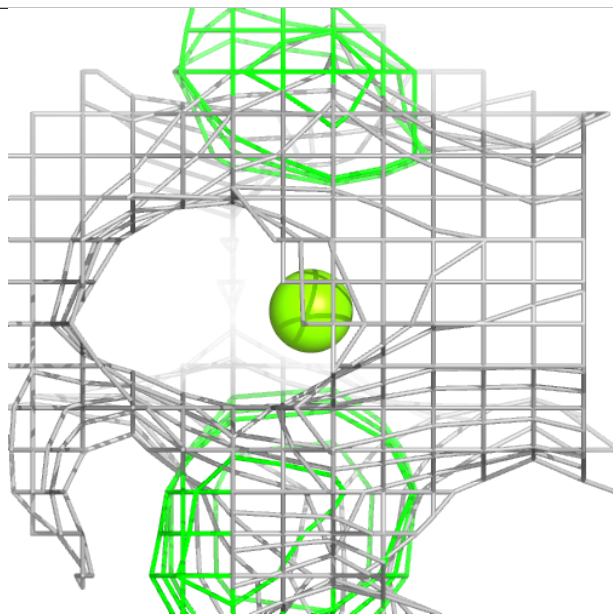
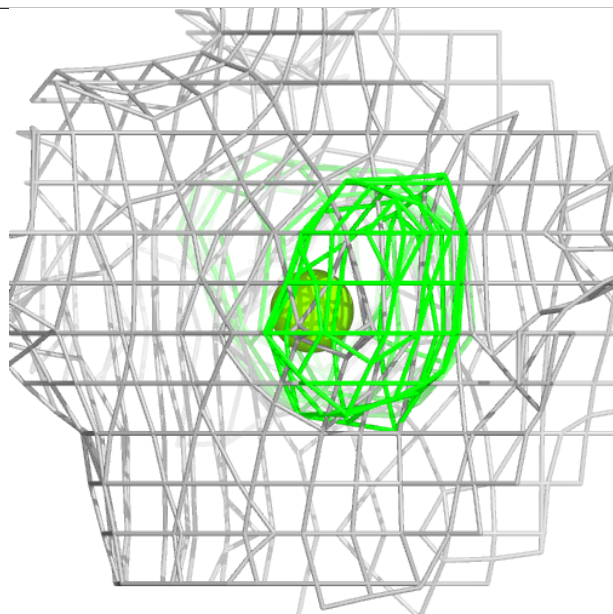
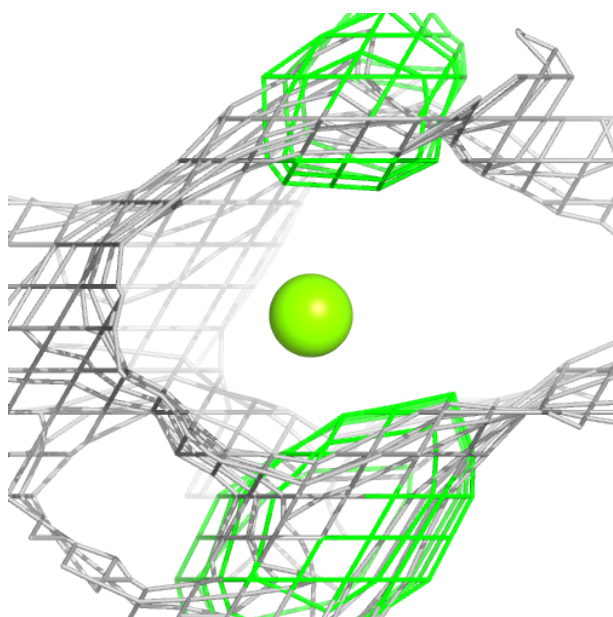
Electron density around MG A 303:

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



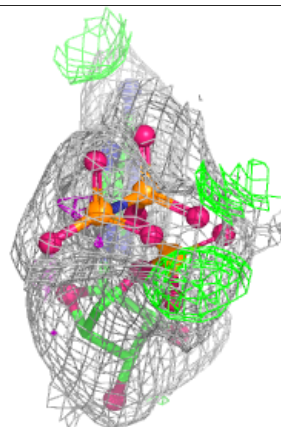
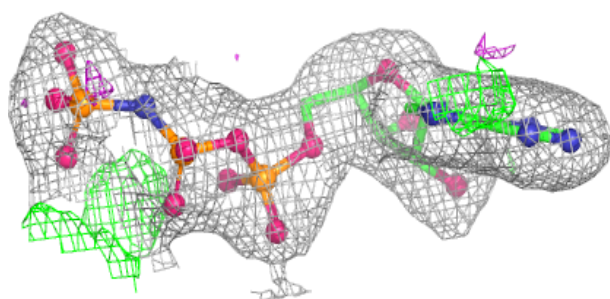
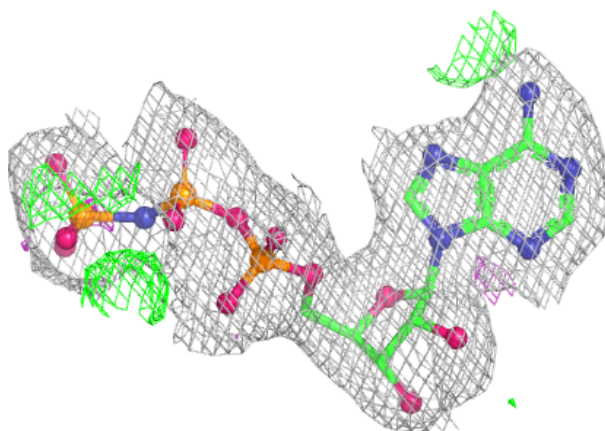
Electron density around MG C 305:

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

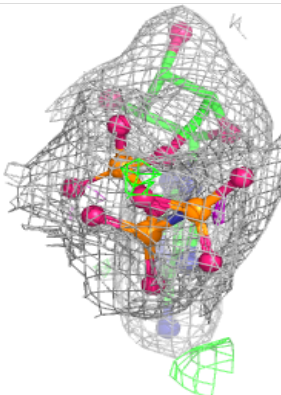
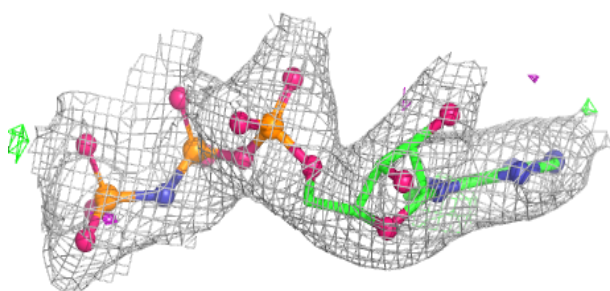
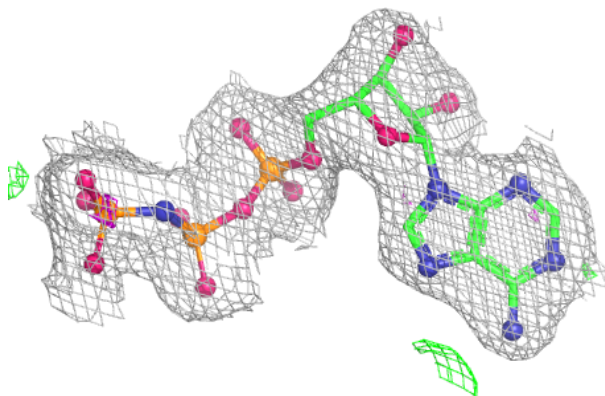


Electron density around ANP E 301:

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

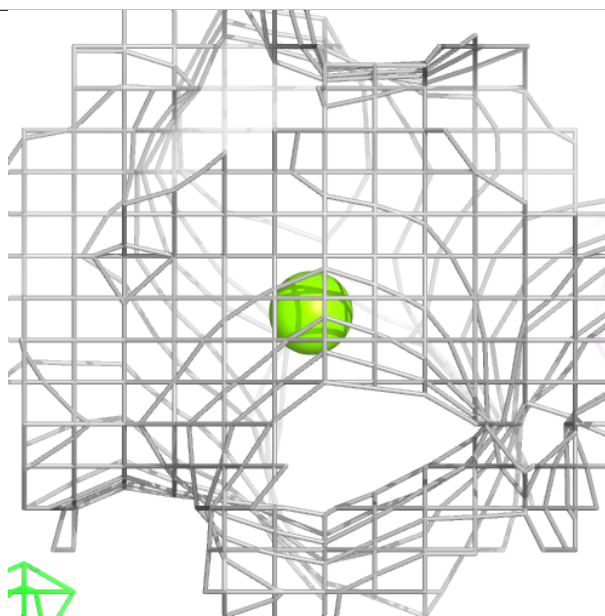
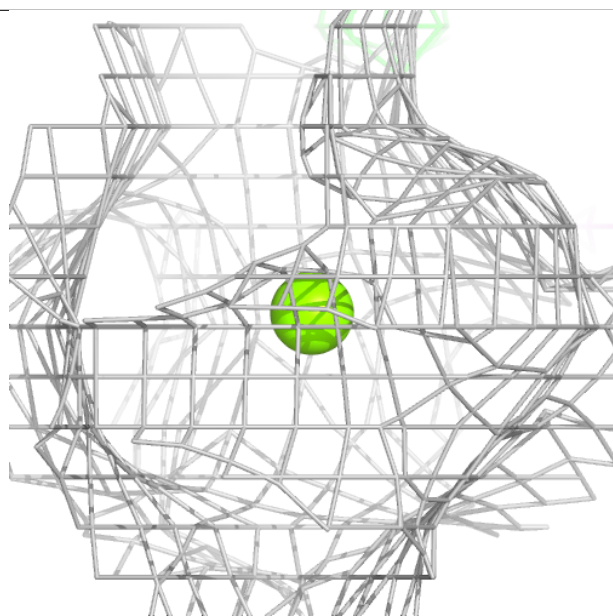
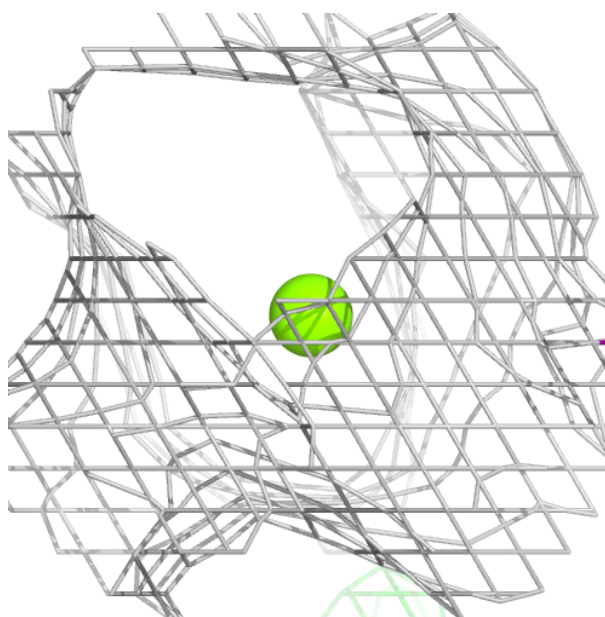
**Electron density around ANP D 301:**

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



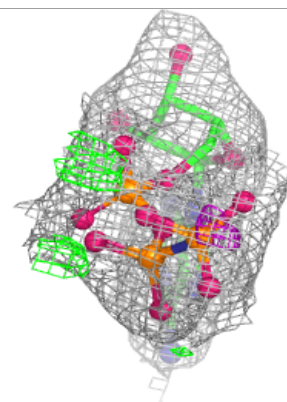
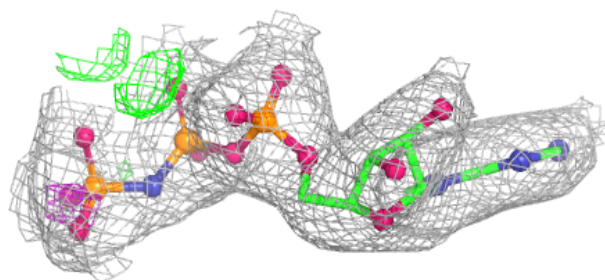
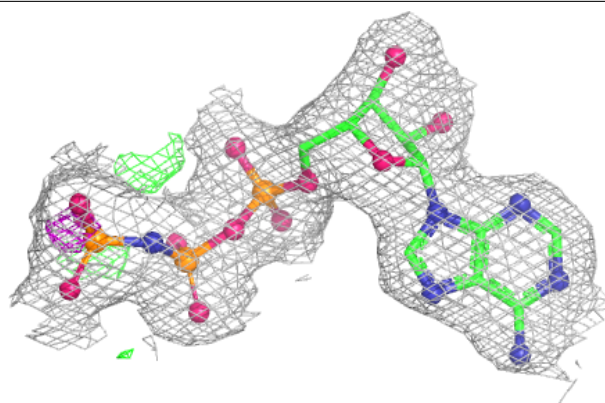
Electron density around MG D 304:

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



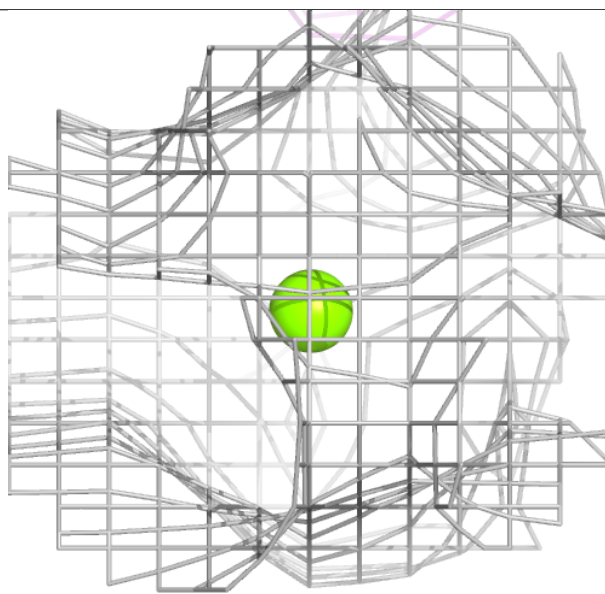
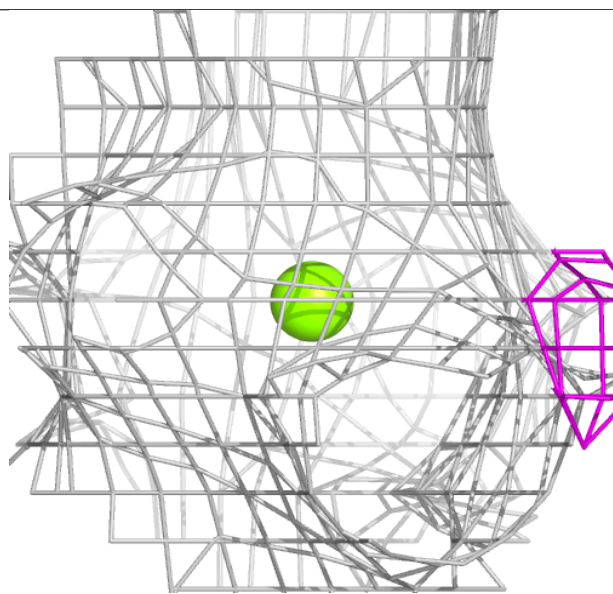
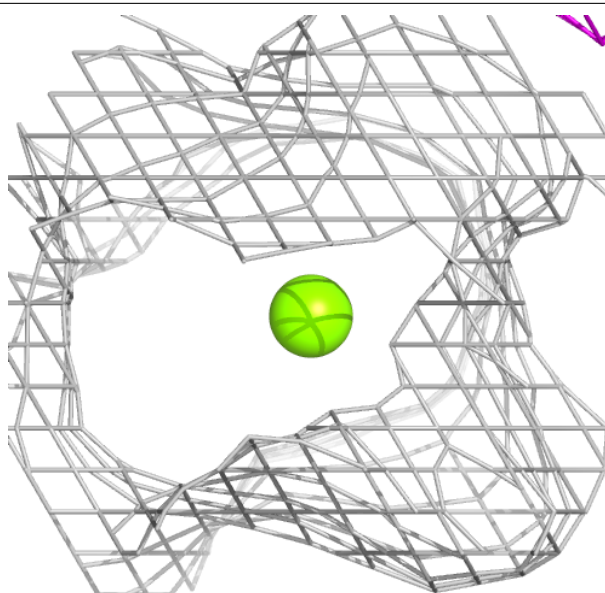
Electron density around ANP C 301:

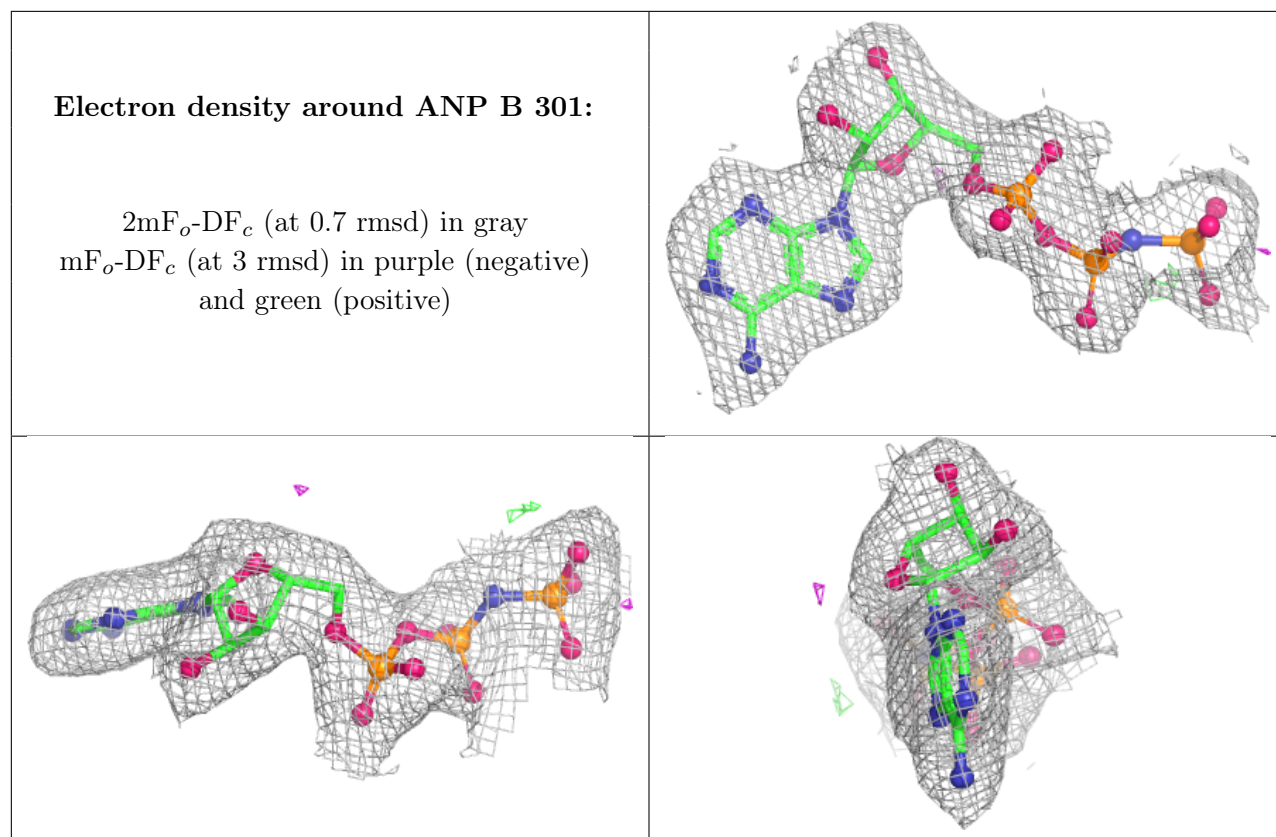
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG B 304:

$2mF_o-DF_c$ (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.