W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2023 – 09:55 AM EDT

PDB ID	:	1PVO
Title	:	X-ray crystal structure of Rho transcription termination factor in complex with ssRNA substrate and ANPPNP
Authors	:	Skordalakes, E.; Berger, J.M.
Deposited on	:	2003-06-27
Resolution	:	3.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

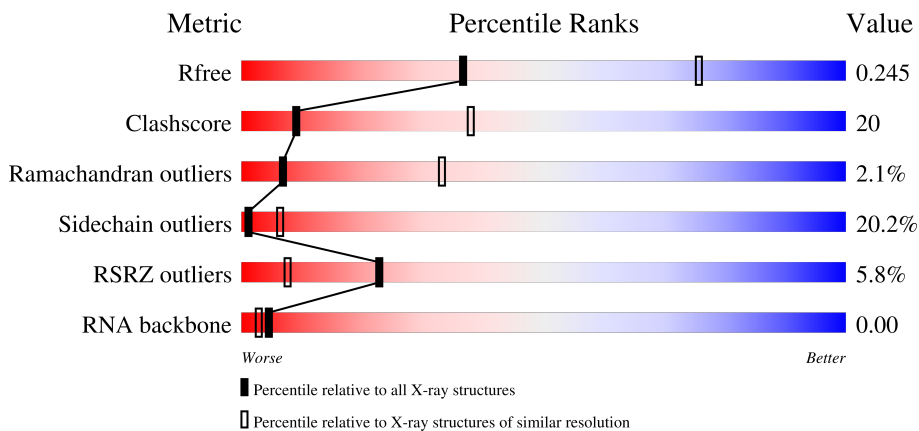|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.245
Clashscore		20
Ramachandran outliers		2.1%
Sidechain outliers		20.2%
RSRZ outliers		5.8%
RNA backbone		0.00

Worse *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=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	G	2	50% 50%
1	H	2	100% / 50% 50%
1	J	2	100% / 100%
1	K	2	100% / 100%

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Mol	Chain	Length	Quality of chain
1	L	2	50% · 50%
2	A	419	7% · 55% · 34% · 9% ·
2	B	419	9% · 43% · 32% · 11% · 15%
2	C	419	3% · 53% · 35% · 9% ·
2	D	419	3% · 47% · 39% · 11% ·
2	E	419	4% · 55% · 35% · 7% ·
2	F	419	6% · 51% · 34% · 11% · ·

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ANP	A	601	X	-	-	-
3	ANP	B	602	X	-	-	-
3	ANP	C	603	X	-	-	-
3	ANP	D	604	X	-	-	-
3	ANP	E	605	X	-	-	-
3	ANP	F	606	X	-	-	-

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 19246 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 RNA chain called 5'-R(P*UP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	2	Total	C	N	O	P	0	0	0
			40	18	5	15	2			
1	H	2	Total	C	N	O	P	0	0	0
			40	18	5	15	2			
1	J	2	Total	C	N	O	P	0	0	0
			40	18	5	15	2			
1	K	2	Total	C	N	O	P	0	0	0
			40	18	5	15	2			
1	L	2	Total	C	N	O	P	0	0	0
			40	18	5	15	2			

- Molecule 2 is a protein called Transcription termination factor rho.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	408	Total	C	N	O	S	0	0	0
			3208	2025	562	604	17			
2	B	358	Total	C	N	O	S	0	0	0
			2813	1776	494	529	14			
2	C	408	Total	C	N	O	S	0	0	0
			3208	2025	562	604	17			
2	D	408	Total	C	N	O	S	0	0	0
			3208	2025	562	604	17			
2	E	407	Total	C	N	O	S	0	0	0
			3201	2020	561	603	17			
2	F	408	Total	C	N	O	S	0	0	0
			3208	2025	562	604	17			

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).

ANP

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

- Molecule 4 is water.

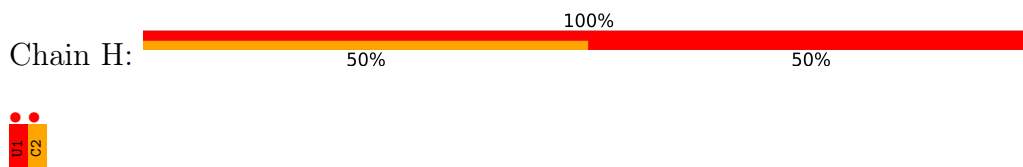| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	C	5	Total	O	0	0
			5	5		
4	D	4	Total	O	0	0
			4	4		
4	E	2	Total	O	0	0
			2	2		
4	F	2	Total	O	0	0
			2	2		

3 Residue-property plots ⓘ

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.
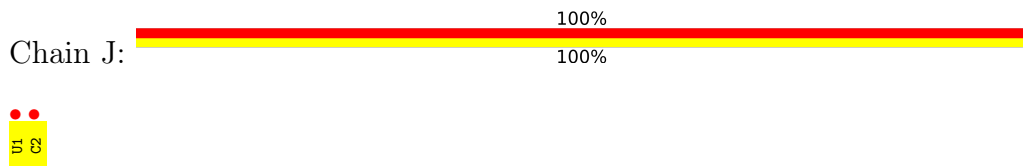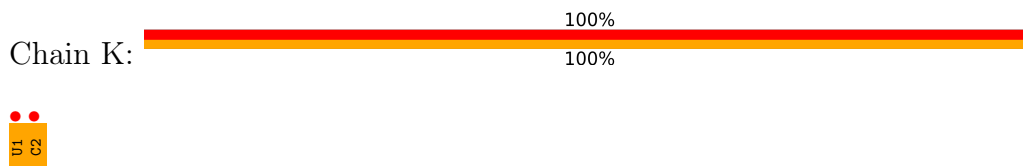
• Molecule 1: 5'-R(P*UP*C)-3'

Chain G:

• Molecule 1: 5'-R(P*UP*C)-3'

Chain H:

• Molecule 1: 5'-R(P*UP*C)-3'

Chain J:
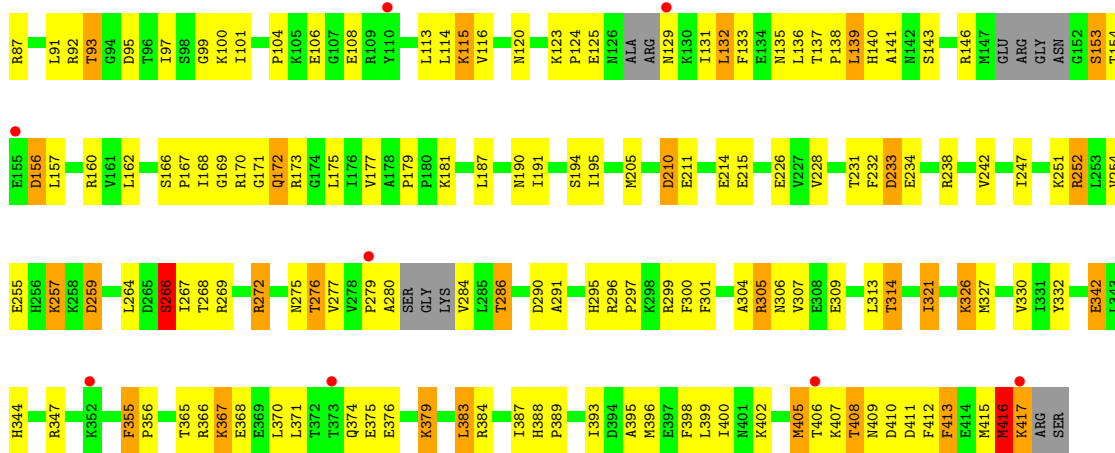
• Molecule 1: 5'-R(P*UP*C)-3'

Chain K:

• Molecule 1: 5'-R(P*UP*C)-3'

Chain L:

• Molecule 2: Transcription termination factor rho

Chain A:

• Molecule 2: Transcription termination factor rho

Chain B:

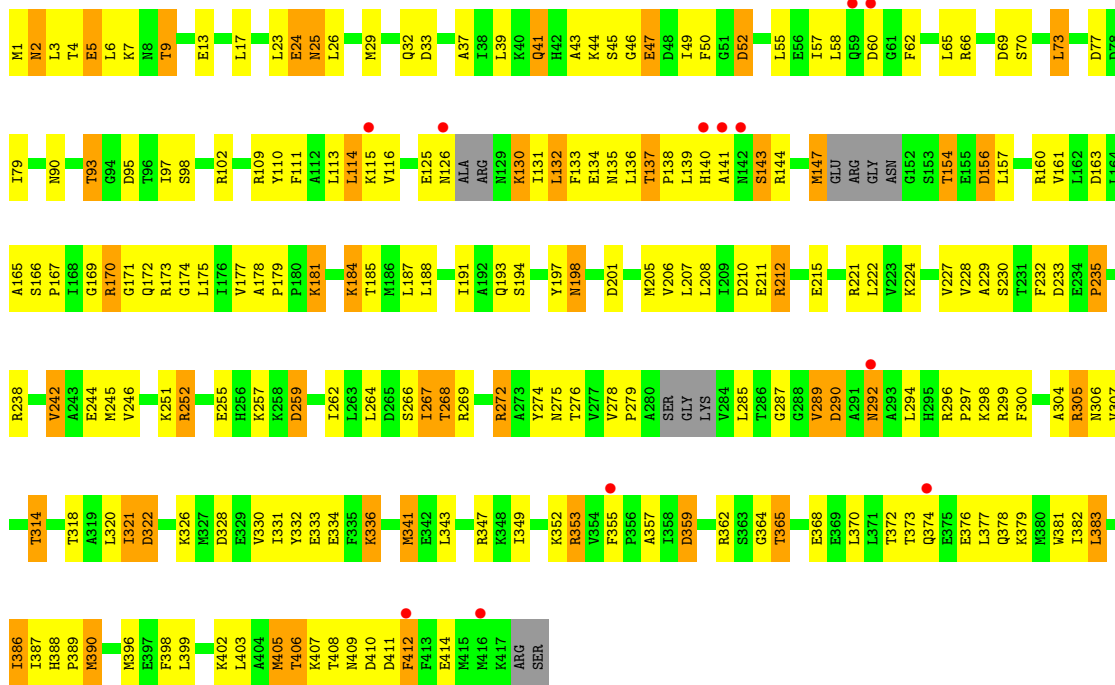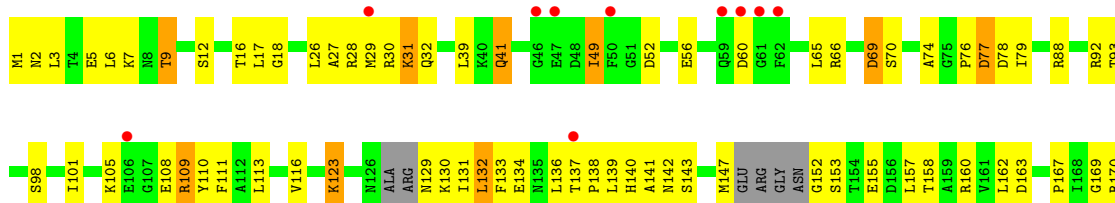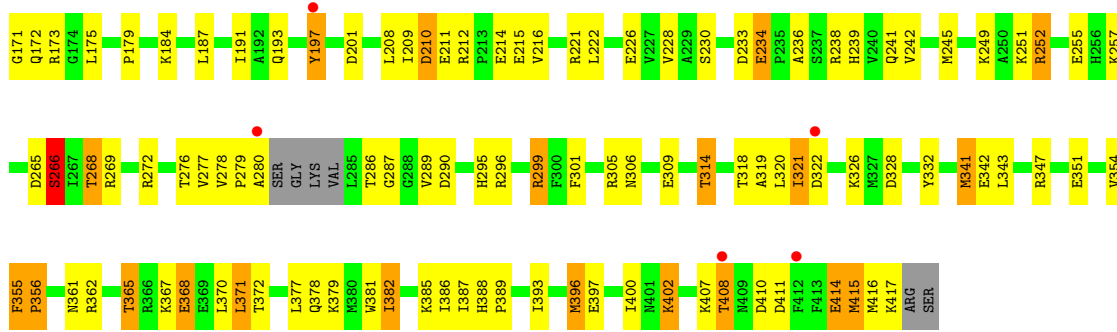• Molecule 2: Transcription termination factor rho

Chain C:

• Molecule 2: Transcription termination factor rho

• Molecule 2: Transcription termination factor rho

G171 Q172 R173 G174 L175 P179 K184 L187 I191 A192 Q193 Y197 D201 L208 I209 D210 E211 R212 P213 E214 E215 V216 R221 L222 E226 V227 V228 A229 S230 D233 E234 P235 A236 S237 R238 H239 V240 Q241 V242 M245 K249 A250 K251 R252 E255 H256 K257

D265 S266 I267 T268 R269 R272 T276 V277 V278 P279 A280 SER GLY LYS VAL L285 T286 G287 G288 V289 D290 H295 R296 R299 F300 F301 R305 N306 E309 T314 T318 A319 L320 I321 D322 K326 M327 D328 Y332 M341 E342 L343 R347 E351 V354

F355 P356 N361 R362 T365 R366 K367 E368 E369 L370 L371 T372 L377 Q378 K379 M380 W381 I382 K385 I386 I387 H388 P389 I393 M396 E397 I400 N401 K402 K407 T408 N409 D410 D411 F412 F413 E414 M416 K417 ARG SER

• **Molecule 2: Transcription termination factor rho**

Chain F:

M1 N2 L3 T4 E5 L6 K7 N8 T9 P10 V11 S12 T16 E19 N20 M21 G22 L23 E24 N25 L26 D33 I34 I35 F36 L39 K40 Q41 K44 S45 G46 E47 D48 I49 F50 G51 D52 G53 V54 L55 E56 I57 L58 Q59 D60 G61 F62 G63 F64 L65 D69 S70 S71 Y72

L73 A74 D77 D78 I79 Y80 R88 R92 T93 I97 I101 R102 P103 E106 Y110 L113 V116 D122 K123 P124 E125 N126 ALA ARG N129 L132 F133 E134 N135 T137 P138 L139 H140 A141 M142 S143 R144 L145 R146 M147 GLU ARG GLY ASN G152 R160 V161

L162 D163 L164 P167 I168 G171 Q172 R173 G174 L175 A178 P179 P180 K181 T185 M186 L187 L188 Q189 Q193 S194 I195 A196 Y197 D201 M205 V206 D210 E211 R212 P213 E214 E218 R221 E226 V227 V228 D233 E244 M245 V246 I247 E248 K249 A250 K251 R252

L253 V254 E255 K258 D259 V260 I261 I262 L263 L264 D265 S266 I267 T268 R269 R272 A273 Y274 N275 T276 V277 V278 P279 A280 SER GLY LYS V284 L285 T286 G287 G288 V289 D290 L294 H295 R296 P297 R298 R299 F300 A303 A304 R305 N306 V307 E308 E309 L313 T314 I315 I316 A319 L320

I321 K326 M327 I331 F335 G339 N340 M341 E342 L343 H344 L345 S346 R347 K348 I349 R353 V354 F355 P356 A357 I358 N361 T365 R366 K367 E368 E369 L370 Q374 E375 E376 L377 W381 I382 L383 R384 K385 I386 I387 H388 P389 M390 G391 E392 I393 E397 I400

L403 A404 M405 T406 K407 T408 N409 D410 D411 F412 F413 E414 M415 M416 K417 ARG SER

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	119.25Å 204.65Å 147.79Å 90.00° 96.54° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 29.88 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.7 (20.00-3.00) 96.3 (29.88-3.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.40 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.271 , 0.304 0.239 , 0.245	Depositor DCC
R_{free} test set	3403 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	89.5	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 114.4	EDS
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	19246	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: ANP

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	G	0.69	0/43	1.40	1/64 (1.6%)
1	H	0.80	0/43	1.34	1/64 (1.6%)
1	J	0.82	0/43	1.05	0/64
1	K	0.98	0/43	1.54	1/64 (1.6%)
1	L	0.69	0/43	1.39	1/64 (1.6%)
2	A	0.42	0/3253	0.71	11/4379 (0.3%)
2	B	0.43	0/2854	0.71	9/3844 (0.2%)
2	C	0.56	0/3253	0.76	7/4379 (0.2%)
2	D	0.51	0/3253	0.75	10/4379 (0.2%)
2	E	0.49	0/3246	0.74	11/4369 (0.3%)
2	F	0.42	0/3253	0.70	14/4379 (0.3%)
All	All	0.48	0/19327	0.74	66/26049 (0.3%)

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
2	B	0	1
2	E	0	3
2	F	1	1
All	All	1	5

There are no bond length outliers.

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	77	ASP	CB-CG-OD2	7.04	124.64	118.30
1	G	1	U	P-O3'-C3'	6.65	127.68	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	95	ASP	CB-CG-OD2	6.63	124.26	118.30
2	A	265	ASP	CB-CG-OD2	6.28	123.95	118.30
2	F	233	ASP	CB-CG-OD2	6.25	123.92	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	F	355	PHE	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	355	PHE	Peptide
2	E	266	SER	Peptide
2	E	355	PHE	Peptide
2	E	371	LEU	Peptide
2	F	24	GLU	Peptide

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	G	40	0	22	0	0
1	H	40	0	22	2	0
1	J	40	0	22	3	0
1	K	40	0	22	4	0
1	L	40	0	22	3	0
2	A	3208	0	3284	116	0
2	B	2813	0	2870	126	0
2	C	3208	0	3284	152	0
2	D	3208	0	3284	149	0
2	E	3201	0	3275	142	0
2	F	3208	0	3284	124	0
3	A	31	0	7	3	0
3	B	31	0	7	0	0
3	C	31	0	7	0	0
3	D	31	0	7	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	31	0	7	0	0
3	F	31	0	7	0	0
4	A	1	0	0	0	0
4	C	5	0	0	0	0
4	D	4	0	0	0	0
4	E	2	0	0	1	0
4	F	2	0	0	0	0
All	All	19246	0	19433	778	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 20.

The worst 5 of 778 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)
2:B:272:ARG:HG3	2:B:272:ARG:HH11	1.01	1.10
2:C:355:PHE:HB2	2:C:356:PRO:HD3	1.26	1.09
2:F:353:ARG:HG3	2:F:353:ARG:HH11	1.06	1.09
2:C:30:ARG:HG2	2:C:30:ARG:HH11	1.14	1.09
2:C:272:ARG:HG3	2:C:272:ARG:HH11	0.92	1.09

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	400/419 (96%)	367 (92%)	30 (8%)	3 (1%)	19	57
2	B	350/419 (84%)	313 (89%)	25 (7%)	12 (3%)	3	20
2	C	400/419 (96%)	361 (90%)	32 (8%)	7 (2%)	8	37
2	D	400/419 (96%)	363 (91%)	27 (7%)	10 (2%)	5	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	399/419 (95%)	370 (93%)	25 (6%)	4 (1%)	15	53
2	F	400/419 (96%)	351 (88%)	35 (9%)	14 (4%)	3	20
All	All	2349/2514 (93%)	2125 (90%)	174 (7%)	50 (2%)	7	33

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	356	PRO
2	C	50	PHE
2	C	355	PHE
2	D	47	GLU
2	D	181	LYS

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	
2	A	350/359 (98%)	271 (77%)	79 (23%)	1	4
2	B	306/359 (85%)	242 (79%)	64 (21%)	1	5
2	C	350/359 (98%)	284 (81%)	66 (19%)	1	8
2	D	350/359 (98%)	273 (78%)	77 (22%)	1	4
2	E	349/359 (97%)	289 (83%)	60 (17%)	2	10
2	F	350/359 (98%)	280 (80%)	70 (20%)	1	7
All	All	2055/2154 (95%)	1639 (80%)	416 (20%)	1	6

5 of 416 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	114	LEU
2	E	9	THR
2	F	368	GLU
2	D	138	PRO
2	D	272	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	306	ASN
2	E	306	ASN
2	D	32	GLN
2	F	41	GLN
2	E	41	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	G	2/2 (100%)	1 (50%)	1 (50%)
1	H	2/2 (100%)	1 (50%)	1 (50%)
1	J	1/2 (50%)	0	0
1	K	2/2 (100%)	1 (50%)	1 (50%)
1	L	2/2 (100%)	1 (50%)	1 (50%)
All	All	9/10 (90%)	4 (44%)	4 (44%)

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	G	2	C
1	H	2	C
1	K	2	C
1	L	2	C

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	G	1	U
1	H	1	U
1	K	1	U
1	L	1	U

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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 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	ANP	B	602	-	29,33,33	4.21	12 (41%)	31,52,52	2.76	16 (51%)
3	ANP	D	604	-	29,33,33	4.28	13 (44%)	31,52,52	2.69	15 (48%)
3	ANP	F	606	-	29,33,33	4.23	13 (44%)	31,52,52	2.69	15 (48%)
3	ANP	E	605	-	29,33,33	4.33	13 (44%)	31,52,52	2.70	15 (48%)
3	ANP	C	603	-	29,33,33	4.25	11 (37%)	31,52,52	2.68	14 (45%)
3	ANP	A	601	-	29,33,33	4.16	14 (48%)	31,52,52	2.87	16 (51%)

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	ANP	B	602	-	3/3/7/8	6/14/38/38	0/3/3/3
3	ANP	D	604	-	2/2/7/8	6/14/38/38	0/3/3/3
3	ANP	F	606	-	2/2/7/8	6/14/38/38	0/3/3/3
3	ANP	E	605	-	2/2/7/8	6/14/38/38	0/3/3/3
3	ANP	C	603	-	3/3/7/8	7/14/38/38	0/3/3/3
3	ANP	A	601	-	3/3/7/8	4/14/38/38	0/3/3/3

The worst 5 of 76 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	605	ANP	C2'-C1'	-14.09	1.32	1.53

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	604	ANP	C2'-C1'	-13.82	1.32	1.53
3	F	606	ANP	C2'-C1'	-13.57	1.33	1.53
3	C	603	ANP	C2'-C1'	-13.53	1.33	1.53
3	A	601	ANP	C2'-C1'	-13.26	1.33	1.53

The worst 5 of 91 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	ANP	C3'-C2'-C1'	5.85	109.79	100.98
3	C	603	ANP	C3'-C2'-C1'	5.79	109.70	100.98
3	B	602	ANP	C3'-C2'-C1'	5.65	109.48	100.98
3	D	604	ANP	C3'-C2'-C1'	5.56	109.34	100.98
3	E	605	ANP	C3'-C2'-C1'	5.47	109.22	100.98

5 of 15 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	601	ANP	C3'
3	A	601	ANP	C2'
3	A	601	ANP	C4'
3	B	602	ANP	C3'
3	B	602	ANP	C1'

5 of 35 torsion outliers are listed below:

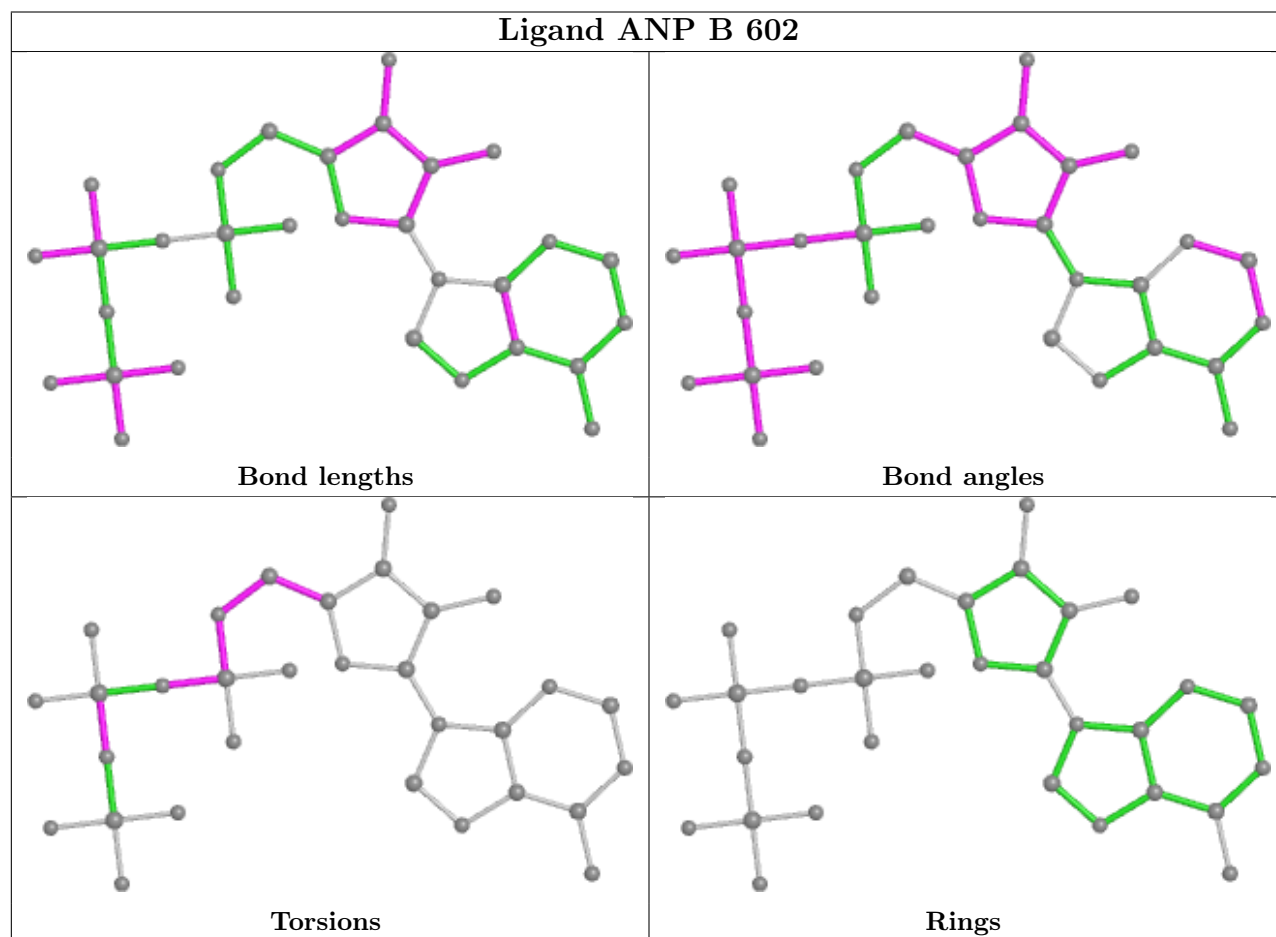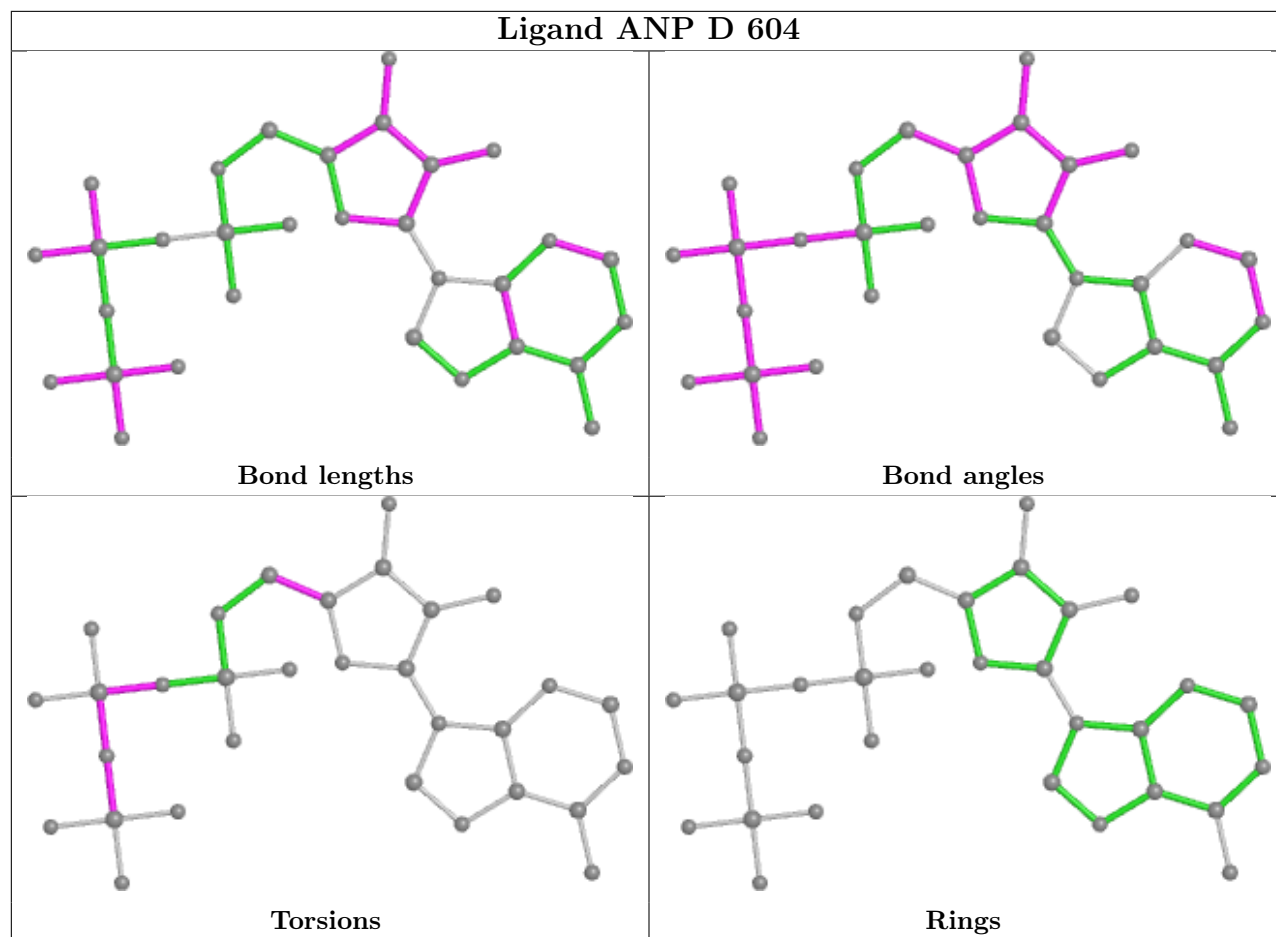| Mol	Chain	Res	Type	Atoms
3	A	601	ANP	PB-N3B-PG-O1G
3	A	601	ANP	PG-N3B-PB-O1B
3	A	601	ANP	C3'-C4'-C5'-O5'
3	B	602	ANP	PG-N3B-PB-O1B
3	B	602	ANP	O4'-C4'-C5'-O5'

There are no ring outliers.
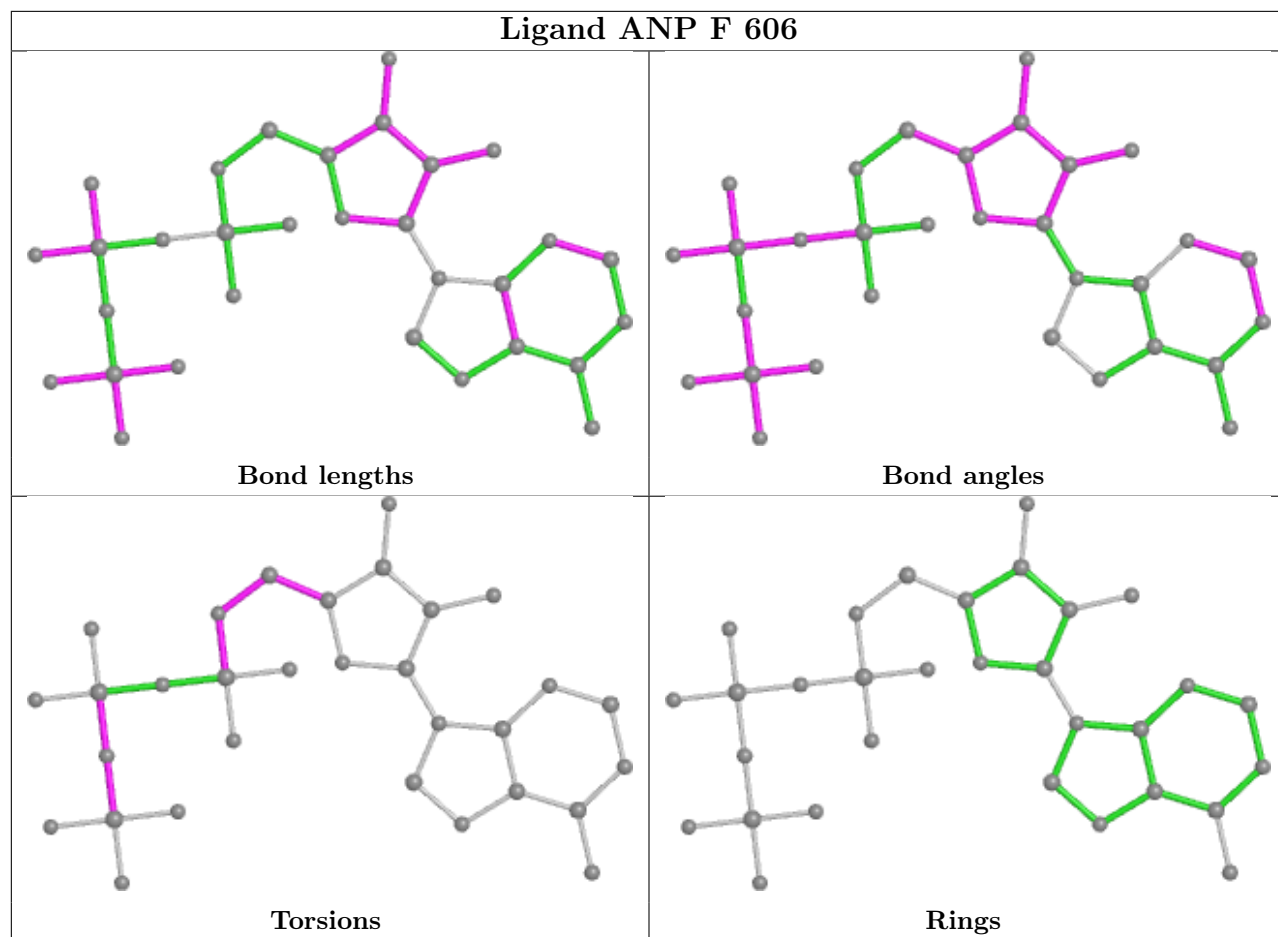
1 monomer is involved in 3 short contacts:

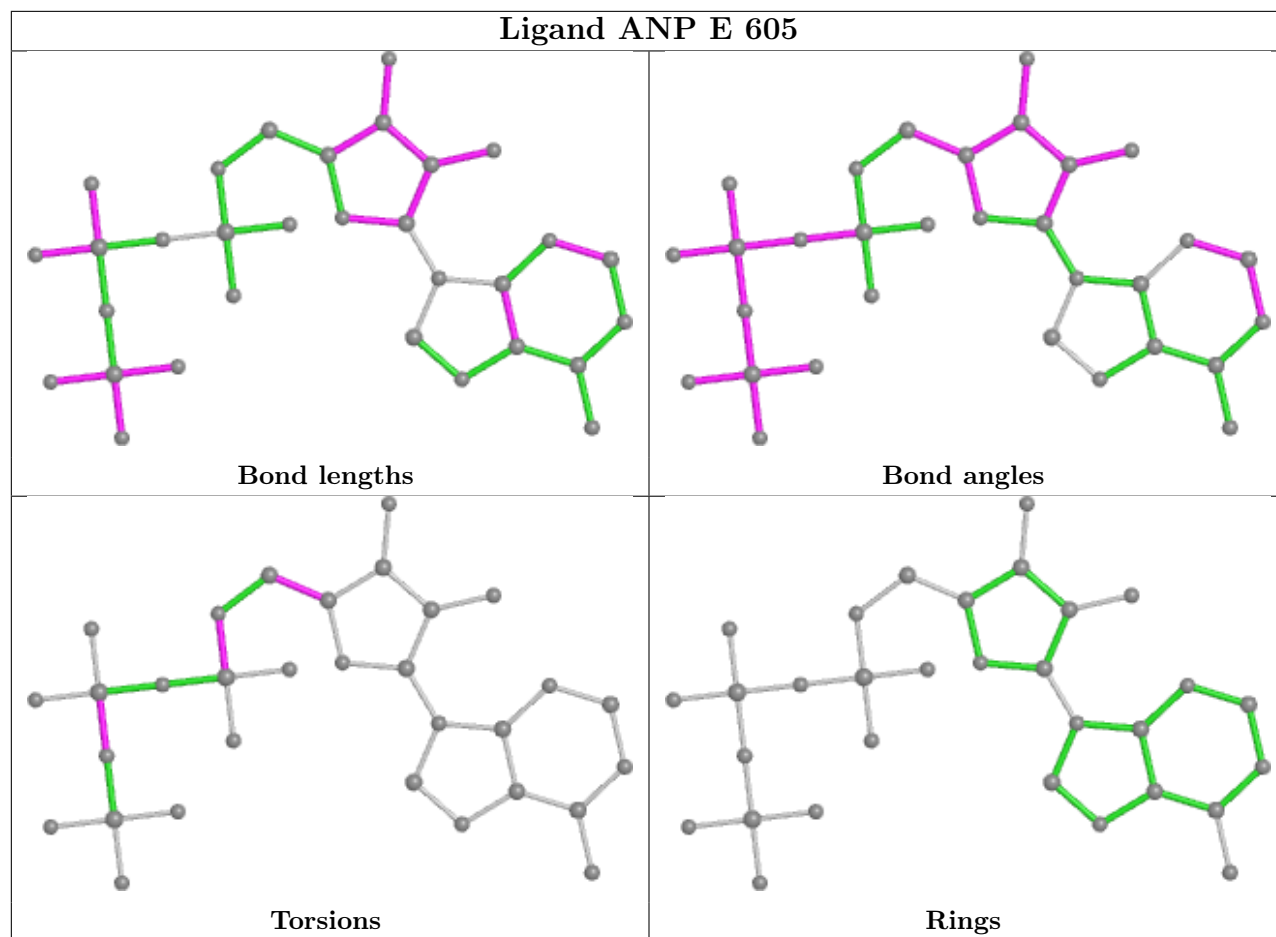| Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	ANP	3	0

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 then 5% of the Mogul distribution of torsion angles is
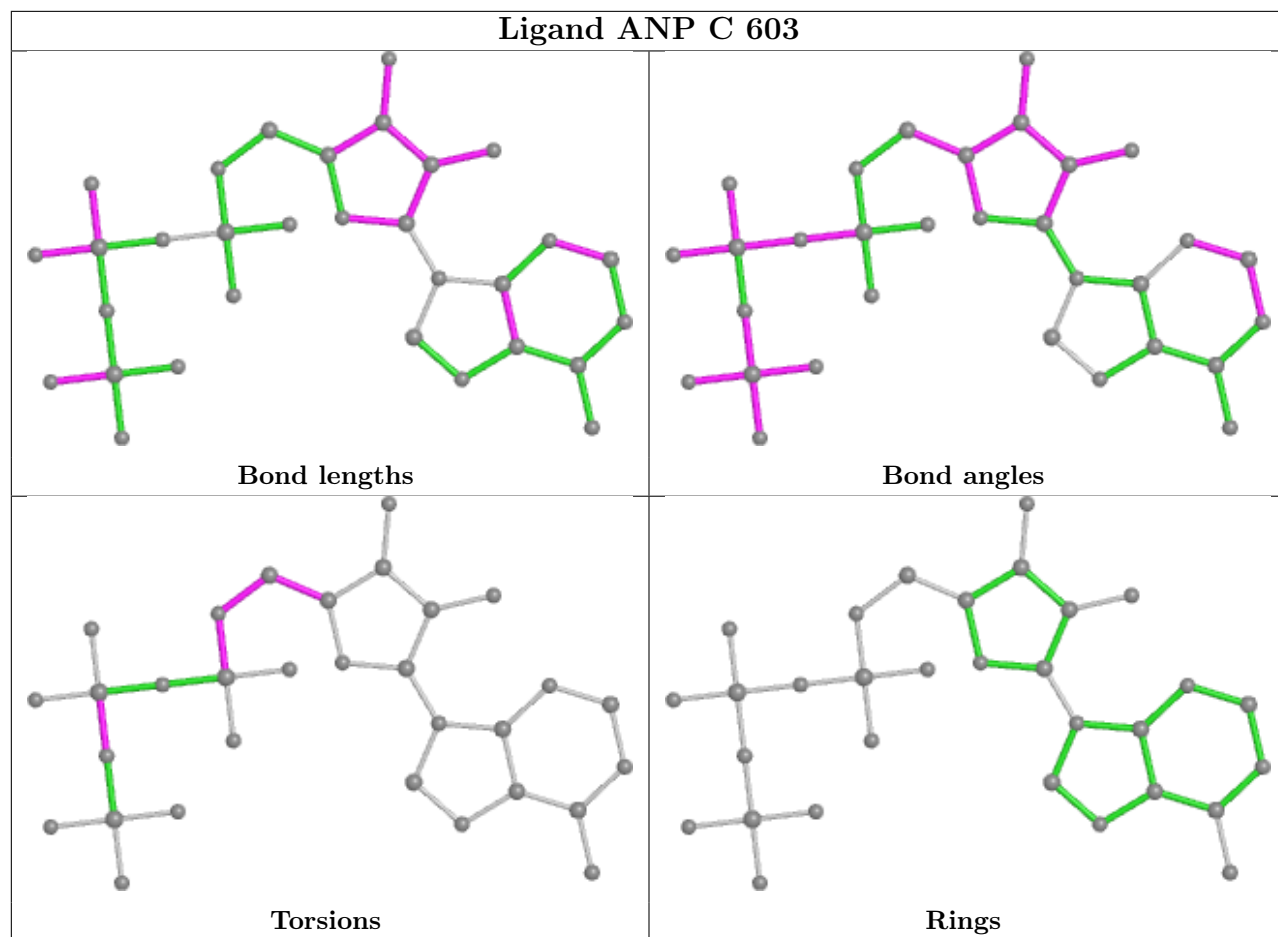
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.
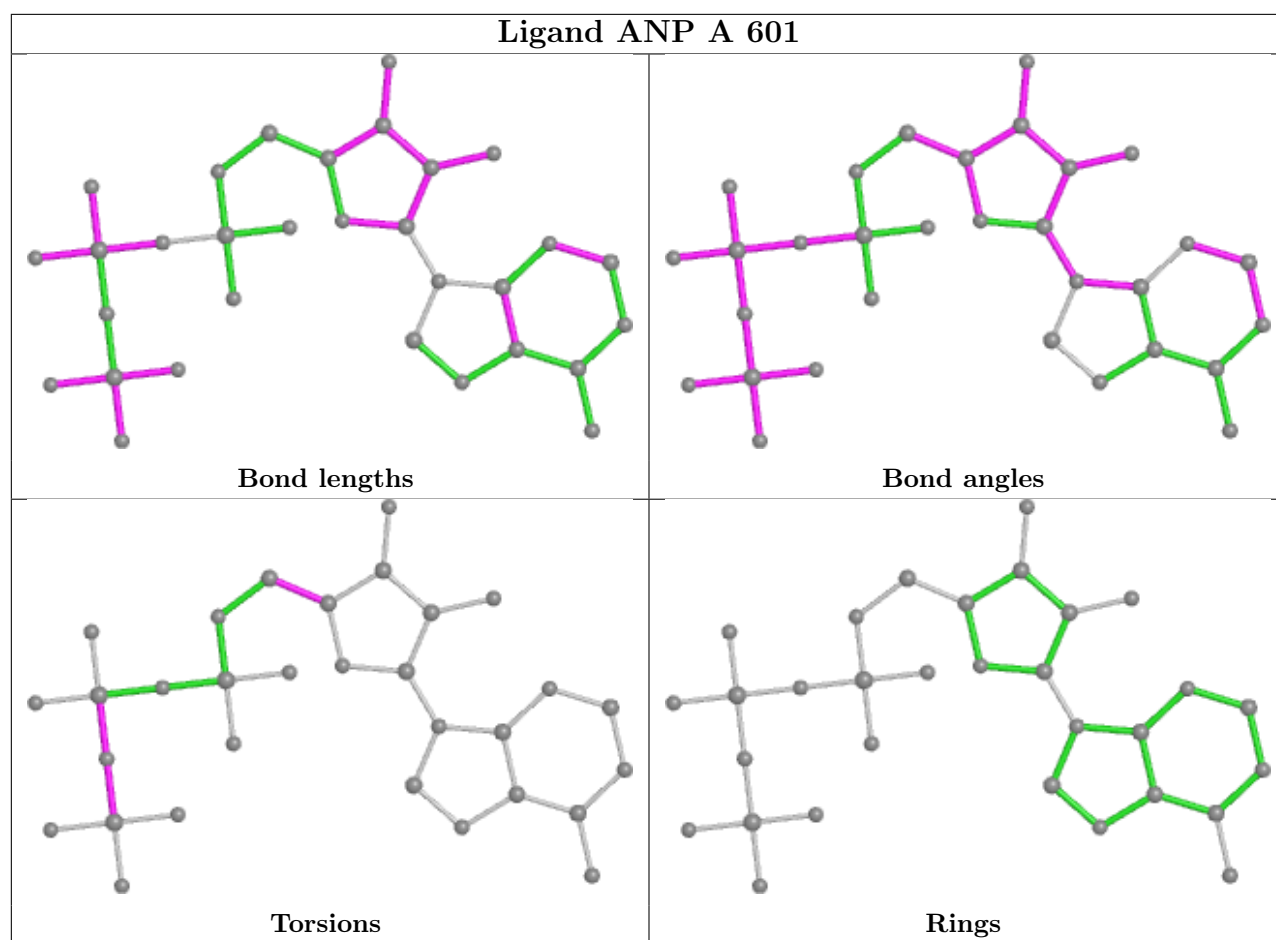

Ligand ANP B 602

Bond lengths

Bond angles

Torsions

Rings

Ligand ANP D 604

Bond lengths

Bond angles

Torsions

Rings

Ligand ANP F 606

Bond lengths

Bond angles

Torsions

Rings

Ligand ANP E 605

Bond lengths

Bond angles

Torsions

Rings

Ligand ANP C 603

Bond lengths

Bond angles

Torsions

Rings

Ligand ANP A 601

Bond lengths

Bond angles

Torsions

Rings

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	G	2/2 (100%)	1.31	0	100	100	150, 150, 150, 150	0
1	H	2/2 (100%)	2.53	2 (100%)	0	0	150, 150, 150, 150	0
1	J	2/2 (100%)	4.25	2 (100%)	0	0	150, 150, 150, 150	0
1	K	2/2 (100%)	3.93	2 (100%)	0	0	150, 150, 150, 150	0
1	L	2/2 (100%)	1.55	0	100	100	150, 150, 150, 150	0
2	A	408/419 (97%)	0.41	30 (7%)	14	4	42, 66, 114, 127	0
2	B	358/419 (85%)	0.53	37 (10%)	6	2	35, 65, 112, 127	0
2	C	408/419 (97%)	0.14	13 (3%)	47	20	20, 43, 96, 103	0
2	D	408/419 (97%)	0.14	12 (2%)	51	23	18, 46, 72, 124	0
2	E	407/419 (97%)	0.10	15 (3%)	41	17	21, 46, 85, 123	0
2	F	408/419 (97%)	0.32	26 (6%)	19	6	39, 65, 105, 119	0
All	All	2407/2524 (95%)	0.28	139 (5%)	23	7	18, 56, 104, 150	0

The worst 5 of 139 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	51	GLY	7.8
2	A	286	THR	6.1
2	A	412	PHE	6.1
2	B	88	ARG	6.0
1	K	2	C	5.7

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

WORLDWIDE
wwPDB
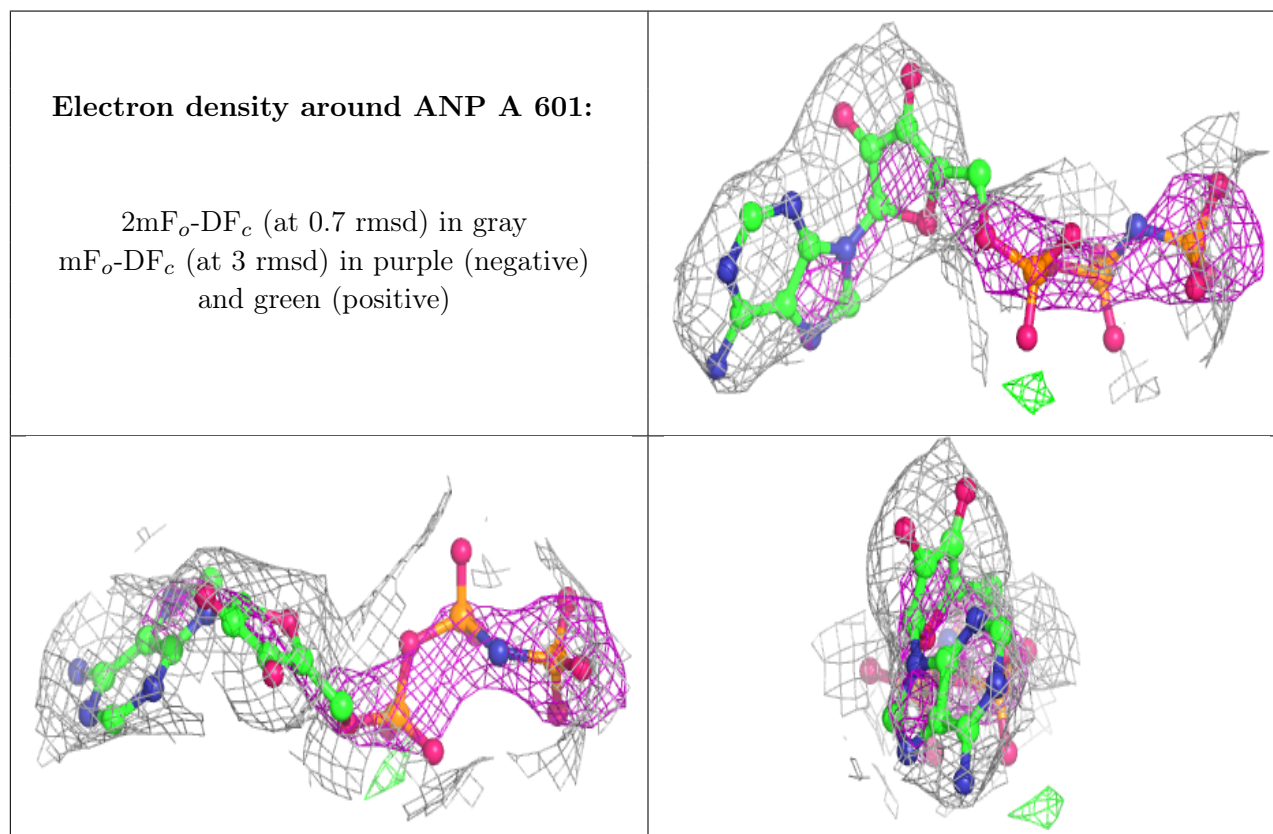PROTEIN DATA BANK

6.3 Carbohydrates (i)
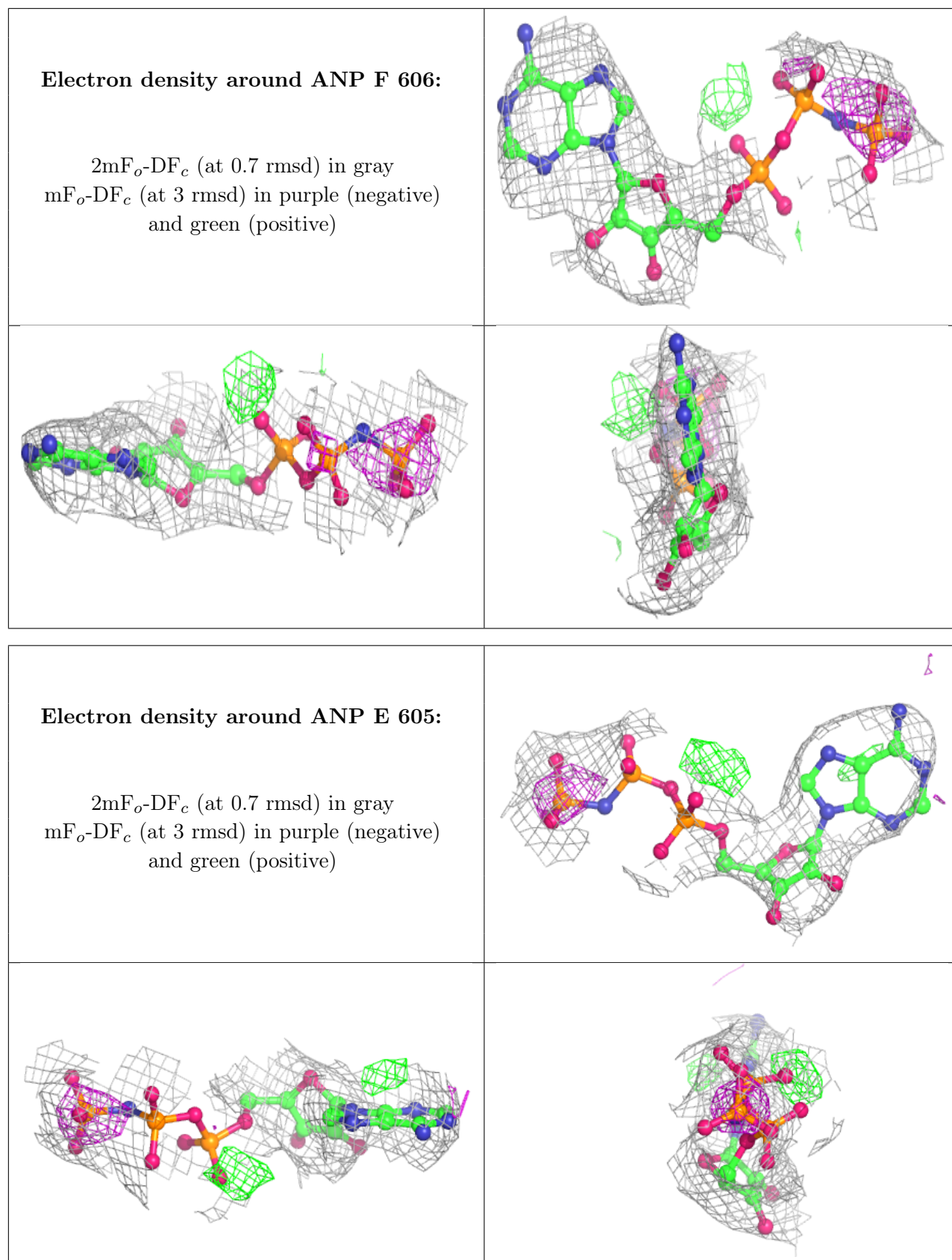
There are no monosaccharides in this entry.

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(Å^2)	Q<0.9
3	ANP	A	601	31/31	0.72	0.32	150,150,150,150	0
3	ANP	F	606	31/31	0.80	0.24	150,150,150,150	0
3	ANP	E	605	31/31	0.83	0.21	150,150,150,150	0
3	ANP	B	602	31/31	0.84	0.17	150,150,150,150	0
3	ANP	C	603	31/31	0.84	0.18	150,150,150,150	0
3	ANP	D	604	31/31	0.86	0.20	150,150,150,150	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.
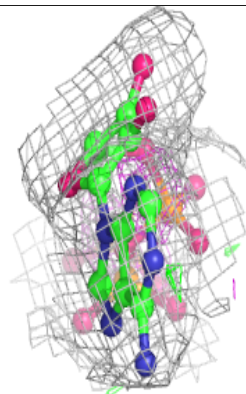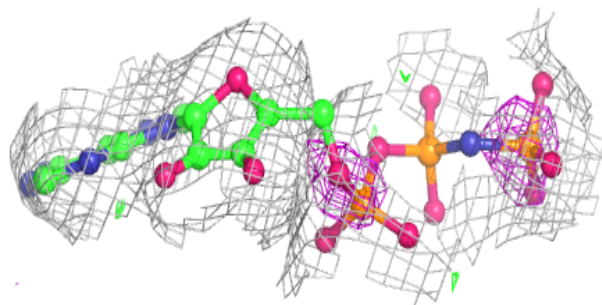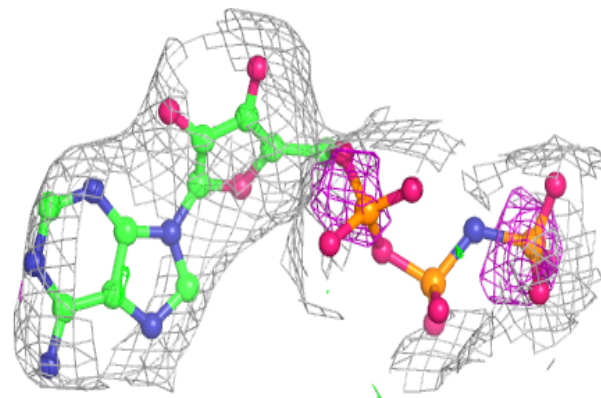

Electron density around ANP A 601:

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

Electron density around ANP F 606:

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

Electron density around ANP E 605:

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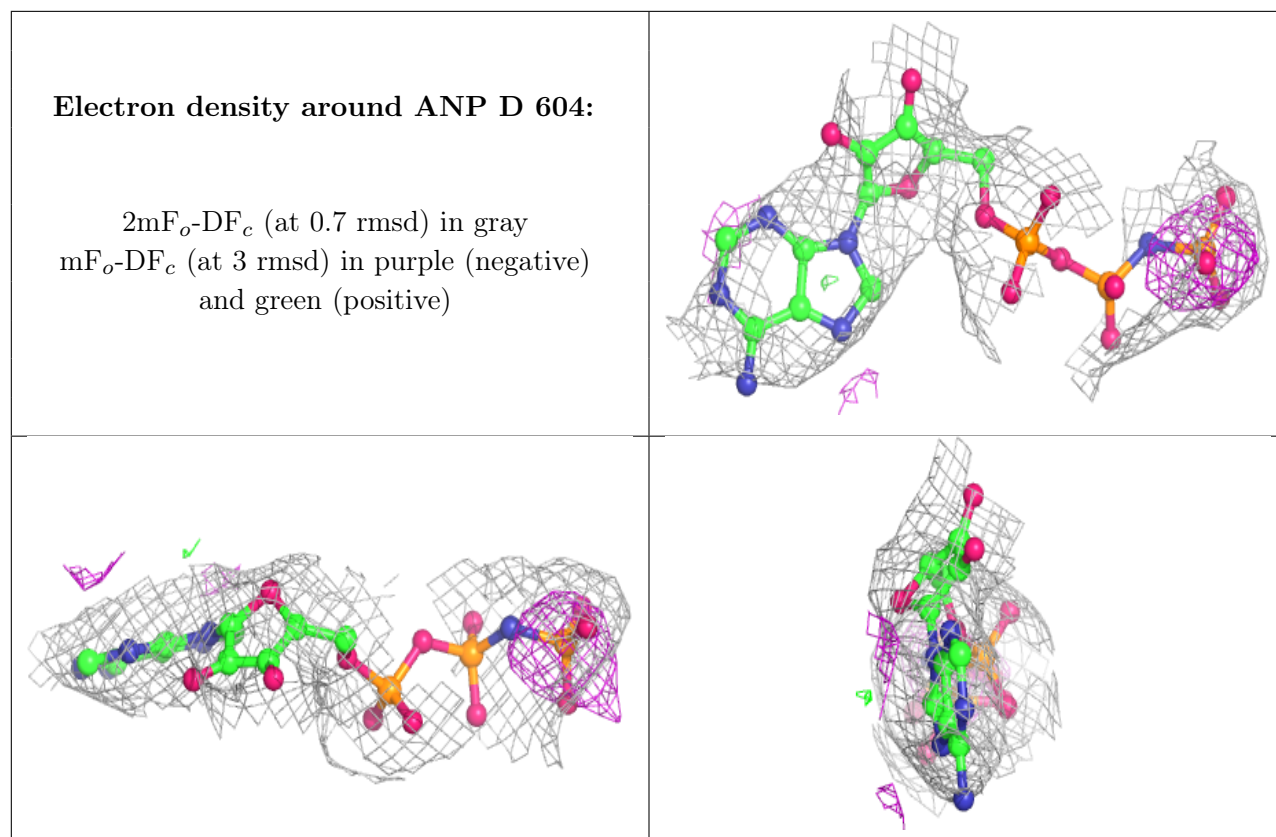and green (positive)

Electron density around ANP B 602:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
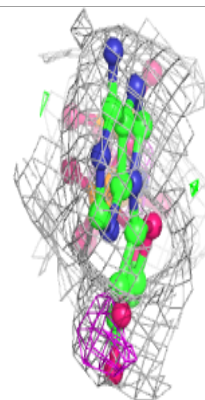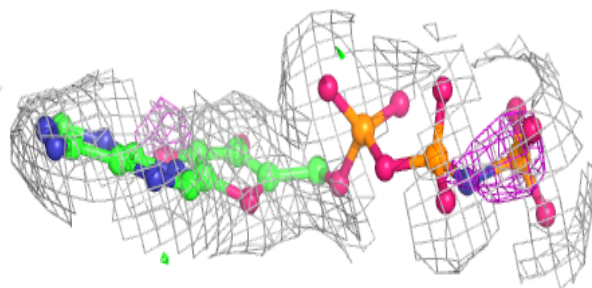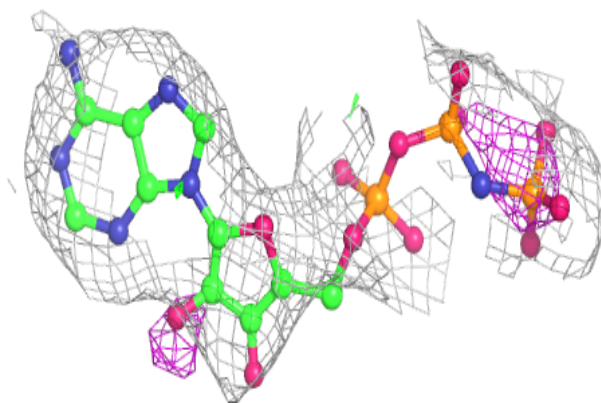
Electron density around ANP C 603:

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

Electron density around ANP D 604:

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

6.5 Other polymers (i)

There are no such residues in this entry.