



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:12 AM UTC

PDB ID : 8ZN7 / pdb_00008zn7
Title : Crystal Structure of Designed Clock Protein KaiC
Authors : Furuike, Y.; Akiyama, S.
Deposited on : 2024-05-26
Resolution : 2.54 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

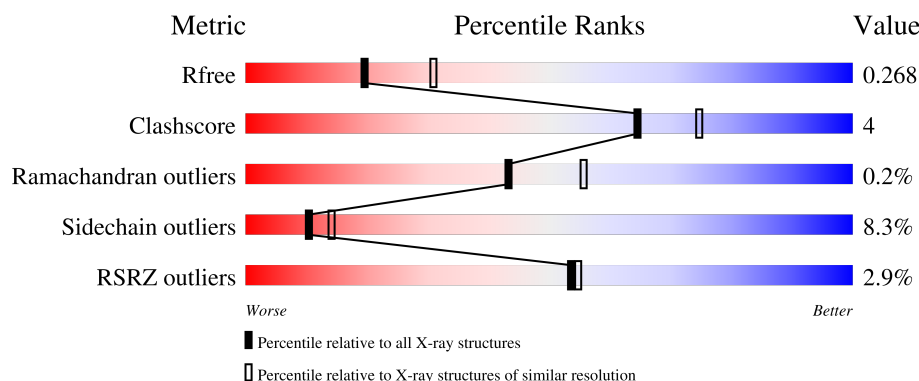
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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 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	512	3% 77% 11% • 10%
1	B	512	2% 77% 13% • 8%
1	C	512	3% 79% 11% • 8%
1	D	512	3% 81% 9% • 9%
1	E	512	3% 81% 9% • 9%

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Mol	Chain	Length	Quality of chain
1	F	512	3% 77% 11% • 10%

2 Entry composition [i](#)

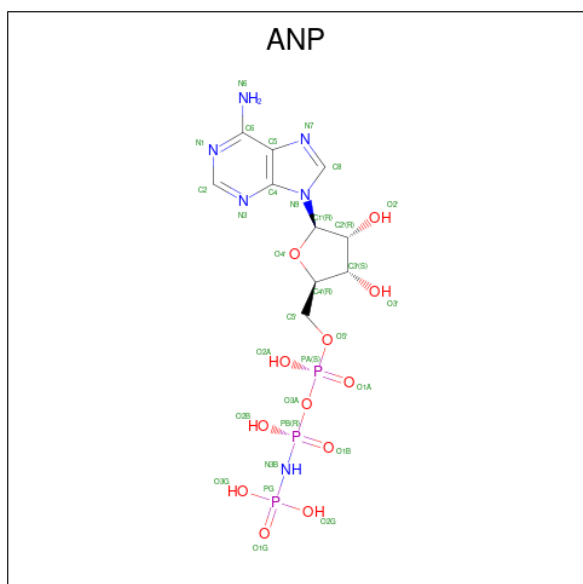
There are 4 unique types of molecules in this entry. The entry contains 20931 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 KaiC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	D	464	Total	C	N	O	P	S	0	0	0
			3344	2120	587	624	1	12			
1	E	466	Total	C	N	O	P	S	0	0	0
			3339	2122	577	626	1	13			
1	B	471	Total	C	N	O	P	S	0	0	0
			3552	2255	627	654	1	15			
1	C	470	Total	C	N	O	P	S	0	0	0
			3494	2218	603	658	1	14			
1	F	460	Total	C	N	O	P	S	0	0	0
			3298	2096	571	616	1	14			
1	A	460	Total	C	N	O	P	S	0	0	0
			3416	2179	593	629	1	14			

- 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	D	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	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
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	C	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	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	2	Total	Mg	0	0
			2	2		
3	E	2	Total	Mg	0	0
			2	2		
3	B	2	Total	Mg	0	0
			2	2		
3	C	2	Total	Mg	0	0
			2	2		
3	F	2	Total	Mg	0	0
			2	2		
3	A	2	Total	Mg	0	0
			2	2		

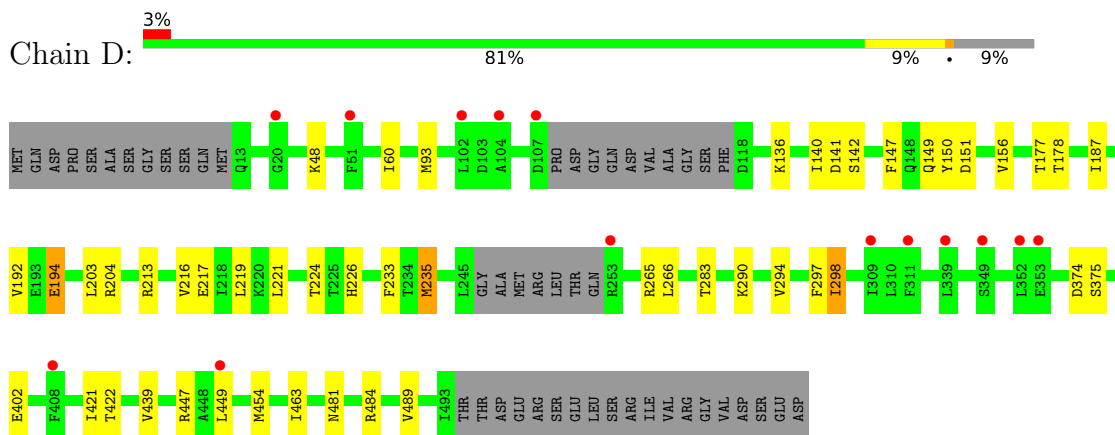
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	11	Total 11	O 11	0	0
4	E	13	Total 13	O 13	0	0
4	B	20	Total 20	O 20	0	0
4	C	15	Total 15	O 15	0	0
4	F	22	Total 22	O 22	0	0
4	A	23	Total 23	O 23	0	0

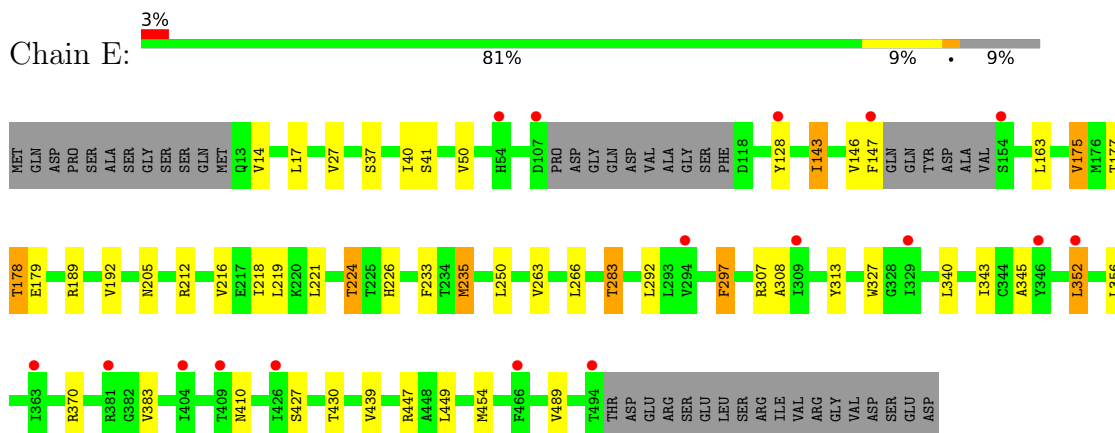
3 Residue-property plots [i](#)

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.

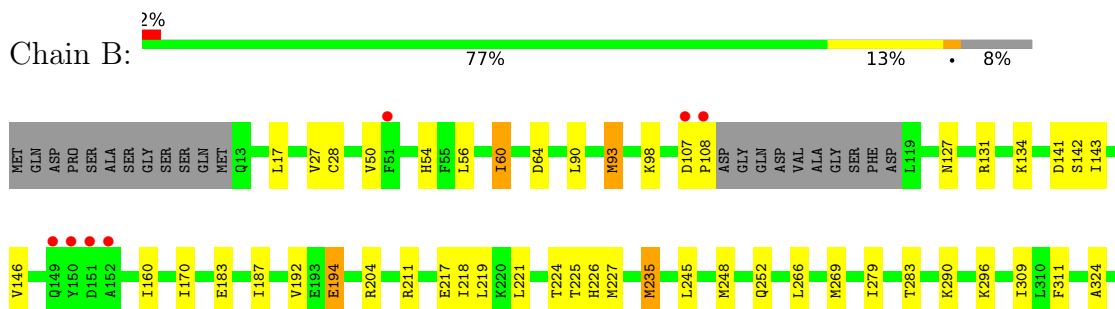
• Molecule 1: KaiC

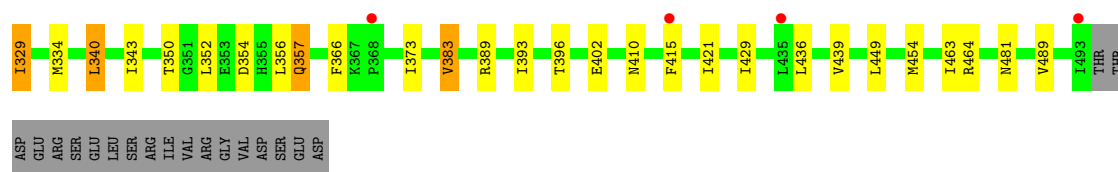


• Molecule 1: KaiC

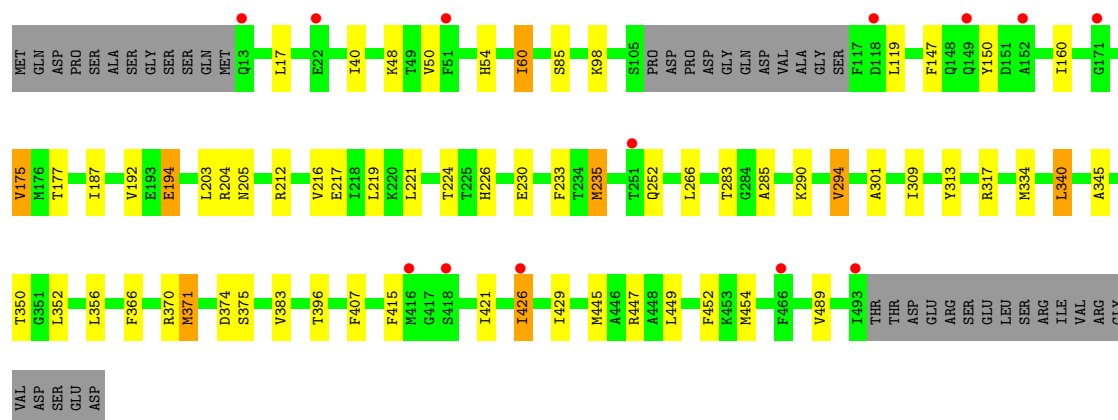


• Molecule 1: KaiC

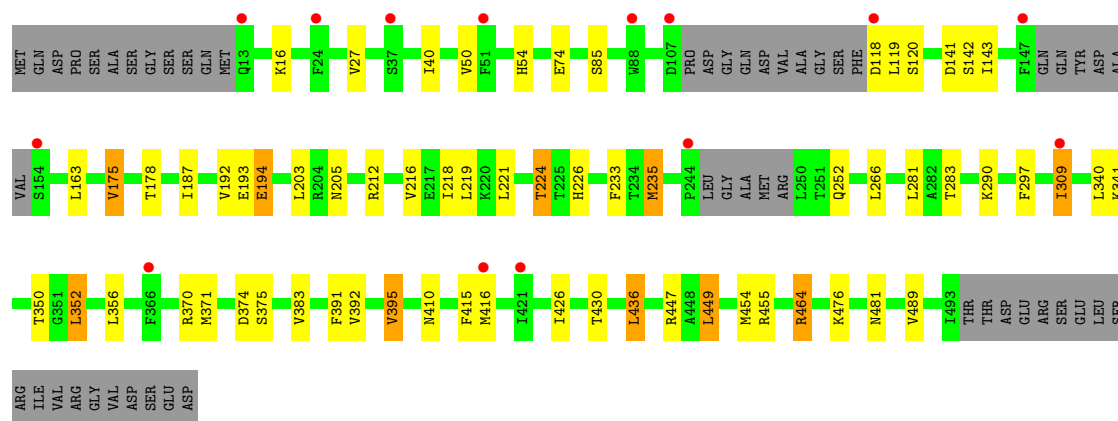




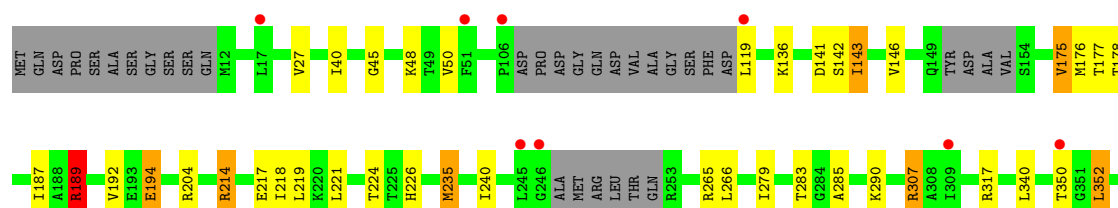
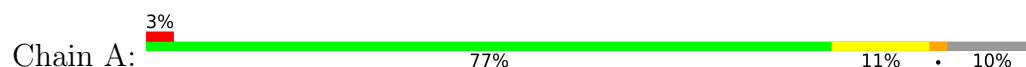
• Molecule 1: KaiC

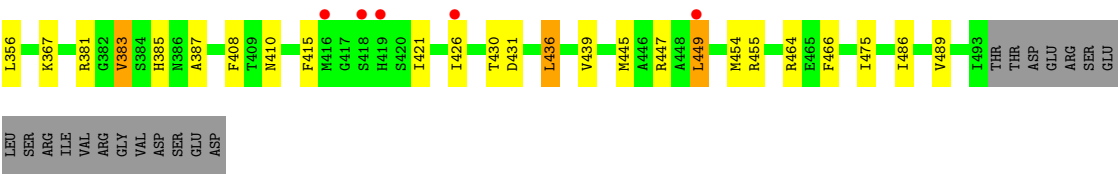


• Molecule 1: KaiC



• Molecule 1: KaiC





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	91.98Å 175.18Å 94.77Å 90.00° 96.93° 90.00°	Depositor
Resolution (Å)	49.19 – 2.54 49.19 – 2.54	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.19-2.54) 99.9 (49.19-2.54)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0415	Depositor
R, R_{free}	0.225 , 0.272 0.223 , 0.268	Depositor DCC
R_{free} test set	4907 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	62.5	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 57.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	20931	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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: SEP, MG, 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	A	0.45	0/3466	0.80	0/4687
1	B	0.44	0/3606	0.80	0/4875
1	C	0.45	0/3545	0.80	0/4801
1	D	0.45	0/3393	0.80	0/4607
1	E	0.46	0/3386	0.80	0/4597
1	F	0.46	0/3345	0.79	0/4543
All	All	0.45	0/20741	0.80	0/28110

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	4
1	F	0	1
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	189	ARG	Sidechain
1	A	214	ARG	Sidechain
1	A	317	ARG	Sidechain
1	A	464	ARG	Sidechain
1	F	464	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3416	0	3282	31	0
1	B	3552	0	3459	34	0
1	C	3494	0	3339	29	0
1	D	3344	0	3091	18	0
1	E	3339	0	3098	19	0
1	F	3298	0	3055	30	0
2	A	62	0	26	2	0
2	B	62	0	26	0	0
2	C	62	0	26	1	0
2	D	62	0	26	1	0
2	E	62	0	26	1	0
2	F	62	0	26	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	A	23	0	0	0	0
4	B	20	0	0	0	0
4	C	15	0	0	0	0
4	D	11	0	0	0	0
4	E	13	0	0	0	0
4	F	22	0	0	1	0
All	All	20931	0	19480	155	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 4.

All (155) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:VAL:HG12	1:B:218:ILE:HD12	1.61	0.81
1:C:50:VAL:HG21	1:C:235:MET:HE1	1.63	0.80
1:A:307:ARG:HB2	1:A:307:ARG:HH21	1.46	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ILE:HD13	1:A:175:VAL:HG13	1.65	0.79
1:F:436:LEU:HD22	1:F:449:LEU:HD22	1.65	0.78
1:F:85:SER:OG	2:F:601:ANP:N6	2.20	0.75
1:F:216:VAL:HG23	1:F:233:PHE:CD2	2.24	0.73
1:C:85:SER:OG	2:C:601:ANP:N6	2.20	0.72
1:A:436:LEU:HD22	1:A:449:LEU:HD22	1.71	0.70
1:A:283:THR:HG23	1:A:410:ASN:HD22	1.57	0.70
1:C:396:THR:HG21	1:C:429:ILE:HG22	1.76	0.68
1:C:60:ILE:HG21	1:C:98:LYS:HB3	1.75	0.68
1:C:216:VAL:HG23	1:C:233:PHE:CD2	2.29	0.67
1:B:283:THR:HG21	1:B:421:ILE:O	1.96	0.66
1:A:189:ARG:HH21	1:A:189:ARG:HG3	1.61	0.66
1:E:179:GLU:OE1	1:E:189:ARG:NH2	2.30	0.64
1:C:40:ILE:HD13	1:C:175:VAL:HG13	1.79	0.64
1:D:216:VAL:HG23	1:D:233:PHE:CD2	2.34	0.63
1:D:187:ILE:HB	1:D:194:GLU:HG2	1.81	0.63
1:B:283:THR:HG23	1:B:410:ASN:HD22	1.64	0.63
1:D:297:PHE:O	1:D:298:ILE:HB	1.98	0.62
1:A:352:LEU:HD22	1:A:383:VAL:HG11	1.80	0.62
1:F:40:ILE:HD13	1:F:175:VAL:HG13	1.81	0.62
1:F:50:VAL:HG21	1:F:235:MET:HE1	1.81	0.62
1:A:50:VAL:HG21	1:A:235:MET:HE1	1.82	0.62
1:D:48:LYS:HD2	1:D:177:THR:HG23	1.82	0.60
1:E:216:VAL:HG23	1:E:233:PHE:CD2	2.37	0.60
1:E:40:ILE:HD13	1:E:175:VAL:HG13	1.83	0.60
1:F:187:ILE:HB	1:F:194:GLU:HG2	1.83	0.59
1:E:221:LEU:HD12	1:E:226:HIS:HB3	1.84	0.59
1:B:221:LEU:HD12	1:B:226:HIS:HB3	1.85	0.58
1:B:187:ILE:HB	1:B:194:GLU:HG2	1.85	0.57
1:D:447:ARG:NH2	2:D:602:ANP:O2'	2.39	0.56
1:A:307:ARG:HH21	1:A:307:ARG:CB	2.17	0.55
1:B:245:LEU:HD21	1:B:393:ILE:HB	1.89	0.55
1:E:50:VAL:HG21	1:E:235:MET:HE1	1.91	0.53
1:C:334:MET:HB3	1:C:340:LEU:HB2	1.91	0.53
1:E:283:THR:HG22	1:E:410:ASN:HD22	1.73	0.53
1:B:396:THR:HG21	1:B:429:ILE:CG2	2.39	0.53
1:F:221:LEU:HD12	1:F:226:HIS:HB3	1.90	0.53
1:B:436:LEU:HG	1:B:449:LEU:HD23	1.91	0.53
1:F:309:ILE:HD12	1:F:341:LYS:CB	2.39	0.53
1:F:392:VAL:HG11	1:F:426:ILE:HG23	1.91	0.53
1:F:464:ARG:NH1	1:F:476:LYS:O	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:ASP:HA	1:A:455:ARG:HD2	1.90	0.52
1:B:60:ILE:HG21	1:B:98:LYS:HB3	1.91	0.52
1:E:41:SER:CB	1:E:178:THR:HG23	2.40	0.52
1:F:415:PHE:HB3	1:A:421:ILE:HD11	1.92	0.52
1:B:309:ILE:HD11	1:B:366:PHE:HB3	1.92	0.52
1:A:45:GLY:O	1:A:214:ARG:NH2	2.42	0.52
1:D:203:LEU:CD2	1:D:216:VAL:HG22	2.39	0.51
1:E:447:ARG:NH2	2:E:602:ANP:O2'	2.43	0.51
1:D:297:PHE:O	1:D:298:ILE:CB	2.59	0.51
1:A:447:ARG:NH2	2:A:602:ANP:O2'	2.43	0.51
1:C:48:LYS:HD2	1:C:177:THR:HG23	1.93	0.51
1:C:309:ILE:HD11	1:C:366:PHE:HB3	1.91	0.51
1:B:127:ASN:O	1:B:131:ARG:HG2	2.10	0.51
1:D:221:LEU:HD12	1:D:226:HIS:HB3	1.93	0.50
1:B:279:ILE:HG13	1:B:396:THR:HG23	1.93	0.50
1:C:187:ILE:HB	1:C:194:GLU:HG2	1.94	0.50
1:F:436:LEU:HD23	1:F:436:LEU:N	2.26	0.50
1:F:352:LEU:HD22	1:F:383:VAL:HG11	1.93	0.50
1:B:211:ARG:NH2	1:C:230:GLU:O	2.44	0.50
1:C:352:LEU:HD22	1:C:383:VAL:HG11	1.92	0.50
1:D:204:ARG:NH2	1:D:217:GLU:OE2	2.45	0.49
1:A:48:LYS:HD2	1:A:177:THR:HG23	1.94	0.49
1:C:426:ILE:HG13	1:C:429:ILE:HD12	1.94	0.49
1:F:203:LEU:HD22	1:F:216:VAL:HG22	1.94	0.49
1:A:383:VAL:HG12	1:A:387:ALA:HB3	1.94	0.49
1:C:204:ARG:NH2	1:C:217:GLU:OE2	2.45	0.49
1:C:294:VAL:HG12	1:C:407:PHE:CE1	2.48	0.49
1:E:297:PHE:CZ	1:E:370:ARG:HB3	2.48	0.49
1:F:283:THR:HG22	1:F:410:ASN:HB3	1.94	0.48
1:A:27:VAL:HG12	1:A:218:ILE:HG12	1.93	0.48
1:A:436:LEU:HD23	1:A:436:LEU:N	2.28	0.48
1:B:107:ASP:N	1:B:108:PRO:HD2	2.29	0.48
1:C:205:ASN:O	1:C:212:ARG:NH1	2.47	0.47
1:B:183:GLU:O	1:B:204:ARG:HD3	2.14	0.47
1:F:74:GLU:OE2	4:F:701:HOH:O	2.21	0.47
1:B:50:VAL:HG21	1:B:235:MET:HE1	1.97	0.46
1:B:463:ILE:HD11	1:A:445:MET:HE3	1.98	0.46
1:F:436:LEU:HD22	1:F:449:LEU:CD2	2.42	0.46
1:F:141:ASP:HA	1:F:142:SER:HA	1.75	0.46
1:B:141:ASP:HA	1:B:142:SER:HA	1.78	0.45
1:B:352:LEU:HD22	1:B:383:VAL:HG11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ARG:NH2	1:A:367:LYS:O	2.49	0.45
1:B:56:LEU:O	1:B:60:ILE:HG12	2.16	0.45
1:B:90:LEU:HA	1:B:93:MET:HG3	1.97	0.45
1:F:193:GLU:OE2	1:F:193:GLU:N	2.46	0.45
1:C:313:TYR:HA	1:C:345:ALA:O	2.17	0.45
1:F:374:ASP:HA	1:F:375:SER:HA	1.78	0.45
1:A:265:ARG:HG2	1:A:475:ILE:HB	1.98	0.45
1:B:311:PHE:HB2	1:B:373:ILE:HD13	1.99	0.45
1:A:204:ARG:NH2	1:A:217:GLU:OE2	2.50	0.45
1:E:205:ASN:O	1:E:212:ARG:NH1	2.49	0.44
1:F:391:PHE:O	1:F:395:VAL:HG23	2.18	0.44
1:B:204:ARG:NH2	1:B:217:GLU:OE2	2.48	0.44
1:D:141:ASP:OD2	1:D:177:THR:HG21	2.17	0.44
1:E:308:ALA:HA	1:E:370:ARG:O	2.17	0.44
1:A:143:ILE:HD13	1:A:176:MET:HE2	1.99	0.44
1:F:297:PHE:CZ	1:F:370:ARG:HD3	2.53	0.44
1:A:187:ILE:HB	1:A:194:GLU:HG2	2.00	0.44
1:C:283:THR:HG21	1:C:421:ILE:HG23	1.99	0.44
1:E:27:VAL:HG12	1:E:218:ILE:HG12	2.00	0.44
1:A:285:ALA:HB2	1:A:415:PHE:HA	2.00	0.44
1:B:27:VAL:HG13	1:B:227:MET:HB2	1.99	0.43
1:D:421:ILE:HG22	1:D:422:THR:HG23	2.00	0.43
1:E:313:TYR:HA	1:E:345:ALA:O	2.18	0.43
1:C:60:ILE:CG2	1:C:98:LYS:HB3	2.45	0.43
1:C:235:MET:HE3	1:C:235:MET:HB3	1.86	0.43
1:E:14:VAL:HB	1:E:224:THR:HG23	1.99	0.43
1:B:334:MET:HB3	1:B:340:LEU:HB2	2.00	0.43
1:F:27:VAL:HG12	1:F:218:ILE:HG13	2.01	0.43
1:A:283:THR:HG21	1:A:421:ILE:O	2.19	0.43
1:A:221:LEU:HD12	1:A:226:HIS:HB3	2.00	0.43
1:F:118:ASP:O	1:F:120:SER:N	2.52	0.43
1:B:28:CYS:SG	1:B:218:ILE:HD13	2.60	0.42
1:B:415:PHE:HB2	1:C:452:PHE:HZ	1.85	0.42
1:F:205:ASN:O	1:F:212:ARG:NH1	2.50	0.42
1:B:350:THR:HB	1:B:354:ASP:HB2	2.02	0.42
1:C:203:LEU:CD2	1:C:216:VAL:HG22	2.49	0.42
1:C:374:ASP:HA	1:C:375:SER:HA	1.86	0.42
1:F:235:MET:HE3	1:F:235:MET:HB3	1.92	0.42
1:F:426:ILE:HG22	1:F:426:ILE:O	2.19	0.42
1:B:357:GLN:HE21	1:B:357:GLN:HA	1.85	0.42
1:C:301:ALA:HB2	1:C:370:ARG:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ASP:HA	1:A:142:SER:HA	1.82	0.42
1:D:463:ILE:HD11	1:C:445:MET:HE3	2.01	0.42
1:B:269:MET:HE3	1:B:464:ARG:HD3	2.01	0.42
1:E:292:LEU:HD13	1:E:327:TRP:CD2	2.55	0.42
1:D:147:PHE:C	1:D:149:GLN:H	2.28	0.41
1:B:389:ARG:O	1:B:393:ILE:HG12	2.20	0.41
1:B:225:THR:HG22	2:A:601:ANP:C2	2.50	0.41
1:D:374:ASP:HA	1:D:375:SER:HA	1.83	0.41
1:F:27:VAL:HG12	1:F:218:ILE:CG1	2.50	0.41
1:A:436:LEU:HD22	1:A:449:LEU:CD2	2.44	0.41
1:F:16:LYS:HE3	1:F:224:THR:HG21	2.01	0.41
1:A:279:ILE:HG23	1:A:408:PHE:CE1	2.56	0.41
1:B:324:ALA:HB1	1:B:329:ILE:HB	2.02	0.41
1:A:307:ARG:HH21	1:A:307:ARG:CG	2.34	0.41
1:E:143:ILE:HG22	1:E:147:PHE:CE2	2.56	0.41
1:E:427:SEP:O	1:E:430:THR:HG22	2.21	0.41
1:D:203:LEU:HD22	1:D:216:VAL:HG22	2.02	0.40
1:D:235:MET:HE3	1:D:235:MET:HB3	1.94	0.40
1:E:27:VAL:HG12	1:E:218:ILE:CG1	2.51	0.40
1:E:352:LEU:HD12	1:E:352:LEU:HA	1.87	0.40
1:C:371:MET:HE3	1:C:371:MET:HB3	1.84	0.40
1:A:27:VAL:HG12	1:A:218:ILE:CG1	2.52	0.40
1:D:60:ILE:CB	1:D:93:MET:HE3	2.50	0.40
1:D:141:ASP:HA	1:D:142:SER:HA	1.72	0.40
1:B:389:ARG:NH2	1:A:381:ARG:HD2	2.37	0.40
1:C:147:PHE:CZ	1:C:160:ILE:HG12	2.56	0.40
1:C:221:LEU:HD12	1:C:226:HIS:HB3	2.03	0.40
1:C:285:ALA:HB2	1:C:415:PHE:HA	2.04	0.40
1:F:281:LEU:HB2	1:F:430:THR:HG21	2.04	0.40

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	
1	A	451/512 (88%)	436 (97%)	15 (3%)	0	100	100
1	B	466/512 (91%)	446 (96%)	20 (4%)	0	100	100
1	C	465/512 (91%)	448 (96%)	16 (3%)	1 (0%)	43	56
1	D	457/512 (89%)	430 (94%)	24 (5%)	3 (1%)	18	25
1	E	459/512 (90%)	441 (96%)	18 (4%)	0	100	100
1	F	451/512 (88%)	439 (97%)	11 (2%)	1 (0%)	43	56
All	All	2749/3072 (90%)	2640 (96%)	104 (4%)	5 (0%)	43	56

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	298	ILE
1	C	150	TYR
1	D	150	TYR
1	F	119	LEU
1	D	151	ASP

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	336/435 (77%)	305 (91%)	31 (9%)	8	10
1	B	359/435 (82%)	328 (91%)	31 (9%)	10	13
1	C	348/435 (80%)	324 (93%)	24 (7%)	14	20
1	D	312/435 (72%)	290 (93%)	22 (7%)	13	19
1	E	313/435 (72%)	285 (91%)	28 (9%)	9	12
1	F	309/435 (71%)	281 (91%)	28 (9%)	9	11
All	All	1977/2610 (76%)	1813 (92%)	164 (8%)	10	14

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	136	LYS
1	D	140	ILE
1	D	156	VAL
1	D	178	THR
1	D	192	VAL
1	D	194	GLU
1	D	213	ARG
1	D	219	LEU
1	D	224	THR
1	D	235	MET
1	D	265	ARG
1	D	266	LEU
1	D	283	THR
1	D	290	LYS
1	D	294	VAL
1	D	402	GLU
1	D	439	VAL
1	D	449	LEU
1	D	454	MET
1	D	481	ASN
1	D	484	ARG
1	D	489	VAL
1	E	17	LEU
1	E	37	SER
1	E	128	TYR
1	E	143	ILE
1	E	146	VAL
1	E	163	LEU
1	E	175	VAL
1	E	177	THR
1	E	178	THR
1	E	192	VAL
1	E	219	LEU
1	E	224	THR
1	E	235	MET
1	E	250	LEU
1	E	263	VAL
1	E	266	LEU
1	E	283	THR
1	E	297	PHE
1	E	307	ARG
1	E	340	LEU
1	E	343	ILE

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Mol	Chain	Res	Type
1	E	352	LEU
1	E	356	LEU
1	E	383	VAL
1	E	439	VAL
1	E	449	LEU
1	E	454	MET
1	E	489	VAL
1	B	17	LEU
1	B	54	HIS
1	B	60	ILE
1	B	64	ASP
1	B	93	MET
1	B	134	LYS
1	B	143	ILE
1	B	146	VAL
1	B	160	ILE
1	B	170	ILE
1	B	192	VAL
1	B	194	GLU
1	B	219	LEU
1	B	224	THR
1	B	235	MET
1	B	248	MET
1	B	252	GLN
1	B	266	LEU
1	B	290	LYS
1	B	296	LYS
1	B	329	ILE
1	B	340	LEU
1	B	343	ILE
1	B	356	LEU
1	B	357	GLN
1	B	383	VAL
1	B	402	GLU
1	B	439	VAL
1	B	454	MET
1	B	481	ASN
1	B	489	VAL
1	C	17	LEU
1	C	54	HIS
1	C	60	ILE
1	C	119	LEU

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Mol	Chain	Res	Type
1	C	175	VAL
1	C	192	VAL
1	C	194	GLU
1	C	219	LEU
1	C	224	THR
1	C	235	MET
1	C	252	GLN
1	C	266	LEU
1	C	290	LYS
1	C	294	VAL
1	C	317	ARG
1	C	340	LEU
1	C	350	THR
1	C	356	LEU
1	C	371	MET
1	C	426	ILE
1	C	447	ARG
1	C	449	LEU
1	C	454	MET
1	C	489	VAL
1	F	54	HIS
1	F	143	ILE
1	F	163	LEU
1	F	175	VAL
1	F	178	THR
1	F	192	VAL
1	F	194	GLU
1	F	219	LEU
1	F	224	THR
1	F	235	MET
1	F	252	GLN
1	F	266	LEU
1	F	290	LYS
1	F	309	ILE
1	F	340	LEU
1	F	350	THR
1	F	352	LEU
1	F	356	LEU
1	F	371	MET
1	F	395	VAL
1	F	416	MET
1	F	436	LEU

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Mol	Chain	Res	Type
1	F	447	ARG
1	F	449	LEU
1	F	454	MET
1	F	455	ARG
1	F	481	ASN
1	F	489	VAL
1	A	119	LEU
1	A	136	LYS
1	A	143	ILE
1	A	146	VAL
1	A	175	VAL
1	A	178	THR
1	A	189	ARG
1	A	192	VAL
1	A	194	GLU
1	A	219	LEU
1	A	224	THR
1	A	235	MET
1	A	240	ILE
1	A	266	LEU
1	A	290	LYS
1	A	307	ARG
1	A	340	LEU
1	A	350	THR
1	A	352	LEU
1	A	356	LEU
1	A	383	VAL
1	A	385	HIS
1	A	426	ILE
1	A	430	THR
1	A	436	LEU
1	A	439	VAL
1	A	449	LEU
1	A	454	MET
1	A	466	PHE
1	A	486	ILE
1	A	489	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	29	HIS

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Mol	Chain	Res	Type
1	D	54	HIS
1	D	256	ASN
1	D	425	HIS
1	E	29	HIS
1	E	205	ASN
1	E	256	ASN
1	E	410	ASN
1	E	450	ASN
1	E	491	HIS
1	B	29	HIS
1	B	62	HIS
1	B	357	GLN
1	B	410	ASN
1	B	450	ASN
1	C	29	HIS
1	C	256	ASN
1	C	365	GLN
1	C	390	GLN
1	C	450	ASN
1	C	491	HIS
1	F	54	HIS
1	F	252	GLN
1	F	256	ASN
1	F	410	ASN
1	F	450	ASN
1	A	15	GLN
1	A	148	GLN
1	A	410	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	SEP	A	427	1	8,9,10	0.58	0	7,12,14	0.77	0
1	SEP	E	427	1	8,9,10	0.59	0	7,12,14	0.64	0
1	SEP	C	427	1	8,9,10	0.63	0	7,12,14	0.71	0
1	SEP	D	427	1	8,9,10	0.61	0	7,12,14	0.66	0
1	SEP	F	427	1	8,9,10	0.63	0	7,12,14	0.66	0
1	SEP	B	427	1	8,9,10	0.63	0	7,12,14	0.70	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
1	SEP	A	427	1	-	1/6/8/10	-
1	SEP	E	427	1	-	0/6/8/10	-
1	SEP	C	427	1	-	1/6/8/10	-
1	SEP	D	427	1	-	0/6/8/10	-
1	SEP	F	427	1	-	0/6/8/10	-
1	SEP	B	427	1	-	1/6/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	427	SEP	N-CA-CB-OG
1	C	427	SEP	N-CA-CB-OG
1	A	427	SEP	N-CA-CB-OG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	427	SEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 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	B	601	3	33,33,33	1.05	3 (9%)	45,52,52	1.00	3 (6%)
2	ANP	F	601	3	33,33,33	1.11	5 (15%)	45,52,52	0.97	1 (2%)
2	ANP	A	602	3	33,33,33	1.12	5 (15%)	45,52,52	0.88	1 (2%)
2	ANP	C	602	3	33,33,33	1.12	5 (15%)	45,52,52	0.94	1 (2%)
2	ANP	F	602	3	33,33,33	1.12	5 (15%)	45,52,52	0.90	2 (4%)
2	ANP	D	602	3	33,33,33	1.12	5 (15%)	45,52,52	0.90	1 (2%)
2	ANP	E	602	3	33,33,33	1.13	5 (15%)	45,52,52	0.87	1 (2%)
2	ANP	C	601	3	33,33,33	1.11	5 (15%)	45,52,52	1.06	3 (6%)
2	ANP	B	602	3	33,33,33	1.10	5 (15%)	45,52,52	0.87	1 (2%)
2	ANP	E	601	3	33,33,33	1.08	5 (15%)	45,52,52	1.06	3 (6%)
2	ANP	A	601	3	33,33,33	1.06	5 (15%)	45,52,52	0.99	2 (4%)
2	ANP	D	601	3	33,33,33	1.08	5 (15%)	45,52,52	0.94	2 (4%)

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	B	601	3	-	5/18/38/38	0/3/3/3
2	ANP	F	601	3	-	6/18/38/38	0/3/3/3
2	ANP	A	602	3	-	4/18/38/38	0/3/3/3
2	ANP	C	602	3	-	5/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ANP	F	602	3	-	4/18/38/38	0/3/3/3
2	ANP	D	602	3	-	4/18/38/38	0/3/3/3
2	ANP	E	602	3	-	1/18/38/38	0/3/3/3
2	ANP	C	601	3	-	7/18/38/38	0/3/3/3
2	ANP	B	602	3	-	6/18/38/38	0/3/3/3
2	ANP	E	601	3	-	3/18/38/38	0/3/3/3
2	ANP	A	601	3	-	3/18/38/38	0/3/3/3
2	ANP	D	601	3	-	6/18/38/38	0/3/3/3

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	602	ANP	PG-O1G	3.61	1.51	1.46
2	E	602	ANP	PG-O1G	3.58	1.51	1.46
2	C	601	ANP	PG-O1G	3.57	1.51	1.46
2	F	602	ANP	PG-O1G	3.51	1.51	1.46
2	B	602	ANP	PG-O1G	3.50	1.51	1.46
2	A	602	ANP	PG-O1G	3.30	1.51	1.46
2	E	601	ANP	PG-O1G	3.28	1.51	1.46
2	D	602	ANP	PG-O1G	3.25	1.51	1.46
2	F	601	ANP	PG-O1G	3.21	1.51	1.46
2	F	601	ANP	PB-O1B	3.15	1.51	1.46
2	B	601	ANP	PG-O1G	3.14	1.50	1.46
2	D	601	ANP	PG-O1G	3.10	1.50	1.46
2	B	601	ANP	PB-O1B	3.07	1.50	1.46
2	D	601	ANP	PB-O1B	3.07	1.50	1.46
2	C	601	ANP	PB-O1B	3.00	1.50	1.46
2	A	602	ANP	PB-O1B	3.00	1.50	1.46
2	B	602	ANP	PB-O1B	3.00	1.50	1.46
2	C	602	ANP	PB-O1B	2.99	1.50	1.46
2	E	601	ANP	PB-O1B	2.97	1.50	1.46
2	D	602	ANP	PB-O1B	2.95	1.50	1.46
2	E	602	ANP	PB-O1B	2.94	1.50	1.46
2	A	601	ANP	PB-O1B	2.93	1.50	1.46
2	A	601	ANP	PG-O1G	2.88	1.50	1.46
2	F	602	ANP	PB-O1B	2.85	1.50	1.46
2	D	601	ANP	PB-O2B	-2.41	1.50	1.56
2	E	601	ANP	PG-O2G	-2.39	1.50	1.56
2	D	601	ANP	PG-O2G	-2.36	1.50	1.56
2	F	602	ANP	PB-O2B	-2.36	1.50	1.56
2	C	601	ANP	PB-O2B	-2.33	1.50	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	602	ANP	PB-O2B	-2.33	1.50	1.56
2	B	602	ANP	PB-O2B	-2.33	1.50	1.56
2	A	601	ANP	PB-O2B	-2.32	1.50	1.56
2	E	602	ANP	PB-O2B	-2.32	1.50	1.56
2	B	601	ANP	PB-O2B	-2.32	1.50	1.56
2	A	602	ANP	PB-O2B	-2.32	1.50	1.56
2	A	601	ANP	PG-O2G	-2.31	1.50	1.56
2	E	601	ANP	PB-O2B	-2.30	1.50	1.56
2	F	601	ANP	PB-O2B	-2.29	1.50	1.56
2	C	601	ANP	PG-O2G	-2.25	1.50	1.56
2	C	602	ANP	PB-O2B	-2.24	1.50	1.56
2	F	601	ANP	PG-O2G	-2.24	1.50	1.56
2	A	602	ANP	PG-O2G	-2.23	1.50	1.56
2	F	602	ANP	PG-O2G	-2.22	1.50	1.56
2	D	601	ANP	PG-O3G	-2.18	1.51	1.56
2	C	602	ANP	PG-O2G	-2.17	1.51	1.56
2	E	601	ANP	PG-O3G	-2.14	1.51	1.56
2	C	602	ANP	PG-O3G	-2.13	1.51	1.56
2	F	602	ANP	PG-O3G	-2.11	1.51	1.56
2	B	602	ANP	PG-O3G	-2.11	1.51	1.56
2	A	602	ANP	PG-O3G	-2.11	1.51	1.56
2	F	601	ANP	PG-O3G	-2.09	1.51	1.56
2	D	602	ANP	PG-O2G	-2.09	1.51	1.56
2	B	602	ANP	PG-O2G	-2.05	1.51	1.56
2	E	602	ANP	PG-O3G	-2.05	1.51	1.56
2	A	601	ANP	PG-O3G	-2.05	1.51	1.56
2	C	601	ANP	PG-O3G	-2.03	1.51	1.56
2	E	602	ANP	PG-O2G	-2.03	1.51	1.56
2	D	602	ANP	PG-O3G	-2.01	1.51	1.56

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	601	ANP	O2B-PB-O1B	4.19	118.86	109.87
2	B	602	ANP	O2B-PB-O1B	4.16	118.78	109.87
2	C	602	ANP	O2B-PB-O1B	4.12	118.70	109.87
2	A	601	ANP	O2B-PB-O1B	4.07	118.60	109.87
2	B	601	ANP	O2B-PB-O1B	4.07	118.59	109.87
2	D	601	ANP	O2B-PB-O1B	4.06	118.58	109.87
2	C	601	ANP	O2B-PB-O1B	4.02	118.50	109.87
2	F	601	ANP	O2B-PB-O1B	4.02	118.49	109.87
2	E	602	ANP	O2B-PB-O1B	4.02	118.49	109.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	602	ANP	O2B-PB-O1B	3.97	118.37	109.87
2	A	602	ANP	O2B-PB-O1B	3.92	118.29	109.87
2	F	602	ANP	O2B-PB-O1B	3.86	118.15	109.87
2	C	601	ANP	O1B-PB-N3B	2.88	116.00	111.77
2	E	601	ANP	O1B-PB-N3B	2.76	115.83	111.77
2	B	601	ANP	O1G-PG-N3B	-2.67	107.84	111.77
2	A	601	ANP	O1G-PG-N3B	-2.52	108.06	111.77
2	C	601	ANP	O3A-PB-N3B	-2.38	99.99	106.59
2	E	601	ANP	O2G-PG-O1G	-2.24	107.82	113.45
2	B	601	ANP	O3A-PB-N3B	-2.16	100.61	106.59
2	D	601	ANP	O3G-PG-O1G	-2.06	108.28	113.45
2	F	602	ANP	O3A-PB-N3B	-2.02	100.98	106.59

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	601	ANP	PB-N3B-PG-O1G
2	D	601	ANP	PG-N3B-PB-O1B
2	D	601	ANP	PA-O3A-PB-O2B
2	D	602	ANP	PB-N3B-PG-O1G
2	D	602	ANP	PG-N3B-PB-O1B
2	D	602	ANP	PA-O3A-PB-O2B
2	E	601	ANP	PB-N3B-PG-O1G
2	E	601	ANP	PG-N3B-PB-O1B
2	E	601	ANP	PA-O3A-PB-O2B
2	E	602	ANP	PB-N3B-PG-O1G
2	B	601	ANP	PB-N3B-PG-O1G
2	B	601	ANP	PG-N3B-PB-O1B
2	B	601	ANP	PA-O3A-PB-O2B
2	B	602	ANP	PB-N3B-PG-O1G
2	B	602	ANP	PG-N3B-PB-O1B
2	B	602	ANP	PA-O3A-PB-O2B
2	B	602	ANP	C5'-O5'-PA-O2A
2	C	601	ANP	PB-N3B-PG-O1G
2	C	601	ANP	PG-N3B-PB-O1B
2	C	601	ANP	PG-N3B-PB-O3A
2	C	601	ANP	PA-O3A-PB-O2B
2	C	601	ANP	O4'-C4'-C5'-O5'
2	C	602	ANP	PB-N3B-PG-O1G
2	C	602	ANP	PG-N3B-PB-O1B
2	C	602	ANP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
2	F	601	ANP	PB-N3B-PG-O1G
2	F	601	ANP	PG-N3B-PB-O1B
2	F	601	ANP	PA-O3A-PB-O2B
2	F	601	ANP	C5'-O5'-PA-O1A
2	F	602	ANP	PB-N3B-PG-O1G
2	F	602	ANP	PG-N3B-PB-O1B
2	F	602	ANP	PA-O3A-PB-O2B
2	A	601	ANP	PB-N3B-PG-O1G
2	A	601	ANP	PG-N3B-PB-O1B
2	A	601	ANP	PA-O3A-PB-O2B
2	A	602	ANP	PB-N3B-PG-O1G
2	A	602	ANP	PG-N3B-PB-O1B
2	A	602	ANP	PA-O3A-PB-O2B
2	C	601	ANP	C3'-C4'-C5'-O5'
2	B	601	ANP	C3'-C4'-C5'-O5'
2	D	601	ANP	C3'-C4'-C5'-O5'
2	B	601	ANP	O4'-C4'-C5'-O5'
2	D	601	ANP	O4'-C4'-C5'-O5'
2	C	602	ANP	PG-N3B-PB-O3A
2	B	602	ANP	C5'-O5'-PA-O3A
2	C	602	ANP	C5'-O5'-PA-O3A
2	F	601	ANP	C5'-O5'-PA-O2A
2	F	601	ANP	C5'-O5'-PA-O3A
2	D	601	ANP	PA-O3A-PB-O1B
2	D	602	ANP	PA-O3A-PB-O1B
2	B	602	ANP	PA-O3A-PB-O1B
2	C	601	ANP	PA-O3A-PB-O1B
2	F	602	ANP	PA-O3A-PB-O1B
2	A	602	ANP	PA-O3A-PB-O1B

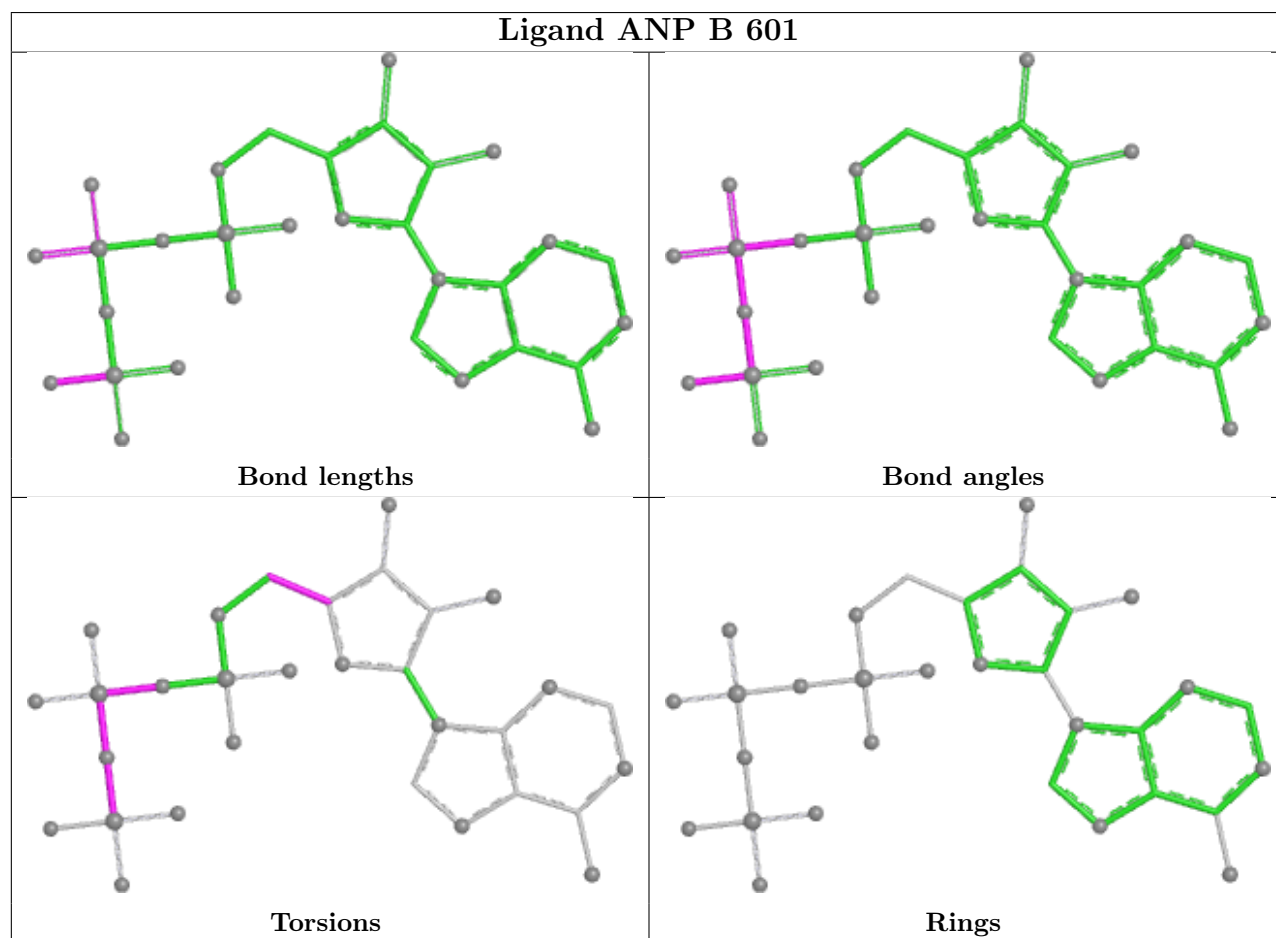
There are no ring outliers.

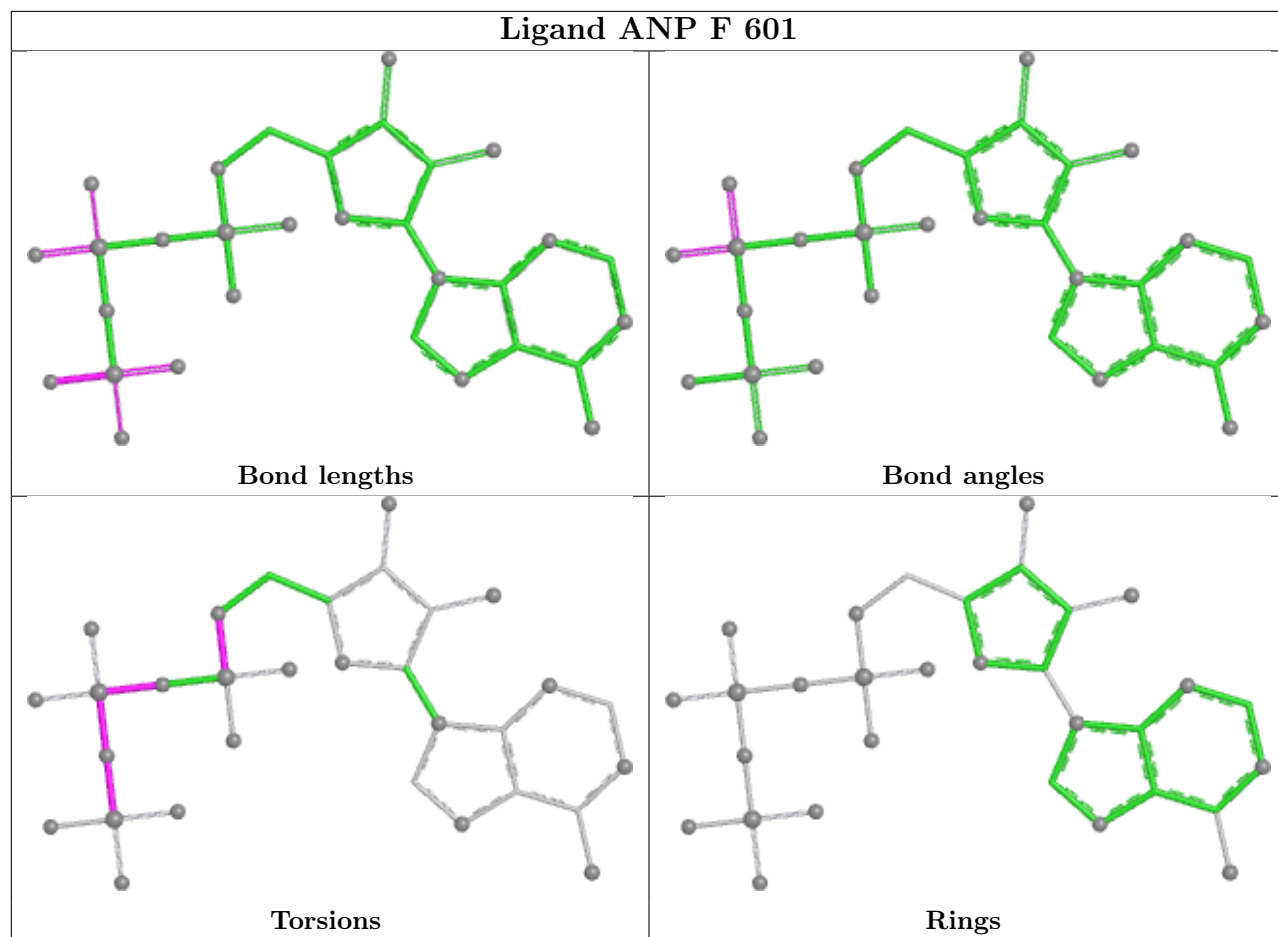
6 monomers are involved in 6 short contacts:

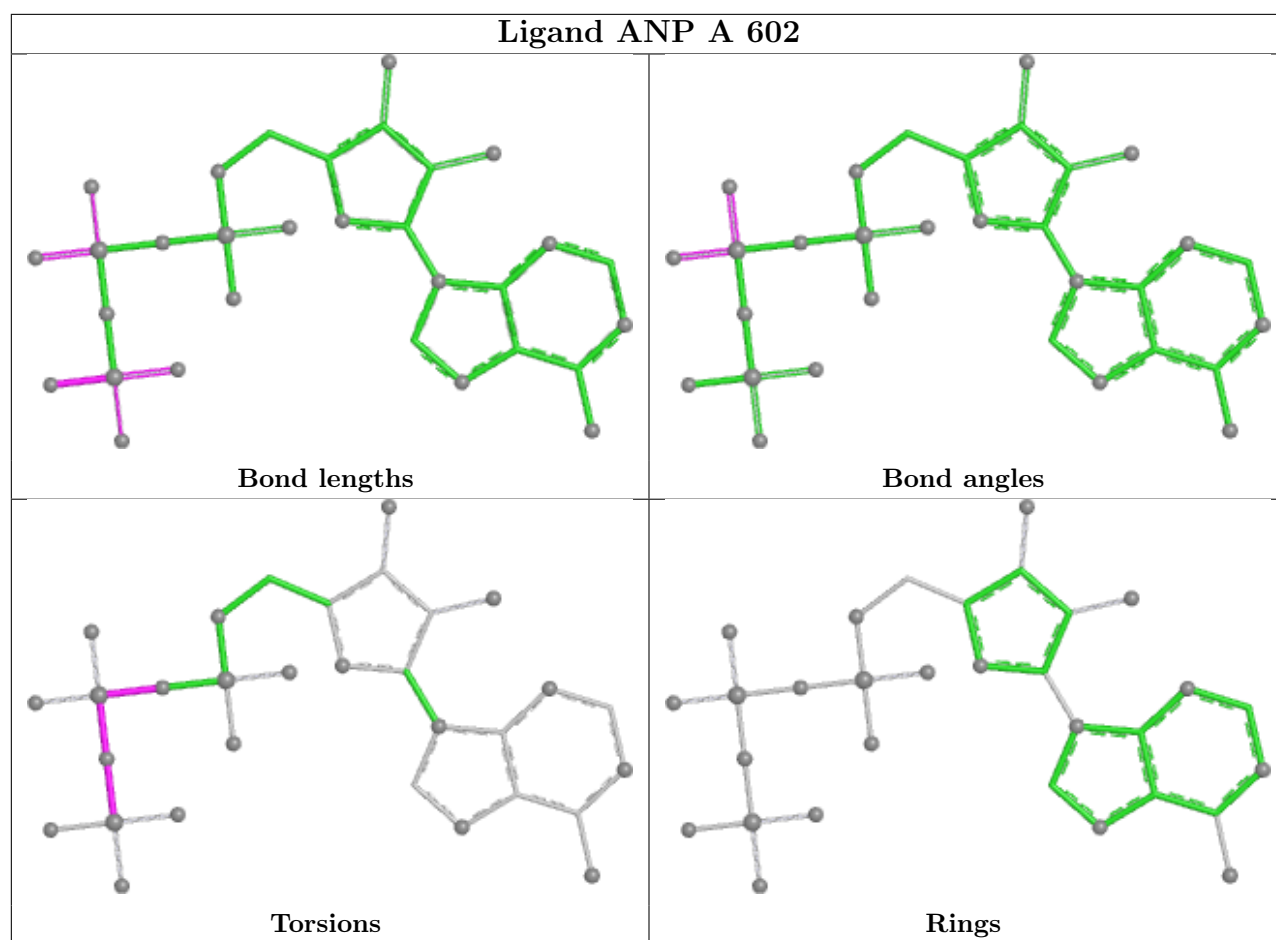
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	601	ANP	1	0
2	A	602	ANP	1	0
2	D	602	ANP	1	0
2	E	602	ANP	1	0
2	C	601	ANP	1	0
2	A	601	ANP	1	0

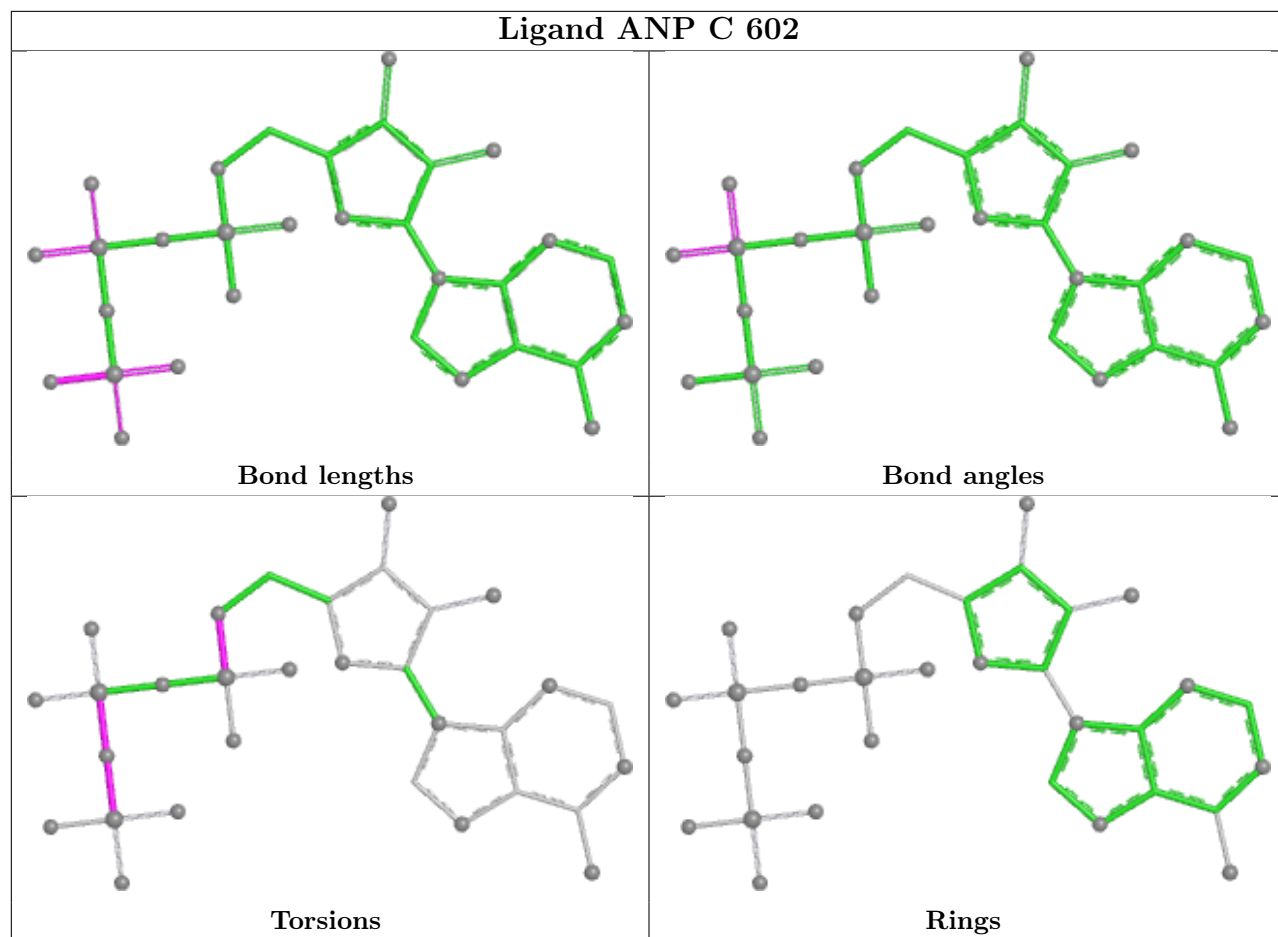
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

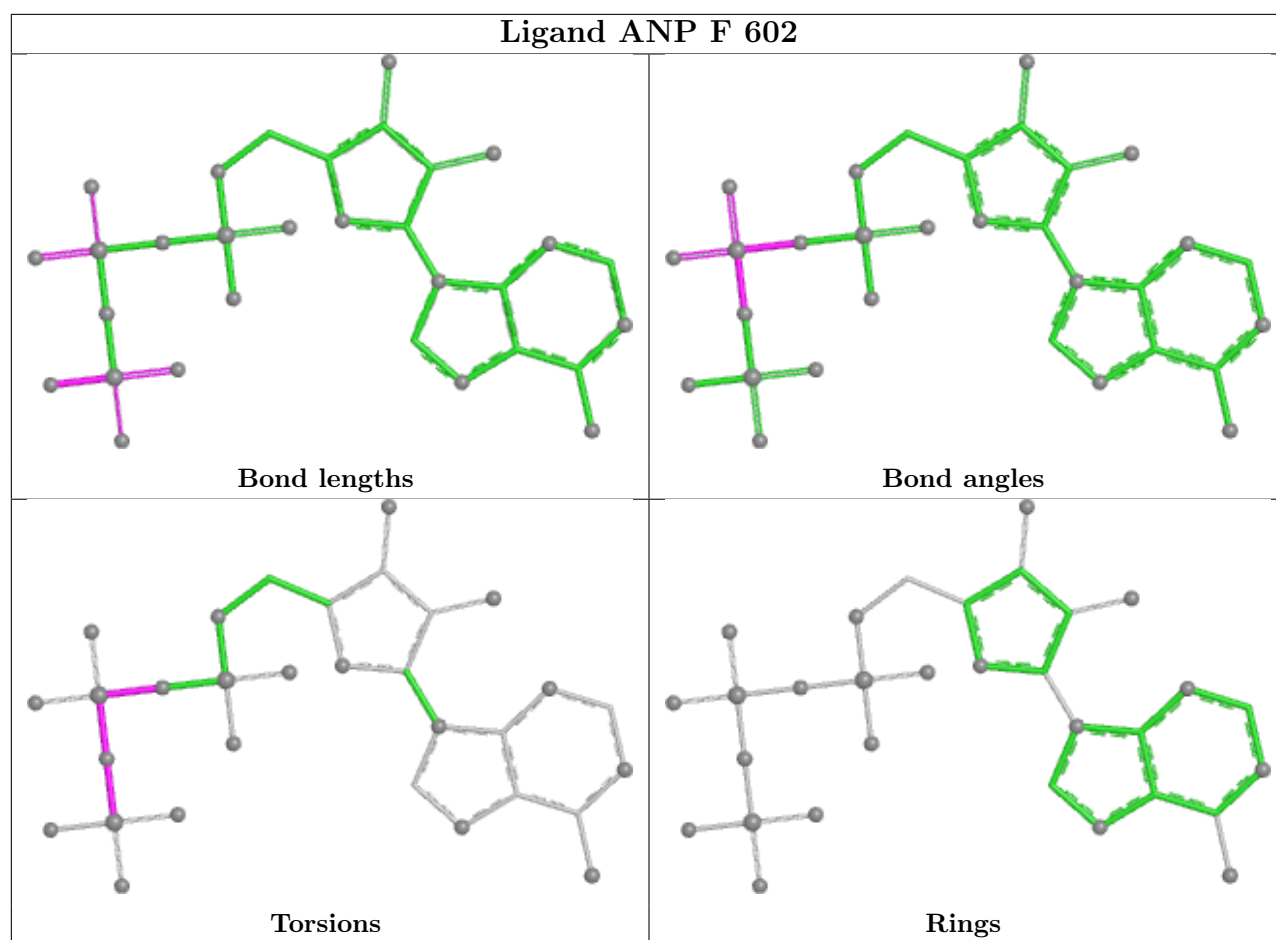
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within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

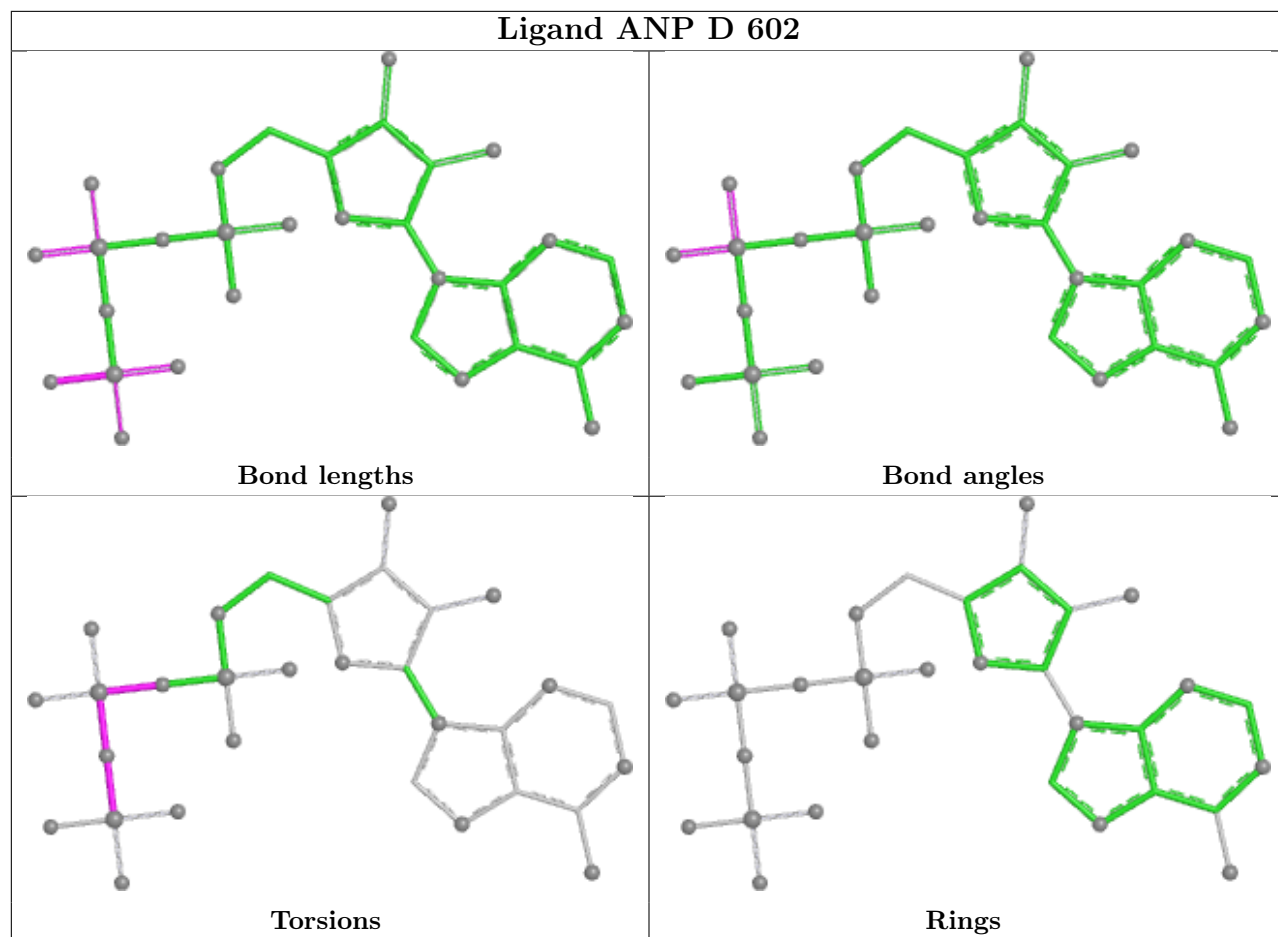


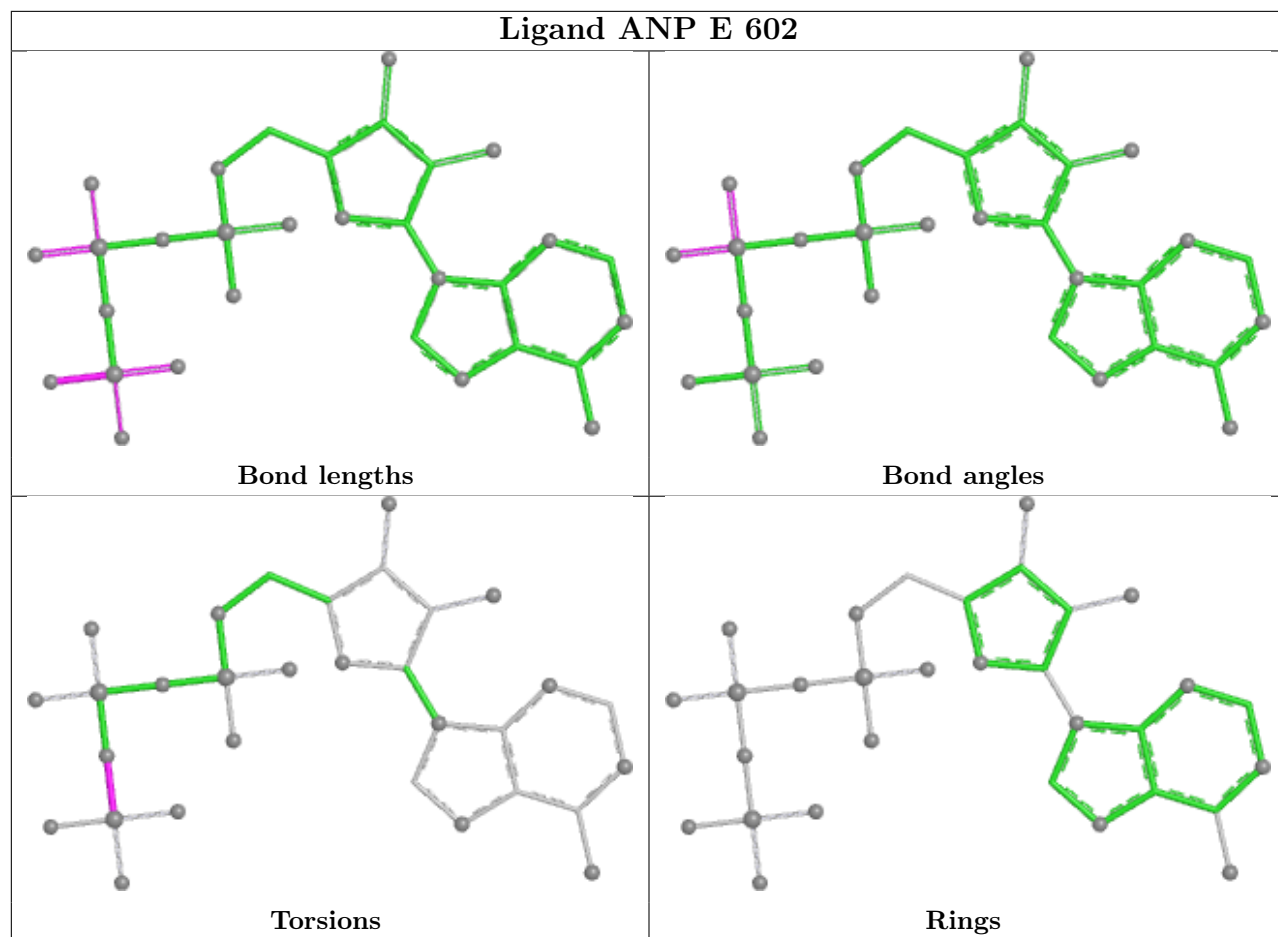


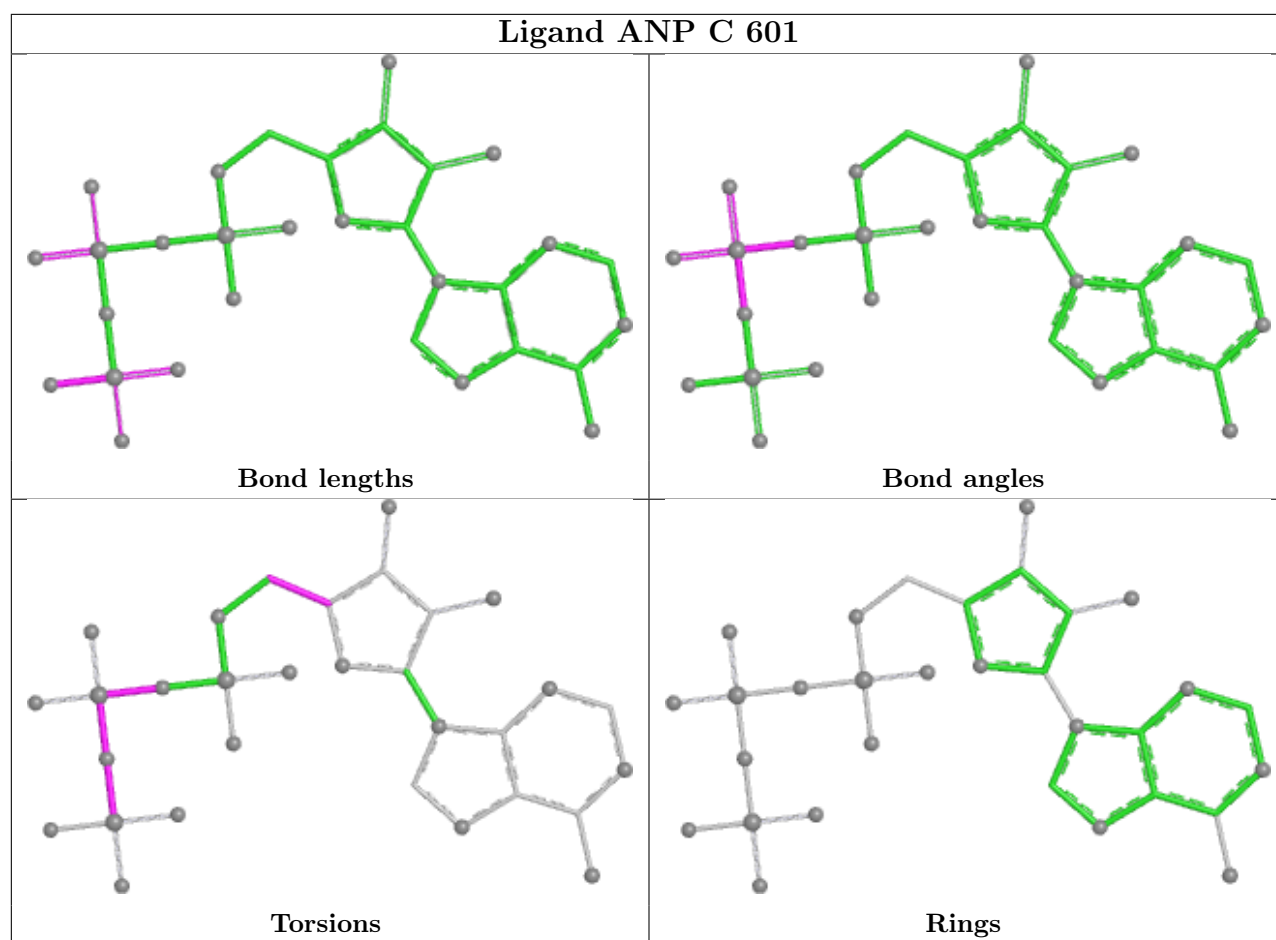


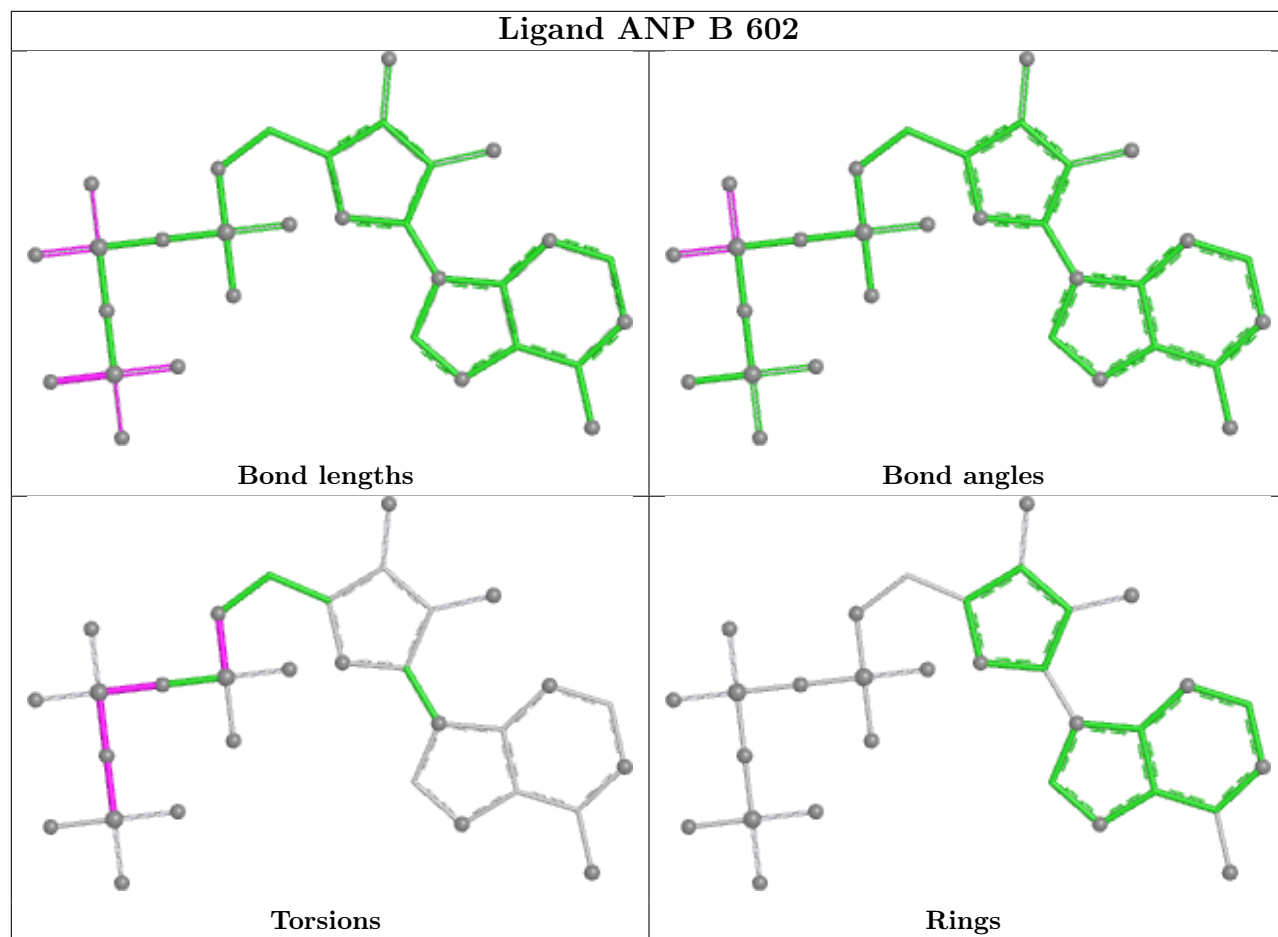


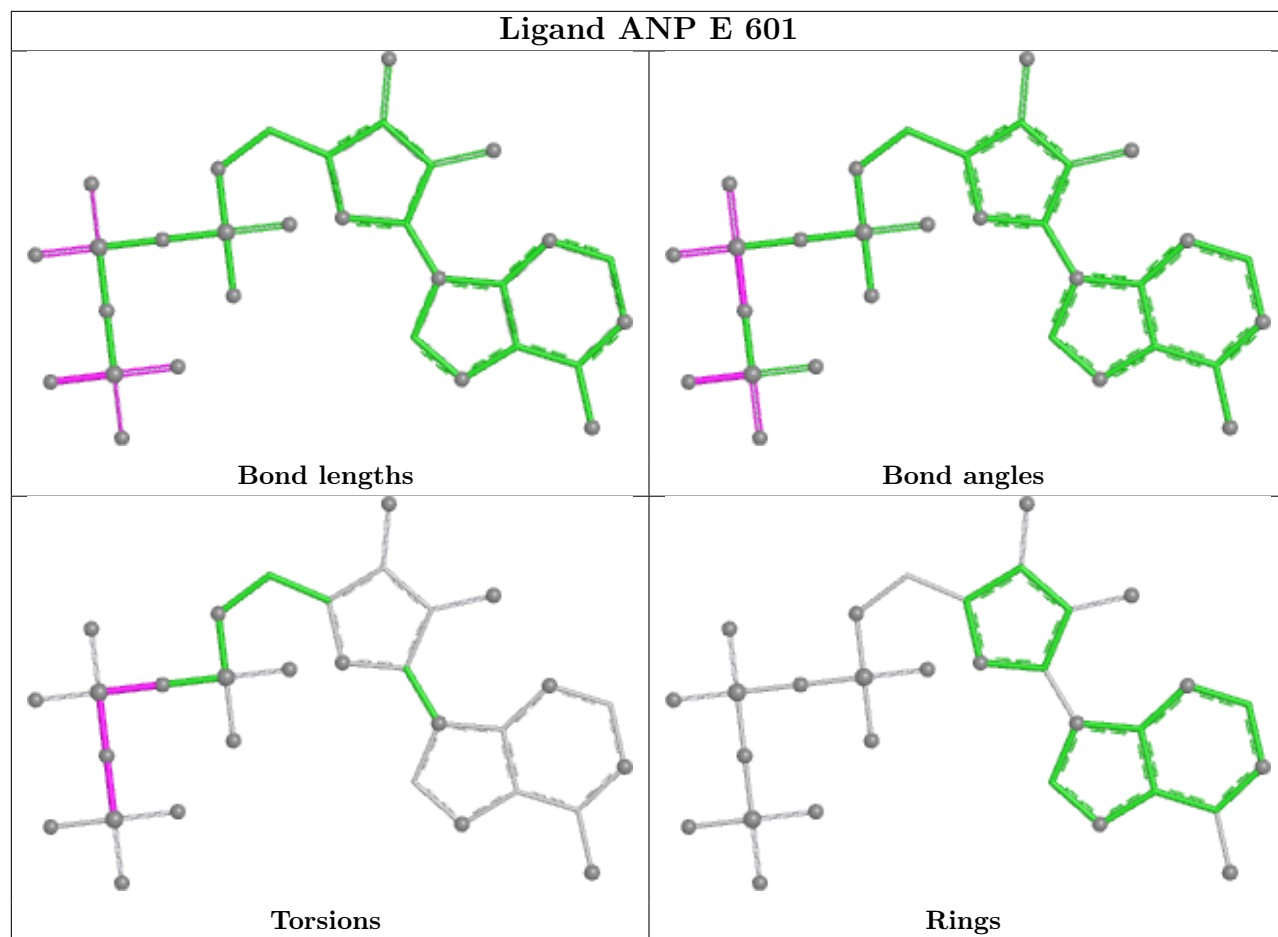


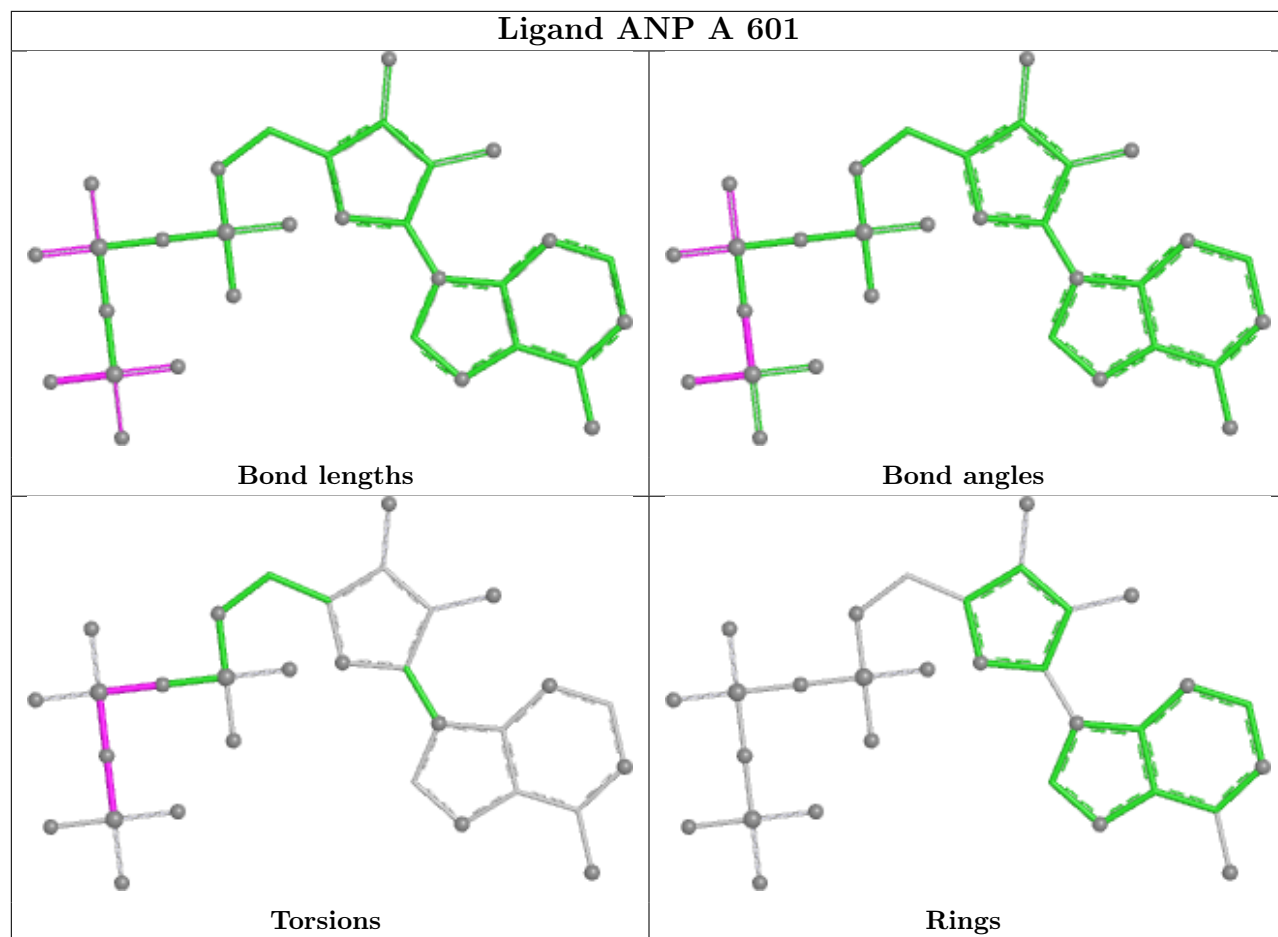


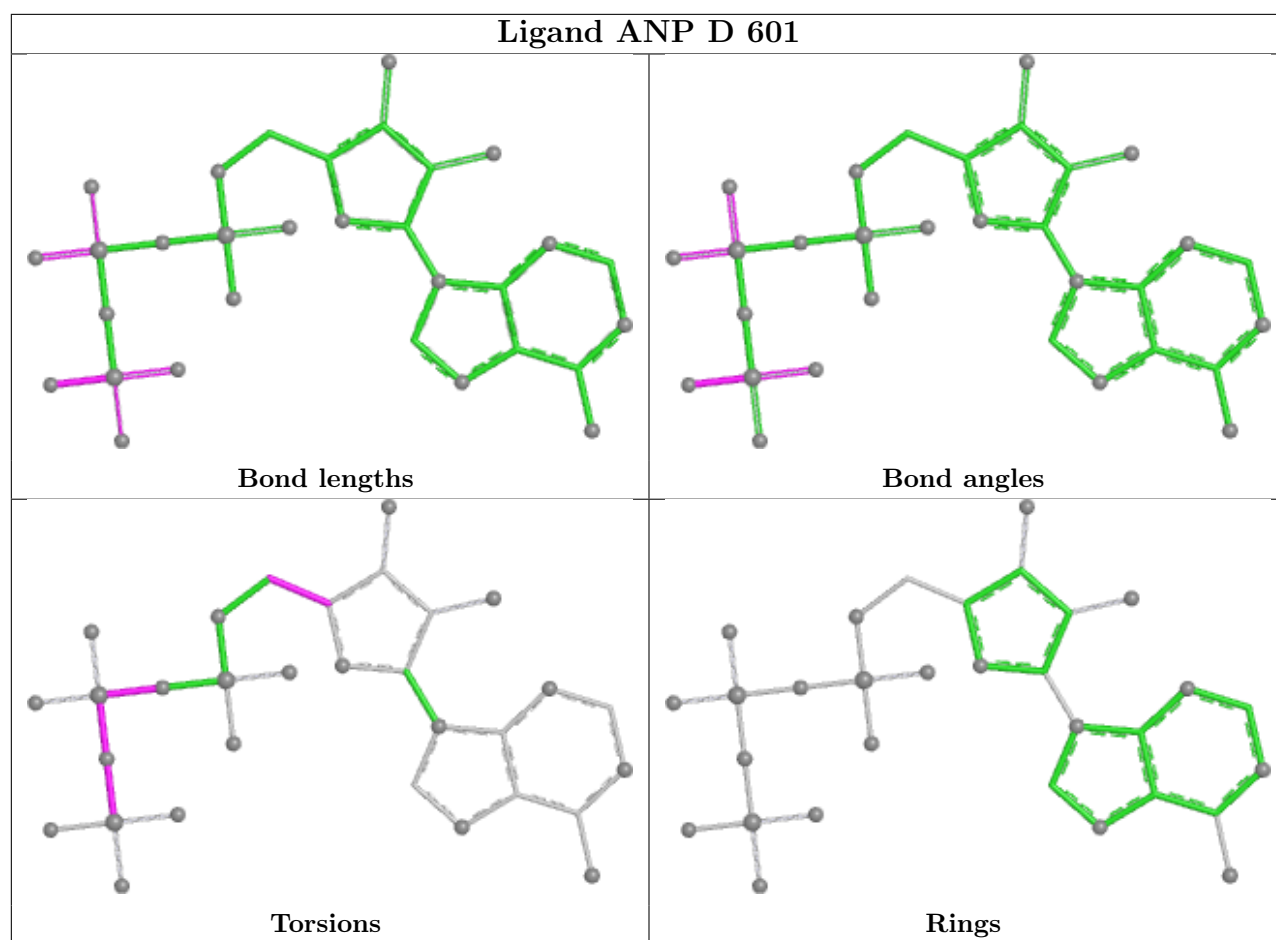












5.7 Other polymers [i](#)

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	459/512 (89%)	0.32	13 (2%) 55 56	37, 59, 86, 115	0
1	B	470/512 (91%)	0.33	11 (2%) 61 62	35, 61, 88, 114	0
1	C	469/512 (91%)	0.31	13 (2%) 55 56	38, 60, 87, 130	0
1	D	463/512 (90%)	0.51	14 (3%) 52 54	43, 74, 100, 128	0
1	E	465/512 (90%)	0.61	17 (3%) 45 46	42, 70, 107, 121	0
1	F	459/512 (89%)	0.42	14 (3%) 51 52	39, 67, 94, 112	0
All	All	2785/3072 (90%)	0.42	82 (2%) 53 55	35, 64, 98, 130	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	107	ASP	3.7
1	B	415	PHE	3.6
1	E	426	ILE	3.5
1	A	51	PHE	3.5
1	A	246	GLY	3.4
1	C	426	ILE	3.3
1	E	329	ILE	3.2
1	C	13	GLN	3.1
1	C	152	ALA	3.1
1	B	149	GLN	3.0
1	D	102	LEU	3.0
1	F	51	PHE	3.0
1	F	421	ILE	2.8
1	F	13	GLN	2.8
1	D	311	PHE	2.8
1	E	346	TYR	2.8
1	A	350	THR	2.8
1	D	353	GLU	2.7
1	A	426	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	309	ILE	2.7
1	D	20	GLY	2.6
1	C	118	ASP	2.6
1	B	493	ILE	2.6
1	C	418	SER	2.6
1	D	107	ASP	2.6
1	E	147	PHE	2.6
1	D	352	LEU	2.6
1	E	404	ILE	2.6
1	B	107	ASP	2.5
1	C	493	ILE	2.5
1	A	309	ILE	2.5
1	F	37	SER	2.5
1	B	150	TYR	2.5
1	F	309	ILE	2.5
1	E	54	HIS	2.4
1	D	104	ALA	2.4
1	B	151	ASP	2.4
1	C	149	GLN	2.4
1	C	251	THR	2.4
1	A	119	LEU	2.4
1	D	339	LEU	2.4
1	A	449	LEU	2.4
1	A	416	MET	2.4
1	F	118	ASP	2.3
1	B	108	PRO	2.3
1	D	349	SER	2.3
1	E	154	SER	2.3
1	A	245	LEU	2.3
1	C	466	PHE	2.3
1	F	147	PHE	2.3
1	C	22	GLU	2.3
1	D	253	ARG	2.3
1	B	368	PRO	2.3
1	E	294	VAL	2.3
1	E	352	LEU	2.2
1	E	363	ILE	2.2
1	A	106	PRO	2.2
1	F	416	MET	2.2
1	F	24	PHE	2.2
1	D	449	LEU	2.2
1	F	366	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	494	THR	2.2
1	F	244	PRO	2.2
1	D	408	PHE	2.2
1	B	51	PHE	2.2
1	B	152	ALA	2.1
1	D	309	ILE	2.1
1	E	128	TYR	2.1
1	E	107	ASP	2.1
1	A	419	HIS	2.1
1	E	409	THR	2.1
1	C	51	PHE	2.1
1	F	154	SER	2.1
1	D	51	PHE	2.1
1	E	466	PHE	2.0
1	B	435	LEU	2.0
1	F	88	TRP	2.0
1	C	416	MET	2.0
1	E	381	ARG	2.0
1	A	17	LEU	2.0
1	C	171	GLY	2.0
1	A	418	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	SEP	A	427	10/11	0.82	0.17	83,89,102,103	0
1	SEP	F	427	10/11	0.85	0.11	74,90,106,108	0
1	SEP	B	427	10/11	0.85	0.14	72,84,104,106	0
1	SEP	E	427	10/11	0.86	0.13	89,96,106,107	0
1	SEP	D	427	10/11	0.86	0.10	75,91,104,106	0
1	SEP	C	427	10/11	0.88	0.10	81,86,101,103	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

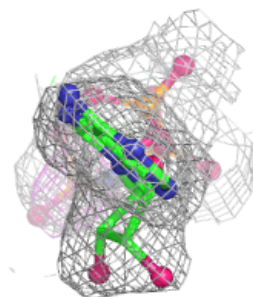
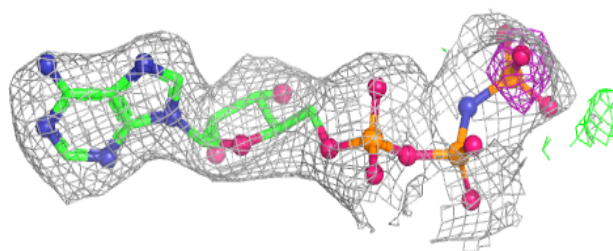
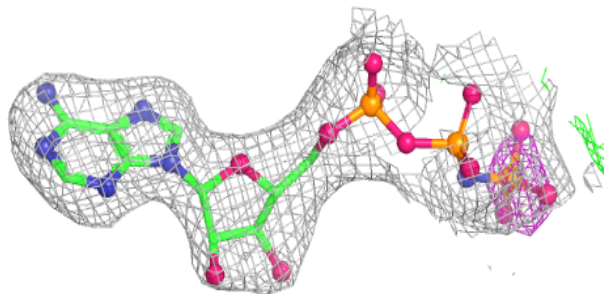
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	D	604	1/1	0.82	0.10	70,70,70,70	0
3	MG	E	604	1/1	0.85	0.08	73,73,73,73	0
3	MG	B	603	1/1	0.88	0.11	51,51,51,51	0
2	ANP	D	602	31/31	0.93	0.08	54,62,91,93	0
2	ANP	E	602	31/31	0.94	0.08	47,59,89,95	0
2	ANP	B	602	31/31	0.94	0.08	46,49,85,85	0
2	ANP	A	602	31/31	0.94	0.08	43,53,81,85	0
3	MG	A	604	1/1	0.94	0.07	56,56,56,56	0
2	ANP	C	602	31/31	0.95	0.07	43,51,78,83	0
2	ANP	F	601	31/31	0.95	0.08	46,53,60,62	0
2	ANP	F	602	31/31	0.95	0.08	42,52,72,75	0
2	ANP	E	601	31/31	0.95	0.08	42,49,63,69	0
2	ANP	D	601	31/31	0.96	0.07	48,58,70,79	0
2	ANP	C	601	31/31	0.96	0.07	48,58,63,64	0
2	ANP	A	601	31/31	0.96	0.07	43,45,50,53	0
2	ANP	B	601	31/31	0.96	0.07	40,50,56,58	0
3	MG	C	604	1/1	0.97	0.03	55,55,55,55	0
3	MG	A	603	1/1	0.98	0.04	45,45,45,45	0
3	MG	E	603	1/1	0.99	0.03	44,44,44,44	0
3	MG	F	603	1/1	0.99	0.06	52,52,52,52	0
3	MG	B	604	1/1	0.99	0.06	51,51,51,51	0
3	MG	C	603	1/1	0.99	0.02	55,55,55,55	0
3	MG	D	603	1/1	1.00	0.07	58,58,58,58	0
3	MG	F	604	1/1	1.00	0.08	47,47,47,47	0

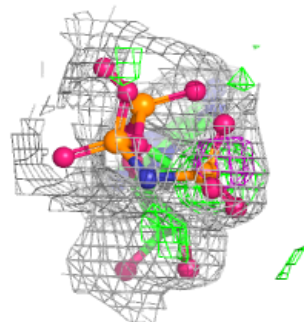
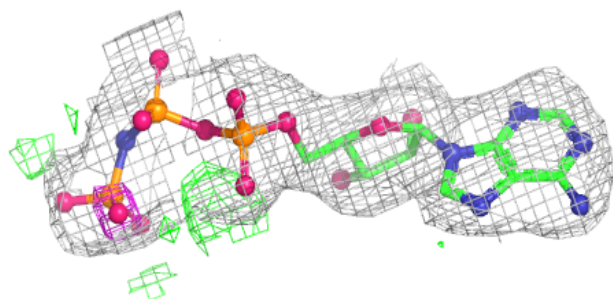
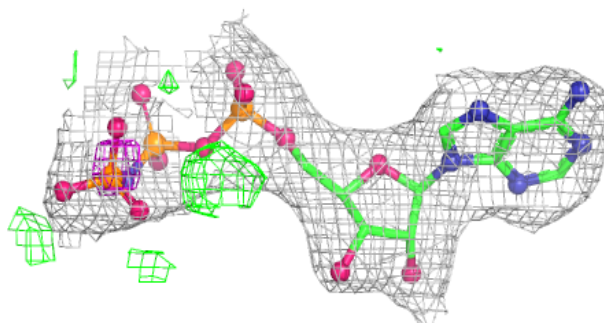
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP D 602:

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

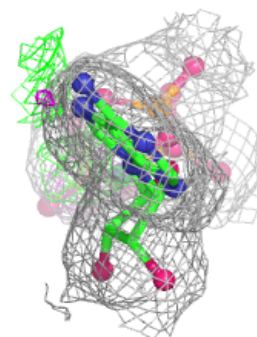
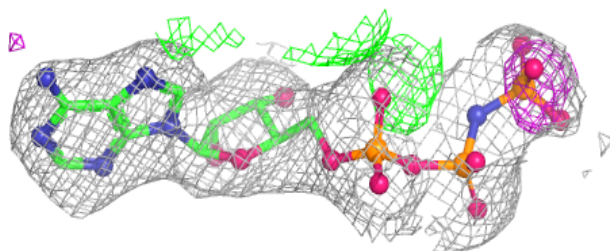
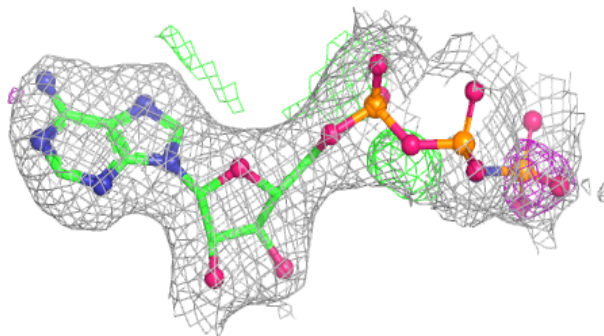
**Electron density around ANP E 602:**

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

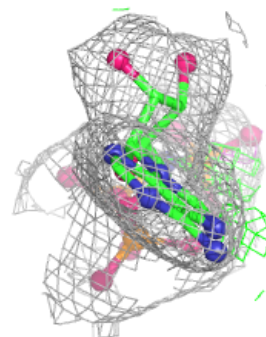
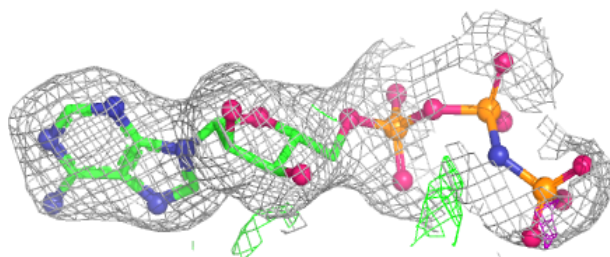
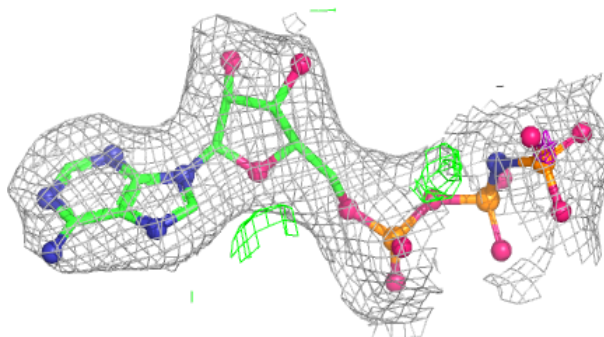


Electron density around ANP B 602:

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

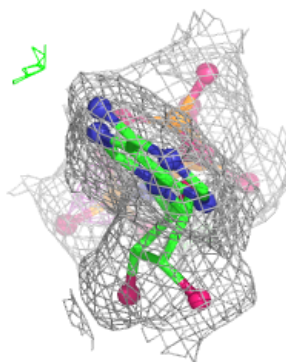
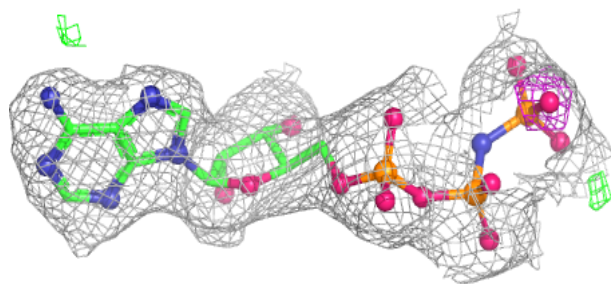
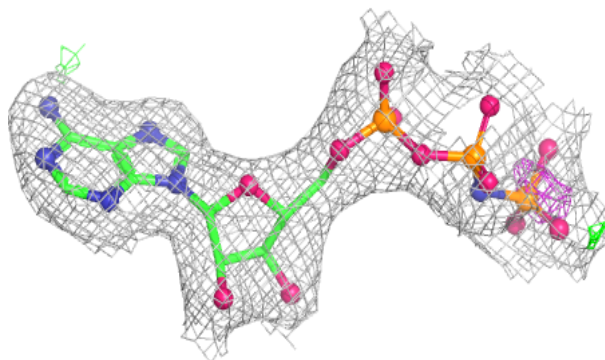
**Electron density around ANP A 602:**

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

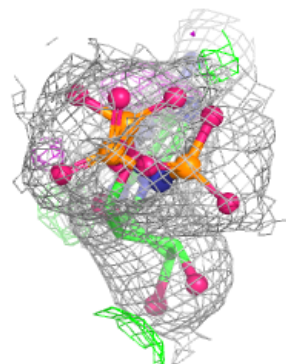
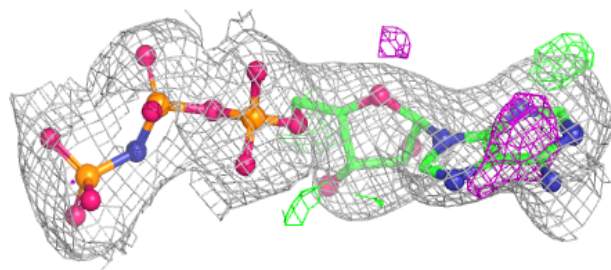
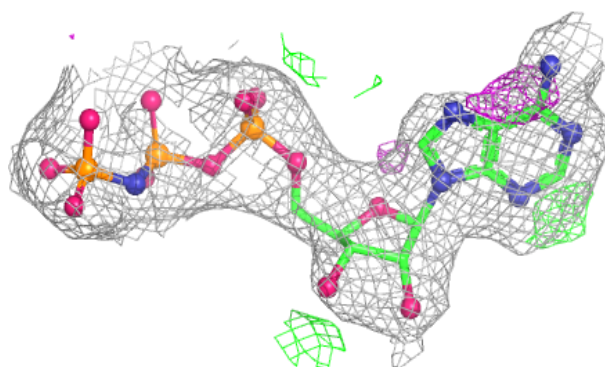


Electron density around ANP C 602:

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

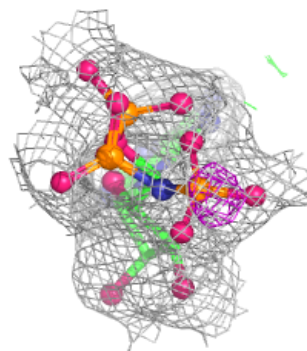
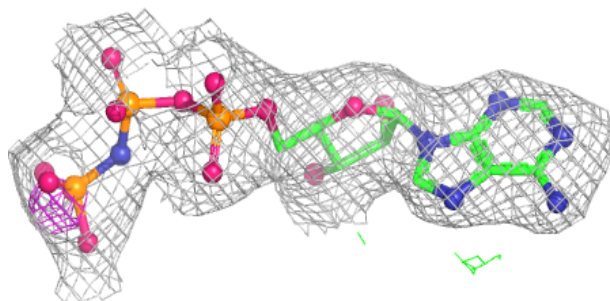
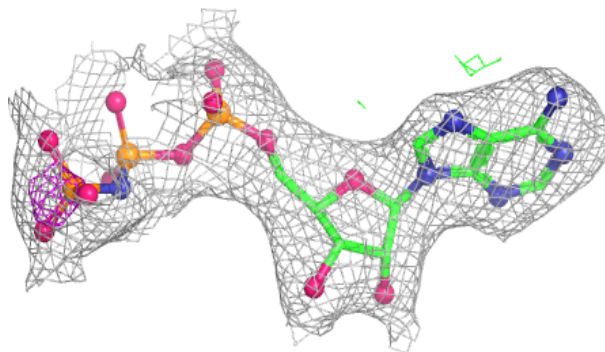
**Electron density around ANP F 601:**

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

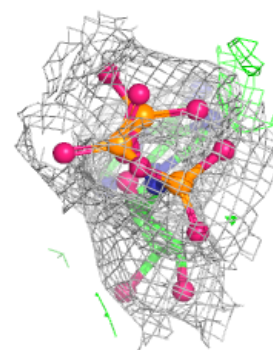
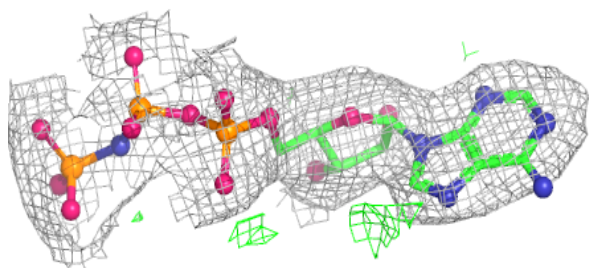
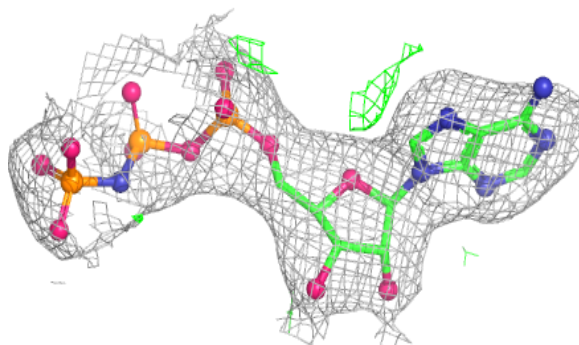


Electron density around ANP F 602:

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

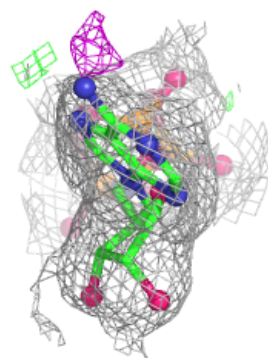
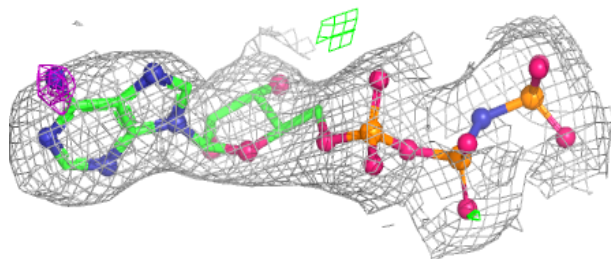
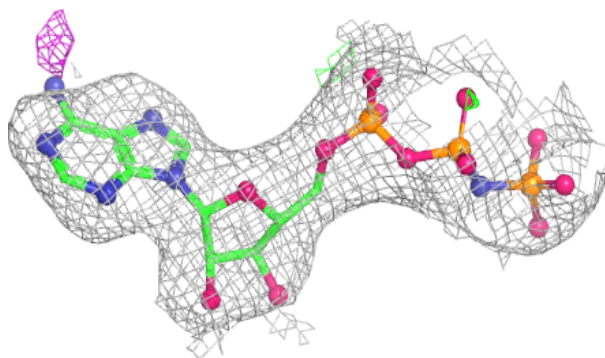
**Electron density around ANP E 601:**

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

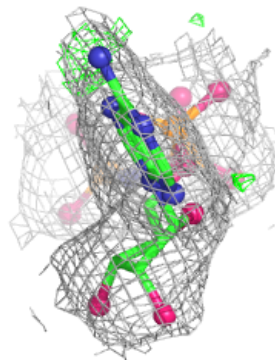
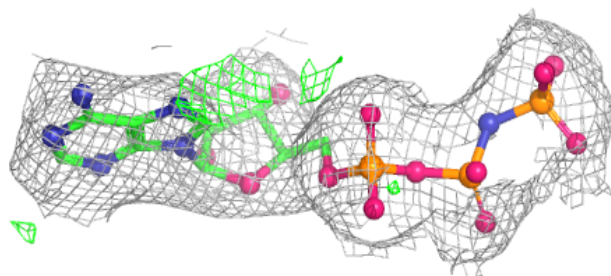
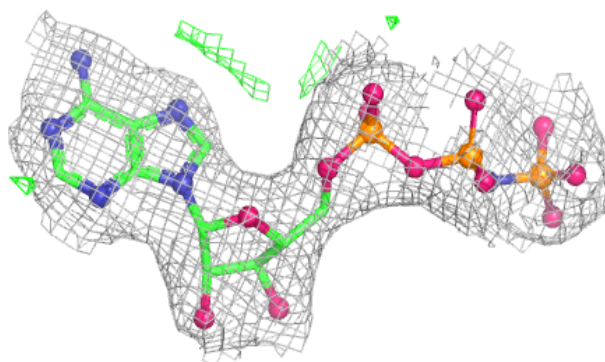


Electron density around ANP D 601:

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

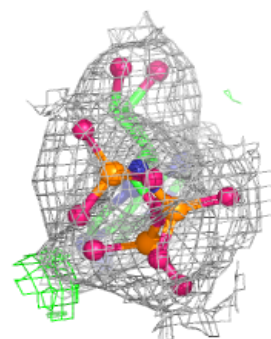
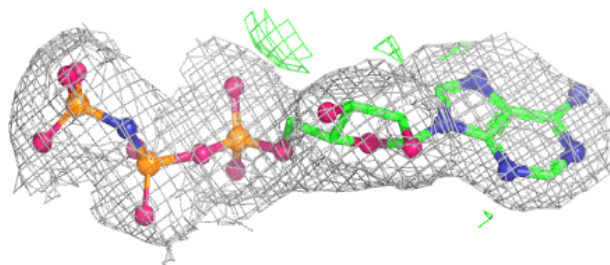
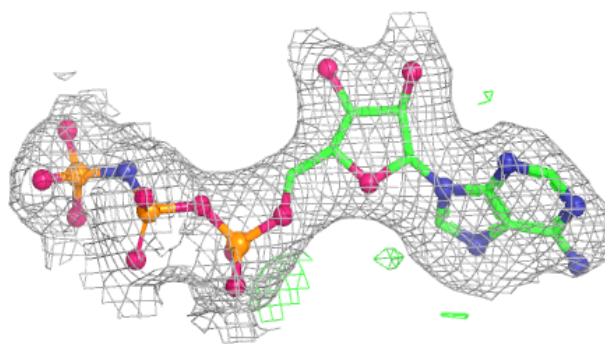
**Electron density around ANP C 601:**

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

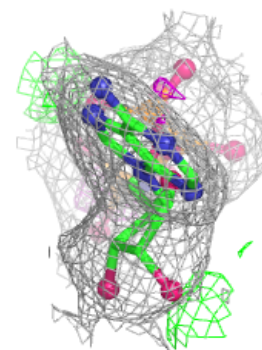
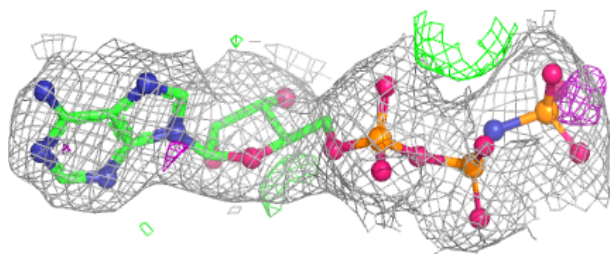
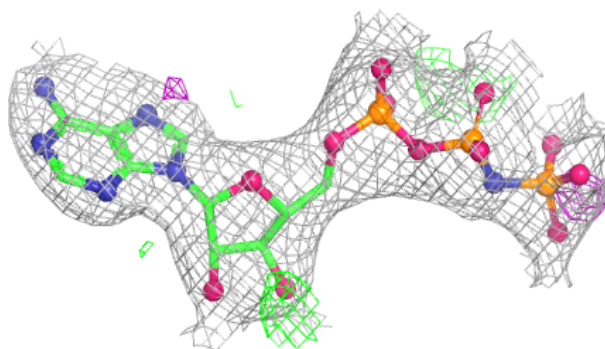


Electron density around ANP A 601:

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

**Electron density around ANP B 601:**

$2mF_o-DF_c$ (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.