



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 11:14 pm BST

PDB ID : 4QHT
Title : Crystal structure of AAA+/ sigma 54 activator domain of the flagellar regulatory protein FlrC from *Vibrio cholerae* in ATP analog bound state
Authors : Dey, S.; Biswas, M.; Sen, U.; Dasgupta, J.
Deposited on : 2014-05-29
Resolution : 2.56 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

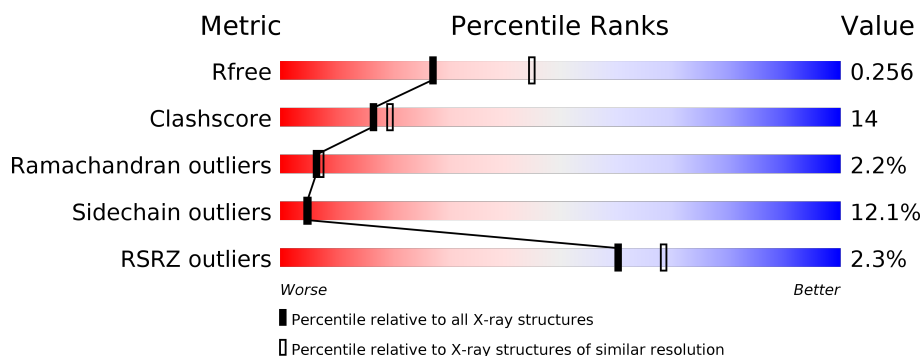
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (2.58-2.54)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	267	<div> <div>2%</div> <div> <div></div> <div>65%</div> <div>21%</div> <div>5%</div> <div>8%</div> </div> </div>
1	B	267	<div> <div>3%</div> <div> <div></div> <div>66%</div> <div>19%</div> <div>5%</div> <div>8%</div> </div> </div>
1	C	267	<div> <div>3%</div> <div> <div></div> <div>70%</div> <div>19%</div> <div>••</div> <div>7%</div> </div> </div>
1	D	267	<div> <div></div> <div> <div></div> <div>69%</div> <div>20%</div> <div>••</div> <div>8%</div> </div> </div>
1	E	267	<div> <div>•</div> <div> <div></div> <div>66%</div> <div>22%</div> <div>••</div> <div>8%</div> </div> </div>
1	F	267	<div> <div>3%</div> <div> <div></div> <div>66%</div> <div>19%</div> <div>6%</div> <div>8%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	267	<div><div><div>%</div><div><div></div></div><div>69%</div><div>19%</div><div>• • 8%</div></div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14136 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 Flagellar regulatory protein C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	S	0	0	0
			1922	1219	342	352	9			
1	B	245	Total	C	N	O	S	0	0	0
			1917	1216	341	351	9			
1	C	248	Total	C	N	O	S	0	0	0
			1935	1226	344	356	9			
1	D	246	Total	C	N	O	S	0	0	0
			1926	1221	342	354	9			
1	E	246	Total	C	N	O	S	0	0	0
			1926	1221	342	354	9			
1	F	245	Total	C	N	O	S	0	0	0
			1917	1216	341	351	9			
1	G	246	Total	C	N	O	S	0	0	0
			1926	1221	342	354	9			

There are 119 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	115	HIS	-	EXPRESSION TAG	UNP A5F6D4
A	116	HIS	-	EXPRESSION TAG	UNP A5F6D4
A	117	HIS	-	EXPRESSION TAG	UNP A5F6D4
A	118	HIS	-	EXPRESSION TAG	UNP A5F6D4
A	119	HIS	-	EXPRESSION TAG	UNP A5F6D4
A	120	HIS	-	EXPRESSION TAG	UNP A5F6D4
A	121	SER	-	EXPRESSION TAG	UNP A5F6D4
A	122	SER	-	EXPRESSION TAG	UNP A5F6D4
A	123	GLY	-	EXPRESSION TAG	UNP A5F6D4
A	124	LEU	-	EXPRESSION TAG	UNP A5F6D4
A	125	VAL	-	EXPRESSION TAG	UNP A5F6D4
A	126	PRO	-	EXPRESSION TAG	UNP A5F6D4
A	127	ARG	-	EXPRESSION TAG	UNP A5F6D4
A	128	GLY	-	EXPRESSION TAG	UNP A5F6D4
A	129	SER	-	EXPRESSION TAG	UNP A5F6D4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	130	HIS	-	EXPRESSION TAG	UNP A5F6D4
A	131	MET	-	EXPRESSION TAG	UNP A5F6D4
B	115	HIS	-	EXPRESSION TAG	UNP A5F6D4
B	116	HIS	-	EXPRESSION TAG	UNP A5F6D4
B	117	HIS	-	EXPRESSION TAG	UNP A5F6D4
B	118	HIS	-	EXPRESSION TAG	UNP A5F6D4
B	119	HIS	-	EXPRESSION TAG	UNP A5F6D4
B	120	HIS	-	EXPRESSION TAG	UNP A5F6D4
B	121	SER	-	EXPRESSION TAG	UNP A5F6D4
B	122	SER	-	EXPRESSION TAG	UNP A5F6D4
B	123	GLY	-	EXPRESSION TAG	UNP A5F6D4
B	124	LEU	-	EXPRESSION TAG	UNP A5F6D4
B	125	VAL	-	EXPRESSION TAG	UNP A5F6D4
B	126	PRO	-	EXPRESSION TAG	UNP A5F6D4
B	127	ARG	-	EXPRESSION TAG	UNP A5F6D4
B	128	GLY	-	EXPRESSION TAG	UNP A5F6D4
B	129	SER	-	EXPRESSION TAG	UNP A5F6D4
B	130	HIS	-	EXPRESSION TAG	UNP A5F6D4
B	131	MET	-	EXPRESSION TAG	UNP A5F6D4
C	115	HIS	-	EXPRESSION TAG	UNP A5F6D4
C	116	HIS	-	EXPRESSION TAG	UNP A5F6D4
C	117	HIS	-	EXPRESSION TAG	UNP A5F6D4
C	118	HIS	-	EXPRESSION TAG	UNP A5F6D4
C	119	HIS	-	EXPRESSION TAG	UNP A5F6D4
C	120	HIS	-	EXPRESSION TAG	UNP A5F6D4
C	121	SER	-	EXPRESSION TAG	UNP A5F6D4
C	122	SER	-	EXPRESSION TAG	UNP A5F6D4
C	123	GLY	-	EXPRESSION TAG	UNP A5F6D4
C	124	LEU	-	EXPRESSION TAG	UNP A5F6D4
C	125	VAL	-	EXPRESSION TAG	UNP A5F6D4
C	126	PRO	-	EXPRESSION TAG	UNP A5F6D4
C	127	ARG	-	EXPRESSION TAG	UNP A5F6D4
C	128	GLY	-	EXPRESSION TAG	UNP A5F6D4
C	129	SER	-	EXPRESSION TAG	UNP A5F6D4
C	130	HIS	-	EXPRESSION TAG	UNP A5F6D4
C	131	MET	-	EXPRESSION TAG	UNP A5F6D4
D	115	HIS	-	EXPRESSION TAG	UNP A5F6D4
D	116	HIS	-	EXPRESSION TAG	UNP A5F6D4
D	117	HIS	-	EXPRESSION TAG	UNP A5F6D4
D	118	HIS	-	EXPRESSION TAG	UNP A5F6D4
D	119	HIS	-	EXPRESSION TAG	UNP A5F6D4
D	120	HIS	-	EXPRESSION TAG	UNP A5F6D4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	121	SER	-	EXPRESSION TAG	UNP A5F6D4
D	122	SER	-	EXPRESSION TAG	UNP A5F6D4
D	123	GLY	-	EXPRESSION TAG	UNP A5F6D4
D	124	LEU	-	EXPRESSION TAG	UNP A5F6D4
D	125	VAL	-	EXPRESSION TAG	UNP A5F6D4
D	126	PRO	-	EXPRESSION TAG	UNP A5F6D4
D	127	ARG	-	EXPRESSION TAG	UNP A5F6D4
D	128	GLY	-	EXPRESSION TAG	UNP A5F6D4
D	129	SER	-	EXPRESSION TAG	UNP A5F6D4
D	130	HIS	-	EXPRESSION TAG	UNP A5F6D4
D	131	MET	-	EXPRESSION TAG	UNP A5F6D4
E	115	HIS	-	EXPRESSION TAG	UNP A5F6D4
E	116	HIS	-	EXPRESSION TAG	UNP A5F6D4
E	117	HIS	-	EXPRESSION TAG	UNP A5F6D4
E	118	HIS	-	EXPRESSION TAG	UNP A5F6D4
E	119	HIS	-	EXPRESSION TAG	UNP A5F6D4
E	120	HIS	-	EXPRESSION TAG	UNP A5F6D4
E	121	SER	-	EXPRESSION TAG	UNP A5F6D4
E	122	SER	-	EXPRESSION TAG	UNP A5F6D4
E	123	GLY	-	EXPRESSION TAG	UNP A5F6D4
E	124	LEU	-	EXPRESSION TAG	UNP A5F6D4
E	125	VAL	-	EXPRESSION TAG	UNP A5F6D4
E	126	PRO	-	EXPRESSION TAG	UNP A5F6D4
E	127	ARG	-	EXPRESSION TAG	UNP A5F6D4
E	128	GLY	-	EXPRESSION TAG	UNP A5F6D4
E	129	SER	-	EXPRESSION TAG	UNP A5F6D4
E	130	HIS	-	EXPRESSION TAG	UNP A5F6D4
E	131	MET	-	EXPRESSION TAG	UNP A5F6D4
F	115	HIS	-	EXPRESSION TAG	UNP A5F6D4
F	116	HIS	-	EXPRESSION TAG	UNP A5F6D4
F	117	HIS	-	EXPRESSION TAG	UNP A5F6D4
F	118	HIS	-	EXPRESSION TAG	UNP A5F6D4
F	119	HIS	-	EXPRESSION TAG	UNP A5F6D4
F	120	HIS	-	EXPRESSION TAG	UNP A5F6D4
F	121	SER	-	EXPRESSION TAG	UNP A5F6D4
F	122	SER	-	EXPRESSION TAG	UNP A5F6D4
F	123	GLY	-	EXPRESSION TAG	UNP A5F6D4
F	124	LEU	-	EXPRESSION TAG	UNP A5F6D4
F	125	VAL	-	EXPRESSION TAG	UNP A5F6D4
F	126	PRO	-	EXPRESSION TAG	UNP A5F6D4
F	127	ARG	-	EXPRESSION TAG	UNP A5F6D4
F	128	GLY	-	EXPRESSION TAG	UNP A5F6D4

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Chain	Residue	Modelled	Actual	Comment	Reference
F	129	SER	-	EXPRESSION TAG	UNP A5F6D4
F	130	HIS	-	EXPRESSION TAG	UNP A5F6D4
F	131	MET	-	EXPRESSION TAG	UNP A5F6D4
G	115	HIS	-	EXPRESSION TAG	UNP A5F6D4
G	116	HIS	-	EXPRESSION TAG	UNP A5F6D4
G	117	HIS	-	EXPRESSION TAG	UNP A5F6D4
G	118	HIS	-	EXPRESSION TAG	UNP A5F6D4
G	119	HIS	-	EXPRESSION TAG	UNP A5F6D4
G	120	HIS	-	EXPRESSION TAG	UNP A5F6D4
G	121	SER	-	EXPRESSION TAG	UNP A5F6D4
G	122	SER	-	EXPRESSION TAG	UNP A5F6D4
G	123	GLY	-	EXPRESSION TAG	UNP A5F6D4
G	124	LEU	-	EXPRESSION TAG	UNP A5F6D4
G	125	VAL	-	EXPRESSION TAG	UNP A5F6D4
G	126	PRO	-	EXPRESSION TAG	UNP A5F6D4
G	127	ARG	-	EXPRESSION TAG	UNP A5F6D4
G	128	GLY	-	EXPRESSION TAG	UNP A5F6D4
G	129	SER	-	EXPRESSION TAG	UNP A5F6D4
G	130	HIS	-	EXPRESSION TAG	UNP A5F6D4
G	131	MET	-	EXPRESSION TAG	UNP A5F6D4

- # ANP

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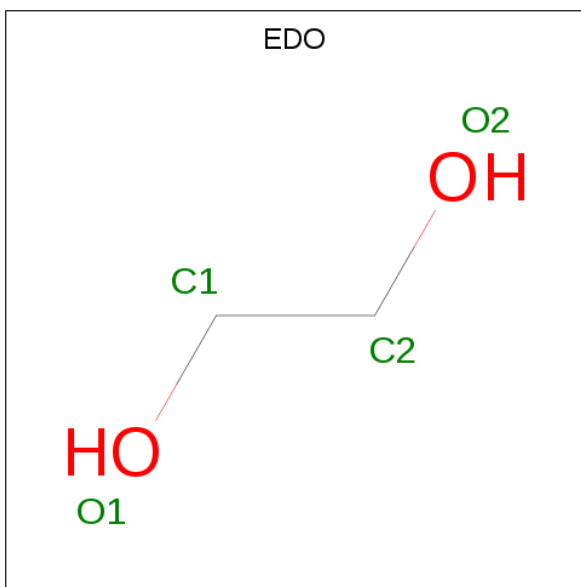
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	F	1	Total	C	N	O	P	0	0
			31	10	6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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

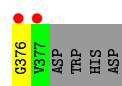
- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		

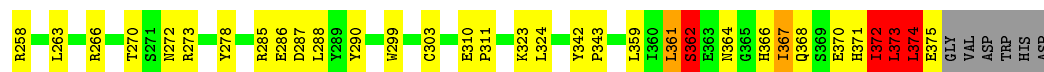
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	56	Total 56	O 56	0	0
5	B	62	Total 62	O 62	0	0
5	C	69	Total 69	O 69	0	0
5	D	54	Total 54	O 54	0	0
5	E	65	Total 65	O 65	0	0
5	F	42	Total 42	O 42	0	0
5	G	47	Total 47	O 47	0	0



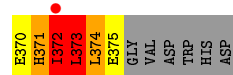
• Molecule 1: Flagellar regulatory protein C

Chain D: 69% 20% 8%



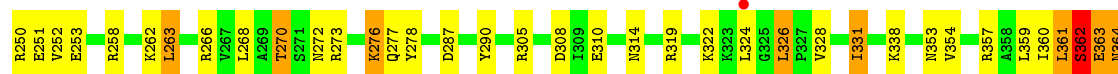
• Molecule 1: Flagellar regulatory protein C

Chain E: 66% 22% 8%



• Molecule 1: Flagellar regulatory protein C

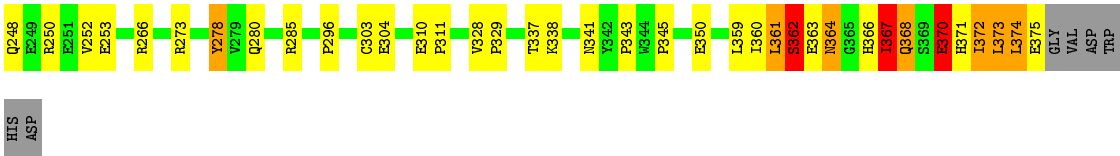
Chain F: 66% 19% 6% 8%



• Molecule 1: Flagellar regulatory protein C

Chain G: 69% 19% 8%





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.96Å 152.56Å 193.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.20 – 2.56 49.20 – 2.56	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.20-2.56) 96.6 (49.20-2.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.54Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.182 , 0.247 0.193 , 0.256	Depositor DCC
R_{free} test set	3902 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	47.6	Xtriage
Anisotropy	0.313	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14136	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.33% 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, EDO

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	0.72	1/1957 (0.1%)	0.65	0/2649
1	B	0.59	0/1952	0.64	0/2642
1	C	0.53	1/1970 (0.1%)	0.63	0/2666
1	D	0.50	0/1961	0.63	0/2654
1	E	0.53	0/1961	0.65	0/2654
1	F	0.44	0/1952	0.62	1/2642 (0.0%)
1	G	0.67	2/1961 (0.1%)	0.66	0/2654
All	All	0.57	4/13714 (0.0%)	0.64	1/18561 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
All	All	0	8

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	370	GLU	CB-CG	-6.31	1.40	1.52
1	G	370	GLU	CB-CG	-5.88	1.41	1.52
1	G	367	ILE	CA-CB	-5.72	1.41	1.54
1	C	367	ILE	CA-CB	-5.46	1.42	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	F	365	GLY	N-CA-C	-6.14	97.76	113.10

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	361	LEU	Peptide
1	B	361	LEU	Peptide
1	B	367	ILE	Peptide
1	C	361	LEU	Peptide
1	D	361	LEU	Peptide

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	1922	0	1967	63	0
1	B	1917	0	1965	73	0
1	C	1935	0	1976	34	0
1	D	1926	0	1971	67	0
1	E	1926	0	1971	56	0
1	F	1917	0	1965	41	0
1	G	1926	0	1971	61	0
2	A	31	0	13	3	0
2	B	31	0	13	4	0
2	C	31	0	13	1	0
2	D	31	0	13	1	0
2	E	31	0	13	1	0
2	F	31	0	13	2	0
2	G	31	0	13	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1	0	0	0	0
4	A	8	0	12	0	0
4	B	4	0	6	2	0
4	C	4	0	6	1	0
4	D	8	0	12	4	0
4	E	8	0	12	0	0
4	F	8	0	12	3	0
4	G	8	0	12	2	0
5	A	56	0	0	5	0
5	B	62	0	0	7	0
5	C	69	0	0	2	0
5	D	54	0	0	3	0
5	E	65	0	0	4	0
5	F	42	0	0	6	0
5	G	47	0	0	5	0
All	All	14136	0	13949	393	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 14.

The worst 5 of 393 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:372:ILE:HD13	1:D:373:LEU:CD1	1.63	1.29
1:B:373:LEU:CD1	1:B:374:LEU:H	1.46	1.29
1:B:291:ARG:NH1	5:B:528:HOH:O	1.62	1.25
1:B:374:LEU:HD12	1:B:374:LEU:C	1.54	1.25
1:B:371:HIS:C	1:B:372:ILE:HD13	1.57	1.22

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	244/267 (91%)	223 (91%)	13 (5%)	8 (3%)	4	3
1	B	243/267 (91%)	224 (92%)	13 (5%)	6 (2%)	5	5
1	C	246/267 (92%)	228 (93%)	12 (5%)	6 (2%)	6	6
1	D	244/267 (91%)	225 (92%)	14 (6%)	5 (2%)	7	8
1	E	244/267 (91%)	227 (93%)	13 (5%)	4 (2%)	9	12
1	F	243/267 (91%)	224 (92%)	15 (6%)	4 (2%)	9	12
1	G	244/267 (91%)	227 (93%)	13 (5%)	4 (2%)	9	12
All	All	1708/1869 (91%)	1578 (92%)	93 (5%)	37 (2%)	6	7

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	LEU
1	A	362	SER
1	A	364	ASN
1	A	373	LEU
1	A	374	LEU

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	208/227 (92%)	181 (87%)	27 (13%)	4	4
1	B	208/227 (92%)	183 (88%)	25 (12%)	5	5
1	C	209/227 (92%)	186 (89%)	23 (11%)	6	6
1	D	209/227 (92%)	188 (90%)	21 (10%)	7	9
1	E	209/227 (92%)	179 (86%)	30 (14%)	3	3
1	F	208/227 (92%)	176 (85%)	32 (15%)	2	2
1	G	209/227 (92%)	190 (91%)	19 (9%)	9	11
All	All	1460/1589 (92%)	1283 (88%)	177 (12%)	5	5

5 of 177 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	232	ILE
1	E	144	LEU
1	G	209	THR
1	D	251	GLU
1	D	362	SER

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

Mol	Chain	Res	Type
1	E	315	HIS
1	G	315	HIS
1	G	130	HIS
1	E	272	ASN
1	F	272	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 7 are monoatomic - leaving 19 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
4	EDO	D	404	-	3,3,3	0.62	0	2,2,2	0.29	0
4	EDO	G	404	-	3,3,3	0.58	0	2,2,2	0.30	0
4	EDO	A	403	-	3,3,3	0.55	0	2,2,2	0.13	0
2	ANP	C	401	3	29,33,33	1.20	3 (10%)	31,52,52	1.23	5 (16%)
4	EDO	C	403	-	3,3,3	0.56	0	2,2,2	0.06	0
2	ANP	A	401	3	29,33,33	1.18	5 (17%)	31,52,52	0.94	3 (9%)
4	EDO	E	403	-	3,3,3	0.47	0	2,2,2	0.38	0
2	ANP	G	401	3	29,33,33	1.21	4 (13%)	31,52,52	1.23	4 (12%)
4	EDO	G	403	-	3,3,3	0.54	0	2,2,2	0.13	0
2	ANP	E	401	3	29,33,33	1.26	5 (17%)	31,52,52	1.07	3 (9%)
4	EDO	B	403	-	3,3,3	0.56	0	2,2,2	0.03	0
2	ANP	D	401	3	29,33,33	1.22	3 (10%)	31,52,52	0.98	2 (6%)
4	EDO	F	403	-	3,3,3	0.56	0	2,2,2	0.26	0
2	ANP	B	401	3	29,33,33	1.19	5 (17%)	31,52,52	1.09	3 (9%)
4	EDO	E	404	-	3,3,3	0.51	0	2,2,2	0.25	0
2	ANP	F	401	3	29,33,33	1.27	5 (17%)	31,52,52	1.03	2 (6%)
4	EDO	D	403	-	3,3,3	0.51	0	2,2,2	0.30	0
4	EDO	F	404	-	3,3,3	0.60	0	2,2,2	0.21	0
4	EDO	A	404	-	3,3,3	0.50	0	2,2,2	0.13	0

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
4	EDO	D	404	-	-	0/1/1/1	-
4	EDO	G	404	-	-	1/1/1/1	-
4	EDO	A	403	-	-	0/1/1/1	-
2	ANP	C	401	3	-	4/14/38/38	0/3/3/3
4	EDO	C	403	-	-	1/1/1/1	-
2	ANP	A	401	3	-	3/14/38/38	0/3/3/3
4	EDO	E	403	-	-	0/1/1/1	-
2	ANP	G	401	3	-	4/14/38/38	0/3/3/3
4	EDO	G	403	-	-	0/1/1/1	-
2	ANP	E	401	3	-	5/14/38/38	0/3/3/3
4	EDO	B	403	-	-	0/1/1/1	-
2	ANP	D	401	3	-	3/14/38/38	0/3/3/3
4	EDO	F	403	-	-	1/1/1/1	-
2	ANP	B	401	3	-	3/14/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	E	404	-	-	0/1/1/1	-
2	ANP	F	401	3	-	2/14/38/38	0/3/3/3
4	EDO	D	403	-	-	1/1/1/1	-
4	EDO	F	404	-	-	0/1/1/1	-
4	EDO	A	404	-	-	1/1/1/1	-

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	ANP	PG-N3B	3.40	1.72	1.63
2	F	401	ANP	PB-O1B	3.30	1.51	1.46
2	D	401	ANP	PB-O1B	3.29	1.51	1.46
2	E	401	ANP	PG-N3B	3.20	1.71	1.63
2	B	401	ANP	PB-O1B	2.98	1.50	1.46

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	ANP	PA-O3A-PB	-3.37	120.74	132.62
2	D	401	ANP	PA-O3A-PB	-3.06	121.83	132.62
2	B	401	ANP	PA-O3A-PB	-2.90	122.40	132.62
2	C	401	ANP	PA-O3A-PB	-2.89	122.42	132.62
2	C	401	ANP	O1G-PG-N3B	-2.78	107.68	111.77

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	401	ANP	PB-N3B-PG-O1G
2	E	401	ANP	PG-N3B-PB-O1B
2	E	401	ANP	PG-N3B-PB-O3A
2	F	401	ANP	PG-N3B-PB-O1B
2	A	401	ANP	PB-N3B-PG-O1G

There are no ring outliers.

15 monomers are involved in 25 short contacts:

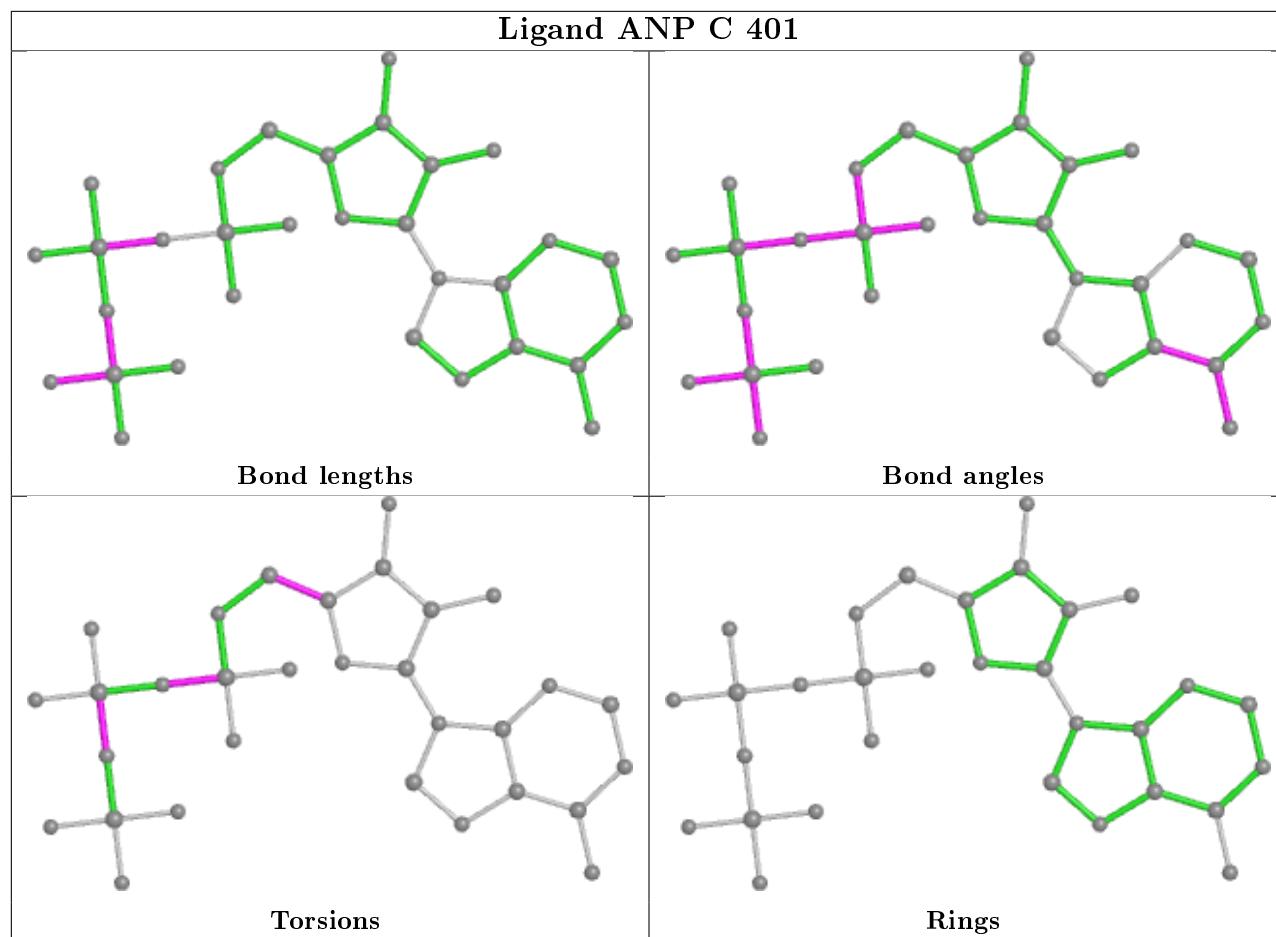
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	404	EDO	2	0
4	G	404	EDO	1	0
2	C	401	ANP	1	0

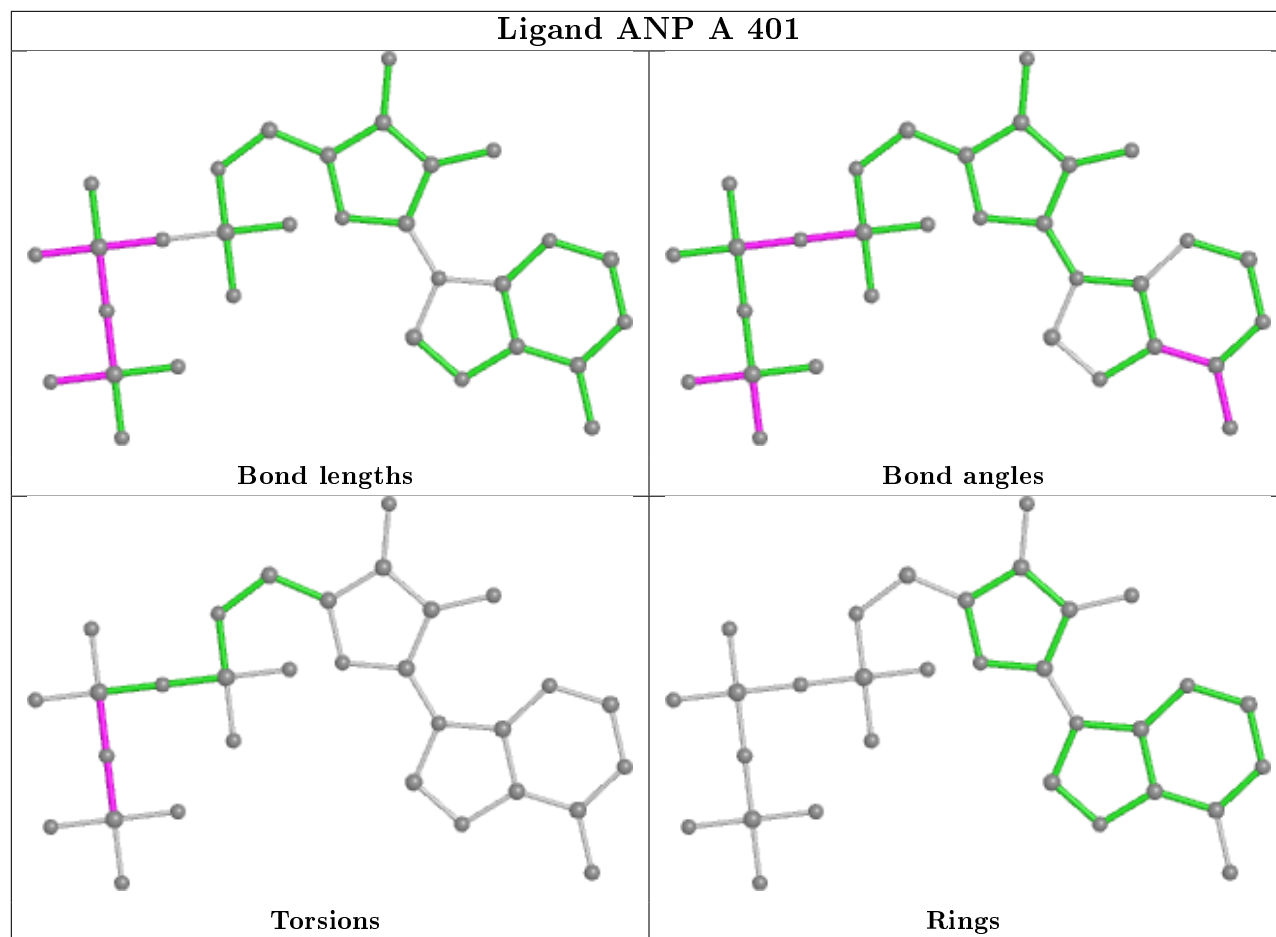
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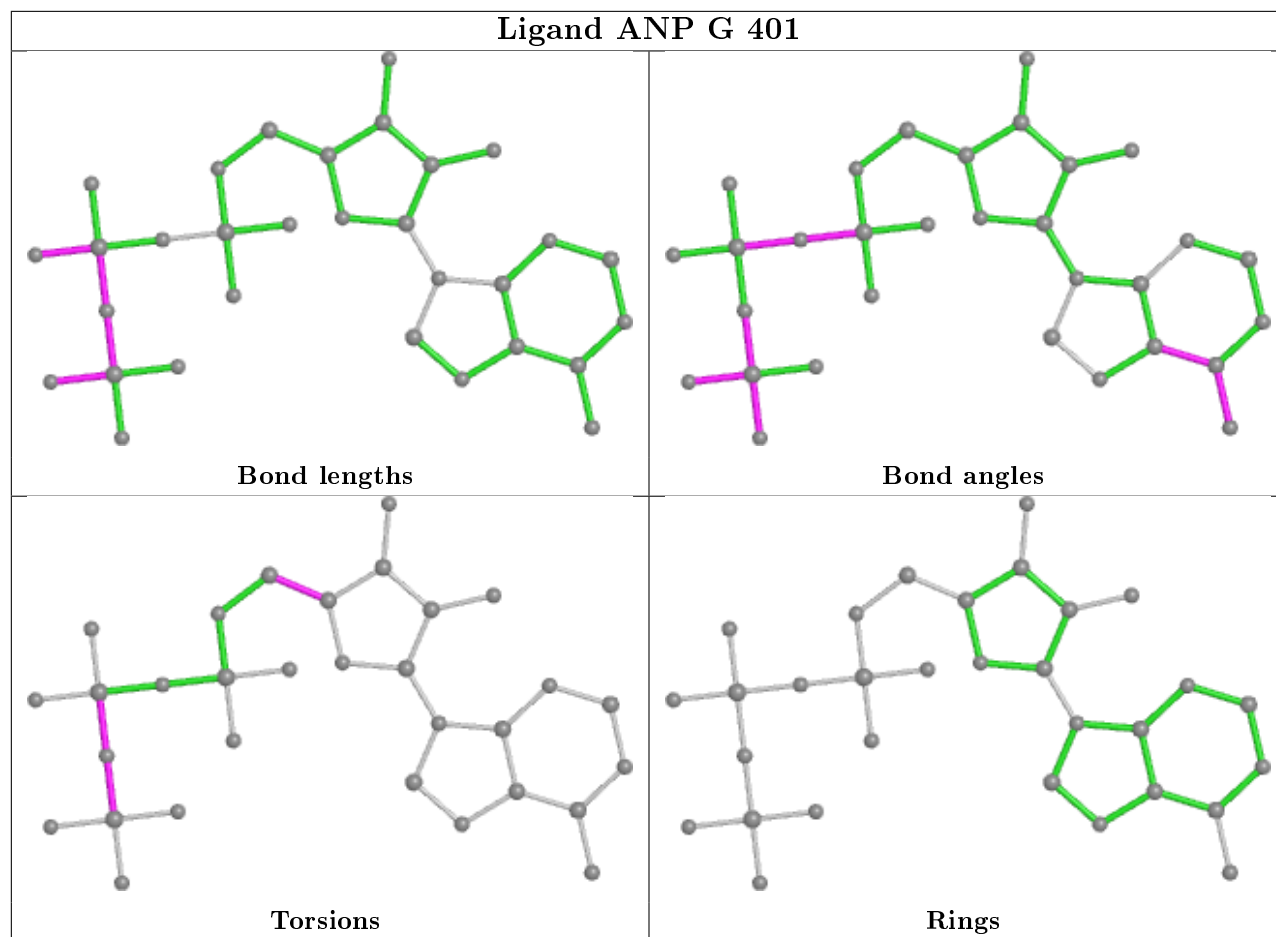
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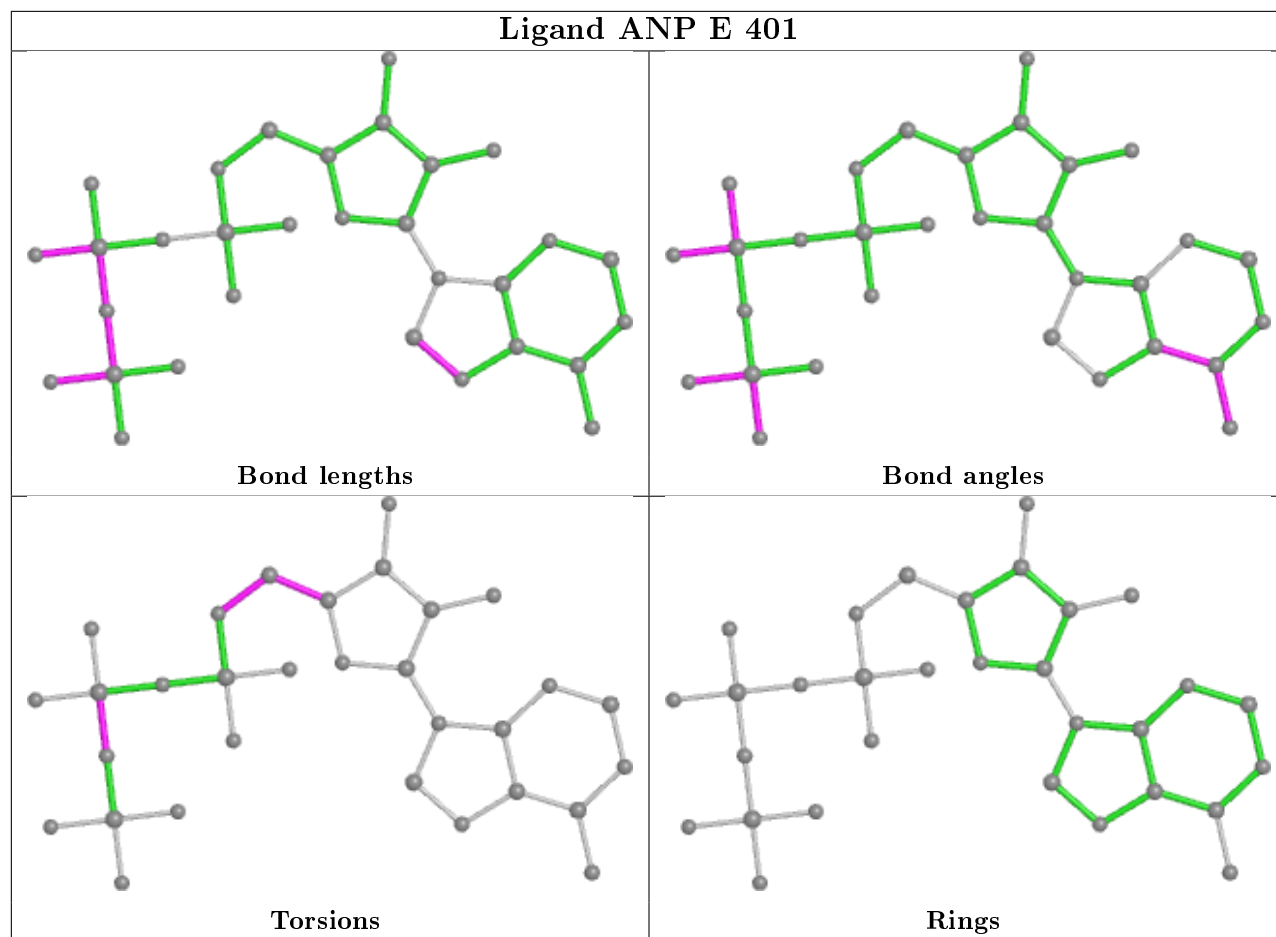
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	403	EDO	1	0
2	A	401	ANP	3	0
2	G	401	ANP	1	0
4	G	403	EDO	1	0
2	E	401	ANP	1	0
4	B	403	EDO	2	0
2	D	401	ANP	1	0
4	F	403	EDO	1	0
2	B	401	ANP	4	0
2	F	401	ANP	2	0
4	D	403	EDO	2	0
4	F	404	EDO	2	0

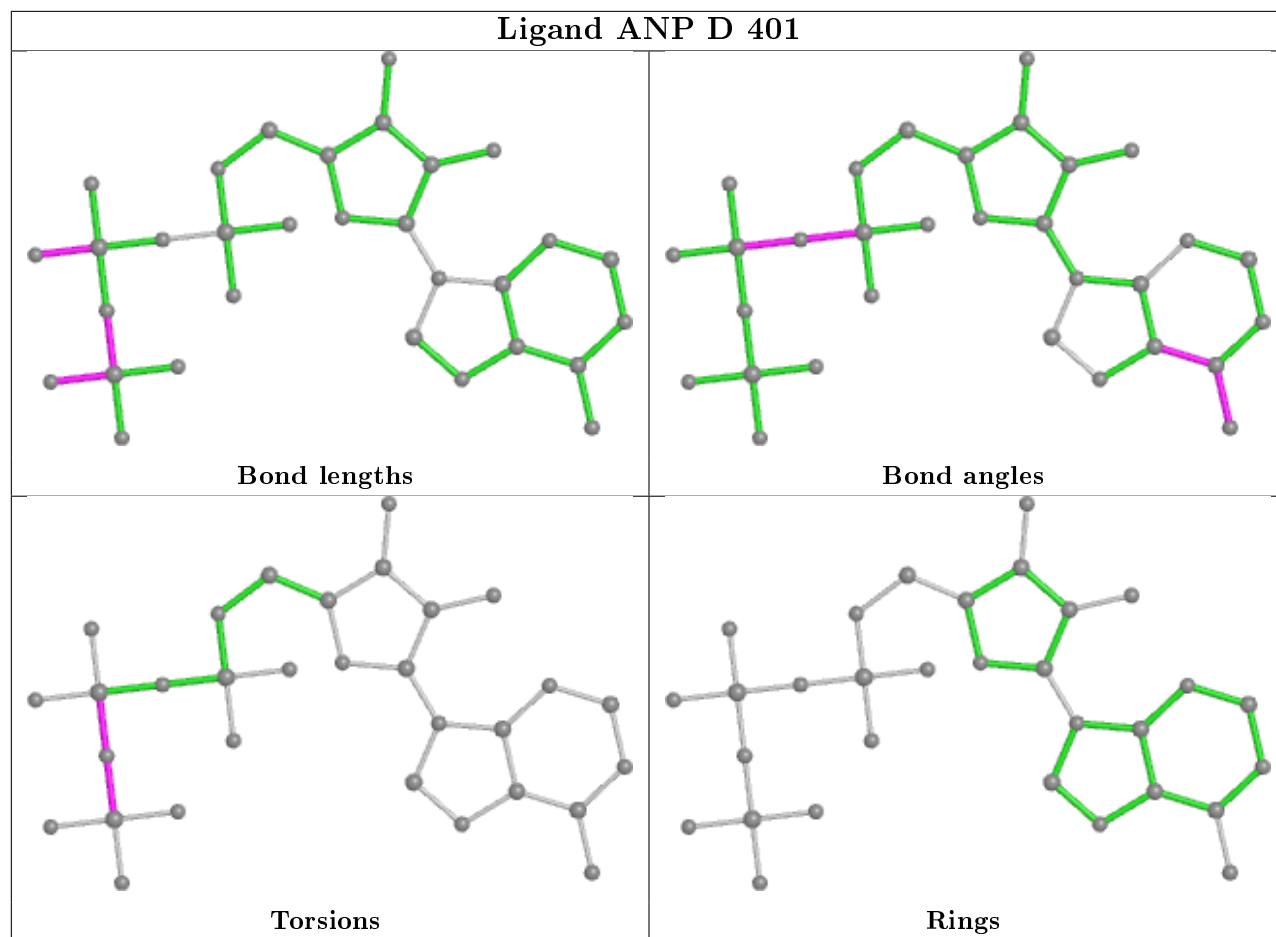
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

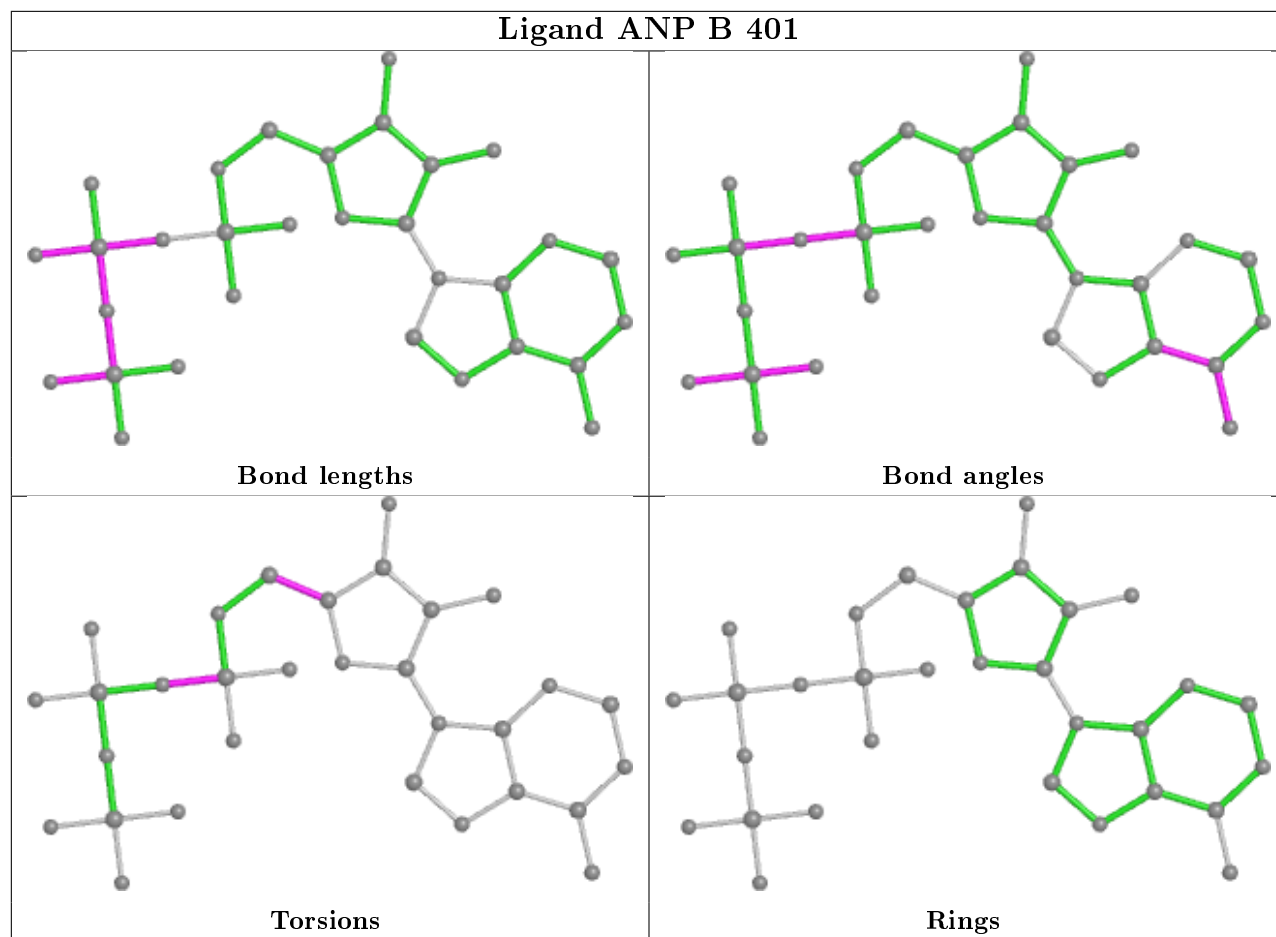


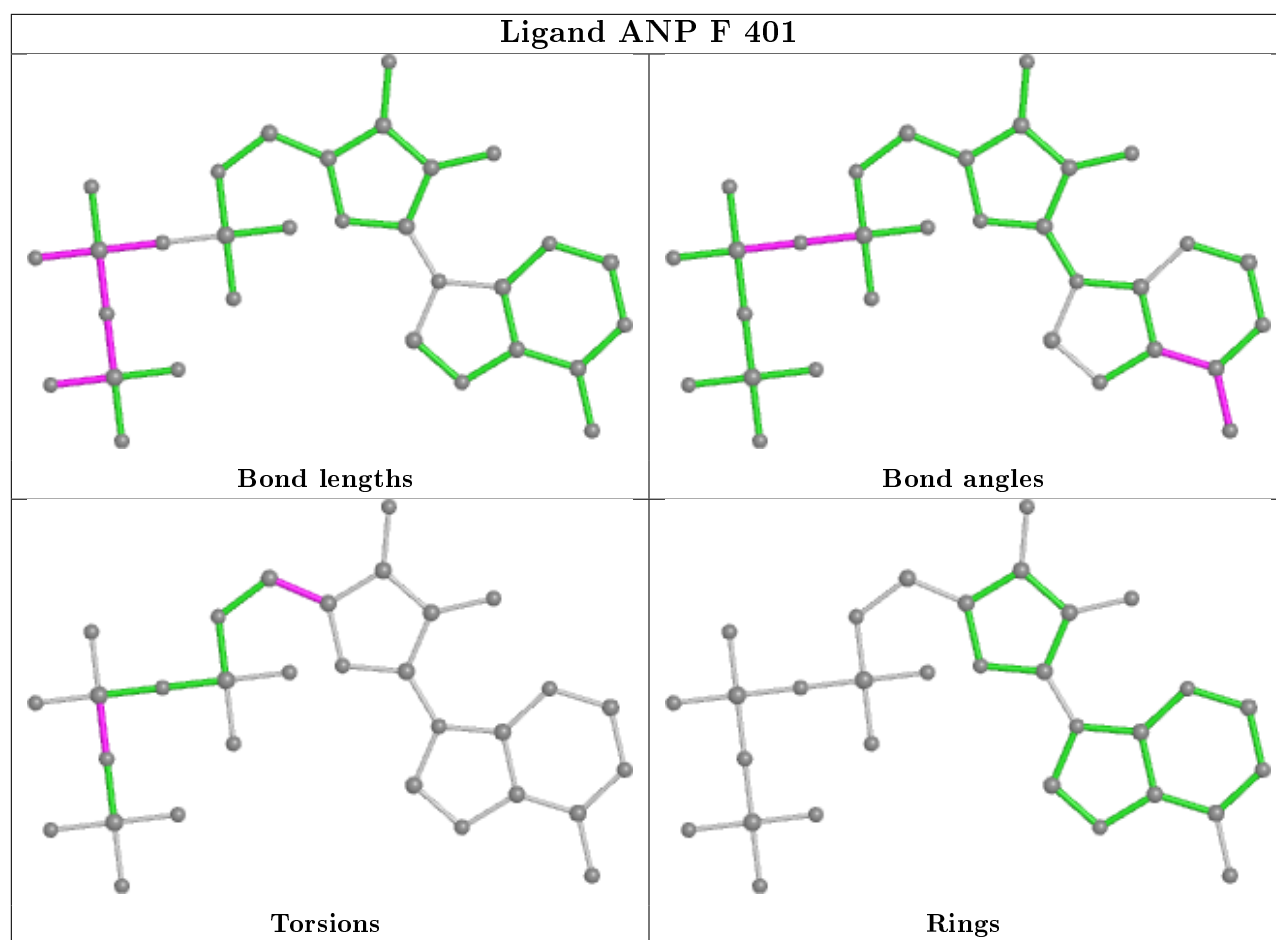












5.7 Other polymers [i](#)

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	246/267 (92%)	-0.20	5 (2%) 65 73	28, 46, 91, 146	0
1	B	245/267 (91%)	-0.15	7 (2%) 51 61	33, 52, 85, 131	0
1	C	248/267 (92%)	-0.20	9 (3%) 42 51	29, 49, 85, 124	0
1	D	246/267 (92%)	-0.14	1 (0%) 92 96	32, 50, 81, 132	0
1	E	246/267 (92%)	-0.24	4 (1%) 72 78	33, 48, 87, 127	0
1	F	245/267 (91%)	-0.13	9 (3%) 41 50	34, 51, 85, 123	0
1	G	246/267 (92%)	-0.26	4 (1%) 72 78	31, 48, 80, 128	0
All	All	1722/1869 (92%)	-0.19	39 (2%) 60 68	28, 49, 86, 146	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	192	PRO	4.8
1	D	130	HIS	4.4
1	C	130	HIS	4.1
1	E	130	HIS	4.1
1	A	130	HIS	4.1

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 carbohydrates in this entry.

6.4 Ligands ⓘ

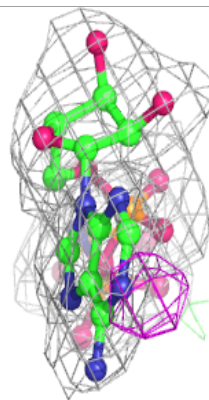
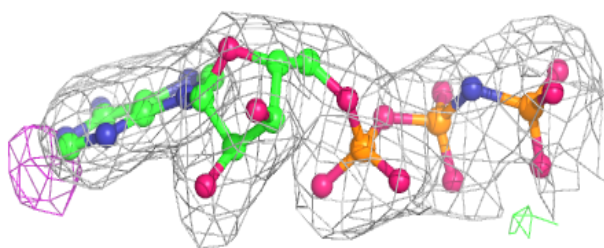
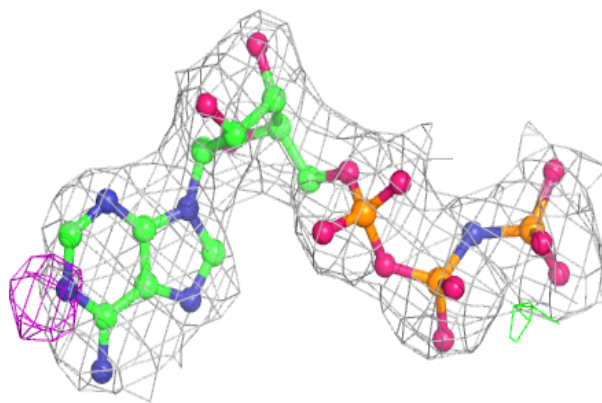
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	D	402	1/1	0.66	0.23	111,111,111,111	0
3	MG	F	402	1/1	0.68	0.10	100,100,100,100	0
3	MG	C	402	1/1	0.71	0.12	94,94,94,94	0
3	MG	E	402	1/1	0.72	0.11	73,73,73,73	0
4	EDO	D	404	4/4	0.73	0.32	57,65,66,68	0
4	EDO	A	404	4/4	0.75	0.27	63,66,66,68	0
3	MG	G	402	1/1	0.77	0.12	86,86,86,86	0
4	EDO	F	404	4/4	0.79	0.26	65,70,71,73	0
4	EDO	E	403	4/4	0.79	0.22	79,81,81,82	0
3	MG	B	402	1/1	0.83	0.08	86,86,86,86	0
4	EDO	F	403	4/4	0.83	0.20	68,68,70,72	0
4	EDO	B	403	4/4	0.85	0.22	56,56,62,62	0
4	EDO	E	404	4/4	0.85	0.23	55,58,64,67	0
4	EDO	G	404	4/4	0.87	0.30	67,72,77,78	0
4	EDO	G	403	4/4	0.89	0.18	67,67,74,74	0
3	MG	A	402	1/1	0.90	0.18	66,66,66,66	0
4	EDO	A	403	4/4	0.90	0.17	63,66,68,69	0
4	EDO	C	403	4/4	0.90	0.20	63,63,68,69	0
4	EDO	D	403	4/4	0.91	0.21	61,68,71,72	0
2	ANP	B	401	31/31	0.94	0.15	37,45,83,120	0
2	ANP	F	401	31/31	0.96	0.13	30,48,74,100	0
2	ANP	G	401	31/31	0.97	0.13	29,40,88,115	0
2	ANP	E	401	31/31	0.97	0.14	36,45,73,99	0
2	ANP	D	401	31/31	0.97	0.13	38,47,79,96	0
2	ANP	A	401	31/31	0.97	0.13	26,38,72,167	0
2	ANP	C	401	31/31	0.98	0.12	33,44,77,122	0

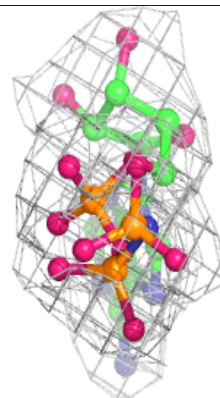
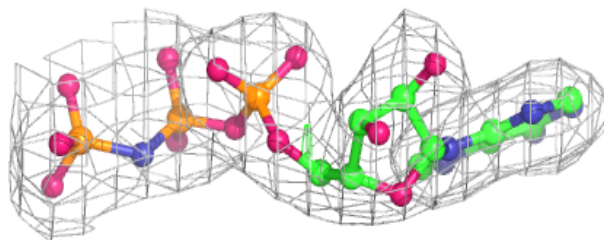
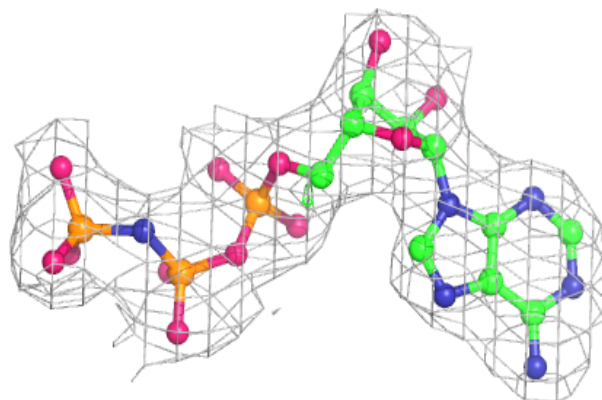
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP B 401:

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

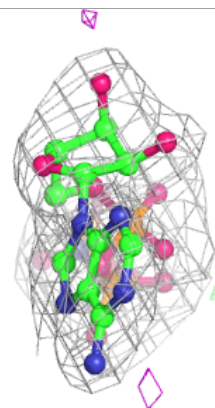
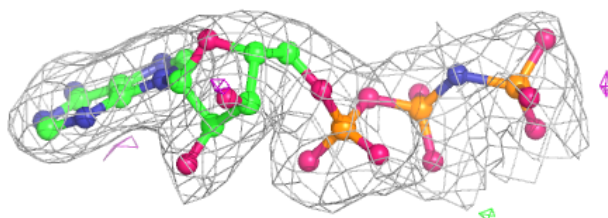
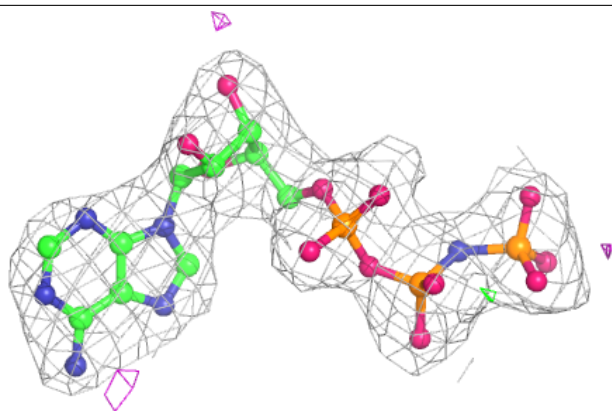
**Electron density around ANP F 401:**

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

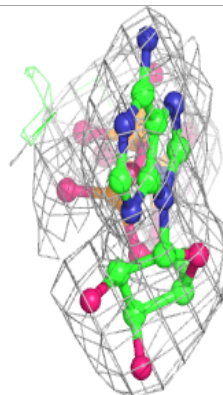
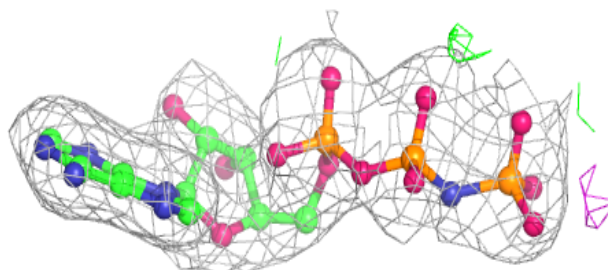
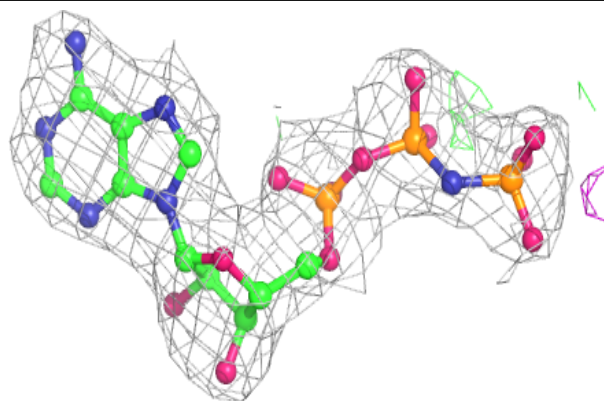


Electron density around ANP G 401:

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

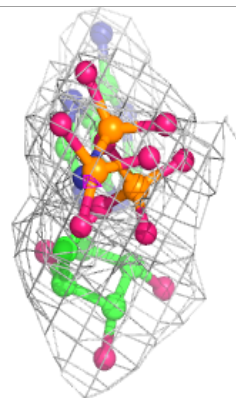
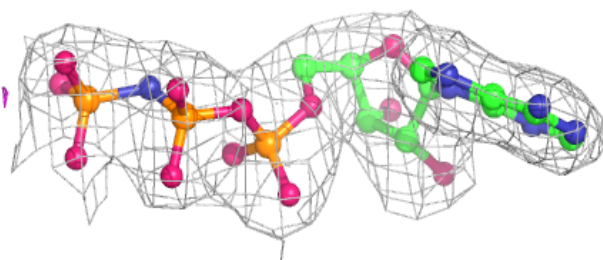
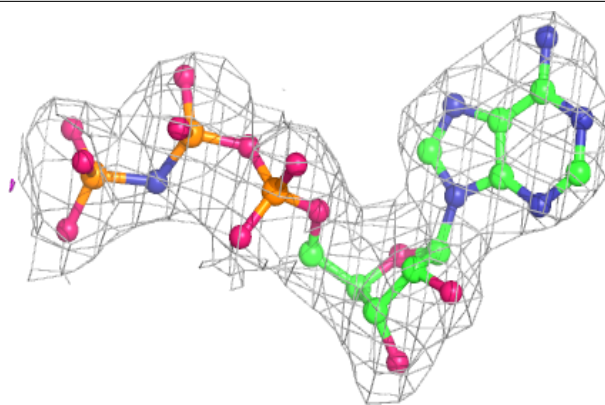
**Electron density around ANP E 401:**

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

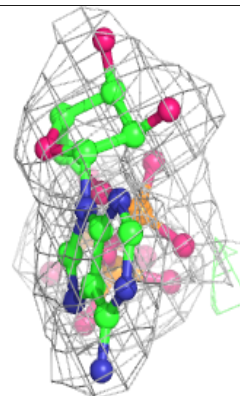
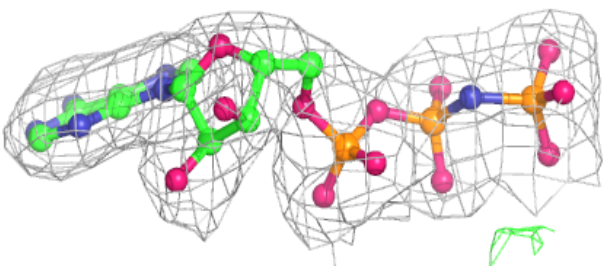
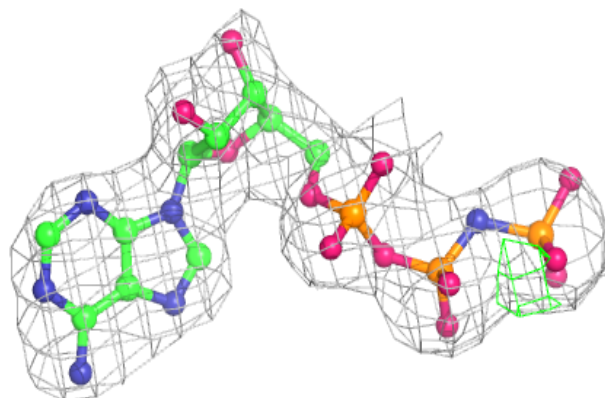


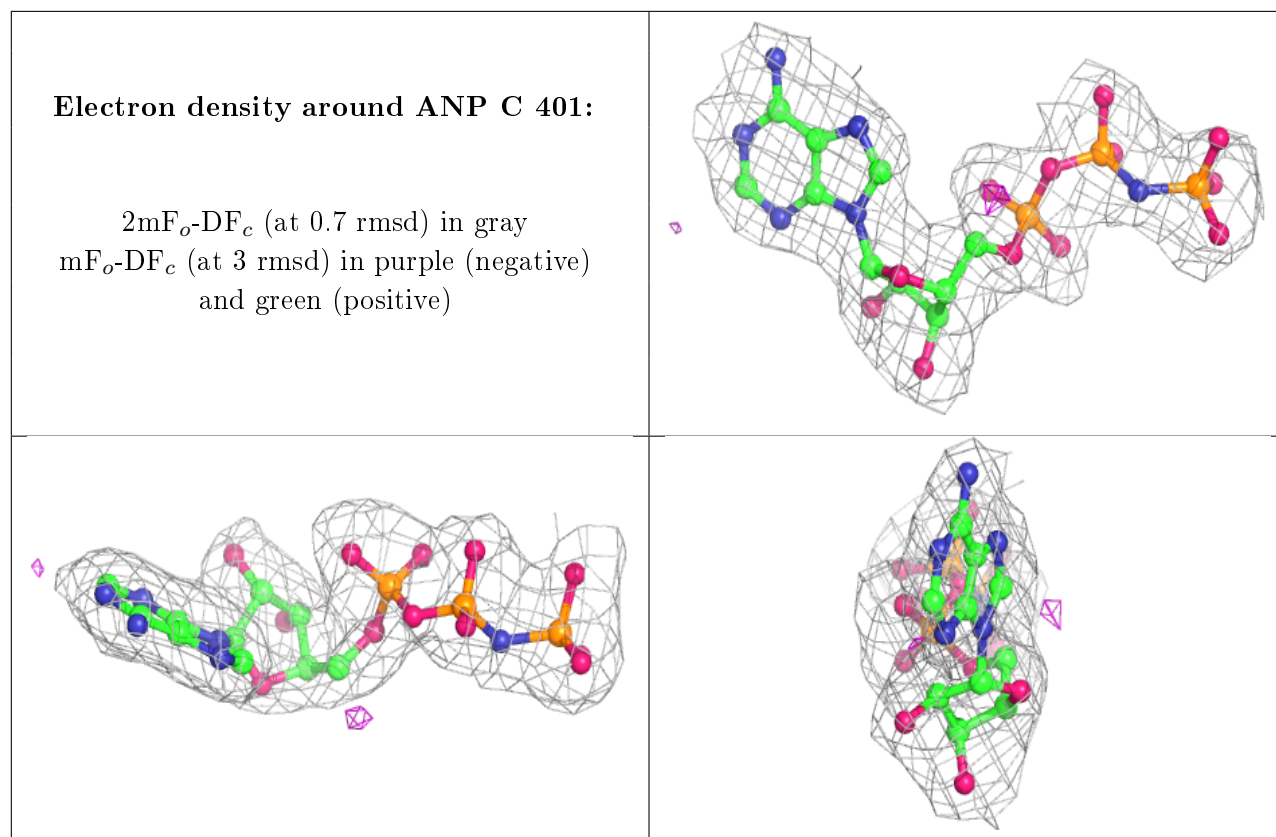
Electron density around ANP D 401:

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

**Electron density around ANP A 401:**

$2mF_o-DF_c$ (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.